

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062920\
 Data File : VX017024.D
 Acq On : 29 Jun 2020 21:57
 Operator : JC/SP
 Sample : L3146-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 200624026-02-VOA

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\82X062920W.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	1.276	28	31	45	rVB	358313	382011	5.56%	1.164%
2	2.428	213	220	223	rBV2	85379	135579	1.97%	0.413%
3	3.014	303	316	334	rBV	2488513	5462670	79.50%	16.640%
4	4.660	572	586	598	rBV	2149361	6871518	100.00%	20.931%
5	4.983	630	639	646	rBV	112583	319141	4.64%	0.972%
6	5.087	646	656	682	rVB	1274843	3826899	55.69%	11.657%
7	5.464	705	718	729	rBV2	158844	461440	6.72%	1.406%
8	5.629	734	745	759	rVB	267016	755844	11.00%	2.302%
9	6.031	801	811	820	rBV	288906	758645	11.04%	2.311%
10	6.117	820	825	830	rVV	33167	86341	1.26%	0.263%
11	6.245	832	846	867	rVV2	196053	859463	12.51%	2.618%
12	6.830	932	942	957	rVV	695110	1663292	24.21%	5.066%
13	7.952	1120	1126	1140	rVB	64388	126777	1.84%	0.386%
14	8.592	1227	1231	1233	rBV	48836	73258	1.07%	0.223%
15	8.622	1233	1236	1241	rVB	53632	83353	1.21%	0.254%
16	8.696	1241	1248	1254	rBV	1461140	2270725	33.05%	6.917%
17	8.763	1254	1259	1268	rVB2	140289	237587	3.46%	0.724%
18	8.848	1268	1273	1279	rBV	107425	167971	2.44%	0.512%
19	9.421	1359	1367	1373	rBV	341616	494637	7.20%	1.507%
20	10.098	1465	1478	1489	rVV	1528224	2251061	32.76%	6.857%
21	10.250	1498	1503	1511	rVV	39899	74760	1.09%	0.228%
22	10.342	1513	1518	1524	rVV	184962	268879	3.91%	0.819%
23	10.421	1524	1531	1542	rVB2	37670	77324	1.13%	0.236%
24	10.683	1569	1574	1578	rBV	132947	180425	2.63%	0.550%
25	11.122	1640	1646	1651	rBV	1420504	1794670	26.12%	5.467%
26	11.415	1688	1694	1699	rVV2	35180	69693	1.01%	0.212%
27	11.793	1741	1756	1760	rBV	49589	92543	1.35%	0.282%
28	11.927	1771	1778	1786	rVB3	94291	139418	2.03%	0.425%
29	12.061	1794	1800	1807	rVB	1265722	1636825	23.82%	4.986%
30	12.128	1807	1811	1816	rBV2	50140	84315	1.23%	0.257%
31	12.280	1830	1836	1841	rBV	54147	86008	1.25%	0.262%
32	12.616	1888	1891	1896	rVB	109280	117908	1.72%	0.359%
33	12.799	1914	1921	1926	rVV	128666	202386	2.95%	0.616%
34	12.945	1933	1945	1950	rBV	298988	413399	6.02%	1.259%

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Sampling : 1 Min Area: 3 % of largest Peak
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35	13.000	1950	1954	1965	rVB2	93430	163164	2.37%	0.497%
36	13.512	2033	2038	2042	rBV	100734	139389	2.03%	0.425%

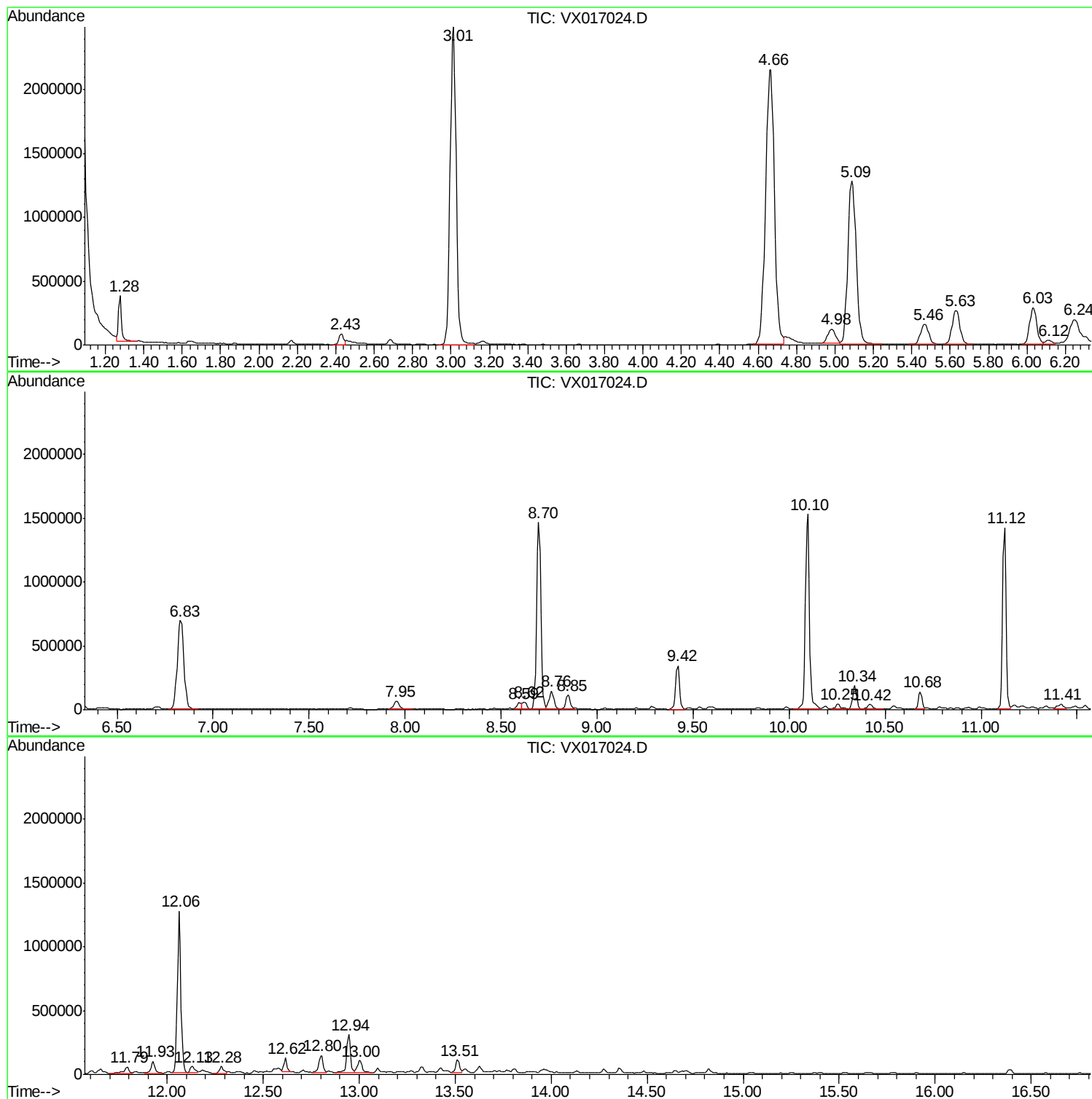
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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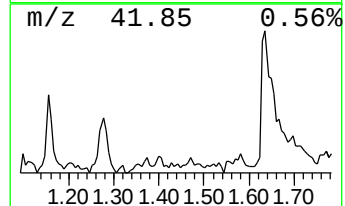
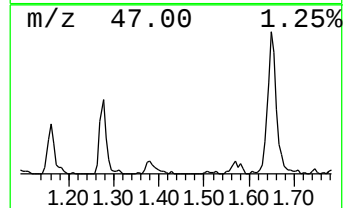
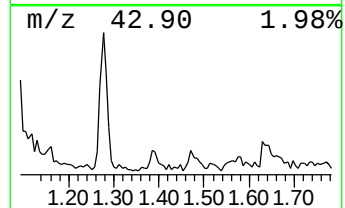
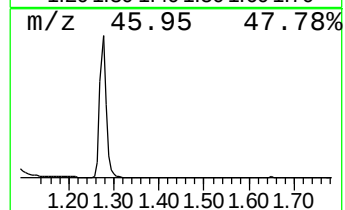
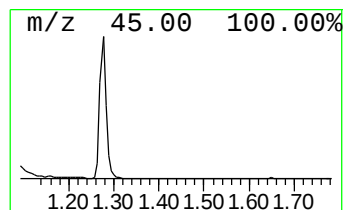
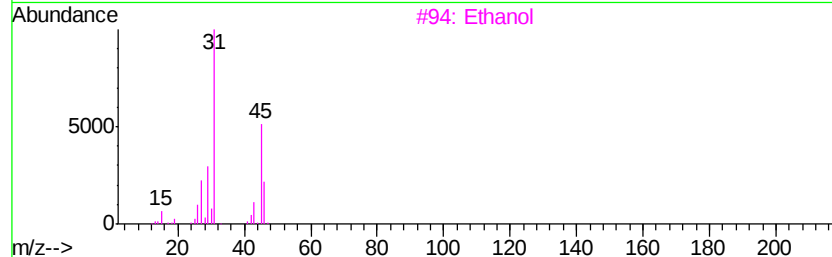
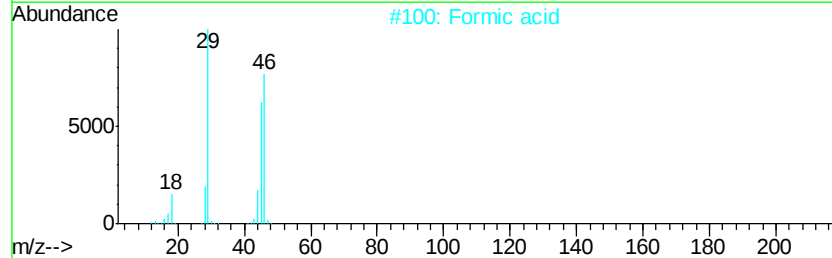
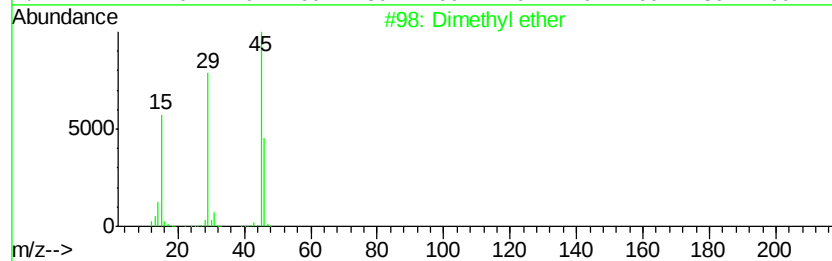
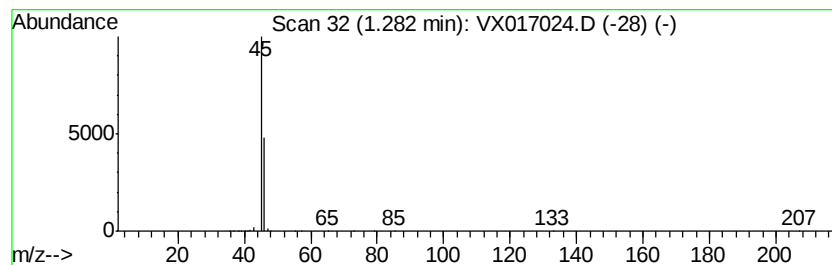
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Quant Title : SW846 8260

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

Peak Number 1 unknown1.28 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.28	25.27 ug/l	382011	Pentafluorobenzene	5.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dimethyl ether	46	C2H6O	000115-10-6	9
2		Formic acid	46	CH2O2	000064-18-6	7
3		Ethanol	46	C2H6O	000064-17-5	7
4		Oxalic acid	90	C2H2O4	000144-62-7	4
5		Methane, nitroso-	45	CH3NO	000865-40-7	3



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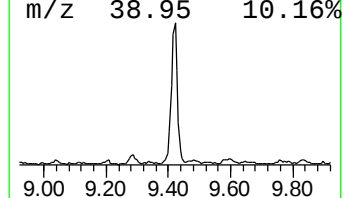
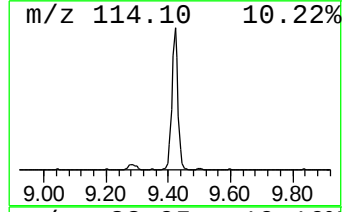
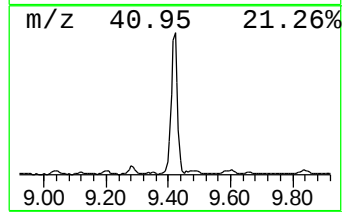
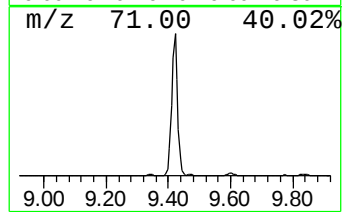
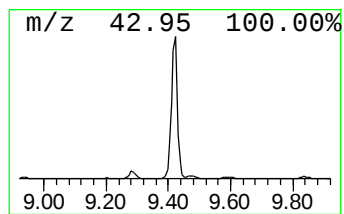
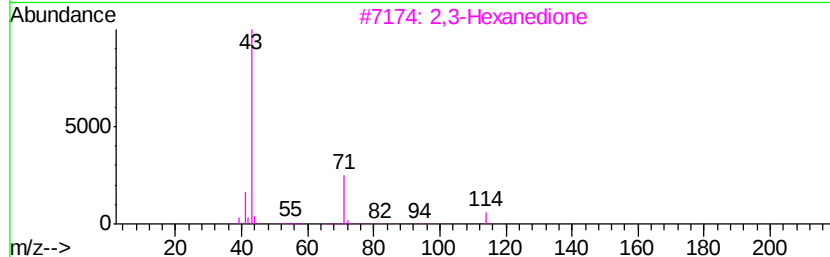
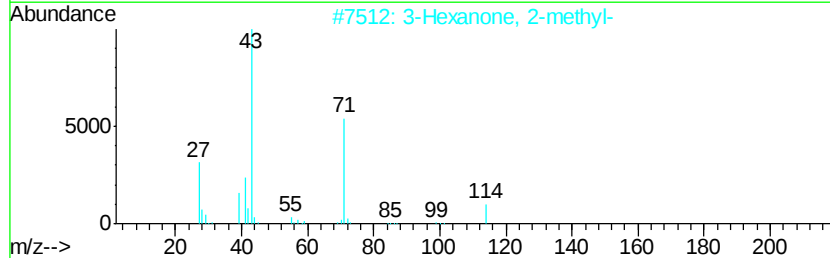
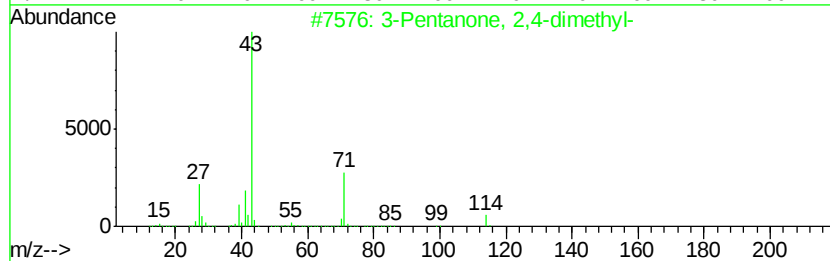
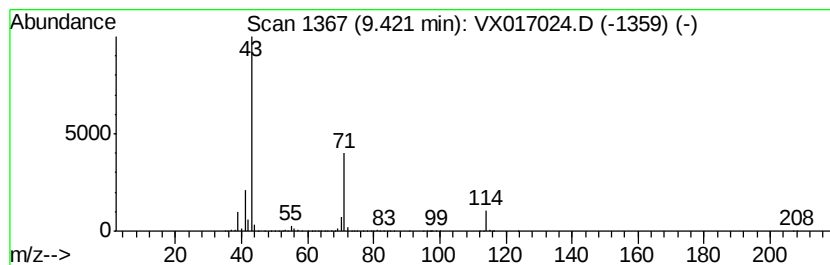
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	10.99 ug/l	494637	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3		2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4		4-Heptanone	114	C7H14O	000123-19-3	59
5		Pyrrolidine	71	C4H9N	000123-75-1	59



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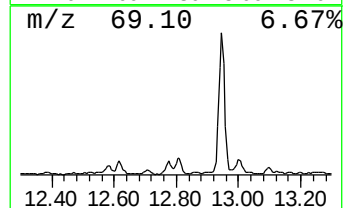
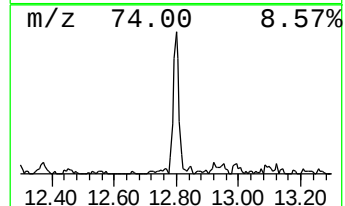
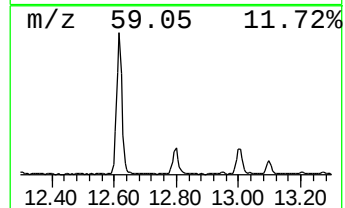
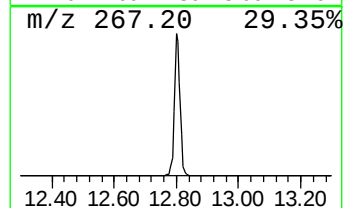
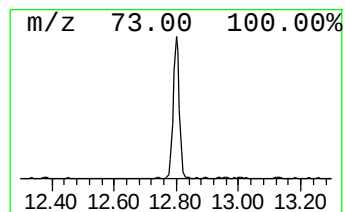
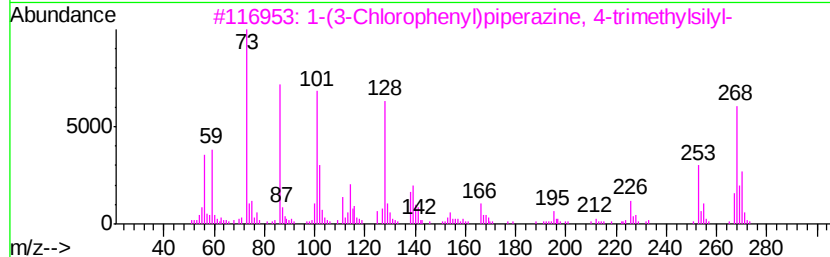
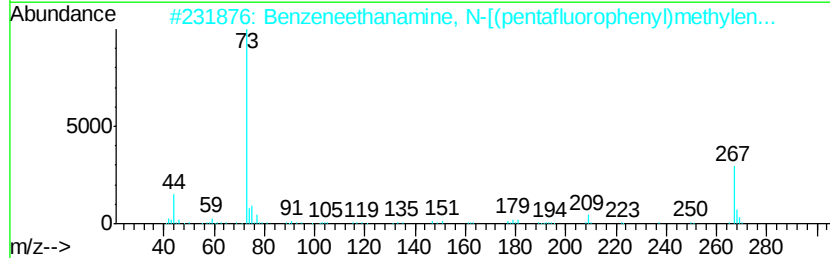
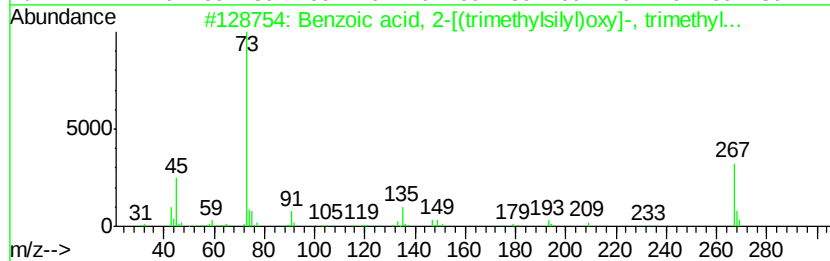
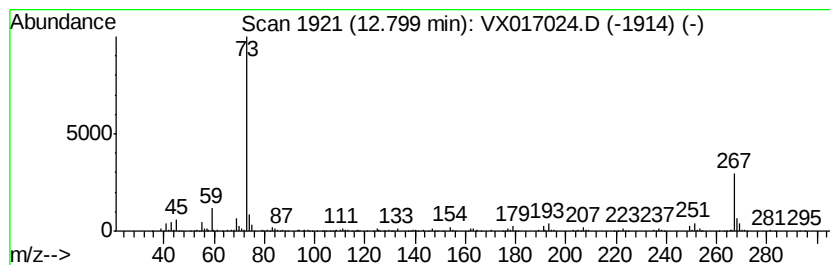
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Peak Number 5 Benzoic acid, 2-[(trimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	6.18 ug/l	202386	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	53
2		Benzenethanamine, N-[(pentafluorophenyl)methyl]...	475	C21H26F5N2Si2	055429-85-1	50
3		1-(3-Chlorophenyl)piperazine, 4-trimethylsilyl-	268	C13H21ClN2Si	1000373-99-3	27
4		1-Boraindane, 3-methyl-1-[1-(triethylsilyl)oxy]-	266	C17H23BSi	190316-36-0	25
5		1-(2-Methoxyethoxy)-2-methyl-2-pyridine...	162	C8H18O3	1000364-24-4	22



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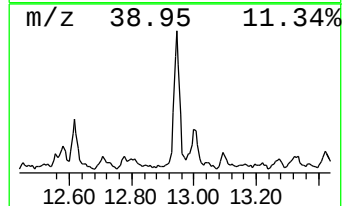
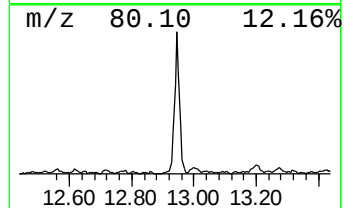
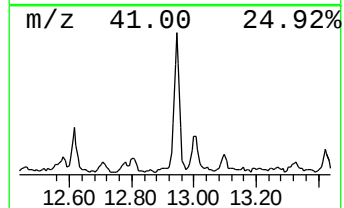
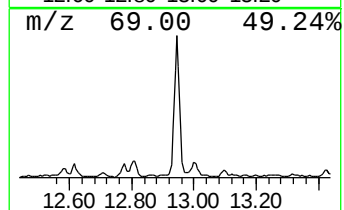
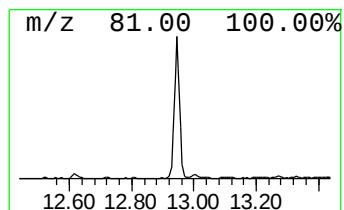
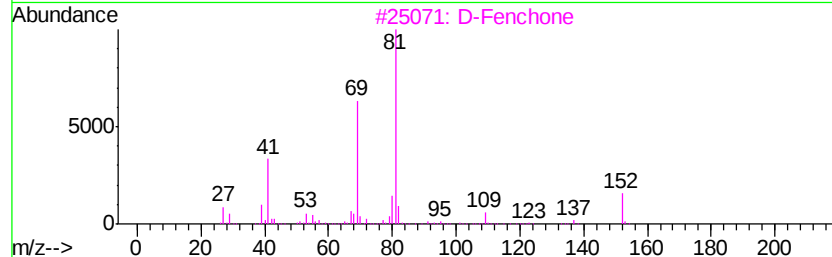
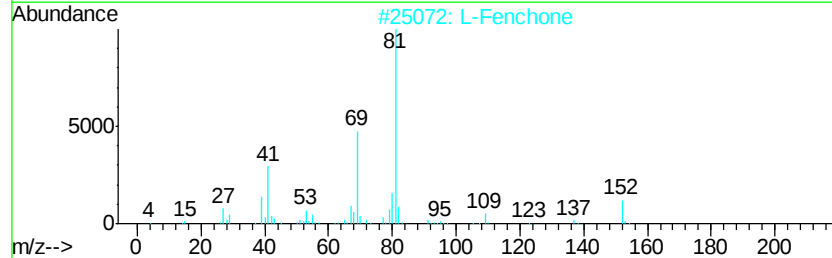
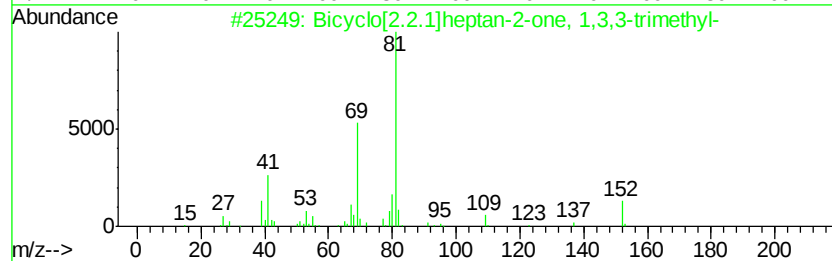
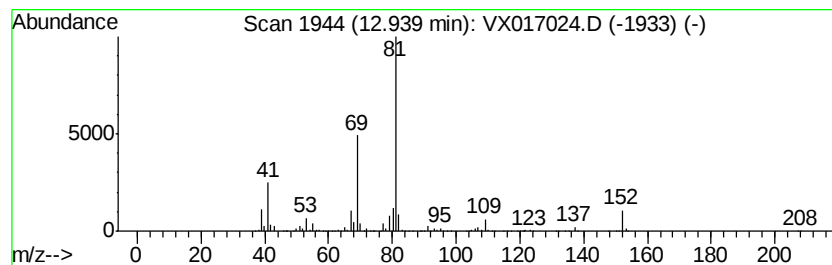
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Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.94	12.63 ug/l	413399	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	91
3	D-Fenchone	152	C10H16O	004695-62-9	90
4	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3N02	1000301-43-3	50
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.28	1.28	25.3	ug/l	382011	1	5.63	755844	50.0
3-Pentanone, 2,4-...	9.42	11.0	ug/l	494637	3	10.10	2251060	50.0
Benzoic acid, 2-[...	12.80	6.2	ug/l	202386	4	12.06	1636830	50.0
Bicyclo[2.2.1]hep...	12.94	12.6	ug/l	413399	4	12.06	1636830	50.0