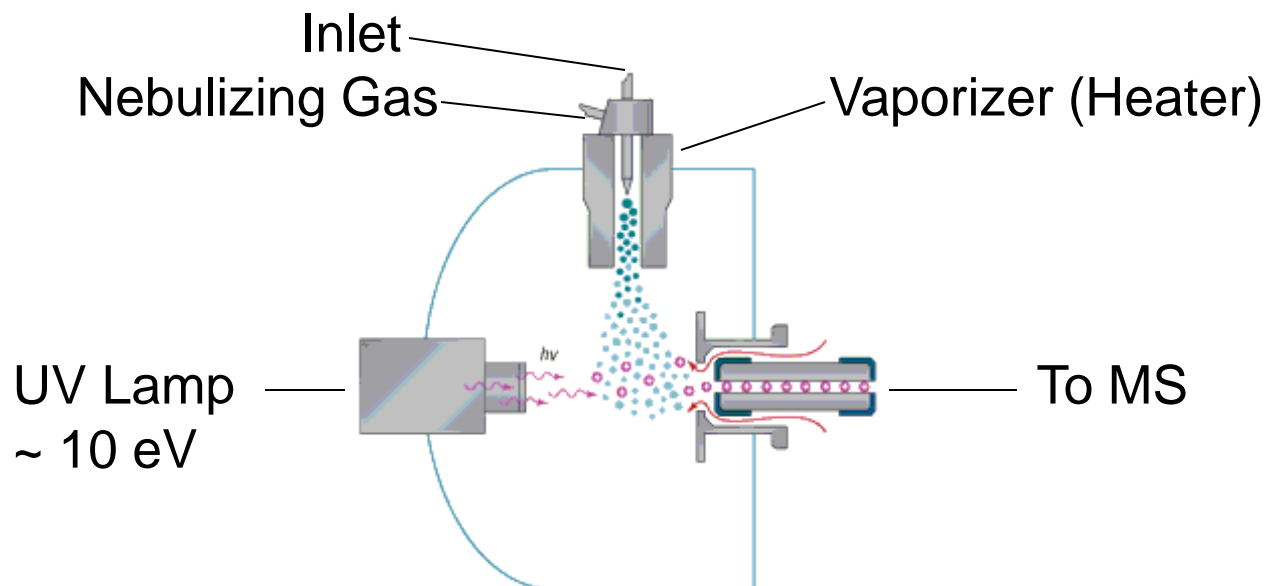


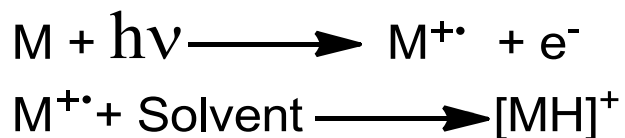
Implementation of APPI Mass Spectrometry for Organometallic compounds

Noam Tal, Tel Aviv University, Israel

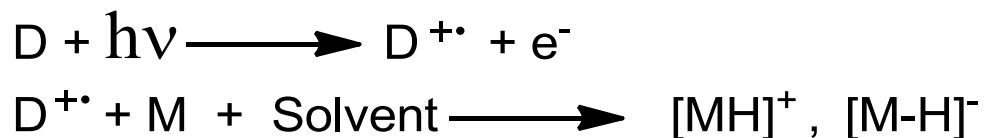
Atm. Pressure Photo Ionization (APPI)



Direct APPI



Dopant/Solvent assisted APPI



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

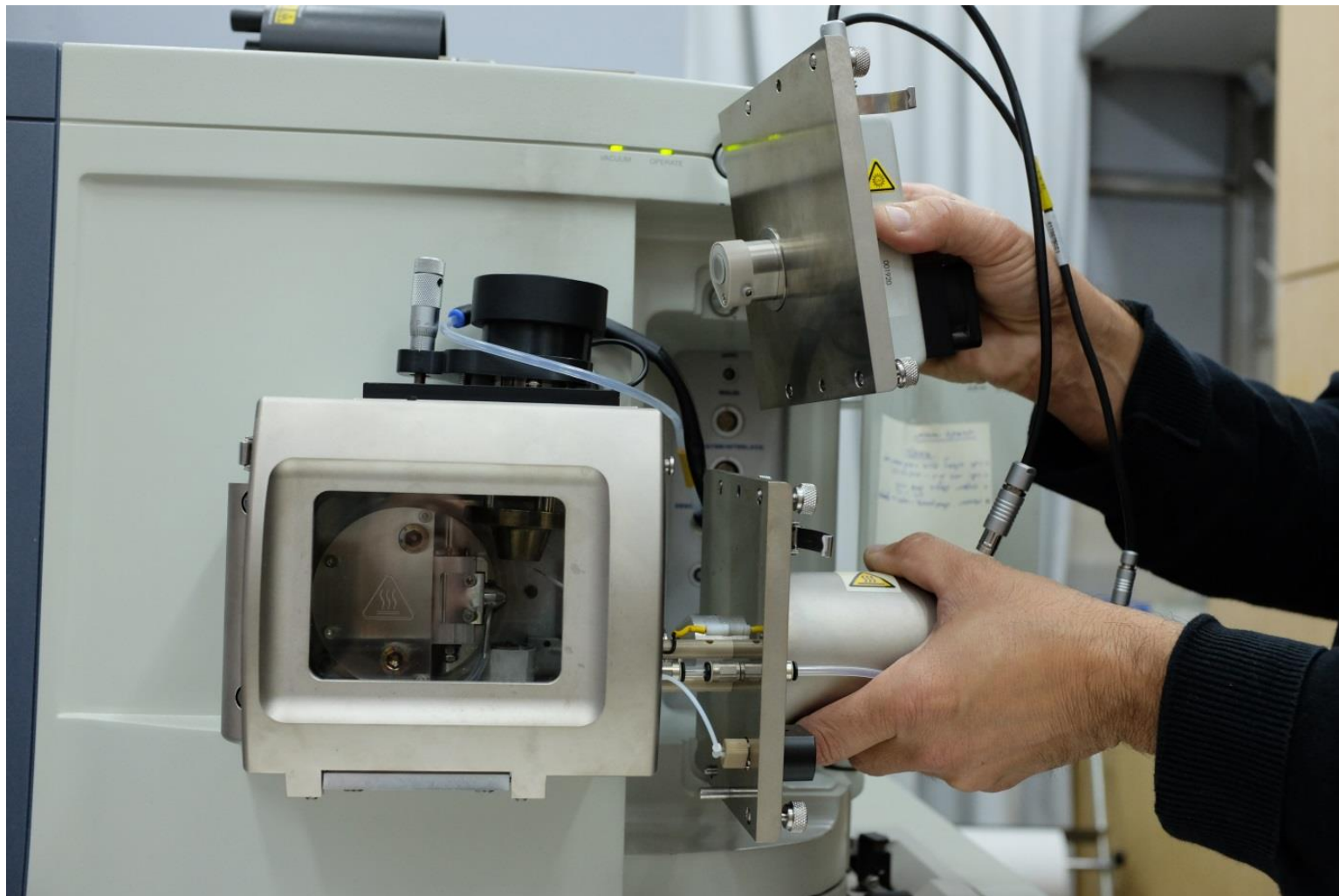
less sensitive

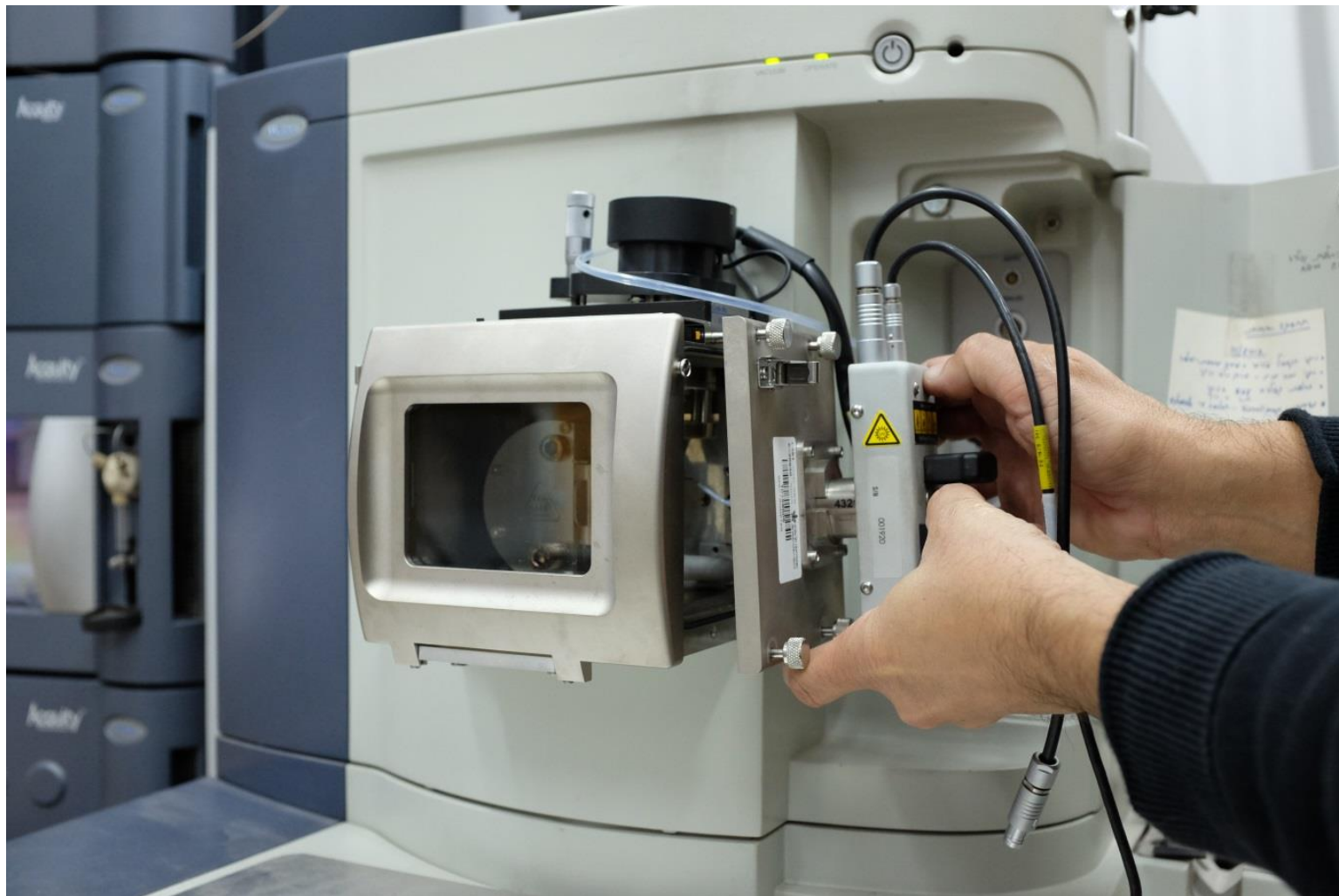
Solvent: Toluene, DCM, Hexane, MeCN, MeOH

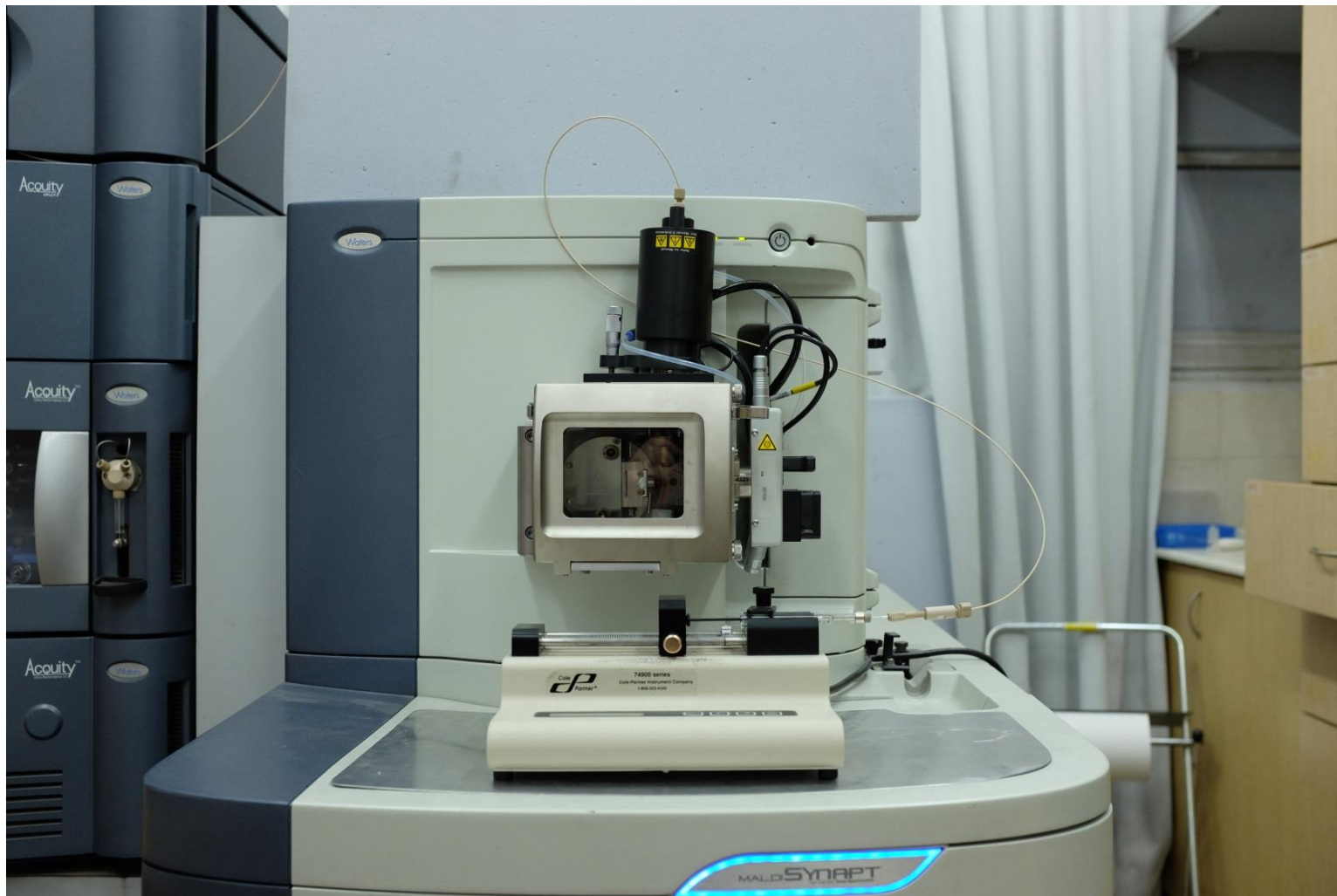
API source

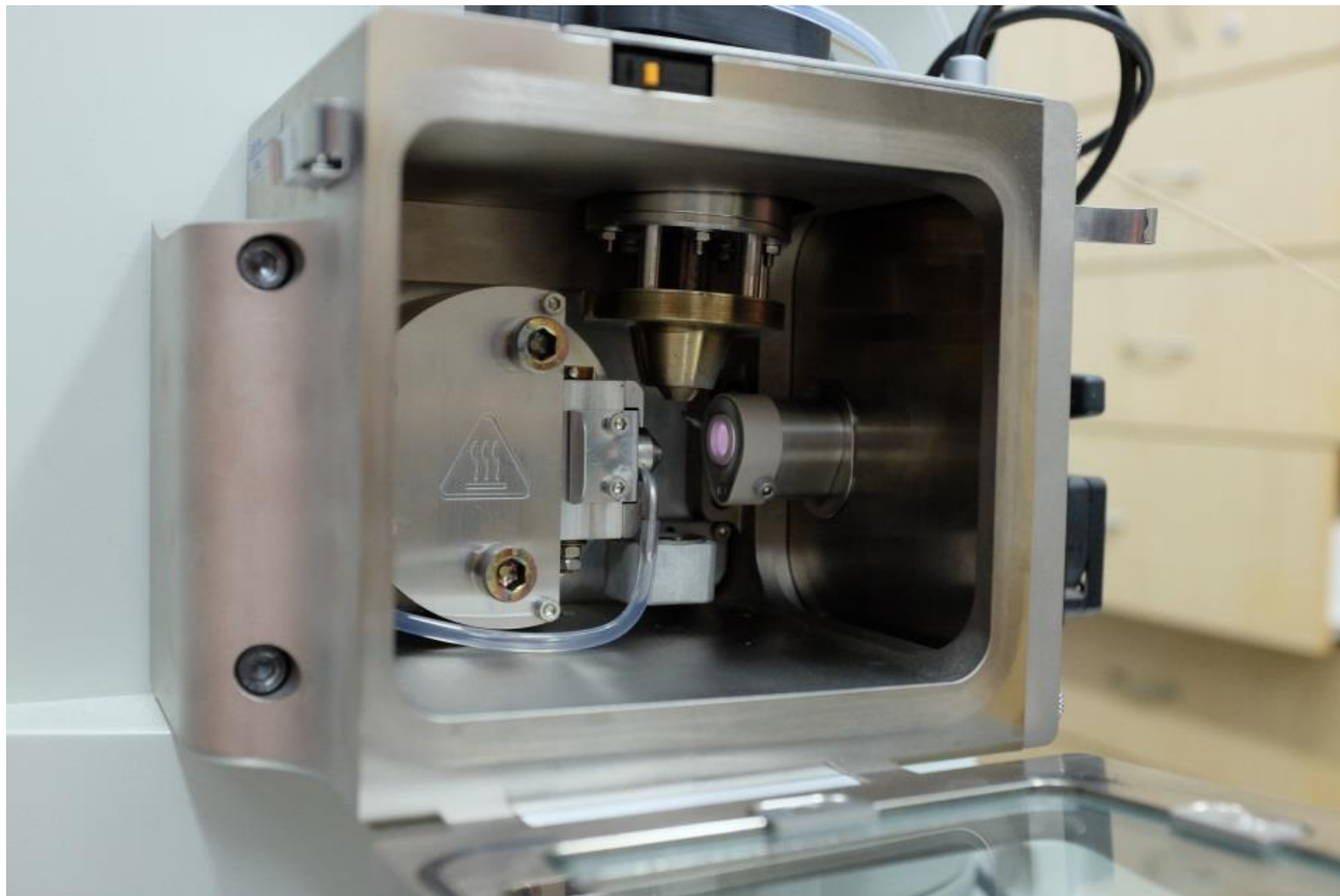








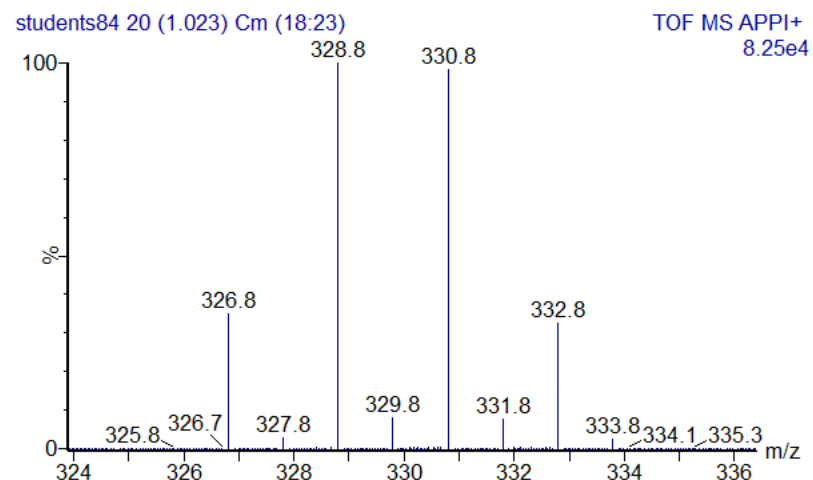
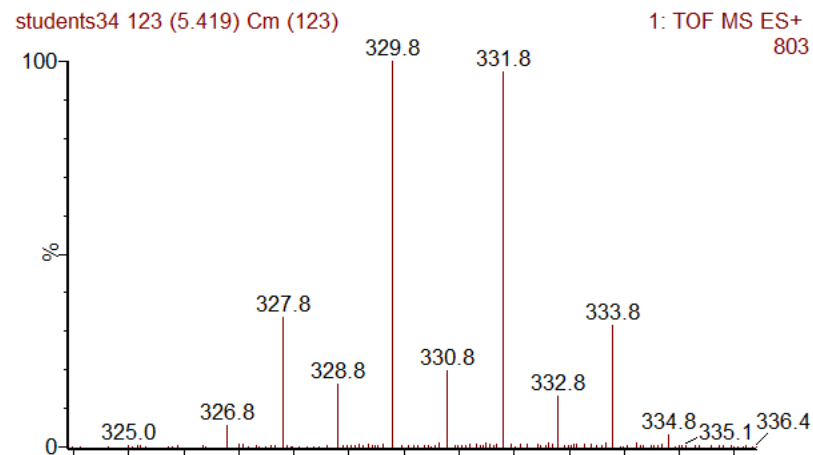
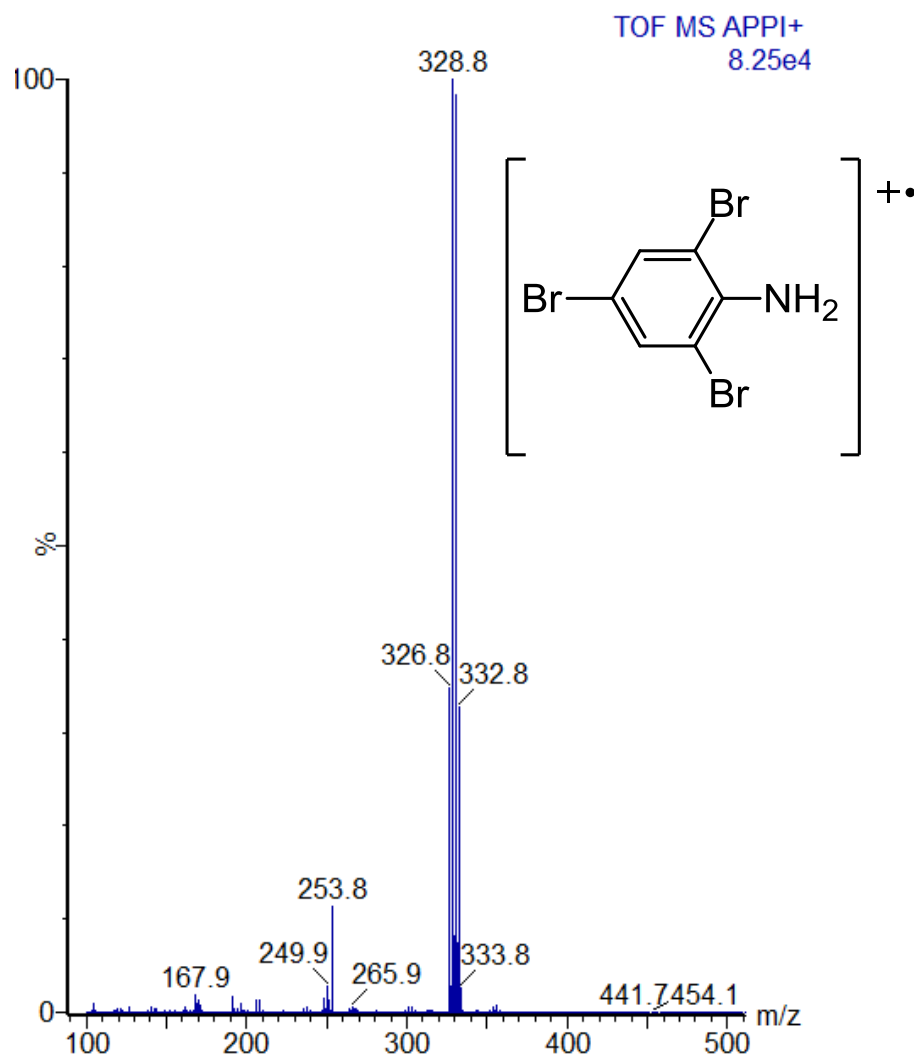




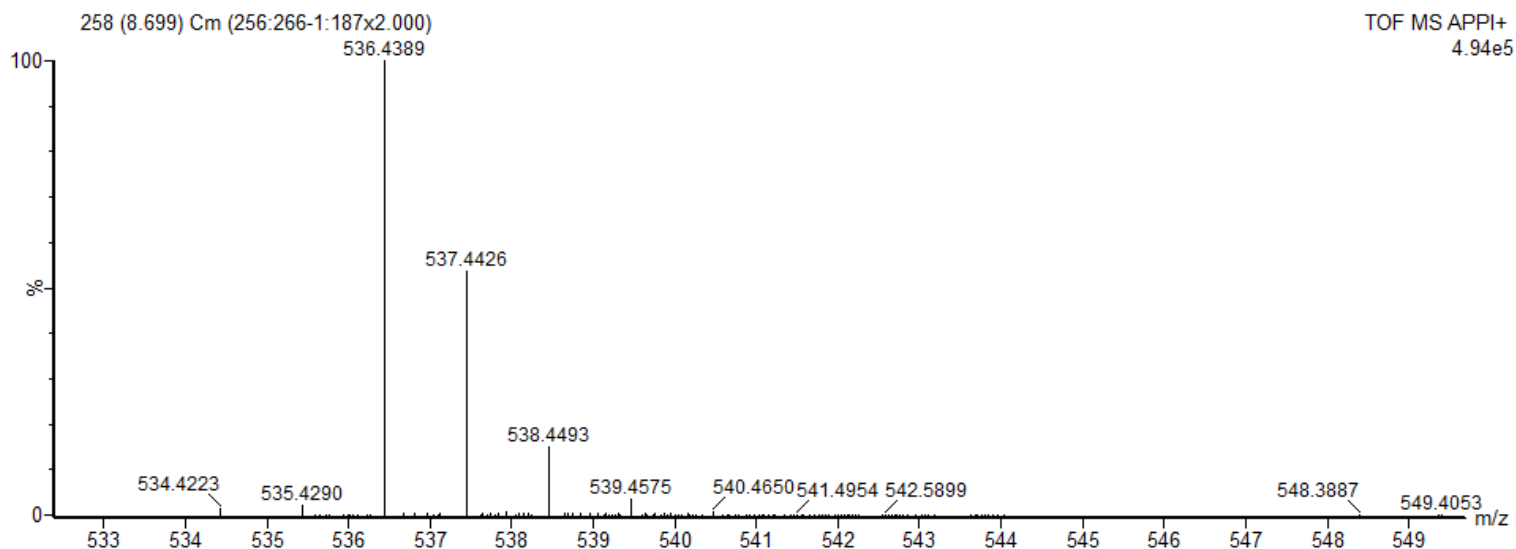
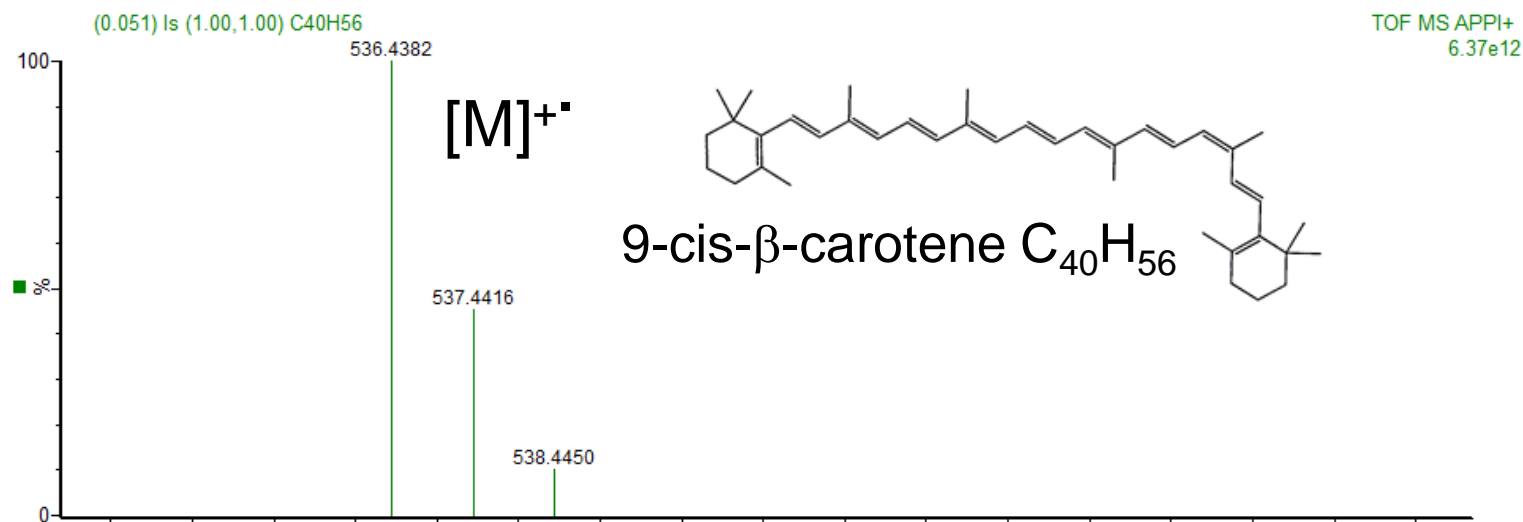
APPI conditions:

- 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 °C
500-750 L/h , 99.9% Dry Nitrogen

Conjugated compounds



Conjugated compounds

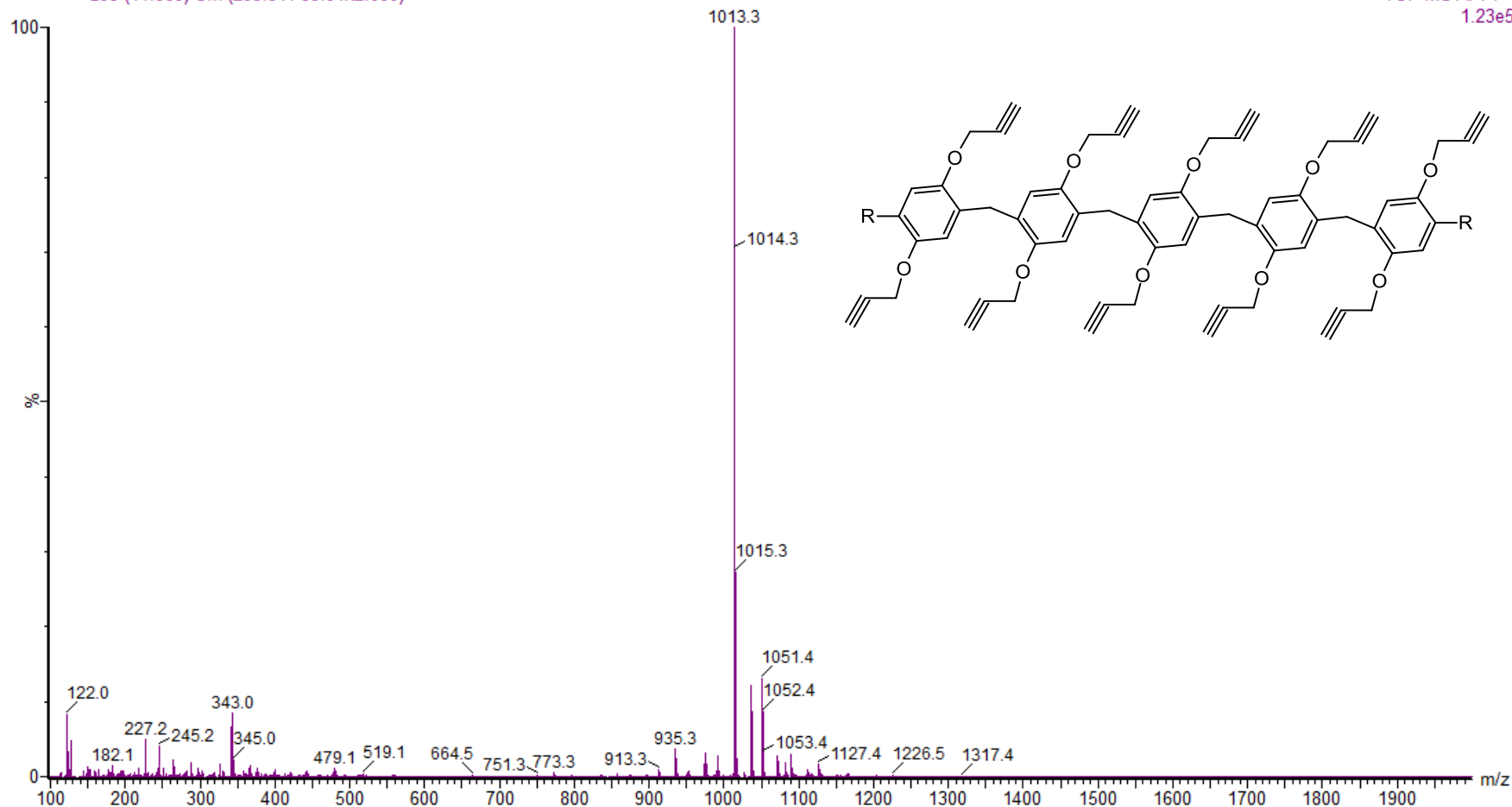


Conjugated compounds

DM1033-1

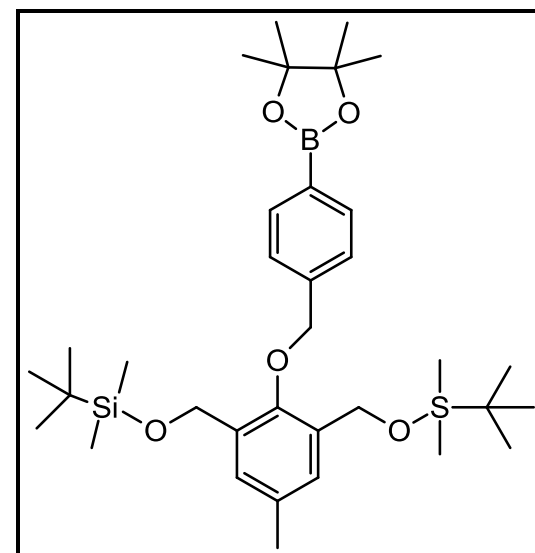
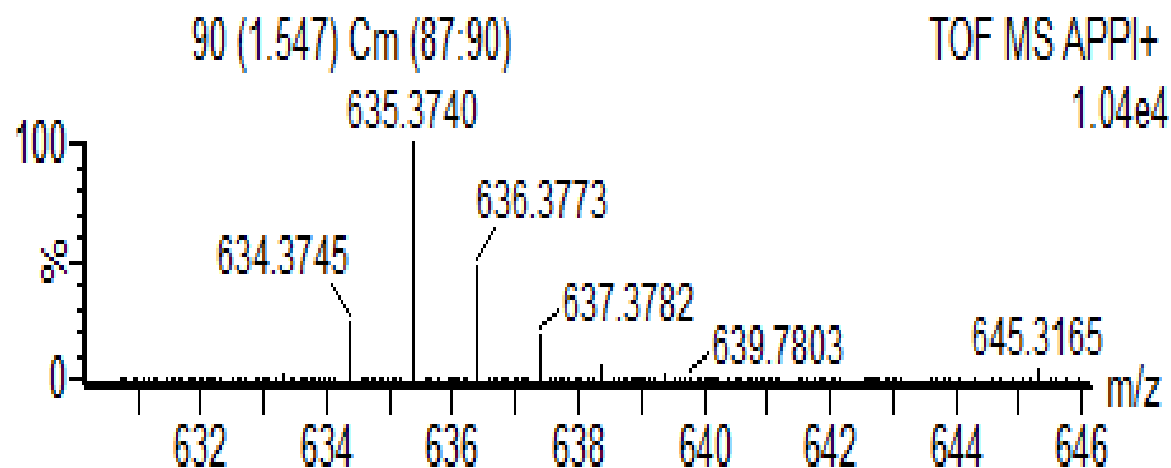
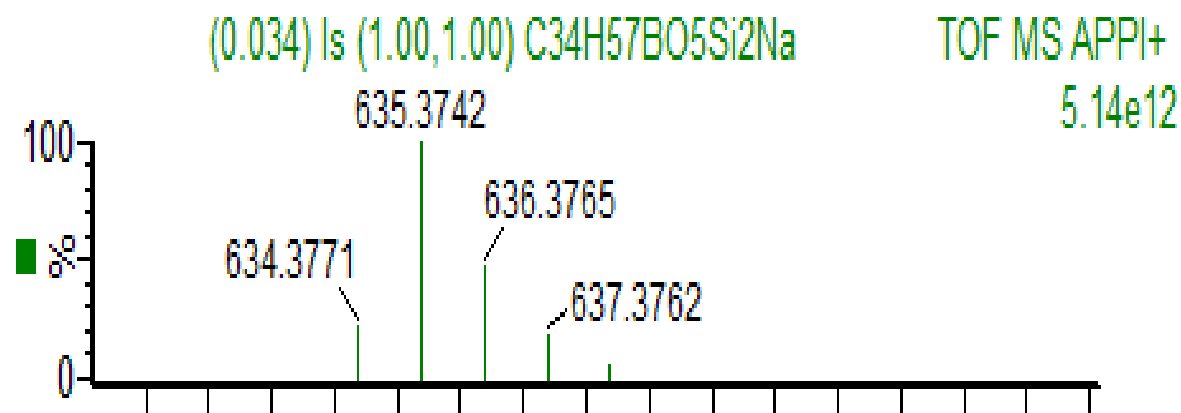
295 (14.860) Cm (295:311-55:91x2.000)

TOF MS APPI+
1.23e5

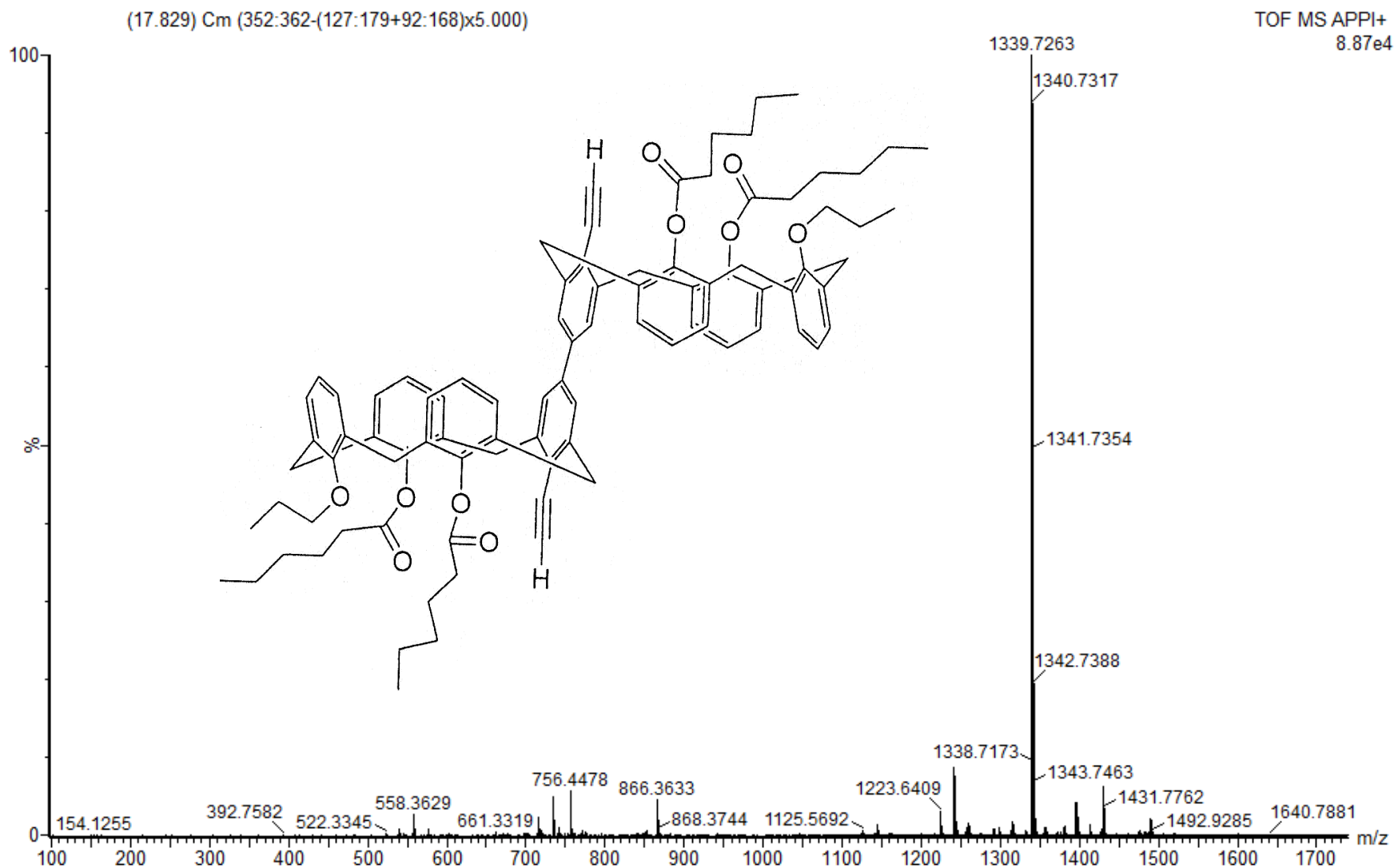


Conjugated compounds

ef 2-41

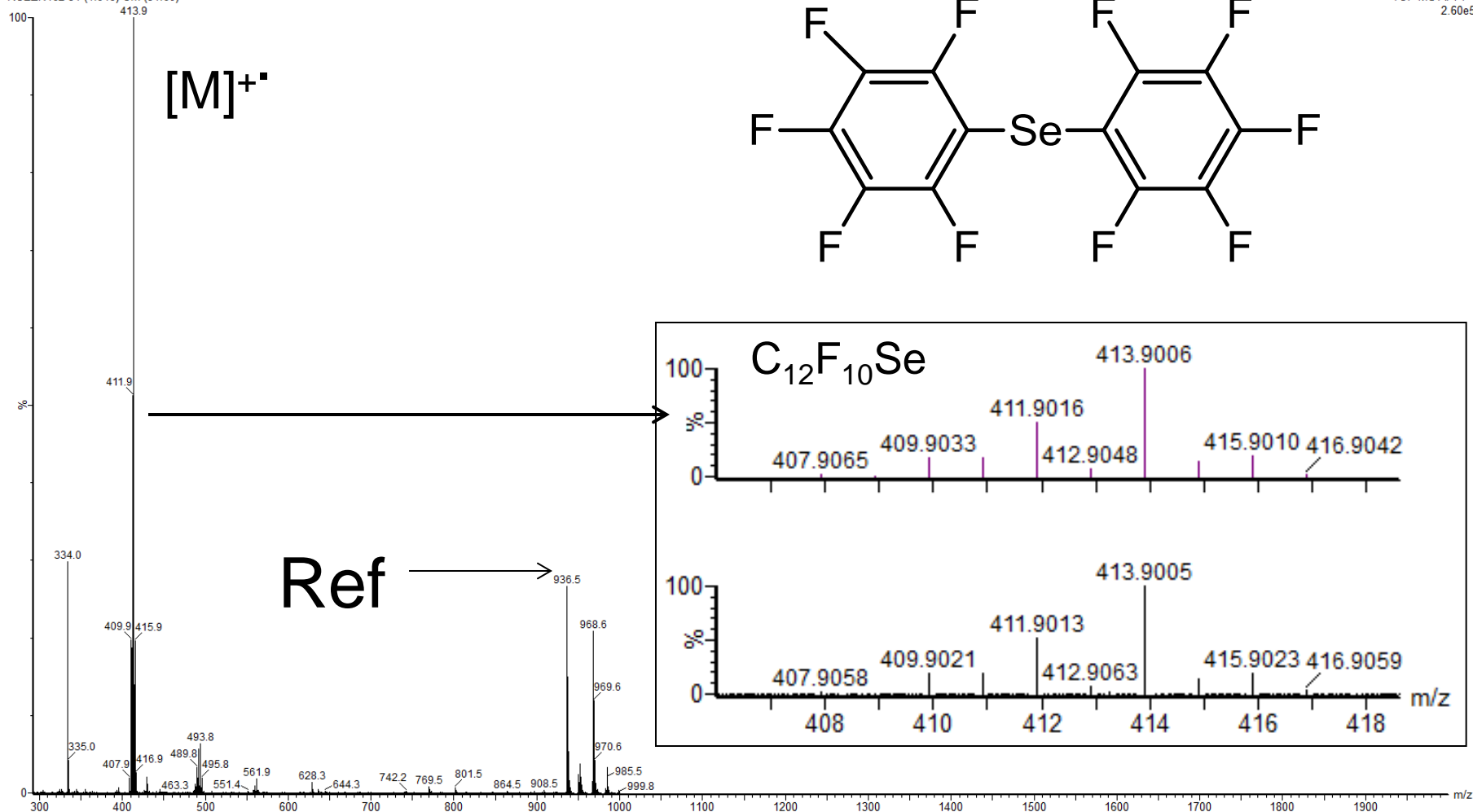


Conjugated compounds

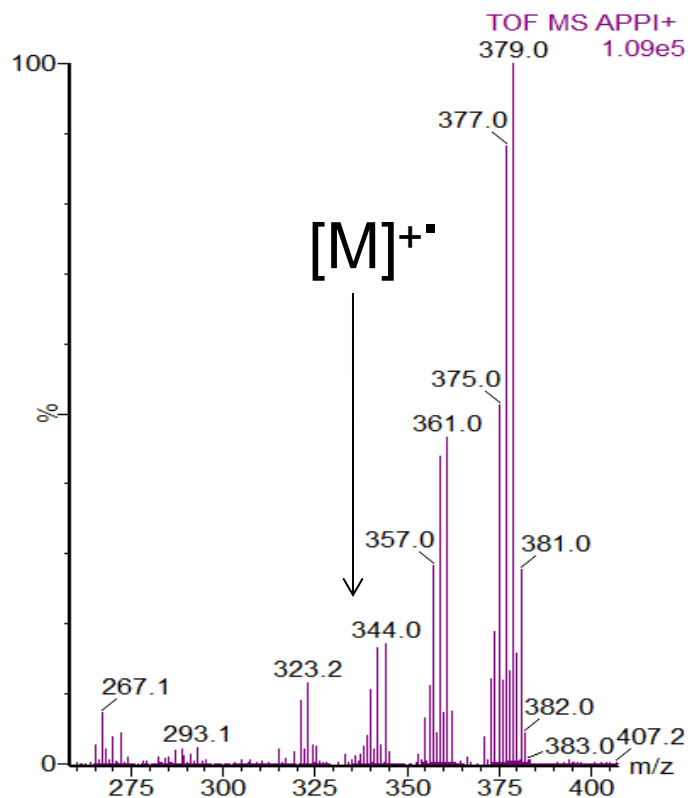
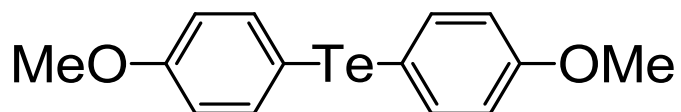


Conjugated compounds

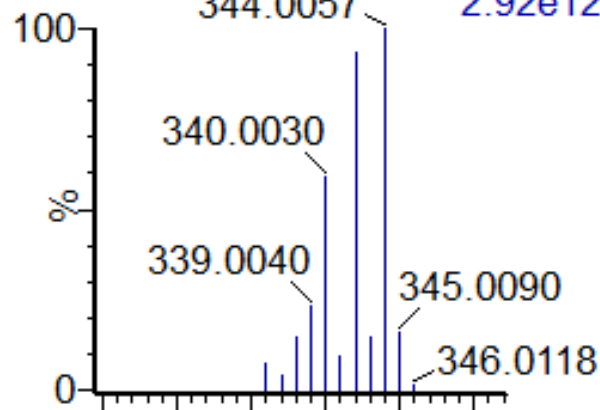
Shay411 Shay Potash
ROZEN162 54 (4.948) Cm (54:60)



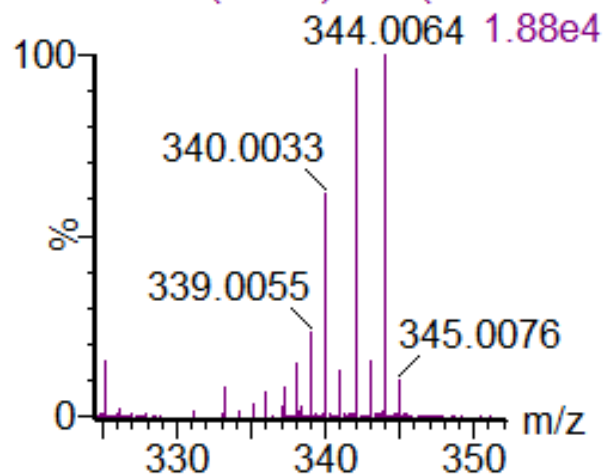
Conjugated compounds



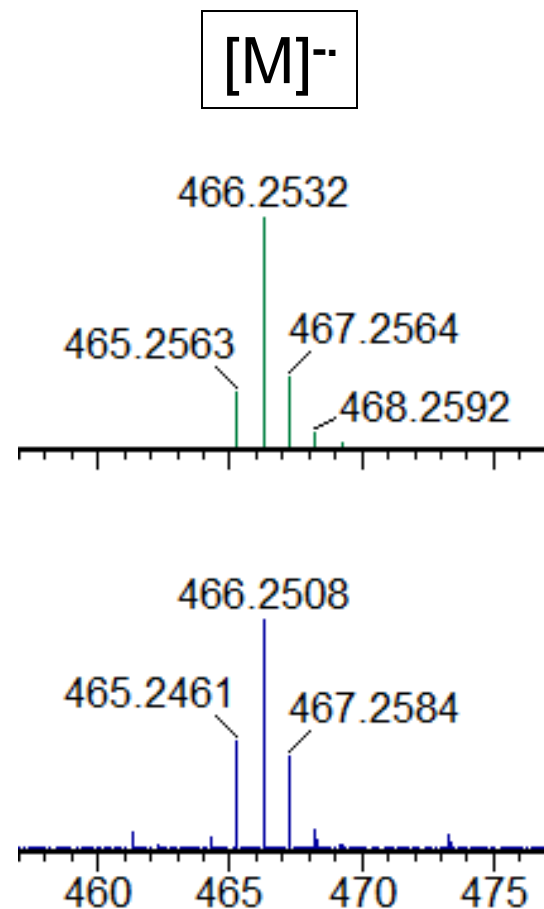
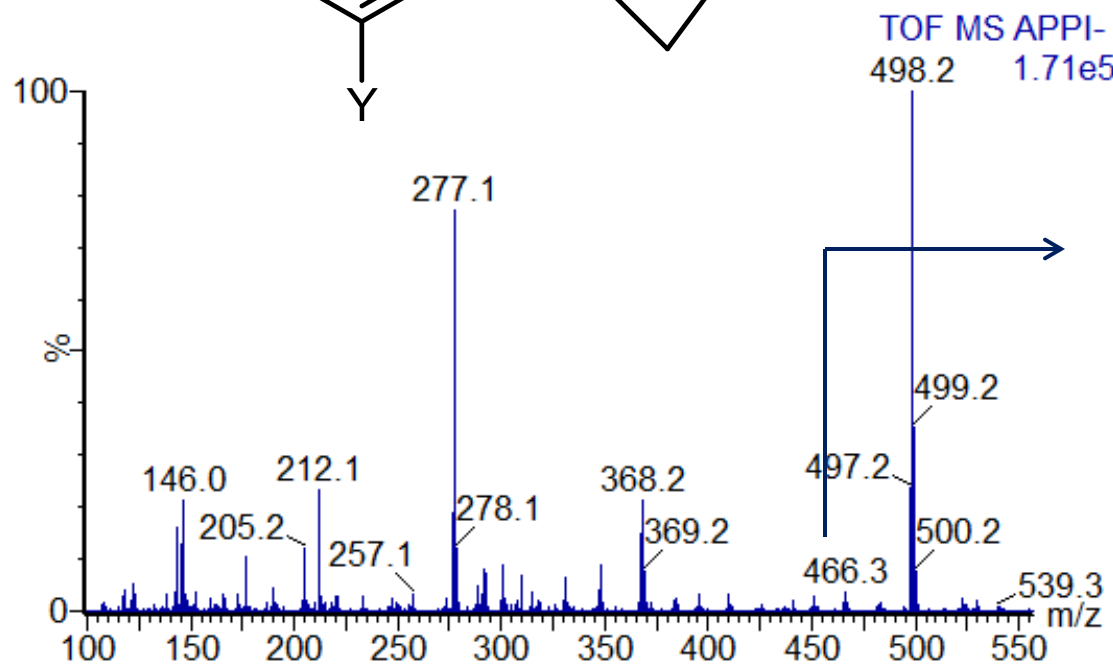
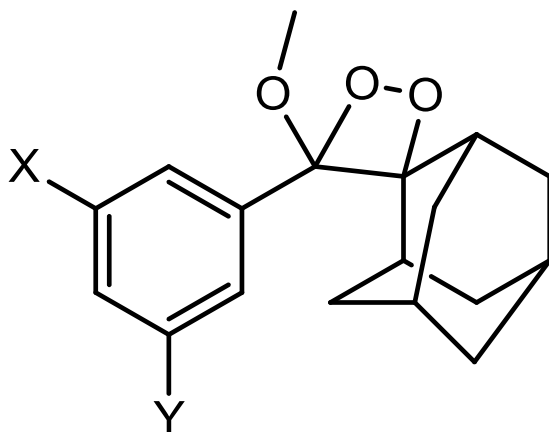
biu142c (0.067) Is (1.00,0.10) C1
344.0057 2.92e12



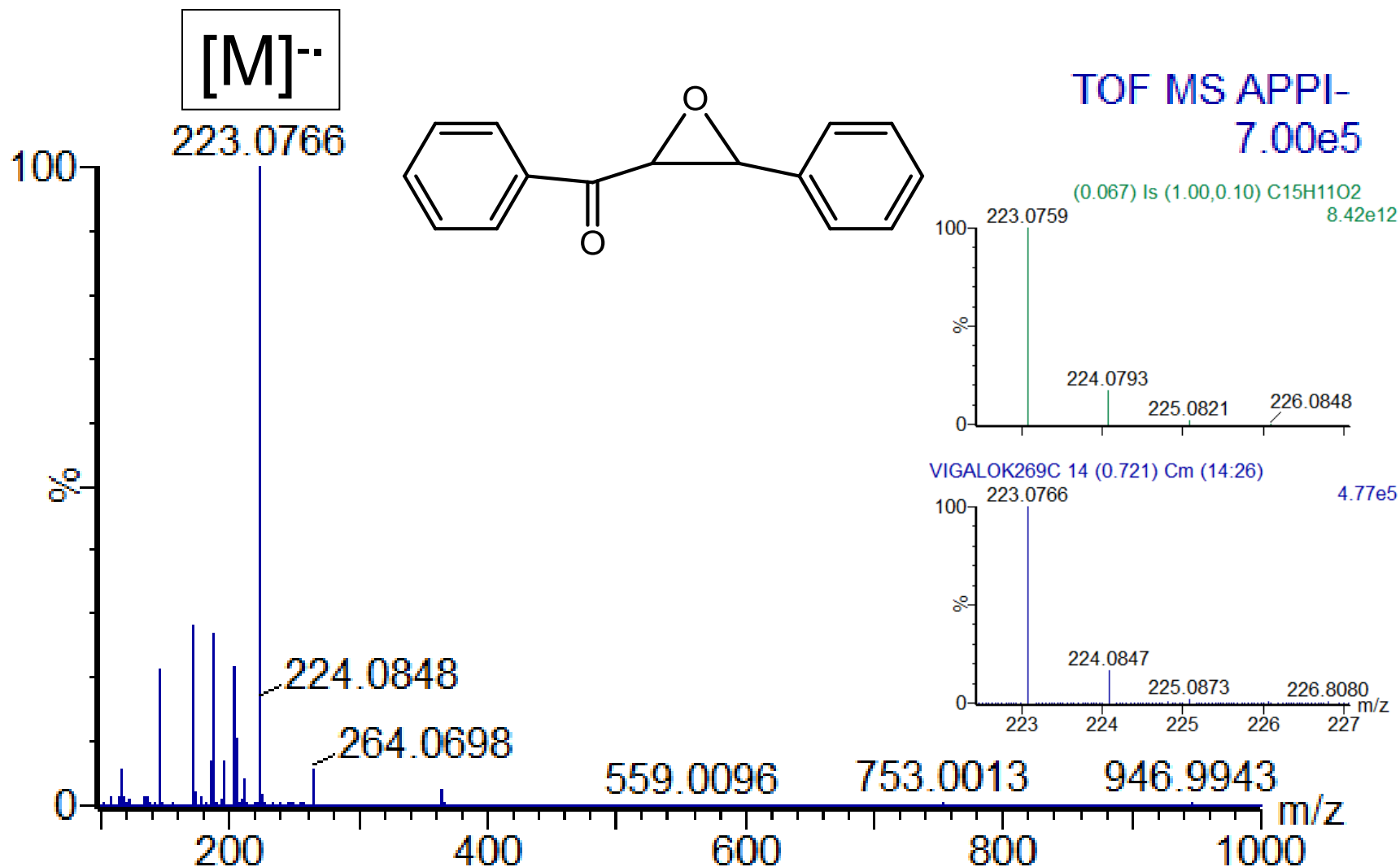
biu142c 93 (4.696) Cm (92:95-22:1)



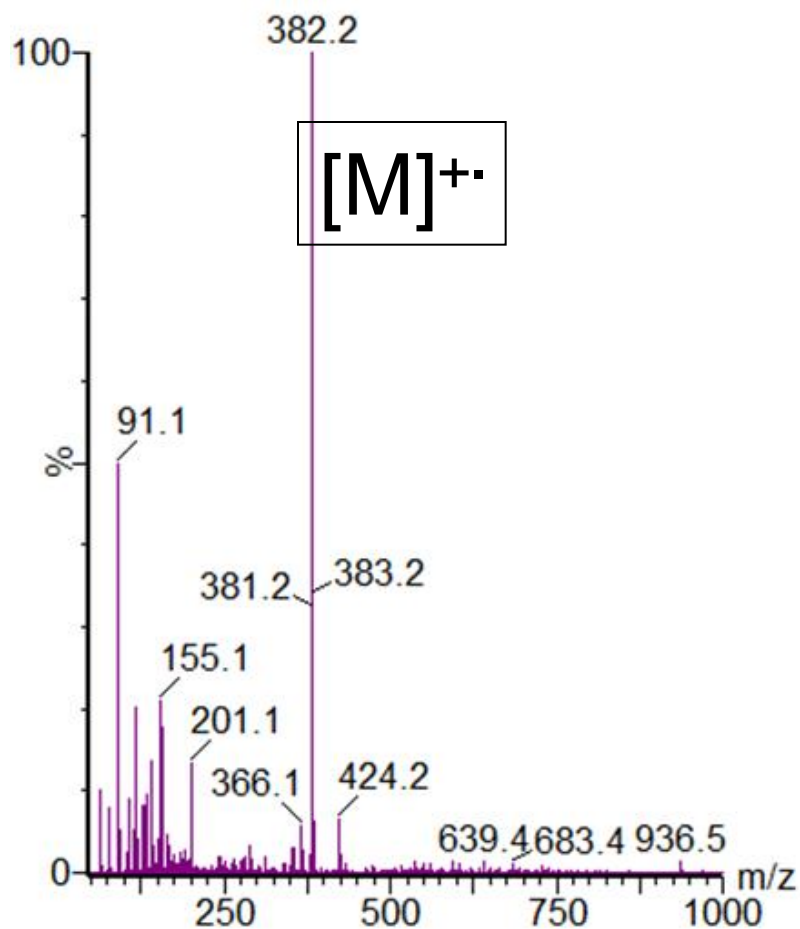
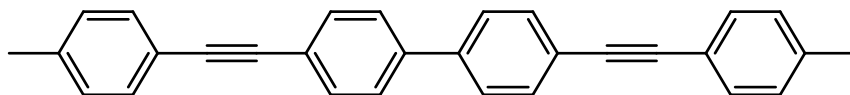
Conjugated compounds



Conjugated compounds



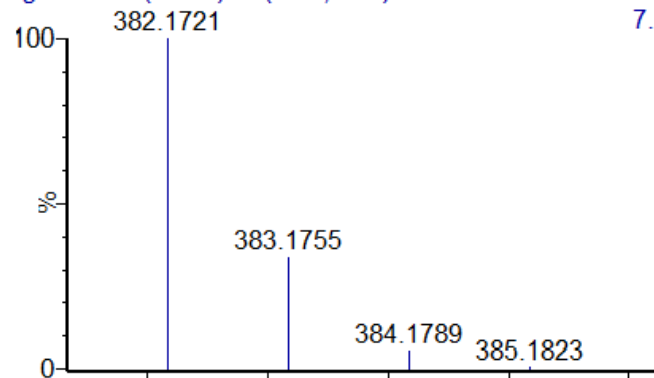
Conjugated compounds



Linear Toly Anat Molad

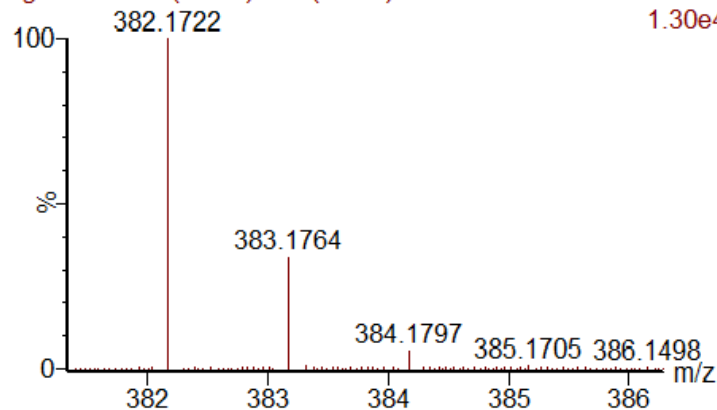
vigaluk95b (0.051) Is (1.00,0.10) C₃₀H₂₂

TOF MS APPI+
7.15e12

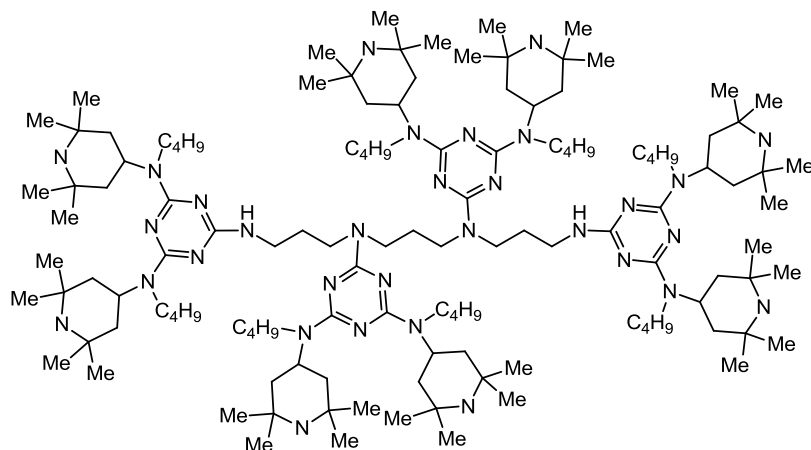


vigaluk95b 84 (2.873) Cm (78:90)

TOF MS APPI+
1.30e4

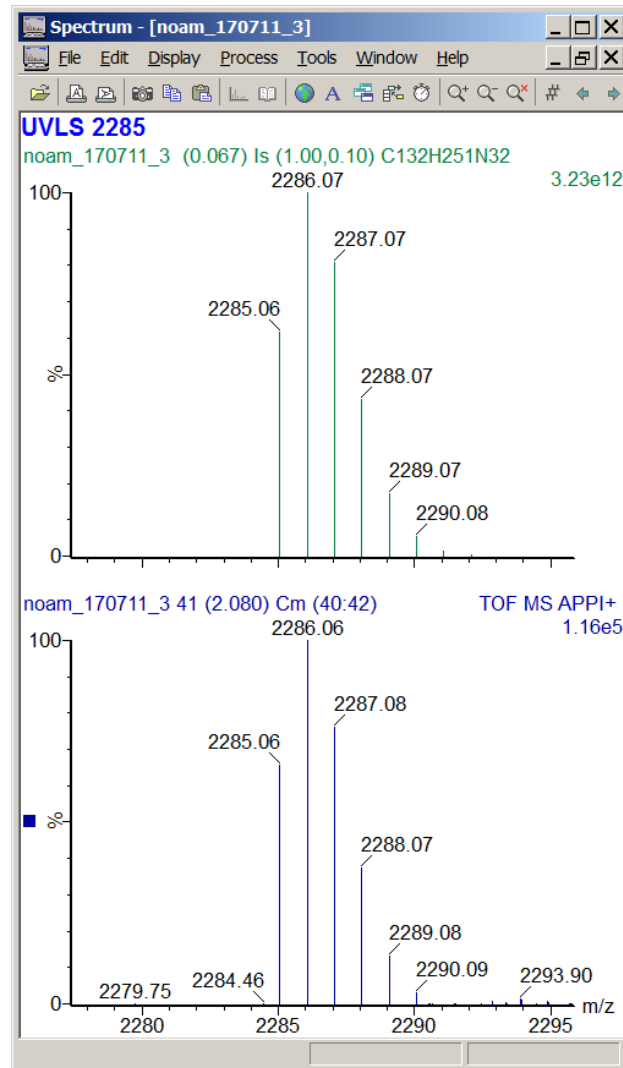
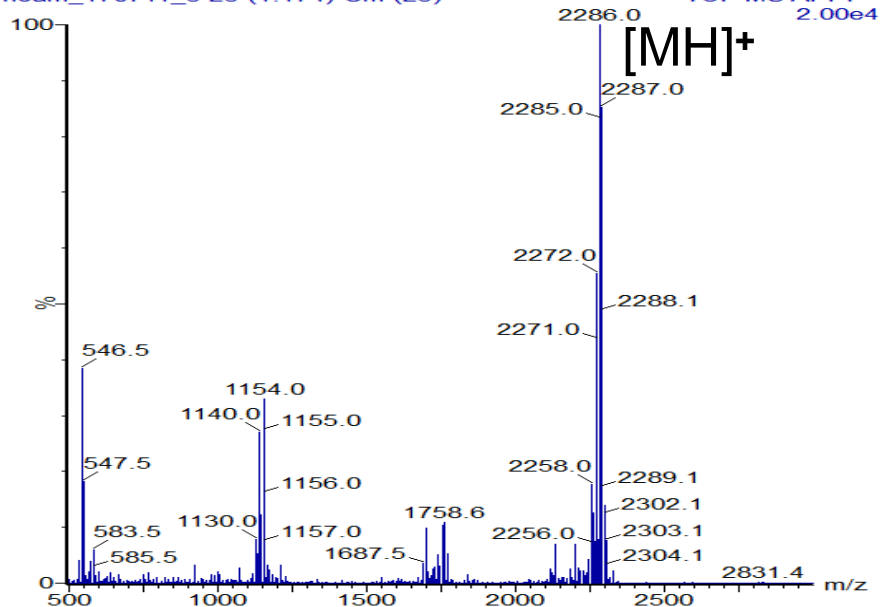


Conjugated compounds



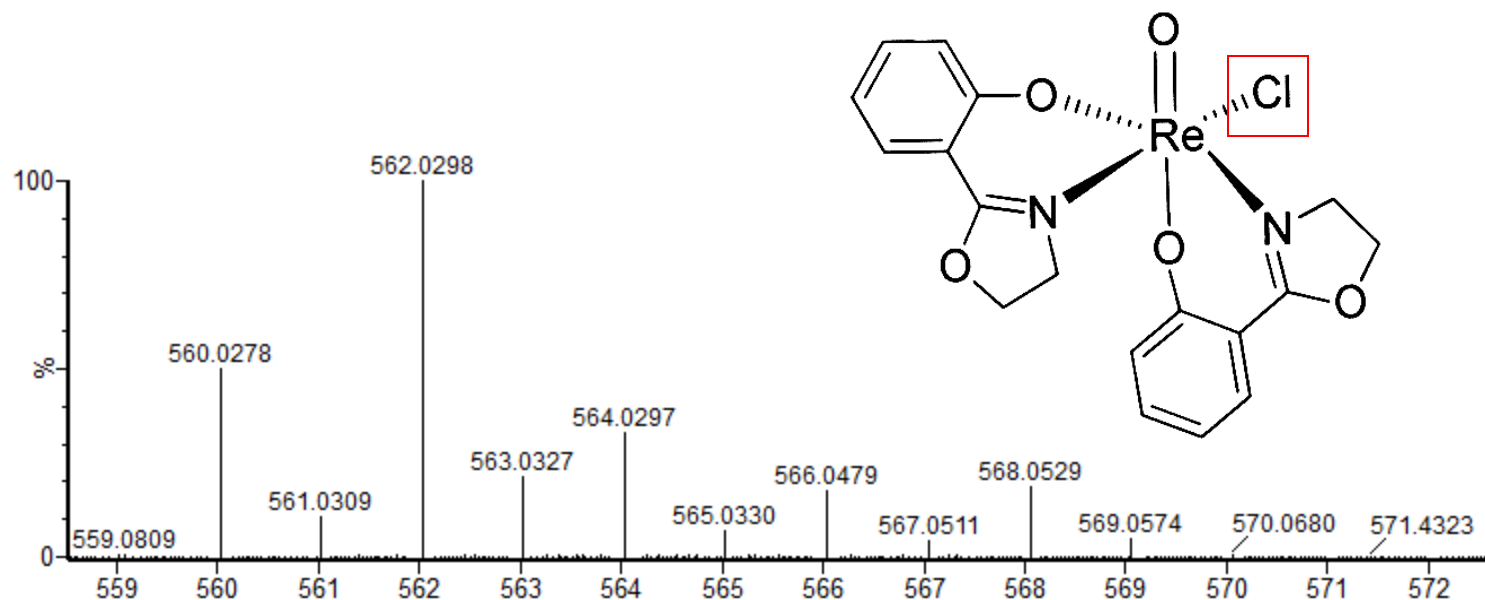
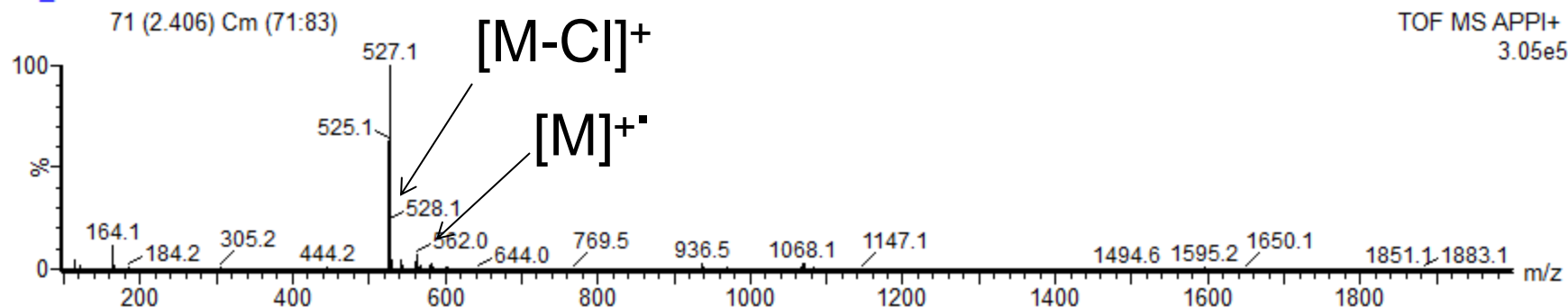
UVLS 2285

noam_170711_3 23 (1.174) Cm (23)

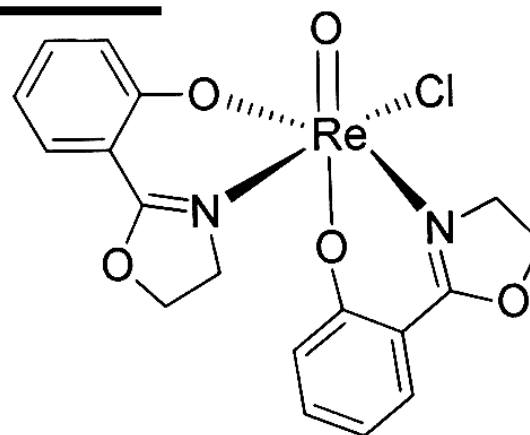
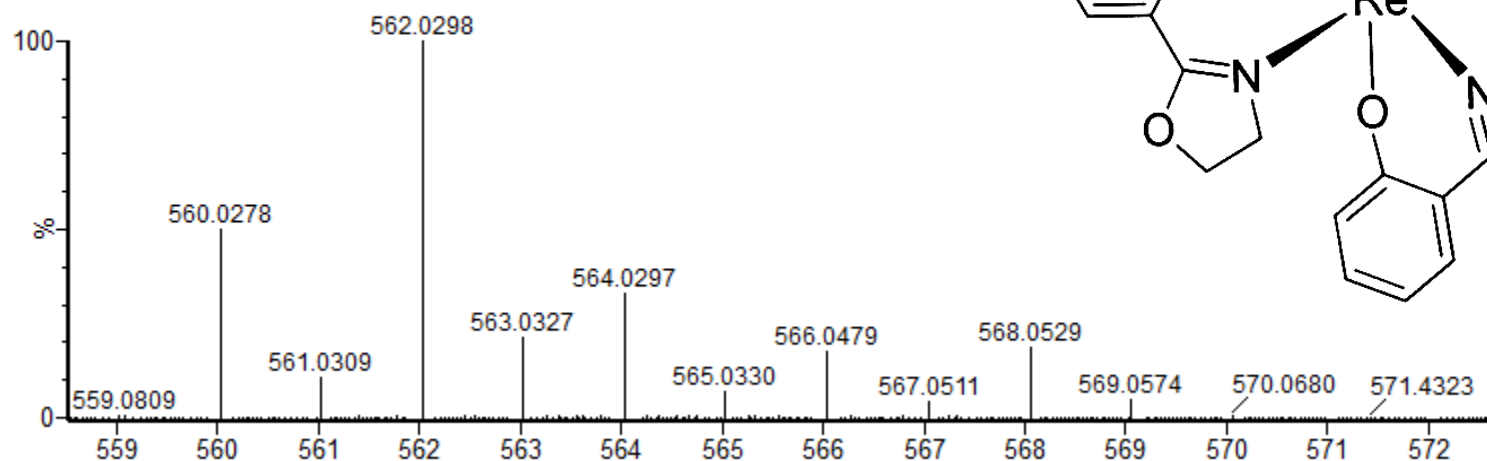


Organometallic

BB_ReS05

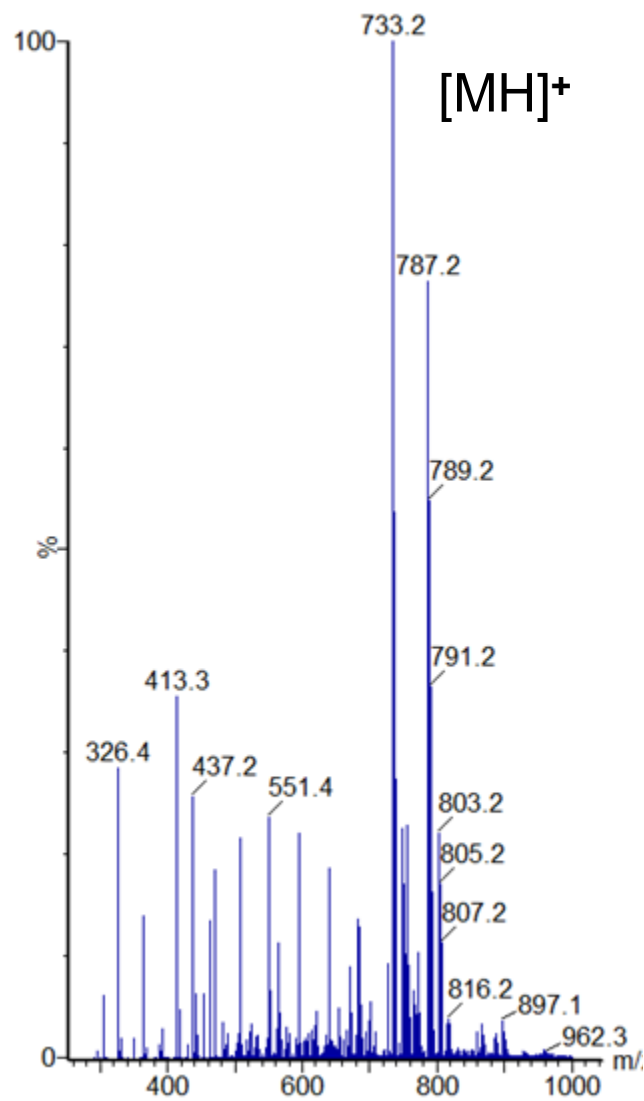


Organometallic



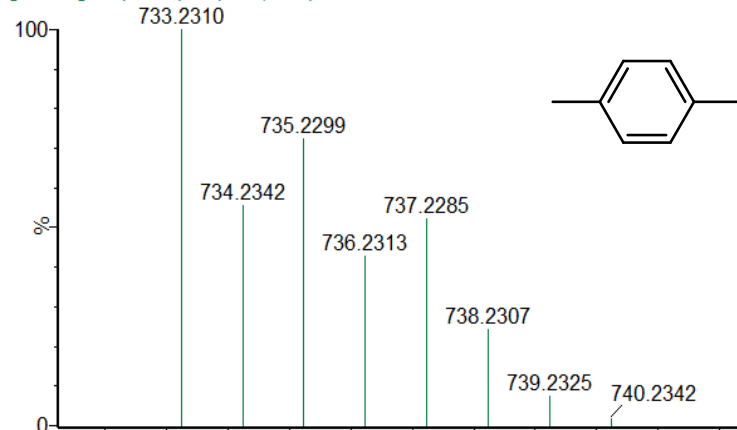
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	Na	Cl	185Re	187Re
562.0298	562.0305	-0.7	-1.2	11.5	C18 H16 N2 O5 Cl 187Re	312.0	0.3	18	16	2	5		1		1
	562.0292	0.6	1.1	12.0	C16 H14 N5 O4 Cl 187Re	313.6	2.0	16	14	5	4		1		1
	562.0294	0.4	0.7	17.0	C23 H16 N4 O9 Cl2	323.2	11.6	23	16	4	9		2		
	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

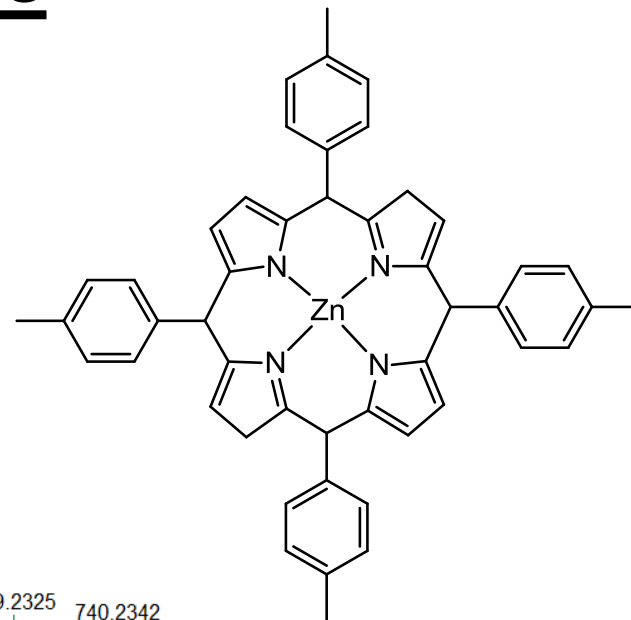
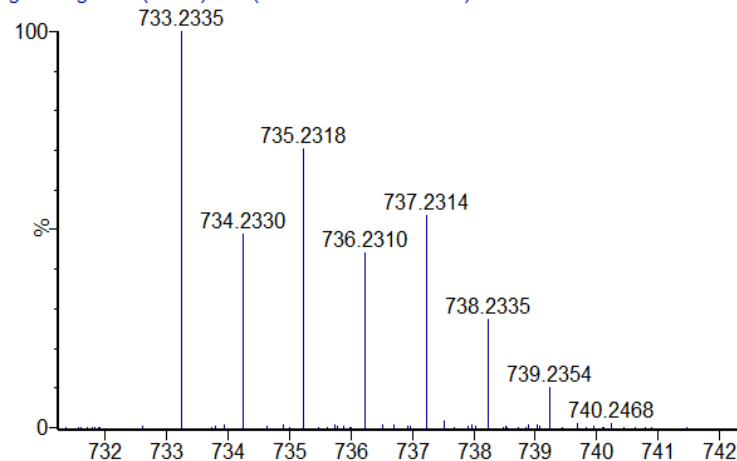


Zn(TTP)

goldberg 5 (0.067) Is (1.00,0.10) C₄₈H₃₆N₄ZnH



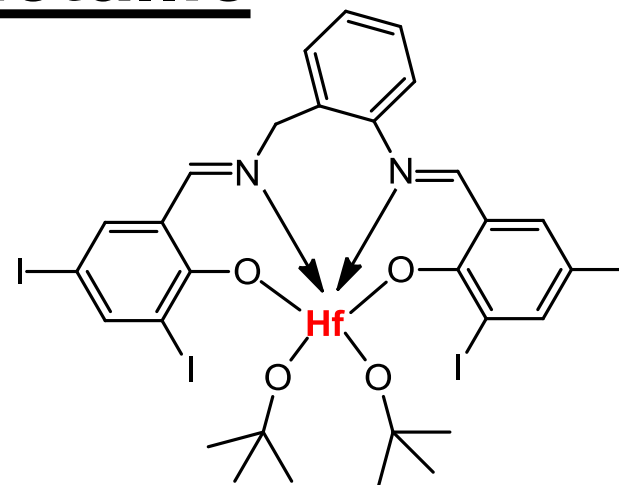
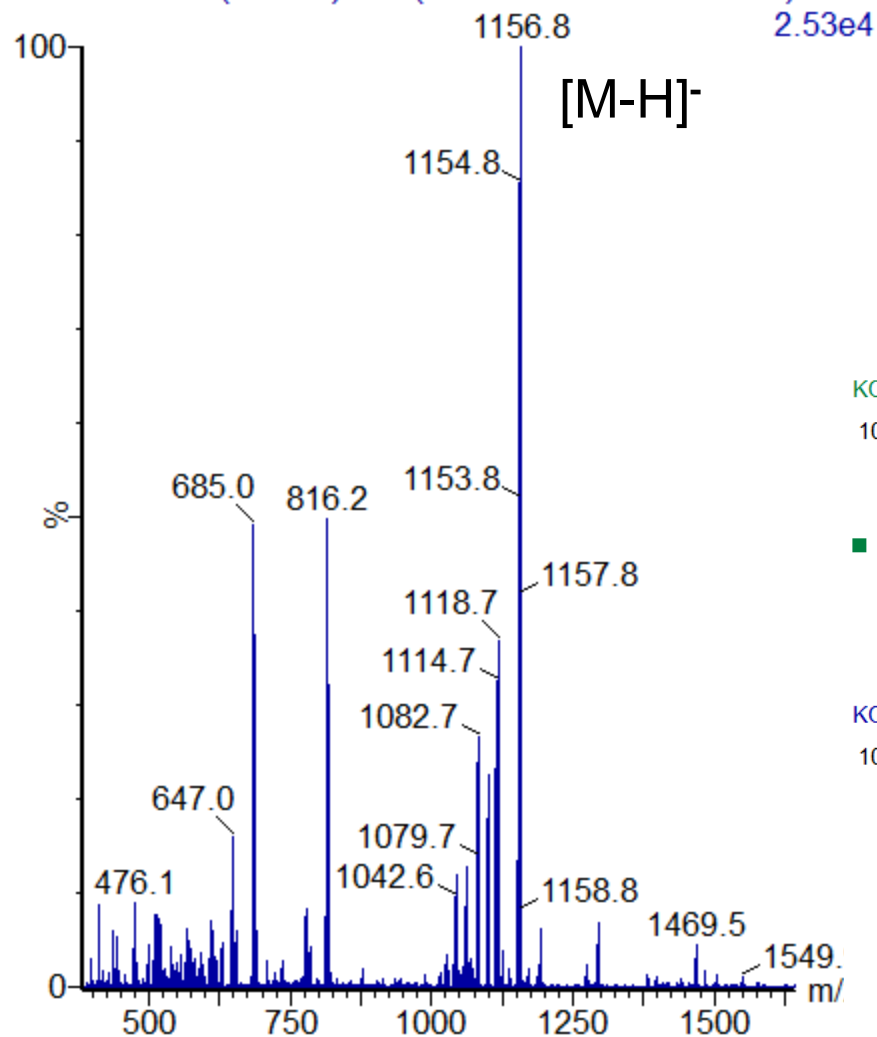
goldberg 5 88 (4.445) Cm (83:88-150:200x10.000)



Organometallic

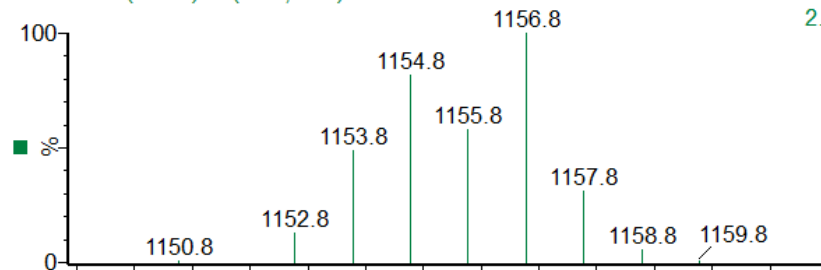
KP-616Hf

KOL112C 389 (19.590) Cm (384:413-119:137x10.000)



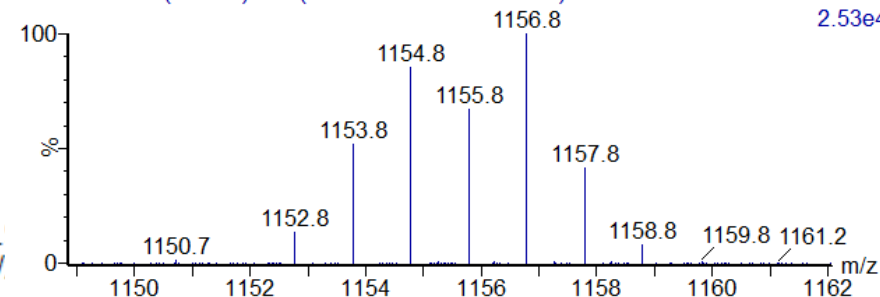
KOL112C (0.067) Is (1.00,0.10) C₂₉H₂₉HfI₄N₂O₄

TOF MS APPI-
2.95e12



KOL112C 389 (19.590) Cm (384:413-119:137x10.000)

TOF MS APPI-
2.53e4

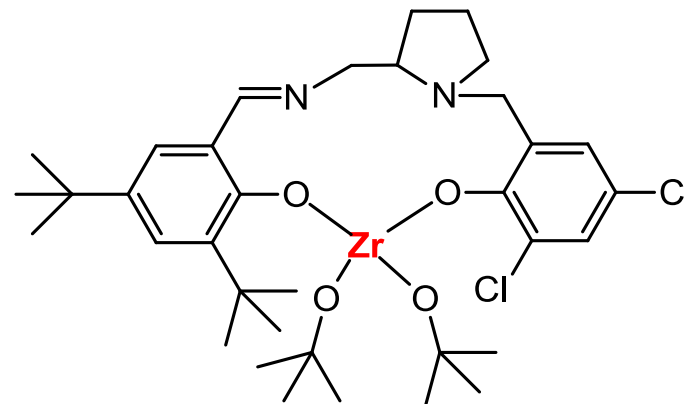
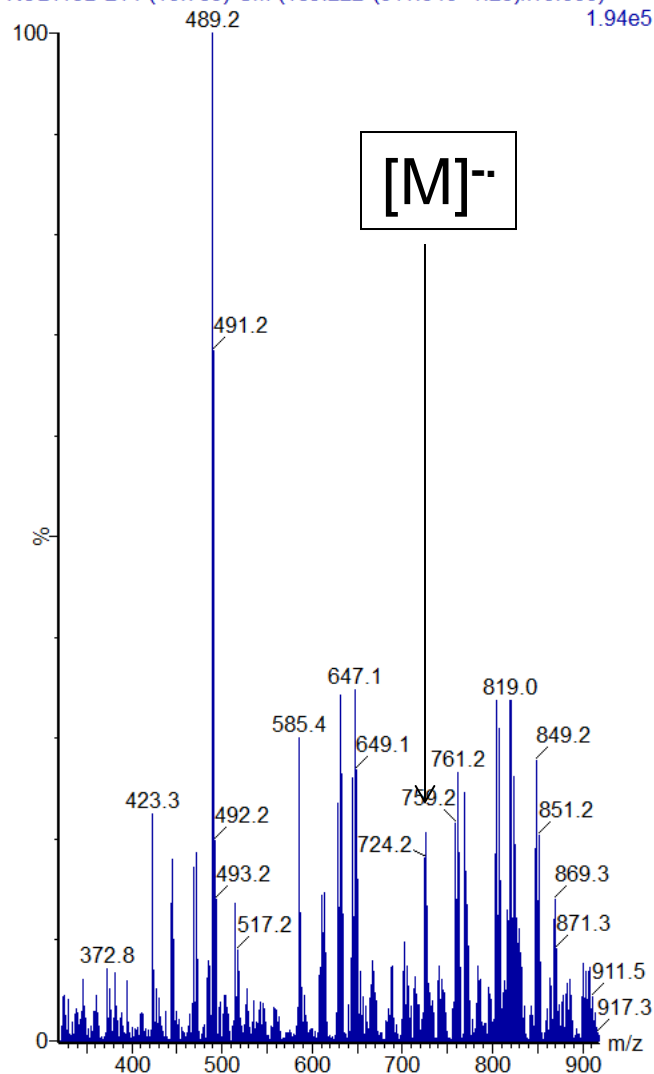


Organometallic

KP-1123Zr

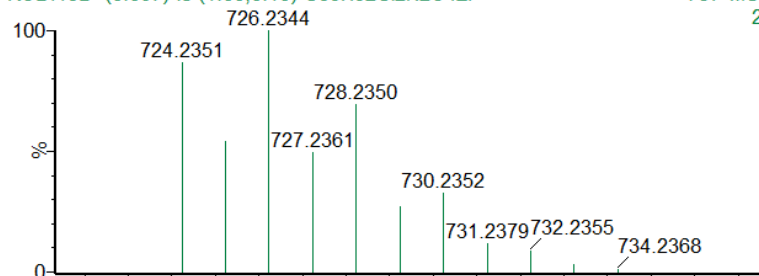
KOL113B 214 (10.785) Cm (189:222-(511:540+1:23)x10.000)

1.94e5



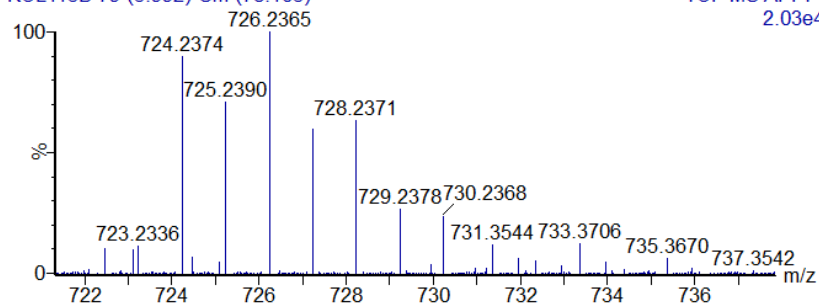
KOL113B (0.067) Is (1.00,0.10) C₃₅H₅₂Cl₂N₂O₄Zr

TOF MS APPI-
2.25e12

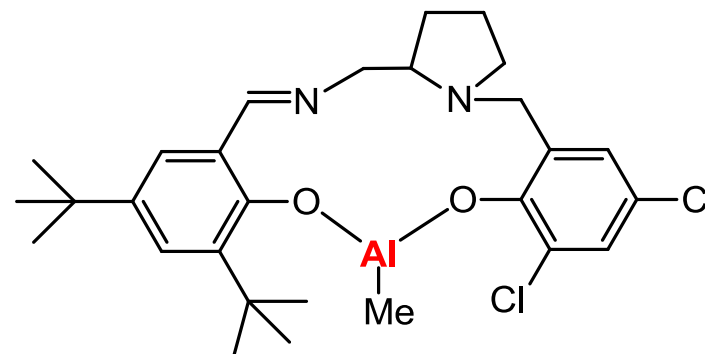
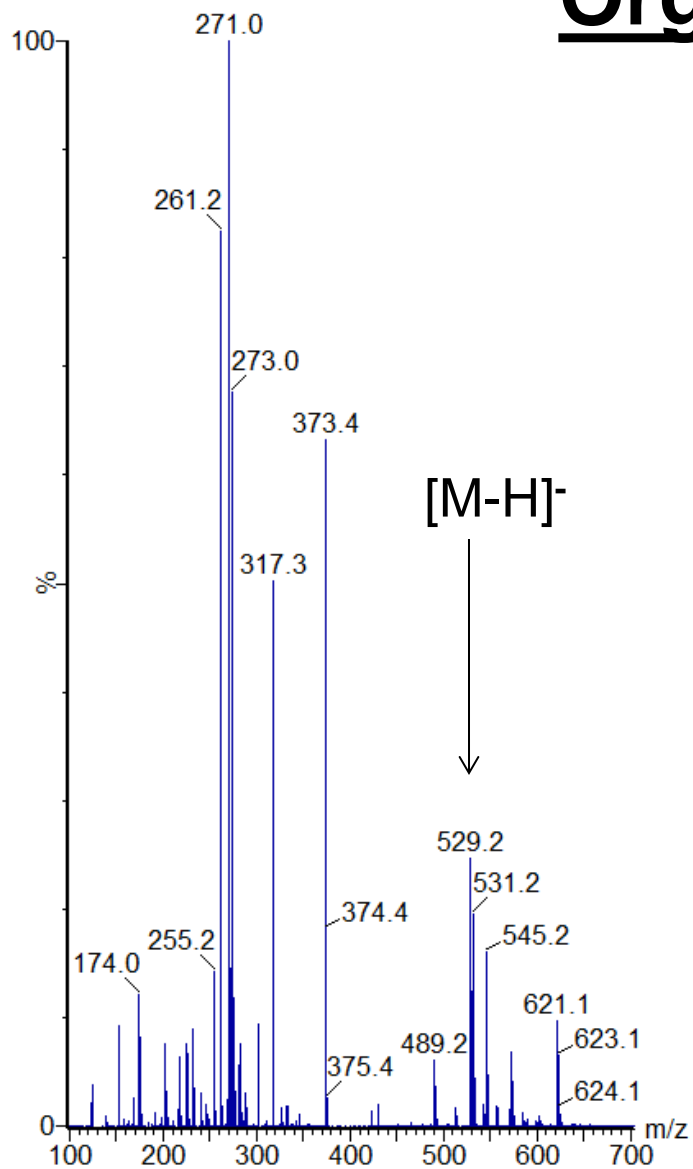


KOL113B 79 (3.992) Cm (78:103)

TOF MS APPI-
2.03e4

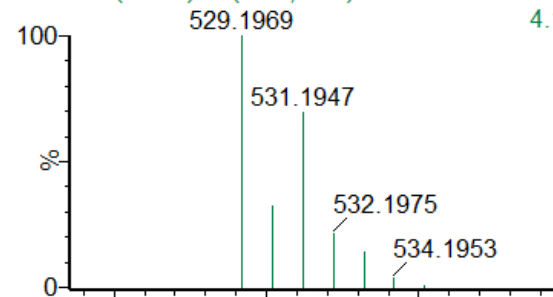


Organometallic

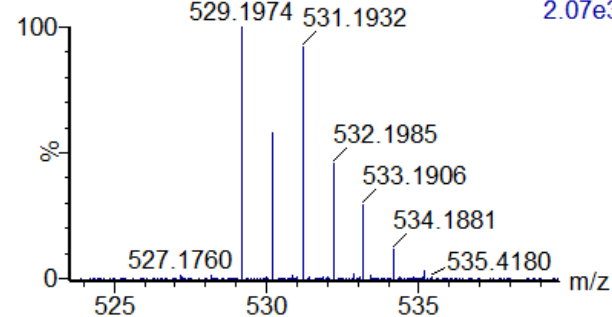


KP-1123AlMe

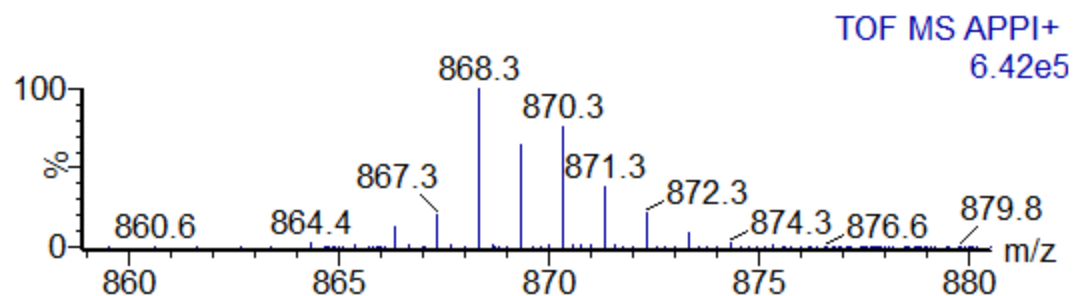
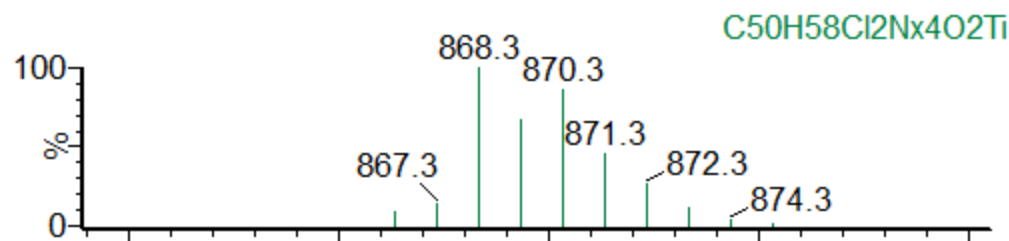
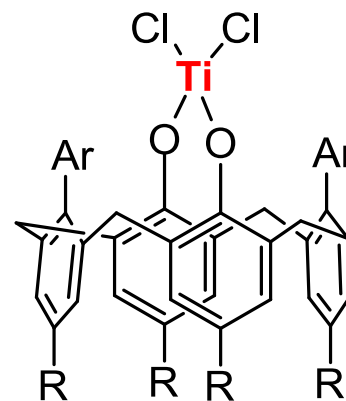
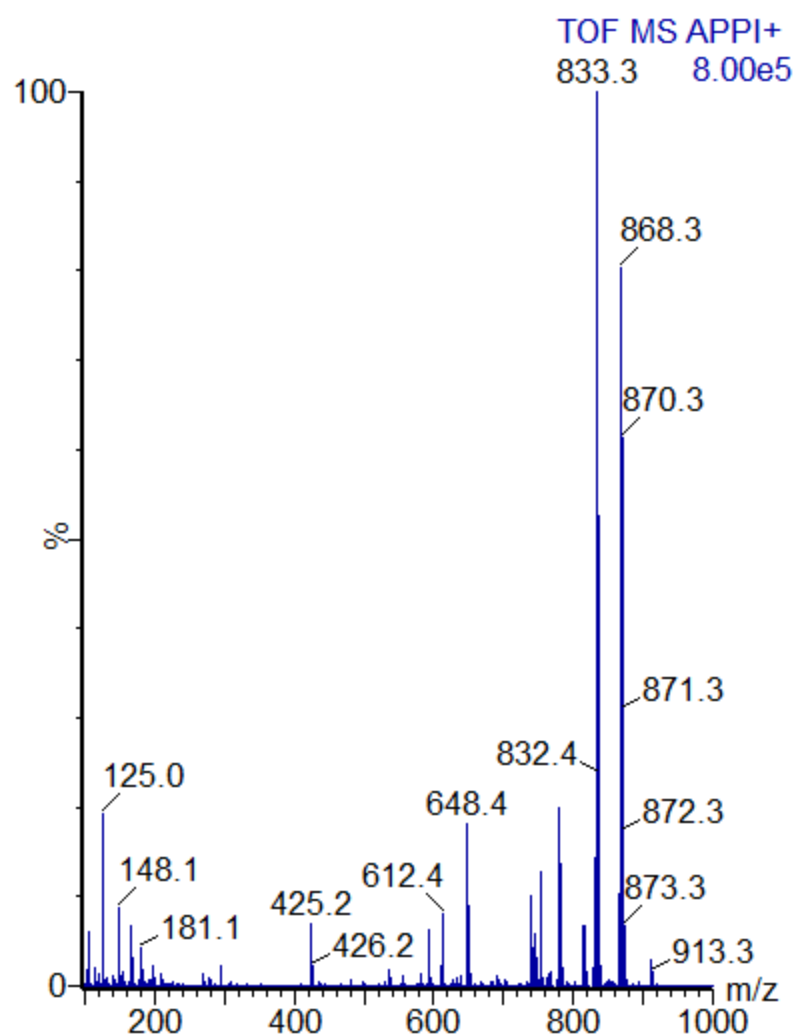
KOL114 (0.067) Is (1.00,0.10) C₂₈H₃₆Cl₂N₂O₂Al 4.14e12



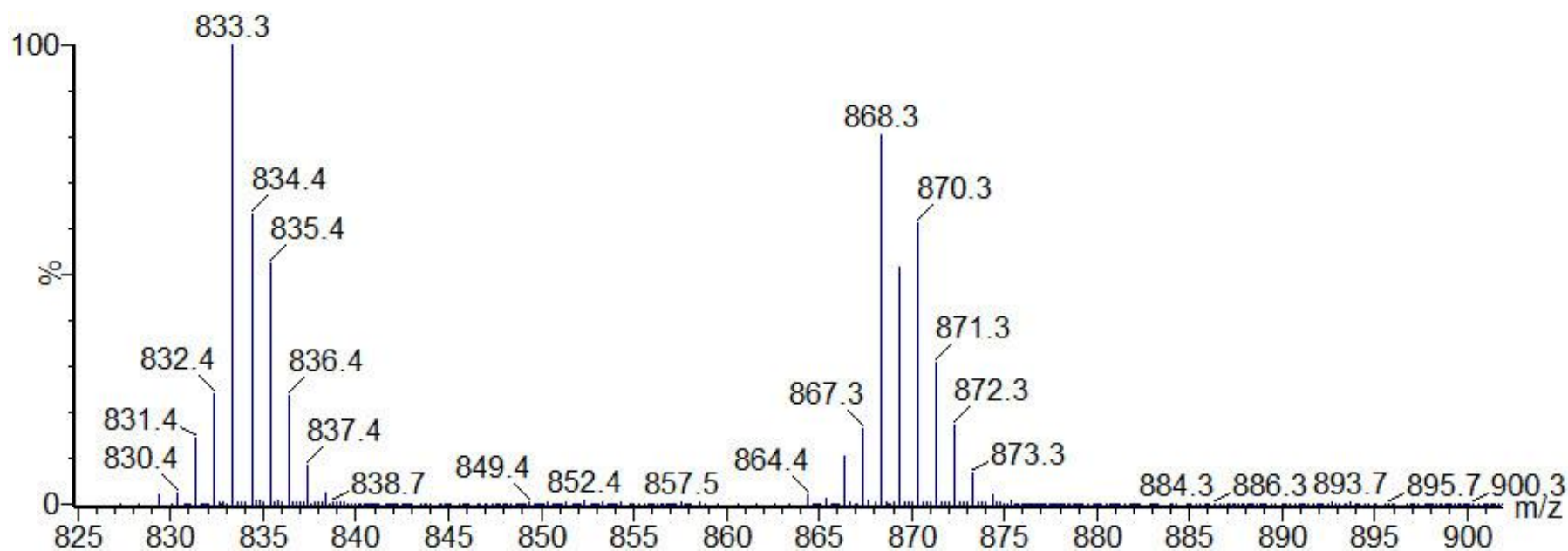
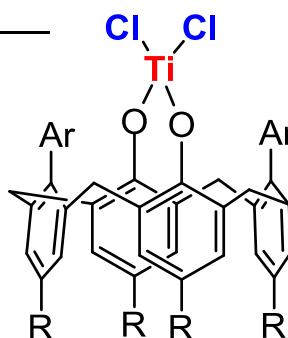
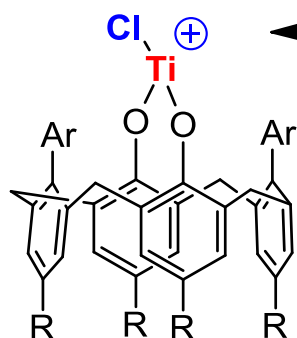
KOL114 616 (31.012) Cm (611:616) TOF MS APPI- 2.07e3



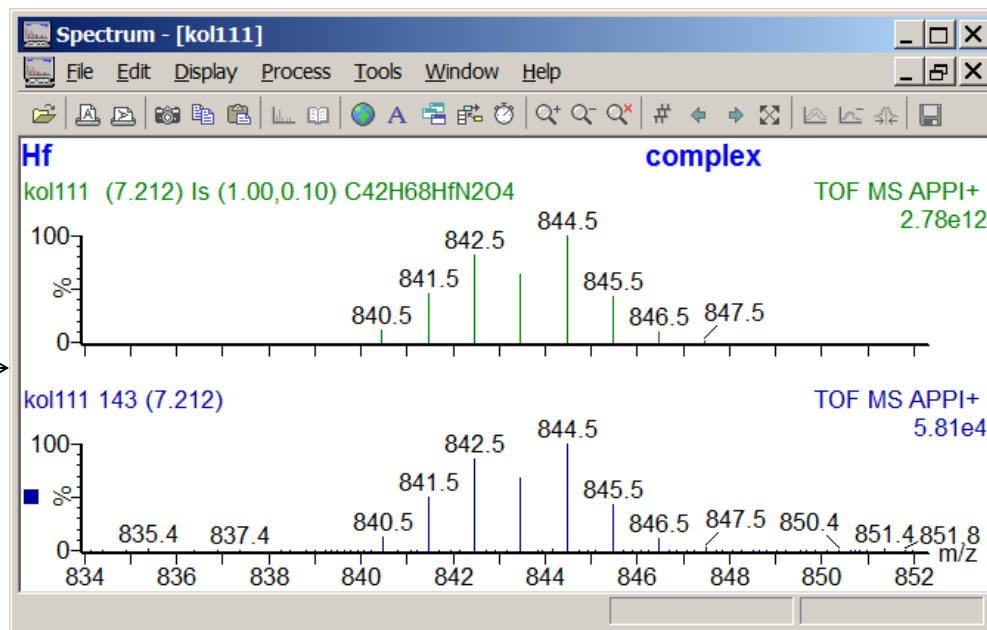
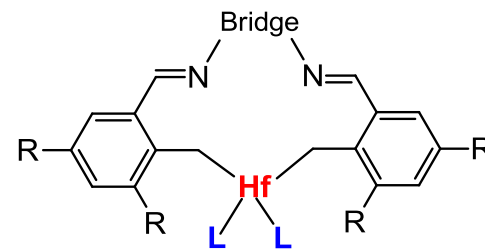
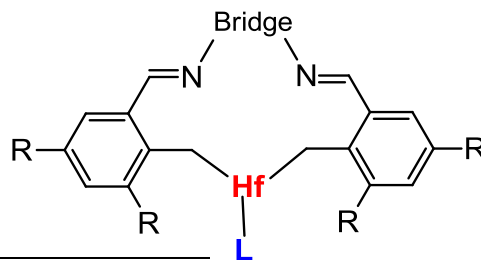
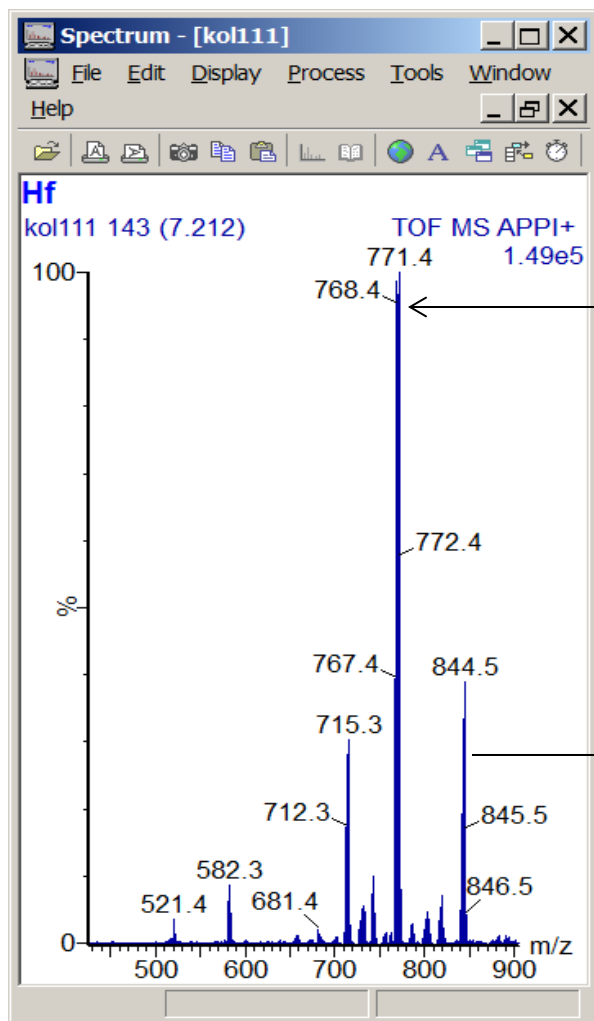
Organometallic



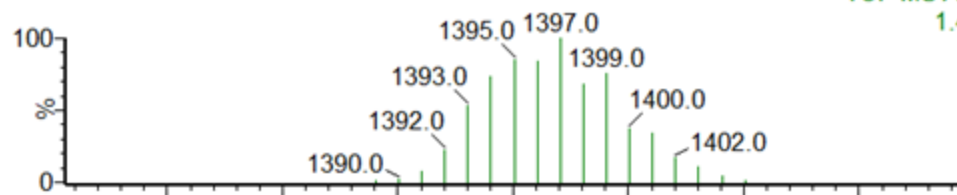
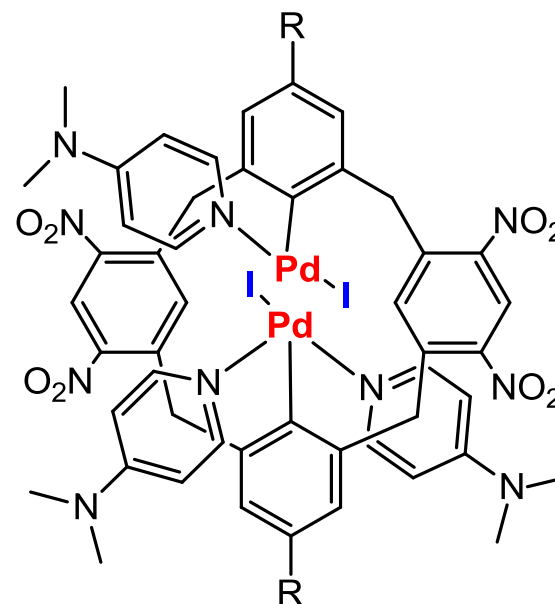
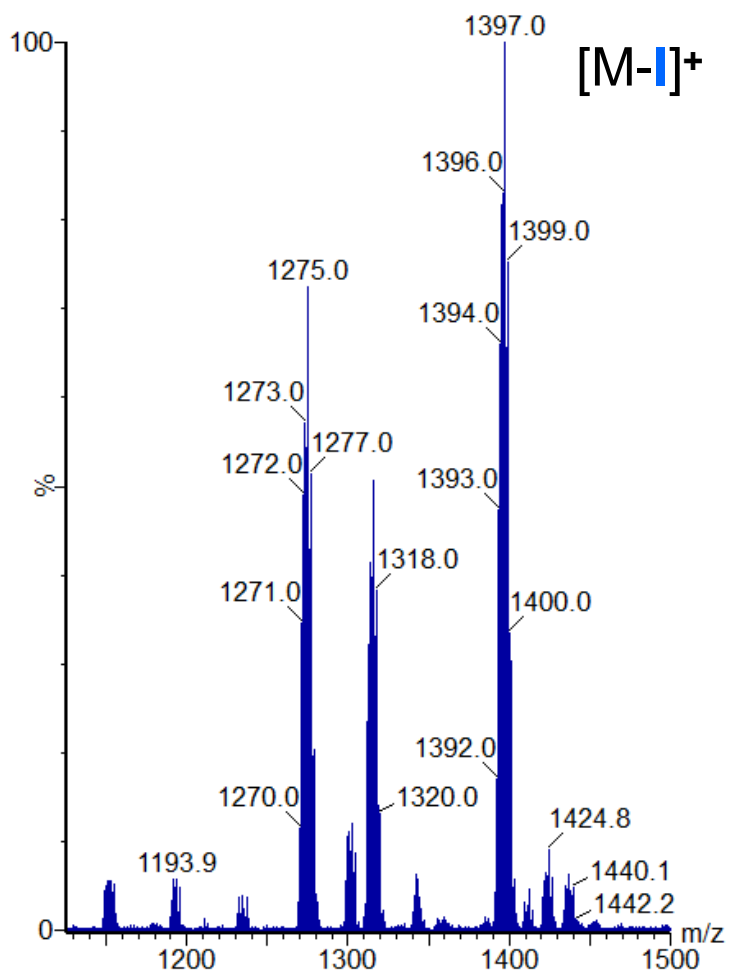
Organometallic



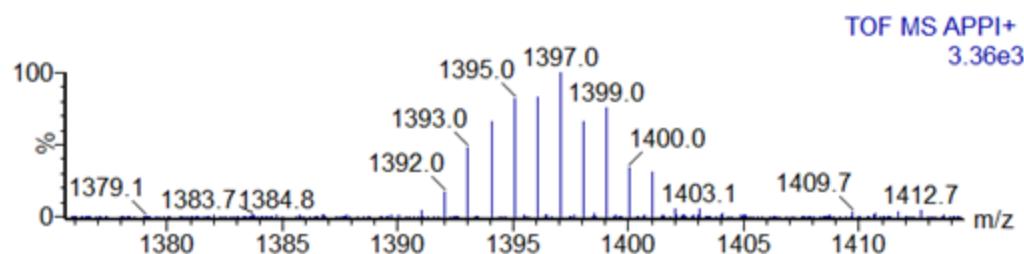
Organometallic



Organometallic

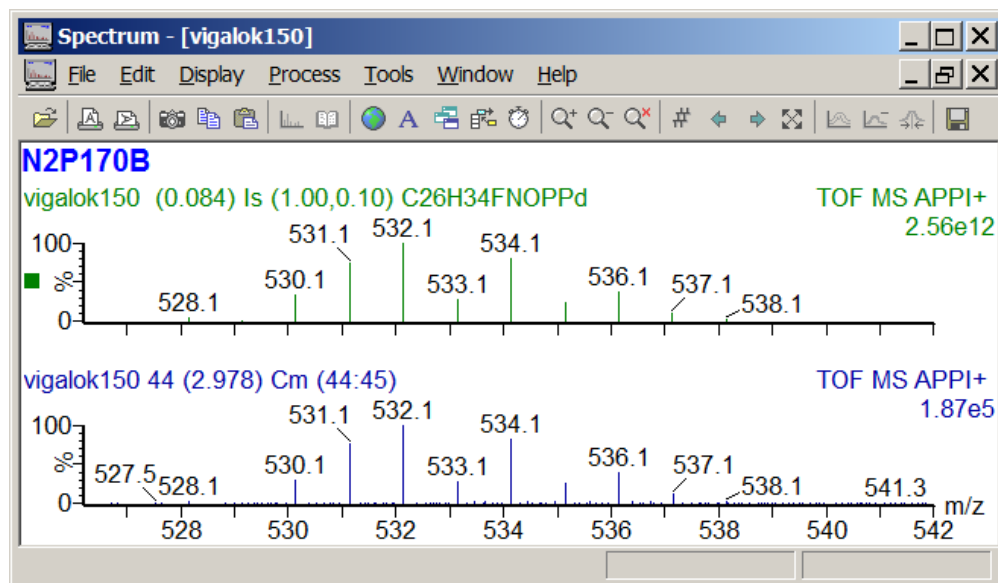
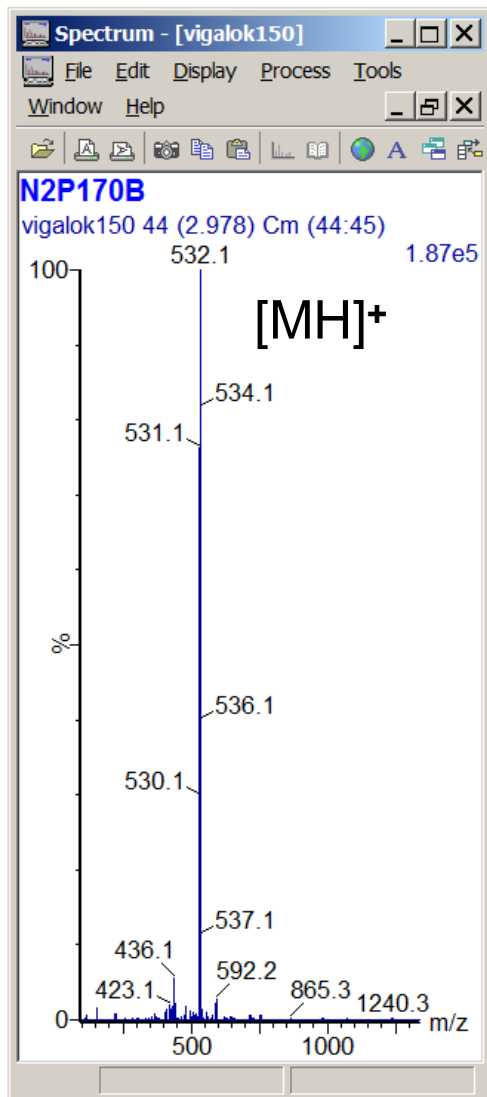
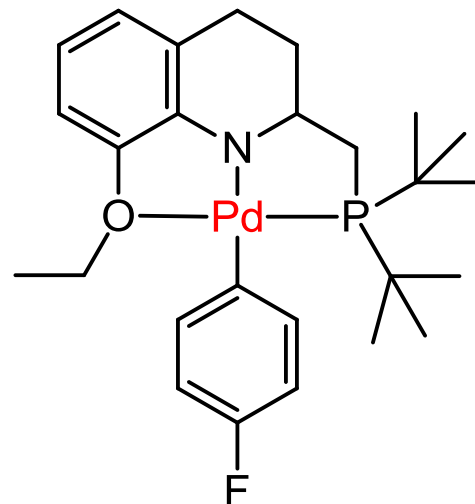


TOF MS APPI+
1.48e12

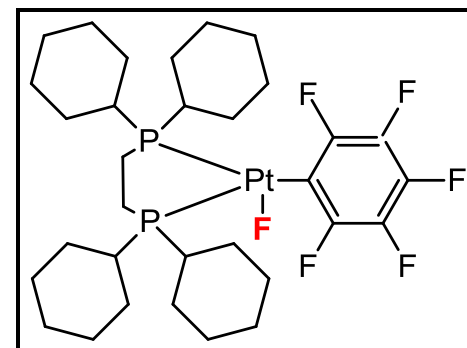
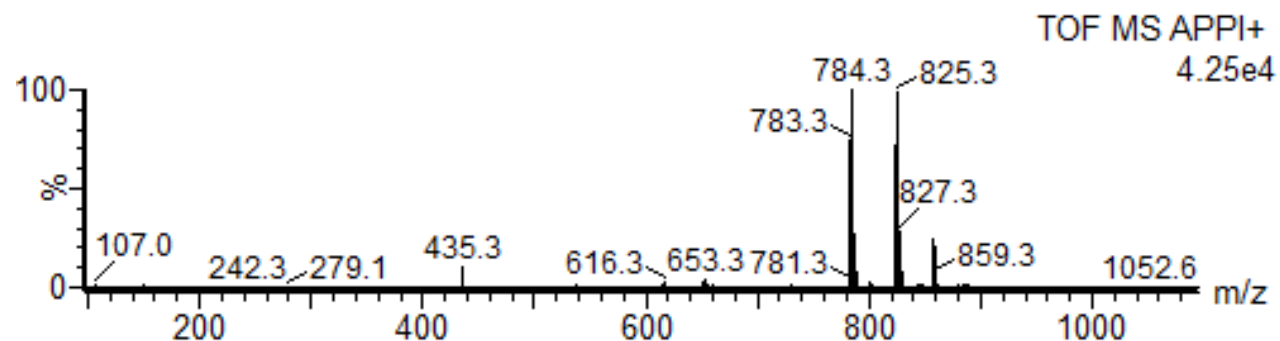
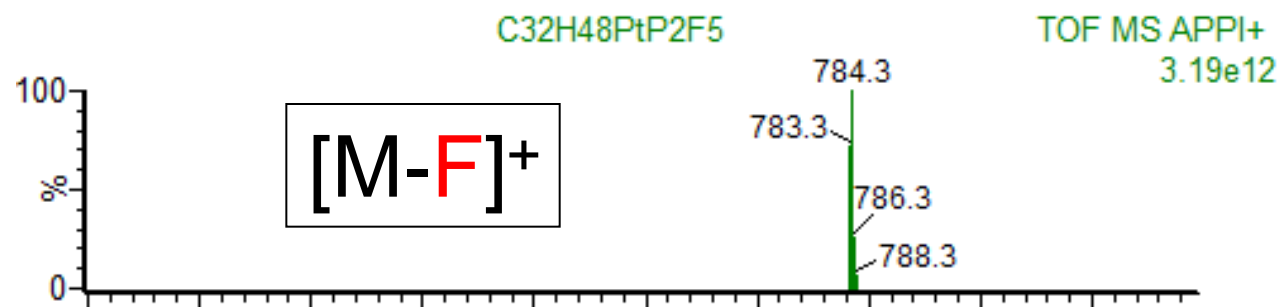
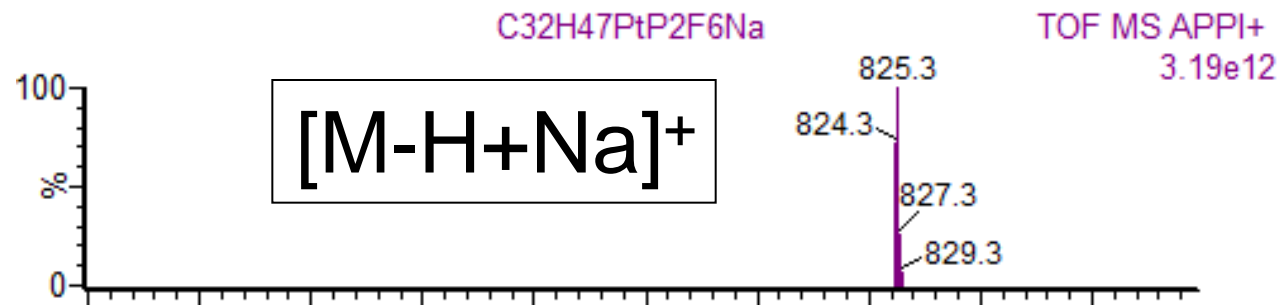


TOF MS APPI+
3.36e3

Organometallic



Organometallic



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