

Supporting Information

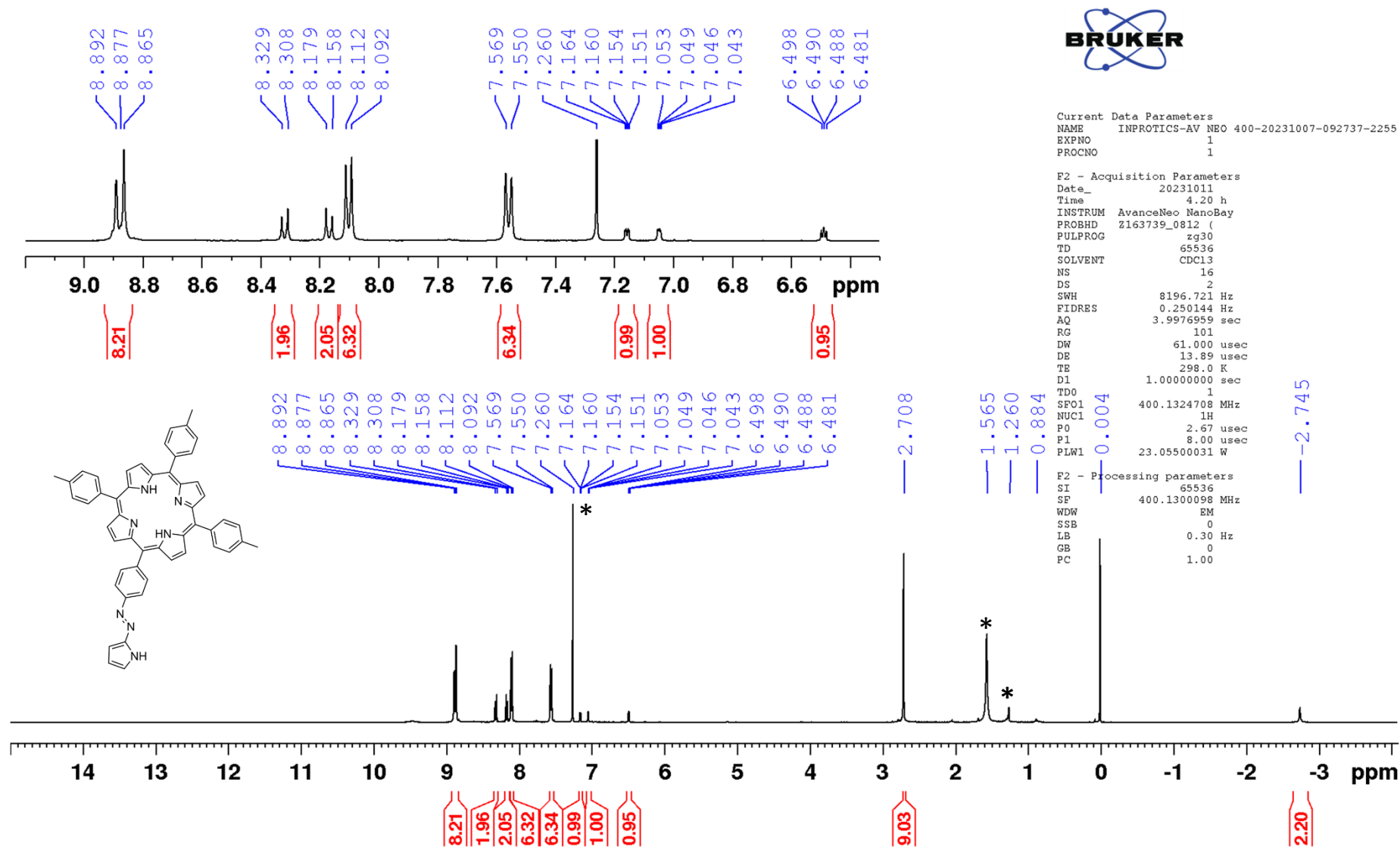
Porphyrin-azoheteroarenes: Synthesis, photophysical, and computational studies

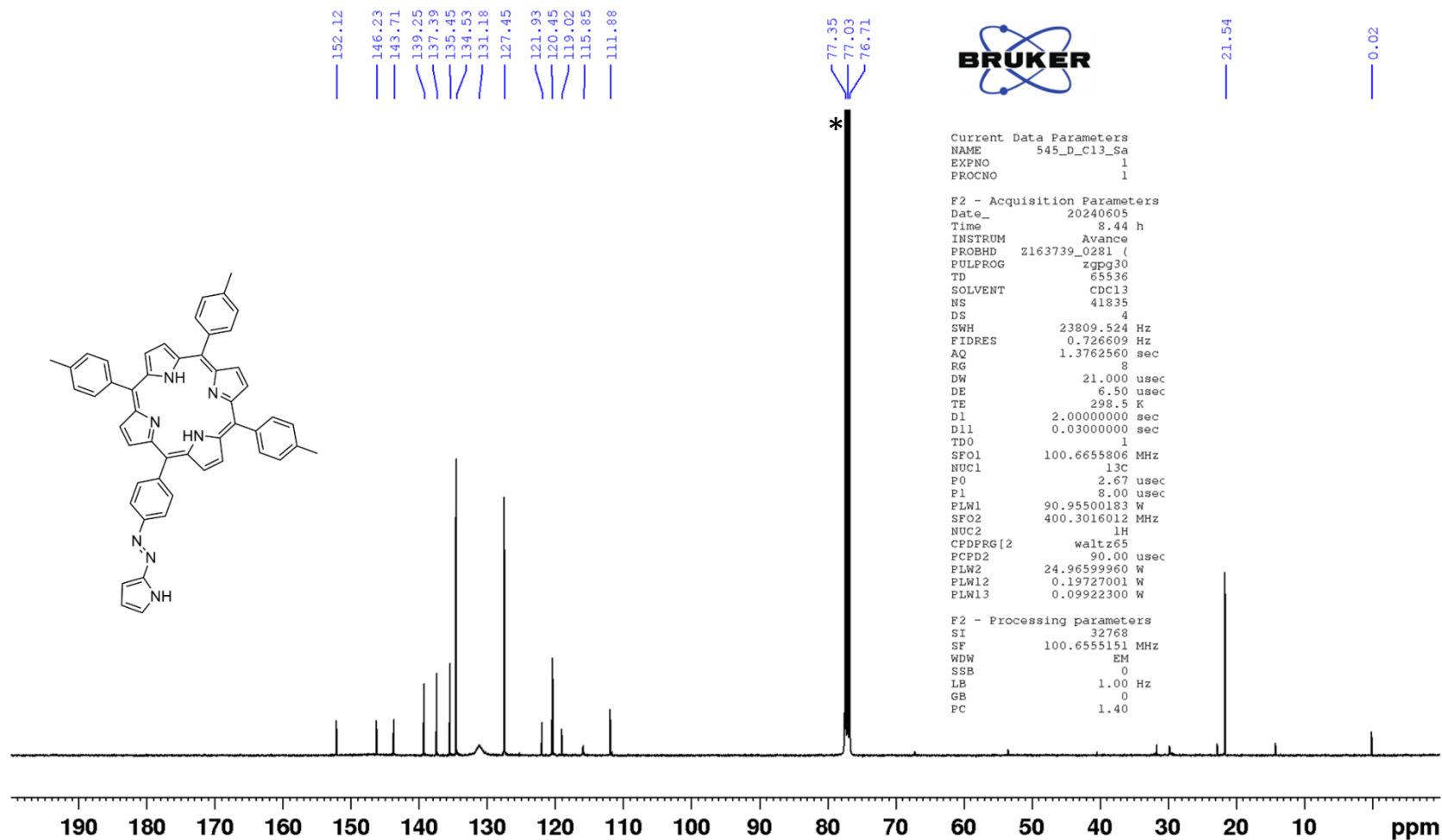
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Analysis Info

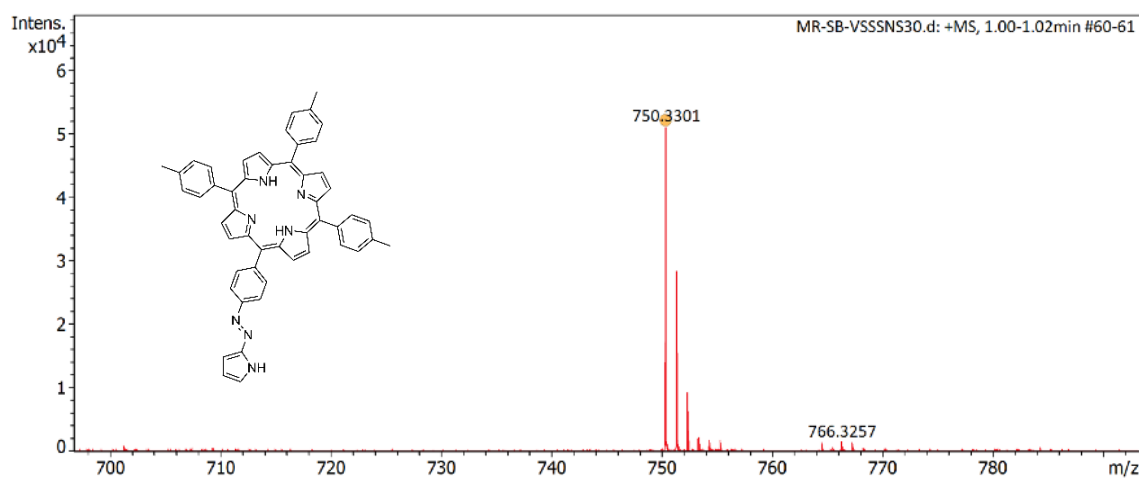
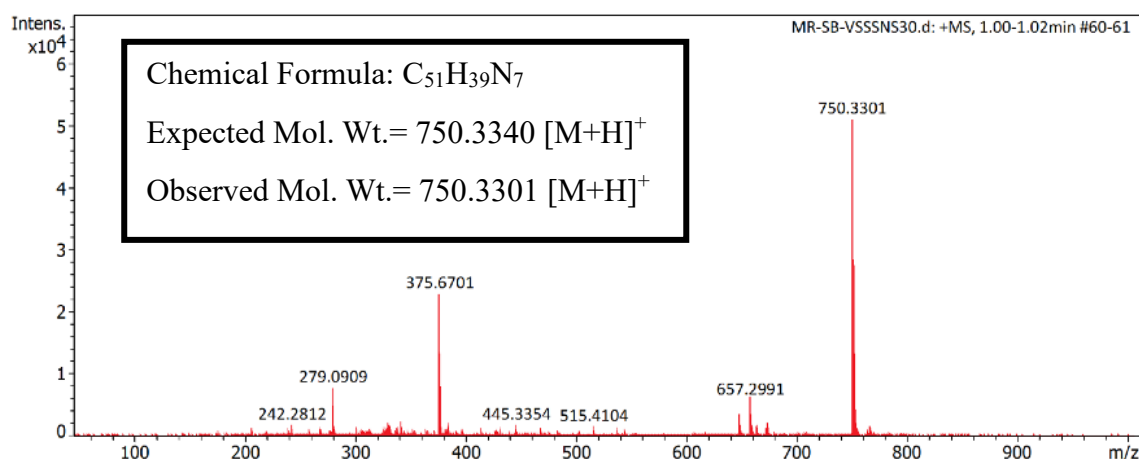
Analysis Name D:\Data\JUNE-24\MR-SB-VSSSNS30.d
 Method Naformat_pos_1000.m
 Sample Name MR-SB-VSSSNS30
 Comment C51H39N7

Acquisition Date 6/17/2024 11:54:19 AM

Operator ssk-in
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
750.3301	1	C ₅₁ H ₄₀ N ₇	750.3340	5.2	34.7	2	100.00	36.0	even	ok

MR-SB-VSSSNS30.d

Bruker Compass DataAnalysis 5.1

printed: 6/18/2024 10:19:08 AM

by: ssk-in

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Figure S3. ES MS spectrum of 4

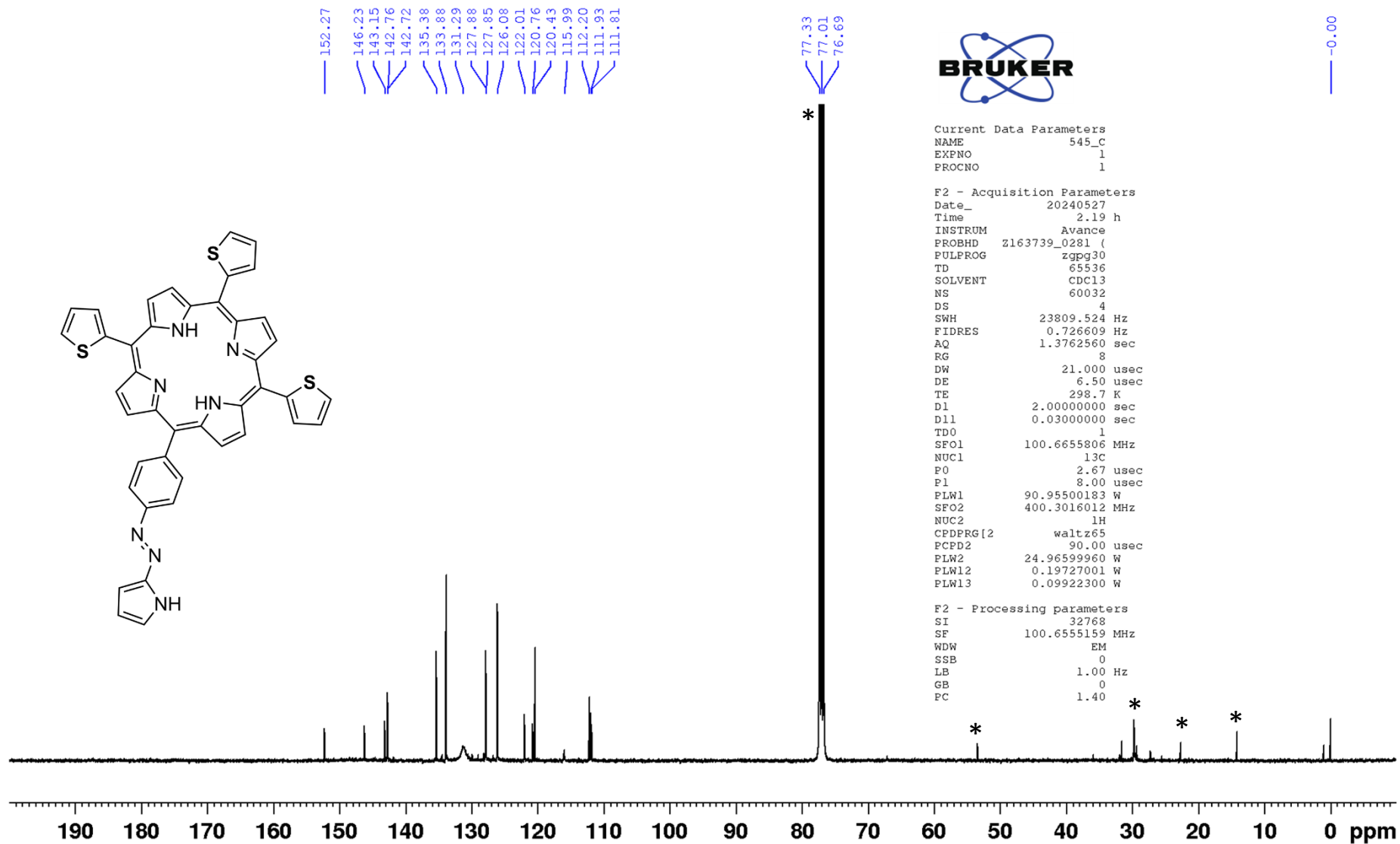


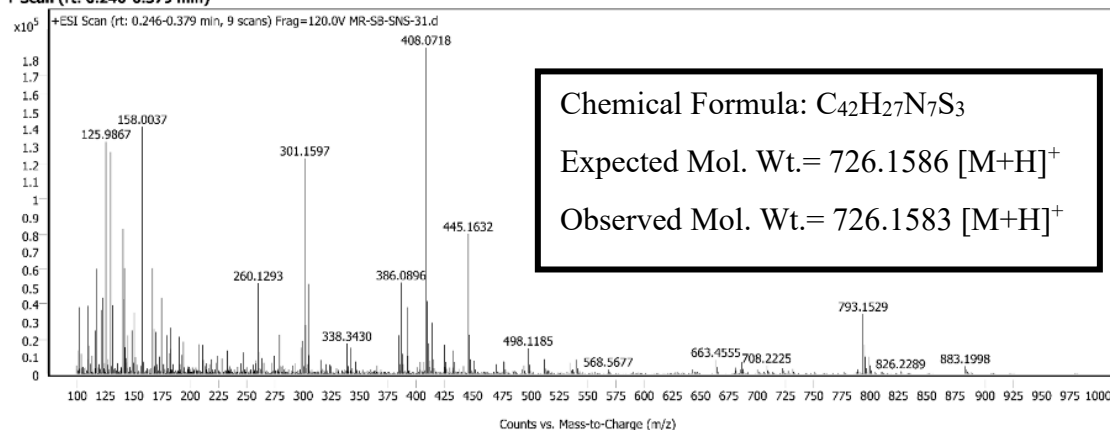
Figure S5. ^{13}C NMR spectrum of **5** (* indicates residual solvent peaks)

Sample Information

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Sample ID		Acq. Time (Local)	5/27/2024 12:00:44 PM (UTC+05:30)
Instrument	LCMSQTOF-G6545B	Method Path (Acq)	D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m
MS Type	QTOF	Version (Acq SW)	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	0.3	IRM Status	Success
Position	P2-B2	Method Path (DA)	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_IITB_1.m
Plate Pos.		Target Source Path	
Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Spectra

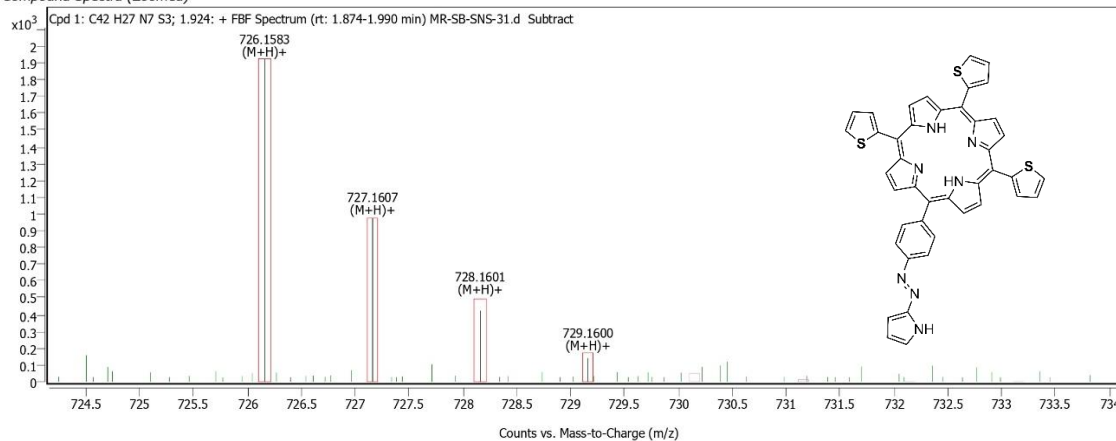
+ Scan (rt: 0.246-0.379 min)

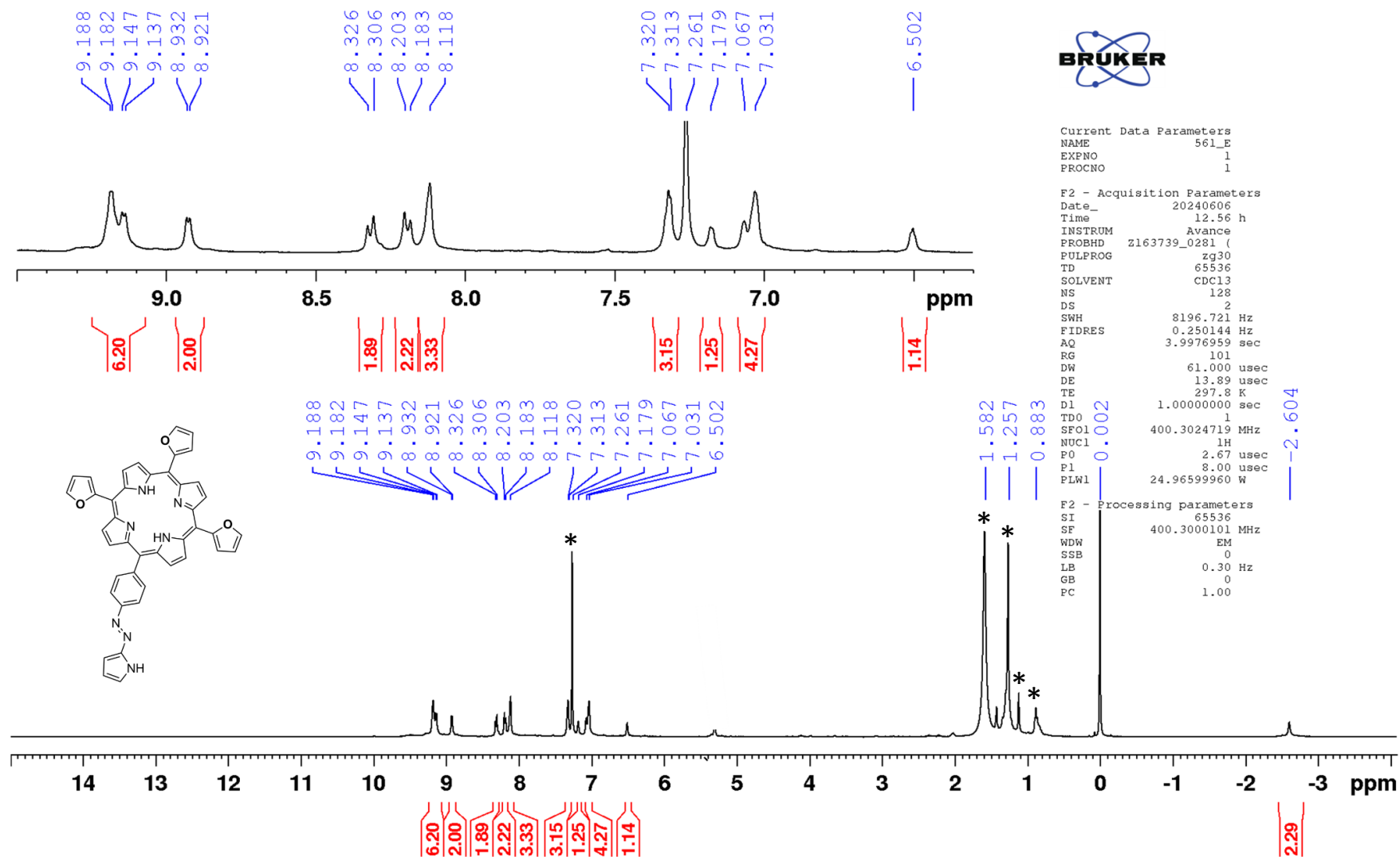
**Compound Details**

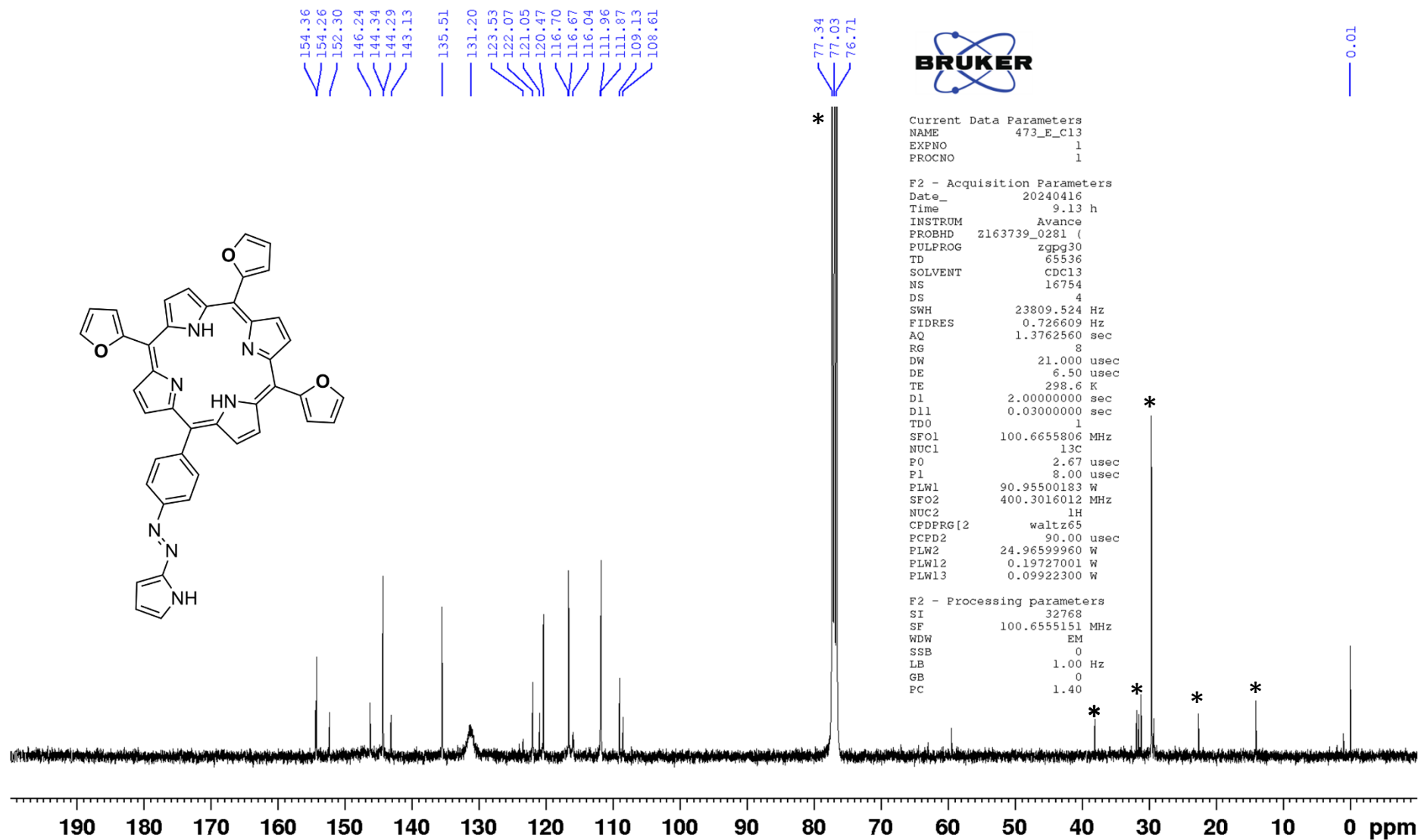
Cpd. 1: C42 H27 N7 S3

Formula	m/z	Observed M/Z	Difference Da	Difference PPM	Score
C42 H27 N7 S3	726.1583	726.158302557461	2.05251770250925	2.83047716432701	96.54

Compound Spectra (Zoomed)


 MassHunter Qual 10.0
 (End of Report)
Figure S6. LCMS QTOF spectrum of 5

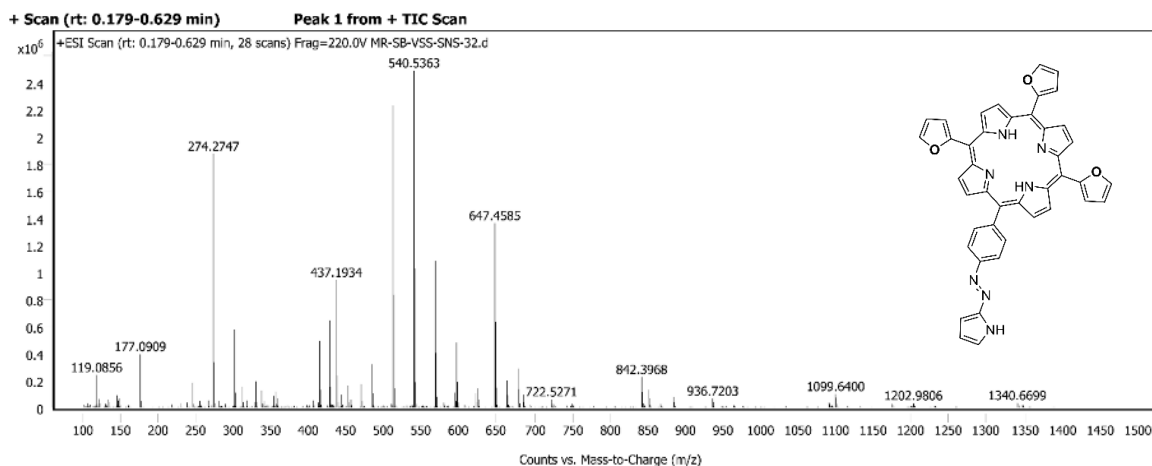




Sample Information

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Sample ID		Acq. Time (Local)	5/30/2024 12:09:32 PM (UTC+05:30)
Instrument	LCMSQTOF-G6545B	Method Path (Acq)	D:\Projects\MASS Data\Methods\A1B1_POS_100-1500_4000_800_220.m
MS Type	QTOF	Version (Acq SW)	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	0.5	IRM Status	Success
Position	PIB1	Method Path (DA)	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_IITB_1.m
Plate Pos.		Target Source Path	
Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Spectra



Compound Details

Cpd. 1: C42 H27 N7 O3

Formula	m/z	Observed M/Z	Difference Da	Difference PPM	Score
C42 H27 N7 O3	678.2248	678.224752295974	-0.135014711645454	-0.199366826925434	99.91

Compound Spectra (Zoomed)

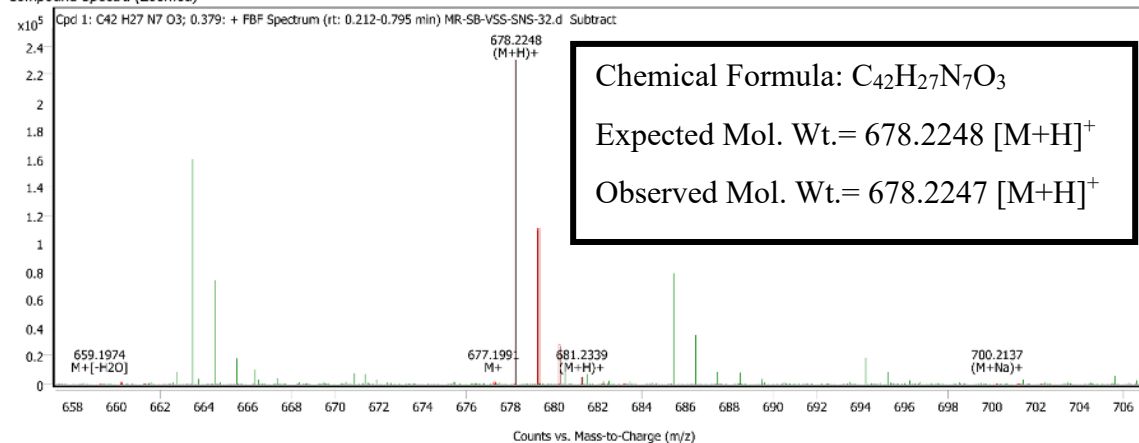
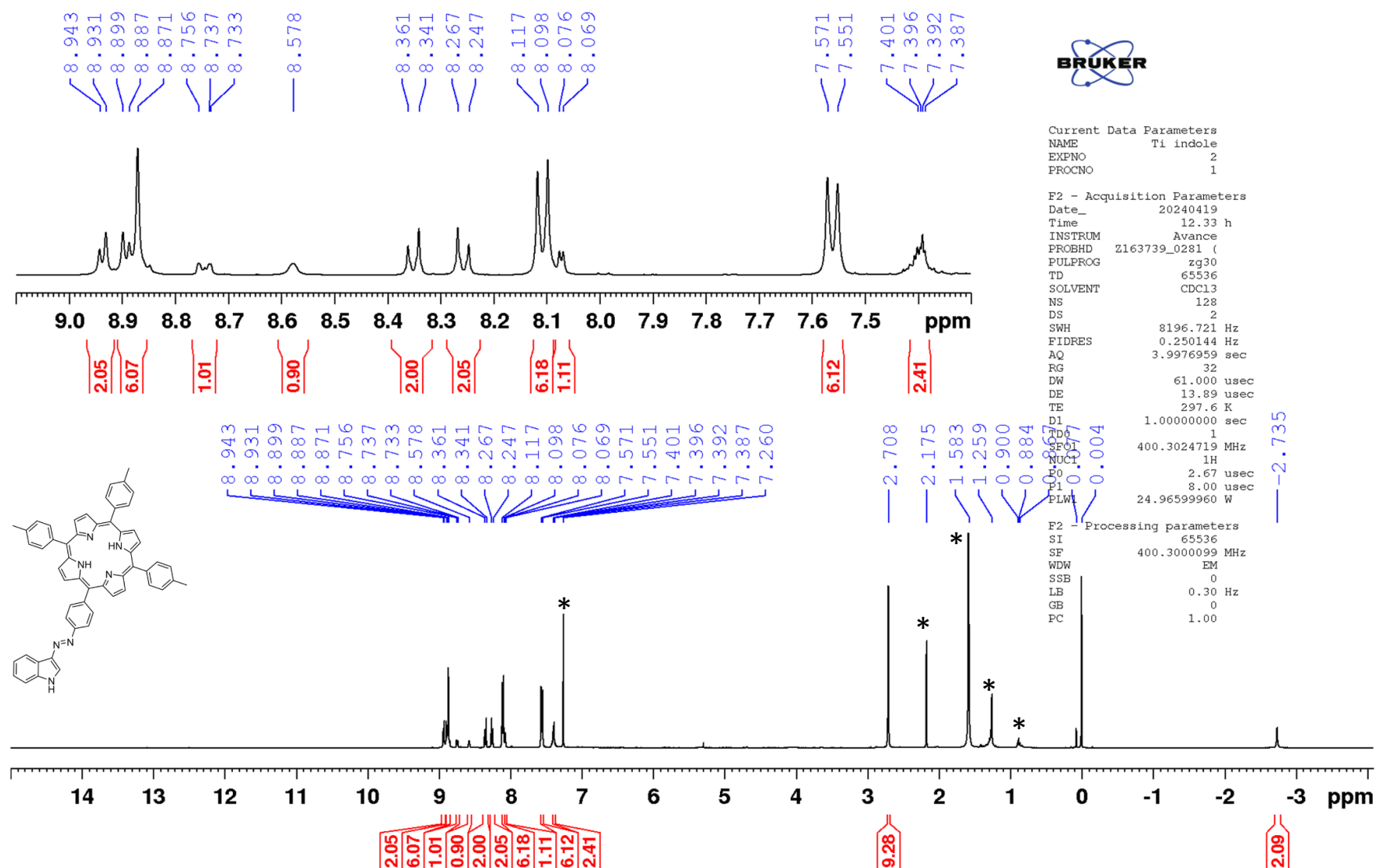
MassHunter Qual 10.0
(End of Report)

Figure S9. LCMS QTOF spectrum of 6



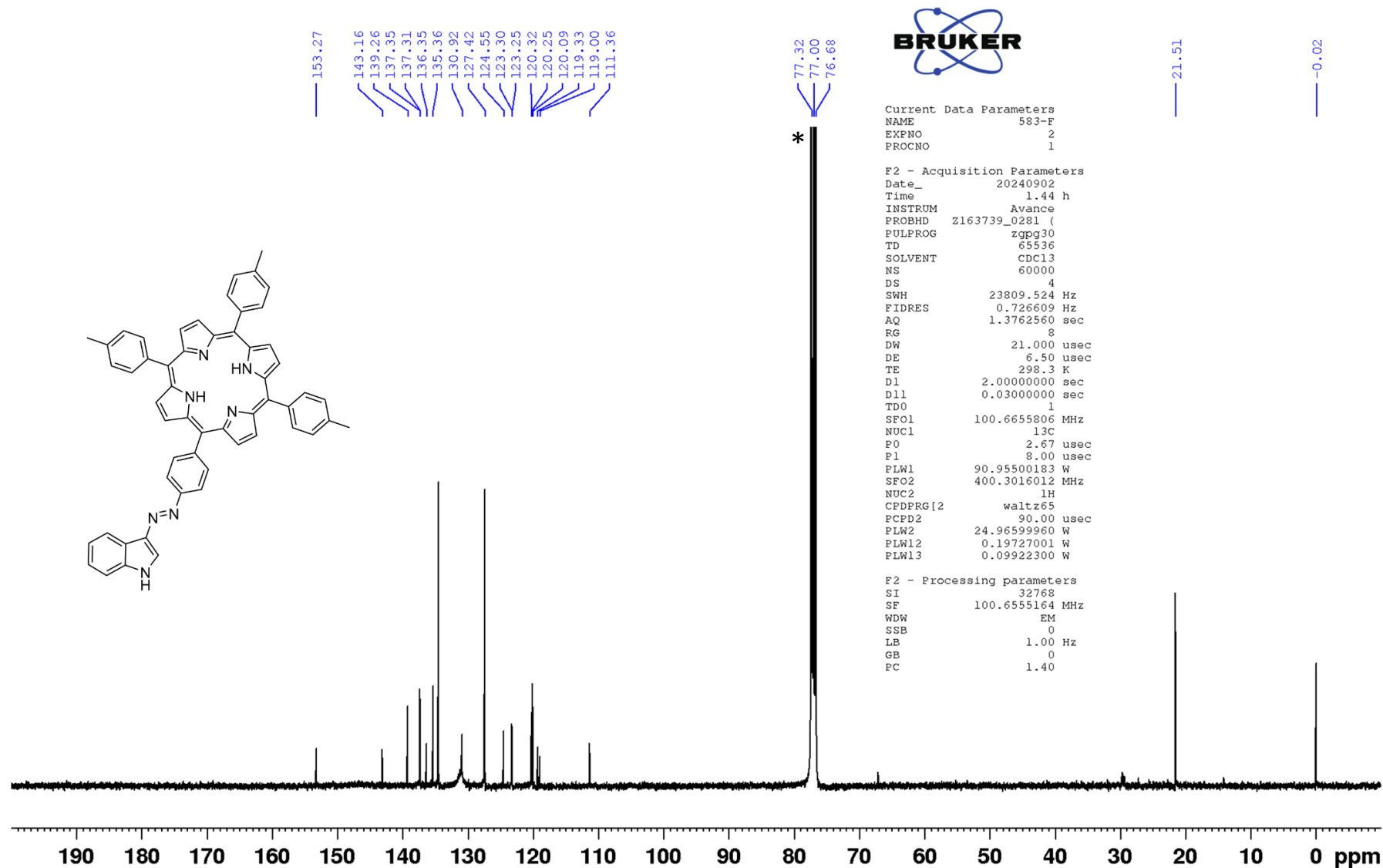
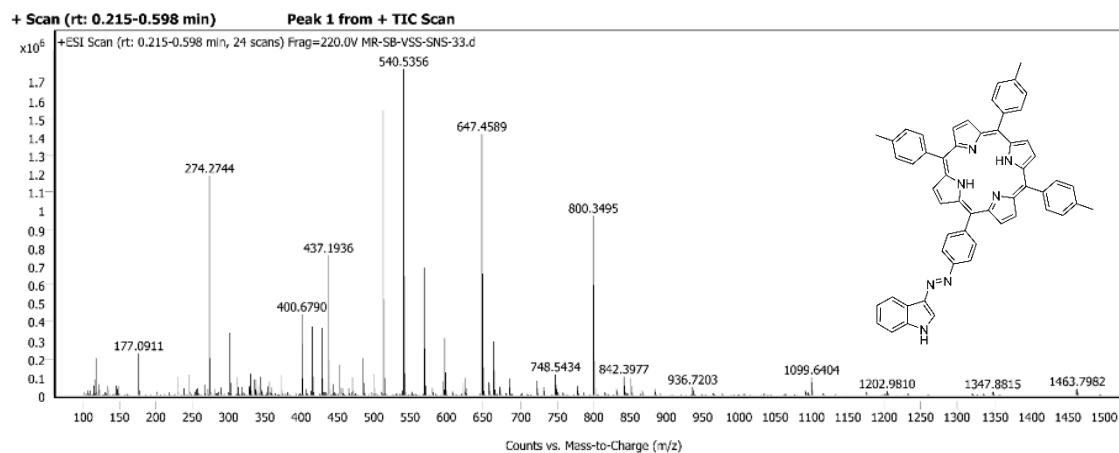


Figure S11. ^{13}C NMR spectrum of **7** (* indicates residual solvent peaks)

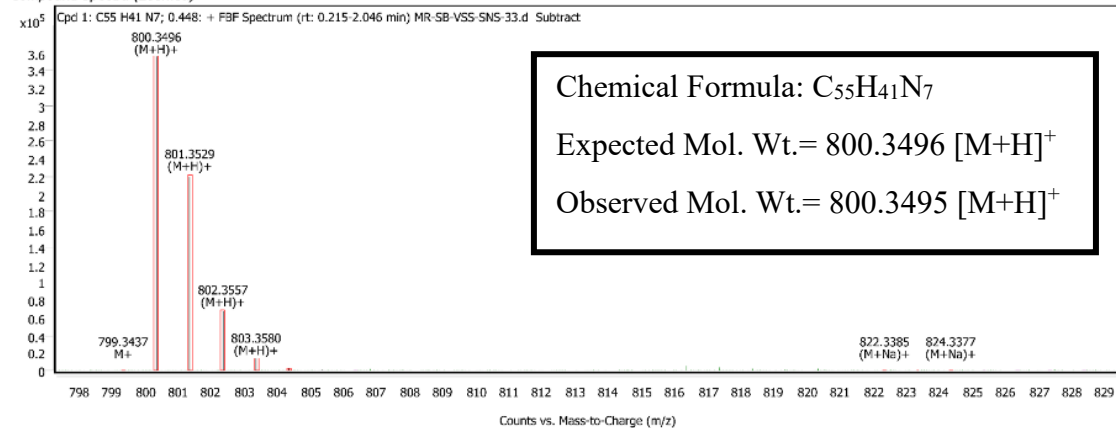
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Sample ID		Acq. Time (Local)	5/30/2024 12:25:55 PM (UTC+05:30)
Instrument	LCMSQTOF-G6545B	Method Path (Acq)	D:\Projects\MASS Data\Methods\A1B1_POS_100-1500_4000_800_220.m
MS Type	QTOF	Version (Acq SW)	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	0.5	IRM Status	Success
Position	P1B1	Method Path (DA)	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_IITB_1.m
Plate Pos.		Target Source Path	
Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Spectra**Compound Details**

Cpd. 1: C55 H41 N7

Formula	m/z	Observed M/Z	Difference Da	Difference PPM	Score
C55 H41 N7	800.3496	800.349585686503	-0.0126728011764499	-0.0158540345896491	99.92

Compound Spectra (Zoomed)

MassHunter Qual 10.0
(End of Report)

Figure S12. LCMS QTOF spectrum of 7

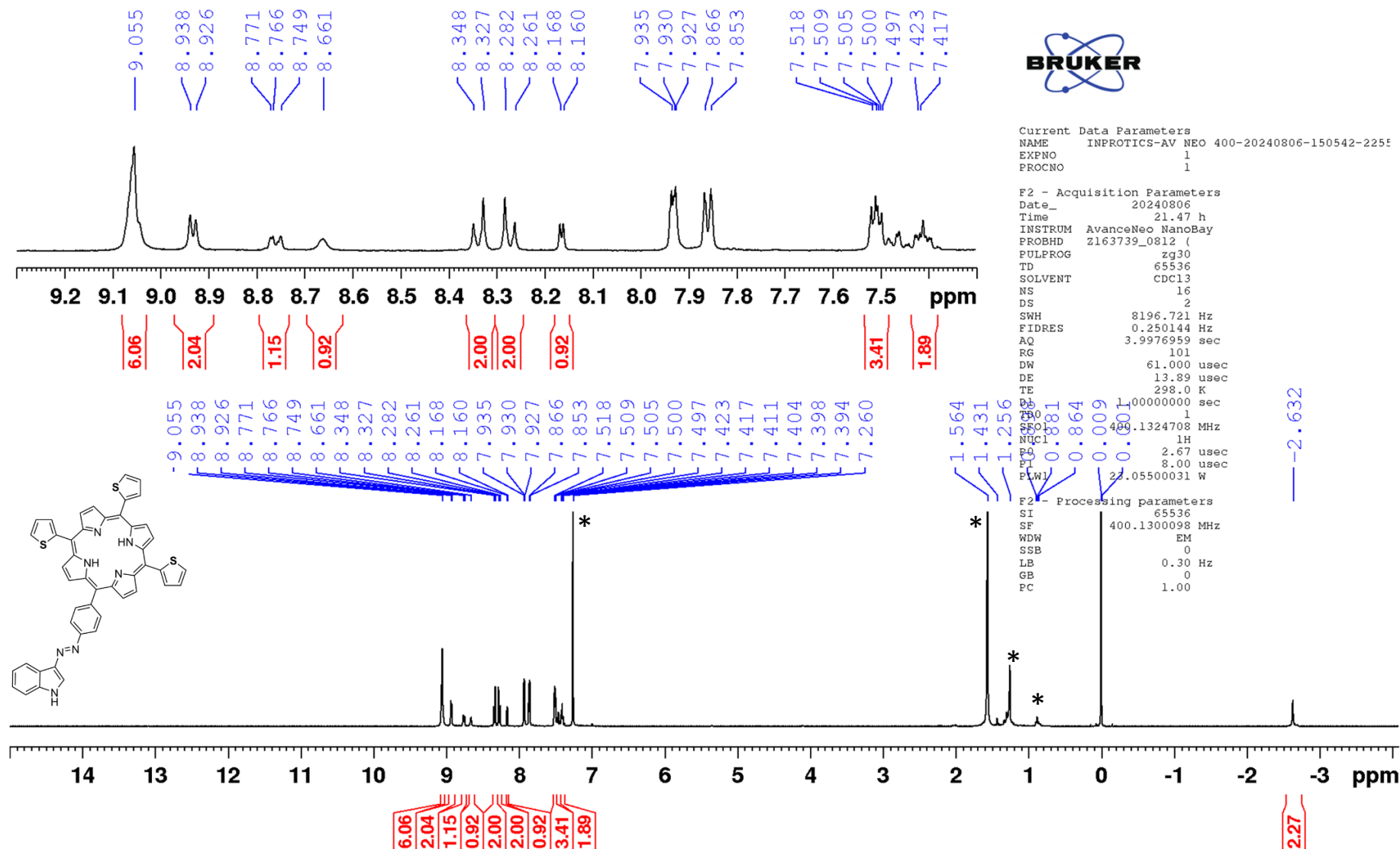


Figure S13. ^1H NMR spectrum of **8** (* indicates residual solvent peaks)

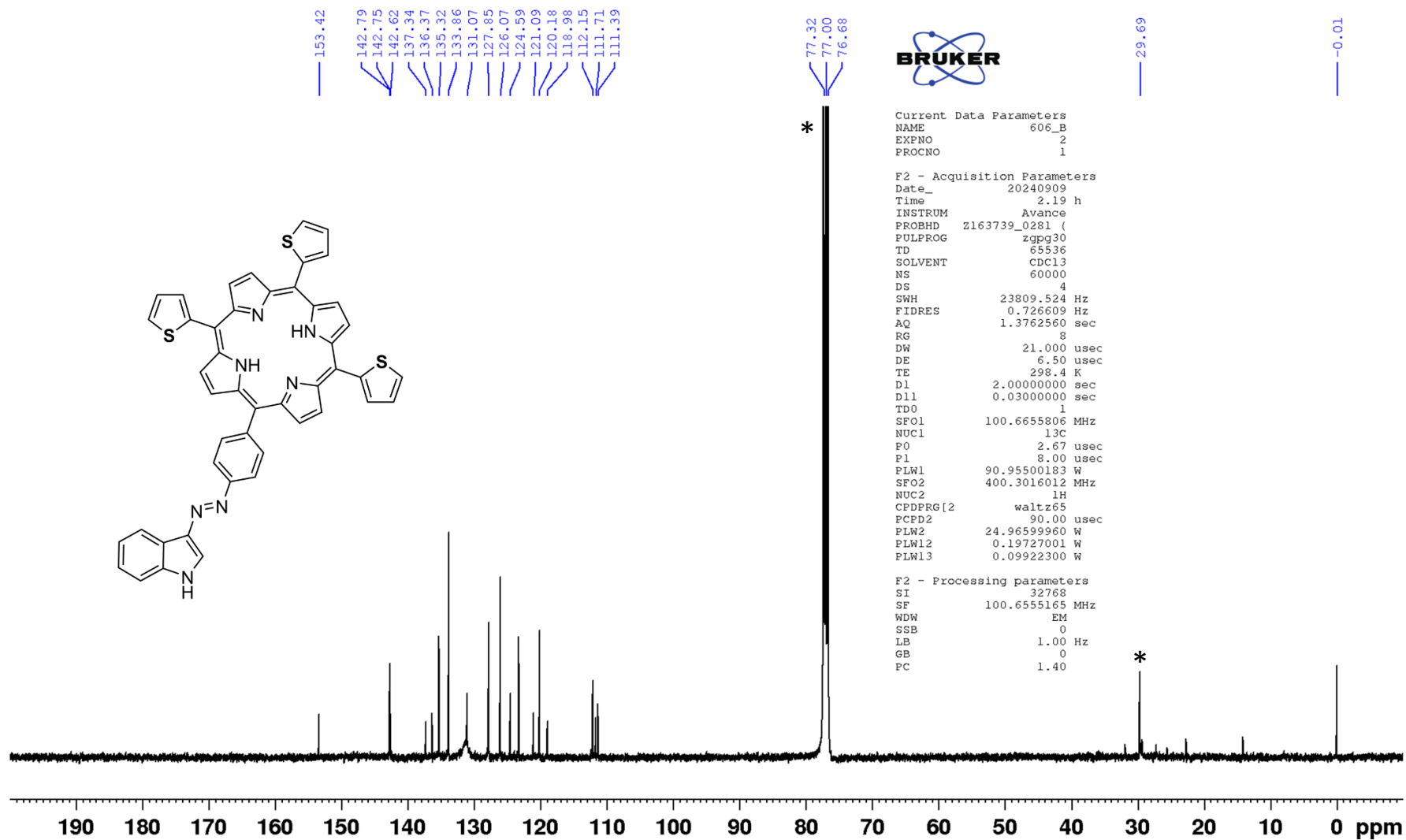


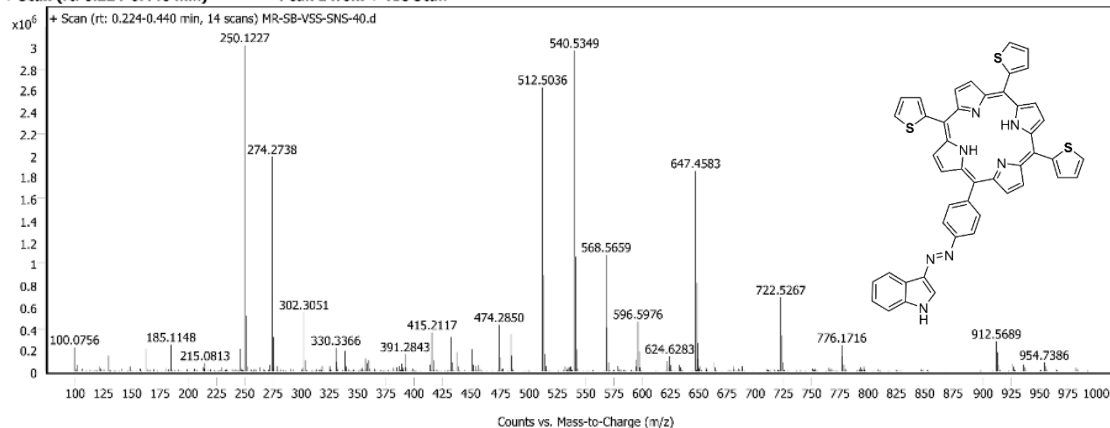
Figure S14. ^{13}C NMR spectrum of **8** (* indicates residual solvent peaks)

Sample Information

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Sample ID		Acq. Time (Local)	29-07-2024 12:13:08 (UTC+05:30)
Instrument	LCMSQTOF-G6545B	Method Path (Acq)	D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m
MS Type	QTOF	Version (Acq SW)	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	6	IRM Status	Success
Position	P2A2	Method Path (DA)	C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_1.m
Plate Pos.		Target Source Path	
Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.224-0.440 min) Peak 1 from + TIC Scan



Compound Details

Cpd. 1: C₄₆H₂₉N₇S₃

Formula	m/z	Observed M/Z	Difference Da	Difference PPM	Score
C ₄₆ H ₂₉ N ₇ S ₃	776.1717	776.171721564506	-0.414049498772329	-0.534143933780154	98.63

Compound Spectra (Zoomed)

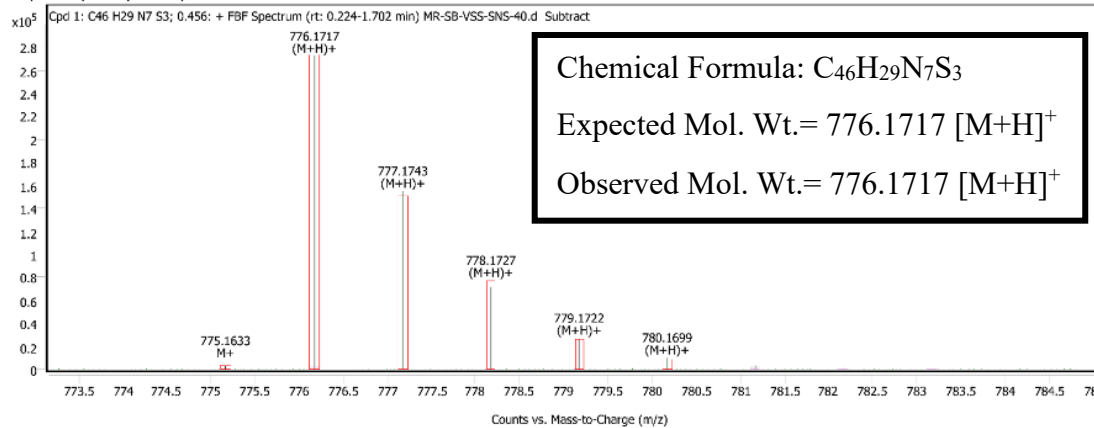
MassHunter Qual 10.0
(End of Report)

Figure S15. LCMS QTOF spectrum of 8

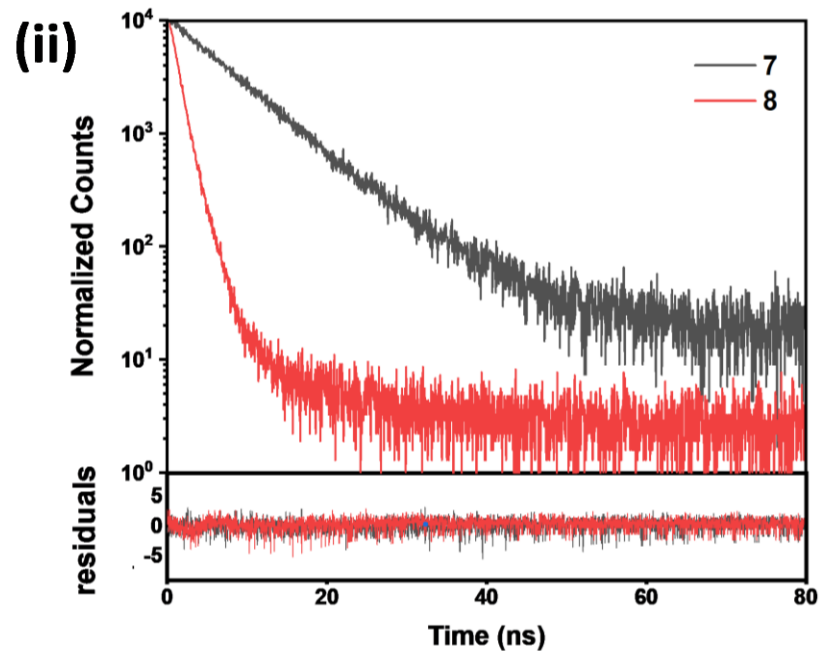
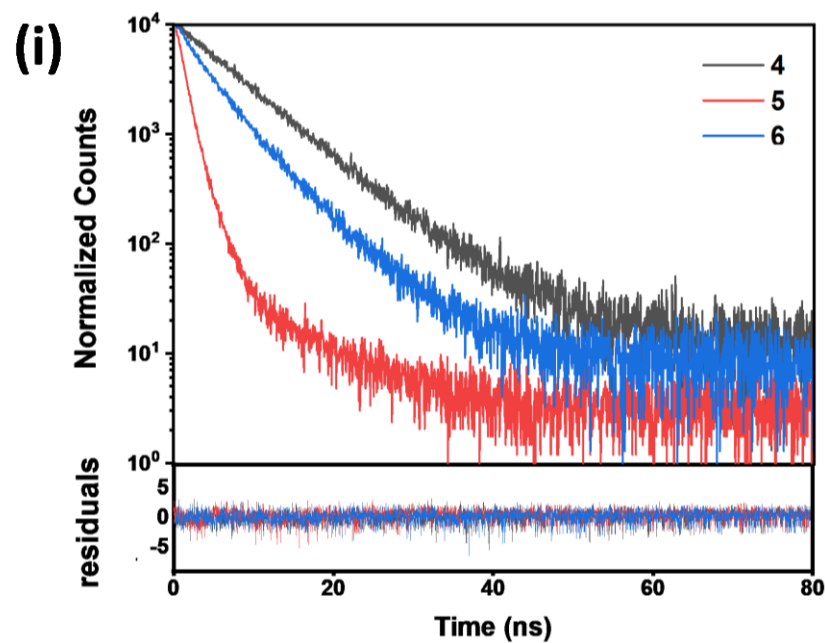


Figure S16. (i) Fluorescence decay profile of hybrids **4** (black line), **5** (red line), and **6** (blue line), (ii) fluorescence decay profile of hybrids **7** (black line) and **8** (red line). All the spectra were recorded in 1×10^{-5} M solution of toluene.

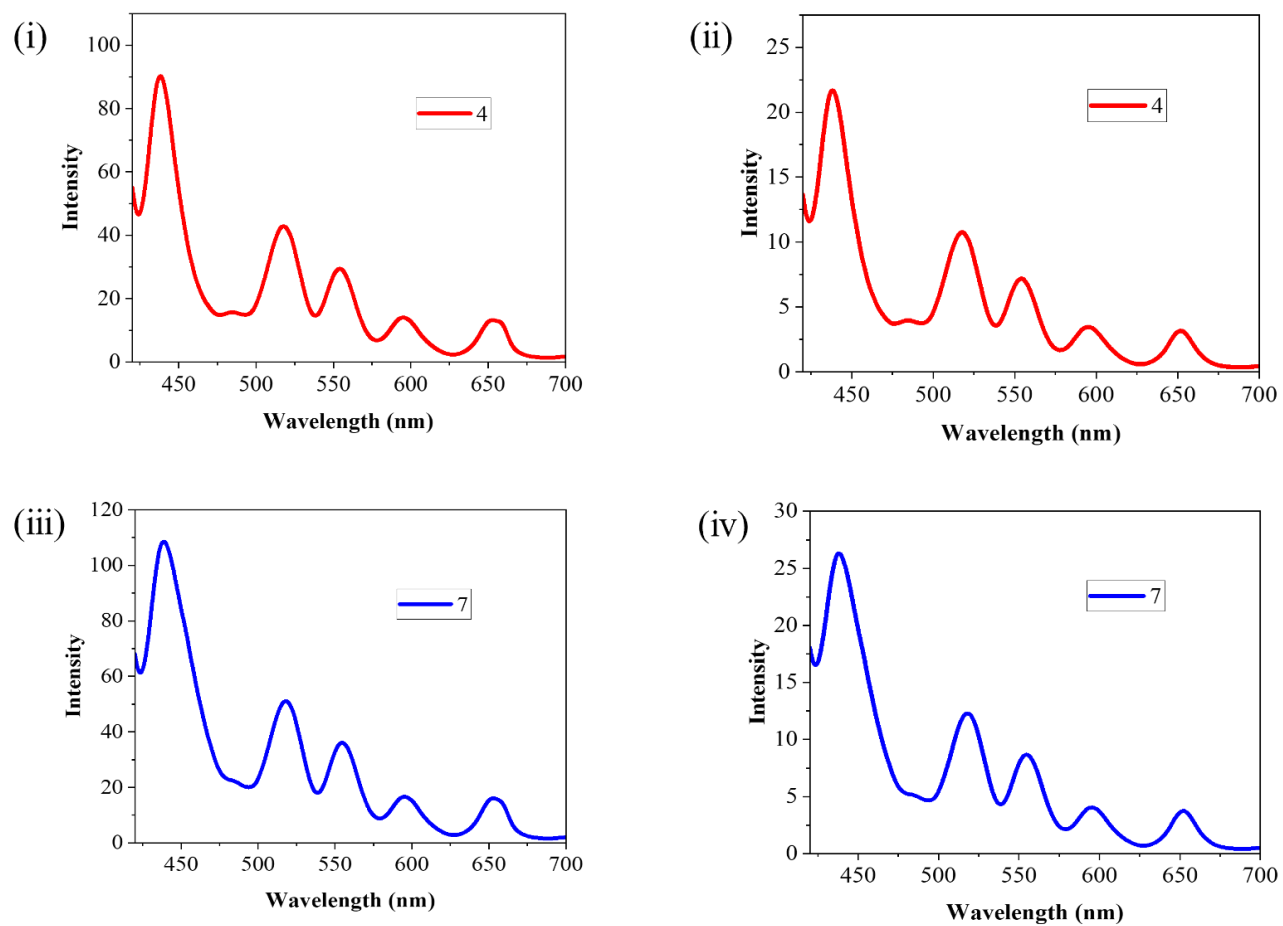


Figure S17. i) Excitation spectra of hybrid **4** ($\lambda_{em} = 660$ nm), ii) **4** ($\lambda_{em} = 725$ nm), iii) **7** ($\lambda_{em} = 660$ nm), iv) **7** ($\lambda_{em} = 725$ nm). All the spectra were recorded in 1×10^{-5} M solution of toluene.

Table S1. The selected dihedral angles (in °) and energies in the lowest energy conformers of the porphyrin-azoheteroarenes

Compound	α in °	β in °	γ in °	HOMO (eV)	LUMO (eV)	Band gap (eV)
4	70-72	68	0.6	-5.68	-1.36	4.31
5	86-90	72	0.5	-5.74	-1.59	4.14
6	54-60	73	2.0	-5.73	-1.45	4.28
7	71-72	68	2.0	-5.64	-1.32	4.32
8	86-89	72	2.4	-5.74	-1.35	4.20

Table S2. Calculated vertical excitation (nm) and oscillator strength (*f*) for the porphyrin-azoheteroarenes

Compound	λ (nm), Oscillator strength(<i>f</i>)
4	407.8 (0.51), 429.7 (0.00), 475.2 (0.16), 522.8 (0.16), 567.6 (0.076)
5	428.5 (0.01), 429.7 (0.176), 439.3 (0.15), 528.4 (0.14), 570.0 (0.045)
6	425.0 (0.09), 427.2 (0.001), 466.1 (0.095), 540.5 (0.22), 590.2 (0.057)
7	414.1 (0.44), 441.0 (0.001), 450.5 (0.18), 518.7 (0.14), 563.4 (0.003)
8	439.9 (0.23), 443.6 (0.01), 444.0 (0.037), 538.6 (0.184), 579.7 (0.07)

Table S3. Optimized Geometries (Cartesian coordinates) of the porphyrin-azoheteroarenes

Optimized geometries (Cartesian coordinates in Å) and energies of porphyrin-arene hybrids (in eV). Notation: E = gas phase energy, Nimag = number of imaginary frequencies.

4 E = -2350.6940 Nimag = 0				5 E = -3194.9985 Nimag = 0			
C1	-2.9109922091	5.6163451410	1.0601519971	C1	-3.4500479349	3.3018004264	0.1595869478
C2	-3.3423026327	4.8900800286	-0.0574458117	C2	-4.7090419946	2.6911717608	0.0939405652
C3	-2.8713039511	7.0057731131	1.0364625099	C3	-2.2119168515	2.6245632288	0.1885208144
C4	-3.2559318806	7.7229559650	-0.1023166736	C4	-5.9820243311	3.3485027430	0.0396119877
C5	-3.6849759617	6.9966597051	-1.2150473759	C5	-6.9524275104	2.3902660056	-0.0375805795
C6	-3.7307001003	5.6041301158	-1.1946984857	C6	-6.3134054001	1.1068371683	-0.0281032366
C7	-3.3854587453	3.3929650094	-0.0326560603	N7	-4.9632845488	1.3416651946	0.0523301081
C8	-4.6577450577	2.8028498222	-0.0209001500	N8	-2.0348840156	1.2748066765	0.2082873439
C9	-2.1632887369	2.6915654252	-0.0178433210	C9	-0.6838162338	1.0824293538	0.2415289814
C10	-5.9189569066	3.4801502908	0.0370935179	C10	0.0208631589	2.3605079823	0.2220561799
C11	-6.9099515024	2.5381933215	0.0298871075	C11	-0.9303044365	3.3193984627	0.1991959011
C12	-6.2966282189	1.2448897611	-0.0354676198	C12	-0.0241807389	-0.1617009127	0.2887947812
N13	-4.9393142401	1.4586368502	-0.0570261511	C13	-6.9417217801	-0.1455894860	-0.0814467436
N14	-2.0090515349	1.3393786601	0.0764363119	C14	1.4708314022	-0.1701347900	0.3644562968
C15	-0.6633155687	1.1205260568	0.0777208175	C15	-0.6570138159	-1.4146006781	0.2860582522
C16	0.0653305492	2.3784388559	-0.0469923815	C16	-6.2816044412	-1.3910179426	-0.0425130008
C17	-0.8670940623	3.3542880974	-0.1084896311	C17	-6.9902227194	-2.6672223020	-0.0738249044
C18	-0.0233753682	-0.1332576083	0.1667620239	C18	-6.0453533195	-3.6276179302	0.0138253385
C19	-6.9482540211	0.0033832193	-0.0722240292	C19	-4.7627885359	-2.9348441888	0.0928384390
C20	1.4701950631	-0.1605146477	0.2459173116	N20	-4.9366195601	-1.5826436569	0.0508709606
C21	-0.6771750617	-1.3746554114	0.1873193057	N21	-2.0074554283	-1.6511516433	0.1858549449
C22	-8.4457417373	0.0312987406	-0.0938322550	C22	-2.2694385954	-2.9962281630	0.2568798188

C23	-6.3049485573	-1.2509561514	-0.0873260178	C23	-1.0064943022	-3.6521948510	0.4090354846
C24	-7.0267918573	-2.5117740067	-0.2203238244	C24	-0.0301962957	-2.6951013982	0.4271846980
C25	-6.0941911667	-3.4893073444	-0.1923166662	C25	-3.5325140022	-3.6090651305	0.2044478267
C26	-4.8050179717	-2.8236517164	-0.0393208109	C26	2.1363064099	0.2763832393	1.5125307274
N27	-4.9617614142	-1.4695485096	0.0053142338	C27	3.5239952293	0.2629421576	1.5788503597
N28	-2.0295476570	-1.5891559971	0.0750024191	C28	4.2840931019	-0.1928064071	0.4960856854
C29	-2.3158312666	-2.9322532558	0.1279620287	C29	3.6256716041	-0.6410111704	-0.6596672115
C30	-1.0631705745	-2.36072413369	0.2935387084	C30	2.2410862023	-0.6305555403	-0.7167458460
C31	-0.0726861166	-2.6656254205	0.3323600354	N31	5.6835225790	-0.1582385043	0.6727213360
C32	-3.5847305295	-3.5238439477	0.0454988648	N32	6.3546933851	-0.5642967501	-0.3195305223
C33	-3.6257004380	-5.0213843986	0.0530585994	C33	7.7161847063	-0.5351830450	-0.1581174529
C34	-2.1389790399	0.3447376553	1.3679523842	N34	8.4876788927	-0.9674636536	-1.2190159309
C35	3.5260949072	0.3174033859	1.4404494324	C35	9.8051361238	-0.8751696746	-0.8989018202
C36	4.2836145902	-0.2107040041	0.3890557351	C36	9.8963550937	-0.3742151871	0.3938653610
C37	3.6229940140	-0.7169344567	-0.7414932336	C37	8.5880256371	-0.1591253472	0.8633236525
C38	2.2389547945	-0.6922641279	-0.8039524866	C38	-3.5549784928	-5.0932688117	0.3079834345
C39	-3.1691318795	-5.7590033709	-1.0468401848	C39	-8.4277559878	-0.1412648191	-0.1580156771
C40	-3.2103828282	-7.1487509226	-1.0414867460	C40	-3.4335680281	4.7888456513	0.2197565567
C41	-3.7028256925	-7.8547848502	0.0619677364	S41	-3.3553510785	-6.1214627841	-1.0954668828
C42	-4.1543998132	-7.1170537173	1.1583638999	C42	-3.5054059847	-7.5559781115	-0.1368003134
C43	-4.1194963531	-5.7241602379	1.1559809186	C43	-3.6986009481	-7.2603498446	1.1805821038
C44	-9.1870535278	-0.3893575006	1.0181548694	C44	-3.7274438137	-5.8567570832	1.4308324607
C45	-10.5768457913	-0.3621078454	1.0008674325	S45	-9.2682757295	-0.1042472808	-1.6938445448
C46	-11.2795768373	0.0813610270	-0.1254049581	C46	-10.8138917914	-0.1235432452	-0.9132823239
C47	-10.5384265120	0.4986395901	-1.2328526230	C47	-10.6892152465	-0.1560175936	-0.4455333023
C48	-9.1451913397	0.4774406752	-1.2190734880	C48	-9.3286884459	-0.1655038796	0.8719903254
C49	-3.2046971531	9.2315115202	-0.1183493377	S49	-3.3820146389	5.7745435242	-1.2266505205
N50	5.6823612199	-0.1832656738	0.5688648671	C50	-3.3825407052	7.2369857952	-0.2988863656
C51	-3.7420064182	-9.3638140015	0.0579426938	C51	-3.4200008645	6.9809158376	1.0401672733
C52	-12.7887917332	0.1040543773	-0.1338831544	C52	-3.4492604552	5.5854389316	1.3326028084
N53	6.3528713884	-0.6576485966	-0.3927745314	H53	-6.1145871372	4.4175733558	0.0576692511
C54	7.7144522060	-0.6357706372	-0.2239400302	H54	-8.0183347323	2.5373721286	-0.0927938067
N55	8.4865322340	-1.1422831473	-1.2506340762	H55	-4.2548358812	0.6188418127	0.0945045795
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C42	-3.9271698741	-7.6041639433	0.1162137885
C43	-4.0966083079	-7.2549517747	1.4238181416
C44	-4.0470267118	-5.8443552042	1.6270780387
S45	-9.3093102255	0.0531473887	-1.7160023221
C46	-10.8382096784	0.1608338214	-0.9097970421
C47	-10.6887572992	0.1939527303	0.4455783603
C48	-9.3225667383	0.1322842186	0.8497798652
S49	-3.1321554670	5.5929824923	-1.6471039791
C50	-3.0056714068	7.1128995726	-0.8264527454
C51	-2.9999080942	6.9522909911	0.5280356728
C52	-3.0994144214	5.5848965086	0.9200328261
C53	8.6442915909	-1.9625383199	-1.7124757168
C54	9.8337517096	-2.2986696567	-2.3407757735
C55	11.0736847508	-2.1321264054	-1.6960003341
C56	11.1504748496	-1.6249393315	-0.4067587868
H57	-5.8813765873	4.4811345830	-0.2791961108
H58	-7.8854842860	2.7032427579	-0.3088459829
H59	-4.2330861420	0.5952749335	-0.0068745850
H60	1.2022913428	2.1879278138	0.2014373344
H61	-0.5721446137	4.1732480661	-0.0581895988
H62	-8.2129498129	-2.6110315515	-0.0818311702
H63	-6.4397774176	-4.6053949885	0.1686571315
H64	-2.7717514448	-1.0239142047	0.1479383912
H65	-1.1589760558	-4.8873470408	0.7373839353
H66	0.8461942768	-3.1171860305	0.7899100944
H67	1.3981841259	0.4112713137	2.5451828180
H68	3.8698459605	0.3061176211	2.8376519131
H69	4.2737128307	-1.4357513357	-1.0416111970
H70	1.8116910419	-1.3466015716	-1.3437052511
H71	10.4223456392	-0.5493814644	2.1630138472
H72	7.9698451578	-0.1976109701	2.5913841459
H73	-3.9205128998	-8.5909068602	-0.3208762235
H74	-4.2515700641	-7.9741209746	2.2172743108
H75	-4.1601818773	-5.3673310158	2.5919621997
H76	-11.7496468319	0.1918904801	-1.4867585360
H77	-11.5198541793	0.2595153518	1.1353534487
H78	-8.9955165183	0.1446627288	1.8813678087
H79	-2.9427719172	8.0277909378	-1.3953672625
H80	-2.9276500076	7.7763890997	1.2254582605
H81	-3.1090711565	5.2493824764	1.9489179453
H82	7.6914677963	-2.0908515962	-2.2109365189
H83	9.8127529960	-2.6974102782	-3.3484587523
H84	11.9848815173	-2.4045453296	-2.2157347696
H85	12.1054957008	-1.4961072090	0.0904146554