Six-armed Structures Based on Benzene Core, Synthesis and Characterization

Via Sonogashira Coupling.

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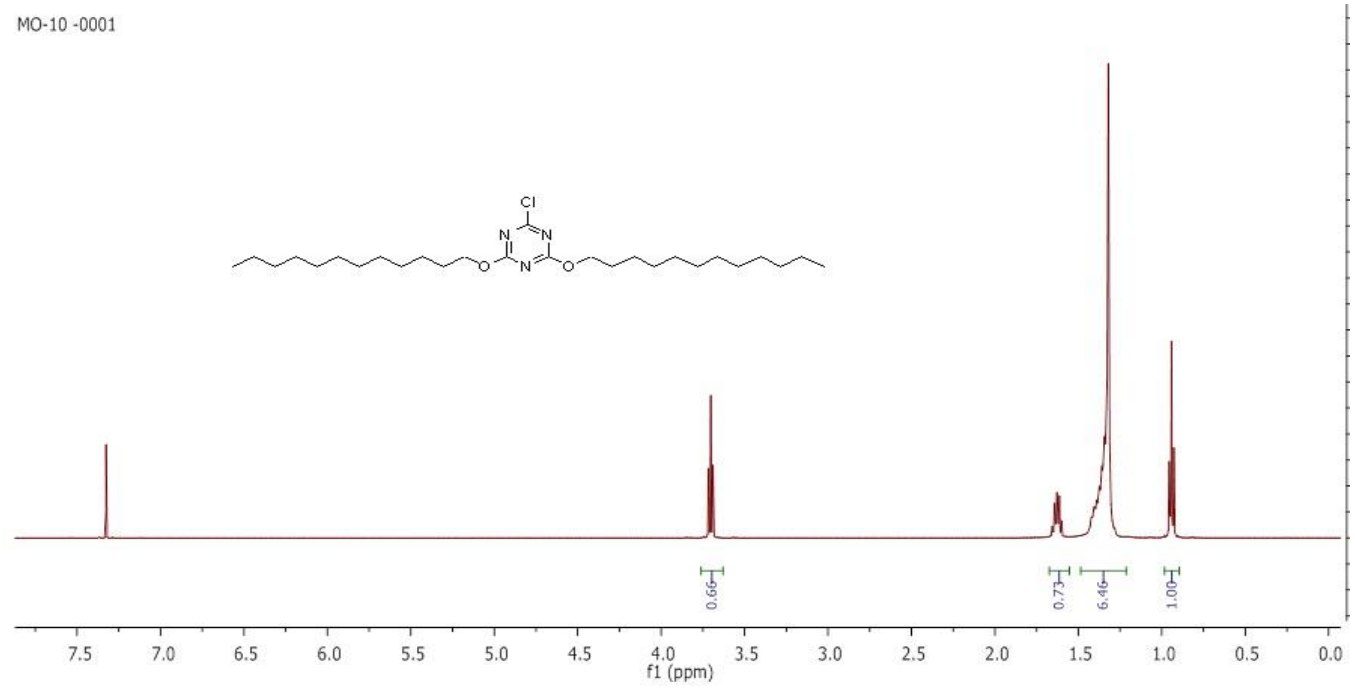
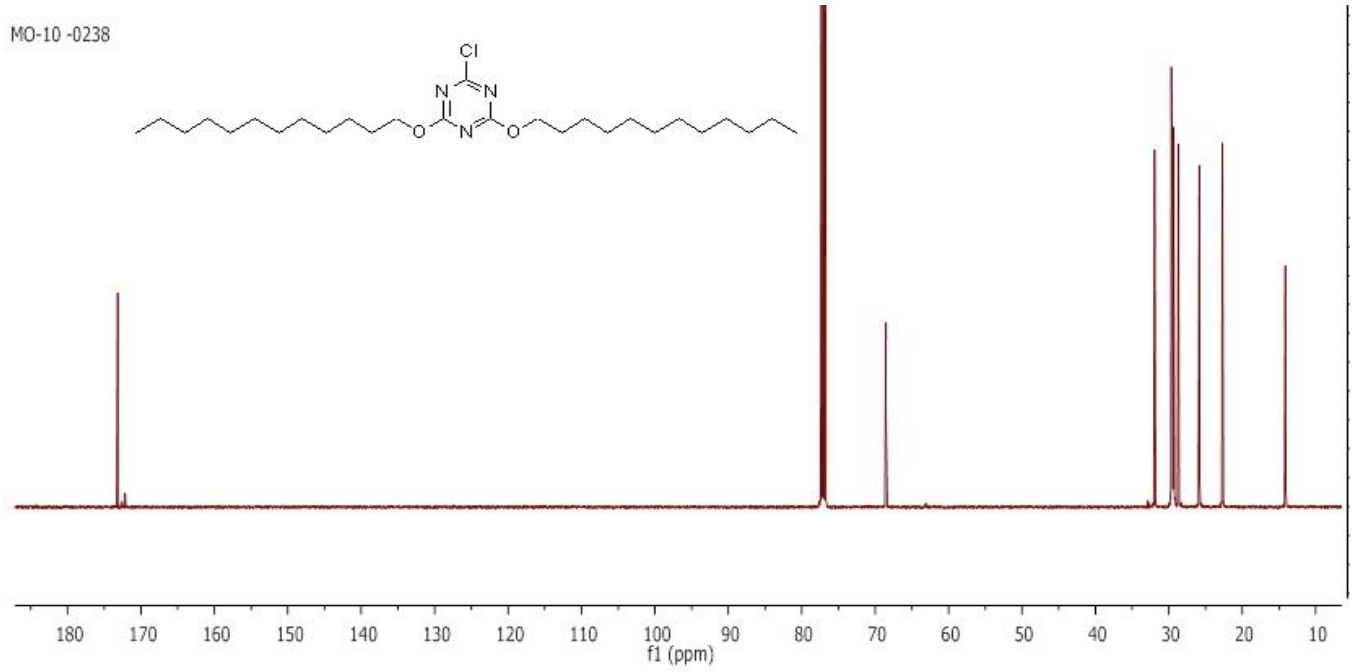
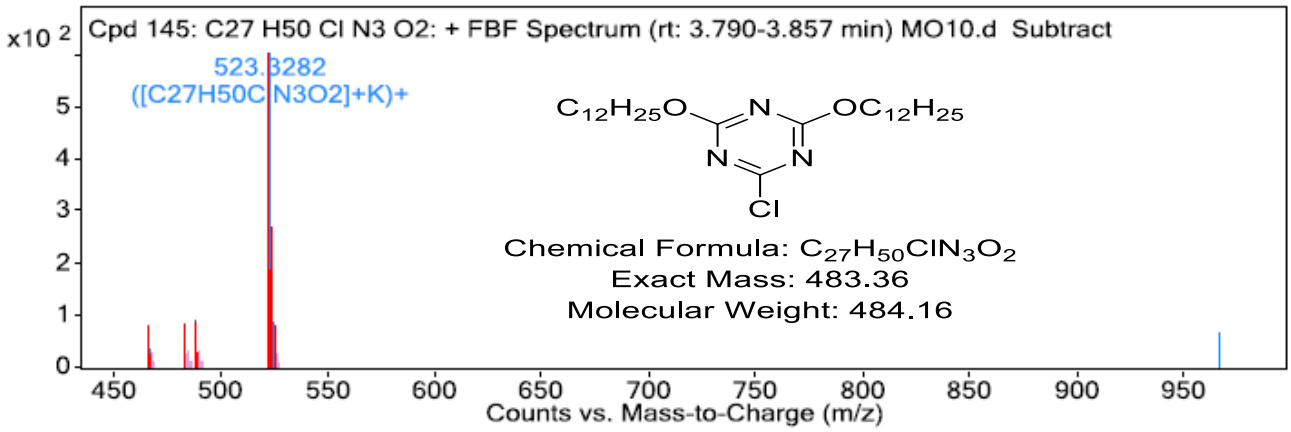
Spectroscopic Date Compound 2



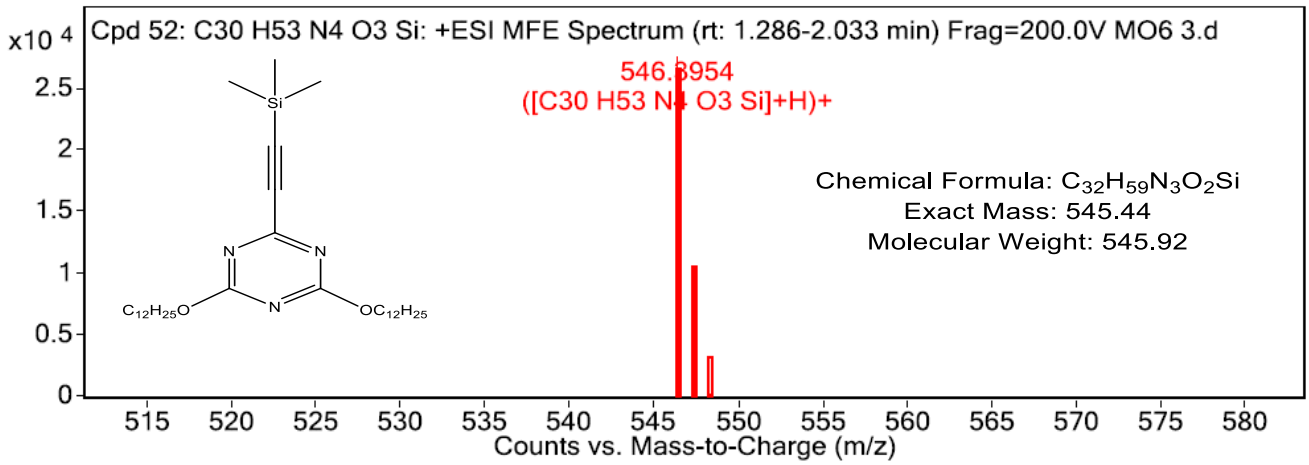




MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
466.3523	1	67.2	C27H50ClN3O2	(M+H)+[-H2O]
467.3546	1	34.54	C27H50ClN3O2	(M+H)+[-H2O]
483.3505	1	80.48	C27H50ClN3O2	M+
488.3443	1	88.06	C27H50ClN3O2	(M+Na)+[-H2O]
489.3308	1	25.27	C27H50ClN3O2	(M+Na)+[-H2O]
522.3373	1	203.35	C27H50ClN3O2	(M+K)+
523.3282	1	602.36	C27H50ClN3O2	(M+K)+
524.3244	1	150	C27H50ClN3O2	(M+K)+
525.3138	1	83.9	C27H50ClN3O2	(M+K)+
966.7171	1	66.27	C27H50ClN3O2	(2M+NH4)+[-H2O]

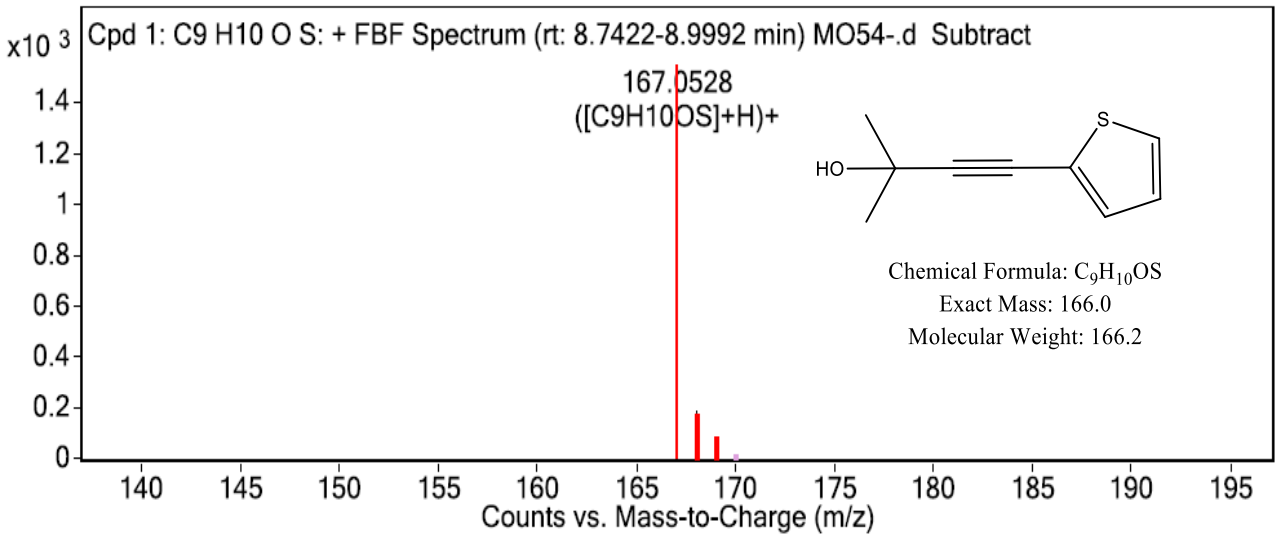
Mass spectroscopic date of compound 3



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
546.3954	1	27568.21	C30 H53 N4 O3 Si	(M+H)+
547.3976	1	9957.84	C30 H53 N4 O3 Si	(M+H)+
548.3977	1	2772.44	C30 H53 N4 O3 Si	(M+H)+

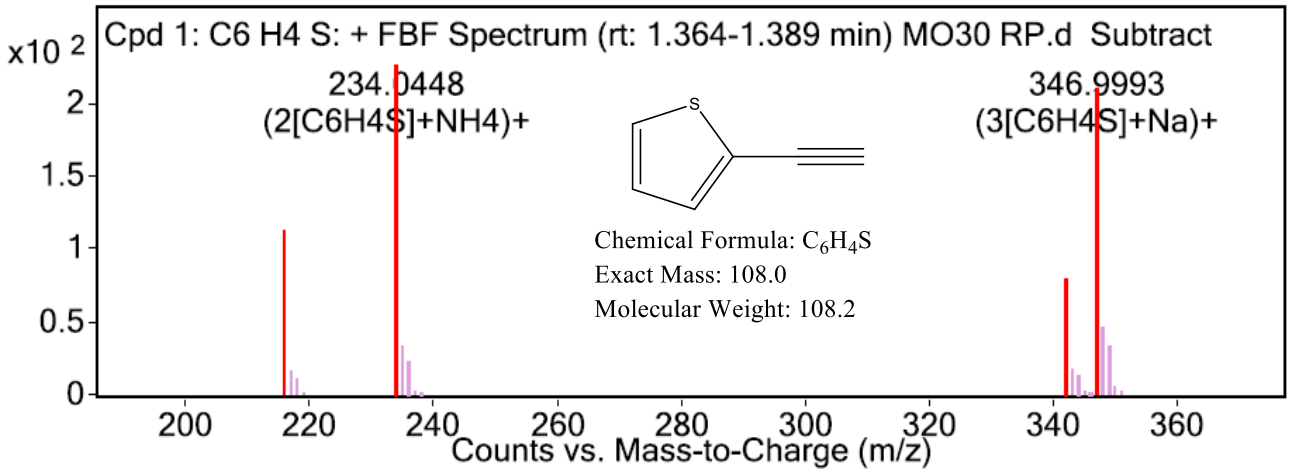
Mass spectroscopic date of compound 5



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
167,0528	1	1546,94	C9H10OS	(M+H)+
168,0567	1	187,62	C9H10OS	(M+H)+
169,0505	1	51,59	C9H10OS	(M+H)+

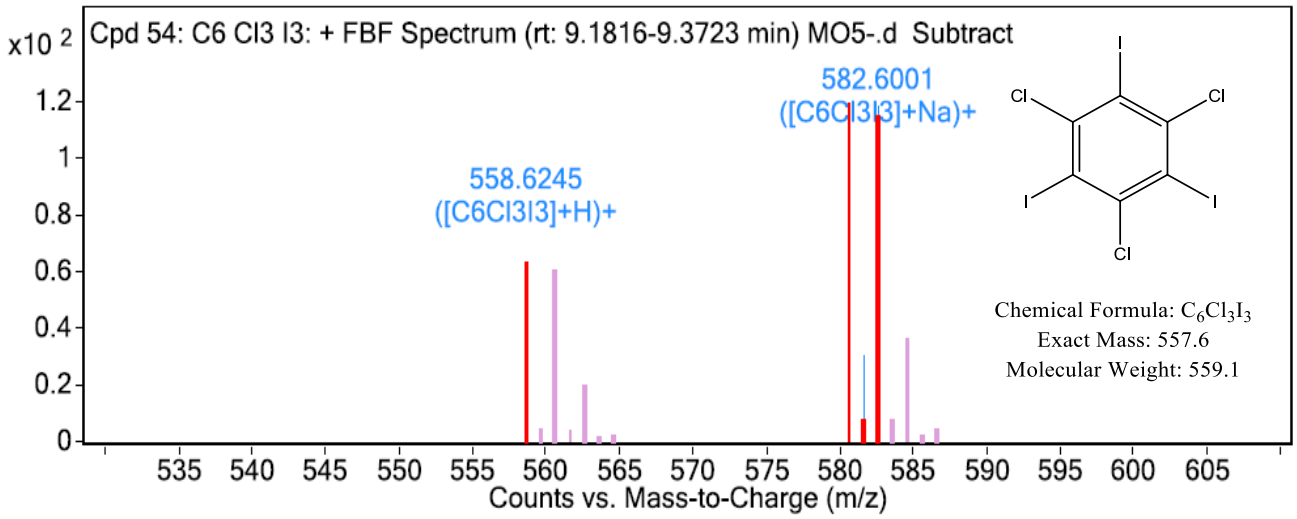
Mass spectroscopic date of compound 6



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
216.0089	1	112.66	C6H4S	2M+
234.0448	1	226.07	C6H4S	(2M+NH4)+
342.035	1	79	C6H4S	(3M+NH4)+
346.9993	1	210.38	C6H4S	(3M+Na)+

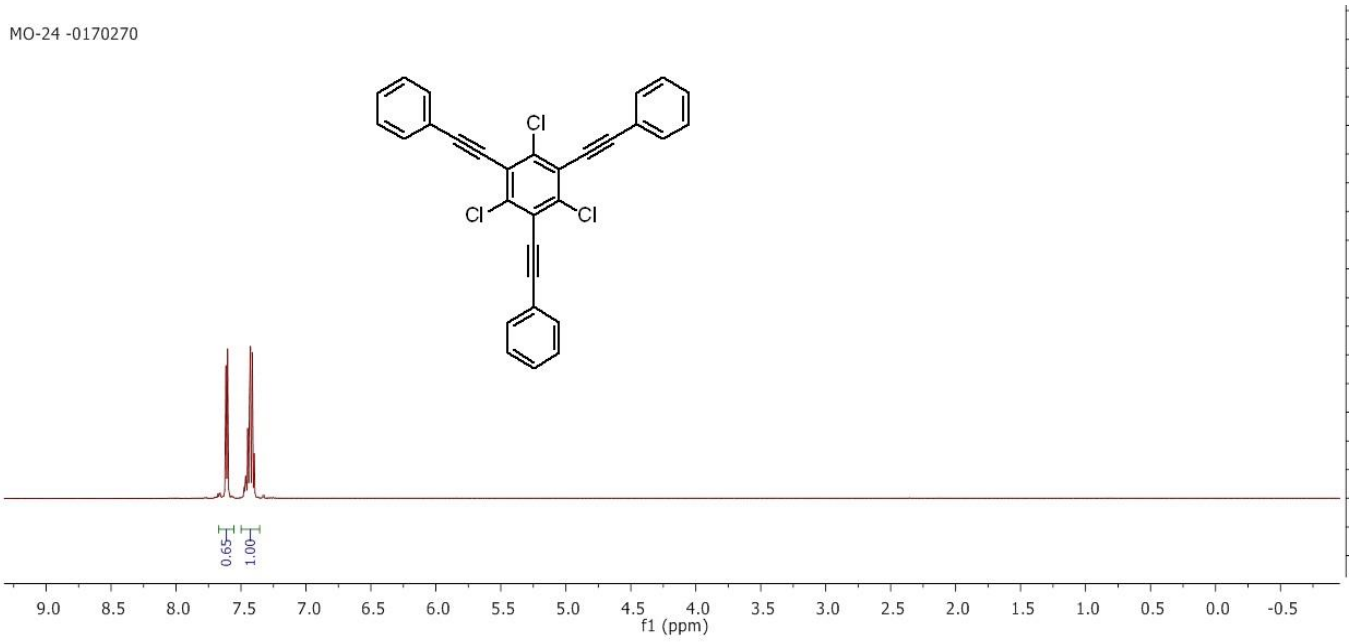
Mass spectroscopic date of compound 8

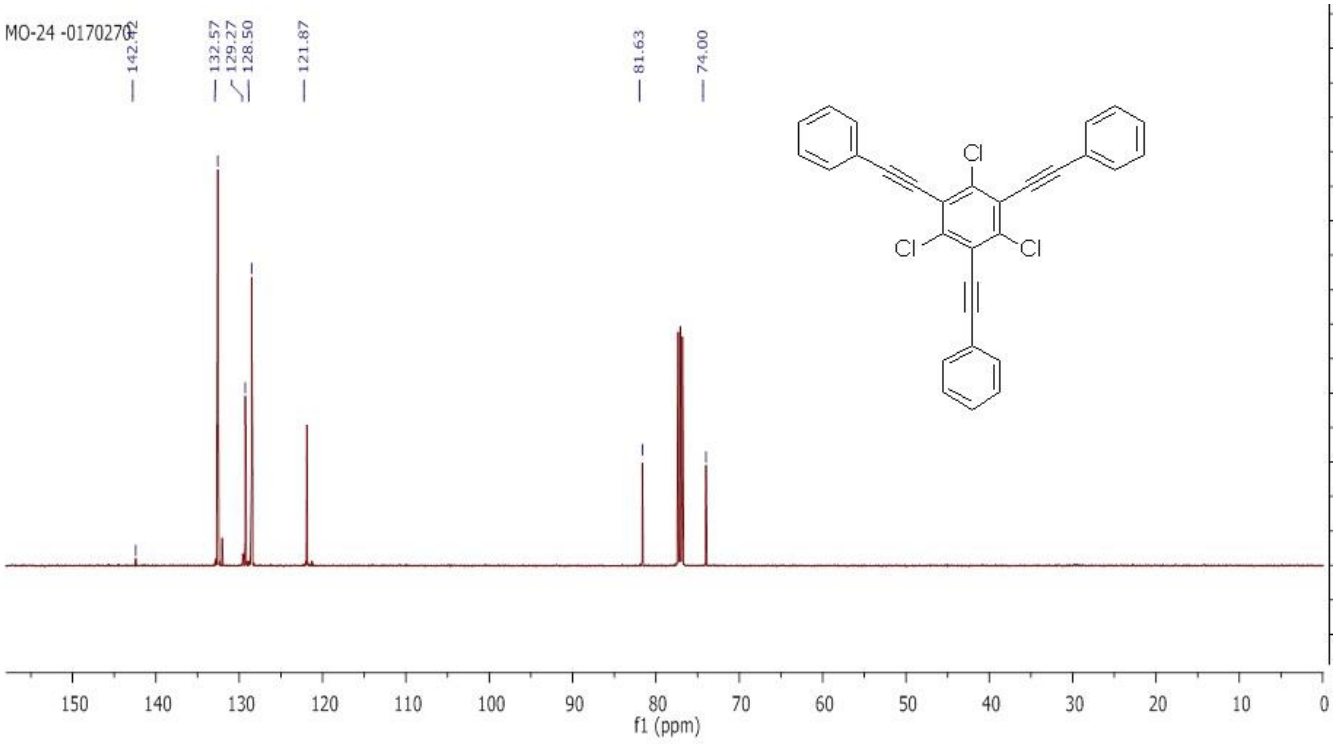


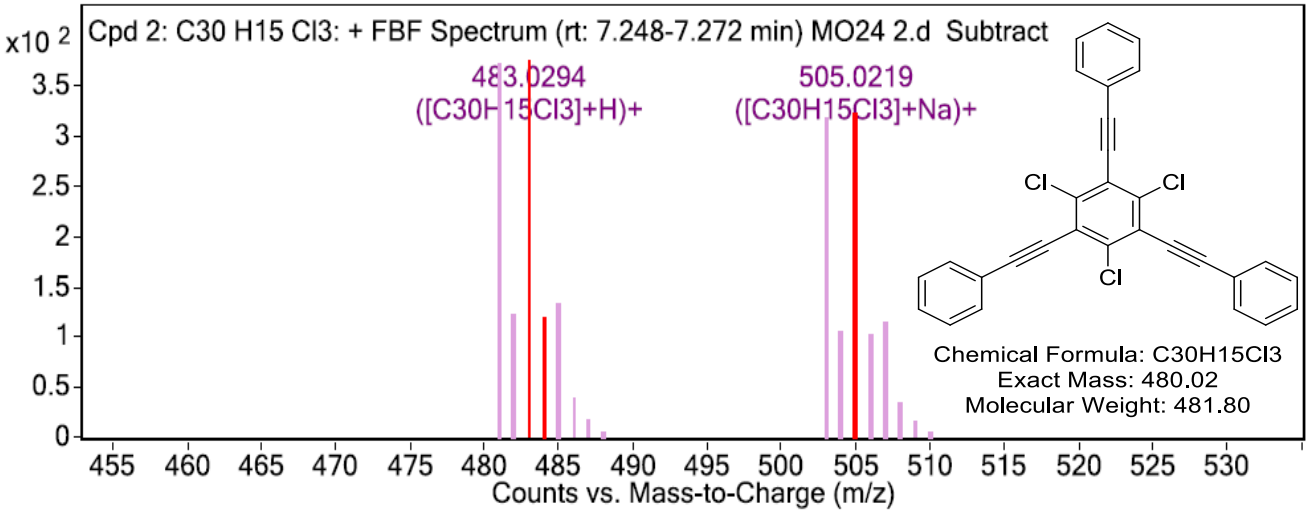
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
558,6245	1	62,64	C6Cl3I3	(M+H)+
580,6046	1	92,71	C6Cl3I3	(M+Na)+
581,6209	1	30,48	C6Cl3I3	(M+Na)+
582,6001	1	118,47	C6Cl3I3	(M+Na)+

Spectroscopic Date of Compound 9a



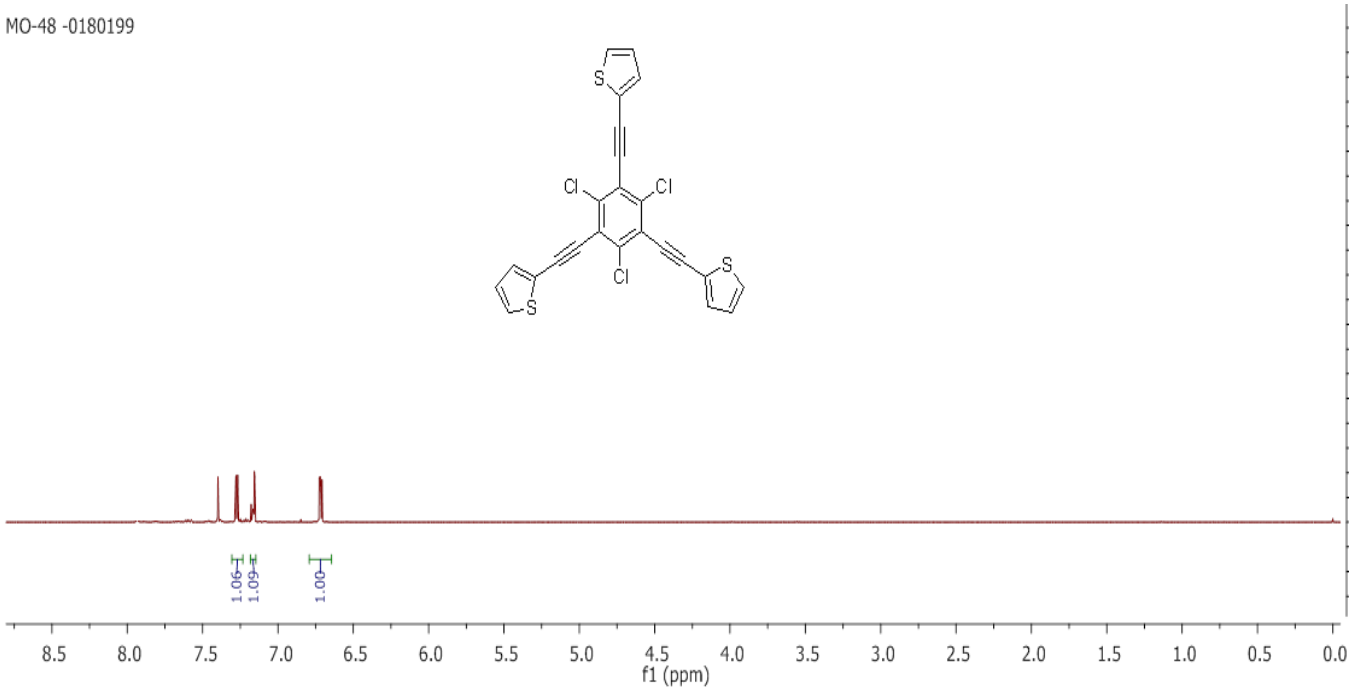


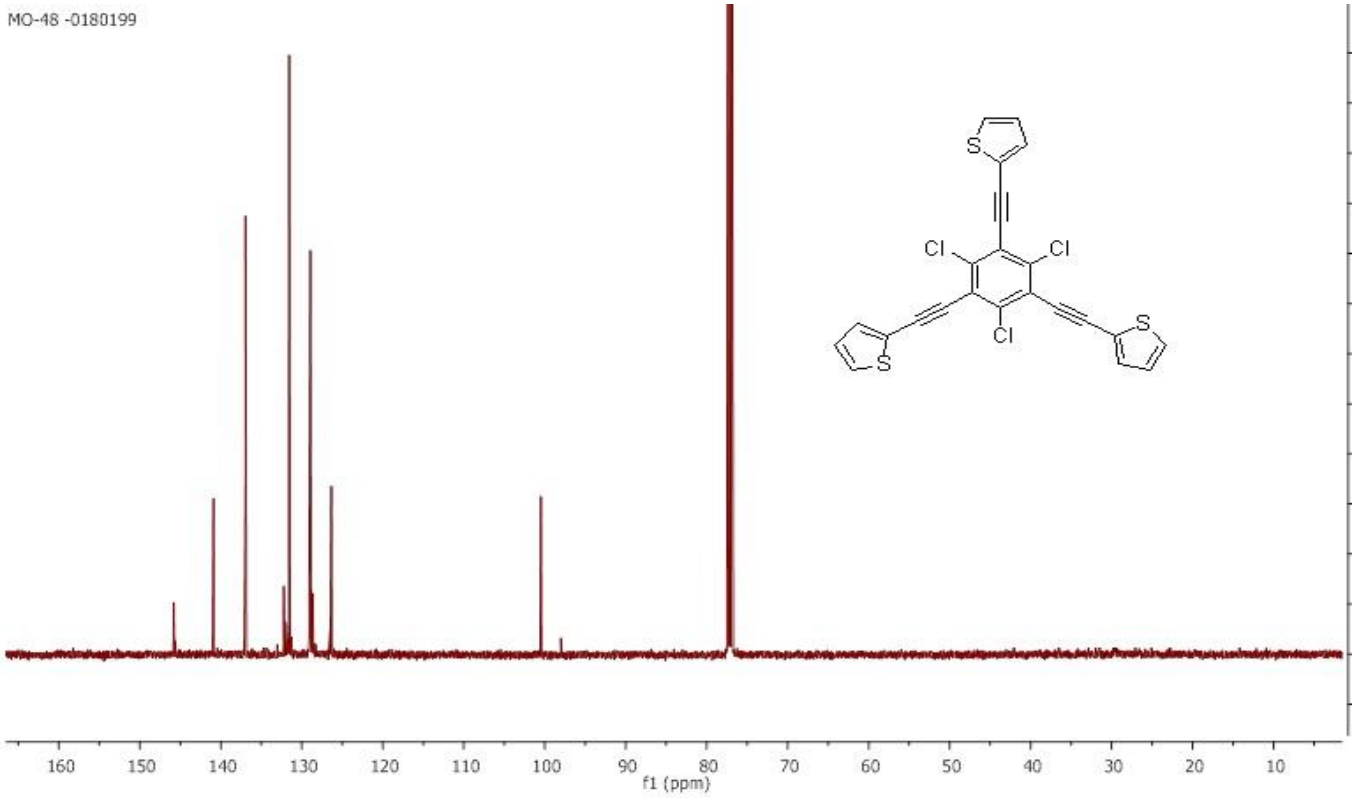


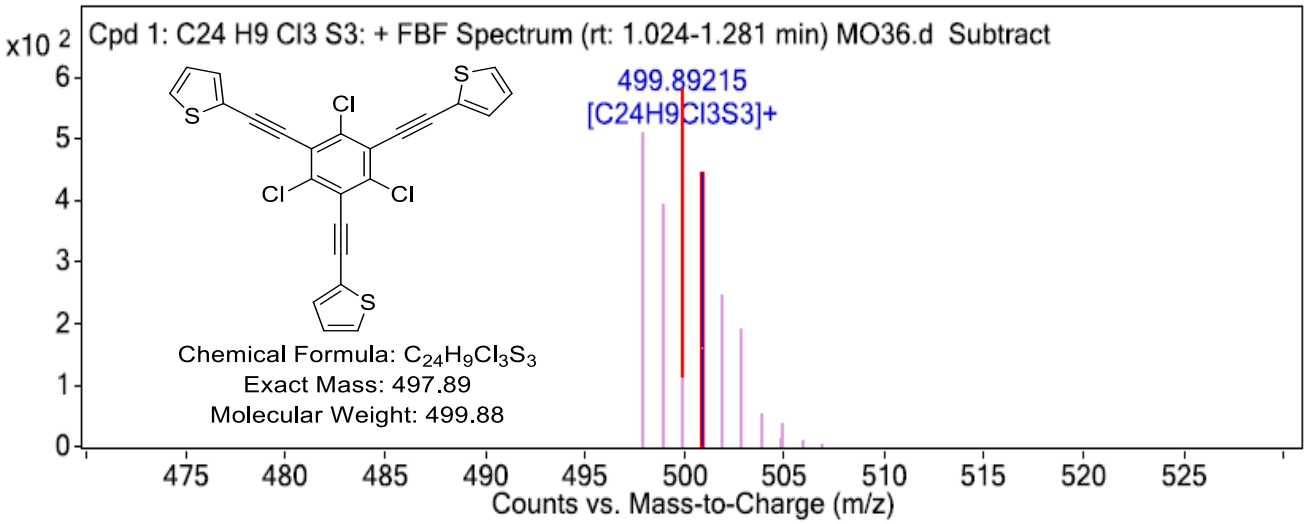
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
483.0294	1	375.58	C30H15Cl3	(M+H)+
484.0249	1	110.95	C30H15Cl3	(M+H)+
505.0219	1	321.7	C30H15Cl3	(M+Na)+

Spectroscopic Data of compound 9b



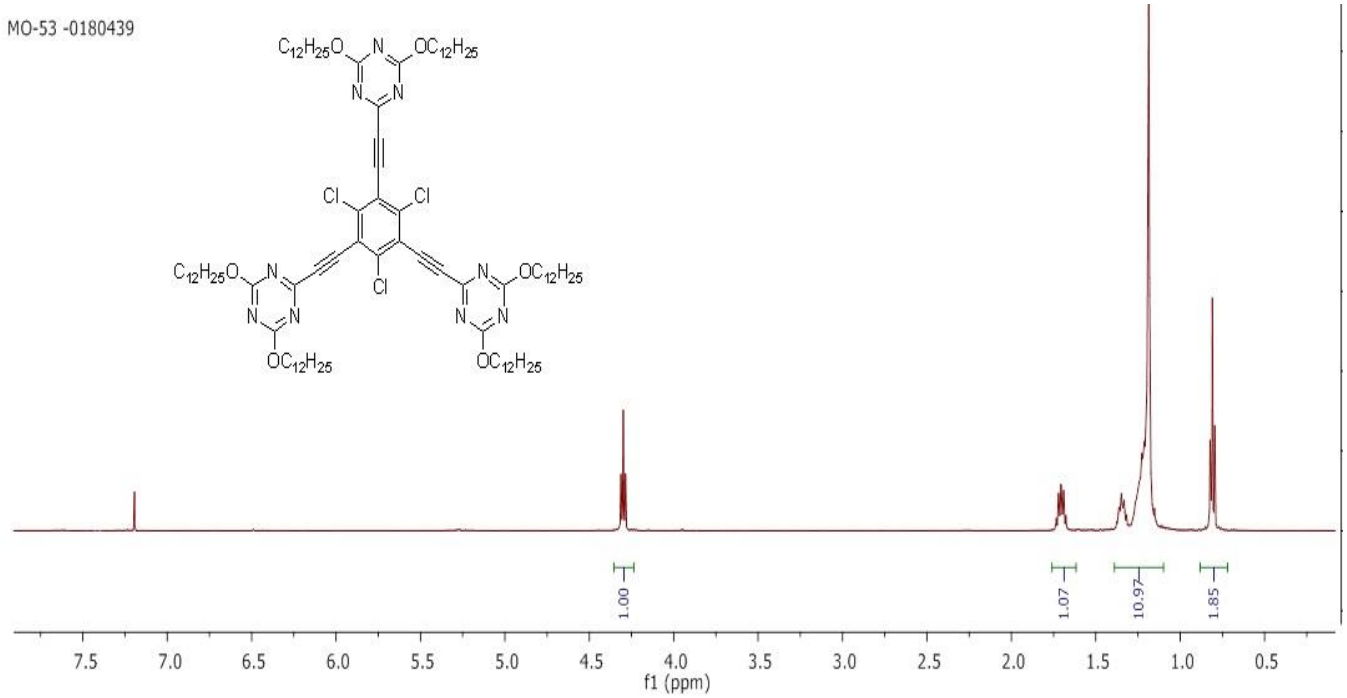


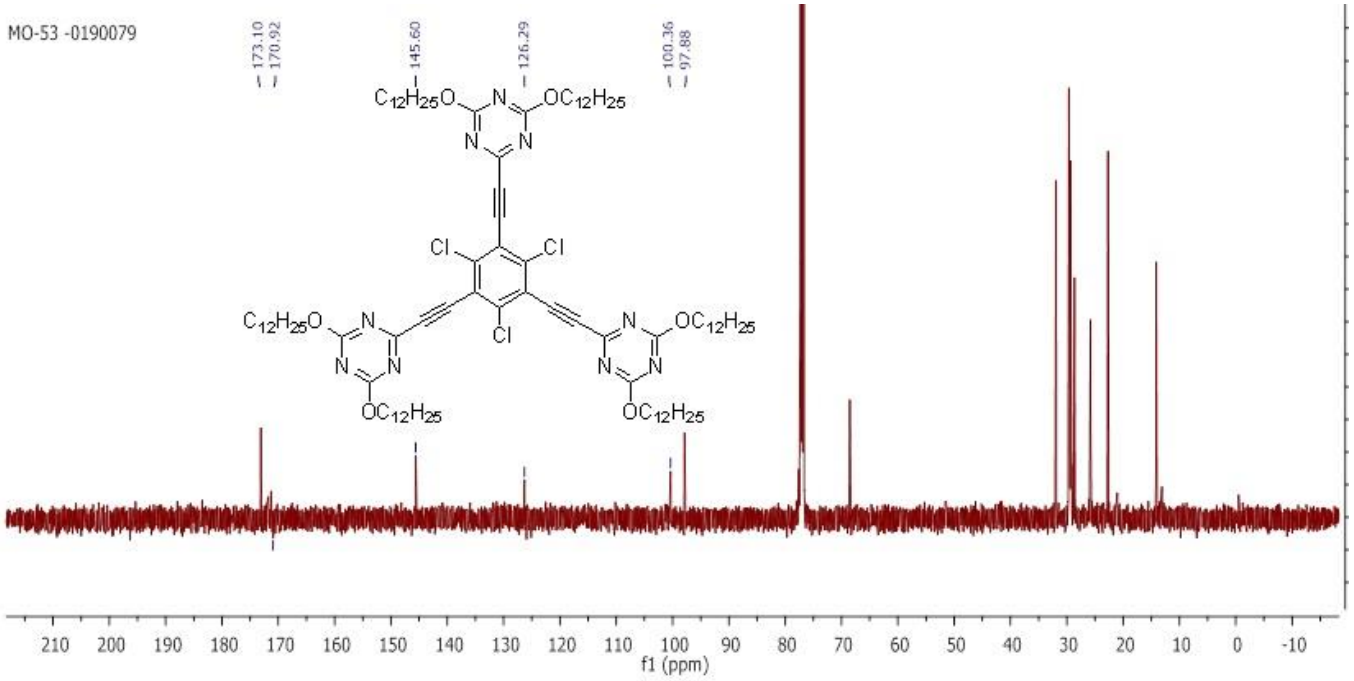


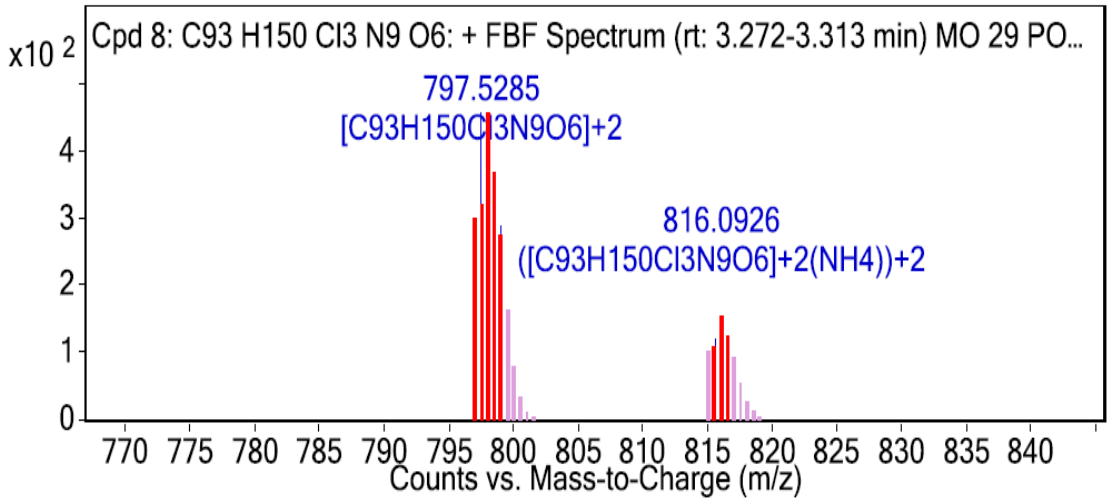
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
499.89215	1	578.54	C24H9Cl3S3	M+
500.88592	1	445.76	C24H9Cl3S3	(M+H)+

Spectroscopic Data of compound 11

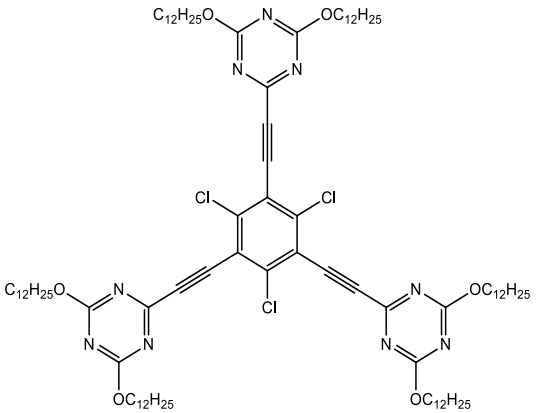






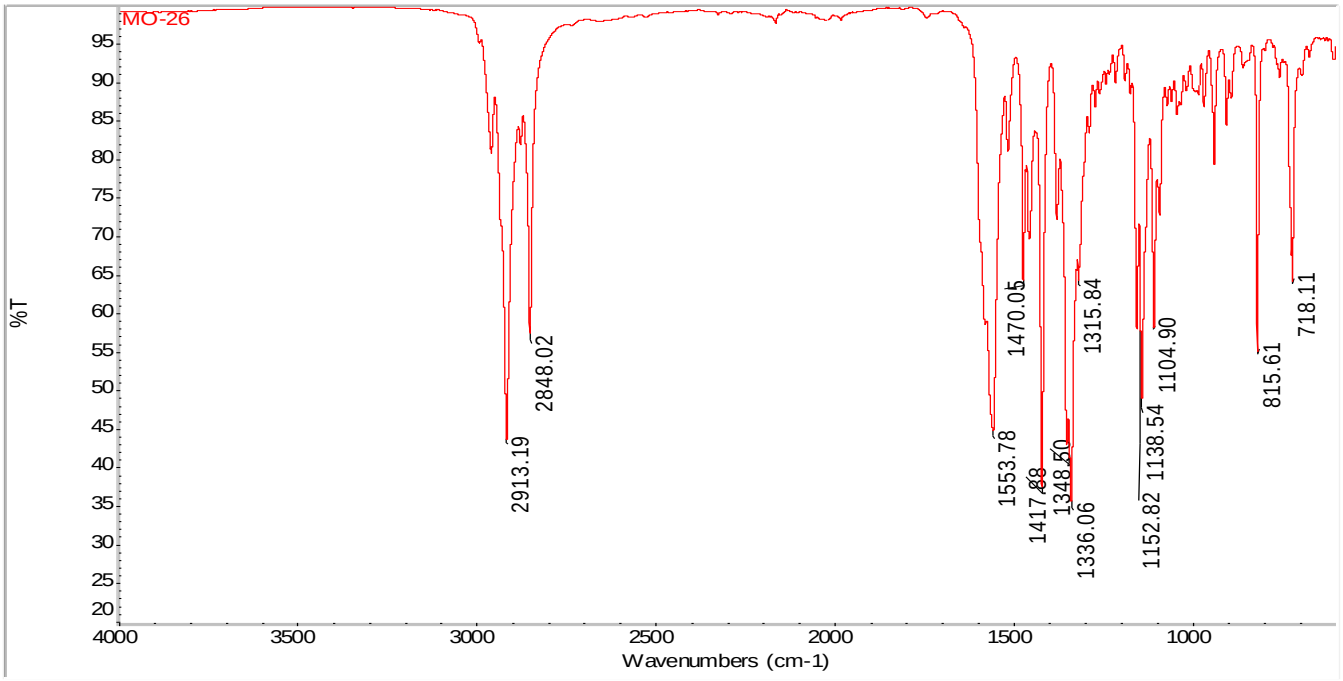
MS Spectrum Peak List

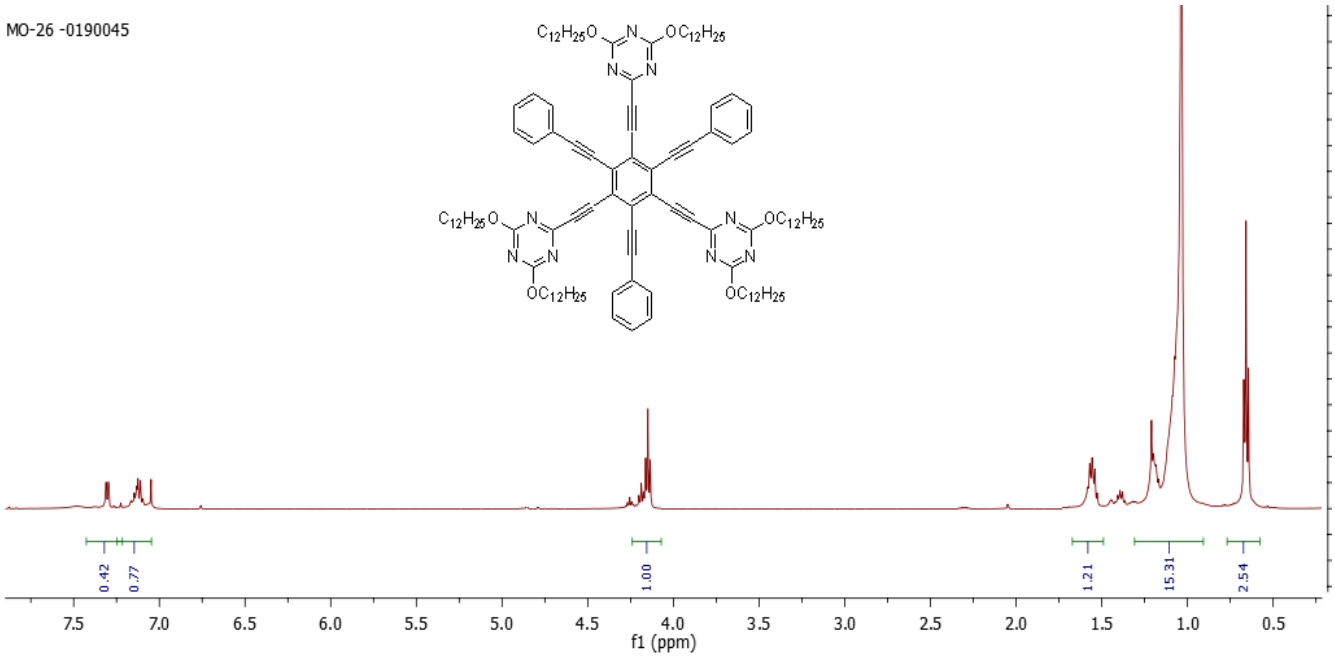
m/z	z	Abund	Formula	Ion
797.0261	2	60.66	C93H150Cl3N9O6	M+2
797.5285	2	458.96	C93H150Cl3N9O6	M+2
798.0225	2	60.68	C93H150Cl3N9O6	M+2
798.5489	2	307.84	C93H150Cl3N9O6	M+2
799.0468	2	289.72	C93H150Cl3N9O6	M+2
815.6095	2	121.01	C93H150Cl3N9O6	(M+2(NH4))+2
816.0926	2	145.71	C93H150Cl3N9O6	(M+2(NH4))+2
816.5787	2	115.34	C93H150Cl3N9O6	(M+2(NH4))+2

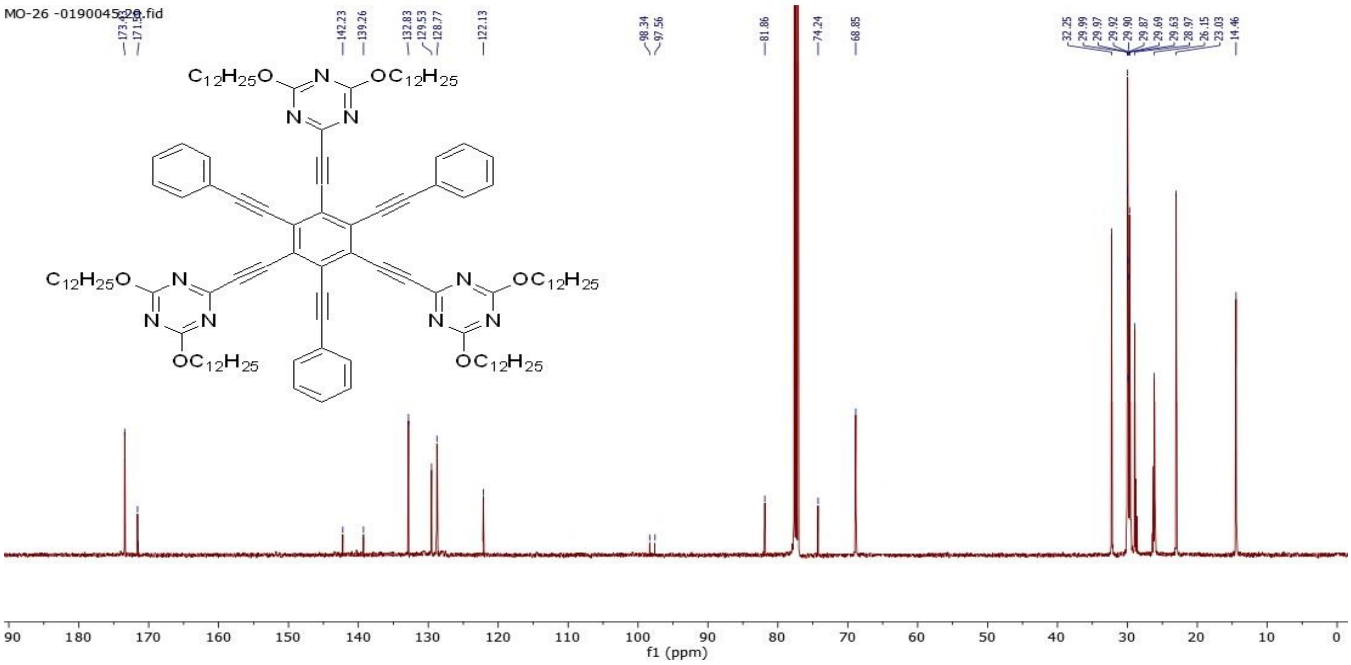


Chemical Formula: $C_{93}H_{150}Cl_3N_9O_6$
Exact Mass: 1594.1
Molecular Weight: 1596.6

Spectroscopic Data of compound 10a



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139.26
132.83
129.53
128.77
122.13
98.34
97.56
81.86
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68.85
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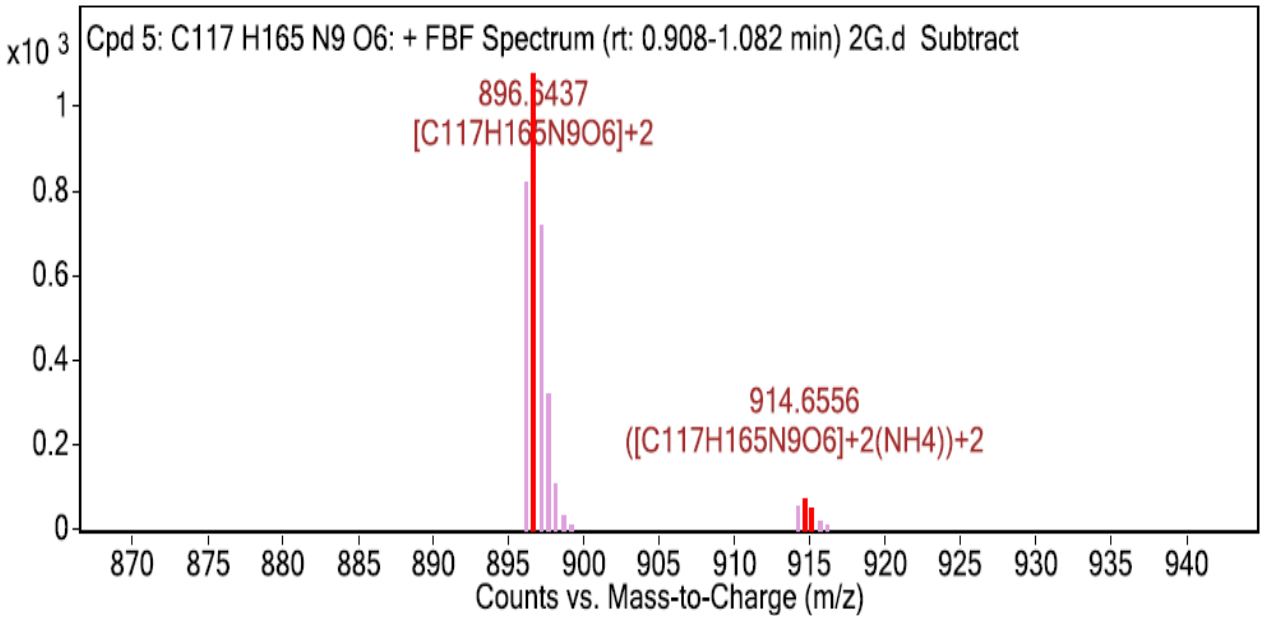
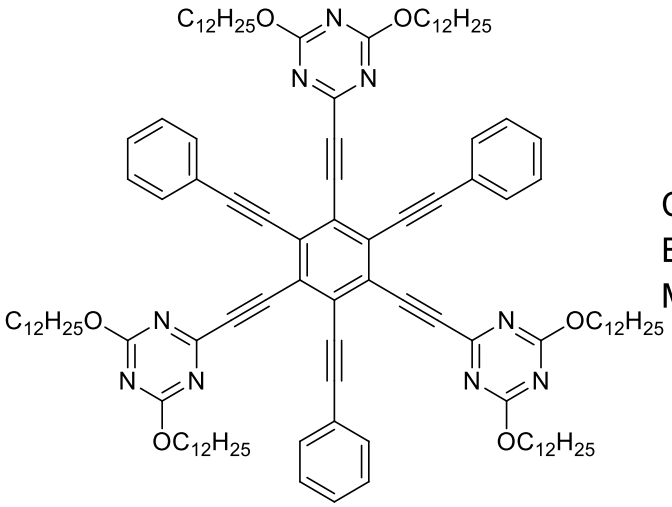
f1 (ppm)



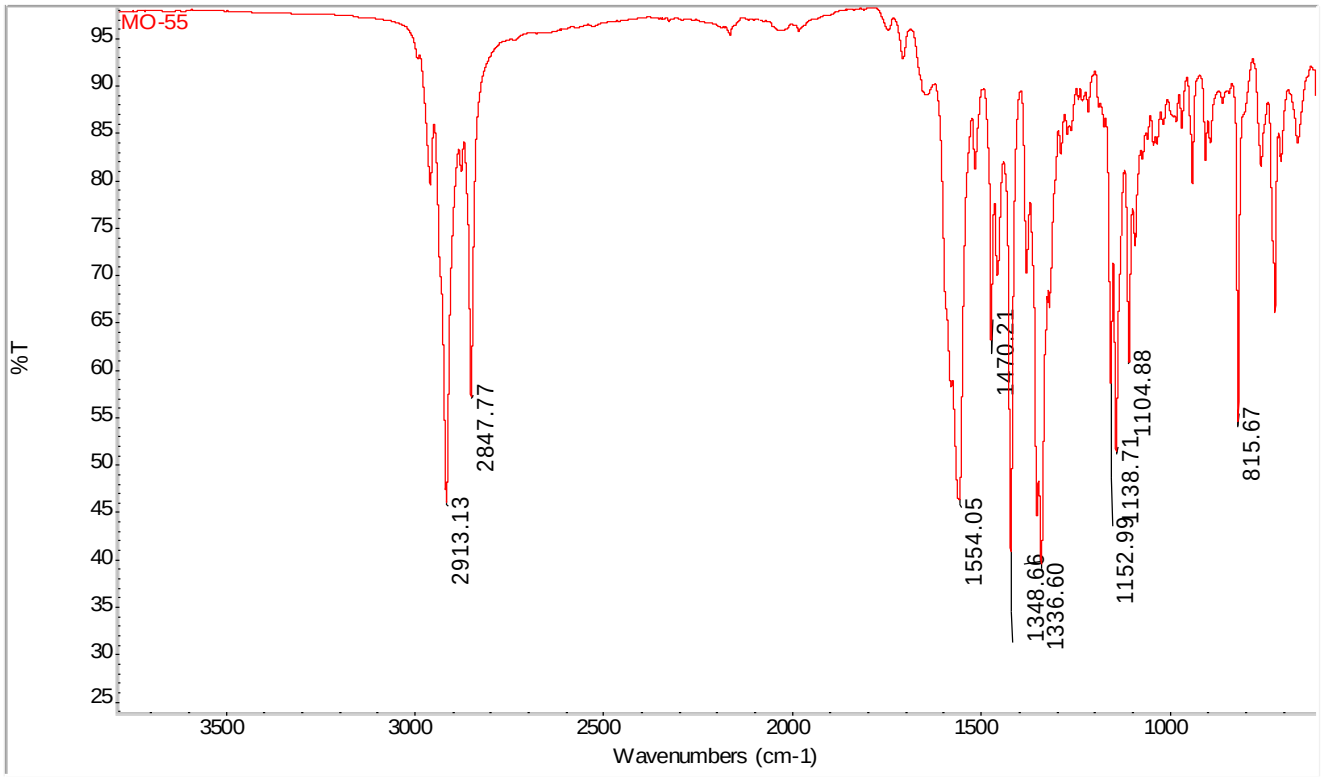
MS Spectrum Peak List

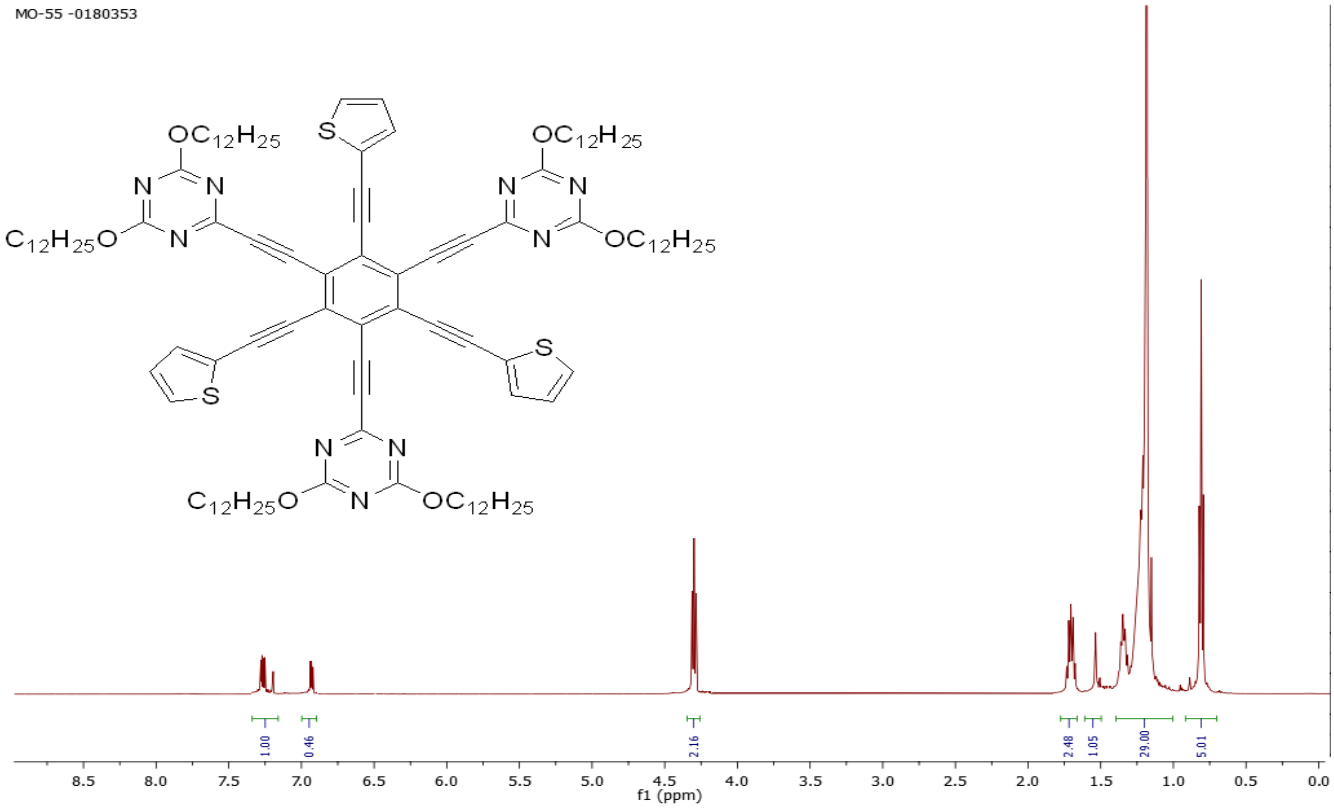
m/z	z	Abund	Formula	Ion
896.6437	2	1077.76	C117H165N9O6	M+2
914.6556	2	61.85	C117H165N9O6	(M+2(NH4))+2
915.1368	2	46.01	C117H165N9O6	(M+2(NH4))+2

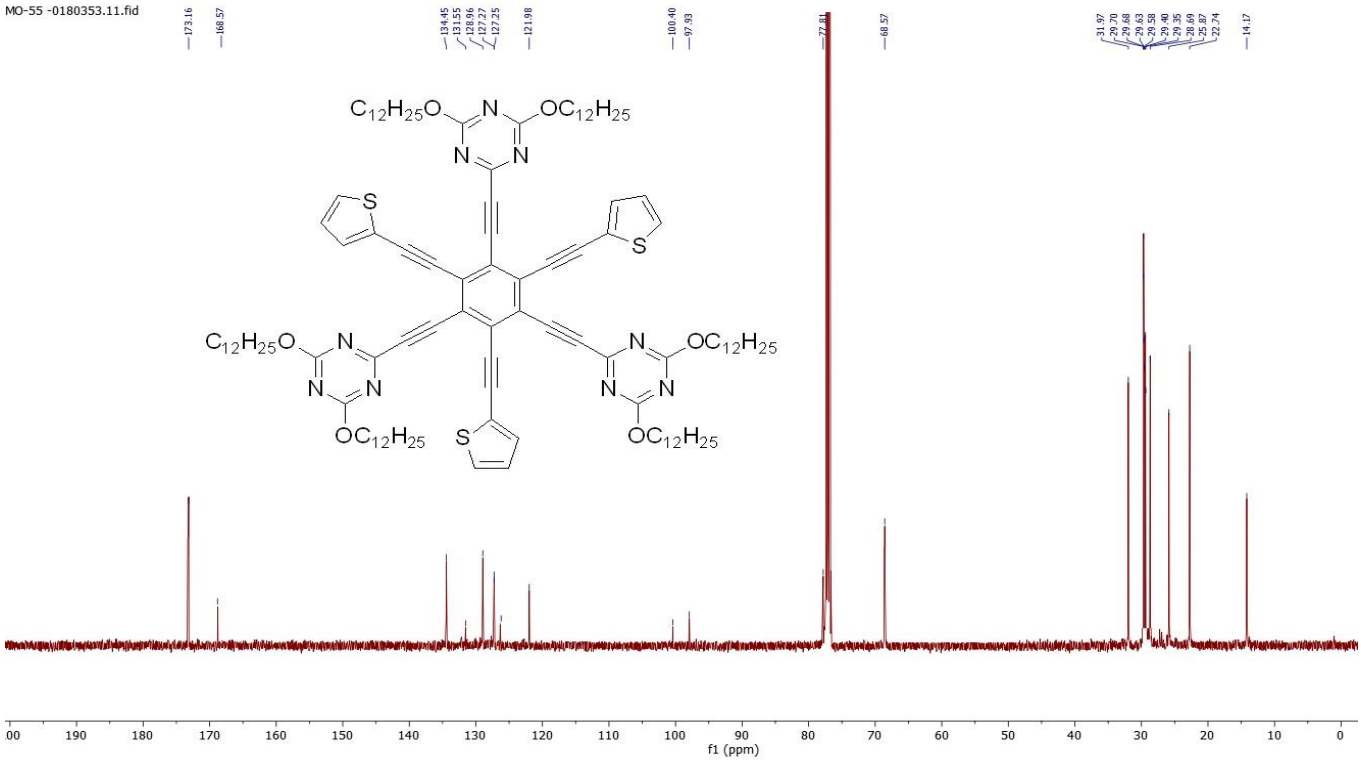


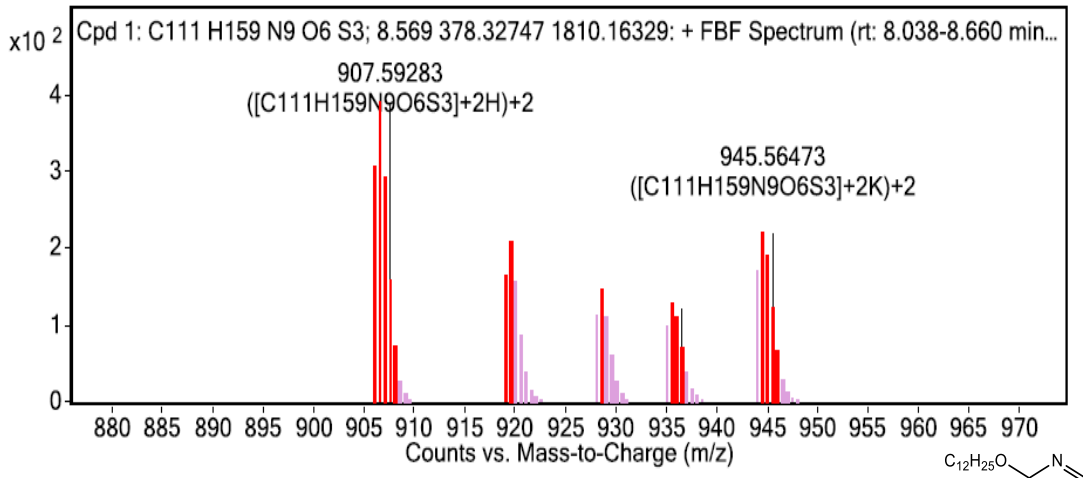
Chemical Formula: $C_{117}H_{165}N_9O_6$
Exact Mass: 1792.29
Molecular Weight: 1793.62

Spectroscopic Data of compound 10b



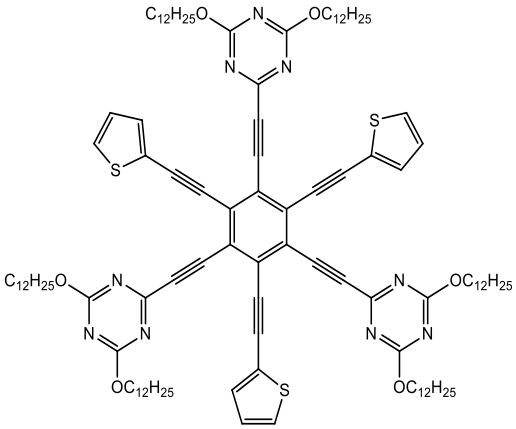






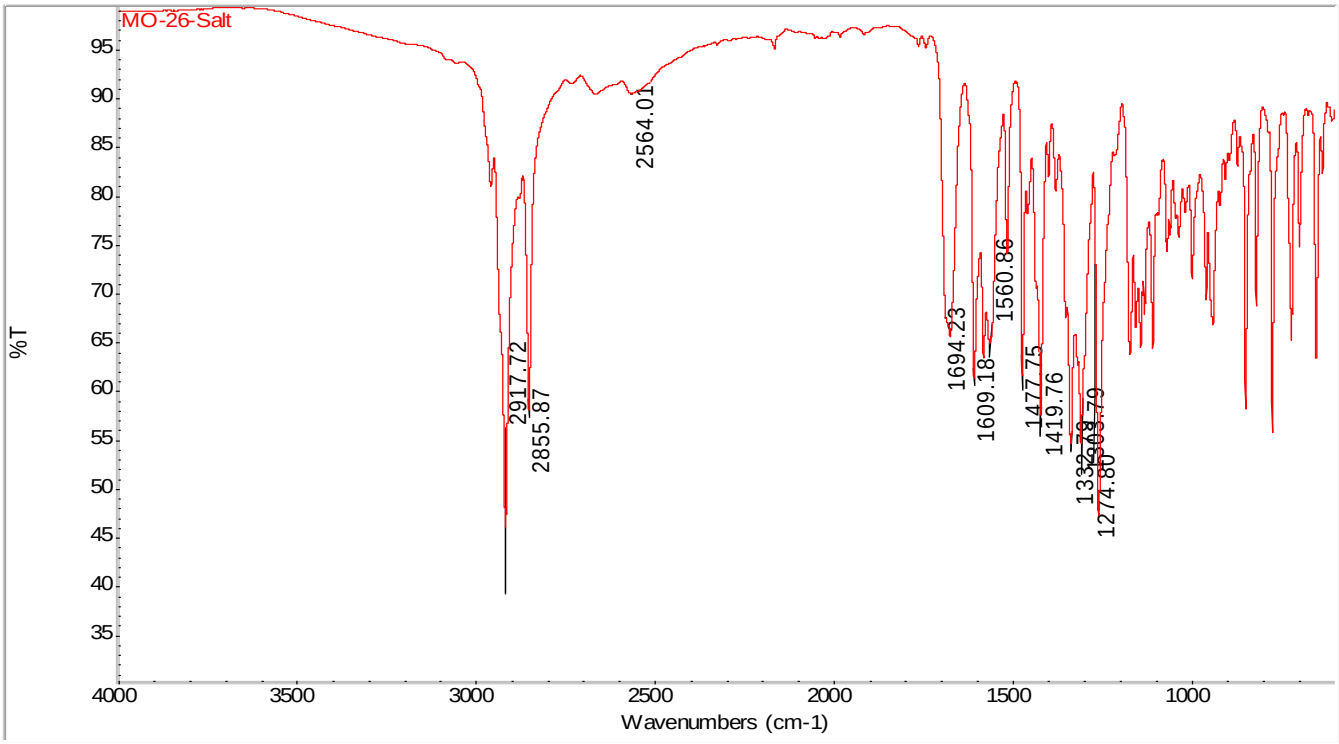
MS Spectrum Peak List

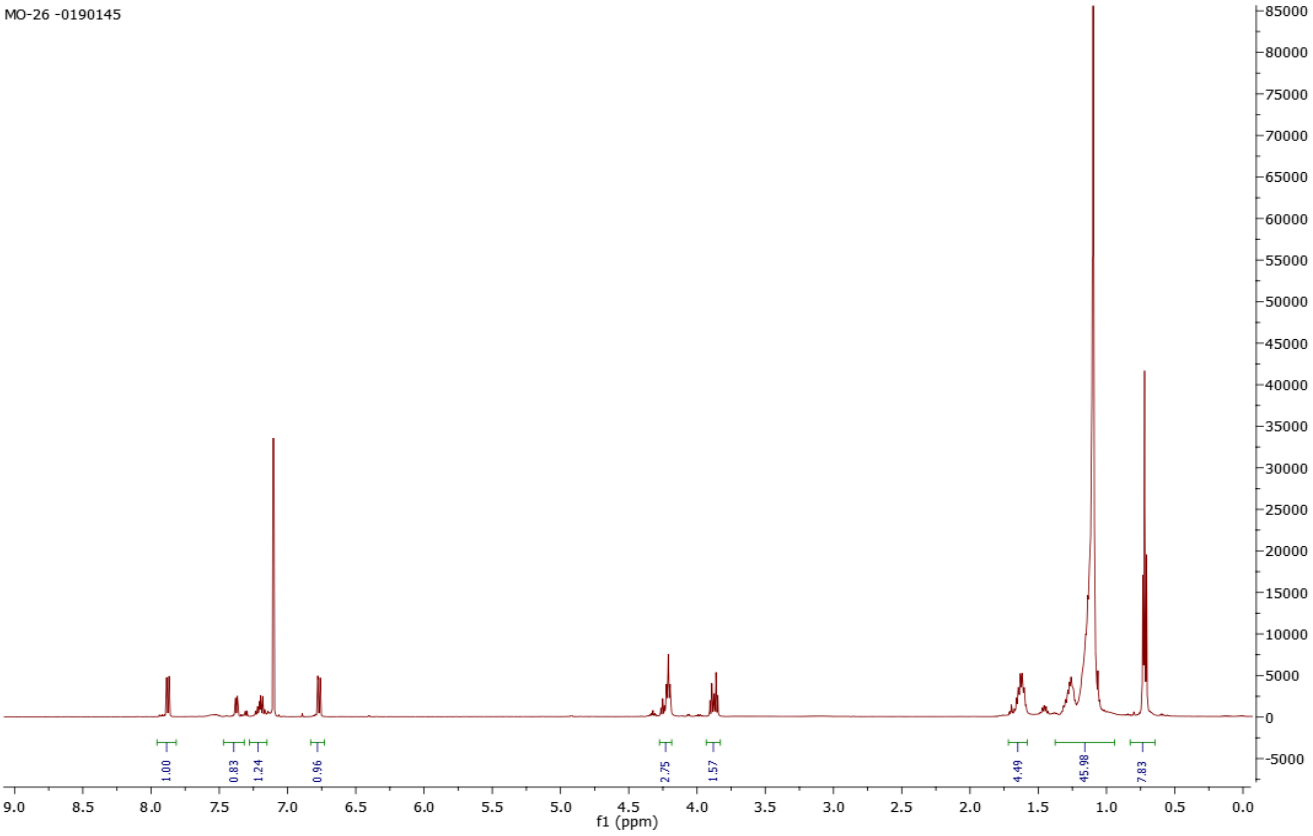
m/z	z	Abund	Formula	Ion
906.09795	2	39.07	C111H159N9O6S3	(M+2H)+2
906.58031	2	282.83	C111H159N9O6S3	(M+2H)+2
907.59283	2	389.09	C111H159N9O6S3	(M+2H)+2
919.06651	2	50.12	C111H159N9O6S3	(M+2Na)+2[-H2O]
919.58689	2	208.09	C111H159N9O6S3	(M+2Na)+2[-H2O]
928.58335	2	145.63	C111H159N9O6S3	(M+2Na)+2
935.53512	2	126.39	C111H159N9O6S3	(M+2K)+2[-H2O]
936.50381	2	120.96	C111H159N9O6S3	(M+2K)+2[-H2O]
944.54631	2	86.46	C111H159N9O6S3	(M+2K)+2
945.56473	2	218.61	C111H159N9O6S3	(M+2K)+2

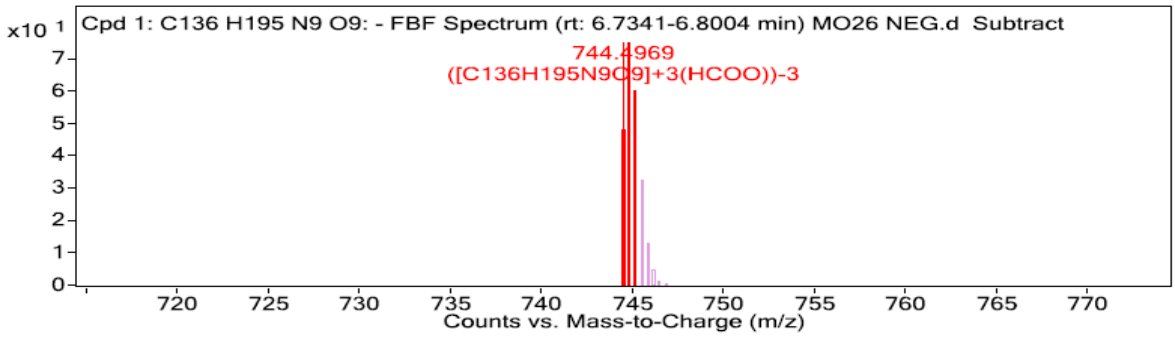


Chemical Formula: $C_{111}H_{159}N_9O_6S_3$
Exact Mass: 1810.2
Molecular Weight: 1811.7

Spectroscopic Data of organic salt 13a

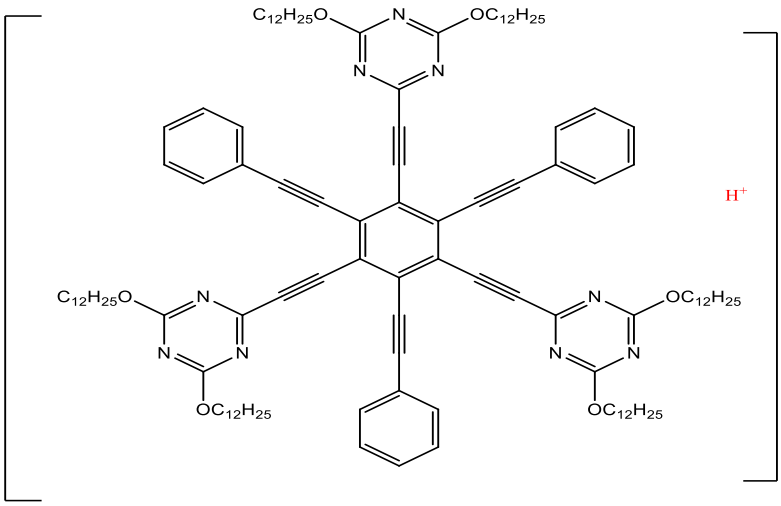


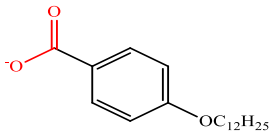




MS Spectrum Peak List

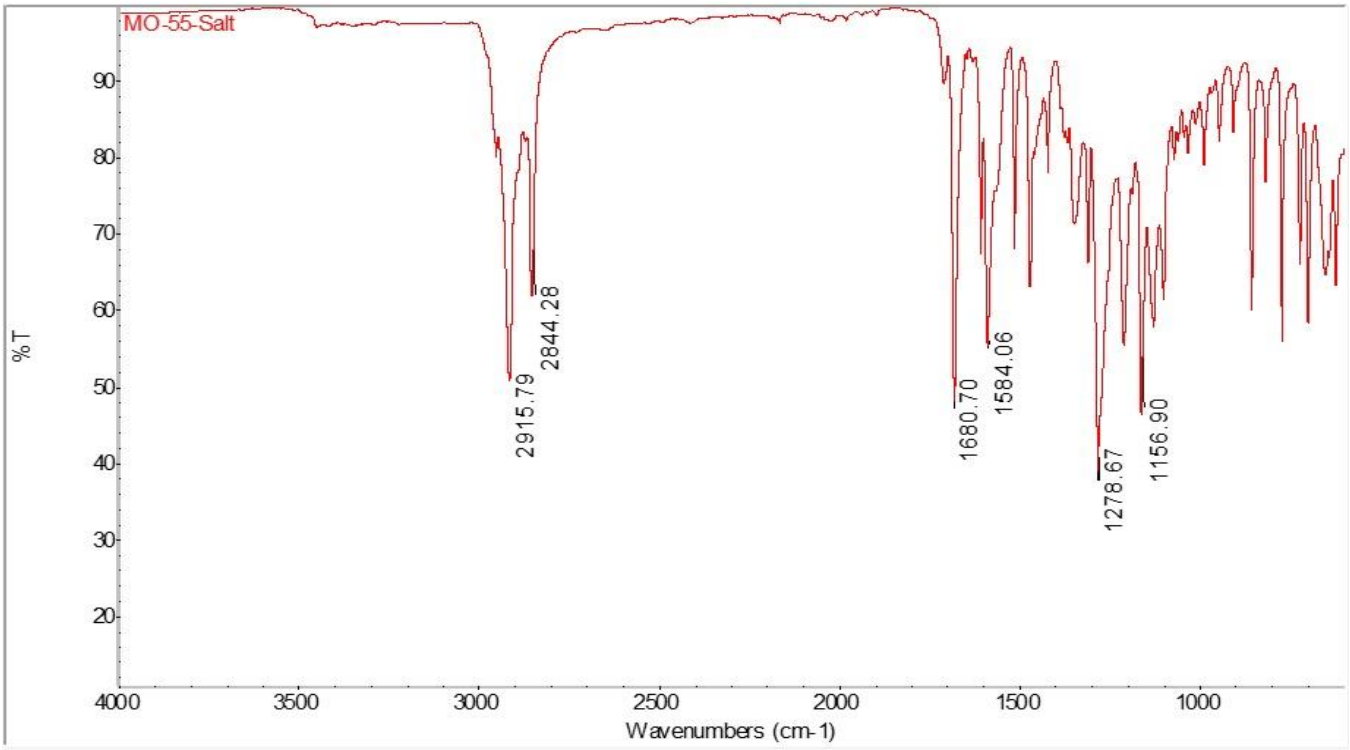
m/z	z	Abund	Formula	Ion
744,4969	3	74,95	C136H195N9O9	(M+3(HCOO))-3
744,849	3	53,33	C136H195N9O9	(M+3(HCOO))-3
745,1874	3	24,88	C136H195N9O9	(M+3(HCOO))-3

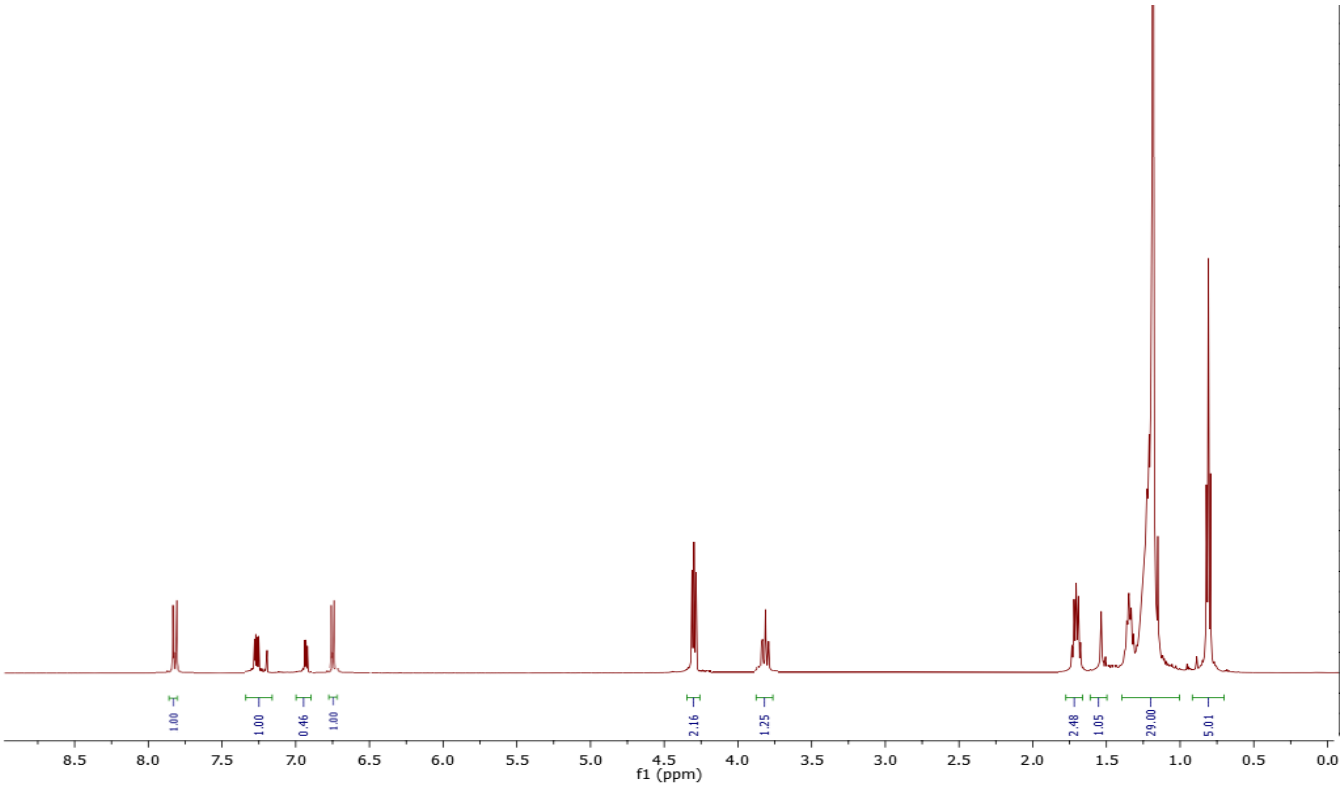




Chemical Formula: $C_{136}H_{195}N_9O_9$
Exact Mass: 2098.51
Molecular Weight: 2100.06

Spectroscopic Data of organic salt 13b





Spectroscopic date of 4-DBA:

