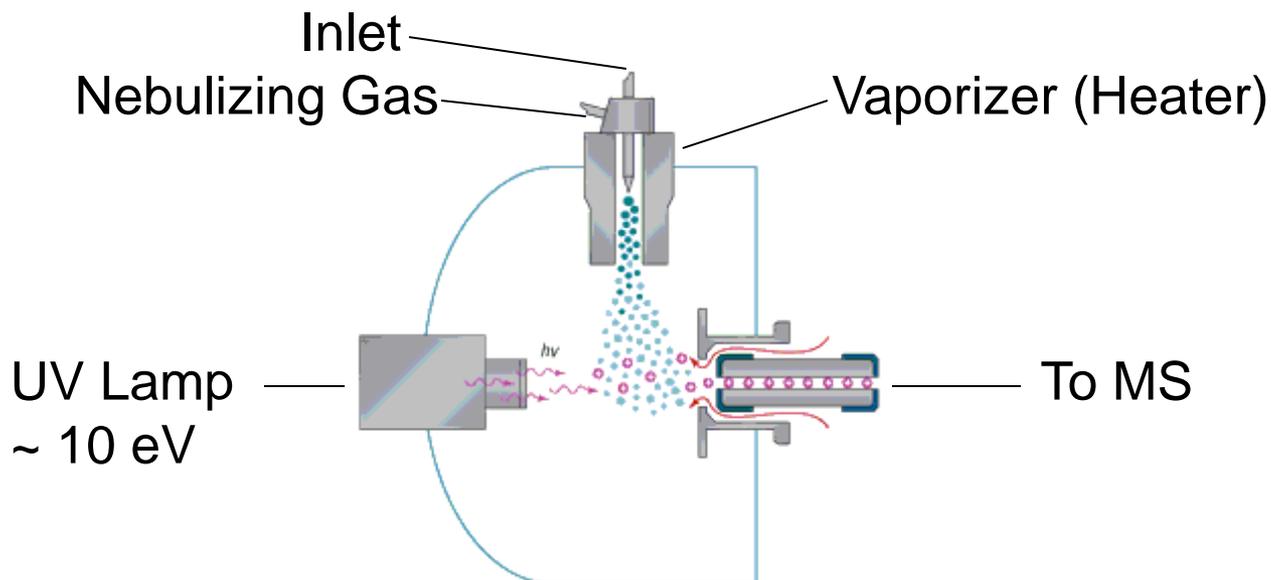


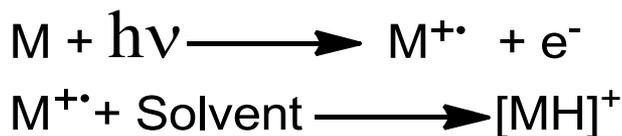
# **Implementation of APPI Mass Spectrometry for Organometallic compounds**

Noam Tal, Tel Aviv University, Israel

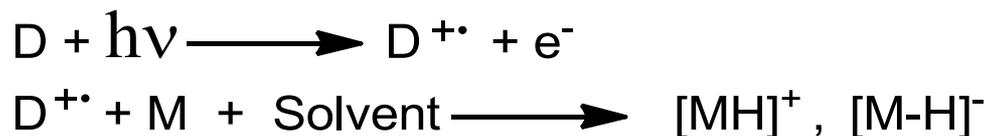
# Atm. Pressure Photo Ionization (APPI)



## 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

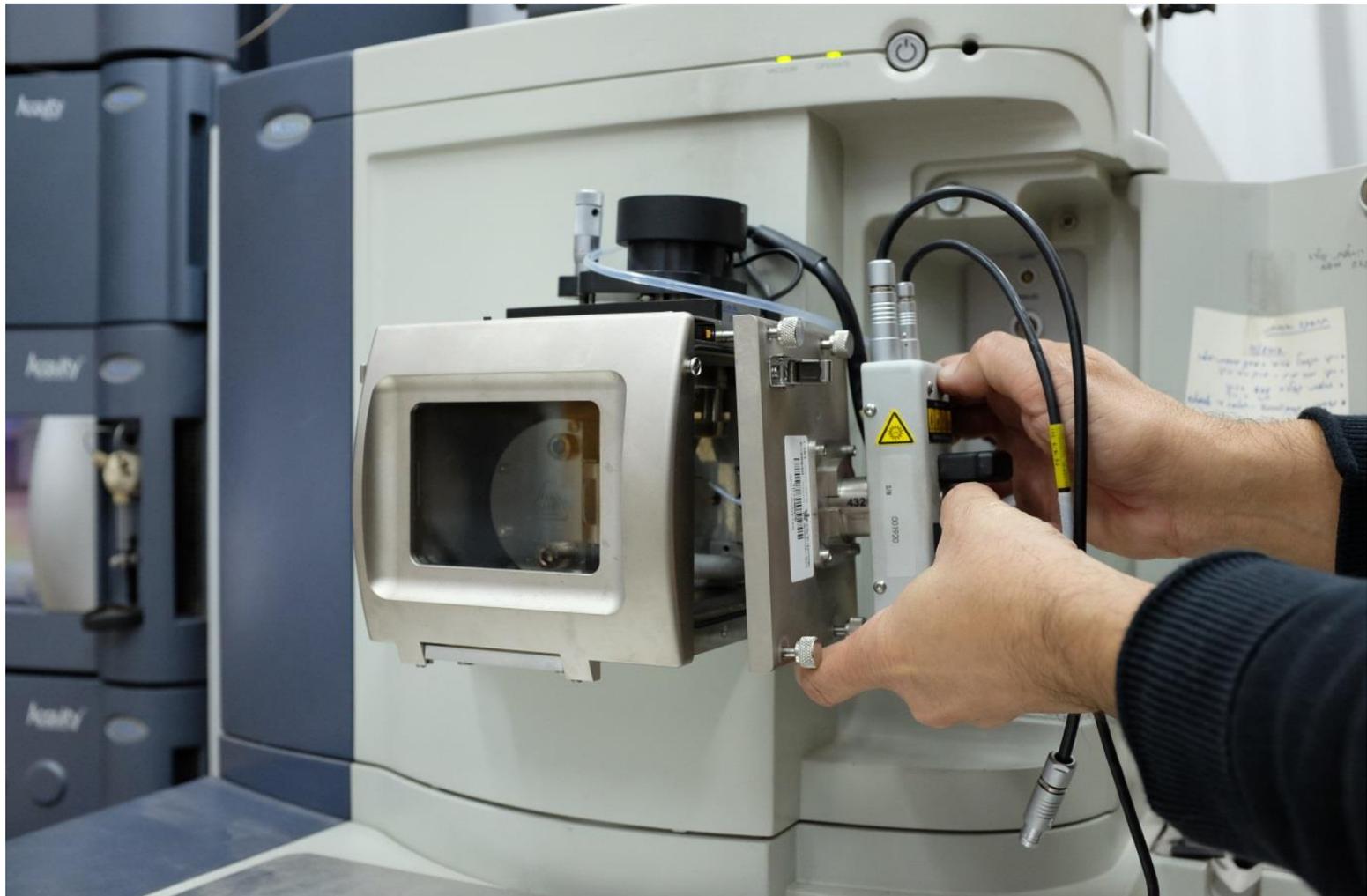
Solvent: Toluene, DCM, Hexane, MeCN, MeOH

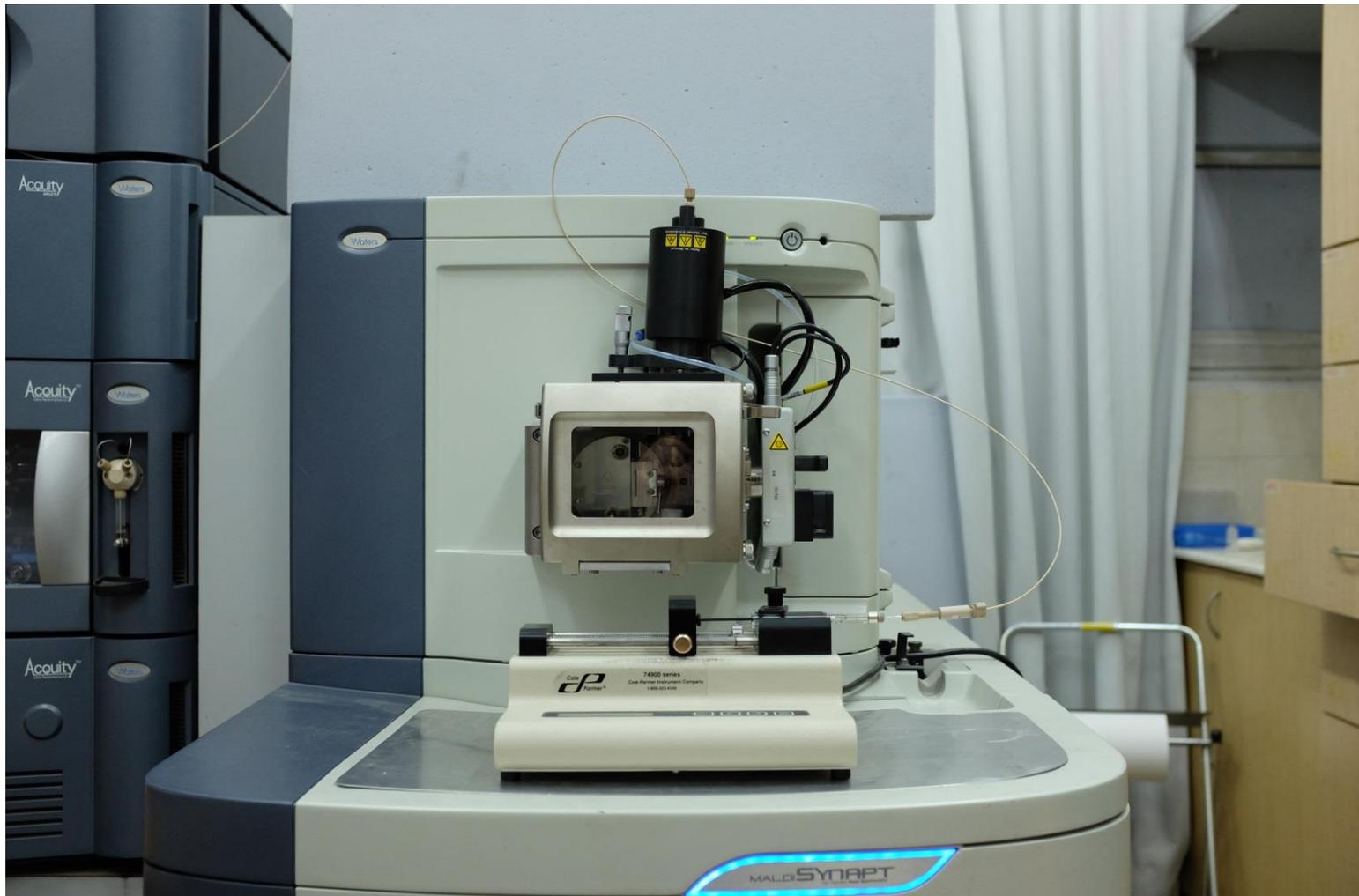
# API source

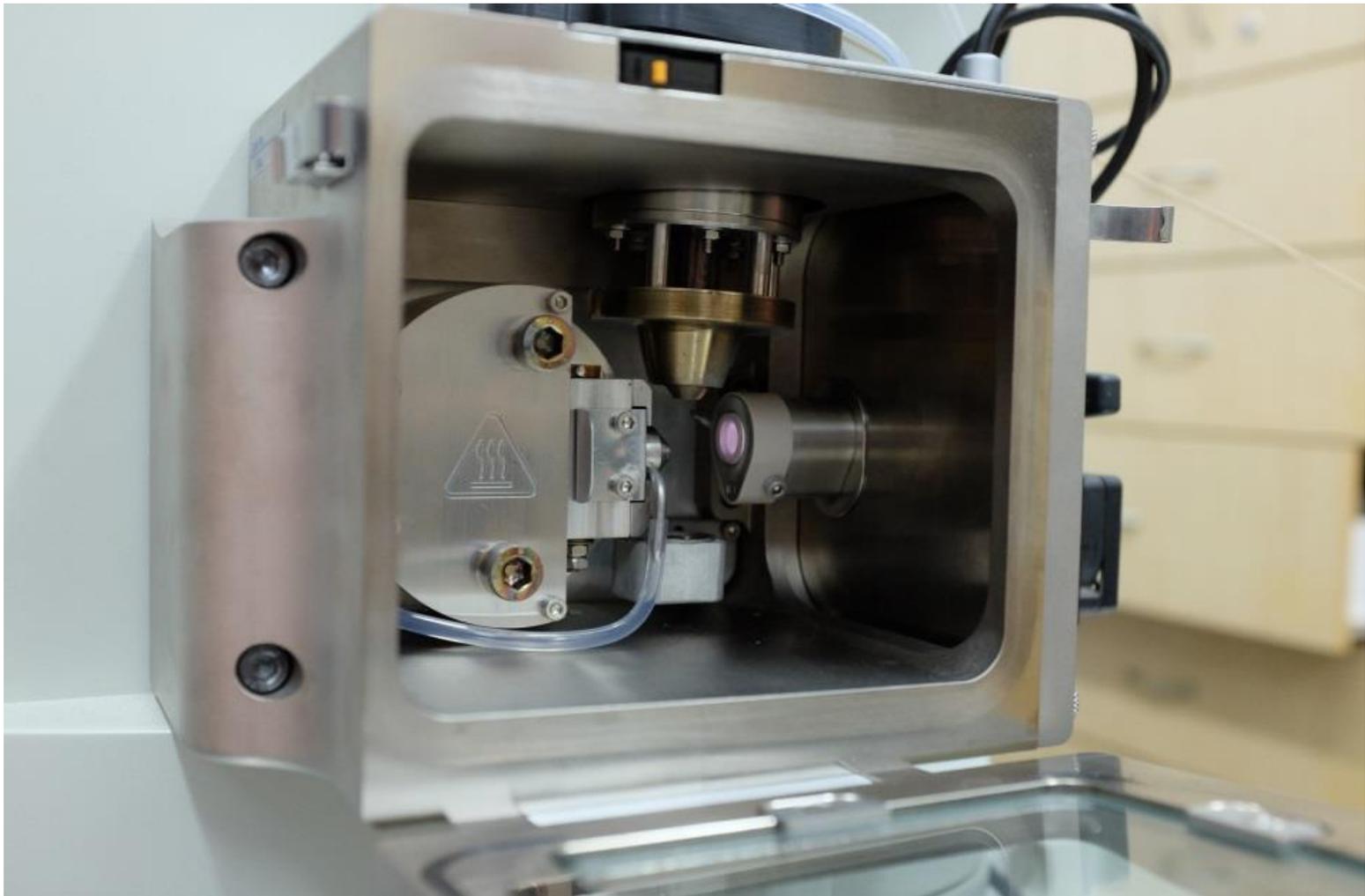








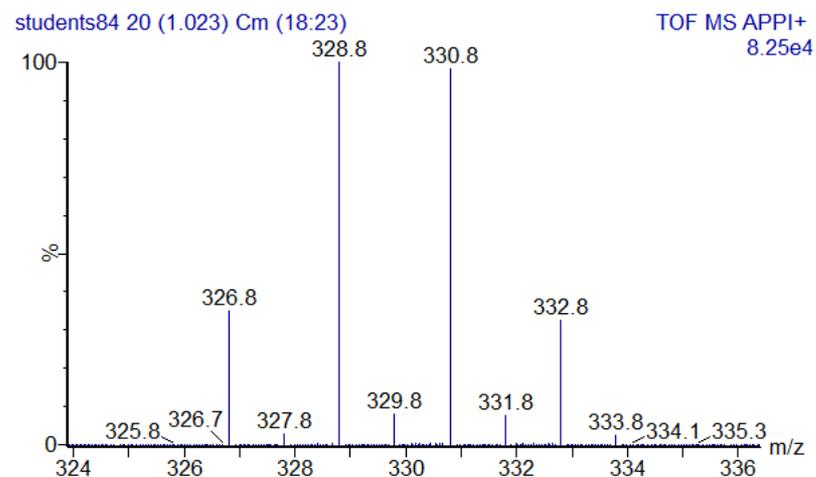
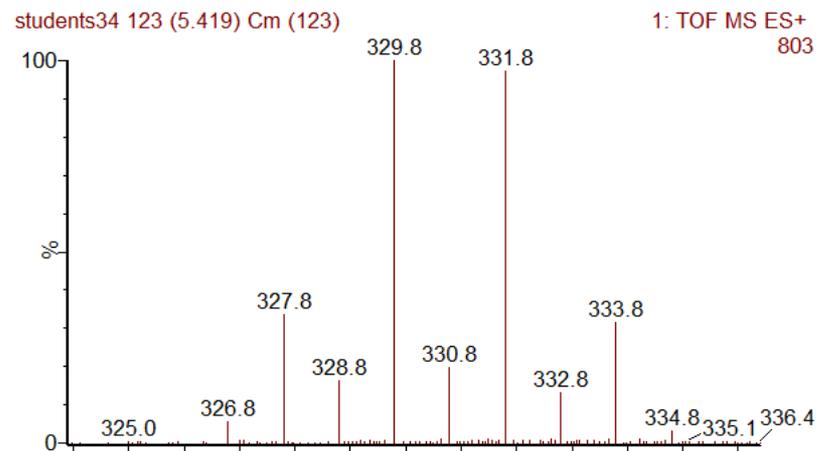
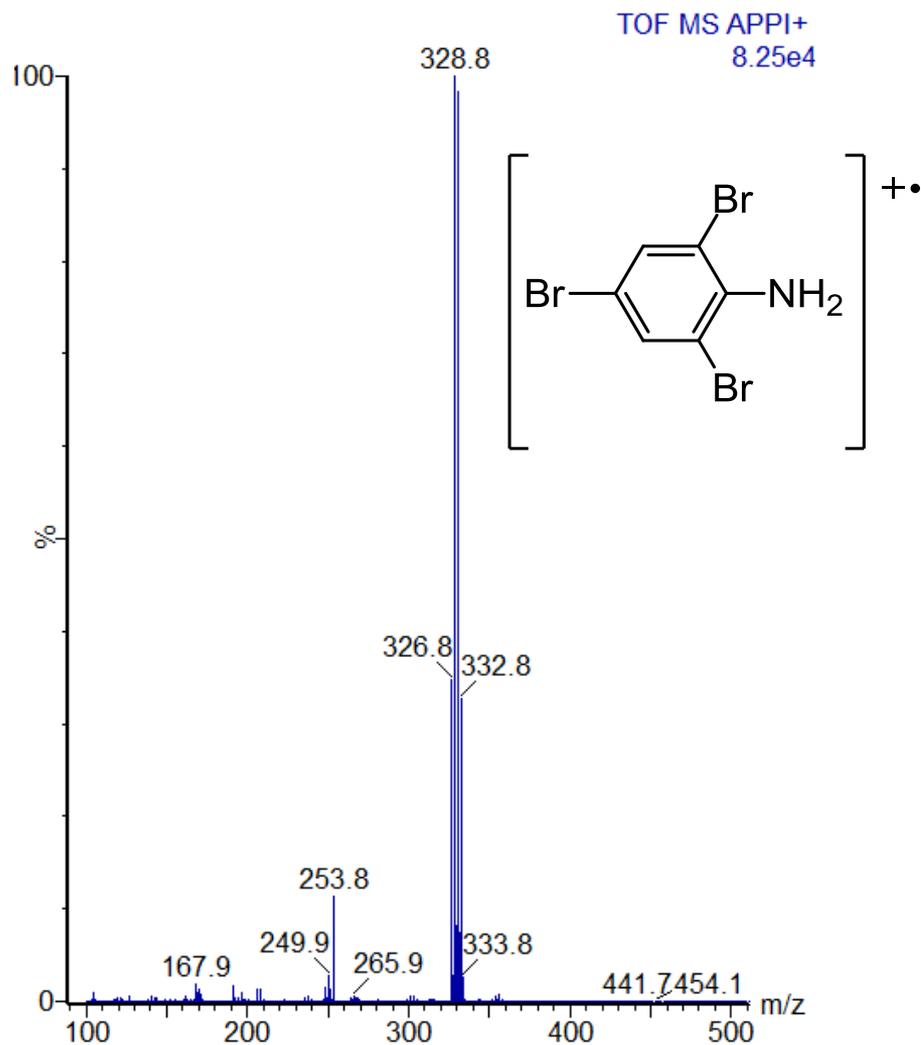




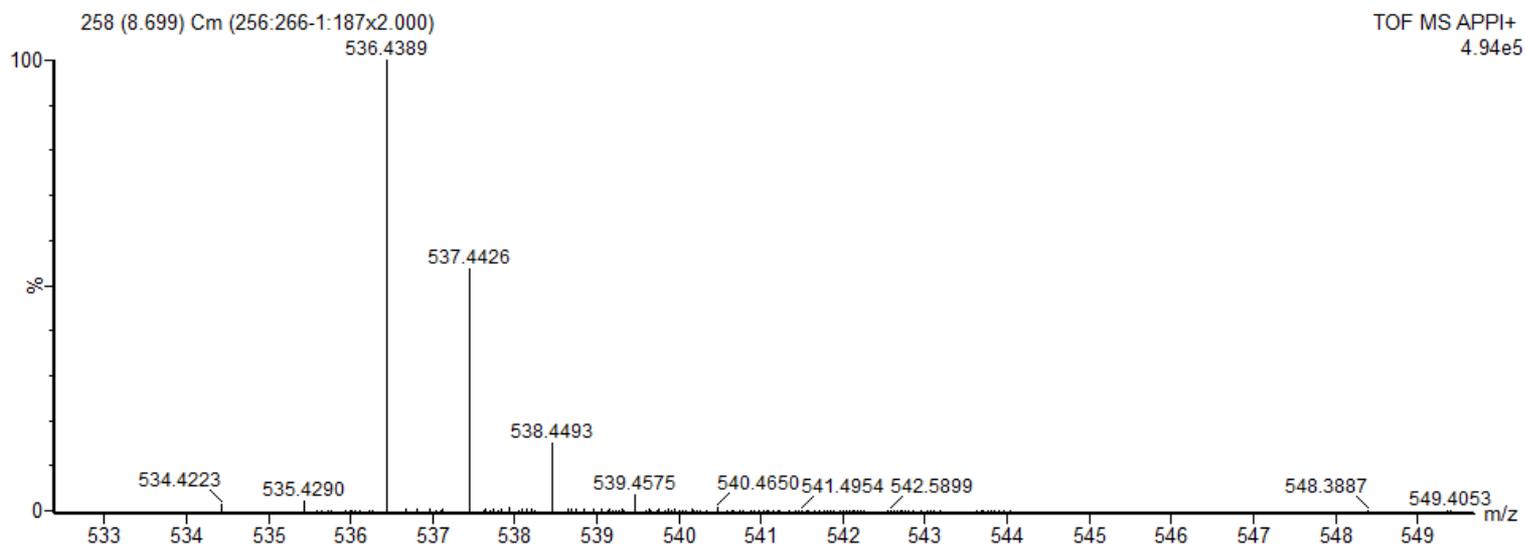
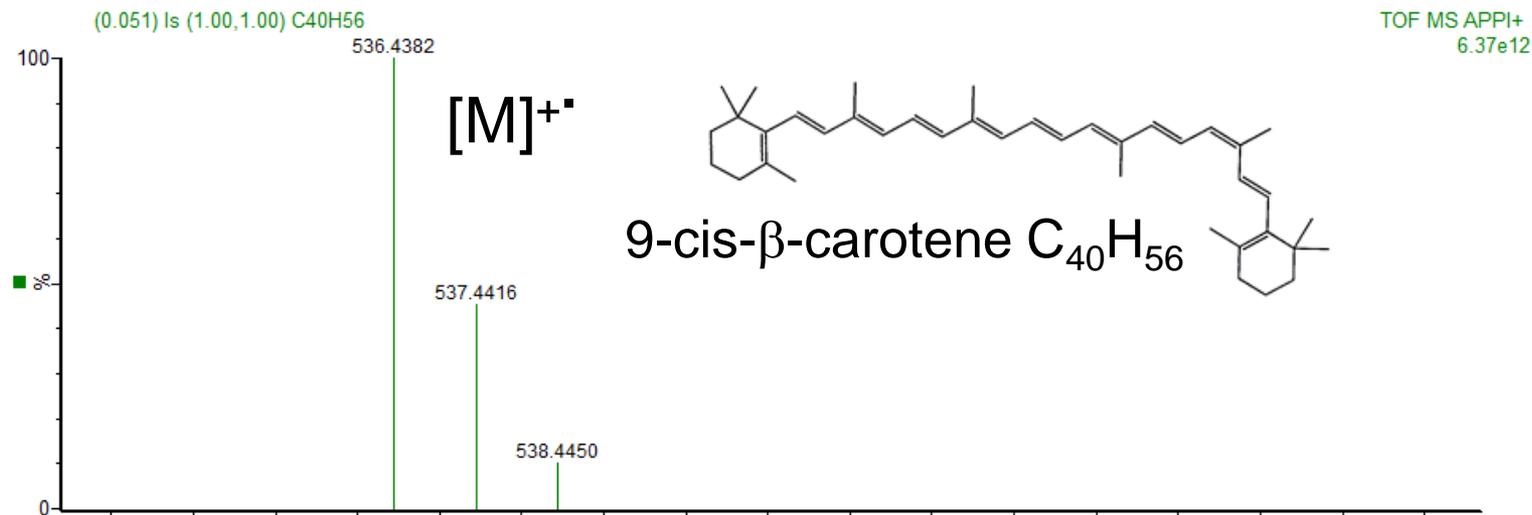
# APPI conditions:

- 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

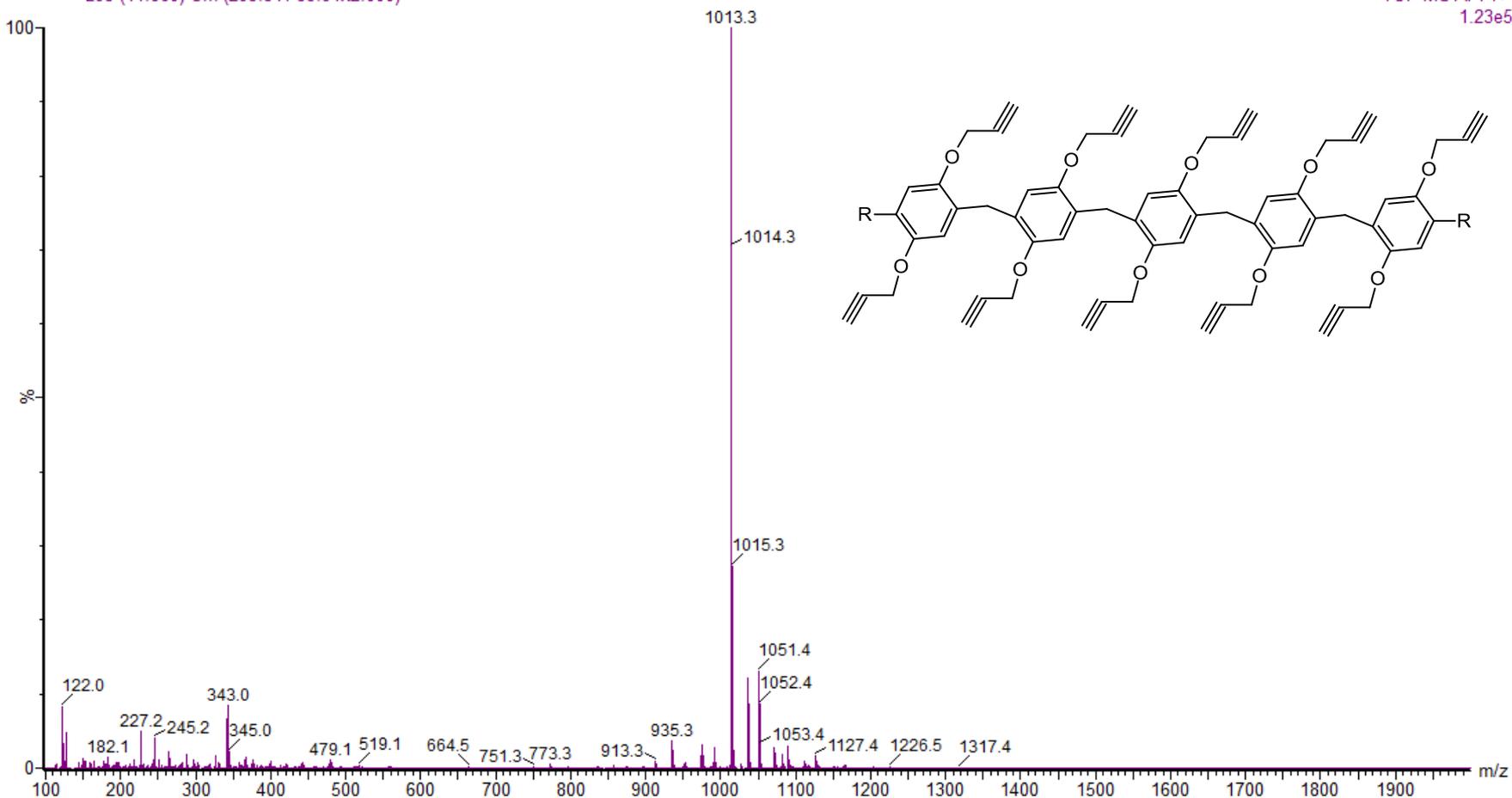


# Conjugated compounds

DM1033-1

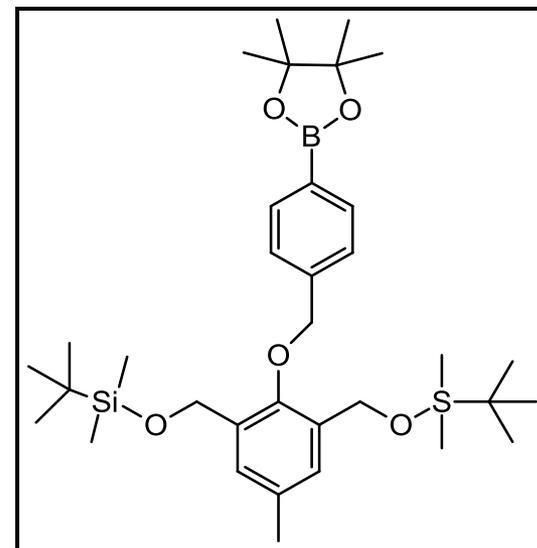
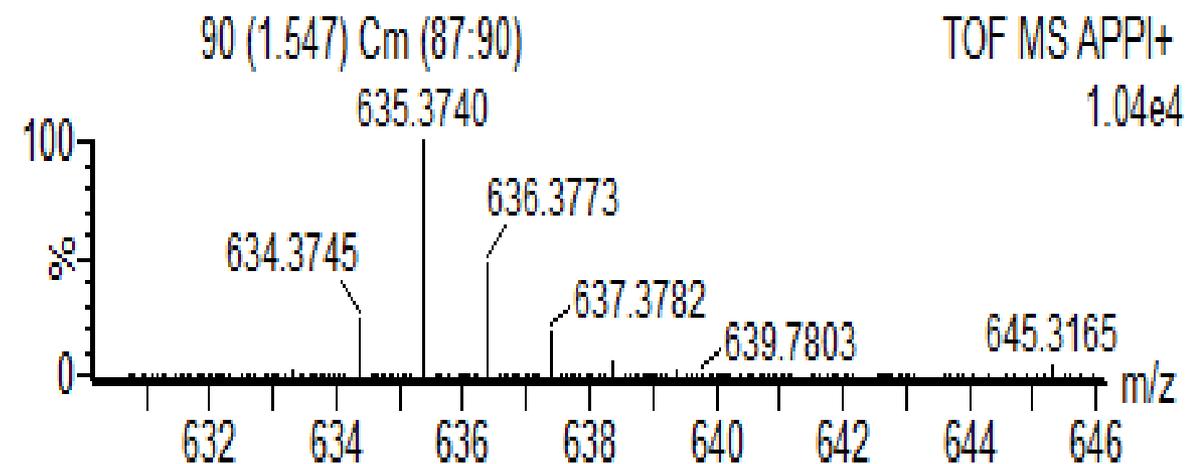
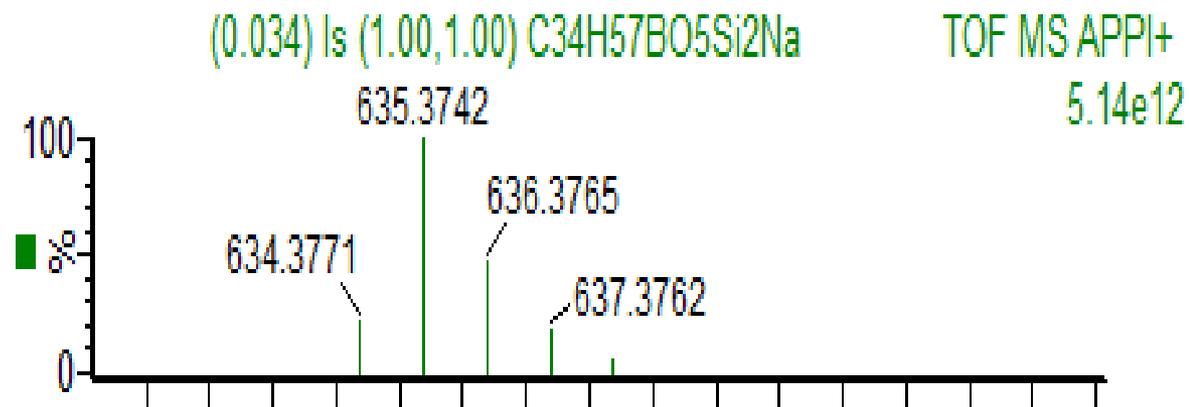
295 (14.860) Cm (295:311-55:91x2.000)

TOF MS APPI+  
1.23e5



# Conjugated compounds

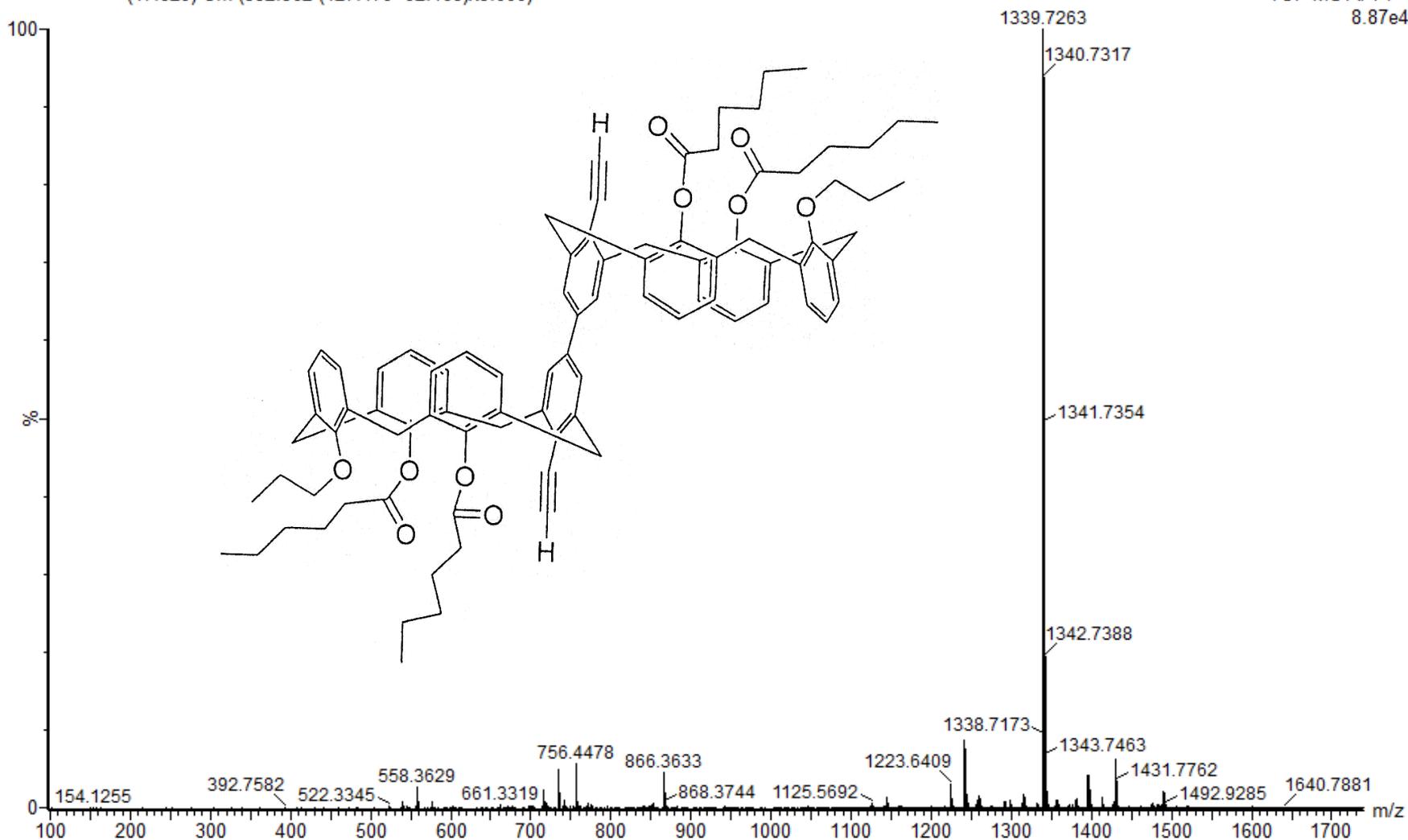
ef 2-41



# Conjugated compounds

(17.829) Cm (352:362-(127:179+92:168)x5.000)

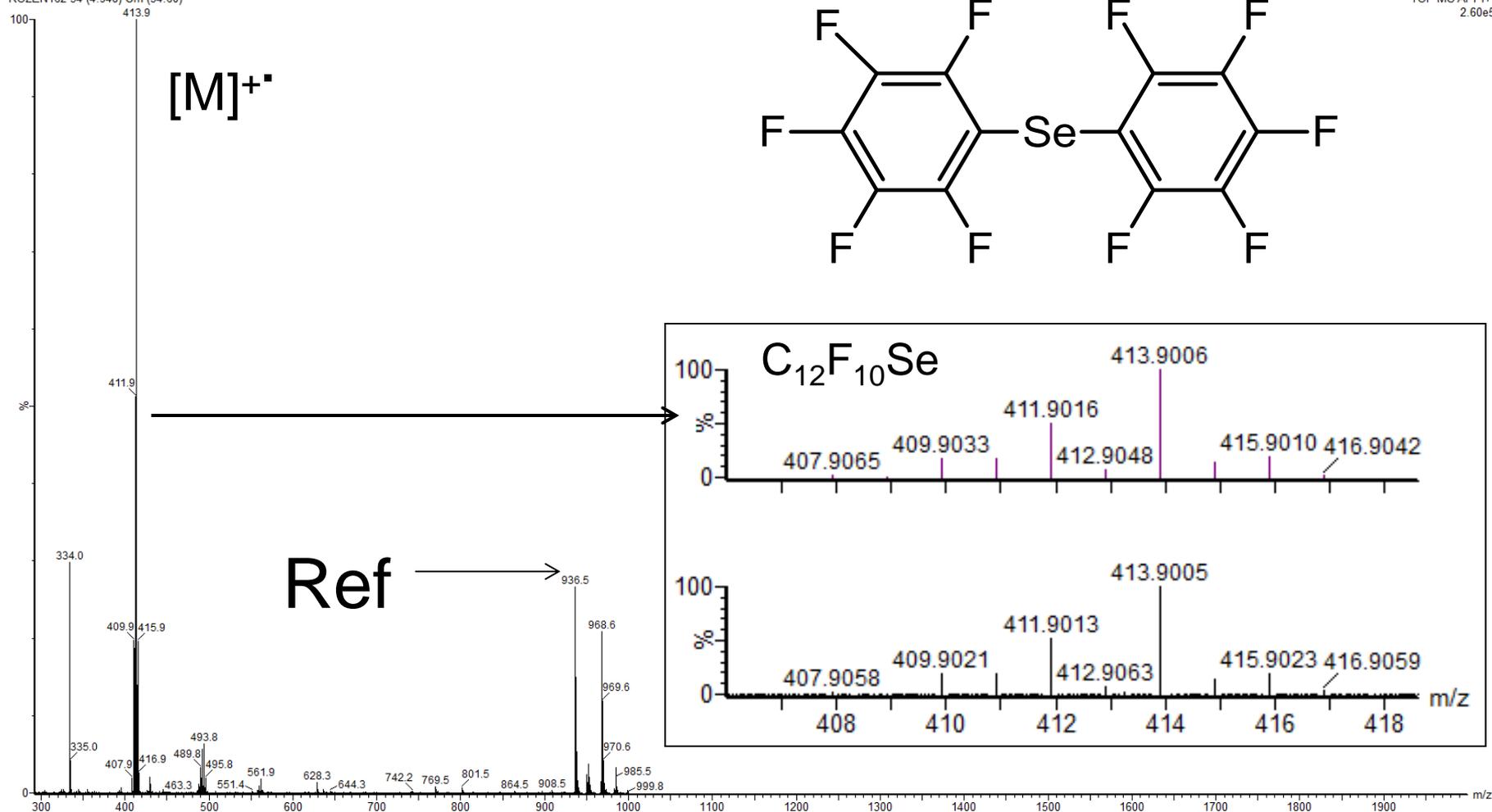
TOF MS APPI+  
8.87e4



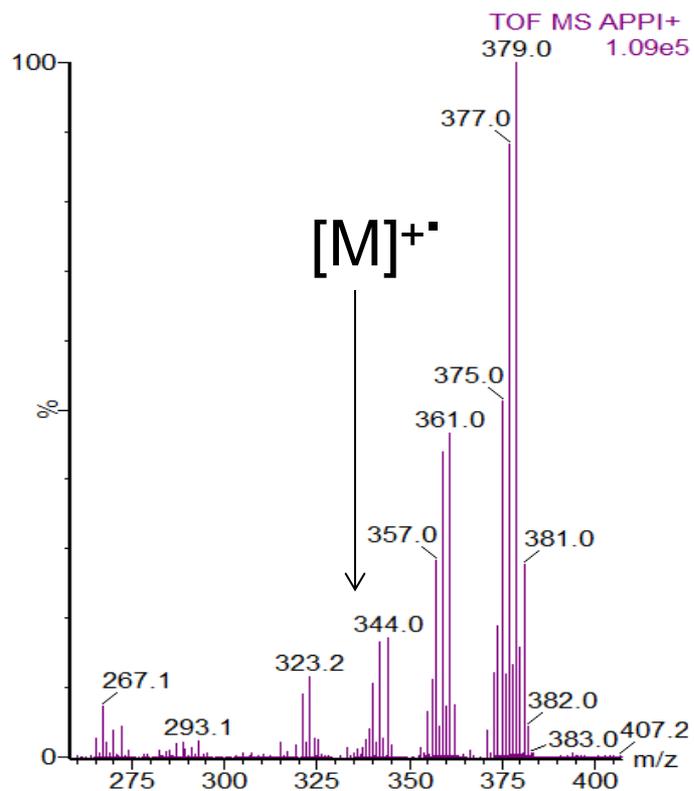
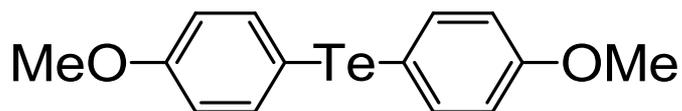
# Conjugated compounds

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

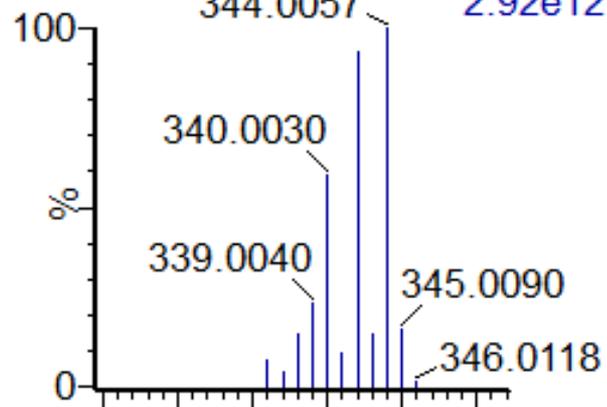
TOF MS APPI+  
2.60e5



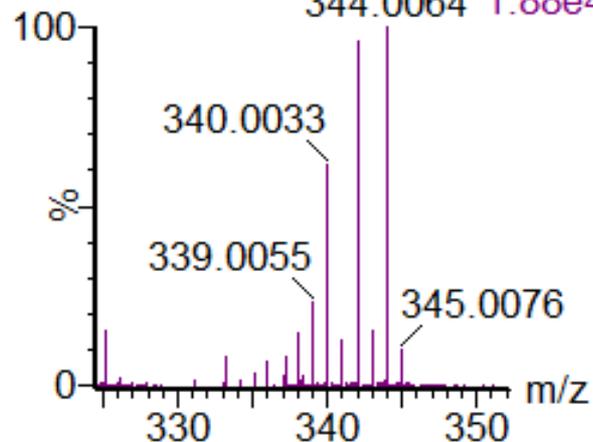
# Conjugated compounds



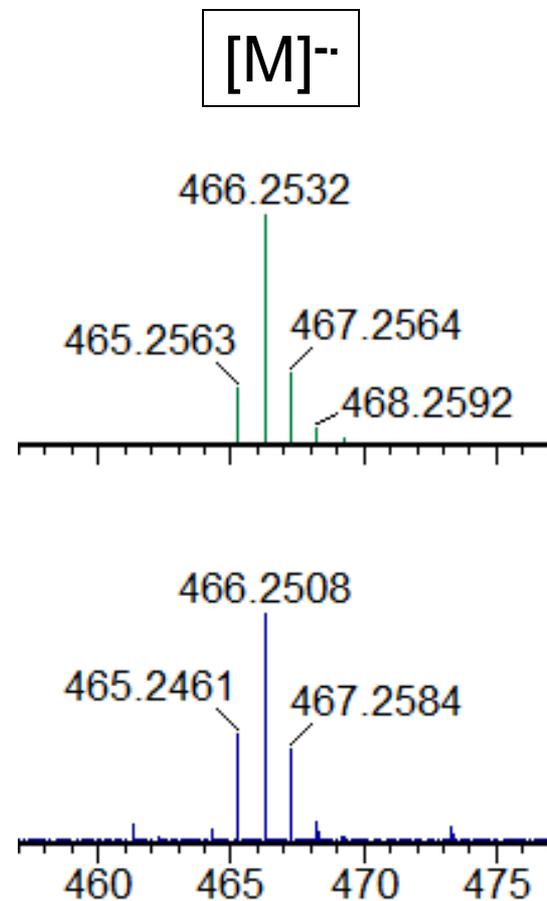
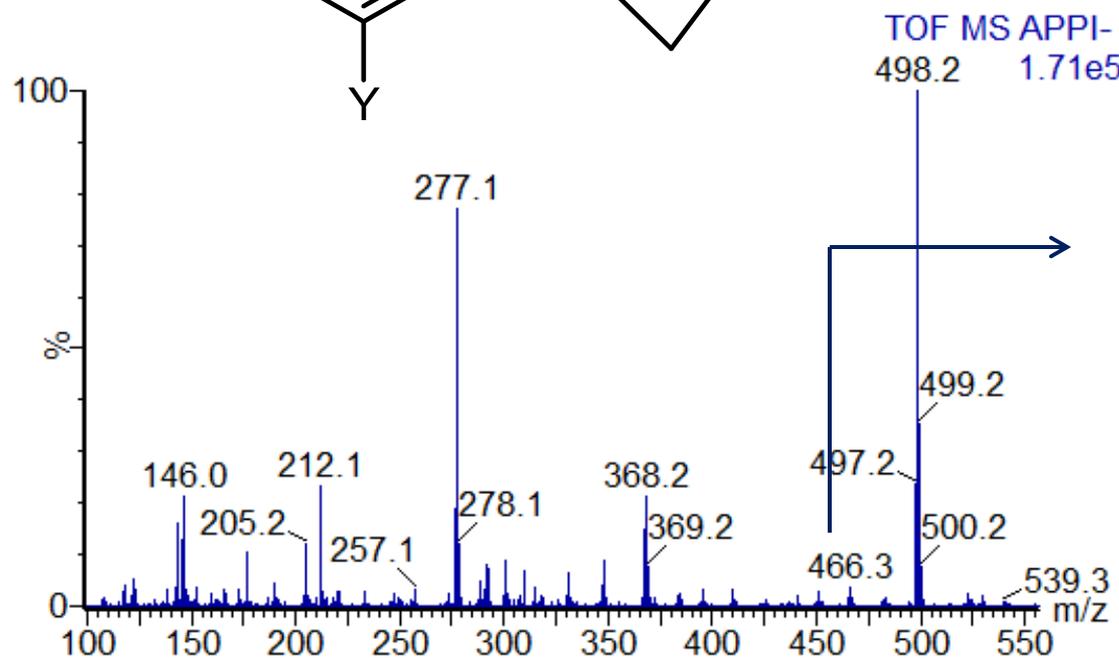
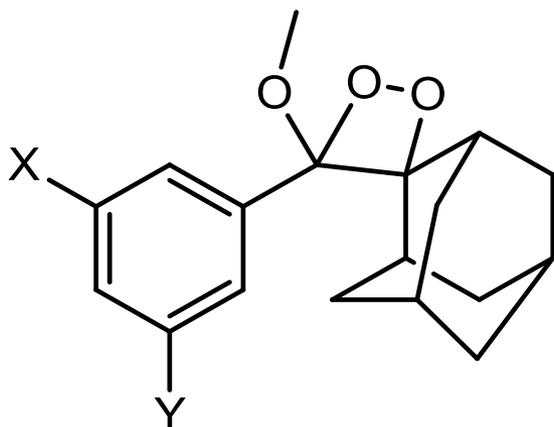
biu142c (0.067) Is (1.00,0.10) C1  
344.0057 2.92e12



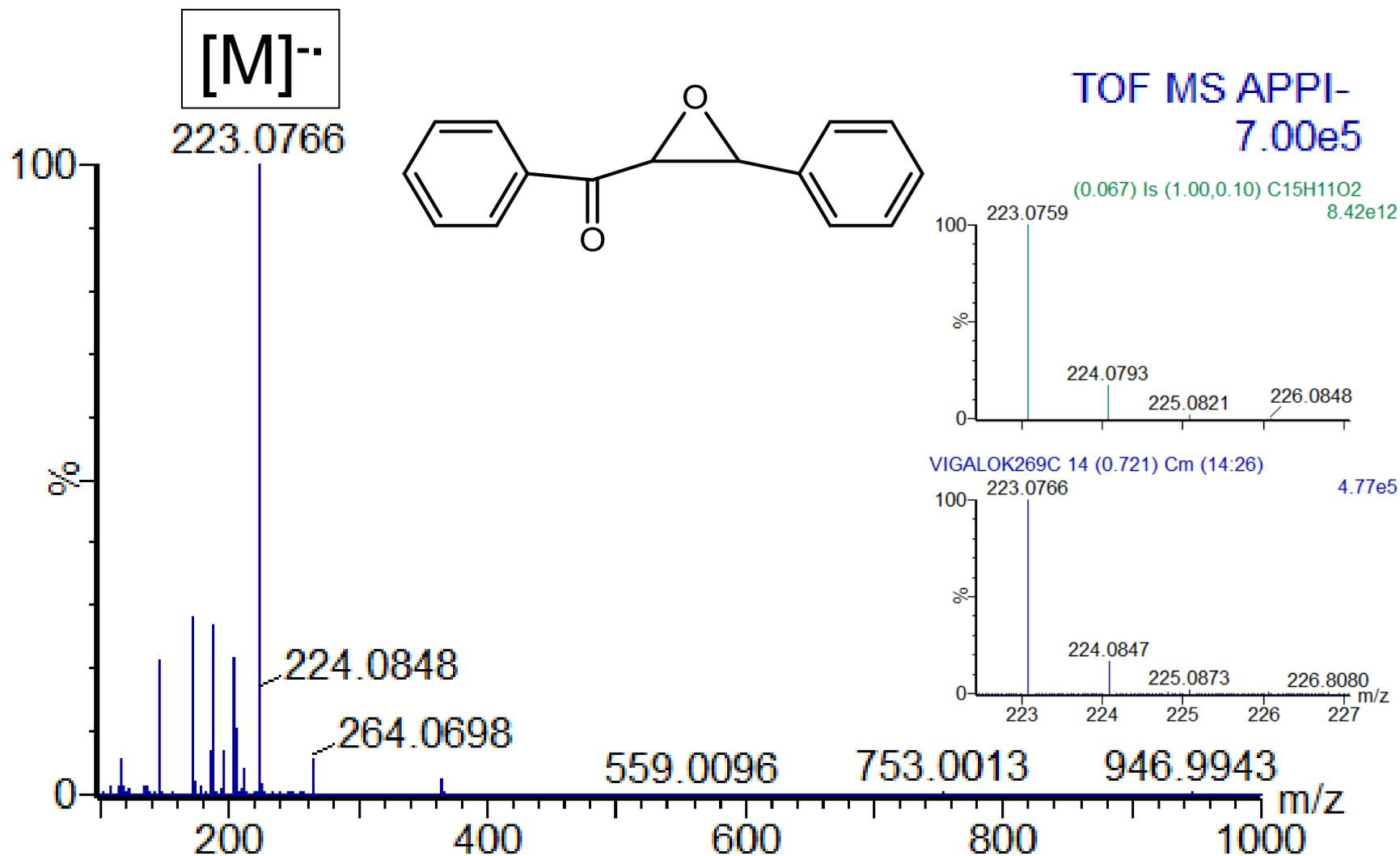
biu142c 93 (4.696) Cm (92:95-22:1)  
344.0064 1.88e4



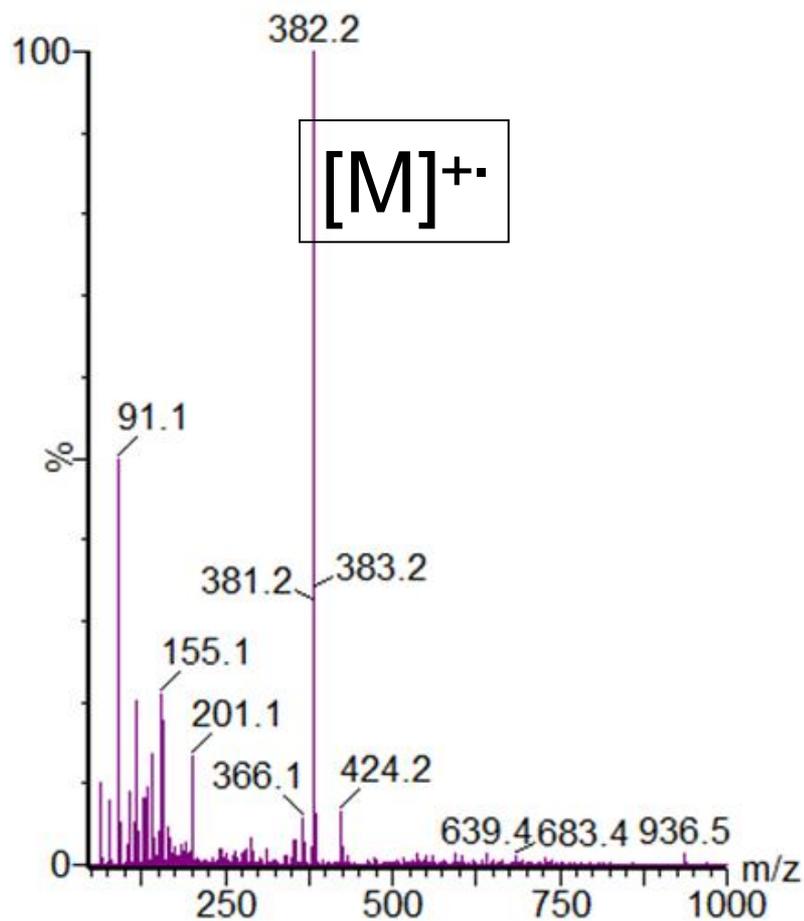
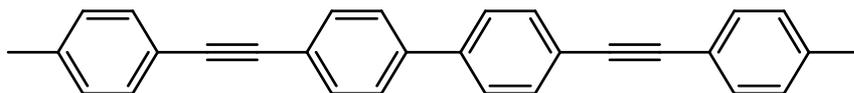
# Conjugated compounds



# Conjugated compounds

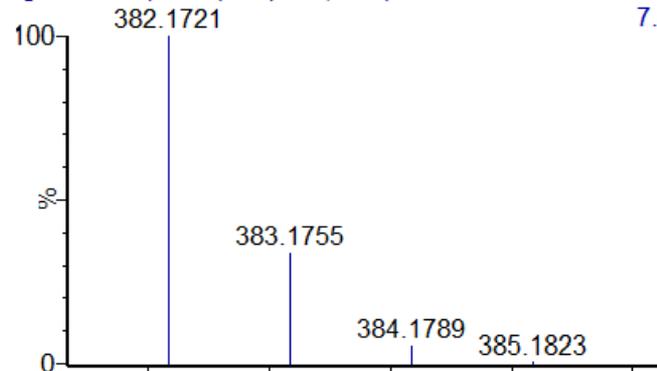


# Conjugated compounds



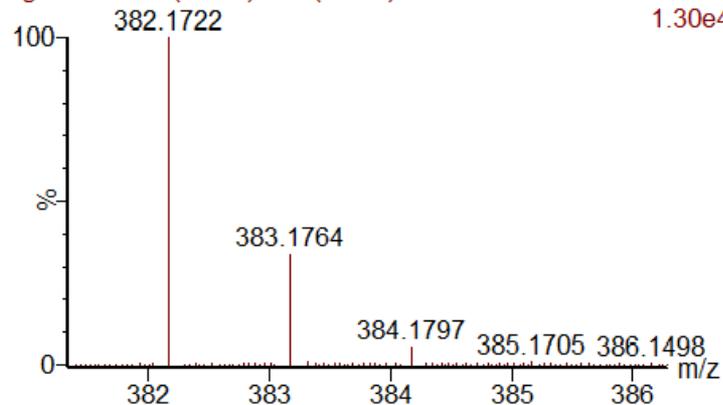
## Linear Toly Anat Molad

vigaluk95b (0.051) Is (1.00,0.10) C<sub>30</sub>H<sub>22</sub> TOF MS APPI+ 7.15e12

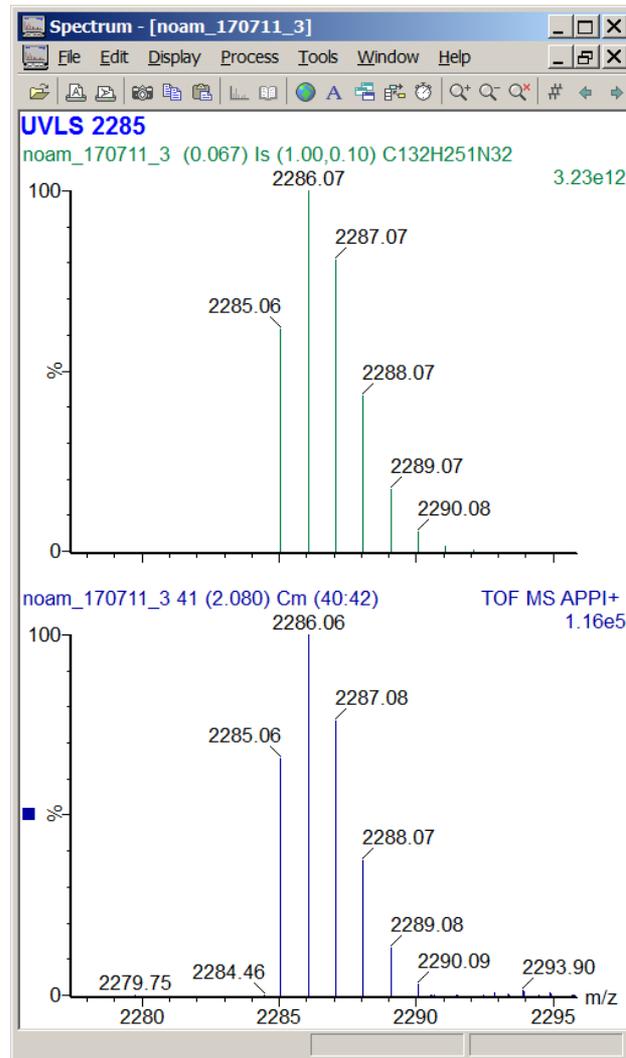
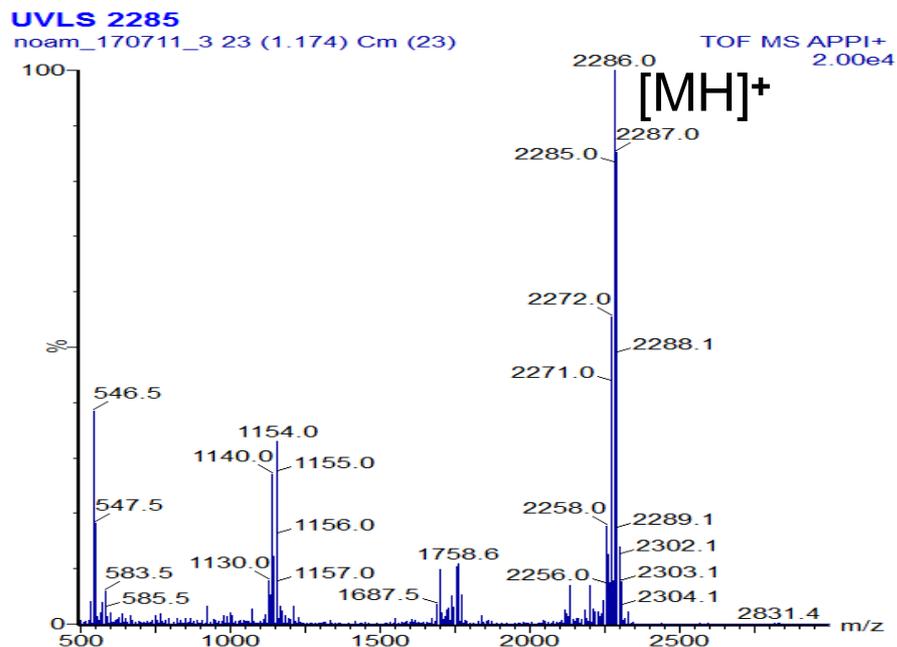
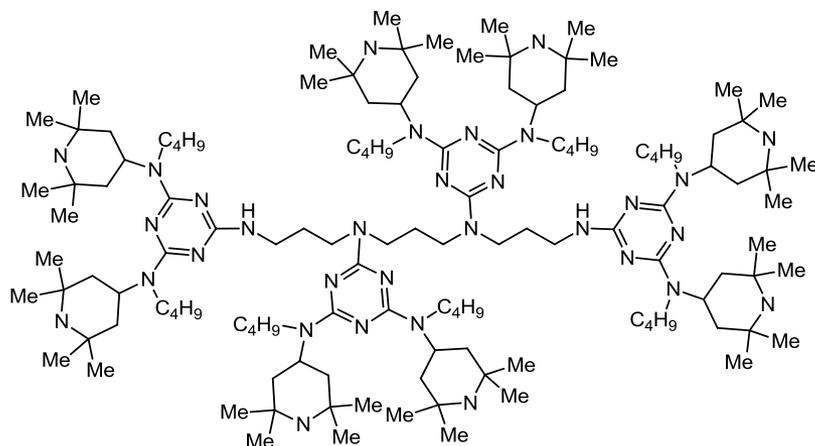


## vigaluk95b 84 (2.873) Cm (78:90)

TOF MS APPI+ 1.30e4

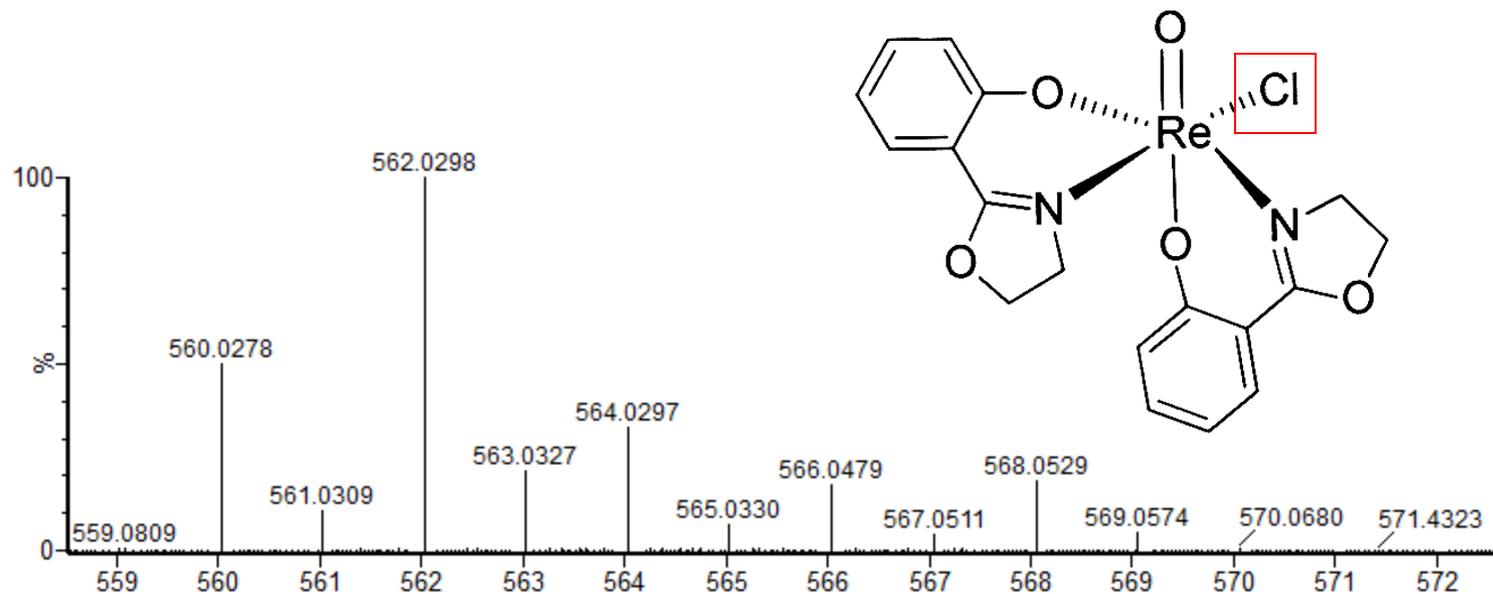
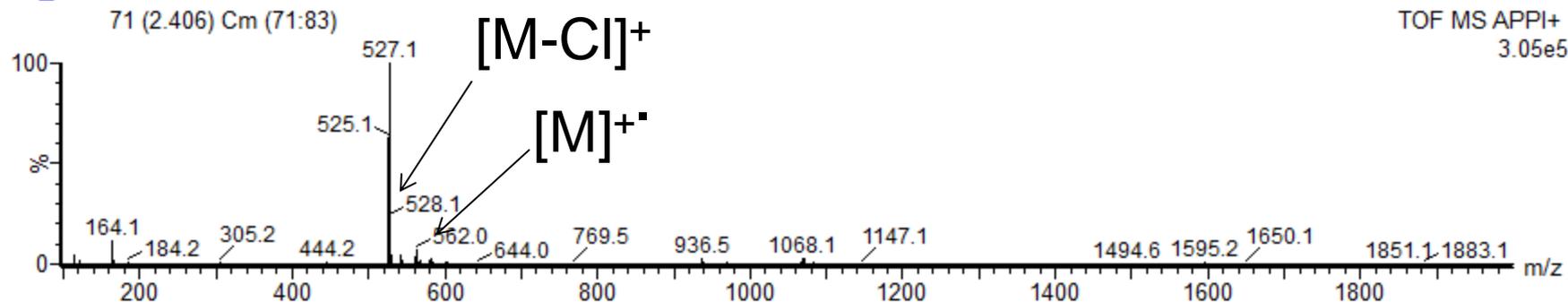


# Conjugated compounds

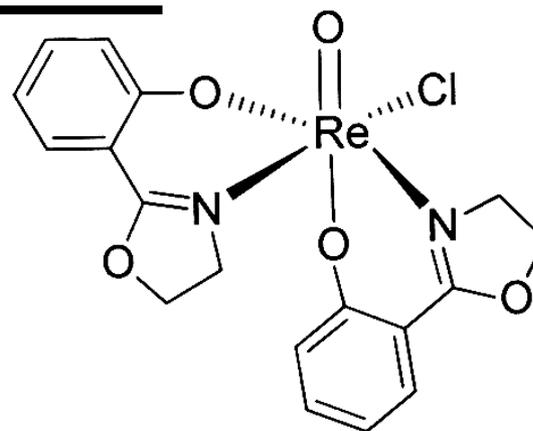
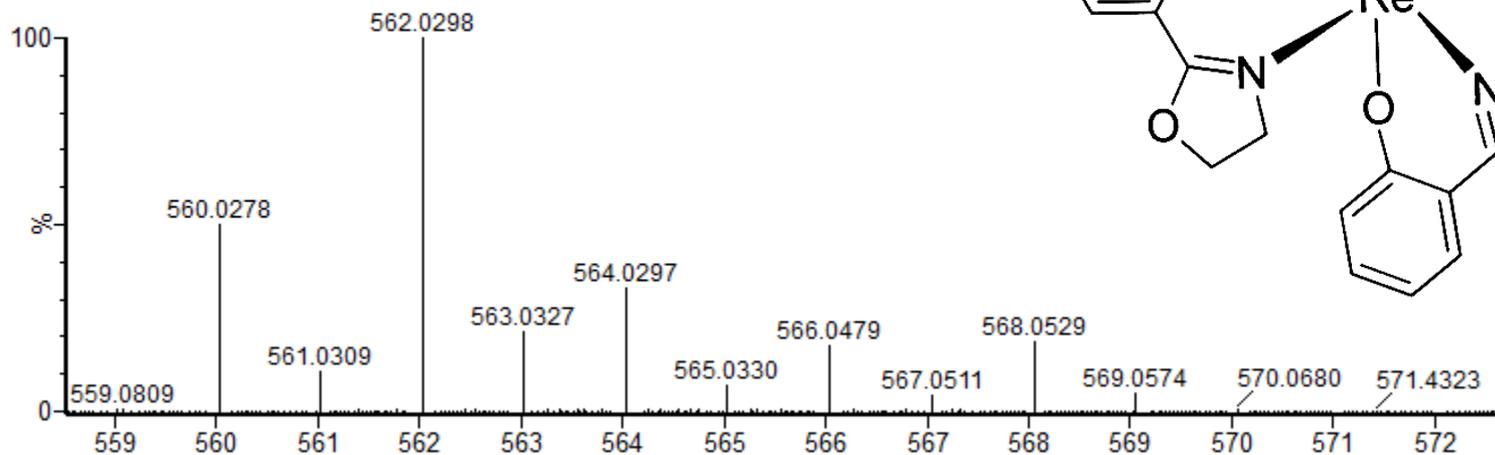


# Organometallic

BB\_ReS05

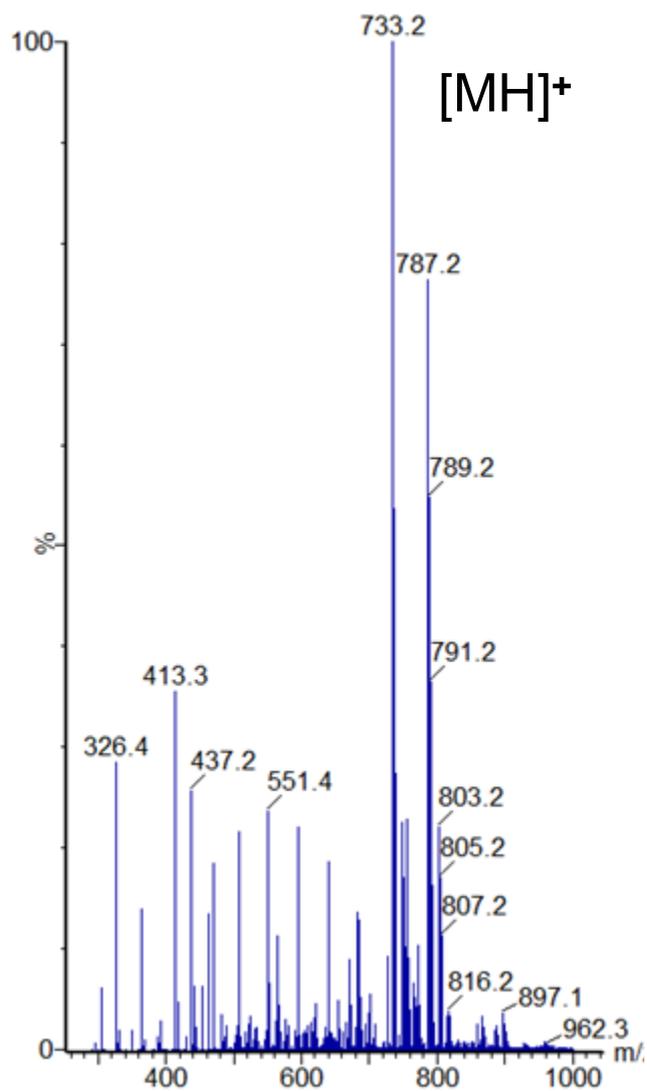


# Organometallic



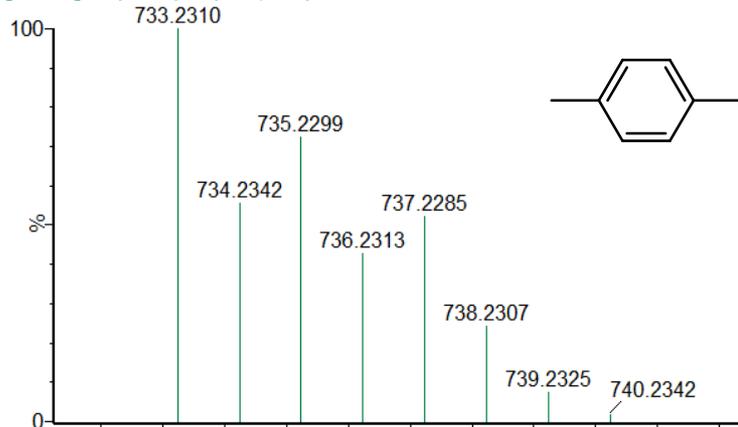
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	Na	Cl	185Re	187Re
562.0298	562.0305	-0.7	-1.2	11.5	C18 H16 N2 O5 Cl 187Re	312.0	0.3	18	16	2	5		1		1
	562.0292	0.6	1.1	12.0	C16 H14 N5 O4 Cl 187Re	313.6	2.0	16	14	5	4		1		1
	562.0294	0.4	0.7	17.0	C23 H16 N4 O9 Cl2	323.2	11.6	23	16	4	9		2	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

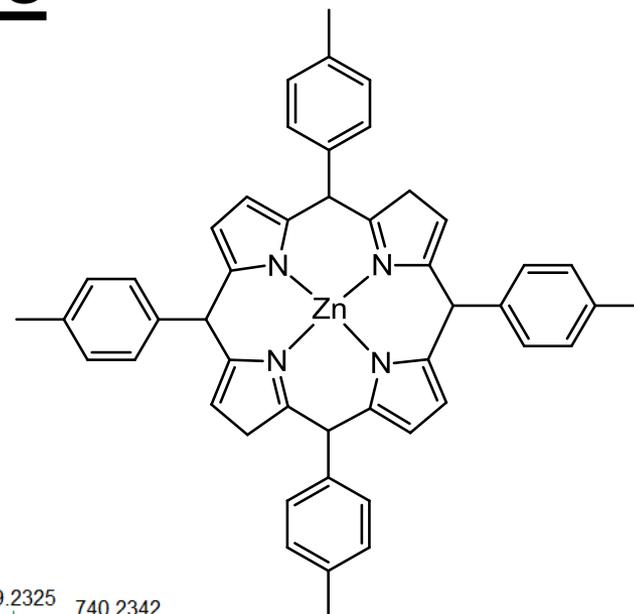
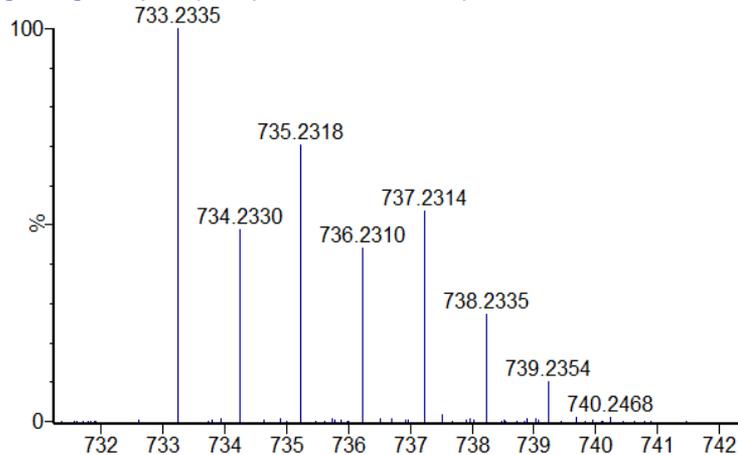


**Zn(TTP)**

goldberg 5 (0.067) Is (1.00,0.10) C<sub>48</sub>H<sub>36</sub>N<sub>4</sub>ZnH



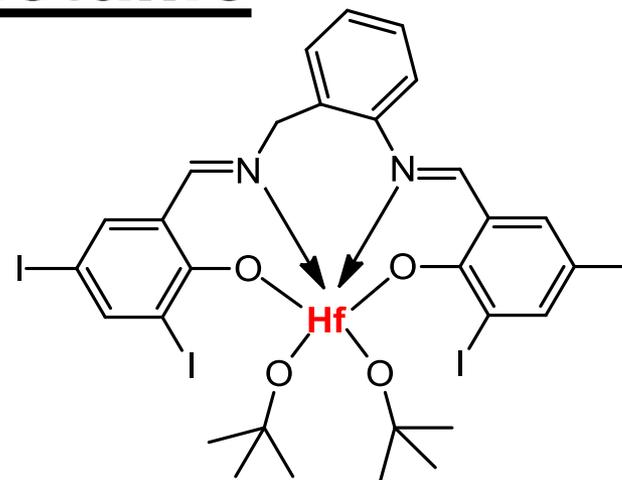
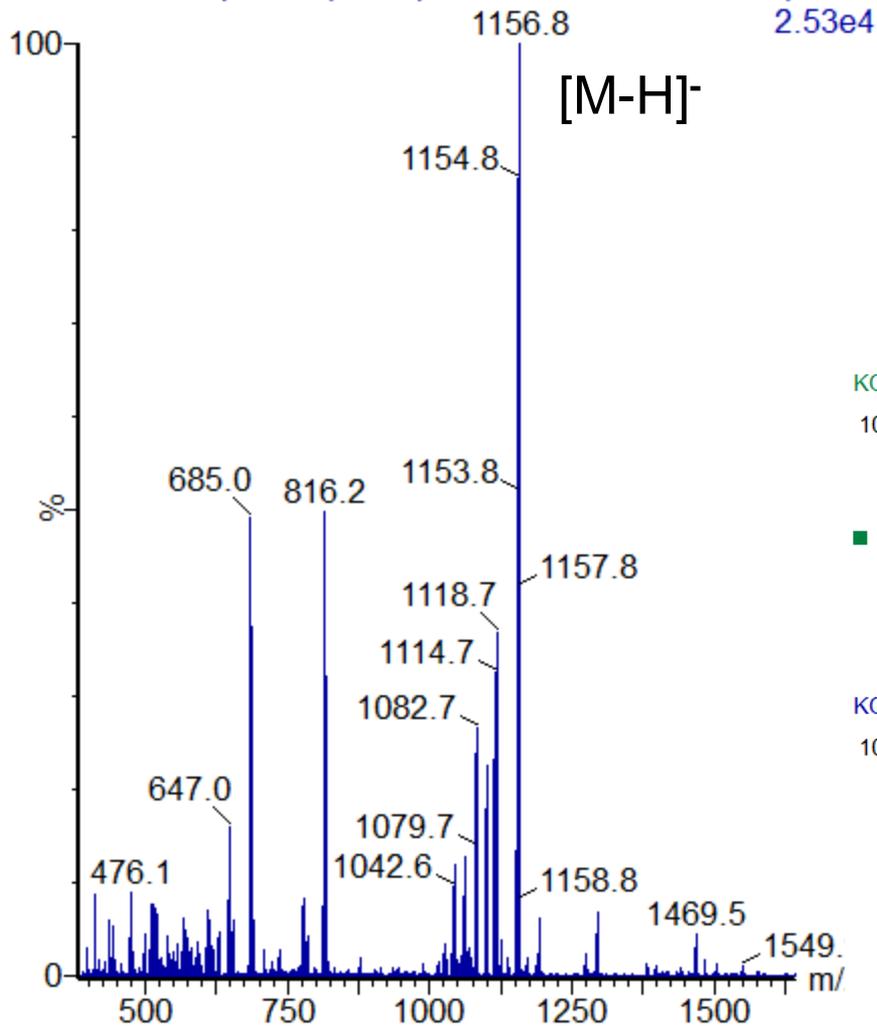
goldberg 5 88 (4.445) Cm (83:88-150:200x10.000)



# Organometallic

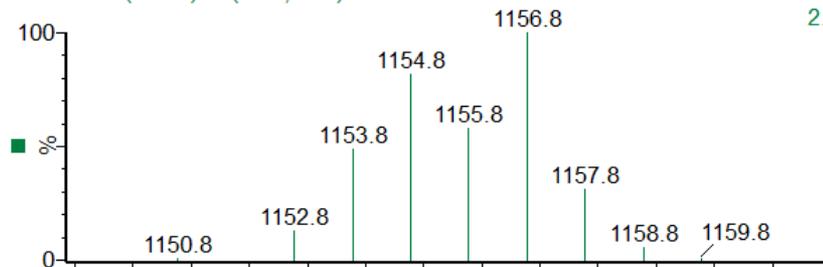
KP-616Hf

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



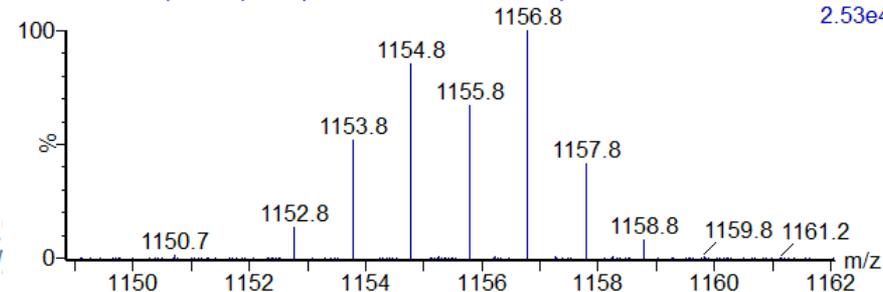
KOL112C (0.067) Is (1.00,0.10) C<sub>29</sub>H<sub>29</sub>HfI<sub>4</sub>N<sub>2</sub>O<sub>4</sub>

TOF MS APPI-  
2.95e12



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

TOF MS APPI-  
2.53e4

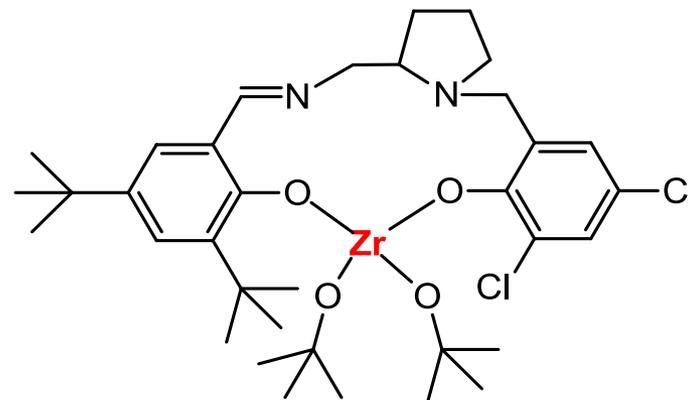
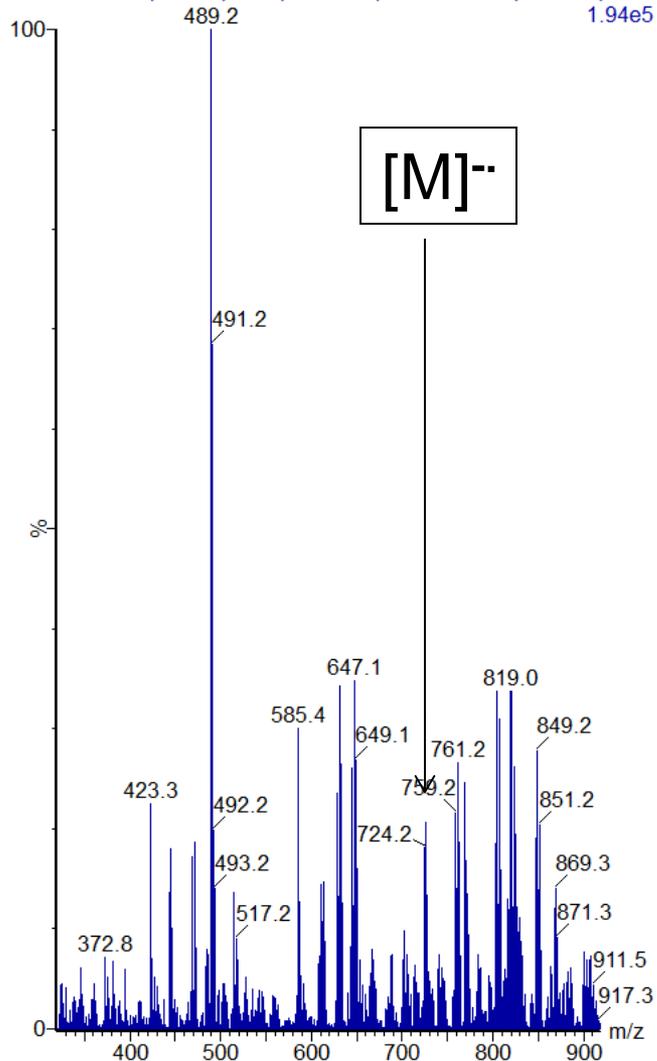


# Organometallic

KP-1123Zr

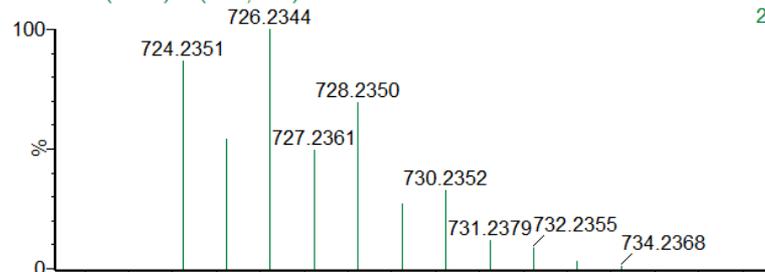
KOL113B 214 (10.785) Cm (189:222-(511:540+1:23)x10.000)

1.94e5



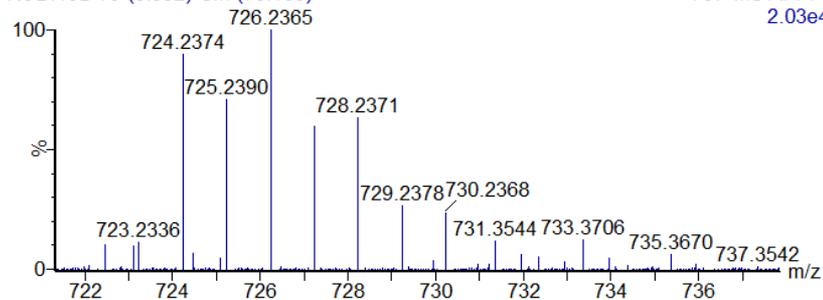
KOL113B (0.067) Is (1.00,0.10) C<sub>35</sub>H<sub>52</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>4</sub>Zr

TOF MS APPI-  
2.25e12

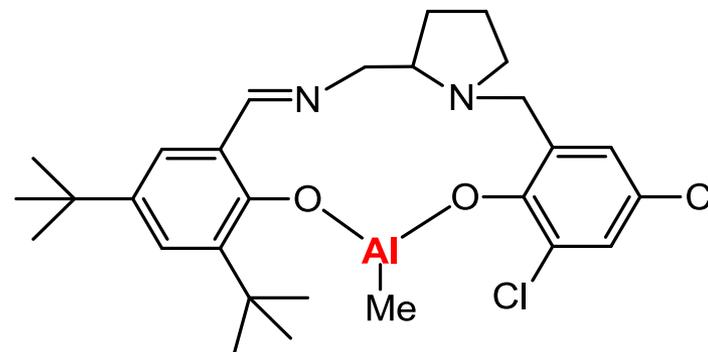
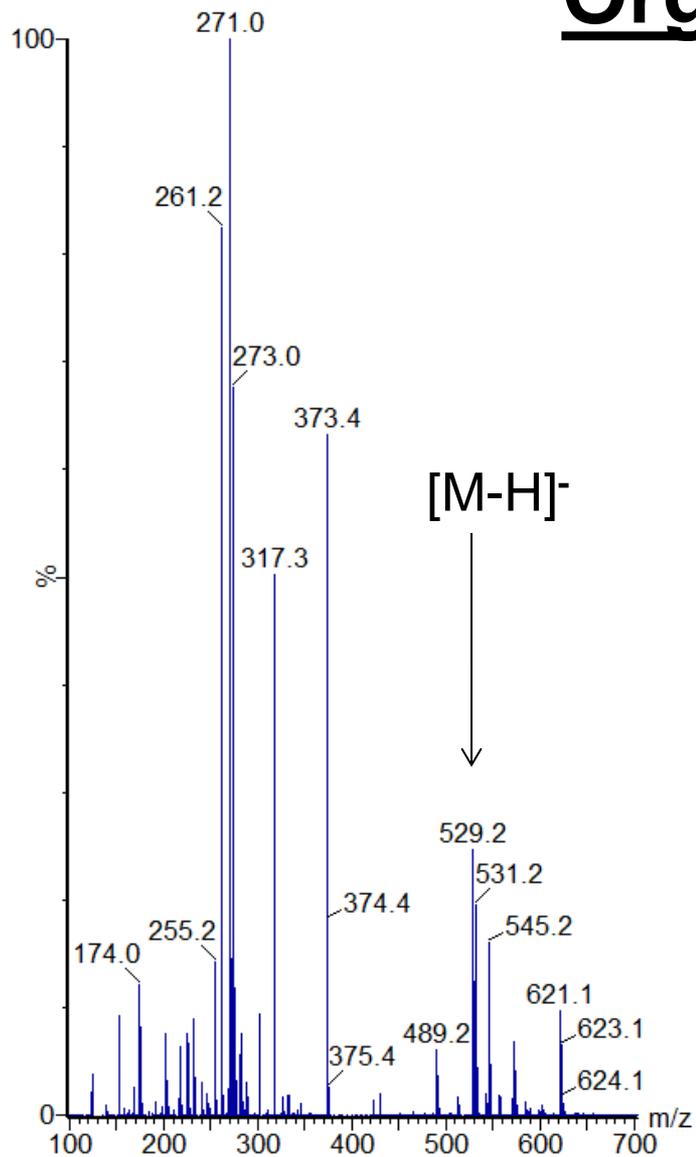


KOL113B 79 (3.992) Cm (78:103)

TOF MS APPI-  
2.03e4

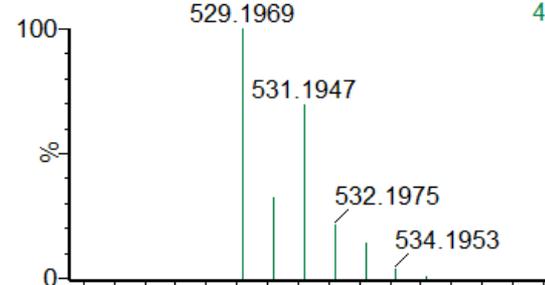


# Organometallic

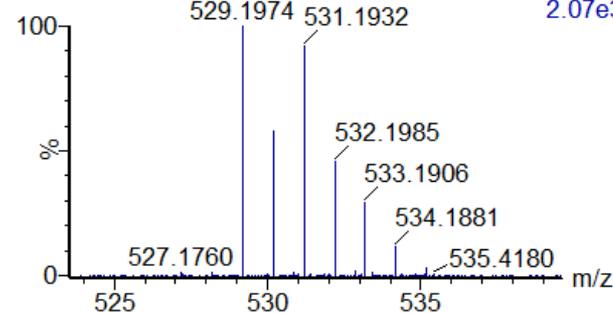


**KP-1123AlMe**

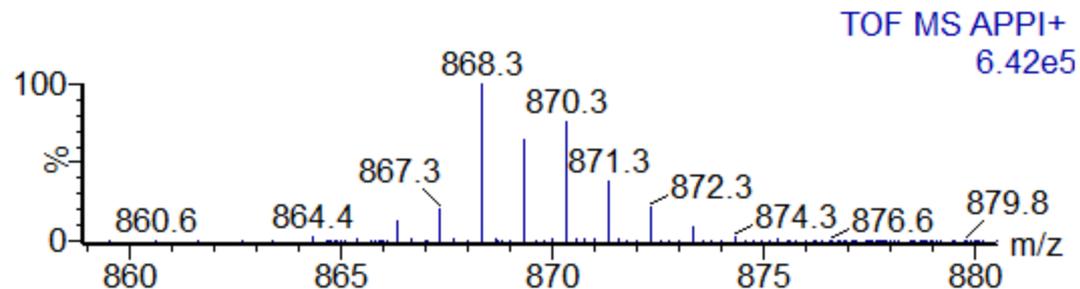
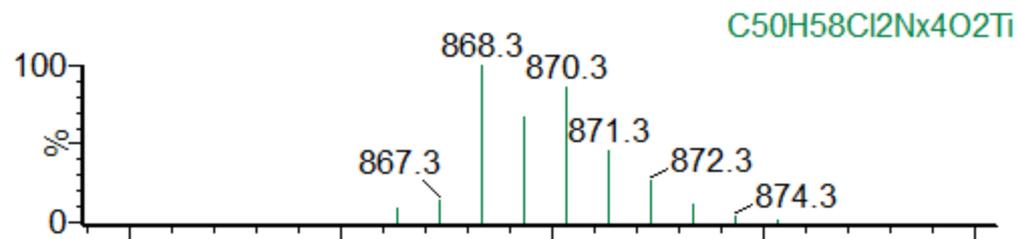
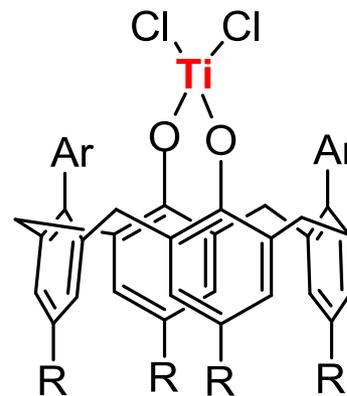
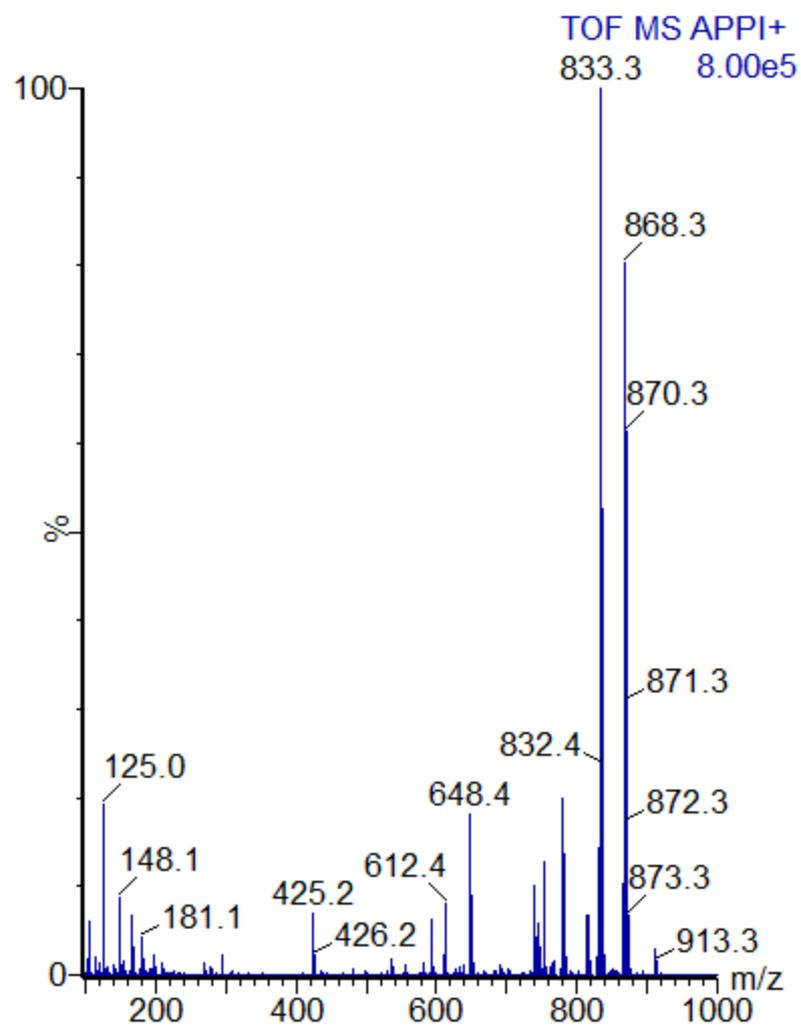
KOL114 (0.067) Is (1.00,0.10) C<sub>28</sub>H<sub>36</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>Al 4.14e12



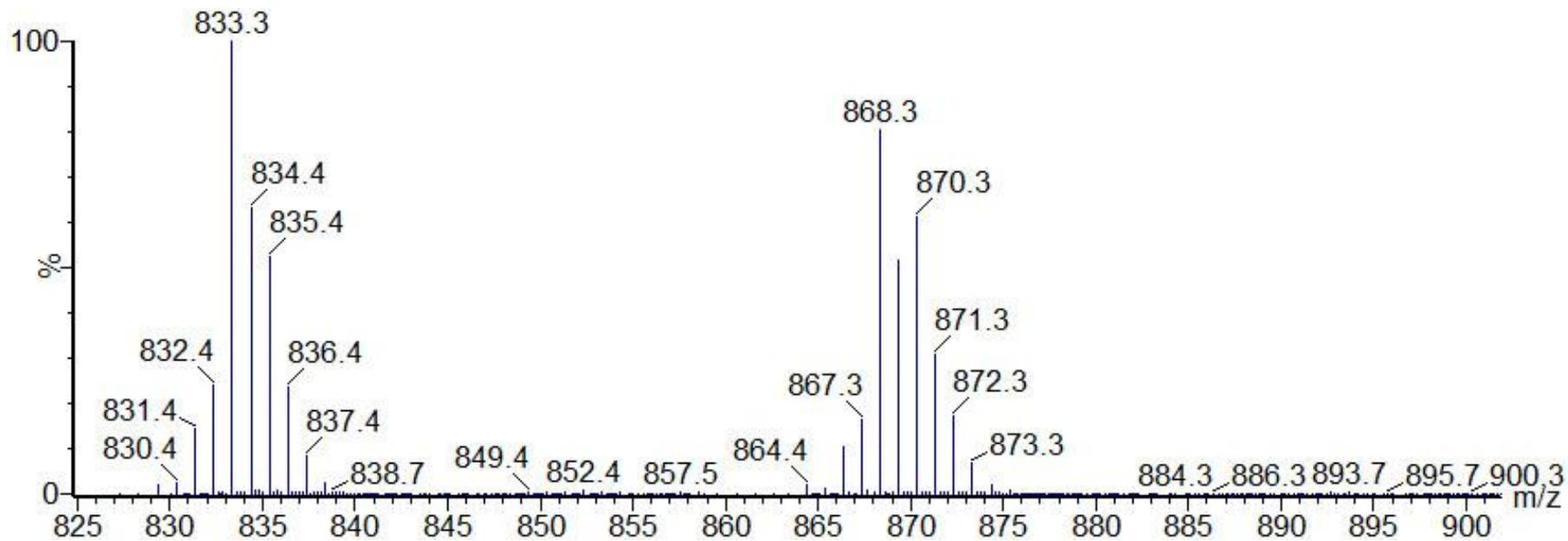
KOL114 616 (31.012) Cm (611:616) TOF MS APPI- 2.07e3



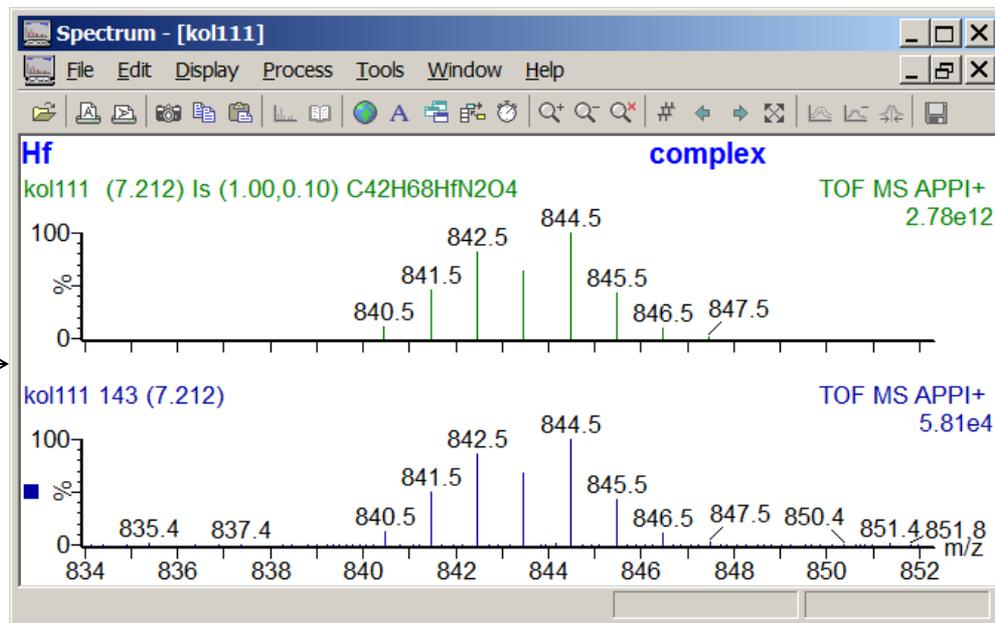
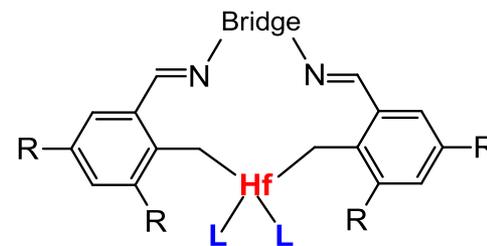
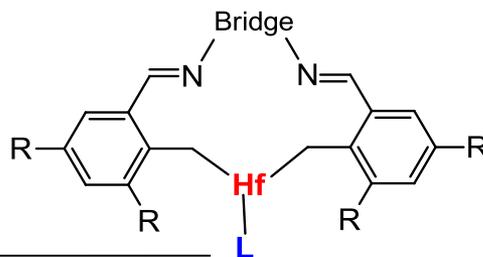
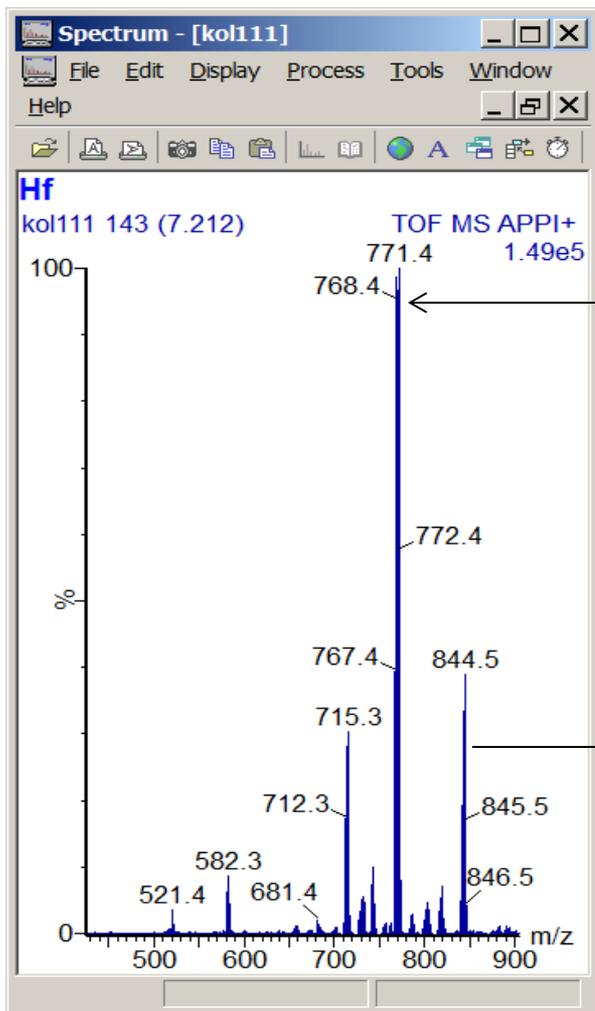
# Organometallic



# Organometallic

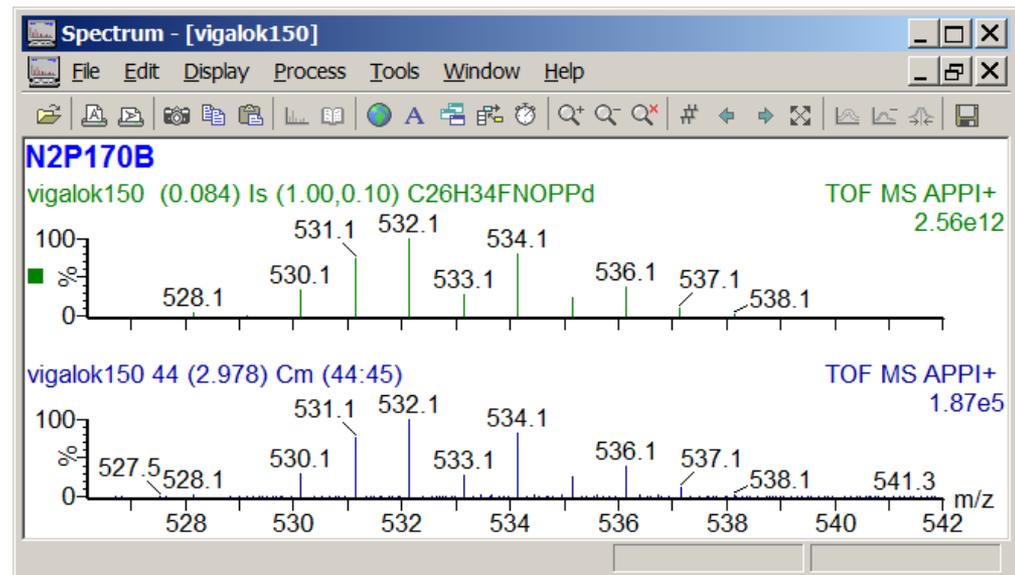
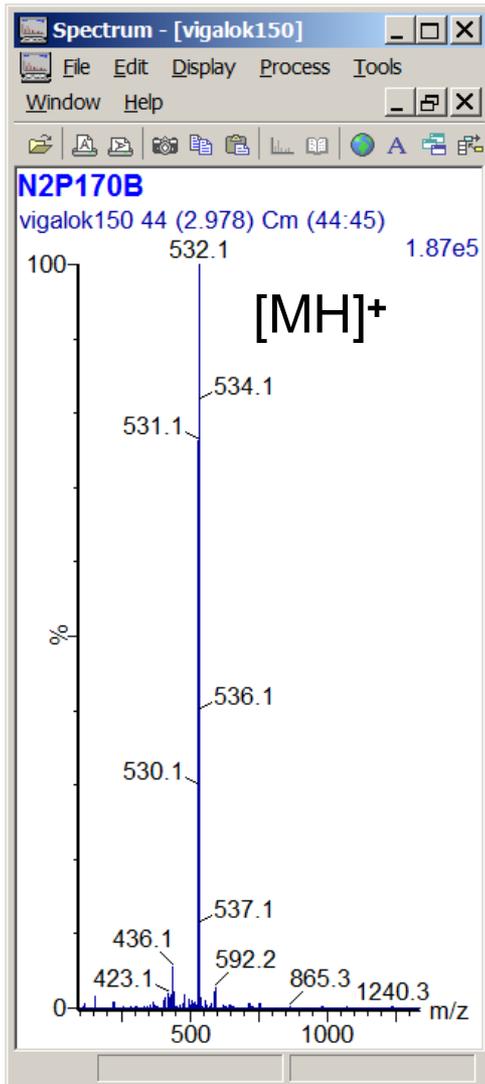
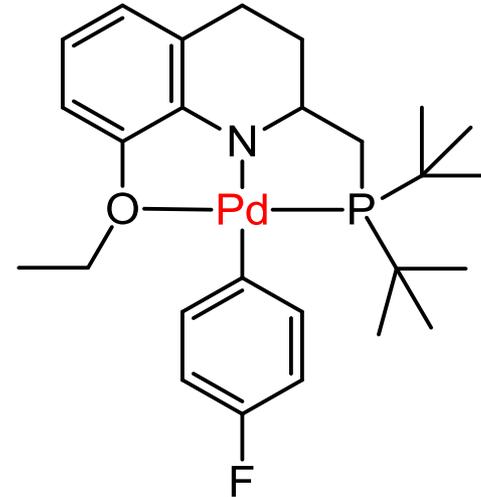


# Organometallic





# Organometallic

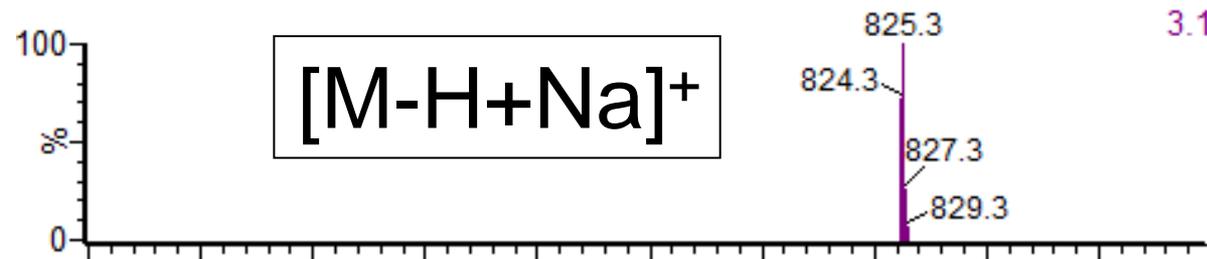


# Organometallic

C<sub>32</sub>H<sub>47</sub>PtP<sub>2</sub>F<sub>6</sub>Na

TOF MS APPI+  
3.19e12

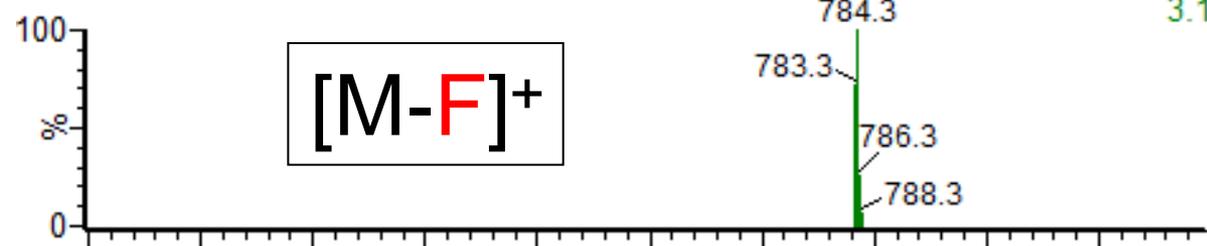
[M-H+Na]<sup>+</sup>



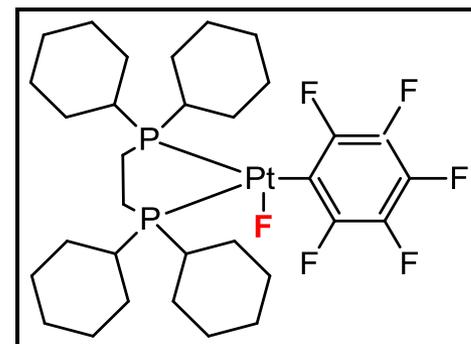
C<sub>32</sub>H<sub>48</sub>PtP<sub>2</sub>F<sub>5</sub>

TOF MS APPI+  
3.19e12

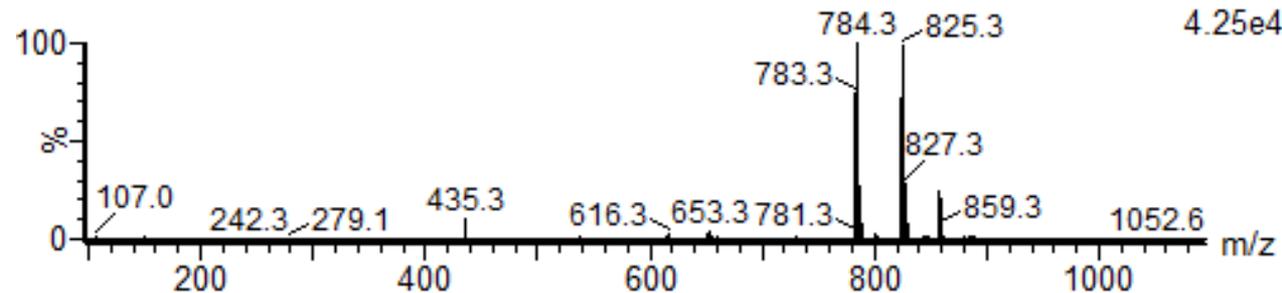
[M-F]<sup>+</sup>



C<sub>32</sub>H<sub>48</sub>PtP<sub>2</sub>F<sub>6</sub>



TOF MS APPI+  
4.25e4



# 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