Supplementary Information

Simplest structure of stable radical showing high-efficiency fluorescence in solution: benzene donors with triarylmethyl radical

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Contents

Table S1. Calculated torsion angles of the aryl rings of the radicals in dichloromethane. Angles out of the brackets are in the D_0 state optimized using UB3LYP/6-31G(d, p). Angles in the brackets are in the D_1 state optimized using TD-UB3LYP/6-31G(d, p).

	PyBTM	PyPBTM	MesPyBTM	Mes_2PyBTM	F_2PyBTM	Mes_2F_2PyBTM
φ_1	48° [35°]	48° [43°]	48° [37°]	48° [37°]	32° [19°]	32° [24°]
φ_2	49° [51°]	48° [45°]	49° [52°]	49° [51°]	53° [52°]	52° [53°]
φ_3	49° [47°]	48° [45°]	49° [47°]	49° [48°]	53° [52°]	52° [49°]
ϕ_4	-	34° [25°]	83° [51°]	84° [50°]	-	87° [49°]
ϕ_5	-	34° [25°]		84° [81°]	-	87° [83°]

φ_1: Torsion angle of pyridyl ring. φ_2 and φ_3: Torsion angles of dichlorophenyl rings. ϕ_4 and ϕ_5: Dihedral angles between mesityl (phenyl) groups and dichlorophenyl groups.

Table S2. PLQYs and photophysical parameters of radicals in chloroform.

	Φ_f / %	τ / ns	k_f / 10^7 s^{-1}	k_{nr} / 10^7 s^{-1}
PyBTM	3	7.6	0.4	12.8
F_2PyBTM	6	18.1	0.3	5.2
PyPBTM	8.6	12	0.7	7.6
MesPyBTM	28	26	1.1	2.8
Mes_2PyBTM	45	39	1.2	1.4
Mes_2F_2PyBTM	69	49	1.4	0.6

Table S3. Stability of PyBTM, MesPyBTM, Mes_2PyBTM, and Mes_2F_2PyBTM in dichloromethane under 370 nm UV irradiation.

Exp. no.	$t_{1/2}$ [s] PyBTM	$t_{1/2}$ [s] MesPyBTM	$t_{1/2}$ [s] Mes_2PyBTM	$t_{1/2}$ [s] Mes_2F_2PyBTM
1	382	240	274	452
2	312	246	276	424
3	368	260	290	414
4	360			
5	254			
6	276			
7	270			
Ave.	317	249	280	430
σ	53	10	9	20

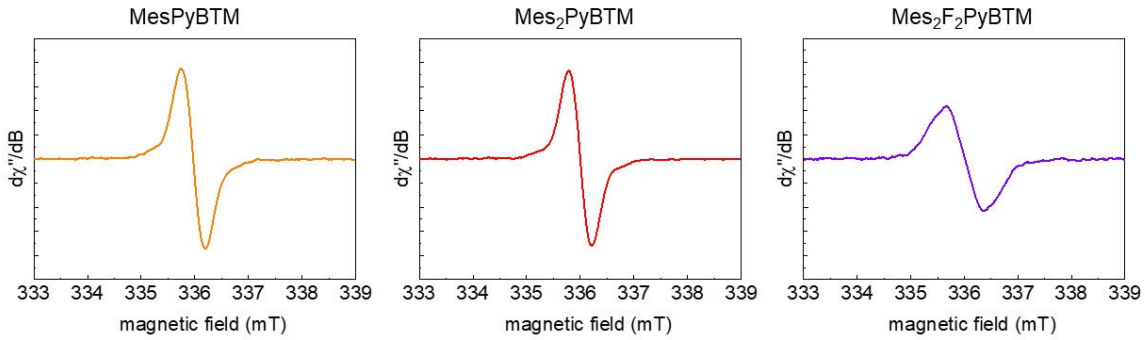


Fig. S1. EPR spectra of MesPyBTM, Mes_2PyBTM, and Mes_2F_2PyBTM in dichloromethane. The *g* factors of the radicals were *ca.* $g = 2.0032 \pm 0.0002$.

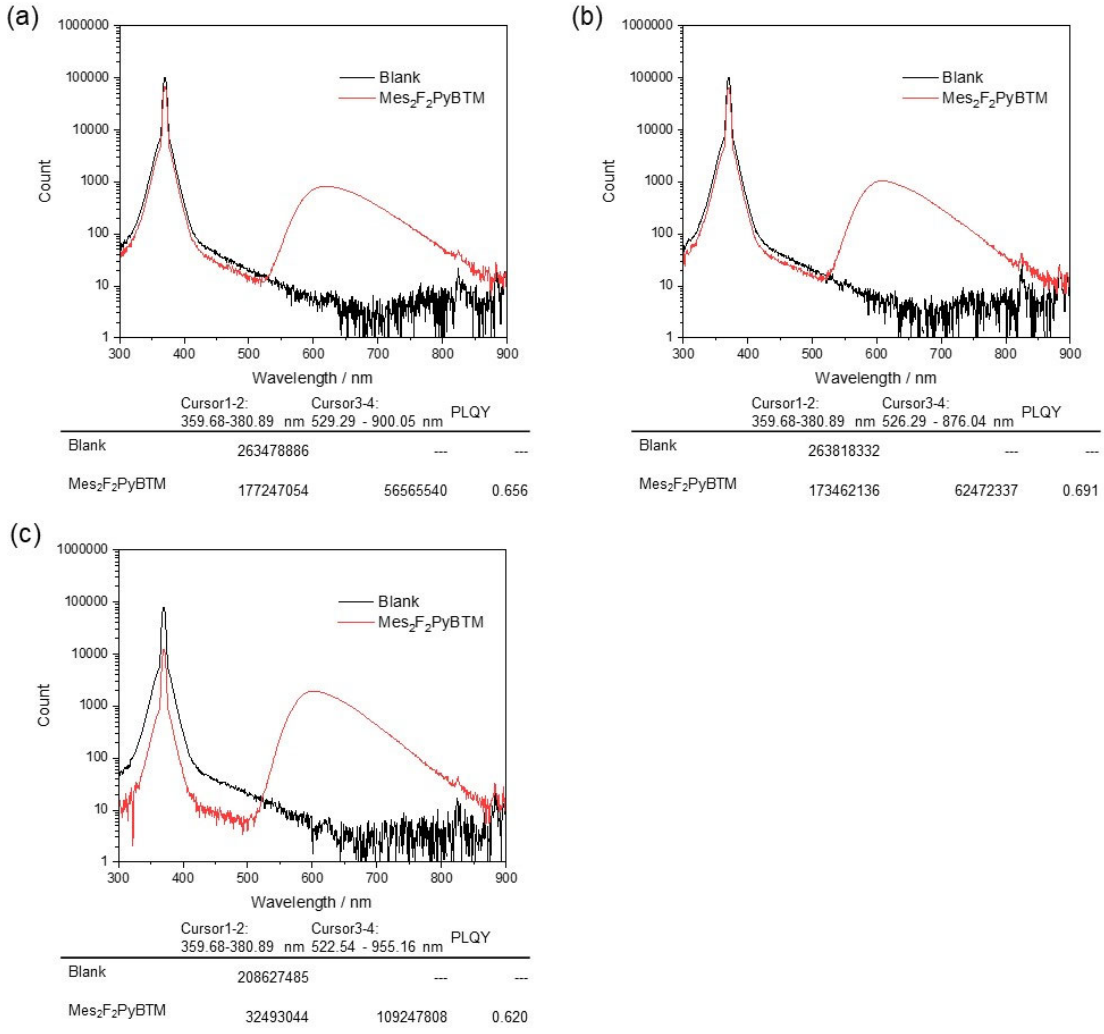


Fig. S2. Absolute photoluminescence quantum yield measurement of Mes_2F_2PyBTMin (a) dichloromethane, (b) chloroform and (c) PMMA film. The PLQYs were 66%, 69% and 62%, respectively.

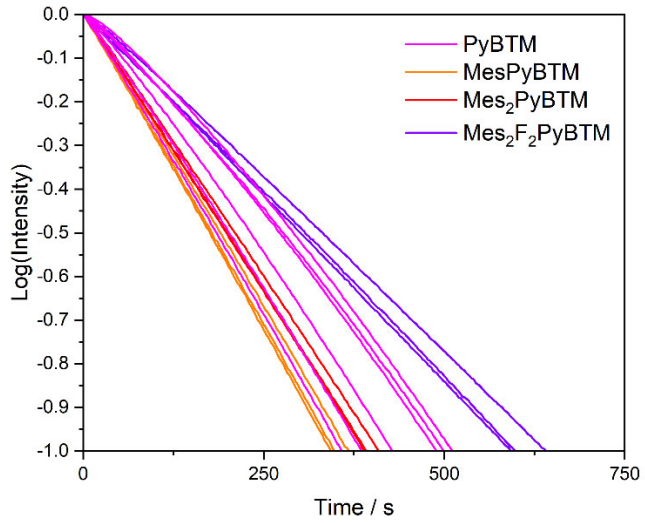


Fig. S3. Plots showing the emission decay of the radicals in dichloromethane under continuous excitation with light at λ_{ex} = 370 nm ± 10 nm. The emission was monitored at the peak emission. The half-lives ($t_{1/2}$, Table S2) were directly determined from raw data. According to the linear approximation, *Log(Intensity)* ≈ −0.3010 × (*Time* / $t_{1/2}$).

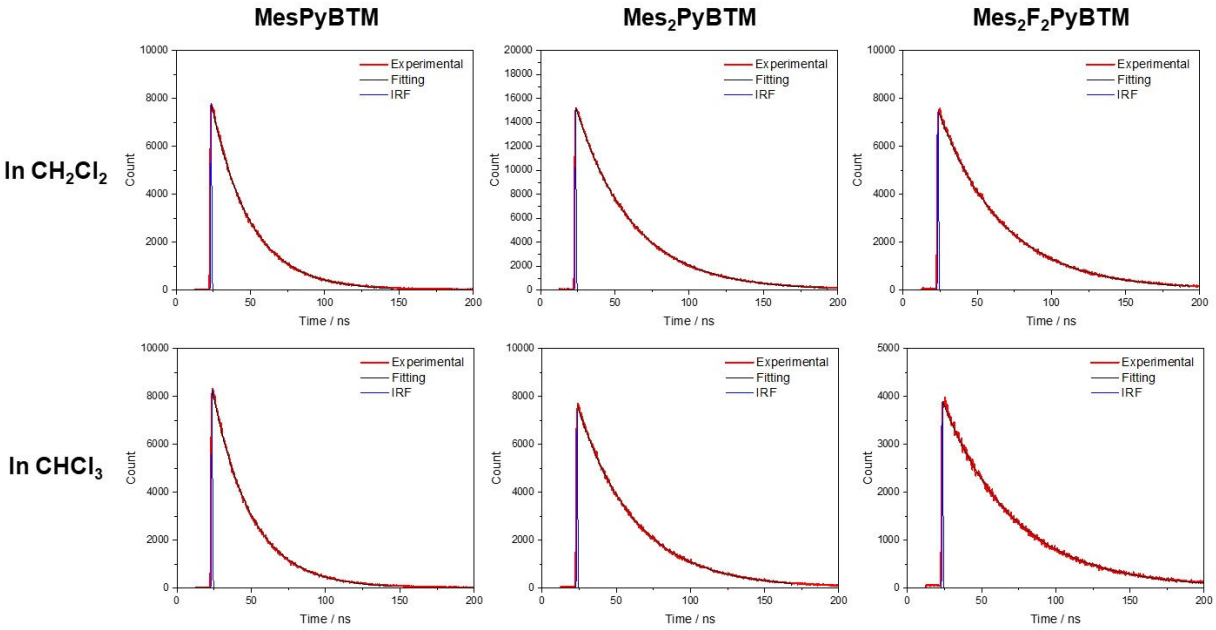


Fig. S4. Photoluminescence decay curves of the radicals excited with a picosecond diode laser with the emission wavelength of 375 nm.

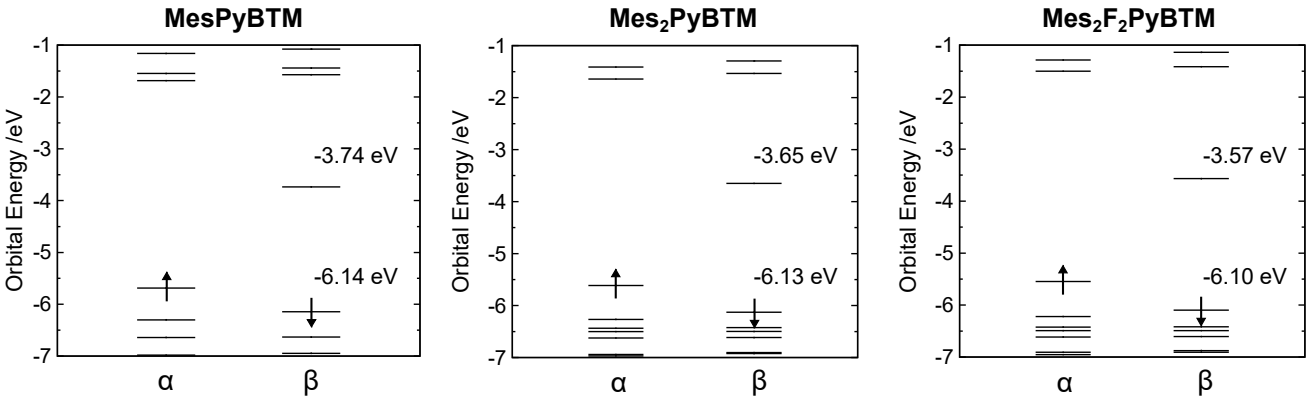


Fig. S5. Calculated orbital levels at the D_1 optimized structure of MesPyBTM, Mes_2PyBTM, and Mes_2F_2PyBTM. Orbital energy levels of the β-HOMO and -LUMO are written.

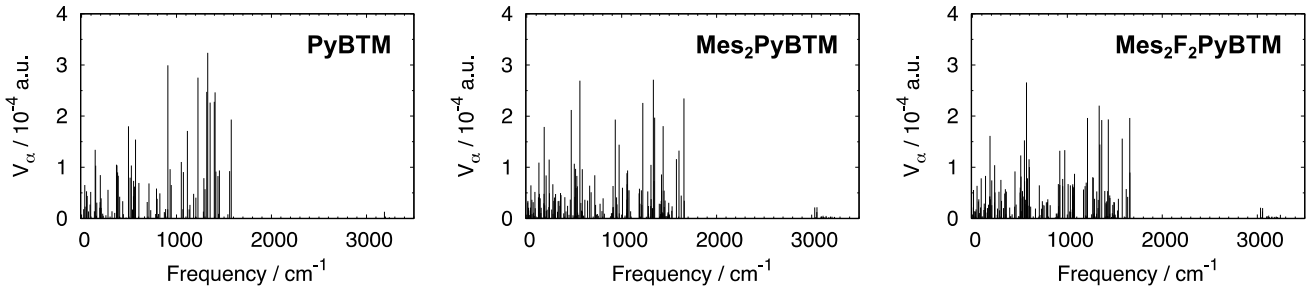


Fig. S6. Calculated off-diagonal vibronic coupling constants (VCCs) between D_1 and D_0 states of PyBTM, Mes_2PyBTM, and Mes_2F_2PyBTM. Square sums of the off-diagonal VCCs, $\sum_\alpha |V_{10,\alpha}|^2$, are 8.45, 7.45, and 6.84×10^{-7} a.u. for PyBTM, Mes_2PyBTM, and Mes_2F_2PyBTM, respectively.

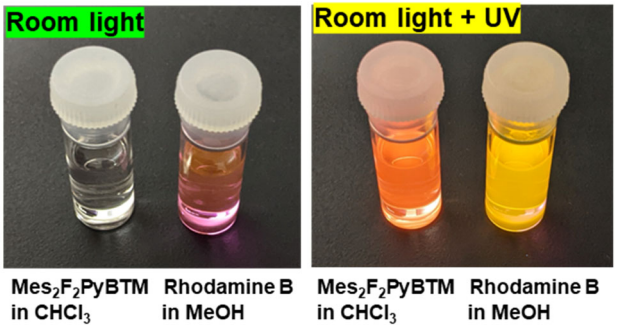


Fig. S7. Pictures of Mes_2F_2PyBTM in chloroform ($A_{365\ nm}$ = 0.10) and rhodamine B in methanol ($A_{365\ nm}$ = 0.10). Mes_2F_2PyBTM showed vivid fluorescence even under room light as well as rhodamine B when irradiated with 365 nm UV light.

Cartesian coordinates of the optimized geometries by DFT calculation

MesPyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.360918	1.750976	2.340760
2	17	0	0.886480	-1.963855	1.979582
3	17	0	0.108016	-1.251533	-2.288973
4	17	0	3.574799	0.596541	-2.125164
5	7	0	2.934101	4.465129	0.431533
6	6	0	-2.381480	0.639557	0.979374
7	1	0	-2.983913	1.094652	1.756840
8	6	0	-0.791465	-0.539997	-0.954203
9	6	0	3.319540	-0.720003	-0.992462
10	6	0	1.961429	4.190527	-0.440601
11	1	0	1.595745	5.008377	-1.054704
12	6	0	1.870498	1.819503	0.173118
13	6	0	4.192080	-1.795845	-1.113710
14	6	0	3.999802	-2.908590	-0.301629
15	6	0	-1.004527	0.826113	0.988763
16	6	0	1.418928	2.916971	-0.599858
17	6	0	2.105107	-1.860087	0.720796
18	6	0	2.958731	-2.953356	0.619653
19	6	0	-2.166942	-0.738470	-0.974092
20	6	0	2.237481	-0.692986	-0.075185
21	6	0	-0.137265	0.250537	0.025139
22	6	0	2.899606	2.157312	1.085479
23	6	0	3.391736	3.457579	1.178177
24	6	0	1.321882	0.457122	0.040830
25	1	0	4.176909	3.682807	1.894063
26	6	0	-2.986770	-0.149134	-0.005346
27	1	0	4.991759	-1.769968	-1.842436
28	6	0	-4.469250	-0.356245	-0.021157
29	6	0	-5.022187	-1.521451	0.550193
30	6	0	-5.307588	0.612814	-0.610983
31	6	0	-6.410244	-1.693841	0.523219
32	6	0	-6.689762	0.396472	-0.617521
33	6	0	-7.262688	-0.747023	-0.052758
34	1	0	-6.834665	-2.592805	0.964363
35	1	0	-7.333929	1.141511	-1.078844
36	1	0	-2.604408	-1.339653	-1.762577
37	1	0	2.822339	-3.812454	1.263508
38	6	0	-4.740296	1.865589	-1.240524
39	1	0	-4.232112	2.495867	-0.502457
40	1	0	-4.001869	1.630190	-2.014498
41	1	0	-5.532600	2.461554	-1.699853
42	6	0	-4.146377	-2.576311	1.188836
43	1	0	-3.470071	-3.037705	0.460827
44	1	0	-3.516603	-2.153649	1.979058
45	1	0	-4.754338	-3.369893	1.629888
46	6	0	-8.760569	-0.941545	-0.042158
47	1	0	-9.026267	-2.002476	-0.063320
48	1	0	-9.207545	-0.512962	0.863504
49	1	0	-9.233244	-0.452756	-0.899030
50	17	0	0.219762	2.733039	-1.864827
51	17	0	3.557576	0.991714	2.217349
52	17	0	5.085441	-4.274400	-0.441280

Mes_2PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.102681	2.093696	2.185968
2	17	0	0.437495	-0.913705	2.156131
3	17	0	-0.437492	-0.913707	-2.156126
4	17	0	2.102681	2.093696	-2.185965
5	7	0	-0.000001	5.657858	0.000001
6	6	0	-3.530066	0.192766	0.952839
7	1	0	-4.277716	0.457974	1.691251
8	6	0	-1.568535	-0.474314	-0.881231
9	6	0	2.321677	0.878779	-0.930965
10	6	0	-0.779256	4.963628	-0.832530
11	1	0	-1.406650	5.527929	-1.516459
12	6	0	0.000000	2.793409	0.000001
13	6	0	3.530066	0.192765	-0.952838
14	6	0	3.773987	-0.848639	-0.050750
15	6	0	-2.321677	0.878779	0.930967
16	6	0	-0.806452	3.571006	-0.866711
17	6	0	1.568537	-0.474313	0.881235
18	6	0	2.770404	-1.172493	0.868813
19	6	0	-2.770402	-1.172493	-0.868810
20	6	0	1.278737	0.585340	-0.015804
21	6	0	-1.278736	0.585340	0.015808
22	6	0	0.806452	3.571007	0.866714
23	6	0	0.779255	4.963629	0.832532
24	6	0	0.000000	1.318992	0.000002
25	1	0	1.406649	5.527931	1.516461
26	6	0	-3.773987	-0.848638	0.050751
27	1	0	4.277716	0.457972	-1.691251
28	6	0	5.071618	-1.595010	-0.069533
29	6	0	5.167407	-2.820425	-0.761629
30	6	0	6.192742	-1.072545	0.608592
31	6	0	6.389576	-3.501254	-0.764410
32	6	0	7.393837	-1.789412	0.580878
33	6	0	7.515791	-3.003137	-0.102357
34	1	0	6.461158	-4.446035	-1.298414
35	1	0	8.255201	-1.388230	1.110045
36	6	0	-5.071619	-1.595007	0.069531
37	6	0	-5.167419	-2.820406	0.761653
38	6	0	-6.192732	-1.072556	-0.608621
39	6	0	-6.389589	-3.501234	0.764430
40	6	0	-7.393828	-1.789421	-0.580911
41	6	0	-7.515793	-3.003130	0.102348
42	1	0	-6.461179	-4.446004	1.298453
43	1	0	-8.255183	-1.388248	-1.110098
44	1	0	-2.933176	-1.960802	-1.594520
45	1	0	2.933178	-1.960802	1.594523
46	6	0	-6.114600	0.233704	-1.366980
47	1	0	-5.894723	1.075960	-0.701796
48	1	0	-5.322151	0.215282	-2.122893
49	1	0	-7.059486	0.445321	-1.873290
50	6	0	-3.981103	-3.402999	1.497023
51	1	0	-3.156513	-3.638309	0.815246
52	1	0	-3.584004	-2.703303	2.240319
53	1	0	-4.260037	-4.323652	2.015244
54	6	0	-8.832707	-3.741750	0.145458
55	1	0	-8.682896	-4.821320	0.238753
56	1	0	-9.436339	-3.422330	1.004122
57	1	0	-9.425606	-3.554685	-0.754582
58	6	0	6.114623	0.233730	1.366925
59	1	0	5.894750	1.075975	0.701724
60	1	0	5.322177	0.215329	2.122841
61	1	0	7.059513	0.445350	1.873226
62	6	0	3.981080	-3.403032	-1.496970
63	1	0	3.156504	-3.638339	-0.815175
64	1	0	3.583964	-2.703347	-2.240267
65	1	0	4.260009	-4.323691	-2.015185
66	6	0	8.832703	-3.741758	-0.145470
67	1	0	8.682890	-4.821331	-0.238739
68	1	0	9.436323	-3.422357	-1.004150
69	1	0	9.425616	-3.554675	0.754557
70	17	0	-1.820044	2.842185	-2.097566
71	17	0	1.820045	2.842187	2.097568

Mes_2F_2PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.075743	2.128842	2.240584
2	17	0	0.460843	-0.665325	2.252825
3	17	0	-0.460843	-0.665325	-2.252824
4	17	0	2.075743	2.128842	-2.240584
5	7	0	0.000000	5.772410	0.000000
6	6	0	-3.515810	0.273944	0.947150
7	1	0	-4.253733	0.500836	1.707813
8	6	0	-1.583277	-0.291565	-0.949113
9	6	0	2.309794	0.963797	-0.940168
10	6	0	-0.967503	5.077488	-0.611541
11	1	0	-1.754775	5.628039	-1.118846
12	6	0	0.000000	2.906772	0.000000
13	6	0	3.515810	0.273943	-0.947151
14	6	0	3.772266	-0.720115	0.004412
15	6	0	-2.309794	0.963798	0.940168
16	6	0	-0.994178	3.690804	-0.625494
17	6	0	1.583277	-0.291565	0.949113
18	6	0	2.784681	-0.993302	0.955769
19	6	0	-2.784681	-0.993302	-0.955769
20	6	0	1.281365	0.716245	0.002875
21	6	0	-1.281365	0.716245	-0.002875
22	6	0	0.994178	3.690804	0.625494
23	6	0	0.967503	5.077488	0.611540
24	6	0	0.000000	1.453923	0.000000
25	1	0	1.754775	5.628039	1.118845
26	6	0	-3.772266	-0.720116	-0.004412
27	1	0	4.253733	0.500836	-1.707813
28	6	0	5.069094	-1.468773	0.003142
29	6	0	5.169844	-2.698655	-0.679910
30	6	0	6.184217	-0.943220	0.688460
31	6	0	6.390930	-3.381386	-0.666143
32	6	0	7.384900	-1.661246	0.676424
33	6	0	7.511586	-2.879895	0.002806
34	1	0	6.466010	-4.330487	-1.191964
35	1	0	8.242137	-1.256888	1.209886
36	6	0	-5.069094	-1.468773	-0.003142
37	6	0	-5.169844	-2.698656	0.679909
38	6	0	-6.184218	-0.943220	-0.688459
39	6	0	-6.390930	-3.381386	0.666142
40	6	0	-7.384901	-1.661246	-0.676423
41	6	0	-7.511586	-2.879895	-0.002805
42	1	0	-6.466009	-4.330488	1.191963
43	1	0	-8.242137	-1.256887	-1.209884
44	1	0	-2.956634	-1.744439	-1.717896
45	1	0	2.956634	-1.744439	1.717896
46	6	0	-6.099928	0.369144	-1.435443
47	1	0	-5.858326	1.201427	-0.765300
48	1	0	-5.318986	0.347650	-2.203289
49	1	0	-7.049012	0.598225	-1.926054
50	6	0	-3.988395	-3.285151	1.419847
51	1	0	-3.150085	-3.491646	0.745541
52	1	0	-3.612243	-2.599997	2.187302
53	1	0	-4.263577	-4.222150	1.910029
54	6	0	-8.827968	-3.620342	0.022970
55	1	0	-8.677702	-4.700288	0.111105
56	1	0	-9.440409	-3.306953	0.877615
57	1	0	-9.412325	-3.428529	-0.881658
58	6	0	6.099928	0.369144	1.435445
59	1	0	5.858325	1.201426	0.765303
60	1	0	5.318986	0.347648	2.203291
61	1	0	7.049011	0.598224	1.926056
62	6	0	3.988395	-3.285150	-1.419849
63	1	0	3.150086	-3.491645	-0.745544
64	1	0	3.612245	-2.599996	-2.187303
65	1	0	4.263578	-4.222148	-1.910031
66	6	0	8.827968	-3.620342	-0.022969
67	1	0	8.677702	-4.700288	-0.111104
68	1	0	9.440409	-3.306953	-0.877616
69	1	0	9.412326	-3.428528	0.881658
70	9	0	1.996381	3.083697	1.286233
71	9	0	-1.996381	3.083697	-1.286233

MesPyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.350352	-1.977429	-2.176034
2	17	0	0.682889	1.766051	-2.059587
3	17	0	0.133918	1.288091	2.260130
4	17	0	3.748714	-0.358443	2.033267
5	7	0	3.029741	-4.519749	-0.071331
6	6	0	-2.363473	-0.792046	-0.883134
7	1	0	-2.961583	-1.296251	-1.630635
8	6	0	-0.770477	0.533628	0.958041
9	6	0	3.331363	0.868767	0.839993
10	6	0	1.930012	-4.215448	0.629870
11	1	0	1.467174	-5.017983	1.198561
12	6	0	1.923825	-1.819519	-0.019454
13	6	0	4.132560	2.005290	0.857162
14	6	0	3.816099	3.065613	0.014800
15	6	0	-0.992561	-0.955277	-0.902845
16	6	0	1.385090	-2.941730	0.688596
17	6	0	1.967283	1.821905	-0.851694
18	6	0	2.724758	2.987925	-0.842611
19	6	0	-2.128036	0.787288	0.929941
20	6	0	2.205245	0.694438	-0.016802
21	6	0	-0.099760	-0.319991	0.024030
22	6	0	3.089103	-2.211067	-0.757031
23	6	0	3.587511	-3.505006	-0.747596
24	6	0	1.359453	-0.499585	-0.006502
25	1	0	4.470267	-3.734100	-1.339114
26	6	0	-2.969848	0.111476	0.017286
27	1	0	4.969080	2.070925	1.541063
28	6	0	-4.414719	0.335732	0.012624
29	6	0	-4.942709	1.680478	-0.030768
30	6	0	-5.327668	-0.783560	0.052461
31	6	0	-6.314155	1.858571	-0.044002
32	6	0	-6.688381	-0.534235	0.062516
33	6	0	-7.214359	0.773431	0.006286
34	1	0	-6.714733	2.865084	-0.114985
35	1	0	-7.376812	-1.370237	0.136828
36	1	0	-2.554932	1.440945	1.679334
37	1	0	2.485317	3.801435	-1.515355
38	6	0	-4.855744	-2.212163	0.172484
39	1	0	-4.578433	-2.629910	-0.801546
40	1	0	-3.985795	-2.304601	0.825448
41	1	0	-5.657344	-2.836735	0.572014
42	6	0	-4.055970	2.896143	-0.148782
43	1	0	-3.655605	3.202719	0.823658
44	1	0	-3.204956	2.720450	-0.809795
45	1	0	-4.629756	3.739107	-0.539156
46	6	0	-8.692209	1.004354	-0.030460
47	1	0	-8.961620	1.960962	0.423890
48	1	0	-9.034892	1.034058	-1.074192
49	1	0	-9.238549	0.199020	0.466037
50	17	0	0.019811	-2.739526	1.791888
51	17	0	3.914249	-1.087378	-1.841121
52	17	0	4.804983	4.519274	0.035623

Mes_2PyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

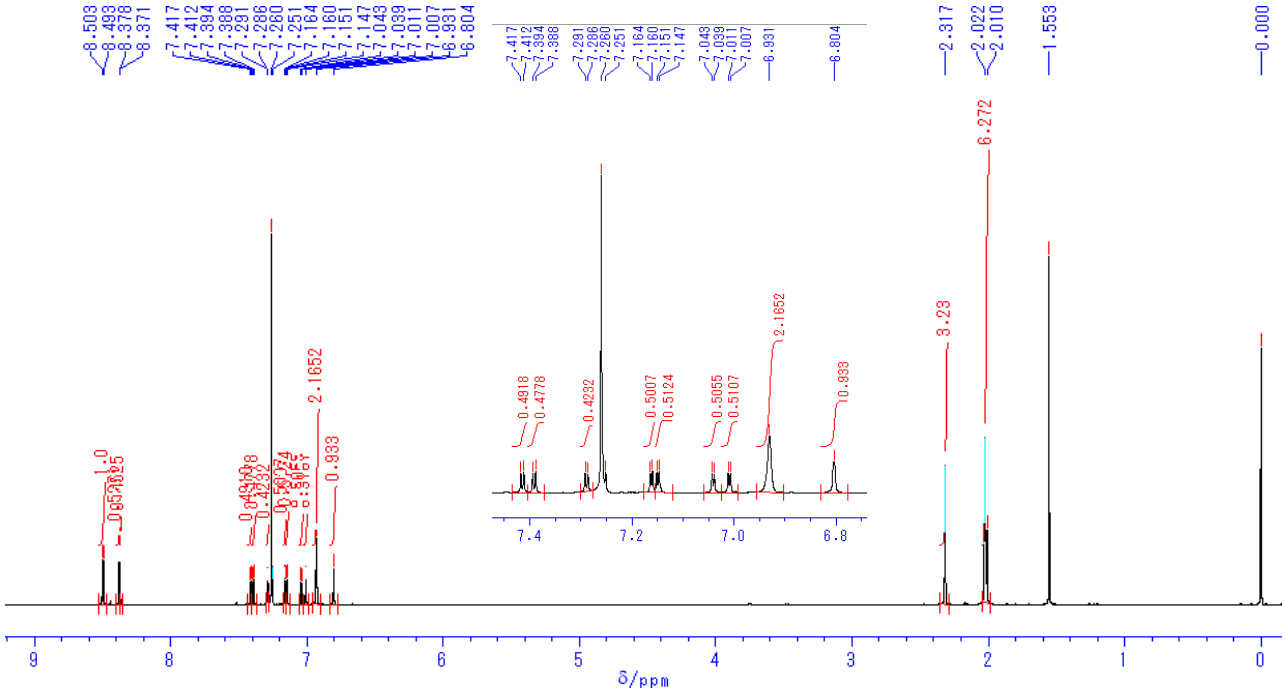
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.156290	2.169138	-2.101216
2	17	0	-0.319551	-0.833275	-2.104119
3	17	0	0.400114	-0.831741	2.200671
4	17	0	-2.219540	2.167648	2.142861
5	7	0	0.119883	5.765098	0.171144
6	6	0	3.521458	0.214780	-0.899409
7	1	0	4.270844	0.469574	-1.637106
8	6	0	1.530463	-0.444372	0.914652
9	6	0	-2.352784	0.932155	0.887208
10	6	0	1.004221	5.007737	0.833307
11	1	0	1.757631	5.525596	1.421488
12	6	0	0.027803	2.848326	0.092238
13	6	0	-3.546494	0.220412	0.872231
14	6	0	-3.734677	-0.848130	-0.012225
15	6	0	2.334596	0.918219	-0.883833
16	6	0	0.982201	3.621460	0.829513
17	6	0	-1.514092	-0.412779	-0.869943
18	6	0	-2.685622	-1.160161	-0.883547
19	6	0	2.668822	-1.222014	0.846251
20	6	0	-1.260094	0.672154	0.012333
21	6	0	1.260656	0.655795	0.035304
22	6	0	-0.880624	3.713870	-0.601827
23	6	0	-0.807136	5.096547	-0.530784
24	6	0	0.003515	1.414401	0.045813
25	1	0	-1.522453	5.691706	-1.092759
26	6	0	3.713833	-0.899666	-0.051684
27	1	0	-4.325974	0.479833	1.579748
28	6	0	-5.012342	-1.628375	-0.023541
29	6	0	-5.090653	-2.865692	0.650301
30	6	0	-6.139178	-1.128086	-0.710450
31	6	0	-6.295054	-3.577831	0.627339
32	6	0	-7.322597	-1.874625	-0.709892
33	6	0	-7.424277	-3.099882	-0.044077
34	1	0	-6.350746	-4.530586	1.149338
35	1	0	-8.186200	-1.488352	-1.246830
36	6	0	4.946642	-1.683837	-0.090634
37	6	0	4.891663	-3.124005	-0.188200
38	6	0	6.231766	-1.028362	-0.029092
39	6	0	6.077157	-3.837569	-0.228668
40	6	0	7.378237	-1.803120	-0.049099
41	6	0	7.335907	-3.208697	-0.156676
42	1	0	6.038769	-4.916890	-0.339311
43	1	0	8.344359	-1.316046	0.041192
44	1	0	2.795623	-2.027601	1.557597
45	1	0	-2.794402	-1.967350	-1.599111
46	6	0	6.376594	0.464597	0.144082
47	1	0	6.301703	0.992082	-0.813244
48	1	0	5.613020	0.879296	0.804858
49	1	0	7.358675	0.697329	0.561066
50	6	0	3.592753	-3.879376	-0.334063
51	1	0	3.110309	-4.048537	0.634843
52	1	0	2.877272	-3.348916	-0.965417
53	1	0	3.780575	-4.861395	-0.773234
54	6	0	8.599793	-4.008724	-0.222631
55	1	0	8.446397	-5.035562	0.116992
56	1	0	8.955366	-4.056346	-1.261164
57	1	0	9.396513	-3.547293	0.366709
58	6	0	-6.084287	0.188262	-1.453406
59	1	0	-5.911747	1.030200	-0.774217
60	1	0	-5.268577	0.204565	-2.183954
61	1	0	-7.020847	0.373395	-1.985458
62	6	0	-3.902122	-3.428935	1.397439
63	1	0	-3.072130	-3.663258	0.721848
64	1	0	-3.514662	-2.716017	2.132901
65	1	0	-4.174252	-4.346912	1.924561
66	6	0	-8.723298	-3.871014	-0.028950
67	1	0	-8.549234	-4.946306	0.072083
68	1	0	-9.355882	-3.563976	0.813353
69	1	0	-9.299290	-3.702190	-0.943666
70	17	0	2.152357	2.829828	1.890990
71	17	0	-2.096513	3.073902	-1.711152

Mes_2F_2PyBTM (D_1 state, UB3LYP/6-31G(d, p))

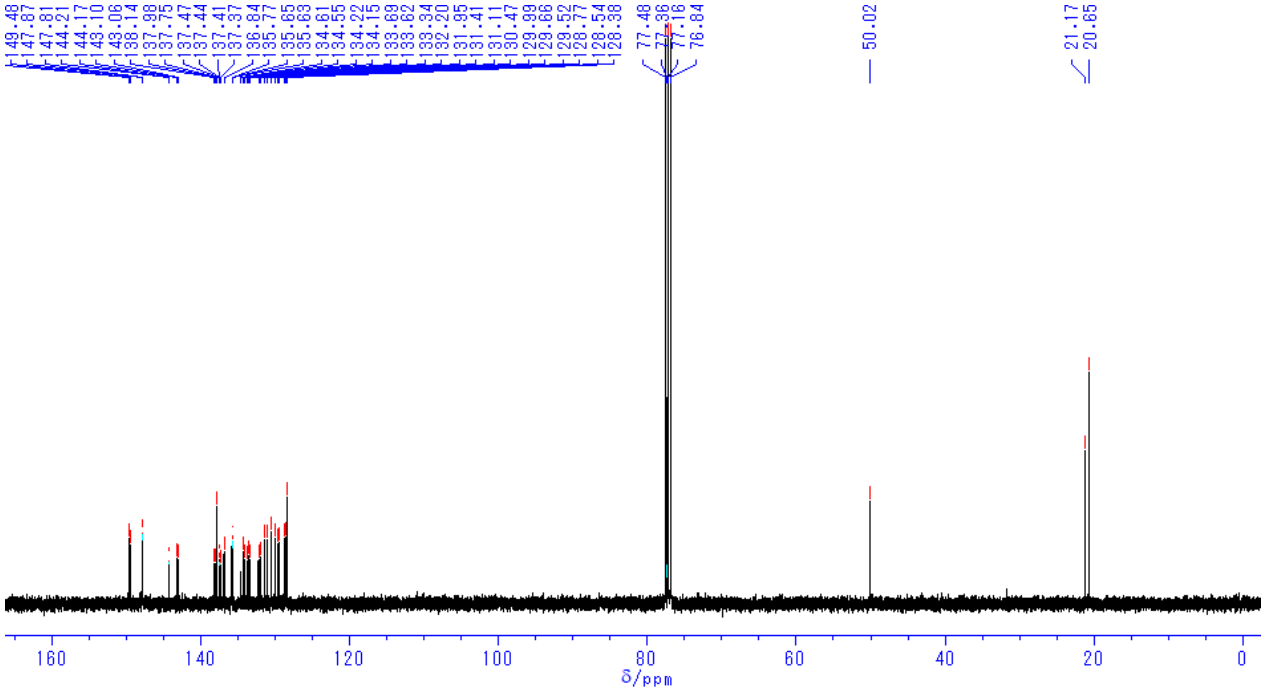
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.117987	2.192359	-2.168490
2	17	0	-0.367752	-0.667442	-2.166342
3	17	0	0.404823	-0.726833	2.206075
4	17	0	-2.169296	2.168638	2.233655
5	7	0	0.178830	5.837638	0.237639
6	6	0	3.523322	0.305186	-0.909203
7	1	0	4.268070	0.552095	-1.654187
8	6	0	1.538421	-0.339706	0.920392
9	6	0	-2.347315	1.009771	0.911963
10	6	0	1.185040	5.057997	0.668101
11	1	0	2.065822	5.541926	1.083987
12	6	0	0.049803	2.926677	0.115261
13	6	0	-3.556262	0.325205	0.874785
14	6	0	-3.776117	-0.692078	-0.061426
15	6	0	2.323317	0.984401	-0.913923
16	6	0	1.143216	3.678399	0.628706
17	6	0	-1.552786	-0.263583	-0.915380
18	6	0	-2.741265	-0.984935	-0.954862
19	6	0	2.693369	-1.096010	0.877091
20	6	0	-1.271078	0.774475	0.011344
21	6	0	1.255783	0.734497	0.018748
22	6	0	-0.976183	3.808195	-0.328802
23	6	0	-0.888791	5.184171	-0.255530
24	6	0	0.004427	1.501993	0.045247
25	1	0	-1.720469	5.776591	-0.630197
26	6	0	3.737746	-0.776268	-0.025204
27	1	0	-4.323428	0.565205	1.602414
28	6	0	-5.072285	-1.440995	-0.101713
29	6	0	-5.188224	-2.688988	0.546138
30	6	0	-6.178368	-0.900212	-0.791268
31	6	0	-6.408743	-3.371688	0.494560
32	6	0	-7.379456	-1.617563	-0.819196
33	6	0	-7.518150	-2.853250	-0.179888
34	1	0	-6.493073	-4.333631	0.995477
35	1	0	-8.227386	-1.199493	-1.357326
36	6	0	4.991447	-1.524891	-0.021193
37	6	0	4.980994	-2.969795	-0.052389
38	6	0	6.257740	-0.828394	0.019963
39	6	0	6.186893	-3.646611	-0.053951
40	6	0	7.427544	-1.568402	0.041875
41	6	0	7.427687	-2.976394	-0.002259
42	1	0	6.182576	-4.730545	-0.117369
43	1	0	8.377704	-1.048708	0.116726
44	1	0	2.833147	-1.878367	1.611149
45	1	0	-2.871616	-1.756353	-1.705400
46	6	0	6.358326	0.673609	0.130175
47	1	0	6.282765	1.156466	-0.850385
48	1	0	5.573859	1.095078	0.761496
49	1	0	7.327795	0.951309	0.549037
50	6	0	3.707135	-3.771659	-0.171332
51	1	0	3.229679	-3.921949	0.803202
52	1	0	2.975859	-3.288806	-0.822317
53	1	0	3.928048	-4.762240	-0.574349
54	6	0	8.710583	-3.747271	-0.023416
55	1	0	8.620073	-4.688621	0.525514
56	1	0	8.970893	-4.005375	-1.059169
57	1	0	9.538740	-3.166299	0.387835
58	6	0	-6.082476	0.429660	-1.505327
59	1	0	-5.876300	1.249313	-0.808521
60	1	0	-5.270954	0.434161	-2.240814
61	1	0	-7.014955	0.658909	-2.027273
62	6	0	-4.021370	-3.295546	1.293406
63	1	0	-3.182748	-3.516886	0.624184
64	1	0	-3.637345	-2.614777	2.060557
65	1	0	-4.315359	-4.227517	1.782903
66	6	0	-8.835165	-3.593329	-0.195659
67	1	0	-8.687534	-4.674598	-0.119025
68	1	0	-9.468822	-3.291706	0.647798
69	1	0	-9.397782	-3.389064	-1.111470
70	9	0	-2.096987	3.281303	-0.884422
71	9	0	2.213701	3.000492	1.127063

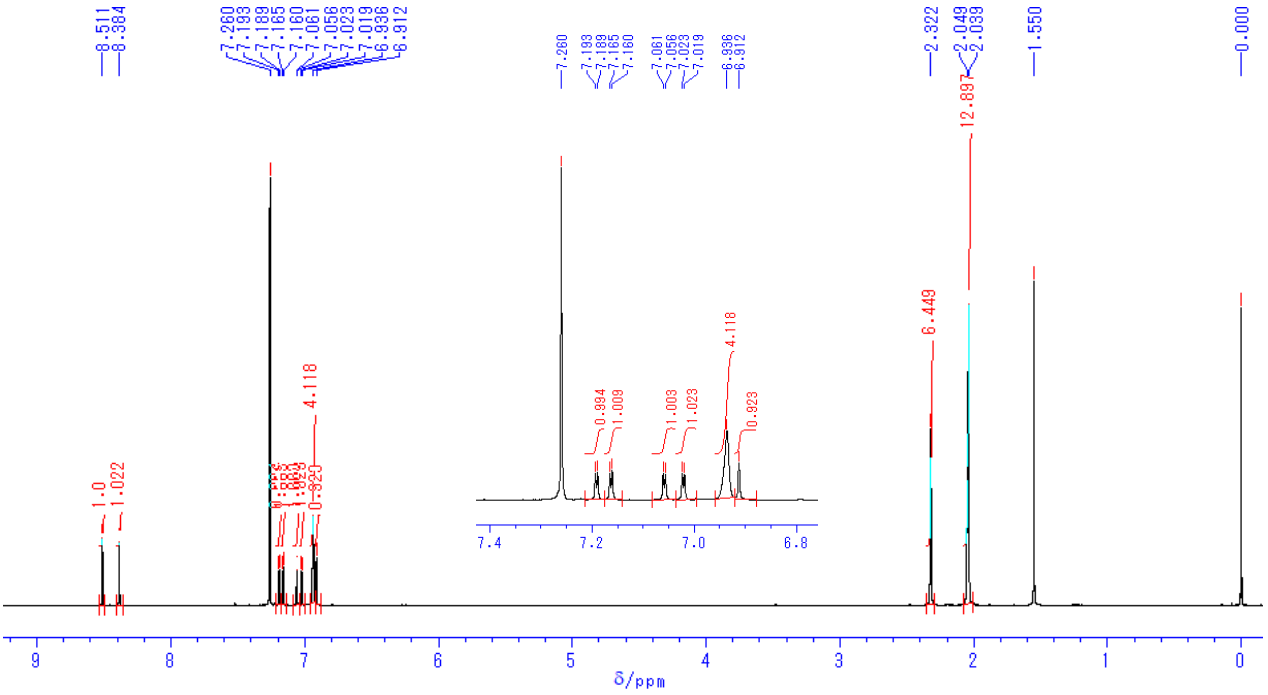
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-MesPyBTM



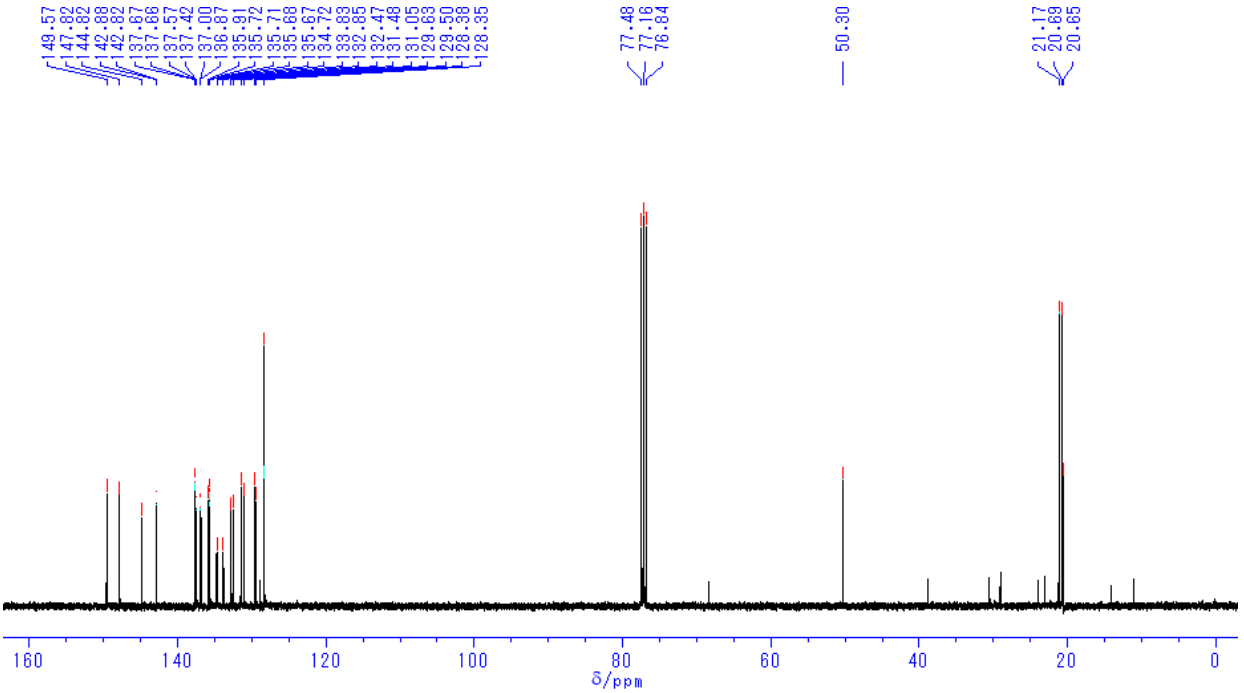
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-MesPyBTM



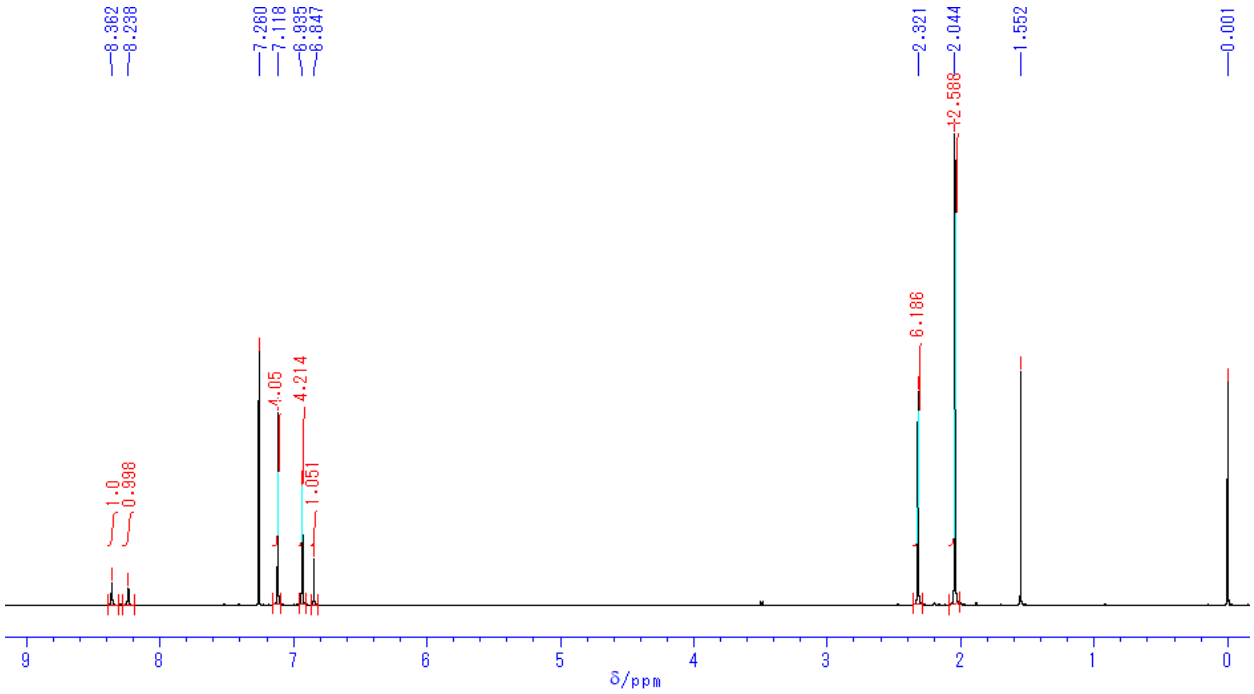
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Mes_2PyBTM



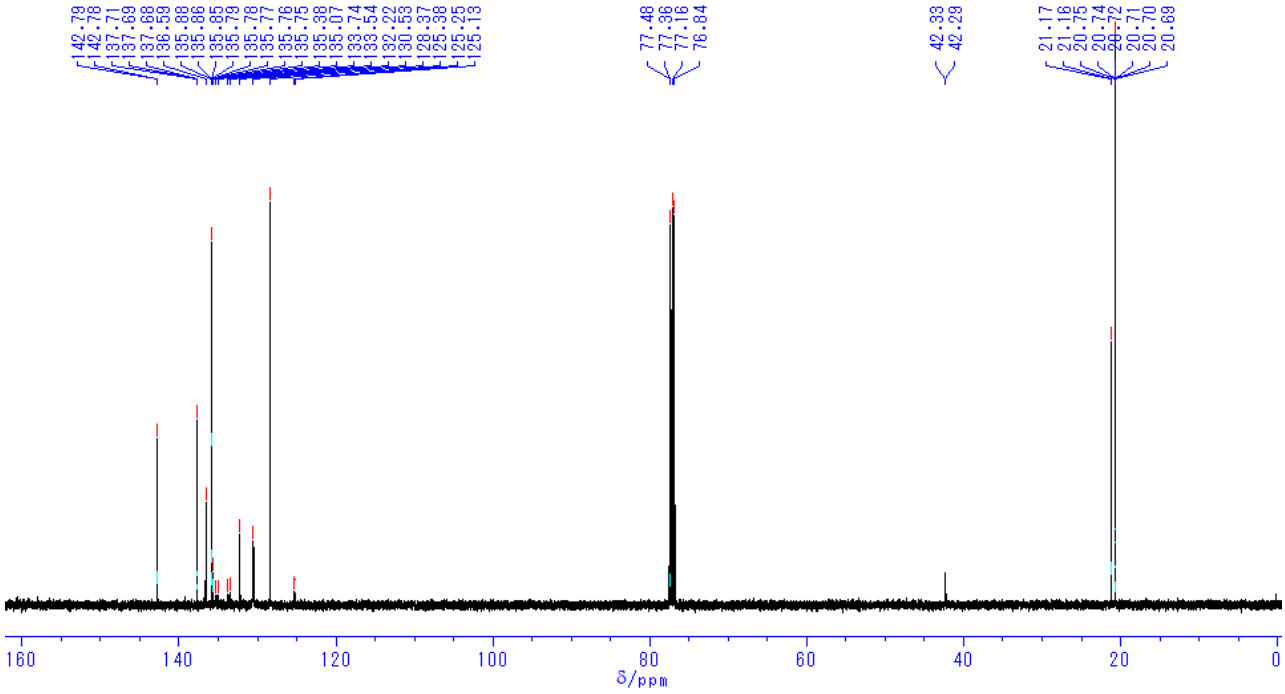
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Mes_2PyBTM



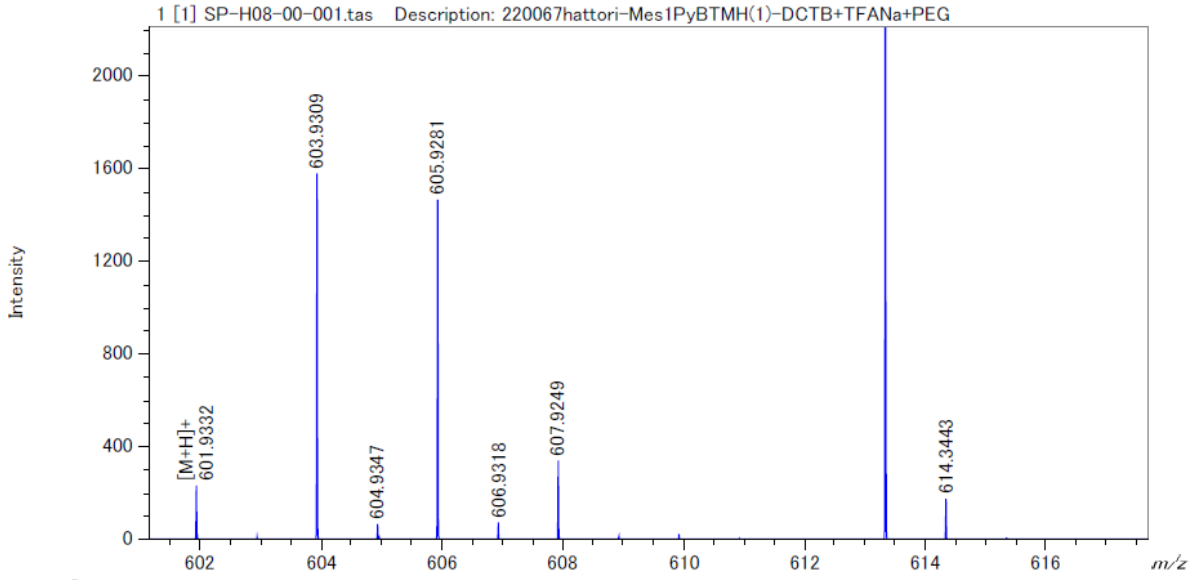
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Mes_2F_2PyBTM

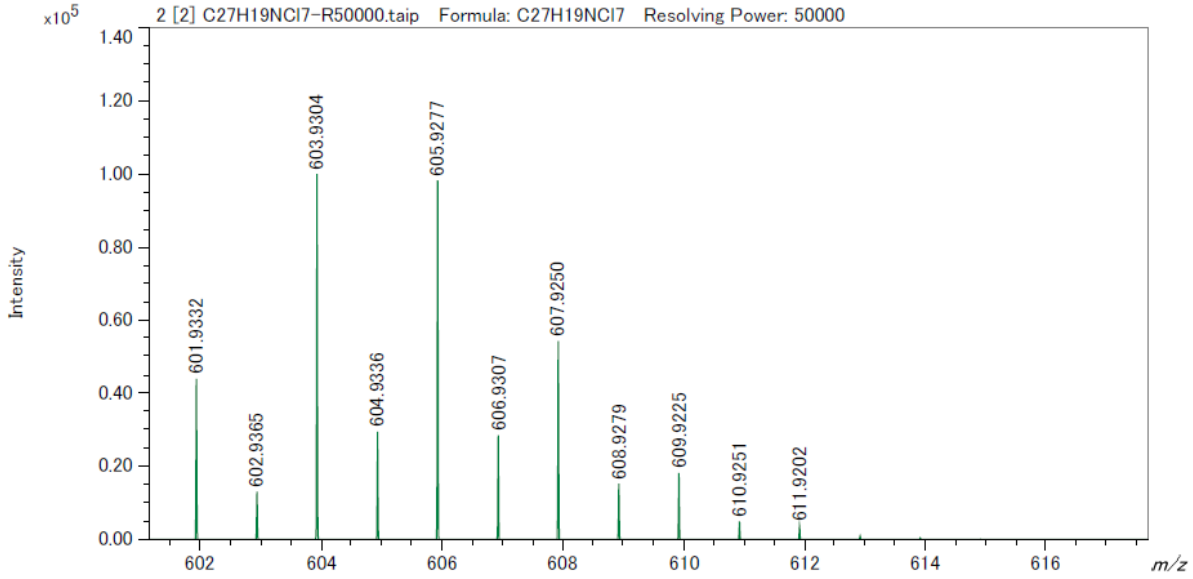


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Mes_2F_2PyBTM



HRMS of αH-MesPyBTM





Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
601.93316 ± 0.00301	5.0 ppm	Odd/Even	+1	−0.5 – 200.0	100

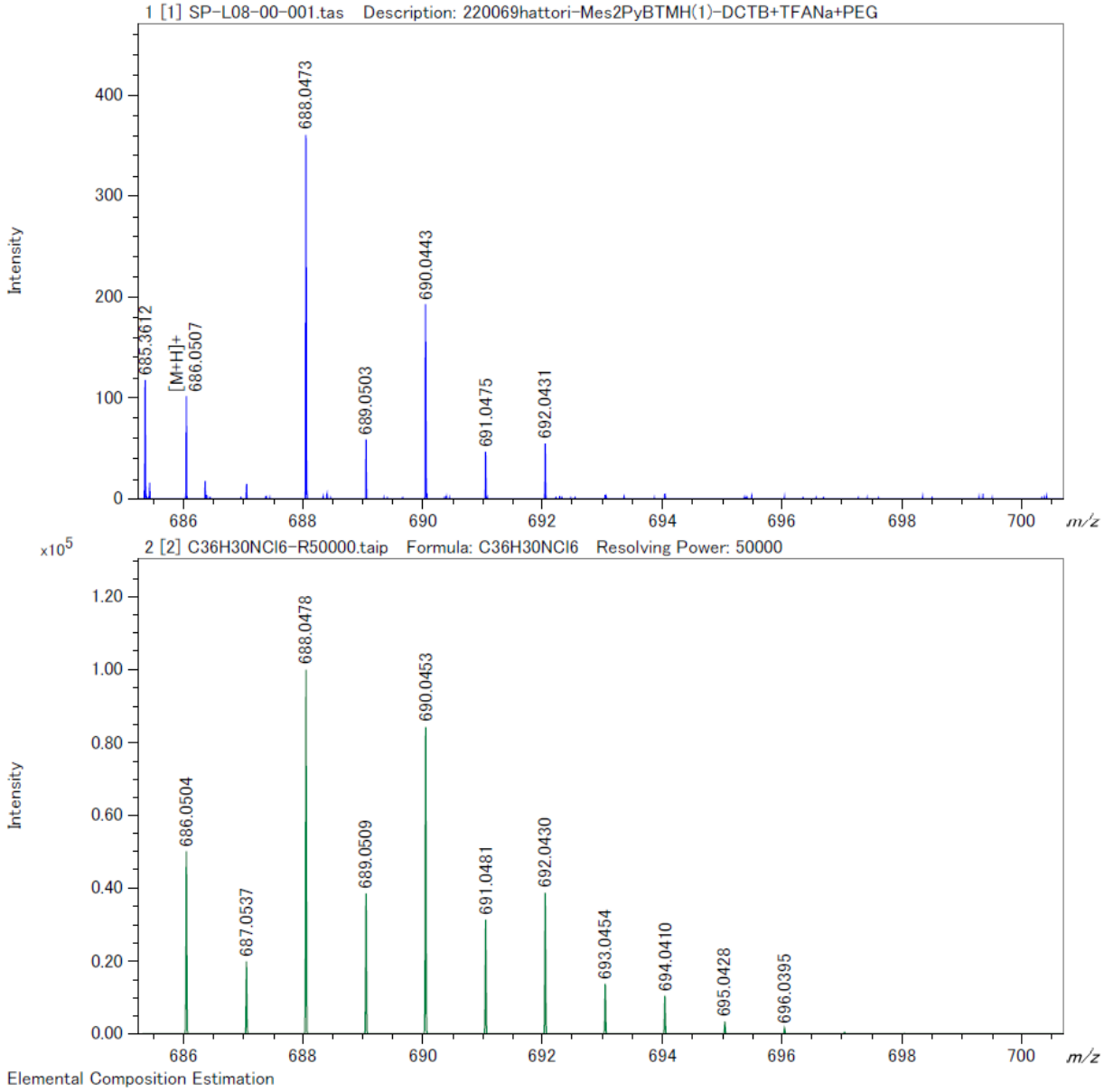
Elements

C 20 – 100 H 10 – 200 N 0 – 10 O 0 – 10 Cl 0 – 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C27 H19 N Cl7	601.93317	15.5	0.00001	−0.00001	−0.02
2	C24 H14 O10 Cl4	601.93356	16.0	0.00040	−0.00040	−0.66
3	C30 H16 O Cl6	601.93268	20.0	0.00048	0.00048	0.79
4	C20 H11 N8 O4 Cl5	601.93404	17.0	0.00088	−0.00088	−1.46
5	C21 H17 N O9 Cl5	601.93405	11.5	0.00089	−0.00089	−1.47
6	C22 H12 N3 O9 Cl4	601.93222	16.5	0.00094	0.00094	1.57
7	C25 H10 N4 O6 Cl4	601.93490	21.0	0.00174	−0.00174	−2.88
8	C28 H14 N3 Cl6	601.93134	20.5	0.00182	0.00182	3.02
9	C21 H24 N O2 Cl8	601.93098	6.5	0.00218	0.00218	3.63
10	C22 H13 N5 O5 Cl5	601.93538	16.5	0.00222	−0.00222	−3.69
11	C20 H10 N6 O8 Cl4	601.93087	17.0	0.00229	0.00229	3.80
12	C31 H11 N2 O Cl5	601.93085	25.0	0.00231	0.00231	3.83
13	C24 H21 O3 Cl7	601.93049	11.0	0.00267	0.00267	4.44

HRMS of αH-Mes_2PyBTM



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
686.05075 ± 0.00343	5.0 ppm	Odd/Even	+1	−0.5 – 200.0	100

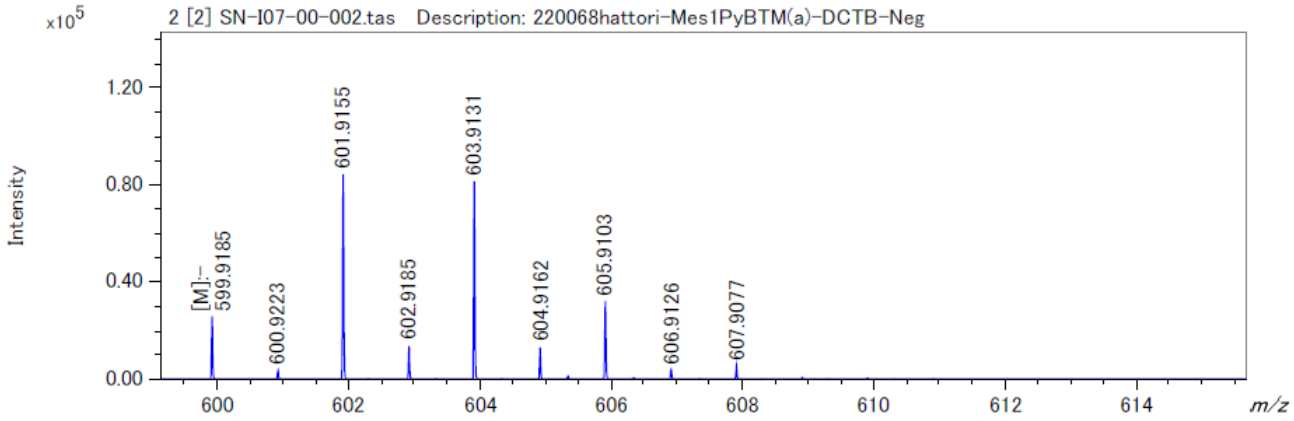
Elements

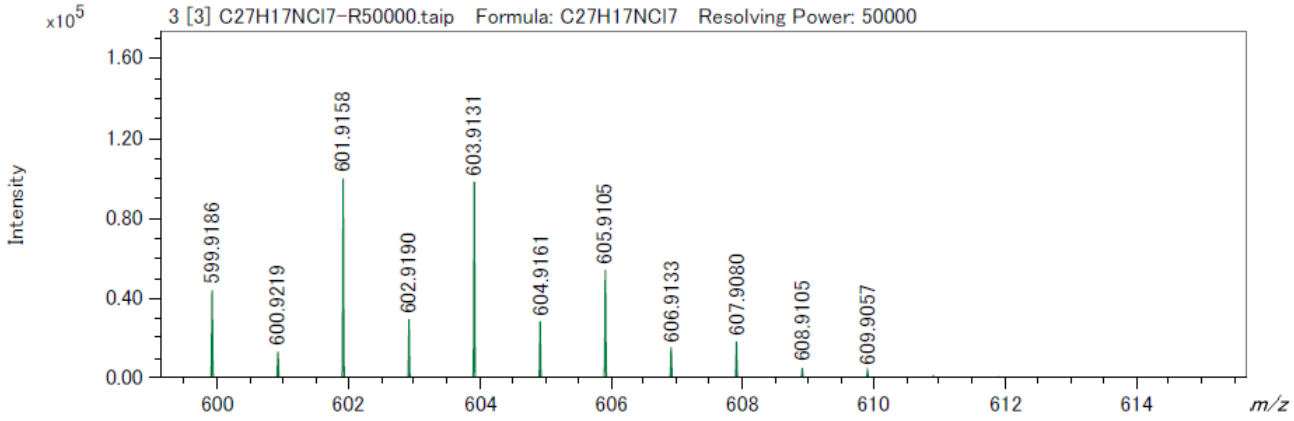
C	20 – 100	H	10 – 200	N	0 – 10	O	0 – 10	Cl	0 – 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C32 H19 N7 O5 Cl3	686.05078	25.5	0.00003	−0.00003	−0.04
2	C33 H25 O10 Cl3	686.05078	20.0	0.00003	−0.00003	−0.05
3	C43 H12 N O9	686.05066	38.5	0.00009	0.00009	0.13
4	C22 H32 N6 O6 Cl6	686.05090	7.0	0.00015	−0.00015	−0.22
5	C26 H43 O Cl9	686.05052	1.0	0.00023	0.00023	0.34
6	C25 H29 N5 O7 Cl5	686.05041	11.5	0.00033	0.00033	0.49
7	C36 H30 N Cl6	686.05039	19.5	0.00035	0.00035	0.52
8	C40 H15 N2 O8 Cl	686.05114	34.0	0.00040	−0.00040	−0.58
9	C35 H16 N6 O6 Cl2	686.05029	30.0	0.00046	0.00046	0.67
10	C29 H22 N8 O4 Cl4	686.05126	21.0	0.00052	−0.00052	−0.75
11	C30 H28 N O9 Cl4	686.05127	15.5	0.00052	−0.00052	−0.76
12	C28 H26 N4 O8 Cl4	686.04993	16.0	0.00082	0.00082	1.20
13	C39 H27 O Cl5	686.04991	24.0	0.00084	0.00084	1.23

HRMS of αMesPyBTM





Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
599.91850 ± 0.00300	5.0 ppm	Odd/Even	1	−0.5 – 200.0	100

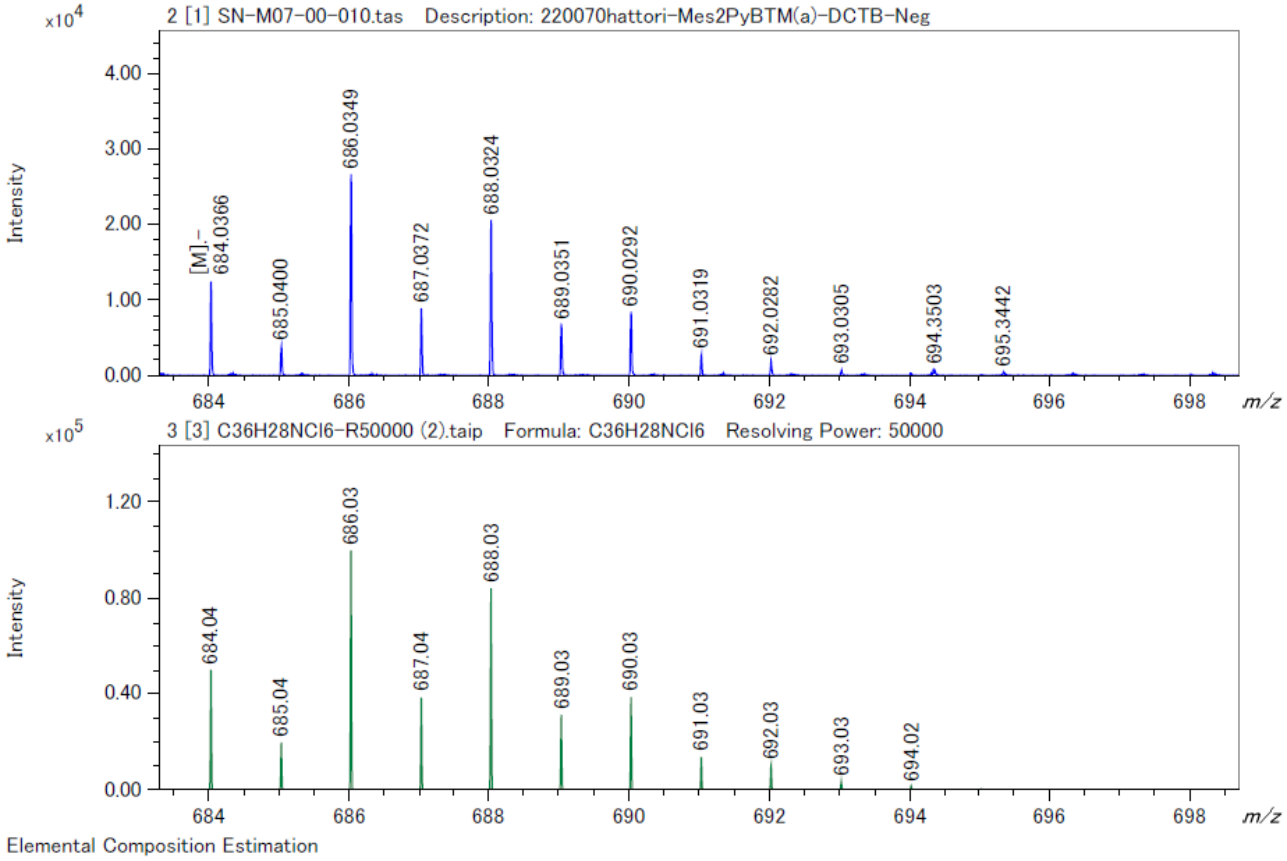
Elements

C 20 – 100 H 10 – 200 N 0 – 10 O 0 – 10 Cl 0 – 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C27 H17 N Cl7	599.91862	16.5	0.00012	−0.00012	−0.20
2	C30 H14 O Cl6	599.91813	21.0	0.00037	0.00037	0.62
3	C24 H12 O10 Cl4	599.91901	17.0	0.00051	−0.00051	−0.84
4	C22 H10 N3 O9 Cl4	599.91766	17.5	0.00084	0.00084	1.39
5	C21 H15 N O9 Cl5	599.91949	12.5	0.00099	−0.00099	−1.66
6	C28 H12 N3 Cl6	599.91679	21.5	0.00171	0.00171	2.85
7	C21 H22 N O2 Cl8	599.91642	7.5	0.00208	0.00208	3.46
8	C22 H11 N5 O5 Cl5	599.92083	17.5	0.00233	−0.00233	−3.89
9	C24 H19 O3 Cl7	599.91594	12.0	0.00256	0.00256	4.27

HRMS of Mes_2PyBTM



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
684.03660 ± 0.00342	5.0 ppm	Odd/Even	1	-0.5 – 200.0	100

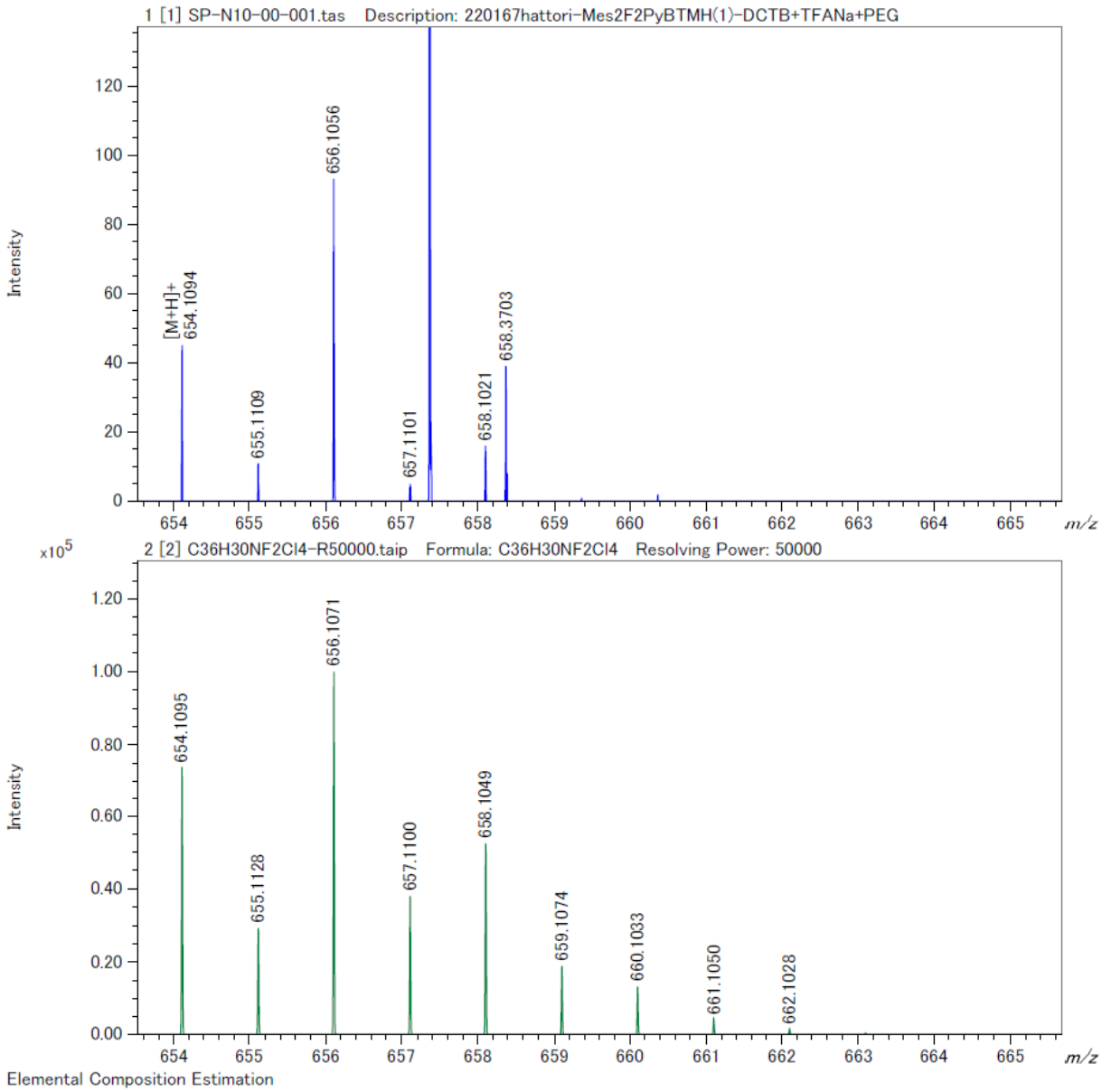
Elements

C 30 – 100 H 0 – 100 N 0 – 5 O 0 – 3 Na 0 – 0 Cl 0 – 8

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C36 H28 N Cl6	684.03584	20.5	0.00076	0.00076	1.11
2	C39 H25 O Cl5	684.03535	25.0	0.00125	0.00125	1.82
3	C49 H12 N Cl2	684.03523	43.5	0.00137	0.00137	2.00
4	C52 H9 O Cl	684.03474	48.0	0.00186	0.00186	2.72
5	C37 H23 N3 Cl5	684.03401	25.5	0.00259	0.00259	3.78
6	C30 H33 N O2 Cl7	684.03365	11.5	0.00295	0.00295	4.32
7	C40 H20 N2 O Cl4	684.03352	30.0	0.00308	0.00308	4.50
8	C50 H7 N3 Cl	684.03340	48.5	0.00320	0.00320	4.68

HRMS of αH-Mes_2F_2PyBTM



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
654.10945 ± 0.00327	5.0 ppm	Odd/Even	+1	−0.5 – 200.0	100

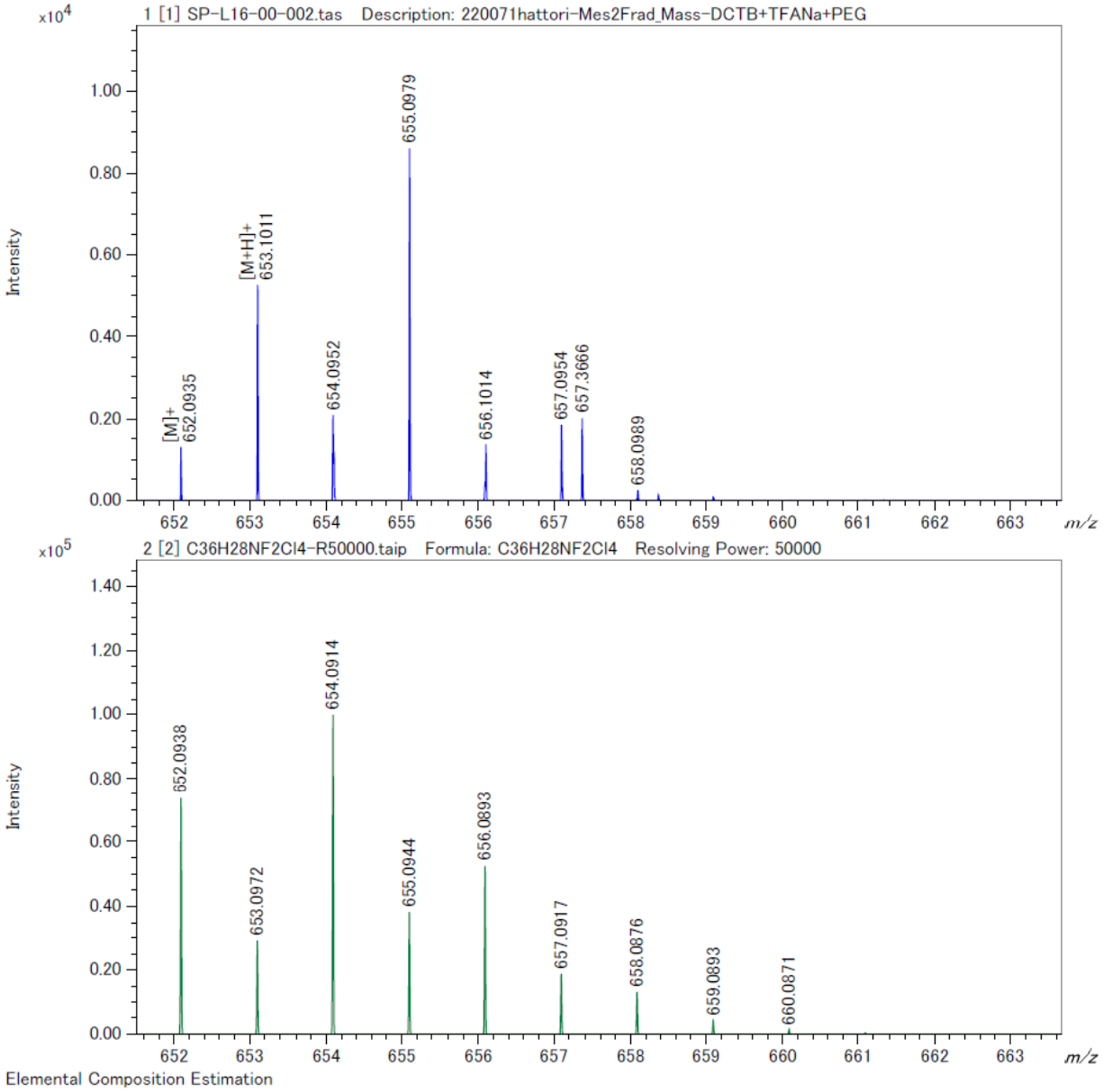
Elements

C 0 – 100 H 0 – 200 N 0 – 10 Cl 0 – 10 F 0 – 3

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C36 H30 N F2 Cl4	654.10949	19.5	0.00004	−0.00004	−0.07
2	C31 H29 N4 F3 Cl4	654.10929	16.0	0.00016	0.00016	0.24
3	C29 H26 N10 Cl4	654.10905	20.0	0.00040	0.00040	0.61
4	C49 H14 N F2	654.10888	42.5	0.00057	0.00057	0.87
5	C44 H13 N4 F3	654.10868	39.0	0.00077	0.00077	1.17
6	C41 H15 N8 Cl	654.11027	38.0	0.00082	−0.00082	−1.26
7	C29 H42 F Cl7	654.10847	5.0	0.00098	0.00098	1.49
8	C42 H10 N10	654.10844	43.0	0.00101	0.00101	1.54
9	C43 H18 N2 F3 Cl	654.11051	34.0	0.00106	−0.00106	−1.62
10	C24 H41 N3 F2 Cl7	654.10828	1.5	0.00117	0.00117	1.80
11	C28 H31 N8 Cl5	654.11088	15.0	0.00143	−0.00143	−2.19
12	C42 H26 F Cl3	654.10786	28.0	0.00159	0.00159	2.43
13	C30 H34 N2 F3 Cl5	654.11112	11.0	0.00167	−0.00167	−2.56

HRMS of Mes_2F_2PyBTM



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
652.09347 ± 0.00326	5.0 ppm	Odd/Even	+1	−0.5 – 200.0	100

Elements

C 0 – 100 H 0 – 200 N 0 – 10 F 0 – 10 Cl 0 – 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C23 H28 N4 F8 Cl4	652.09348	6.0	0.00001	−0.00001	−0.02
2	C26 H26 N7 F4 Cl4	652.09344	13.5	0.00003	0.00003	0.05
3	C29 H24 N10 Cl4	652.09340	21.0	0.00007	0.00007	0.11
4	C31 H27 N4 F3 Cl4	652.09364	17.0	0.00017	−0.00017	−0.26
5	C18 H27 N7 F9 Cl4	652.09328	2.5	0.00019	0.00019	0.29
6	C28 H29 N F7 Cl4	652.09368	9.5	0.00021	−0.00021	−0.32
7	C21 H25 N10 F5 Cl4	652.09324	10.0	0.00023	0.00023	0.35
8	C49 H12 N F2	652.09323	43.5	0.00024	0.00024	0.37
9	C36 H28 N F2 Cl4	652.09384	20.5	0.00037	−0.00037	−0.57
10	C41 H13 N F7	652.09307	32.5	0.00040	0.00040	0.61
11	C44 H11 N4 F3	652.09303	40.0	0.00044	0.00044	0.68
12	C36 H12 N4 F8	652.09287	29.0	0.00060	0.00060	0.92
13	C39 H10 N7 F4	652.09283	36.5	0.00064	0.00064	0.98