Supporting Information

MANUSCRIPT TITLE: Identification of Environmental Liquid Crystal Monomers: A Class of New Persistent Organic Pollutants–Fluorinated Biphenyls and Analogs–Emitted from E-Waste Dismantling

AUTHORS: Mingshan Zhu,[†] Mingjie Shen,[†] Xinxin Liang, Hui Chen, Chunyou Zhu, Bibai Du, Dan Luo, Shenyu Lan, Zhiqing Feng, and Lixi Zeng*

ADDRESS: *Guangdong Key Laboratory of Environmental Pollution and Health, School of Environment, Guangdong-Hongkong-Macau Joint Laboratory of Collaborative Innovation for Environmental Quality, Jinan University, Guangzhou 511443, China*

[†]M.Z. and M.S. contributed equally to this work.

NO. OF TABLES: 3

NO. OF FIGURES: 3

NO. OF PAGES: 12

*Corresponding authors

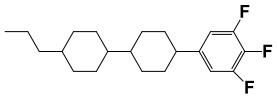
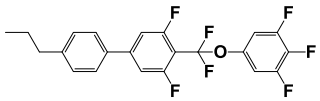
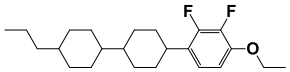
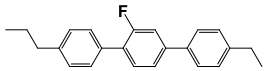
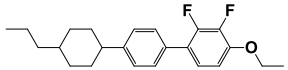
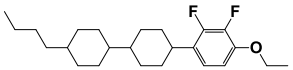
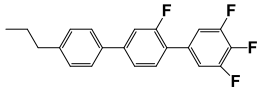
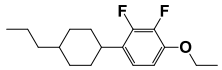
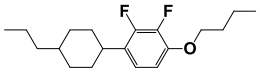
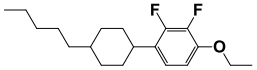
***Dr. Lixi Zeng**

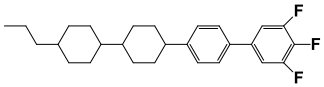
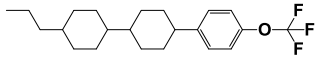
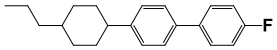
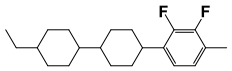
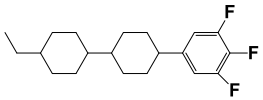
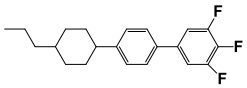
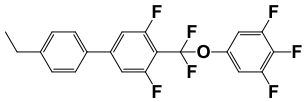
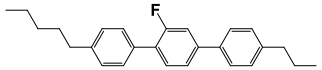
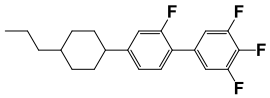
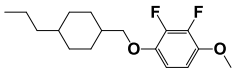
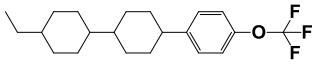
Guangdong Key Laboratory of Environmental Pollution and Health, School of Environment, Jinan University, Guangzhou 510632, China

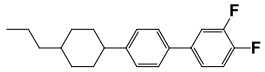
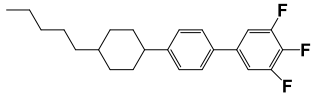
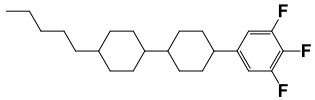
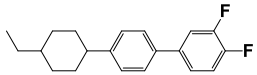
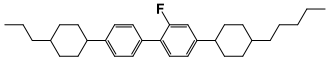
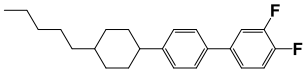
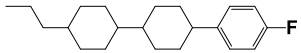
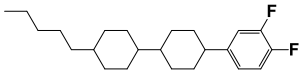
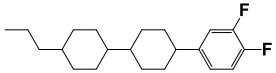
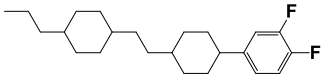
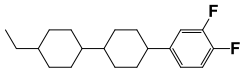
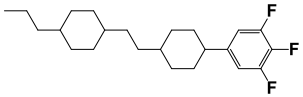
Phone: +(86)-20-37336629

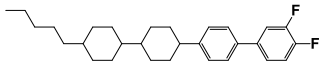
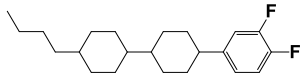
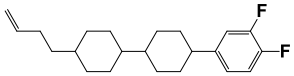
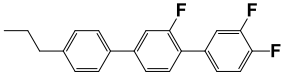
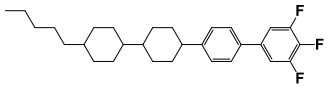
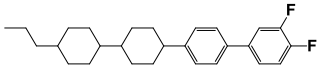
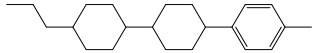
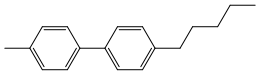
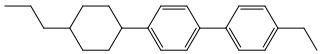
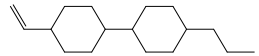
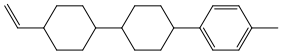
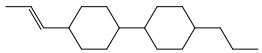
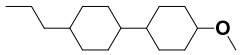
E-mail: lxzeng@jnu.edu.cn

Table S1. Full names, abbreviations, chemical structures, formulas, molecular weight (MW), and logK_{ow} of 46 target LCMs.

Class	No.	Full Name	Abbreviation	Chemical Structure	Formula	MW	logK_{ow} [a]
Fluorinated Biphenyls & Analogs	1	1,2,3-trifluoro-5-[3-(3-propylcyclohexyl) cyclohexyl]benzene	TPrCB		$C_{21}H_{29}F_3$	338.46	9.50
	2	4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-propyl-biphenyl	DTMDPB		$C_{22}H_{15}F_7O$	428.35	9.10
	3	1-Ethoxy-2,3-difluoro-4-[(trans,trans)-4'-propyl[1,1'-bicyclohexyl]-4-yl]benzene	EDPBB		$C_{23}H_{34}F_2O$	364.52	9.87
	4	4''-Ethyl-2'-fluoro-4-propyl-1,1':4',1''-terphenyl	EFPT		$C_{23}H_{23}F$	318.44	8.29
	5	4-Ethoxy-2,3-difluoro-4'-(trans-4-propylcyclohexyl)biphenyl	EDPB		$C_{23}H_{28}F_2O$	358.47	8.95
	6	1-[4-(4-butylcyclohexyl)cyclohexyl]-4-ethoxy-2,3-difluoro-benzene	BCEDB		$C_{24}H_{36}F_2O$	378.54	10.36
	7	2',3,4,5-Tetrafluoro-4''-propyl-1,1':4',1''-terphenyl	TePT		$C_{21}H_{16}F_4$	344.35	7.85
	8	1-Ethoxy-2,3-difluoro-4-(trans-4-propylcyclohexyl)benzene	EDPrB		$C_{17}H_{24}F_2O$	282.37	7.18
	9	1-Butoxy-2,3-difluoro-4-(trans-4-propylcyclohexyl)benzene	BDPrB		$C_{19}H_{28}F_2O$	310.43	8.16
	10	1-Ethoxy-2,3-difluoro-4-(trans-4-pentylcyclohexyl)benzene	EDPeB		$C_{19}H_{28}F_2O$	310.43	8.16

	11	3,4,5-trifluoro-4'-[(trans,trans)-4'-propyl[1,1'-bicyclohexyl]-4-yl]biphenyl	TPrBB		$C_{27}H_{33}F_3$	414.56	11.26
	12	4-[trans-4-(trans-4-Propylcyclohexyl)cyclohexyl]-1-(trifluoromethoxy)benzene	PCTB		$C_{22}H_{31}F_3O$	368.48	9.94
	13	4-fluoro-4'-(trans-4-propylcyclohexyl)biphenyl	FPB		$C_{21}H_{25}F$	296.43	8.17
	14	1-[(trans,trans)-4'-Ethyl[1,1'-bicyclohexyl]-4-yl]-2,3-difluoro-4-methyl-benzene	EBDMB		$C_{21}H_{30}F_2$	320.47	9.35
	15	3,4,5-Trifluoro-1-[trans-4'-(trans-4"-ethylcyclohexyl)cyclohexyl]benzene	TECB		$C_{20}H_{27}F_3$	324.43	9.01
	16	3,4,5-Trifluoro-4'-(trans-4-propylcyclohexyl)biphenyl	TrPrB		$C_{21}H_{23}F_3$	332.41	8.57
	17	4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4'-ethyl-biphenyl	DTMDEB		$C_{21}H_{13}F_7O$	414.32	8.61
	18	4"-Propyl-2'-fluoro-4-pentyl-1,1':4',1"-terphenyl	PFPT		$C_{26}H_{29}F$	360.52	9.76
	19	2',3,4,5-Tetrafluoro-4'-(trans-4-propylcyclohexyl)biphenyl	TePrB		$C_{21}H_{22}F_4$	350.40	8.78
	20	2,3-Difluoro-1-methoxy-4-[(trans-4-propylcyclohexyl)methoxy]benzene	DMPMB		$C_{17}H_{24}F_2O_2$	298.37	6.23
	21	1-[4-(4-ethylcyclohexyl)cyclohexyl]-4-(trifluoromethoxy)benzene	ECTB		$C_{21}H_{29}F_3O$	354.46	9.45

	22	3,4-Difluoro-4'-(trans-4-propylcyclohexyl) biphenyl	DPrB		$C_{21}H_{24}F_2$	314.42	8.37
	23	3,4,5-Trifluoro-4'-(trans-4-pentylcyclohexyl)biphenyl	TrPeB		$C_{23}H_{27}F_3$	360.46	9.56
	24	3,4,5-Trifluoro-1-[trans-4'-(trans-4"-pentylcyclohexyl)cyclohexyl]benzene	TPeCB		$C_{23}H_{33}F$	366.51	10.48
	25	3,4-Difluoro-4'-(trans-4-ethylcyclohexyl)biphenyl	DEB		$C_{20}H_{22}F_2$	300.39	7.88
	26	2-Fluoro-4-(trans-4-pentylcyclohexyl)-4'-(trans-4-propylcyclohexyl)biphenyl	FPePrB		$C_{32}H_{45}F$	448.71	13.37
	27	3,4-Difluoro-4'-(trans-4-pentylcyclohexyl)biphenyl	DPeB		$C_{23}H_{28}F_2$	342.47	9.36
	28	1-Fluoro-4-[4-(4-propylcyclohexyl)cyclohexyl] benzene	FPCB		$C_{21}H_{31}F$	302.48	9.10
	29	1,2-Difluoro-4-[4-(4-pentylcyclohexyl) cyclohexyl]benzene	DPeCB		$C_{23}H_{34}F_2$	348.52	10.28
	30	1,2-Difluoro-4-[trans-4-(trans-4-propylcyclohexyl)cyclohexyl]benzene	DPrCB		$C_{21}H_{30}F_2$	320.47	9.30
	31	1,2-Difluoro-4-[trans-4-[2-(trans-4-propylcyclohexyl)ethyl]cyclohexyl]benzene	DPrECB		$C_{23}H_{34}F_2$	348.52	10.28
	32	1,2-Difluoro-4-[trans-4-(trans-4-ethylcyclohexyl) cyclohexyl]benzene	DECB		$C_{20}H_{28}F_2$	306.44	8.81
	33	1,2,3-Trifluoro-5-[trans-4-[2-(trans-4-propylcyclohexyl)ethyl]cyclohexyl]benzene	TPrECB		$C_{23}H_{33}F_3$	366.51	10.48

	34	3,4-Difluoro-4'-[(trans,trans)-4'-pentyl[1,1'-bicyclohexyl]-4-yl]biphenyl	DPeBB		$C_{29}H_{38}F_2$	424.62	12.04
	35	3,4-Difluoro-1-[4-(trans-4-butylcyclohexyl)cyclohexyl]benzene	DBCB		$C_{22}H_{32}F_2$	334.49	9.79
	36	4-[(trans,trans)-4'-(3-Buten-1-yl)[1,1'-bicyclohexyl]-4-yl]-1,2-difluoro-benzene	BBDB		$C_{22}H_{30}F_2$	332.48	9.65
	37	2',3,4-Trifluoro-4''-propyl-1,1':4',1''-terphenyl	TrPT		$C_{21}H_{17}F_3$	326.36	6.83
	38	3,4,5-Trifluoro-4'-[(trans,trans)-4'-pentyl[1,1'-bicyclohexyl]-4-yl]biphenyl	TPeBB		$C_{29}H_{37}F_3$	442.61	12.24
	39	3,4-Difluoro-4'-[(trans,trans)-4'-propyl[1,1'-bicyclohexyl]-4-yl]biphenyl	DPrBB		$C_{27}H_{34}F_2$	396.57	11.06
Biphenyls & Analogs	1	1-Methyl-4-[4-(4-propylcyclohexyl)cyclohexyl]benzene	MPCB		$C_{22}H_{34}$	298.51	9.44
	2	4'-Methyl-4-pentyl-biphenyl	MPB		$C_{18}H_{22}$	238.37	6.82
	3	4-Ethyl-4'-(trans-4-propylcyclohexyl)biphenyl	EPB		$C_{23}H_{30}$	306.49	9.01
	4	trans,trans-4-Propyl-4'-vinyl-bicyclohexyl	PVB		$C_{17}H_{30}$	234.43	8.03
	5	1-[(trans,trans)-4'-Ethenyl[1,1'-bicyclohexyl]-4-yl]-4-methyl-benzene	EBMB		$C_{21}H_{30}$	282.47	8.82
	6	trans,trans-4-Propenyl-4'-propyl-bicyclohexyl	PPB		$C_{18}H_{32}$	248.45	8.45
	7	trans,trans-4-Methoxy-4'-propyl-bicyclohexyl	MOPB		$C_{16}H_{30}O$	238.42	6.42

[a] Estimated by the US Environmental Protection Agency (EPA) EPI Suite 4.1.

Table S2. Optimized EI-MS/MS parameters for 46 LCMs

No.	Abbr.	MS confirmation		MS quantitation		RT[b] (min)
		Transition	CE[a] (eV)	Transition	CE (eV)	
1	PVB	234.1−>109.1	6	205.1−>81.0	15	11.289
2	MOPB	206.1−>123.0	6	163.1−>81.0	12	11.863
3	PPB	205.1−>80.9	15	248.1−>81.0	18	12.589
4	EDPrB	156.0−>127.1	21	282.1−>169.1	21	13.299
5	MPB	181.1−>165.1	15	238.1−>181.1	15	14.055
6	DMPMB	298.1−>160.0	9	160.0−>145.0	12	14.825
7	BDPrB	310.1−>254.1	6	254.1−>156.0	9	15.512
8	EDPeB	310.1−>197.0	9	184.0−>156.0	12	15.625
9	ECTB	354.1−>188.1	18	188.1−>91.0	21	16.250
10	TECB	145.0−>125.1	21	324.1−>189.1	9	16.295
11	DECB	306.1−>140.1	12	140.1−>138.9	18	16.583
12	DTMDEB	252.0−>183.0	18	267.0−>252.0	21	17.186
13	DEB	300.1−>229.1	15	229.1−>214.1	18	17.250
14	PCTB	368.1−>188.1	9	188.1−>119.1	18	17.632
15	TPrCB	158.1−>132.0	24	338.1−>203.0	9	17.704
16	EBMB	282.1−>157.1	9	118.1−>117.1	12	17.711
17	TePrB	239.0−>219.0	18	350.1−>251.9	12	17.762
18	FPCB	302.1−>122.1	9	122.1−>121.1	18	17.899
19	DPrCB	320.1−>140.1	12	140.1−>114.1	18	18.059
20	EBDMB	320.2−>154.1	15	154.0−>153.1	12	18.236
21	TPrBB	234.1−>219.0	24	221.1−>201.1	21	18.255
22	TrPrB	234.0−>233.1	15	332.1−>247.1	15	18.259
23	DTMDPB	252.1−>183.0	21	281.1−>252.1	24	18.599
24	DPrB	216.1−>201.1	21	314.1−>216.1	15	18.823
25	FPB	296.1−>211.1	15	211.1−>196.0	18	18.847
26	TePT	315.1−>275.0	24	344.1−>315.1	18	19.041
27	MPCB	298.1−>118.1	9	118.1−>117.1	12	19.577
28	TrPT	297.0−>275.0	24	326.1−>297.0	18	19.762
29	BBDB	179.1−>164.0	18	332.2−>179.1	12	19.806
30	DBCB	127.0−>101.0	21	334.1−>83.2	18	19.890
31	TPrECB	366.1−>213.1	6	213.1−>145.1	15	20.939
32	DPrECB	348.1−>140.1	15	140.1−>114.1	21	21.406
33	TPeCB	366.1−>231.2	9	145.1−>125.0	21	21.502
34	DPeCB	348.1−>140.0	15	140.0−>114.1	21	21.991
35	TrPeB	234.1−>219.1	24	247.1−>232.1	15	22.199
36	DPeB	216.1−>201.1	21	342.0−>216.1	12	22.983
37	EPB	193.1−>178.1	15	306.1−>193.1	21	23.381
38	EDPBB	364.1−>184.1	9	184.1−>156.0	9	24.320
39	EFPT	289.1−>274.1	21	318.1−>289.1	18	24.795
40	EDPB	231.9−>183.0	21	358.1−>245.1	18	25.782

41	BCEDB	378.0−>184.1	9	184.1−>156.0	9	26.928
42	PFPT	360.1−>303.1	18	303.1−>274.0	21	30.942
43	DPrBB	216.2−>201.0	24	396.2−>216.2	18	32.585
44	TPeBB	442.3−>234.1	15	221.1−>201.1	21	35.101
45	DPeBB	216.1−>201.0	24	424.1−>216.1	15	35.820
46	FPePrB	448.3−>350.2	15	448.2−>97.0	21	42.720
47	BPh-d10	164.1−>160.1	24	164.1−>162.1	18	7.080
48	$^{13}C_{12}$-BDE-77	388.6−>229.0	24	497.6−>338.0	24	22.502
49	$^{13}C_{6}$-BTBPE	362.9−>337.0	15	362.9−>362.8	3	24.805

[a] CE: Collision energy (eV); [b] RT: Retention time (min).

Table S3. QA/QC data, including detection of limit (LOD), matrix spike recovery (RE, n = 3), and matrix effect (ME, n = 3), for 46 LCMs in dust samples.

No.	Abbr.	LOD (ng/g)	Spike level (10 or 20 ng/g)[a]		Spike level (100 ng/g)		ME (%)
			RE (%)	RSD (%)	RE (%)	RSD (%)	
1	PVB	2.04	86	6	87	6	82
2	MOPB	6.38	87	7	89	7	81
3	PPB	6.67	80	6	85	10	81
4	EDPrB	0.92	94	4	81	8	92
5	MPB	1.69	106	10	101	10	103
6	DMPMB	1.23	109	4	104	5	100
7	BDPrB	1.03	105	4	100	10	94
8	EDPeB	0.67	91	10	90	7	87
9	ECTB	0.41	101	6	92	7	82
10	TECB	1.60	82	7	80	6	90
11	DECB	4.69	91	7	88	6	86
12	DTMDEB	1.08	110	7	109	9	96
13	DEB	0.65	102	5	98	6	92
14	PCTB	1.80	98	6	103	5	93
15	TPrCB	0.59	101	8	103	8	89
16	EBMB	0.67	104	9	96	9	86
17	TePrB	0.66	92	10	103	7	92
18	FPCB	2.86	94	6	88	8	89
19	DPrCB	3.80	85	5	83	6	91
20	EBDMB	4.11	91	9	88	7	94
21	TPrBB	4.48	107	10	97	11	86
22	TrPrB	2.70	94	10	95	11	92
23	DTMDPB	0.41	108	8	107	6	99
24	DPrB	1.12	108	9	106	8	85
25	FPB	0.93	103	7	104	7	96
26	TePT	1.42	119	11	116	11	98
27	MPCB	5.36	107	10	89	9	97
28	TrPT	6.98	107	5	101	5	100
29	BBDB	5.45	101	6	105	5	109
30	DBCB	6.12	104	7	94	7	94
31	TPrECB	9.80	90	12	99	10	105
32	DPrECB	1.36	109	9	106	10	105
33	TPeCB	3.90	99	7	96	6	108
34	DPeCB	6.67	107	10	105	7	114
35	TrPeB	3.66	108	6	110	7	112
36	DPeB	1.90	109	4	110	3	110
37	EPB	3.43	106	7	94	8	108
38	EDPBB	2.78	91	10	93	8	108

39	EFPT	2.03	111	8	112	7	99
40	EDPB	1.85	90	7	93	8	107
41	BCEDB	2.78	107	9	105	5	99
42	PFPT	1.82	109	10	100	8	108
43	DPrBB	2.30	101	9	107	8	115
44	TPeBB	3.30	90	7	93	5	100
45	DPeBB	7.14	104	4	108	6	106
46	FPePrB	11.9	89	6	92	7	112

[a] The low spiked level was set as 10 ng/g for LCMs, with the exception of FPePrBb (20 ng/g) due to its high LOD.

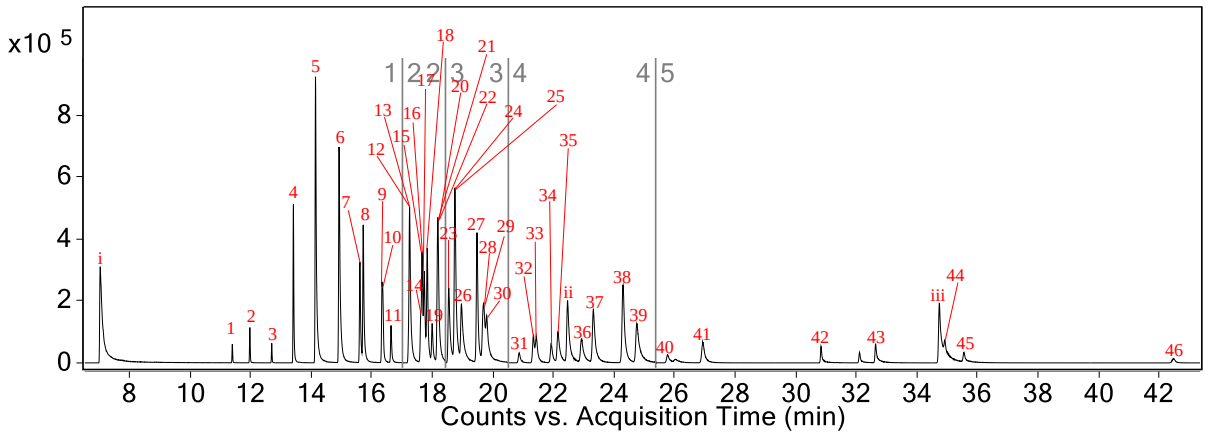


Figure S1. Total ion chromatogram (TIC) of 46 LCMs and three internal standards (IS) using GC-EI-MS/MS analysis (100 ng/mL for each analyte): 1. PVB, 2. MOPB, 3. PPB, 4. EDPrB, 5. MPB, 6. DMPMB, 7. BDPrB, 8. EDPeB, 9. ECTB, 10. TECB, 11. DECB, 12. DTMDEB, 13. DEB, 14. PCTB, 15. TPrCB, 16. EBMB, 17. TePrB, 18. FPCB, 19. DPrCB, 20. EBDMB, 21. TPrBB, 22. TrPrB, 23. DTMDPB, 24.DPrB, 25. FPB, 26. TePT, 27. MPCB, 28. TrPT, 29. BBDB, 30. DBCB, 31. TPrECB, 32. DPrECB, 33. TPeCB, 34. DPeCB, 35. TrPeB, 36. DPeB, 37. EPB, 38. EDPBB, 39. EFPT, 40. EDPB, 41. BCEDB, 42. PFPT, 43. DPrBB, 44. TPeBB, 45. DPeBB, 46. FPePrB; i. BPh-d10, ii. $^{13}C_{12}$-BDE-77, iii. $^{13}C_{6}$-BTBPE

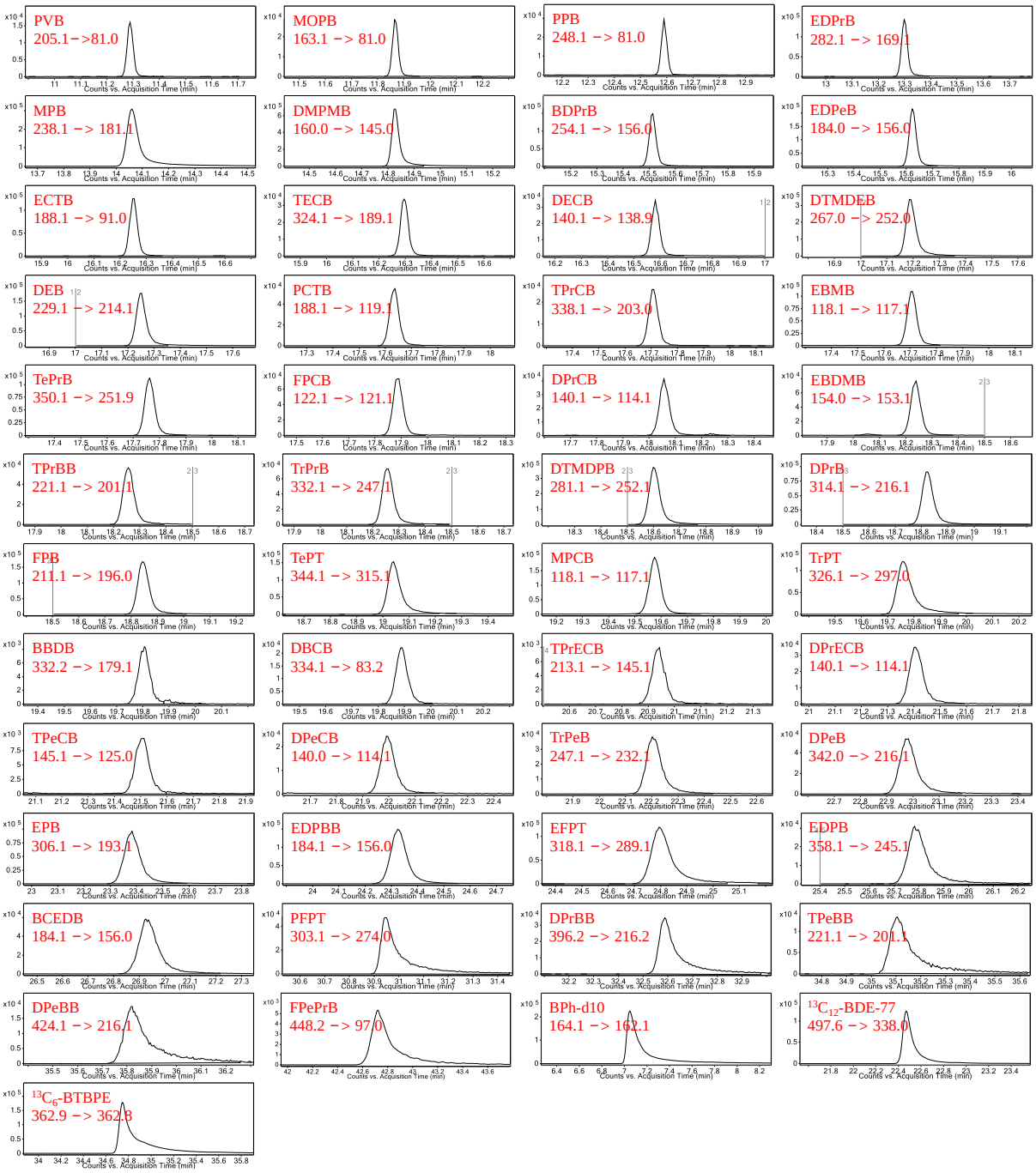


Figure S2. Extracted GC-MS/MS MRM chromatograms of 46 LCMs and three internal standards.

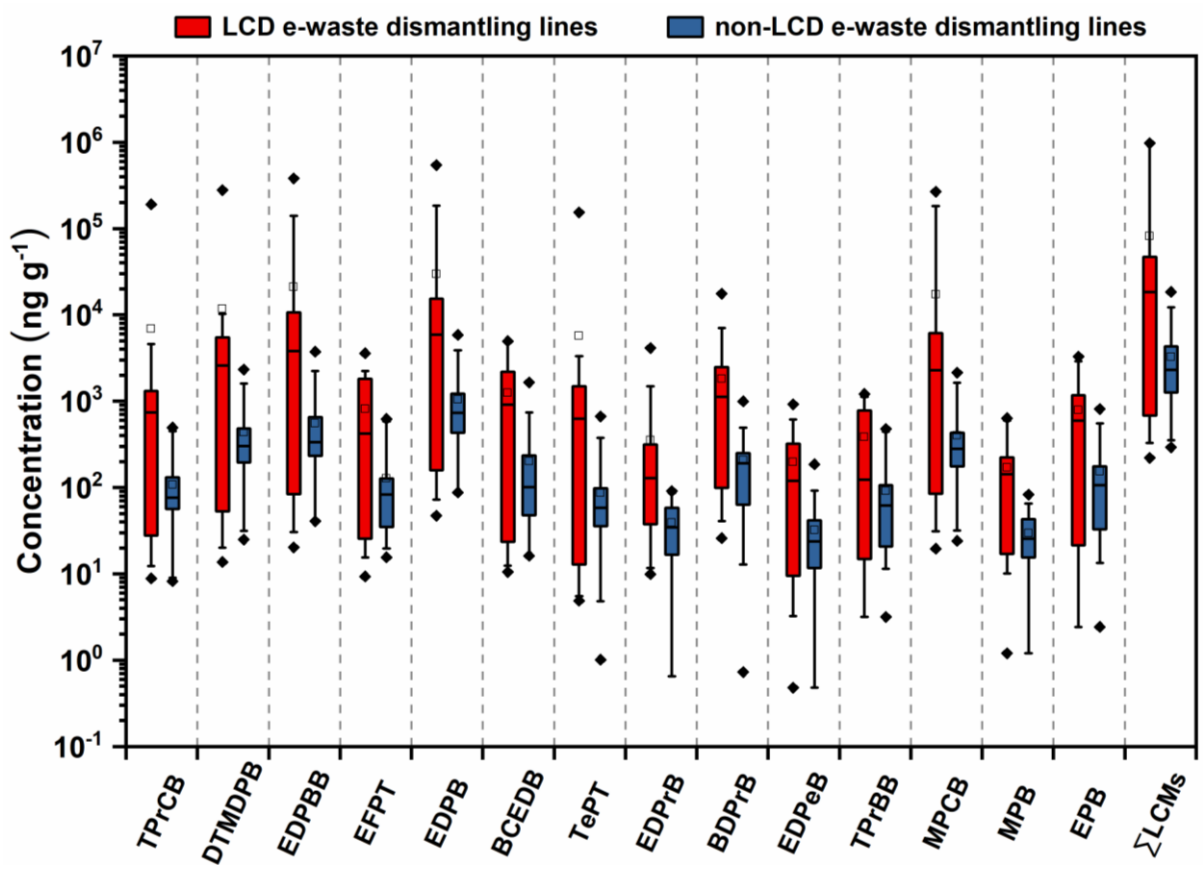


Figure S3. Comparing the measured concentrations of 14 main LCMs and $\sum_{40}$LCMs in two types of dust samples collected from LCD and non-LCD e-waste dismantling lines.