

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010320\
 Data File : VX014402.D
 Acq On : 03 Jan 2020 15:50
 Operator : JC/SP
 Sample : K6476-05
 Misc : 6.98g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WP022SB455_191227-12-14

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	43	rBV	505407	656567	26.19%	3.609%
2	1.265	59	62	67	rBV	34675	46053	1.84%	0.253%
3	1.674	106	129	130	rBV9	93952	494898	19.74%	2.721%
4	3.009	342	348	355	rBV	16028	39750	1.59%	0.219%
5	5.490	744	755	771	rBV2	238141	760891	30.36%	4.183%
6	5.648	771	781	797	rVB	500055	1427785	56.96%	7.849%
7	6.057	836	848	864	rBV2	284561	813184	32.44%	4.470%
8	6.849	967	978	993	rBV	721369	1814856	72.40%	9.977%
9	8.709	1276	1283	1293	rBV	1579610	2506601	100.00%	13.779%
10	8.825	1297	1302	1305	rVV3	15177	27380	1.09%	0.151%
11	10.111	1507	1513	1522	rBV	1501715	2150168	85.78%	11.820%
12	11.135	1676	1681	1691	rBV	1311013	1682793	67.13%	9.251%
13	12.074	1830	1835	1843	rVB	1706590	2103724	83.93%	11.565%
14	12.391	1878	1887	1890	rBV4	25207	55339	2.21%	0.304%
15	12.470	1895	1900	1904	rBV5	23403	29582	1.18%	0.163%
16	14.964	2304	2309	2313	rBV2	101860	131110	5.23%	0.721%
17	15.110	2328	2333	2334	rBV4	20312	30892	1.23%	0.170%
18	15.147	2334	2339	2345	rVV	1768607	2291962	91.44%	12.599%
19	15.415	2378	2383	2389	rVB	279149	390478	15.58%	2.147%
20	15.573	2405	2409	2416	rVB3	52863	97861	3.90%	0.538%
21	15.756	2433	2439	2451	rVB4	108912	263829	10.53%	1.450%
22	15.970	2470	2474	2483	rVB9	25347	58636	2.34%	0.322%
23	16.128	2494	2500	2509	rVB3	40509	107126	4.27%	0.589%
24	16.238	2513	2518	2525	rVB2	47651	89571	3.57%	0.492%
25	16.445	2545	2552	2557	rBV2	59948	120107	4.79%	0.660%

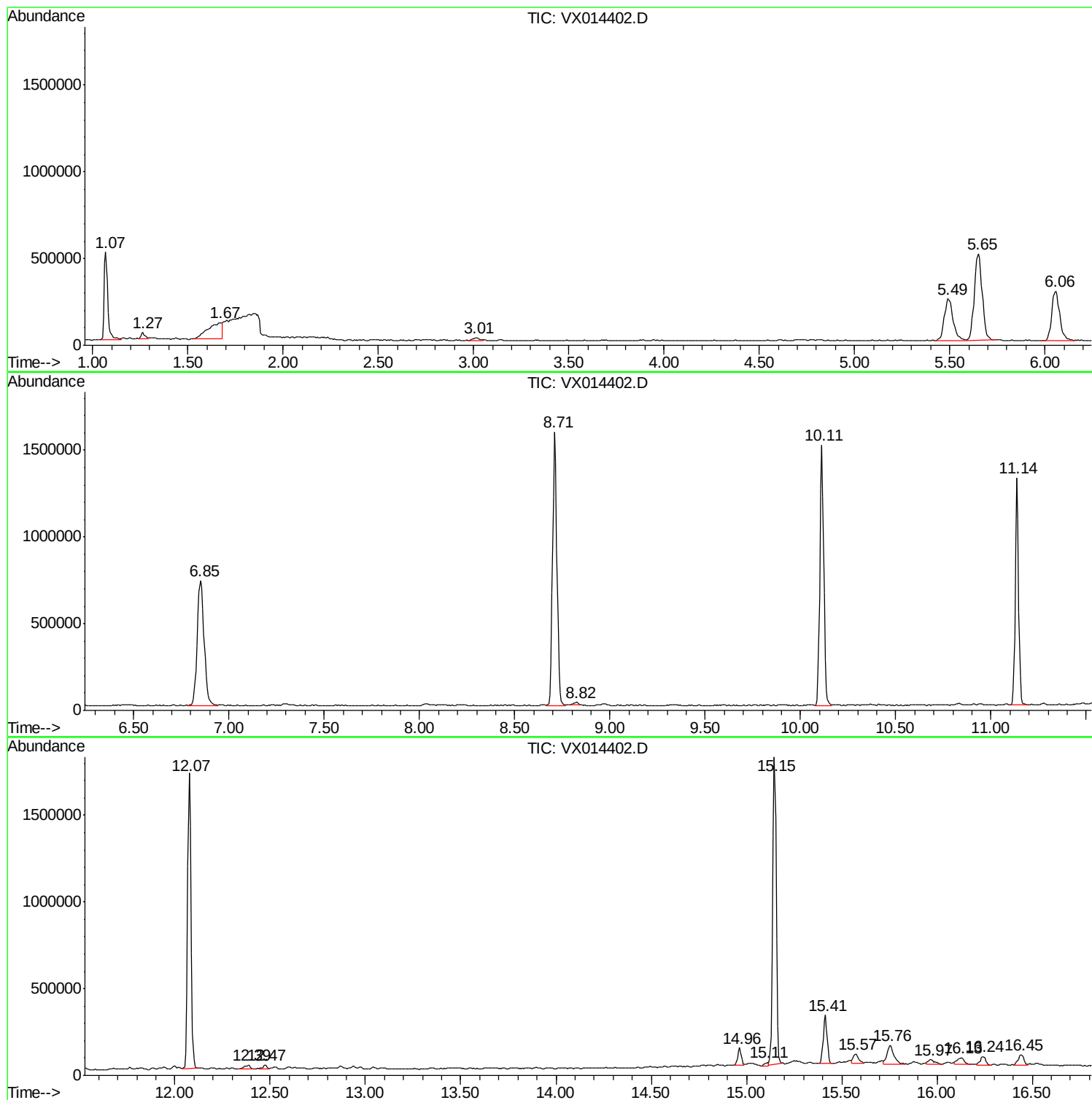
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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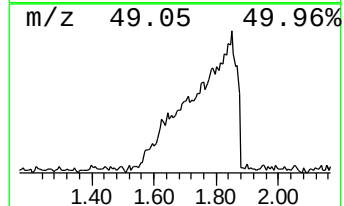
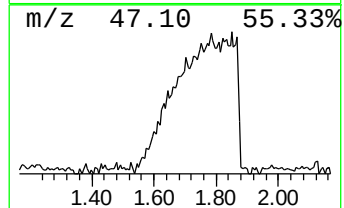
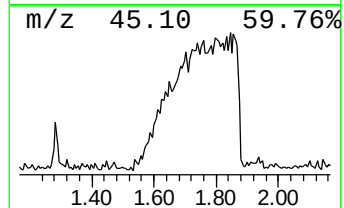
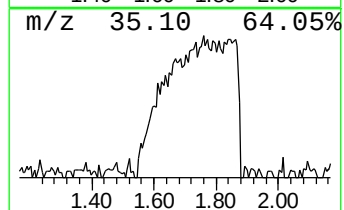
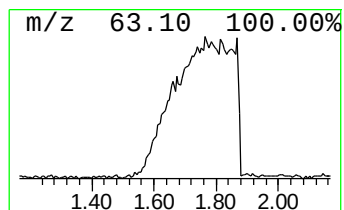
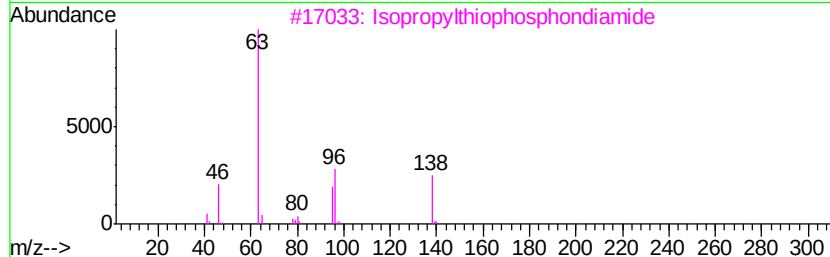
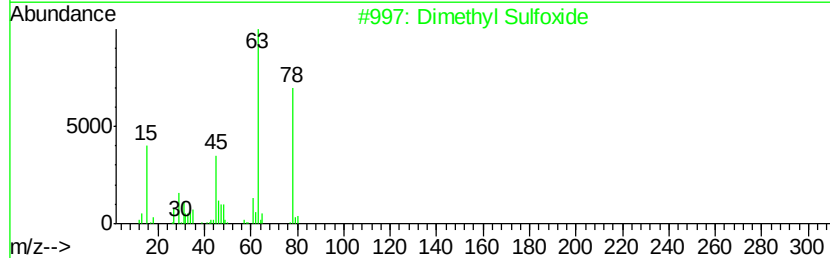
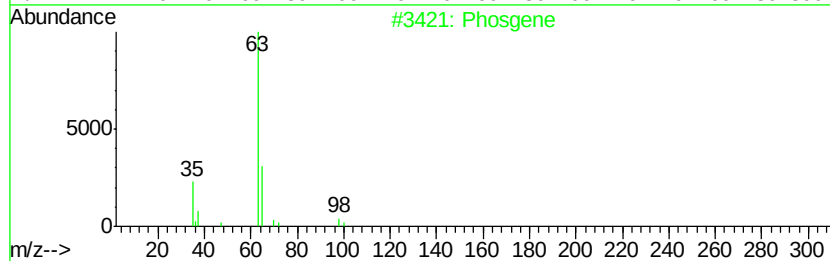
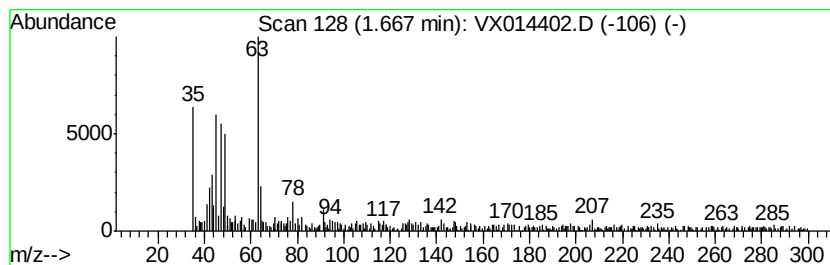
Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown1.67 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	17.33 ug/l	494898	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosgene	98	CCl2O	000075-44-5	43
2		Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	35
3		Isopropylthiophosphondiamide	138	C3H11N2PS	1000306-03-6	23
4		2-Anilino-4-(methylamino)-6-(pip...	363	C18H17N7O2	1000225-97-3	20
5		(Z)-1-Chloro-2-(methylsulfonyl)e...	140	C3H5ClO2S	115584-12-8	17



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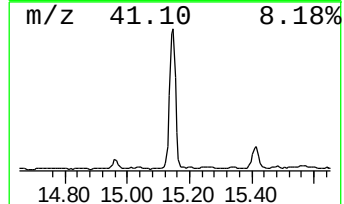
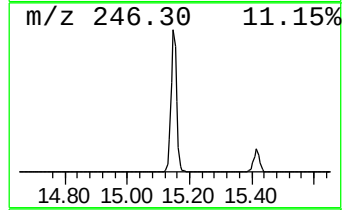
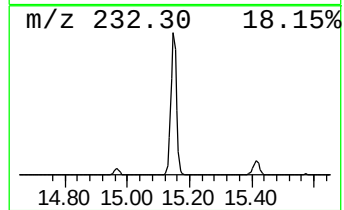
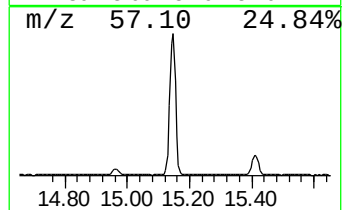
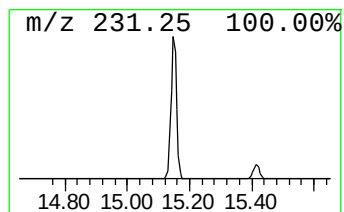
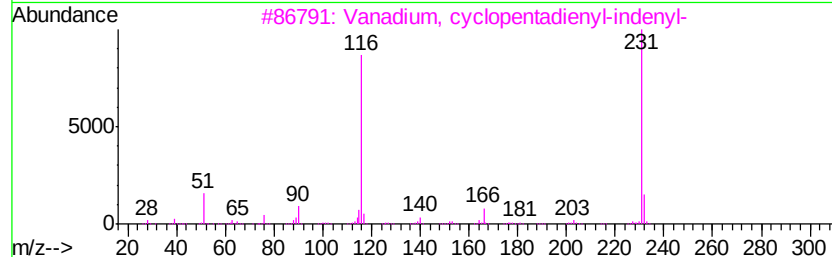
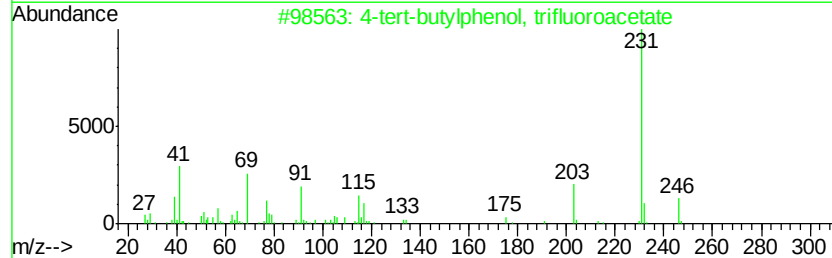
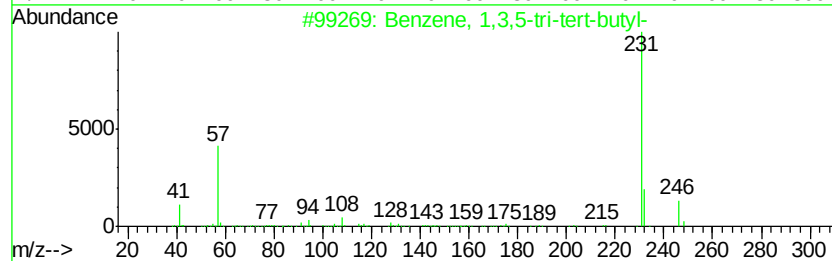
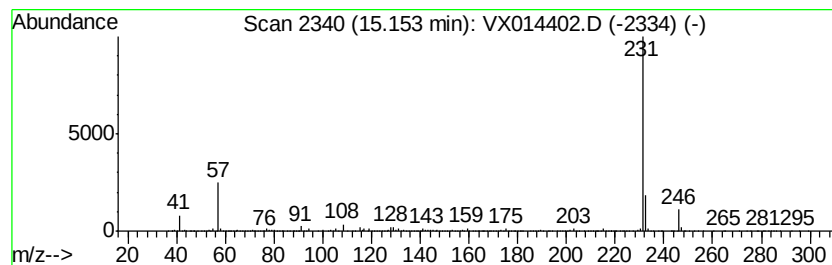
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Peak Number 3 Benzene, 1,3,5-tri-tert-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	54.47 ug/l	2291960	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1,3,5-tri-tert-butyl-	246 C18H30	001460-02-2 90
2		4-tert-butylphenol, trifluoroace...	246 C12H13F3O2	1000376-51-5 72
3		Vanadium, cyclopentadienyl-indenyl-	231 C14H12V	1000152-33-3 64
4		Benzene, 1,2,4,5-tetrakis(1-meth...	246 C18H30	000635-11-0 56
5		Benzene, hexaethyl-	246 C18H30	000604-88-6 56



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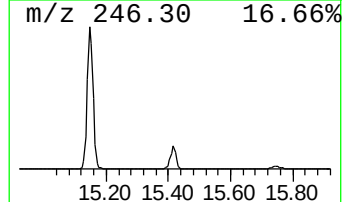
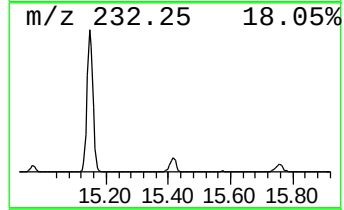
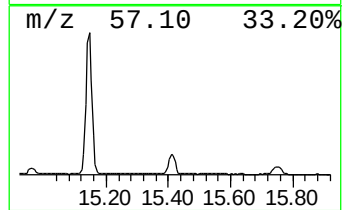
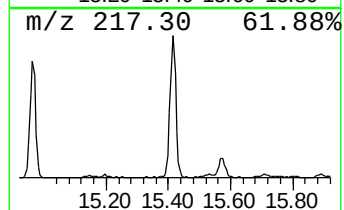
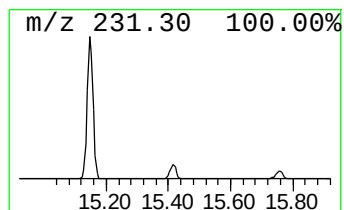
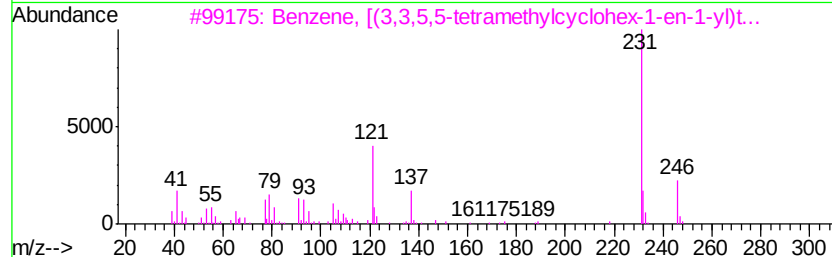
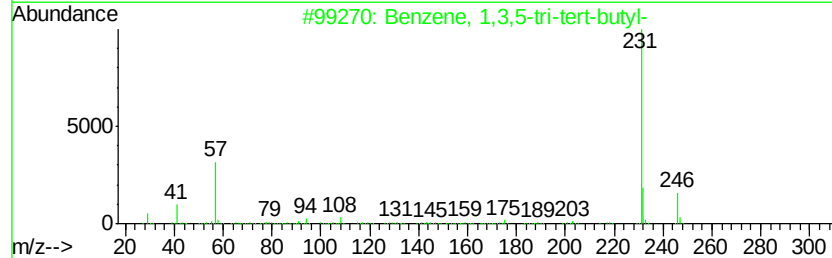
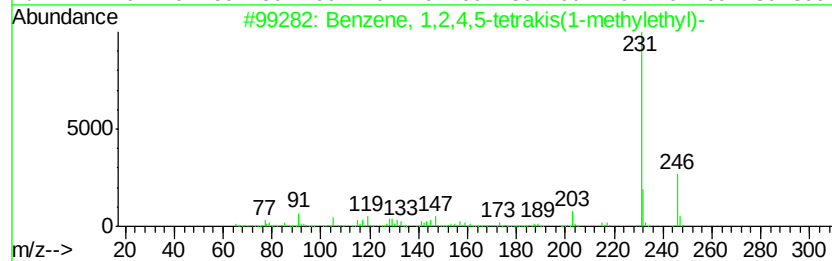
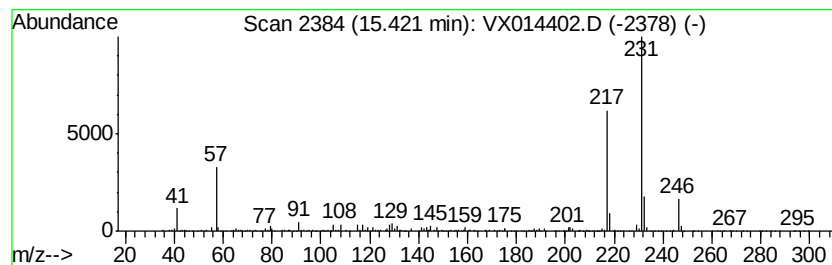
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 Peak Number 4 Benzene, 1,2,4,5-tetrakis(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.42	9.28 ug/l	390478	1,4-Dichlorobenzene-d4	12.07		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,4,5-tetrakis(1-meth...	246	C18H30	000635-11-0	89
2		Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	64
3		Benzene, [(3,3,5,5-tetramethylcy...	246	C16H22S	102108-78-1	47
4		Benzene, hexaethyl-	246	C18H30	000604-88-6	45
5		Cannabichromene	314	C21H30O2	020675-51-8	43



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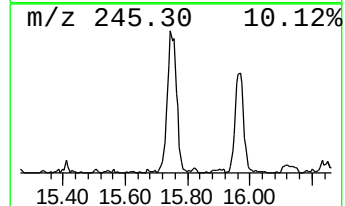
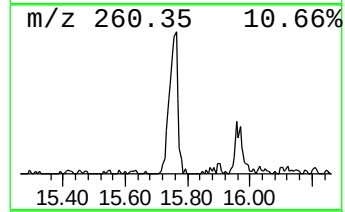
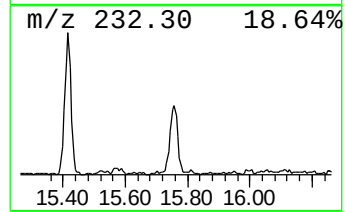
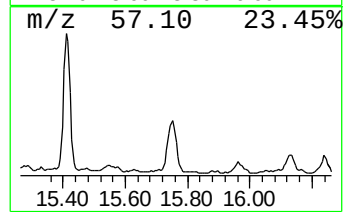
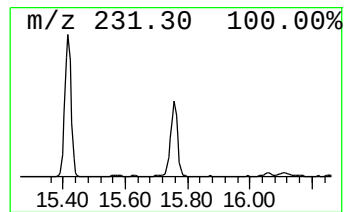
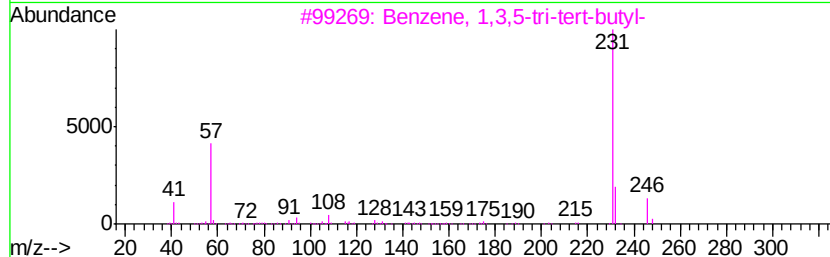
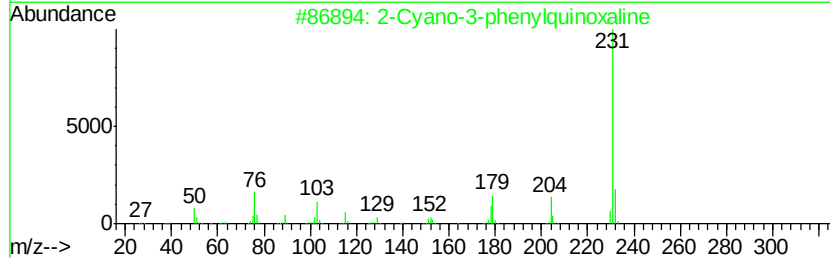
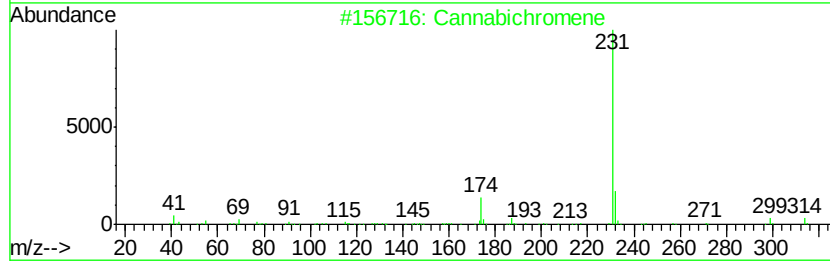
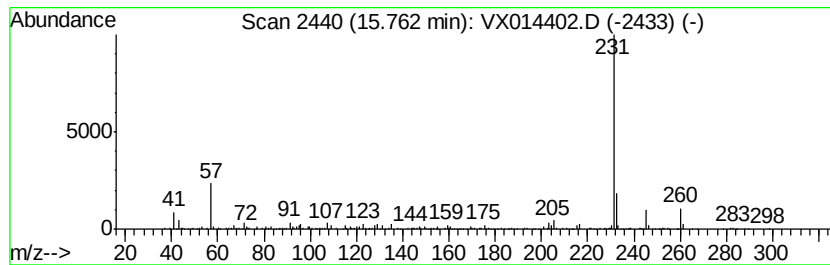
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Peak Number 5 Cannabichromene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.76	6.27 ug/l	263829	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cannabichromene	314	C21H30O2	020675-51-8	59
2	2-Cyano-3-phenylquinoxaline	231	C15H9N3	059393-45-2	59
3	Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	45
4	Benzene, 1,2,4,5-tetrakis(1-meth...	246	C18H30	000635-11-0	45
5	6-[2-Benzylpiperidino]-3-nitropi...	322	C18H18N4O2	093683-77-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1,3,5-tr...	15.15	54.5	ug/l	2291960	4	12.07	2103720	50.0
Benzene, 1,2,4,5-...	15.42	9.3	ug/l	390478	4	12.07	2103720	50.0
Cannabichromene	15.76	6.3	ug/l	263829	4	12.07	2103720	50.0