

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031822\
 Data File : VX027528.D
 Acq On : 18 Mar 2022 15:19
 Operator : JC/MD
 Sample : N2002-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 220316043-02-VOA

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
 Title : SW846 8260

Signal : TIC: VX027528.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.544	71	75	81	rBV	93340	118201	4.57%	0.636%
2	1.593	81	83	89	rBV	34481	57013	2.20%	0.307%
3	2.380	206	212	231	rBV	333965	689657	26.66%	3.708%
4	2.538	231	238	252	rVV	156767	316042	12.22%	1.699%
5	2.965	299	308	327	rVB	1185969	2586818	100.00%	13.909%
6	4.574	558	572	602	rBV2	686836	2404869	92.97%	12.930%
7	5.007	631	643	663	rBV3	229600	751672	29.06%	4.042%
8	5.391	694	706	722	rBV2	212104	619227	23.94%	3.329%
9	5.556	722	733	746	rVV	345633	986275	38.13%	5.303%
10	5.958	789	799	811	rBV	212087	564389	21.82%	3.035%
11	6.239	837	845	856	rVB2	18565	53056	2.05%	0.285%
12	6.763	921	931	949	rBV	529933	1273248	49.22%	6.846%
13	7.464	1039	1046	1056	rBV2	14758	32502	1.26%	0.175%
14	8.653	1234	1241	1248	rBV	1095982	1719211	66.46%	9.244%
15	10.055	1461	1471	1484	rBV	1166886	1567954	60.61%	8.430%
16	11.085	1634	1640	1646	rBV	945148	1230551	47.57%	6.616%
17	11.506	1705	1709	1716	rVB	25351	35781	1.38%	0.192%
18	12.024	1788	1794	1802	rBV	1307263	1593408	61.60%	8.567%
19	12.104	1802	1807	1811	rBV4	20685	28895	1.12%	0.155%
20	12.579	1881	1885	1896	rVB2	45597	63903	2.47%	0.344%
21	12.768	1906	1916	1919	rBV	36472	62434	2.41%	0.336%
22	12.805	1919	1922	1929	rVB3	17513	26428	1.02%	0.142%
23	12.908	1931	1939	1943	rBV	194094	254620	9.84%	1.369%
24	12.951	1943	1946	1959	rVB4	29501	78838	3.05%	0.424%
25	13.213	1985	1989	1996	rVB5	20430	37528	1.45%	0.202%
26	13.335	2005	2009	2013	rBV	35779	49487	1.91%	0.266%
27	13.475	2027	2032	2034	rBV2	78940	105949	4.10%	0.570%
28	13.512	2034	2038	2045	rVV	427378	567604	21.94%	3.052%
29	13.591	2045	2051	2060	rVV2	184922	290201	11.22%	1.560%
30	13.731	2070	2074	2079	rBV	199337	247442	9.57%	1.330%
31	13.780	2079	2082	2086	rVB	31570	37248	1.44%	0.200%
32	14.097	2128	2134	2146	rBV	86027	148302	5.73%	0.797%

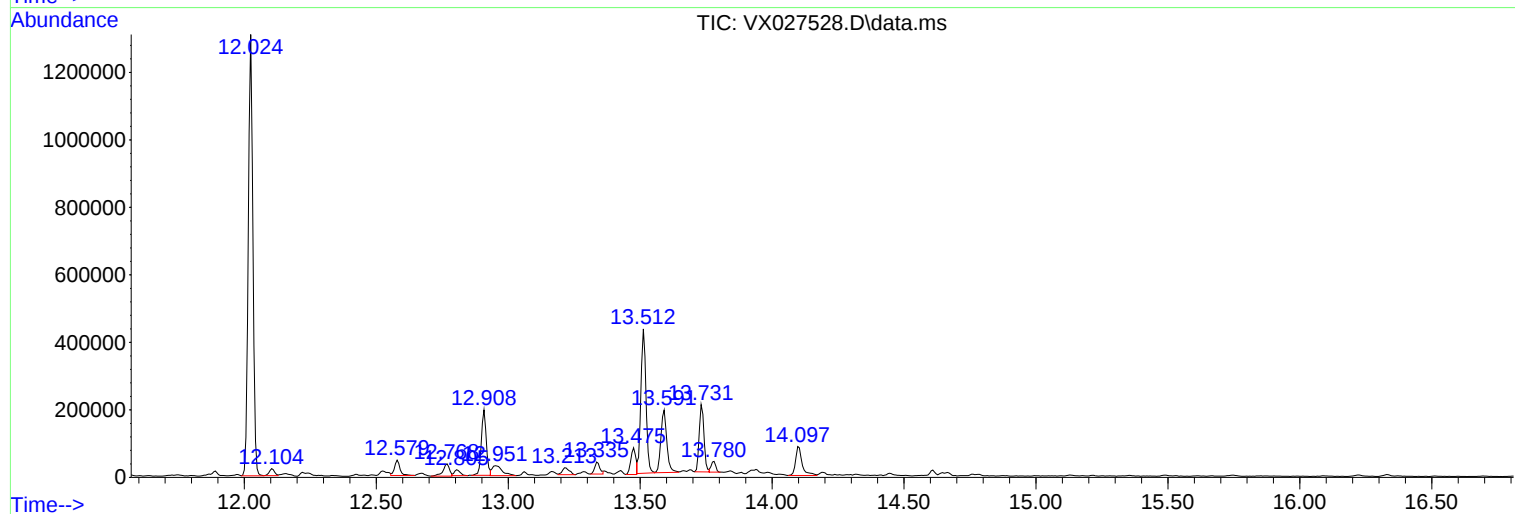
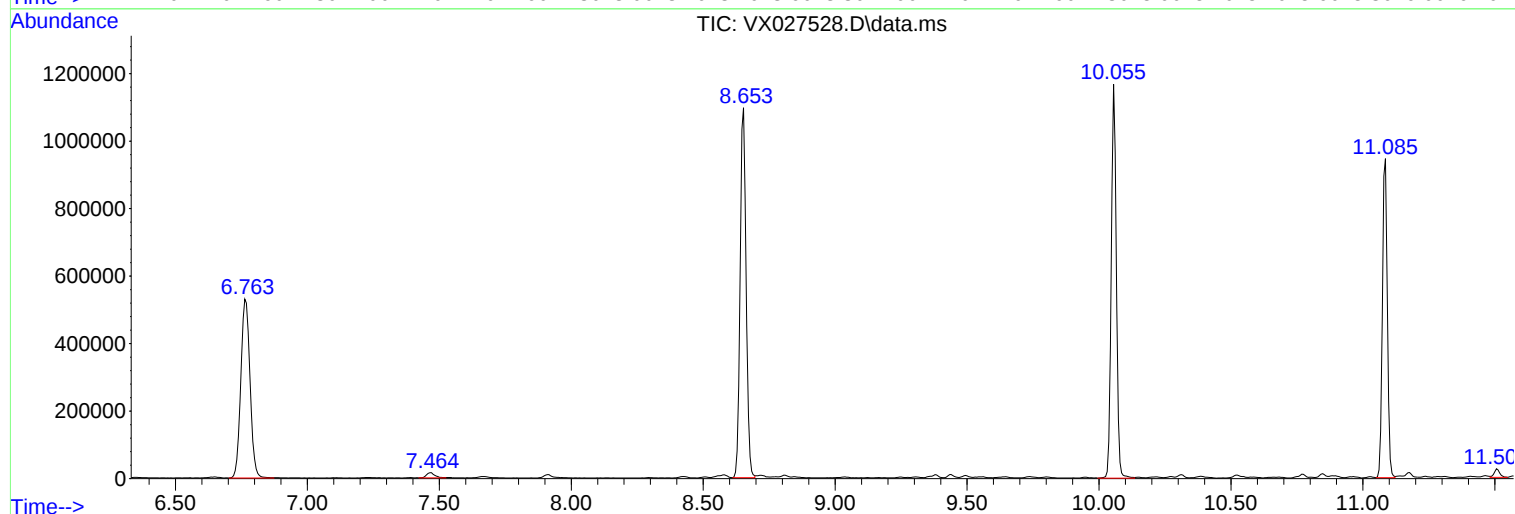
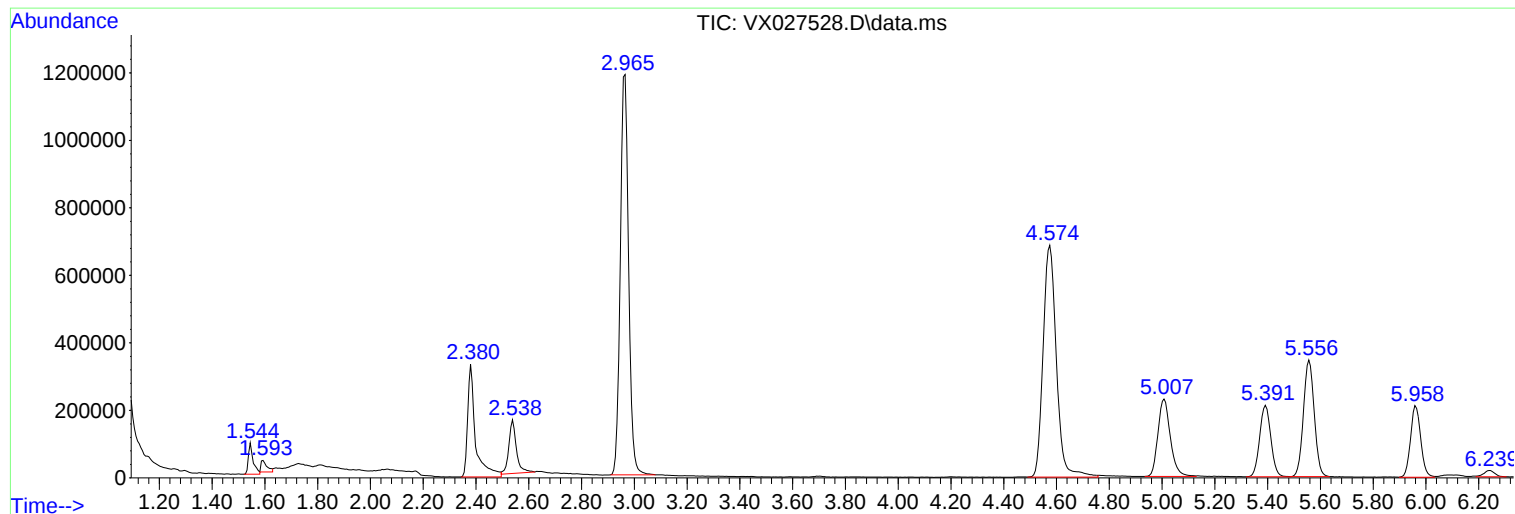
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ClientSampleId :
220316043-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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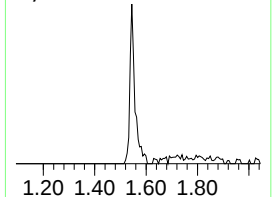
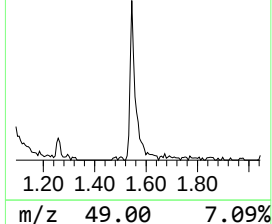
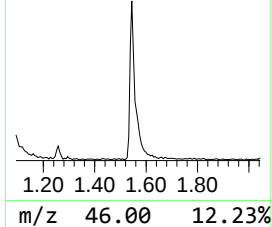
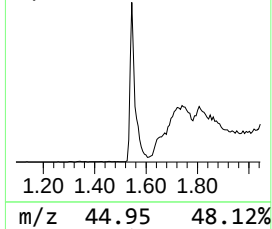
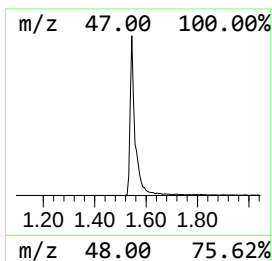
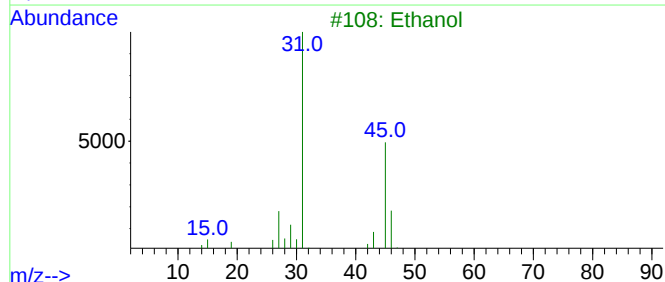
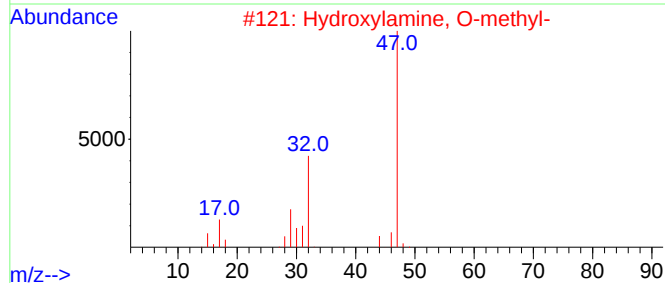
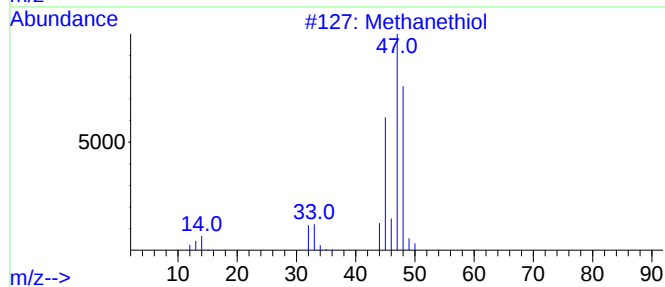
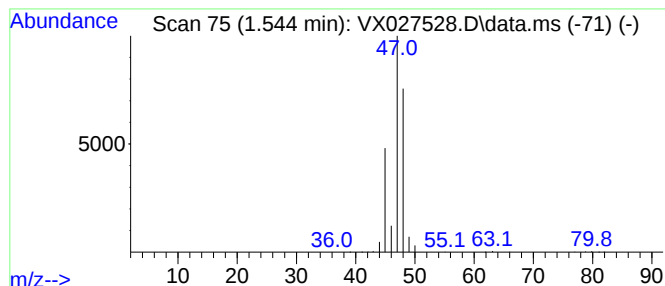
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.544	5.99 ug/l	118201	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
3			Ethanol	46	C2H6O	000064-17-5	4
4			Ethane, fluoro-	48	C2H5F	000353-36-6	4
5			Divinyl sulphone	118	C4H6O2S	000077-77-0	4



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ClientSampleId :
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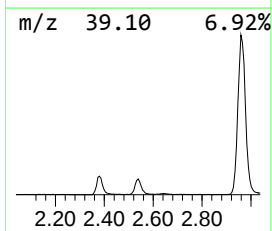
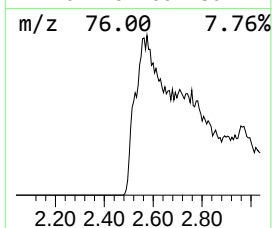
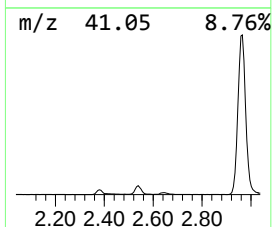
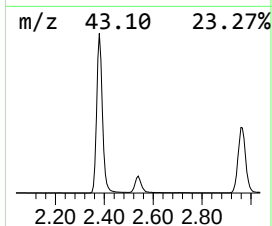
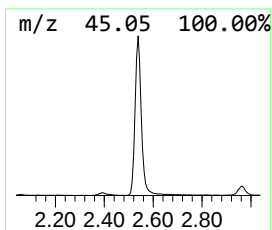
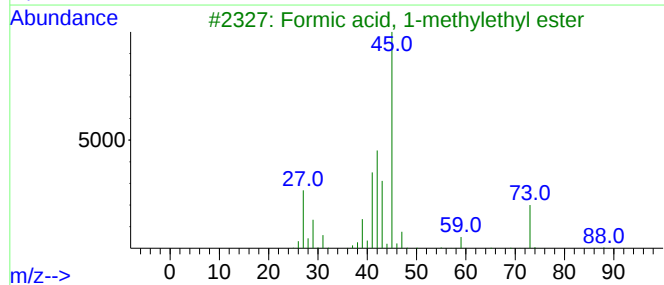
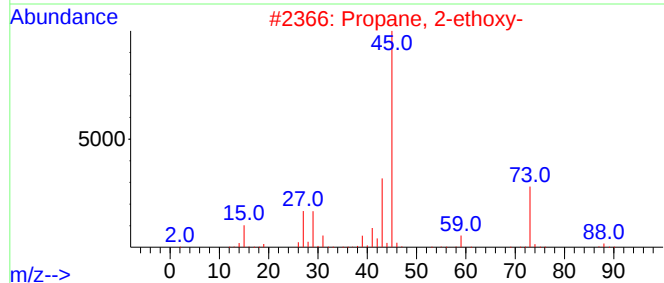
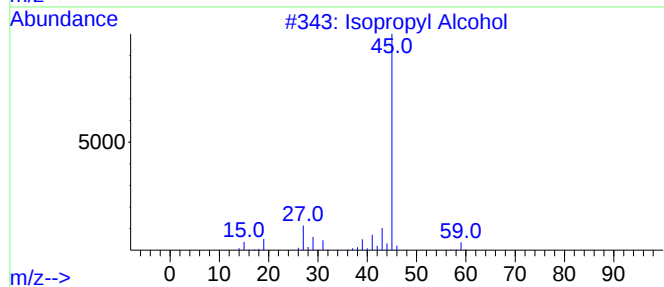
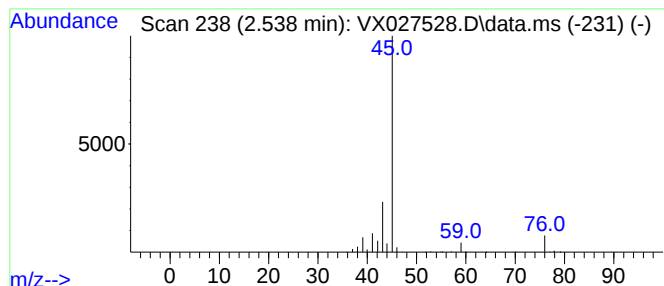
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.538	16.02 ug/l	316042	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	39
4			2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
5			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9



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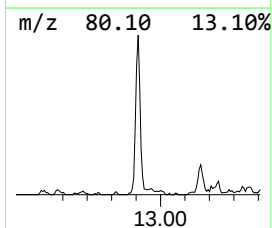
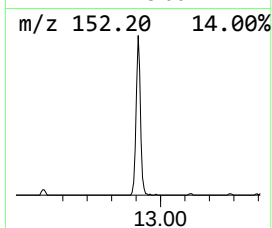
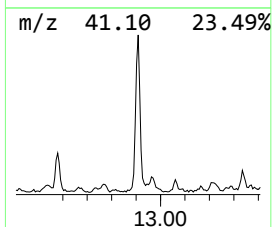
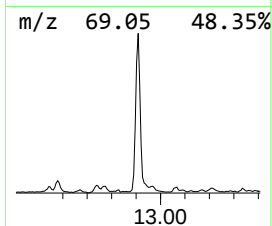
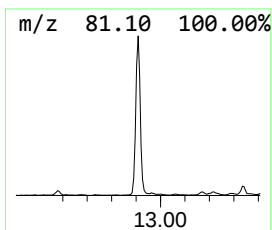
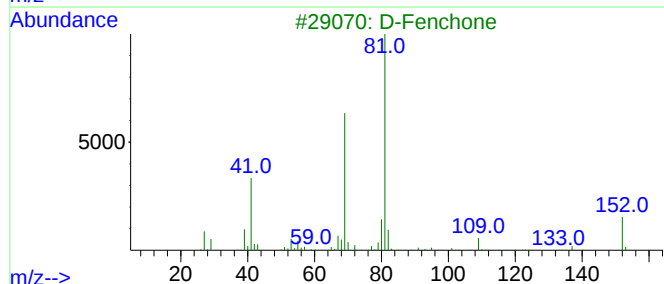
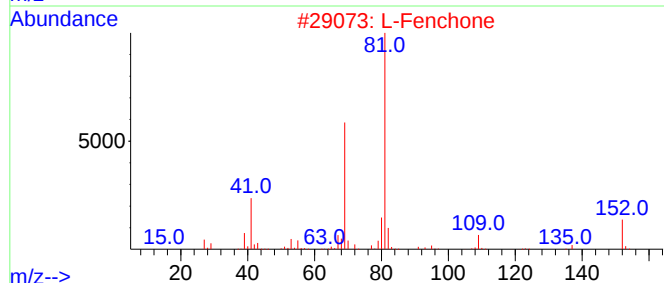
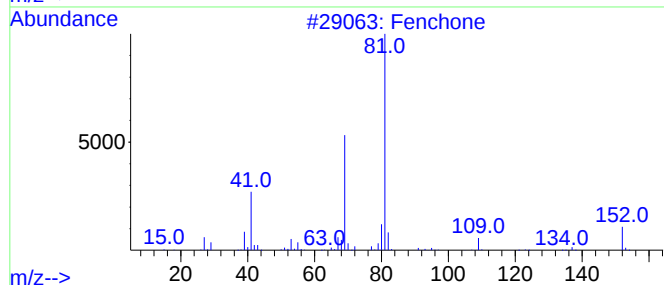
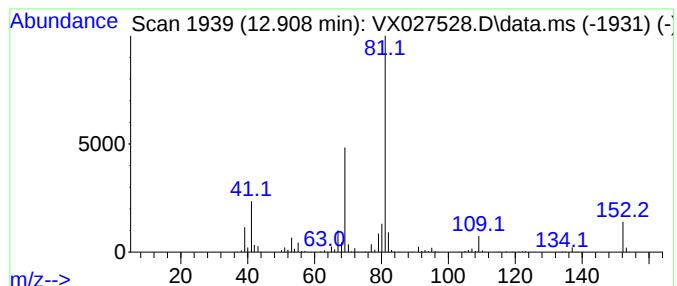
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Fenchone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	7.99 ug/l	254620	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-	124	C8H12O	001767-84-6	42
5			2-Cyclopentene-1-carboxylic acid	140	C8H12O2	068317-73-7	40



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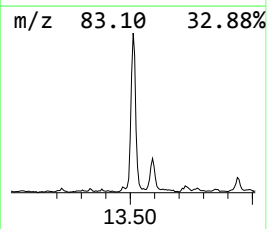
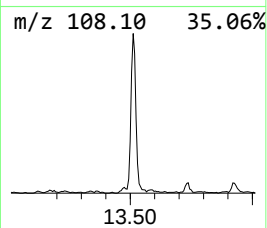
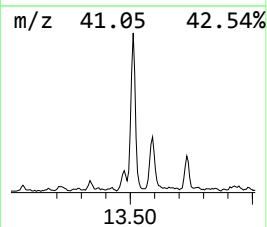
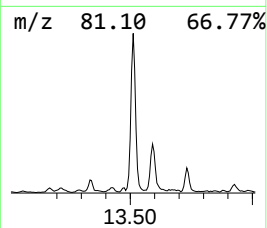
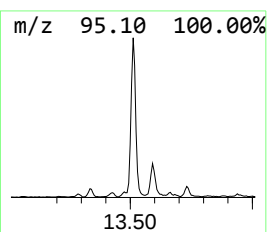
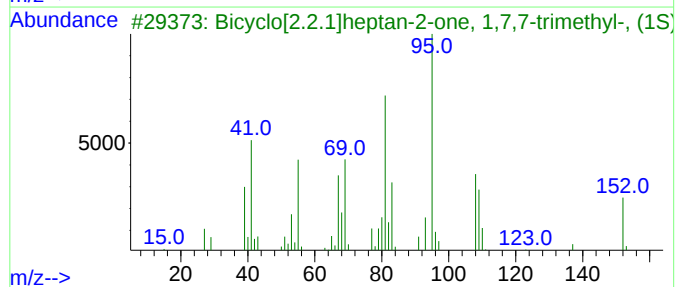
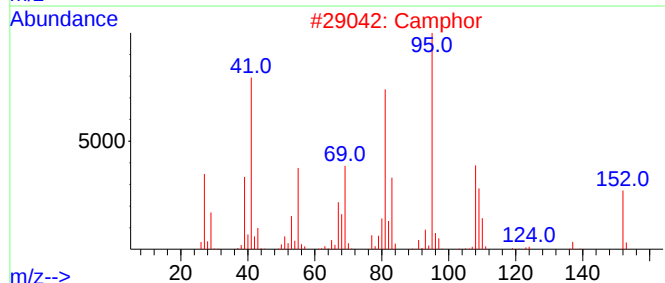
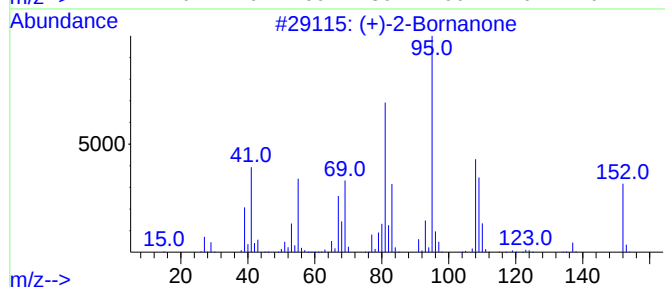
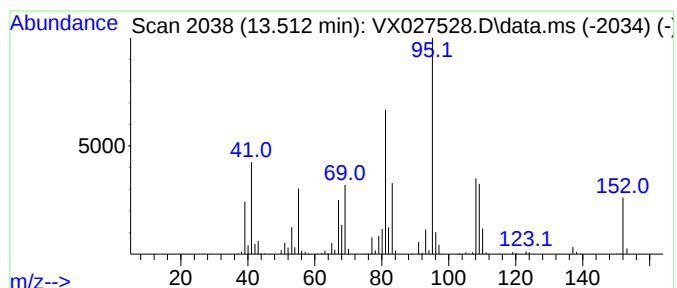
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	17.81 ug/l	567604	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2			Camphor	152	C10H16O	000076-22-2	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			1-Adamantanol	152	C10H16O	000768-95-6	46



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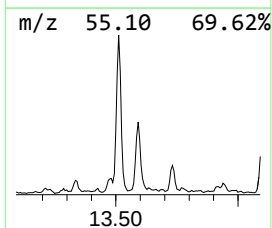
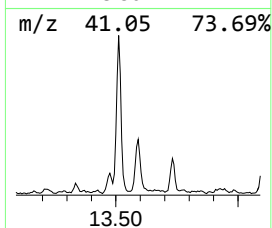
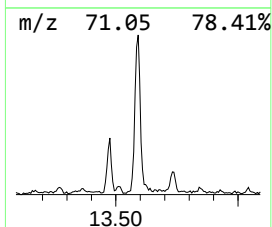
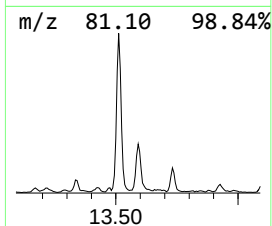
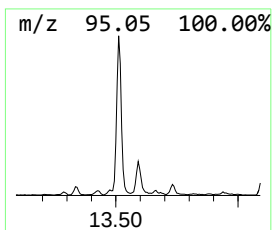
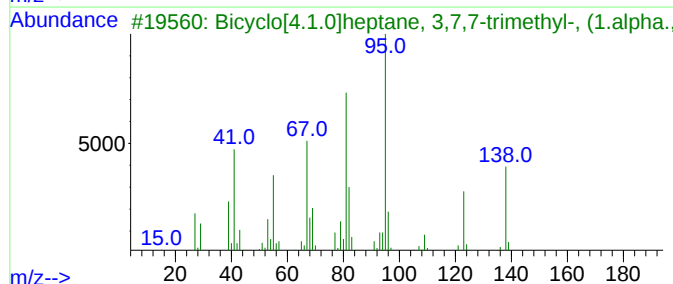
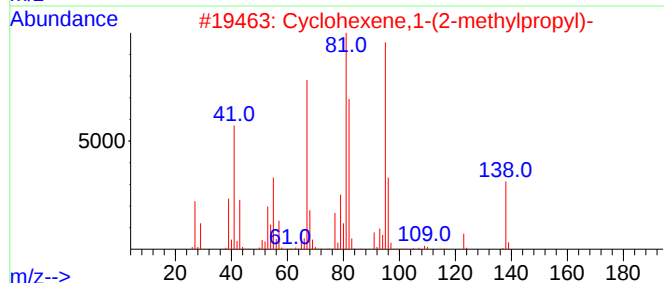
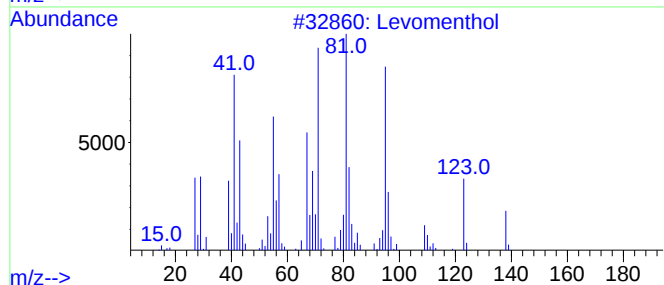
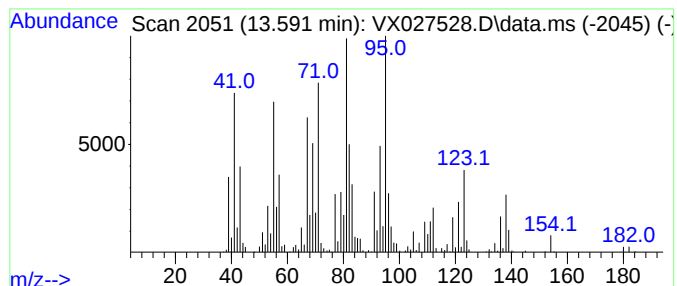
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Levomenthol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	9.11 ug/l	290201	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levomenthol	156	C10H20O	002216-51-5	72
2			Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	60
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	53
4			Ethyl L-menthyl carbonate	228	C13H24O3	035106-15-1	49
5			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	49



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.544	6.0	ug/l	118201	1	5.556	986275	50.0
Isopropyl Alcohol	2.538	16.0	ug/l	316042	1	5.556	986275	50.0
Fenchone	12.908	8.0	ug/l	254620	4	12.024	1593410	50.0
(+)-2-Bornanone	13.512	17.8	ug/l	567604	4	12.024	1593410	50.0
Levomenthol	13.591	9.1	ug/l	290201	4	12.024	1593410	50.0