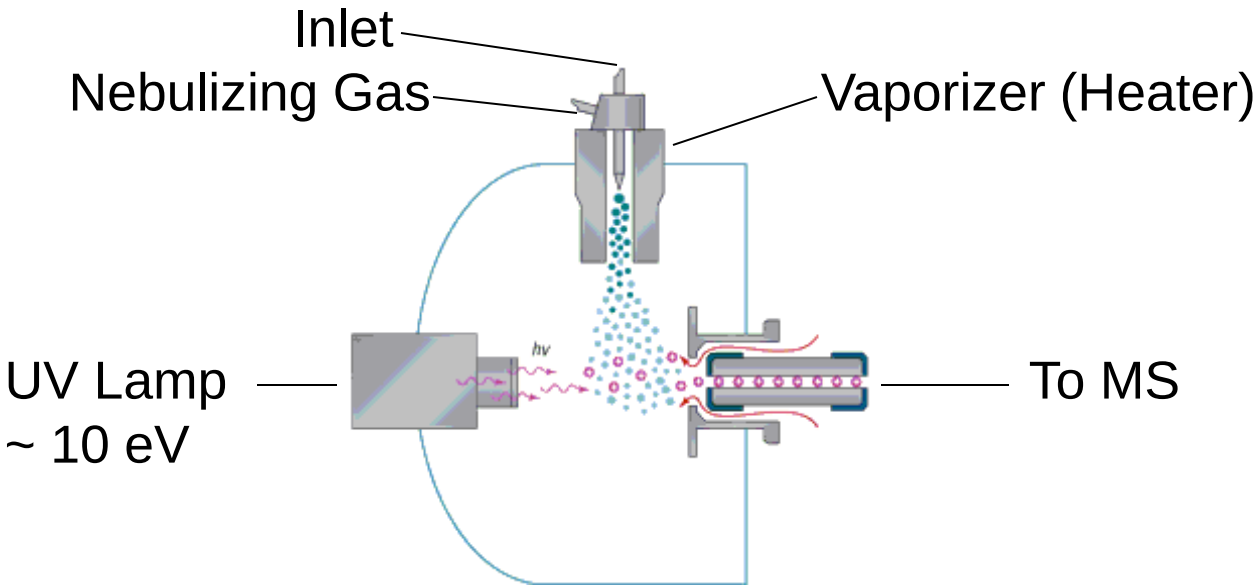
Implementation of APPI Mass Spectrometry for Organometallic compounds

Noam Tal, Tel Aviv University, Israel

Atm. Pressure Photo Ionization (APPI)



Direct APPI

$$M + h\nu \longrightarrow M^{+\bullet} + e^-$$

$$M^{+\bullet} + \text{Solvent} \longrightarrow [MH]^+$$

Dopant/Solvent assisted APPI

$$D + h\nu \longrightarrow D^{+\bullet} + e^-$$

$$D^{+\bullet} + M + \text{Solvent} \longrightarrow [MH]^+ , [M\text{-}H]^-$$

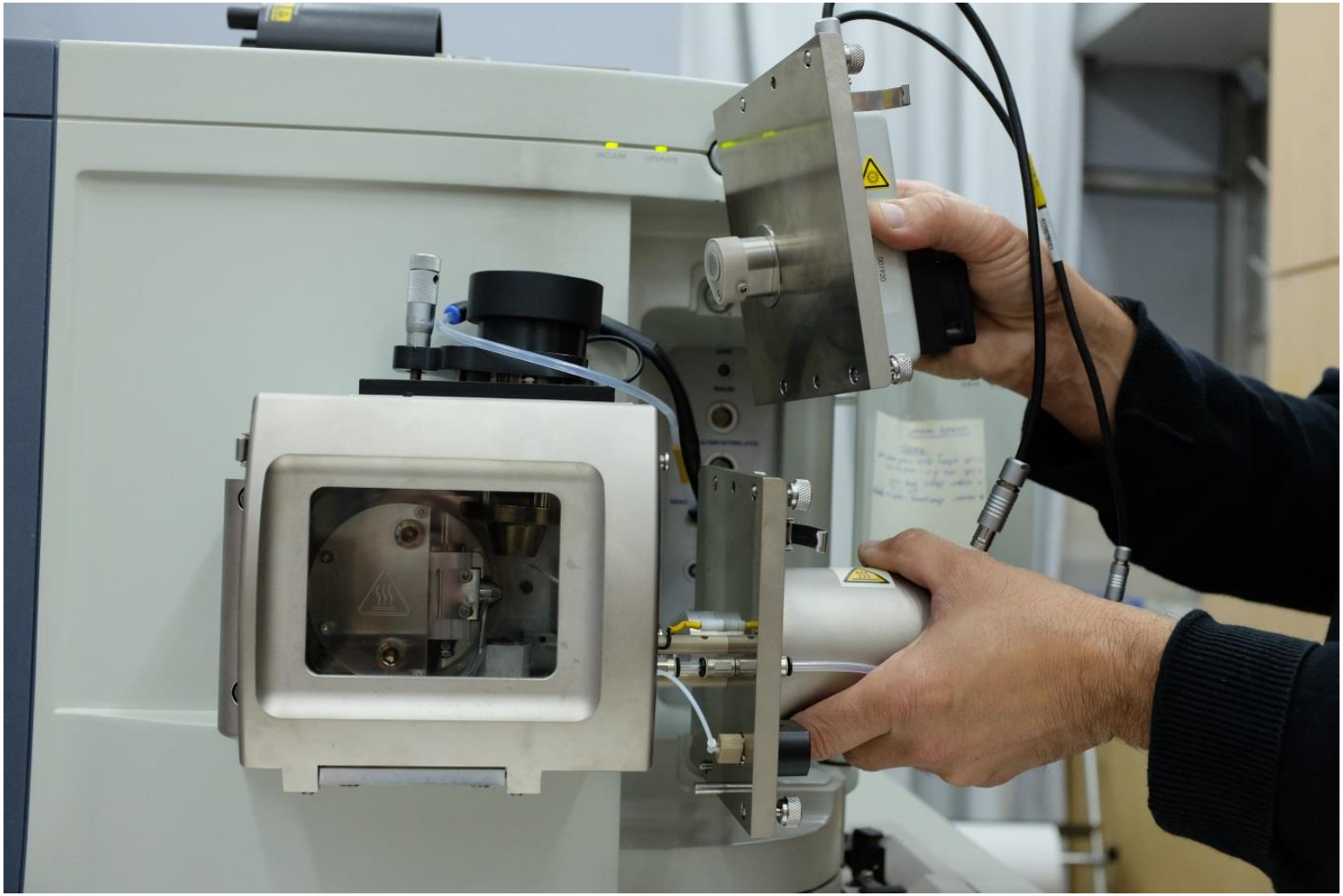
D = Photosensitizer: Toluene, Acetone

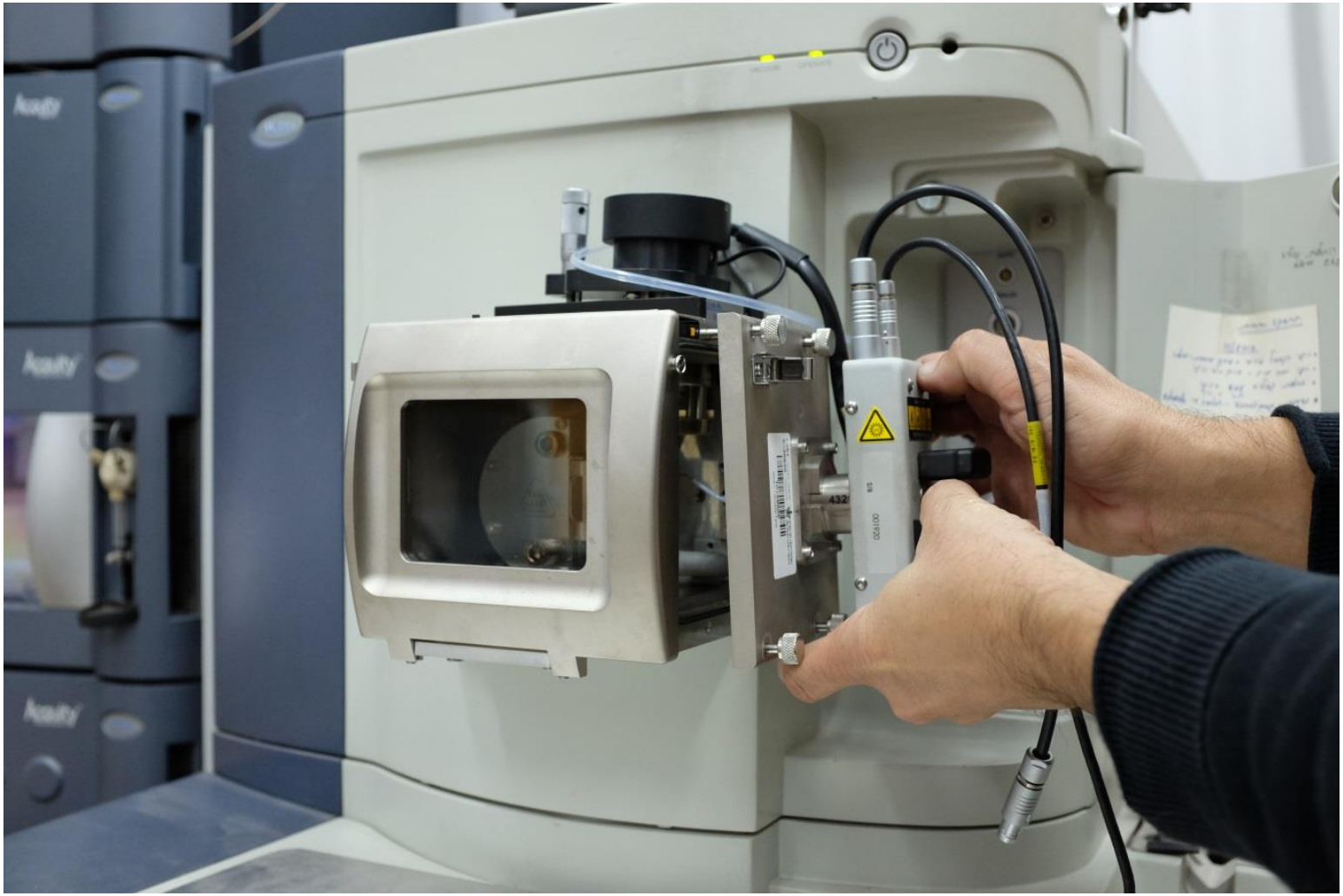
	APCI	APPI
Sensitivity:	Pos >> Neg	Pos ~= Neg
Mass range	~1200 Da	~2500 Da
Aliphatic:	Yes	Limited
Conjugated:	Yes	Excellent
Organometallic:	Limited	Excellent
Conditions:	Sensitive	less sensitive

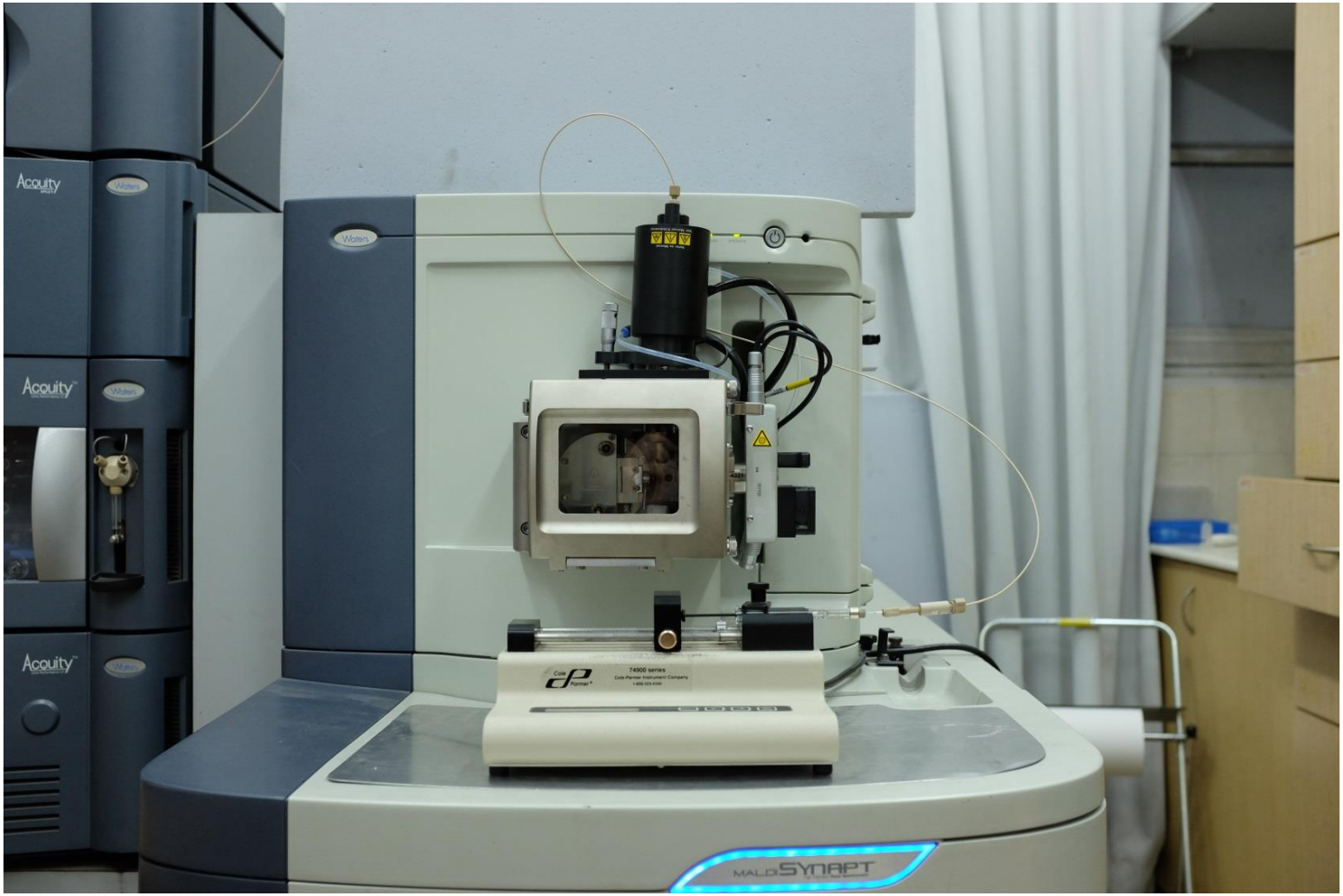
Solvent: Toluene, DCM, Hexane, MeCN, MeOH

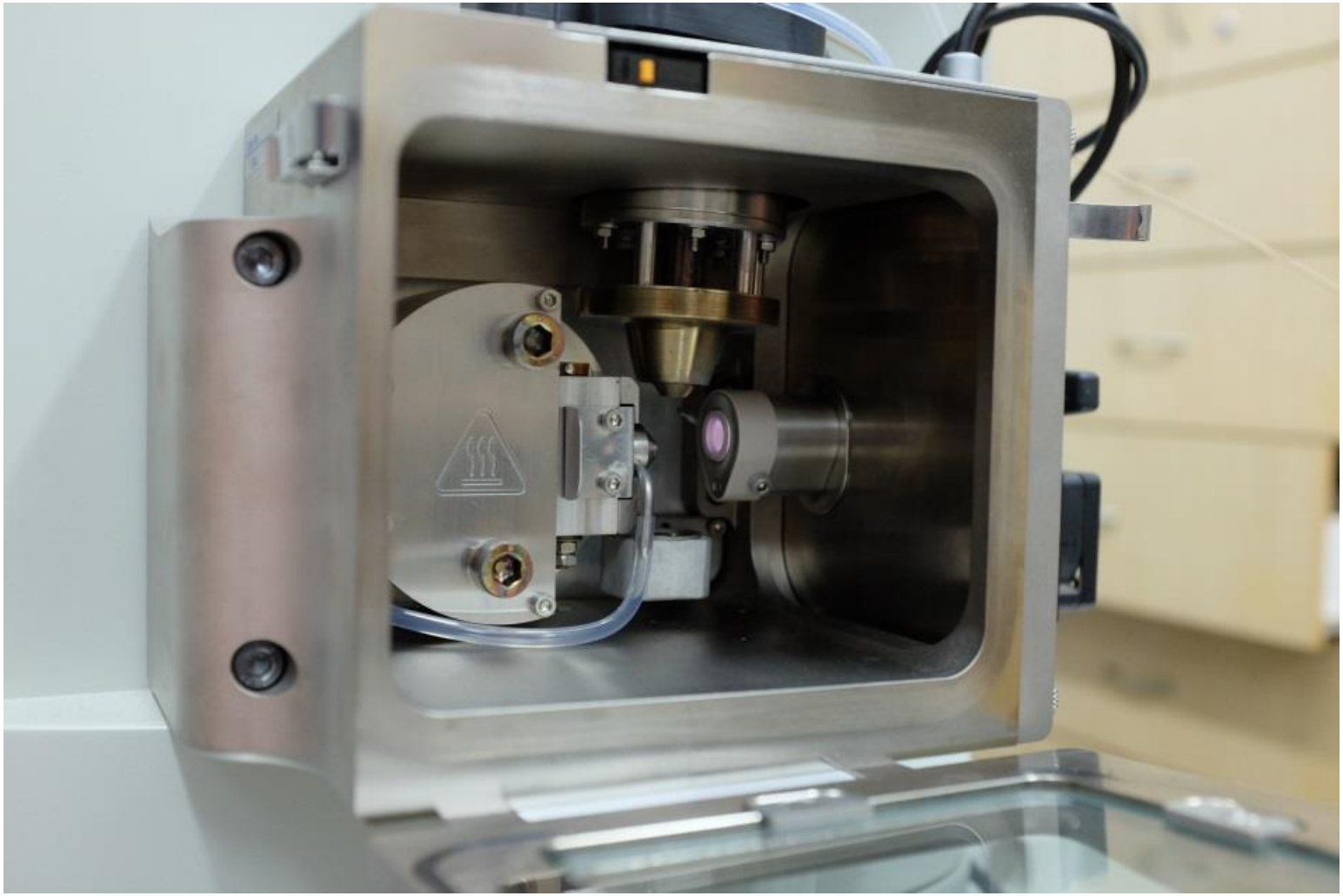
API source


4321
S/N
001920






Acquity
Waters
Acquity
Waters
Acquity
Waters
Waters
74900 series
MALDI SYNAPT

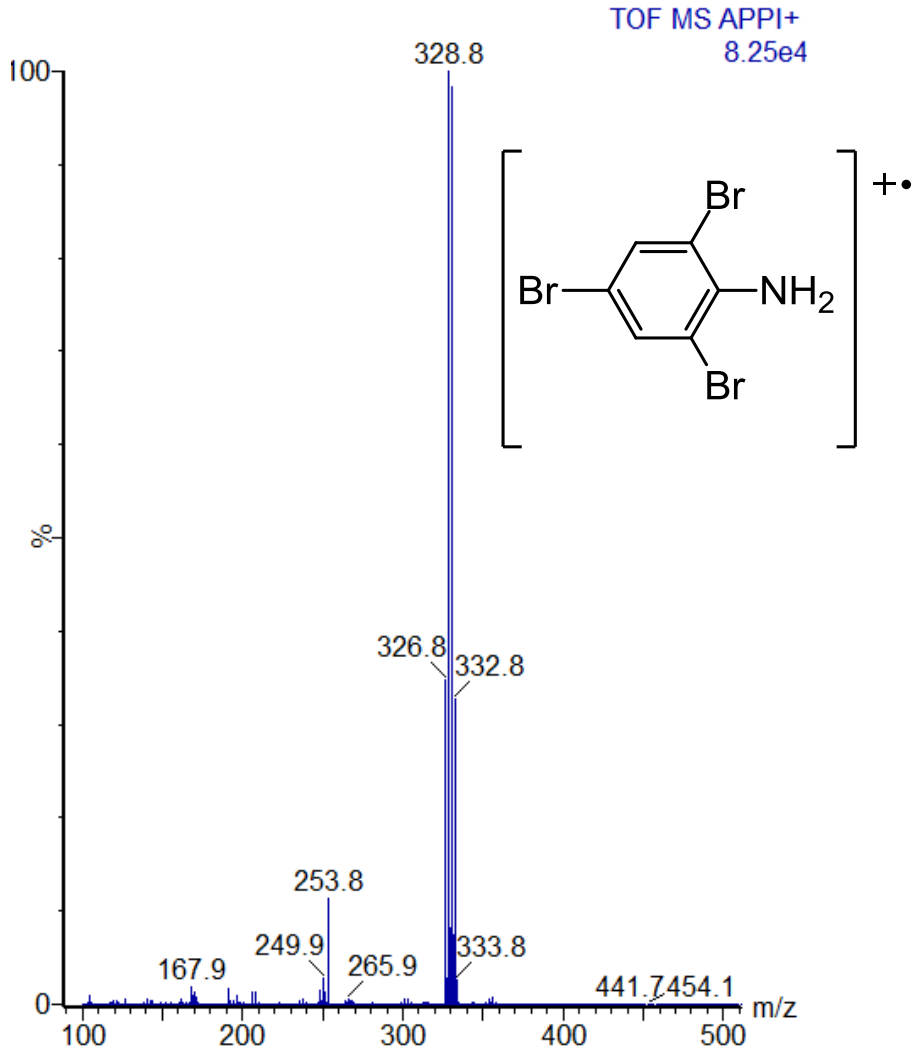


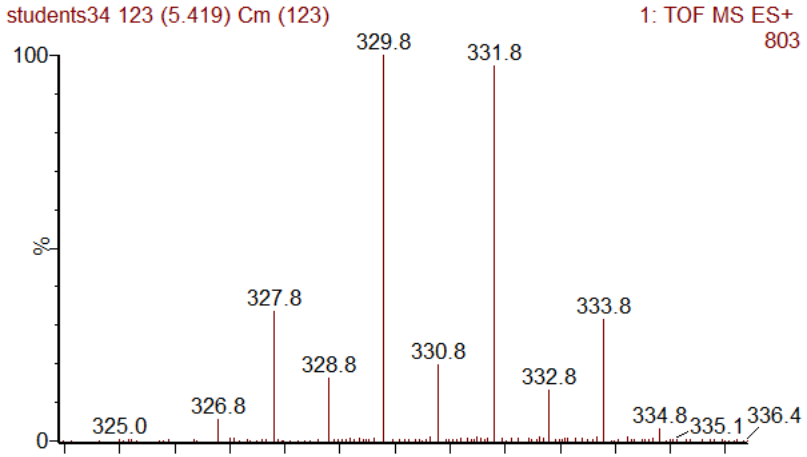
APPI conditions:

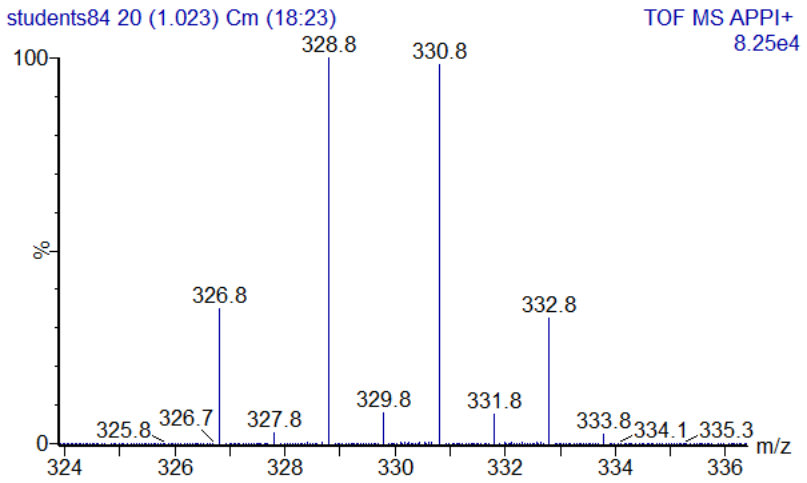
- UV Lamp: Syagen 10.6 ev krypton discharge Lamp
- Repeller 0.8-1.2 KV
- Sampling Cone 40
- Extraction Cone 4
- DCM/MeCN + 1-10%Toluene, Acetone
- Desolvation: 300-400 ^{o}C

  500-750 L/h , 99.9% Dry Nitrogen

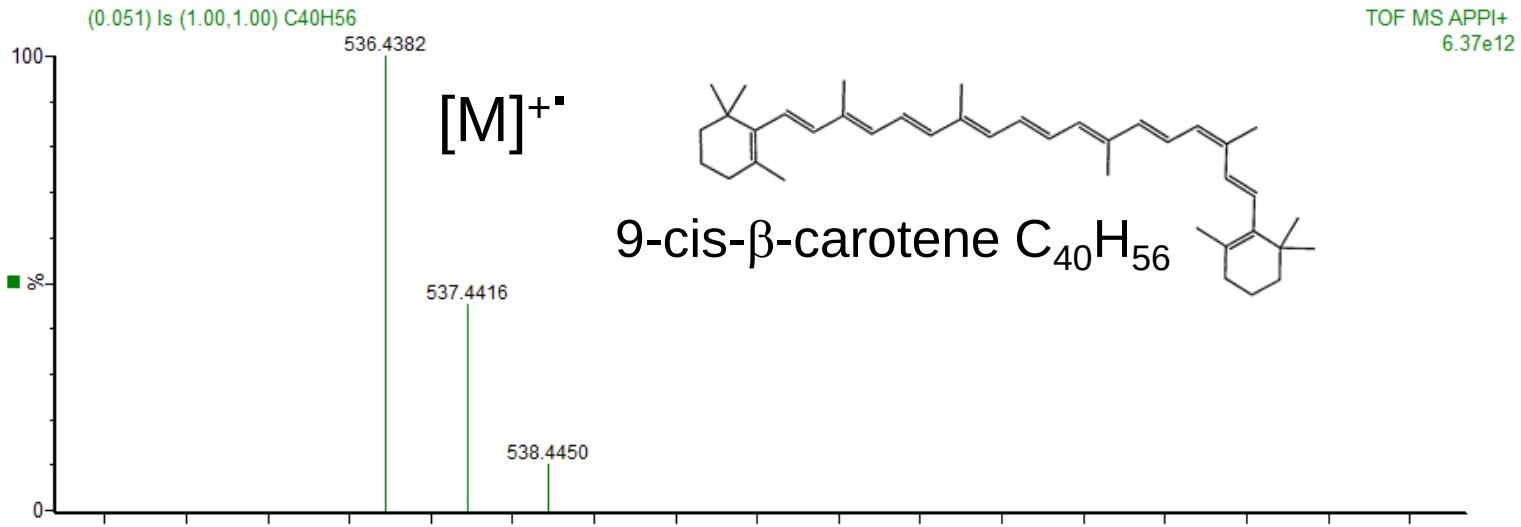
Conjugated compounds

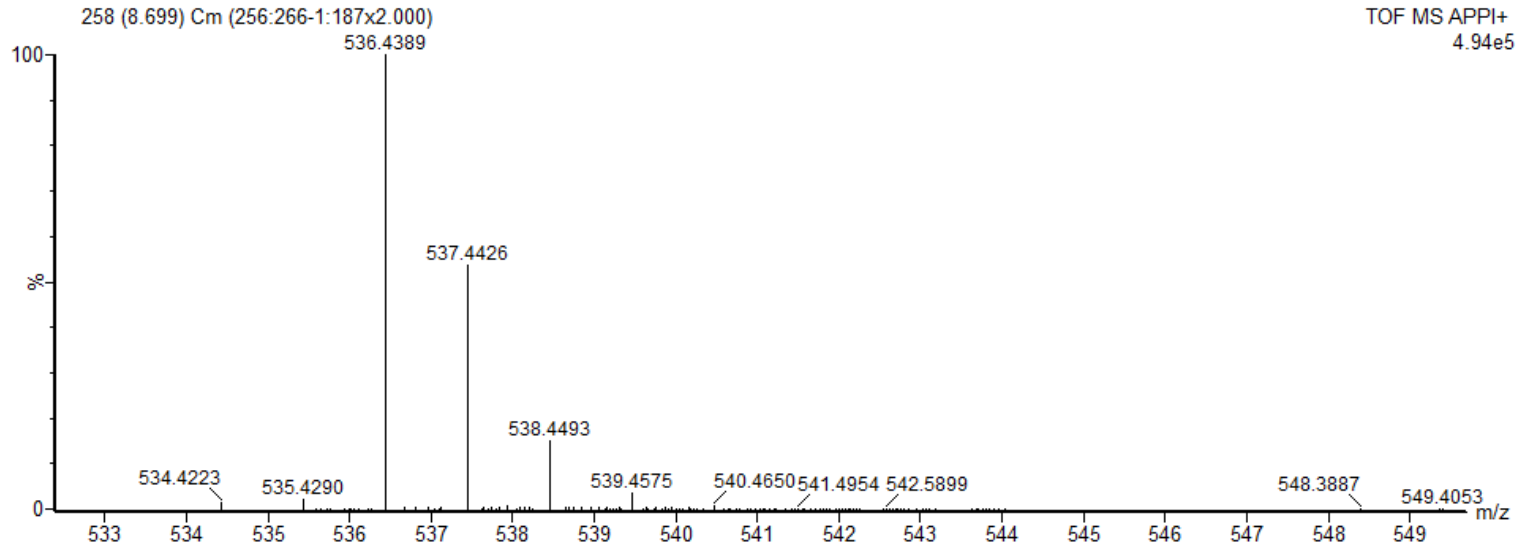




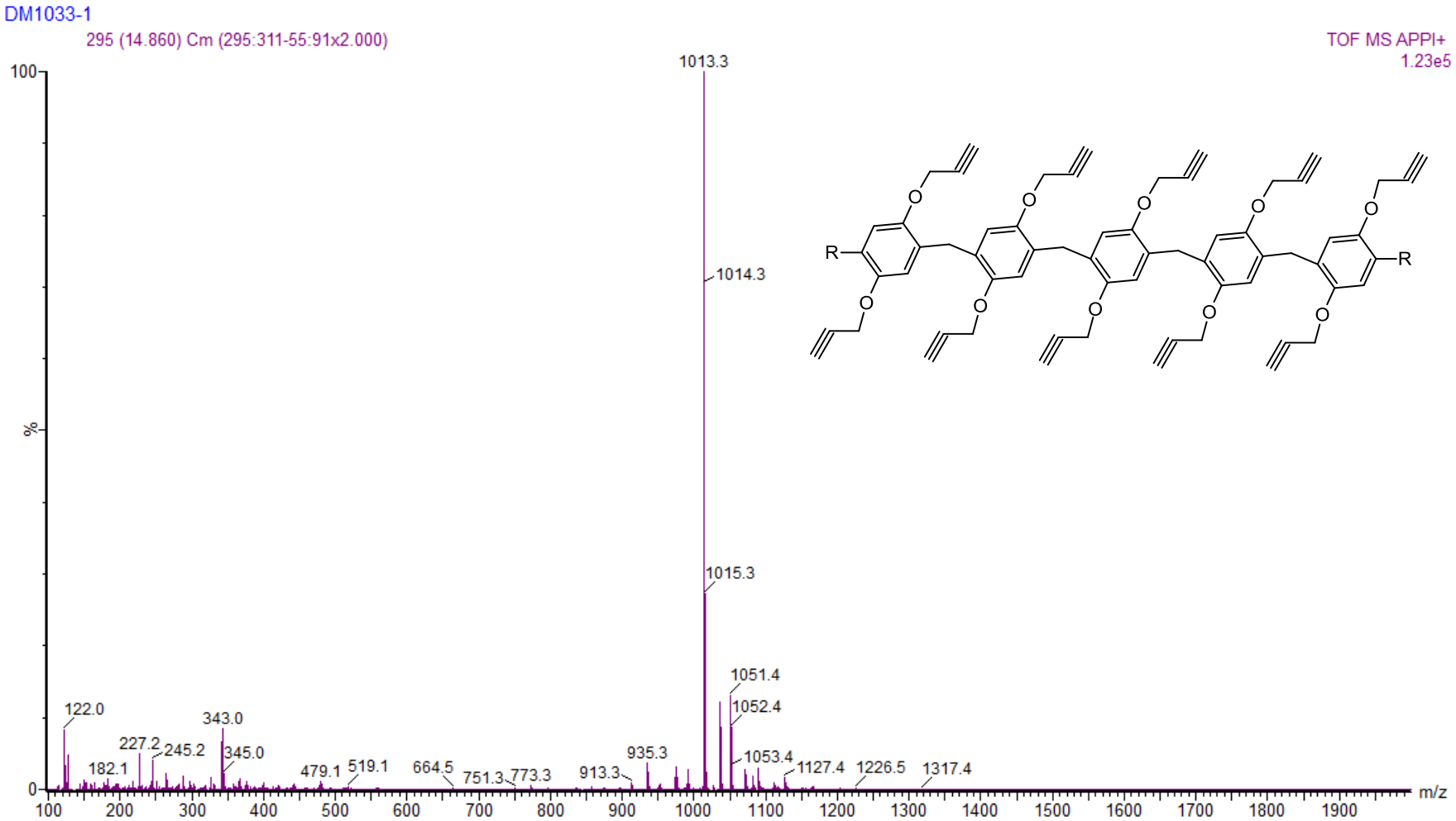


Conjugated compounds



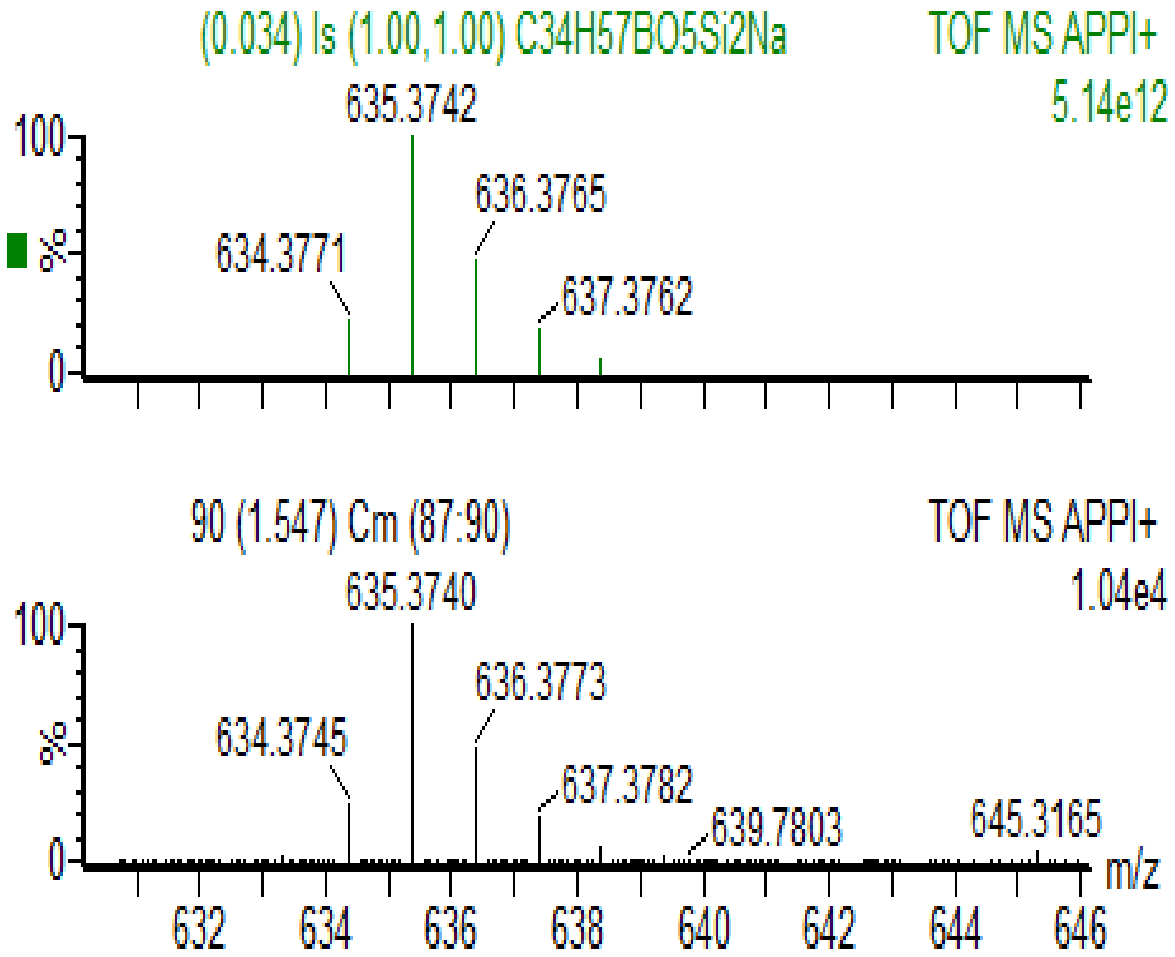


Conjugated compounds

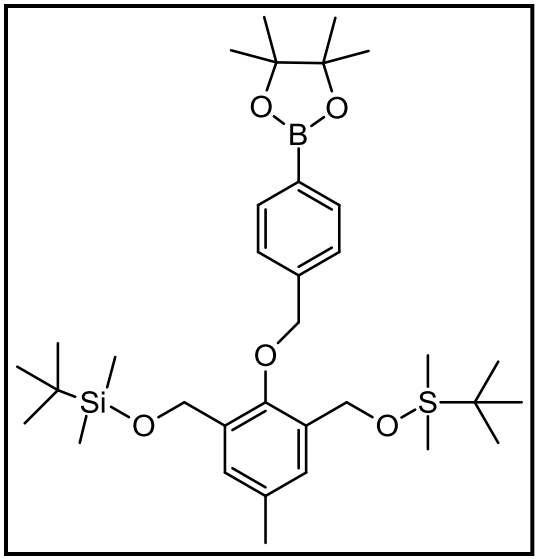


Conjugated compounds

ef 2-41



$C_{34}H_{57}BSi_2O_5Na$



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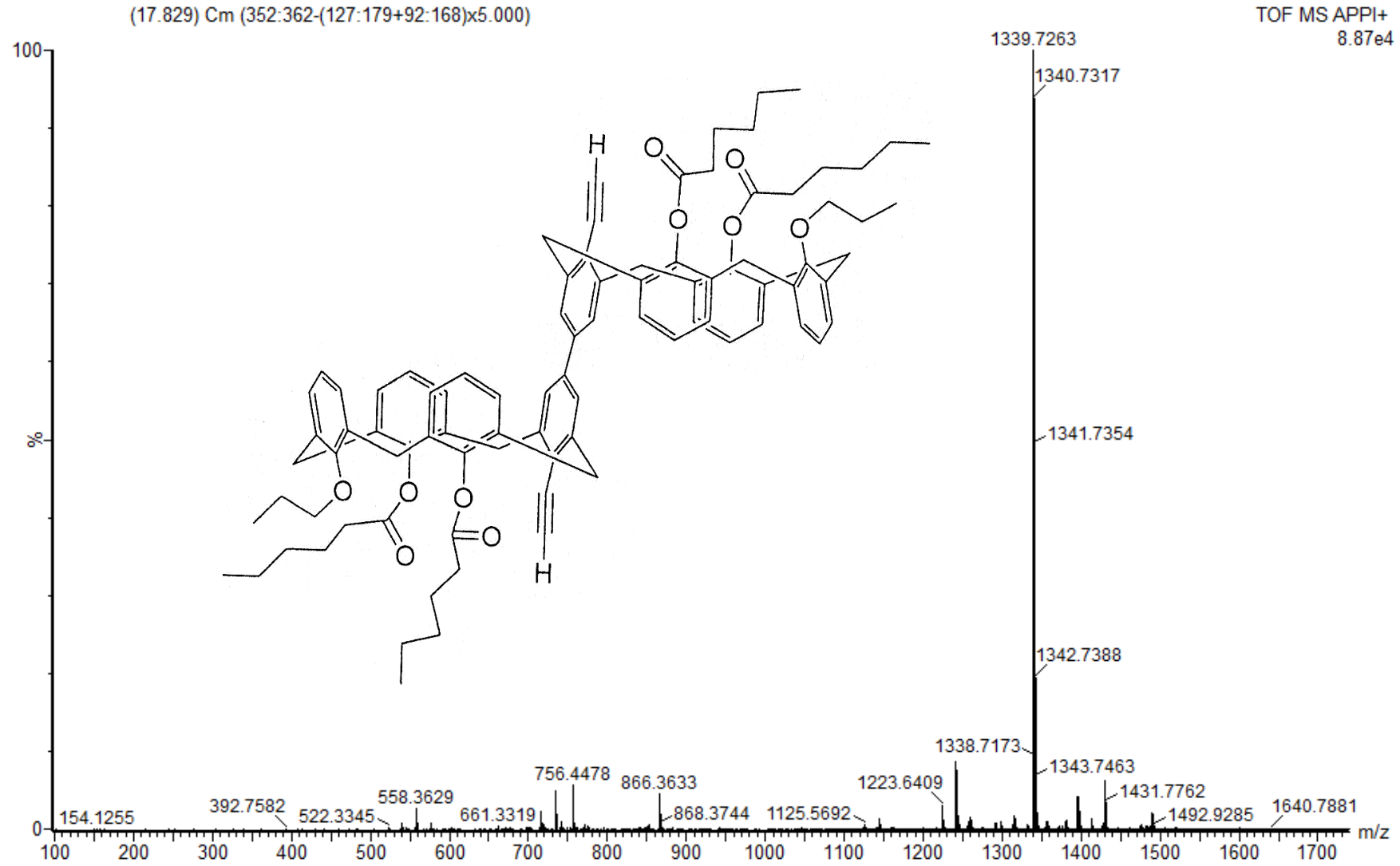

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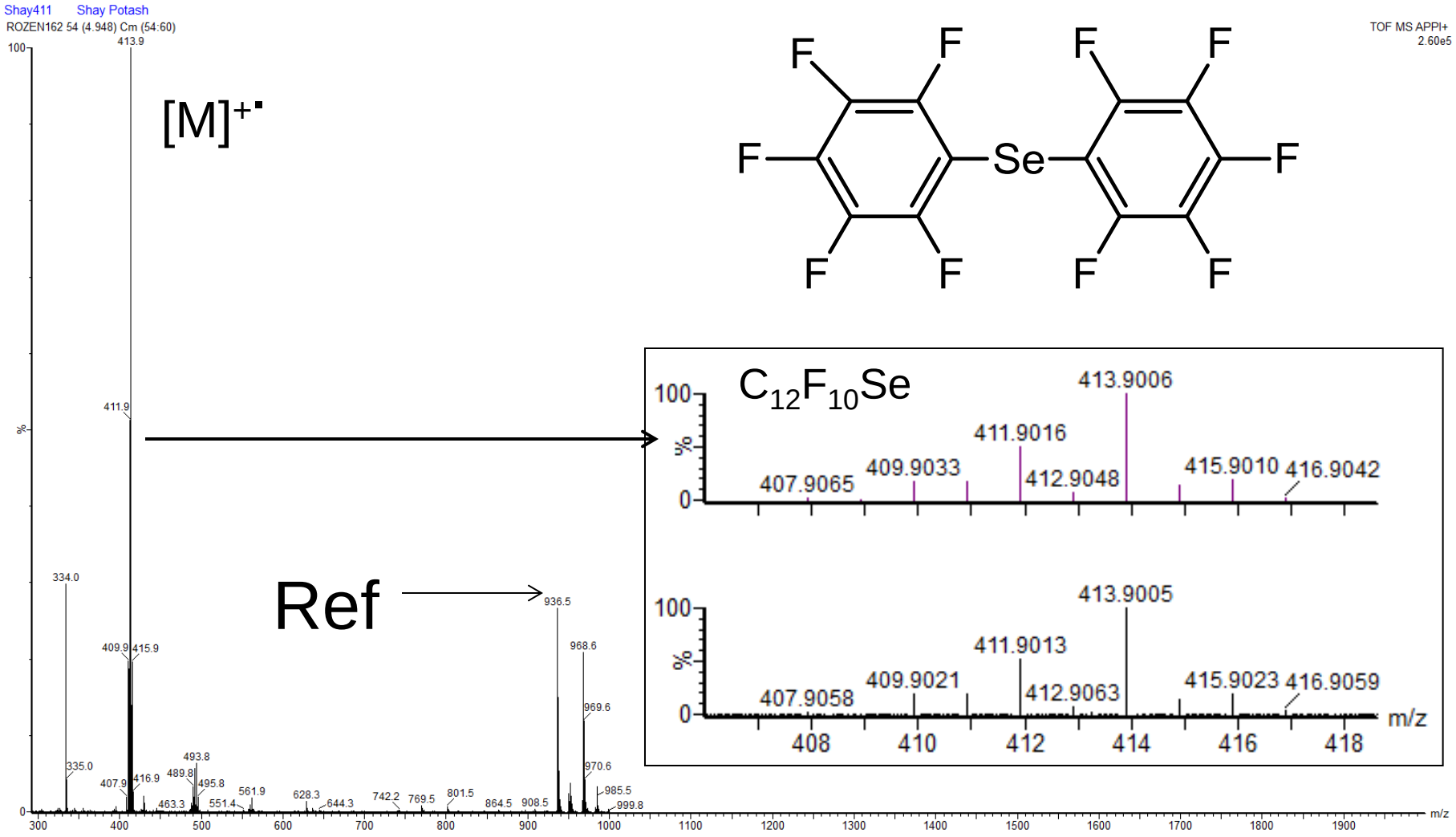
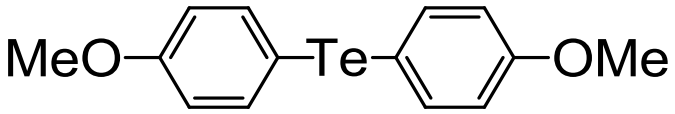
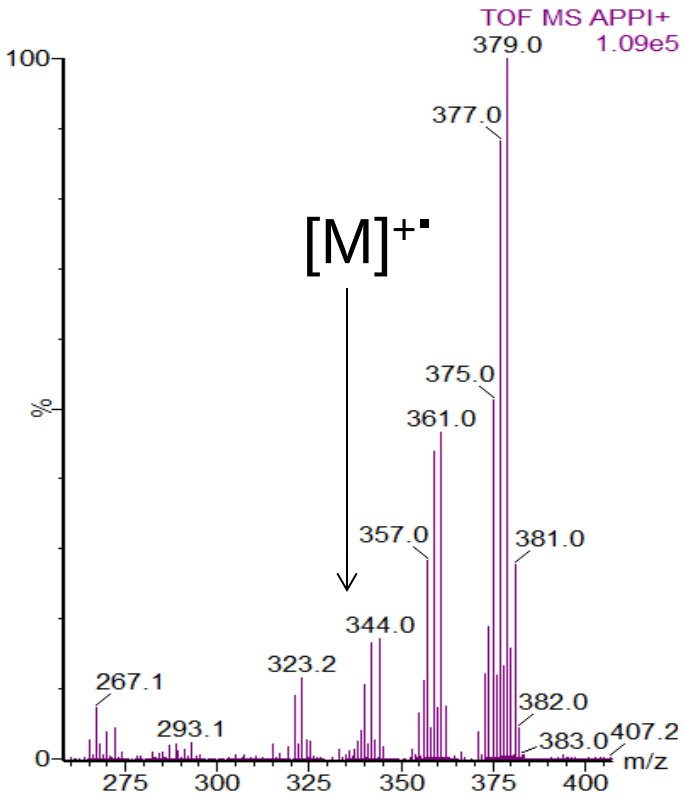
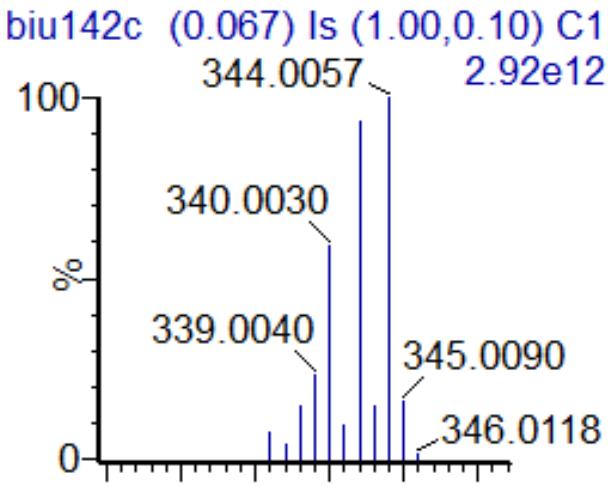
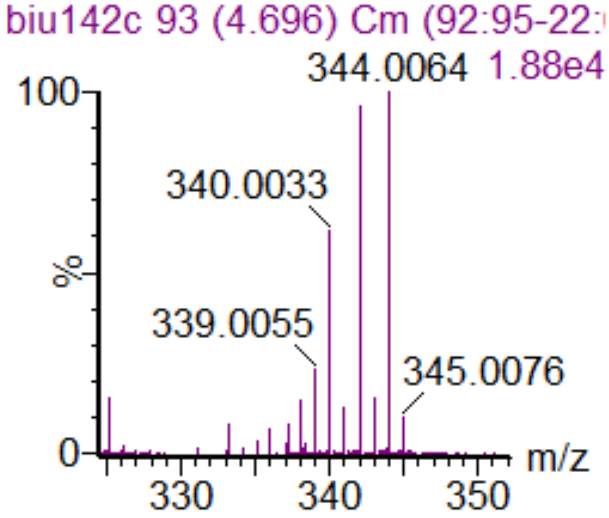


Conjugated compounds









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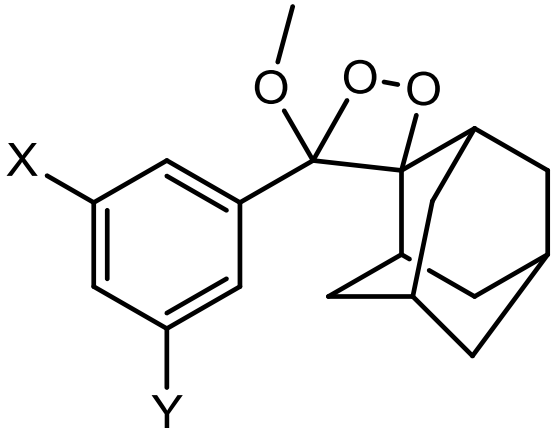

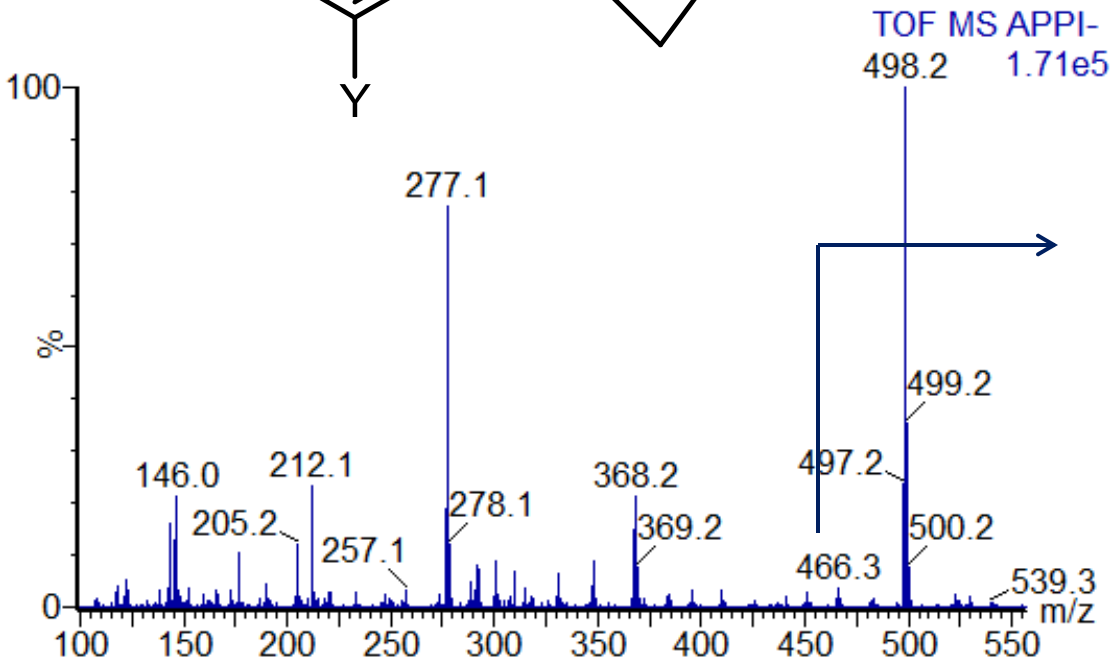

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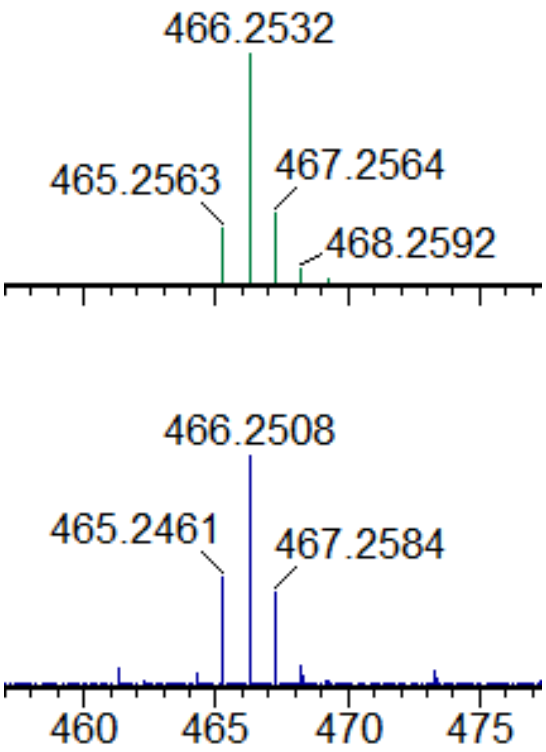

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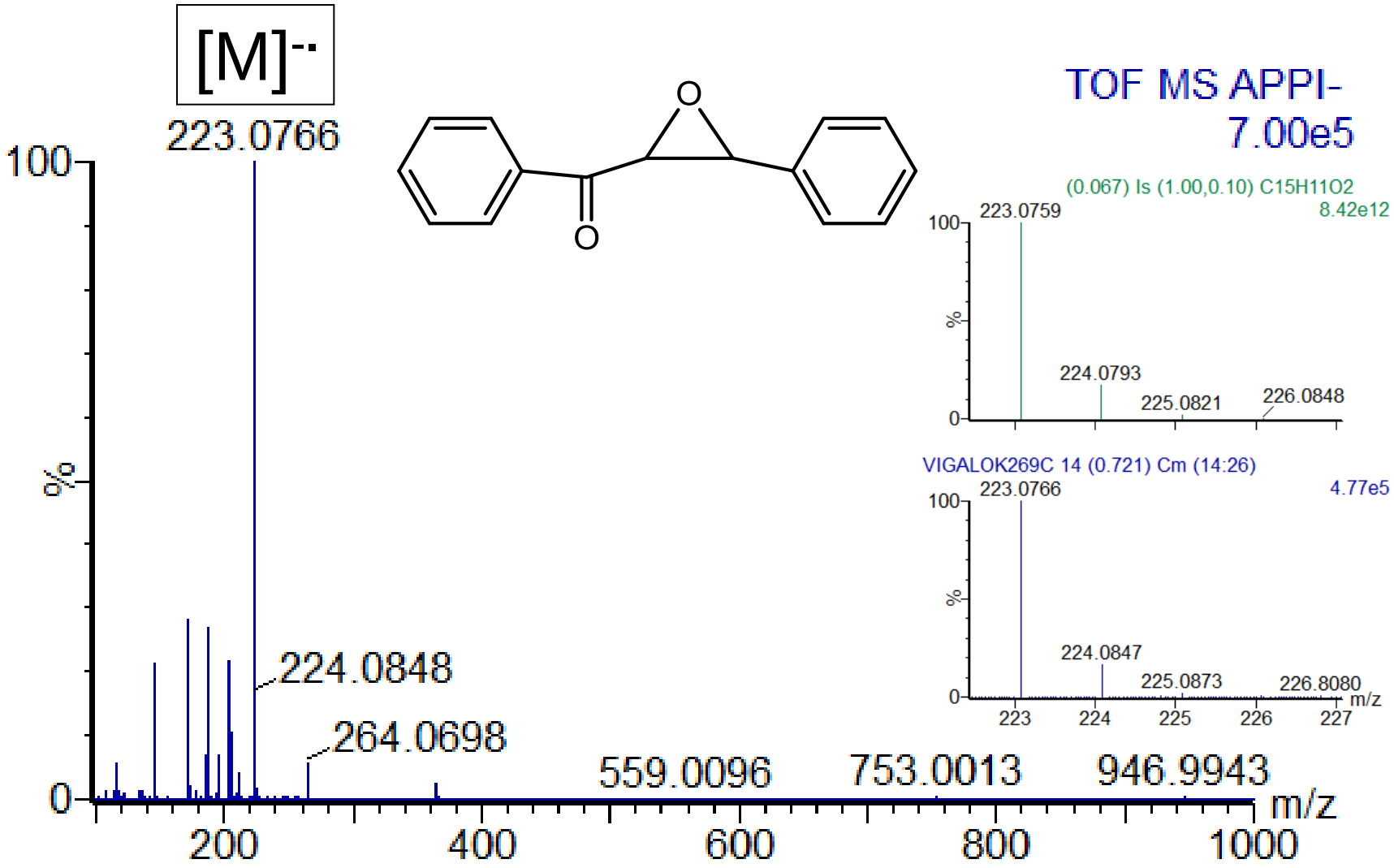

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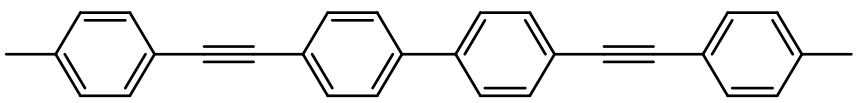

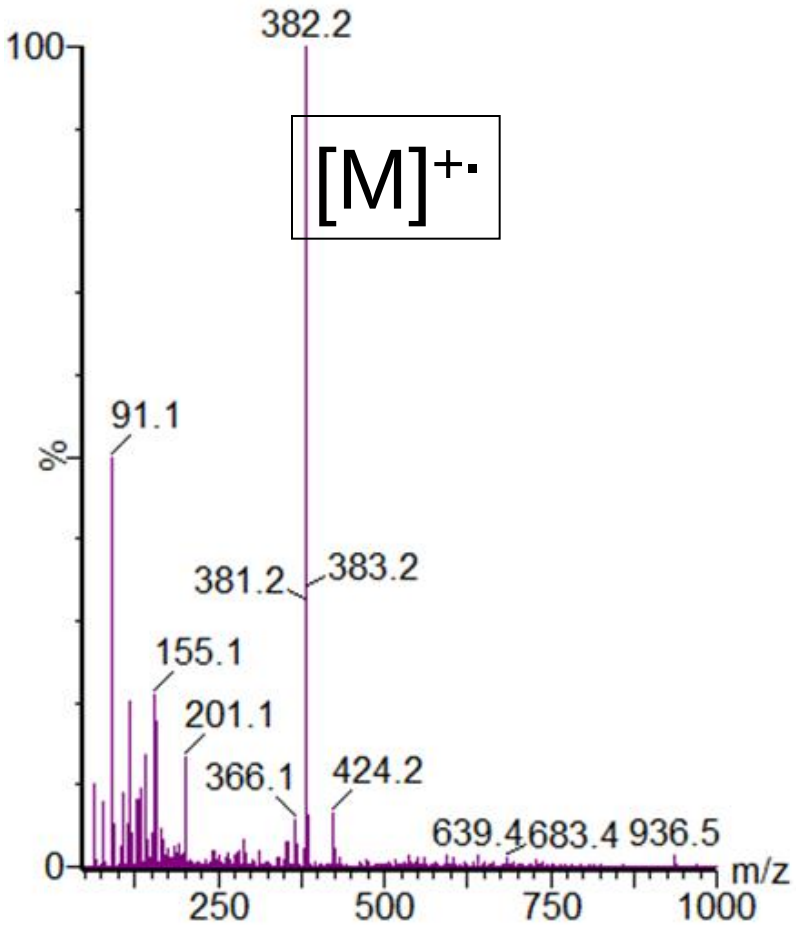

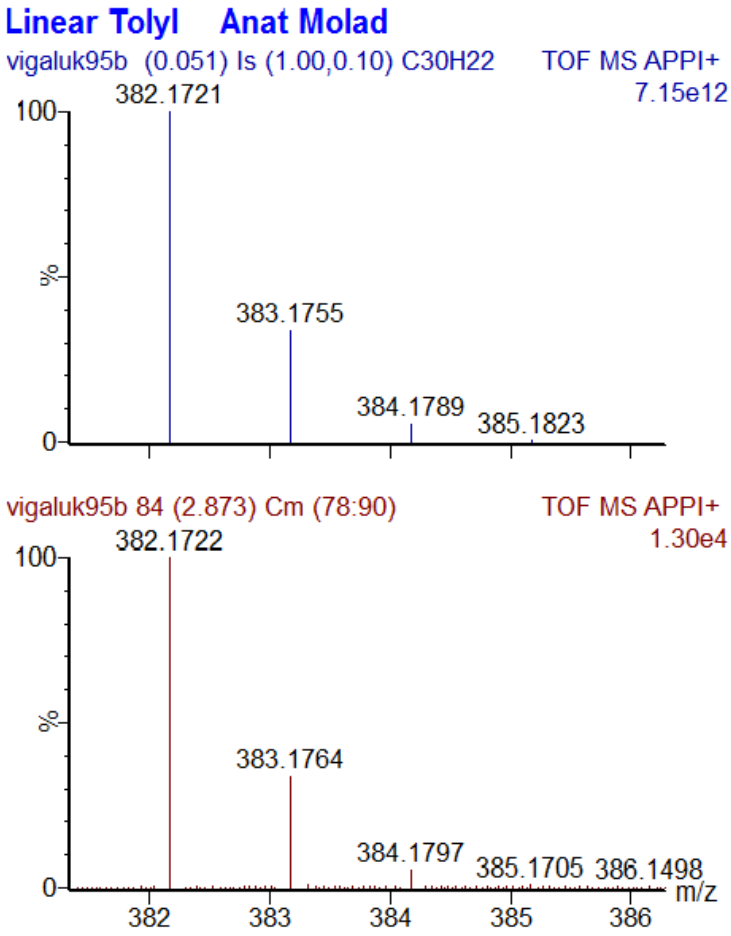

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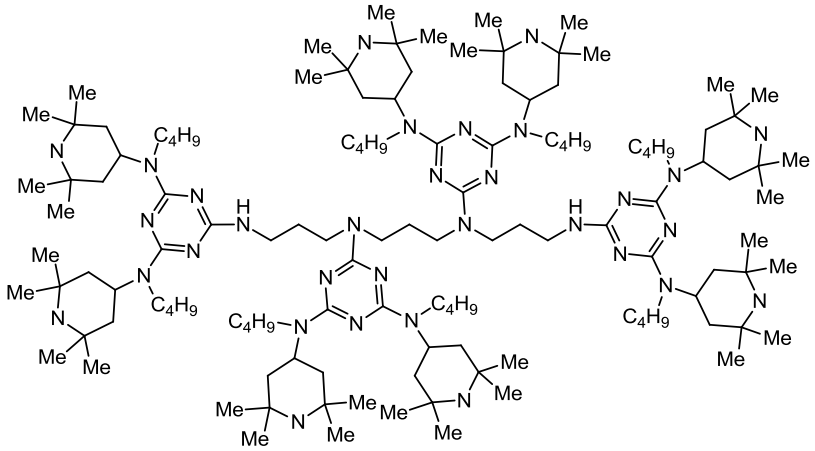
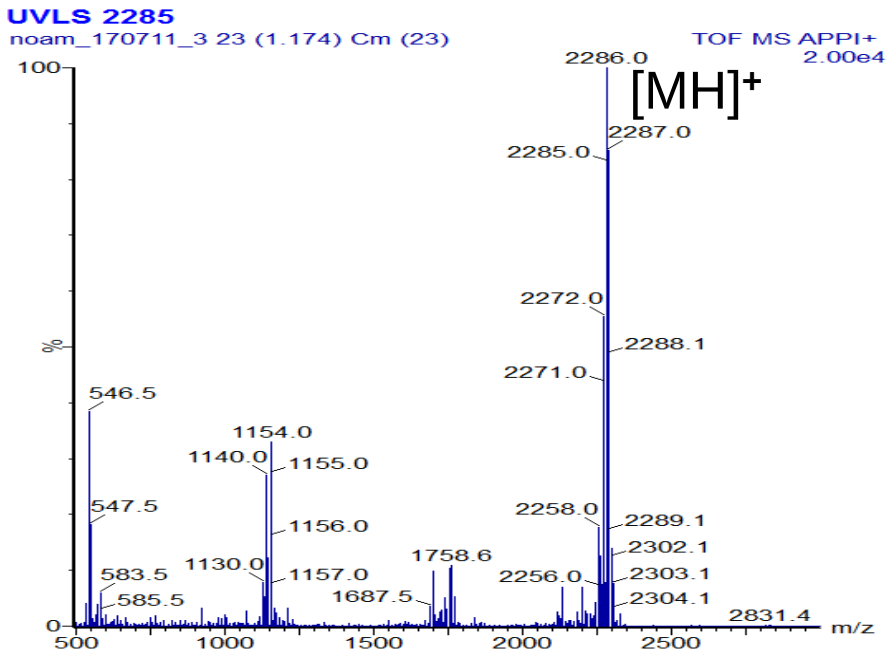
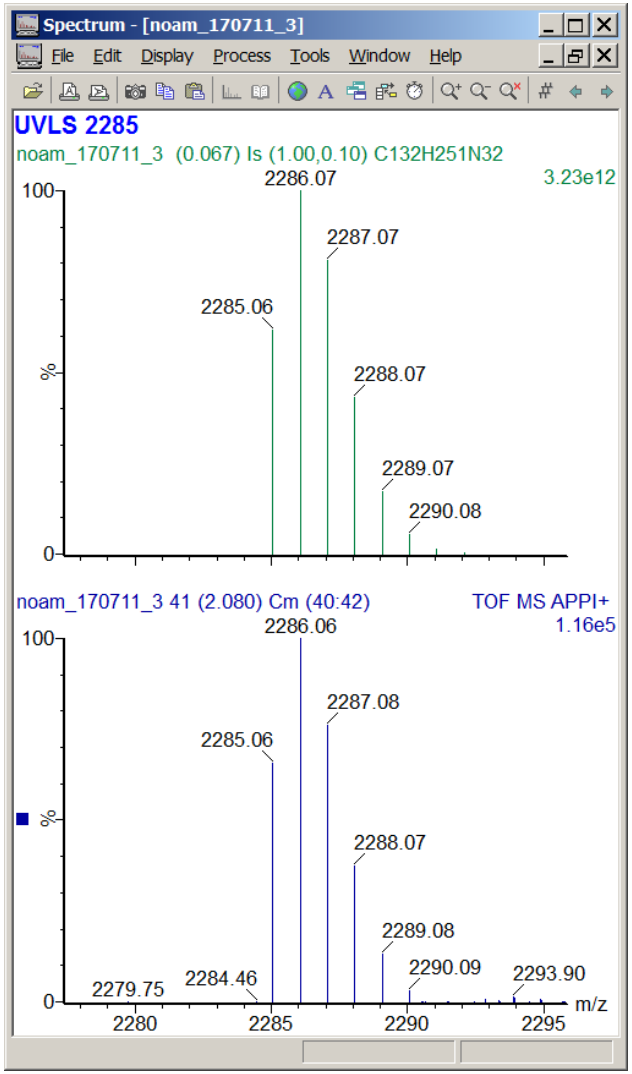
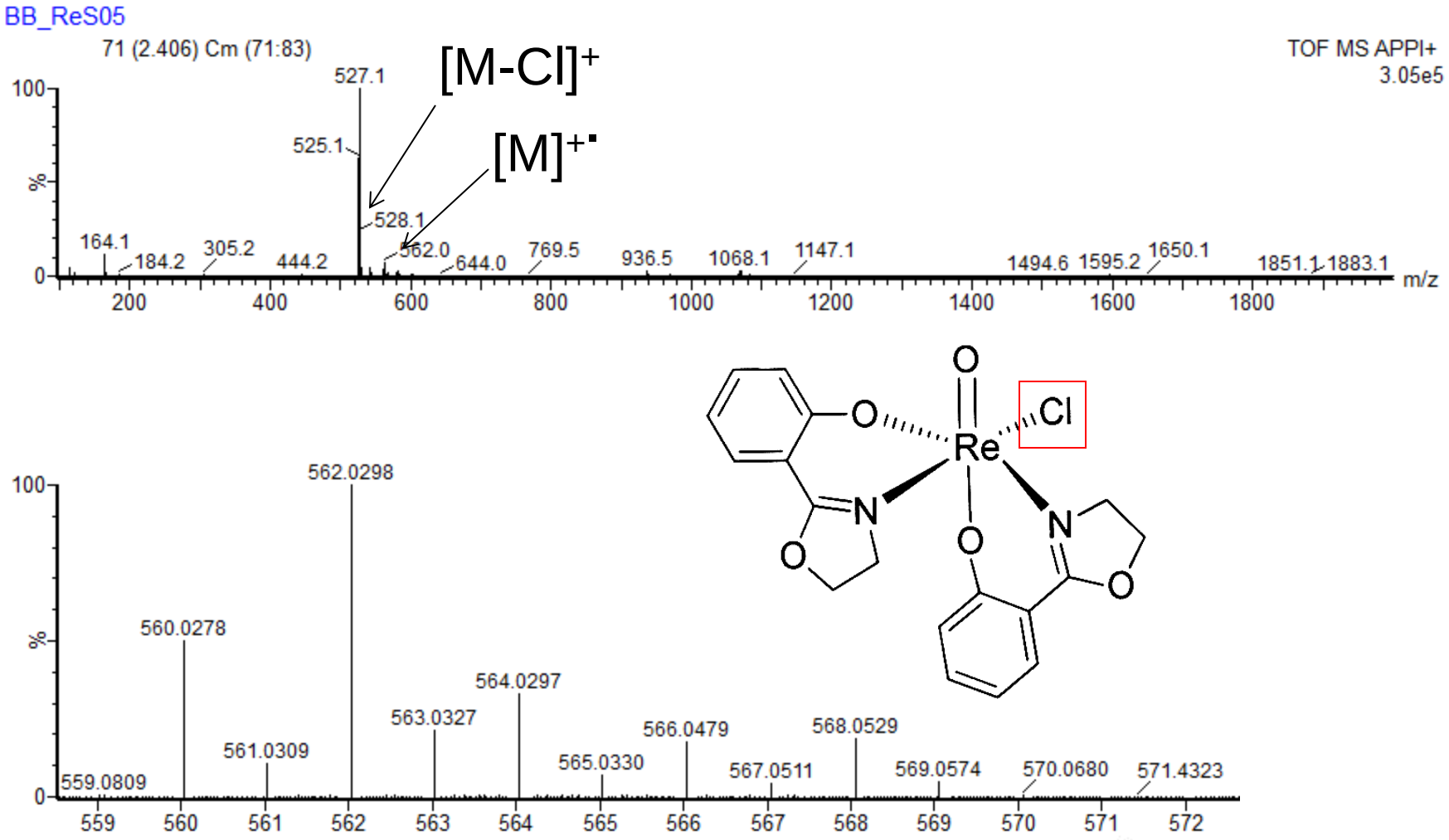






Organometallic



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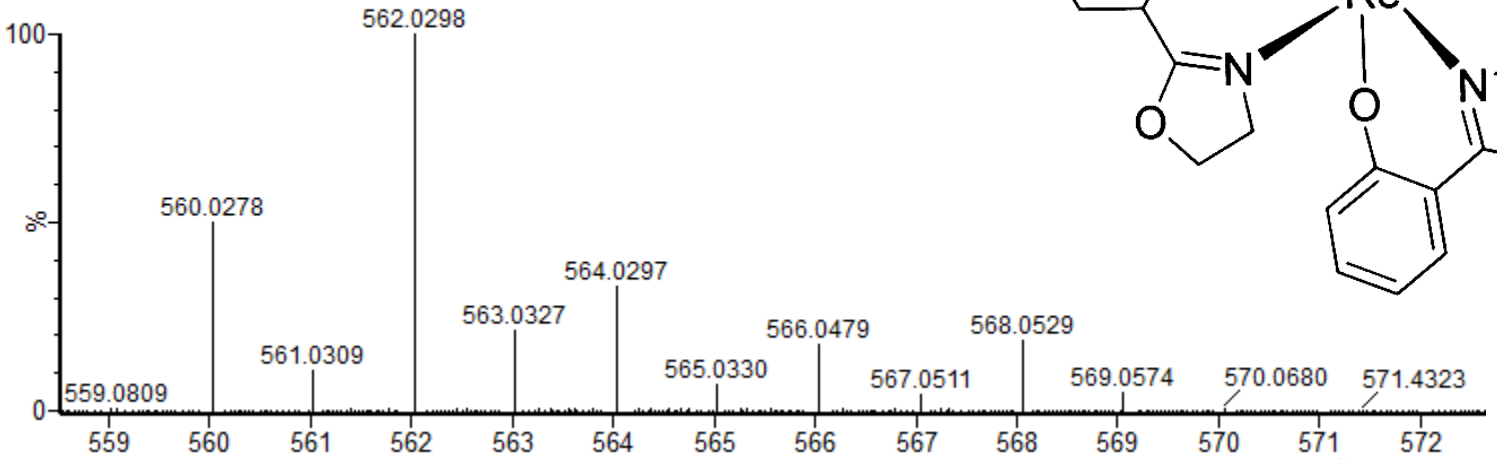
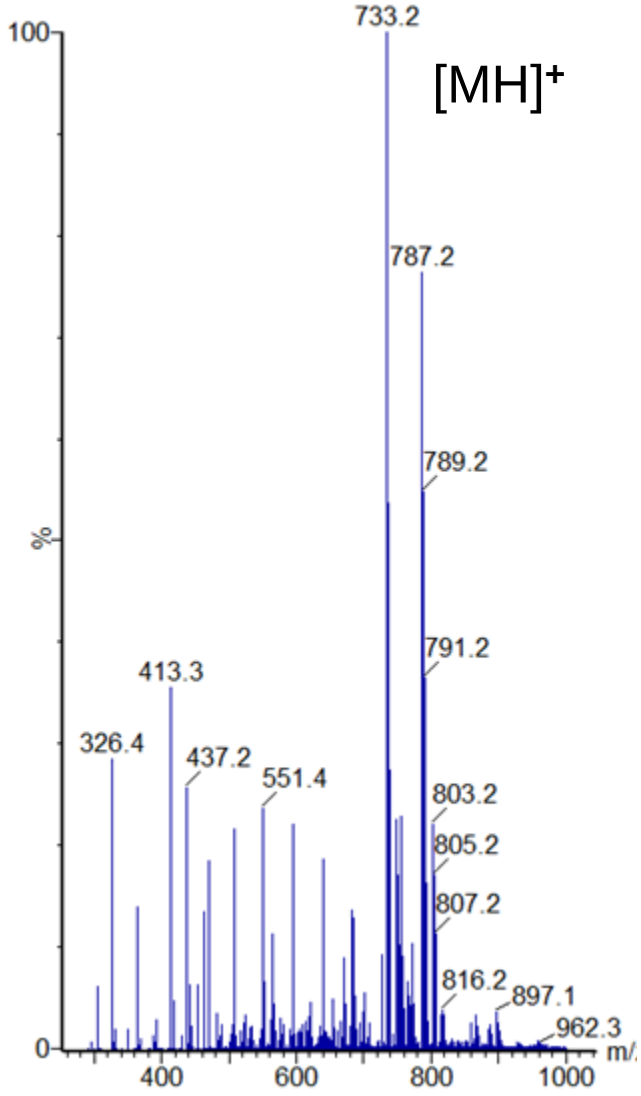
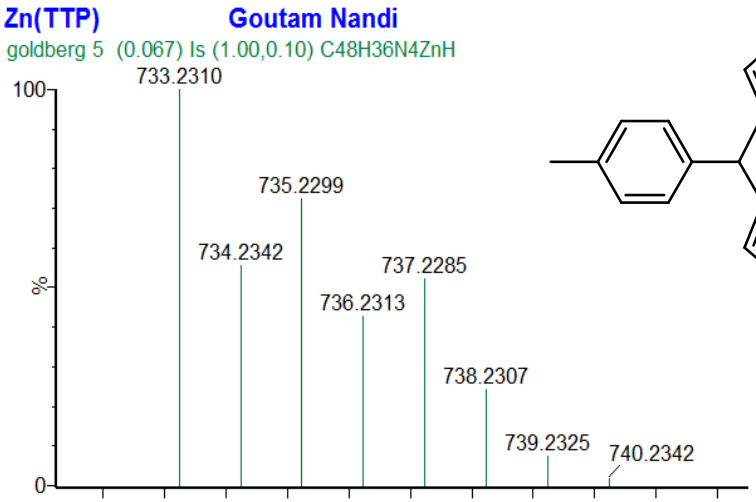
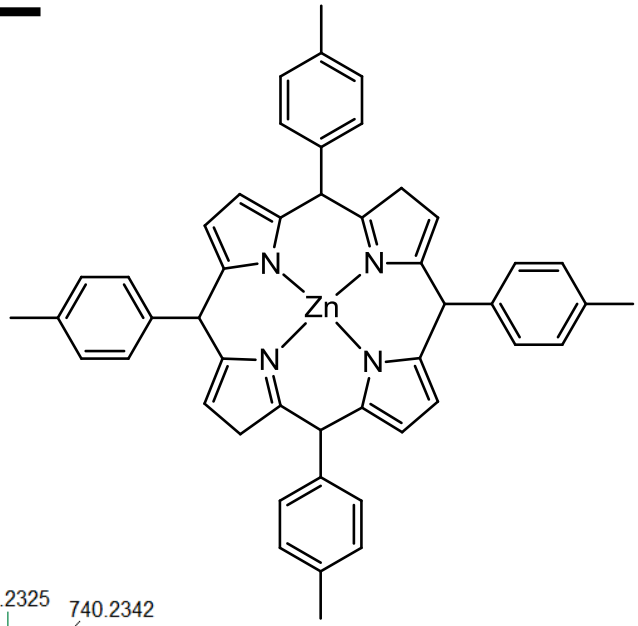


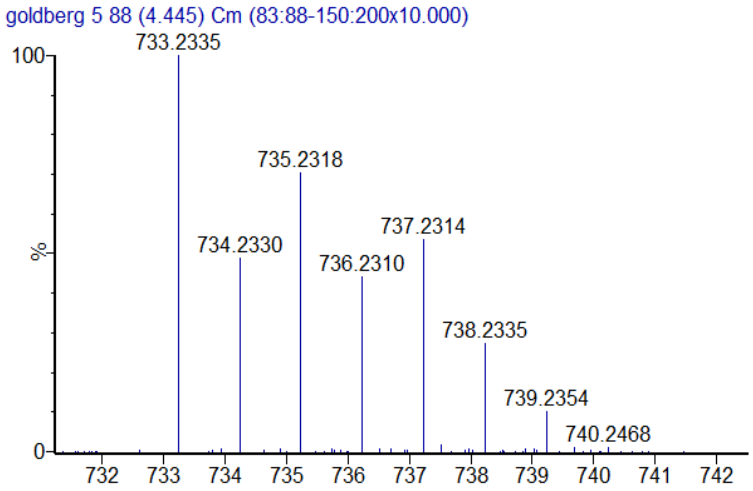
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	Na	Cl	185Re	187Re
562.0298	562.0305	-0.7	-1.2	11.5	C18 H16 N2 O5 Cl 187Re	312.0	0.3	18	16	2	5		1		1
	562.0292	0.6	1.1	12.0	C16 H14 N5 O4 Cl 187Re	313.6	2.0	16	14	5	4		1		1
	562.0294	0.4	0.7	17.0	C23 H16 N4 O9 Cl2	323.2	11.6	23	16	4	9		2		
	562.0295	0.3	0.5	11.5	C15 H14 N6 O4 Cl 185Re	314.5	2.9	15	14	6	4		1	1	
	562.0297	0.1	0.2	18.5	C24 H15 N5 O6 Na Cl2	323.0	11.3	24	15	5	6	1	2		
	562.0298	0.0	0.0	7.5	C17 H19 O6 Na Cl 185Re	314.3	2.7	17	19		6	1	1	1	

Organometallic

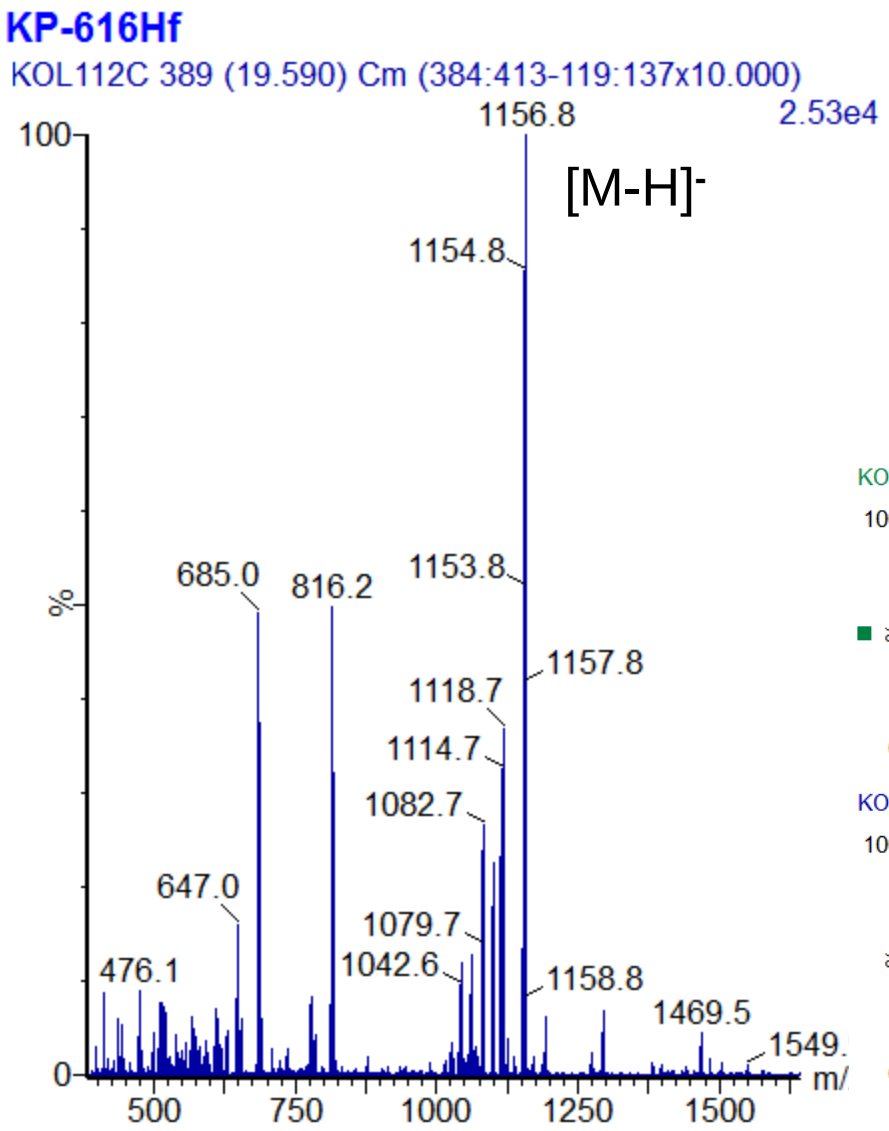


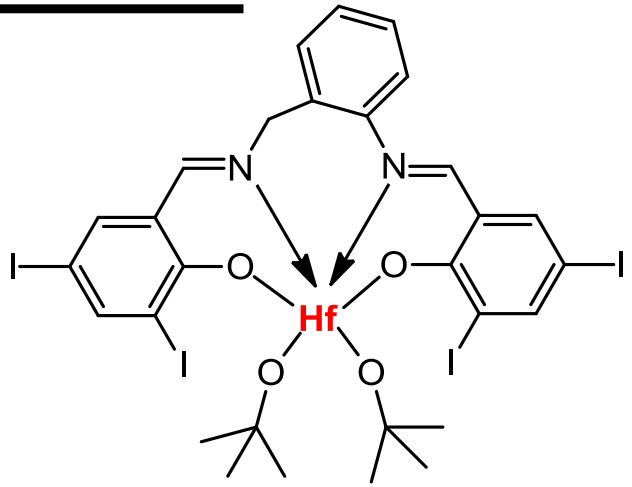


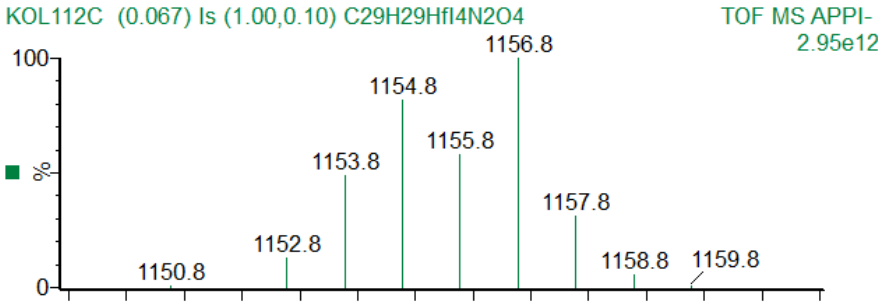


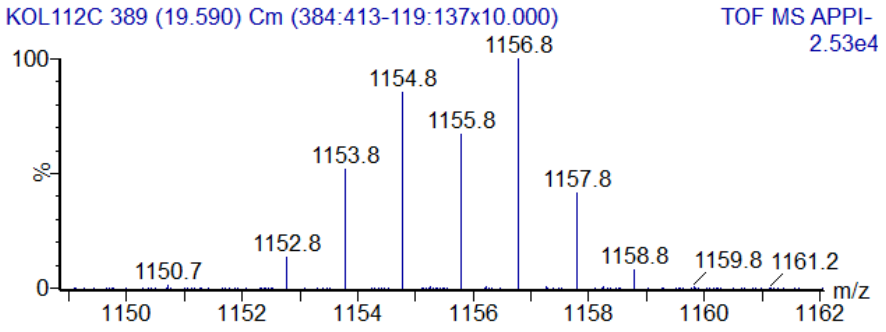


Organometallic









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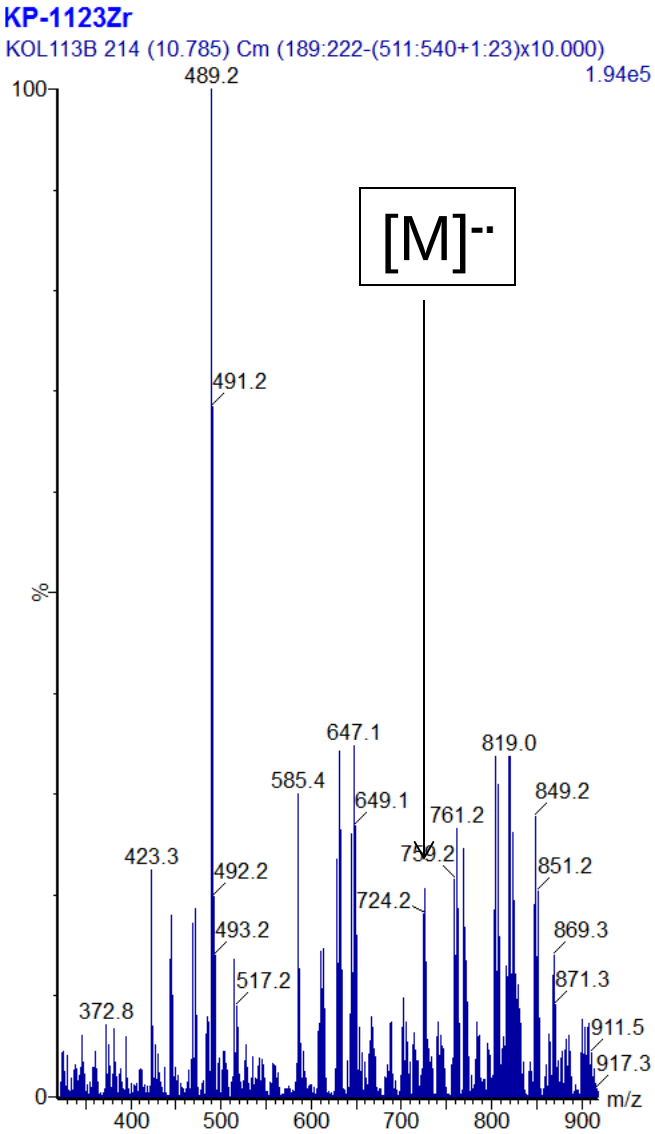
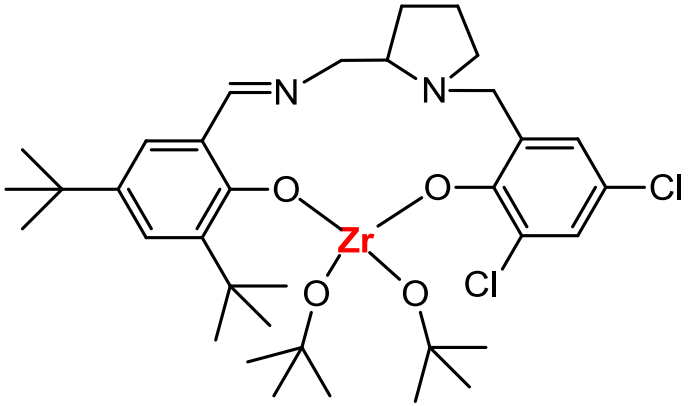
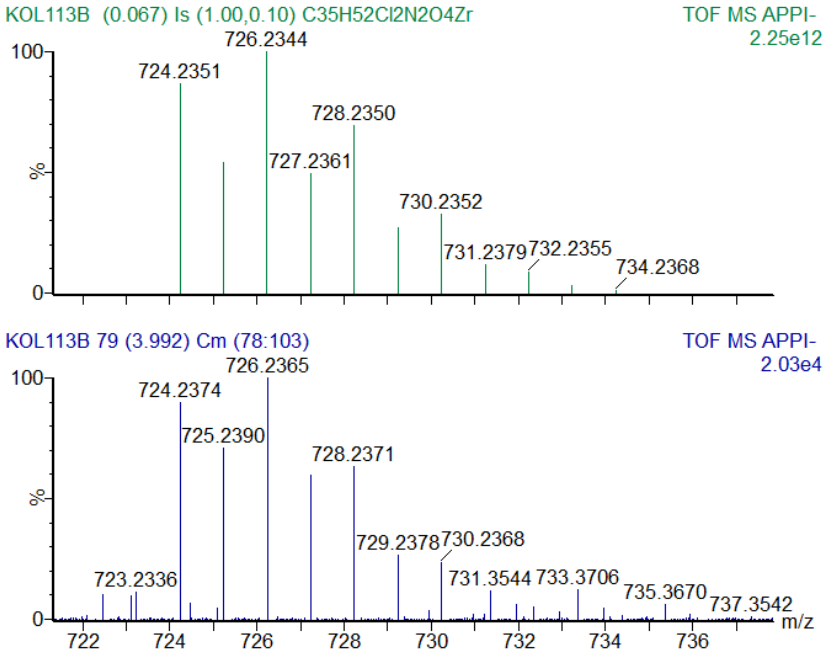
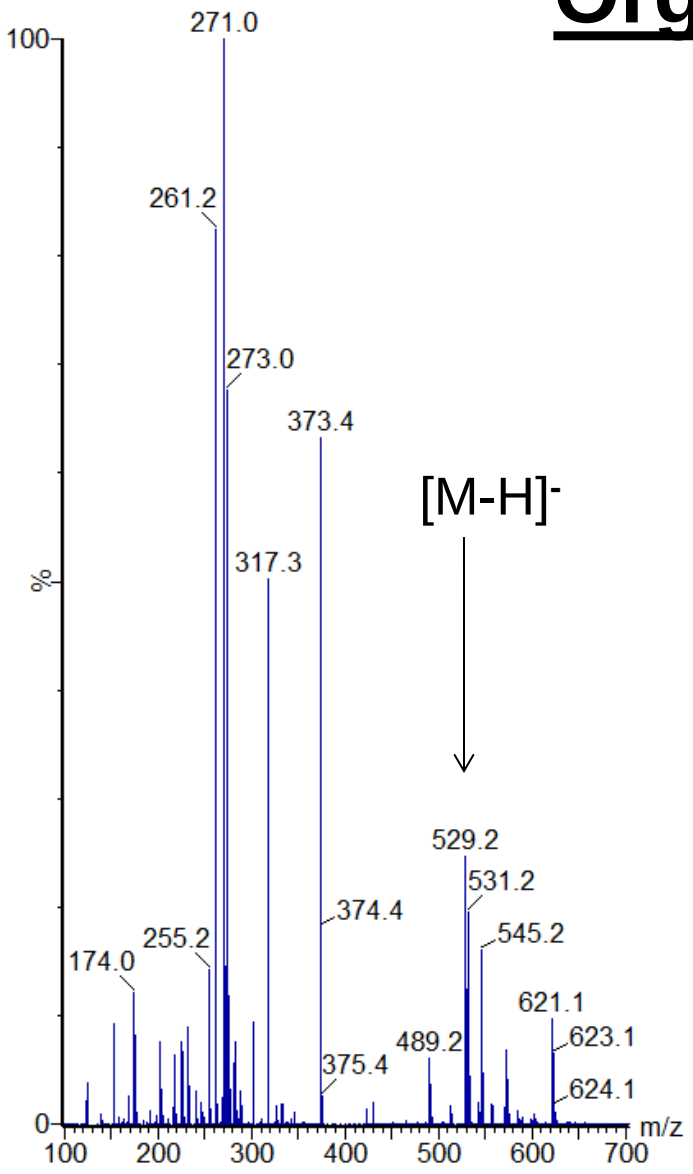
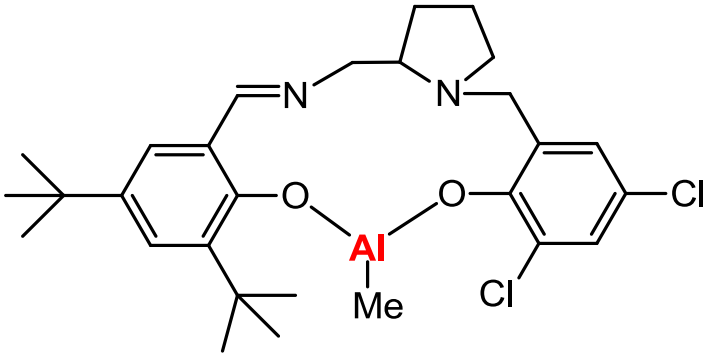






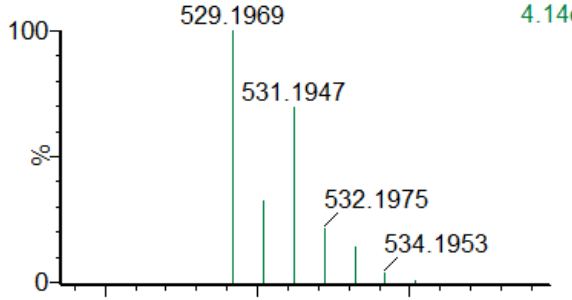
Organometallic



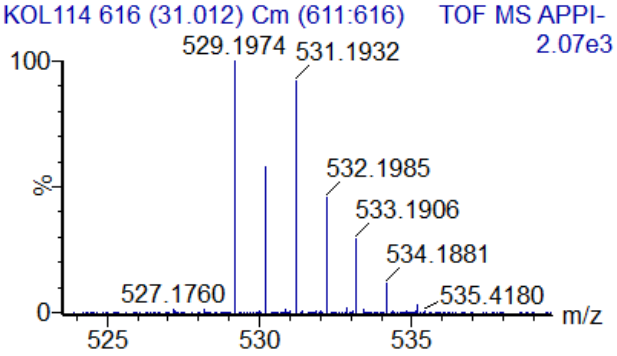


KP-1123AlMe

KOL114 (0.067) Is (1.00,0.10) C28H36Cl2N2O2Al 4.14e12



KOL114 616 (31.012) Cm (611:616) TOF MS APPI- 2.07e3



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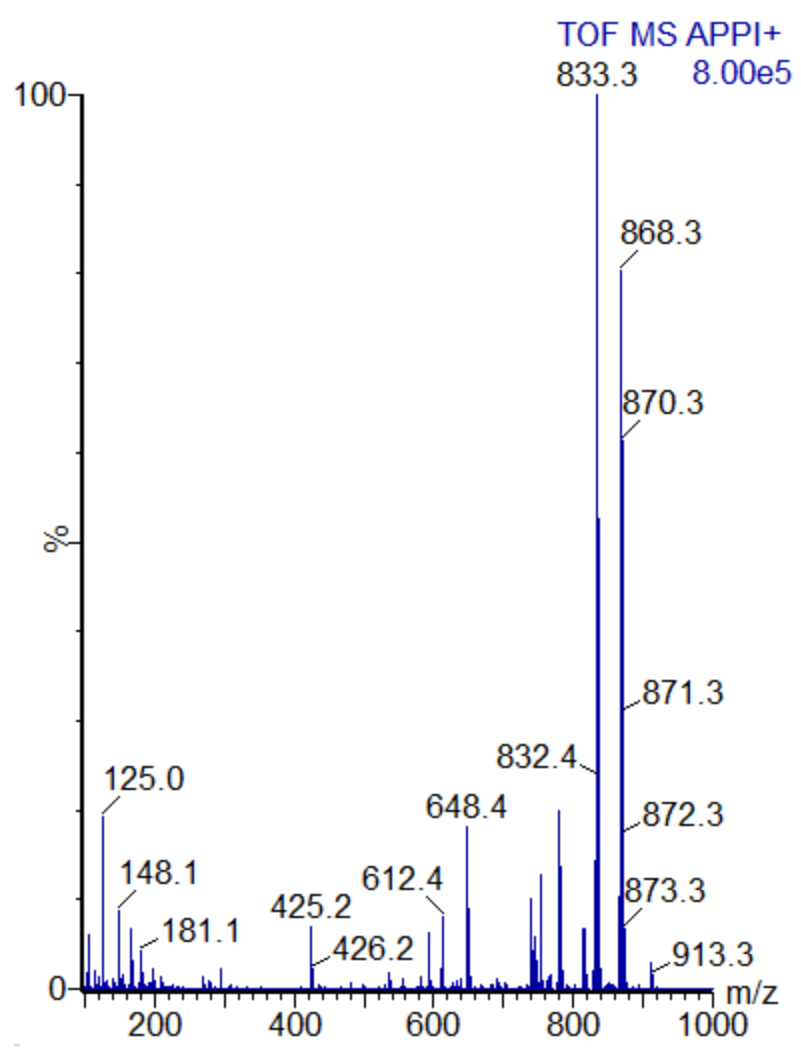

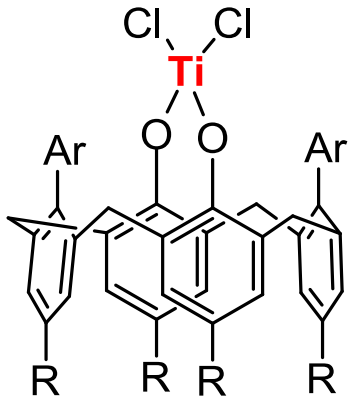

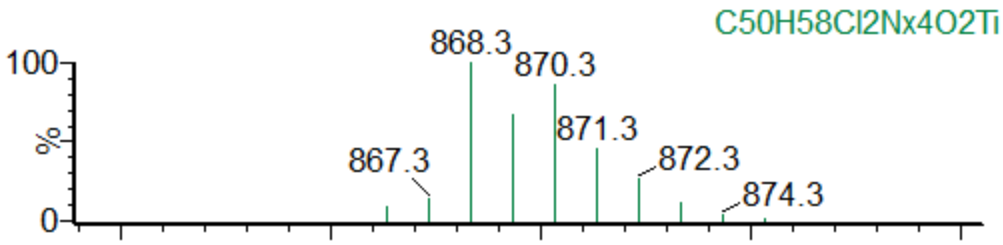

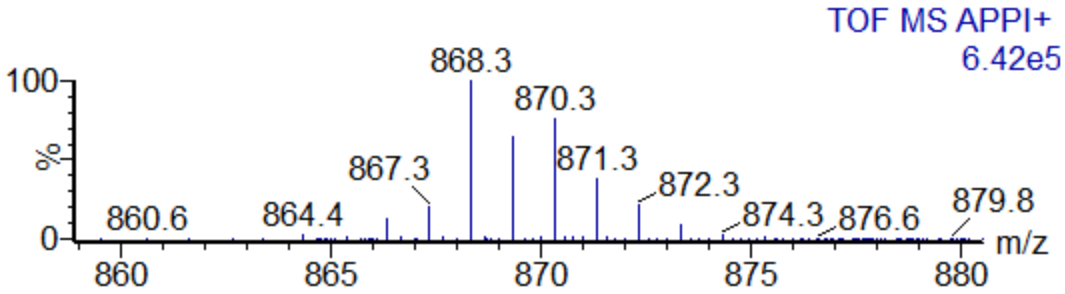

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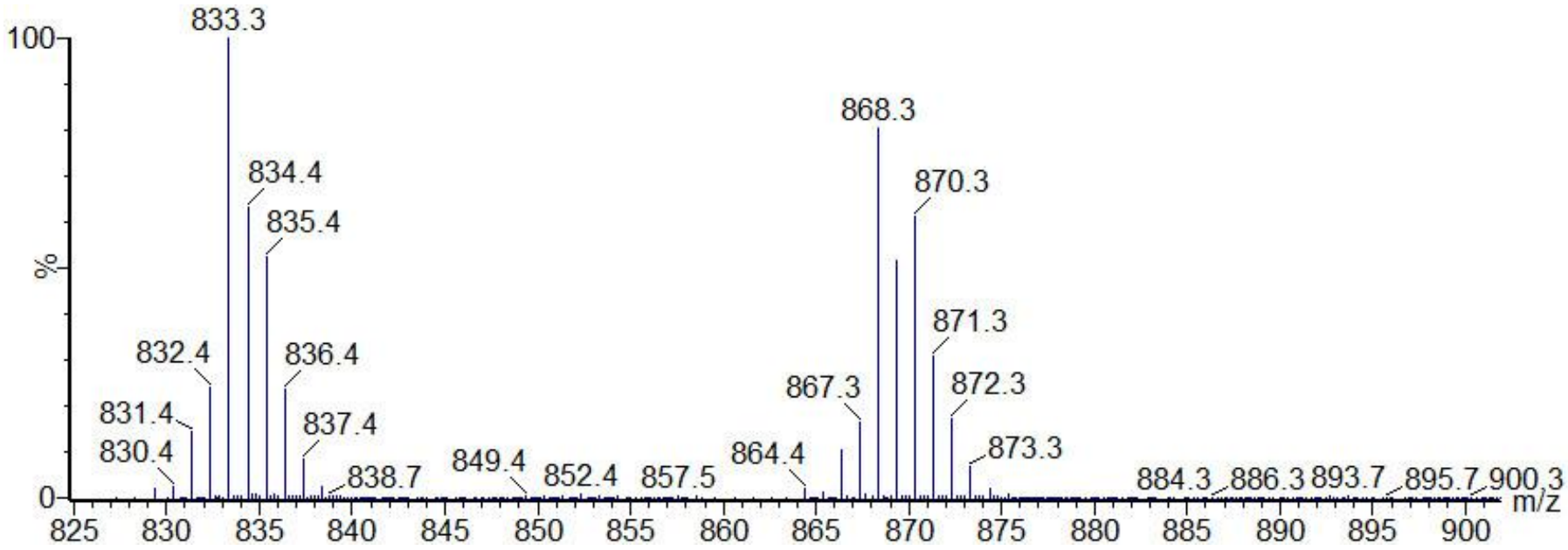
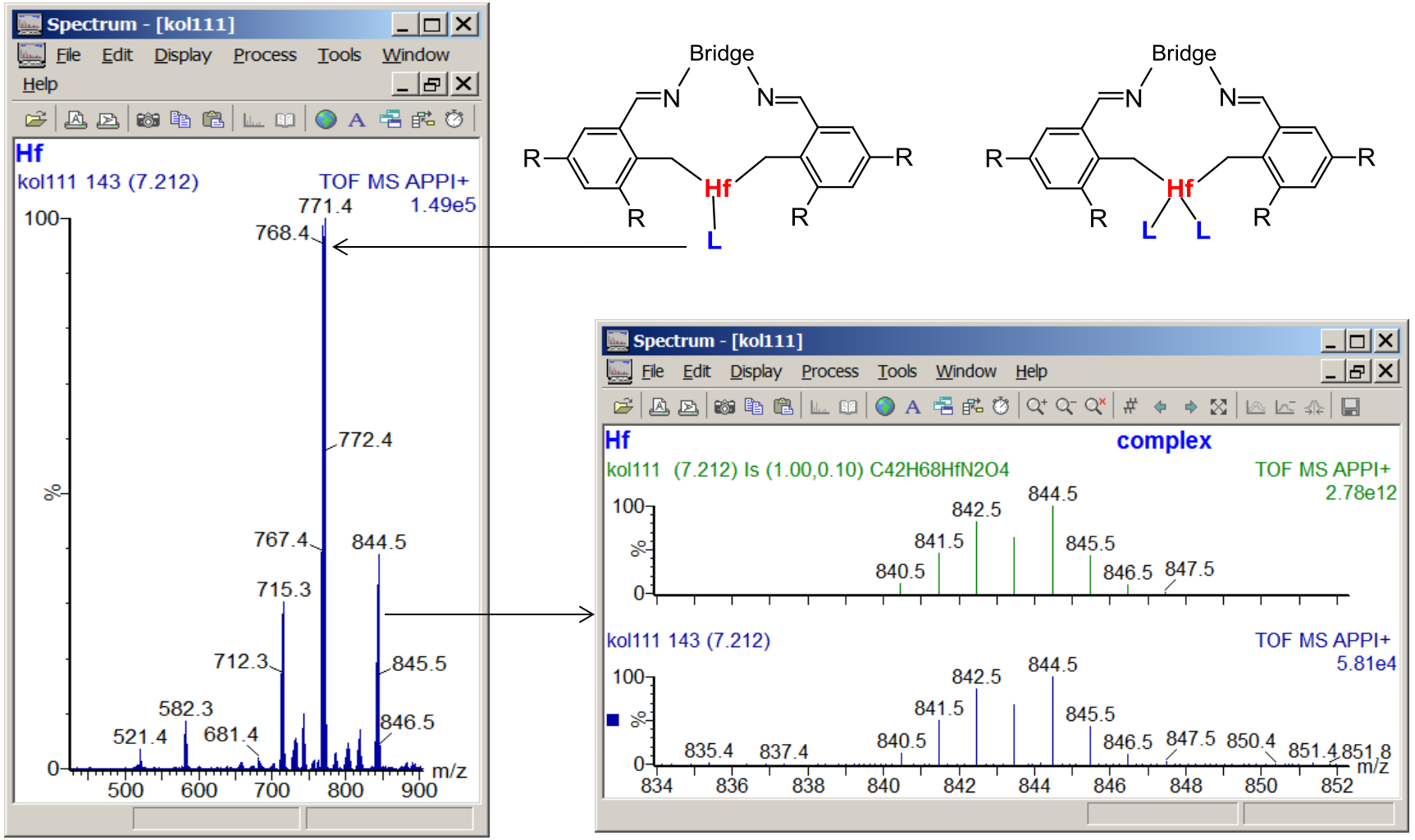


Organometallic



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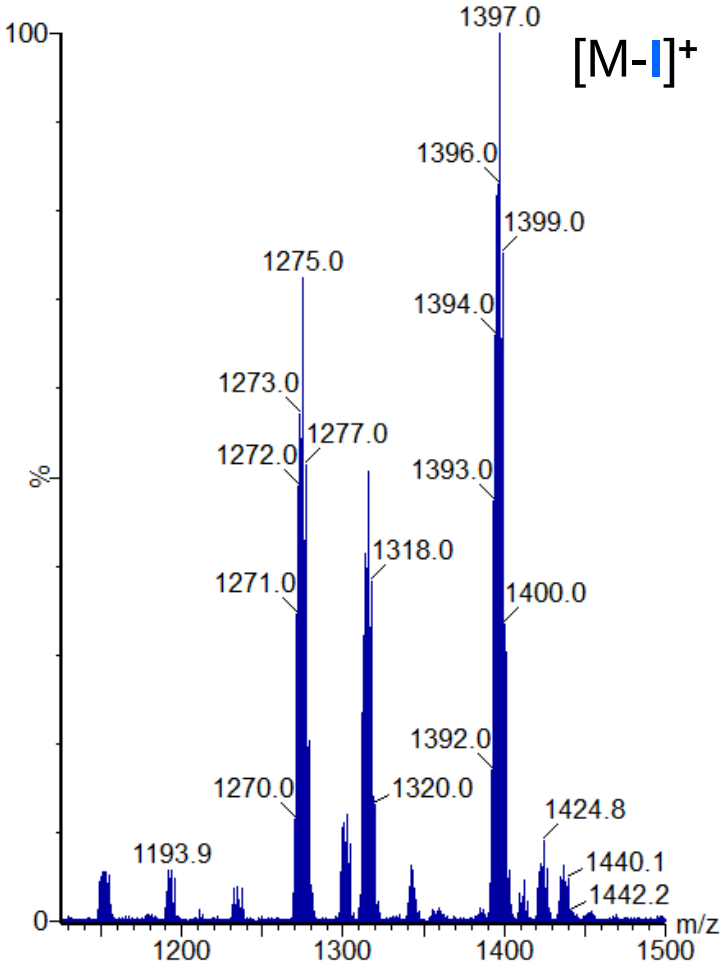
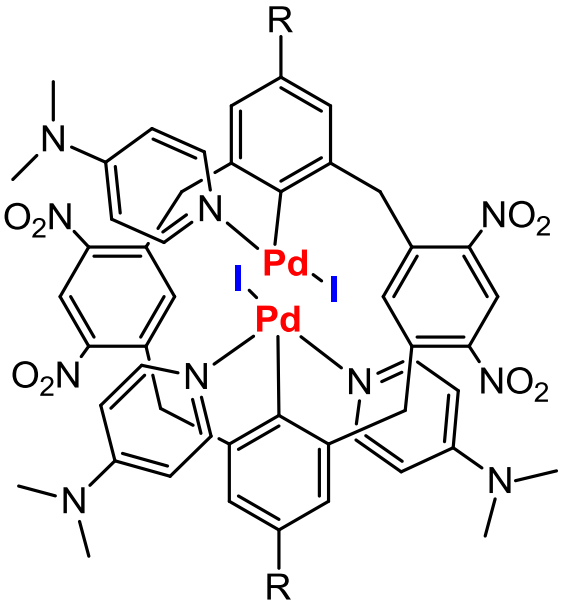
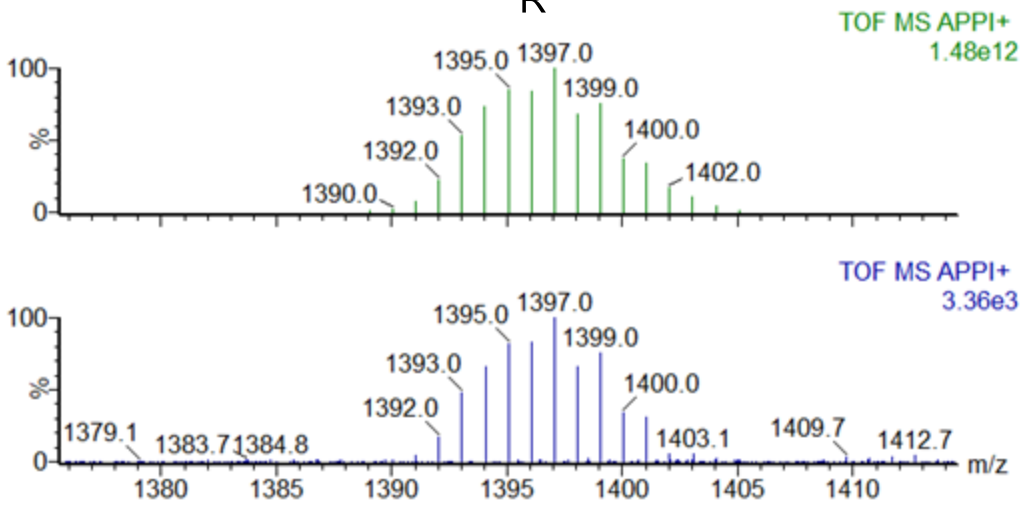
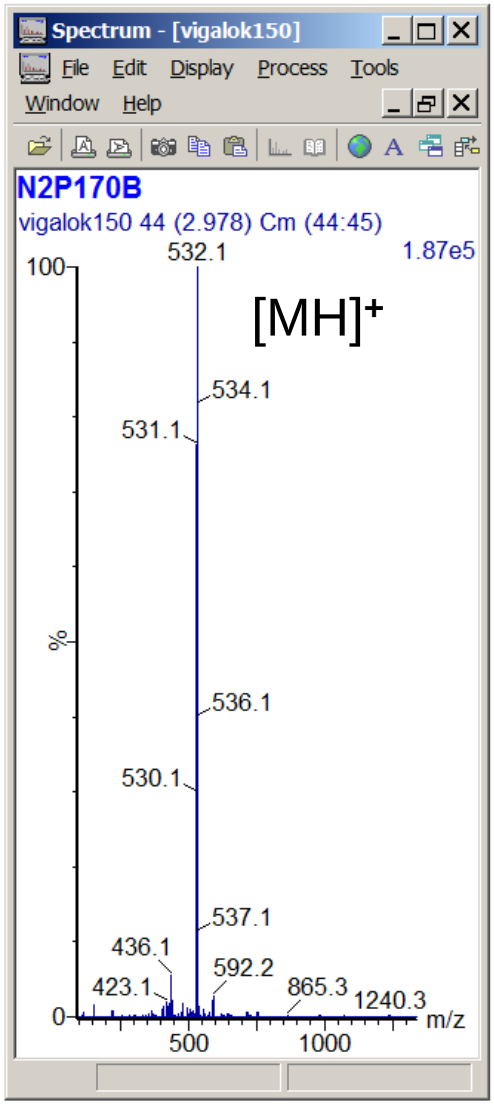
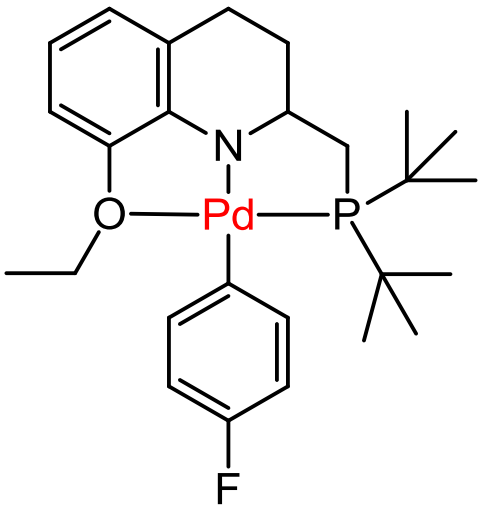


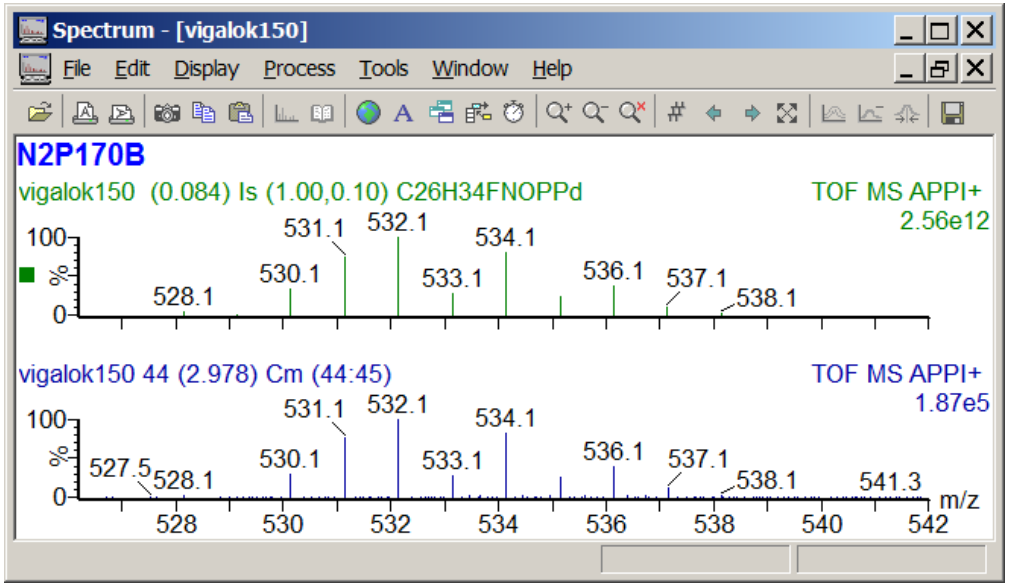




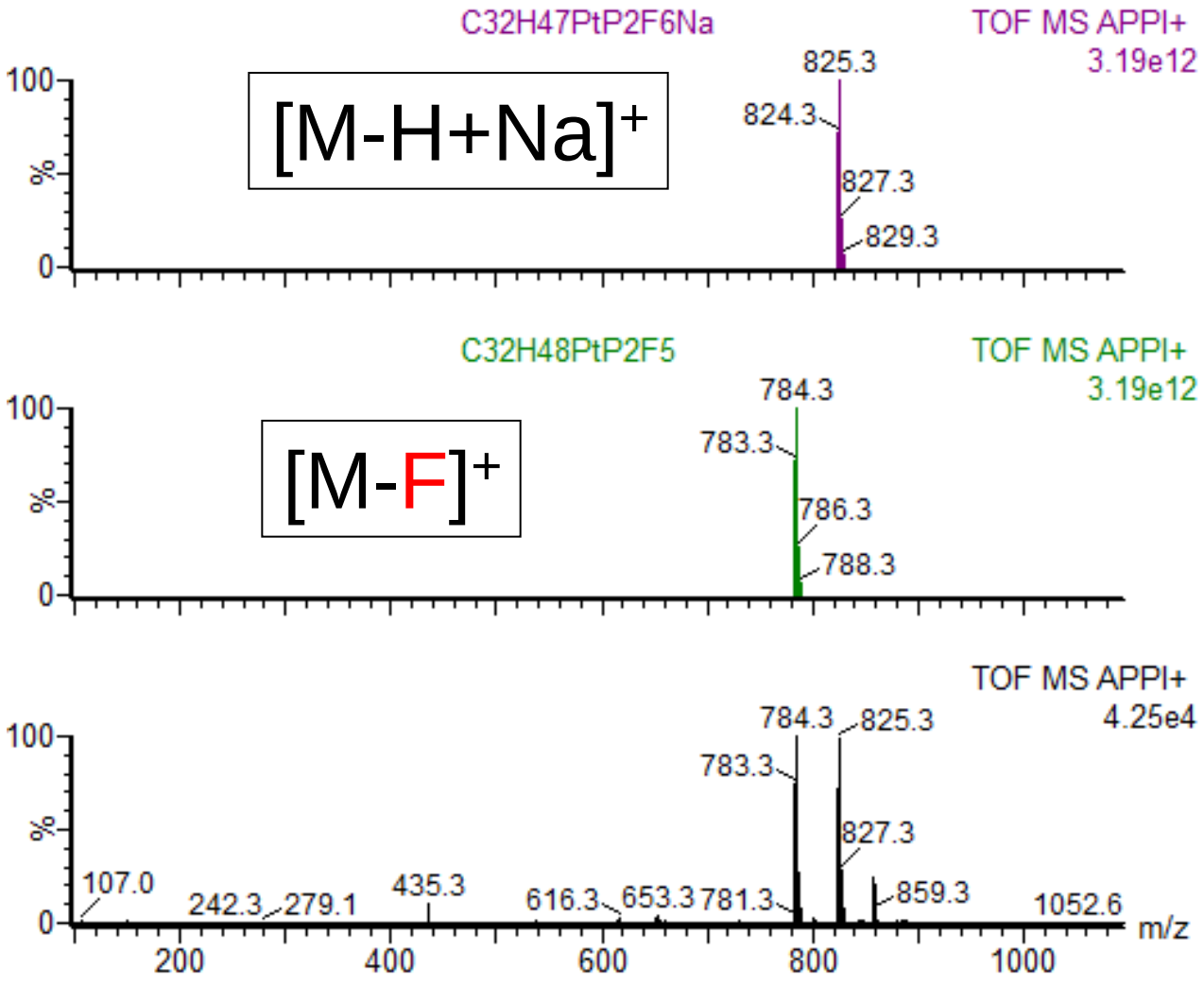
Organometallic



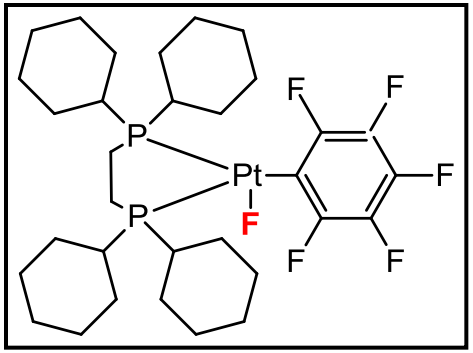




Organometallic



$C_{32}H_{48}PtP_2F_6$



Summary

1. APPI is suitable to conjugated and organometallic compounds that can't be analyzed using ESI, and decompose in EI.

2. High sensitivity both in positive and negative modes

3. Provides additional information compared to ESI.
   (labile ligands or counter ions)

4. Broaden capabilities of API source