Persistent, bioaccumulative, and toxic properties of liquid crystal monomers and their detection in indoor residential dust

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Liquid crystal monomers (LCMs) are used widely in liquid crystal displays (LCDs), which are dramatically changing the world due to the provision of convenient communication. However, there are essentially no published reports on the fate and/or effects of LCMs in the environment. Of 362 currently produced LCMs, 87 were identified as persistent and bioaccumulative (P&B) chemicals, which indicated that these chemicals would exhibit resistance to degradation and exhibit mobility after entering the environment. Following exposure to mixtures of LCM collected from 6 LCD devices, significant modulation of 5 genes, *CYP1A4*, *PDK4*, *FGF19*, *LBFABP*, and *THRSP*, was observed in vitro. Modulation of expressions of mRNAs coding for these genes has frequently been reported for toxic (T) persistent organic pollutants (POPs). In LCM mixtures, 33 individual LCMs were identified by use of mass spectrometry and screened for in 53 samples of dust from indoor environments. LCMs were detectable in 47% of analyzed samples, and 17 of the 33 LCMs were detectable in at least 1 sample of dust. Based on chemical properties, including P&B&T of LCMs and their ubiquitous detection in dust samples, the initial screening information suggests a need for studies to determine status and trends in concentrations of LCMs in various environmental matrices as well as tissues of humans and wildlife. There is also a need for more comprehensive in vivo studies to determine toxic effects and potencies of LCMs during chronic, sublethal exposures.

liquid crystal displays (LCDs) | liquid crystal monomers (LCMs) | persistence (P) | bioaccumulation (B) | toxic (T)

The demand for liquid crystal displays (LCDs) has increased since the 1990s with rapid increases in the use of personal computers, digital cameras, digital televisions, mobile phones, and intelligent electronic products (1). Liquid crystal monomers (LCMs) have been widely used in LCDs, which rely on the optical properties of certain liquid crystalline substances in the presence or absence of an electric field. A consulting business reported that in 2018, the global shipment of LCD panels rose to 198 million m^2 (2). With an increasing number of LCD panels being put into production worldwide, the demand for LCM materials is rapidly increasing. Old LCD devices eventually become electronic waste (e-waste), which is typically discarded—at best in proper e-waste sites—and thus poses serious environmental concerns and challenges. However, environmental behavior, fate, and adverse effects of LCMs have not been reported, and even the specific physical–chemical properties of LCMs have not been very well studied.

LCMs represent a state of matter that flows similar to a liquid but consists of anisotropic compounds (3, 4). At typical ambient temperatures, properties of LCMs are intermediate between liquid and solid states (5). LCMs were first discovered by Reinitzer (6), and since then, thousands of LCMs, with various chemical structures, have been synthesized and commercialized. Typical LCMs are considered to have the following properties: 1) most have aromatic nuclei that are polarizable, planar, and rigid; 2) the central group in the molecule usually contains a multiple bond along the long axis of the molecule or a system of conjugated double bonds that makes the molecule rigid and planar; and 3) the length of the molecule is generally greater than its diameter (7). Manufacturers can enhance performances of LCMs by changing the terminal functional group by introducing a side chain or replacing phenyl groups with a cyclohexyl ring (8). These chemical moieties can result in various structures for LCMs, which can exhibit differential persistence and bioaccumulation potentials (P&B) once they enter the environment.

To the best of our knowledge, current research and legislation/regulations on handling and disposal of e-waste focuses primarily on metals or metalloids, flame retardants, and ozone-depleting substances, but no regulations exist for LCM materials (9). Even though key materials in LCDs are mixed LCMs, there are essentially no published reports on occurrences or hazards posed by LCMs (10, 11). Information regarding structures of LCMs is normally kept confidential among manufacturers of LCs or LCDs. Thus, studies of effects of LCMs on biota are relatively rare (10). A large producer of LCMs once claimed that those used

Significance

Liquid crystal devices, such as smartphones, televisions, and tablet computers, have become integral tools of modern society; however, people do not know the environmental effects of liquid crystal monomers (LCMs). The present study conducted an extensive survey on industries producing LCMs and generated a list containing 362 current-produced LCMs. Eighty-seven out of 362 LCMs showed potential as P&B chemicals, indicating that these LCMs would exhibit resistance to degradation and high mobility after entering the environment. Beyond that, we observed that exposure to LCMs resulted in adverse effects during in vitro screening, by use of cell culture and toxicogenomic evaluation, that were similar to effects observed for other persistent organic pollutants, and that some LCMs were detectable in samples of indoor dust.

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The authors declare no competing interest.

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commercially were not harmful to fish during short-term exposures to relatively high concentrations, relative to what would be expected to occur in surface waters (10). However, the absence of acute effects does not necessarily mean that LCMs have no persistent, bioaccumulative, and/or chronic toxic (T) properties (10, 12).

In silico screening of substances to determine if they are P&B typically relies on quantitative structure property relationships (QSPRs) to predict P&B properties, and various jurisdictions have different criteria set as thresholds to determine if a substance is considered to be P and/or B (13). In previous studies, investigators have successfully identified P and B organic chemicals (14, 15) and pharmaceuticals (16, 17) in commerce. Estimation Programs Interface (EPI) Suite software has effectively estimated physical chemical parameter values for a range of chemicals classes (18). By use of these techniques, in 2018, our research group published a viewpoint based on a list covering more than 300 LCMs, and we challenged environmental chemists to pay attention to potential P&B LCMs (11). We also noted that identification and quantification of LCMs in environmental media has not been reported, and emissions and fates of LCMs remained largely unknown.

Current releases or concentrations of LCMs in various compartments used to produce commercial LCDs are not known, although potential adverse effects on wildlife and the general environment have been suggested (19, 20). In this study, the primary objectives were to 1) provide a list of the 362 LCMs previously reported in our viewpoint article, where P&B properties were discussed; 2) examine mRNA expression of 43 genes following exposure of chicken embryonic hepatocytes (CEHs) to 6 LCM mixtures from largely produced and used LCD devices; 3) identify chemical structures of LCMs in these collected mixtures; and 4) investigate occurrences of LCMs identified in LCD devices in indoor dust.

Results and Discussion

The workflow of this entire study is summarized in Fig. 1, which includes calculation of P&B properties of 362 LCMs, toxicity assessment of LCM mixtures from LCD devices, identification of chemical structures in LCM mixtures, and occurrence of LCMs in dust samples.

Current Status of Use and Production of LCD and LCM around the World. At the core of the global, modern display industry, LCD panels are almost exclusively produced in 3 Asian countries: China, Japan, and South Korea. At present, China is the world's largest producer of the latest generation LCD panels. The distribution of manufacturers of LCMs and LCDs around the world and in China are illustrated in *SI Appendix*, Figs. S2 and S3, respectively.

In 2017, global demand for thin film transistor-LC (TFT-LC) materials was 960 tons, of which the demand in mainland China was 320 metric tons (21). With an increasing number of LCD panel production lines in mainland China, the demand for TFT-LC materials is rapidly increasing. The top 3 positions for production of high-performance TFT-LC materials were held by 3 large firms in the global LC materials market (21), while the upstream materials for LCDs, such as monomers and intermediate products, were mainly produced in China.

During production of LCD devices, LCMs are simply filled into the space between polarizers and are not chemically bonded to any base material. This means that throughout the life cycle of LCM-containing devices, they exhibit greater potentials to be released into the environment. That is, they can be released during production; through wastewater; or during active use, disposal, or recycling. For many years, huge amounts of globally produced e-waste have been dismantled, disposed, and introduced into environments (5). It is likely that during these relatively low-tech recycling practices of recovering metal or indium from LCD devices, LCMs could enter local environments (19).

Assessment of P&B Properties for 362 LCMs. Since information on compositions of mixed LCMs is normally confidential business information, and relative proportions of LCMs in these devices are constantly updated, it is difficult to study the chemical properties of LCMs. Ten industries that produce LCMs were presently surveyed, and a list containing 362 commercial LCMs was developed. These 362 current-use LCMs were screened by use of the QSPRs program and expert judgment of persistence and bioaccumulation (13, 14, 16).

All 362 LCMs were individually evaluated to identify if they were P or B or both by use of the US Environmental Protection Agency's (US EPA) EPI Suite software (18) (Table 1), along with details of the regulation, guidance document, or publication that provided the screening criteria. For LCMs that exhibited log K_{ow} values greater than 5 or bioconcentration factor (BCF) values greater than 1,000, the chemical was considered to be B. The US EPA established that BCF values between 100 and 1,000 indicate a moderate level of concern based on potential B of chemicals under the proposed rule for P&B chemicals (22). The BCF cutoff value of 1,000 for a high level of concern for bioaccumulation potential has been used over the years; in the context of the Stockholm Convention, criteria were listed in Annex D to identify whether a chemical is considered bioaccumulative, with the first criterion being a log K_{ow} >5 (23). LCM chemicals with high log K_{ow} values were considered to be

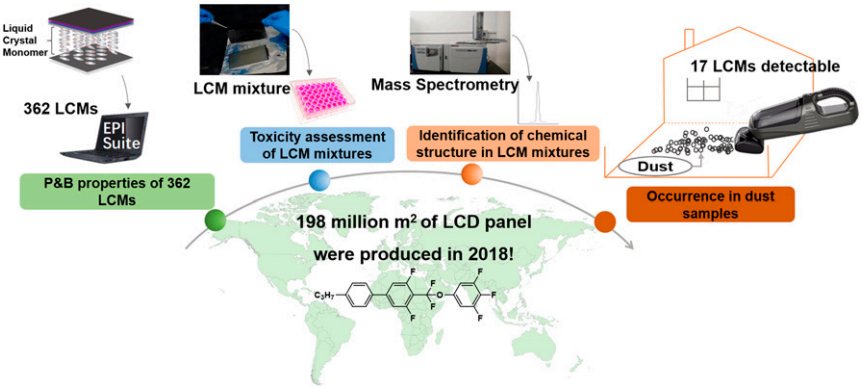

Fig. 1. Workflow of the present study, which includes calculation of P&B properties of 362 LCMs (Fig. 2), toxicity assessment of LCM mixtures from LCD devices (Fig. 3), identification of chemical structure in LCM mixtures (Fig. 4), and detection of LCMs in dust samples (Fig. 5).

Table 1. Persistence and bioaccumulation characteristics of 362 LCMs

Characteristics	Number	Percent	Notes
Log K_{ow}* > 5	340	93.9	Indicates tendency to adsorb to sediments and to bioaccumulate.
BCF > 1,000	202	55.8	BCF is an estimate of bioaccumulation potential.
BCF > 5,000	68	18.8	
AO$t_{1/2}$[†] > 2 d	1	0.3	AO$t_{1/2}$ indicates stability to atmospheric oxidation.
Log K_{aw}[‡] > −5 and log K_{aw} < −1	205	56.6	K_{aw} describes air–water partitioning. Compounds with log K_{aw} > −5 and < −1 have long-range transport potential.
$t_{1/2,\ w}$[§] ≥ 60 d	171	47.2	/
Combined Log K_{ow} > 5, Log K_{aw} > −5 and < −1,and $t_{1/2,w}$ ≥ 60 d	87	24.0	/
Combined Log K_{ow} > 5,Log K_{aw} > −5 and < −1, BCF > 5,000 and $t_{1/2,w}$ ≥ 180 d	10	2.8	The number of substances with all 3 characteristics combined is much smaller.

*Log K_{ow}, octanol–water partition coefficient.
[†]AO$t_{1/2}$, atmospheric oxidation half-life.
[‡]Log K_{aw}, atmosphere–water partition coefficient.
[§]$t_{1/2,w}$, biodegradation half-life in water.

potentially B, even though many QSPRs suggest that BCF decreased with log K_{ow} > 6 (13). Generally, a chemical compound is considered potentially P if the values from BIOWIN[1] or BIOWIN[5] models are less than 0.5 (not readily biodegradable) (24). In accordance with the rules of thumb (13) (e.g., persistent being more halogenated, more branched, and nitroaromatic and biodegradable being straight-chain aliphatic compounds, esters, acids, and hydroxyl functional groups), if chemicals had some of these functional groups, they were considered to be potential P chemicals. Combined with biodegradation half-life values in water ($t_{1/2}$ ≥ 60 d) and aerobic biodegradable values (BIOWIN[1] or BIOWIN[5]), probable P&B chemicals were selected. Of these P&B chemicals, LCMs were considered to be very persistent and very bioaccumulative (vPvB) if BCF values were greater than 5,000 and half-lives in water were greater than 180 d (Fig. 2).

Based on these criteria, of the 362 chemicals, a significant proportion were predicted to be B; 340 were estimated to have log K_{ow} ≥ 5, and 202 were estimated to have BCF of >1,000 (*SI Appendix*, Table S1) (13). A total of 205 LCMs were rated as potentially susceptible to long-range atmospheric transport (log K_{aw} ≥ −5 and ≤ −1). Chemicals were considered to be potentially P if degradation half-lives in water exceeded 60 d (16). By using the following 3 properties—1) log K_{ow} ≥ 5, 2) log K_{aw} ≥ −5 and ≤ −1, and 3) $t_{1/2}$ ≥ 60 d—87 LCMs were classified as potentially P&B (Fig. 2). All LCMs that were classified as P&B were fluorinated, which is consistent with generally greater P&B characteristics of halogenated compounds (13).

Of the 87 LCMs classified as P&B, a C≡C triple bond was apparent in 16.4%, while 29.9% included an ester group, and 43.7% were biphenyl/triphenyl compounds. To reduce the list of 87 to a more manageable number, 10 priority substances were selected for further evaluation that satisfied the following properties: log K_{ow} ≥ 5, BCF > 5,000, BIOWIN[1] < 0.5, and $t_{1/2,w}$ ≥ 180 d (*SI Appendix*, Table S2).

All LCMs listed in *SI Appendix*, Table S2, are fluorinated with various central and terminal groups. The first and second chemicals, 4″-ethyl-2′,3,4,5-tetrafluoro-1,1′:4′,1″-terphenyl (Chemical Abstracts Service Registry Number [CASRN] 326894-55-7) and 2′,3,4,5-tetrafluoro-4″-propyl-1,1′:4′,1″-terphenyl (CASRN 205806-87-7), are triphenyl homologs with similar estimated properties. Both have an estimated log K_{ow} > 7, log K_{aw} between −5 and −1, and $t_{1/2,w}$ = 180 d, which indicates that these chemicals are predicted to be potentially vP and vB. The 4 fluorine atoms have an electron-withdrawing effect and at the terminus of chemicals can easily show the formation of an accumulative effect; the electron cloud migration is large, thus showing a large dielectric anisotropy. Therefore, polyfluorinated triphenyls are used in high-performance TFT-LC materials as medium polar substances to enhance electrical conductivity. However, toxic potencies estimated by ECOSAR indicated that these chemicals might exhibit acute effects, and estimated BIOWIN[1] and BIOWIN[5] of approximately −0.26 and −0.18 showed that these chemicals are not readily biodegradable.

The third and fourth chemicals, 1-ethoxy-2,3-difluoro-4-(4-ethylcyclohexyl) benzene (CASRN 415915-41-2) and 1-ethoxy-2,3-difluoro-4-(4-propylcyclohexyl) benzene (CASRN 174350-05-1), are phenyl cyclohexyl LCs, which are ideal display materials because they have high chemical and photochemical stability. Both fluorine atoms and the oxygen atom in the ethoxyl group form a p–π conjugated structure with the phenyl ring, increasing electron cloud density and dipole moment. In addition, the transstructure of cyclohexyl can develop close packing in the molecular

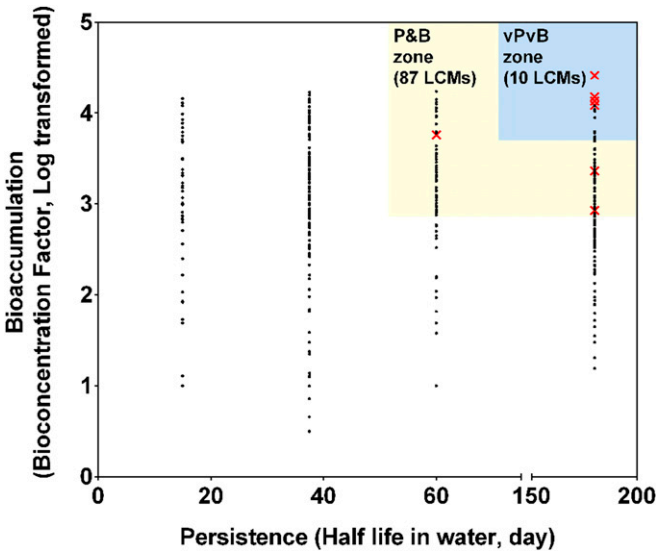

Fig. 2. Distribution persistence (half-life in water) and bioaccumulation (BCF) of 362 LCMs compared to typical POPs, i.e., PBDEs (BDE-47, BDE-99, BDE-154, and BDE-183), hexabromocyclododecane (HBCDD), and PCBs (CB-157 and CB-189). The black dots represent individual LCMs, and the red crosses represent the POPs.

structure, thus exhibiting a greater clearing point than biphenyl LCs. Both the third and fourth chemicals have estimated BCFs > 10,000 and log K_{ow} values of ~7, which indicates potentially large B. When all of the estimates from BIOWIN were considered, they were both suggested to be P. Both were predicted to have an $AOt_{1/2}$ value of < 1 d, reflecting the predicted instability of the chemicals toward atmospheric oxidation by OH-radical reactions.

Currently, fates and effects of LCMs in the environment are rarely studied. Thermotropic LCs (4-n-pentyl-4′-cyanobiphenyl, 4-cyano-4′-n-heptyl-biphenyl, 4-cyano-4′-n-oxyoctyl-biphenyl and 4-cyano-4″-n-pentyl-terphenyl) were toxic to fungal spores (12). All these LCs were included in our database, with the chemical 4-n-pentyl-4′-cyanobiphenyl predicted to have a log K_{ow} value of ~5.8, log K_{aw} of −3.25, BCF > 3,000, and $AOt_{1/2}$ > 1 d, which was indicative of potential for bioaccumulation and long-range atmospheric transport. Due to the absence of the central group, biphenyl and triphenyl chemicals are more stable than other LCMs and, thus, exhibit lesser susceptibility to microbial degradation and enhanced possibility for persistence and bioaccumulation (*SI Appendix*, Table S1).

Electrical and electronic equipment is widely used in the world, but there are no standards and few relevant research reports on recycling of LCMs in e-waste (10, 12). Thus, potential environmental effects of LCMs are poorly measured and difficult to predict. This study has yielded some probable P&B LC substances that should be considered for further study and monitoring of concentrations in various environmental matrices.

Investigation of Toxicity of Mixtures of LCM from Current-Use LCD Devices. PCR array technology is a reliable approach to investigate adverse effects of environmental contaminants (25, 26). To investigate whether exposure to mixtures of LCM from $n = 6$ current-use LCD devices resulted in changes in expressions of selected mRNAs in CEHs, an avian ToxChip, which measures the expression of mRNAs coding for 43 genes from 9 biological pathways including bile acids/cholesterol regulation, cell cycle, DNA repair, glucose metabolism, immune response, oxidative stress, the thyroid hormone pathway, lipid homeostasis, and xenobiotic metabolism, was used (*SI Appendix*, Table S3). Five genes, *CYP1A4*, *FGF19*, *LBFABP*, *PDK4*, and *THRSP*, were significantly dysregulated following exposure to 2 units per mL LCM mixtures (note that 1 unit represents the amount of LCM mixture that was dissolved from 1 in. of LCD devices) (Fig. 3*A*). These 5 gene targets were involved in xenobiotic metabolism, bile acids/cholesterol regulation, lipid homeostasis, glucose metabolism, and the thyroid hormone pathway, respectively.

Expression of *CYP1A4* is modulated by the aryl hydrocarbon receptor (AhR), which is the main receptor that interacts with, and binds to, 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) and other dioxin-like chemicals (27). Here we observed significant up-regulation of *CYP1A4* in CEHs following exposure to LCM mixtures 2, 3, 4, and 6 (Fig. 3*B*), which might indicate that LCM mixtures could act like dioxin-like compounds to induce hepatic cytochrome P450-dependent arachidonic acid epoxygenation. *FGF19*, which is associated with bile acids/cholesterol regulation, was up-regulated in CEH following exposure to LCM mixtures 2, 3, 4, and 6 (Fig. 3*B*). *FGF19* plays an important role in digestion and absorption of lipids from the small intestine and is involved with regulation of bile acid biosynthesis, gallbladder filling, and glucose and metabolism of lipids (28). *LBFABP* is associated with lipid homeostasis and was significantly up-regulated in CEH following exposure to mixtures 2, 3, 4, and 6. *LBFABP* encodes the liver basic fatty acid binding protein, which is involved in binding, transport, and metabolism of long-chain fatty acids and lipids such as cholesterol and bile acids (29). *PDK4*, which is associated with metabolism of glucose, was significantly ($P < 0.05$)

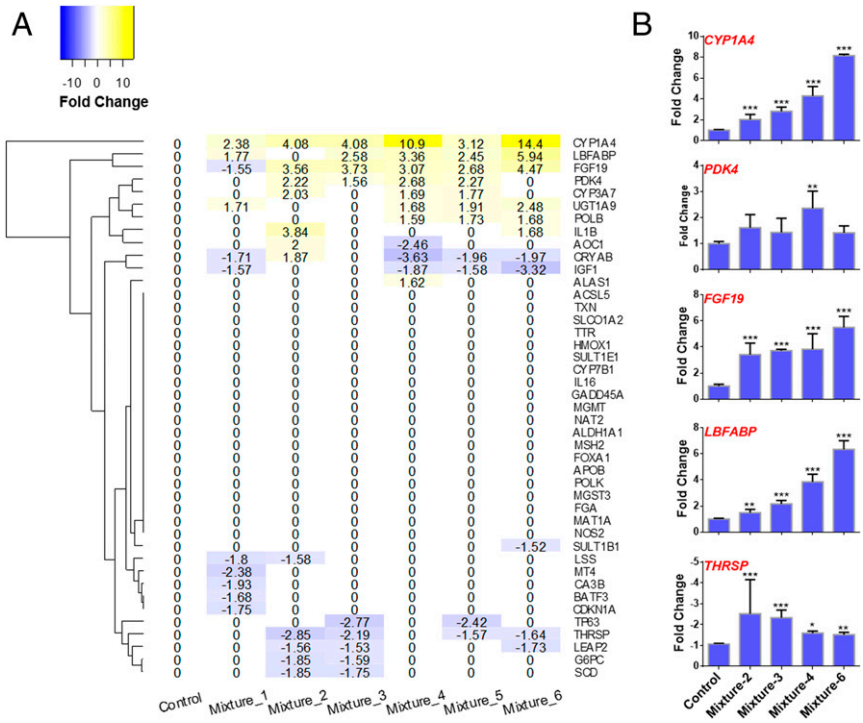

Fig. 3. Alteration of mRNA expression in CEHs exposed to LCM mixtures of 6 current-use LCD devices. (*A*) Transcriptional profiles of 43 genes on the Avian ToxChip PCR array following exposure to 2 units/mL mixtures of LCM (note that 1 unit represents the amount of LCM mixture that was dissolved from 1 in. of LCD devices). (*B*) Confirmation of alteration of mRNA expression of 5 target genes (*CYP1A4*, *PDK4*, *FGF19*, *LBFABP*, and *THRSP*; error bars for each point are the SD of 3 replicates) by use of real-time PCR (pairwise *P* values were determined for each treatment compared to the DMSO vehicle control group; $*P < 0.05$; $**P < 0.01$; $***P < 0.001$).

up-regulated following exposure to LCM mixture 4. *PDK4* is associated with conversion of glucose to acetyl-CoA, which is associated with energy generation and maintaining the balance between metabolisms of carbohydrates and lipids (30). *PDK4* was also dysregulated in CEH following exposure to a toxic organophosphate ester (OPE) contaminant, TDCIPP (31). *THRSP*, which is associated with the thyroid hormone pathway, was down-regulated following exposure to LCM mixtures 2, 3, 4, and 6. The thyroid hormone pathway plays an important role in normal central nervous system development in birds, among many other critical roles (32). Similar alterations of *THRSP* were also previously reported for organic flame retardants, including *PBDEs*, *TPHP*, and *EHDPP*, which were identified as potent competitors for thyroxine binding to TTR (33, 34).

Among 43 genes associated with 9 biological pathways represented on the ToxChip, multiple genes were responsive to mixtures that contained LCMs and provided some initial insight regarding mechanisms of toxicity of LCMs. These genes/pathways were previously reported to be responsive following exposure to other halogenated environmental contaminants, i.e., dioxin-like compounds (*CYP1A4*) (33, 34) and flame retardants (*FGF19*, *LBFABP*, *PDK4*, and *THRSP*) (26).

Identification of Chemical Structures of LCMs in Current-Use LCD Devices. As key materials in electronic displays, individual LCMs could not satisfy the complex and diverse requirements of displays; thus, mixtures of LCMs are carefully balanced in LCDs. Here specific chemical structures of LCMs were further identified in 6 LCM mixtures that were used for toxicity assessment in *Investigation of Toxicity of Mixtures of LCM from Current-Use LCD Devices*.

Eluates containing a mixture of LCMs were analyzed in full-scan mode by gas chromatography-mass spectrometry (GC-MS). Using the mass spectrogram, the preliminary chemical structures could be predicted and matched with peaks. Based on the predicted structures, 10 pure chemicals were purchased and analyzed by GC-MS. Based on retention times and fragment ions, 10 LCMs were identified, and LC-Q Exactive MS was used to verify exact masses from which molecular formulae could be derived by comparing the detected mass with the exact mass.

All 33 LCMs in the mixtures were identified and structures written, based on fundamentals of mass spectrometry similar to those suggested previously (Fig. 4 and *SI Appendix*, Fig. S5) (35–39). Mass spectra of LCMs 5, 9, 13, 16, 31, and 33 have been published previously (35, 40). In our study, the 33 LCMs could be placed into 3 major categories, and mass spectra of those 3 classes of LC chemicals (*SI Appendix*, Tables S4–S6) and mass spectra and possible fragmentation pathways are shown in *SI Appendix*, Fig. S4.

All 33 identified LCMs were on our list of LCMs (*SI Appendix*, Table S1), and properties of the 33 LCs, identified by electron impact ionization (EI) mass spectra, are in *SI Appendix*, Table S7. All 33 LCMs have estimated log $K_{ow} > 5$, and more than 50% have BCF > 1,000, which indicates that after entering into the environment, most of the identified LCMs in phones have potential for bioaccumulation. Of the 33 identified LCMs, 25 were predicted to have $t_{1/2,w} \geq 60$ d, 28 had an estimated BIOWIN^1 < 0.5, and all 33 LCMs had an estimated BIOWIN^5 < 0.5, which indicates significant persistence of LCMs currently used in LCDs. Fourteen LCMs had predicted log $K_{aw} \geq -5$ and ≤ -1, which indicated potential for long-range atmospheric transport. Based on these 3 properties (log $K_{ow} \geq 5$, BCF > 1,000, and biodegradation $t_{1/2,w} \geq 60$ d), 9 LCMs were classified as potential P&B.

Most of the LCMs in LCDs of frequently used smartphones were predicted to exhibit bioaccumulation or persistence in the environment (*SI Appendix*, Table S7). Of the 33 LCMs, 26 were fluorinated, which indicates generally longer persistence and bioaccumulative potential of those halogenated LCMs to cause

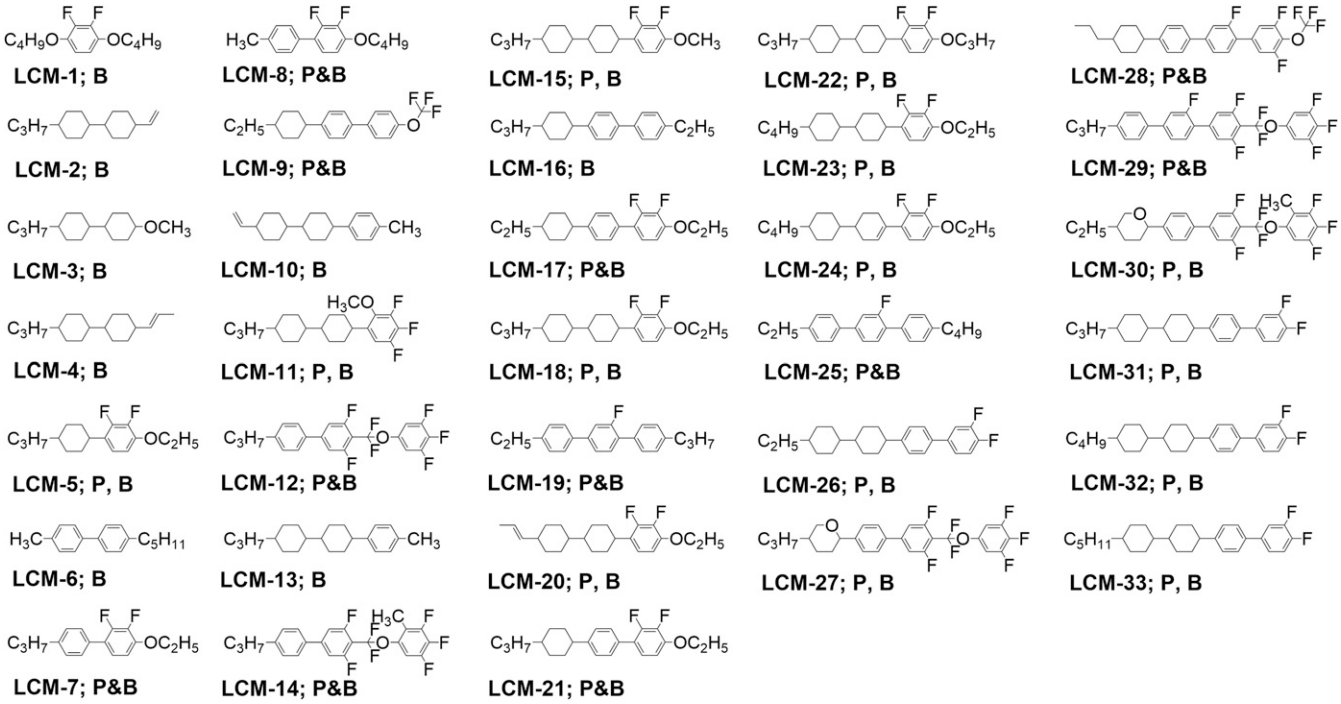

Fig. 4. Chemical structures and P&B properties of 33 LCMs that were identified in the LCM mixtures of 6 commercial LCD devices. In this figure, P refers to persistence (a chemical was considered P if the value for the BIOWIN^1 or BIOWIN^5 models was less than 0.5 or the chemical molecule had certain functional groups [e.g., persistent: highly halogenated, highly branched]). B refers to bioaccumulation, and a chemical was considered to be B if log $K_{ow} > 5$ or BCF values were greater than 1,000. P&B refers to persistence and bioaccumulation (i.e., those chemicals with log K_{ow} and $t_{1/2}$ values greater than 5 and 60 d, respectively, and log *K*aw values between −5 and −1). Specific information (i.e., full name and chemical properties) for all 33 LCMs can be found in *SI Appendix*, Table S7.

adverse environmental effects if they enter the environment. The 1-(4-propylcyclohexyl)-4-vinylcyclohexane (LCM-2, CASRN 116020-44-1), which was detected in all 6 LCDs of the commercial cellphones studied, has an estimated log K_{ow} and BCF of ~8 and 4,000 respectively, which is indicative of potential for bioaccumulation. The 1-ethoxy-2,3-difluoro-4-(4-propylphenyl) benzene (LCM-7, CASRN 157248-24-3), 4-ethoxy-4'-(4-ethylcyclohexyl)-2,3-difluorobiphenyl (LCM-17, CASRN 323178-01-4), 1-ethoxy-2,3-difluoro-4-(4-(4-propylcyclohexyl) cyclohexyl) benzene (LCM-18, CASRN 123560-48-5), 4-ethoxy-2,3-difluoro-4'-(4-propylcyclohexyl) biphenyl (LCM-21, CASRN 189750-98-9), and 1-(4-(4-butylcyclohexyl) cyclohexyl)-4-ethoxy-2,3-difluorobenzene (LCM-23, CASRN 473257-15-7), which were detected in 4 of 6 commercial LCDs, were all predicted to be P&B.

We suggest that further studies should be conducted on these 33 LCMs that are currently being used in commercial LCDs to determine their status and trends in concentrations in various environmental matrices as well as tissues of humans and wildlife.

Screening of 33 Identified LCMs in Indoor Dust Samples. To our knowledge, no quantitative analytical methods exist for LCMs in environmental matrices. In our study, preparation and extraction of samples for the determination of LCMs in dust were similar to those for extracting brominated flame retardants from sediments (41, 42). Because of its efficiency, reproducibility, minimization of solvent use, and minimal background interference, accelerated solvent extraction (ASE) was used to extract LCMs from dust (43). When samples were analyzed by GC-MS/MS, the relative abundance and retention times were used to initially identify the 33 target LCMs. Details of validation parameters and spike recoveries for determination of LCMs are provided in *SI Appendix*, Table S8. Seventeen LCMs, including LCM-2, LCM-3, LCM-5, LCM-6, LCM-7, LCM-10, LCM-12, LCM-13, LCM-15, LCM-17, LCM-18, LCM-20, LCM-21, LCM-22, LCM-23, LCM-28, and LCM-30, were detected in 47% of samples of indoor dust, whereas the others were not quantifiable in any of the analyzed samples (Fig. 5*A* and *SI Appendix*, Table S9). Among the 53 samples of dust, concentrations of Σ_{33}LCM ranged from 0.13 to 2,213 ng/g, dry mass (dm), and more than 80% of the total sum concentration of LCMs comprised LCM-15, LCM-18, LCM-20, and LCM-23. In the present study, concentrations of LCMs varied among sources of dust. For example, the mean Σ_{33}LCM concentration in dust from the laboratory building was 374 ng/g, dm, compared to dust from the canteen (3.64 ng/g, dm). The rank order (from lowest to highest) of mean concentrations of Σ_{33}LCM in dust from buildings was canteen < dormitory < teaching building < hotel < electronic product maintenance center < residence < laboratory building.

Among the 17 LCMs detected in the 53 analyzed dust samples, LCM-5, LCM-7, LCM-12, LCM-15, LCM-17, LCM-18, LCM-20, LCM-21, LCM-22, LCM-23, LCM-28, and LCM-30 were fluorinated chemical compounds (*SI Appendix*, Table S9). This pattern of LCMs was generally comparable with predictions that fluorinated LCMs exhibited greater potential for P&B. Fluorinated LCMs, especially LCM-12, were detected in all 7 sampling spaces (Fig. 5*A*); however, there was no obvious trend that concentrations of fluorinated LCMs in the same area were greater than unfluorinated LCMs.

To study characteristics of LCMs relative to other contaminants in indoor dust, concentrations of OPEs, polybrominated diphenyl ethers (PBDEs), and novel brominated flame retardants (NBFRs) were also measured. Details of analysis methods used for OPEs, PBDEs, and NBFRs are described in *SI Appendix*. Compared to concentrations of conventional contaminants in the same indoor dust samples (Fig. 5*B*), concentrations of Σ_{33}LCM were less than those of ΣOPEs, ΣPBDEs, and ΣNBFRs. Unlike conventional flame retardants, applications of most LCMs are limited to electronic equipment, and large-scale use of LCMs has been relatively recent. This could help explain the lesser concentrations of LCMs compared to additive flame retardants in the dust samples (Fig. 5*B*).

Comparison with Typical Persistent Organic Pollutants and Significance. Persistent organic pollutants (POPs) defined under the Stockholm Convention (44) and the list of carcinogens from the World Health Organization have informed elimination and/or production and use restriction for flame retardant additives such as 2,2′,4,4′-tetrabromodiphenyl ether (BDE-47) (in 2009), 2,3,3′,4,4′,5′-hexachlorobiphenyl (CB-157) (in 2004), and hexabromocyclododecane (HBCDD) (in 2013). It has been confirmed that these flame-retardant additives are persistent in the environment and have a strong potential to bioaccumulate and biomagnify in organisms (45). These chemicals have potential for long-range environmental transport and have been detected in tissues of humans from many regions (46). There is evidence of potential toxic effects in aquatic organisms, including mammals (47, 48). Similar to PBDEs and polychlorinated biphenyls (PCBs), LC chemicals, which were predicted to have potential P and B based on our findings, are all halogenated. Due to the lack of experimental data regarding LCMs, we used estimated properties (degradation half-life in water, BCFs, and fish chronic toxicity values) to compare LCMs with PBDEs, HBCDD, and PCBs. In this study, we selected the 5 most frequently detected brominated flame retardants (BDE-47, BDE-99,

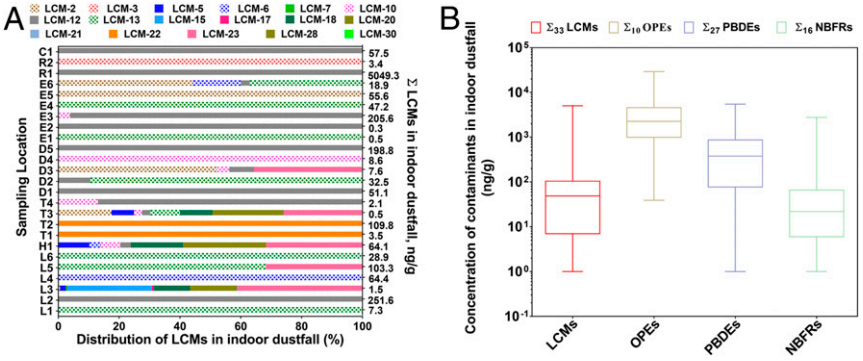

Fig. 5. Screening identified 33 LCMs in samples of indoor dust that were collected from 7 indoor spaces in Nanjing, China. (*A*) Distribution pattern of LCMs that had detectable concentrations (n = 25 samples) in indoor dust samples at different sampling spaces (C, R, E, D, T, H, and L represent the sampling spaces: canteen, residence, electronic product maintenance center, dormitory, teaching building, hotel, and laboratory building, respectively). (*B*) Box plot showing the total log-transformed concentrations (ng/g) of 33 LCMs compared to typically monitored environmental contaminants (i.e., Σ_{10}OPEs, Σ_{27}PBDEs, and Σ_{16}NBFRs in n = 53 dust samples from n = 7 sampling spaces). The upper, middle, and lower lines in the box represent the 75th, 50th, and 25th centiles, respectively, whereas the lower and upper bars represent the minimum and maximum values, respectively.

BDE-154, BDE-183, and HBCDD) and 2 polychlorinated biphenyls (CB-157 and CB-189) in the environment to compare with the 362 LCMs (Fig. 2).

All selected PBDEs and PCBs have an estimated half-life in water ($t_{1/2,w}$) of 180 d and 2.0 ≤ log BCF ≤ 4.5 (800 ≤ BCF ≤ 15,000 L/kg, wet mass [wm]); HBCDD has an estimated half-life in water of 60 d and BCF of 5,759 L/kg, wm. LCMs were classified as P&B if the biodegradation half-life values in water exceeded 60 d and BCF ≥ 1,000. Therefore, predicted properties for P&B LCMs are generally similar to those of PBDEs, HBCDD, and PCBs, indicating the potential for LCMs to persist and accumulate in the environment and human beings.

The present study assessed P&B characteristics of LCMs as described by Mackay et al. (49) and Howard et al. (13). Only intensive properties such as degradation half-lives and partition coefficients are meaningfully ranked because they are independent of any consideration of quantity of chemical produced or emitted to the environment. From the systematic evaluation of essentially all 362 commercial LCMs, we demonstrated that over 90% are predicted to be potential P or B chemicals (11). Most of these chemicals have rigid and persistent structures (e.g., diphenyl/triphenyl backbone structure or with halogen substitution) that appear to be persistent and possibly bioaccumulative, similar to POPs including PCBs, PBDEs, and HBCDD (50–53). In addition, we found that 17 of the 33 identified LCMs from 6 models of largely produced LCD devices were detected in indoor dust samples, and most of these were fluorinated and estimated to be bioaccumulative and persistent. Overall, these findings raise concerns regarding the environmental behavior, fate, and adverse effects of LCMs (11) and suggest that future studies on this unique class of chemicals are warranted.

Materials and Methods

Database for the Evaluation of the P&B Properties of LCMs. To address the question of how many LCMs are currently being produced, we surveyed 18 LCM-producing industries in China and compiled lists of all their commercial LCM products from their official websites. A product list containing 362 commercial LCMs was used to compile chemical properties and make assessments of individual LCMs (*SI Appendix*, Table S1). Since some of the chemicals have no CASRNs, LCMs were entered into the database using Simplified Molecular Input Line Entry Specification (SMILES) notations. Physical–chemical properties were estimated using EPI Suite software (18). Parameters used to make predictions of characteristics used to screen for P&B were CASRN, chemical name, molecular mass, vapor pressure (VP), AO $t_{1/2}$ (atmospheric oxidation half-life) (AOPWIN), log K_{aw} (air–water partition coefficients), log K_{ow} (octanol–water partition coefficients) (KOWWIN), log K_{oa} (octanol-air partition coefficients) (KOAWIN), BCF, BIOWIN^1 and BIOWIN^5 (2 biodegradation estimates), and degradation half-lives ($t_{1/2}$) in water, soil, and sediment (fugacity). The properties that were relevant to the determination of P&B included log K_{ow}, BCF, and BIOWIN^1 and BIOWIN^5. Once the properties were estimated and added to the database, they were used to rank potential P&B chemicals. We used EPI Suite software (18) to estimate physical–chemical properties of LCMs, such as octanol–water partition coefficients (log K_{ow}) and biodegradation half-lives in environmental media ($t_{1/2}$); the software has been well studied and has been reviewed by Ng et al. (54). The training datasets of EPI Suite software (18) contained biphenyls, esters, nitriles, alkynes, halobenzenes, etc., and therefore, the main structures of the LCMs studied are within the applicability domain of EPI Suite.

Software Used to Predict P&B Properties of LCMs. Molecular structures, SMILES notations, CASRNs, and names of the LCM products were obtained from Cambridge Soft Corporation ChemDraw (55) and the Royal Society of Chemistry ChemSpider database (56). EPI Suite software, developed by the US EPA and Syracuse Research Corp., was used for estimation of physical–chemical properties and environmental fate of 362 LCMs (18). EPI Suite uses 11 separate linear–free energy relationships to estimate properties from first and second principles. A plot of comparisons to typical POPs was generated by R software (version 3.5.1). EPI Suite software and R software are open source and available free of cost.

Preparation of LCM Mixtures. LCD panels of 6 frequently used smartphone models used in the present study were purchased from local smartphone maintenance shops in Nanjing, Jiangsu province, eastern China. Production volumes in China during 2018 of all these brands of smartphones were reported to be greater than 100 million units (57). LCD panels were brought into our laboratory and dismantled manually (*SI Appendix*, Fig. S1). LCM layers between polarizers in LCD devices were dissolved with acetone and washed into a 500-mL precleaned beaker, then transferred into a 15-mL disposable borosilicate glass tube (16 × 100 mm; VWR International). Then, solvent containing LCMs was blown down to dryness by use of a gentle stream of high-purity nitrogen and then redissolved in 1 mL acetone. To help ensure complete isolation of LCMs from LCD devices, dissolutions were repeated a second time. Results demonstrated that more than 90% of LCMs were isolated from LCD devices by the first dissolution. LCM mixtures were stored at −20 °C until further instrumental analysis (solvent exchanged with 2,2,4-trimethyl pentane [TMP]) or toxicity assessment (solvent exchanged with dimethyl sulfoxide [DMSO]).

Preparation of CEHs. Detailed information on the preparation of CEHs can be found elsewhere (58, 59). Briefly, fertilized and unincubated eggs of white leghorn chicken (*Gallus gallus domesticus*) were purchased from the Canadian Food Inspection Agency and incubated at 37.5 °C for 19 d. Day 19 embryos were rapidly decapitated, and livers were removed and pooled in culture dishes. Hepatocytes were separated and cell aggregations reduced with Percoll and DNase I, respectively. Cells were centrifuged and suspended in fresh medium containing 1 μg/mL of insulin and thyroxine. Cell suspensions were distributed into 48-well plates (25 μL cell suspension into 500 μL fresh medium). Plates were incubated at 37.5 °C under an atmosphere containing 5% CO_2 for 24 h prior to chemical administration. To determine the dose–response relationships for viability of CEHs, after 24 h, they were dosed with the DMSO solvent control (2.5 μL/well; $n = 3$) or mixtures of LCMs at nominal concentrations of 2, 1, 0.5, 0.25, 0.125, or 0.0625 units per mL (note that 1 unit represents the amount of LCM mixture that was dissolved from 1 in. of LCD devices). For toxicogenomic evaluation using the avian ToxChip PCR array or targeted real-time PCR, a nominal concentration of 2 units per mL was used. Following dosing, cells were incubated for an additional 24 h.

Identification of Chemical Structures of 33 LCMs in LCM Mixtures. Identification of the chemical structure of the LCMs followed the procedures summarized in *Identification of Chemical Structures of LCMs in Current-Use LCD Devices*. First, LCMs in mixtures from LCD devices were screened in full scan mode with a scan range of mass-to-charge ratio (*m/z*) 50 to 650 by use of a ThermoFisher Scientific Trace 1300 GC coupled with an ISQ LT single quadrupole mass analyzer (GC-MS; ThermoFisher Scientific). The GC-MS was equipped with a DB-5HT column (15 m × 250 μm × 0.10 μm; J&W Scientific). The GC temperature ramp started from 80 °C, hold 3 min, ramp 20 °C/min to 160 °C, hold 1 min, ramp 10 °C/min to 240 °C, hold 3 min, ramp 10 °C/min to 300 °C, hold 10 min. The injection volume was 1 μL. Ultrahigh-purity helium was used as the carrier gas at a flow rate of 1.2 mL min^{-1}. Ionization was operated in heated EI mode. The MS transfer line temperature was set at 300 °C. The ion source temperature was 230 °C.

After mass spectra were acquired for all LCMs, chemical structures were elucidated following previous publications. Specifically, Leclercq et al. reported mass spectra of various classes of LCM (35–39). By analyzing mass spectra, MS fragmentation pathways of LCMs were determined. By combining MS fragmentation pathways, similar to Leclercq and coworkers, with fundamentals of mass spectrometry, structures of LCMs corresponding to each peak of the gas chromatogram were proposed. Structures were further verified by comparing to structures of LCMs that had been established previously. As a result, 33 LCMs were positively identified for subsequent examination in $n = 6$ currently produced LCD devices.

For full identification of LCMs, the ideal way would be to obtain pure authentic standards for comparison of retention times and/or mass spectra. However, only 10 of the 33 LCMs are commercially available as pure standards. These were 4′-methyl-4-pentylbiphenyl (CASRN 64835-63-8, purity > 98%), 4-propyl-4′-vinylbicyclohexyl (CASRN 116020-44-1, purity > 98%), 4-[difluoro-(3,4,5-trifluorophenoxy)-methyl]-3,5-difluoro-4′-propylbiphenyl (CASRN 303186-20-1, purity > 98%), 1-ethoxy-2,3-difluoro-4-(4-propylcyclohexyl) benzene (CASRN 174350-05-1, purity > 98%), 4-propenyl-4′-propylbicyclohexyl (CASRN 279246-65-0), 4′-propyl-4-(p-tolyl)-bicyclohexyl (CASRN 84656-75-7, > 98%), 4-ethyl-4′-(4-propylcyclohexyl)-biphenyl (CASRN 84540-37-4, purity 98%), 1-methoxy-4-(4-propylcyclohexyl)cyclohexane (CASRN 97398-80-6), 4-(4-methylphenyl)-4′-vinylbicyclohexyl (CASRN 155041-85-3, purity 98%), and 4″-ethyl-2′-fluoro-4-propyl-1,1′:4′,1″-terphenyl (CASRN 95759-44-7, > 99%). These authentic,

native standards were purchased from Tokyo Chemical Industry Co., Ltd. (TCI), J&K (Acceleration Scientific and Industrial Development Thereby Serving Humanity), or Beijing Bayi Space LCD Technology Co., Ltd. For the 10 LCMs where we had authentic standards, their high-resolution molecular weights were confirmed by use of a Q Exactive Focus quadrupole orbitrap mass spectrometer (ThermoFisher Scientific) equipped with a Dionex UltiMate 3000 UHPLC system (ThermoFisher Scientific). This UHPLC-Q-Orbitrap/MS was equipped with a Hypersil GOLD-C18 Selectivity column (1.9 μm; 100 mm × 2.1 mm; ThermoFisher Scientific). The injection volume was 5 μL. Pure water (A) and methanol (B) were used as mobile phases. Initially, 5% of B was increased to 95% in 5 min, then increased to 100% at 7 min and held static for 8 min, followed by a decrease to the initial conditions of 5% of B held for 8 min to allow for equilibration. The rate of flow was 0.40 mL/min. Temperature of the column was maintained at 35 °C. The ionization was operated in heated ESI mode. The spray voltage was set at 3.5 kV in positive mode. The ion transfer capillary temperature was set at 320 °C, and the probe heater temperature was set at 425 °C. Full-scan mode was conducted with a scan range of *m/z* 120 to 1,000. The mass spectrometer was controlled by Xcalibur 4.1 software (ThermoFisher Scientific).

Collection of Indoor Dust Samples and Analysis. To identify and quantify LCMs in indoor environments, 53 sampling points in 7 indoor spaces, including laboratory building, hotel, teaching building, dormitory, electronic product maintenance center, residence, and canteen, were established in Nanjing city, eastern China, from which dust was collected during winter of 2018 (November to December). The 53 samples were numbered L1-14, H1-4, T1-12, D1-10, E1-7, R1-4, and C1-2. A whirlwind car dust collector (CARCHAT DIVI-V401) was used to collect samples of dust, which were subsequently sealed in polyethylene zip bags, transported to the laboratory, and then sieved using a 10-mesh sieve to remove larger materials. Sieved dust samples were transferred into precleaned dark brown glass bottles and kept in a refrigerator at −80 °C for further analyses.

Sieved dust (50 mg) was mixed with diatomaceous earth (treated at 600 °C for 8 h) and extracted by ASE (DIONEX 350; ThermoFisher Scientific) with an organic phase (50:50 cyclohexane:ethyl acetate). Oven temperature was 100 °C, and pressure was 1,500 psi. ASE extracts were concentrated to 1 mL by use of a gentle stream of nitrogen. To remove obvious impurities, samples were transferred into a glass column, coupled with a Syringe Filter (13 mm × 0.22 μm, PTFE membrane; ANPEL). Each sample was collected into a centrifuge tube, the solvent removed by evaporation to dryness, and then reconstituted in 7 mL of 50:50 cyclohexane:ethyl acetate. The extract was subjected to gel permeation chromatography (AutoClean GPC; LabTech) that was operated using 50:50 cyclohexane:ethyl acetate at a flow rate of 5 mL/min. The collected fraction was reevaporated to ∼0.5 mL and further cleaned-up on an Si SPE cartridge (500 mg × 6 mL; CNW Technologies). The fraction was collected and evaporated to dryness, then dissolved into 200 μL of TMP and transferred to a glass GC vial with insert and cap, and stored at 4 °C until GC-MS/MS analysis.

The analytical instrument was a ThermoFisher Scientific Trace1300 GC, coupled with a TSQ 9000 triple-quadrupole mass spectrometer (ThermoFisher Scientific). The GC column used for separation was TG-SQC (15 m × 0.25 mm × 0.25 μm) (ThermoFisher Scientific). A volume of 1 μL of sample was injected, split-less with an injector temperature of 285 °C. Helium was used as the carrier gas with a constant flow rate of 1.0 mL/min. Oven temperature was programmed as follows: the initial temperature was held at 80 °C for 3 min, 20 °C/min to 120 °C, 5 °C/min to 280 °C (held for 1 min), and then ramped to 300 °C at 10 °C/min and held for 3 min. Mass spectrometer parameters were as follows: the ion source temperature and transfer line temperature were 280 °C and 290 °C, respectively, and the ion source filament voltage was 70 eV. The mass spectrometer was operated in the EI mode, and analysis was performed in selected-reaction monitoring mode.

Data Availability Statement. More details on experimental procedures and datasets can be found in *SI Appendix*, which includes 9 supporting figures and 5 supporting tables. The supporting figures and tables contain detailed information on persistence, bioaccumulation, and toxicity data for 362 commercial LCMs (*SI Appendix*, Table S1); predicted properties of 10 LCMs that were identified to be vPvB in the environment (*SI Appendix*, Table S2); RefSeq accession numbers and gene descriptions for the 43 target genes and 2 housekeeping genes on the fourth generation Avian ToxChip PCR array (*SI Appendix*, Table S3); relative abundances of characteristic ions in the EI mass spectra of LCMs in the LCDs of 6 models of largely produced commercial smartphones (*SI Appendix*, Tables S4–S6); property data for the 33 LCMs that were identified from the LCDs of 6 models of largely produced commercial smartphones (*SI Appendix*, Table S7); ion pairs and collision energy, spiked recoveries, and validation parameters for determination of individual LCMs (*SI Appendix*, Table S8); limit of detection, blank concentration, detected frequency, arithmetic means, and ranges (ng/mL) of LCMs in indoor dust samples (*SI Appendix*, Table S9); collection of LCMs from LCD devices in the laboratory (*SI Appendix*, Fig. S1); distribution of manufacturers of LCs and LCDs in the world (*SI Appendix*, Fig. S2) and China (*SI Appendix*, Fig. S3); the possible fragmentation pathways of LCMs in LCDs from 6 models of largely produced commercial smartphones under electron impact ionization (EI) source (*SI Appendix*, Fig. S4); and total ion chromatogram of the LCM mixtures from 6 dismantled LCDs devices by use of GC-EI-MS (full scan mode) (*SI Appendix*, Fig. S5).

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Supporting Information

Persistent, Bioaccumulative and Toxic Properties of Liquid Crystal Monomers (LCMs) and their Detection in Indoor Residential Dust

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1 More Details on Experimental Procedures

1.1 Uncertainty Associated with Estimation of Properties

We used EPI Suite software (1) to estimate physical-chemical properties of LCMs, such as octanol-water partition coefficients (log K_{ow}) and biodegradation half-lives in environmental media ($t_{1/2}$); the software has been well studied and has been reviewed by Ng et al.(2) The training datasets of EPI Suite software(1) contained biphenyls, esters, nitriles, alkynes, halobenzenes etc. and therefore, the main structures of LCMs studied are within the applicability domain of EPI Suite. However, due to the lack of the actual values for the new contaminants, it was impossible to compare estimated with experimental values.

1.2 Cell viability and expressions of mRNA for 43 genes in CEHs following exposure to n=6 LCM mixture extracts

The ViaLight^{TM} Plus BioAssay kit was used to measure adenosine triphosphate (ATP) in CEHs exposed to LCM extracts for 24 h. Based on results of previous studies, TDCIPP at a nominal concentration of 300 μM was used as a positive control (3). Following the 24-h incubation period, plates were maintained at room temperature for no less than 5 min. Then, CEH medium was gently aspirated from each well and fresh medium and cell lysis reagent were successively added into each well and mixed well. A 100 μL aliquot of this medium/lysis reagent mixture was transferred to a luminometer plate, and incubated for 2 min at room temperature. The mixture was then mixed with 100 μL of ATP monitoring reagent plus, and immediately measured for intensity of luciferase luminescence by use of the Luminoskan Ascent.

To determine effects on gene expression, extracts containing LCMs were investigated at 2 units/mL. After exposure for 24 h, variations in expression of mRNAs were investigated by use of the 4th generation custom chicken RT^2 Profiler PCR Array (ToxChip) (3, 4). The 96-well ToxChip contained 43 target genes and 5 control genes in duplicate. Biological functions of these 43 target genes are described in Table S3, and the 5 control genes were: 1 positive PCR control (PPC), 1 reverse transcription control (RTC), 2 housekeeping genes, and 1 genomic DNA control.

Isolation of total RNA from CEH has been described previously (5). In brief, plates were removed from the -80 ^{o}C freezer, and cell lysis reagent was added into each well. Then, 200 ng of RNA was reverse-transcribed to

complimentary DNA (cDNA) using the QuantiTect Reverse Transcription kit (Qiagen) and cDNA was gently mixed with the RT2 SYBR Green Mastermix (Qiagen). A 25 μL aliquot of this mixture was immediately added to each well on the 96-well ToxChip. All arrays were measured in the Agilent MX3005 (Agilent Technologies, Santa Clara, CA, U.S.A.) using thermal profiles reported previously (3, 4). There was no amplification in the genomic DNA contamination well (cycle threshold [Ct] ≥ 35), and the PPC and RTC controls also met appropriate QA/QC criteria of ΔCt ≤ 5; ΔCt = Ct values of RTC – Ct values of PPC. These results ensured robust analyses of mRNA expression. Following exposure of CEHs to extracts containing LCMs, relative Cts of the two housekeeping genes did not vary significantly (ANOVA, $p > 0.05$).

Based on results from the ToxChip, real-time RT-PCR was used to confirm and further quantify mRNA expression levels of five genes, including *CYP1A4*, *FGF19*, *LBFABP*, *PKD4*, and *THRSP*. Briefly, 5 μL of cDNA, RT2 primer assays for the target and housekeeping genes (Qiagen), and RT2 SYBR Green Mastermix (Qiagen) were mixed together to obtain a final volume of 25 μL. Reaction conditions for PCR were 5 °C for 10 min, followed by 40 cycles of 95 °C for 30 s and 60 °C for 1 min. During the reaction, no amplification was observed in the no template controls for any of the assays, which indicated that contamination did not happen during reactions. *EEF1A1* was used as a housekeeping gene, the expression of which was invariable across all treatment groups.

1.3 QA&QC for screening of the 33 identified LCMs in indoor dust samples

During identification and quantification of LCMs in dust, strict analytic procedures to ensure quality control were implemented. For every 11 samples, a laboratory blank was analyzed, reflecting possible background contamination in the clean laboratory. Since authentic standards of all LCMs were not available and in particular, no mass labelled internal standards were available, 4'-ethylbiphenyl-4-carbonitril and 4'-(octyloxy)-4-biphenylcarbonitrile (Beijing Bayi Space LCD Technology Co., Ltd.) were used as internal standards and added to all samples before extraction. Since some of the LCMs were present in the blanks, a value equal to three times the RSD (relative standard deviation) of the blank measurement was set as the limit of quantification (LOQ). For chemicals that were not detected in blanks, LODs were based on a signal to noise ratio of 3. Due to the lack of standards, the concentration of 23 LCMs were semi-quantified by referencing to a standard compound with similar structure. Microsoft Excel 2016, R software (version

3.5.1) and GraphPad Prism 6 were used for statistical analysis and presentation of experimental data in this paper.

1.4 Analysis methods for polybrominated diphenyl ethers (PBDEs), novel brominated flame retardants (NBFRs) and organophosphate (OPEs).

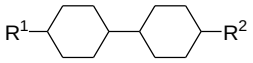
BDE-30, BDE-181, $^{13}C_{12}$-*syn*-DDC-CO, $^{13}C_{12}$-*anti*-DDC-CO, and $^{13}C_{12}$-BDE-209 (Wellington Laboratories, Guelph, Canada) were use as the internal standards for 27 PBDEs and 16 NBFRs. The sample preparation and extraction process for the determination of PBDEs and NBFRs were same as the LCMs. GC-MS (ThermoFisher Scientific Trace 1300， San Jose, CA, USA) equipped with the negative chemical ionization mode (NCI) and DB-5HT column (15 m × 0.25 mm ×0.1μm，J&W Scientific, Folsom, USA), was used for analyzing the samples. The oven temperature was set to 60 ℃ for 3 min, then ramped at 50 ℃/min to 250 ℃, and then 25 ℃/min to 320 ℃ (hold for 15 min). The temperature of the transfer line, the ion source and the inlet were set at 280 ℃, 250 ℃ and 240 ℃, respectively. Helium was used as the carrier gas at a flow rate of 0.85 ml/min, and methane was used as the chemical-ionization moderating gas at a flow rate of 1.5 ml/min.

d_{12}-TCEP, d_{15}-TDCIPP, d_{15}-TEP, d_{27}-TNBP, and d_{15}-TPHP (Sigma-Aldrich, AK Scientific, and TCI America, USA) were used as the internal standards for 10 OPEs. The sample preparation and extraction process for the determination of OPEs are briefly outlined here. Approximately 50 mg of sieved dust was accurately weighed and spiked with 10ng of 5 internal standards. A total of 0.5g $NaSO_4$ and 0.1g NaCl were added to remove water followed by extraction in glass test tubes using ultrasonic solvent extraction for 10 min at room temperature. The solvent was 2 mL 50:50 cyclohexane: dichloromethane. After centrifugation at 4500 g for 5 min, supernatant was transferred into clean glass test tubes. These steps were repeated twice yielding approximately 6 mL supernatant, which was then concentrated to 100 μL by a gentle stream of nitrogen and re-dissolved in 0.4 mL acetone. The prepared sample was further cleaned-up on a Si SPE cartridge (500 mg × 6 mL, CNW Technologies, Shanghai, China). The fraction was collected and solvent evaporated to dryness, and then dissolved into 100 μL of 2,2,4-trimethyl pentane (TMP). The TMP solution was transferred to a glass GC vial with insert and cap and stored at 4 ℃ until analysis. GC-MS (ThermoFisher Scientific Trace 1300, San Jose, CA, USA) equipped with the electron impact ionization mode (EI) and TG-5MS column (30 m × 0.32 mm ×0.25 μm), was used for analyzing the samples. The oven temperature was set to 50 ℃ for 3 min, then

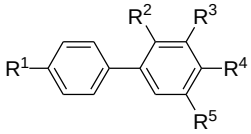
ramped at 20 ℃/min to 100 ℃ (held for 3 min), and then 12 ℃/min to 230 ℃ (held for 15 min), then 5 ℃/min raised to 260 ℃, then 10 ℃/min raised to 300 ℃ (held for 14 min). The temperature of the transfer line, the ion source and the inlet were set at 300 ℃, 230 ℃ and 285 ℃, respectively. Helium was used as the carrier gas at a flow rate of 1.2 ml/min.

2 Further discussion of the details on mass spectra and possible fragmentation pathways for LCMs.

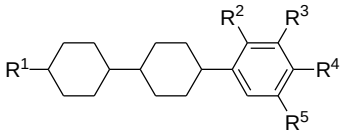
The molecular ions are present in all instances. 33 chemicals roughly could be divided into three major categories, i.e. bicyclohexyl derivatives, bicyclohexylphenyl derivatives and biphenyl derivatives, respectively. The mass spectra of the three classes of liquid crystal chemicals are collected in Tables S4-6.



(Bicyclohexyl derivatives)



(Biphenyl derivatives)



(Bicyclohexylphenyl derivatives)

In the mass spectra of the bicyclohexyl derivatives 1-3 (Table S4), the ions $[R^1C_6H_8]^+$ appears itself as an odd-electron ion at m/z ($80+R^1$). These derivatives also yield characteristic ions at m/z 109, 95, 81 and 69. The bicyclohexylphenyl derivatives 9-16 (Table S5) produce characteristic ions $[CH_2{=}CHC_6HR^2R^3R^4R^5]^+$ at m/z ($100+R^2+R^3+R^4+R^5$) and the satellite ions at m/z ($87+R^2+R^3+R^4+R^5$) by EI. The ions $[CH_2{=}CHC_6HR^2R^3R^5\text{-}OH]^+$ at m/z ($117+R^2+R^3+R^5$) and the satellite ions at m/z ($104+R^2+R^3+R^5$) show higher relative abundances when R^4 correspond to alkoxyl group. Additional low mass alkenyl ions are found at m/z 83, m/z 69 and m/z 55.

The most common chemicals of the identified commercial LCMs are biphenyl derivatives. Due to the various substituent group, the fragment ions appear different pattern (see Table S6). The alkoxyl- and –fluoro-biphenyl derivatives 7-8 (Table S6a) yield $[R^1C_6H_4C_6HR^2R^3R^5\text{-}OH]^+$ ions at m/z ($166+R^1+R^2+R^3+R^5$), the mass spectra also contain peaks at m/z 152 and 151, attributed to biphenyl ions. The cyclohexylbiphenyl derivatives17 and 21-23 (Table S6b) produce characteristic ions at m/z ($176+R^2+R^3+R^4+R^5$) and their satellites at ±13u. The former ions, $[H_2C{=}CHC_6H_4C_6HR^2R^3R^4R^5]^+$, are formed by loss of the neutral fragments $[R^1C_4H_7]$ from the molecular ions. The satellites at m/z ($189+R^2+R^3+R^4+R^5$) and ($163+R^2+R^3+R^4+R^5$) correspond to the (iso)propenylbiphenyl $[H_4C_3C_6H_4C_6HR^2R^3R^4R^5]^+$, and tropylium- or benzyl-like $[H_2CC_6H_4C_6HR^2R^3R^4R^5]^+$ ions, respectively.

The EI mass spectra of the bicyclohexyl biphenyls 24-27 (Table S6d) yield peaks of ions at m/z 216 and satellites at ±13u. The major fragmentation pathways are identical with or analogous to those of the monocyclohexylbiphenyl derivatives. Table S6e exhibits fragments of difluoro-(phenoxy)-methylbiphenyl derivatives 28-31, these compounds give the base peak at m/z ($199+R^1+R^2+R^3+R^5$) and additional ions at m/z ($213+R^2+R^3+R^5$). Compound 6 gives peaks at m/z 238(28%), 181(100%), 165(24%) and 152(5%); compound 32 gives peaks at m/z 375(100%), 346(29%) and 173(16%); and compound 33 gives peaks at m/z 407(45%), 394(60%) and 381(29%) (not tabulated).

The accurate quantitative analysis of the LCMs in smartphones was not possible because authentic and pure analytical standards are not currently commercially available, except those of 2, 3, 5, 6, 9, 10, 17 and 29.

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

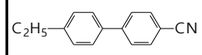
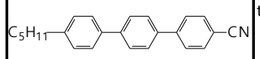
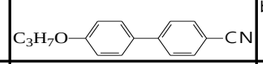
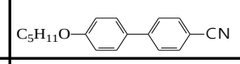
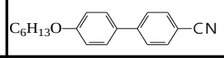
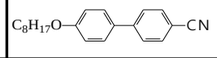
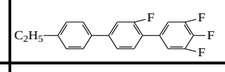
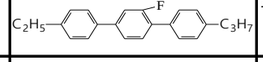
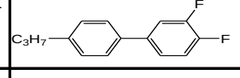
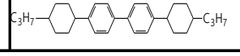
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
1	0058743-75-2		4'-Ethylbiphenyl-4-carbonitril	C(#N)c(ccc(c(ccc(c1)CC)c1)c2)c2	207.3	0.0000145	1.94E-03	2.252	-3.62	4.34	7.96	340.5	2.53	1.0105	0.1776	37.5	75.0	337.5	2.60E-01	Mysid 96-hr LC50	Neutral Organics
2	0054211-46-0		4-Cyano-4''-pentyl-p-terphenyl	C(#N)c(ccc(c(ccc(c(ccc(c1)CCCCC)c1)c2)c2)c3)c3	325.5	1.02E-09	1.36E-07	0.88	-4.37	7.58	11.95	6917	3.84	1.0627	0.0071	37.5	75.0	337.5	5.75E-05	Mysid 96-hr LC50	Neutral Organics
3	0052709-86-1		4'-Propoxy-4-biphenylcarbonitrile	C(#N)c(ccc(c(ccc(OCCC)c1)c1)c2)c2	237.3	2.76E-06	3.67E-04	0.435	-4.77	4.37	9.14	353.5	2.55	1.0735	0.438	37.5	75.0	337.5	2.79E-01	Mysid 96-hr LC50	Neutral Organics
4	0052364-71-3		4-Cyano-4'-pentyloxybiphenyl	C(#N)c(ccc(c(ccc(OCCCCC)c1)c1)c2)c2	265.4	4.98E-07	6.64E-05	0.383	-4.52	5.35	9.87	1572	3.20	1.1686	0.4534	15.0	30.0	135.0	2.10E-02	Mysid 96-hr LC50	Neutral Organics
5	0041424-11-7		4'-(Hexyloxy)-4-biphenylcarbonitrile	C(#N)c(ccc(c(ccc(OCCCCCC)c1)c1)c2)c2	279.4	2.1E-07	2.80E-05	0.365	-4.40	5.84	10.24	3315	3.52	1.1619	0.4611	37.5	75.0	337.5	6.00E-03	Mysid 96-hr LC50	Neutral Organics
6	0052364-73-5		4'-(Octyloxy)-4-biphenylcarbonitrile	C(#N)c(ccc(c(ccc(OCCCCCCC)c1)c1)c2)c2	307.4	3.68E-08	4.90E-06	0.333	-4.15	6.82	10.97	622.7	2.79	1.1485	0.4765	37.5	75.0	337.5	4.33E-04	Mysid 96-hr LC50	Neutral Organics
7	00326894-55-7		4''-Ethyl-2',3,4,5-tetrafluoro-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CC)cc3)cc2)cc(F)c(F)c1	330.3	7.85E-07	1.05E-04	1.594	-2.45	7.36	9.81	8853	3.95	-2.595	-0.1824	180.0	360.0	1620.8	1.06E-04	Mysid 96-hr LC50	Neutral Organics
8	0095759-44-7		4''-Ethyl-2'-fluoro-4-propyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CC)cc3)cc2)ccc(CCC)cc1	318.4	3.61E-08	4.82E-06	0.842	-2.36	8.29	10.65	3106	3.49	-0.1047	-0.1886	60.0	120.0	541.7	8.06E-06	Mysid 96-hr LC50	Neutral Organics
9	00118164-49-1		3,4-difluoro-4'-propyl-1,1'-Biphenyl	c1(c2cc(F)c(F)cc2)ccc(CCC)cc1	232.3	0.000387	5.15E-02	1.764	-1.35	5.69	7.04	2627	3.42	-0.9283	0.1075	60.0	120.0	541.7	7.00E-03	Mysid 96-hr LC50	Neutral Organics
10	0085600-56-2		4,4'-Bis(4-propylcyclohexyl)biphenyl	c1(c4ccc(C3CCC(CCC)CC3)cc4)ccc(C2CCC(CCC)CC2)cc1	402.7	4.94E-10	6.59E-08	0.281	-0.43	12.19	12.62	38.08	1.58	0.6652	-0.0584	60.0	120.0	541.7	2.33E-10	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

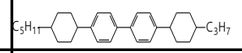
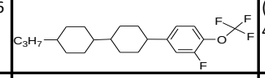
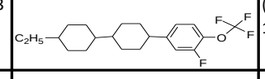
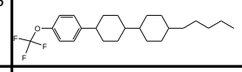
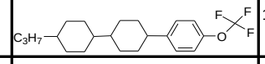
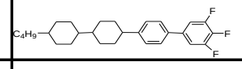
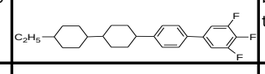
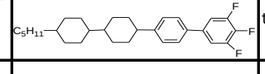
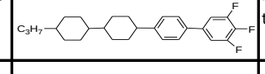
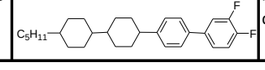
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
11	0080955-71-1		4-(4-Pentylcyclohexyl)-4'-(4-propylcyclohexyl)biphenyl	c1(c4ccc(C3CCC(CCCCC)CC3)cc4)ccc(C2CCC(CCC)CC2)cc1	430.7	1.05E-10	1.40E-08	0.262	-0.18	13.17	13.35	12.57	1.10	0.7603	-0.043	37.5	75.0	337.5	1.69E-11	Mysid 96-hr LC50	Neutral Organics
12	00137810-19-6		4-[3-Fluoro-4-(trifluoromethoxy)phenyl]-4'-propyl-1,1'-bi(cyclohexyl)	c1(OC(F)(F)F)c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)cc1	386.5	3.36E-06	4.48E-04	0.293	0.13	10.14	10.01	383.3	2.58	-0.5803	0.1364	180.0	360.0	1620.8	6.08E-08	Mysid 96-hr LC50	Neutral Organics
13	00139395-96-3		4-Ethyl-4'-[3-fluoro-4-(trifluoromethoxy)phenyl]-1,1'-bi(cyclohexyl)	c1(OC(F)(F)F)c(F)cc(C2CCC(C3CCC(CC)CC3)CC2)cc1	372.5	6.69E-06	8.92E-04	0.305	0.01	9.65	9.64	667	2.82	-0.5736	0.1287	180.0	360.0	1620.8	2.25E-07	Mysid 96-hr LC50	Neutral Organics
14	00133914-49-5		4-pentyl-4'-[4-(trifluoromethoxy)phenyl]-1,1'-Bicyclohexyl	c1(C2CCC(C3CCC(CCCCC)CC3)CC2)ccc(OC(F)(F)F)cc1	396.5	4.88E-07	6.51E-05	0.189	0.31	10.93	10.62	158.6	2.20	0.3334	0.1961	60.0	120.0	541.7	7.33E-09	Mysid 96-hr LC50	Neutral Organics
15	00133937-72-1		4-Propyl-4'-[4-(trifluoromethoxy)phenyl]-1,1'-bi(cyclohexyl)	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(OC(F)(F)F)cc1	368.5	0.0000028	3.74E-04	0.199	0.07	9.94	9.88	480.5	2.68	0.2383	0.1808	180.0	360.0	1620.8	1.00E-07	Mysid 96-hr LC50	Neutral Organics
16	00NA		4'-(4'-butyl[1,1'-bicyclohexyl]-4-yl)-3,4,5-trifluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)c(F)c4)ccc(C2CCC(C3CCC(CCCC)CC3)CC2)cc1	428.6	4.85E-09	6.46E-07	0.331	-0.39	11.75	12.14	62.36	1.80	-1.7234	-0.1274	180.0	360.0	1620.8	8.21E-10	Mysid 96-hr LC50	Neutral Organics
17	00137529-40-9		4'-(4'-ethyl[1,1'-bicyclohexyl]-4-yl)-3,4,5-trifluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)c(F)c4)ccc(C2CCC(C3CCC(CC)CC3)CC2)cc1	400.5	2.35E-08	3.14E-06	0.362	-0.64	10.77	11.41	188.9	2.28	-1.8184	-0.1428	180.0	360.0	1620.8	1.13E-08	Mysid 96-hr LC50	Neutral Organics
18	00137529-43-2		4'-(4'-pentyl[1,1'-bicyclohexyl]-4-yl)-3,4,5-trifluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)c(F)c4)ccc(C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	442.6	2.27E-09	3.02E-07	0.317	-0.27	12.24	12.51	35.83	1.55	-1.73	-0.1197	180.0	360.0	1620.8	2.21E-10	Mysid 96-hr LC50	Neutral Organics
19	00137529-41-0		4'-(4'-propyl[1,1'-bicyclohexyl]-4-yl)-3,4,5-trifluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)c(F)c4)ccc(C2CCC(C3CCC(CCC)CC3)CC2)cc1	414.6	1.16E-08	1.55E-06	0.346	-0.52	11.26	11.78	108.5	2.04	-1.8251	-0.1351	180.0	360.0	1620.8	3.05E-09	Mysid 96-hr LC50	Neutral Organics
20	00136609-96-6		4'-(4'-pentyl[1,1'-bicyclohexyl]-4-yl)-3,4-difluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)cc4)ccc(C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	424.6	1.54E-09	2.06E-07	0.313	-0.34	12.04	12.38	44.93	1.65	-0.9115	-0.0754	180.0	360.0	1620.8	3.67E-10	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

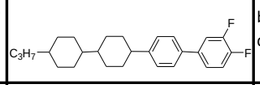
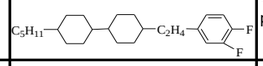
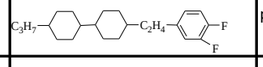
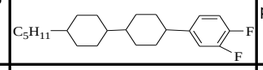
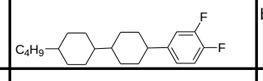
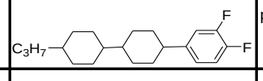
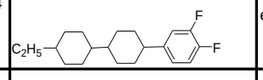
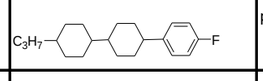
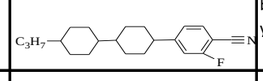
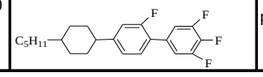
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
21	00119990-81-7		4'-(4'-propyl[1,1'-bicyclohexyl]-4-yl)-3,4-difluoro-1,1'-Biphenyl	c1(c4cc(F)c(F)cc4)ccc(C2CCC(C3CCC(CCC)CC3)CC2)cc1	396.6	9.13E-09	1.22E-06	0.341	-0.58	11.06	11.64	136.1	2.13	-1.0066	-0.0907	180.0	360.0	1620.8	5.05E-09	Mysid 96-hr LC50	Neutral Organics
22	00117923-21-4		4-[2-(3,4-Difluorophenyl)ethyl]-4'-pentyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(CCC2CCC(C3CCC(CCCCC)CC3)CC2)cc1	376.6	4.27E-07	5.70E-05	0.298	1.02	11.26	10.24	108.5	2.04	-0.8886	0.0506	60.0	120.0	541.7	2.77E-09	Mysid 96-hr LC50	Neutral Organics
23	00117943-37-0		4-[2-(3,4-Difluorophenyl)ethyl]-4'-propyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(CCC2CCC(C3CCC(CCC)CC3)CC2)cc1	348.5	2.46E-06	3.28E-04	0.323	0.78	10.28	9.50	328.7	2.52	-0.9837	0.0352	180.0	360.0	1620.8	3.78E-08	Mysid 96-hr LC50	Neutral Organics
24	00118164-51-5		4-(3,4-Difluorophenyl)-4'-pentyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	348.5	2.46E-06	3.28E-04	0.328	0.78	10.28	9.50	328.7	2.52	-0.8753	0.1182	60.0	120.0	541.7	3.78E-08	Mysid 96-hr LC50	Neutral Organics
25	0082832-58-4		4-(3,4-Difluorophenyl)-4'-butyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(C2CCC(C3CCC(CCCC)CC3)CC2)cc1	334.5	5.84E-06	7.78E-04	0.343	0.65	9.79	9.14	572.1	2.76	-0.8686	0.1105	60.0	120.0	541.7	1.39E-07	Mysid 96-hr LC50	Neutral Organics
26	0082832-57-3		4-(3,4-Difluorophenyl)-4'-propyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)cc1	320.5	0.0000138	1.84E-03	0.359	0.53	9.30	8.77	995.7	3.00	-0.9703	0.1028	180.0	360.0	1620.8	5.12E-07	Mysid 96-hr LC50	Neutral Organics
27	00118164-50-4		4-(3,4-Difluorophenyl)-4'-ethyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(C2CCC(C3CCC(CC)CC3)CC2)cc1	306.4	0.0000323	4.30E-03	0.377	0.41	8.81	8.40	1733	3.24	-0.9637	0.0951	180.0	360.0	1620.8	1.88E-06	Mysid 96-hr LC50	Neutral Organics
28	0082832-27-7		4-(4-Fluoro-phenyl)-4'-propyl-bicyclohexyl	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(F)cc1	302.5	0.0000137	1.82E-03	0.348	0.46	9.10	8.64	1248	3.10	-0.1518	0.1472	60.0	120.0	541.7	8.37E-07	Mysid 96-hr LC50	Neutral Organics
29	0093743-04-5		2-Fluoro-4-[4'-propyl-1,1'-bi(cyclohexyl)-4-yl]benzonitrile	C(#N)c1c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)cc1	327.5	3.12E-07	4.16E-05	0.371	-1.55	8.64	10.19	2081	3.32	0.1433	0.1362	60.0	120.0	541.7	3.13E-06	Mysid 96-hr LC50	Neutral Organics
30	00173837-36-0		2,3',4',5'-Tetrafluoro-4-(4-pentylcyclohexyl)biphenyl	c1(c2c(F)cc(C3CCC(CCCCC)CC3)cc2)cc(F)c(F)c(F)c1	378.5	3.96E-07	5.29E-05	0.515	-0.59	9.76	10.35	592.7	2.77	-2.5095	-0.0235	180.0	360.0	1620.8	1.72E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

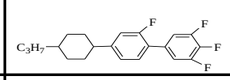
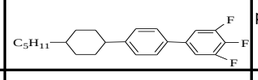
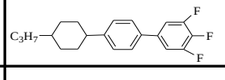
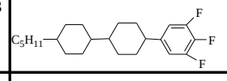
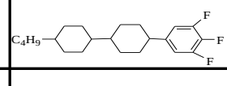
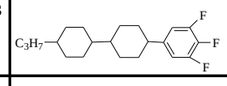
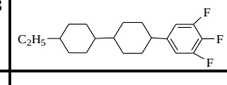
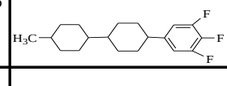
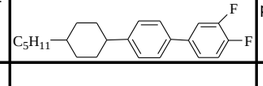
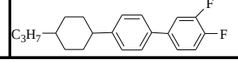
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
31	00173837-35-9		2,3',4',5'-Tetrafluoro-4-(4-propylcyclohexyl)biphenyl	c1(c2c(F)cc(C3CCC(CCC)CC3)cc2)cc(F)c(F)c(F)c1	350.4	0.0000022	2.93E-04	0.596	-0.83	8.78	9.61	1795	3.25	-2.6046	-0.0389	180.0	360.0	1620.8	2.34E-06	Mysid 96-hr LC50	Neutral Organics
32	00137019-95-5		3,4,5-Trifluoro-4'-(4-pentylcyclohexyl)biphenyl	c1(c3cc(F)c(F)c(F)c3)ccc(C2CCC(CCCCC)CC2)cc1	360.5	3.72E-07	4.95E-05	0.512	-0.65	9.56	10.21	743.1	2.87	-1.6909	0.0209	180.0	360.0	1620.8	2.83E-07	Mysid 96-hr LC50	Neutral Organics
33	00132123-39-8		3,4,5-Trifluoro-4'-(4-propylcyclohexyl)biphenyl	c1(c3cc(F)c(F)c(F)c3)ccc(C2CCC(CCC)CC2)cc1	332.4	2.06E-06	2.75E-04	0.592	-0.90	8.57	9.47	2251	3.35	-1.786	0.0055	180.0	360.0	1620.8	3.85E-06	Mysid 96-hr LC50	Neutral Organics
34	00137644-54-3		4-Pentyl-4'-(3,4,5-trifluorophenyl)-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(C2CCC(C3CCC(CCCCC)CC3)CC2)c1	366.5	2.91E-06	3.88E-04	0.323	0.85	10.48	9.64	262.2	2.42	-1.6938	0.0738	180.0	360.0	1620.8	2.29E-08	Mysid 96-hr LC50	Neutral Organics
35	00NA		4-Butyl-4'-(3,4,5-trifluorophenyl)-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(C2CCC(C3CCC(CCCC)CC3)CC2)c1	352.5	5.86E-06	7.82E-04	0.338	0.72	9.99	9.27	456.3	2.66	-1.6871	0.0661	180.0	360.0	1620.8	8.47E-08	Mysid 96-hr LC50	Neutral Organics
36	00131819-23-3		4-Propyl-4'-(3,4,5-trifluorophenyl)-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)c1	338.5	0.0000139	1.85E-03	0.354	0.60	9.50	8.90	794.2	2.90	-1.7889	0.0584	180.0	360.0	1620.8	3.12E-07	Mysid 96-hr LC50	Neutral Organics
37	00139215-80-8		4-Ethyl-4'-(3,4,5-trifluorophenyl)-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(C2CCC(C3CCC(CC)CC3)CC2)c1	324.4	0.0000326	4.35E-03	0.371	0.48	9.01	8.54	1382	3.14	-1.7822	0.0507	180.0	360.0	1620.8	1.15E-06	Mysid 96-hr LC50	Neutral Organics
38	00281680-30-6		4-Methyl-4'-(3,4,5-trifluorophenyl)-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(C2CCC(C3CCC(C)CC3)CC2)c1	310.4	0.0000783	1.04E-02	0.396	0.35	8.52	8.17	2406	3.38	-1.7755	0.0431	180.0	360.0	1620.8	4.22E-06	Mysid 96-hr LC50	Neutral Organics
39	00134412-17-2		3,4-Difluoro-4'-(4-pentylcyclohexyl)biphenyl	c1(c3cc(F)c(F)cc3)ccc(C2CCC(CCCCC)CC2)cc1	342.5	3.48E-07	4.64E-05	0.502	-0.72	9.36	10.08	931.6	2.97	-0.8724	0.0652	60.0	120.0	541.7	4.66E-07	Mysid 96-hr LC50	Neutral Organics
40	0085312-59-0		3,4-Difluoro-4'-(4-propylcyclohexyl)biphenyl	c1(c3cc(F)c(F)cc3)ccc(C2CCC(CCC)CC2)cc1	314.4	1.66E-06	2.21E-04	0.578	-0.97	8.37	9.34	2822	3.45	-0.9675	0.0499	180.0	360.0	1620.8	6.30E-06	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

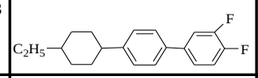
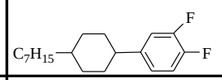
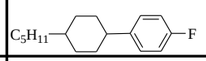
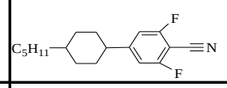
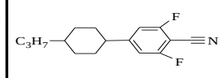
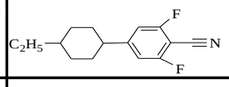
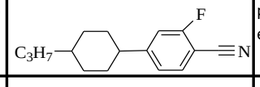
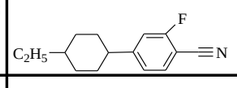
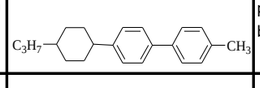
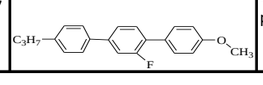
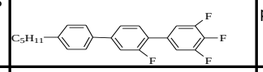
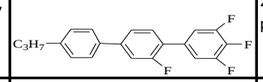
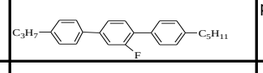
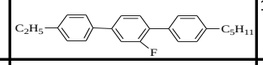
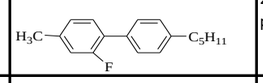
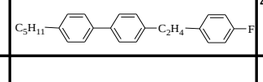
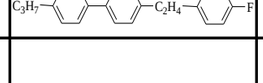
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
41	00134412-18-3		3,4-Difluoro-4'-(4-Ethylcyclohexyl)biphenyl	c1(c3cc(F)c(F)cc3)ccc(C2CCC(CC)CC2)cc1	300.4	3.96E-06	5.27E-04	0.626	-1.09	7.88	8.97	4911	3.69	-0.9608	0.0422	180.0	360.0	1620.8	2.31E-05	Mysid 96-hr LC50	Neutral Organics
42	00139136-72-4		1,2-Difluoro-4-(4-heptylcyclohexyl)benzene	c1(F)c(F)cc(C2CCC(CCCCCCC)CC2)cc1	294.4	0.0000896	1.19E-02	0.475	0.64	8.57	7.93	2251	3.35	-0.8495	0.2741	60.0	120.0	541.7	3.41E-06	Mysid 96-hr LC50	Neutral Organics
43	0076802-61-4		1-Fluoro-4-(4-pentylcyclohexyl)benzene	c1(C2CCC(CCCCC)CC2)ccc(F)cc1	248.4	0.000557	7.43E-02	0.517	0.33	7.39	7.06	8546	3.93	-0.0176	0.3031	37.5	75.0	337.5	7.34E-05	Mysid 96-hr LC50	Neutral Organics
44	0088308-37-6		2,6-difluoro-4-(4-pentylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CCCCC)CC2)cc1F	291.4	0.0000116	1.55E-03	0.562	-1.62	7.14	8.76	11360	4.06	-0.5411	0.2478	60.0	120.0	541.7	1.72E-04	Mysid 96-hr LC50	Neutral Organics
45	00167306-96-9		2,6-difluoro-4-(4-propylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CCC)CC2)cc1F	263.3	0.0000632	8.43E-03	0.66	-1.87	6.16	8.03	5367	3.73	-0.6361	0.2324	180.0	360.0	1620.8	2.00E-03	Mysid 96-hr LC50	Neutral Organics
46	00208844-07-9		2,6-difluoro-4-(4-ethylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CC)CC2)cc1F	249.3	0.000156	2.08E-02	0.723	-1.99	5.67	7.66	2545	3.41	-0.6295	0.2247	180.0	360.0	1620.8	8.00E-03	Mysid 96-hr LC50	Neutral Organics
47	00106021-42-5		2-fluoro-4-(4-propylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CCC)CC2)cc1	245.3	0.0000511	6.81E-03	0.671	-1.93	5.96	7.89	3958	3.60	0.1824	0.2768	60.0	120.0	541.7	4.00E-03	Mysid 96-hr LC50	Neutral Organics
48	00112026-71-8		2-fluoro-4-(4-ethylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CC)CC2)cc1	231.3	0.000127	1.69E-02	0.736	-2.06	5.47	7.53	1877	3.27	0.1891	0.2691	60.0	120.0	541.7	1.30E-02	Mysid 96-hr LC50	Neutral Organics
49	00173306-43-9		4-Methyl-4'-(4-propylcyclohexyl)-1,1'-biphenyl	c1(c2ccc(C3CCC(CCC)CC3)cc2)ccc(C)cc1	292.5	5.87E-07	7.82E-05	0.459	-1.06	8.52	9.58	2392	3.38	0.7176	0.1301	37.5	75.0	337.5	3.92E-06	Mysid 96-hr LC50	Neutral Organics
50	00953049-25-7		2'-Fluoro-4-methoxy-4''-propyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CCC)cc3)c2)ccc(OC)cc1	320.4	3.19E-08	4.25E-06	0.467	-3.76	7.33	11.09	9150	3.96	-0.0284	0.0565	60.0	120.0	541.7	1.12E-04	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
51	00326894-64-8		2',3,4,5-Tetrafluoro-4''-pentyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CCCCC)cc3)cc2)cc(F)c(F)c(F)c1	372.4	6.02E-08	8.02E-06	0.981	-2.08	8.83	10.91	1680	3.23	-2.5066	-0.1593	180.0	360.0	1620.8	2.12E-06	Mysid 96-hr LC50	Neutral Organics
52	00205806-87-7		2',3,4,5-Tetrafluoro-4''-propyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CCC)cc3)cc2)cc(F)c(F)c(F)c1	344.4	3.35E-07	4.47E-05	1.325	-2.33	7.85	10.18	5087	3.71	-2.6017	-0.1747	180.0	360.0	1620.8	2.89E-05	Mysid 96-hr LC50	Neutral Organics
53	0095759-51-6		2'-fluoro-4-pentyl-4''-propyl-1,1': 4', 1''-Terphenyl	c1(c2c(F)cc(c3ccc(CCC)cc3)cc2)ccc(CCCCC)cc1	360.5	2.55E-09	3.40E-07	0.633	-2.00	9.76	11.76	589.3	2.77	-0.0163	-0.1655	60.0	120.0	541.7	1.61E-07	Mysid 96-hr LC50	Neutral Organics
54	0095759-59-4		4''-Ethyl-2'-fluoro-4-pentyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CC)cc3)cc2)ccc(CCCCC)cc1	346.5	6.2E-09	8.27E-07	0.689	-2.12	9.27	11.39	1026	3.01	-0.0096	-0.1732	60.0	120.0	541.7	5.95E-07	Mysid 96-hr LC50	Neutral Organics
55	00NA		2-Fluoro-4-methyl-4'-pentyl-biphenyl	c1(c2c(F)cc(C)cc2)ccc(CCCCC)cc1	256.4	0.0000219	2.91E-03	0.821	-1.13	7.02	8.15	13060	4.12	0.0333	0.1588	37.5	75.0	337.5	2.12E-04	Mysid 96-hr LC50	Neutral Organics
56	00NA		4-[2-(4-fluorophenyl)ethyl]-4'-pentyl-1,1'-biphenyl	c1(c2ccc(CCc3ccc(F)cc3)cc2)ccc(CCCCC)cc1	346.5	1.79E-08	2.39E-06	0.568	-2.10	9.22	11.32	1093	3.04	0.045	-0.2211	60.0	120.0	541.7	6.94E-07	Mysid 96-hr LC50	Neutral Organics
57	00131739-10-1		4-[2-(4-fluorophenyl)ethyl]-4'-propyl-1,1'-biphenyl	c1(c2ccc(CCc3ccc(F)cc3)cc2)ccc(CCC)cc1	318.4	1.03E-07	1.38E-05	0.669	-2.34	8.23	10.57	3310	3.52	-0.05	-0.2365	60.0	120.0	541.7	9.40E-06	Mysid 96-hr LC50	Neutral Organics
58	00NA		4-Fluoro-4'-pentyl-biphenyl	c1(c2ccc(CCCCC)cc2)ccc(F)cc1	242.3	0.0000597	7.96E-03	1.06	-1.17	6.47	7.64	8616	3.94	-0.0147	0.1673	37.5	75.0	337.5	8.98E-04	Mysid 96-hr LC50	Neutral Organics
59	0052364-72-4		4'-(Heptyloxy)-4-biphenylcarbonitrile	C(#N)c1ccc(c2ccc(OCCCCCCC)cc2)cc1	293.4	8.81E-08	1.17E-05	0.348	-4.28	6.33	10.61	6991	3.85	1.1552	0.4688	37.5	75.0	337.5	1.58E-03	Mysid 96-hr LC50	Neutral Organics
60	0052709-87-2		4'-(Butyloxy)-4-biphenylcarbonitrile	C(#N)c1ccc(c2ccc(OCCCC)cc2)cc1	251.3	1.18E-06	1.57E-04	0.404	-4.65	4.86	9.51	745.5	2.87	1.1752	0.4457	15.0	30.0	135.0	7.70E-02	Mysid 96-hr LC50	Neutral Organics

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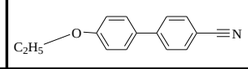
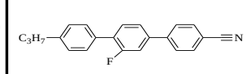
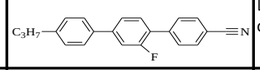
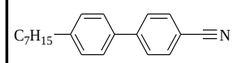
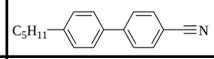
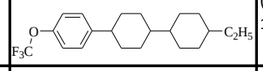
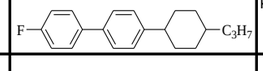
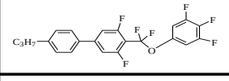
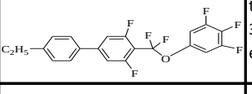
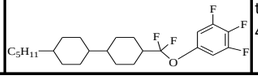
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
61	0058743-78-5		4'-(Ethyloxy)-4-biphenylcarbonitrile	C(#N)c1ccc(c2ccc(OCC)cc2)cc1	223.3	6.43E-06	8.57E-04	0.527	-4.89	3.88	8.77	167.6	2.22	1.0802	0.4303	37.5	75.0	337.5	1.01E+00	Mysid 96-hr LC50	Neutral Organics
62	00116831-09-5		3'-Fluoro-4''-propyl-[1,1':4',1''-terphenyl]-4-carbonitrile	c1(c2c(F)cc(c3ccc(C(#N))cc3)cc2)ccc(CCC)cc1	315.4	6.61E-09	8.82E-07	1.306	-4.55	6.80	11.35	14200	4.15	0.1491	-0.0526	60.0	120.0	541.7	4.75E-04	Mysid 96-hr LC50	Neutral Organics
63	00127523-43-7		2'-Fluoro-4''-propyl-[1,1':4',1''-terphenyl]-4-carbonitrile	c1(c2c(F)cc(c3ccc(CCC)cc3)cc2)ccc(C(#N))cc1	315.4	6.61E-09	8.82E-07	1.24	-4.55	6.80	11.35	14200	4.15	0.1491	-0.0526	60.0	120.0	541.7	4.75E-04	Mysid 96-hr LC50	Neutral Organics
64	0041122-71-8		4'-Heptyl-4-biphenylcarbonitrile	C(#N)c1ccc(c2ccc(CCCCCCC)cc2)cc1	277.4	2.38E-07	3.17E-05	0.909	-3.01	6.80	9.81	14200	4.15	1.0856	0.216	37.5	75.0	337.5	4.18E-04	Mysid 96-hr LC50	Neutral Organics
65	0040817-08-1		4'-Pentyl-4-biphenylcarbonitrile	C(#N)c1ccc(c2ccc(CCCCC)cc2)cc1	249.4	1.33E-06	1.77E-04	1.197	-3.25	5.82	9.07	3193	3.50	1.0989	0.2007	15.0	30.0	135.0	6.00E-03	Mysid 96-hr LC50	Neutral Organics
66	00135734-59-7		4-Ethyl-4'-[4-(trifluoromethoxy)phenyl]-1,1'-bi(cyclohexyl)	c1(C2CCC(C3CCC(CC)CC3)CC2)ccc(OC(F)(F)F)cc1	354.5	6.66E-06	8.87E-04	0.205	-0.06	9.45	9.51	836.2	2.92	0.245	0.1731	60.0	120.0	541.7	3.71E-07	Mysid 96-hr LC50	Neutral Organics
67	0087260-24-0		4-Fluoro-4'-(4-propylcyclohexyl)biphenyl	c1(c2ccc(C3CCC(CCC)CC3)cc2)ccc(F)cc1	296.4	1.65E-06	2.20E-04	0.544	-1.03	8.17	9.20	3537	3.55	-0.1489	0.0942	60.0	120.0	541.7	1.03E-05	Mysid 96-hr LC50	Neutral Organics
68	00303186-20-1		4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl	C(F)(F)(c3c(F)cc(c2ccc(CCC)cc2)cc3F)Oc1cc(F)c(F)c(F)c1	428.4	3.41E-07	4.55E-05	0.478	-2.87	9.10	11.97	1241	3.09	-3.5037	-0.1178	180.0	360.0	1620.8	1.17E-06	Mysid 96-hr LC50	Neutral Organics
69	00303186-19-8		4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-ethylbiphenyl	C(F)(F)(c3c(F)cc(c2ccc(CC)cc2)cc3F)Oc1cc(F)c(F)c(F)c1	414.3	6.7E-07	8.94E-05	0.509	-2.99	8.61	11.60	2161	3.34	-3.497	-0.1255	180.0	360.0	1620.8	4.34E-06	Mysid 96-hr LC50	Neutral Organics
70	00208338-52-7		4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-4'-pentyl-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(OC(F)(F)C2CCC(C3CCC(CCCCC)CC3)CC2)c1	432.5	8.36E-07	1.11E-04	0.273	0.30	11.53	11.24	80.22	1.90	-1.8319	0.1972	180.0	360.0	1620.8	1.53E-09	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

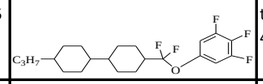
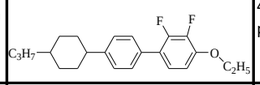
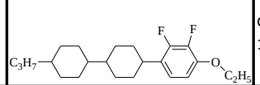
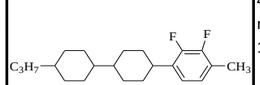
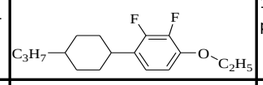
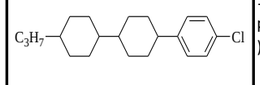
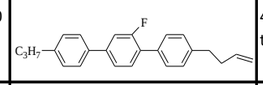
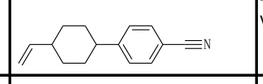
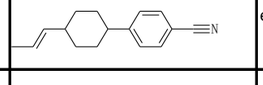
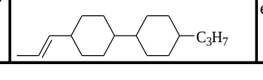
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
71	00208338-50-5		4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-4'-propyl-1,1'-bi(cyclohexyl)	c1(F)c(F)c(F)cc(OC(F)(F)C2CCC(C3CCC(CCC)CC3)CC2)c1	404.5	0.0000046	6.13E-04	0.295	0.05	10.55	10.50	243	2.39	-1.927	0.1819	180.0	360.0	1620.8	2.11E-08	Mysid 96-hr LC50	Neutral Organics
72	00189750-98-9		4-Ethoxy-2,3-difluoro-4'-(4-propylcyclohexyl)biphenyl	c1(c3c(F)c(F)c(OCC)cc3)ccc(C2CCC(CCC)CC2)cc1	358.5	1.16E-07	1.55E-05	0.36	-2.07	8.95	11.02	1480	3.17	-0.8565	0.1556	180.0	360.0	1620.8	1.50E-06	Mysid 96-hr LC50	Neutral Organics
73	00123560-48-5		4-(4-Ethoxy-2,3-difluorophenyl)-4'-propyl-1,1'-bi(cyclohexyl)	c1(OCC)c(F)c(F)c(C2CCC(C3CCC(CCC)CC3)CC2)cc1	364.5	9.29E-07	1.24E-04	0.238	-0.57	9.87	10.44	522.2	2.72	-0.8594	0.2086	180.0	360.0	1620.8	1.22E-07	Mysid 96-hr LC50	Neutral Organics
74	00174350-06-2		4-(2,3-Difluoro-4-methylphenyl)-4'-propyl-1,1'-bi(cyclohexyl)	c1(C)c(F)c(F)c(C2CCC(C3CCC(CCC)CC3)CC2)cc1	334.5	0.000005	6.67E-04	0.35	0.57	9.85	9.28	537	2.73	-0.9223	0.0943	180.0	360.0	1620.8	1.19E-07	Mysid 96-hr LC50	Neutral Organics
75	00174350-05-1		1-Ethoxy-2,3-difluoro-4-(4-propylcyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(CCC)CC2)cc1	282.4	0.000165	2.20E-02	0.334	-0.96	7.18	8.14	10830	4.04	-0.8203	0.3492	180.0	360.0	1620.8	1.48E-04	Mysid 96-hr LC50	Neutral Organics
76	00NA		1-chloro-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(CL)cc1	318.9	2.52E-06	3.36E-04	0.363	0.27	9.54	9.27	756.3	2.88	0.468	0.087	60.0	120.0	54.2	2.61E-07	Mysid 96-hr LC50	Neutral Organics
77	00915956-24-0		4-(3-Buten-1-yl)-2'-fluoro-4''-propyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(CCC)cc3)cc2)ccc(CCC=C)cc1	344.5	6.68E-09	8.91E-07	0.266	-2.25	9.14	11.39	1196	3.08	-0.1171	-0.1985	60.0	120.0	54.2	8.59E-07	Mysid 96-hr LC50	Neutral Organics
78	0096184-42-8		4-(4-Vinylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(C=C)CC2)cc1	211.3	0.000133	1.78E-02	0.277	-2.25	5.13	7.38	1125	3.05	1.0086	0.2882	37.5	75.0	337.5	3.10E-02	Mysid 96-hr LC50	Neutral Organics
79	0096184-40-6		4-(4-(prop-1-enyl)cyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(C=CC)CC2)cc1	225.3	0.0000428	5.70E-03	0.155[Cis-isomer]	-2.06	5.54	7.60	2106	3.32	1.0019	0.2407	37.5	75.0	337.5	1.10E-02	Mysid 96-hr LC50	Neutral Organics
80	00279246-65-0		4-(4-(prop-1-enyl)cyclohexyl)benzonitrile	C1(C=CC)CCC(C2CCC(CCC)CC2)CC1	248.5	0.00146	1.95E-01	0.127[Cis-isomer]	1.81	8.45	6.65	2599	3.42	0.6293	0.2926	37.5	75.0	337.5	4.08E-06	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

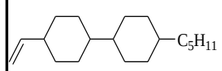
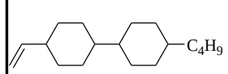
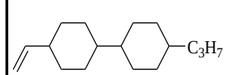
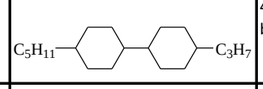
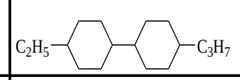
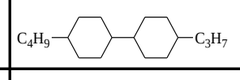
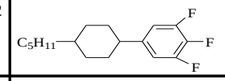
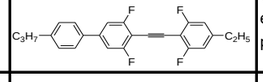
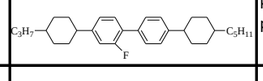
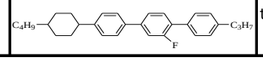
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
81	00129738-34-7		4-Pentyl-4'-vinyl-1,1'-bi(cyclohexyl)	C(=C)C1CCC(C2CCC(CCCCC)CC2)CC1	262.5	0.00068	9.06E-02	0.188	1.86	9.02	7.17	1367	3.14	0.731	0.3555	15.0	30.0	135.0	9.05E-07	Mysid 96-hr LC50	Neutral Organics
82	00153429-47-1		4-Butyl-4'-vinyl-1,1'-bi(cyclohexyl)	C(=C)C1CCC(C2CCC(CCCC)CC2)CC1	248.5	0.0017	2.26E-01	0.193	1.73	8.53	6.80	2378	3.38	0.7377	0.3478	15.0	30.0	135.0	3.29E-06	Mysid 96-hr LC50	Neutral Organics
83	00477557-80-5		4-Propyl-4'-vinyl-1,1'-bi(cyclohexyl)	C(=C)C1CCC(C2CCC(CCC)CC2)CC1	234.4	0.00434	5.78E-01	0.198	1.61	8.03	6.42	4139	3.62	0.6359	0.3401	37.5	75.0	337.5	1.19E-05	Mysid 96-hr LC50	Neutral Organics
84	0092263-41-7		4-Pentyl-4'-propyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCCCC)CC2)CCC(CCC)CC1	278.5	0.000261	3.48E-02	0.314	2.39	9.64	7.26	673.2	2.83	0.7234	0.3884	15.0	30.0	135.0	1.72E-07	Mysid 96-hr LC50	Neutral Organics
85	0096624-41-8		4-Ethyl-4'-propyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCC)CC2)CCC(CC)CC1	236.4	0.00403	5.38E-01	0.359	2.02	8.17	6.15	3549	3.55	0.635	0.3654	37.5	75.0	337.5	8.27E-06	Mysid 96-hr LC50	Neutral Organics
86	0096624-52-1		4-Butyl-4'-propyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCCC)CC2)CCC(CCC)CC1	264.5	0.000626	8.35E-02	0.328	2.26	9.15	6.89	1172	3.07	0.7301	0.3808	15.0	30.0	135.0	6.27E-07	Mysid 96-hr LC50	Neutral Organics
87	00131819-22-2		1,2,3-Trifluoro-5-(4-pentylcyclohexyl)benzene	c1(F)c(F)c(F)cc(C2CCC(CCCCC)CC2)c1	284.4	0.000615	8.19E-02	0.529	0.46	7.79	7.33	5437	3.74	-1.6547	0.2144	180.0	360.0	1620.8	2.80E-05	Mysid 96-hr LC50	Neutral Organics
88	00NA		3,5-Difluoro-4-[2-(2,6-difluoro-4-ethylphenyl)ethynyl]-4'-propyl-1,1'-biphenyl	C(c3c(F)cc(c2ccc(CCC)cc2)cc3F)#Cc1c(F)cc(CC)cc1F	396.4	1.09E-08	1.45E-06	0.271	-3.01	9.16	12.17	1167	3.07	-2.5718	-0.3931	180.0	360.0	1620.8	9.31E-07	Mysid 96-hr LC50	Neutral Organics
89	0099896-05-6		2-Fluoro-4'-(4-pentylcyclohexyl)-4-(4-propylcyclohexyl)biphenyl	c1(c4c(F)cc(C3CCC(CCC)CC3)cc4)ccc(C2CCC(CCCCC)CC2)cc1	448.7	1.19E-10	1.58E-08	0.269	-0.12	13.37	13.49	10.03	1.00	-0.0583	-0.0874	60.0	120.0	541.7	1.02E-11	Mysid 96-hr LC50	Neutral Organics
90	00915021-67-9		4''-(4-Butylcyclohexyl)-2'-fluoro-4-propyl-1,1':4',1''-terphenyl	c1(c2c(F)cc(c3ccc(C4CCC(CCC)CC4)cc3)cc2)ccc(CCC)cc1	428.6	3.5E-11	4.66E-09	0.384	-1.74	11.96	13.70	49.46	1.69	-0.0487	-0.2309	60.0	120.0	541.7	4.68E-10	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

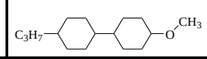
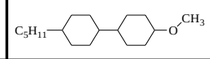
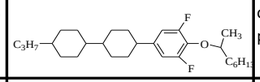
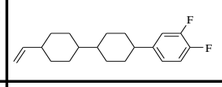
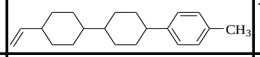
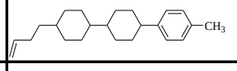
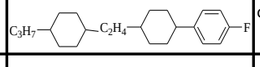
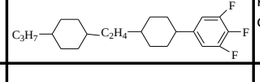
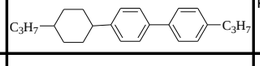
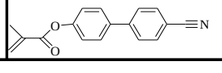
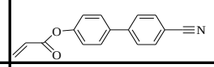
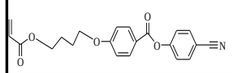
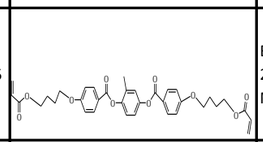
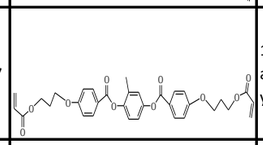
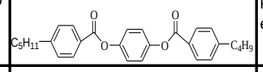
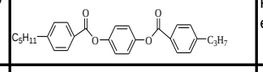
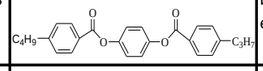
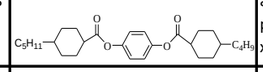
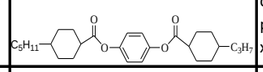
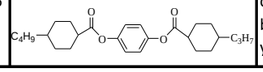
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
91	0097398-80-6		4-Methoxy-4'-propyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCC)CC2)CCC(OC)CC1	238.4	0.0033	4.40E-01	0.245	-0.44	6.42	6.86	8041	3.91	0.2867	0.3116	37.5	75.0	337.5	1.00E-03	Mysid 96-hr LC50	Neutral Organics
92	00102714-95-4		4-Methoxy-4'-pentyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCCCC)CC2)CCC(OC)CC1	266.5	0.000434	5.78E-02	0.23	-0.20	7.41	7.61	8417	3.93	0.3818	0.3269	15.0	30.0	135.0	7.59E-05	Mysid 96-hr LC50	Neutral Organics
93	00185207-90-3		4-[3,5-Difluoro-4-(2-octanyloxy)phenyl]-4'-propyl-1,1'-bi(cyclohexyl)	c1(F)c(OC(C)CCCCCC)c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)c1	448.7	9.08E-09	1.21E-06	0.192	0.16	12.74	12.58	20.42	1.31	-0.791	0.1056	180.0	360.0	1620.8	5.71E-11	Mysid 96-hr LC50	Neutral Organics
94	00142400-92-8		4-(3,4-Difluorophenyl)-4'-vinyl-1,1'-bi(cyclohexyl)	c1(F)c(F)cc(C2CCC(C3CCC(C=C)CC3)CC2)cc1	304.4	0.0000348	4.64E-03	0.203	0.28	8.67	8.39	2021	3.31	-0.9627	0.0698	180.0	360.0	1620.8	2.71E-06	Mysid 96-hr LC50	Neutral Organics
95	00155041-85-3		4-(4-Methylphenyl)-4'-vinyl-1,1'-bi(cyclohexyl)	c1(C2CCC(C3CCC(C=C)CC3)CC2)ccc(C)cc1	282.5	0.0000126	1.68E-03	0.188	0.19	8.82	8.63	1713	3.23	0.7224	0.1501	37.5	75.0	337.5	1.69E-06	Mysid 96-hr LC50	Neutral Organics
96	00129738-42-7		4-(3-Buten-1-yl)-4'-(4-methylphenyl)-1,1'-bi(cyclohexyl)	c1(C2CCC(C3CCC(CCC=C)CC3)CC2)ccc(C)cc1	310.5	2.25E-06	2.99E-04	0.178	0.44	9.80	9.37	565.6	2.75	0.7091	0.1654	37.5	75.0	337.5	1.26E-07	Mysid 96-hr LC50	Neutral Organics
97	0091162-04-8		1-Fluoro-4-{4-[2-(4-propylcyclohexyl)ethyl]cyclohexyl}benzene	c1(C2CCC(CCC3CCC(CCC)CC3)CC2)ccc(F)cc1	330.5	2.44E-06	3.26E-04	0.319	0.71	10.08	9.37	412.1	2.62	-0.1651	0.1625	60.0	120.0	541.7	6.20E-08	Mysid 96-hr LC50	Neutral Organics
98	00131819-24-4		1,2,3-Trifluoro-5-{4-[2-(4-propylcyclohexyl)ethyl]cyclohexyl}benzene	c1(F)c(F)c(F)cc(C2CCC(CCC3CCC(CCC)CC3)CC2)c1	366.5	2.91E-06	3.88E-04	0.323	0.85	10.48	9.64	262.2	2.42	-1.8022	0.0738	180.0	360.0	1620.8	2.29E-08	Mysid 96-hr LC50	Neutral Organics
99	00122957-72-6		4-Propyl-4'-(4-propylcyclohexyl)biphenyl	c1(c2ccc(C3CCC(CCC)CC3)cc2)ccc(CCC)cc1	320.5	0.0000001	1.34E-05	0.418	-0.81	9.50	10.31	789.6	2.90	0.7043	-0.0007	37.5	75.0	337.5	2.92E-07	Mysid 96-hr LC50	Neutral Organics
100	00NA		2-methyl-2-Propenoic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester	C(#N)c1ccc(c2ccc(OC(=O)C(=C)C)cc2)cc1	263.3	5.84E-07	7.78E-05	0.52	-5.79	3.80	9.59	150	2.18	1.1034	0.4228	37.5	75.0	337.5	2.16E+00	Green Algae 96-hr EC50	Methacrylates

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
101	0067483-58-3		2-Propenoic acid, 4'-cyano[1,1'-biphenyl]-4-yl ester	C(#N)c1ccc(c2ccc(OC(=O)C=C)cc2)cc1	249.3	9.94E-07	1.32E-04	0.919	-5.98	3.26	9.24	65.31	1.82	1.1101	0.4703	37.5	75.0	337.5	3.26E-01	Mysid 96-hr LC50	Acrylates
102	00NA		4-cyanophenyl 4-(4-(acryloyloxy)butoxy)benzoate	C(#N)c1cc(OC(=O)c2ccc(OCCCCOC(=O)C=C)cc2)ccc1	365.4	1.28E-08	1.71E-06	0.247	-9.06	4.04	13.10	215.5	2.33	1.3609	0.8614	37.5	75.0	337.5	2.09E-01	Mysid 96-hr LC50	Acrylates + Esters
103	00132900-75-5		Benzoic acid, 4-[4-[(1-oxo-2-propenyl)oxy]butoxy]-, 2-Methyl-1,4-phenylene ester	O=C(c3ccc(OCCCCOC(=O)C=C)cc3)Oc1c(C)cc(OC(=O)c2ccc(OCCCCOC(=O)C=C)cc2)cc1	616.7	2.01E-15	2.68E-13	0.119	-13.38	8.22	21.60	847.6	2.93	1.4692	1.2073	60.0	120.0	541.7	9.11E-04	Mysid 96-hr LC50	Acrylates + Esters
104	00174063-87-7		1,4-Bis-[4-(3-acryloyloxypropyloxy)benzoyloxy]-2-methylbenzene	O=C(c3ccc(OCCCOC(=O)C=C)cc3)Oc1c(C)cc(OC(=O)c2ccc(OCCCOC(=O)C=C)cc2)cc1	588.6	1.13E-14	1.51E-12	0.122	-13.63	7.24	20.87	10140	4.01	1.4825	1.1919	37.5	75.0	337.5	6.00E-03	Mysid 96-hr LC50	Acrylates + Esters
105	00199540-46-0		4-Butylbenzoic acid 4-[(4-pentylbenzoyl)oxy]phenyl ester	O=C(c3ccc(CCCCC)cc3)Oc1ccc(OC(=O)c2ccc(CCCC)cc2)cc1	444.6	1.3E-10	1.73E-08	0.549	-4.96	9.31	14.27	248.9	2.40	1.2105	0.3121	15.0	30.0	135.0	8.36E-05	Mysid 96-hr LC50	Esters
106	00199540-45-9		4-Propylbenzoic acid 4-[(4-pentylbenzoyl)oxy]phenyl ester	O=C(c3ccc(CCCCC)cc3)Oc1ccc(OC(=O)c2ccc(CCC)cc2)cc1	430.6	3.27E-10	4.36E-08	0.592	-5.08	8.82	13.90	1711	3.23	1.1087	0.3044	37.5	75.0	337.5	2.06E-04	Mysid 96-hr LC50	Esters
107	00199540-44-8		4-Propylbenzoic acid 4-[(4-butylbenzoyl)oxy]phenyl ester	O=C(c3ccc(CCCC)cc3)Oc1ccc(OC(=O)c2ccc(CCC)cc2)cc1	416.5	8.18E-10	1.09E-07	0.642	-5.20	8.33	13.53	2977	3.47	1.1154	0.2968	37.5	75.0	337.5	5.05E-04	Mysid 96-hr LC50	Esters
108	00175784-02-8		4-Butylcyclohexanecarboxylic acid 4-[[(4-pentylcyclohexyl)carbonyl]oxy]phenyl ester	O=C(C3CCC(CCCCC)CC3)Oc1ccc(OC(=O)C2CCC(CCCC)CC2)cc1	456.7	2.21E-09	2.94E-07	0.339	-2.87	10.68	13.55	53.08	1.73	1.0954	0.6282	15.0	30.0	135.0	6.37E-06	Mysid 96-hr LC50	Esters
109	00175784-01-7		4-Propylcyclohexanecarboxylic acid 4-[[(4-pentylcyclohexyl)carbonyl]oxy]phenyl ester	O=C(C3CCC(CCCCC)CC3)Oc1ccc(OC(=O)C2CCC(CCC)CC2)cc1	442.6	5.61E-09	7.48E-07	0.355	-2.99	10.19	13.18	364.8	2.56	0.9936	0.6205	15.0	30.0	135.0	1.57E-05	Mysid 96-hr LC50	Esters
110	00175784-00-6		4-Propylcyclohexanecarboxylic acid 4-[[(4-butylcyclohexyl)carbonyl]oxy]phenyl ester	O=C(C3CCC(CCCC)CC3)Oc1ccc(OC(=O)C2CCC(CCC)CC2)cc1	428.6	1.42E-08	1.89E-06	0.373	-3.12	9.70	12.82	634.9	2.80	1.0003	0.6128	15.0	30.0	135.0	3.86E-05	Mysid 96-hr LC50	Esters

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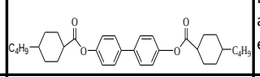
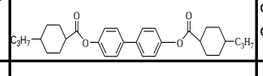
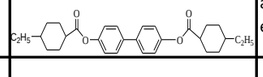
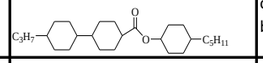
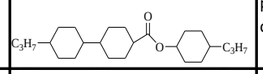
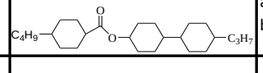
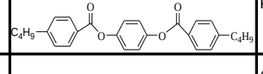
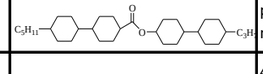
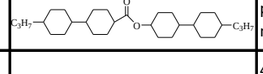
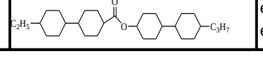
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
111	00398138-22-2		4-Butylcyclohexanecarboxylic acid [1,1'-biphenyl]-4,4'-diyl ester	c1(c4ccc(OC(=O)C3CCC(CCCC)CC3)cc4)ccc(OC(=O)C2CCC(CCCC)CC2)cc1	518.7	1.54E-12	2.05E-10	0.318	-4.11	11.27	15.38	107.4	2.03	1.0658	0.427	15.0	30.0	135.0	2.35E-06	Mysid 96-hr LC50	Esters
112	00398138-21-1		4-Propylcyclohexanecarboxylic acid [1,1'-biphenyl]-4,4'-diyl ester	c1(c4ccc(OC(=O)C3CCC(CCC)CC3)cc4)ccc(OC(=O)C2CCC(CCC)CC2)cc1	490.7	1.01E-11	1.34E-09	0.348	-4.36	10.29	14.65	325.2	2.51	0.8623	0.4116	37.5	75.0	337.5	1.43E-05	Mysid 96-hr LC50	Esters
113	00190731-46-5		4-Ethylcyclohexanecarboxylic acid [1,1'-biphenyl]-4,4'-diyl ester	c1(c4ccc(OC(=O)C3CCC(CC)CC3)cc4)ccc(OC(=O)C2CCC(CC)CC2)cc1	462.6	6.49E-11	8.65E-09	0.383	-4.60	9.31	13.91	985.1	2.99	0.8757	0.3963	37.5	75.0	337.5	8.73E-05	Mysid 96-hr LC50	Esters
114	00102714-87-4		4-Pentylcyclohexanecarboxylic acid 4'-propyl[1,1'-bicyclohexyl]-4-yl ester	O=C(C3CCC(C2CCC(CCC)CC2)CC3)OC1CCC(CCCCC)CC1	404.7	2.37E-08	3.16E-06	0.236	-0.26	11.38	11.64	94.88	1.98	0.8375	0.4607	37.5	75.0	337.5	1.49E-06	Mysid 96-hr LC50	Esters
115	0083242-83-5		4-propylcyclohexyl -4'-propyl[1,1'-bicyclohexyl]-4-carboxylate	O=C(C3CCC(C2CCC(CCC)CC2)CC3)OC1CCC(CCC)CC1	376.6	1.41E-07	1.88E-05	0.252	-0.50	10.40	10.90	287.4	2.46	0.7424	0.4453	37.5	75.0	337.5	8.94E-06	Mysid 96-hr LC50	Esters
116	00NA		4-Butylcyclohexanecarboxylic acid 4'-propyl[1,1'-bicyclohexyl]-4-yl ester	O=C(C3CCC(CCCC)CC3)OC1CCC(C2CCC(CCC)CC2)CC1	390.7	5.81E-08	7.74E-06	0.244	-0.38	10.89	11.27	165.1	2.22	0.8442	0.453	15.0	30.0	135.0	3.65E-06	Mysid 96-hr LC50	Esters
117	0079892-74-3		4-Butylbenzoic acid 1,4-phenylene ester	O=C(c3ccc(CCCC)cc3)Oc1ccc(OC(=O)c2ccc(CCCC)cc2)cc1	430.6	3.27E-10	4.36E-08	0.592	-5.08	8.82	13.90	1711	3.23	1.2171	0.3044	15.0	30.0	135.0	2.06E-04	Mysid 96-hr LC50	Esters
118	00NA		4-(4-propylcyclohexyl)cyclohexyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCCCC)CC4)CC3)OC1CCC(C2CCC(CCC)CC2)CC1	486.8	1.08E-10	1.44E-08	0.184	0.13	14.07	13.95	4.575	0.66	0.7984	0.3201	37.5	75.0	337.5	1.09E-08	Mysid 96-hr LC50	Esters
119	00NA		4-(4-propylcyclohexyl)cyclohexyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCC)CC4)CC3)OC1CCC(C2CCC(CCC)CC2)CC1	458.8	6.56E-10	8.74E-08	0.193	-0.12	13.09	13.21	13.86	1.14	0.7033	0.3047	37.5	75.0	337.5	6.62E-08	Mysid 96-hr LC50	Esters
120	00NA		4-(4-propylcyclohexyl)cyclohexyl 4-(4-ethylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CC)CC4)CC3)OC1CCC(C2CCC(CCC)CC2)CC1	444.8	1.6E-09	2.14E-07	0.198	-0.25	12.60	12.85	24.12	1.38	0.71	0.297	37.5	75.0	337.5	1.63E-07	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

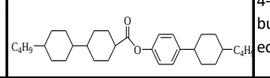
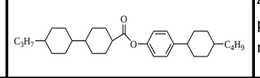
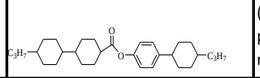
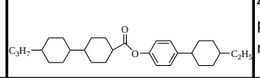
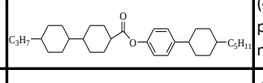
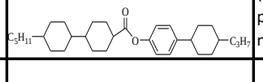
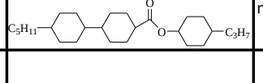
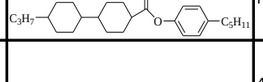
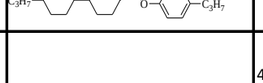
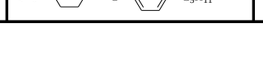
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
121	00184652-93-5		4-(4-butylcyclohexyl)phenyl 4-(4-butylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCCC)CC4)CC3)Oc1ccc(C2CCC(CCCC)CC2)cc1	480.8	4.36E-11	5.82E-09	0.228	-0.65	13.15	13.80	12.97	1.11	0.9644	0.2449	15.0	30.0	135.0	6.20E-08	Mysid 96-hr LC50	Esters
122	00115978-59-1		4-(4-butylcyclohexyl)phenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCC)CC4)CC3)Oc1ccc(C2CCC(CCCC)CC2)cc1	466.8	1.06E-10	1.42E-08	0.235	-0.77	12.65	13.42	22.57	1.35	0.8626	0.2372	37.5	75.0	337.5	1.53E-07	Mysid 96-hr LC50	Esters
123	0088038-92-0		4-(4-propylcyclohexyl)phenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCC)CC4)CC3)Oc1ccc(C2CCC(CCC)CC2)cc1	452.7	2.58E-10	3.44E-08	0.243	-0.89	12.16	13.05	39.27	1.59	0.7609	0.2296	37.5	75.0	337.5	3.77E-07	Mysid 96-hr LC50	Esters
124	00202830-70-4		4-(4-ethylcyclohexyl)phenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCC)CC4)CC3)Oc1ccc(C2CCC(CC)CC2)cc1	438.7	4.87E-10	6.49E-08	0.251	-1.02	11.67	12.69	68.35	1.84	0.7675	0.2219	37.5	75.0	337.5	9.28E-07	Mysid 96-hr LC50	Esters
125	00131790-57-3		4-(4-pentylcyclohexyl)phenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCC)CC4)CC3)Oc1ccc(C2CCC(CCCC)CC2)cc1	480.8	4.36E-11	5.82E-09	0.228	-0.65	13.15	13.80	12.97	1.11	0.8559	0.2449	37.5	75.0	337.5	6.20E-08	Mysid 96-hr LC50	Esters
126	0091545-93-6		4-(4-propylcyclohexyl)phenyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C4CCC(CCCCC)CC4)CC3)Oc1ccc(C2CCC(CC)CC2)cc1	480.8	4.36E-11	5.82E-09	0.228	-0.65	13.15	13.80	12.97	1.11	0.8559	0.2449	37.5	75.0	337.5	6.20E-08	Mysid 96-hr LC50	Esters
127	0094732-93-1		4-propylcyclohexyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C2CCC(CCCCC)CC2)CC3)OC1CCC(CCC)CC1	404.7	2.37E-08	3.16E-06	0.236	-0.26	11.38	11.64	94.88	1.98	0.8375	0.4607	37.5	75.0	337.5	1.49E-06	Mysid 96-hr LC50	Esters
128	0084078-44-4		4-pentylphenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C2CCC(CCC)CC2)CC3)Oc1ccc(CCCCC)cc1	398.6	8.22E-09	1.10E-06	0.309	-1.03	10.46	11.49	268.9	2.43	0.895	0.3026	37.5	75.0	337.5	8.46E-06	Mysid 96-hr LC50	Esters
129	0097564-42-6		4-propylphenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C2CCC(CCC)CC2)CC3)Oc1ccc(CCC)cc1	370.6	4.77E-08	6.36E-06	0.336	-1.28	9.48	10.76	814.3	2.91	0.8	0.2872	37.5	75.0	337.5	5.07E-05	Mysid 96-hr LC50	Esters
130	0070602-95-8		4-pentylphenyl 4-butylcyclohexanecarboxylate	O=C(C2CCC(CCCC)CC2)Oc1ccc(CCCCC)cc1	330.5	6.56E-07	8.75E-05	0.462	-1.29	8.26	9.55	811.2	2.91	1.0359	0.4509	15.0	30.0	135.0	4.54E-04	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

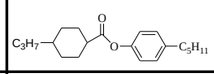
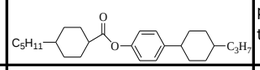
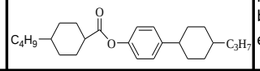
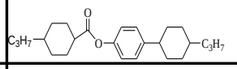
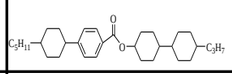
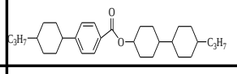
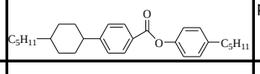
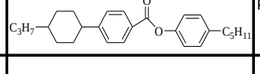
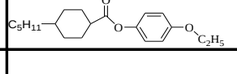
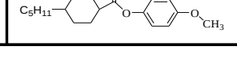
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
131	0076025-60-0		4-pentylphenyl 4-propylcyclohexanecarboxylate	O=C(C2CCC(CCC)CC2)Oc1ccc(CCCCC)cc1	316.5	1.57E-06	2.10E-04	0.492	-1.41	7.77	9.18	5575	3.75	0.9342	0.4432	15.0	30.0	135.0	1.10E-03	Mysid 96-hr LC50	Esters
132	0083242-82-4		4-(4-propylcyclohexyl)phenyl 4-pentylcyclohexanecarboxylate	O=C(C3CCC(CCCCC)CC3)Oc1ccc(C2CCC(CCC)CC2)cc1	398.6	8.22E-09	1.10E-06	0.314	-1.03	10.46	11.49	268.9	2.43	0.895	0.3855	37.5	75.0	337.5	8.46E-06	Mysid 96-hr LC50	Esters
133	0084540-35-2		4-(4-propylcyclohexyl)phenyl 4-butylcyclohexanecarboxylate	O=C(C3CCC(CCCC)CC3)Oc1ccc(C2CCC(CCC)CC2)cc1	384.6	1.98E-08	2.65E-06	0.328	-1.15	9.97	11.12	467.9	2.67	0.9017	0.3778	37.5	75.0	337.5	2.07E-05	Mysid 96-hr LC50	Esters
134	0084207-06-7		4-(4-propylcyclohexyl)phenyl 4-propylcyclohexanecarboxylate	c1(C3CCC(CCC)CC3)ccc(OC(=O)C2CCC(CCC)CC2)cc1	370.6	4.77E-08	6.36E-06	0.343	-1.28	9.48	10.76	814.3	2.91	0.8	0.3702	37.5	75.0	337.5	5.07E-05	Mysid 96-hr LC50	Esters
135	00947536-74-5		4-(4-propylcyclohexyl)cyclohexyl 4-(4-pentylcyclohexyl)benzoate	O=C(c3ccc(C4CCC(CCCCC)CC4)cc3)OC1CCC(C2CCC(CCC)CC2)CC1	480.8	4.36E-11	5.82E-09	0.208	-0.92	13.38	14.30	9.908	1.00	0.8559	0.2449	37.5	75.0	337.5	3.95E-08	Mysid 96-hr LC50	Esters
136	0086603-66-9		4-(4-propylcyclohexyl)cyclohexyl 4-(4-propylcyclohexyl)benzoate	O=C(c3ccc(C4CCC(CCC)CC4)cc3)OC1CCC(C2CCC(CCC)CC2)CC1	452.7	2.58E-10	3.44E-08	0.22	-1.17	12.40	13.57	30.01	1.48	0.7609	0.2296	37.5	75.0	337.5	2.40E-07	Mysid 96-hr LC50	Esters
137	0081929-44-4		4-pentylphenyl 4-(4-pentylcyclohexyl)benzoate	O=C(c3ccc(C2CCC(CCCCC)CC2)cc3)Oc1ccc(CCCCC)cc1	420.6	5.84E-10	7.78E-08	0.347	-1.83	10.76	12.59	48.67	1.69	1.0477	0.2428	15.0	30.0	135.0	5.07E-06	Mysid 96-hr LC50	Esters
138	0081929-40-0		4-pentylphenyl 4-(4-propylcyclohexyl)benzoate	O=C(c3ccc(C2CCC(CCC)CC2)cc3)Oc1ccc(CCCCC)cc1	392.6	3.03E-09	4.03E-07	0.382	-2.08	9.77	11.85	582.2	2.77	0.9526	0.2275	37.5	75.0	337.5	3.06E-05	Mysid 96-hr LC50	Esters
139	0067679-63-4		4-ethoxyphenyl 4-pentylcyclohexanecarboxylate	O=C(C2CCC(CCCCC)CC2)Oc1ccc(OCC)cc1	318.5	1.33E-06	1.78E-04	0.284	-2.81	6.81	9.62	14540	4.16	1.0105	0.6883	15.0	30.0	135.0	7.00E-03	Mysid 96-hr LC50	Esters
140	0067589-52-0		4-methoxyphenyl 4-pentylcyclohexanecarboxylate	O=C(C2CCC(CCCCC)CC2)Oc1ccc(OC)cc1	304.4	3.18E-06	4.24E-04	0.331	-2.93	6.32	9.25	6894	3.84	1.0171	0.6806	15.0	30.0	135.0	1.70E-02	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

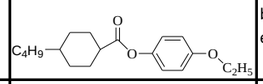
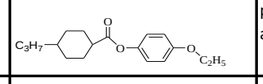
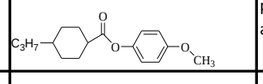
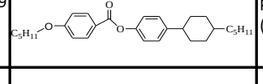
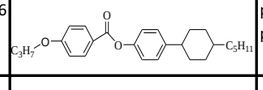
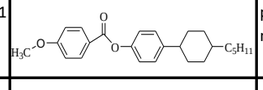
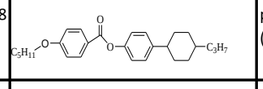
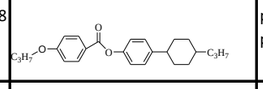
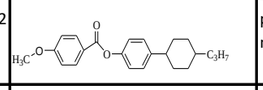
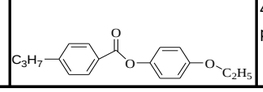
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
141	0067589-47-3		4-ethoxyphenyl 4-butylcyclohexanecarboxylate	O=C(C2CCC(CCCC)CC2)Oc1ccc(OCC)cc1	304.4	3.18E-06	4.24E-04	0.295	-2.93	6.32	9.25	6894	3.84	1.0171	0.6806	15.0	30.0	135.0	1.70E-02	Mysid 96-hr LC50	Esters
142	0067589-39-3		4-ethoxyphenyl 4-propylcyclohexanecarboxylate	O=C(C2CCC(CCC)CC2)Oc1ccc(OCC)cc1	290.4	7.55E-06	1.01E-03	0.307	-3.05	5.83	8.88	3269	3.51	0.9154	0.6729	37.5	75.0	337.5	4.00E-02	Mysid 96-hr LC50	Esters
143	0067589-38-2		4-methoxyphenyl 4-propylcyclohexanecarboxylate	O=C(C2CCC(CCC)CC2)Oc1ccc(OC)cc1	276.4	0.0000178	2.37E-03	0.362	-3.18	5.34	8.52	1550	3.19	0.9221	0.6652	37.5	75.0	337.5	9.70E-02	Mysid 96-hr LC50	Esters
144	001233010-35-9		4-(4-pentylcyclohexyl)phenyl 4-(pentyloxy)benzoate	O=C(c3ccc(OCCCCC)cc3)Oc1ccc(C2CCC(CCCCC)CC2)cc1	436.6	2.2E-10	2.94E-08	0.196	-3.10	10.29	13.39	82.38	1.92	1.1173	0.4956	15.0	30.0	135.0	1.28E-05	Mysid 96-hr LC50	Esters
145	001233010-58-6		4-(4-pentylcyclohexyl)phenyl 4-propoxybenzoate	O=C(c3ccc(OCCC)cc3)Oc1ccc(C2CCC(CCCCC)CC2)cc1	408.6	1.29E-09	1.71E-07	0.209	-3.34	9.31	12.65	985.4	2.99	1.0222	0.4802	37.5	75.0	337.5	7.71E-05	Mysid 96-hr LC50	Esters
146	001229648-08-1		4-(4-pentylcyclohexyl)phenyl 4-methoxybenzoate	O=C(c3ccc(OC)cc3)Oc1ccc(C2CCC(CCCCC)CC2)cc1	380.5	6.56E-09	8.75E-07	0.257	-3.59	8.32	11.91	2985	3.48	1.0356	0.4649	37.5	75.0	337.5	4.64E-04	Mysid 96-hr LC50	Esters
147	001233010-34-8		4-(4-propylcyclohexyl)phenyl 4-(pentyloxy)benzoate	O=C(c3ccc(OCCCCC)cc3)Oc1ccc(C2CCC(CCC)CC2)cc1	408.6	1.29E-09	1.71E-07	0.207	-3.34	9.31	12.65	985.4	2.99	1.0222	0.4802	37.5	75.0	337.5	7.71E-05	Mysid 96-hr LC50	Esters
148	001233010-42-8		4-(4-propylcyclohexyl)phenyl 4-propoxybenzoate	O=C(c3ccc(OCCC)cc3)Oc1ccc(C2CCC(CCC)CC2)cc1	380.5	6.56E-09	8.75E-07	0.221	-3.59	8.32	11.91	2985	3.48	0.9271	0.4649	37.5	75.0	337.5	4.64E-04	Mysid 96-hr LC50	Esters
149	001229648-09-2		4-(4-propylcyclohexyl)phenyl 4-methoxybenzoate	O=C(c3ccc(OC)cc3)Oc1ccc(C2CCC(CCC)CC2)cc1	352.5	3.15E-08	4.20E-06	0.276	-3.84	7.34	11.18	9040	3.96	0.9405	0.4495	37.5	75.0	337.5	3.00E-03	Mysid 96-hr LC50	Esters
150	0053132-08-4		4-ethoxyphenyl 4-propylbenzoate	O=C(c2ccc(CCC)cc2)Oc1ccc(OCC)cc1	284.4	2.74E-06	3.65E-04	0.371	-4.10	5.15	9.25	1155	3.06	0.9729	0.5148	37.5	75.0	337.5	1.45E-01	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

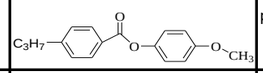
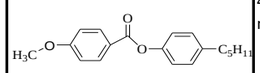
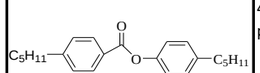
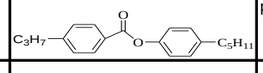
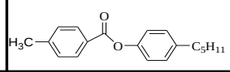
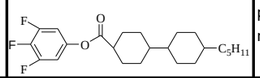
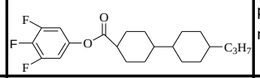
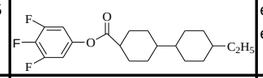
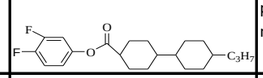
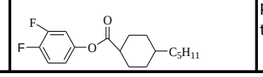
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
151	0050649-61-1		4-methoxyphenyl 4-propylbenzoate	O=C(c2ccc(CCC)cc2)Oc1ccc(OC)cc1	270.3	6.39E-06	8.52E-04	0.455	-4.22	4.66	8.88	547.7	2.74	0.9796	0.5072	37.5	75.0	337.5	3.49E-01	Mysid 96-hr LC50	Esters
152	0038444-13-2		4-pentylphenyl 4-methoxybenzoate	O=C(c2ccc(OC)cc2)Oc1ccc(CCCCC)cc1	298.4	1.17E-06	1.56E-04	0.365	-3.97	5.64	9.61	2436	3.39	1.0747	0.5225	15.0	30.0	135.0	6.00E-02	Mysid 96-hr LC50	Esters
153	0074305-48-9		4-pentylphenyl 4-pentylbenzoate	O=C(c2ccc(CCCCC)cc2)Oc1ccc(CCCCC)cc1	338.5	9.92E-08	1.32E-05	0.576	-2.21	8.07	10.28	1009	3.00	1.0868	0.3005	15.0	30.0	135.0	6.71E-04	Mysid 96-hr LC50	Esters
154	0050649-60-0		4-pentylphenyl 4-propylbenzoate	O=C(c2ccc(CCC)cc2)Oc1ccc(CCCCC)cc1	310.4	5.6E-07	7.47E-05	0.68	-2.46	7.09	9.55	12070	4.08	0.9917	0.2852	15.0	30.0	135.0	4.00E-03	Mysid 96-hr LC50	Esters
155	0050649-59-7		4-pentylphenyl 4-methylbenzoate	O=C(c2ccc(C)cc2)Oc1ccc(CCCCC)cc1	282.4	3.09E-06	4.12E-04	0.785	-2.70	6.10	8.80	4947	3.69	1.0051	0.4159	15.0	30.0	135.0	2.30E-02	Mysid 96-hr LC50	Esters
156	00175859-25-3		3,4,5-trifluorophenyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	c1(F)c(F)c(F)cc(OC(=O)C2CCC(C3CCC(CCCCC)CC3)CC2)c1	410.5	1.54E-07	2.06E-05	0.361	-1.12	9.53	10.65	766.3	2.88	-1.5953	0.3088	180.0	360.0	1620.8	5.07E-05	Mysid 96-hr LC50	Esters
157	00132123-45-6		3,4,5-trifluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	c1(F)c(F)c(F)cc(OC(=O)C2CCC(C3CCC(CCC)CC3)CC2)c1	382.5	8.66E-07	1.16E-04	0.399	-1.36	8.55	9.91	2321	3.37	-1.6903	0.2934	180.0	360.0	1620.8	3.05E-04	Mysid 96-hr LC50	Esters
158	00181943-55-5		3,4,5-trifluorophenyl 4-(4-ethylcyclohexyl)cyclohexanecarboxylate	c1(F)c(F)c(F)cc(OC(=O)C2CCC(C3CCC(CC)CC3)CC2)c1	368.4	2.04E-06	2.72E-04	0.421	-1.49	8.06	9.55	4039	3.61	-1.6837	0.2857	180.0	360.0	1620.8	7.47E-04	Mysid 96-hr LC50	Esters
159	0094840-77-4		3,4-difluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	c1(F)c(F)cc(OC(=O)C2CCC(C3CCC(CCC)CC3)CC2)cc1	364.5	8.12E-07	1.08E-04	0.402	-1.43	8.35	9.78	2910	3.46	-0.8718	0.3378	180.0	360.0	1620.8	4.25E-04	Mysid 96-hr LC50	Esters
160	0089203-80-5		3,4-difluorophenyl 4-pentylcyclohexanecarboxylate	c1(F)c(F)cc(OC(=O)C2CCC(CCCCC)CC2)cc1	310.4	0.0000246	3.28E-03	0.645	-1.57	6.64	8.21	11210	4.05	-0.7376	0.4938	60.0	120.0	541.7	9.00E-03	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

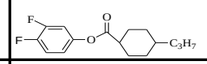
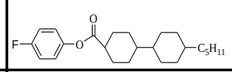
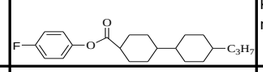
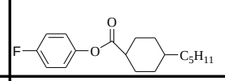
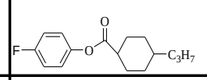
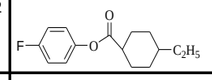
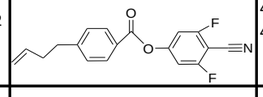
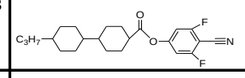
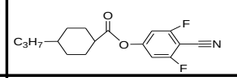
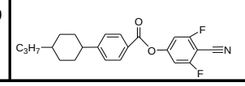
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
161	0094737-80-1		3,4-difluorophenyl 4-propylcyclohexanecarboxylate	c1(F)c(F)cc(OC(=O)C2CCC(CCC)CC2)cc1	282.3	0.000145	1.93E-02	0.778	-1.81	5.66	7.47	2520	3.40	-0.8327	0.4784	60.0	120.0	541.7	5.40E-02	Mysid 96-hr LC50	Esters
162	0088878-50-6		4-fluorophenyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C2CCC(CCCCC)CC2)CC3)Oc1ccc(F)cc1	374.5	1.35E-07	1.81E-05	0.352	-1.25	9.13	10.38	1204	3.08	0.0419	0.3975	37.5	75.0	337.5	9.91E-05	Mysid 96-hr LC50	Esters
163	0081701-13-5		4-fluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	O=C(C3CCC(C2CCC(CCC)CC2)CC3)Oc1ccc(F)cc1	346.5	6.61E-07	8.82E-05	0.388	-1.50	8.15	9.65	3648	3.56	-0.0532	0.3822	60.0	120.0	541.7	5.92E-04	Mysid 96-hr LC50	Esters
164	0079912-83-7		4-fluorophenyl 4-pentylcyclohexanecarboxylate	O=C(C2CCC(CCCCC)CC2)Oc1ccc(F)cc1	292.4	0.0000244	3.26E-03	0.61	-1.64	6.44	8.08	8266	3.92	0.081	0.5381	37.5	75.0	337.5	1.30E-02	Mysid 96-hr LC50	Esters
165	0079912-81-5		4-fluorophenyl 4-propylcyclohexanecarboxylate	O=C(C2CCC(CCC)CC2)Oc1ccc(F)cc1	264.3	0.000141	1.88E-02	0.728	-1.88	5.46	7.34	1859	3.27	-0.0141	0.5227	37.5	75.0	337.5	7.40E-02	Mysid 96-hr LC50	Esters
166	00100633-61-2		4-fluorophenyl 4-ethylcyclohexanecarboxylate	O=C(C2CCC(CC)CC2)Oc1ccc(F)cc1	250.3	0.00036	4.80E-02	0.805	-2.01	4.97	6.98	881.5	2.95	-0.0074	0.5151	37.5	75.0	337.5	1.79E-01	Mysid 96-hr LC50	Esters
167	00208528-35-2		4-cyano-3,5-difluorophenyl 4-(but-3-enyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCC=C)cc2)cc1F	313.3	6.5E-07	8.66E-05	0.319	-4.88	4.88	9.76	767	2.89	-0.4857	0.2918	180.0	360.0	162.1	2.66E-01	Mysid 96-hr LC50	Esters
168	00145804-13-3		4-cyano-3,5-difluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(C3CCC(CCC)CC3)CC2)cc1F	389.5	2.46E-08	3.28E-06	0.406	-3.45	7.89	11.34	4851	3.69	-0.5767	0.3268	180.0	360.0	162.1	1.07E-03	Mysid 96-hr LC50	Esters
169	00170447-78-6		4-cyano-3,5-difluorophenyl 4-propylcyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(CCC)CC2)cc1F	307.3	4.13E-06	5.50E-04	0.795	-3.83	5.21	9.04	1266	3.10	-0.5376	0.4674	60.0	120.0	541.7	1.39E-01	Mysid 96-hr LC50	Esters
170	00186320-72-9		4-cyano-3,5-difluorophenyl 4-(4-propylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CCC)CC3)cc2)cc1F	383.4	8.41E-09	1.12E-06	0.543	-4.49	7.21	11.70	10500	4.02	-0.5191	0.2517	180.0	360.0	162.1	4.00E-03	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

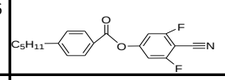
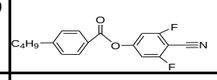
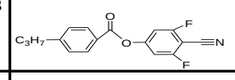
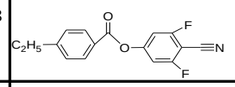
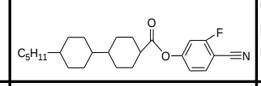
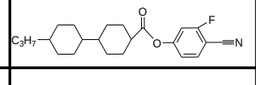
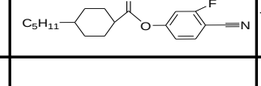
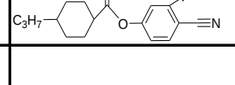
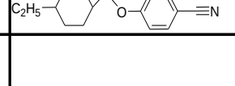
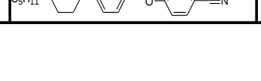
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
171	00123843-69-6		4-cyano-3,5-difluorophenyl 4-pentylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCCCC)cc2)cc1F	329.4	2.58E-07	3.44E-05	1.042	-4.63	5.50	10.13	1990	3.30	-0.3849	0.3247	60.0	120.0	541.7	8.50E-02	Mysid 96-hr LC50	Esters
172	00337367-02-9		4-cyano-3,5-difluorophenyl 4-butylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCCC)cc2)cc1F	315.3	6.06E-07	8.08E-05	1.208	-4.75	5.01	9.76	943.6	2.98	-0.3783	0.3171	60.0	120.0	541.7	2.07E-01	Mysid 96-hr LC50	Esters
173	00193275-43-3		4-cyano-3,5-difluorophenyl 4-propylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCC)cc2)cc1F	301.3	1.42E-06	1.89E-04	1.438	-4.87	4.52	9.39	447.5	2.65	-0.48	0.3094	180.0	360.0	162.1	5.02E-01	Mysid 96-hr LC50	Esters
174	00337367-01-8		4-cyano-3,5-difluorophenyl 4-ethylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CC)cc2)cc1F	287.3	3.29E-06	4.38E-04	1.761	-5.00	4.03	9.03	212.2	2.33	-0.4733	0.3017	180.0	360.0	162.1	1.22E+00	Mysid 96-hr LC50	Esters
175	0094353-27-2		4-cyano-3-fluorophenyl 4-(4-pentylcyclohexyl)cyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	399.6	3.86E-09	5.15E-07	0.368	-3.27	8.68	11.95	2008	3.30	0.3369	0.3866	37.5	75.0	337.5	2.50E-04	Mysid 96-hr LC50	Esters
176	0094353-26-1		4-cyano-3-fluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(C3CCC(CCC)CC3)CC2)cc1	371.5	1.93E-08	2.58E-06	0.408	-3.51	7.69	11.20	6082	3.78	0.2419	0.3712	60.0	120.0	541.7	1.50E-03	Mysid 96-hr LC50	Esters
177	0090525-59-0		4-cyano-3-fluorophenyl 4-pentylcyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(CCCCC)CC2)cc1	317.4	5.93E-07	7.90E-05	0.661	-3.65	5.99	9.64	4153	3.62	0.3761	0.5271	37.5	75.0	337.5	3.30E-02	Mysid 96-hr LC50	Esters
178	0090525-57-8		4-cyano-3-fluorophenyl 4-propylcyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(CCC)CC2)cc1	289.4	3.27E-06	4.37E-04	0.801	-3.90	5.01	8.91	934	2.97	0.281	0.5118	60.0	120.0	541.7	1.92E-01	Mysid 96-hr LC50	Esters
179	0090525-56-7		4-cyano-3-fluorophenyl 4-ethylcyclohexanecarboxylate	C(#N)c1c(F)cc(OC(=O)C2CCC(CC)CC2)cc1	275.3	7.63E-06	1.02E-03	0.896	-4.02	4.52	8.54	442.9	2.65	0.2877	0.5041	60.0	120.0	541.7	4.64E-01	Mysid 96-hr LC50	Esters
180	0092118-84-8		4-cyano-3-fluorophenyl 4-(4-pentylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CCCCC)CC3)cc2)cc1	393.5	1.3E-09	1.74E-07	0.477	-4.31	7.99	12.30	4348	3.64	0.3945	0.3114	60.0	120.0	541.7	9.03E-04	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

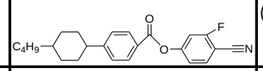
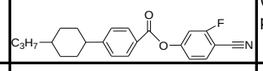
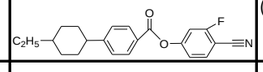
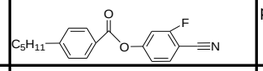
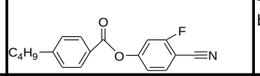
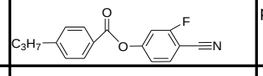
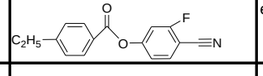
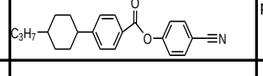
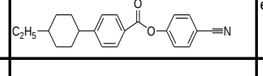
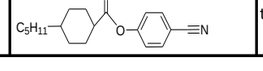
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
181	0092118-83-7		4-cyano-3-fluorophenyl 4-(4-butylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CCCC)CC3)cc2)cc1	379.5	3.13E-09	4.17E-07	0.509	-4.43	7.50	11.93	7567	3.88	0.4012	0.3037	60.0	120.0	541.7	2.00E-03	Mysid 96-hr LC50	Esters
182	0092118-82-6		4-cyano-3-fluorophenyl 4-(4-propylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CCC)CC3)cc2)cc1	365.5	7.48E-09	9.98E-07	0.546	-4.56	7.01	11.57	13170	4.12	0.2994	0.2961	60.0	120.0	541.7	5.00E-03	Mysid 96-hr LC50	Esters
183	0092118-81-5		4-cyano-3-fluorophenyl 4-(4-ethylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CC)CC3)cc2)cc1	351.4	1.78E-08	2.37E-06	0.588	-4.68	6.52	11.20	9279	3.97	0.3061	0.2884	60.0	120.0	541.7	1.30E-02	Mysid 96-hr LC50	Esters
184	0086786-89-2		4-cyano-3-fluorophenyl 4-pentylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCCCC)cc2)cc1	311.4	2.35E-07	3.13E-05	1.054	-4.69	5.30	9.99	1468	3.17	0.4336	0.3691	37.5	75.0	337.5	1.17E-01	Mysid 96-hr LC50	Esters
185	0086776-52-5		4-cyano-3-fluorophenyl 4-butylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCCC)cc2)cc1	297.3	5.51E-07	7.35E-05	1.224	-4.82	4.81	9.63	695.9	2.84	0.4403	0.3614	37.5	75.0	337.5	2.85E-01	Mysid 96-hr LC50	Esters
186	0086776-51-4		4-cyano-3-fluorophenyl 4-propylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CCC)cc2)cc1	283.3	1.29E-06	1.72E-04	1.46	-4.94	4.32	9.26	330	2.52	0.3385	0.3537	60.0	120.0	541.7	6.90E-01	Mysid 96-hr LC50	Esters
187	0086776-50-3		4-cyano-3-fluorophenyl 4-ethylbenzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(CC)cc2)cc1	269.3	2.99E-06	3.99E-04	1.794	-5.06	3.83	8.89	156.5	2.19	0.3452	0.346	60.0	120.0	541.7	1.67E+00	Mysid 96-hr LC50	Esters
188	0081930-17-8		4-cyanophenyl 4-(4-propylcyclohexyl)benzoate	O=C(c3ccc(C2CCC(CCC)CC2)cc3)Oc1ccc(C(#N))cc1	347.5	6.66E-09	8.87E-07	0.549	-4.62	6.81	11.43	14430	4.16	1.118	0.3404	37.5	75.0	337.5	8.00E-03	Mysid 96-hr LC50	Esters
189	0073592-83-3		4-cyanophenyl 4-(4-ethylcyclohexyl)benzoate	O=C(c3ccc(C2CCC(CC)CC2)cc3)Oc1ccc(C(#N))cc1	333.4	1.58E-08	2.11E-06	0.591	-4.75	6.32	11.07	6844	3.84	1.1247	0.3327	37.5	75.0	337.5	1.80E-02	Mysid 96-hr LC50	Esters
190	0062439-35-4		4-cyanophenyl 4-pentylcyclohexanecarboxylate	C(#N)c1ccc(OC(=O)C2CCC(CCCCC)CC2)cc1	299.4	5.56E-07	7.41E-05	0.665	-3.72	5.79	9.51	3063	3.49	1.1946	0.5715	15.0	30.0	135.0	4.50E-02	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

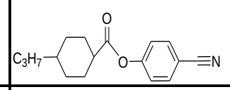
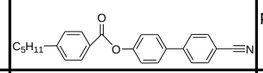
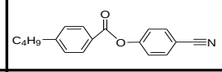
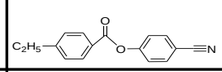
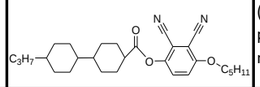
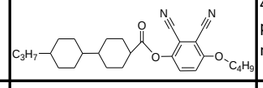
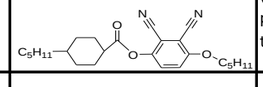
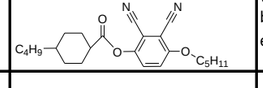
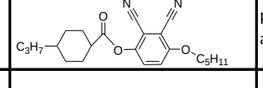
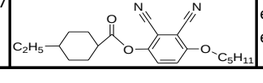
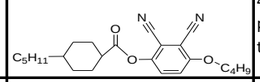
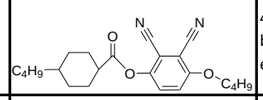
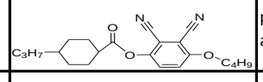
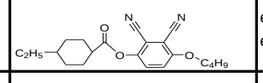
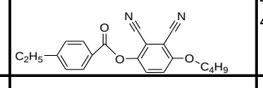
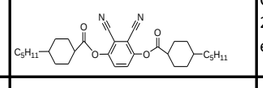
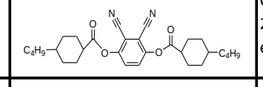
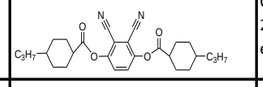
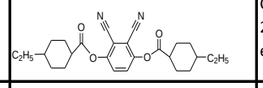
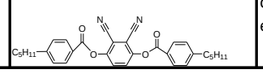
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
191	0062439-33-2		4-cyanophenyl 4-propylcyclohexanecarboxylate	C(#N)c1ccc(OC(=O)C2CCC(CCC)CC2)cc1	271.4	3.07E-06	4.09E-04	0.807	-3.96	4.81	8.77	688.9	2.84	1.0995	0.5561	37.5	75.0	337.5	2.63E-01	Mysid 96-hr LC50	Esters
192	0059443-80-0		4'-Cyano-4-biphenylyl 4-pentylbenzoate	C(#N)c1ccc(c2ccc(OC(=O)c3ccc(CCCCC)cc3)cc2)cc1	369.5	1.43E-10	1.90E-08	0.881	-5.88	6.87	12.75	15780	4.20	1.2159	0.2199	37.5	75.0	337.5	7.00E-03	Mysid 96-hr LC50	Esters
193	0038690-77-6		4-cyanophenyl 4-butylbenzoate	O=C(c2ccc(CCCC)cc2)Oc1ccc(C(#N))cc1	279.3	5.01E-07	6.68E-05	1.237	-4.88	4.61	9.49	513.2	2.71	1.2588	0.4058	15.0	30.0	135.0	3.92E-01	Mysid 96-hr LC50	Esters
194	0056131-48-7		4-cyanophenyl 4-ethylbenzoate	O=C(c2ccc(CC)cc2)Oc1ccc(C(#N))cc1	251.3	2.32E-06	3.10E-04	1.821	-5.13	3.63	8.76	115.4	2.06	1.1638	0.3904	37.5	75.0	337.5	2.28E+00	Mysid 96-hr LC50	Esters
195	0090681-46-2		2,3-dicyano-4-(pentyloxy)phenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	C(#N)c3c(C(#N))c(OCCCCC)ccc3OC(=O)C1CCC(C2CCC(CCC)CC2)CC1	464.7	2.5E-12	3.33E-10	0.268	-6.33	9.09	15.42	1265	3.10	1.5549	0.5334	37.5	75.0	337.5	1.33E-04	Mysid 96-hr LC50	ters + Phthalonitriles
196	00NA		4-butoxy-2,3-dicyanophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	C(#N)c3c(C(#N))c(OCCCC)ccc3OC(=O)C1CCC(C2CCC(CCC)CC2)CC1	450.6	5.8E-12	7.73E-10	0.278	-6.45	8.59	15.04	2201	3.34	1.5615	0.5257	37.5	75.0	337.5	3.29E-04	Mysid 96-hr LC50	ters + Phthalonitriles
197	0075941-52-5		2,3-dicyano-4-(pentyloxy)phenyl 4-pentylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCCC)ccc2OC(=O)C1CCC(CCCCC)CC1	410.6	8.06E-11	1.07E-08	0.358	-6.47	7.38	13.85	2193	3.34	1.689	0.6894	15.0	30.0	135.0	3.00E-03	Mysid 96-hr LC50	ters + Phthalonitriles
198	0075941-51-4		2,3-dicyano-4-(pentyloxy)phenyl 4-butylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCCC)ccc2OC(=O)C1CCC(CCCC)CC1	396.5	1.86E-10	2.47E-08	0.376	-6.59	6.89	13.48	689.4	2.84	1.6957	0.6817	15.0	30.0	135.0	7.00E-03	Mysid 96-hr LC50	ters + Phthalonitriles
199	0075941-50-3		2,3-dicyano-4-(pentyloxy)phenyl 4-propylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCCC)ccc2OC(=O)C1CCC(CCC)CC1	382.5	4.5E-10	6.00E-08	0.396	-6.71	6.40	13.11	7740	3.89	1.594	0.674	37.5	75.0	337.5	1.80E-02	Mysid 96-hr LC50	ters + Phthalonitriles
200	001234032-17-7		2,3-dicyano-4-(pentyloxy)phenyl 4-ethylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCCC)ccc2OC(=O)C1CCC(CC)CC1	368.5	1.09E-09	1.45E-07	0.418	-6.84	5.91	12.75	3670	3.57	1.6006	0.6663	37.5	75.0	337.5	4.40E-02	Mysid 96-hr LC50	ters + Phthalonitriles

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
201	00NA		4-butoxy-2,3-dicyanophenyl 4-pentylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCC)ccc2OC(=O)C1CCC(CCCCC)CC1	396.5	1.86E-10	2.47E-08	0.376	-6.59	6.89	13.48	689.4	2.84	1.6957	0.6817	15.0	30.0	135.0	7.00E-03	Mysid 96-hr LC50	ters + Phthalonitriles
202	0075941-46-7		4-butoxy-2,3-dicyanophenyl 4-butylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCC)ccc2OC(=O)C1CCC(CCCC)CC1	382.5	4.5E-10	6.00E-08	0.396	-6.71	6.40	13.11	7740	3.89	1.7024	0.674	15.0	30.0	135.0	1.80E-02	Mysid 96-hr LC50	ters + Phthalonitriles
203	00NA		4-butoxy-2,3-dicyanophenyl 4-propylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCC)ccc2OC(=O)C1CCC(CCC)CC1	368.5	1.09E-09	1.45E-07	0.418	-6.84	5.91	12.75	3670	3.57	1.6006	0.6663	37.5	75.0	337.5	4.40E-02	Mysid 96-hr LC50	ters + Phthalonitriles
204	00NA		4-butoxy-2,3-dicyanophenyl 4-ethylcyclohexanecarboxylate	C(#N)c2c(C(#N))c(OCCCC)ccc2OC(=O)C1CCC(CC)CC1	354.5	2.61E-09	3.48E-07	0.442	-6.96	5.42	12.38	1741	3.24	1.6073	0.6586	37.5	75.0	337.5	1.08E-01	Mysid 96-hr LC50	ters + Phthalonitriles
205	00NA		4-butoxy-2,3-dicyanophenyl 4-ethylbenzoate	C(#N)c2c(C(#N))c(OCCCC)ccc2OC(=O)c1ccc(CC)cc1	348.4	8.82E-10	1.18E-07	0.587	-8.00	4.73	12.73	615	2.79	1.6649	0.5006	37.5	75.0	337.5	3.90E-01	Mysid 96-hr LC50	ters + Phthalonitriles
206	0075414-73-2		4-pentyl-Cyclohexanecarboxylic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)C2CCC(CCCCC)CC2)ccc3OC(=O)C1CCC(CCCCC)CC1	520.7	2.64E-13	3.53E-11	0.34	-6.78	10.26	17.04	84.77	1.93	1.6789	0.614	15.0	30.0	135.0	1.60E-05	Mysid 96-hr LC50	ters + Phthalonitriles
207	0075414-72-1		4-butyl-Cyclohexanecarboxylic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)C2CCC(CCCC)CC2)ccc3OC(=O)C1CCC(CCCC)CC1	492.7	1.63E-12	2.18E-10	0.373	-7.02	9.28	16.30	1014	3.01	1.6922	0.5986	15.0	30.0	135.0	9.76E-05	Mysid 96-hr LC50	ters + Phthalonitriles
208	00NA		4-propyl-Cyclohexanecarboxylic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)C2CCC(CCC)CC2)ccc3OC(=O)C1CCC(CCC)CC1	464.6	9.95E-12	1.33E-09	0.414	-7.27	8.30	15.57	3071	3.49	1.4887	0.5832	37.5	75.0	337.5	5.94E-04	Mysid 96-hr LC50	ters + Phthalonitriles
209	00NA		4-ethyl-Cyclohexanecarboxylic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)C2CCC(CC)CC2)ccc3OC(=O)C1CCC(CC)CC1	436.6	5.97E-11	7.95E-09	0.465	-7.52	7.32	14.84	9302	3.97	1.5021	0.5678	37.5	75.0	337.5	4.00E-03	Mysid 96-hr LC50	ters + Phthalonitriles
210	0075942-28-8		4-Pentylbenzoic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)c2ccc(CCCCC)cc2)ccc3OC(=O)c1ccc(CCCCC)cc1	508.6	3.68E-14	4.90E-12	0.55	-8.86	8.89	17.75	397.5	2.60	1.794	0.2979	37.5	75.0	337.5	2.10E-04	Mysid 96-hr LC50	ters + Phthalonitriles

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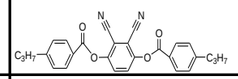
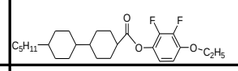
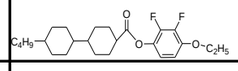
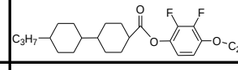
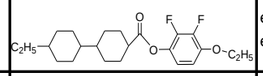
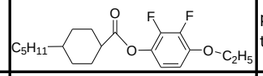
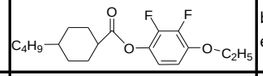
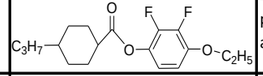
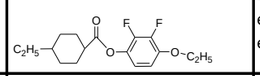
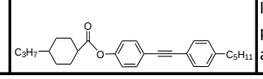
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
211	0078333-30-9		4-Propylbenzoic acid 2,3-dicyano-1,4-phenylene ester	C(#N)c3c(C(#N))c(OC(=O)c2ccc(CCC)cc2)ccc3OC(=O)c1ccc(CCC)cc1	452.5	1.11E-12	1.48E-10	0.775	-9.36	6.93	16.29	17350	4.24	1.6038	0.2671	60.0	120.0	541.7	8.00E-03	Mysid 96-hr LC50	ters + Phthalonitriles
212	00126163-43-7		4'-Pentyl-[1,1'-bicyclohexyl]-4-carboxylic acid 4-ethoxy-2,3-difluorophenyl ester	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	436.6	1.01E-08	1.35E-06	0.258	-2.29	9.90	12.19	503.9	2.70	-0.6658	0.4589	60.0	120.0	541.7	2.66E-05	Mysid 96-hr LC50	Esters
213	00NA		4-ethoxy-2,3-difluorophenyl 4-(4-butylcyclohexyl)cyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(C3CCC(CCCC)CC3)CC2)cc1	422.6	2.42E-08	3.23E-06	0.267	-2.41	9.41	11.82	876.9	2.94	-0.6591	0.4513	60.0	120.0	541.7	6.55E-05	Mysid 96-hr LC50	Esters
214	00NA		4-ethoxy-2,3-difluorophenyl 4-(4-propylcyclohexyl)cyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(C3CCC(CCC)CC3)CC2)cc1	408.5	5.76E-08	7.68E-06	0.277	-2.54	8.92	11.46	1526	3.18	-0.7608	0.4436	180.0	0.4	1620.8	1.61E-04	Mysid 96-hr LC50	Esters
215	00NA		4-ethoxy-2,3-difluorophenyl 4-(4-ethylcyclohexyl)cyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(C3CCC(CC)CC3)CC2)cc1	394.5	1.36E-07	1.82E-05	0.287	-2.66	8.43	11.09	2656	3.42	-0.7542	0.4359	180.0	0.4	1620.8	3.95E-04	Mysid 96-hr LC50	Esters
216	00NA		4-ethoxy-2,3-difluorophenyl 4-pentylcyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(CCCCC)CC2)cc1	354.4	1.76E-06	2.34E-04	0.374	-2.67	7.21	9.88	10450	4.02	-0.6267	0.5995	60.0	120.0	541.7	4.00E-03	Mysid 96-hr LC50	Esters
217	00NA		4-ethoxy-2,3-difluorophenyl 4-butylcyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(CCCC)CC2)cc1	340.4	4.11E-06	5.49E-04	0.394	-2.80	6.72	9.52	12670	4.10	-0.62	0.5918	60.0	120.0	541.7	9.00E-03	Mysid 96-hr LC50	Esters
218	00NA		4-ethoxy-2,3-difluorophenyl 4-propylcyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(CCC)CC2)cc1	326.4	9.57E-06	1.28E-03	0.415	-2.92	6.23	9.15	6010	3.78	-0.7217	0.5842	180.0	0.4	1620.8	2.10E-02	Mysid 96-hr LC50	Esters
219	00NA		4-ethoxy-2,3-difluorophenyl 4-ethylcyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(CC)CC2)cc1	312.4	0.0000221	2.95E-03	0.439	-3.04	5.74	8.78	2850	3.46	-0.7151	0.5765	60.0	120.0	541.7	5.10E-02	Mysid 96-hr LC50	Esters
220	00NA		4-(2-(4-pentylphenyl)ethynyl)phenyl 4-propylcyclohexanecarboxylate	c1(C#Cc3ccc(CCCCC)cc3)ccc(OC(=O)C2CCC(CCC)CC2)cc1	416.6	2.05E-10	2.73E-08	0.219	-3.38	9.80	13.18	563.9	2.75	0.8865	0.1782	37.5	75.0	337.5	3.07E-05	Mysid 96-hr LC50	Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

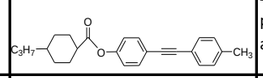
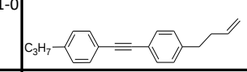
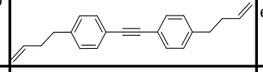
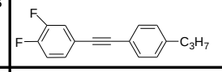
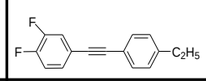
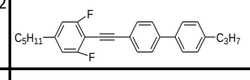
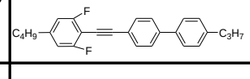
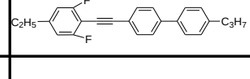
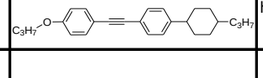
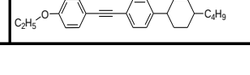
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
221	00NA		4-(2-p-tolylethynyl)phenyl 4-propylcyclohexanecarboxylate	c1(C#Cc3ccc(C)cc3)ccc(OC(=O)C2CCC(CCC)CC2)cc1	360.5	6.09E-09	8.11E-07	0.244	-3.87	7.84	11.71	5173	3.71	0.8048	0.2936	37.5	75.0	337.5	1.11E-03	Mysid 96-hr LC50	Esters
222	001262505-01-0		1-(but-3-enyl)-4-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCC=C)cc2)ccc(CCC)cc1	274.4	1.47E-06	1.96E-04	0.169	-2.05	7.44	9.49	8121	3.91	0.7262	-0.0321	37.5	75.0	337.5	7.16E-05	Mysid 96-hr LC50	Neutral Organics
223	00202652-64-0		1,2-bis(4-(but-3-enyl)phenyl)ethyne	c1(C#Cc2ccc(CCC=C)cc2)ccc(CCC=C)cc1	286.4	6.74E-07	8.99E-05	0.12	-2.05	7.79	9.84	5443	3.74	0.7205	-0.0496	37.5	75.0	337.5	2.83E-05	Mysid 96-hr LC50	Neutral Organics
224	00121118-73-8		1,2-difluoro-4-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2cc(F)c(F)cc2)ccc(CCC)cc1	256.3	0.0000524	6.98E-03	0.33	-2.20	5.95	8.15	3940	3.60	-0.9398	0.0361	180.0	360.0	1620.8	4.00E-03	Mysid 96-hr LC50	Neutral Organics
225	00145698-43-7		4-(2-(4-ethylphenyl)ethynyl)-1,2-difluorobenzene	c1(C#Cc2cc(F)c(F)cc2)ccc(CC)cc1	242.3	0.00013	1.74E-02	0.344	-2.32	5.46	7.78	1868	3.27	-0.9331	0.0284	60.0	120.0	541.7	1.40E-02	Mysid 96-hr LC50	Neutral Organics
226	001149373-93-2		4-[2-(2,6-Difluoro-4-pentylphenyl)ethynyl]-4'-propyl-1,1'-biphenyl	C(c3c(F)cc(CCCCC)cc3F)#Cc1ccc(c2ccc(CCC)cc2)cc1	402.5	6.51E-10	8.68E-08	0.24	-2.78	10.23	13.01	347.9	2.54	-0.8463	-0.2814	180.0	360.0	1620.8	5.01E-08	Mysid 96-hr LC50	Neutral Organics
227	00221526-79-0		4-[2-(2,6-Difluoro-4-butylphenyl)ethynyl]-4'-propyl-1,1'-biphenyl	C(c3c(F)cc(CCCC)cc3F)#Cc1ccc(c2ccc(CCC)cc2)cc1	388.5	1.48E-09	1.97E-07	0.247	-2.90	9.74	12.64	605.4	2.78	-0.8396	-0.289	180.0	360.0	1620.8	1.86E-07	Mysid 96-hr LC50	Neutral Organics
228	00221526-72-3		4-[2-(2,6-Difluoro-4-ethylphenyl)ethynyl]-4'-propyl-1,1'-biphenyl	C(c3c(F)cc(CC)cc3F)#Cc1ccc(c2ccc(CCC)cc2)cc1	360.5	7.61E-09	1.01E-06	0.264	-3.15	8.76	11.91	1834	3.26	-0.9347	-0.3044	180.0	360.0	1620.8	2.54E-06	Mysid 96-hr LC50	Neutral Organics
229	00116903-49-2		1-propoxy-4-(2-(4-(4-propylcyclohexyl)phenyl)ethynyl)benzene	c1(C#Cc2ccc(C3CCC(CCC)CC3)cc2)ccc(OCCC)cc1	360.5	7.61E-09	1.01E-06	0.162	-2.93	9.30	12.23	989.1	3.00	0.7625	0.1806	37.5	75.0	337.5	5.67E-07	Mysid 96-hr LC50	Neutral Organics
230	00199795-20-5		1-(2-(4-(4-butylcyclohexyl)phenyl)ethynyl)-4-ethoxybenzene	c1(C#Cc2ccc(C3CCC(CCCC)CC3)cc2)ccc(OCC)cc1	360.5	7.61E-09	1.01E-06	0.169	-2.93	9.30	12.23	989.1	3.00	0.8709	0.1806	37.5	75.0	337.5	5.67E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

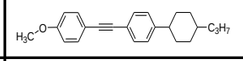
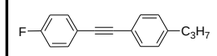
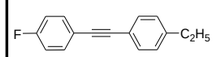
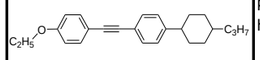
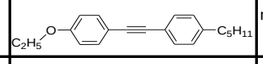
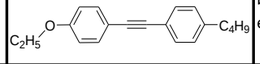
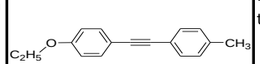
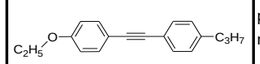
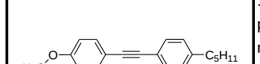
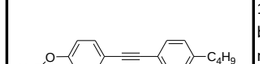
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
231	00116903-47-0		1-methoxy-4-(2-(4-(4-propylcyclohexyl)phenyl)ethynyl)benzene	c1(C#Cc2ccc(C3CCC(CCC)CC3)cc2)ccc(OC)cc1	332.5	4.29E-08	5.72E-06	0.19	-3.18	8.32	11.50	2996	3.48	0.7758	0.1652	37.5	75.0	337.5	7.71E-06	Mysid 96-hr LC50	Neutral Organics
232	00145698-32-4		1-fluoro-4-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCC)cc2)ccc(F)cc1	238.3	0.0000471	6.27E-03	0.321	-2.27	5.75	8.02	2906	3.46	-0.1212	0.0804	60.0	120.0	541.7	6.00E-03	Mysid 96-hr LC50	Neutral Organics
233	00160083-17-0		1-(2-(4-ethylphenyl)ethynyl)-4-fluorobenzene	c1(C#Cc2ccc(CC)cc2)ccc(F)cc1	224.3	0.000116	1.54E-02	0.335	-2.39	5.26	7.65	1378	3.14	-0.1145	0.0727	60.0	120.0	541.7	2.30E-02	Mysid 96-hr LC50	Neutral Organics
234	00167633-81-0		1-ethoxy-4-(2-(4-(4-propylcyclohexyl)phenyl)ethynyl)benzene	c1(C#Cc2ccc(C3CCC(CCC)CC3)cc2)ccc(OCC)cc1	346.5	1.81E-08	2.41E-06	0.173	-3.06	8.81	11.87	1721	3.24	0.7692	0.1729	37.5	75.0	337.5	2.09E-06	Mysid 96-hr LC50	Neutral Organics
235	0095480-29-8		1-ethoxy-4-(2-(4-pentylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCCCC)cc2)ccc(OCC)cc1	292.4	6.37E-07	8.49E-05	0.205	-3.19	7.11	10.30	11780	4.07	0.9033	0.2459	37.5	75.0	337.5	1.89E-04	Mysid 96-hr LC50	Neutral Organics
236	0085583-83-1		1-(2-(4-butylphenyl)ethynyl)-4-ethoxybenzene	c1(C#Cc2ccc(CCCC)cc2)ccc(OCC)cc1	278.4	1.24E-06	1.65E-04	0.21	-3.32	6.62	9.94	10780	4.03	0.91	0.2383	37.5	75.0	337.5	6.89E-04	Mysid 96-hr LC50	Neutral Organics
237	00116903-46-9		1-ethoxy-4-(2-p-tolylethynyl)benzene	c1(C#Cc2ccc(C)cc2)ccc(OCC)cc1	236.3	0.0000153	2.04E-03	0.227	-3.69	5.14	8.83	1149	3.06	0.8216	0.3614	37.5	75.0	337.5	3.30E-02	Mysid 96-hr LC50	Neutral Organics
238	0039969-29-4		1-ethoxy-4-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCC)cc2)ccc(OCC)cc1	264.4	2.88E-06	3.85E-04	0.216	-3.44	6.13	9.57	5111	3.71	0.8083	0.2306	37.5	75.0	337.5	3.00E-03	Mysid 96-hr LC50	Neutral Organics
239	0039969-28-3		1-methoxy-4-(2-(4-pentylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCCCC)cc2)ccc(OC)cc1	278.4	1.24E-06	1.65E-04	0.228	-3.32	6.62	9.94	10780	4.03	0.91	0.2383	37.5	75.0	337.5	6.89E-04	Mysid 96-hr LC50	Neutral Organics
240	0035684-12-9		1-(2-(4-butylphenyl)ethynyl)-4-methoxybenzene	c1(C#Cc2ccc(CCCC)cc2)ccc(OC)cc1	264.4	2.88E-06	3.85E-04	0.235	-3.44	6.13	9.57	5111	3.71	0.9167	0.2306	15.0	30.0	135.0	3.00E-03	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

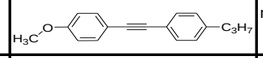
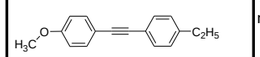
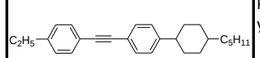
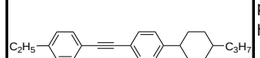
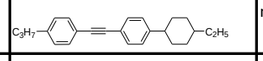
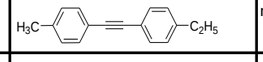
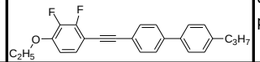
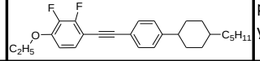
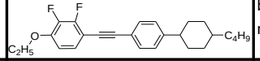
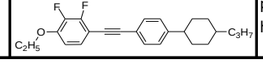
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
241	0039969-26-1		1-methoxy-4-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2ccc(CCC)cc2)ccc(OC)cc1	250.3	6.67E-06	8.89E-04	0.243	-3.56	5.63	9.19	2424	3.38	0.8149	0.2229	37.5	75.0	337.5	9.00E-03	Mysid 96-hr LC50	Neutral Organics
242	0063221-88-5		1-(2-(4-ethylphenyl)ethynyl)-4-methoxybenzene	c1(C#Cc2ccc(CC)cc2)ccc(OC)cc1	236.3	0.0000153	2.04E-03	0.25	-3.69	5.14	8.83	1149	3.06	0.8216	0.2152	37.5	75.0	337.5	3.30E-02	Mysid 96-hr LC50	Neutral Organics
243	00NA		1-ethyl-4-(2-(4-(4-pentylcyclohexyl)phenyl)ethynyl)benzene	c1(C#Cc2ccc(C3CCC(CCCCC)CC3)cc2)ccc(CC)cc1	358.6	8.32E-09	1.11E-06	0.211	-1.54	10.26	11.80	335.8	2.53	0.7946	-0.0645	37.5	75.0	337.5	4.09E-08	Mysid 96-hr LC50	Neutral Organics
244	00202205-77-4		1-ethyl-4-(2-(4-(4-propylcyclohexyl)phenyl)ethynyl)benzene	c1(C#Cc2ccc(C3CCC(CCC)CC3)cc2)ccc(CC)cc1	330.5	4.69E-08	6.25E-06	0.223	-1.79	9.28	11.07	1017	3.01	0.6995	-0.0798	37.5	75.0	337.5	5.56E-07	Mysid 96-hr LC50	Neutral Organics
245	00100558-65-4		1-(2-(4-(4-ethylcyclohexyl)phenyl)ethynyl)-4-propylbenzene	c1(C#Cc2ccc(C3CCC(CC)CC3)cc2)ccc(CCC)cc1	330.5	4.69E-08	6.25E-06	0.223	-1.79	9.28	11.07	1017	3.01	0.6995	-0.0798	37.5	75.0	337.5	5.56E-07	Mysid 96-hr LC50	Neutral Organics
246	0022692-80-4		1-(2-(4-ethylphenyl)ethynyl)-4-methylbenzene	c1(C#Cc2ccc(CC)cc2)ccc(C)cc1	220.3	0.0000393	5.24E-03	0.32	-2.41	5.61	8.02	2334	3.37	0.752	0.1086	37.5	75.0	337.5	9.00E-03	Mysid 96-hr LC50	Neutral Organics
247	00126163-06-2		4-[(4-Ethoxy-2,3-difluorophenyl)ethynyl]-4'-propyl-1,1'-biphenyl	C(c3c(F)c(F)c(OCC)cc3)#Cc1ccc(c2ccc(CCC)cc2)cc1	376.5	3.23E-09	4.31E-07	0.231	-4.42	8.29	12.71	3103	3.49	-0.8651	-0.0517	180.0	360.0	1620.8	9.51E-06	Mysid 96-hr LC50	Neutral Organics
248	00124770-59-8		1-Ethoxy-2,3-difluoro-4-[[4-(4-pentylcyclohexyl)phenyl]ethynyl]benzene	C(c3c(F)c(F)c(OCC)cc3)#Cc1ccc(C2CCC(CCCCC)CC2)cc1	410.6	4.16E-09	5.55E-07	0.184	-2.68	10.20	12.88	361.6	2.56	-0.7729	0.0995	180.0	360.0	1620.8	5.61E-08	Mysid 96-hr LC50	Neutral Organics
249	00NA		1-Ethoxy-2,3-difluoro-4-[[4-(4-butylcyclohexyl)phenyl]ethynyl]benzene	C(c3c(F)c(F)c(OCC)cc3)#Cc1ccc(C2CCC(CCCC)CC2)cc1	396.5	9.6E-09	1.28E-06	0.189	-2.80	9.70	12.50	629.3	2.80	-0.7662	0.0919	180.0	360.0	1620.8	2.08E-07	Mysid 96-hr LC50	Neutral Organics
250	00123560-57-6		1-Ethoxy-2,3-difluoro-4-[[4-(4-propylcyclohexyl)phenyl]ethynyl]benzene	C(c3c(F)c(F)c(OCC)cc3)#Cc1ccc(C2CCC(CCC)CC2)cc1	382.5	2.28E-08	3.04E-06	0.194	-2.92	9.21	12.13	1095	3.04	-0.868	0.0842	180.0	360.0	1620.8	7.70E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

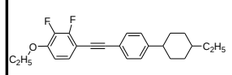
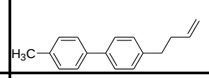
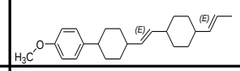
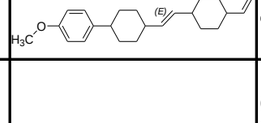
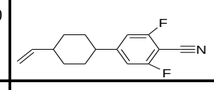
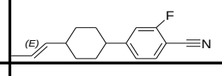
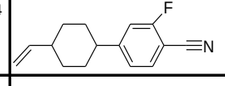
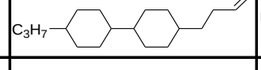
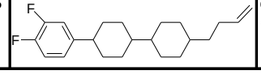
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
251	00NA		1-Ethoxy-2,3-difluoro-4-[[4-(4-ethylcyclohexyl)phenyl]ethynyl]benzene	C(c3c(F)c(F)c(OCC)cc3)#Cc1ccc(C2CCC(CC)CC2)cc1	368.5	5.4E-08	7.20E-06	0.199	-3.04	8.72	11.76	1906	3.28	-0.8613	0.0765	180.0	360.0	1620.8	2.85E-06	Mysid 96-hr LC50	Neutral Organics
252	00NA		4-Methyl-4'-(but-3-enyl)-biphenyl	c1(c2ccc(CCC=C)cc2)ccc(C)cc1	222.3	0.0000548	7.31E-03	0.289	-1.45	6.19	7.64	5626	3.75	0.751	0.1702	37.5	75.0	337.5	1.78E-03	Mysid 96-hr LC50	Neutral Organics
253	00NA		1-methoxy-4-(4-((E)-2-(4-((E)-prop-1-enyl)cyclohexyl)vinyl)cyclohexyl)benzene	c1(C2CCC(C=CC3CCC(C=CC)CC3)CC2)ccc(OC)cc1	338.5	2.21E-07	2.94E-05	0.0658 [Cis-isomer]	-0.70	9.53	10.23	766.1	2.88	0.773	0.1441	37.5	75.0	337.5	2.86E-07	Mysid 96-hr LC50	Neutral Organics
254	00174079-87-9		(E)-1-methoxy-4-(4-(2-(4-vinylcyclohexyl)vinyl)cyclohexyl)benzene	c1(C2CCC(C=CC3CCC(C=C)CC3)CC2)ccc(OC)cc1	324.5	6.77E-07	9.03E-05	0.0808 [Cis-isomer]	-0.89	9.12	10.01	1220	3.09	0.7796	0.1916	37.5	75.0	337.5	8.50E-07	Mysid 96-hr LC50	Neutral Organics
255	00NA		(E)-1-methyl-4-(4-(2-(4-vinylcyclohexyl)vinyl)cyclohexyl)benzene	c1(C2CCC(C=CC3CCC(C=C)CC3)CC2)ccc(C)cc1	308.5	1.91E-06	2.55E-04	0.0955 [Cis-isomer]	0.38	9.58	9.20	720.9	2.86	0.71	0.085	37.5	75.0	337.5	2.25E-07	Mysid 96-hr LC50	Neutral Organics
256	00337366-98-0		2,6-difluoro-4-(4-vinylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(C=C)CC2)cc1F	247.3	0.000169	2.25E-02	0.274	-2.12	5.53	7.65	2069	3.32	-0.6285	0.1995	180.0	360.0	1620.8	1.20E-02	Mysid 96-hr LC50	Neutral Organics
257	00NA		(E)-2-fluoro-4-(4-(prop-1-enyl)cyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(C=CC)CC2)cc1	243.3	0.0000432	5.76E-03	0.155 [Cis-isomer]	-1.99	5.74	7.73	2855	3.46	0.1834	0.1963	60.0	120.0	541.7	7.00E-03	Mysid 96-hr LC50	Neutral Organics
258	00157453-50-4		2-fluoro-4-(4-vinylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(C=C)CC2)cc1	229.3	0.000137	1.83E-02	0.275	-2.18	5.33	7.51	1526	3.18	0.1901	0.2438	60.0	120.0	541.7	1.90E-02	Mysid 96-hr LC50	Neutral Organics
259	00153429-48-2		1-(but-3-enyl)-4-(4-propylcyclohexyl)cyclohexane	C1(C2CCC(CCC=C)CC2)CCC(CCC)CC1	262.5	0.00068	9.06E-02	0.187	1.86	9.02	7.17	1367	3.14	0.6226	0.3555	37.5	75.0	337.5	9.05E-07	Mysid 96-hr LC50	Neutral Organics
260	00155266-68-5		4-(4-(4-(but-3-enyl)cyclohexyl)cyclohexyl)-1,2-difluorobenzene	c1(F)c(F)cc(C2CCC(C3CCC(CCC=C)CC3)CC2)cc1	332.5	6.29E-06	8.39E-04	0.191	0.53	9.65	9.12	667.3	2.82	-0.976	0.0852	180.0	360.0	1620.8	2.01E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

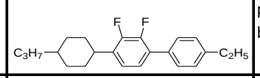
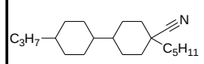
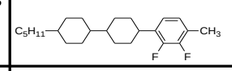
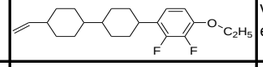
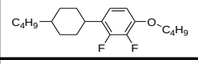
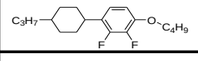
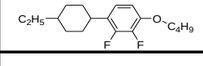
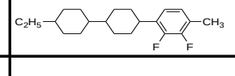
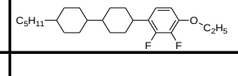
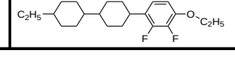
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
261	00943538-31-6		4'-Ethyl-2,3-difluoro-4-(4-propylcyclohexyl)-1,1'-biphenyl	c1(c2c(F)c(F)c(C3CCC(CCC)CC3)cc2)ccc(CC)cc1	342.5	3.13E-07	4.17E-05	0.537	-0.80	9.41	10.21	874.3	2.94	-0.9261	-0.0971	180.0	360.0	1620.8	3.99E-07	Mysid 96-hr LC50	Neutral Organics
262	00NA		1-pentyl-4-(4-propylcyclohexyl)cyclohexanecarbonitrile	C(#N)C1(CCCCC)CCC(C2CCC(CCC)CC2)CC1	303.5	1.25E-06	1.66E-04	0.352	-1.28	8.63	9.91	2117	3.33	0.8345	0.4409	37.5	75.0	337.5	3.03E-06	Mysid 96-hr LC50	Neutral Organics
263	00208717-25-3		2,3-difluoro-1-methyl-4-(4-(4-pentylcyclohexyl)cyclohexyl)benzene	c1(C)c(F)c(F)c(C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	362.6	1.05E-06	1.40E-04	0.321	0.82	10.83	10.01	177.3	2.25	-0.8273	0.1097	180.0	360.0	1620.8	8.78E-09	Mysid 96-hr LC50	Neutral Organics
264	00NA		1-ethoxy-2,3-difluoro-4-(4-(4-vinylcyclohexyl)cyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(C3CCC(C=C)CC3)CC2)cc1	348.5	2.34E-06	3.12E-04	0.158	-0.83	9.24	10.07	1060	3.03	-0.8518	0.1756	180.0	360.0	1620.8	6.48E-07	Mysid 96-hr LC50	Neutral Organics
265	00NA		1-butoxy-4-(4-butylcyclohexyl)-2,3-difluorobenzene	c1(OCCCC)c(F)c(F)c(C2CCC(CCCC)CC2)cc1	324.5	0.0000117	1.56E-03	0.27	-0.59	8.66	9.25	2054	3.31	-0.6235	0.3722	60.0	120.0	541.7	3.01E-06	Mysid 96-hr LC50	Neutral Organics
266	00208709-55-1		1-butoxy-2,3-difluoro-4-(4-propylcyclohexyl)benzene	c1(OCCCC)c(F)c(F)c(C2CCC(CCC)CC2)cc1	310.4	0.0000275	3.66E-03	0.28	-0.71	8.16	8.87	3575	3.55	-0.7252	0.3645	60.0	120.0	541.7	1.11E-05	Mysid 96-hr LC50	Neutral Organics
267	00NA		1-butoxy-4-(4-ethylcyclohexyl)-2,3-difluorobenzene	c1(OCCCC)c(F)c(F)c(C2CCC(CC)CC2)cc1	296.4	0.0000659	8.79E-03	0.291	-0.83	7.67	8.50	6222	3.79	-0.7185	0.3568	60.0	120.0	541.7	4.05E-05	Mysid 96-hr LC50	Neutral Organics
268	00174350-08-4		1-(4-(4-ethylcyclohexyl)cyclohexyl)-2,3-difluoro-4-methylbenzene	c1(C)c(F)c(F)c(C2CCC(C3CCC(CC)CC3)CC2)cc1	320.5	0.0000118	1.58E-03	0.367	0.45	9.35	8.90	934.5	2.97	-0.9157	0.0866	180.0	360.0	1620.8	4.39E-07	Mysid 96-hr LC50	Neutral Organics
269	00124728-81-0		1-ethoxy-2,3-difluoro-4-(4-(4-pentylcyclohexyl)cyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(C3CCC(CCCCC)CC3)CC2)cc1	392.6	1.66E-07	2.21E-05	0.224	-0.33	10.85	11.18	172.4	2.24	-0.7643	0.2239	180.0	360.0	1620.8	8.88E-09	Mysid 96-hr LC50	Neutral Organics
270	00253199-08-5		1-ethoxy-4-(4-(4-ethylcyclohexyl)cyclohexyl)-2,3-difluorobenzene	c1(OCC)c(F)c(F)c(C2CCC(C3CCC(CC)CC3)CC2)cc1	350.5	2.18E-06	2.91E-04	0.246	-0.70	9.38	10.08	908.8	2.96	-0.8527	0.2009	180.0	360.0	1620.8	4.49E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

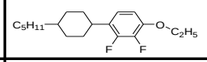
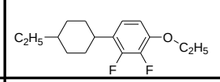
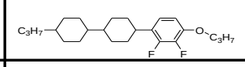
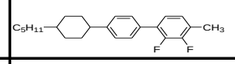
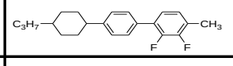
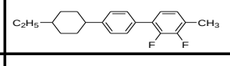
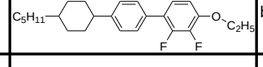
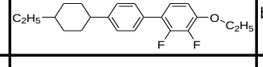
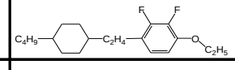
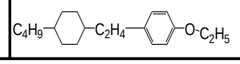
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
271	00124729-02-8		1-ethoxy-2,3-difluoro-4-(4-pentylcyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(CCCCC)CC2)cc1	310.4	0.0000275	3.66E-03	0.307	-0.71	8.16	8.87	3575	3.55	-0.7252	0.3645	60.0	120.0	541.7	1.11E-05	Mysid 96-hr LC50	Neutral Organics
272	00415915-41-2		1-ethoxy-4-(4-ethylcyclohexyl)-2,3-difluorobenzene	c1(OCC)c(F)c(F)c(C2CCC(CC)CC2)cc1	268.4	0.000433	5.77E-02	0.349	-1.08	6.69	7.77	12080	4.08	-0.8136	0.3415	180.0	360.0	1620.8	5.41E-04	Mysid 96-hr LC50	Neutral Organics
273	00473257-14-6		2,3-difluoro-1-propoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(OCCC)c(F)c(F)c(C2CCC(C3CCC(CCC)CC3)CC2)cc1	378.6	3.93E-07	5.24E-05	0.217	-0.45	10.36	10.81	300.1	2.48	-0.8661	0.2163	180.0	360.0	1620.8	3.29E-08	Mysid 96-hr LC50	Neutral Organics
274	00NA		2,3-Difluoro-4-methyl-4'-(4-pentylcyclohexyl)-1,1'-biphenyl	c1(c3c(F)c(F)c(C)cc3)ccc(C2CCC(CCCCC)CC2)cc1	356.5	1.32E-07	1.76E-05	0.491	-0.68	9.90	10.58	502.4	2.70	-0.8244	0.0567	180.0	360.0	1620.8	1.08E-07	Mysid 96-hr LC50	Neutral Organics
275	00364765-44-6		2,3-Difluoro-4-methyl-4'-(4-propylcyclohexyl)-1,1'-biphenyl	c1(c3c(F)c(F)c(C)cc3)ccc(C2CCC(CCC)CC2)cc1	328.5	7.41E-07	9.87E-05	0.564	-0.92	8.92	9.84	1522	3.18	-0.9195	0.0414	180.0	360.0	1620.8	1.47E-06	Mysid 96-hr LC50	Neutral Organics
276	00NA		2,3-Difluoro-4-methyl-4'-(4-ethylcyclohexyl)-1,1'-biphenyl	c1(c3c(F)c(F)c(C)cc3)ccc(C2CCC(CC)CC2)cc1	314.4	1.74E-06	2.32E-04	0.61	-1.05	8.43	9.48	2648	3.42	-0.9128	0.0337	180.0	360.0	1620.8	5.40E-06	Mysid 96-hr LC50	Neutral Organics
277	00123560-47-4		2,3-Difluoro-4-ethoxy-4'-(4-pentylcyclohexyl)-1,1'-biphenyl	c1(c3c(F)c(F)c(OCC)cc3)ccc(C2CCC(CCCCC)CC2)cc1	386.5	2.42E-08	3.23E-06	0.328	-1.83	9.93	11.76	488.6	2.69	-0.7614	0.171	180.0	360.0	1620.8	1.10E-07	Mysid 96-hr LC50	Neutral Organics
278	00323178-01-4		2,3-Difluoro-4-ethoxy-4'-(4-ethylcyclohexyl)-1,1'-biphenyl	c1(c3c(F)c(F)c(OCC)cc3)ccc(C2CCC(CC)CC2)cc1	344.5	2.77E-07	3.69E-05	0.378	-2.20	8.46	10.66	2575	3.41	-0.8498	0.148	180.0	360.0	1620.8	5.53E-06	Mysid 96-hr LC50	Neutral Organics
279	00NA		1-Ethoxy-2,3-difluoro-4-[2-(4-butylcyclohexyl)ethyl]benzene	c1(OCC)c(F)c(F)c(CCC2CCC(CCCC)CC2)cc1	324.5	0.0000117	1.56E-03	0.29	-0.59	8.66	9.25	2054	3.31	-0.7319	0.2893	60.0	120.0	541.7	3.01E-06	Mysid 96-hr LC50	Neutral Organics
280	00NA		1-Ethoxy-4-[2-(4-butylcyclohexyl)ethyl]benzene	CCCCC(CC1)CCC1CCc2ccc(cc2)OCC	288.5	0.0000115	1.54E-03	0.206	-0.72	8.26	8.98	3229	3.51	0.9052	0.378	37.5	75.0	337.5	8.02E-06	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

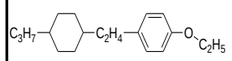
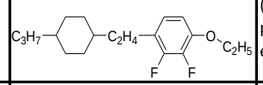
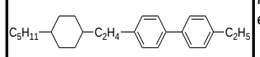
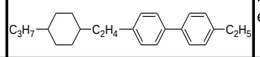
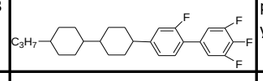
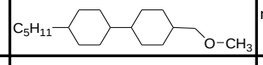
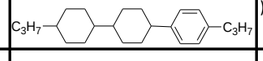
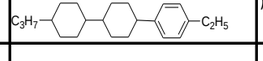
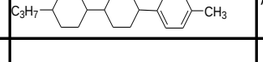
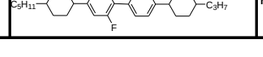
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
281	00NA		1-Ethoxy-4-[2-(4-propylcyclohexyl)ethyl]benzene	c1(OCC)ccc(CCC2CCC(CCC)CC2)cc1	274.5	0.0000271	3.61E-03	0.212	-0.84	7.76	8.60	5619	3.75	0.8035	0.3703	37.5	75.0	337.5	2.93E-05	Mysid 96-hr LC50	Neutral Organics
282	00NA		1-Ethoxy-2,3-difluoro-4-[2-(4-propylcyclohexyl)ethyl]benzene	FC1=C(CCC2CCC(CCC)CC2)C=CC(OCC)=C1F	310.4	0.0000275	3.66E-03	0.302	-0.71	8.16	8.87	3575	3.55	-0.8336	0.2816	180.0	360.0	1620.8	1.11E-05	Mysid 96-hr LC50	Neutral Organics
283	0085872-01-1		4-Ethyl-4'-[2-(4-pentylcyclohexyl)ethyl]biphenyl	c1(c2ccc(CCC3CCC(CCCCC)CC3)cc2)ccc(CC)cc1	362.6	8.33E-09	1.11E-06	0.352	-0.44	10.98	11.42	149.8	2.18	0.7927	-0.0606	37.5	75.0	337.5	5.83E-09	Mysid 96-hr LC50	Neutral Organics
284	00NA		4-Ethyl-4'-[2-(4-propylcyclohexyl)ethyl]biphenyl	c1(c2ccc(CCC3CCC(CCC)CC3)cc2)ccc(CC)cc1	334.6	4.11E-08	5.48E-06	0.389	-0.69	9.99	10.68	453.7	2.66	0.6976	-0.0759	37.5	75.0	337.5	7.93E-08	Mysid 96-hr LC50	Neutral Organics
285	00188289-44-3		2,3',4',5'-Tetrafluoro-4-[4'-propyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	c1(c2c(F)cc(C3CCC(C4CCC(CCC)CC4)CC3)cc2)cc(F)c(F)c(F)c1	432.6	1.28E-08	1.71E-06	0.347	-0.45	11.46	11.91	86.57	1.94	-2.6437	-0.1795	180.0	360.0	1620.8	1.84E-09	Mysid 96-hr LC50	Neutral Organics
286	0088416-89-1		1-(methoxymethyl)-4-(4-pentylcyclohexyl)cyclohexane	C1(C2CCC(CCCCC)CC2)CCC(COC)CC1	280.5	0.000184	2.45E-02	0.234	-0.07	7.90	7.97	4836	3.69	0.3751	0.3346	15.0	30.0	135.0	2.08E-05	Mysid 96-hr LC50	Neutral Organics
287	0084656-77-9		1-propyl-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(CCC)cc1	326.6	8.71E-07	1.16E-04	0.296	0.69	10.43	9.74	278.7	2.45	0.7014	0.0522	37.5	75.0	337.5	2.37E-08	Mysid 96-hr LC50	Neutral Organics
288	0084656-76-8		1-ethyl-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(CC)cc1	312.5	2.08E-06	2.78E-04	0.308	0.56	9.94	9.38	485	2.69	0.7081	0.0445	37.5	75.0	337.5	8.71E-08	Mysid 96-hr LC50	Neutral Organics
289	0084656-75-7		1-methyl-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(C2CCC(C3CCC(CCC)CC3)CC2)ccc(C)cc1	298.5	4.94E-06	6.59E-04	0.314	0.44	9.44	9.00	844	2.93	0.7148	0.183	37.5	75.0	337.5	3.19E-07	Mysid 96-hr LC50	Neutral Organics
290	00106349-49-9		2-Fluoro-4-(4-pentylcyclohexyl)-4'-(4-propylcyclohexyl)biphenyl	c1(c4c(F)cc(C3CCC(CCCCC)CC3)cc4)ccc(C2CCC(CCC)CC2)cc1	448.7	1.19E-10	1.58E-08	0.269	-0.12	13.37	13.49	10.03	1.00	-0.0583	-0.0874	60.0	120.0	541.7	1.02E-11	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

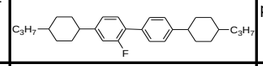
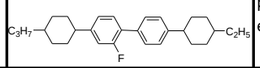
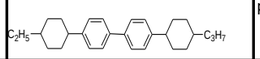
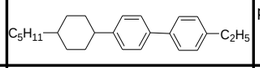
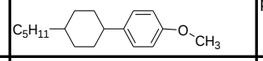
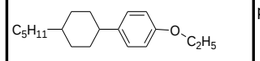
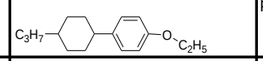
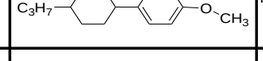
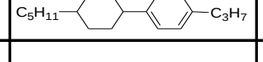
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
291	00102714-93-2		2-Fluoro-4,4'-bis(4-propylcyclohexyl)biphenyl	c1(c4c(F)cc(C3CCC(CCC)CC3)cc4)ccc(C2CCC(CCC)CC2)cc1	420.7	6.96E-10	9.28E-08	0.289	-0.36	12.39	12.75	30.37	1.48	-0.1534	-0.1027	180.0	360.0	1620.8	1.41E-10	Mysid 96-hr LC50	Neutral Organics
292	00708264-04-4		2-Fluoro-4-(4-propylcyclohexyl)-4'-(4-ethylcyclohexyl)biphenyl	c1(c4c(F)cc(C3CCC(CCC)CC3)cc4)ccc(C2CCC(CC)CC2)cc1	406.6	1.29E-09	1.72E-07	0.301	-0.49	11.90	12.39	52.86	1.72	-0.1467	-0.1104	180.0	360.0	1620.8	5.21E-10	Mysid 96-hr LC50	Neutral Organics
293	00300545-17-9		4-(4-Ethylcyclohexyl)-4'-(4-propylcyclohexyl)biphenyl	c1(c4ccc(C3CCC(CCC)CC3)cc4)ccc(C2CCC(CC)CC2)cc1	388.6	1.21E-09	1.62E-07	0.292	-0.55	11.70	12.25	66.27	1.82	0.6719	-0.0661	60.0	120.0	541.7	8.63E-10	Mysid 96-hr LC50	Neutral Organics
294	0079709-85-6		4-Ethyl-4'-(4-pentylcyclohexyl)biphenyl	c1(c2ccc(C3CCC(CCCCC)CC3)cc2)ccc(CC)cc1	334.6	4.11E-08	5.48E-06	0.395	-0.69	9.99	10.68	453.7	2.66	0.806	0.007	37.5	75.0	337.5	7.93E-08	Mysid 96-hr LC50	Neutral Organics
295	0084952-30-7		1-Methoxy-4-(4-pentylcyclohexyl)benzene	c1(C2CCC(CCCCC)CC2)ccc(OC)cc1	260.4	0.0000637	8.50E-03	0.241	-0.97	7.27	8.24	9780	3.99	0.9186	0.4456	15.0	30.0	135.0	1.07E-04	Mysid 96-hr LC50	Neutral Organics
296	0084540-32-9		1-Ethoxy-4-(4-pentylcyclohexyl)benzene	c1(C2CCC(CCCCC)CC2)ccc(OCC)cc1	274.5	0.0000271	3.61E-03	0.215	-0.84	7.76	8.60	5619	3.75	0.9119	0.4533	15.0	30.0	135.0	2.93E-05	Mysid 96-hr LC50	Neutral Organics
297	0080944-44-1		1-Ethoxy-4-(4-propylcyclohexyl)benzene	c1(C2CCC(CCC)CC2)ccc(OCC)cc1	246.4	0.000155	2.07E-02	0.228	-1.09	6.78	7.87	13850	4.14	0.8168	0.4379	37.5	75.0	337.5	3.88E-04	Mysid 96-hr LC50	Neutral Organics
298	0081936-32-5		1-Methoxy-4-(4-propylcyclohexyl)benzene	c1(C2CCC(CCC)CC2)ccc(OC)cc1	232.4	0.000396	5.28E-02	0.257	-1.21	6.29	7.50	6570	3.82	0.8235	0.4302	37.5	75.0	337.5	1.40E-03	Mysid 96-hr LC50	Neutral Organics
299	0082991-48-8		1-(4-Pentylcyclohexyl)-4-propylbenzene	c1(C2CCC(CCCCC)CC2)ccc(CCC)cc1	272.5	0.0000317	4.23E-03	0.411	0.55	8.72	8.17	1908	3.28	0.8356	0.2082	37.5	75.0	337.5	2.11E-06	Mysid 96-hr LC50	Neutral Organics
300	0082991-47-7		1-Ethyl-4-(4-propylcyclohexyl)benzene	c1(C2CCC(CCC)CC2)ccc(CC)cc1	230.4	0.000463	6.17E-02	0.489	0.18	7.25	7.07	10060	4.00	0.7472	0.1851	37.5	75.0	337.5	1.01E-04	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

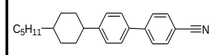
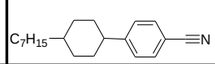
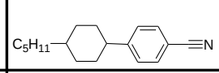
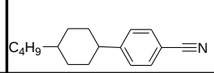
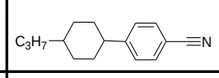
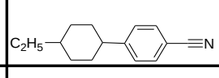
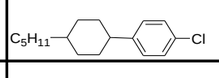
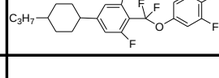
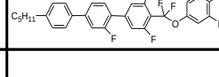
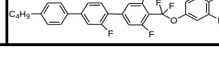
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
301	0068065-81-6		4-(4-pentylcyclohexyl)-4'-cyanobiphenyl	C(#N)c1ccc(c2ccc(C3CCC(CCCCC)CC3)cc2)cc1	331.5	6.17E-09	8.22E-07	0.501	-2.87	8.50	11.37	2441	3.39	1.0598	0.143	37.5	75.0	337.5	4.67E-06	Mysid 96-hr LC50	Neutral Organics
302	0061204-03-3		4-(4-Heptylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(CCCCCCC)CC2)cc1	283.5	1.61E-06	2.14E-04	0.5	-1.51	7.72	9.23	5897	3.77	1.0827	0.3519	37.5	75.0	337.5	3.40E-05	Mysid 96-hr LC50	Neutral Organics
303	0062788-05-0		4-(4-Pentylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(CCCCC)CC2)cc1	255.4	9.07E-06	1.21E-03	0.576	-1.75	6.74	8.49	12980	4.11	1.0961	0.3365	15.0	30.0	135.0	4.52E-04	Mysid 96-hr LC50	Neutral Organics
304	0061204-00-0		4-(4-Butylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(CCCC)CC2)cc1	241.4	0.0000213	2.85E-03	0.623	-1.88	6.25	8.13	6156	3.79	1.1027	0.3288	15.0	30.0	135.0	1.64E-03	Mysid 96-hr LC50	Neutral Organics
305	00313552-83-9		4-(4-Propylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(CCC)CC2)cc1	227.4	0.0000504	6.72E-03	0.679	-2.00	5.76	7.76	2919	3.47	1.001	0.3211	37.5	75.0	337.5	6.00E-03	Mysid 96-hr LC50	Neutral Organics
306	0073592-81-1		4-(4-Ethylcyclohexyl)benzonitrile	C(#N)c1ccc(C2CCC(CC)CC2)cc1	213.3	0.000123	1.64E-02	0.746	-2.12	5.27	7.39	1384	3.14	1.0077	0.3134	37.5	75.0	337.5	2.10E-02	Mysid 96-hr LC50	Neutral Organics
307	00189887-50-1		1-Chloro-4-(4-pentylcyclohexyl)benzene	c1(C2CCC(CCCCC)CC2)ccc(Cl)cc1	264.8	0.0000914	1.22E-02	0.551	0.13	7.84	7.71	5178	3.71	0.6021	0.243	37.5	75.0	337.5	2.32E-05	Mysid 96-hr LC50	Neutral Organics
308	00208338-62-9		2-(difluoro(3,4,5-trifluorophenoxy)methyl)-1,3-difluoro-5-(4-propylcyclohexyl)benzene	C(F)(F)(c3c(F)cc(C2CCC(CCC)CC2)cc3F)Oc1cc(F)c(F)c(F)c1	434.4	2.16E-06	2.88E-04	0.305	-1.38	10.03	11.41	438.1	2.64	-3.5066	0.018	180.0	360.0	1620.8	9.46E-08	Mysid 96-hr LC50	Neutral Organics
309	00916156-32-6		4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-2',3,5-trifluoro-4''-pentyl-1,1':4',1''-terphenyl	C(F)(F)(c4c(F)cc(c2c(F)cc(c3ccc(CCCCC)cc3)cc2)cc4F)Oc1cc(F)c(F)c(F)c1	550.5	5.22E-11	6.96E-09	0.408	-3.67	12.05	15.72	44.68	1.65	-4.2634	-0.3404	180.0	360.0	1620.8	4.69E-10	Mysid 96-hr LC50	Neutral Organics
310	00914087-74-4		4''-Butyl-4-[difluoro(3,4,5-trifluorophenoxy)methyl]-2',3,5-trifluoro-1,1':4',1''-terphenyl	C(F)(F)(c4c(F)cc(c2c(F)cc(c3ccc(CCCC)cc3)cc2)cc4F)Oc1cc(F)c(F)c(F)c1	536.5	1.2E-10	1.60E-08	0.431	-3.80	11.56	15.36	77.75	1.89	-4.2567	-0.348	180.0	360.0	1620.8	1.76E-09	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

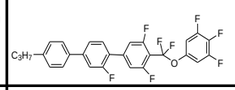
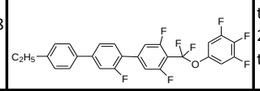
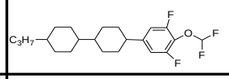
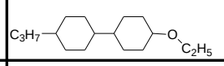
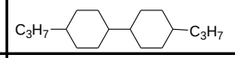
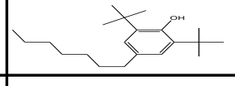
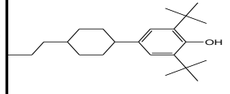
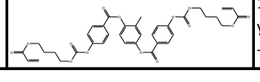
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
311	00303186-36-9		4''-Propyl-4-[difluoro(3,4,5-trifluorophenoxy)methyl]-2',3,5-trifluoro-1,1':4',1''-terphenyl	C(F)(F)(c4c(F)cc(c2c(F)cc(c3ccc(CCC)cc3)cc2)cc4F)Oc1cc(F)c(F)c(F)c1	522.4	2.73E-10	3.64E-08	0.457	-3.92	11.07	14.99	135.3	2.13	-4.3585	-0.3557	180.0	360.0	1620.8	6.56E-09	Mysid 96-hr LC50	Neutral Organics
312	001047653-92-8		4''-Ethyl-4-[difluoro(3,4,5-trifluorophenoxy)methyl]-2',3,5-trifluoro-1,1':4',1''-terphenyl	C(F)(F)(c4c(F)cc(c2c(F)cc(c3ccc(CC)cc3)cc2)cc4F)Oc1cc(F)c(F)c(F)c1	508.4	6.22E-10	8.30E-08	0.486	-4.04	10.58	14.62	235.5	2.37	-4.3518	-0.3634	180.0	360.0	1620.8	2.45E-08	Mysid 96-hr LC50	Neutral Organics
313	00NA		2-(difluoromethoxy)-1,3-difluoro-5-(4-(4-propylcyclohexyl)cyclohexyl)benzene	c1(F)c(OC(F)F)c(F)cc(C2CCC(C3CCC(CCC)CC3)CC2)c1	386.5	2.85E-06	3.80E-04	0.313	-0.10	9.74	9.84	606.9	2.78	-0.8698	0.0775	180.0	360.0	1620.8	1.86E-07	Mysid 96-hr LC50	Neutral Organics
314	0095756-62-0		1-ethoxy-4-(4-propylcyclohexyl)cyclohexane	C1(C2CCC(CCC)CC2)CCC(OCC)CC1	252.4	0.00127	1.70E-01	0.219	-0.32	6.91	7.23	16960	4.23	0.28	0.3193	37.5	75.0	337.5	2.76E-04	Mysid 96-hr LC50	Neutral Organics
315	0086503-59-5		1-propyl-4-(4-propylcyclohexyl)cyclohexane	C1(C2CCC(CCC)CC2)CCC(CCC)CC1	250.5	0.00156	2.08E-01	0.343	2.14	8.66	6.52	2039	3.31	0.6283	0.3731	37.5	75.0	337.5	2.28E-06	Mysid 96-hr LC50	Neutral Organics
316	00NA		4-Ethyl-4'-pentyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCCCC)CC2)CCC(CC)CC1	264.5	0.000626	8.35E-02	0.328	2.26	9.15	6.89	1172	3.07	0.7301	0.3808	15.0	30.0	135.0	6.27E-07	Mysid 96-hr LC50	Neutral Organics
317	00NA		4-Ethyl-4'-butyl-1,1'-bi(cyclohexyl)	C1(C2CCC(CCCC)CC2)CCC(CC)CC1	250.5	0.00156	2.08E-01	0.343	2.14	8.66	6.52	2039	3.31	0.7367	0.3731	15.0	30.0	135.0	2.28E-06	Mysid 96-hr LC50	Neutral Organics
318	00765956-84-1		2,6-di-tert-butyl-4-heptylphenol	C(C)(C)(C)c1c(O)c(C(C)(C)C)cc(CCCCCCC)c1	304.5	7.73E-07	1.03E-04	0.42	-3.03	7.98	11.01	2654	3.42	0.5136	0.2163	37.5	75.0	337.5	2.27E-04	Fish (SW) 96-hr LC50	Phenols
319	00400031-56-3		2,6-di-tert-butyl-4-(4-propylcyclohexyl)phenol	C(C)(C)(C)c1c(O)c(C(C)(C)C)cc(C2CCC(CCC)CC2)c1	330.6	1.1E-07	1.46E-05	0.339	-3.15	8.70	11.85	1174	3.07	0.3928	0.1279	60.0	120.0	541.7	6.10E-05	Fish (SW) 96-hr LC50	Phenols
320	00187585-64-4		2-Methyl-1,4-phenylene bis[4-[[[4-[(1-oxo-2-propen-1-yl)oxy]butoxy]carbonyl]oxy]-benzoate]	O=C(c3ccc(OC(=O)OCCCCOC(=O)C=C)cc3)Oc1c(C)cc(OC(=O)c2ccc(OC(=O)OCCCCOC(=O)C=C)cc2)cc1	704.7	1.33E-19	1.77E-17	0.274	-13.67	6.98	20.65	786	2.90	1.1635	0.5549	60.0	120.0	541.7	1.10E-02	Mysid 96-hr LC50	Acrylates + Esters

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

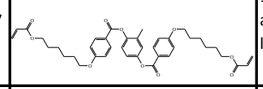
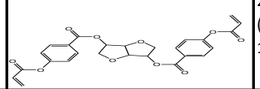
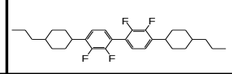
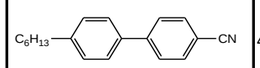
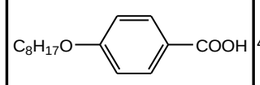
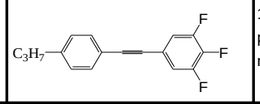
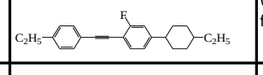
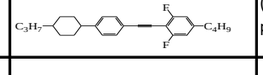
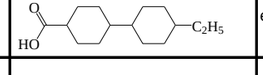
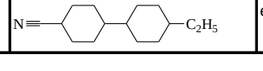
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
321	00125248-71-7		1,4-Bis-[4-(6-acryloyloxyhexyloxy)benzoyloyy]-2-methylbenzene	O=C(c3ccc(OCCCCCCOC(=O)C=C)cc3)Oc1c(C)cc(OC(=O)c2ccc(OCCCCCCOC(=O)C=C)cc2)cc1	672.8	6.16E-17	8.22E-15	0.112	-12.89	10.19	23.08	92.39	1.97	1.4425	1.238	60.0	120.0	541.7	2.39E-05	Mysid 96-hr LC50	Acrylates + Esters
322	00NA		2,5-Bis-O-[4-(acryloyloxy)benzoyl]-1,4:3,6-dianhydrohexitol	O=C(c4ccc(OC(=O)C=C)cc4)OC1C2C(C(OC(=O)c3ccc(OC(=O)C=C)cc3)CO2)OC1	494.5	1.19E-11	1.59E-09	0.207	-15.68	1.81	17.49	7.246	0.86	0.5141	0.8111	37.5	75.0	337.5	2.96E+00	Mysid 96-hr LC50	Acrylates + Esters
323	00NA		2,2',3,3'-tetrafluoro-4-(4-propylcyclohexyl)-4'-(4-propylcyclohexyl)biphenyl	c1(c4c(F)c(F)c(C3CCC(CCC)CC3)cc4)c(F)c(F)c(C2CCC(CCC)CC2)cc1	474.6	9.92E-10	1.32E-07	0.338	-0.16	12.99	13.15	15.41	1.19	-2.609	-0.2358	180.0	360.0	1620.8	3.05E-11	Mysid 96-hr LC50	Neutral Organics
324	0041122-70-7		4-cyano-4'-hexylbiphenyl	C(#N)c(cc2)ccc2c1ccc(CCCCCC)cc1	263.4	5.63E-07	7.51E-05	1.033	-3.13	6.09	9.22	4.84E+03	3.69	1.0923	0.3394	15.0	30.0	135.0	1.52E-03	Mysid 96-hr LC50	Neutral Organics
325	002493-84-7		4-(octyloxy)benzoic acid	O=C(c1ccc(OCCCCCCCC)cc1)O	250.3	3.15E-06	4.20E-04	0.404	-5.72	5.39	11.11	10	1.00	1.0456	0.9974	15.0	30.0	135.0	1.77E-01	Mysid 96-hr LC50	Neutral Organics
326	00NA		1,2,3-trifluoro-5-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2cc(F)c(F)c(F)c2)ccc(CCC)cc1	274.3	0.0000584	7.79E-03	0.329	-2.13	6.15	8.28	5342	3.73	-1.7583	-0.0083	180.0	360.0	1620.8	2.00E-03	Mysid 96-hr LC50	Neutral Organics
327	00NA		4-(4-ethylcyclohexyl)-1-(2-(4-ethylphenyl)ethynyl)-2-fluorobenzene	C(c3c(F)cc(C2CCC(CC)CC2)cc3)#Cc1ccc(CC)cc1	334.5	1.24E-07	1.65E-05	0.227	-1.84	8.99	10.83	1412	3.15	-0.1123	-0.1319	60.0	120.0	541.7	1.25E-06	Mysid 96-hr LC50	Neutral Organics
328	00NA		1-(2-(4-butyl-2,6-difluorophenyl)ethynyl)-4-(4-propylcyclohexyl)benzene	C(c3c(F)cc(CCCC)cc3F)#Cc1ccc(C2CCC(CCC)CC2)cc1	394.6	1.05E-08	1.40E-06	0.205	-1.41	10.66	12.07	213.6	2.33	-0.8425	-0.1532	180.0	360.0	1620.8	1.50E-08	Mysid 96-hr LC50	Neutral Organics
329	0084976-67-0		4-(4-ethylcyclohexyl)cyclohexanecarboxylic acid	O=C(O)C1CCC(C2CCC(CC)CC2)CC1	238.4	0.0000177	2.36E-03	0.409	-3.76	5.95	9.71	10	1.00	0.7068	0.4416	15.0	30.0	135.0	3.60E-02	Mysid 96-hr LC50	Neutral Organics
330	00NA		4-(4-ethylcyclohexyl)cyclohexanecarbonitrile	C(#N)C1CCC(C2CCC(CC)CC2)CC1	219.4	0.000204	2.73E-02	0.446	-2.02	5.72	7.74	2761	3.44	0.9501	0.3886	37.5	75.0	337.5	6.00E-03	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

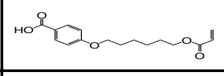
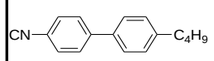
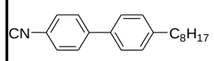
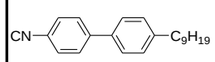
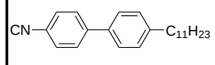
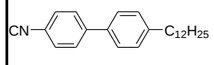
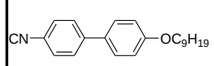
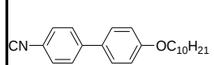
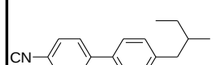
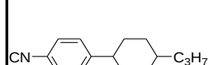
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
331	0083883-26-5		4-(6-(acryloyloxy)hexyloxy)benzoic acid	O=C(O)c1ccc(OCCCCCCOC(=O)C=C)cc1	292.3	2.27E-07	3.02E-05	0.307	-8.87	4.31	13.18	3.162	0.50	1.0913	1.1063	37.5	75.0	337.5	1.27E+00	Mysid 96-hr LC50	Acrylates
332	0052709-83-8		4-cyano-4'-butylbiphenyl	C(#N)c(ccc(c(ccc(c1)CCCC)c1)c2)c2	235.33	3.11E-06	4.14E-04	1.42E+00	-3.38	5.32	8.70	1514	3.18	1.1056	0.193	15.0	30.0	135.0	2.00E-02	Mysid 96-hr LC50	Neutral Organics
333	0052709-84-9		4-cyano-4'-octylbiphenyl	C(#N)c(ccc(c(ccc(c1)CCCCCCCC)c1)c2)c2	291.44	9.98E-08	1.33E-05	0.812	-2.88	7.29	10.17	2432	3.39	1.0789	0.2237	37.5	75.0	337.5	1.14E-04	Mysid 96-hr LC50	Neutral Organics
334	0052709-85-0		4-cyano-4'-nonylbiphenyl	C(#N)c(ccc(c(ccc(c1)CCCCCCCCC)c1)c2)c2	305.47	4.17E-08	5.56E-06	0.733	-2.76	7.78	10.54	1397	3.15	1.0722	0.2314	37.5	75.0	337.5	3.12E-05	Mysid 96-hr LC50	Neutral Organics
335	0065860-74-4		4-cyano-4'-undecylbiphenyl	C(#N)c(ccc(c(ccc(c1)CCCCCCCCCC)c1)c2)c2	333.52	7.17E-09	9.55E-07	0.614	-2.51	8.76	11.27	461.3	2.66	1.0589	0.2468	37.5	75.0	337.5	2.31E-06	Mysid 96-hr LC50	Neutral Organics
336	0057125-49-2		4-cyano-4'-dodecylbiphenyl	C(#N)c(ccc(c(ccc(c1)CCCCCCCCCCC)c1)c2)c2	347.55	3.52E-09	4.70E-07	0.568	-2.39	9.25	11.64	265.1	2.42	1.0522	0.2545	37.5	75.0	337.5	6.27E-07	Mysid 96-hr LC50	Neutral Organics
337	0058932-13-1		4-cyano-4'-nonoxybiphenyl	C(#N)c(ccc(c(ccc(OCCCCCCCCC)c1)c1)c2)c2	321.47	1.83E-08	2.44E-06	0.319	-4.03	7.31	11.34	2365	3.37	1.1418	0.4841	37.5	75.0	337.5	1.18E-04	Mysid 96-hr LC50	Neutral Organics
338	0070247-25-5		4'-(decyloxy)-4-biphenylcarbonitrile	C(#N)c(ccc(c(ccc(OCCCCCCCCCC)c1)c1)c2)c2	335.49	7.63E-09	1.02E-06	0.306	-3.91	7.8	11.71	1359	3.13	1.1352	0.4918	37.5	75.0	337.5	3.20E-05	Mysid 96-hr LC50	Neutral Organics
339	0063799-11-1		4'-(2-methylbutyl)-4-biphenylcarbonitrile	C(#N)c1ccc(cc1)c2ccc(cc2)CC(CC)C	249.36	2.03E-06	2.71E-04	1.161	-3.25	5.74	8.99	2856	3.46	0.9905	0.0516	37.5	75.0	337.5	7.00E-03	Mysid 96-hr LC50	Neutral Organics
340	0061203-99-4		4-(4-propylcyclohexyl)benzonitrile	C(#N)c(ccc(c1)C(CCC(C2)CCC)C2)c1	227.35	5.04E-05	6.72E-03	0.679	-2.00	5.76	7.76	2919	3.47	1.001	0.3211	37.5	75.0	337.5	6.00E-03	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

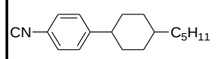
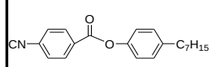
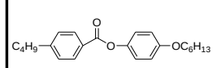
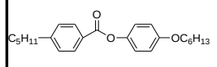
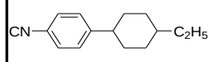
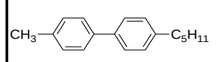
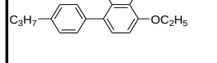
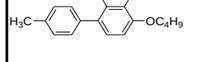
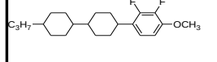
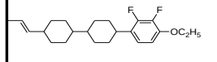
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
341	0061204-01-1		4-(trans-4-amylcyclohexyl)benzonitrile	C(#N)c(ccc(c1)C(CCC(C2)CCCCC)C2)c1	255.41	9.07E-06	1.21E-03	0.576	-1.75	6.74	8.49	12980	4.11	1.0961	0.3365	15.0	30.0	135.0	4.52E-04	Mysid 96-hr LC50	Neutral Organics
342	0038690-76-5		4-cyanophenyl 4-heptylbenzoate	O=C(Oc(ccc(C(#N))c1)c1)c(ccc(c2)CCCCCCC)c2	321.42	3.81E-08	5.07E-06	0.83	-4.51	6.09	10.60	4813	3.68	1.2388	0.4288	15.0	30.0	135.0	2.70E-02	Mysid 96-hr LC50	Esters
343	0038454-28-3		4-(hexyloxy)phenyl 4-butylbenzoate	O=C(Oc(ccc(OCCCCCC)c1)c1)c(ccc(c2)CCCC)c2	354.49	3.65E-08	4.87E-06	0.272	-3.48	7.6	11.08	1708	3.23	1.1564	0.5533	15.0	30.0	135.0	1.70E-03	Mysid 96-hr LC50	Esters
344	0050802-52-3		4-hexyloxyphenyl 4-pentylbenzoate	O=C(Oc(ccc(OCCCCCC)c1)c1)c(ccc(c2)CCCCC)c2	368.52	1.81E-08	2.42E-06	0.263	-3.36	8.09	11.45	981.6	2.99	1.1497	0.561	15.0	30.0	135.0	6.97E-04	Mysid 96-hr LC50	Esters
345	0072928-54-2		1-cyano-4-(trans-4-ethylcyclohexyl)benzene	C(#N)c(ccc(c1)C(CCC(C2)CC)C2)c1	213.33	0.000123	1.64E-02	0.746	-2.12	5.27	7.39	1384	3.14	1.0077	0.3134	37.5	75.0	337.5	2.10E-02	Mysid 96-hr LC50	Neutral Organics
346	0064835-63-8		4'-methyl-4-pentylbiphenyl	c(ccc(c(ccc(c1)C)c1)c2)(c2)CCCCC	238.38	2.17E-05	2.89E-03	0.78	-1.20	6.82	8.02	14590	4.16	0.8518	0.2031	15.0	30.0	135.0	3.41E-04	Mysid 96-hr LC50	Neutral Organics
347	157248-24-3		1-ethoxy-2,3-difluoro-4-(4-propylphenyl)benzene	Fc1c(F)c(OCC)ccc1c2ccc(CCC)cc2	276.33	2.24E-05	0.00299	0.618	-2.453	6.26	8.713	6264	3.797	-0.8174	0.2133	180	360	1621	0.00182	Mysid 96-hr LC50	Neutral Organics
348	NA		1-butoxy-2,3-difluoro-4-(4-methylphenyl)benzene	Cc1ccc(c2ccc(OCCCC)c(F)c2F)cc1	276.3	0.0000224	2.99E-03	0.506	-2.45	6.26	8.71	6264	3.80	-0.709	0.3595	60.0	120.0	541.7	1.82E-03	Mysid 96-hr LC50	Neutral Organics
349	431947-34-1		2,3-difluoro-1-methoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(F)c(OC)ccc1C(CC3)CCC3C2CCC(CCC)CC2	350.5	2.18E-06	0.000291	0.27	-0.696	9.38	10.076	908.8	2.958	-0.8527	0.2009	180	360	1621	4.49E-07	Mysid 96-hr LC50	Neutral Organics
350	NA		1-ethoxy-2,3-difluoro-4-(4-(4-(prop-1-enyl)cyclohexyl)cyclohexyl)benzene	CC=CC1CCC(C2CCC(c3ccc(OCC)c(F)c3F)CC2)CC1	362.51	7.67E-07	0.000102	0.109	-0.63	9.65	10.28	665.6	2.823	-0.8584	0.1281	180	360	1621	2.18E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

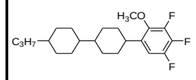
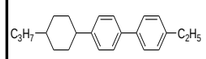
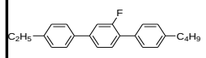
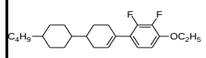
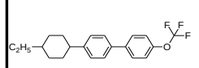
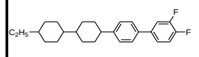
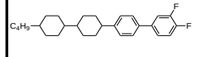
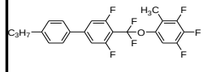
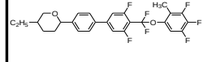
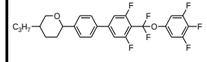
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
351	NA		1,2,3-trifluoro-4-methoxy-5-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(OC)c(C(CC3)CCC3C2CCC(CCC)CC2)cc(F)c1F	368.49	2.33E-06	0.00031	0.348	-0.63	9.58	10.21	724.9	2.86	-1.6713	0.1565	180	360	1621	2.73E-07	Mysid 96-hr LC50	Neutral Organics
352	84540-37-4		1-ethyl-4-(4-(4-propylcyclohexyl)phenyl)benzene	CCCC1CCC(c2ccc(c3ccc(CC)cc3)cc2)CC1	306.5	2.43E-07	3.24E-05	0.441	-0.935	9.01	9.945	1374	3.138	0.711	-0.0084	37.5	75	338	1.07E-06	Mysid 96-hr LC50	Neutral Organics
353	825633-75-8		4-butyl-4''-ethyl-2'-fluoro-1,1':4',1''-terphenyl	Fc1cc(c3ccc(CC)cc3)ccc1c2ccc(CCCC)cc2	332.5	1.5E-08	2E-006 (	0.758	-2.24	8.78	11.02	1785	3.25	-0.003	-0.1809	60.0	120.0	541.7	2.19E-06	Mysid 96-hr LC50	Neutral Organics
354	NA		1-(4-(4-butylcyclohexyl)cyclohex-1-enyl)-4-ethoxy-2,3-difluorobenzene	Fc1c(F)c(OCC)ccc1C(CC3)=CCC3C2CCC(CCCC)CC2	376.53	2.62E-07	3.49E-05	0.085	-0.762	10.28	11.042	330.4	2.519	-0.8114	0.2185	60	120	542	4.13E-08	Mysid 96-hr LC50	Neutral Organics
355	650634-92-7		4-(4-ethylcyclohexyl)-4'-(trifluoromethoxy)biphenyl	FC(F)(F)Oc(cc3)ccc3c(cc2)ccc2C1CCC(CC)CC1	348.4	9.51E-07	1.27E-04	0.325	-1.56	8.53	10.09	2370	3.38	0.2478	0.1201	60.0	120.0	541.7	4.57E-06	Mysid 96-hr LC50	Neutral Organics
356	NA		3,4-difluoro-4'-[4'-ethyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CC)CC4)CC3)cc2)ccc1F	382.54	2.20E-08	2.94E-06	0.357	-0.706	10.57	11.276	236.8	2.374	-0.9999	-0.0984	180	360	1621	1.87E-08	Mysid 96-hr LC50	Neutral Organics
357	NA		3,4-difluoro-4'-[4'-butyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CCCC)CC4)CC3)cc2)ccc1F	410.6	3.76E-09	5.02E-07	0.326	-0.461	11.55	12.011	78.19	1.893	-0.9048	-0.083	180	360	1621	1.36E-09	Mysid 96-hr LC50	Neutral Organics
358	NA		4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl	FC(F)(Oc3cc(F)c(F)c(F)c3C)c(c(F)c2)c(F)cc2c1ccc(CCC)cc1	442.4	1.37E-07	1.82E-05	0.426	-2.83	9.65	12.48	669.5	2.83	-3.4557	-0.1263	180.0	360.0	1620.8	2.70E-07	Mysid 96-hr LC50	Neutral Organics
359	NA		4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-ethyl-tetrahydro-2h-pyran)-yl]-biphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4C)c(c(F)c2)c(F)cc2c1ccc(C3OCC(CC)CC3)cc1	512.47	1.21E-09	1.61E-07	0.183	-5.647	10.1	15.747	403.7	2.606	-3.8911	-0.2158	180	360	1621	9.15E-08	Mysid 96-hr LC50	Neutral Organics
360	NA		4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-propyl-tetrahydro-2h-pyran)-yl]-biphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4)c(c(F)c2)c(F)cc2c1ccc(C3OCC(CC)CC3)cc1	512.47	1.23E-09	1.64E-07	0.187	-5.566	10.04	15.606	430.1	2.634	-3.9458	-0.1996	180	360	1621	1.07E-07	Mysid 96-hr LC50	Neutral Organics

Table S1. 362 Commercial LCMs with Persistence and Bioaccumulation Potential

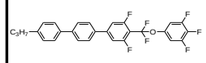
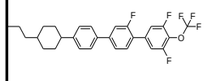
Number	CASRN	Molstructure	Name	SMILES	Mol Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
361	NA		4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4"-propyl-1,1':4',1"-terphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4)c(c(F)c2)c(F)cc2c1ccc(c3ccc(CCC)cc3)cc1	504.5	2.26E-10	3.01E-08	0.415	-3.99	10.87	14.86	169.7	2.23	-3.5399	-0.3114	180.0	360.0	1620.8	1.10E-08	Mysid 96-hr LC50	Neutral Organics
362	524709-77-1		4-trifluoromethoxy-3,5-difluoro-2'-fluoro-4"-(4-propylcyclohexyl)-1,1':4',1"-terphenyl	CCCC1CCC(c2ccc(c3ccc(c4cc(F)c(OC(F)(F)F)c(F)c4)c(F)c3)cc2)CC1	492.5	4.19E-10	5.59E-08	0.463	-2.35	11.39	13.74	94.43	1.98	-2.2507	-0.1988	180.0	360.0	1620.8	2.58E-09	Mysid 96-hr LC50	Neutral Organics

Table S2. Properties of ten liquid crystal monomers (LCMs) that were identified to be very persistent and very bioaccumulative (vPvB) in the environment.

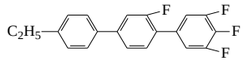
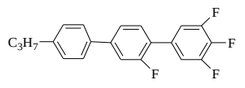
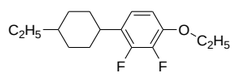
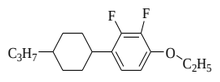
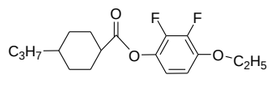
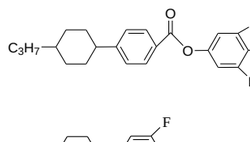
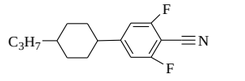
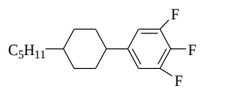
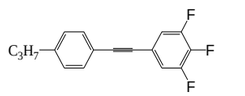
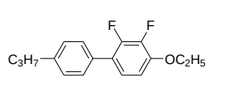
Number	CASRN	Mol. structure	Name	SMILES	Mol. Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR (lowest LC50 value for all species)	ECOSAR (species, duration, end point, predicted mg/L)	ECOSAR Class
1	00326894-55-7		4"-ethyl-2',3,4,5-tetrafluoro-1,1':4',1"-terphenyl	c1(c2c(F)cc(c3ccc(CC)cc3)cc2)cc(F)c(F)c(F)c1	331.33	7.85E-07	0.000105	1.59	-2.45	7.36	9.81	8853	3.947	-2.60	-0.18	180.0	360.0	1620.8	1.06E-04	Mysid 96-hr LC50	Neutral Organics
2	00205806-87-7		2',3,4,5-tetrafluoro-4"-propyl-1,1':4',1"-terphenyl	c1(c2c(F)cc(c3ccc(CCC)cc3)cc2)cc(F)c(F)c(F)c1	344.35	3.35E-07	4.47E-05	1.33	-2.33	7.85	10.18	5087	3.706	-2.60	-0.17	180.0	360.0	1620.8	2.89E-05	Mysid 96-hr LC50	Neutral Organics
3	00415915-41-2		1-ethoxy-2,3-difluoro-4-(4-ethylcyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(CC)CC2)cc1	268.35	0.000433	0.0577	0.35	-1.08	6.69	7.77	12080	4.082	-0.81	0.34	180.0	360.0	1620.8	5.41E-04	Mysid 96-hr LC50	Neutral Organics
4	00174350-05-1		1-ethoxy-2,3-difluoro-4-(4-propylcyclohexyl)benzene	c1(OCC)c(F)c(F)c(C2CCC(CCC)CC2)cc1	282.38	0.000165	0.022	0.33	-0.96	7.18	8.14	10830	4.035	-0.82	0.35	180.0	360.0	1620.8	1.48E-04	Mysid 96-hr LC50	Neutral Organics
5	00NA		4-ethoxy-2,3-difluorophenyl 4-propylcyclohexanecarboxylate	c1(OCC)c(F)c(F)c(OC(=O)C2CCC(CCC)CC2)cc1	326.39	9.57E-06	0.00128	0.42	-2.92	6.23	9.15	6010	3.779	-0.72	0.58	180.0	0.4	1620.8	2.10E-02	Mysid 96-hr LC50	Esters
6	00186320-72-9		4-cyano-3,5-difluorophenyl 4-(4-propylcyclohexyl)benzoate	C(#N)c1c(F)cc(OC(=O)c2ccc(C3CCC(CCC)CC3)cc2)cc1F	383.44	8.41E-09	1.12E-06	0.54	-4.49	7.21	11.70	10500	4.021	-0.52	0.25	180.0	360.0	162.1	4.00E-03	Mysid 96-hr LC50	Esters
7	00167306-96-9		2,6-difluoro-4-(4-propylcyclohexyl)benzonitrile	C(#N)c1c(F)cc(C2CCC(CCC)CC2)cc1F	263.33	6.32E-05	0.00843	0.66	-1.87	6.16	8.03	5367	3.73	-0.64	0.23	180.0	360.0	1620.8	2.00E-03	Mysid 96-hr LC50	Neutral Organics
8	00131819-22-2		1,2,3-Trifluoro-5-(4-pentylcyclohexyl)benzene	c1(F)c(F)c(F)cc(C2CCC(CCCCC)CC2)c1	284.37	0.000615	0.0819	0.53	0.46	7.79	7.33	5437	3.735	-1.65	0.21	180.0	360.0	1620.8	2.80E-05	Mysid 96-hr LC50	Neutral Organics
9	00NA		1,2,3-trifluoro-5-(2-(4-propylphenyl)ethynyl)benzene	c1(C#Cc2cc(F)c(F)c(F)c2)ccc(CCC)cc1	274.29	5.84E-05	0.00779	0.33	-2.13	6.15	8.28	5342	3.728	-1.76	-0.01	180.0	360.0	1620.8	2.00E-03	Mysid 96-hr LC50	Neutral Organics
10	157248-24-3		1-ethoxy-2,3-difluoro-4-(4-propylphenyl)benzene	Fc1c(F)c(OCC)ccc1c2ccc(CCC)cc2	276.33	2.24E-05	0.00299	0.62	-2.45	6.26	8.71	6264	3.797	-0.82	0.21	180	360	1621	0.00182	Mysid 96-hr LC50	Neutral Organics

Table S3. Pathway, RefSeq accession numbers and gene descriptions for the 43 target genes and 2 housekeeping genes on the 4th generation Avian ToxChip PCR array.

Pathway	Gene Symbol	RefSeq Accession	Description
Bile acids/cholesterol regulation	*CYP7B1*	XM_418276	Cytochrome P450, family 7, subfamily B, polypeptide 1
	FGF19	NM_204674	Fibroblast growth factor 19
	NR5A2	NM_205078	Nuclear receptor subfamily 5, group A, member 2
Cell cycle	*CDKN1A*	NM_204396	Cdk inhibitor CIP1 (p21)
	RBP2	NM_001277417	Retinol binding protein 2, cellular
	ECE1	NM_204717	Endothelin converting enzyme 1
	ROCK1	NM_001199448	Rho-associated, coiled-coil containing protein kinase 1
	TP53	NM_205264	Tumor protein p53
DNA repair	*GADD45A*	NM_001044678	Growth arrest and DNA-damage-inducible, alpha
	MGMT	XM_421823	O-6-methylguanine-DNA methyltransferase
	MSH2	XM_426110	MutS homolog 2, colon cancer, nonpolyposis type 1 (E. coli)
	SIRT3	NM_001199493	Sirtuin (silent mating type information regulation 2 homolog) 3 (S. cerevisiae)
	XPC	XM_004944606	Xeroderma pigmentosum, complementation group C
	POLB	XM_004947614	Polymerase (DNA directed), beta
	POLK	NM_204183	Polymerase (DNA directed) kappa
	DDB2	NM_001039301	Damage-specific DNA binding protein 2, 48kDa
	XRCC5	XM_004942890	X-ray repair complementing defective repair in Chinese hamster cells 5 (double-strand-break rejoining; Ku autoantigen, 80kDa)
	APEX1	NM_001184759	APEX nuclease (multifunctional DNA repair enzyme) 1
Glucose metabolism	*PDK4*	NM_001199909	Pyruvate dehydrogenase kinase, isozyme 4
	G6pc	XM_003642817	Glucose-6-phosphatase-like
Immune response	*BATF3*	XM_419428	Basic leucine zipper transcription factor, ATF-like 3
	IL16	NM_204352	Interleukin 16 (lymphocyte chemoattractant factor)
	LEAP2	NM_001001606	Liver expressed antimicrobial peptide 2
Lipid homeostasis	*LBFABP*	NM_204634	Liver basic fatty acid binding protein
	ACSL5	NM_001031237	Acyl-CoA synthetase long-chain family member 5
	SLCO1A2	XM_416421	Solute carrier organic anion transporter family, member 1A2
	SCD	NM_204890	Stearoyl-CoA desaturase (delta-9-desaturase)
Oxidative stress	*MT4*	NM_205275	Metallothionein 4
	MGST3	NM_001277533	Microsomal glutathione S-transferase 3
	OGG1	NM_001277838	8-oxoguanine DNA glycosylase
	TXN	NM_205453	Thioredoxin
Thyroid hormone pathway	*DIO1*	NM_001097614	Deiodinase, iodothyronine, type I
	TTR	NM_205335	Transthyretin
	THRSP	NM_213577	Thyroid hormone responsive (SPOT14 homolog, rat)
	IGF1	NM_001004384	Insulin-like growth factor 1 (somatomedin C)
Xenobiotic metabolism	*CYP3A7*	NM_001001751	Cytochrome P450 A 37
	CYP1A4	NM_205147	Cytochrome P450 1A4
	UGT1A9	XM_001234353	UDP glucuronosyltransferase 1 family, polypeptide A9
	SULT1B1	NM_204545	Sulfotransferase family, cytosolic, 1B, member 1
	ALAS1	NM_001018012	Aminolevulinate, delta-, synthase 1
	SULT1E1	XM_420616	Sulfotransferase family 1E, estrogen-preferring, member 1

	FGA	NM_001271911	Fibrinogen alpha chain
	MAT1A	NM_001199519	Methionine adenosyltransferase I, alpha
Control	*EEF1A1*	NM_204157	Eukaryotic translation elongation factor 1 alpha 1
	RPL4	NM_001007479	Ribosomal protein L4

Table S4. Relative abundances of characteristic ions in the EI mass spectra of bicyclohexyl derivatives [a]

No.	R^1	R^2	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %					
					80+R^1	206	109	95	81	69
1	Pr	OMe	238	81	40	63	35	31	100	52
2	Pr	Vinyl	234	69	37	6	86	64	93	100
3	Pr	Propenyl	248	81	58	6	51	47	100	71

[a] Pr=*n*-propyl, Me=methyl.

[b] m/z of base peak.

Table S5. Relative abundances of characteristic ions in the EI mass spectra of bicyclohexylphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %												
								117+R^2+R^3+R^5	114+R^2+R^3+R^4+R^5	113+R^2+R^3+R^4+R^5	104+R^2+R^3+R^5	100+R^2+R^3+R^4+R^5	87+R^2+R^3+R^4+R^5	107	95	91	83	81	69	67	55
9	Vinyl	H	H	Me	H	282	118	4	26	33	7	100	96	10	15	28	2	23	5	34	11
10	Pr	H	H	Me	H	299	118	3	9	19	2	100	51	2	5	12	14	12	20	7	10
11	Pr	F	F	OMe	H	350	350	1	6	11	1	79	57	2	6	—	24	11	34	8	16
12	Pr	F	F	OEt	H	364	364	35	4	7	41	47	18	2	7	3	24	12	33	9	16
13	Propenyl	F	F	OEt	H	362	362	14	17	3	48	52	19	7	11	5	19	15	29	17	19
14	Pr	F	F	OPr	H	379	156	100	6	2	73	6	4	3	10	—	35	19	50	15	25
15	Bu	F	F	OEt	H	378	378	39	5	8	44	54	21	2	8	2	37	14	19	10	19
16	Pr	OMe	F	F	F	368	368	—	4	9	—	66	51	2	7	8	36	17	51	13	21

[a,b] See Table S4.

[c] Et=ethyl, Bu=n-butyl.

Table S6a. Relative abundances of characteristic ions in the EI mass spectra of biphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %							
								166+R^1+R^2+R^3+R^5	247	219	170	152	151	115	91
7	Pr	F	F	OEt	H	276	219	26	36	100	11	1	5	2	1
8	Me	F	F	OBu	H	276	220	100	1	20	10	1	5	2	3

Table S6b. Relative abundances of characteristic ions in the EI mass spectra of biphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %											
								189+R^2+R^3+R^4+R^5	176+R^2+R^3+R^4+R^5	163+R^2+R^3+R^4+R^5	161+R^2+R^3+R^4+R^5	245	232	152	151	115	91	81	55
17	Pr-Cy	H	H	Et	H	306	306	23	19	16	38	—	—	3	1	3	2	3	3
21	Et-Cy	F	F	OEt	H	344	344	19	13	9	29	28	27	1	2	3	1	3	4
22	Pr-Cy	F	F	OEt	H	358	358	15	11	6	19	19	22	1	2	3	2	4	4
23	Et-Cy	H	H	OCF_3	H	348	348	51	53	22	6	—	—	6	2	6	2	3	4

Table S6c. Relative abundances of characteristic ions in the EI mass spectra of biphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %					
								M-15	289	274	183	137	91
18	Et	H	F	Ph-Pr	H	318	289	5	100	26	4	18	2
19	Et	H	F	Ph-Bu	H	332	289	4	100	29	4	10	2

Table S6d. Relative abundances of characteristic ions in the EI mass spectra of biphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %									
								229	216	203	183	151	111	97	83	69	55
24	Et-biCy	H	F	F	H	382	382	6	37	26	4	2	10	8	5	27	11
25	Pr-biCy	H	F	F	H	396	396	5	36	26	4	1	4	5	14	22	11
26	Bu-biCy	H	F	F	H	410	410	5	34	26	3	1	3	10	21	12	13
27	Pe-biCy	H	F	F	H	424	424	5	34	29	3	2	5	16	16	12	13

Table S6e. Relative abundances of characteristic ions in the EI mass spectra of biphenyl derivatives [a,c]

No.	R^1	R^2	R^3	R^4	R^5	RMM m/z	B.p.[b] m/z	Relative abundances of characteristic ions / %									
								199+R^1+R^2+R^3+R^5	213+R^2+R^3+R^5	228+R^2+R^3+R^5	200+R^2+R^3+R^5	219	207	183	170	126	69	55
28	Pr	H	F	X[d]	F	442	281	100	24	—	1	1	—	3	—	2	—	—
29	Pr	H	F	Y[e]	F	428	281	100	27	—	1	1	—	3	—	4	1	—
30	Et-Z[f]	H	F	X[d]	F	512	351	100	2	11	5	1	2	—	2	—	2	3
31	Pr-Z[f]	H	F	Y[e]	F	512	365	100	3	15	8	2	2	—	3	—	5	6

[a,b] See Table S4.

[c] Et=ethyl, Bu=n-butyl, Cy=cyclohexyl, Pe=pentyl, Ph=phenyl, biCy=bicyclohexyl.

[d] X= difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl.

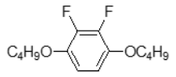
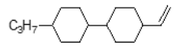
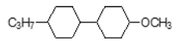
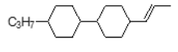
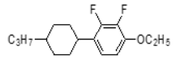
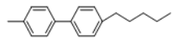
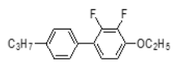
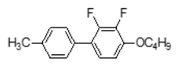
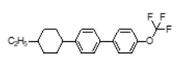
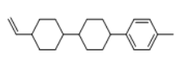
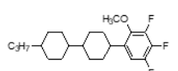
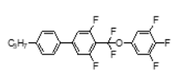
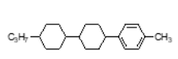
[e] Y= difluoro(3,4,5-trifluorophenoxy)methyl.

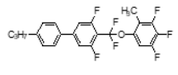
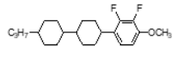
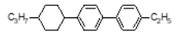
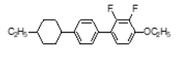
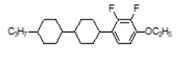
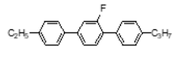
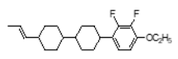
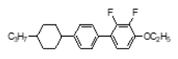
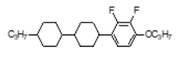
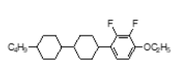
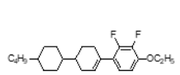
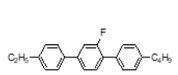
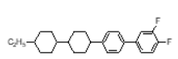
[f] Z= 2,5-tetrahydro-2H-pyran.

[g] W= 4-trifluoromethoxy-3,5-difluorophenyl.

[i] V= 3,5-difluoro-4-[difluoro(3,4,5-trifluorophenoxy)methyl]-phenyl.

Table S7. Property data for the 33 liquid crystal monomers (LCMs) that were identified from the liquid crystal displays (LCDs) of six models of largely produced commercial smartphones.

Abbreviation	CASRN	Mol. structure	Name	SMILES	Mol. Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
LCM-1	NA		1,4-dibutoxy-2,3-difluorobenzene	Fc1c(F)c(OCCCC)ccc1OCCCC	258.3	1.20E-03	1.61E-01	0.33	-2.24	5.50	7.74	1983	3.297	-0.515	0.6826	37.5	75	338	1.40E-02	Mysid 96-hr LC50	Neutral Organics
LCM-2	116020-44-1		1-(4-propylcyclohexyl)-4-vinylcyclohexane	C=CC(CC2)CCC2C1CCC(CCC)CC1	234.4	4.34E-03	5.78E-01	0.20	1.61	8.03	6.42	4139	3.617	0.6359	0.3401	37.5	75	338	1.19E-05	Mysid 96-hr LC50	Neutral Organics
LCM-3	97398-80-6		1-methoxy-4-(4-propylcyclohexyl)cyclohexane	CCCC1CCC(C2CCC(OC)CC2)CC1	238.4	3.30E-03	4.40E-01	0.25	-0.44	6.42	6.86	8041	3.905	0.2867	0.3116	37.5	75	338	1.00E-03	Mysid 96-hr LC50	Neutral Organics
LCM-4	279246-65-0		1-(prop-1-enyl)-4-(4-propylcyclohexyl)cyclohexane	CC=CC(CC2)CCC2C1CCC(CCC)CC1	248.5	1.46E-03	1.95E-01	0.13	1.81	8.45	6.65	2599	3.415	0.6293	0.2926	37.5	75	338	4.08E-06	Mysid 96-hr LC50	Neutral Organics
LCM-5	174350-05-1		1-ethoxy-2,3-difluoro-4-(4-propylcyclohexyl)benzene	Fc1c(F)c(C2CCC(CCC)CC2)ccc1OCC	282.4	1.65E-04	2.20E-02	0.33	-0.96	7.18	8.14	1.083	4.035	-0.82	0.3492	180	360	1621	1.48E-04	Mysid 96-hr LC50	Neutral Organics
LCM-6	64835-63-8		4-methyl-4'-pentylbiphenyl	Cc1ccc(c2ccc(CCCCC)cc2)cc1	238.4	2.17E-05	2.89E-03	0.78	-1.20	6.82	8.02	14590	4.164	0.8518	0.2031	15	30	135	3.41E-04	Mysid 96-hr LC50	Neutral Organics
LCM-7	157248-24-3		1-ethoxy-2,3-difluoro-4-(4-propylphenyl)benzene	Fc1c(F)c(OCC)ccc1c2ccc(CCC)cc2	276.3	2.24E-05	2.99E-03	0.62	-2.45	6.26	8.71	6264	3.797	-0.817	0.2133	180	360	1621	1.82E-03	Mysid 96-hr LC50	Neutral Organics
LCM-8	NA		1-butoxy-2,3-difluoro-4-(4-methylphenyl)benzene	Cc1ccc(c2ccc(OCCCC)c(F)c2F)cc1	276.3	2.24E-05	2.99E-03	0.51	-2.45	6.26	8.71	6264	3.797	-0.709	0.3595	60	120	542	1.82E-03	Mysid 96-hr LC50	Neutral Organics
LCM-9	650634-92-7		4-(4-ethylcyclohexyl)-4'-(trifluoromethoxy)biphenyl	FC(F)(F)Oc(cc3)ccc3c(cc2)ccc2C1CCC(CC)CC1	348.4	9.51E-07	1.27E-04	0.33	-1.56	8.53	10.09	2370	3.375	0.2478	0.1201	60	120	542	4.57E-06	Mysid 96-hr LC50	Neutral Organics
LCM-10	155041-85-3		1-methyl-4-(4-(4-vinylcyclohexyl)cyclohexyl)benzene	Cc(cc3)ccc3C(CC2)CCC2C1CCC(C=C)CC1	282.5	1.26E-05	1.68E-03	0.19	0.19	8.82	8.63	1713	3.234	0.7224	0.1501	37.5	75	338	1.69E-06	Mysid 96-hr LC50	Neutral Organics
LCM-11	NA		1,2,3-trifluoro-4-methoxy-5-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(OC)c(C(CC3)CCC3C2CCC(CCC)CC2)cc(F)c1F	368.5	2.33E-06	3.10E-04	0.35	-0.63	9.58	10.21	724.9	2.86	-1.671	0.1565	180	360	1621	2.73E-07	Mysid 96-hr LC50	Neutral Organics
LCM-12	303186-20-1		4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl	FC(F)(Oc3cc(F)c(F)c(F)c3)c(c(F)c2)c(F)cc2c1ccc(CCC)cc1	428.4	3.41E-07	4.55E-05	0.48	-2.87	9.10	11.97	1241	3.094	-3.504	-0.1178	180	360	1621	1.17E-06	Mysid 96-hr LC50	Neutral Organics
LCM-13	84656-75-7		1-methyl-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Cc(cc3)ccc3C(CC2)CCC2C1CCC(CCC)CC1	298.5	4.94E-06	6.59E-04	0.31	0.44	9.44	9.00	844	2.926	0.7148	0.183	37.5	75	338	3.19E-07	Mysid 96-hr LC50	Neutral Organics

Abbreviation	CASRN	Mol. structure	Name	SMILES	Mol. Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
LCM-14	1690317-23-7		4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl	FC(F)(Oc3cc(F)c(F)c(F)c3C)c(c(F)c2)c(F)cc2c1ccc(CCC)cc1	442.4	1.37E-07	1.82E-05	0.43	-2.83	9.65	12.48	669.5	2.826	-3.456	-0.1263	180	360	1621	2.70E-07	Mysid 96-hr LC50	Neutral Organics
LCM-15	431947-34-1		2,3-difluoro-1-methoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(F)c(OC)ccc1C(CC3)CCC3C2CCC(CCC)CC2	350.5	2.18E-06	2.91E-04	0.27	-0.70	9.38	10.08	908.8	2.958	-0.853	0.2009	180	360	1621	4.49E-07	Mysid 96-hr LC50	Neutral Organics
LCM-16	84540-37-4		1-ethyl-4-(4-(4-propylcyclohexyl)phenyl)benzene	CCCC1CCC(c2ccc(c3ccc(CC)cc3)cc2)CC1	306.5	2.43E-07	3.24E-05	0.44	-0.94	9.01	9.95	1374	3.138	0.711	-0.0084	37.5	75	338	1.07E-06	Mysid 96-hr LC50	Neutral Organics
LCM-17	323178-01-4		4-ethoxy-4'-(4-ethylcyclohexyl)-2,3-difluorobiphenyl	Fc1c(F)c(OCC)ccc1c(cc3)ccc3C2CCC(CC)CC2	344.5	2.77E-07	3.69E-05	0.38	-2.20	8.46	10.66	2575	3.411	-0.85	0.148	180	360	1621	5.53E-06	Mysid 96-hr LC50	Neutral Organics
LCM-18	123560-48-5		1-ethoxy-2,3-difluoro-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(F)c(OCC)ccc1C(CC3)CCC3C2CCC(CCC)CC2	364.5	9.29E-07	1.24E-04	0.24	-0.57	9.87	10.44	522.2	2.718	-0.859	0.2086	180	360	1621	1.22E-07	Mysid 96-hr LC50	Neutral Organics
LCM-19	95759-44-7		4''-ethyl-2'-fluoro-4-propyl-1,1':4',1''-terphenyl	Fc1cc(c3ccc(CC)cc3)ccc1c2ccc(CCC)cc2	318.4	3.61E-08	4.82E-06	0.84	-2.36	8.29	10.65	3106	3.492	-0.105	-0.1886	60	120	542	8.06E-06	Mysid 96-hr LC50	Neutral Organics
LCM-20	NA		1-ethoxy-2,3-difluoro-4-(4-(4-(prop-1-enyl)cyclohexyl)cyclohexyl)benzene	CC=CC1CCC(C2CCC(c3ccc(OCC)c(F)c3F)CC2)CC1	362.5	7.67E-07	1.02E-04	0.11	-0.63	9.65	10.28	665.6	2.823	-0.858	0.1281	180	360	1621	2.18E-07	Mysid 96-hr LC50	Neutral Organics
LCM-21	189750-98-9		4-ethoxy-2,3-difluoro-4'-(4-propylcyclohexyl)biphenyl	Fc1c(F)c(OCC)ccc1c(cc3)ccc3C2CCC(CCC)CC2	358.5	1.16E-07	1.55E-05	0.36	-2.07	8.95	11.02	1480	3.17	-0.857	0.1556	180	360	1621	1.50E-06	Mysid 96-hr LC50	Neutral Organics
LCM-22	473257-14-6		2,3-difluoro-1-propoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene	Fc1c(F)c(OCCC)ccc1C(CC3)CCC3C2CCC(CCC)CC2	378.6	3.93E-07	5.24E-05	0.22	-0.45	10.36	10.81	300.1	2.477	-0.866	0.2163	180	360	1621	3.29E-08	Mysid 96-hr LC50	Neutral Organics
LCM-23	473257-15-7		1-(4-(4-butylcyclohexyl)cyclohexyl)-4-ethoxy-2,3-difluorobenzene	Fc1c(F)c(OCC)ccc1C(CC3)CCC3C2CCC(CCCC)CC2	378.6	3.93E-07	5.24E-05	0.23	-0.45	10.36	10.81	300.1	2.477	-0.758	0.2163	180	360	1621	3.29E-08	Mysid 96-hr LC50	Neutral Organics
LCM-24	NA		1-(4-(4-butylcyclohexyl)cyclohex-1-enyl)-4-ethoxy-2,3-difluorobenzene	Fc1c(F)c(OCC)ccc1C(CC3)=CCC3C2CCC(CCCC)CC2	376.5	2.62E-07	3.49E-05	0.09	-0.76	10.28	11.04	330.4	2.519	-0.811	0.2185	60	120	542	4.13E-08	Mysid 96-hr LC50	Neutral Organics
LCM-25	825633-75-8		4-butyl-4''-ethyl-2'-fluoro-1,1':4',1''-terphenyl	Fc1cc(c3ccc(CC)cc3)ccc1c2ccc(CCCC)cc2	332.5	1.50E-08	2E-006	0.76	-2.24	8.78	11.02	1785	3.252	-0.003	-0.1809	60	120	542	2.19E-06	Mysid 96-hr LC50	Neutral Organics
LCM-26	139195-63-4		3,4-difluoro-4'-[4'-ethyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CC)CC4)CC3)cc2)ccc1F	382.5	2.20E-08	2.94E-06	0.36	-0.71	10.57	11.28	236.8	2.374	-1	-0.0984	180	360	1621	1.87E-08	Mysid 96-hr LC50	Neutral Organics

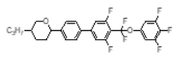
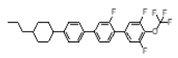
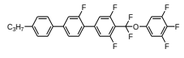
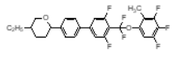
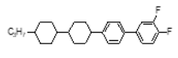
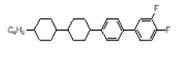
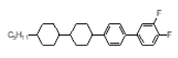
Abbreviation	CASRN	Mol. structure	Name	SMILES	Mol. Wt	Vapor Pressure estimate (mmHg)	Vapor Pressure estimate (Pa)	Atmospheric Oxidation $t_{1/2}$ (d)	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF (L/kg wet-wt)	LogBCF	BIOWIN[1]	BIOWIN[5]	Half-time in water(d)	Half-time in Soil(d)	Half-time in sediment (d)	ECOSAR(lowest LC50 value for all species)	ECOSAR(species, duration, end point, predicted mg/L)	ECOSAR Class
LCM-27	NA		4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-propyl-tetrahydro-2H-pyran)-yl]-biphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4)c(c(F)c2)c(F)cc2c1ccc(C3OCC(CCC)CC3)cc1	512.5	1.23E-09	1.64E-07	0.19	-5.57	10.04	15.61	430.1	2.634	-3.946	-0.1996	180	360	1621	1.07E-07	Mysid 96-hr LC50	Neutral Organics
LCM-28	524709-77-1		4-trifluoromethoxy-3,5-difluoro-2'-fluoro-4"-(4-propylcyclohexyl)-1,1':4',1"-terphenyl	CCCC1CCC(c2ccc(c3ccc(c4cc(F)c(OC(F)(F)F)c(F)c4)c(F)c3)cc2)CC1	492.5	4.19E-10	5.59E-08	0.46	-2.35	11.39	13.74	94.43	1.975	-2.251	-0.1988	180	360	1621	2.58E-09	Mysid 96-hr LC50	Neutral Organics
LCM-29	303186-36-9		4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-2'-fluoro-4"-propyl-1,1':4',1"-terphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4)c(c(F)c2)c(F)cc2c1ccc(c3ccc(CCC)cc3)cc1F	522.4	2.73E-10	3.64E-08	0.46	-3.92	11.07	14.99	135.3	2.131	-4.359	-0.3557	180	360	1621	6.56E-09	Mysid 96-hr LC50	Neutral Organics
LCM-30	1700444-88-7		4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-ethyl-tetrahydro-2H-pyran)-yl]-biphenyl	FC(F)(Oc4cc(F)c(F)c(F)c4C)c(c(F)c2)c(F)cc2c1ccc(C3OCC(CC)CC3)cc1	512.5	1.21E-09	1.61E-07	0.18	-5.65	10.10	15.75	403.7	2.606	-3.891	-0.2158	180	360	1621	9.15E-08	Mysid 96-hr LC50	Neutral Organics
LCM-31	119990-81-7		3,4-difluoro-4'-[4'-propyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CCC)CC4)CC3)cc2)ccc1F	396.6	9.13E-09	1.22E-06	0.34	-0.58	11.06	11.64	136.1	2.134	-1.007	-0.0907	180	360	1621	5.05E-09	Mysid 96-hr LC50	Neutral Organics
LCM-32	119990-82-8		3,4-difluoro-4'-[4'-butyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CCCC)CC4)CC3)cc2)ccc1F	410.6	3.76E-09	5.02E-07	0.33	-0.46	11.55	12.01	78.19	1.893	-0.905	-0.083	180	360	1621	1.36E-09	Mysid 96-hr LC50	Neutral Organics
LCM-33	136609-96-6		3,4-difluoro-4'-[4'-pentyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl	Fc1cc(c2ccc(C3CCC(C4CCC(CCCCC)CC4)CC3)cc2)ccc1F	424.6	1.54E-09	2.06E-07	0.31	-0.34	12.04	12.38	44.93	1.652	-0.912	-0.0754	180	360	1621	3.67E-10	Mysid 96-hr LC50	Neutral Organics

Table S8. Ion pairs and collision energy, spiked recoveries and validation parameters for determination of individual liquid crystal monomer (LCMs).

Name	CASRN	MS Quantitation		MS Confirming		Spiked Recovery (%, Dust)	Standard Working Curve	
		Transition	Collision Energy (eV)	Transition	Collision Energy (eV)		Linearity (ng/mL)	R^2
LCM-1	NA	146.0->98.0	15	258.1->146.0	10	64.6~81.8	/	/
LCM-2	116020-44-1	205.2->81.1	10	234.2->109.1	5	72.4~95.9	1~100	0.9990
LCM-3	97398-80-6	163.2->81.1	10	206.2->123.0	5	121.7~163.0	1~100	0.9977
LCM-4	279246-65-0	205.2->81.1	15	248.2->123.1	5	41.3~62.7	1~100	0.9994
LCM-5	174350-05-1	282.1->169.0	15	156.0->107.0	25	98.9~107.1	1~100	0.9990
LCM-6	64835-63-8	181.1->165.0	20	238.1->181.1	10	90.9~103.4	1~100	0.9994
LCM-7	157248-24-3	219.1->170.0	25	276.1->219.0	15	98.3~126.8	/	/
LCM-8	NA	276.1->220.1	10	220.1->170.1	35	99.8~127.7	/	/
LCM-9	650634-92-7	264.0->167.1	25	348.1->277.0	10	81.2~132.9	/	/
LCM-10	155041-85-3	282.2->157.1	10	118.1->117.1	10	106.1~117.9	1~100	0.9997
LCM-11	NA	188.0->119.0	15	368.2->188.0	10	76.4~110.0	/	/
LCM-12	303186-20-1	252.0->183.0	15	281.1->252.0	20	104.4~132.5	1~100	0.9996
LCM-13	84656-75-7	118.1->117.1	10	298.2->118.1	10	42.3~117.6	1~100	0.9994
LCM-14	1690317-23-7	281.0->252.0	20	252.0->183.0	15	73.3~90.5	/	/
LCM-15	431947-34-1	170.0->127.0	20	350.2->170.0	10	70.0~88.9	/	/
LCM-16	84540-37-4	193.1->178.1	15	306.2->193.1	20	93.8~113.6	1~100	0.9996
LCM-17	323178-01-4	344.1->245.0	15	232.0->183.0	20	67.2~84.8	/	/
LCM-18	123560-48-5	184.1->156.0	10	364.2->156.0	15	78.0~102.0	/	/
LCM-19	95759-44-7	318.1->289.1	15	289.1->274.1	20	85.0~97.1	1~100	0.9998

LCM-20	NA	184.0->156.0	10	362.2->223.1	10	79.8~99.0	/	/
LCM-21	189750-98-9	358.1->245.0	15	232.0->183.0	20	66.9~88.1	/	/
LCM-22	473257-14-6	378.2->184.1	10	156.0->107.0	25	92.3~114.4	/	/
LCM-23	473257-15-7	184.1->156.0	10	378.2->184.1	10	84.4~109.8	/	/
LCM-24	NA	143.0->75.1	25	376.2->195.0	20	74.4~125.4	/	/
LCM-25	825633-75-8	289.1->274.1	20	332.1->289.1	15	99.1~126.7	/	/
LCM-26	139195-63-4	382.2->216.1	10	216.1->201.0	20	85.8~110.0	/	/
LCM-27	NA	492.1->393.9	15	365.1->239.0	25	46.1~59.6	/	/
LCM-28	524709-77-1	394.0->325.0	20	407.1->391.9	15	44.7~55.6	/	/
LCM-29	303186-36-9	375.1->345.9	25	173.1->163.1	5	115.6~156.0	/	/
LCM-30	1700444-88-7	267.0->170.0	25	351.1->239.0	25	142.9~178.5	/	/
LCM-31	119990-81-7	396.2->216.1	10	216.1->201.0	20	97.3~127.4	/	/
LCM-32	119990-82-8	203.0->183.0	15	410.2->216.0	10	107.5~133.5	/	/
LCM-33	136609-96-6	424.2->216.1	10	216.0->200.9	20	105.5~129.2	/	/

Table S9. Limits of detection (LODs), blank concentrations, detected frequencies, arithmetic means and ranges (ng/mL) of liquid crystal monomers (LCMs) in indoor dust samples.

Abbreviation	CASRN	LOD[a] (ng/mL）	Blank Concentration ± SD[b] (ng/mL）	DF[c] (%)	Mean ± SD (ng/mL）	Range （ng/mL）
LCM-1	NA[d]	1.079	ND[e]	0	ND	ND
LCM-2	116020-44-1	6.708	0.27±0.60	9	1.09±4.06	ND~25.71
LCM-3	97398-80-6	0.566	ND	2	1.23±8.94	ND~65.05
LCM-4	279246-65-0	0.297	ND	0	ND	ND
LCM-5	174350-05-1	1.997	0.23±0.15	6	0.59±3.42	ND~24.56
LCM-6	64835-63-8	0.977	0.33±0.11	6	0.16±0.74	ND~4.69
LCM-7	157248-24-3	3.245	0.03±0.04	2	0.11±0.78	ND~5.66
LCM-8	NA	3.678	0.01±0.01	0	ND	ND
LCM-9	650634-92-7	0.002	ND	0	ND	ND
LCM-10	155041-85-3	0.050	ND	11	0.10±0.33	ND~1.75
LCM-11	NA	2.754	0.39±0.36	0	ND	ND
LCM-12	303186-20-1	0.892	0.70±0.21	25	0.54±2.16	ND~15.48
LCM-13	84656-75-7	4.524	0.79±1.19	15	1.79±5.09	ND~25.13
LCM-14	1690317-23-7	4.112	0.01±0.01	0	ND	ND
LCM-15	431947-34-1	6.708	0.42±0.94	2	6.67±48.55	ND~353.42
LCM-16	84540-37-4	0.123	ND	0	ND	ND
LCM-17	323178-01-4	3.429	0.01±0.01	2	0.15±1.12	ND~8.17
LCM-18	123560-48-5	4.475	0.43±0.63	6	3.07±20.97	ND~152.68
LCM-19	95759-44-7	0.398	0.01±0.00	0	ND	ND

Abbreviation	CASRN	LOD[a] (ng/mL）	Blank Concentration ± SD[b] (ng/mL）	DF[c] (%)	Mean ± SD (ng/mL）	Range （ng/mL）
LCM-20	NA	6.708	0.52±1.17	6	4.09±27.13	ND~197.41
LCM-21	189750-98-9	1.604	0.01±0.00	2	0.07±0.52	ND~3.81
LCM-22	473257-14-6	0.014	0.00±0.00	4	ND±0.02	ND~0.14
LCM-23	473257-15-7	4.611	0.43±0.66	9	10.41±71.30	ND~519.39
LCM-24	NA	0.002	ND	0	ND	ND
LCM-25	825633-75-8	2.974	ND	0	ND	ND
LCM-26	139195-63-4	0.002	ND	0	ND	ND
LCM-27	NA	0.002	ND	0	ND	ND
LCM-28	524709-77-1	0.002	ND	2	0.00±0.01	ND~0.04
LCM-29	303186-36-9	6.708	ND	0	ND	ND
LCM-30	1700444-88-7	0.002	ND	8	ND	ND~0.01
LCM-31	119990-81-7	6.708	ND	0	ND	ND
LCM-32	119990-82-8	6.708	ND	0	ND	ND
LCM-33	136609-96-6	0.002	ND	0	ND	ND

[a] “LOD” means limit of detection, [b] “SD” means standard deviation, [c] “DF” means detection frequency, [d] “NA” means not available, [e] “ND” means not detectable.

Figure S1. Collection of Liquid Crystal Monomers (LCMs) from Liquid Crystal Display (LCD) devices in our Laboratory. A: dismantle the LCD devices; B: wash down the LCMs from LCD device by use of acetone.

A B

Figure S2. Distribution of manufacturers of liquid crystals (LCs) and liquid crystal displays (LCDs) worldwide. The data were collected from public databases available on the internet and official websites of companies. In the statistical process, because the retrieval was not comprehensive enough, there were necessarily some omissions and inaccuracies in the factory locations.

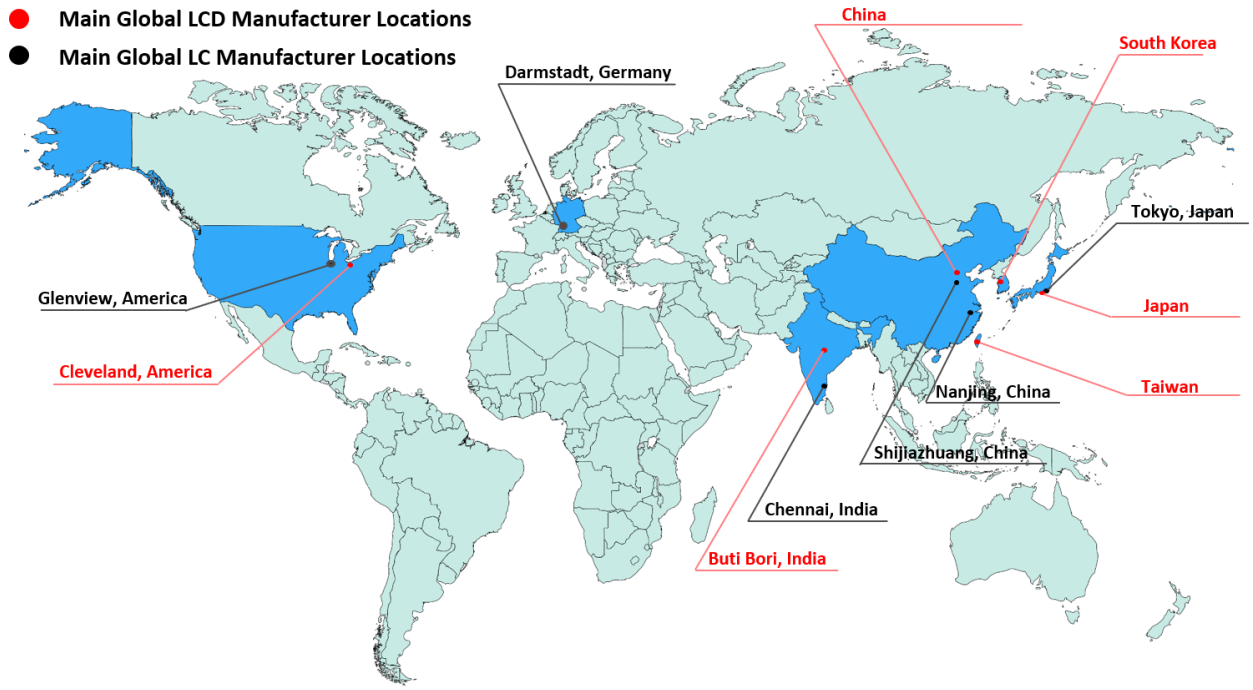
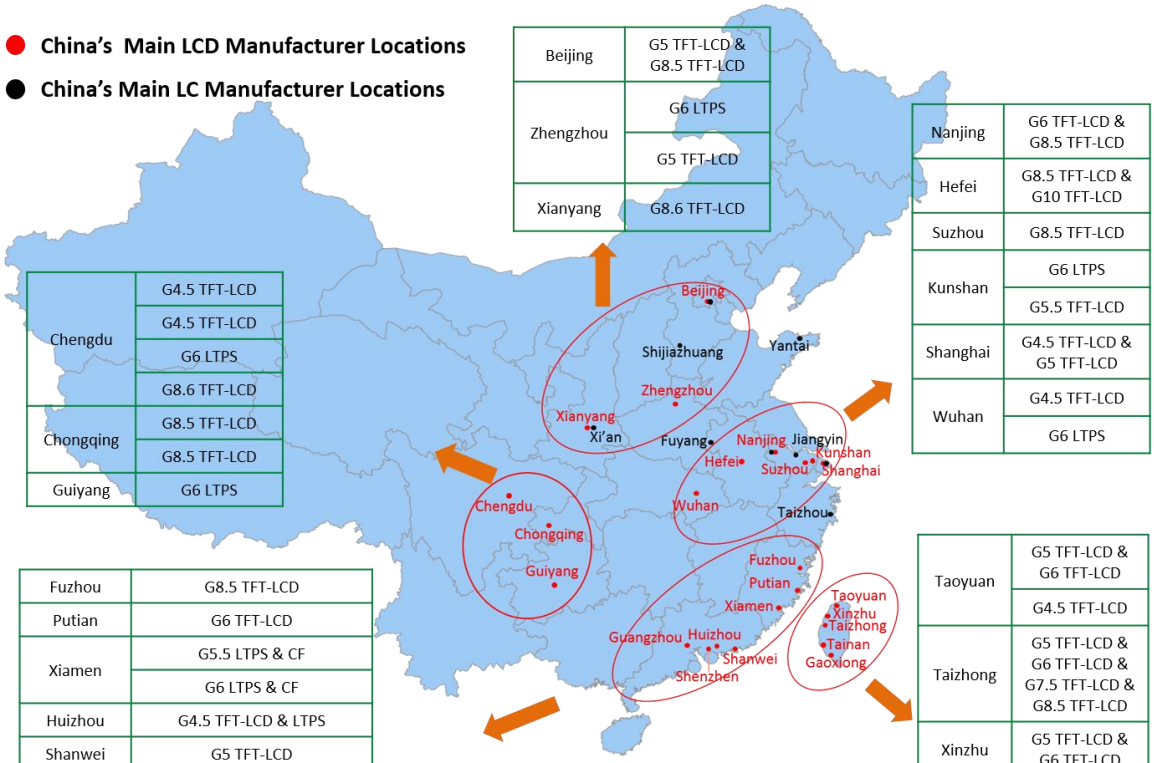


Figure S3. Distribution of manufacturers of liquid crystals (LCs) and liquid crystal displays (LCDs) in China. The data were collected from public databases available on the internet and official websites of companies. In the statistical process, because the retrieval was not comprehensive enough, there were necessarily some omissions and inaccuracies in the factory location.



Beijing	G5 TFT-LCD & G8.5 TFT-LCD
Zhengzhou	G6 LTPS
	G5 TFT-LCD
Xianyang	G8.6 TFT-LCD

Nanjing	G6 TFT-LCD & G8.5 TFT-LCD
Hefei	G8.5 TFT-LCD & G10 TFT-LCD
Suzhou	G8.5 TFT-LCD
Kunshan	G6 LTPS
	G5.5 TFT-LCD
Shanghai	G4.5 TFT-LCD & G5 TFT-LCD
Wuhan	G4.5 TFT-LCD
	G6 LTPS

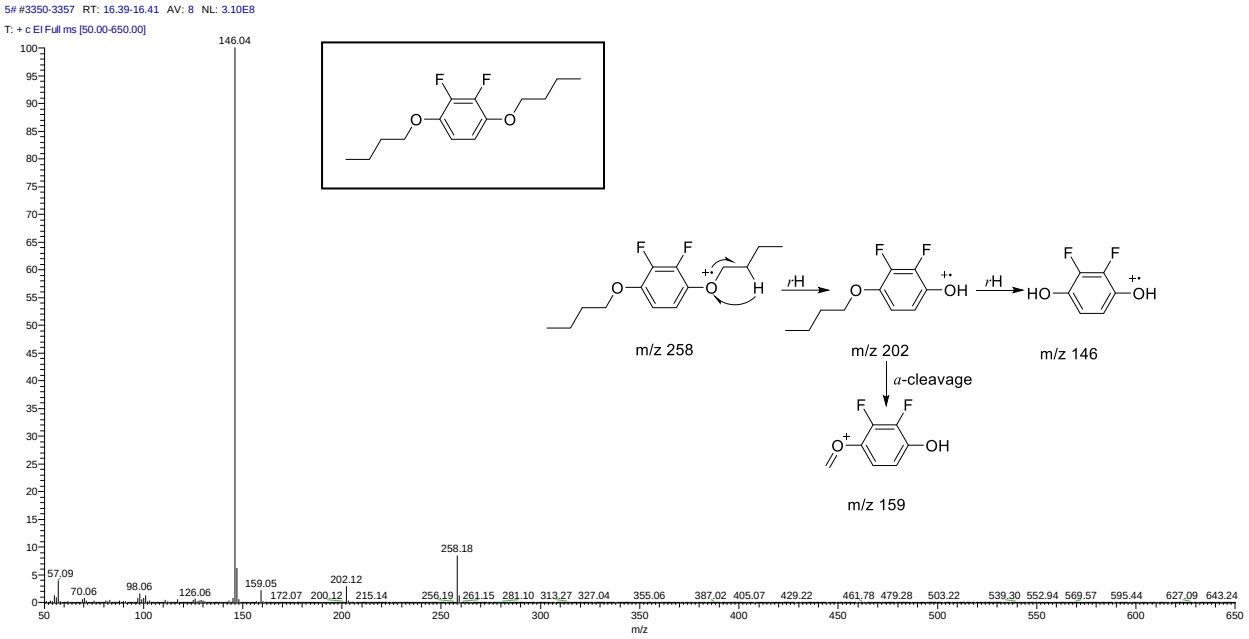
Chengdu	G4.5 TFT-LCD
	G4.5 TFT-LCD
	G6 LTPS
	G8.6 TFT-LCD
Chongqing	G8.5 TFT-LCD
	G8.5 TFT-LCD
Guiyang	G6 LTPS

Fuzhou	G8.5 TFT-LCD
Putian	G6 TFT-LCD
Xiamen	G5.5 LTPS & CF
	G6 LTPS & CF
Huizhou	G4.5 TFT-LCD & LTPS
Shanwei	G5 TFT-LCD
Shenzhen	G8.5 TFT-LCD & G11 TFT-LCD
	G5.5 LTPS
	G5.5 TFT-LCD
Guangzhou	G8.5 TFT-LCD

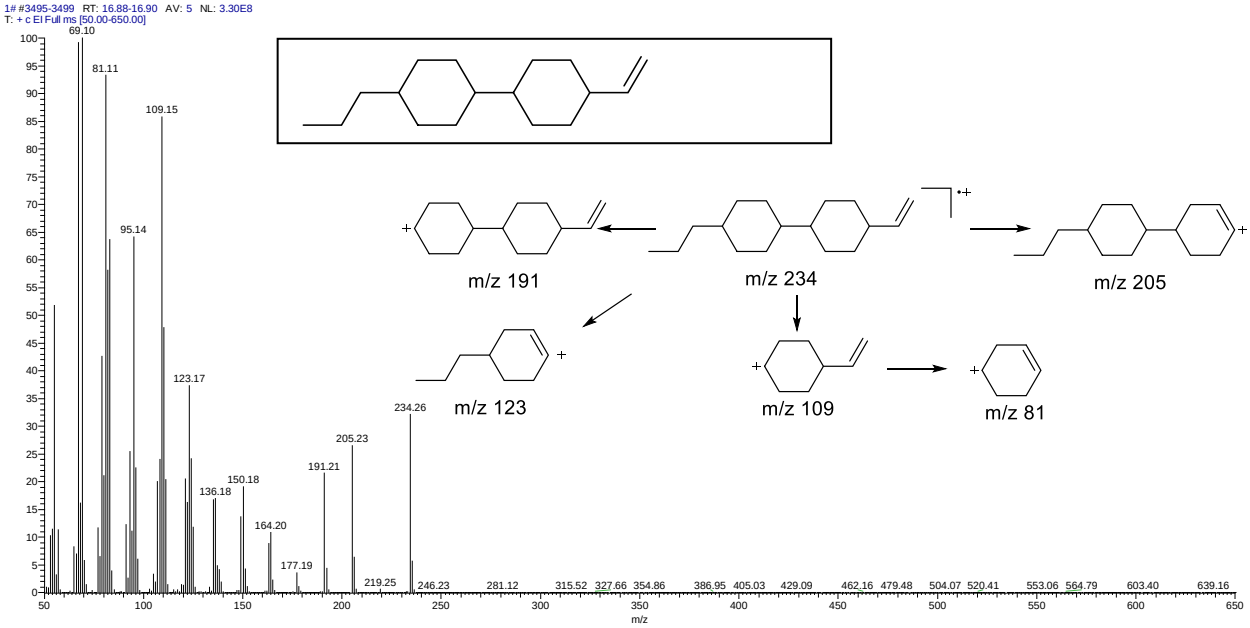
Taoyuan	G5 TFT-LCD & G6 TFT-LCD
	G4.5 TFT-LCD
Taizhong	G5 TFT-LCD & G6 TFT-LCD & G7.5 TFT-LCD & G8.5 TFT-LCD
Xinzhu	G5 TFT-LCD & G6 TFT-LCD
Tainan	G5 TFT-LCD & G5.5 TFT-LCD & G6 TFT-LCD & G7.5 TFT-LCD
Gaoxiong	G8.5 TFT-LCD & G8.6 TFT-LCD

Figure S4. Possible fragmentation pathways of liquid crystal monomers (LCMs) in liquid crystal displays from six models of largely produced commercial smartphones under electron impact ionization (EI) source.

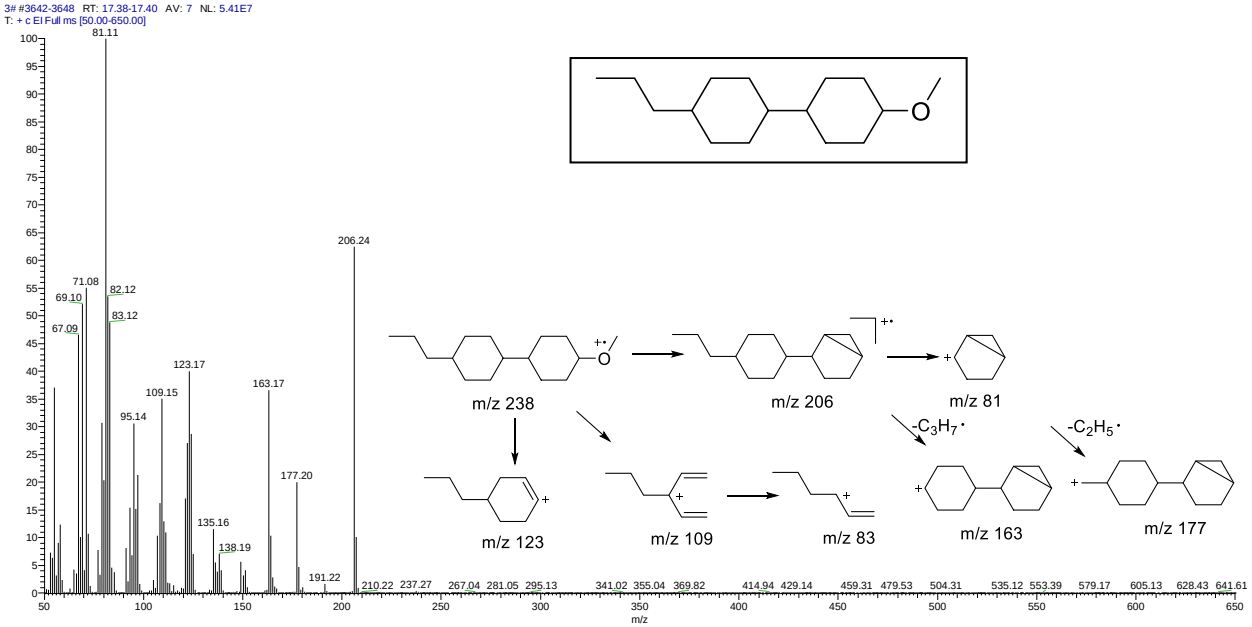
1) 1,4-dibutoxy-2,3-difluorobenzene (LCM-1):



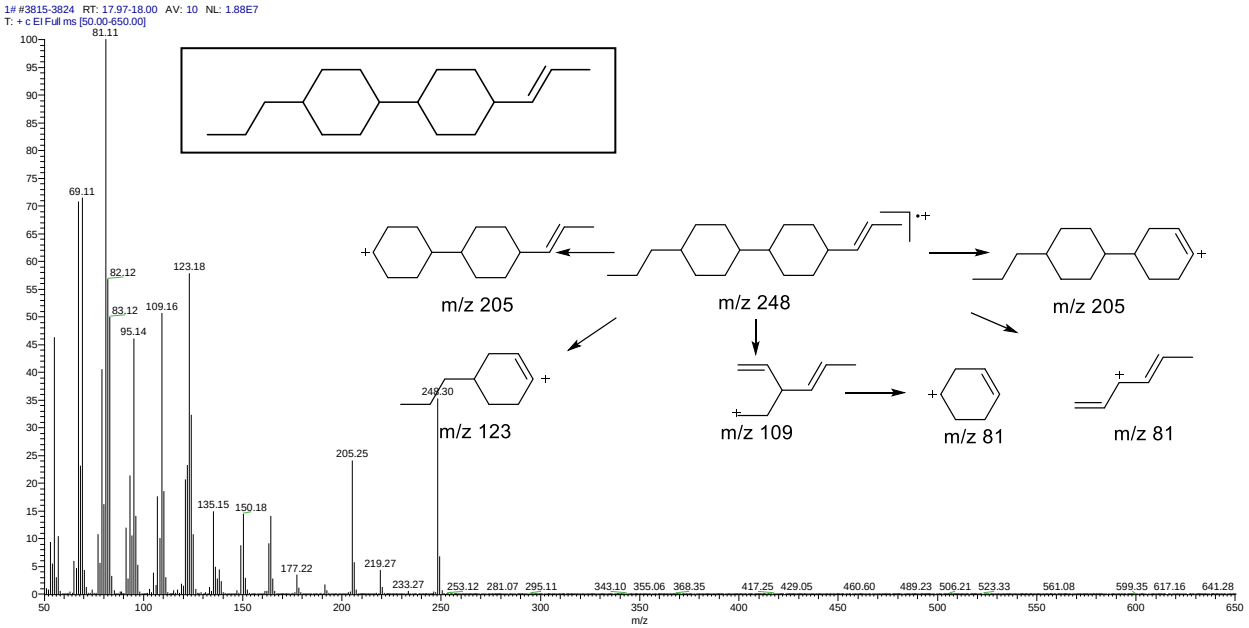
2) 1-(4-propylcyclohexyl)-4-vinylcyclohexane (LCM-2):



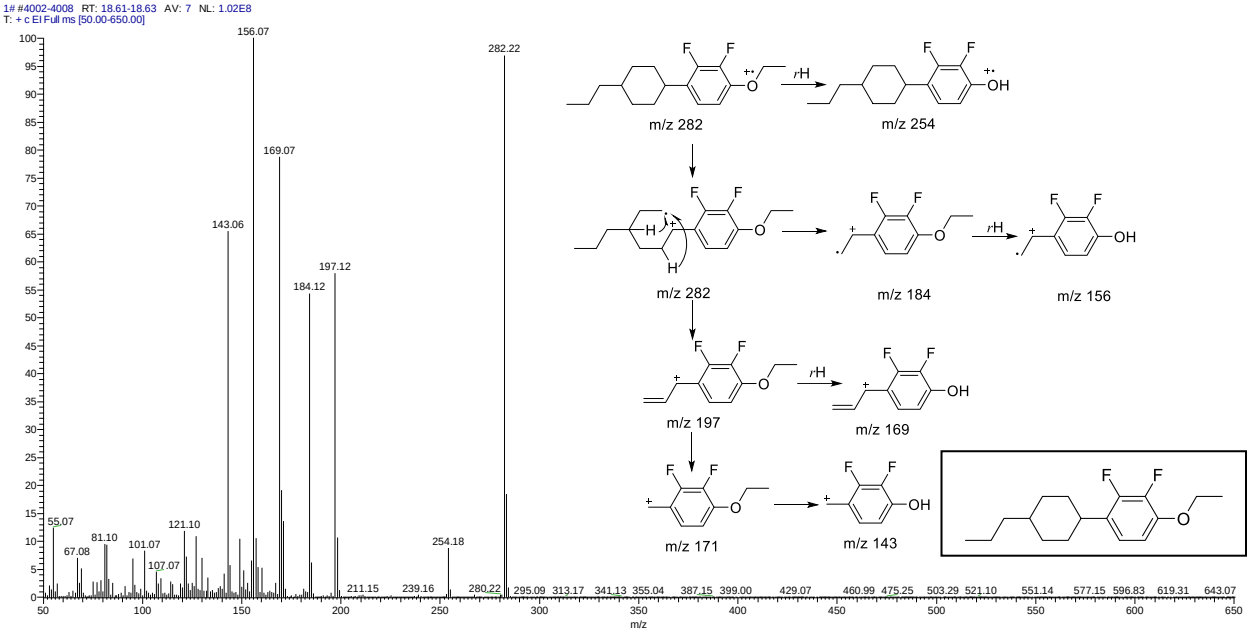
3) 1-methoxy-4-(4-propylcyclohexyl)cyclohexane (LCM-3):



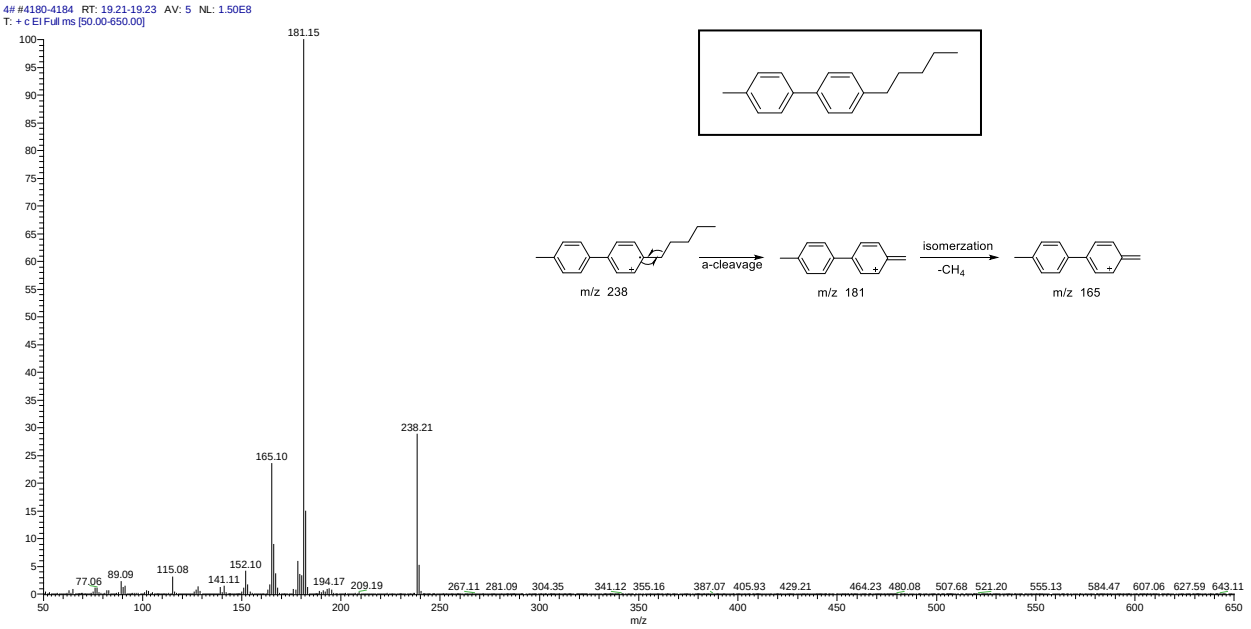
4) 1-(prop-1-enyl)-4-(4-propylcyclohexyl)cyclohexane (LCM-4):



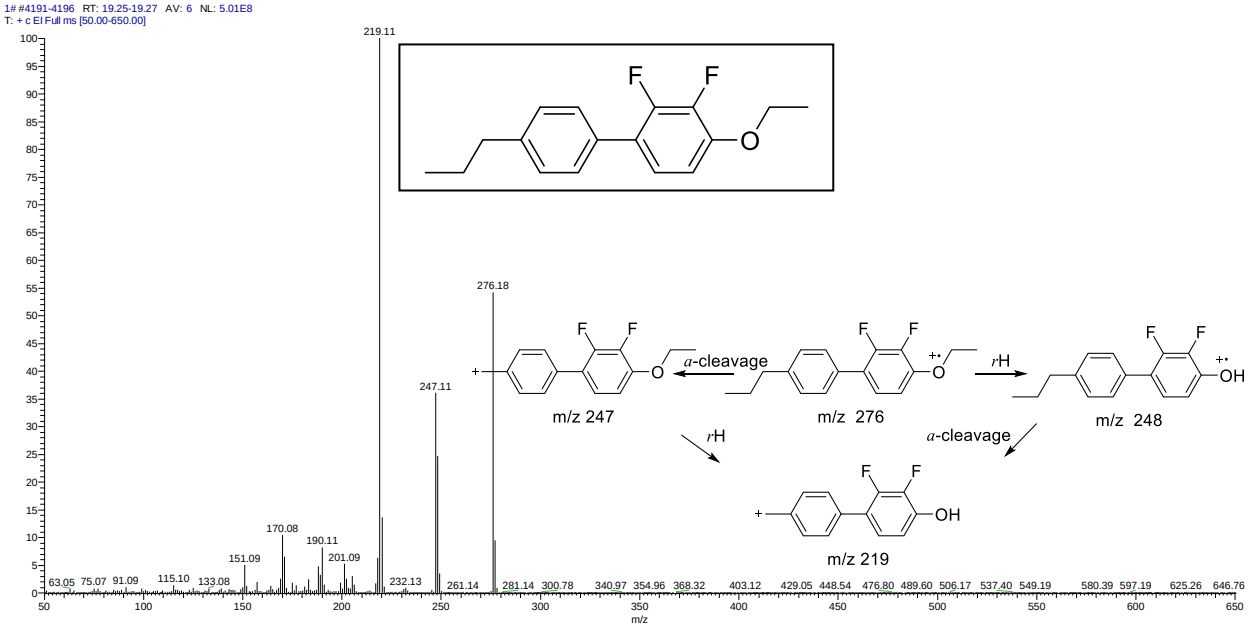
5) 1-ethoxy-2,3-difluoro-4-(4-propylcyclohexyl)benzene (LCM-5):



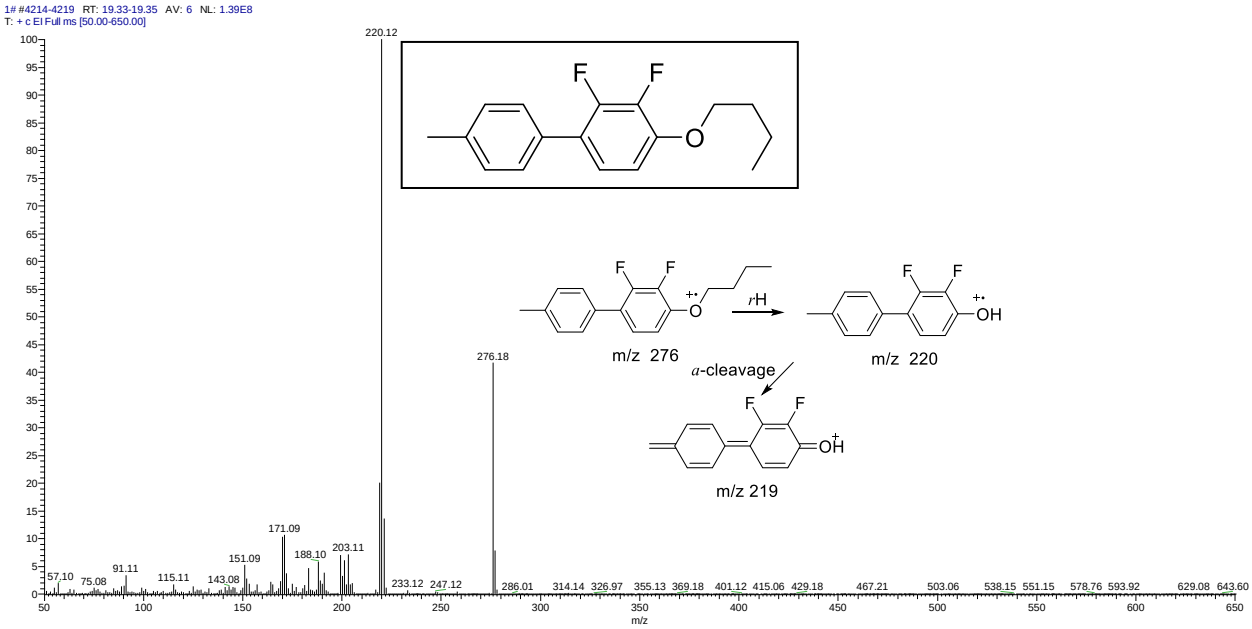
6) 4-methyl-4'-pentylbiphenyl (LCM-6):



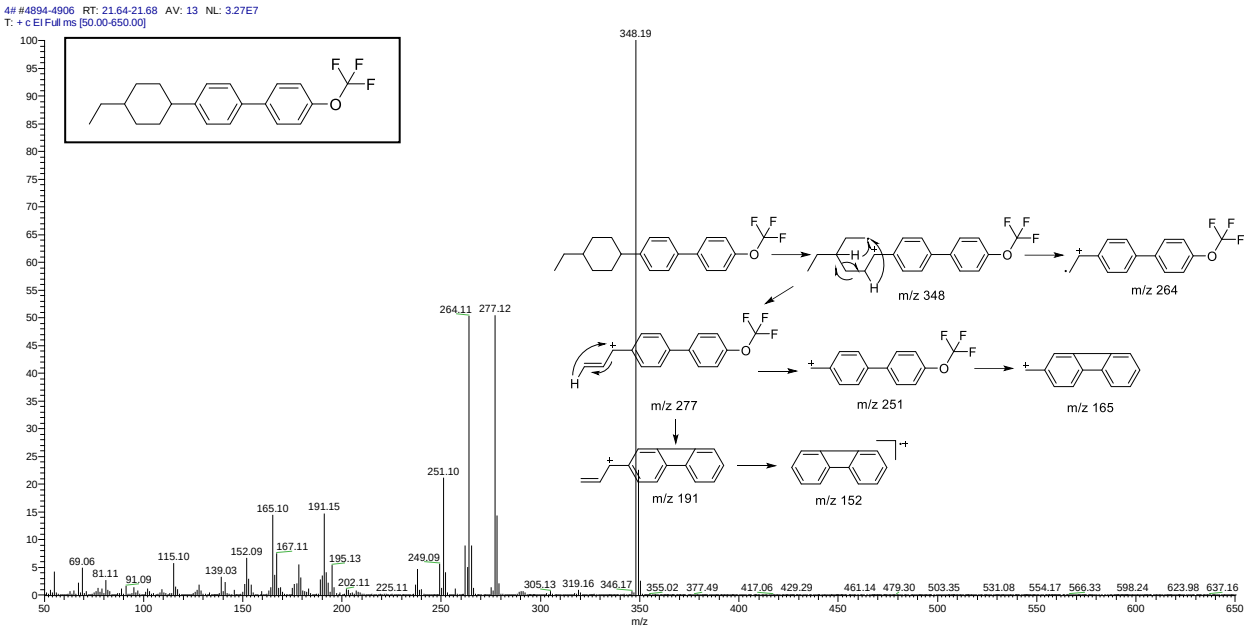
7) 1-ethoxy-2,3-difluoro-4-(4-propylphenyl)benzene (LCM-7):



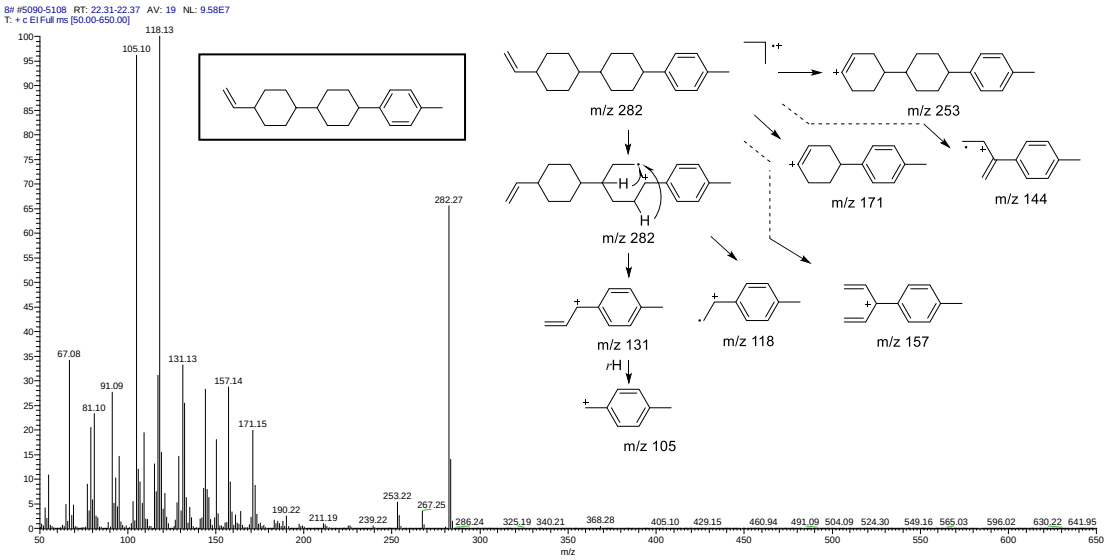
8) 1-butoxy-2,3-difluoro-4-(4-methylphenyl)benzene (LCM-8):



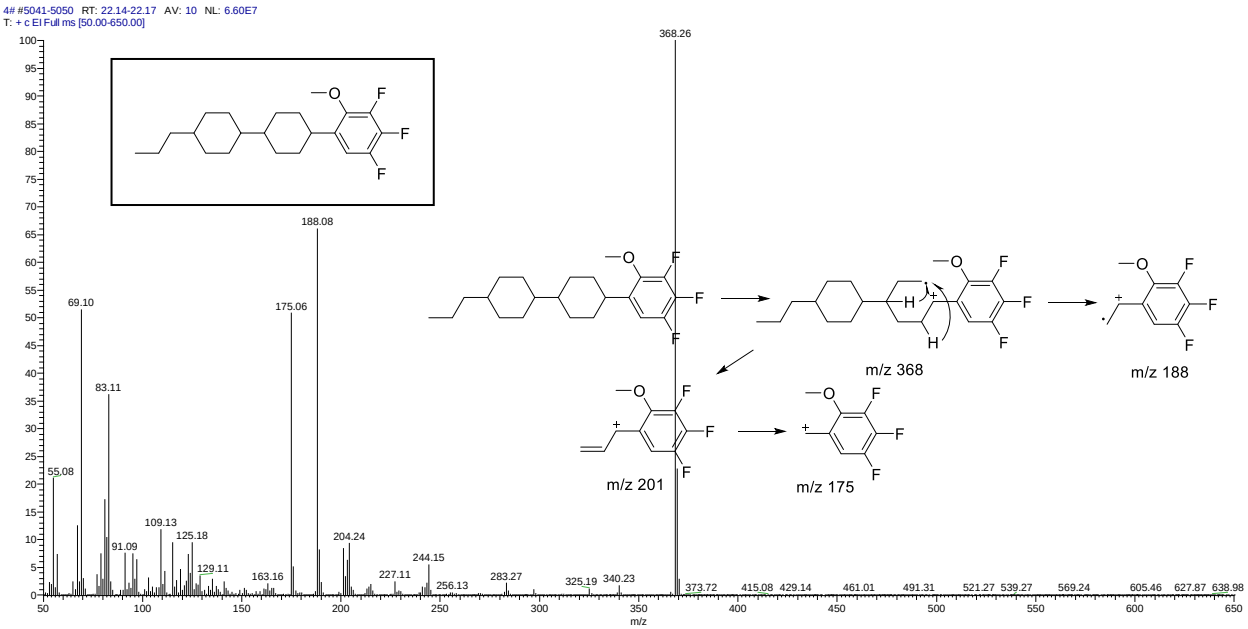
9) 4-(4-ethylcyclohexyl)-4'-(trifluoromethoxy)biphenyl (LCM-9):



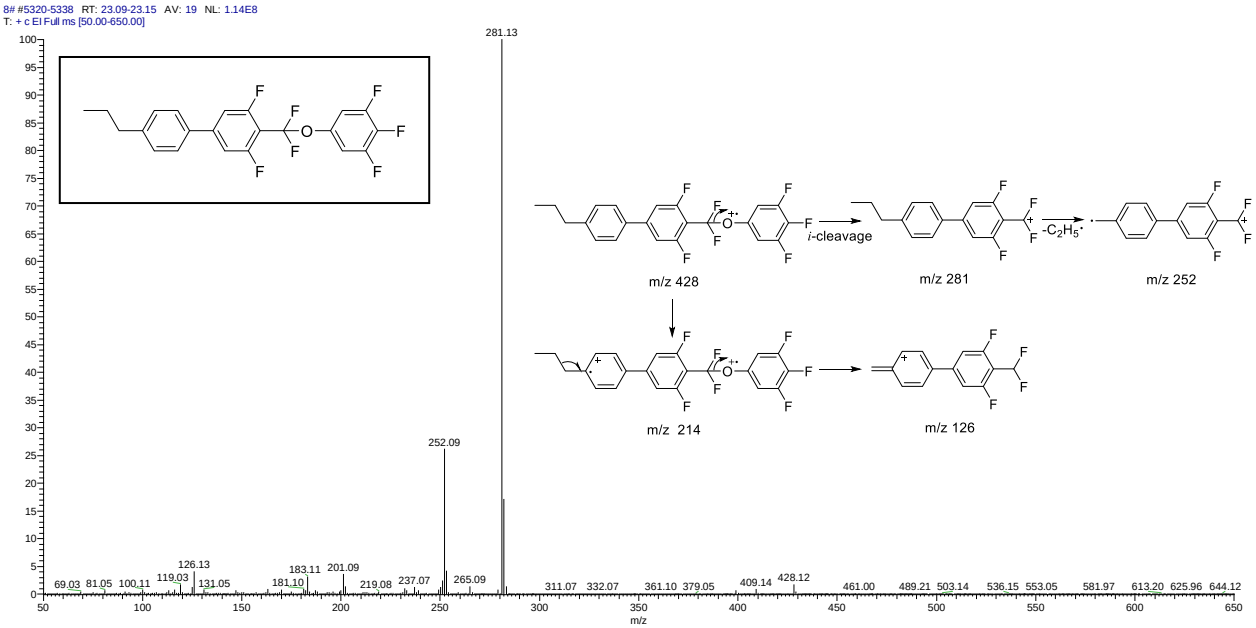
10) 1-methyl-4-(4-(4-vinylcyclohexyl)cyclohexyl)benzene (LCM-10):



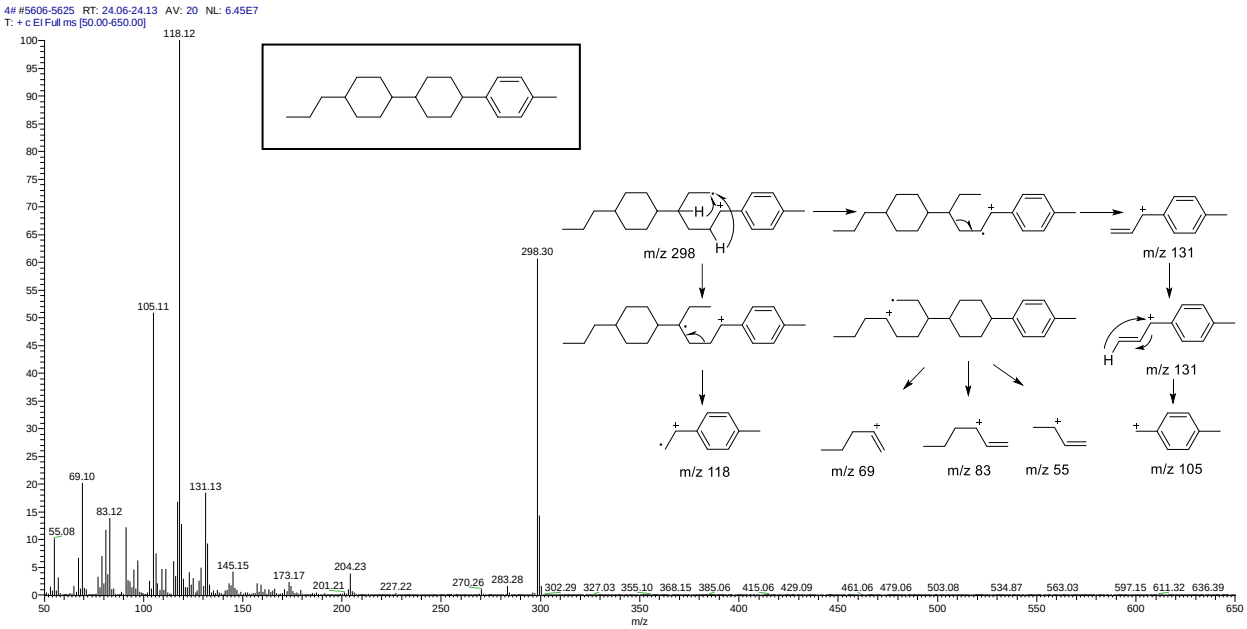
11) 1,2,3-trifluoro-4-methoxy-5-(4-(4-propylcyclohexyl)cyclohexyl)benzene (LCM-11):



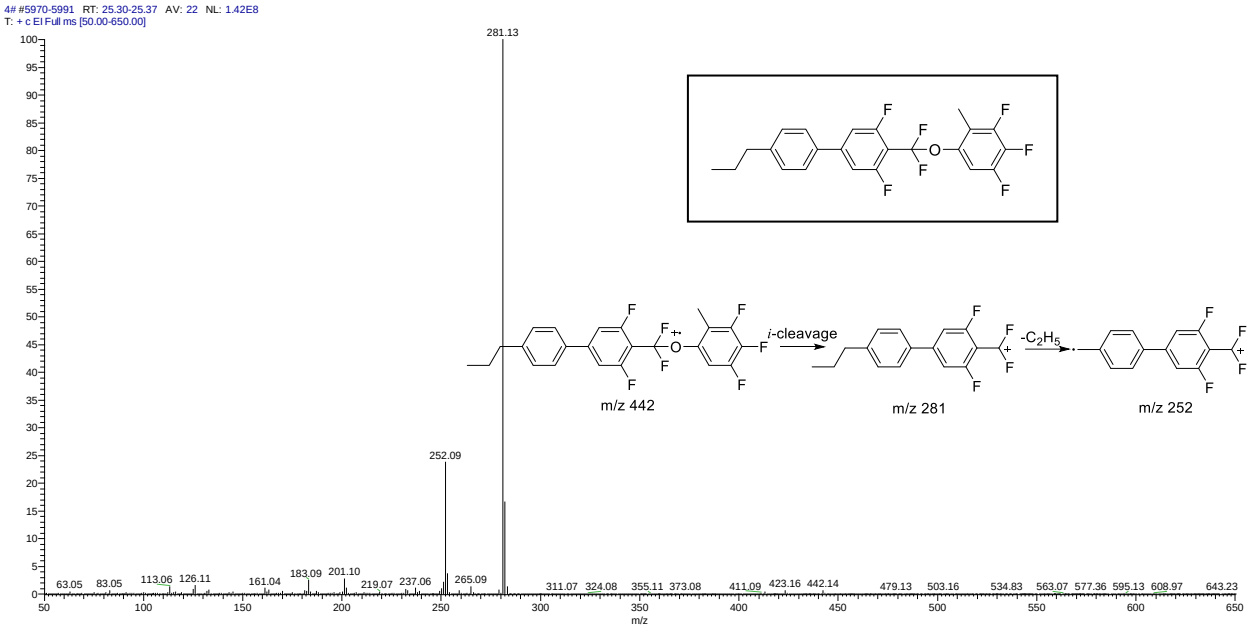
12) 4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl (LCM-12):



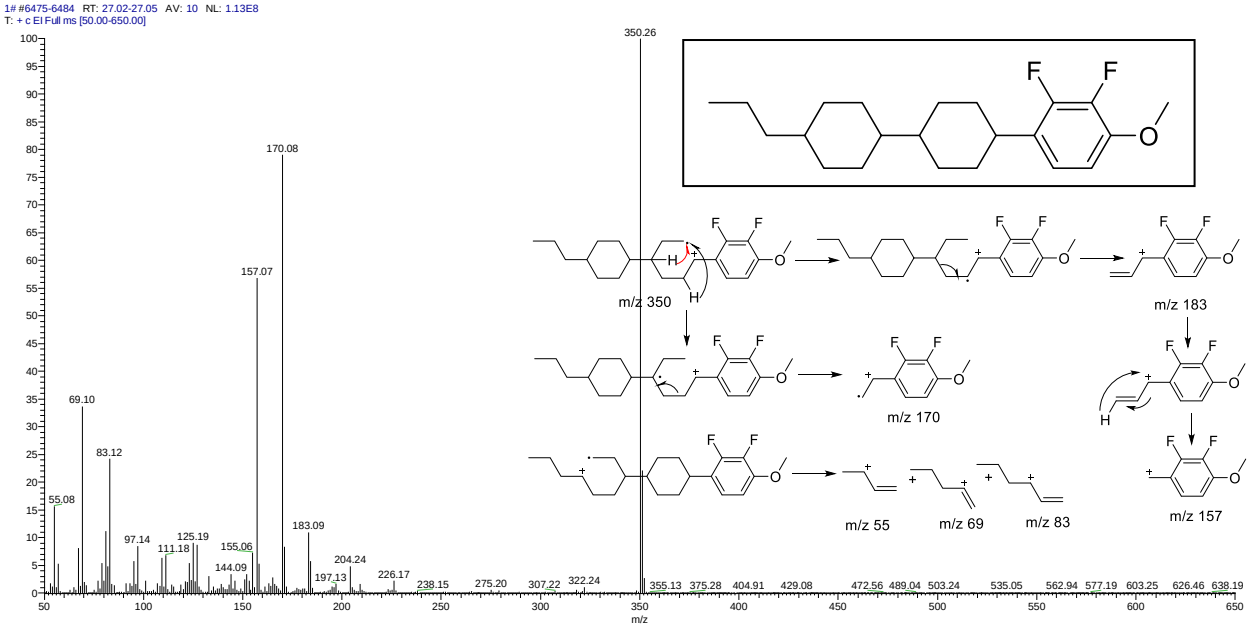
13) 1-methyl-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene (LCM-13):



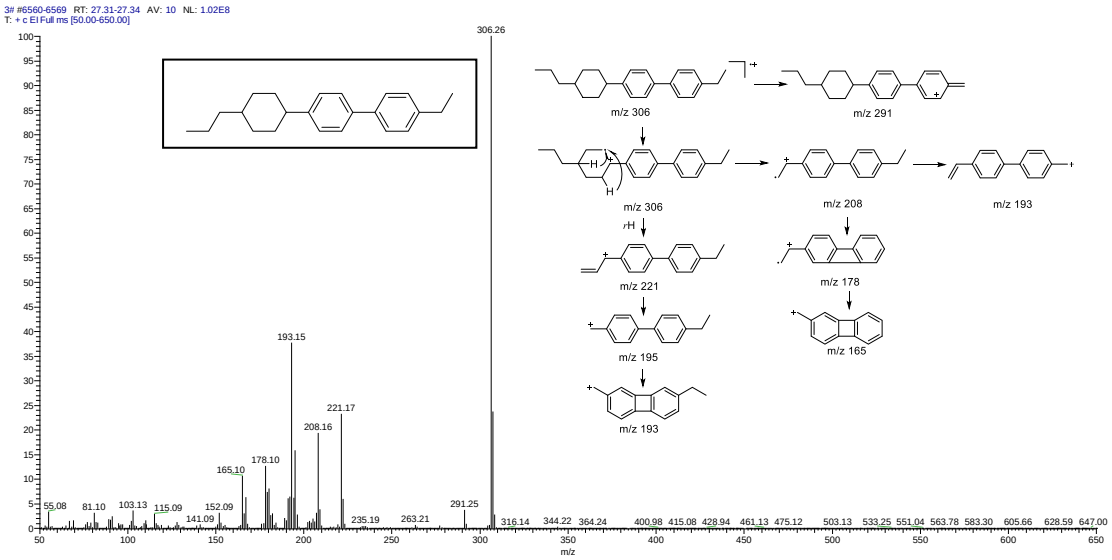
14) 4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propylbiphenyl (LCM-14)：



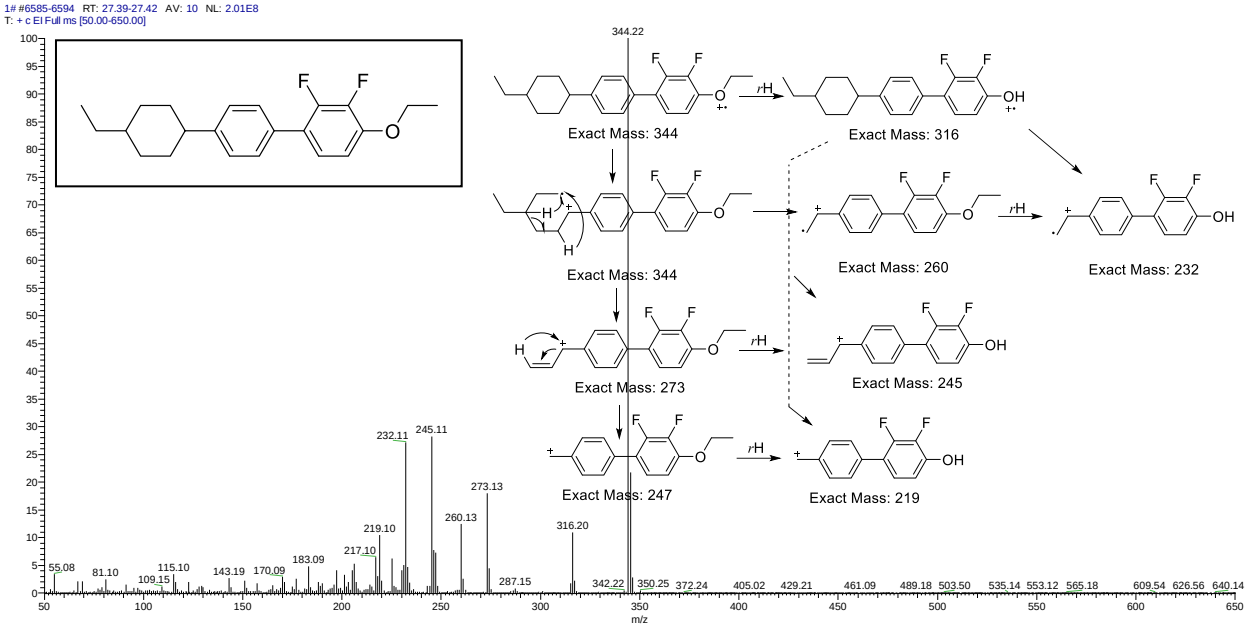
15) 2,3-difluoro-1-methoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene (LCM-15):



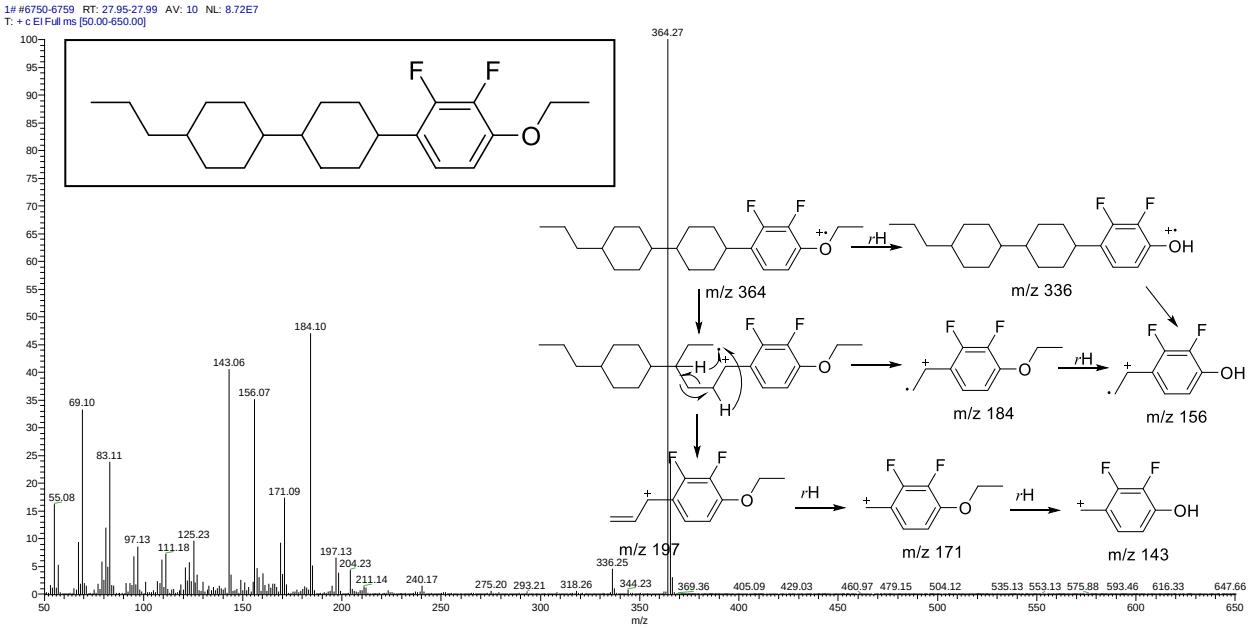
16) 1-ethyl-4-(4-(4-propylcyclohexyl)phenyl)benzene (LCM-16):



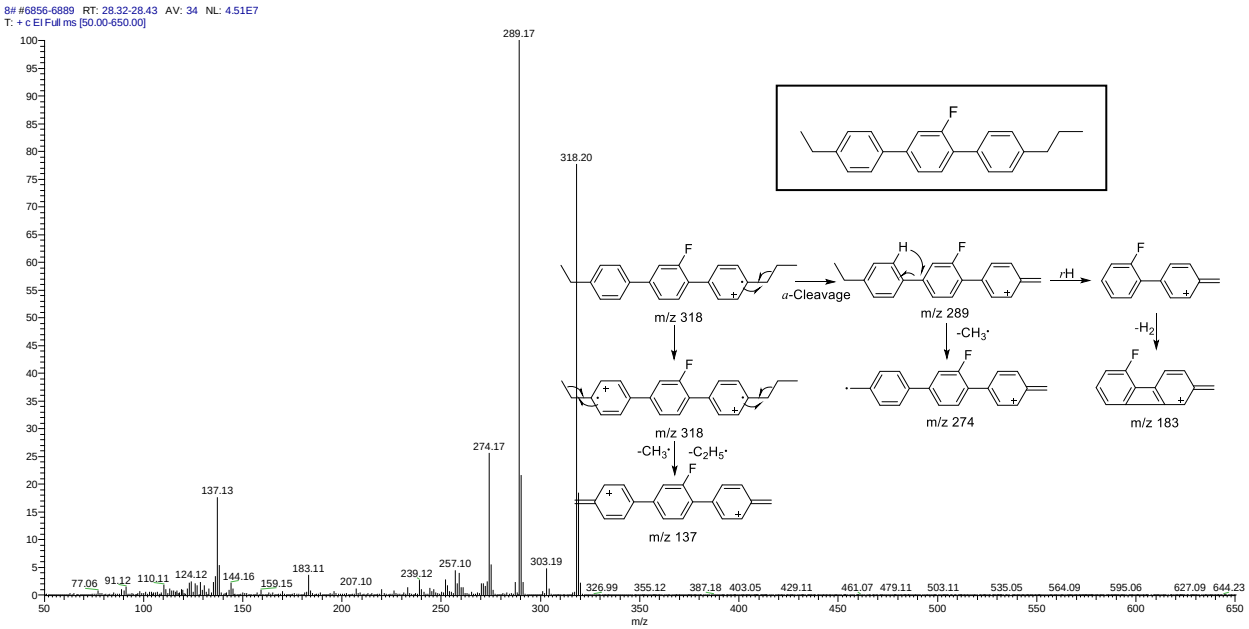
17) 4-ethoxy-4'-(4-ethylcyclohexyl)-2,3-difluorobiphenyl (LCM-17):



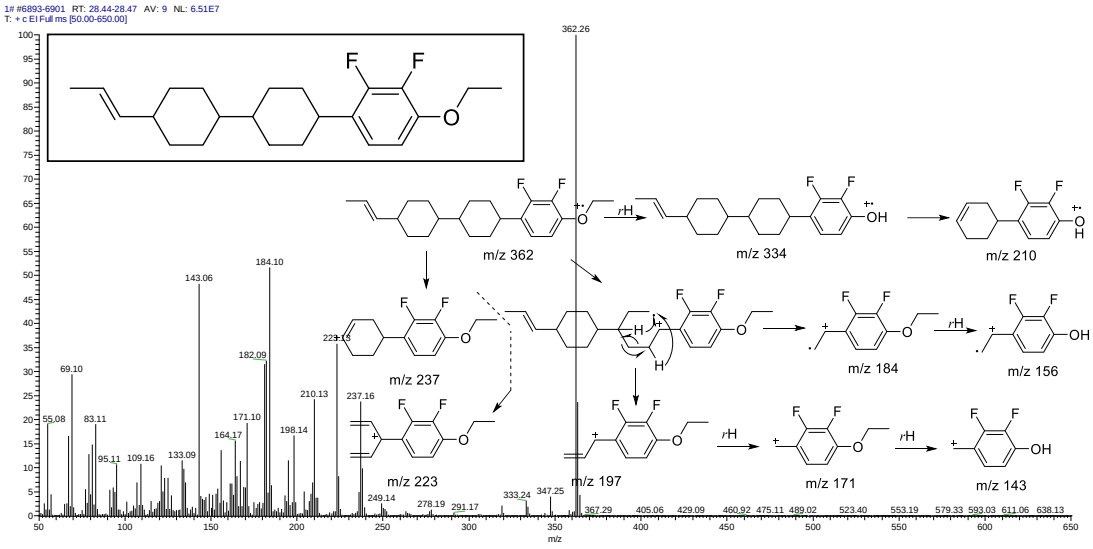
18) 1-ethoxy-2,3-difluoro-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene (LCM-18):



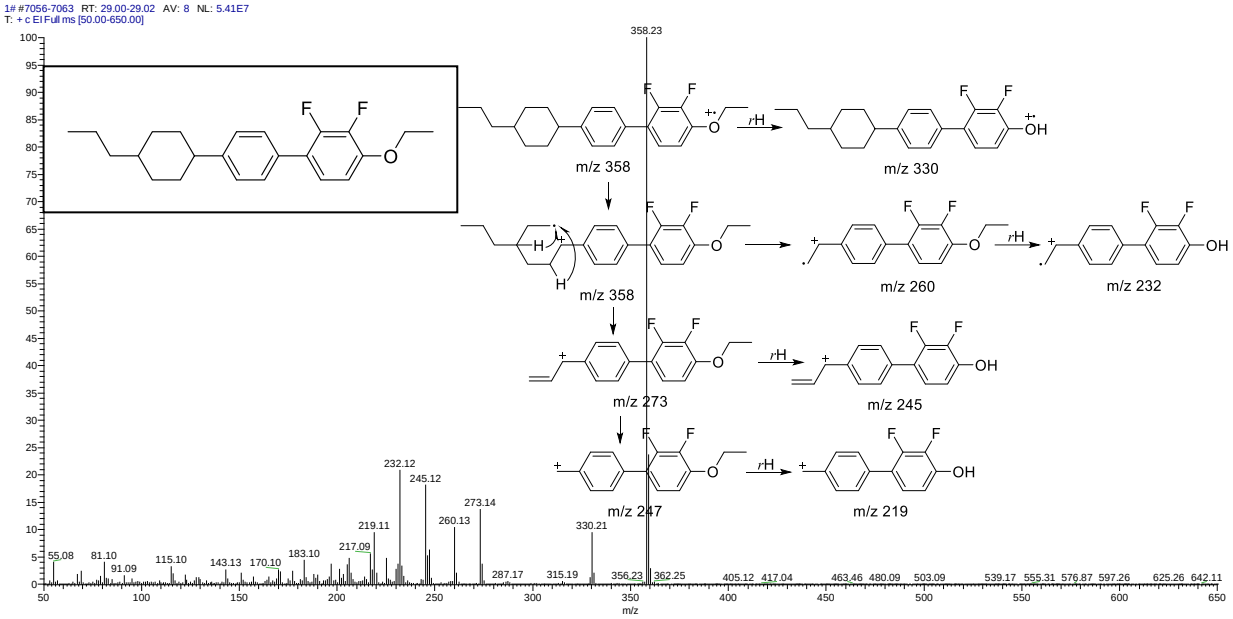
19) 4"-ethyl-2'-fluoro-4-propyl-1,1':4',1"-terphenyl (LCM-19):



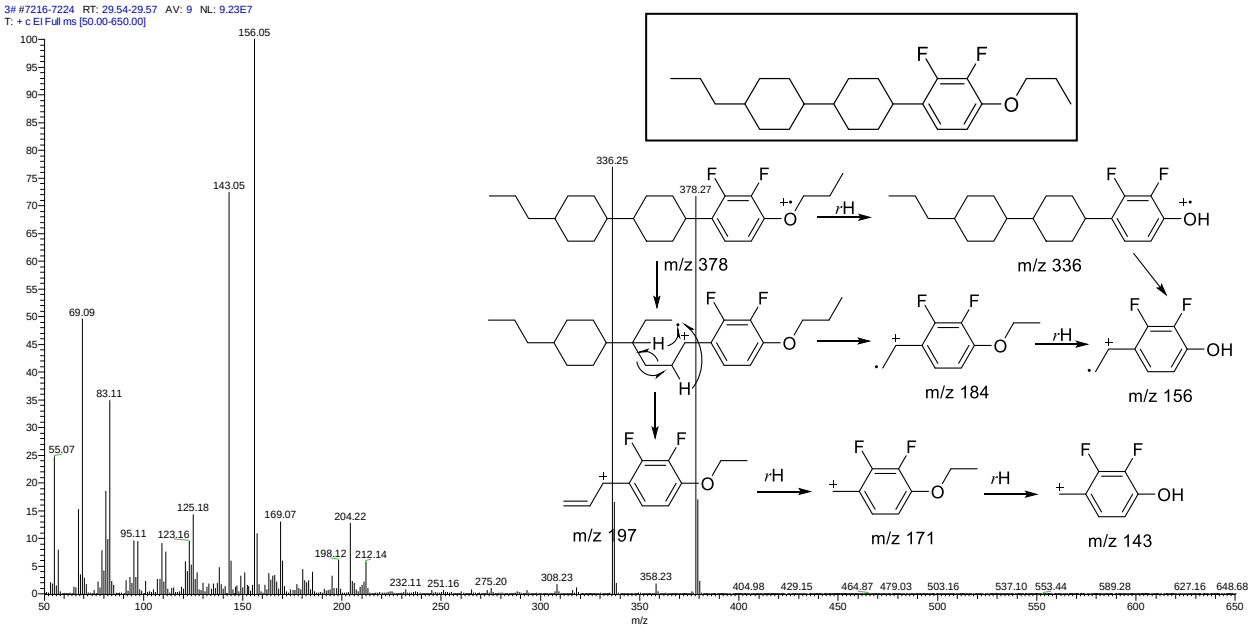
20) 1-ethoxy-2,3-difluoro-4-(4-(4-(prop-1-enyl)cyclohexyl)cyclohexyl)benzene (LCM-20):



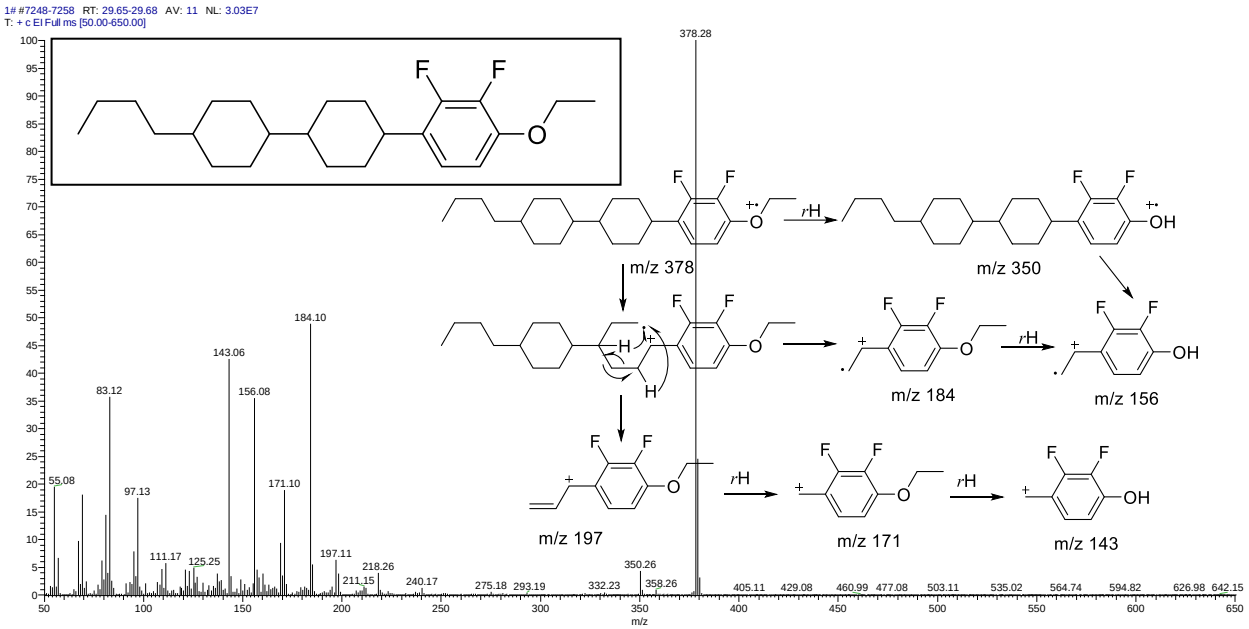
21) 4-ethoxy-2,3-difluoro-4'-(4-propylcyclohexyl)biphenyl (LCM-21):



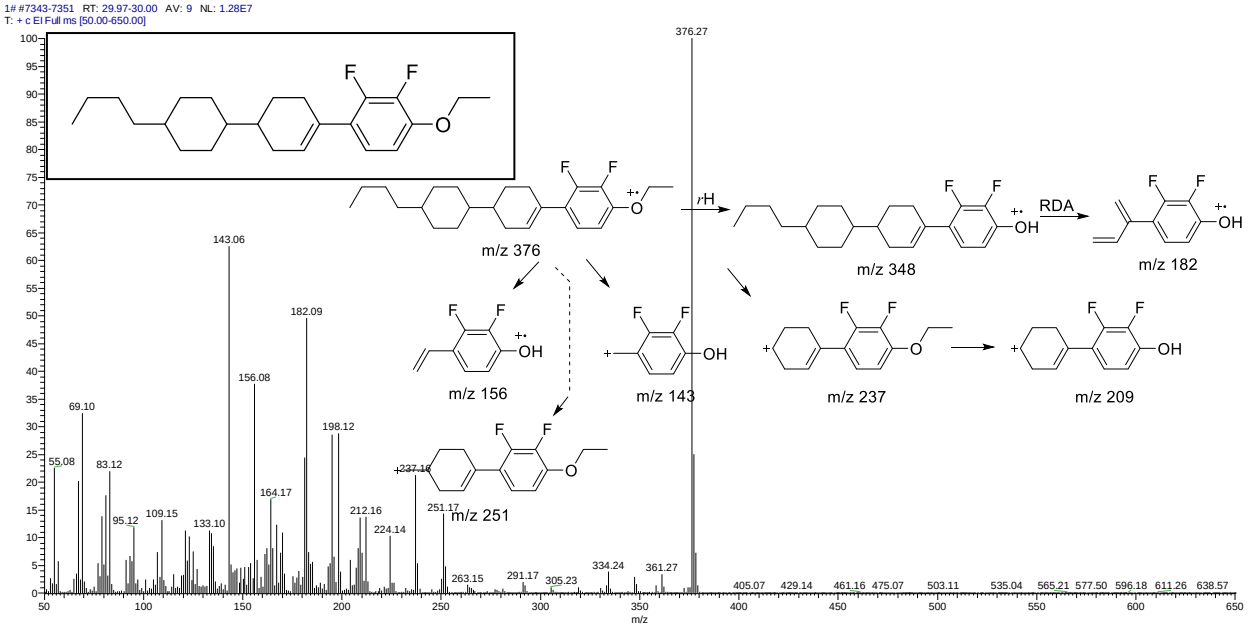
22) 2,3-difluoro-1-propoxy-4-(4-(4-propylcyclohexyl)cyclohexyl)benzene (LCM-22):



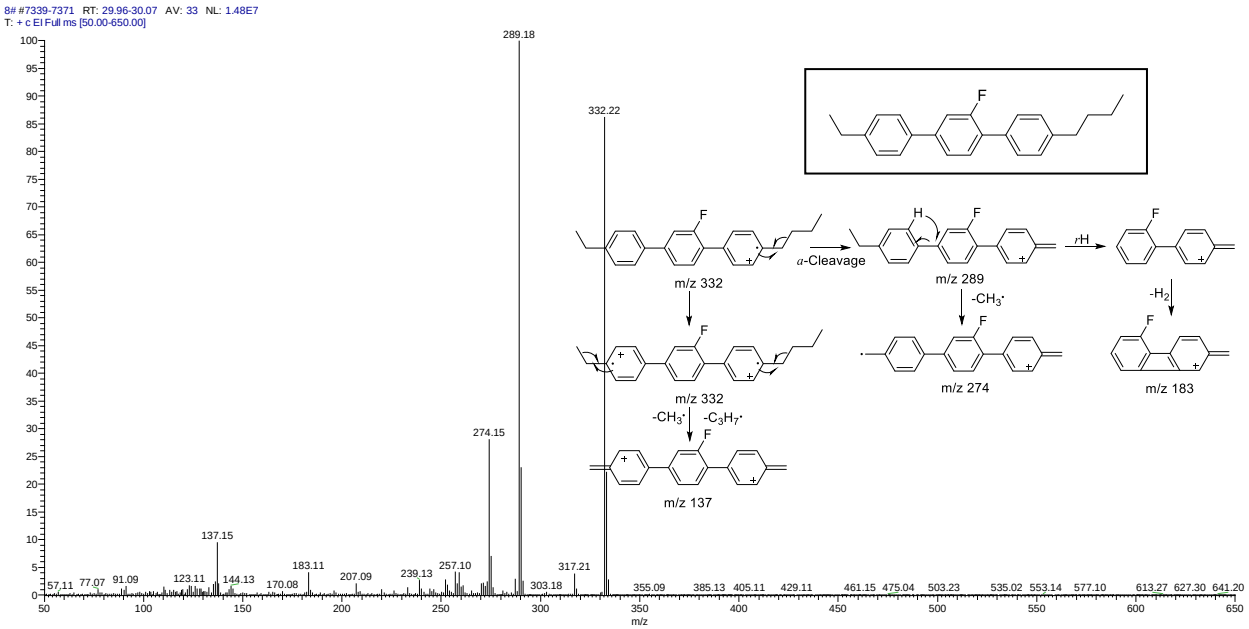
23) 1-(4-(4-butylcyclohexyl)cyclohexyl)-4-ethoxy-2,3-difluorobenzene (LCM-23):



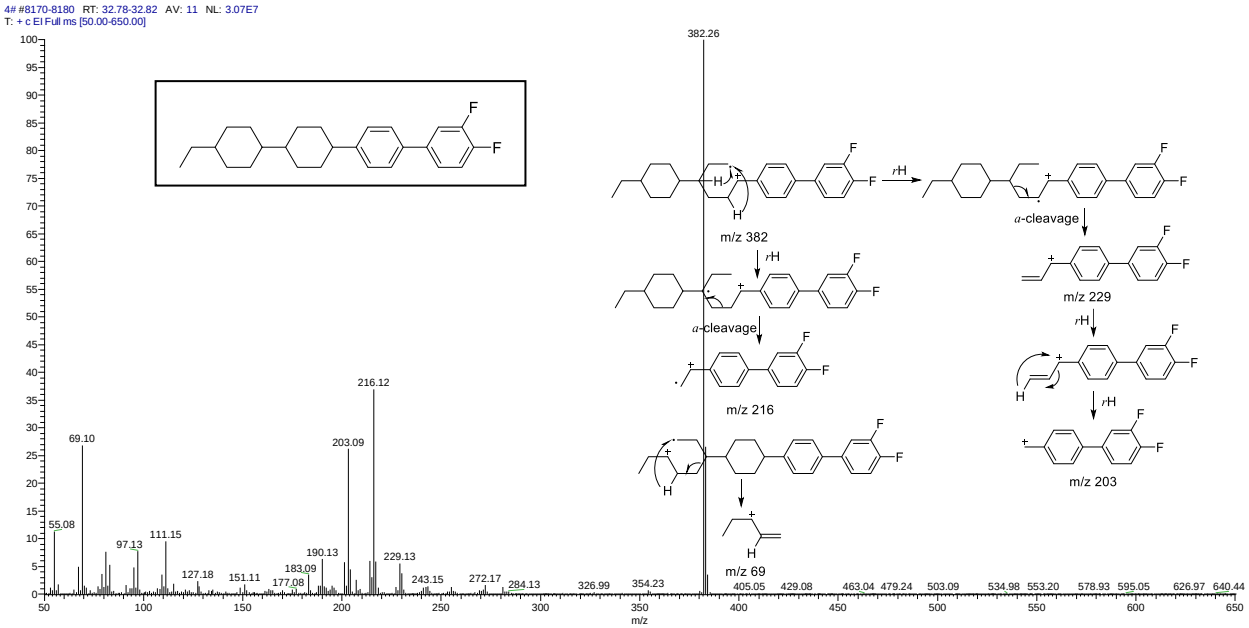
24) 1-(4-(4-butylcyclohexyl)cyclohex-1-enyl)-4-ethoxy-2,3-difluorobenzene (LCM-24):



25) 4-butyl-4"-ethyl-2'-fluoro-1,1':4',1"-terphenyl (LCM-25):

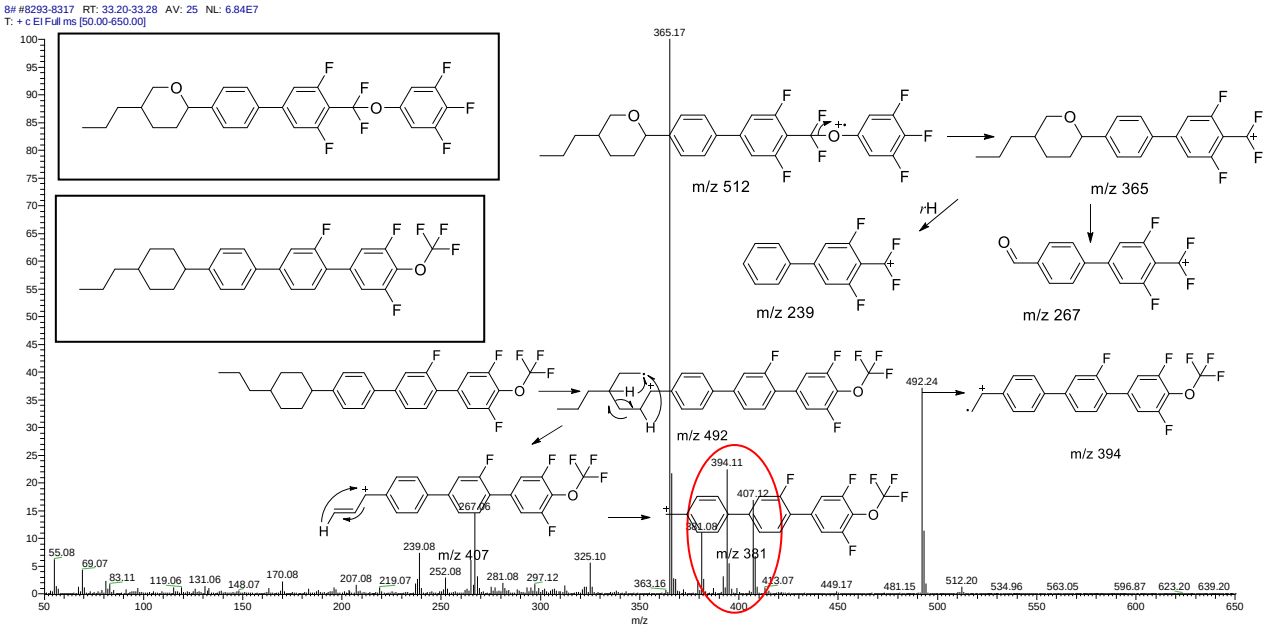


26) 3,4-difluoro-4'-[4'-ethyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl (LCM-26):

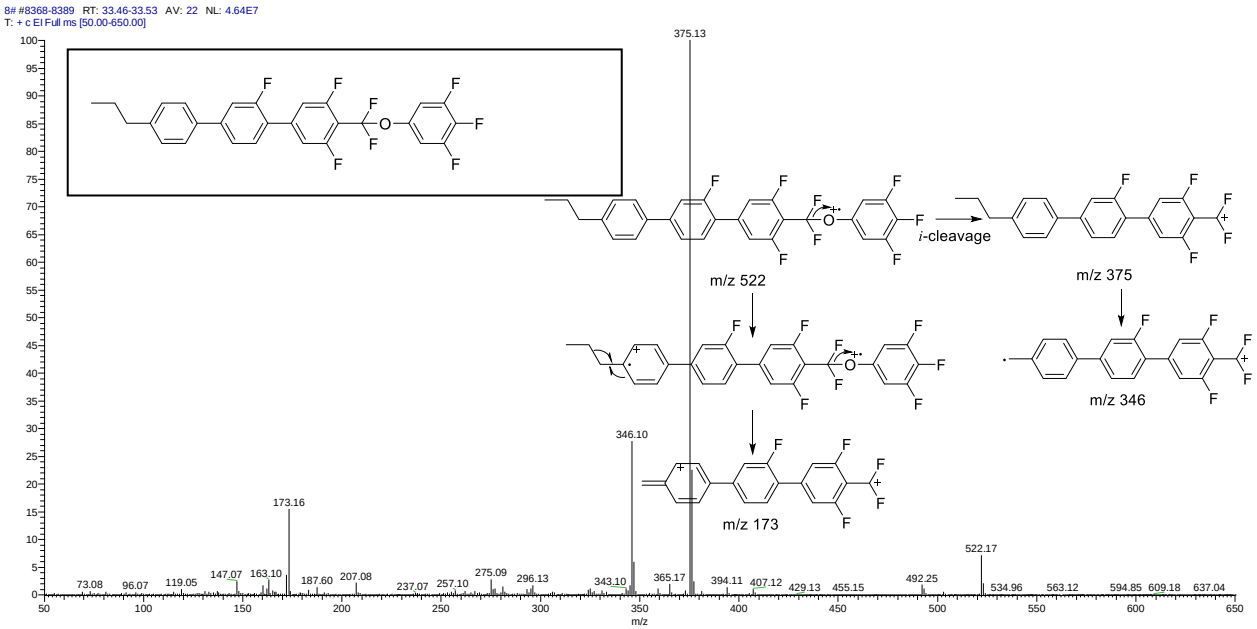


27) 4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-propyl-tetrahydro-2H-pyran)-yl]-biphenyl (LCM-27)

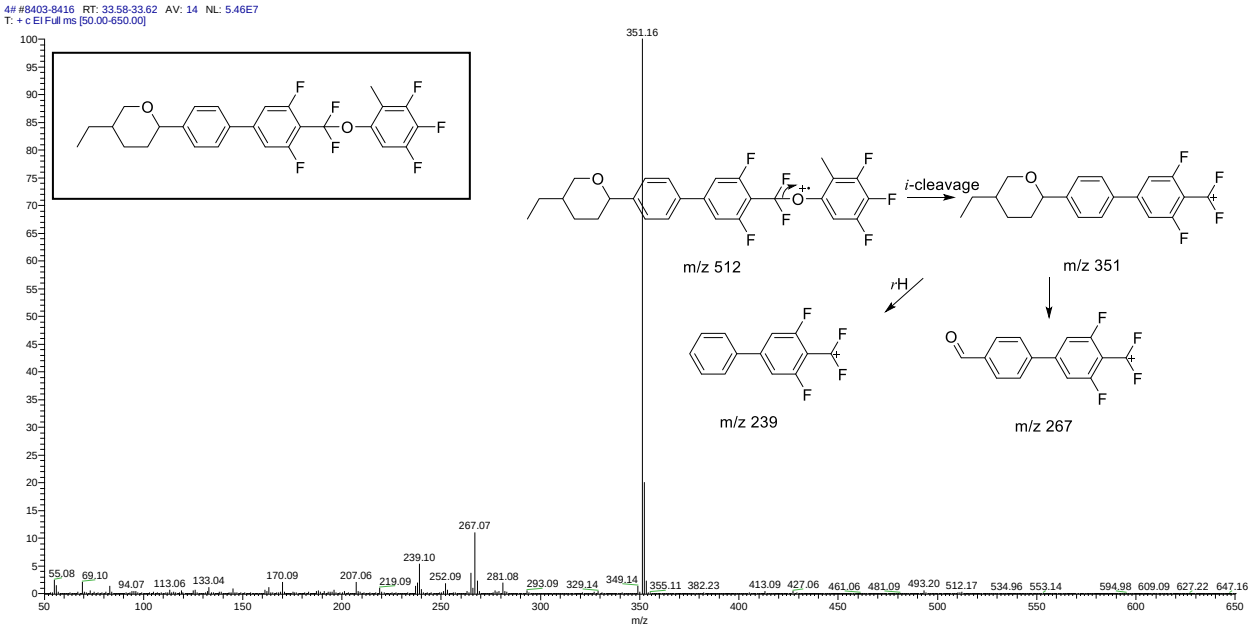
and 4-trifluoromethoxy-3,5-difluoro-2'-fluoro-4''-(4-propylcyclohexyl)-1,1':4',1''-terphenyl (LCM-28):



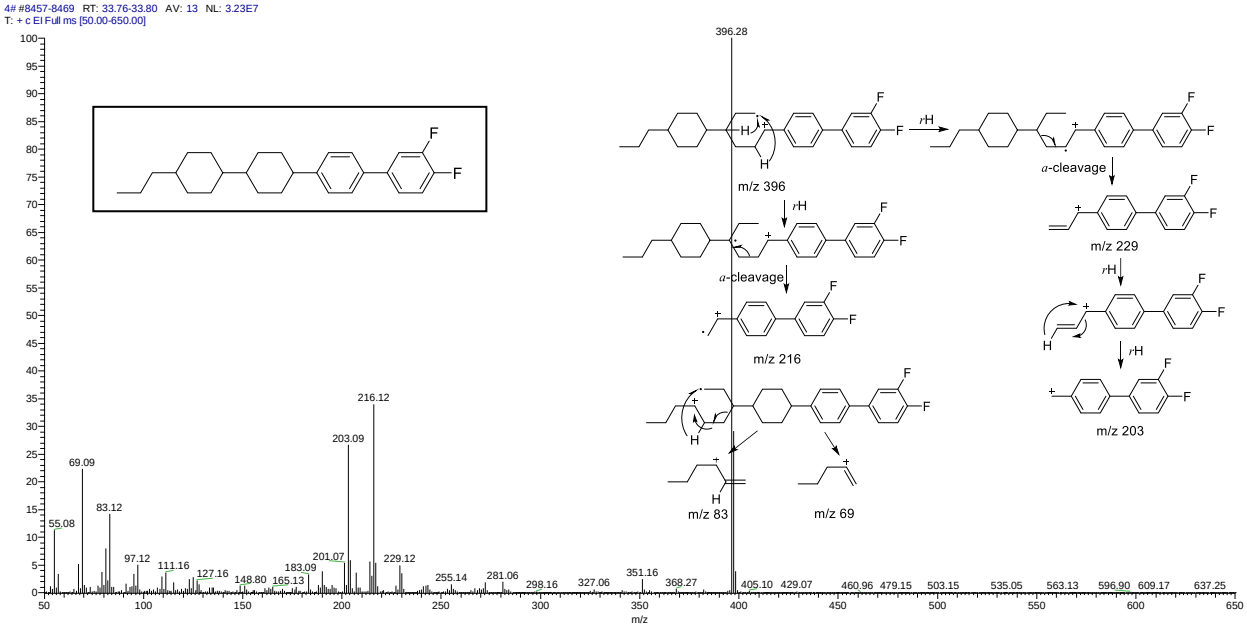
28) 4-[difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-2'-fluoro-4''-propyl-1,1':4',1''-terphenyl (LCM-29):



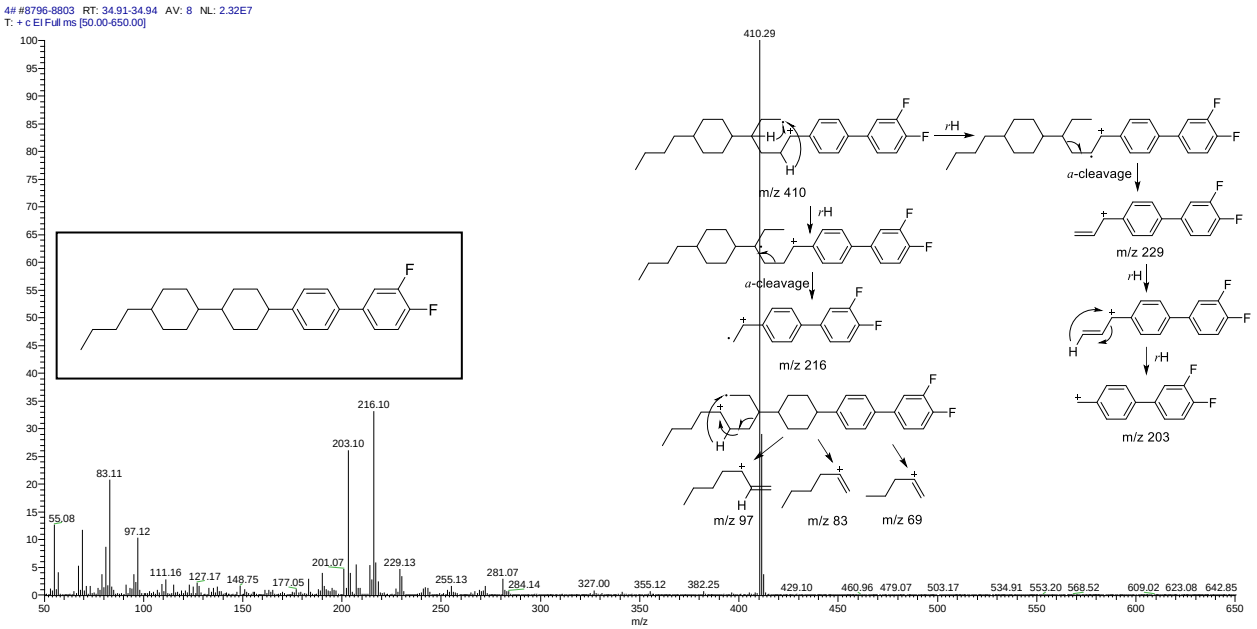
29) 4-[difluoro(2-methyl-3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-[(5-ethyl-tetrahydro-2H-pyran)-yl]-biphenyl (LCM-30):



30) 3,4-difluoro-4'-[4'-propyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl (LCM-31):



31) 3,4-difluoro-4'-[4'-butyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl (LCM-32):



32) 3,4-difluoro-4'-[4'-pentyl-1,1'-bi(cyclohexyl)-4-yl]biphenyl (LCM-33):

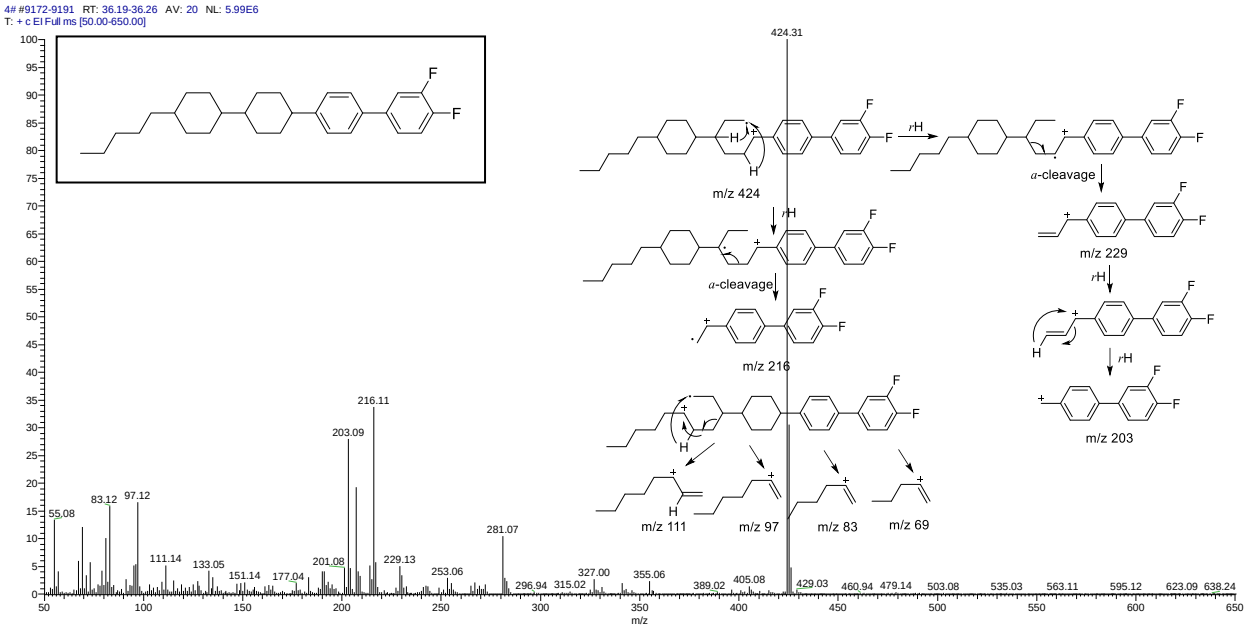
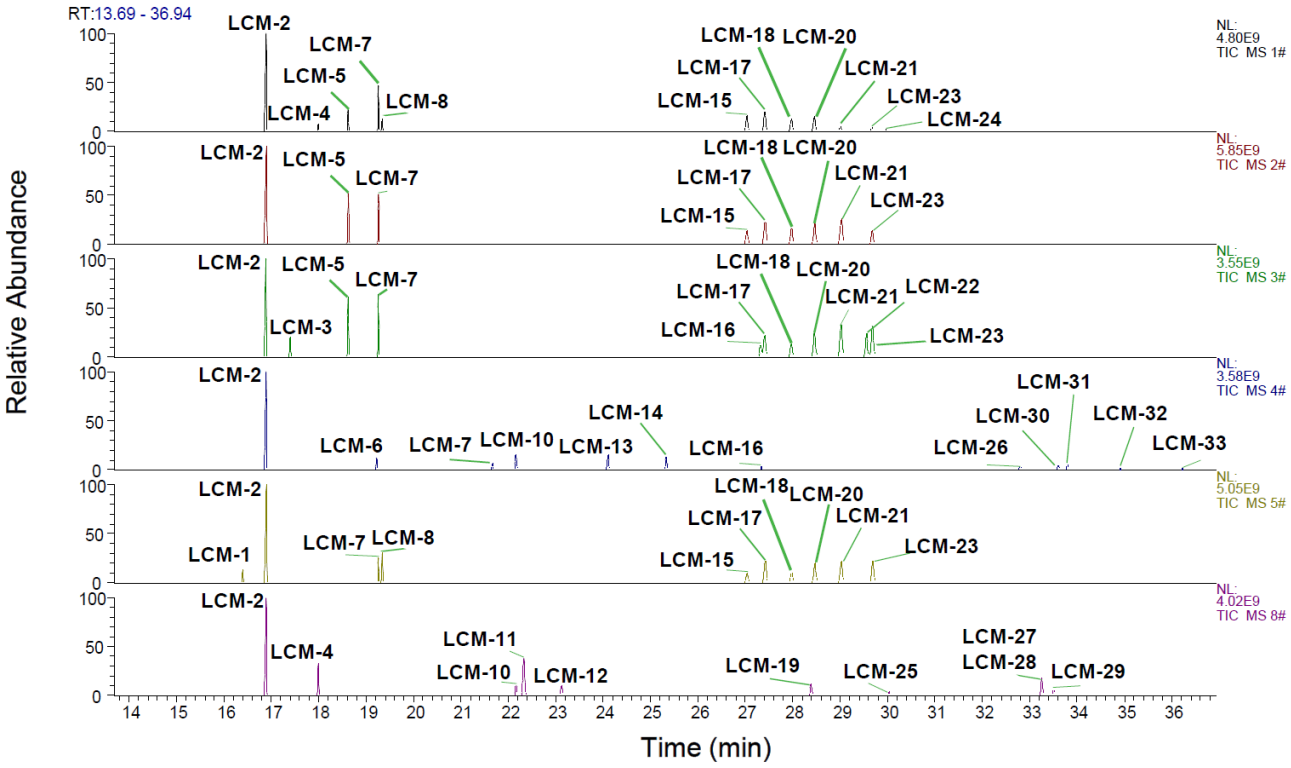


Figure S5. Total Ion Chromatogram (TIC) of the liquid crystal monomer (LCM) mixtures from six dismantled liquid crystal devices (LCDs) by use of GC-EI-MS (Full scan mode).



Reference:

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2. Ng CA, Scheringer M, Fenner K, & Hungerbuhler K (2011) A Framework for Evaluating the Contribution of Transformation Products to Chemical Persistence in the Environment. *Environ Sci Technol* 45(1):111-117.
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5. Su GY, Crump D, Letcher RJ, & Kennedy SW (2014) Rapid in Vitro Metabolism of the Flame Retardant Triphenyl Phosphate and Effects on Cytotoxicity and mRNA Expression in Chicken Embryonic Hepatocytes. *Environ Sci Technol* 48(22):13511-13519.