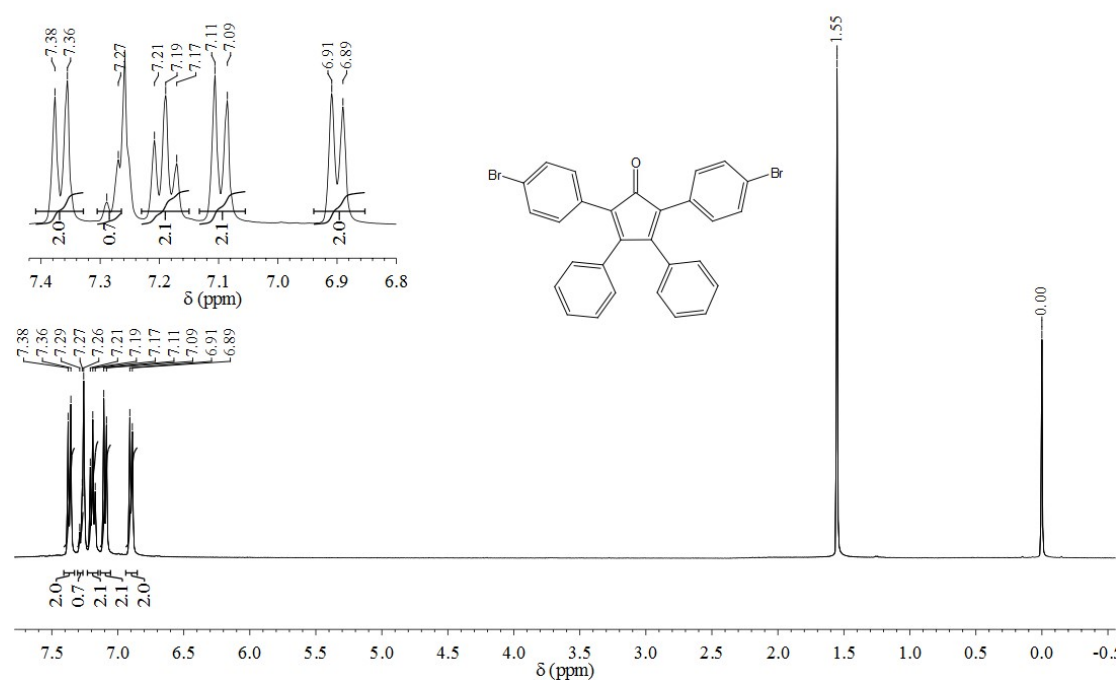


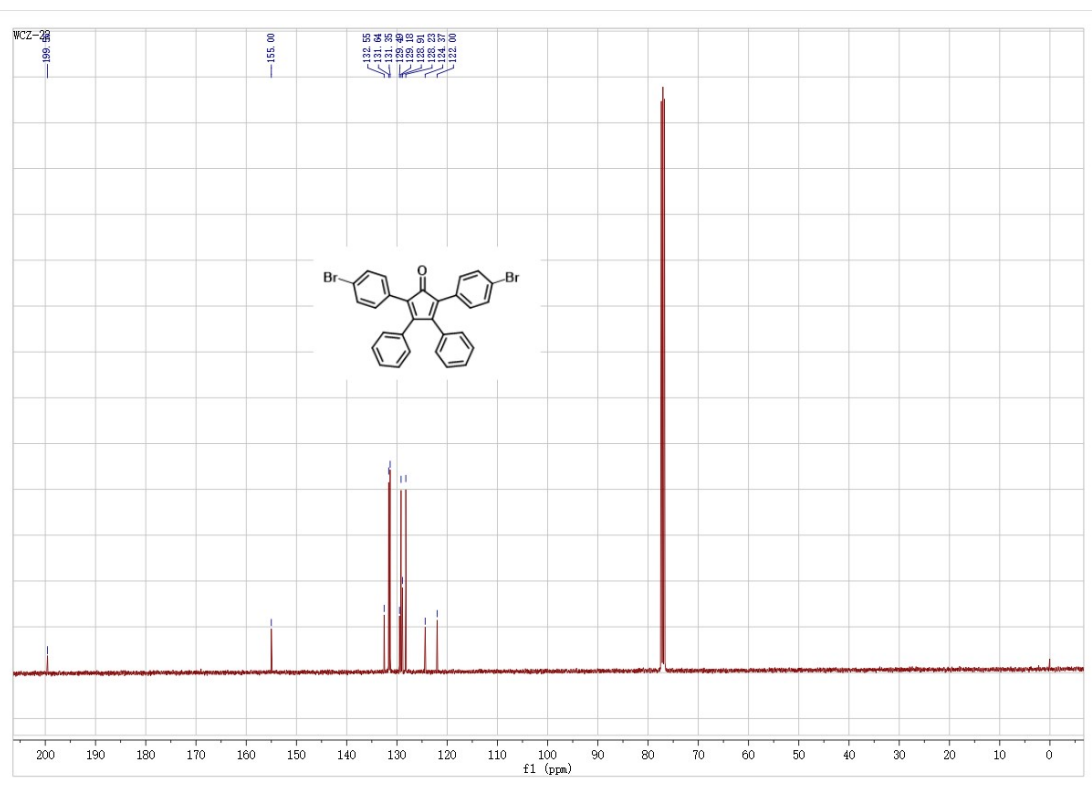
## Position-dependent hexaarylbenzene AIEgens: synthesis, characterization and optical properties

Wen-Xuan Zhao, Li-Feng Yang, Dan Yu, Fei-Yu Chen, Ling Liang, Jing-Yi, Cao, Guang, Yang, Shu-

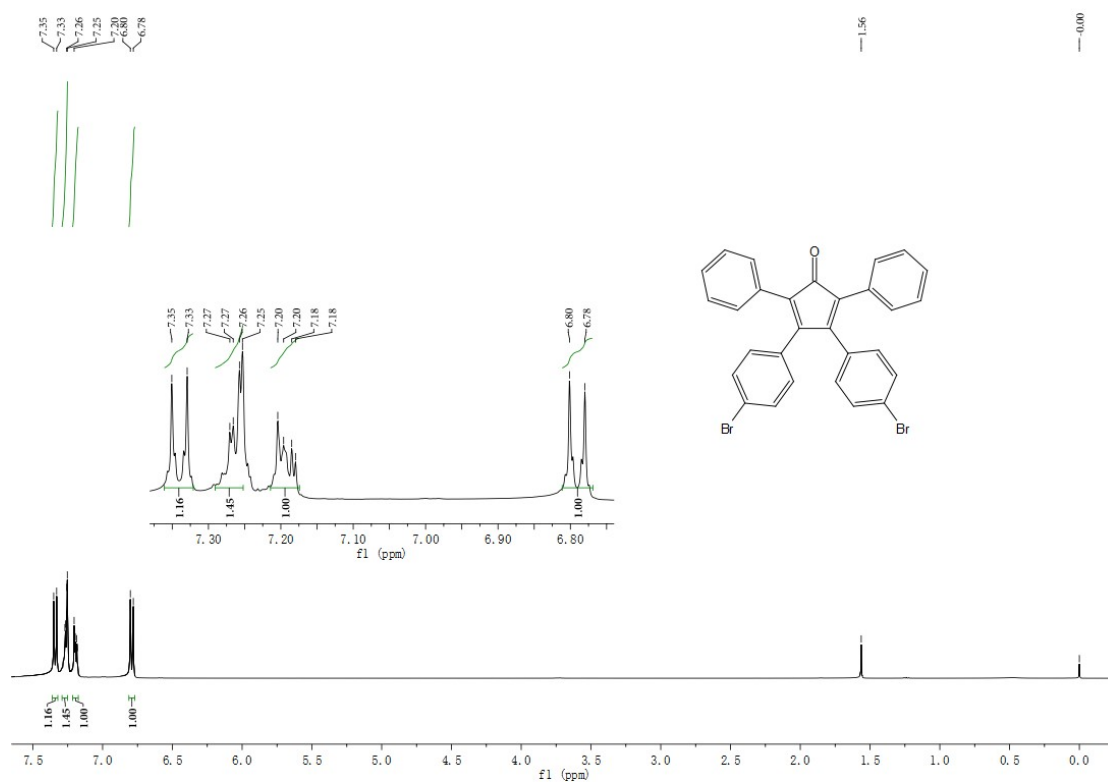
Hai Chen, Takehiko Yamato,\* Carl Redshaw, and Chuan-Zeng Wang\*



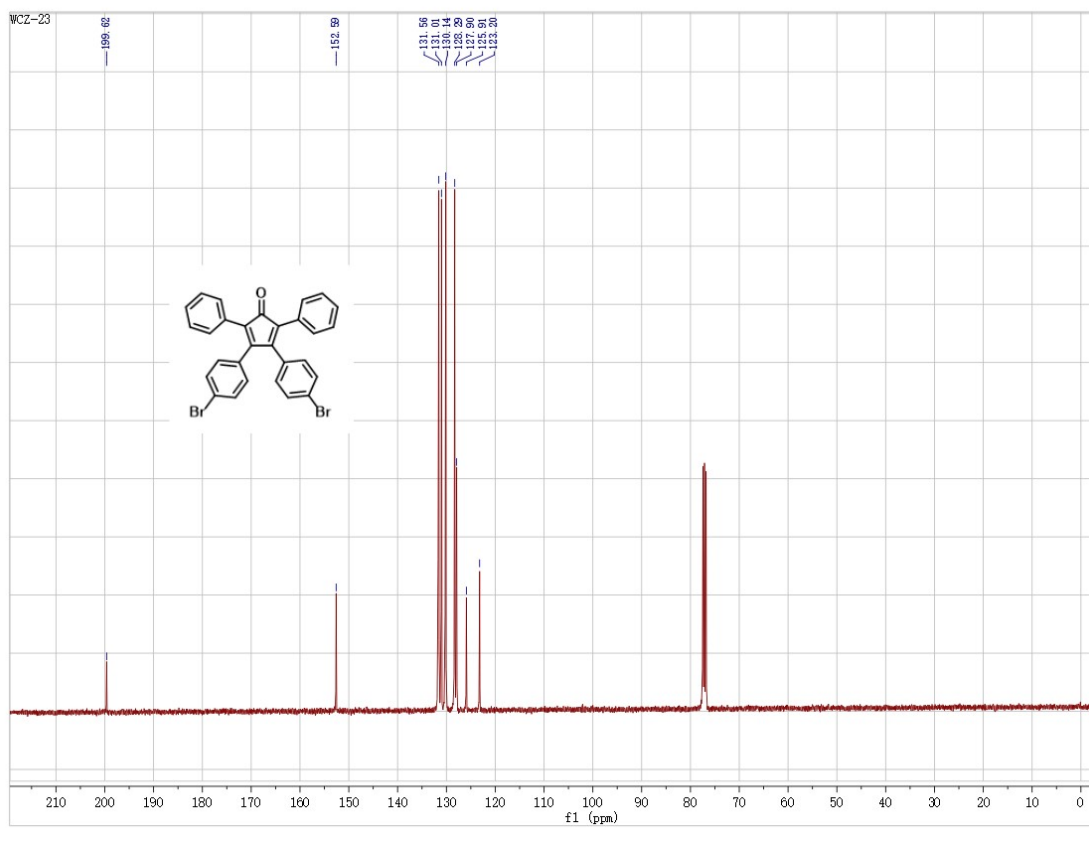
**Figure S1.**  $^1\text{H-NMR}$  spectrum of **3a** (400 MHz,  $\text{CDCl}_3$ ).



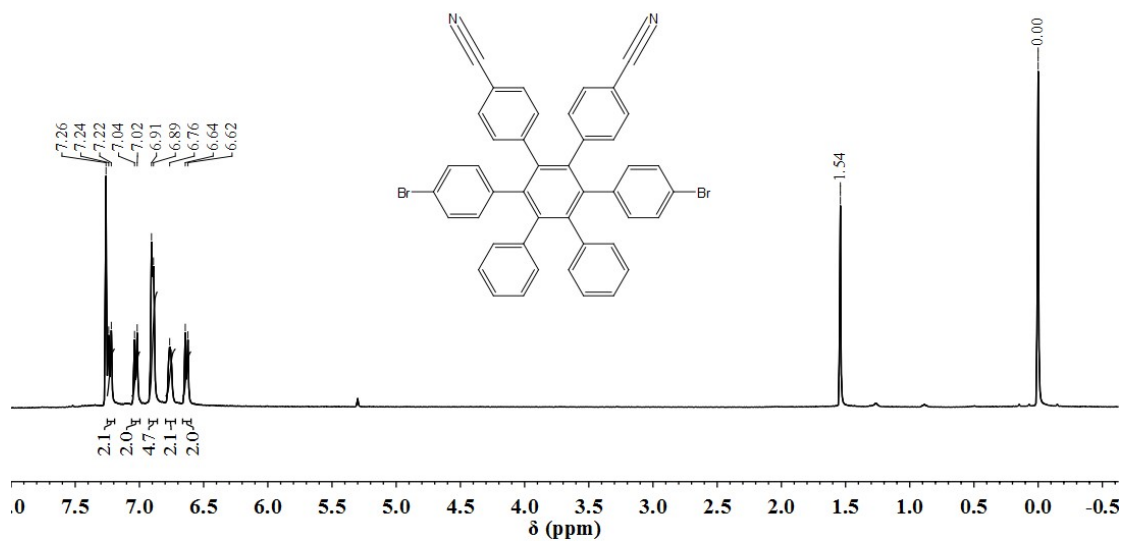
**Figure S2.**  $^{13}\text{C}$ -NMR spectrum of **3a** (100 MHz,  $\text{CDCl}_3$ ).



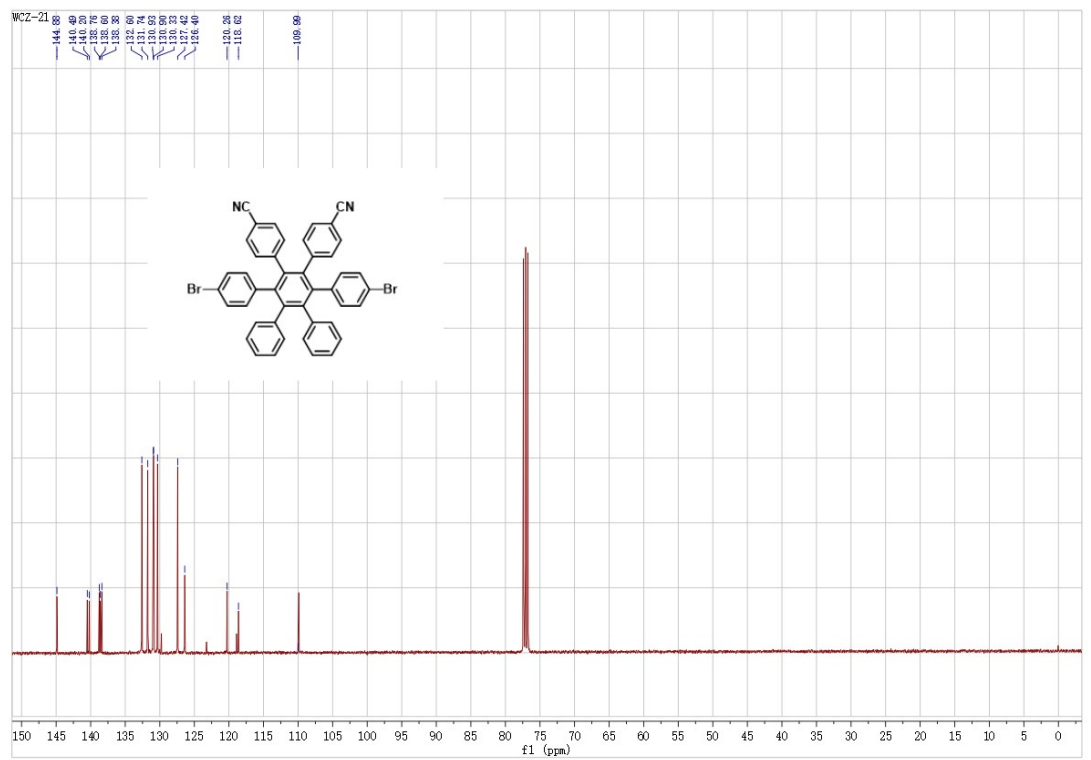
**Figure S3.**  $^1\text{H}$ -NMR spectrum of **3b** (400 MHz,  $\text{CDCl}_3$ ).



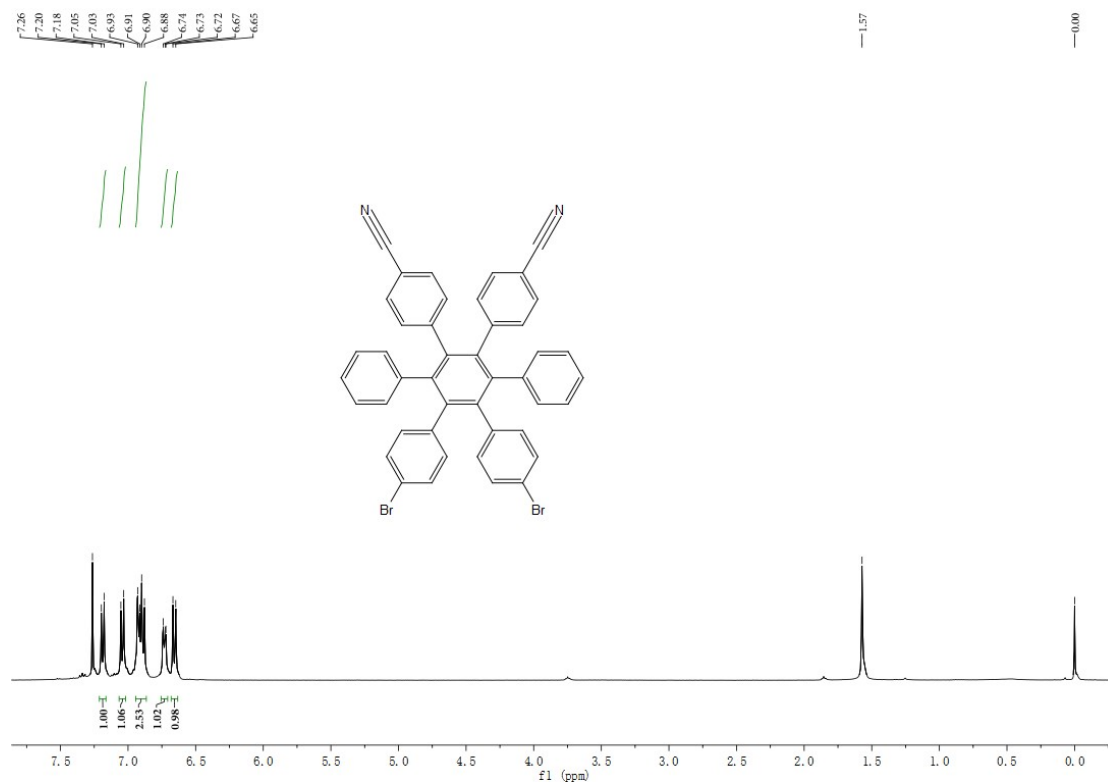
**Figure S4.**  $^{13}\text{C}$ -NMR spectrum of **3b** (100 MHz,  $\text{CDCl}_3$ ).



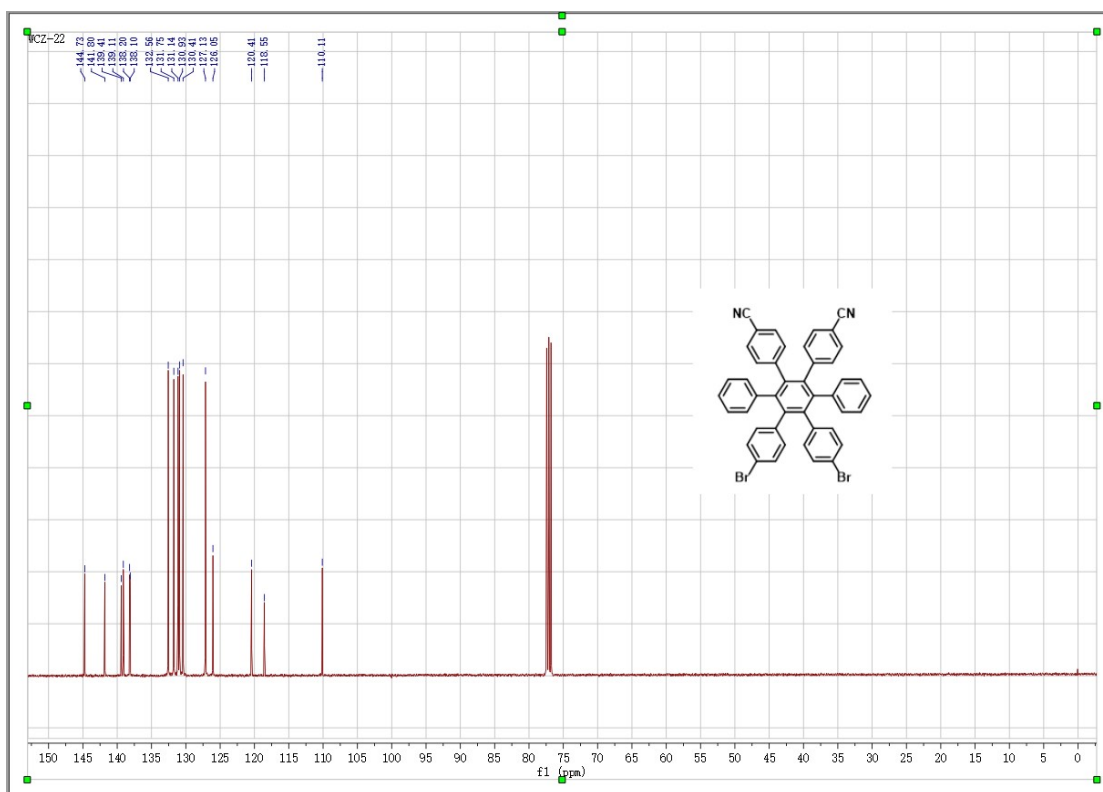
**Figure S5.**  $^1\text{H}$ -NMR spectrum of compound **4a** (400 MHz,  $\text{CDCl}_3$ ).



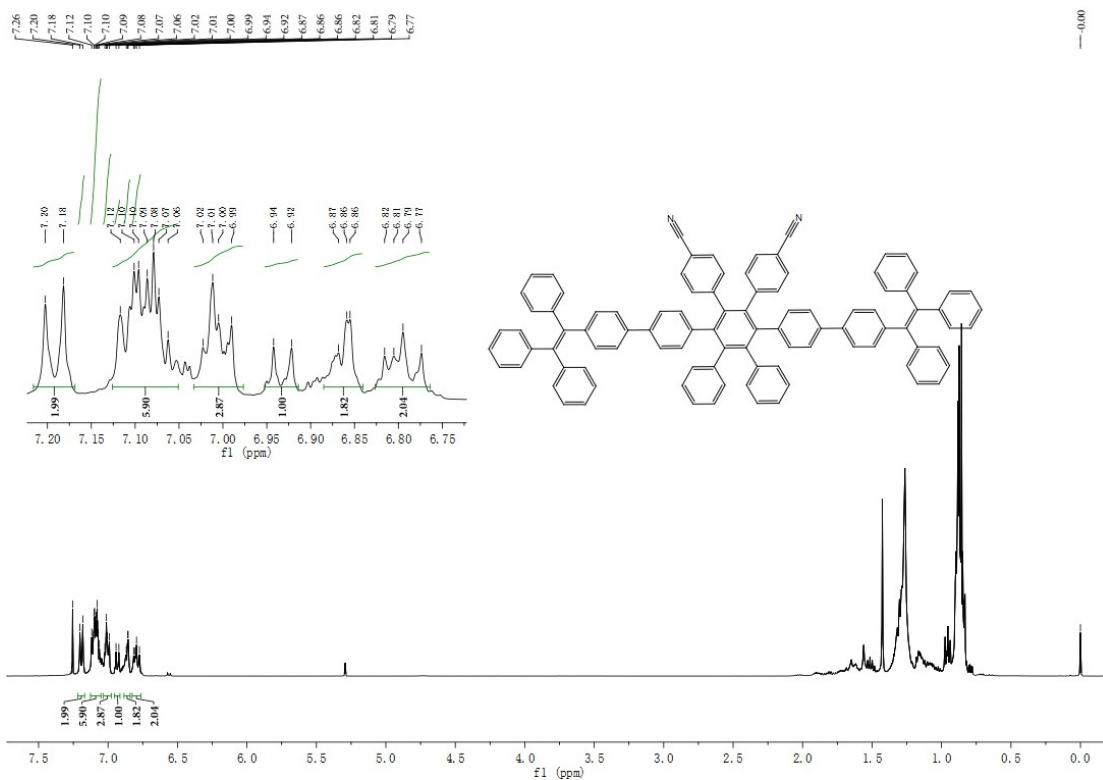
**Figure S6.**  $^{13}\text{C-NMR}$  spectrum of **4a** (100 MHz,  $\text{CDCl}_3$ ).



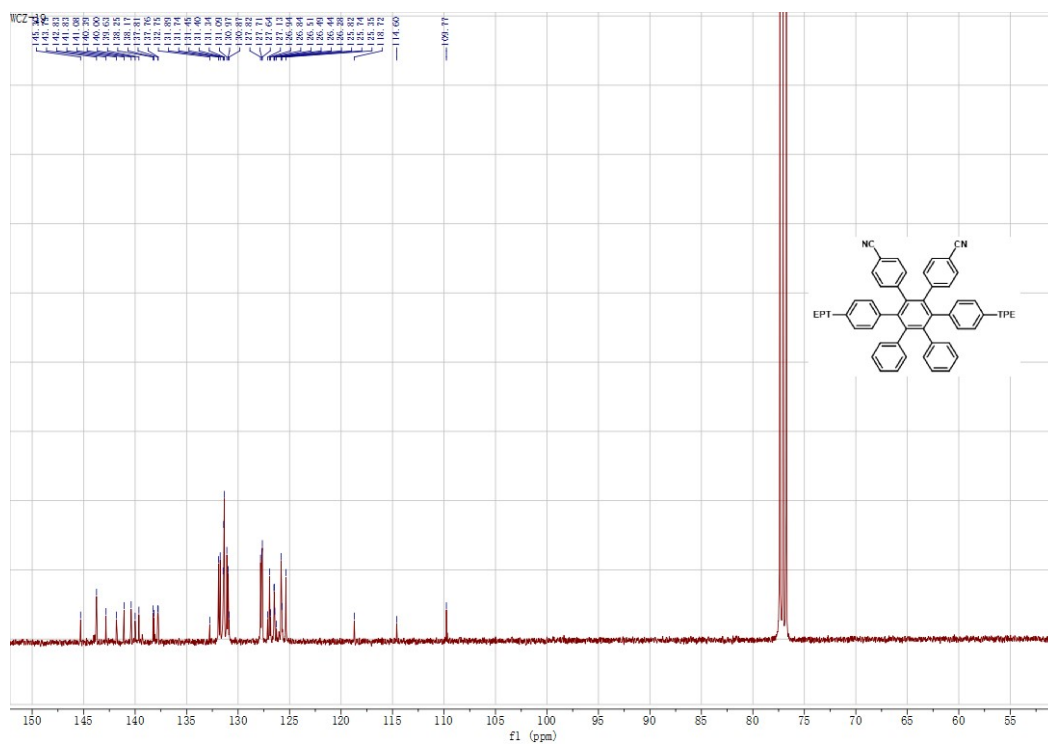
**Figure S7.**  $^1\text{H-NMR}$  spectrum of compound **4b** (400 MHz,  $\text{CDCl}_3$ ).



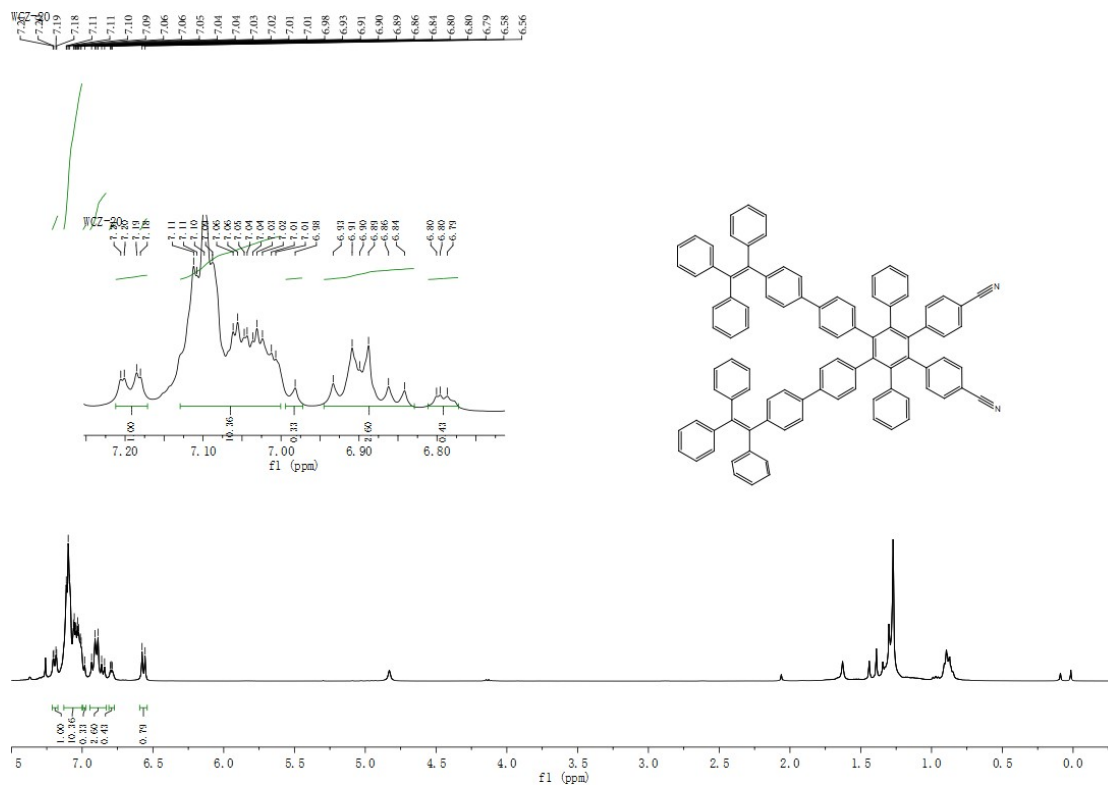
**Figure S8.**  $^{13}\text{C-NMR}$  spectrum of **4b** (100 MHz,  $\text{CDCl}_3$ ).



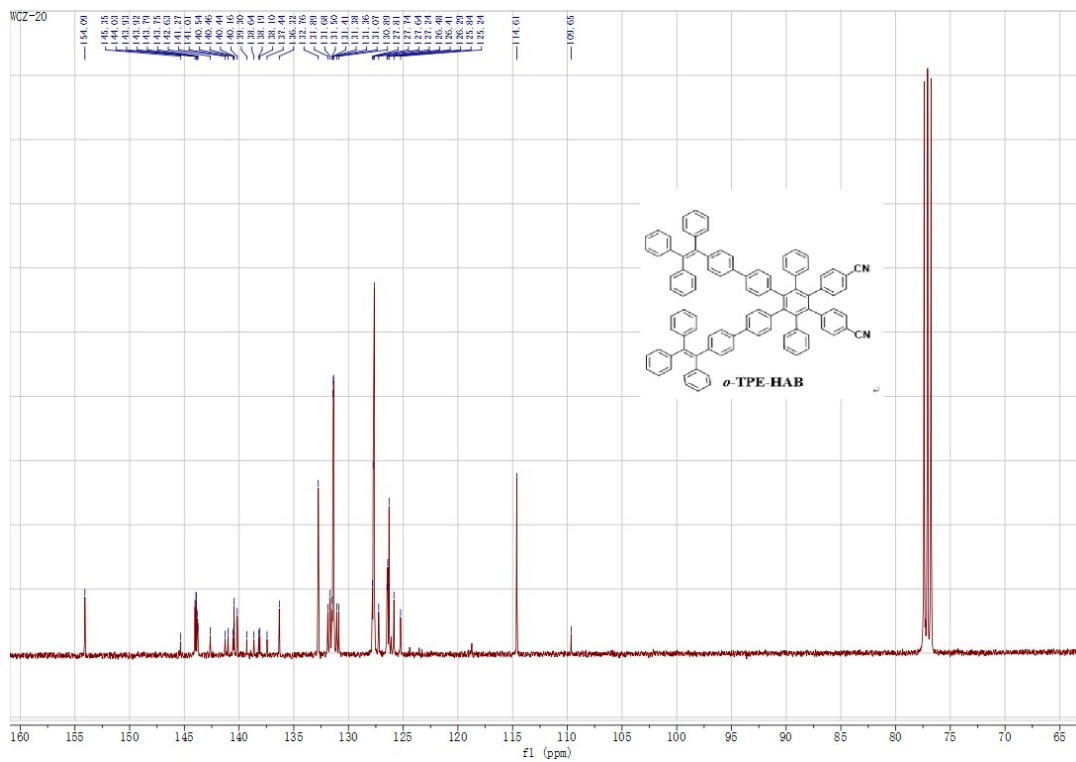
**Figure S9.**  $^1\text{H-NMR}$  spectrum of *p*-TPE-HAB (400 MHz, 293 K,  $\text{CDCl}_3$ ).



**Figure S10.** <sup>13</sup>C-NMR spectrum of *p*-TPE-HAB (100 MHz, 293 K, CDCl<sub>3</sub>).



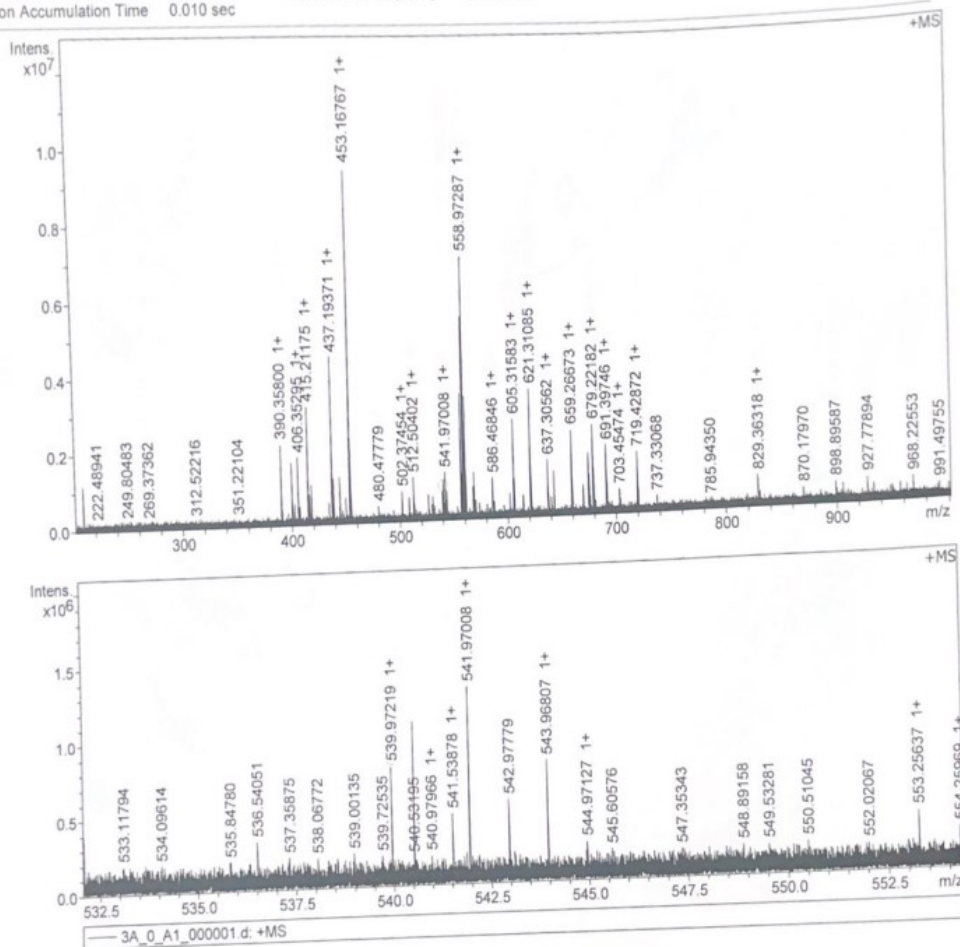
**Figure S11.** <sup>1</sup>H-NMR spectrum of *o*-TPE-HAB (400 MHz, 293 K, CDCl<sub>3</sub>).



**Figure S12.** <sup>13</sup>C-NMR spectrum of *o*-TPE-HAB (100 MHz, 293 K, CDCl<sub>3</sub>).

**Acquisition Parameter**

Acquisition Mode	Single MS	Acquired Scans	9	Calibration Date	Fri Nov 10 05:21:59 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2097152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	4194304
Broadband High Mass	1000.0 m/z	Laser Power	27.2 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.010 sec				

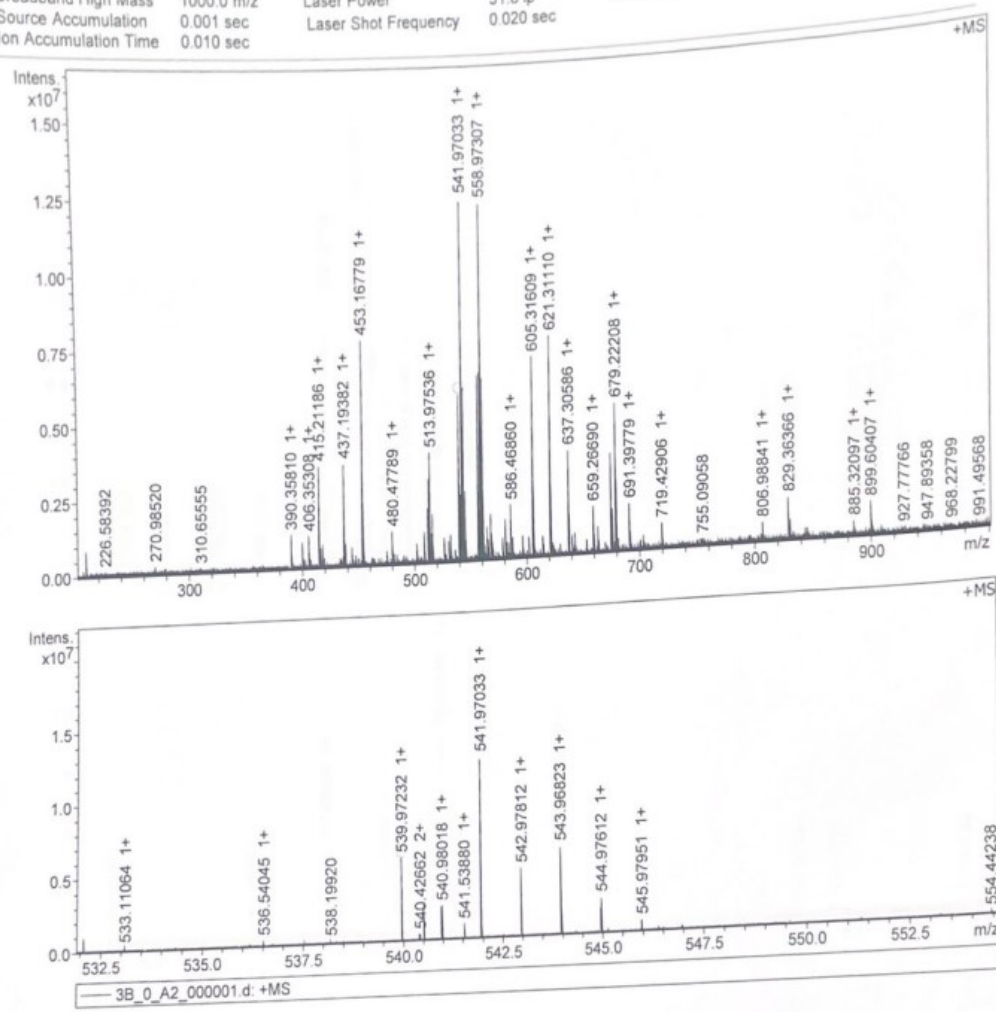


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
539.972193	1	C <sub>29</sub> H <sub>18</sub> Br <sub>2</sub> O	100.00	539.971891	-0.6	0.0	84.4	20.0	odd	ok

**Figure S13.** High resolution MS spectrum of **3a**.



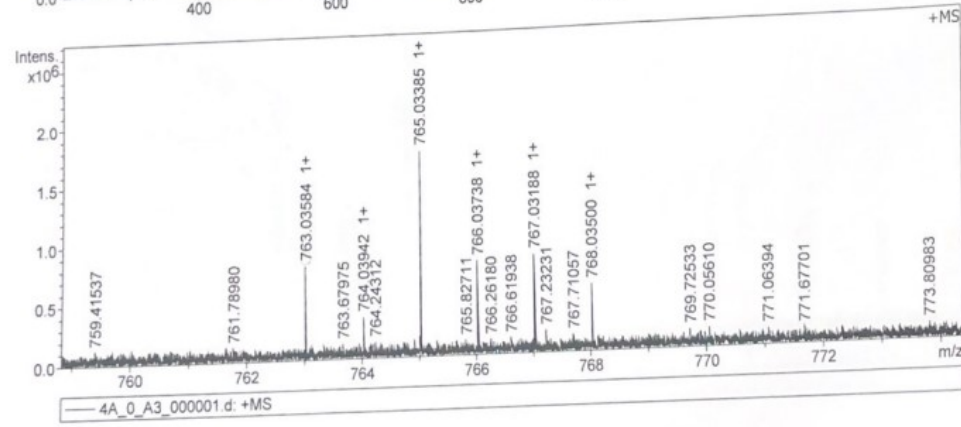
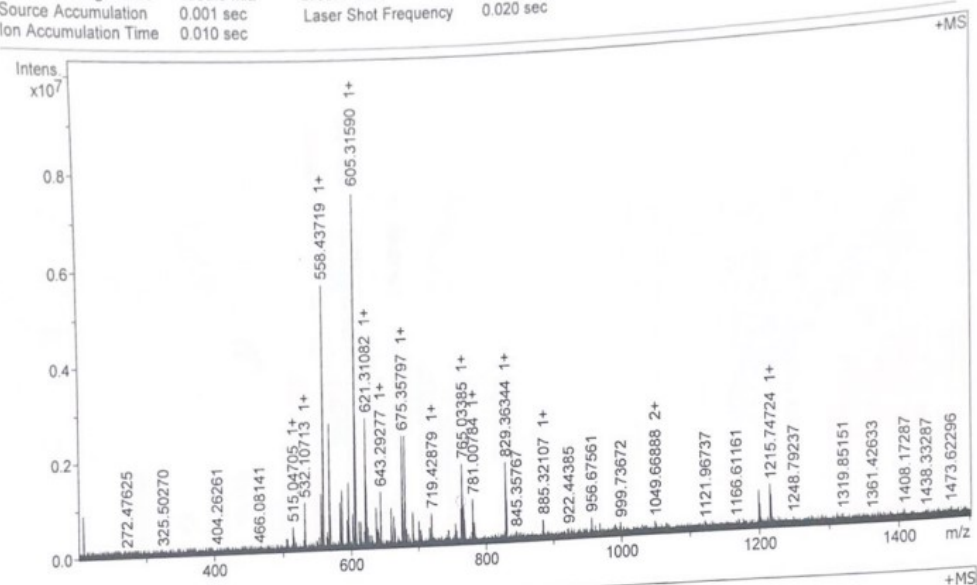
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 Polarity: Positive  
 Broadband Low Mass: 202.1 m/z  
 Broadband High Mass: 1000.0 m/z  
 Source Accumulation: 0.001 sec  
 Ion Accumulation Time: 0.010 sec  
 Acquired Scans: 3  
 No. of Cell Fills: 1  
 No. of Laser Shots: 10  
 Laser Power: 31.8 lp  
 Laser Shot Frequency: 0.020 sec  
 Calibration Date: Fri Nov 10 05:21:59 2023  
 Data Acquisition Size: 2097152  
 Data Processing Size: 4194304  
 Apodization: Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
539.972317	1	C <sub>29</sub> H <sub>18</sub> Br <sub>2</sub> O	100.00	539.971891	0.8	-0.3	22.9	20.0	odd	ok

**Figure S14.** High resolution MS spectrum of **3b**.

**Acquisition Parameter**  
 Acquisition Mode: Single MS  
 Polarity: Positive  
 Broadband Low Mass: 202.1 m/z  
 Broadband High Mass: 1500.0 m/z  
 Source Accumulation: 0.001 sec  
 Ion Accumulation Time: 0.010 sec  
 Acquired Scans: 3  
 No. of Cell Fills: 1  
 No. of Laser Shots: 10  
 Laser Power: 31.8 lp  
 Laser Shot Frequency: 0.020 sec  
 Calibration Date: Fri Nov 10 05:21:59 2023  
 Data Acquisition Size: 2097152  
 Data Processing Size: 4194304  
 Apodization: Sine-Bell Multiplication



— 4A\_0\_A3\_000001.d: +MS

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
763.035837	1	C44H26Br2N2Na	100.00	763.035494	0.5	0.1	49.7	31.5	even	ok

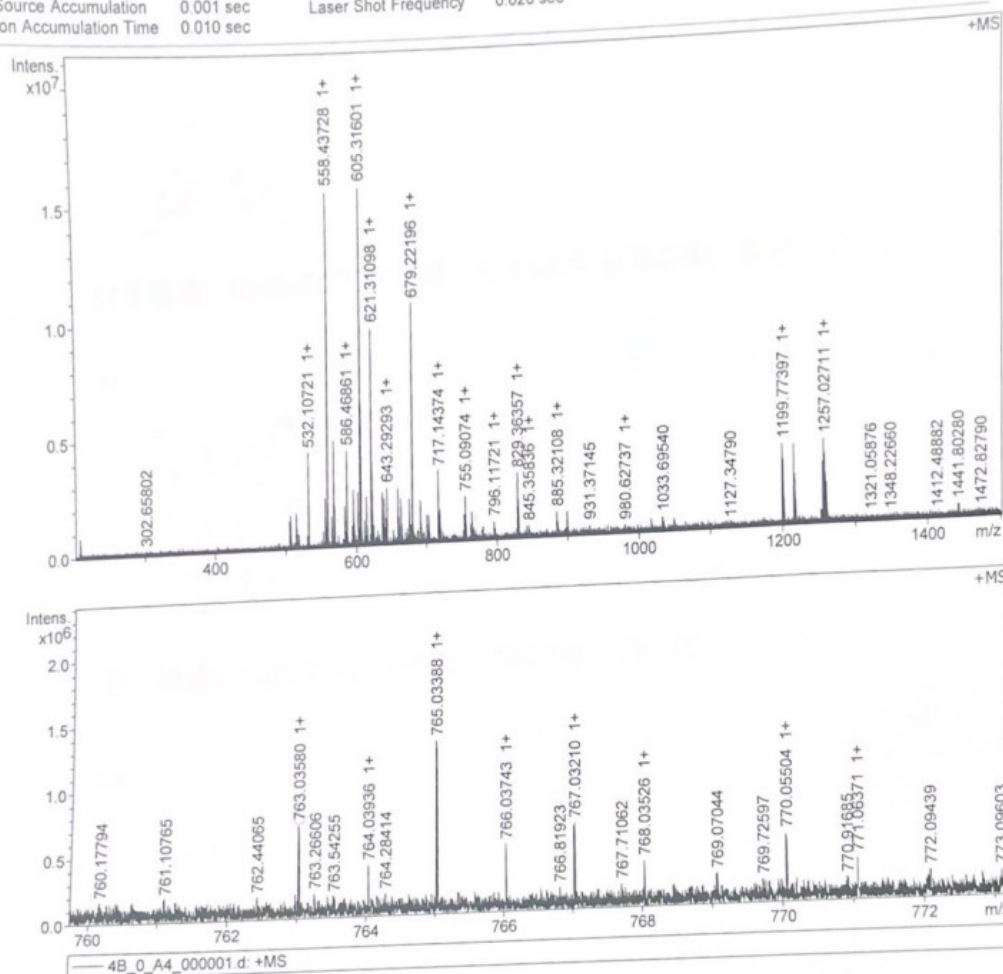
**Figure S15.** High resolution MS spectrum of **4a**.

**Acquisition Parameter**

Acquisition Mode Single MS  
 Polarity Positive  
 Broadband Low Mass 202.1 m/z  
 Broadband High Mass 1500.0 m/z  
 Source Accumulation 0.001 sec  
 Ion Accumulation Time 0.010 sec

Acquired Scans 5  
 No. of Cell Fills 1  
 No. of Laser Shots 10  
 Laser Power 31.8 lp  
 Laser Shot Frequency 0.020 sec

Calibration Date Fri Nov 10 05 21 59 2023  
 Data Acquisition Size 2097152  
 Data Processing Size 4194304  
 Apodization Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
763.03580	1	C <sub>44</sub> H <sub>26</sub> Br <sub>2</sub> N <sub>2</sub> Na	100.00	763.035494	0.4	-0.0	53.6	31.5	even	ok

**Figure S16.** High resolution MS spectrum of **4b**.

**Analysis Info**

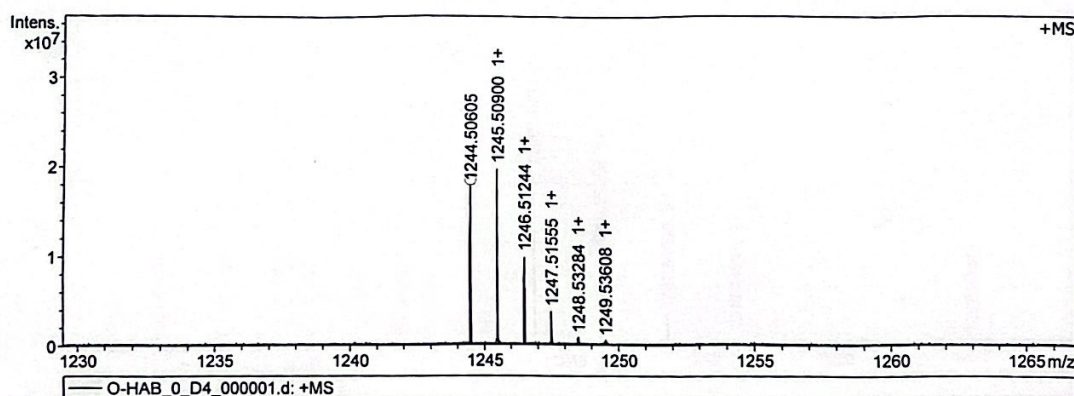
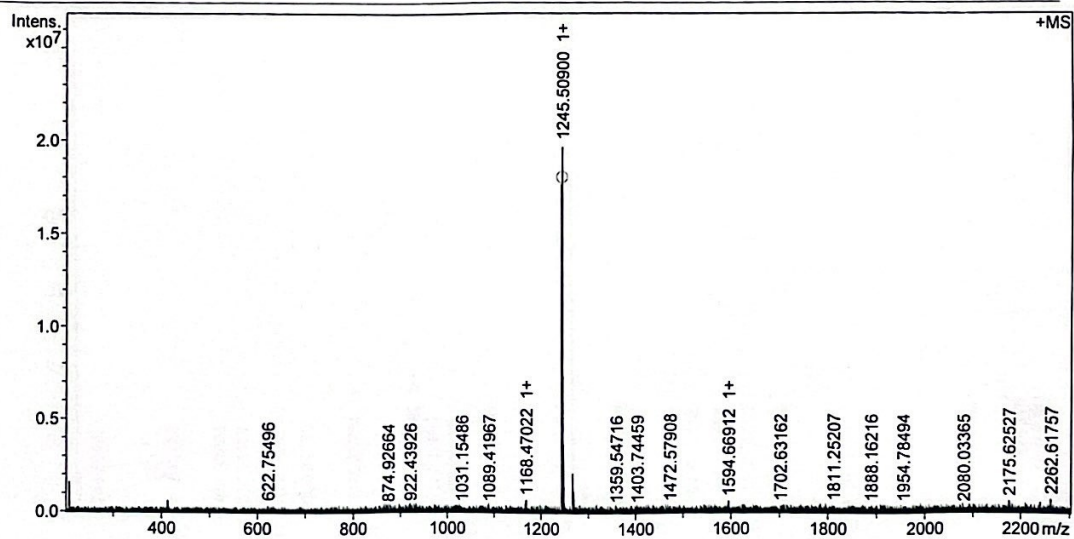
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 Sample Name MURU-N-ESI  
 Comment

Acquisition Date 2/22/2024 5:19:24 PM

Operator  
 Instrument solariX

**Acquisition Parameter**

Acquisition Mode	Single MS	Acquired Scans	6	Calibration Date	Fri Nov 10 05:21:59 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2097152
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Broadband High Mass	2300.0 m/z	Laser Power	19.4 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.010 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
1244.506054	1	C96H64N2	100.00	1244.506401	-0.3	0.5	24.8	66.0	odd	ok

**Figure S17.** High resolution MS spectrum of *p*-TPE-HAB.

# MALDI,P-HAB,20240222

## Analysis Info

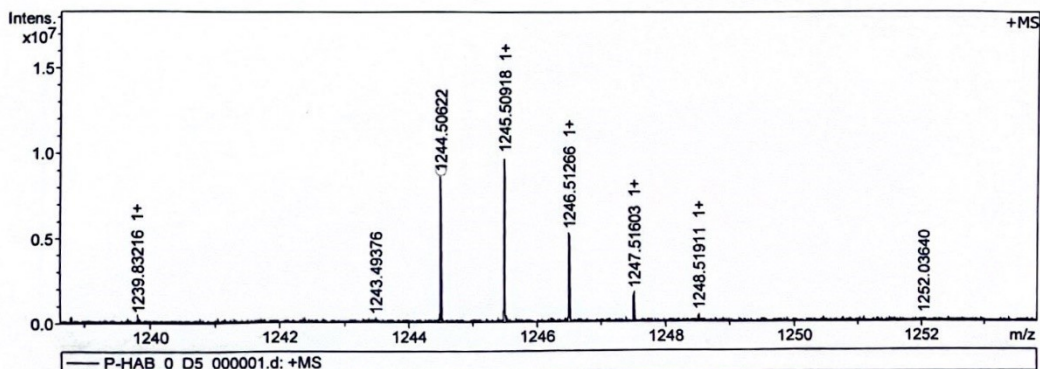
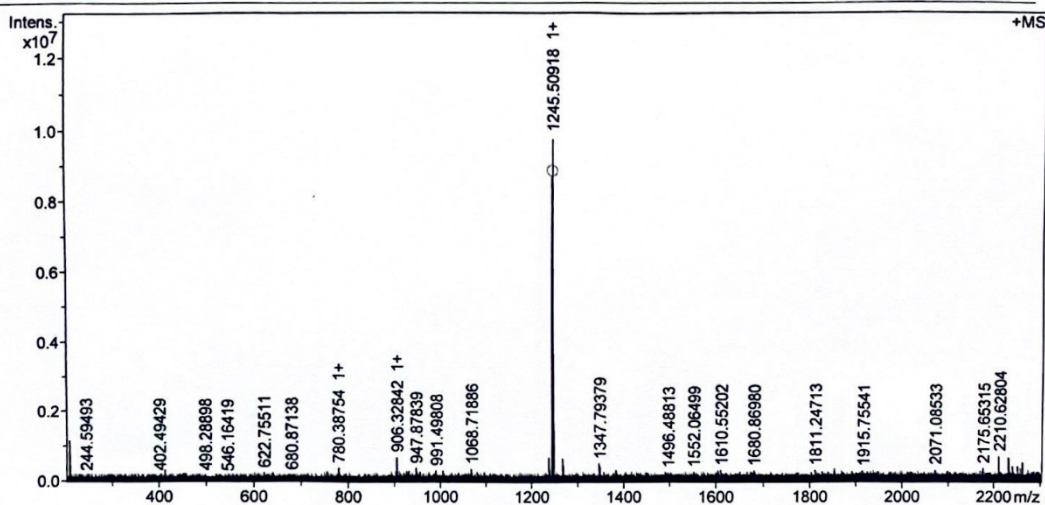
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 Comment

Acquisition Date 2/22/2024 5:20:21 PM

Operator  
 Instrument solariX

## Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	5	Calibration Date	Fri Nov 10 05:21:59 2023
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2097152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	4194304
Broadband High Mass	2300.0 m/z	Laser Power	26.8 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.010 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
1244.506217	1	C96H64N2	100.00	1244.506401	0.1	0.3	27.2	66.0	odd	ok

Figure S18. High resolution MS spectrum of *o*-TPE-HAB.



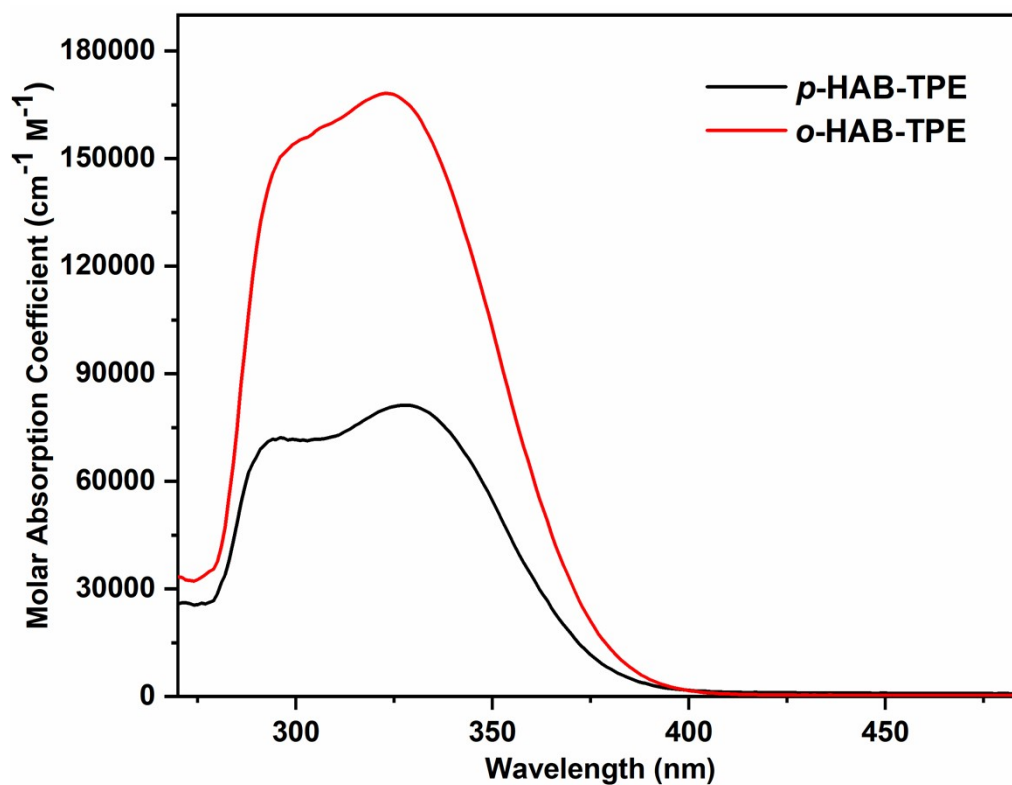


Figure S19. UV-Vis absorption spectra of compounds *p*-TPE-HAB and *o*-TPE-HAB.

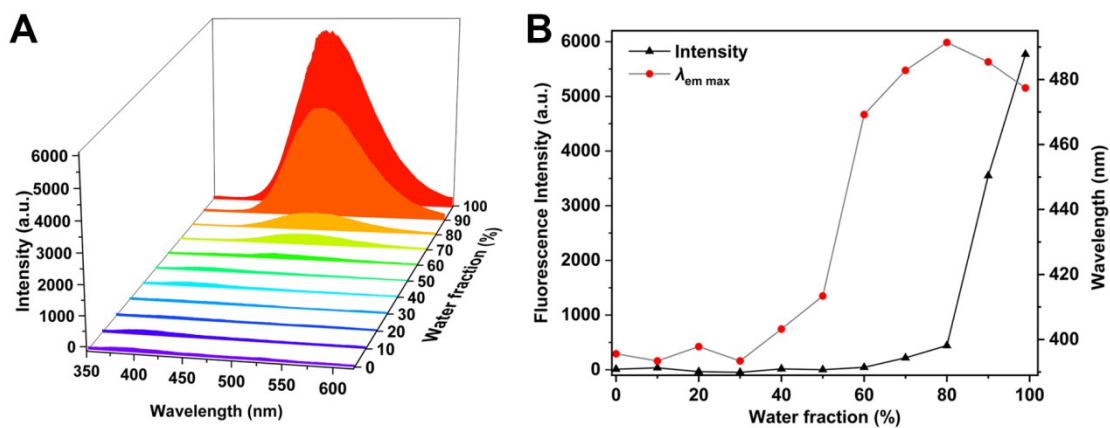


Figure S20. (A) The fluorescence spectra of *o*-TPE-HAB in mixed H<sub>2</sub>O/THF solutions ( $1 \times 10^{-6}$  M); (B) Plots of maximum emission wavelength and emission intensity at different water fractions (0–99 vol%) for *o*-TPE-HAB.

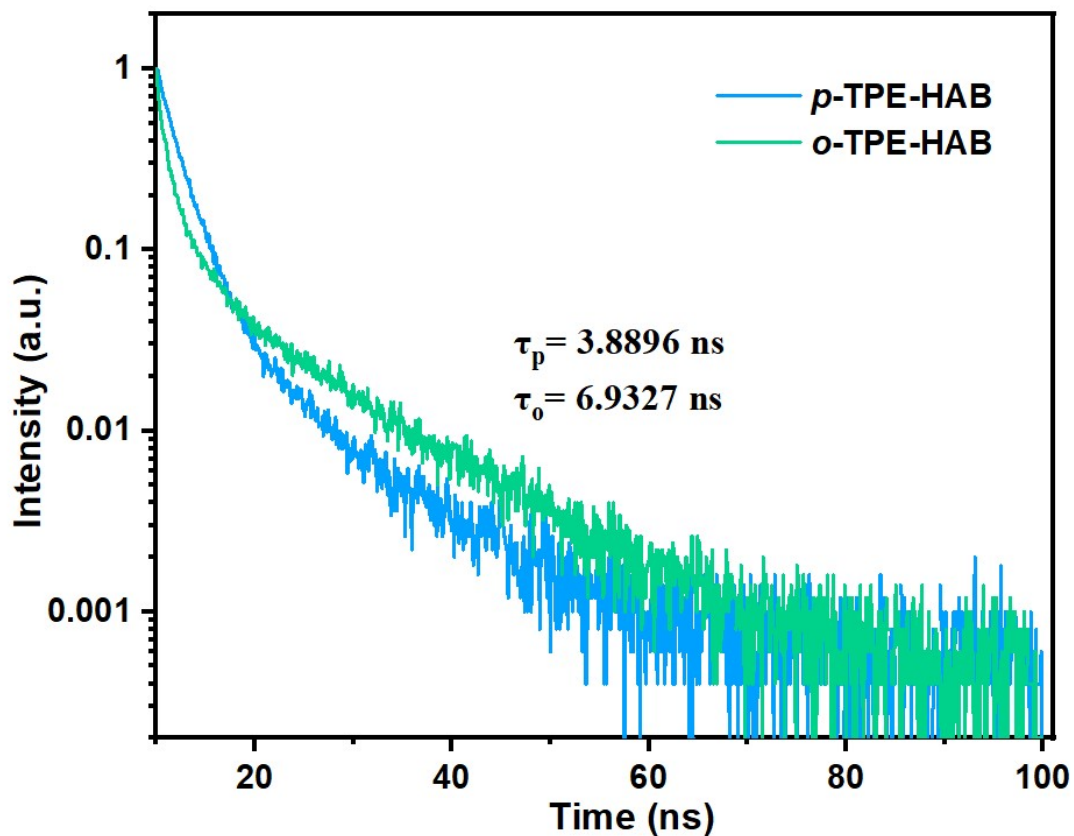


Figure S21. Decay curves of *p*-TPE-HAB and *o*-TPE-HAB in THF solution.

Table S1. Cartesian coordinates of the optimized geometry of *p*-TPE-HAB

C	0.639247	-1.486922	-0.108831
C	-0.754816	-1.431604	-0.108267
C	-1.403916	-0.197153	-0.103477
C	-0.658891	0.982730	-0.098048
C	0.734834	0.927345	-0.098133
C	1.383979	-0.307558	-0.103922
C	1.557441	2.229221	-0.092132
C	1.932825	2.822812	-1.297104
C	1.927645	2.814877	1.119137
C	2.677384	4.002673	-1.291566
H	1.640922	2.361719	-2.251792
C	2.672431	3.994200	1.124596
H	1.631603	2.346638	2.069089
C	3.047007	4.588376	-0.080831
H	2.972861	4.470748	-2.241694
H	2.964356	4.456005	2.079054
C	-1.375918	2.345611	-0.092676
C	-1.699003	2.968672	-1.297928
C	-1.702090	2.957457	1.118304
C	-2.349305	4.202995	-1.292963

H	-1.442420	2.486581	-2.252389
C	-2.351812	4.191708	1.123192
H	-1.447196	2.466032	2.068476
C	-2.675806	4.814362	-0.082519
H	-2.604339	4.693848	-2.243312
H	-2.609001	4.674174	2.077422
C	-2.942700	-0.135977	-0.103741
C	-3.639314	-0.101888	-1.311545
C	-3.640162	-0.114252	1.104684
C	-5.033404	-0.047269	-1.311688
H	-3.089971	-0.119366	-2.263994
C	-5.033899	-0.059168	1.104466
H	-3.090689	-0.141079	2.056868
C	-5.730615	-0.026069	-0.103798
H	-5.582452	-0.020849	-2.264049
H	-5.583869	-0.042026	2.056680
C	-1.576656	-2.733962	-0.114778
C	-1.951226	-3.316463	-1.325402
C	-1.946979	-3.331152	1.090810
C	-2.695090	-4.496761	-1.331203
H	-1.659228	-2.846279	-2.275616
C	-2.691070	-4.510911	1.084935
H	-1.651578	-2.871655	2.045220
C	-3.064832	-5.093993	-0.126150
H	-2.989925	-4.956092	-2.285787
H	-2.983089	-4.981805	2.034912
H	-3.651265	-6.024158	-0.130538
C	1.355693	-2.850106	-0.114752
C	1.679272	-3.462900	-1.325125
C	1.680843	-3.472501	1.091116
C	2.329047	-4.697499	-1.330386
H	1.423495	-2.972494	-2.275557
C	2.330038	-4.707028	1.085777
H	1.425560	-2.989171	2.045327
C	2.654528	-5.319411	-0.125050
H	2.584471	-5.180257	-2.284769
H	2.586422	-5.197807	2.035976
H	3.166493	-6.292553	-0.129014
C	2.922778	-0.368365	-0.104291
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C	3.619710	-0.390855	-1.313008
C	5.014006	-0.456456	1.102794
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C	5.013435	-0.446254	-1.313367



H	3.069789	-0.365399	-2.264972
C	5.710645	-0.479454	-0.105392
H	5.563471	-0.482286	2.054930
H	5.562988	-0.463983	-2.265812
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C	-7.952074	0.426964	1.047458
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H	-7.442454	-0.613306	-2.162972
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H	-9.884128	0.792446	1.954764
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C	7.960970	-0.192235	-1.253892
C	7.931924	-0.945859	1.041651
C	9.355048	-0.247164	-1.254216
H	7.423416	0.127284	-2.158428
C	9.325651	-1.001206	1.041105
H	7.370675	-1.220773	1.946482
C	10.037307	-0.651461	-0.106777
H	9.915874	0.028193	-2.159089
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C	-11.596108	0.205939	-0.104649
C	-12.321764	-0.872275	0.279336
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C	-14.572191	-1.160957	-0.868596
C	-14.541908	-0.380487	1.417943
C	-15.965953	-1.098568	-0.871362
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C	-15.935316	-0.317686	1.414950
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H	-17.745927	-0.627721	0.268288
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C	12.621228	-2.190040	-1.892980
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C	13.271375	-3.357247	-2.294735
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C	13.263353	-4.147378	-0.011412
H	12.354804	-2.831136	1.448688
C	13.592535	-4.335736	-1.354010
H	13.530498	-3.505780	-3.353006
H	13.516331	-4.919229	0.730021
H	14.104793	-5.255817	-1.670511
C	11.592823	1.656842	0.727196
C	11.250117	1.838642	2.066869
C	11.293090	2.646302	-0.210004
C	10.608745	3.010136	2.470249
H	11.486520	1.059240	2.805712
C	10.651445	3.817283	0.193271
H	11.563346	2.502710	-1.266243
C	10.309587	3.999411	1.533560
H	10.339036	3.153467	3.526590
H	10.415078	4.597278	-0.545114
H	9.803929	4.922715	1.851283
C	13.839994	0.294572	0.278752
C	14.552337	0.657294	-0.864149
C	14.521388	-0.131834	1.419408
C	15.946103	0.594990	-0.866719
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H	16.507555	0.881434	-1.767754
H	16.452108	-0.530574	2.315420
H	17.725749	0.119924	0.271692
C	-3.393397	6.176945	-0.076781
C	3.869076	5.890591	-0.074462
N	-3.927676	7.191449	-0.072509
N	4.481144	6.860149	-0.069720

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Table S2. Cartesian coordinates of the optimized geometry of *o*-TPE-HAB

C	-3.909247	-0.725489	0.032079
C	-3.920193	0.669515	0.014287
C	-5.133257	1.357719	0.022666
C	-6.336151	0.650867	0.047648
C	-6.325136	-0.743807	0.064955
C	-5.111602	-1.432059	0.057567
C	-7.675409	1.411066	0.056811
C	-8.265523	1.770087	1.268459
C	-8.298829	1.740408	-1.147390
C	-9.478426	2.459485	1.276644
H	-7.774294	1.511010	2.217572
C	-9.511677	2.429225	-1.139120
H	-7.833385	1.457176	-2.102606
C	-10.101347	2.789149	0.072967
H	-9.943291	2.742841	2.232025
H	-10.003257	2.688923	-2.088003
C	-7.652419	-1.524295	0.092516
C	-8.270411	-1.892051	-1.102499
C	-8.237092	-1.863286	1.313360
C	-9.472451	-2.599825	-1.077426
H	-7.809713	-1.625371	-2.064726
C	-9.439087	-2.570478	1.338348
H	-7.749672	-1.573164	2.255458
C	-10.056634	-2.939130	0.142881
H	-9.959294	-2.890062	-2.019705
H	-9.900133	-2.837784	2.300355
C	-5.099779	-2.971891	0.076957
C	-5.111781	-3.684779	-1.121738
C	-5.077449	-3.654036	1.294083
C	-5.100265	-5.079780	-1.104082
H	-5.129008	-3.147492	-2.081043

C	-5.066415	-5.048706	1.311664
H	-5.068048	-3.091735	2.239084
C	-5.077427	-5.761655	0.112501
H	-5.109280	-5.641639	-2.049267
H	-5.048824	-5.586607	2.270740
H	-5.068528	-6.861133	0.126602
C	-2.569656	-1.485110	0.023452
C	-1.979855	-1.845554	-1.187926
C	-1.946013	-1.813189	1.227881
C	-0.765858	-2.533029	-1.195655
H	-2.470895	-1.586828	-2.137232
C	-0.732544	-2.500918	1.220084
H	-2.411269	-1.528938	2.182885
C	-0.142204	-2.860533	0.008232
H	-0.300795	-2.816725	-2.150839
H	-0.240795	-2.759635	2.169148
C	-2.592443	1.449227	-0.012763
C	-2.006257	1.786583	-1.232517
C	-1.975519	1.817937	1.183344
C	-0.803792	2.493656	-1.256926
H	-2.492374	1.496479	-2.175264
C	-0.773101	2.524426	1.158865
H	-2.437864	1.551781	2.144955
C	-0.187371	2.862667	-0.061349
H	-0.342028	2.759922	-2.218705
H	-0.286641	2.815150	2.101368
C	-5.145439	2.897557	0.003917
C	-5.135076	3.609937	1.202928
C	-5.167244	3.580208	-1.212935
C	-5.145309	5.004955	1.185831
H	-5.117523	3.072257	2.162008
C	-5.177952	4.974888	-1.229944
H	-5.175470	3.018307	-2.158184
C	-5.166588	5.687345	-0.030492
H	-5.136687	5.566421	2.131254
H	-5.195145	5.513189	-2.188804
H	-5.174836	6.786833	-0.044148
C	1.140060	3.642932	-0.088035
C	1.944976	3.689381	1.050022
C	1.537423	4.303922	-1.250967
C	3.147928	4.395623	1.025505
H	1.632277	3.168286	1.966494
C	2.739870	5.010370	-1.275259
H	0.902582	4.267206	-2.148144

C	3.545393	5.055914	-0.137072
H	3.782605	4.431750	1.922736
H	3.053311	5.531418	-2.191631
C	1.197705	-3.619595	-0.000038
C	1.807114	-3.972332	1.203880
C	1.802406	-3.954196	-1.212307
C	3.020605	-4.660702	1.196282
H	1.330639	-3.709110	2.159353
C	3.015842	-4.641984	-1.219824
H	1.321751	-3.675918	-2.161427
C	3.624815	-4.995622	-0.015455
H	3.500684	-4.939103	2.145576
H	3.492672	-4.905826	-2.175069
C	-11.440297	3.549896	0.081750
C	-11.383589	-3.720161	0.170812
N	-12.437206	4.116307	0.088290
N	-12.371568	-4.301674	0.191608
C	4.873066	5.835749	-0.164302
C	4.882632	7.174160	0.048138
C	4.964409	-5.755235	-0.024098
C	4.980281	-7.110332	-0.029196
C	6.194404	5.092109	-0.433867
C	6.626360	4.890022	-1.744514
C	6.959464	4.620044	0.633398
C	7.823835	4.217010	-1.988602
H	6.023856	5.262237	-2.585755
C	8.156405	3.946786	0.389278
H	6.618650	4.779450	1.666710
C	8.588844	3.745585	-0.921799
H	8.164440	4.058176	-3.021996
H	8.759582	3.574616	1.230194
H	9.532578	3.214970	-1.114004
C	5.939845	7.795748	0.979550
C	5.810948	7.670850	2.362665
C	7.026770	8.484410	0.439592
C	6.769202	8.233326	3.206373
H	4.954708	7.127897	2.788454
C	7.984503	9.047133	1.283172
H	7.128158	8.582809	-0.650974
C	7.855943	8.921259	2.666660
H	6.667629	8.134358	4.296800
H	8.841238	9.589947	0.857929
H	8.611194	9.364793	3.331493
C	3.839917	8.075628	-0.638668

C0	2.875029	8.732753	0.124483
C	3.860247	8.234718	-2.024848
C	1.930917	9.550045	-0.497738
H	2.858986	8.607865	1.216906
C	2.916037	9.051455	-2.646897
H	4.621085	7.716451	-2.626362
C	1.951531	9.709491	-1.883270
H	1.170546	10.068396	0.104168
H	2.931791	9.177033	-3.739351
H	1.207388	10.353467	-2.373858
C	6.290520	-4.972277	-0.026956
C	6.889134	-4.609596	1.179421
C	6.893121	-4.625287	-1.236785
C	8.090930	-3.900970	1.176735
H	6.414681	-4.883218	2.132976
C	8.094385	-3.916419	-1.239395
H	6.420919	-4.911306	-2.187845
C	8.693559	-3.554561	-0.032556
H	8.562951	-3.615511	2.127973
H	8.569551	-3.642796	-2.192717
H	9.640671	-2.995899	-0.034857
C	6.324365	-7.861972	-0.037828
C	6.941659	-8.201283	1.165932
C	6.924956	-8.203281	-1.250270
C	8.158936	-8.882932	1.158014
H	6.468426	-7.932774	2.121544
C	8.142176	-8.884348	-1.258110
H	6.438083	-7.935589	-2.199265
C	8.759041	-9.224558	-0.053891
H	8.645235	-9.150749	2.107187
H	8.615769	-9.153474	-2.213492
H	9.718532	-9.761648	-0.060316
C	3.658846	-7.901155	-0.026387
C	3.054118	-8.253477	-1.232785
C	3.066196	-8.264961	1.183418
C	1.857380	-8.970612	-1.230144
H	3.521107	-7.967240	-2.186321
C	1.869498	-8.981513	1.185983
H	3.543156	-7.987005	2.134494
C	1.265226	-9.334718	-0.020877
H	1.380998	-9.248675	-2.181398
H	1.402168	-9.268375	2.139286
H	0.321918	-9.899780	-0.018611

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