Supporting Information for

Electron-donating arene-substituted pentacenedione derivatives: a study of structural, electronic, and electrochemical properties

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1. NMR Spectra of Compounds 3a and 5a-d

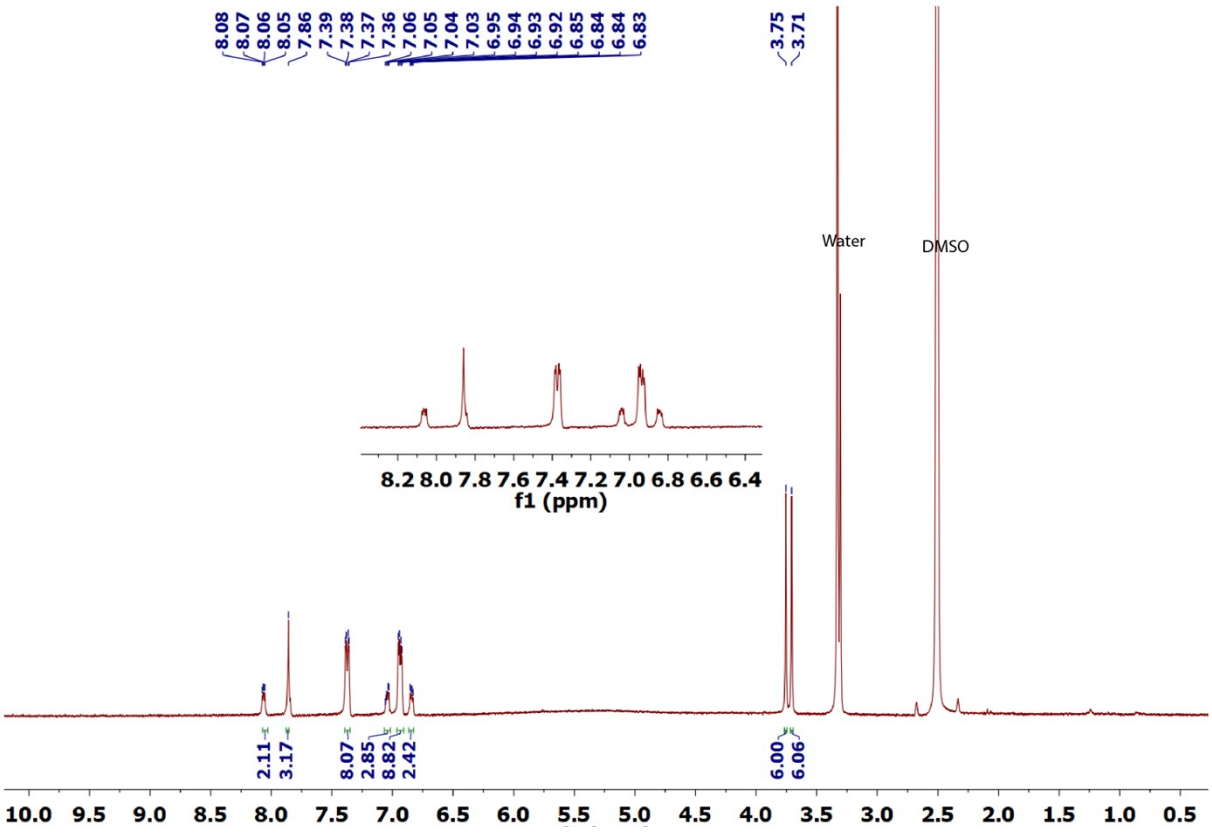


Fig. S-1 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3a**.

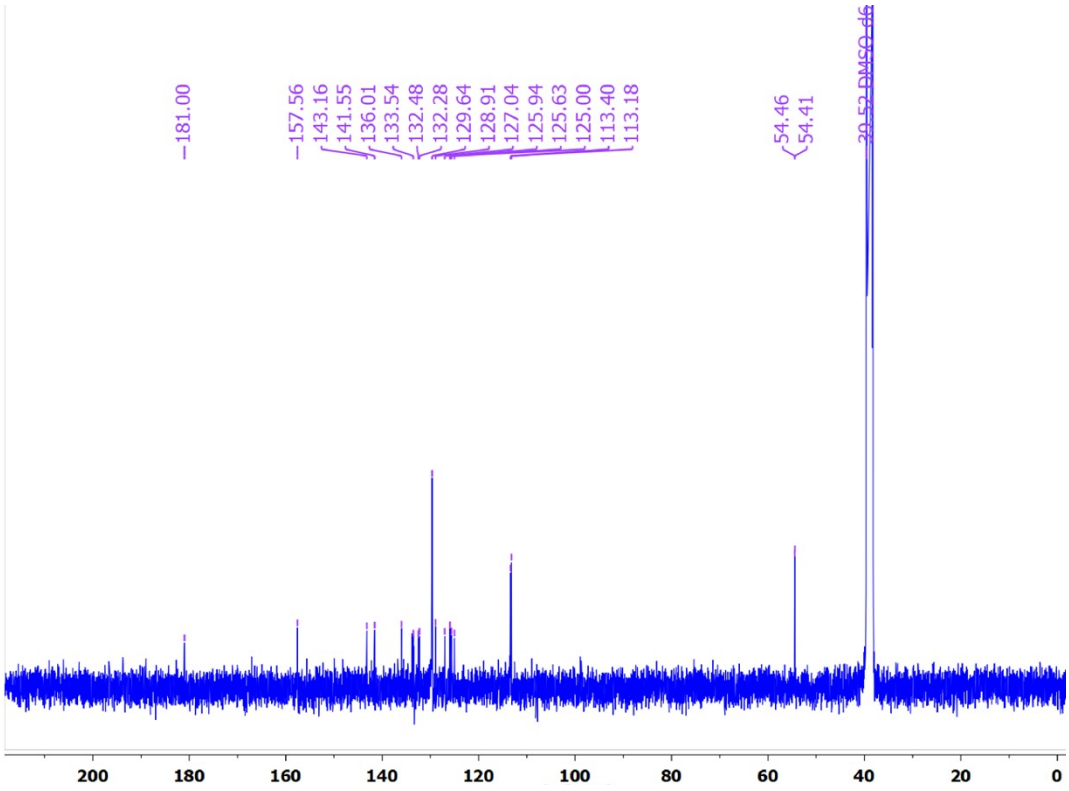


Fig. S-2 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **3a**.

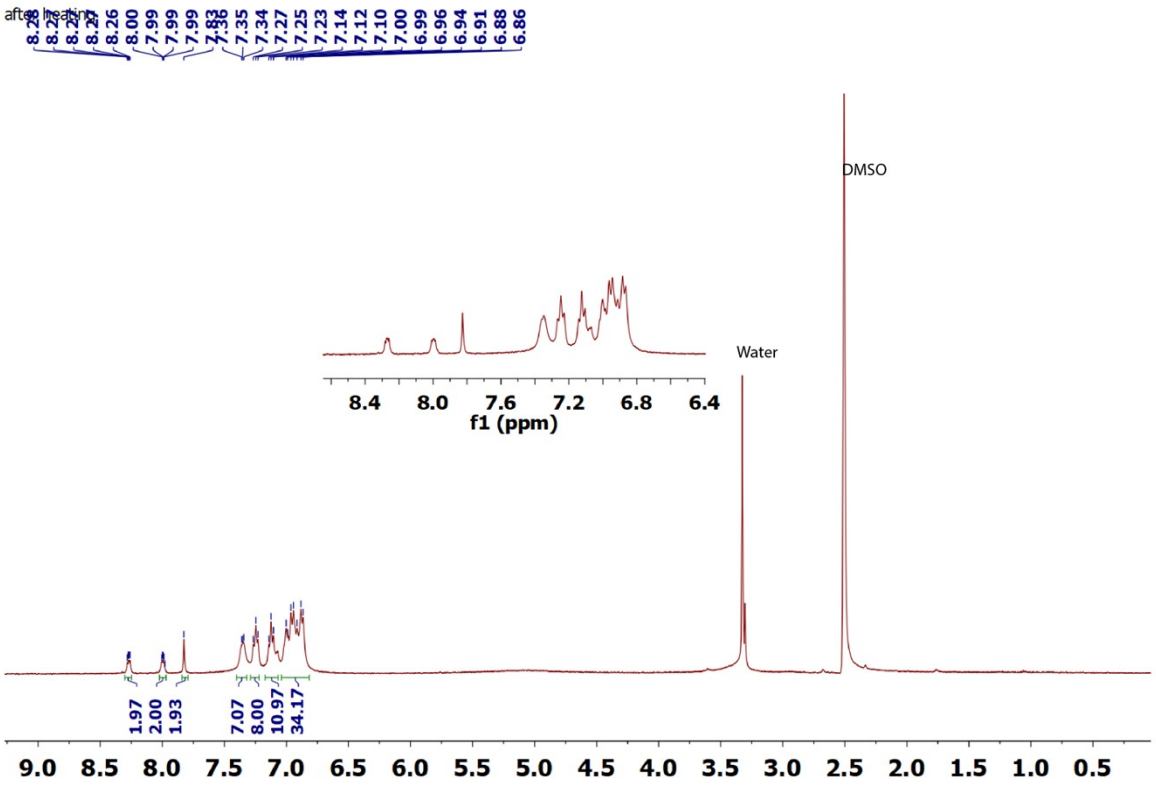


Fig. S-3 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5a**.

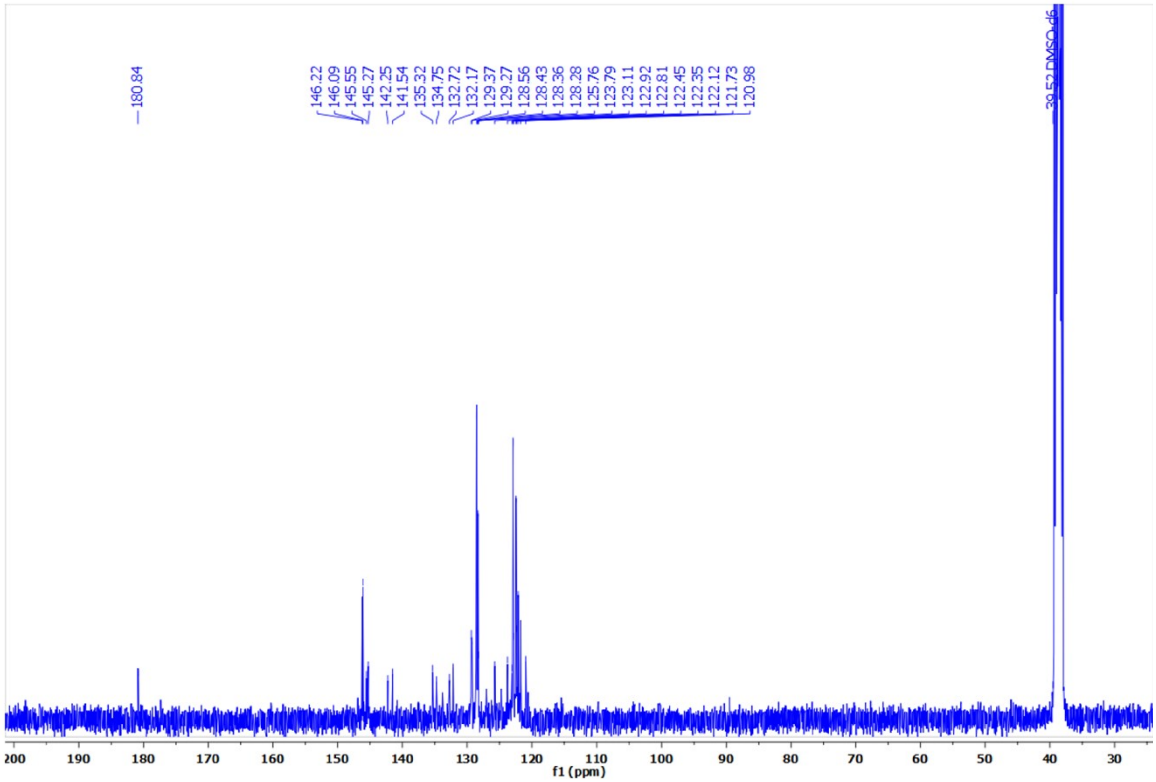


Fig. S-4 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5a**.

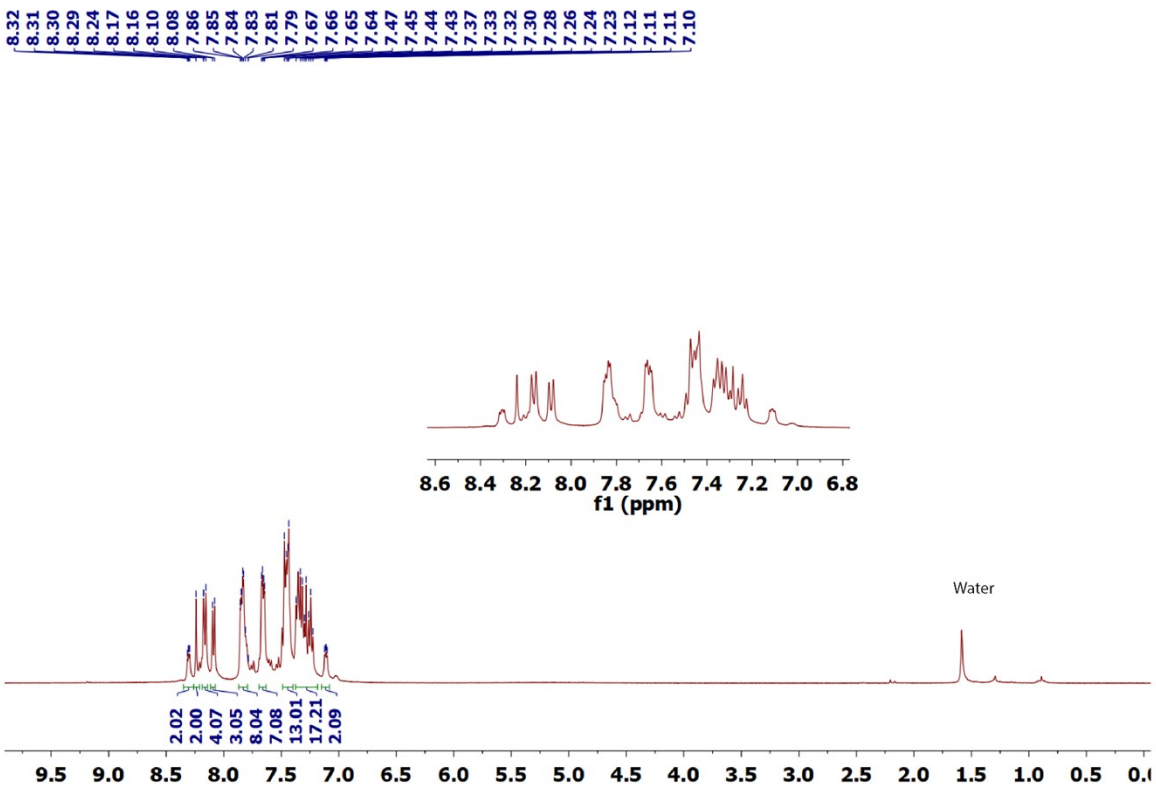


Fig. S-5 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5b**.

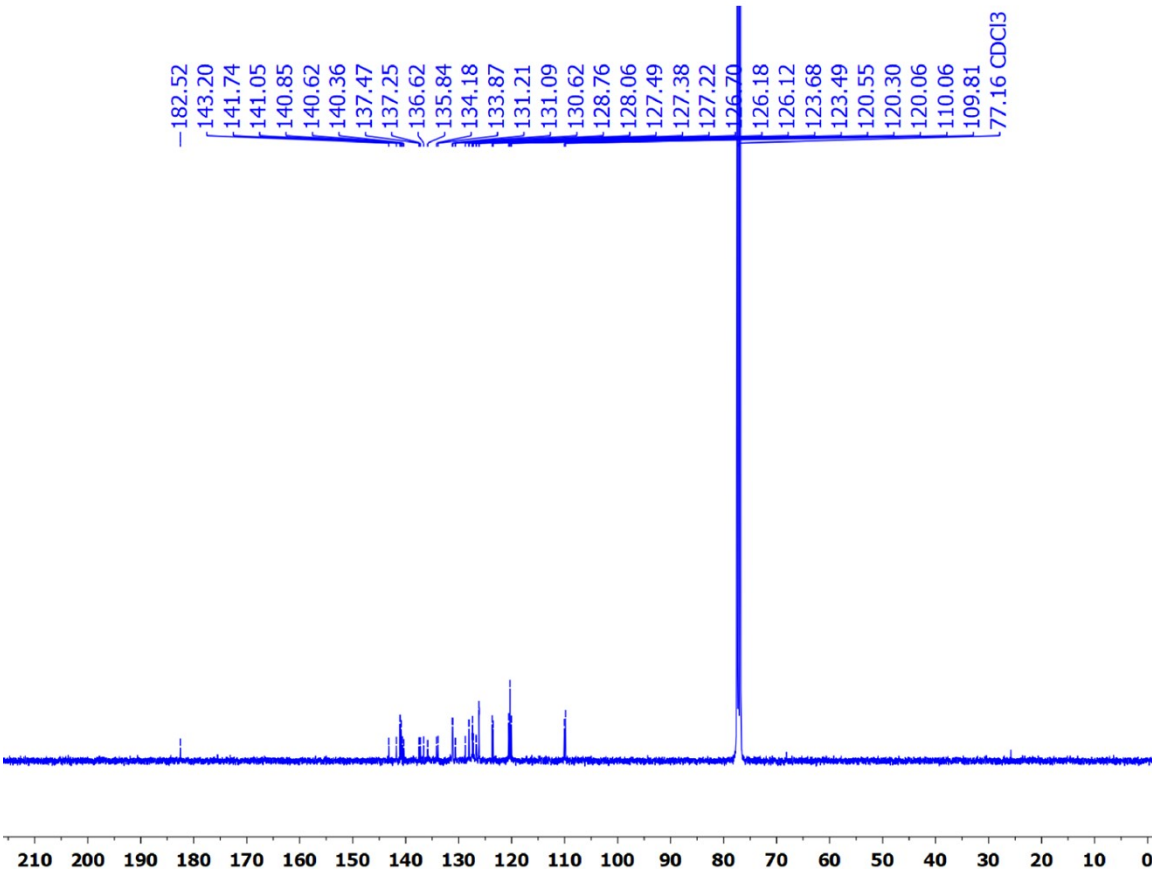


Fig. S-6 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5b**.

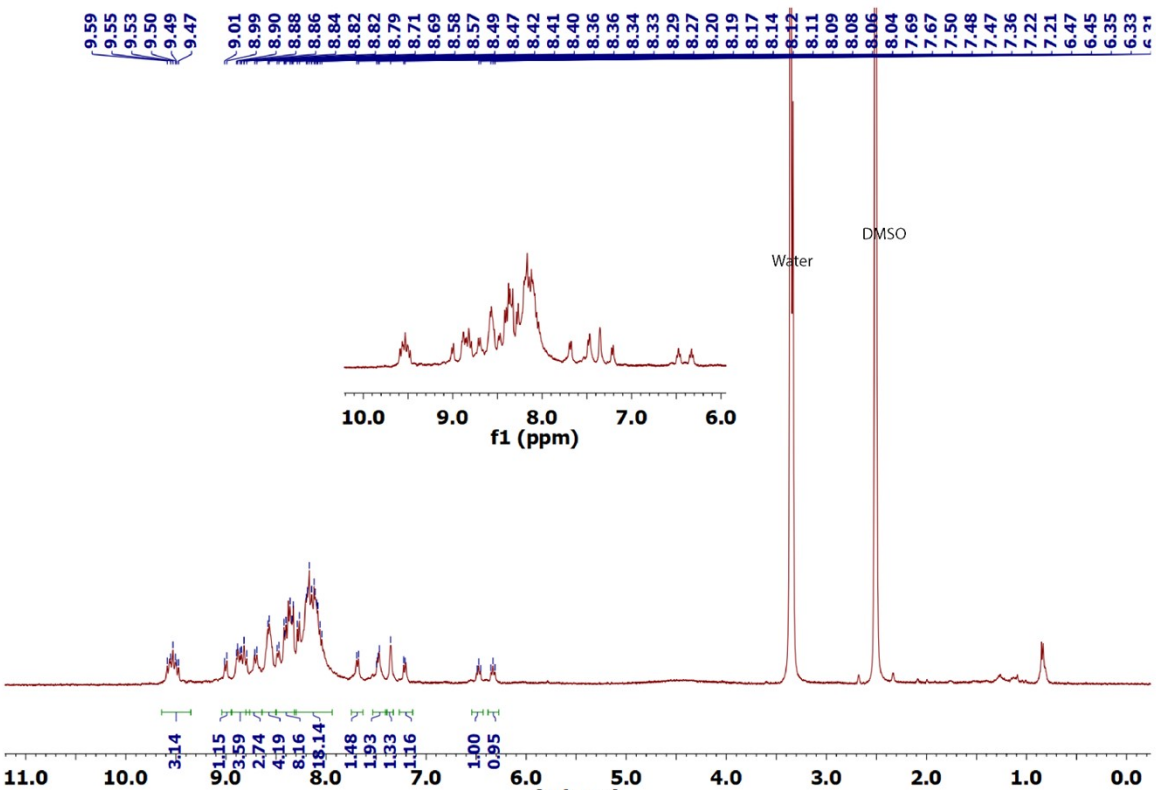


Fig. S-7 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5c**

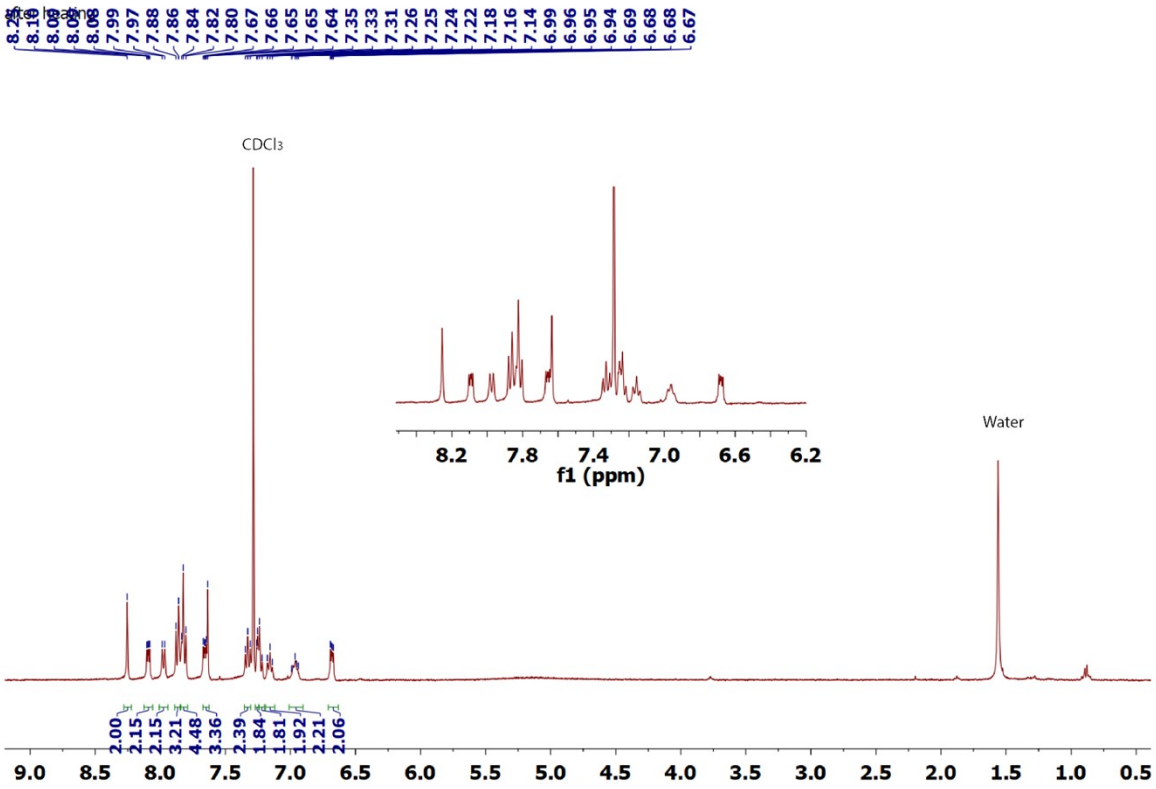


Fig. S-8 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5d**.

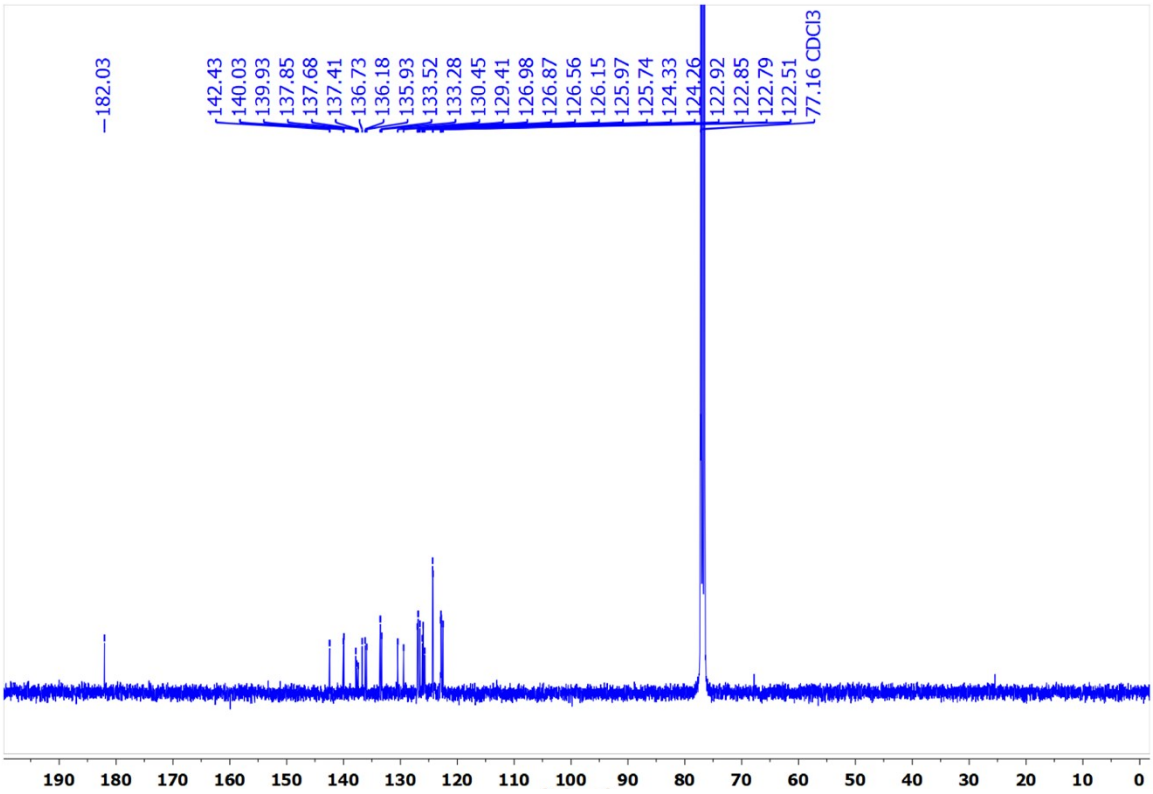
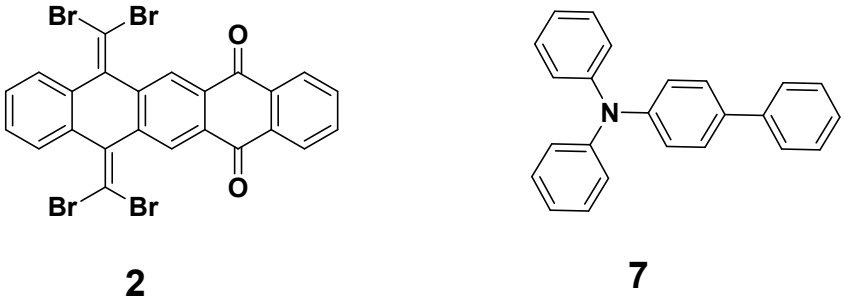


Fig. S-9 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5d**.

2. UV-Vis Titrations of Compounds **2** and TPA **7** with TFA

The UV-vis of a solution of **2** and TPA derivative **7** in $CHCl_3$ was measured. One equivalent of TFA was add each time to the solution and the UV-Vis data was collected.



2 **7**

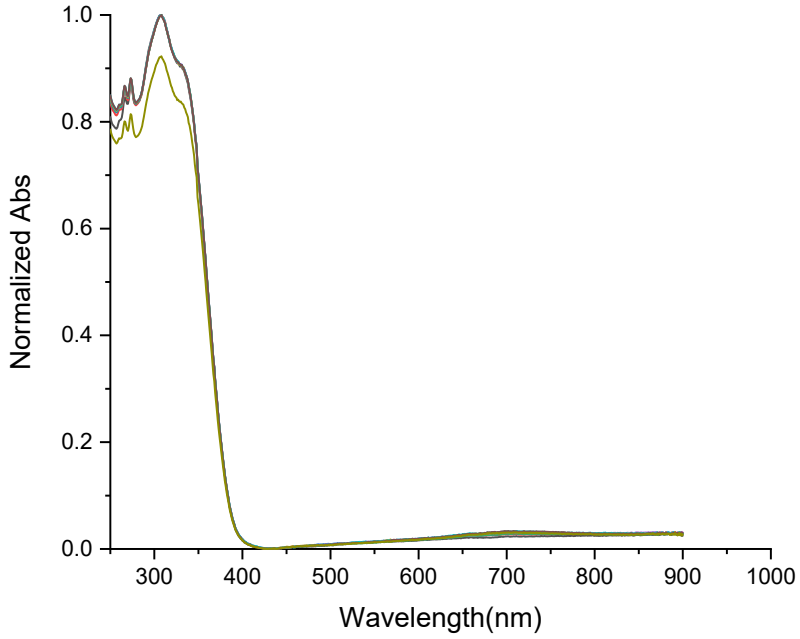
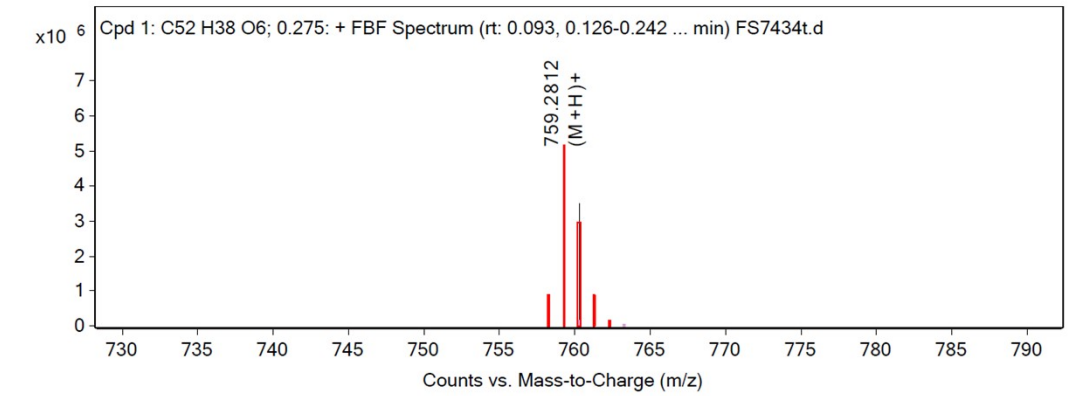


Fig. S-10 Normalized absorption spectra of **2** and **7** (46.50 μM in CHCl3) mixed with TFA (up to 8 mole equivalents).

High-Resolution Mass Spectra for Compounds 3a and 5a-c

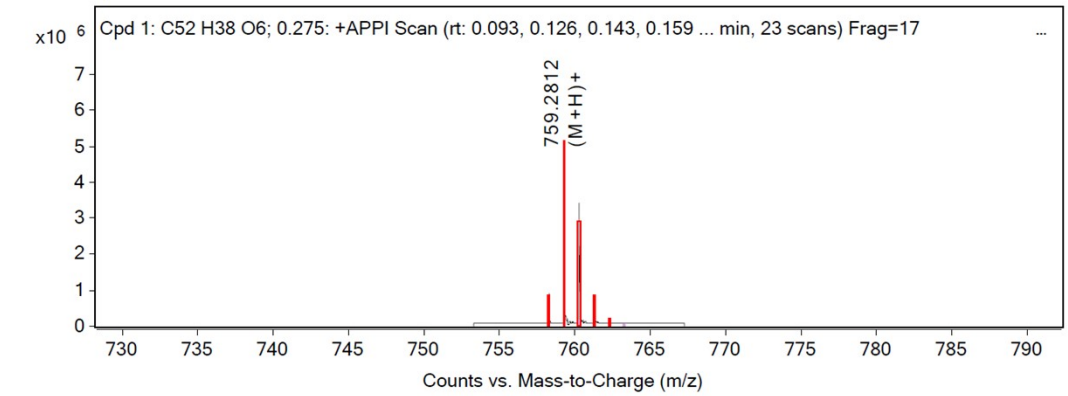
Target Compound Screening Report



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Ion/Isotope
758.2683	1	879758.06	M+
759.2812	1	5164614.5	(M+H)+
760.2833	1	3503861.25	(M+H)+
761.283	1	383746.66	(M+H)+
762.2936	1	71024.84	(M+H)+

MS Zoomed Spectrum



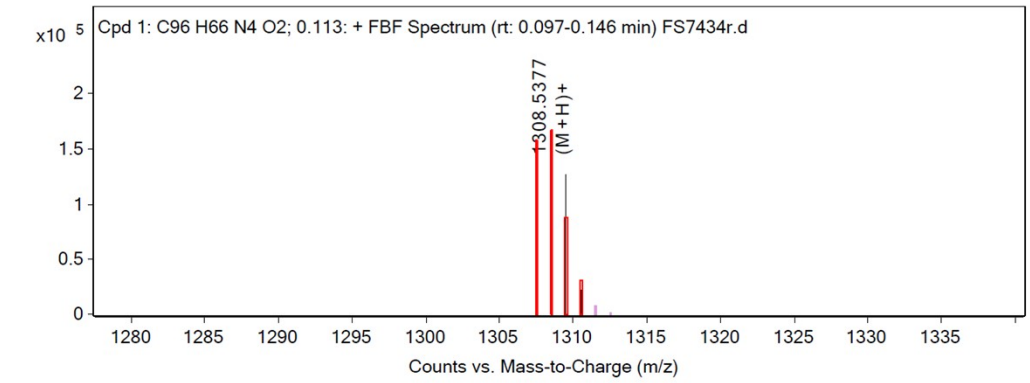
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
758.2683	1	879758.06	M+	-2.64
759.2799		5116371.58		
759.2812	1	5164614.5	(M+H)+	-9.31
760.2833	1	3503861.25	(M+H)+	-7.58
761.283	1	383746.66	(M+H)+	-3.04
762.2936	1	71024.84	(M+H)+	-12.9

--- End Of Report ---

Fig. S-11 High-resolution mass spectrum (LC-TOF, positive mode) of compound **3a.**

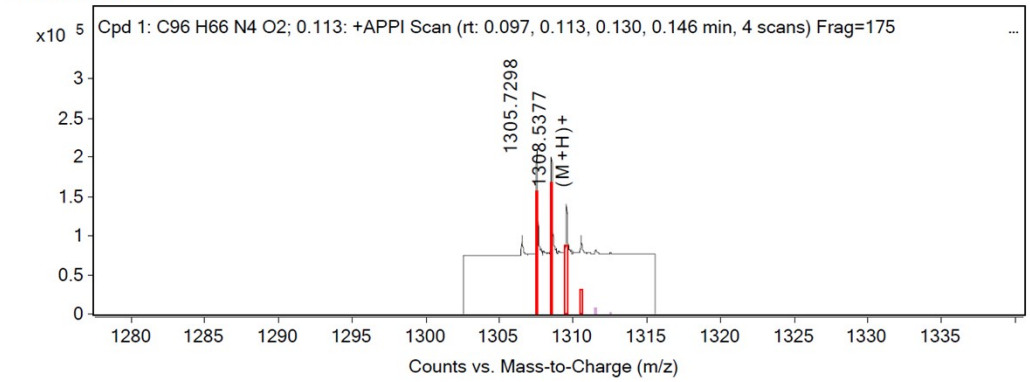
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
1307.5336	1	138185.13	(M+H)+
1308.5377	1	156451.55	(M+H)+
1309.5414	1	126036.31	(M+H)+
1310.5714	1	21983.62	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
1305.7298		209506.9		
1307.5336	1	138185.13	(M+H)+	-5.9
1308.5377	1	156451.55	(M+H)+	-6.55
1309.5414	1	126036.31	(M+H)+	-6.87
1310.5714	1	21983.62	(M+H)+	-27.27

--- End Of Report ---

Fig. S-12 High-resolution mass spectrum (LC-TOF, positive mode) of compound **5a.**

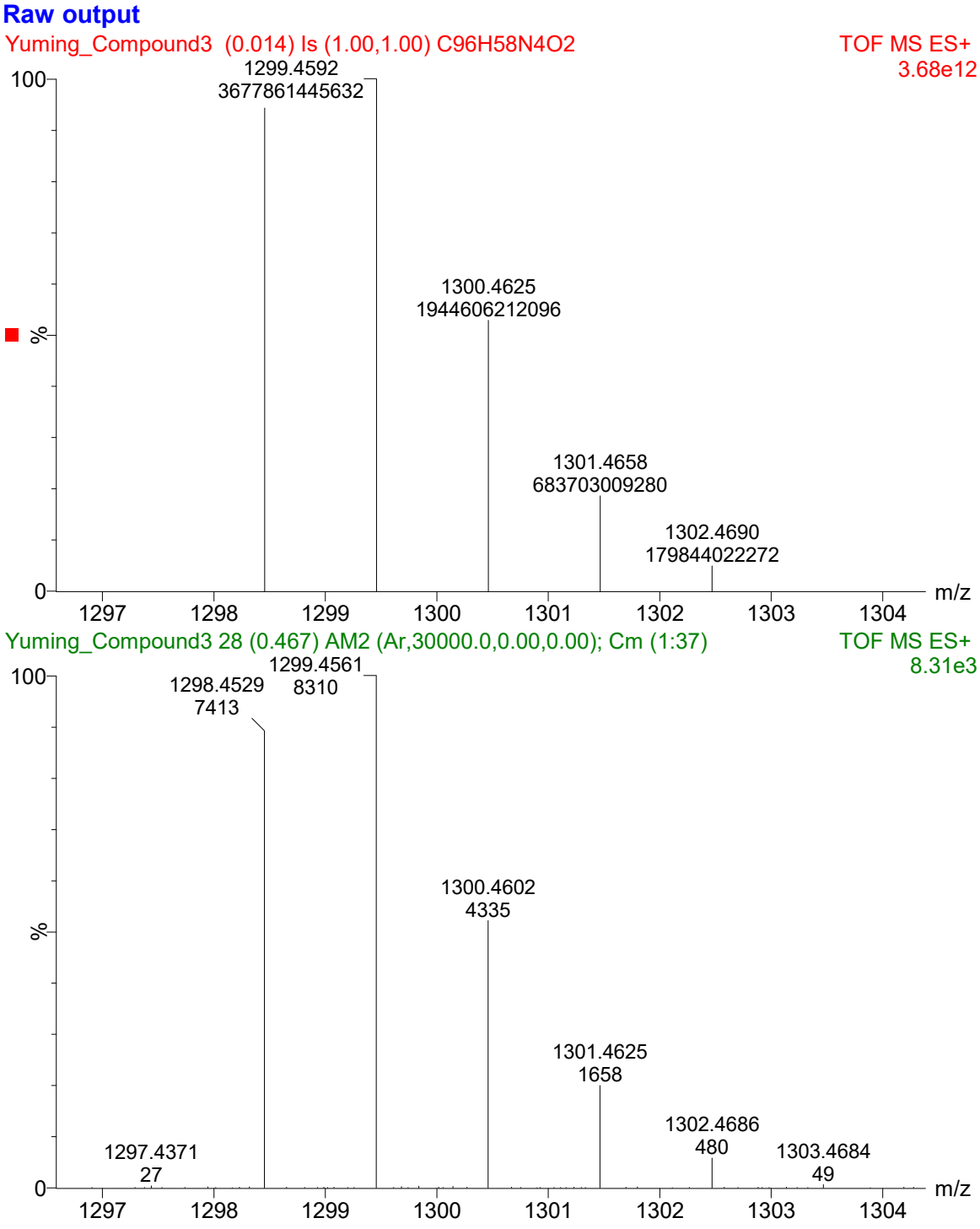
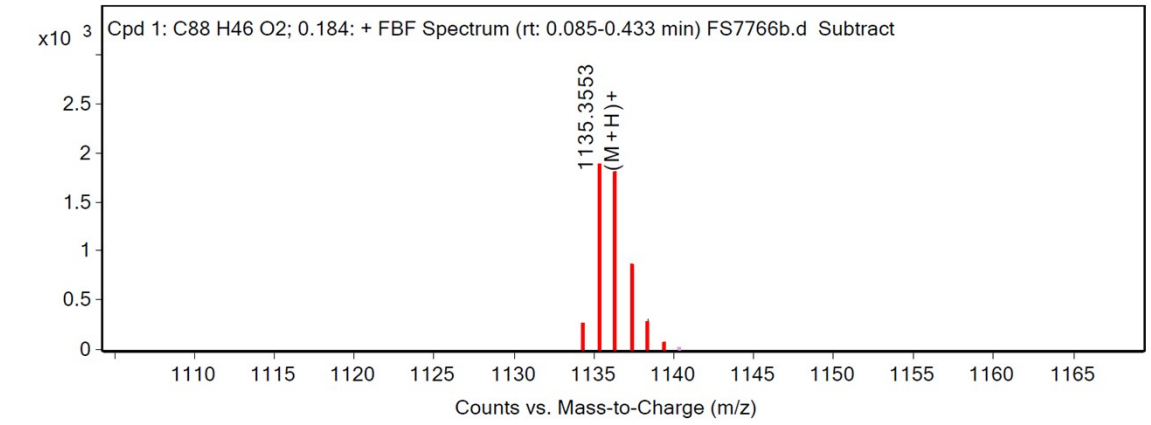


Fig. S-13 High-resolution mass spectrum (positive mode) of compound 5b was mesured using a cyclic IMS cyclic ion mobility mass spectrometer (Wilmslow, UK).

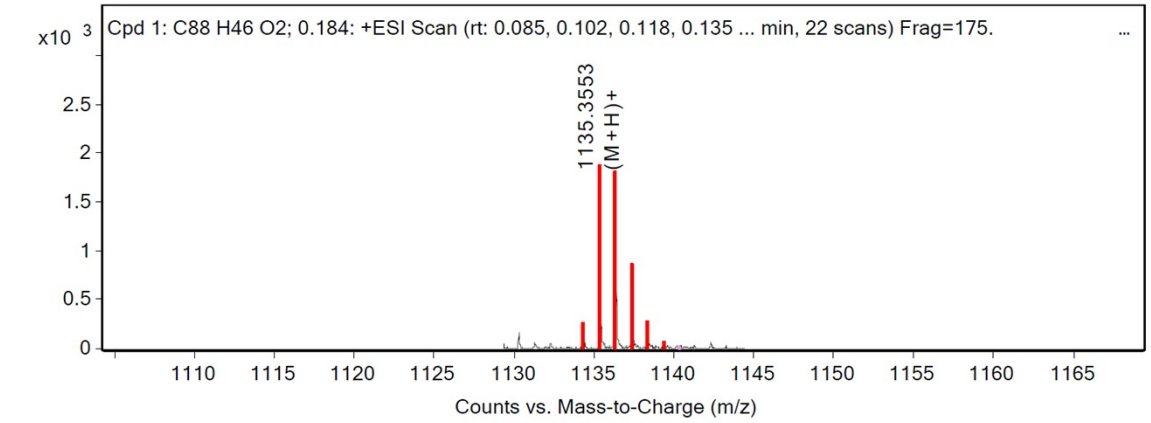
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
1134.3477	1	258.56	(M+H)+[-H]
1135.3553	1	1880.6	(M+H)+
1136.3585	1	1677.68	(M+H)+
1137.3597	1	823.66	(M+H)+
1138.3642	1	311.19	(M+H)+
1139.3618	1	28.66	(M+H)+

MS Zoomed Spectrum



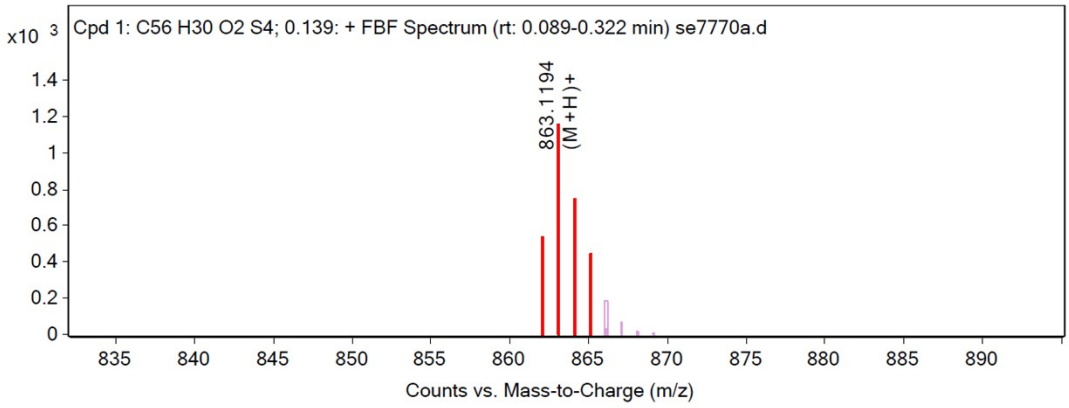
MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
1134.3477	1	258.56	(M+H)+[-H]	1.35
1135.3551		1879.88		
1135.3553	1	1880.6	(M+H)+	1.51
1136.3585	1	1677.68	(M+H)+	1.69
1137.3597	1	823.66	(M+H)+	3.61
1138.3642	1	311.19	(M+H)+	2.52
1139.3618	1	28.66	(M+H)+	7.54

--- End Of Report ---

Fig. S-14 High-resolution mass spectrum (LC-TOF, positive mode) of compound **5c.**

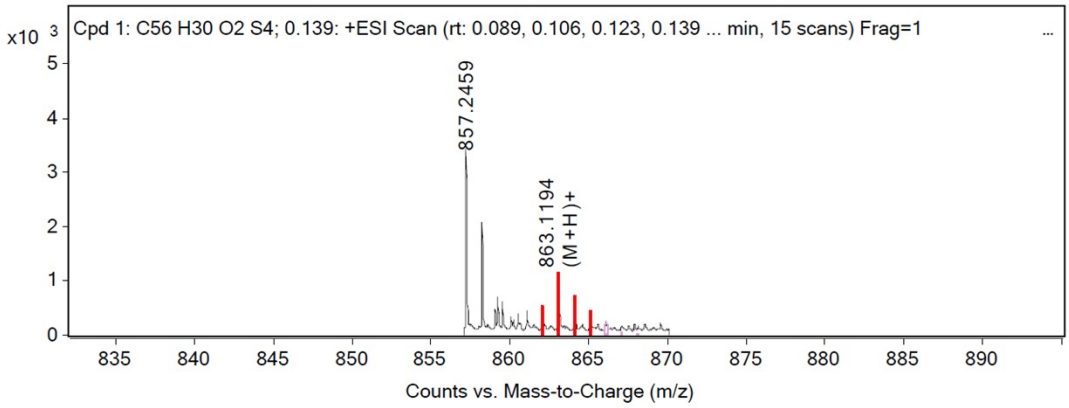
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
862.11	1	535.71	M+
863.1194	1	1157.65	(M+H)+
864.1226	1	701.45	(M+H)+
865.1191	1	433.22	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
857.2459		3420.65		
862.11	1	535.71	M+	2.71
863.1194	1	1157.65	(M+H)+	0.9
864.1226	1	701.45	(M+H)+	0.79
865.1191	1	433.22	(M+H)+	2.91

--- End Of Report ---

Fig. S-15 High-resolution mass spectrum (LC-TOF, positive mode) of compound **5d.**

Cartesian coordinates and optimized **5a** in gas phase: *E*(RB3LYP) = -4067.5408 hartees; Dipole Moment = 1.865279Debye; Basis Set = 6-31G(d,p).

O	3.41700	-4.27290	-2.56700
O	5.32330	0.78200	-2.95070
C	3.83620	-3.12350	-2.68610
C	5.27160	-2.85850	-2.99710
C	6.13630	-3.94160	-3.19030
H	5.72920	-4.94340	-3.10710
C	7.47990	-3.72210	-3.48050
H	8.14670	-4.56600	-3.63100
C	7.97180	-2.41550	-3.57740
H	9.02040	-2.24550	-3.80300
C	7.11910	-1.33240	-3.38360
H	7.47640	-0.31080	-3.45100
C	5.76630	-1.54310	-3.09390
C	4.87600	-0.36150	-2.88730
C	3.44080	-0.62670	-2.60500
C	2.57000	0.45120	-2.43100
H	2.98050	1.44700	-2.52200
C	1.21030	0.25370	-2.15930
C	0.20790	1.34130	-1.97260
C	-1.07010	1.02450	-2.67060
C	-1.74610	1.98880	-3.43230
H	-1.35800	3.00090	-3.46510
C	-2.89180	1.65710	-4.14790
H	-3.39840	2.41370	-4.73980
C	-3.37100	0.34580	-4.11980
H	-4.25360	0.07310	-4.69100
C	-2.70380	-0.62580	-3.37820
H	-3.06810	-1.64440	-3.38530
C	-1.55350	-0.30500	-2.64230
C	-0.74600	-1.28690	-1.86480
C	0.71420	-1.07650	-2.07950
C	1.58950	-2.15020	-2.27420
H	1.22840	-3.17010	-2.23100
C	2.94510	-1.94500	-2.52190
C	0.40210	2.45730	-1.21080
C	1.74600	2.82760	-0.65580
C	2.16380	2.37590	0.60320
H	1.51530	1.71960	1.17680
C	3.40730	2.72540	1.12120
H	3.72040	2.33370	2.08270
C	4.26610	3.57930	0.40830
C	2.60570	3.68470	-1.35970
C	3.83630	4.06870	-0.83600
C	-0.70700	3.35800	-0.77700
C	-0.54420	4.75450	-0.74110
H	0.39460	5.19240	-1.06320
C	-1.55250	5.59620	-0.28570

H	-1.39490	6.66920	-0.27300
C	-2.77150	5.07010	0.17210
C	-1.92490	2.84310	-0.29460
C	-2.93820	3.67460	0.16430
C	-1.24890	-2.23140	-1.02040
C	-2.71930	-2.48220	-0.85640
C	-3.45200	-1.79410	0.12130
H	-2.95140	-1.05370	0.73870
C	-4.80350	-2.05160	0.32890
H	-5.34770	-1.50720	1.09300
C	-5.47360	-3.01500	-0.44270
C	-3.39120	-3.45620	-1.61020
C	-4.74600	-3.71560	-1.41740
C	-0.38530	-3.04040	-0.10900
C	-0.50670	-4.43880	-0.04140
H	-1.25970	-4.94190	-0.63940
C	0.32970	-5.19930	0.76620
H	0.23420	-6.27960	0.78110
C	1.31500	-4.58410	1.55590
C	0.56270	-2.43130	0.73140
C	1.40060	-3.18240	1.54690
N	-3.80100	5.92350	0.64130
H	-3.86600	3.24440	0.52530
H	-2.08220	1.77020	-0.28470
C	-4.58330	5.54890	1.76930
C	-3.97760	4.98010	2.90100
C	-5.97310	5.74790	1.76820
C	-4.75020	4.61010	3.99980
H	-2.90310	4.83110	2.91160
C	-6.73450	5.39170	2.87920
H	-6.44770	6.18240	0.89480
C	-6.13110	4.81670	3.99930
H	-4.26550	4.17110	4.86720
H	-7.80870	5.55240	2.86160
H	-6.72880	4.53340	4.86020
C	-4.05190	7.16450	-0.00760
C	-4.29640	8.32440	0.74460
C	-4.06370	7.24670	-1.40930
C	-4.55430	9.53510	0.10490
H	-4.28340	8.26900	1.82790
C	-4.30430	8.46580	-2.03940
H	-3.88340	6.35240	-1.99620
C	-4.55550	9.61620	-1.28900
H	-4.74120	10.42290	0.70230
H	-4.30970	8.51160	-3.12470
H	-4.74970	10.56280	-1.78370
H	-5.24690	-4.46070	-2.02600
H	-2.85270	-4.00330	-2.37950
N	-6.85420	-3.27390	-0.24150
C	-7.34190	-4.60940	-0.29180
C	-8.53780	-4.90680	-0.96450
C	-6.63460	-5.64980	0.33170

C	-9.01580	-6.21510	-1.00250
H	-9.08660	-4.10870	-1.45300
C	-7.11120	-6.95780	0.27200
H	-5.71380	-5.42600	0.85990
C	-8.30530	-7.24940	-0.39010
H	-9.94290	-6.42730	-1.52730
H	-6.55120	-7.75050	0.75990
H	-8.67730	-8.26850	-0.42810
C	-7.75450	-2.19870	-0.00450
C	-8.77170	-2.32130	0.95580
C	-7.64200	-0.99990	-0.72710
C	-9.65900	-1.27030	1.17760
H	-8.86090	-3.24180	1.52260
C	-8.52250	0.05220	-0.48400
H	-6.86210	-0.89840	-1.47430
C	-9.53900	-0.07590	0.46450
H	-10.44000	-1.38280	1.92420
H	-8.41960	0.97280	-1.05130
H	-10.22730	0.74360	0.64580
N	5.53690	3.93090	0.92600
H	4.47920	4.73390	-1.40120
H	2.30840	4.05580	-2.33680
C	6.65640	4.06780	0.05560
C	7.59170	5.09400	0.26480
C	6.84070	3.18470	-1.02050
C	8.69300	5.22390	-0.57900
H	7.45070	5.78500	1.08910
C	7.93320	3.33940	-1.87120
H	6.12710	2.39010	-1.20660
C	8.86990	4.35190	-1.65490
H	9.40730	6.02290	-0.40100
H	8.04790	2.65160	-2.70380
H	9.72350	4.46280	-2.31670
C	5.70820	4.11720	2.32650
C	4.78180	4.87220	3.06320
C	6.80790	3.55200	2.99110
C	4.94960	5.04630	4.43540
H	3.93380	5.31760	2.55360
C	6.97740	3.74710	4.36030
H	7.52450	2.96420	2.42750
C	6.04900	4.49010	5.09230
H	4.22330	5.63350	4.99020
H	7.83400	3.30270	4.85910
H	6.18080	4.63410	6.16020
H	0.66100	-1.35060	0.72510
H	2.13810	-2.68660	2.16860
N	2.20580	-5.36800	2.33040
C	2.58450	-4.94500	3.63280
C	3.91880	-5.04240	4.06000
C	1.62470	-4.42250	4.51520
C	4.27720	-4.63340	5.34270
H	4.66740	-5.43870	3.38260

C	1.99700	-3.99930	5.78920
H	0.59050	-4.35230	4.19530
C	3.32270	-4.10540	6.21430
H	5.31410	-4.71550	5.65590
H	1.24090	-3.59790	6.45800
H	3.60780	-3.78160	7.21050
C	2.78320	-6.53920	1.76090
C	2.92930	-7.70290	2.53250
C	3.21050	-6.54620	0.42300
C	3.50110	-8.84590	1.97740
H	2.59380	-7.70370	3.56430
C	3.76230	-7.70170	-0.12670
H	3.10680	-5.65530	-0.18770
C	3.91680	-8.85540	0.64450
H	3.60740	-9.73790	2.58830
H	4.08370	-7.68860	-1.16410
H	4.35420	-9.75050	0.21270

Crystallographic Data and Detailed Refinements for 3a

Table S-1. Crystal data and structure refinement of **3a**

Identification code	Ey-MOME(**3a**)
Empirical formula	$C_{52}H_{38}O_6$
Formula weight	758.82
Temperature/K	100(2)
Crystal system	monoclinic
Space group	*Ia*
a/Å	7.32520(10)
b/Å	22.6642(2)
c/Å	23.2798(2)
β/°	92.4510(10)
Volume/Å^3	3861.37(7)
Z	4
ρ_{calc}g/cm^3	1.305
μ/mm^{-1}	0.676
F(000)	1592.0
Crystal size/mm^3	0.1 × 0.03 × 0.03
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	5.444 to 158.436
Index ranges	$-9 \le h \le 9$, $-28 \le k \le 27$, $-29 \le l \le 29$
Reflections collected	49012
Independent reflections	7972 [R_{int} = 0.0557, R_{sigma} = 0.0368]
Data/restraints/parameters	7972/2/527
Goodness-of-fit on F^2	1.056
Final *R* indexes [*I*>=2σ (I)]	R_1 = 0.0434, wR_2 = 0.1115
Final *R* indexes [all data]	R_1 = 0.0449, wR_2 = 0.1127
Largest diff. peak/hole / e Å^{-3}	0.35/-0.19
Flack parameter	-0.06(11)

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) of **3a**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6961(4)	4087.2(10)	3521.0(9)	39.8(5)
O2	6299(4)	4690.8(10)	5740.3(10)	43.2(6)
O3	6067(3)	-615.5(9)	3803.5(10)	36.7(5)
O4	-555(3)	2794.9(11)	3166.3(11)	43.0(6)
O5	4128(4)	218.1(10)	7429.1(10)	42.4(5)
O6	1300(4)	4274.3(10)	6870.0(11)	44.8(6)
C1	6930(4)	2104.2(12)	4606.5(12)	26.8(5)
C2	6740(4)	2737.6(12)	4750.6(12)	27.1(5)
C3	6784(4)	3176.0(12)	4331.9(12)	28.3(6)
C4	6709(4)	3767.3(12)	4483.1(12)	27.8(6)
C5	6839(4)	4224.2(13)	4023.1(13)	31.3(6)
C6	6808(4)	4855.4(13)	4206.0(14)	31.9(6)
C7	6940(5)	5294.4(14)	3791.3(15)	39.0(7)
C8	6956(5)	5882.4(15)	3956.0(17)	45.1(8)
C9	6861(5)	6036.0(14)	4529.2(17)	44.4(8)
C10	6711(5)	5603.8(14)	4945.4(15)	38.1(7)
C11	6678(4)	5011.9(13)	4783.9(13)	31.6(6)
C12	6502(4)	4552.5(13)	5239.1(13)	31.7(6)
C13	6579(4)	3922.9(12)	5062.1(12)	28.2(5)
C14	6517(4)	3486.4(13)	5481.4(12)	29.3(6)
C15	6609(4)	2892.0(12)	5335.8(12)	27.7(6)
C16	6628(4)	2384.8(12)	5746.6(12)	27.9(5)
C17	8016(4)	1936.0(12)	5600.0(12)	28.0(6)
C18	9168(4)	1674.6(13)	6016.6(13)	30.8(6)
C19	10493(4)	1278.3(13)	5861.7(14)	34.8(6)
C20	10678(4)	1135.3(13)	5289.2(14)	34.2(6)
C21	9547(4)	1391.2(12)	4864.3(13)	30.8(6)
C22	8208(4)	1794.6(12)	5017.2(12)	27.8(6)
C23	5934(4)	1841.7(12)	4179.3(12)	28.4(6)
C24	6069(4)	1196.8(13)	4062.5(13)	29.7(6)
C25	5342(4)	802.2(13)	4450.7(13)	32.6(6)
C26	5360(4)	201.4(14)	4352.8(13)	34.4(6)
C27	6097(4)	-15.4(13)	3854.9(13)	31.1(6)
C28	6791(4)	366.6(13)	3454.2(13)	32.7(6)
C29	6783(4)	973.5(13)	3565.0(13)	32.2(6)
C30	6636(5)	-860.6(14)	3278.1(15)	41.1(7)
C31	4326(4)	2134.5(12)	3886.9(12)	27.7(6)

Atom	*x*	*y*	*z*	U(eq)
C32	4102(4)	2192.5(13)	3293.7(13)	32.7(6)
C33	2492(5)	2409.7(13)	3037.0(13)	34.0(6)
C34	1075(4)	2576.2(12)	3373.9(13)	33.0(6)
C35	1263(4)	2513.8(13)	3968.2(13)	33.3(6)
C36	2856(4)	2298.5(13)	4218.0(13)	30.9(6)
C37	-683(6)	2947.8(19)	2576.6(17)	52.3(9)
C38	5441(4)	2311.1(12)	6172.6(12)	28.4(6)
C39	5170(4)	1742.1(13)	6481.4(12)	29.2(6)
C40	5195(4)	1195.0(14)	6213.8(13)	32.8(6)
C41	4856(4)	671.1(13)	6511.0(14)	34.4(6)
C42	4489(4)	696.9(14)	7091.0(14)	34.8(6)
C43	4445(5)	1236.2(15)	7365.0(14)	38.6(7)
C44	4770(5)	1746.5(14)	7064.4(14)	34.6(6)
C45	4349(5)	-354.4(14)	7196.1(17)	44.3(8)
C46	4254(4)	2811.5(12)	6353.7(12)	29.6(6)
C47	2493(4)	2889.3(13)	6137.6(13)	34.0(6)
C48	1442(5)	3374.3(14)	6299.3(14)	38.0(7)
C49	2179(5)	3780.0(13)	6688.4(13)	35.6(7)
C50	3934(5)	3700.0(14)	6924.8(13)	36.1(7)
C51	4952(5)	3221.0(13)	6758.2(13)	34.1(6)
C52	-491(5)	4390.6(16)	6633.7(18)	49.2(9)

Table S-3. Selected Bond Distances (Å)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C5	1.216(4)	C17	C22	1.407(4)
O2	C12	1.223(4)	C18	C19	1.381(4)
O3	C27	1.365(3)	C19	C20	1.384(5)
O3	C30	1.422(4)	C20	C21	1.390(4)
O4	C34	1.362(4)	C21	C22	1.398(4)
O4	C37	1.415(4)	C23	C24	1.491(4)
O5	C42	1.373(4)	C23	C31	1.491(4)
O5	C45	1.418(4)	C24	C25	1.393(4)
O6	C49	1.368(4)	C24	C29	1.387(4)
O6	C52	1.425(5)	C25	C26	1.381(4)
C1	C2	1.482(4)	C26	C27	1.389(4)
C1	C22	1.486(4)	C27	C28	1.385(4)
C1	C23	1.347(4)	C28	C29	1.400(4)
C2	C3	1.393(4)	C31	C32	1.390(4)
C2	C15	1.414(4)	C31	C36	1.401(4)
C3	C4	1.387(4)	C32	C33	1.389(5)
C4	C5	1.496(4)	C33	C34	1.380(4)
C4	C13	1.401(4)	C34	C35	1.392(4)
C5	C6	1.493(4)	C35	C36	1.371(4)
C6	C7	1.393(4)	C38	C39	1.494(4)
C6	C11	1.399(4)	C38	C46	1.500(4)
C7	C8	1.387(5)	C39	C40	1.388(4)
C8	C9	1.384(6)	C39	C44	1.401(4)
C9	C10	1.385(5)	C40	C41	1.402(4)
C10	C11	1.393(4)	C41	C42	1.389(5)
C11	C12	1.495(4)	C42	C43	1.380(5)
C12	C13	1.487(4)	C43	C44	1.378(4)
C13	C14	1.392(4)	C46	C47	1.375(5)
C14	C15	1.392(4)	C46	C51	1.403(4)
C15	C16	1.495(4)	C47	C48	1.403(5)
C16	C17	1.488(4)	C48	C49	1.384(5)
C16	C38	1.357(4)	C49	C50	1.388(5)
C17	C18	1.391(4)	C50	C51	1.382(4)

Table S-4. Selected Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C27	O3	C30	117.4(2)	C21	C22	C1	125.1(3)
C34	O4	C37	117.0(3)	C21	C22	C17	119.7(3)
C42	O5	C45	118.4(3)	C1	C23	C24	122.0(3)
C49	O6	C52	118.0(3)	C1	C23	C31	122.2(2)
C2	C1	C22	112.0(2)	C31	C23	C24	114.2(2)
C23	C1	C2	122.8(3)	C25	C24	C23	118.7(3)
C23	C1	C22	125.0(2)	C29	C24	C23	122.7(3)
C3	C2	C1	121.8(3)	C29	C24	C25	118.4(3)
C3	C2	C15	120.1(2)	C26	C25	C24	121.3(3)
C15	C2	C1	118.0(2)	C25	C26	C27	119.6(3)
C4	C3	C2	120.6(3)	O3	C27	C26	114.8(3)
C3	C4	C5	118.9(3)	O3	C27	C28	124.6(3)
C3	C4	C13	119.5(2)	C28	C27	C26	120.5(3)
C13	C4	C5	121.6(3)	C27	C28	C29	119.1(3)
O1	C5	C4	121.4(3)	C24	C29	C28	121.1(3)
O1	C5	C6	121.4(3)	C32	C31	C23	123.6(3)
C6	C5	C4	117.2(3)	C32	C31	C36	117.4(3)
C7	C6	C5	119.0(3)	C36	C31	C23	118.5(3)
C7	C6	C11	119.7(3)	C33	C32	C31	121.5(3)
C11	C6	C5	121.3(3)	C34	C33	C32	119.9(3)
C8	C7	C6	119.7(3)	O4	C34	C33	124.5(3)
C9	C8	C7	120.6(3)	O4	C34	C35	116.0(3)
C8	C9	C10	120.4(3)	C33	C34	C35	119.5(3)
C9	C10	C11	119.5(3)	C36	C35	C34	120.3(3)
C6	C11	C12	121.1(3)	C35	C36	C31	121.4(3)
C10	C11	C6	120.2(3)	C16	C38	C39	124.1(3)
C10	C11	C12	118.7(3)	C16	C38	C46	120.6(2)
O2	C12	C11	121.0(3)	C39	C38	C46	115.3(2)
O2	C12	C13	121.2(3)	C40	C39	C38	123.4(3)
C13	C12	C11	117.8(3)	C40	C39	C44	116.7(3)
C4	C13	C12	120.9(2)	C44	C39	C38	119.8(3)
C14	C13	C4	120.1(3)	C39	C40	C41	121.9(3)
C14	C13	C12	119.0(3)	C42	C41	C40	119.3(3)
C15	C14	C13	120.9(3)	O5	C42	C41	125.0(3)
C2	C15	C16	115.3(2)	O5	C42	C43	115.2(3)
C14	C15	C2	118.7(2)	C43	C42	C41	119.7(3)
C14	C15	C16	126.0(3)	C44	C43	C42	120.1(3)
C17	C16	C15	111.5(2)	C43	C44	C39	122.3(3)
C38	C16	C15	125.0(3)	C47	C46	C38	122.7(3)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C38	C16	C17	123.3(2)	C47	C46	C51	118.0(3)
C18	C17	C16	122.1(3)	C51	C46	C38	119.3(3)
C18	C17	C22	119.5(3)	C46	C47	C48	121.3(3)
C22	C17	C16	118.3(3)	C49	C48	C47	119.5(3)
C19	C18	C17	120.5(3)	O6	C49	C48	124.8(3)
C18	C19	C20	120.2(3)	O6	C49	C50	115.1(3)
C19	C20	C21	120.5(3)	C48	C49	C50	120.1(3)
C20	C21	C22	119.7(3)	C51	C50	C49	119.5(3)
C17	C22	C1	115.3(3)	C50	C51	C46	121.5(3)

Table S-5. Selected Torsion Angles

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C5	C6	C7	-0.6(5)	C17	C16	C38	C46	171.4(3)
O1	C5	C6	C11	-179.7(3)	C17	C18	C19	C20	-0.4(4)
O2	C12	C13	C4	176.4(3)	C18	C17	C22	C1	-179.1(3)
O2	C12	C13	C14	-3.5(5)	C18	C17	C22	C21	0.3(4)
O3	C27	C28	C29	-178.4(3)	C18	C19	C20	C21	0.5(5)
O4	C34	C35	C36	-179.8(3)	C19	C20	C21	C22	-0.2(4)
O5	C42	C43	C44	-179.4(3)	C20	C21	C22	C1	179.2(3)
O6	C49	C50	C51	-178.5(3)	C20	C21	C22	C17	-0.2(4)
C1	C2	C3	C4	-176.3(3)	C22	C1	C2	C3	135.0(3)
C1	C2	C15	C14	177.0(3)	C22	C1	C2	C15	-41.7(4)
C1	C2	C15	C16	-1.6(4)	C22	C1	C23	C24	-2.1(5)
C1	C23	C24	C25	71.2(4)	C22	C1	C23	C31	162.9(3)
C1	C23	C24	C29	-113.1(3)	C22	C17	C18	C19	0.0(4)
C1	C23	C31	C32	128.0(3)	C23	C1	C2	C3	-49.9(4)
C1	C23	C31	C36	-59.9(4)	C23	C1	C2	C15	133.4(3)
C2	C1	C22	C17	43.0(3)	C23	C1	C22	C17	-131.9(3)
C2	C1	C22	C21	-136.4(3)	C23	C1	C22	C21	48.7(4)
C2	C1	C23	C24	-176.5(3)	C23	C24	C25	C26	177.3(3)
C2	C1	C23	C31	-11.5(4)	C23	C24	C29	C28	-176.2(3)
C2	C3	C4	C5	177.4(3)	C23	C31	C32	C33	172.8(3)
C2	C3	C4	C13	-0.3(4)	C23	C31	C36	C35	-173.2(3)
C2	C15	C16	C17	42.3(3)	C24	C23	C31	C32	-65.9(4)
C2	C15	C16	C38	-132.6(3)	C24	C23	C31	C36	106.1(3)
C3	C2	C15	C14	0.2(4)	C24	C25	C26	C27	-0.8(5)
C3	C2	C15	C16	-178.3(3)	C25	C24	C29	C28	-0.5(5)
C3	C4	C5	O1	1.9(5)	C25	C26	C27	O3	179.3(3)
C3	C4	C5	C6	-178.2(3)	C25	C26	C27	C28	-0.8(5)
C3	C4	C13	C12	179.8(3)	C26	C27	C28	C29	1.6(5)
C3	C4	C13	C14	-0.3(4)	C27	C28	C29	C24	-1.0(5)
C4	C5	C6	C7	179.6(3)	C29	C24	C25	C26	1.4(5)
C4	C5	C6	C11	0.5(4)	C30	O3	C27	C26	174.0(3)
C4	C13	C14	C15	0.9(4)	C30	O3	C27	C28	-6.0(4)
C5	C4	C13	C12	2.1(4)	C31	C23	C24	C25	-94.9(3)
C5	C4	C13	C14	-178.0(3)	C31	C23	C24	C29	80.8(4)
C5	C6	C7	C8	-178.5(3)	C31	C32	C33	C34	0.3(4)
C5	C6	C11	C10	177.9(3)	C32	C31	C36	C35	-0.7(4)
C5	C6	C11	C12	-2.1(4)	C32	C33	C34	O4	179.9(3)
C6	C7	C8	C9	0.6(5)	C32	C33	C34	C35	-1.2(4)
C6	C11	C12	O2	-176.4(3)	C33	C34	C35	C36	1.2(4)

A	B	C	D	Angle/°
C6	C11	C12	C13	3.5(4)
C7	C6	C11	C10	-1.1(5)
C7	C6	C11	C12	178.9(3)
C7	C8	C9	C10	-1.3(6)
C8	C9	C10	C11	0.7(5)
C9	C10	C11	C6	0.4(5)
C9	C10	C11	C12	-179.5(3)
C10	C11	C12	O2	3.6(5)
C10	C11	C12	C13	-176.5(3)
C11	C6	C7	C8	0.6(5)
C11	C12	C13	C4	-3.5(4)
C11	C12	C13	C14	176.6(3)
C12	C13	C14	C15	-179.2(3)
C13	C4	C5	O1	179.6(3)
C13	C4	C5	C6	-0.5(4)
C13	C14	C15	C2	-0.9(4)
C13	C14	C15	C16	177.5(3)
C14	C15	C16	C17	-136.1(3)
C14	C15	C16	C38	49.0(5)
C15	C2	C3	C4	0.4(4)
C15	C16	C17	C18	136.1(3)
C15	C16	C17	C22	-41.1(3)
C15	C16	C38	C39	164.1(3)
C15	C16	C38	C46	-14.3(5)
C16	C17	C18	C19	-177.2(3)
C16	C17	C22	C1	-1.9(4)
C16	C17	C22	C21	177.6(3)
C16	C38	C39	C40	-37.6(4)
C16	C38	C39	C44	146.0(3)
C16	C38	C46	C47	94.9(4)
C16	C38	C46	C51	-84.9(4)
C17	C16	C38	C39	-10.2(5)
C34	C35	C36	C31	-0.2(5)
C36	C31	C32	C33	0.6(4)
C37	O4	C34	C33	-10.5(5)
C37	O4	C34	C35	170.5(3)
C38	C16	C17	C18	-48.9(4)
C38	C16	C17	C22	133.9(3)
C38	C39	C40	C41	-177.1(3)
C38	C39	C44	C43	177.7(3)
C38	C46	C47	C48	-177.5(3)
C38	C46	C51	C50	177.9(3)
C39	C38	C46	C47	-83.6(3)
C39	C38	C46	C51	96.6(3)
C39	C40	C41	C42	-0.2(5)
C40	C39	C44	C43	1.0(5)
C40	C41	C42	O5	179.7(3)
C40	C41	C42	C43	0.6(5)
C41	C42	C43	C44	-0.2(5)
C42	C43	C44	C39	-0.7(5)
C44	C39	C40	C41	-0.6(4)
C45	O5	C42	C41	7.8(5)
C45	O5	C42	C43	-173.0(3)
C46	C38	C39	C40	140.8(3)
C46	C38	C39	C44	-35.6(4)
C46	C47	C48	C49	-0.7(5)
C47	C46	C51	C50	-1.9(4)
C47	C48	C49	O6	178.8(3)
C47	C48	C49	C50	-1.3(5)
C48	C49	C50	C51	1.6(5)
C49	C50	C51	C46	0.1(5)
C51	C46	C47	C48	2.2(4)
C52	O6	C49	C48	-1.5(5)
C52	O6	C49	C50	178.5(3)

2. Crystallographic Data and Detailed Refinements for 5c

Table S-6. Crystal data and structure refinement

Identification code	Ey-pyrene
Empirical formula	$C_{108.85}H_{90.7}Cl_{0.7}O_{3.75}$
Formula weight	1483.52
Temperature/K	100(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	13.5911(3)
b/Å	14.1632(4)
c/Å	23.9764(6)
α/°	94.222(2)
β/°	93.435(2)
γ/°	106.380(2)
Volume/Å^3	4400.2(2)
Z	2
ρ_{calc}g/cm^3	1.120
μ/mm^{-1}	0.698
F(000)	1571.0
Crystal size/mm^3	0.395 × 0.088 × 0.074
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	6.534 to 159.038
Index ranges	$-17 \le h \le 16$, $-18 \le k \le 18$, $-30 \le l \le 30$
Reflections collected	100508
Independent reflections	18467 [R_{int} = 0.0499, R_{sigma} = 0.0330]
Data/restraints/parameters	18467/789/1247
Goodness-of-fit on F^2	1.269
Final *R* indexes [*I*>=2σ (I)]	R_1 = 0.1026, wR_2 = 0.3072
Final *R* indexes [all data]	R_1 = 0.1345, wR_2 = 0.3434
Largest diff. peak/hole / e Å^{-3}	0.61/-0.43

Table S-7. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	3691.4(15)	6946.6(15)	4897.8(8)	67.3(5)
O2	6922.2(15)	5461.6(16)	4926.3(8)	67.4(5)
C1	4447(2)	6647.2(19)	4904.8(11)	58.9(6)
C2	5062(2)	6638.3(19)	5439.1(11)	59.8(6)
C3	4789(3)	7008(2)	5941.1(11)	68.3(7)
C4	5352(3)	7019(2)	6437.5(12)	72.4(7)
C5	6199(3)	6649(2)	6443.2(12)	70.5(7)
C6	6477(2)	6266(2)	5954.6(11)	64.9(6)
C7	5915(2)	6265.8(19)	5444.0(11)	58.7(6)
C8	6222(2)	5851(2)	4916.0(10)	57.2(6)
C9	5664(2)	5928.6(19)	4379.4(10)	56.6(6)
C10	5961(2)	5577(2)	3878.8(10)	57.3(6)
C11	5444(2)	5611(2)	3368.9(10)	57.5(6)
C12	5663(2)	5176(2)	2820.6(10)	61.1(6)
C13	4705(2)	4696(2)	2452.7(10)	58.7(6)
C14	4534(2)	3772(2)	2155.0(10)	62.4(6)
C15	3621(2)	3332(2)	1830.4(11)	66.9(7)
C16	2870(2)	3828(2)	1790.2(11)	67.6(7)
C17	3031(2)	4741(2)	2084.1(11)	62.6(6)
C18	3926(2)	5177(2)	2424.4(10)	58.2(6)
C19	4098(2)	6097(2)	2806.7(10)	57.7(6)
C20	4614(2)	6027.4(19)	3363.2(10)	57.6(6)
C21	4295(2)	6342.1(19)	3864.0(10)	57.4(6)
C22	4814(2)	6302.1(18)	4373.6(10)	56.3(6)
C23	6611(2)	5232(2)	2655.1(11)	67.4(7)
C24	7608(2)	5769(2)	2993.0(12)	66.8(7)
C25	8072(2)	6742(3)	2900.5(13)	73.3(8)
C26	9045(3)	7248(3)	3158.5(14)	77.5(8)
C27	9592(2)	6805(2)	3499.8(13)	72.9(8)
C28	10619(3)	7299(3)	3751.0(14)	79.3(8)
C29	11133(3)	6822(3)	4069.9(15)	81.9(9)
C30	10699(2)	5809(3)	4177.6(13)	73.5(8)
C31	11232(3)	5313(3)	4504.2(15)	84.7(9)
C32	10783(3)	4352(3)	4616.0(17)	88.7(10)
C33	9783(3)	3867(3)	4394.8(15)	84.1(9)
C34	9225(2)	4328(3)	4059.0(14)	75.6(8)
C35	8202(2)	3834(3)	3819.5(13)	73.3(8)

Atom	*x*	*y*	*z*	U(eq)
C36	7685(2)	4291(2)	3480.1(13)	70.9(7)
C37	8128(2)	5289(2)	3348.8(11)	62.2(6)
C38	9130(2)	5802(2)	3599.3(12)	69.1(7)
C39	9684(2)	5314(3)	3944.4(12)	71.6(8)
C40	6785(2)	4830(3)	2081.6(12)	72.0(7)
C41	7266(3)	4081(3)	2039.5(14)	82.3(9)
C42	7458(3)	3669(3)	1529.7(15)	89.7(10)
C43	7194(3)	4026(3)	1034.4(15)	88.0(10)
C44	7380(3)	3630(4)	493.0(17)	101.3(12)
C45	7169(3)	4022(4)	26.2(17)	107.5(14)
C46	6744(3)	4828(4)	34.8(14)	96.3(12)
C47	6529(3)	5253(4)	-445.2(16)	111.8(15)
C48	6107(3)	6019(5)	-423.6(16)	120.0(18)
C49	5897(3)	6431(4)	86.2(15)	106.0(14)
C50	6103(3)	6036(4)	583.5(14)	92.3(11)
C51	5879(3)	6418(3)	1118.3(13)	83.6(9)
C52	6092(2)	6037(3)	1593.3(13)	75.9(8)
C53	6534(2)	5225(3)	1592.3(12)	72.1(8)
C54	6746(2)	4825(3)	1063.2(12)	78.9(9)
C55	6529(3)	5235(3)	562.3(13)	84.0(9)
C56	3864(2)	6921(2)	2686.9(11)	62.0(6)
C57	3441(2)	7116(2)	2126.8(11)	61.6(6)
C58	4147(2)	7620(2)	1771.5(12)	68.0(7)
C59	3830(2)	7951(2)	1287.4(12)	70.0(7)
C60	2791(2)	7834(2)	1141.0(12)	67.5(7)
C61	2442(3)	8221(3)	657.4(13)	77.8(8)
C62	1445(3)	8112(3)	531.6(15)	85.0(9)
C63	675(3)	7606(3)	877.6(14)	80.1(8)
C64	-373(3)	7478(3)	758.3(17)	94.2(11)
C65	-1092(3)	6979(4)	1091.7(19)	99.9(12)
C66	-790(3)	6581(3)	1558.4(17)	90.4(10)
C67	249(2)	6690(2)	1701.1(14)	74.1(8)
C68	594(2)	6307(2)	2188.8(13)	73.6(8)
C69	1603(2)	6442(2)	2327.5(12)	68.6(7)
C70	2382(2)	6956(2)	1986.8(11)	61.2(6)
C71	2057(2)	7324(2)	1493.3(11)	63.8(6)
C72	997(2)	7203(2)	1358.6(12)	70.4(7)
C73	4091(3)	7820(2)	3100.0(12)	72.8(8)
C74	3254(3)	8094(3)	3311.1(13)	80.1(9)
C75	3392(4)	8885(3)	3704.5(15)	93.1(11)
C76	4295(6)	9455(11)	3903(7)	78(3)

Atom	*x*	*y*	*z*	U(eq)
C76A	4465(11)	9458(11)	3882(8)	97(4)
C77	4416(8)	10269(12)	4312(8)	81(2)
C77A	4767(19)	10289(14)	4308(9)	108(4)
C78	5363(9)	10802(10)	4518(7)	81(3)
C78A	5750(20)	10831(15)	4445(9)	121(5)
C79	6266(8)	10673(10)	4295(6)	82(2)
C79A	6620(18)	10629(12)	4236(10)	115(4)
C80	7222(10)	11229(11)	4478(8)	109(3)
C80A	7610(20)	11160(15)	4360(11)	142(6)
C81	8118(8)	11055(10)	4295(7)	111(4)
C81A	8435(19)	10930(17)	4131(13)	161(6)
C82	8019(7)	10256(10)	3885(7)	107(4)
C82A	8278(16)	10147(17)	3694(13)	156(6)
C83	7022(7)	9658(12)	3672(7)	86(3)
C83A	7226(14)	9563(17)	3561(12)	119(4)
C84	6918(7)	8787(11)	3281(6)	80(3)
C84A	6976(12)	8745(17)	3112(11)	111(5)
C85	5984(8)	8201(10)	3081(7)	86(3)
C85A	5987(9)	8183(13)	3024(9)	91(4)
C86	5081(3)	8392(2)	3269.3(13)	75.9(8)
C87	5160(7)	9227(11)	3690(6)	72(2)
C87A	5369(12)	9247(12)	3663(9)	94(4)
C88	6158(6)	9823(9)	3891(6)	73(2)
C88A	6408(15)	9808(14)	3794(10)	115(4)
O3	1065(6)	3774(7)	3059(3)	221(3)
C102	1060(8)	2699(8)	3015(6)	222(5)
C103	-56(9)	2143(8)	2907(6)	235(5)
C104	-543(8)	2763(8)	2565(5)	211(4)
C105	142(8)	3763(6)	2679(3)	169(3)
O4	7547(5)	8505(5)	4899(2)	174(2)
Cl3	9430(15)	9266(18)	5179(9)	262(7)
Cl4	7903(15)	9054(16)	5978(9)	262(7)
C107	8198(5)	8018(5)	4520(3)	128.0(18)
C108	9122(7)	8066(9)	4854(3)	190(4)
C109	8765(9)	8030(11)	5429(4)	212(4)
C110	8138(8)	8709(8)	5463(3)	183(3)
C111	8741(18)	9895(15)	5597(10)	107(8)
Cl1	9760(30)	11120(20)	2829(14)	238(8)
Cl2	8080(20)	11880(20)	2552(13)	238(8)
C106	9300(30)	12170(20)	2930(20)	119(14)
Cl5	8100(50)	10910(30)	1260(30)	380(30)

Atom	*x*	*y*	*z*	U(eq)
Cl6	7540(30)	8960(20)	1706(13)	234(12)
C118	7400(60)	9640(30)	1130(20)	230(30)
C89	387(5)	4142(6)	1144(3)	145(2)
C90	304(4)	4149(5)	544(2)	130.1(18)
C91	77(4)	4992(5)	298(2)	126.5(18)
C92	4842(5)	10375(5)	158(3)	146(2)
C93	5222(15)	11319(11)	394(6)	141(3)
C94	5259(11)	10832(8)	716(4)	141(3)
C95	4872(7)	11736(6)	893(3)	168(3)
C96	6189(11)	11389(8)	2638(5)	185(4)
C97	5252(15)	10609(8)	2394(4)	192(6)
C98	4288(18)	10741(7)	2515(4)	221(8)
C99	3270(15)	9992(7)	2307(4)	211(7)
C100	2328(15)	10161(10)	2462(6)	224(7)
C101	1350(11)	9343(8)	2402(5)	198(5)
C112	7435(18)	9240(15)	1184(14)	311(16)
C113	8204(18)	10150(20)	1008(14)	315(13)
C114	9298(16)	10140(20)	1183(12)	312(12)
C115	10000(14)	10890(17)	847(8)	243(8)
C116	11110(16)	10940(20)	1037(11)	282(11)
C117	11714(14)	11524(17)	605(9)	237(9)

Table S-8. Selected Bond Distances (Å)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.217(3)	C63	C72	1.422(5)
O2	C8	1.228(3)	C64	C65	1.371(6)
C1	C2	1.490(4)	C65	C66	1.381(6)
C1	C22	1.494(3)	C66	C67	1.394(5)
C2	C3	1.389(4)	C67	C68	1.433(5)
C2	C7	1.403(4)	C67	C72	1.417(5)
C3	C4	1.372(4)	C68	C69	1.348(4)
C4	C5	1.394(4)	C69	C70	1.440(4)
C5	C6	1.372(4)	C70	C71	1.423(4)
C6	C7	1.403(4)	C71	C72	1.417(4)
C7	C8	1.487(3)	C73	C74	1.411(5)
C8	C9	1.481(4)	C73	C86	1.380(5)
C9	C10	1.391(3)	C74	C75	1.372(5)
C9	C22	1.399(4)	C75	C76	1.303(9)
C10	C11	1.384(4)	C75	C76A	1.475(13)
C11	C12	1.492(3)	C76	C77	1.423(10)
C11	C20	1.413(4)	C76	C87	1.419(9)
C12	C13	1.486(4)	C76A	C77A	1.447(11)
C12	C23	1.354(4)	C76A	C87A	1.461(13)
C13	C14	1.395(4)	C77	C78	1.338(11)
C13	C18	1.412(4)	C77A	C78A	1.342(15)
C14	C15	1.382(4)	C78	C79	1.419(11)
C15	C16	1.396(4)	C78A	C79A	1.410(16)
C16	C17	1.380(4)	C79	C80	1.344(12)
C17	C18	1.383(4)	C79	C88	1.455(10)
C18	C19	1.490(4)	C79A	C80A	1.342(15)
C19	C20	1.493(3)	C79A	C88A	1.466(13)
C19	C56	1.340(4)	C80	C81	1.400(13)
C20	C21	1.386(3)	C80A	C81A	1.389(19)
C21	C22	1.387(4)	C81	C82	1.414(13)
C23	C24	1.506(4)	C81A	C82A	1.429(17)
C23	C40	1.507(4)	C82	C83	1.420(10)
C24	C25	1.385(5)	C82A	C83A	1.438(14)
C24	C37	1.405(4)	C83	C84	1.461(10)
C25	C26	1.395(5)	C83	C88	1.387(10)
C26	C27	1.373(5)	C83A	C84A	1.472(14)
C27	C28	1.444(5)	C83A	C88A	1.391(15)
C27	C38	1.427(5)	C84	C85	1.343(10)
C28	C29	1.345(5)	C84A	C85A	1.351(13)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C29	C30	1.438(5)	C85	C86	1.420(10)
C30	C31	1.390(5)	C85A	C86	1.488(13)
C30	C39	1.419(4)	C86	C87	1.472(9)
C31	C32	1.379(6)	C86	C87A	1.426(10)
C32	C33	1.391(5)	C87	C88	1.414(9)
C33	C34	1.390(5)	C87A	C88A	1.414(13)
C34	C35	1.432(5)	O3	C102	1.516(10)
C34	C39	1.414(5)	O3	C105	1.501(9)
C35	C36	1.357(4)	C102	C103	1.495(10)
C36	C37	1.437(4)	C103	C104	1.500(10)
C37	C38	1.422(4)	C104	C105	1.455(10)
C38	C39	1.425(5)	O4	C107	1.560(8)
C40	C41	1.396(5)	O4	C110	1.496(9)
C40	C53	1.400(5)	Cl3	Cl3[1]	2.46(6)
C41	C42	1.386(4)	Cl3	C111	1.767(9)
C42	C43	1.391(6)	Cl4	C111	1.752(9)
C43	C44	1.441(4)	C107	C108	1.430(8)
C43	C54	1.426(5)	C108	C109	1.489(9)
C44	C45	1.336(7)	C109	C110	1.455(10)
C45	C46	1.417(7)	Cl1	C106	1.778(9)
C46	C47	1.390(6)	Cl2	C106	1.771(9)
C46	C55	1.432(5)	Cl5	C118	1.775(9)
C47	C48	1.362(8)	Cl6	C118	1.768(9)
C48	C49	1.395(6)	C89	C90	1.437(8)
C49	C50	1.400(5)	C90	C91	1.469(8)
C50	C51	1.439(5)	C91	C91[2]	1.434(10)
C50	C55	1.410(6)	C92	C92[3]	1.437(11)
C51	C52	1.347(5)	C92	C93	1.356(16)
C52	C53	1.439(5)	C92	C94	1.451(11)
C53	C54	1.430(4)	C93	C95	1.459(14)
C54	C55	1.423(5)	C94	C95	1.557(12)
C56	C57	1.504(4)	C96	C97	1.484(17)
C56	C73	1.501(4)	C97	C98	1.42(2)
C57	C58	1.399(4)	C98	C99	1.52(2)
C57	C70	1.408(4)	C99	C100	1.43(2)
C58	C59	1.373(4)	C100	C101	1.49(2)
C59	C60	1.395(4)	C112	C113	1.518(13)
C60	C61	1.429(4)	C113	C114	1.525(13)
C60	C71	1.419(4)	C114	C115	1.530(13)
C61	C62	1.333(5)	C115	C116	1.529(12)
C62	C63	1.437(5)	C116	C117	1.505(13)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C63	C64	1.393(5)			

[1]2-X,2-Y,1-Z; [2]-X,1-Y,-Z; [3]1-X,2-Y,-Z

Table S-9. Selected Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C2	121.6(2)	C58	C57	C70	119.0(2)
O1	C1	C22	121.1(2)	C70	C57	C56	122.9(2)
C2	C1	C22	117.3(2)	C59	C58	C57	121.6(3)
C3	C2	C1	119.5(2)	C58	C59	C60	121.3(3)
C3	C2	C7	119.4(2)	C59	C60	C61	122.6(3)
C7	C2	C1	121.1(2)	C59	C60	C71	118.3(3)
C4	C3	C2	120.6(3)	C71	C60	C61	119.1(3)
C3	C4	C5	120.2(3)	C62	C61	C60	121.4(3)
C6	C5	C4	120.5(3)	C61	C62	C63	121.5(3)
C5	C6	C7	119.7(3)	C64	C63	C62	123.0(3)
C2	C7	C6	119.7(2)	C64	C63	C72	118.5(3)
C2	C7	C8	120.9(2)	C72	C63	C62	118.5(3)
C6	C7	C8	119.4(2)	C65	C64	C63	121.8(4)
O2	C8	C7	120.7(2)	C64	C65	C66	120.3(4)
O2	C8	C9	121.1(2)	C65	C66	C67	120.6(4)
C9	C8	C7	118.2(2)	C66	C67	C68	122.2(3)
C10	C9	C8	119.1(2)	C66	C67	C72	119.5(3)
C10	C9	C22	120.0(2)	C72	C67	C68	118.3(3)
C22	C9	C8	120.8(2)	C69	C68	C67	121.4(3)
C11	C10	C9	121.1(2)	C68	C69	C70	121.7(3)
C10	C11	C12	124.1(2)	C57	C70	C69	122.7(2)
C10	C11	C20	118.7(2)	C57	C70	C71	119.3(2)
C20	C11	C12	117.1(2)	C71	C70	C69	118.0(3)
C13	C12	C11	112.0(2)	C60	C71	C70	120.5(3)
C23	C12	C11	125.4(3)	C72	C71	C60	119.6(3)
C23	C12	C13	122.6(2)	C72	C71	C70	119.9(3)
C14	C13	C12	122.3(2)	C67	C72	C63	119.4(3)
C14	C13	C18	119.1(2)	C67	C72	C71	120.7(3)
C18	C13	C12	118.5(2)	C71	C72	C63	120.0(3)
C15	C14	C13	120.9(2)	C74	C73	C56	118.2(3)
C14	C15	C16	119.5(3)	C86	C73	C56	122.4(3)
C17	C16	C15	120.0(3)	C86	C73	C74	119.4(3)
C16	C17	C18	121.1(3)	C75	C74	C73	122.0(4)
C13	C18	C19	116.6(2)	C74	C75	C76A	116.5(6)
C17	C18	C13	119.3(2)	C76	C75	C74	123.4(6)
C17	C18	C19	123.9(2)	C75	C76	C77	122.2(7)
C18	C19	C20	111.9(2)	C75	C76	C87	116.5(8)
C56	C19	C18	126.8(2)	C87	C76	C77	121.2(7)
C56	C19	C20	121.4(2)	C77A	C76A	C75	124.6(11)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	C20	C19	117.8(2)	C77A	C76A	C87A	110.8(11)
C21	C20	C11	120.0(2)	C87A	C76A	C75	124.6(9)
C21	C20	C19	122.2(2)	C78	C77	C76	119.4(8)
C20	C21	C22	120.9(2)	C78A	C77A	C76A	123.7(14)
C9	C22	C1	121.4(2)	C77	C78	C79	122.7(8)
C21	C22	C1	119.3(2)	C77A	C78A	C79A	125.5(13)
C21	C22	C9	119.2(2)	C78	C79	C88	118.1(7)
C12	C23	C24	124.9(2)	C80	C79	C78	123.6(8)
C12	C23	C40	123.0(3)	C80	C79	C88	118.0(8)
C24	C23	C40	112.0(2)	C78A	C79A	C88A	115.4(12)
C25	C24	C23	118.0(3)	C80A	C79A	C78A	127.0(13)
C25	C24	C37	119.4(3)	C80A	C79A	C88A	117.3(15)
C37	C24	C23	122.2(3)	C79	C80	C81	124.0(9)
C24	C25	C26	120.7(3)	C79A	C80A	C81A	124.2(16)
C27	C26	C25	122.0(3)	C80	C81	C82	118.4(8)
C26	C27	C28	123.1(3)	C80A	C81A	C82A	121.0(15)
C26	C27	C38	118.1(3)	C81	C82	C83	119.6(8)
C38	C27	C28	118.8(3)	C81A	C82A	C83A	115.2(15)
C29	C28	C27	120.7(3)	C82	C83	C84	119.6(8)
C28	C29	C30	122.3(3)	C88	C83	C82	119.9(7)
C31	C30	C29	122.4(3)	C88	C83	C84	119.9(7)
C31	C30	C39	119.6(3)	C82A	C83A	C84A	119.7(14)
C39	C30	C29	118.0(3)	C88A	C83A	C82A	122.5(12)
C32	C31	C30	121.1(3)	C88A	C83A	C84A	117.4(11)
C31	C32	C33	119.6(3)	C85	C84	C83	120.7(9)
C34	C33	C32	121.4(4)	C85A	C84A	C83A	117.5(14)
C33	C34	C35	122.1(3)	C84	C85	C86	120.3(9)
C33	C34	C39	119.1(3)	C84A	C85A	C86	126.7(14)
C39	C34	C35	118.7(3)	C73	C86	C85	124.7(6)
C36	C35	C34	120.9(3)	C73	C86	C85A	121.5(7)
C35	C36	C37	122.0(3)	C73	C86	C87	115.0(4)
C24	C37	C36	122.7(3)	C73	C86	C87A	126.2(7)
C24	C37	C38	119.6(3)	C85	C86	C87	120.3(7)
C38	C37	C36	117.7(3)	C87A	C86	C85A	112.2(10)
C37	C38	C27	120.1(3)	C76	C87	C86	123.6(7)
C37	C38	C39	120.3(3)	C88	C87	C76	118.8(7)
C39	C38	C27	119.6(3)	C88	C87	C86	117.6(7)
C30	C39	C38	120.6(3)	C86	C87A	C76A	111.2(10)
C34	C39	C30	119.2(3)	C88A	C87A	C76A	126.7(10)
C34	C39	C38	120.2(3)	C88A	C87A	C86	122.1(10)
C41	C40	C23	118.9(3)	C83	C88	C79	119.9(7)

Atom	Atom	Atom	Angle/°
C41	C40	C53	119.0(3)
C53	C40	C23	122.0(3)
C42	C41	C40	122.8(3)
C41	C42	C43	119.6(3)
C42	C43	C44	122.0(4)
C42	C43	C54	119.1(3)
C54	C43	C44	118.8(4)
C45	C44	C43	120.8(4)
C44	C45	C46	122.4(3)
C45	C46	C55	118.8(4)
C47	C46	C45	123.3(4)
C47	C46	C55	117.9(4)
C48	C47	C46	121.8(4)
C47	C48	C49	121.2(4)
C48	C49	C50	119.3(5)
C49	C50	C51	121.5(4)
C49	C50	C55	119.6(3)
C55	C50	C51	118.9(3)
C52	C51	C50	120.8(4)
C51	C52	C53	122.2(3)
C40	C53	C52	123.3(3)
C40	C53	C54	119.0(3)
C54	C53	C52	117.7(3)
C43	C54	C53	120.4(3)
C55	C54	C43	119.6(3)
C55	C54	C53	120.0(3)
C50	C55	C46	120.1(4)
C50	C55	C54	120.4(3)
C54	C55	C46	119.5(4)
C19	C56	C57	126.2(2)
C19	C56	C73	122.6(2)
C73	C56	C57	111.0(2)
C58	C57	C56	117.3(3)
C83	C88	C87	120.7(7)
C87	C88	C79	119.1(7)
C83A	C88A	C79A	119.2(12)
C83A	C88A	C87A	123.1(11)
C87A	C88A	C79A	117.4(12)
C105	O3	C102	103.3(8)
C103	C102	O3	103.8(8)
C102	C103	C104	106.5(8)
C105	C104	C103	104.9(7)
C104	C105	O3	110.5(7)
C110	O4	C107	104.2(6)
C108	C107	O4	106.6(5)
C107	C108	C109	101.7(7)
C110	C109	C108	105.3(8)
C109	C110	O4	102.7(7)
Cl4	C111	Cl3	109.6(12)
Cl2	C106	Cl1	106.8(13)
Cl6	C118	Cl5	112.3(15)
C89	C90	C91	119.2(5)
C91[1]	C91	C90	121.5(6)
C92[2]	C92	C94	126.2(9)
C93	C92	C92[2]	140.6(11)
C92	C93	C95	125.6(13)
C92	C94	C95	112.7(9)
C98	C97	C96	117.1(12)
C97	C98	C99	122.8(10)
C100	C99	C98	119.6(11)
C99	C100	C101	120.9(12)
C112	C113	C114	110.0(17)
C113	C114	C115	105.8(16)
C116	C115	C114	107.3(15)
C117	C116	C115	102.8(15)

[1]-X,1-Y,-Z; [2]1-X,2-Y,-Z

Table S-10. Selected Torsion Angles

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	C3	-2.0(4)	C51	C52	C53	C54	0.0(5)
O1	C1	C2	C7	178.2(3)	C52	C53	C54	C43	179.4(3)
O1	C1	C22	C9	-178.0(3)	C52	C53	C54	C55	0.6(5)
O1	C1	C22	C21	1.2(4)	C53	C40	C41	C42	-3.6(5)
O2	C8	C9	C10	-1.8(4)	C53	C54	C55	C46	180.0(3)
O2	C8	C9	C22	174.9(3)	C53	C54	C55	C50	-0.1(5)
C1	C2	C3	C4	-179.1(3)	C54	C43	C44	C45	2.1(6)
C1	C2	C7	C6	-179.9(3)	C55	C46	C47	C48	-1.3(7)
C1	C2	C7	C8	-1.1(4)	C55	C50	C51	C52	1.5(6)
C2	C1	C22	C9	3.8(4)	C56	C19	C20	C11	-135.0(3)
C2	C1	C22	C21	-176.9(2)	C56	C19	C20	C21	46.0(4)
C2	C3	C4	C5	-0.7(5)	C56	C57	C58	C59	-171.0(3)
C2	C7	C8	O2	-174.7(3)	C56	C57	C70	C69	-10.7(4)
C2	C7	C8	C9	5.7(4)	C56	C57	C70	C71	168.6(2)
C3	C2	C7	C6	0.3(4)	C56	C73	C74	C75	177.7(3)
C3	C2	C7	C8	179.1(3)	C56	C73	C86	C85	-0.4(10)
C3	C4	C5	C6	-0.3(5)	C56	C73	C86	C85A	3.8(10)
C4	C5	C6	C7	1.3(5)	C56	C73	C86	C87	-178.2(9)
C5	C6	C7	C2	-1.3(4)	C56	C73	C86	C87A	-179.1(13)
C5	C6	C7	C8	179.9(3)	C57	C56	C73	C74	71.7(3)
C6	C7	C8	O2	4.1(4)	C57	C56	C73	C86	-107.0(3)
C6	C7	C8	C9	-175.5(2)	C57	C58	C59	C60	2.8(5)
C7	C2	C3	C4	0.7(5)	C57	C70	C71	C60	0.9(4)
C7	C8	C9	C10	177.7(2)	C57	C70	C71	C72	-177.5(3)
C7	C8	C9	C22	-5.5(4)	C58	C57	C70	C69	179.8(3)
C8	C9	C10	C11	178.3(2)	C58	C57	C70	C71	-0.9(4)
C8	C9	C22	C1	0.8(4)	C58	C59	C60	C61	176.3(3)
C8	C9	C22	C21	-178.5(2)	C58	C59	C60	C71	-2.8(5)
C9	C10	C11	C12	-174.8(3)	C59	C60	C61	C62	-179.0(3)
C9	C10	C11	C20	1.2(4)	C59	C60	C71	C70	0.9(4)
C10	C9	C22	C1	177.5(2)	C59	C60	C71	C72	179.3(3)
C10	C9	C22	C21	-1.8(4)	C60	C61	C62	C63	0.3(6)
C10	C11	C12	C13	140.7(3)	C60	C71	C72	C63	-1.0(4)
C10	C11	C12	C23	-41.9(4)	C60	C71	C72	C67	179.5(3)
C10	C11	C20	C19	177.3(2)	C61	C60	C71	C70	-178.1(3)
C10	C11	C20	C21	-3.6(4)	C61	C60	C71	C72	0.3(4)
C11	C12	C13	C14	-135.5(3)	C61	C62	C63	C64	-179.9(4)
C11	C12	C13	C18	41.7(3)	C61	C62	C63	C72	-1.0(6)
C11	C12	C23	C24	-1.6(5)	C62	C63	C64	C65	179.1(4)

A	B	C	D	Angle/°
C11	C12	C23	C40	-176.2(3)
C11	C20	C21	C22	3.4(4)
C12	C11	C20	C19	-6.4(4)
C12	C11	C20	C21	172.7(2)
C12	C13	C14	C15	177.9(2)
C12	C13	C18	C17	180.0(2)
C12	C13	C18	C19	-4.8(3)
C12	C23	C24	C25	-92.8(4)
C12	C23	C24	C37	94.1(4)
C12	C23	C40	C41	-118.6(4)
C12	C23	C40	C53	65.2(4)
C13	C12	C23	C24	175.5(3)
C13	C12	C23	C40	1.0(5)
C13	C14	C15	C16	1.4(4)
C13	C18	C19	C20	-37.1(3)
C13	C18	C19	C56	141.1(3)
C14	C13	C18	C17	-2.7(4)
C14	C13	C18	C19	172.4(2)
C14	C15	C16	C17	-1.6(4)
C15	C16	C17	C18	-0.5(4)
C16	C17	C18	C13	2.7(4)
C16	C17	C18	C19	-172.2(3)
C17	C18	C19	C20	137.9(3)
C17	C18	C19	C56	-44.0(4)
C18	C13	C14	C15	0.7(4)
C18	C19	C20	C11	43.3(3)
C18	C19	C20	C21	-135.8(3)
C18	C19	C56	C57	-4.3(5)
C18	C19	C56	C73	-178.6(3)
C19	C20	C21	C22	-177.6(2)
C19	C56	C57	C58	-94.4(4)
C19	C56	C57	C70	96.0(3)
C19	C56	C73	C74	-113.2(3)
C19	C56	C73	C86	68.1(4)
C20	C11	C12	C13	-35.4(3)
C20	C11	C12	C23	142.1(3)
C20	C19	C56	C57	173.7(3)
C20	C19	C56	C73	-0.6(4)
C20	C21	C22	C1	-180.0(2)
C20	C21	C22	C9	-0.7(4)
C22	C1	C2	C3	176.1(3)
C62	C63	C72	C67	-179.2(3)
C62	C63	C72	C71	1.3(5)
C63	C64	C65	C66	-0.5(7)
C64	C63	C72	C67	-0.2(5)
C64	C63	C72	C71	-179.7(3)
C64	C65	C66	C67	0.8(6)
C65	C66	C67	C68	178.6(3)
C65	C66	C67	C72	-0.9(6)
C66	C67	C68	C69	-178.3(3)
C66	C67	C72	C63	0.6(5)
C66	C67	C72	C71	-179.9(3)
C67	C68	C69	C70	-1.5(5)
C68	C67	C72	C63	-178.9(3)
C68	C67	C72	C71	0.6(5)
C68	C69	C70	C57	179.2(3)
C68	C69	C70	C71	0.0(4)
C69	C70	C71	C60	-179.8(3)
C69	C70	C71	C72	1.7(4)
C70	C57	C58	C59	-0.9(4)
C70	C71	C72	C63	177.4(3)
C70	C71	C72	C67	-2.1(4)
C71	C60	C61	C62	0.0(5)
C72	C63	C64	C65	0.2(6)
C72	C67	C68	C69	1.1(5)
C73	C56	C57	C58	80.5(3)
C73	C56	C57	C70	-89.2(3)
C73	C74	C75	C76	1.7(13)
C73	C74	C75	C76A	2.1(12)
C73	C86	C87	C76	-1(2)
C73	C86	C87	C88	178.3(12)
C73	C86	C87A	C76A	1(2)
C73	C86	C87A	C88A	-177.4(17)
C74	C73	C86	C85	-179.1(9)
C74	C73	C86	C85A	-174.9(10)
C74	C73	C86	C87	3.1(10)
C74	C73	C86	C87A	2.2(14)
C74	C75	C76	C77	-179.9(15)
C74	C75	C76	C87	0(2)
C74	C75	C76A	C77A	-177.3(18)
C74	C75	C76A	C87A	1(3)
C75	C76	C77	C78	177.2(18)

A	B	C	D	Angle/°
C22	C1	C2	C7	-3.6(4)
C22	C9	C10	C11	1.5(4)
C23	C12	C13	C14	47.0(4)
C23	C12	C13	C18	-135.8(3)
C23	C24	C25	C26	-173.6(3)
C23	C24	C37	C36	-9.1(4)
C23	C24	C37	C38	171.8(2)
C23	C40	C41	C42	-179.9(3)
C23	C40	C53	C52	-0.2(5)
C23	C40	C53	C54	178.3(3)
C24	C23	C40	C41	66.3(4)
C24	C23	C40	C53	-109.9(3)
C24	C25	C26	C27	1.7(5)
C24	C37	C38	C27	1.5(4)
C24	C37	C38	C39	-177.6(2)
C25	C24	C37	C36	177.9(3)
C25	C24	C37	C38	-1.3(4)
C25	C26	C27	C28	177.1(3)
C25	C26	C27	C38	-1.5(4)
C26	C27	C28	C29	-178.1(3)
C26	C27	C38	C37	-0.1(4)
C26	C27	C38	C39	179.0(3)
C27	C28	C29	C30	0.0(5)
C27	C38	C39	C30	-1.6(4)
C27	C38	C39	C34	178.3(3)
C28	C27	C38	C37	-178.8(2)
C28	C27	C38	C39	0.4(4)
C28	C29	C30	C31	179.6(3)
C28	C29	C30	C39	-1.2(5)
C29	C30	C31	C32	177.8(3)
C29	C30	C39	C34	-177.9(3)
C29	C30	C39	C38	2.0(4)
C30	C31	C32	C33	0.6(5)
C31	C30	C39	C34	1.3(4)
C31	C30	C39	C38	-178.8(3)
C31	C32	C33	C34	0.4(5)
C32	C33	C34	C35	178.8(3)
C32	C33	C34	C39	-0.5(5)
C33	C34	C35	C36	-178.1(3)
C33	C34	C39	C30	-0.4(4)
C33	C34	C39	C38	179.7(3)
C75	C76	C87	C86	-1(3)
C75	C76	C87	C88	179.9(16)
C75	C76A	C77A	C78A	-177(2)
C75	C76A	C87A	C86	-2(3)
C75	C76A	C87A	C88A	176(2)
C76	C77	C78	C79	8(3)
C76	C87	C88	C79	-2(3)
C76	C87	C88	C83	-177(2)
C76A	C77A	C78A	C79A	-6(4)
C76A	C87A	C88A	C79A	7(4)
C76A	C87A	C88A	C83A	-179(3)
C77	C76	C87	C86	179.7(18)
C77	C76	C87	C88	0(3)
C77	C78	C79	C80	176.9(19)
C77	C78	C79	C88	-10(3)
C77A	C76A	C87A	C86	176.3(19)
C77A	C76A	C87A	C88A	-6(4)
C77A	C78A	C79A	C80A	179(3)
C77A	C78A	C79A	C88A	6(4)
C78	C79	C80	C81	174(2)
C78	C79	C88	C83	-178.6(19)
C78	C79	C88	C87	7(3)
C78A	C79A	C80A	C81A	-179(3)
C78A	C79A	C88A	C83A	180(3)
C78A	C79A	C88A	C87A	-6(4)
C79	C80	C81	C82	1(3)
C79A	C80A	C81A	C82A	6(5)
C80	C79	C88	C83	-5(3)
C80	C79	C88	C87	-179.8(18)
C80	C81	C82	C83	0(3)
C80A	C79A	C88A	C83A	6(4)
C80A	C79A	C88A	C87A	180(2)
C80A	C81A	C82A	C83A	-7(4)
C81	C82	C83	C84	-175.2(18)
C81	C82	C83	C88	-4(3)
C81A	C82A	C83A	C84A	179(3)
C81A	C82A	C83A	C88A	7(4)
C82	C83	C84	C85	179.0(18)
C82	C83	C88	C79	7(3)
C82	C83	C88	C87	-179.1(18)
C82A	C83A	C84A	C85A	176(3)

A	B	C	D	Angle/°
C34	C35	C36	C37	-0.6(4)
C35	C34	C39	C30	-179.7(3)
C35	C34	C39	C38	0.4(4)
C35	C36	C37	C24	179.2(3)
C35	C36	C37	C38	-1.6(4)
C36	C37	C38	C27	-177.8(2)
C36	C37	C38	C39	3.1(4)
C37	C24	C25	C26	-0.3(4)
C37	C38	C39	C30	177.5(2)
C37	C38	C39	C34	-2.6(4)
C38	C27	C28	C29	0.4(4)
C39	C30	C31	C32	-1.4(5)
C39	C34	C35	C36	1.2(4)
C40	C23	C24	C25	82.3(3)
C40	C23	C24	C37	-90.9(3)
C40	C41	C42	C43	1.9(6)
C40	C53	C54	C43	0.8(5)
C40	C53	C54	C55	-178.0(3)
C41	C40	C53	C52	-176.4(3)
C41	C40	C53	C54	2.1(5)
C41	C42	C43	C44	179.7(4)
C41	C42	C43	C54	1.2(6)
C42	C43	C44	C45	-176.4(4)
C42	C43	C54	C53	-2.5(5)
C42	C43	C54	C55	176.3(3)
C43	C44	C45	C46	-0.8(7)
C43	C54	C55	C46	1.1(5)
C43	C54	C55	C50	-178.9(3)
C44	C43	C54	C53	178.9(3)
C44	C43	C54	C55	-2.2(5)
C44	C45	C46	C47	179.3(4)
C44	C45	C46	C55	-0.3(6)
C45	C46	C47	C48	179.0(5)
C45	C46	C55	C50	-179.8(4)
C45	C46	C55	C54	0.1(5)
C46	C47	C48	C49	1.8(8)
C47	C46	C55	C50	0.5(6)
C47	C46	C55	C54	-179.5(4)
C47	C48	C49	C50	-1.4(7)
C48	C49	C50	C51	-178.6(4)
C48	C49	C50	C55	0.6(6)
C82A	C83A	C88A	C79A	-7(5)
C82A	C83A	C88A	C87A	179(3)
C83	C84	C85	C86	-3(3)
C83A	C84A	C85A	C86	11(4)
C84	C83	C88	C79	177.9(16)
C84	C83	C88	C87	-8(3)
C84	C85	C86	C73	-178.3(12)
C84	C85	C86	C87	-1(2)
C84A	C83A	C88A	C79A	-179(2)
C84A	C83A	C88A	C87A	7(5)
C84A	C85A	C86	C73	173(2)
C84A	C85A	C86	C87A	-5(3)
C85	C86	C87	C76	-179.1(17)
C85	C86	C87	C88	0(2)
C85A	C86	C87A	C76A	177.8(17)
C85A	C86	C87A	C88A	0(3)
C86	C73	C74	C75	-3.6(5)
C86	C87	C88	C79	178.2(14)
C86	C87	C88	C83	4(3)
C86	C87A	C88A	C79A	-176(2)
C86	C87A	C88A	C83A	-2(4)
C87	C76	C77	C78	-3(3)
C87A	C76A	C77A	C78A	5(3)
C88	C79	C80	C81	2(3)
C88	C83	C84	C85	8(3)
C88A	C79A	C80A	C81A	-6(4)
C88A	C83A	C84A	C85A	-11(4)
O3	C102	C103	C104	33.2(15)
C102	O3	C105	C104	17.4(10)
C102	C103	C104	C105	-22.4(15)
C103	C104	C105	O3	2.7(13)
C105	O3	C102	C103	-30.4(11)
O4	C107	C108	C109	29.6(10)
Cl3[1]	Cl3	C111	Cl4	-174.8(17)
C107	O4	C110	C109	-21.2(10)
C107	C108	C109	C110	-44.7(12)
C108	C109	C110	O4	40.7(12)
C110	O4	C107	C108	-5.8(9)
C89	C90	C91	C91[2]	-176.1(7)
C92[3]	C92	C93	C95	-149.7(14)
C92[3]	C92	C94	C95	170.4(9)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C49	C50	C51	C52	-179.3(4)	C96	C97	C98	C99	-178.4(8)
C49	C50	C55	C46	-0.2(6)	C97	C98	C99	C100	177.8(10)
C49	C50	C55	C54	179.9(4)	C98	C99	C100	C101	-163.3(11)
C50	C51	C52	C53	-1.0(5)	C112	C113	C114	C115	164(3)
C51	C50	C55	C46	179.0(3)	C113	C114	C115	C116	177(2)
C51	C50	C55	C54	-1.0(5)	C114	C115	C116	C117	169(2)
C51	C52	C53	C40	178.5(3)					

[1]2-X,2-Y,1-Z; [2]-X,1-Y,-Z; [3]1-X,2-Y,-Z