

Supplementary Material
Aerosol and Air Quality Research (AAQR)
Mechanical treatment of MSWI fly ash: a way forward to inhibit PCB
reformation

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Table S1. Short and elementary analysis of fly ash (MFA), silica (SiO₂) and activated carbon (AC).

Fly ash (wt.%)															
Elements	C	O	Na	Cl	Ca	Cu	Fe	Si	Cr	Mn	Al	Ti	Ni	As	Zn
0 h	10.5	30.8	11.2	16.6	0.4	0.1	0.1	28.4	0.0	0.0	0.1	0.6	0.0	3.2	0.0
1 h	5.4	32.3	7.6	10.8	0.0	0.2	6.0	36.4	1.0	0.7	0.2	0.0	0.2	1.4	0.0
2 h	5.0	35.8	7.0	9.8	0.0	0.2	8.6	36.2	1.2	1.1	0.3	0.0	0.3	2.5	0.0
4 h	4.5	35.2	6.6	8.8	0.0	0.2	9.6	35.1	1.3	1.2	0.3	0.3	0.4	2.3	0.0
8 h	5.4	32.2	5.8	9.0	0.0	0.2	9.1	35.0	1.8	1.2	0.2	0.3	0.4	2.5	0.0
Activated Carbon (wt.%)															
Elements	C	H	O	N	S	Zn	Cu	Pb	Mn	Si	Ti	Fe	Cr	Ca	
	93	1.5	1.7	0.2	0.2	0.0	0.0	0.0	0.2	1.5	2.7	3.4	0.4	1.1	
	Moisture		Ash		Volatiles		Fixed carbon								
	1.7		2.1		7.4		89								
Silica (wt.%)															
Elements	Zn	Cu	Ca	Mn	Mg	Ni	Fe	Cr							
	n.d.	n.d.	0.2	n.d.	0.1	0.0	0.0	0.0							

S1. Chemicals

$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (purity >99.0%), n-Hexane (purity 95.0%), Diethyl ether, Anhydrous Na_2SO_4 , NaCl (purity > 99.5%), NaOH and HCl of analytical grade reagents (AR), were procured from Aladdin Chemistry Co. Ltd. SiO_2 (AR) was obtained from Sinopharm Chemical Reagent Co., Ltd, China.

Table S2. BET surface area and average particle size of 0, 1, 2, 4 and 8 h milled fly ash.

Time, h	0 h	1 h	2 h	4 h	8 h
BET($\text{m}^2 \text{g}^{-1}$)	2.54	5.62	5.73	5.85	6.29
Average particle size, dp (nm)	23.6	10.7	10.4	9.06	9.54

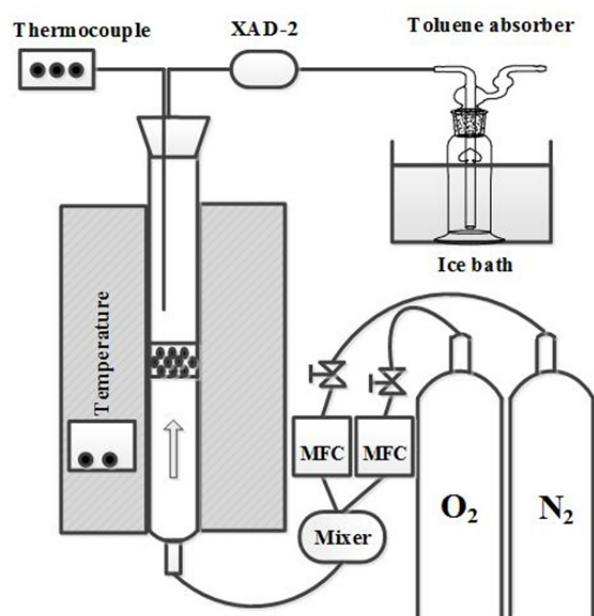


Fig. S1. De-novo testing apparatus.

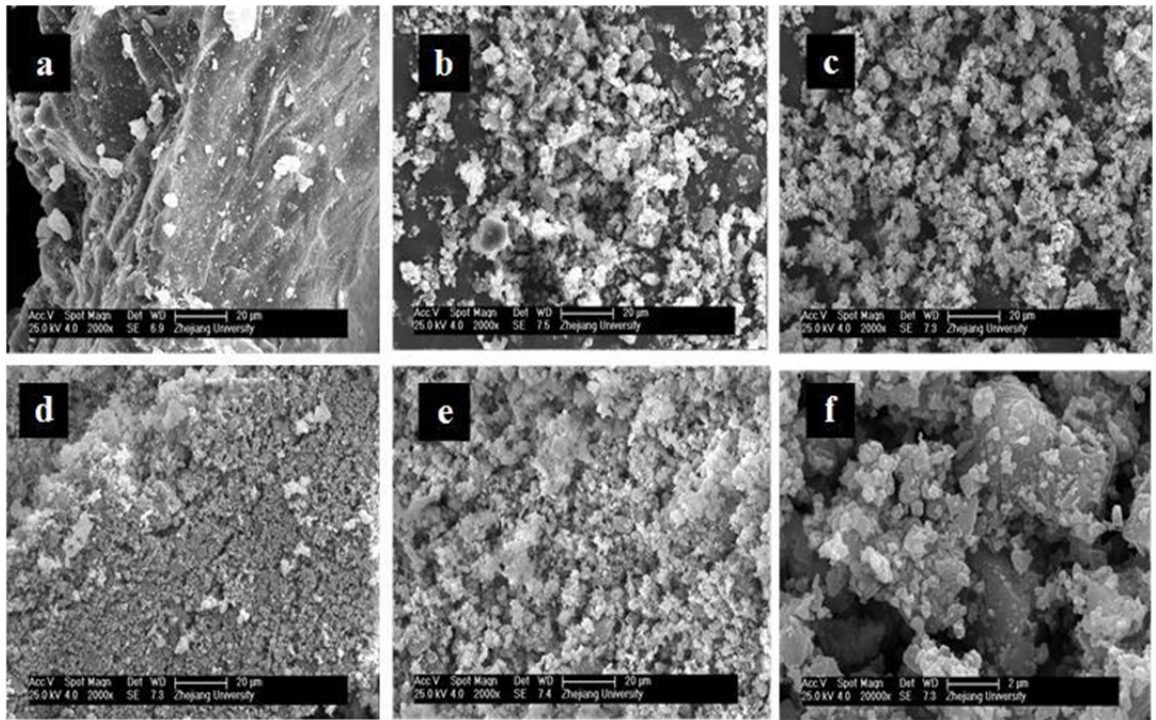


Fig. S2. SEM micrographs a-e for 0, 1, 2, 4 and 8 h milled fly ash magnified at $\times 2000$ (1k), f Eight hours milled fly ash magnified at $\times 20000$ (1k).

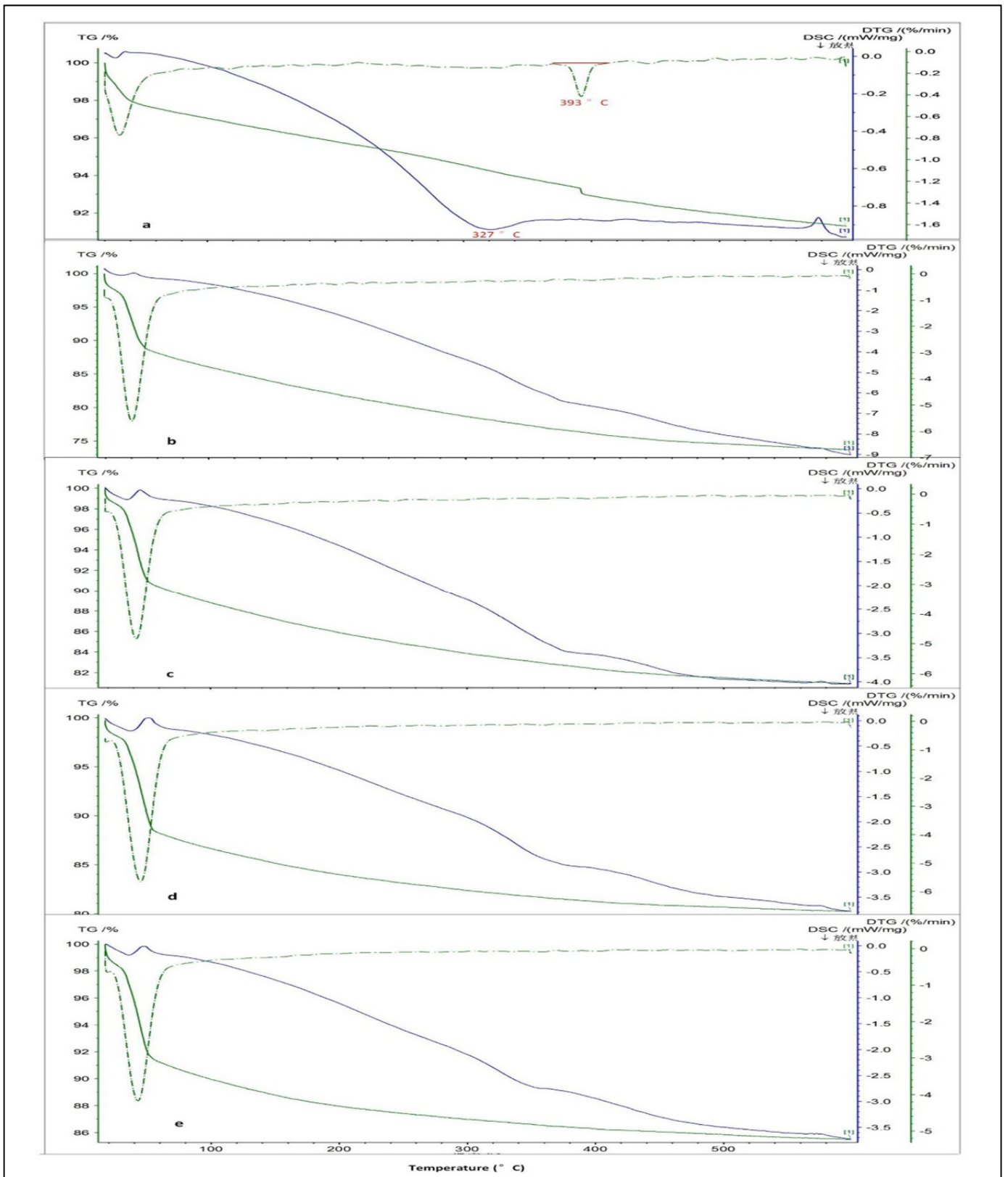


Fig. S3. TGA/DSC and DTG curves of milled samples (0, 1, 2, 4 and 8 h) of fly ash.

Equ. S1.

Average chlorination degree is defined as the sum of the products of the mole fraction f_j and the number of chlorine atoms n_j for each homologue:

$$d_c = \sum_{j=4}^8 f_j \times n_j \quad (\text{S1})$$

Equ. S2.

$$G0-G (1, 2, 4 \text{ or } 8)/G0 \times 100 \text{ OR } S0-S (1, 2, 4, \text{ or } 8)/S0 \times 100 \quad (\text{S2})$$

While:

G and S stands for gas and solid phase values in 0, 1, 2, 4 and 8 h milled samples, respectively.

Table S3. PCB content in gas and solid phase of MFA.

Time, h	PCB Content (ng g ⁻¹)				
	0h	1h	2h	4h	8h
∑PCB (Gas)	2353	1174	1472	138	85
∑PCB (Solid)	2833	809	1649	99	83
∑PCB (Gas + Solid)	5185	1983	2646	236	168

Table S4. PCB homologues (ng g⁻¹) in gas and solid phase of MFA.

ng g ⁻¹	0h		1h		2h		4h		8h	
	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)
H1CB	145	224	97	148	138	181	14	21	13	16
H2CB	418	466	215	265	357	388	27	23	21	20
H3CB	490	514	311	101	344	437	65	33	31	29
H4CB	609	784	435	174	484	506	26	18	15	17
H5CB	136	84	43	53	98	82	5	3	3	2
H6CB	92	78	32	33	25	26	1	0	0	0
H7CB	99	89	19	15	14	16	1	0	0	0
H8CB	78	92	12	10	7	6	0	0	0	0
H9CB	103	180	7	7	4	5	0	0	0	0
H10CB	182	322	2	3	2	2	0	0	0	0
Total-PCB	2353	2833	1174	809	1472	1649	138	99	85	83

Table S5. PCB homologues (ng g⁻¹) in gas and solid phase of MFA.

% homologues	0h		1h		2h		4h		8h	
	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)	(gas)	(solid)
H1CB	6	8	8	18	9	11	10	21	15	19
H2CB	18	16	18	33	24	23	20	24	25	24
H3CB	21	18	26	13	23	27	47	33	37	34
H4CB	26	28	37	22	33	31	19	18	18	20
H5CB	6	3	4	7	7	5	3	3	3	2
H6CB	4	3	3	4	2	2	1	0	1	0
H7CB	4	3	2	2	1	1	0	0	0	0
H8CB	3	3	1	1	0	0	0	0	0	0
H9CB	4	6	1	1	0	0	0	0	0	0
H10CB	8	11	0	0	0	0	0	0	0	0
	100	100	100	100	100	100	100	100	100	100

Table S6. Data for relationship of milling with de no formation.

Time, h	*PCDD/F	*PCB	I-TEQ for PCB	Cl-PCB	Particle size, <i>dp</i>	BET	**Cl	**C	**Cu	**Fe	**Cr	**Ni
0 h	5065	5185	1	9	23.6	2.54	16.6	10.5	0.1	0.1	0	0
1 h	1765	1983	0	6	10.7	5.62	10.8	5.4	0.2	6	1	0.2
2 h	40	2646	1	6	10.4	5.73	9.8	5	0.2	8.6	1.2	0.3
4 h	60	236	0	6	9.06	5.85	8.8	4.5	0.2	9.6	1.3	0.4
8 h	325	168	0	5	9.54	6.29	9	5.4	0.2	9.1	1.8	0.4

* = PCDD/F and PCB values are sum of gas and solid phase of MFA in ng g⁻¹

**=values are obtained by XRF analysis (wt.%)

Table S7. Percent isomer distributions of PCB in 0, 1, 2, 4 and 8 h milled MFA samples.

Time, h		0 h	1h	2h	4h	8h	MIN	MAX	Average	SD (%)
M1CB	#1	9	7	6	12	16	6	16	10	42
M1CB	#2	56	59	44	50	46	44	59	51	13
M1CB	#3	36	34	50	38	38	34	50	39	16
D2CB	#4	1	2	1	3	*n.d	1	3	2	44
D2CB	#10	1	2	1	3	n.d	1	3	2	40
D2CB	#7 #9	1	2	2	3	2	1	3	2	33
D2CB	#6	6	11	11	5	n.d	5	11	8	43
D2CB	#5 #8	14	17	17	11	15	11	17	15	16
D2CB	#14	0	1	1	1	6	0	6	2	125
D2CB	#11	37	28	28	53	49	28	53	39	29
D2CB	#13	13	22	21	7	14	7	22	16	40
D2CB	#12	n.d	n.d	n.d	n.d	n.d	-	-	-	-
D2CB	#15	26	14	16	14	n.d	14	26	17	32
T3CB	#19	2	2	2	1	1	1	2	2	13
T3CB	#30	n.d	n.d	n.d	n.d	n.d	-	-	-	-
T3CB	#18	11	11	16	13	11	11	16	12	17
T3CB	#17	6	6	7	6	8	6	8	7	13
T3CB	#24#27	1	1	1	1	2	1	2	1	24
T3CB	#32	8	11	11	10	12	8	12	11	14
T3CB	#34	0	1	n.d	n.d	n.d	0	1	0	36
T3CB	#23 #29	1	1	1	0	n.d	0	1	1	34
T3CB	#26	4	8	3	3	3	3	8	4	58
T3CB	#25	1	4	2	2	2	1	4	2	53
T3CB	#28 #31	36	33	36	42	38	33	42	37	9
T3CB	#21,20,33	10	2	5	9	12	2	12	8	52
T3CB	#22	3	8	4	6	7	3	8	6	36
T3CB	#36	6	0	2	n.d	n.d	0	6	3	99
T3CB	#39	0	0	0	n.d	n.d	0	0	0	30
T3CB	#38	3	4	3	n.d	n.d	3	4	3	22
T3CB	#35	2	2	2	1	1	1	2	2	29
T3CB	#37	6	5	4	3	4	3	6	5	24
T4CB	#54	n.d	n.d	n.d	n.d	n.d	0	0	-	-
T4CB	#50	n.d	n.d	n.d	n.d	n.d	0	0	-	-
T4CB	#53	0	0	0	2	2	0	2	1	85
T4CB	#51	12	2	13	1	3	1	13	6	91
T4CB	#45	1	0	0	2	2	0	2	1	72
T4CB	#46,69,73	0	2	0	0	1	0	2	1	122
T4CB	#52	2	1	2	8	9	1	9	4	81
T4CB	#43	n.d	n.d	n.d	n.d	n.d	0	0	-	-
T4CB	#49	4	6	n.d	5	6	4	6	6	16
T4CB	#47,48,75,65	16	7	15	8	11	7	16	12	34
T4CB	#62	n.d	26	n.d	n.d	n.d	26	26	26	-
T4CB	#44	3	4	1	11	12	1	12	6	84

T4CB	#59	n.d	n.d	n.d	n.d	n.d	0	0	-	-
T4CB	#42	1	2	2	5	8	1	8	3	77
T4CB	#41,71,72	1	1	1	5	6	1	6	3	95
T4CB	#64,68	46	23	51	12	6	6	51	28	74
T4CB	#40	0	0	1	1	1	0	1	1	48
T4CB	#57	0	1	0	0	0	0	1	0	102
T4CB	#67	0	0	0	0	0	0	0	0	37
T4CB	#58	0	n.d	n.d	n.d	n.d	0	0	0	-
T4CB	#63	0	2	0	1	0	0	2	1	104
T4CB	#61	2	2	3	8	6	2	8	4	61
T4CB	#74	n.d	n.d	n.d	n.d	n.d	0	0	-	-
T4CB	#70,76	3	3	3	15	8	3	15	6	84
T4CB	#66,80	3	n.d	3	7	6	3	7	5	45
T4CB	#55	0	1	0	0	0	0	1	0	51
T4CB	#56	1	2	1	6	5	1	6	3	73
T4CB	#78	0	2	0	0	1	0	2	1	89
T4CB	#81	0	3	0	0	1	0	3	1	133
T4CB	#77	1	2	1	2	1	1	2	1	36
T4CB	#60	1	1	1	1	3	1	3	1	68
T4CB	#79	0	0	0	0	0	0	0	0	55
P5CB	#104	3	1	0	1	5	0	5	2	109
P5CB	#123	1	2	2	1	0	0	2	1	40
P5CB	#118	13	5	13	15	10	5	15	11	35
P5CB	#114	2	1	1	0	0	0	2	1	90
P5CB	#105	7	5	6	4	6	4	7	6	22
P5CB	#126	16	8	5	3	3	3	16	7	81
P5CB	#96,103	1	0	1	1	1	0	1	1	42
P5CB	#100	2	0	1	1	1	0	2	1	59
P5CB	#94	2	3	2	1	1	1	3	2	56
P5CB	#98,102,121	0	1	1	1	9	0	9	2	149
P5CB	#93,95	1	2	1	5	3	1	5	3	65
P5CB	#88	1	0	1	1	0	0	1	1	46
P5CB	#91	1	15	11	2	3	1	15	6	98
P5CB	#92	1	0	1	1	1	0	1	1	24
P5CB	#84,89,90	1	2	1	2	6	1	6	2	93
P5CB	#101,113	1	8	7	6	8	1	8	6	50
P5CB	#99	0	12	9	4	2	0	12	5	88
P5CB	#112,119	2	0	1	1	1	0	2	1	48
P5CB	#83	2	2	2	2	2	2	2	2	12
P5CB	#109	1	1	1	1	0	0	1	1	45
P5CB	#87,111,115, 116,117,125	2	1	1	1	3	1	3	2	69
P5CB	#97	3	4	3	3	2	2	4	3	27
P5CB	#120	1	2	2	1	1	1	2	1	33
P5CB	#85	2	3	3	2	3	2	3	3	21
P5CB	#110	3	3	3	6	7	3	7	4	47
P5CB	#82	1	4	3	2	1	1	4	2	73
P5CB	#124	1	1	1	1	1	1	1	1	11
P5CB	#108	2	2	2	2	2	2	2	2	12
P5CB	#107	1	1	1	1	1	1	1	1	12
P5CB	#106	13	4	13	15	10	4	15	11	38
P5CB	#122	6	1	1	10	1	1	10	4	114
P5CB	#127	7	5	3	4	6	3	7	5	30
H6CB	#155	3	2	1	27	5	1	27	8	31
H6CB	#167	5	3	3	3	5	3	5	4	40
H6CB	#156	13	7	7	8	4	4	13	8	32
H6CB	#157	7	4	4	4	8	4	8	5	47
H6CB	#169	11	5	4	6	n.d	4	11	6	135
H6CB	#150	2	0	0	n.d	n.d	0	2	1	64
H6CB	#152	1	0	2	n.d	n.d	0	2	1	102

H6CB	#148	1	0	0	n.d	n.d	0	1	0	54
H6CB	#145	1	0	1	n.d	n.d	0	1	1	77
H6CB	#154	1	0	0	n.d	n.d	0	1	1	101
H6CB	#136	3	0	0	n.d	3	0	3	2	97
H6CB	#151	2	0	0	n.d	n.d	0	2	1	31
H6CB	#135	0	1	0	n.d	n.d	0	1	0	102
H6CB	#144	1	0	0	n.d	n.d	0	1	1	96
H6CB	#147	2	0	0	n.d	2	0	2	1	57
H6CB	#139,149	0	4	3	3	n.d	0	4	3	89
H6CB	#140	2	0	0	n.d	2	0	2	1	12
H6CB	#143	2	2	2	n.d	2	2	2	2	21
H6CB	#133,134	1	1	1	n.d	1	1	1	1	37
H6CB	#131,165	2	4	5	n.d	5	2	5	4	117
H6CB	#142,146,161	2	2	2	3	15	2	15	5	55
H6CB	#153,168	2	8	6	13	7	2	13	7	47
H6CB	#132	2	3	3	6	5	2	6	4	35
H6CB	#141	2	2	2	4	3	2	4	2	45
H6CB	#137	2	3	3	2	1	1	3	2	49
H6CB	#130	3	5	5	2	7	2	7	4	94
H6CB	#163,164	2	3	3	5	16	2	16	6	73
H6CB	#138	5	11	8	n.d	0	0	11	6	49
H6CB	#158,160	4	2	3	6	2	2	6	3	80
H6CB	#129	7	13	14	2	1	1	14	7	64
H6CB	#166	1	1	1	0	2	0	2	1	13
H6CB	#159	1	1	1	1	1	1	1	1	68
H6CB	#162	2	7	10	2	5	2	10	5	31
H6CB	#128	5	3	3	3	n.d	3	5	4	31
H7CB	#188	1	1	0	3	1	0	3	1	109
H7CB	#189	20	7	9	9	11	7	20	11	47
H7CB	#184	0	2	4	29	26	0	29	12	115
H7CB	#179	1	2	2	1	3	1	3	2	56
H7CB	#176	1	2	2	4	2	1	4	2	52
H7CB	#186	0	1	0	4	1	0	4	1	121
H7CB	#178	1	1	1	1	2	1	2	1	51
H7CB	#175	1	3	2	2	3	1	3	2	32
H7CB	#182,187	1	2	1	4	7	1	7	3	83
H7CB	#183	1	2	2	1	5	1	5	2	76
H7CB	#185	0	1	0	2	1	0	2	1	73
H7CB	#174	4	3	4	2	3	2	4	3	26
H7CB	#181	2	2	1	2	n.d	n.d	2	2	28
H7CB	#177	1	2	2	2	1	1	2	2	27
H7CB	#171	7	10	10	4	2	2	10	7	58
H7CB	#173	4	7	5	2	4	2	7	4	42
H7CB	#172,192	6	8	7	4	3	3	8	6	37
H7CB	#180,193	8	10	8	10	6	6	10	8	18
H7CB	#191	4	4	3	6	3	3	6	4	32
H7CB	#170,190	38	30	35	9	17	9	38	26	48
O8CB	#202	1	7	2	4	n.d	n.d	7	4	80
O8CB	#205	18	7	8	17	n.d	n.d	18	13	50
O8CB	#200	1	6	4	7	n.d	n.d	7	5	52
O8CB	#204	1	2	1	6	n.d	n.d	6	3	79
O8CB	#197	1	2	3	13	n.d	n.d	13	5	103
O8CB	#199	3	3	5	5	n.d	n.d	5	4	26
O8CB	#198	3	4	3	8	n.d	n.d	8	4	46
O8CB	#201	3	6	4	8	n.d	n.d	8	5	35
O8CB	#196,203	17	16	17	10	n.d	n.d	17	15	22
O8CB	#195	21	15	18	4	n.d	n.d	21	15	51
O8CB	#194	30	32	34	19	n.d	n.d	34	29	23
N9CB	#206	76	50	54	48	56	48	76	57	20
N9CB	#207	16	28	27	40	41	16	41	30	33

N9CB	#208	8	22	19	12	3	3	22	13	61
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Table S8(a). Percent reduction efficiencies of PCB isomers (Gas phase) in differently milled samples.

Time, h	Isomers	Initial value	Percent reduction efficiency after milling in gas phase			
		(ng/g) 0 h	1 h	2 h	4 h	8 h
M1CB	#1	15.6	58.7	5.0	0.8	0.0
M1CB	#2	72.3	22.5	7.5	0.9	0.2
M1CB	#3	57.3	39.2	-128.6	0.9	0.0
Mono-CB		145.2	33.0	-41.4	0.9	0.1
D2CB	#4	5.0	9.1	37.2	0.7	0.2
D2CB	#10	5.5	9.1	37.2	0.7	0.2
D2CB	#7 #9	4.7	-10.0	-30.8	0.8	0.4
D2CB	#6	20.7	-18.2	-37.2	1.0	0.1
D2CB	#5 #8	59.4	38.3	-44.3	0.9	0.3
D2CB	#14	1.2	16.6	-714.4	1.0	0.2
D2CB	#11	148.3	59.8	-89.0	0.9	0.1
D2CB	#13	61.9	23.1	-47.1	1.0	0.4
D2CB	#12	n.d.	n.d.	n.d.	n.d.	n.d.
D2CB	#15	111.5	72.2	-116.4	0.9	0.3
Di-CB		418.3	48.6	-66.0	0.9	0.2
T3CB	#19	7.2	5.1	16.9	0.8	0.5
T3CB	#30	n.d.	n.d.	n.d.	n.d.	n.d.
T3CB	#18	44.6	5.8	-6.3	0.8	0.6
T3CB	#17	23.7	6.3	8.5	0.8	0.5
T3CB	#24 #27	4.6	-9.3	22.0	0.8	0.5
T3CB	#32	35.3	-12.3	17.6	0.8	0.5
T3CB	#34	2.2	40.9	n.d.	n.d.	n.d.
T3CB	#23 #29	5.4	61.9	50.4	0.8	n.d.
T3CB	#26	23.3	45.4	20.5	0.8	0.5
T3CB	#25	6.3	-14.2	31.7	0.8	0.6
T3CB	#28 #31	156.9	29.7	-21.5	0.8	0.5
T3CB	#21, 20,33	55.0	95.7	-1360.8	0.8	0.5
T3CB	#22	24.4	-13.7	90.8	-0.6	0.5
T3CB	#36	29.1	97.7	-2708.9	n.d.	n.d.
T3CB	#39	0.9	-28.9	24.5	n.d.	n.d.
T3CB	#38	16.6	13.9	25.9	n.d.	n.d.
T3CB	#35	11.5	49.5	-2.1	0.9	0.3
T3CB	#37	43.5	77.1	-33.9	0.8	0.5
Tri-CB		490.4	36.6	-10.4	0.8	0.5
T4CB	#54	n.d.	*--	n.d.	n.d.	n.d.
T4CB	#50	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#53	2.5	20.9	12.9	0.7	0.6
T4CB	#51	73.5	83.7	-350.7	1.0	0.3
T4CB	#45	2.9	20.5	28.6	0.7	0.4
T4CB	#46,69,73	1.1	-747.6	99.2	0.9	-9.6
T4CB	#52	11.7	33.5	9.2	0.7	0.5
T4CB	#43	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#49	25.7	-36.9	n.d.	n.d.	0.5
T4CB	#47,48,75,65	93.6	52.8	-98.2	1.0	0.4
T4CB	#62	n.d.	--	n.d.	n.d.	n.d.
T4CB	#44	15.4	21.4	75.5	0.1	0.5
T4CB	#59	n.d.	--	n.d.	n.d.	n.d.

T4CB	#42	8.8	-37.2	42.0	0.8	0.4
T4CB	#41,71,72	5.9	53.0	-100.6	0.8	0.5
T4CB	#64,68	288.9	53.3	-88.3	1.0	0.4
T4CB	#40	4.4	59.0	-63.9	0.9	0.1
T4CB	#57	0.5	-628.1	86.8	0.9	0.4
T4CB	#67	1.3	-18.3	22.0	0.9	0.3
T4CB	#58	0.1	n.d.	n.d.	n.d.	n.d.
T4CB	#63	0.8	-410.3	82.6	0.8	0.2
T4CB	#61	12.3	39.2	-63.4	0.8	0.4
T4CB	#74	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#70,76	17.0	21.9	1.4	0.8	0.4
T4CB	#66,80	16.8	71.7	-173.1	0.8	0.4
T4CB	#55	1.6	-51.9	56.4	0.9	0.5
T4CB	#56	8.4	37.8	-18.2	0.7	0.6
T4CB	#78	2.9	-147.5	83.2	1.0	0.4
T4CB	#81	1.4	-718.4	90.8	1.0	0.4
T4CB	#77	6.2	45.2	-60.4	0.9	0.4
T4CB	#60	4.1	53.1	-43.1	1.0	-8.4
T4CB	#79	1.0	-115.1	53.5	0.9	0.4
Tetra-CB		608.6	28.5	-11.3	0.9	0.4
P5CB	#104	3.0	93.4	-153.1	1.0	-8.6
P5CB	#123	2.3	68.9	-255.8	1.0	0.6
P5CB	#118	20.0	88.5	-488.2	0.9	0.3
P5CB	#114	0.1	-187.2	-0.4	1.0	0.7
P5CB	#105	8.9	76.6	-34.9	1.0	0.3
P5CB	#126	15.9	77.8	-23.2	1.0	0.6
P5CB	#96,103	1.3	78.9	-273.3	1.0	-1.5
P5CB	#100	2.2	95.5	-714.9	0.9	-0.3
P5CB	#94	1.2	0.0	-93.7	1.0	-1.7
P5CB	#98,102,121	0.2	-76.4	-318.0	1.0	0.0
P5CB	#93,95	1.2	33.9	8.3	0.7	0.3
P5CB	#88	0.4	76.9	-627.9	0.9	0.5
P5CB	#91	0.8	-686.7	-39.8	1.0	0.3
P5CB	#92	1.1	85.2	-262.8	1.0	-0.4
P5CB	#84,89,90	2.2	72.4	-26.1	0.9	0.3
P5CB	#101,113	1.5	-116.0	-100.4	1.0	0.2
P5CB	#99	0.5	-806.5	-62.3	1.0	0.2
P5CB	#112,119	2.8	93.2	-417.4	1.0	0.0
P5CB	#83	3.4	71.3	-112.2	0.9	0.3
P5CB	#109	1.5	71.2	-282.4	1.0	0.6
P5CB	#87,111,115,116, 117,125	2.4	84.7	-113.5	1.0	-0.5
P5CB	#97	4.7	68.9	-127.2	1.0	0.3
P5CB	#120	1.8	62.1	-213.8	1.0	-0.2
P5CB	#85	3.4	60.4	-115.7	1.0	0.3
P5CB	#110	4.0	74.9	-210.7	0.9	0.3
P5CB	#82	0.6	-157.4	-154.7	1.0	0.6
P5CB	#124	1.2	89.2	-899.3	1.0	-0.1
P5CB	#108	3.4	71.3	-112.2	0.9	0.3
P5CB	#107	1.5	50.4	23.0	1.0	-0.9
P5CB	#106	20.0	88.5	-488.2	0.9	0.3
P5CB	#122	9.3	95.2	-0.6	-0.5	1.0
P5CB	#127	8.8	76.6	-34.9	1.0	0.3
Penta-CB		131.7	68.0	-131.6	95.4	36.6

H6CB	#155	4.5	82.9	57.0	0.3	n.d.
H6CB	#167	4.8	79.5	34.1	1.0	0.1
H6CB	#156	11.4	79.1	26.4	1.0	0.6
H6CB	#157	5.8	74.6	37.8	1.0	0.5
H6CB	#169	6.9	78.6	30.0	1.0	-0.1
H6CB	#150	1.9	98.0	63.8	0.4	n.d.
H6CB	#152	1.1	83.2	-338.4	1.0	n.d.
H6CB	#148	1.3	96.1	42.2	0.9	n.d.
H6CB	#145	1.0	91.5	-310.1	1.0	n.d.
H6CB	#154	0.1	-31.0	62.6	n.d.	n.d.
H6CB	#136	2.1	92.9	71.5	0.8	n.d.
H6CB	#151	1.3	84.9	72.6	0.9	-2.0
H6CB	#135	0.5	60.1	50.5	1.0	n.d.
H6CB	#144	2.5	92.5	86.2	0.9	n.d.
H6CB	#147	1.5	95.3	39.9	0.9	n.d.
H6CB	#139,149	0.6	-107.9	36.7	1.0	0.6
H6CB	#140	1.8	97.5	-336.5	1.0	n.d.
H6CB	#143	1.4	62.7	-0.5	1.0	-0.8
H6CB	#133,134	0.7	54.4	35.7	0.9	0.4
H6CB	#131,165	3.0	55.6	2.8	1.0	0.7
H6CB	#142,146,161	1.2	43.3	26.6	1.0	-0.3
H6CB	#153,168	3.0	13.3	53.1	0.9	0.3
H6CB	#132	2.0	55.0	-4.8	0.9	0.4
H6CB	#141	1.8	57.8	48.1	0.9	0.0
H6CB	#137	2.2	55.7	27.0	1.0	0.1
H6CB	#130	3.4	60.7	-3.2	1.0	0.6
H6CB	#163,164	2.5	62.3	22.8	1.0	0.0
H6CB	#138	5.9	35.5	50.0	n.d.	n.d.
H6CB	#158,160	4.1	93.7	-255.9	0.9	1.0
H6CB	#129	8.3	52.6	3.9	1.0	0.3
H6CB	#166	0.6	73.2	18.8	1.0	-3.3
H6CB	#159	1.0	63.7	34.4	1.0	0.3
H6CB	#162	1.4	-129.5	25.9	1.0	0.5
H6CB	#128	4.7	79.5	34.1	1.0	0.1
Hexa-CB		96.2	66.0	23.3	1.0	0.5
H7CB	#188	0.5	66.5	71.0	0.6	0.9
H7CB	#189	15.1	91.0	4.6	1.0	0.3
H7CB	#184	0.2	-40.6	-137.6	0.7	0.4
H7CB	#179	0.7	29.6	51.6	0.9	0.1
H7CB	#176	0.8	59.3	10.5	1.0	-2.6
H7CB	#186	0.3	20.2	82.7	0.8	0.6
H7CB	#178	0.6	59.0	41.1	1.0	-5.8
H7CB	#175	1.2	59.9	36.4	0.9	0.3
H7CB	#182,187	0.7	50.4	34.4	0.9	0.0
H7CB	#183	1.2	71.3	13.3	n.d.	n.d.
H7CB	#185	0.5	67.6	55.5	0.7	0.8
H7CB	#174	4.5	84.9	11.3	1.0	0.1
H7CB	#181	1.9	75.7	64.3	0.8	n.d.
H7CB	#177	1.2	85.0	-107.0	1.0	0.4
H7CB	#171	8.8	85.4	-14.4	1.0	0.7
H7CB	#173	4.4	69.5	44.9	1.0	-0.1
H7CB	#172,192	6.1	76.4	39.6	1.0	0.4
H7CB	#180,193	7.4	77.2	43.4	1.0	0.4
H7CB	#191	4.4	81.3	51.3	0.9	0.8
H7CB	#170,190	38.7	82.0	24.8	1.0	-0.6

Hepta-CB		99.0	80.6	25.7	1.0	0.3
O8CB	#202	0.8	14.4	75.4	1.0	n.d.
O8CB	#205	11.2	91.8	47.8	1.0	n.d.
O8CB	#200	1.3	51.7	55.3	1.0	n.d.
O8CB	#204	0.4	33.5	80.1	0.9	n.d.
O8CB	#197	1.5	80.1	30.5	0.9	n.d.
O8CB	#199	3.0	86.8	14.2	1.0	n.d.
O8CB	#198	2.5	80.9	55.5	0.9	n.d.
O8CB	#201	2.7	75.2	53.6	1.0	n.d.
O8CB	#196,203	15.4	85.4	50.7	1.0	n.d.
O8CB	#195	15.4	87.1	36.4	1.0	n.d.
O8CB	#194	23.6	86.7	19.9	1.0	n.d.
Octa-CB		77.6	85.0	40.6	1.0	n.d.
N9CB	#208	10.3	81.5	52.6	1.0	n.d.
N9CB	#206	71.3	95.4	30.8	1.0	-0.8
N9CB	#207	21.8	89.6	50.4	1.0	-0.5
Nona-CB		103.3	92.8	42.3	1.0	-0.7
D10CB	#209	182.2	98.7	9.9	1.0	n.d.

*Highlighted isomers are dl-PCB

Table S8(b). Percent reduction efficiencies of PCB isomers (Solid phase) in differently milled samples.

Time, h	Isomers	Initial value	Percent Reduction Efficiency after milling			
		(ng/g)	in solid phase			
		0 h	1 h	2 h	4 h	8 h
M1CB	#1	16.0	33.3	-26.7	80.9	-22.2
M1CB	#2	134.0	33.3	1.5	87.7	30.5
M1CB	#3	74.2	35.2	-65.7	90.3	30.4
Mono-CB		224.2	33.9	-22.3	88.3	24.0
D2CB	#4	3.7	-22.1	-53.4	93.9	n.d.
D2CB	#10	5.8	13.4	-53.4	93.9	n.d.
D2CB	#7 #9	6.9	26.1	-53.8	92.1	58.7
D2CB	#6	31.9	5.8	-70.8	97.8	n.d.
D2CB	#5 #8	65.0	28.1	-54.9	96.9	-53.3
D2CB	#14	1.9	1.4	-4.2	78.8	-490.7
D2CB	#11	178.3	58.0	-32.8	86.4	33.5
D2CB	#13	56.8	-4.2	-50.8	98.3	-218.7
D2CB	#12	n.d.	n.d.	n.d.	n.d.	n.d.
D2CB	#15	115.7	68.0	-36.1	94.3	n.d.
Di-CB		466.1	43.2	-46.5	94.0	13.8
T3CB	#19	9.3	95.2	-2060.2	94.5	25.1
T3CB	#30	n.d.	n.d.	n.d.	n.d.	n.d.
T3CB	#18	64.2	92.6	-1527.4	94.8	40.7
T3CB	#17	32.5	91.3	-1183.7	94.7	-35.7
T3CB	#24 #27	6.5	92.1	-1304.7	93.7	-69.4
T3CB	#32	49.1	90.2	-1061.4	94.1	-28.4
T3CB	#34	1.5	18.0	-17.8	n.d.	n.d.
T3CB	#23	2.7	86.8	-729.3	95.7	n.d.
T3CB	#26	15.0	-44.7	22.5	95.1	11.7
T3CB	#25	7.8	-25.9	2.7	94.2	1.5
T3CB	#28 #31	209.3	88.3	-505.8	90.6	34.0
T3CB	#21, 20,33	48.4	85.4	61.0	-12.0	-27.5
T3CB	#22	3.1	-32.5	-679.6	93.4	9.8
T3CB	#36	29.0	99.4	-270.3	n.d.	n.d.

T3CB	#39	1.0	68.3	-347.9	n.d.	n.d.
T3CB	#38	12.5	74.1	-296.5	n.d.	n.d.
T3CB	#35	6.6	51.9	-94.8	91.1	16.2
T3CB	#37	15.6	20.6	-28.6	93.2	-28.1
Tri-CB		514.1	80.3	-331.4	92.5	12.2
T4CB	#54	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#50	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#53	3.9	92.5	-792.9	92.1	-149.3
T4CB	#51	98.4	99.6	-16522.7	99.6	-131.2
T4CB	#45	4.2	91.5	-696.0	92.8	-55.5
T4CB	#46,69,73	1.1	-68.5	14.4	95.0	-14.7
T4CB	#52	15.3	91.2	-782.7	90.6	-44.7
T4CB	#43	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#49	34.7	94.0	-475.0	93.1	-52.0
T4CB	#47,48,75,65	125.2	99.8	-22706.9	97.5	-49.4
T4CB	#62	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#44	21.8	29.8	85.9	16.0	-41.1
T4CB	#59	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#42	11.3	87.3	-465.8	91.4	-138.1
T4CB	#71,72	10.5	85.8	1.4	52.0	-78.2
T4CB	#64,68	355.7	98.9	-6150.1	99.2	91.4
T4CB	#40	2.0	75.6	-605.0	93.6	13.0
T4CB	#57	0.6	-27.9	84.3	-0.5	n.d.
T4CB	#67	1.6	79.3	-208.1	92.5	n.d.
T4CB	#58	0.3	n.d.	n.d.	n.d.	n.d.
T4CB	#63	1.2	-333.9	91.3	73.0	n.d.
T4CB	#61	21.0	72.5	-150.4	90.4	45.1
T4CB	#74	n.d.	n.d.	n.d.	n.d.	n.d.
T4CB	#70,76	22.8	78.2	-226.1	75.2	73.9
T4CB	#66,80	24.4	n.d.	n.d.	99.7	36.9
T4CB	#55	1.7	46.3	-36.2	91.8	n.d.
T4CB	#56	9.0	29.2	-1.3	85.8	-16.7
T4CB	#78	1.9	-48.6	51.6	96.3	-365.9
T4CB	#81	1.6	-486.0	87.2	98.0	-1296.6
T4CB	#77	7.4	-29.4	38.9	92.4	71.2
T4CB	#60	4.5	11.7	0.0	88.9	28.8
T4CB	#79	1.4	48.5	-54.7	96.5	n.d.
Tetra-CB		783.5	77.8	-190.6	96.5	5.8
P5CB	#104	2.4	87.1	45.9	75.7	-375.9
P5CB	#123	0.9	11.8	-3.0	97.0	n.d.
P5CB	#118	9.0	70.9	-244.7	95.5	n.d.
P5CB	#114	4.3	89.6	-11.9	98.5	-86.1
P5CB	#105	5.6	54.6	-222.5	98.4	-50.9
P5CB	#126	18.7	80.0	-34.7	98.3	4.1
P5CB	#96	1.3	86.1	2.2	82.2	n.d.
P5CB	#100	1.4	89.8	-2.5	77.7	n.d.
P5CB	#94	2.2	18.6	-17.4	98.8	n.d.
P5CB	#98,102,121	0.1	-571.2	-12.4	94.3	-1053.9
P5CB	#93,95	1.3	-0.7	-23.2	90.3	n.d.
P5CB	#88	1.5	88.9	-91.4	93.4	n.d.
P5CB	#91	1.8	-347.7	-26.7	99.6	-138.9
P5CB	#92	0.0	-580.8	-30.2	91.4	n.d.
P5CB	#84,89,90	0.5	-54.5	-32.1	94.7	-332.2

P5CB	#101,113	0.3	-1556.9	-23.5	96.8	19.8
P5CB	#99	0.1	-4851.6	-25.3	98.5	n.d.
P5CB	#112,119	0.6	61.2	-28.1	89.8	n.d.
P5CB	#83	1.0	-27.4	-18.3	96.4	n.d.
P5CB	#109	0.6	-43.6	35.1	97.2	n.d.
P5CB	#87,111,115,116, 117,125	2.7	77.1	-8.0	97.0	-450.1
P5CB	#97	1.3	-54.5	-34.3	96.8	n.d.
P5CB	#120	0.5	-87.4	-35.1	94.1	n.d.
P5CB	#85	0.7	-124.8	-36.3	96.9	-30.8
P5CB	#110	2.5	40.7	-53.0	92.0	3.9
P5CB	#82	0.6	-312.6	50.0	97.1	n.d.
P5CB	#124	0.5	-33.1	61.2	88.2	n.d.
P5CB	#108	1.0	-27.4	-18.3	96.4	n.d.
P5CB	#107	0.9	82.8	-575.0	96.4	n.d.
P5CB	#106	9.0	79.1	-380.5	95.5	n.d.
P5CB	#122	4.4	88.1	-27.8	98.1	7.2
P5CB	#127	5.6	54.6	-25.1	96.0	-50.9
		83.3	97.0	-55.3	96.8	33.0
H6CB	#155	0.4	-134.5	68.6	44.3	n.d.
H6CB	#167	4.3	75.8	21.2	98.3	n.d.
H6CB	#156	12.1	79.0	21.4	98.0	n.d.
H6CB	#157	6.1	78.2	20.3	98.1	n.d.
H6CB	#169	11.8	87.2	24.0	96.1	n.d.
H6CB	#150	0.9	93.9	8.5	n.d.	n.d.
H6CB	#152	1.1	98.4	26.8	n.d.	n.d.
H6CB	#148	0.5	89.0	-74.9	n.d.	n.d.
H6CB	#145	0.1	27.1	58.9	n.d.	n.d.
H6CB	#154	1.5	89.4	97.7	n.d.	n.d.
H6CB	#136	3.7	98.3	64.7	n.d.	n.d.
H6CB	#151	1.5	92.7	47.1	n.d.	n.d.
H6CB	#135	0.1	-125.9	25.6	n.d.	n.d.
H6CB	#144	0.1	43.5	24.3	n.d.	n.d.
H6CB	#147	1.7	94.7	39.2	n.d.	n.d.
H6CB	#139,149	0.2	-644.8	33.5	98.1	n.d.
H6CB	#140	1.8	99.3	-105.3	n.d.	n.d.
H6CB	#143	1.2	48.4	21.1	n.d.	n.d.
H6CB	#133,134	0.7	56.0	21.0	n.d.	n.d.
H6CB	#131,165	0.3	-470.5	16.7	n.d.	n.d.
H6CB	#142,146,161	1.6	56.1	9.4	96.3	n.d.
H6CB	#153,168	0.9	-203.6	39.4	95.7	n.d.
H6CB	#132	1.0	1.6	15.4	96.0	n.d.
H6CB	#141	0.9	26.1	27.6	94.4	n.d.
H6CB	#137	1.4	29.5	17.3	98.8	n.d.
H6CB	#130	1.8	6.6	21.4	99.0	n.d.
H6CB	#163,164	1.9	37.4	28.7	95.5	n.d.
H6CB	#138	3.4	-5.1	35.6	97.5	n.d.
H6CB	#158,160	2.9	59.2	39.4	98.0	n.d.
H6CB	#129	4.7	4.9	25.8	99.6	n.d.
H6CB	#166	0.8	70.1	27.6	99.0	n.d.
H6CB	#159	1.3	72.7	12.9	98.1	n.d.
H6CB	#162	2.1	20.0	-72.9	99.6	n.d.
H6CB	#128	4.2	75.8	21.2	98.3	n.d.
Hexa-CB		78.4	58.4	21.5	98.2	n.d.
H7CB	#188	0.7	94.4	-57.6	86.2	n.d.

H7CB	#189	22.2	95.0	-21.1	98.3	n.d.
H7CB	#184	0.3	-49.2	-37.1	83.7	n.d.
H7CB	#179	0.4	16.9	24.5	n.d.	n.d.
H7CB	#176	0.6	32.7	22.6	92.0	n.d.
H7CB	#186	0.2	75.3	36.2	48.7	n.d.
H7CB	#178	0.4	51.6	44.5	93.4	n.d.
H7CB	#175	0.8	46.5	10.4	98.9	n.d.
H7CB	#182,187	0.6	38.3	37.6	94.2	n.d.
H7CB	#183	0.8	46.6	28.6	98.8	n.d.
H7CB	#185	0.4	68.5	82.5	87.3	n.d.
H7CB	#174	2.8	85.0	-59.9	98.7	n.d.
H7CB	#181	1.6	84.2	41.6	n.d.	n.d.
H7CB	#177	1.2	57.7	34.8	97.6	n.d.
H7CB	#171	4.6	57.8	12.7	99.3	n.d.
H7CB	#173	3.1	68.7	10.2	99.7	n.d.
H7CB	#172,192	4.7	71.7	13.7	99.1	n.d.
H7CB	#180,193	7.1	76.8	17.2	97.1	n.d.
H7CB	#191	3.5	82.3	14.0	98.7	n.d.
H7CB	#170,190	33.0	89.6	-58.4	99.3	n.d.
Hepta-CB		89.0	83.1	-5.4	97.9	n.d.
O8CB	#202	0.4	-118.2	85.9	99.4	n.d.
O8CB	#205	20.0	97.4	-9.9	98.4	n.d.
O8CB	#200	1.1	45.3	47.0	98.6	n.d.
O8CB	#204	0.3	32.0	52.2	96.7	n.d.
O8CB	#197	1.0	78.5	-14.6	97.6	n.d.
O8CB	#199	2.7	92.0	-39.7	98.7	n.d.
O8CB	#198	2.8	85.1	48.2	99.4	n.d.
O8CB	#201	3.0	81.2	50.8	97.6	n.d.
O8CB	#196,203	13.7	90.9	9.8	99.4	n.d.
O8CB	#195	19.9	93.2	17.4	99.7	n.d.
O8CB	#194	26.5	85.4	49.4	99.3	n.d.
Octa-CB		91.6	88.9	37.3	99.1	n.d.
N9CB	#208	11.6	89.6	23.8	98.7	n.d.
N9CB	#206	144.6	97.3	26.3	99.3	n.d.
N9CB	#207	23.7	92.5	17.8	98.9	n.d.
Nona-CB		179.9	96.2	23.6	99.1	n.d.
Deca-CB #209		322.3	99.0	27.7	87.4	n.d.

**Highlighted isomers are dl-PCB*