

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041422\
 Data File : VX028113.D
 Acq On : 14 Apr 2022 17:35
 Operator : JC/MD
 Sample : N2406-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 220413003-02-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\82X041222W.M
 Title : SW846 8260

Signal : TIC: VX028113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.538	70	74	83	rBV	124549	161854	4.71%	0.897%
2	2.374	205	211	218	rBV	409925	656857	19.12%	3.639%
3	2.428	218	220	229	rVV3	14317	40468	1.18%	0.224%
4	2.532	229	237	246	rVB	84644	171397	4.99%	0.949%
5	2.953	295	306	325	rBV	1162170	2516640	73.24%	13.942%
6	4.568	556	571	585	rBV2	1038513	3436005	100.00%	19.035%
7	5.001	630	642	659	rBV2	249490	788252	22.94%	4.367%
8	5.391	694	706	718	rBV	152598	449818	13.09%	2.492%
9	5.556	720	733	748	rVB	238053	678268	19.74%	3.757%
10	5.952	789	798	809	rBV	166092	432669	12.59%	2.397%
11	6.239	832	845	857	rVB3	22260	65317	1.90%	0.362%
12	6.763	921	931	945	rBV	382390	899779	26.19%	4.985%
13	7.458	1039	1045	1061	rVB2	31753	69496	2.02%	0.385%
14	8.580	1220	1229	1234	rBV2	17499	34935	1.02%	0.194%
15	8.653	1234	1241	1248	rVV	787182	1253174	36.47%	6.942%
16	9.378	1353	1360	1365	rBV	52766	79906	2.33%	0.443%
17	10.055	1461	1471	1483	rBV	878824	1182196	34.41%	6.549%
18	10.195	1489	1494	1503	rBV2	33424	59599	1.73%	0.330%
19	10.305	1507	1512	1519	rVV2	43361	68426	1.99%	0.379%
20	11.085	1634	1640	1646	rBV	667421	875356	25.48%	4.849%
21	11.506	1704	1709	1715	rVB4	22325	34533	1.01%	0.191%
22	11.750	1738	1749	1754	rVB	19409	35036	1.02%	0.194%
23	11.890	1768	1772	1780	rVB	33570	44659	1.30%	0.247%
24	12.024	1788	1794	1801	rVB	891822	1113656	32.41%	6.169%
25	12.104	1801	1807	1811	rBV3	42311	64502	1.88%	0.357%
26	12.579	1882	1885	1889	rVB	30471	36213	1.05%	0.201%
27	12.768	1907	1916	1919	rBV4	31531	53763	1.56%	0.298%
28	12.908	1927	1939	1944	rBV	438106	583377	16.98%	3.232%
29	12.963	1944	1948	1958	rVB5	32908	68779	2.00%	0.381%
30	13.213	1985	1989	1996	rVV5	25287	45710	1.33%	0.253%
31	13.335	2005	2009	2020	rBV	72267	115783	3.37%	0.641%
32	13.475	2027	2032	2034	rBV2	93929	130189	3.79%	0.721%
33	13.512	2034	2038	2045	rVB	817854	1033005	30.06%	5.723%
34	13.591	2045	2051	2060	rBV2	163608	251222	7.31%	1.392%
35	13.731	2070	2074	2078	rBV	94386	116555	3.39%	0.646%
36	13.774	2078	2081	2086	rVB	118918	157156	4.57%	0.871%

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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\82X041222W.M
Title : SW846 8260

37	13.939	2101	2108	2113	rBV4	28679	66303	1.93%	0.367%
38	14.097	2129	2134	2146	rBV	119230	180570	5.26%	1.000%

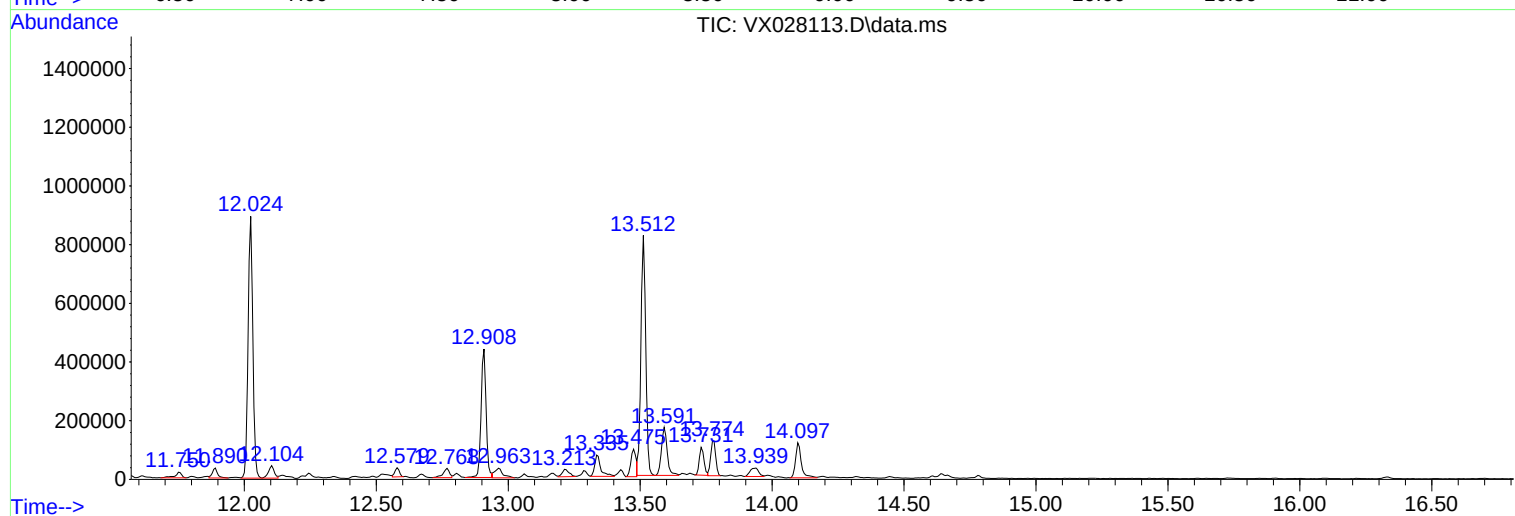
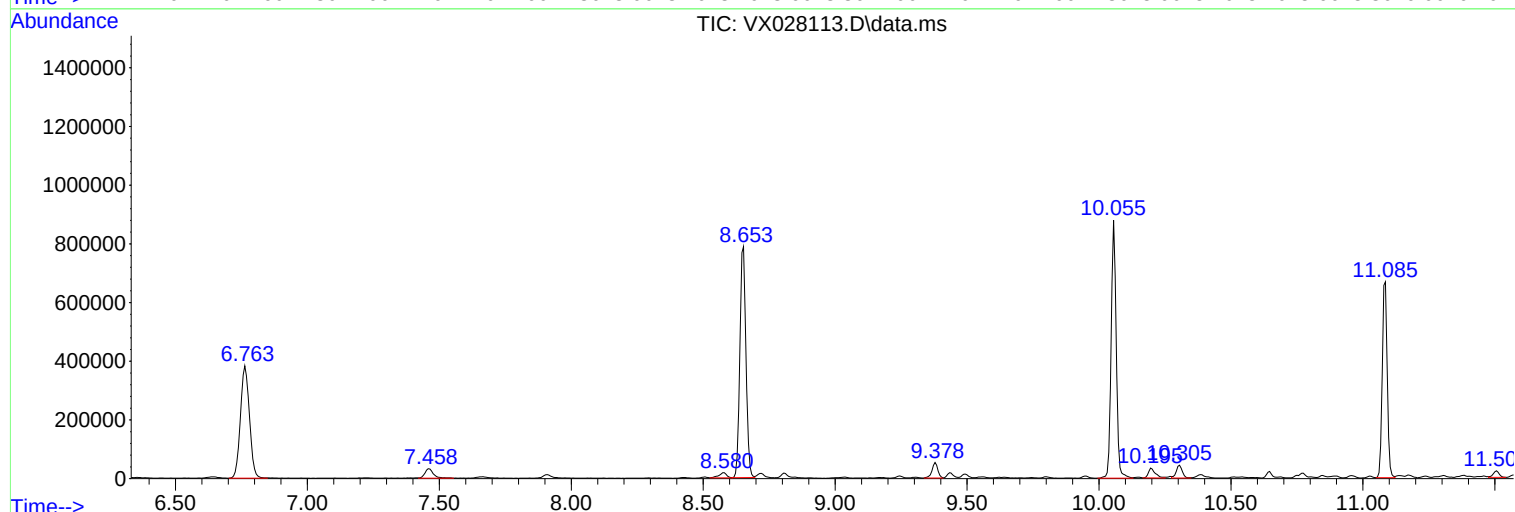
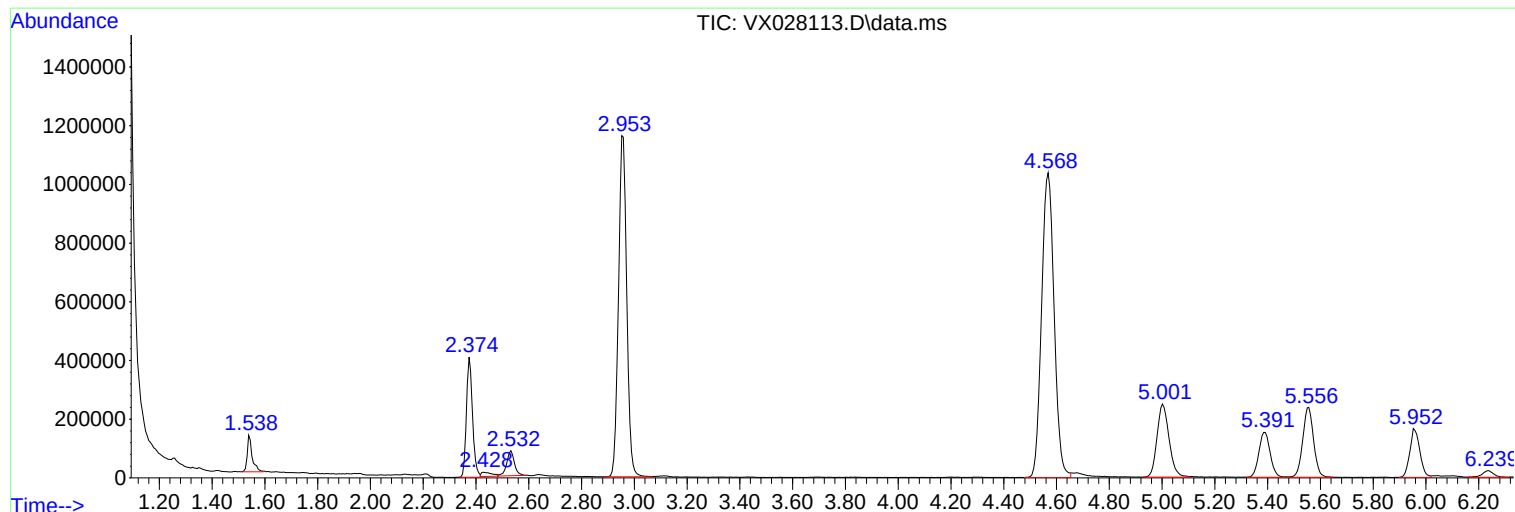
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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



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MSVOA_X
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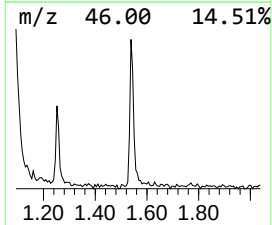
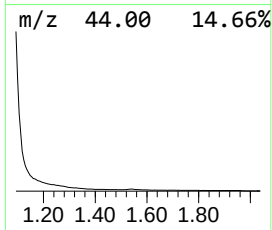
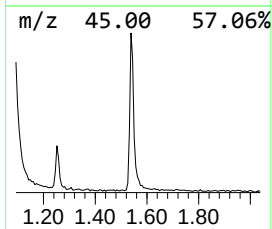
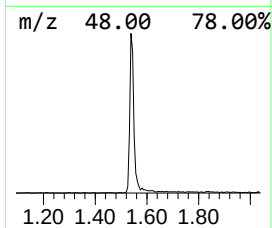
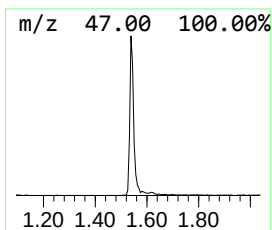
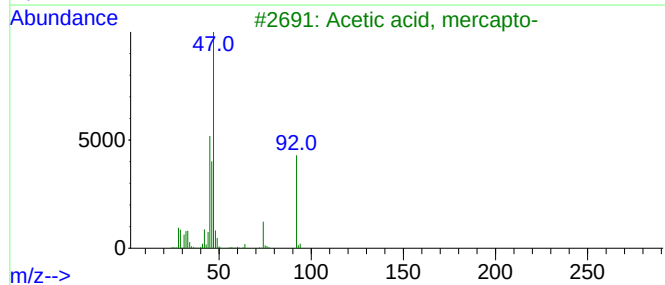
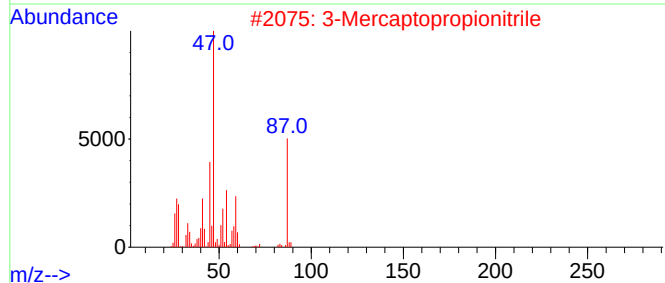
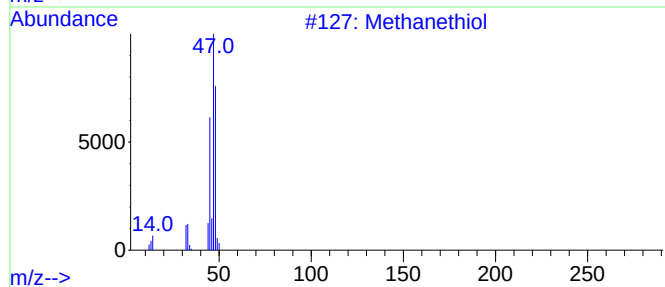
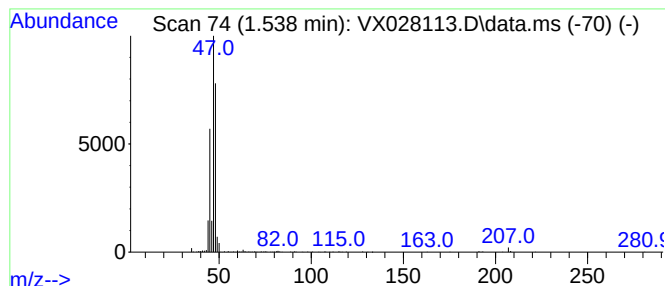
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

Peak Number 1 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.538	11.93 ug/l	161854	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	37
3			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	28
4			Methoxyacetyl chloride	108	C3H5ClO2	038870-89-2	9
5			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	9



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Instrument :
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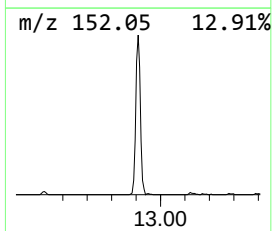
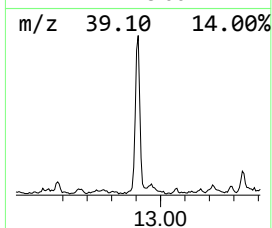
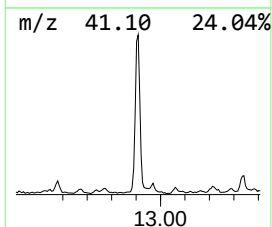
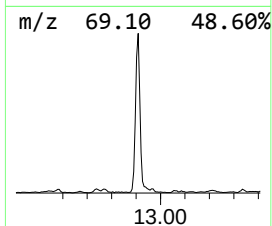
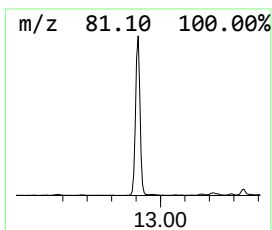
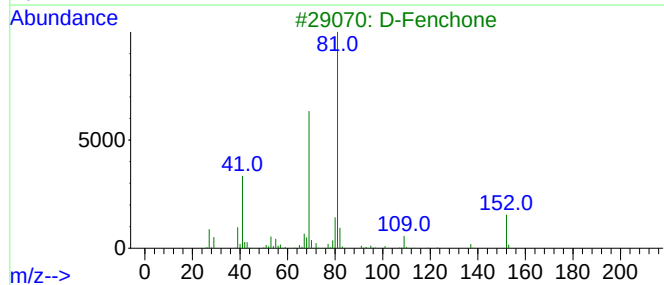
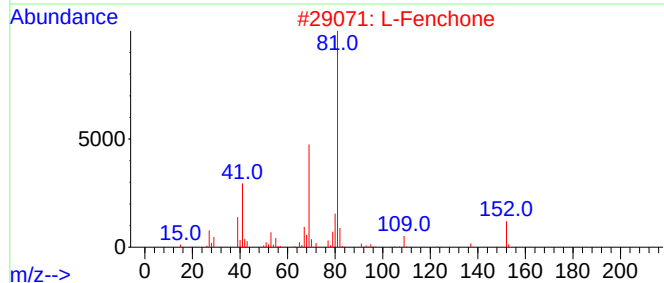
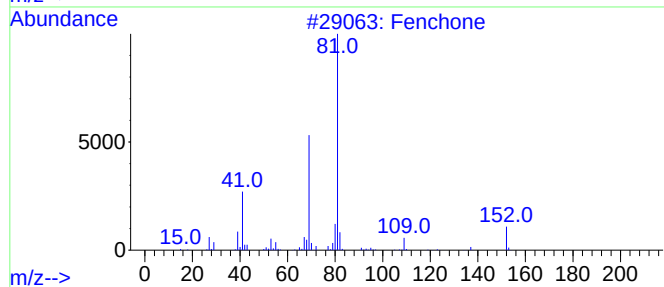
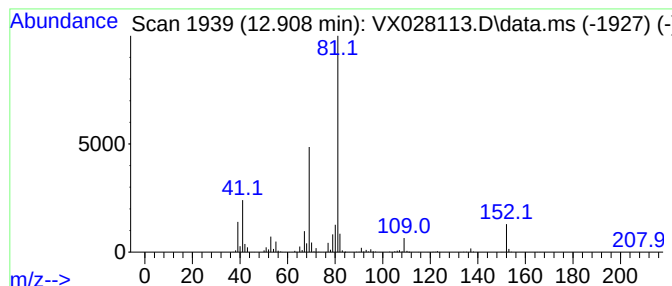
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	26.19 ug/l	583377	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	95
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-	124	C8H12O	001767-84-6	45
5			2-Cyclopentene-1-carboxylic acid	140	C8H12O2	068317-73-7	42



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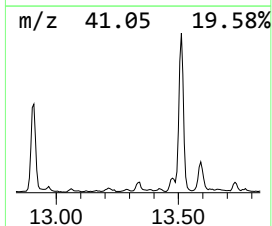
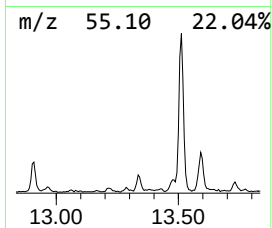
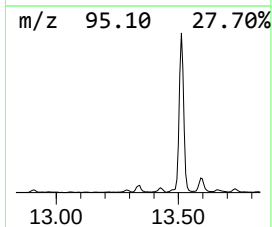
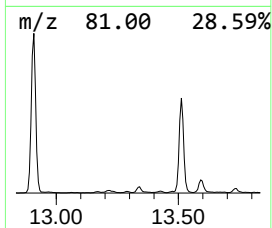
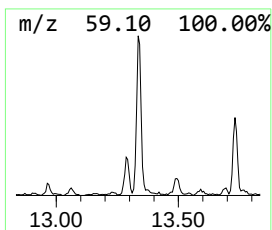
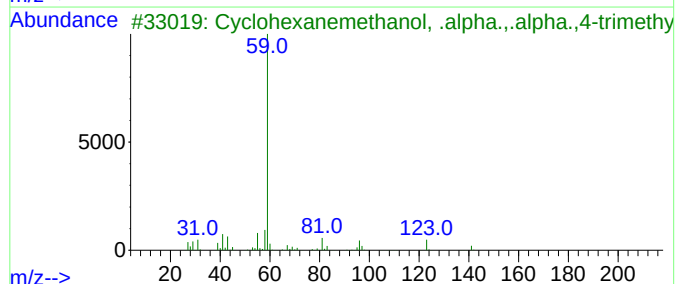
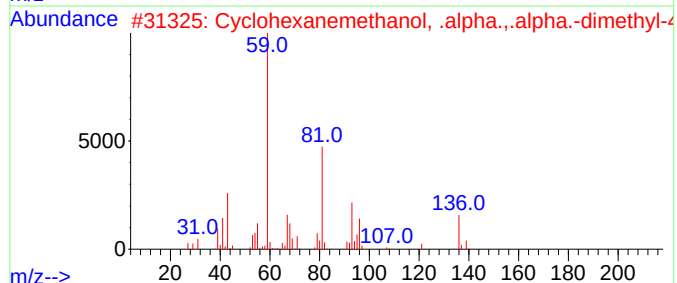
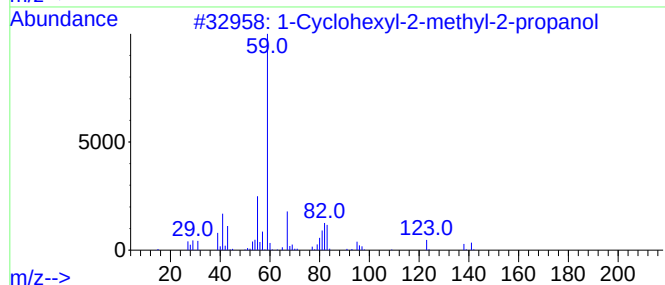
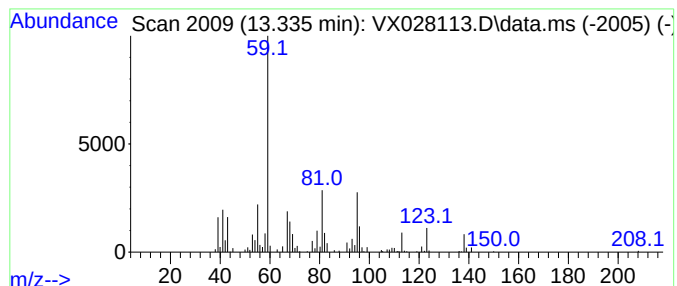
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Cyclohexyl-2-methyl-2-pro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	5.20 ug/l	115783	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	50
2			Cyclohexanemethanol, .alpha.,.al...	154	C10H18O	007299-42-5	40
3			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	38
4			trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	38
5			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	38



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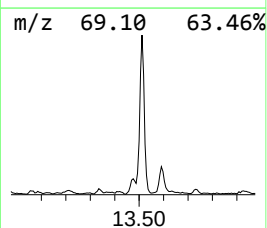
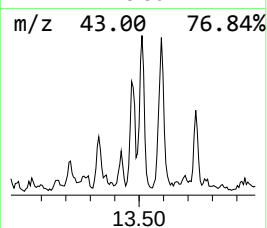
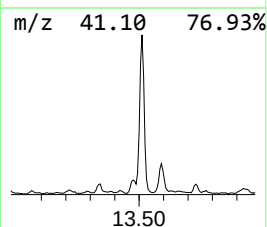
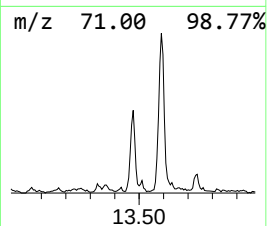
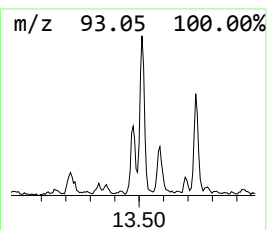
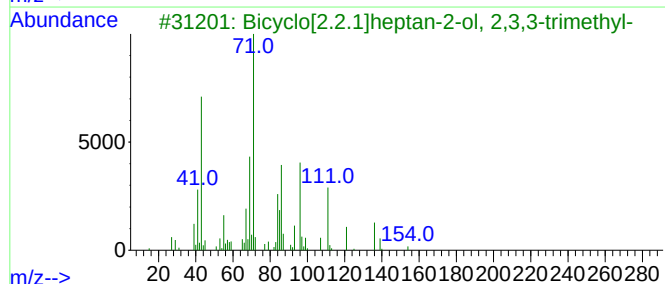
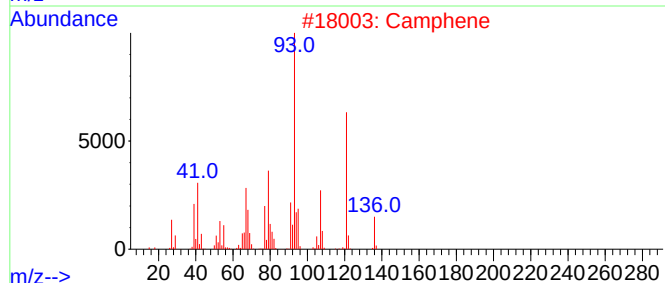
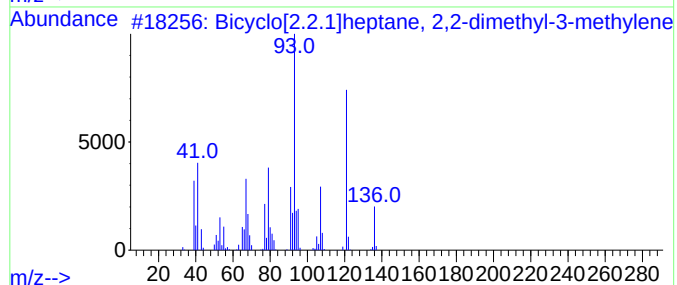
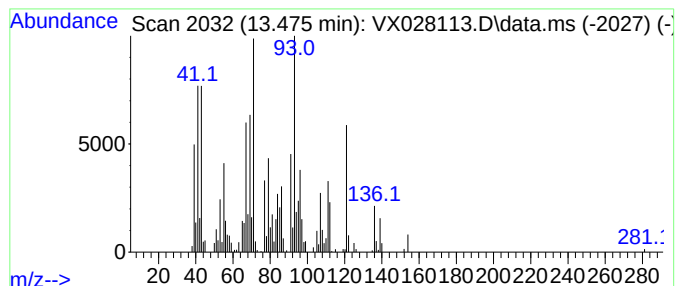
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	5.85 ug/l	130189	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	59
2			Camphene	136	C10H16	000079-92-5	56
3			Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	46
4			Bicyclo[3.1.0]hexan-2-ol, 2-meth...	154	C10H18O	017699-16-0	43
5			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	41



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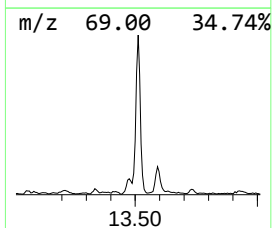
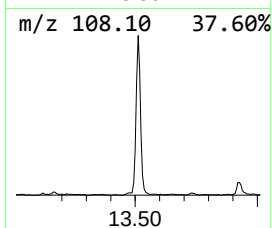
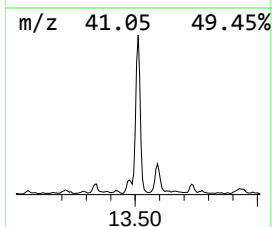
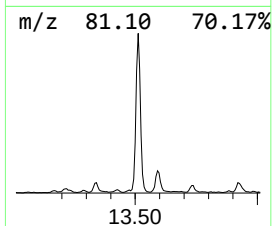
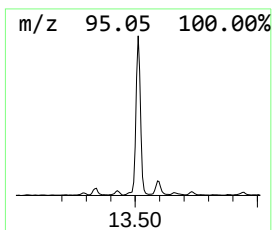
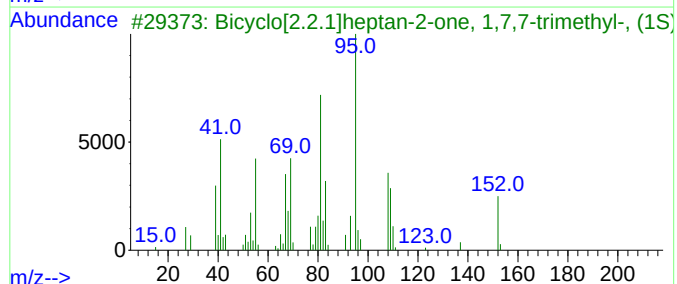
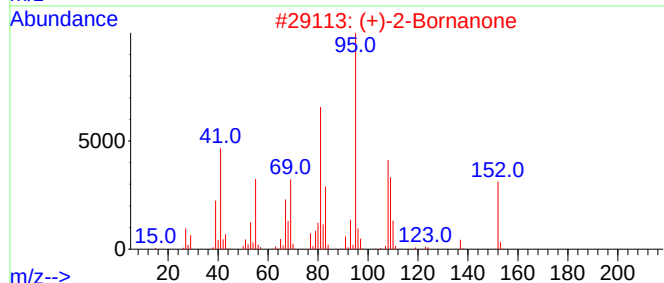
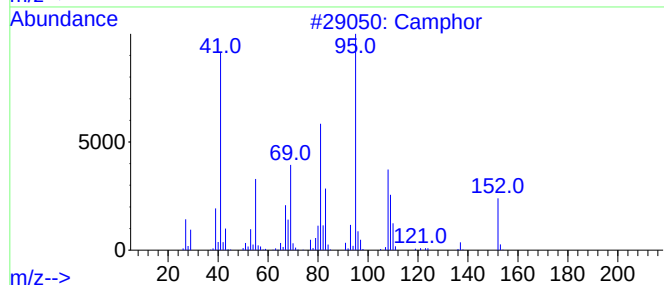
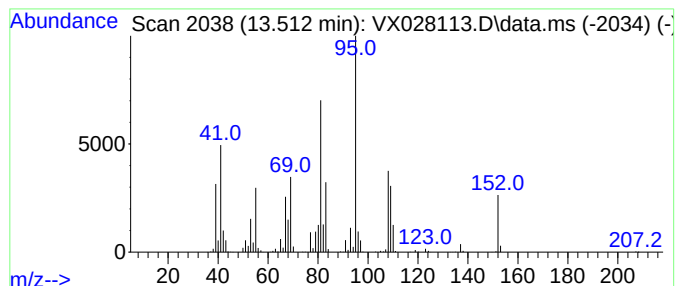
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

Peak Number 5 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	46.38 ug/l	1033010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5			1-Adamantanol	152	C10H16O	000768-95-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041422\
Data File : VX028113.D
Acq On : 14 Apr 2022 17:35
Operator : JC/MD
Sample : N2406-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
220413003-02-VOA

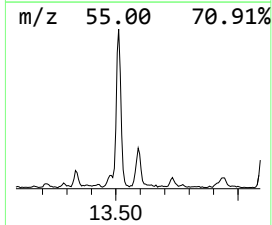
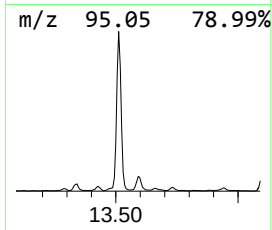
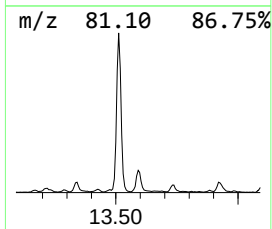
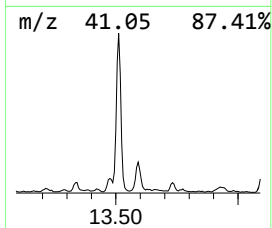
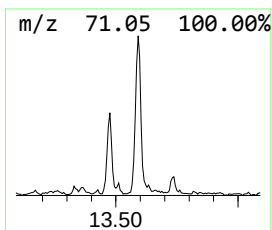
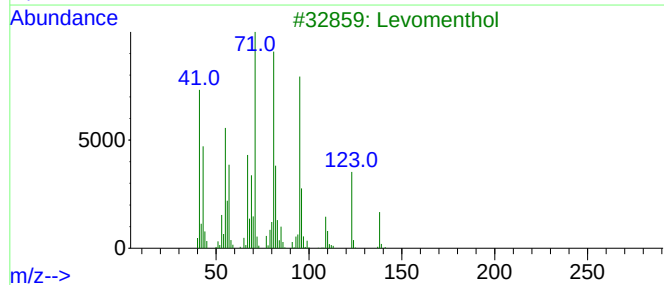
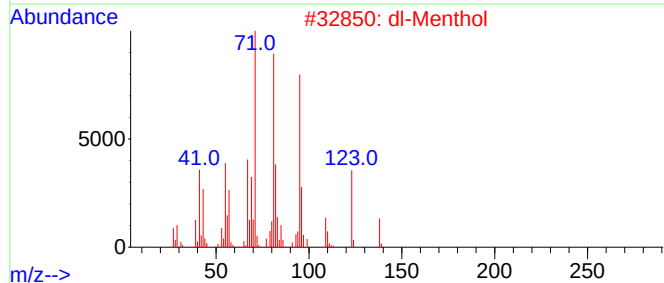
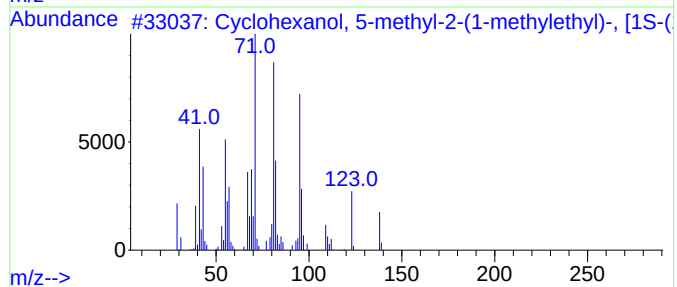
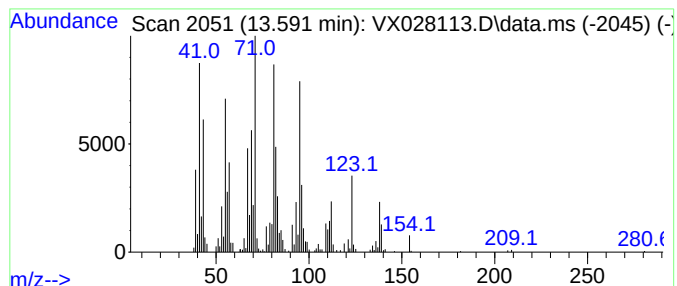
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Quant Title : SW846 8260

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

Peak Number 6 dl-Menthol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	11.28 ug/l	251222	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	91
2			dl-Menthol	156	C10H20O	000089-78-1	90
3			Levomenthol	156	C10H20O	002216-51-5	90
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	83
5			d-Menthol	156	C10H20O	015356-60-2	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041422\
Data File : VX028113.D
Acq On : 14 Apr 2022 17:35
Operator : JC/MD
Sample : N2406-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
220413003-02-VOA

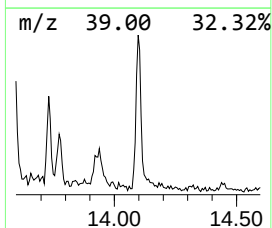
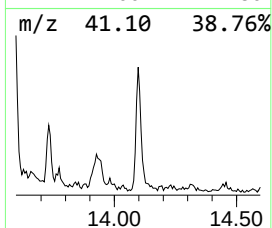
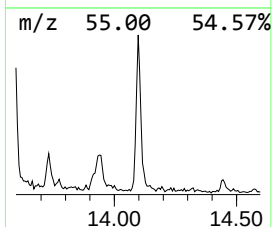
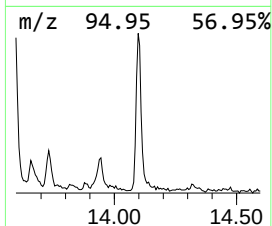
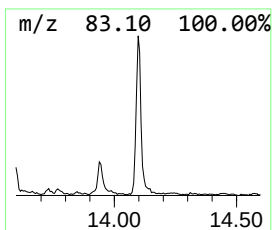
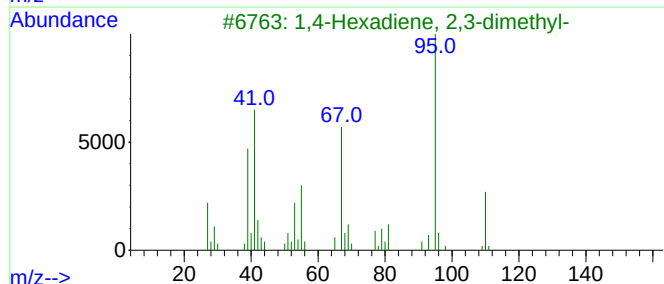
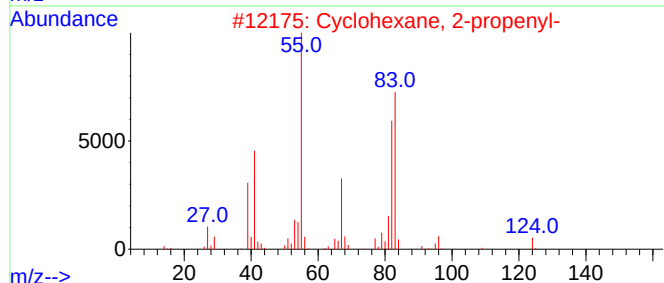
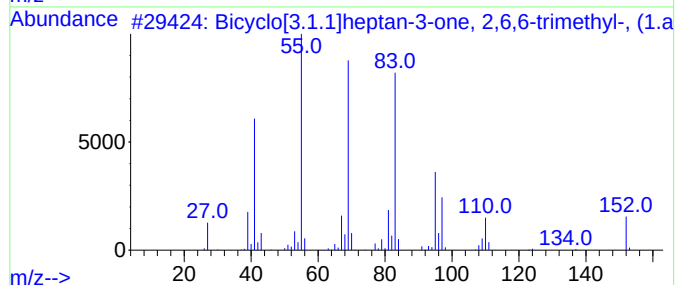
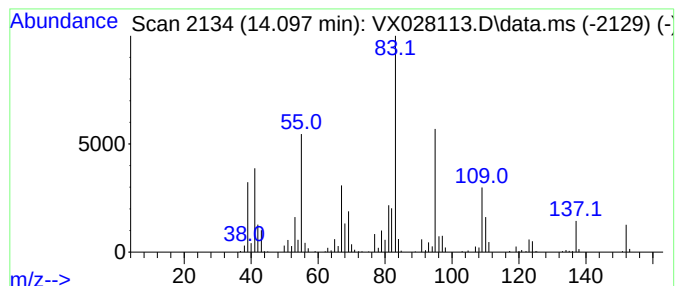
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.097 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	8.11 ug/l	180570	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	49
2			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38
3			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	35
4			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	35
5			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041422\
Data File : VX028113.D
Acq On : 14 Apr 2022 17:35
Operator : JC/MD
Sample : N2406-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
220413003-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.538	11.9	ug/l	161854	1	5.556	678268	50.0
Fenchone	12.908	26.2	ug/l	583377	4	12.024	1113660	50.0
1-Cyclohexyl-2-...	13.335	5.2	ug/l	115783	4	12.024	1113660	50.0
Bicyclo[2.2.1]h...	13.475	5.8	ug/l	130189	4	12.024	1113660	50.0
Camphor	13.512	46.4	ug/l	1033010	4	12.024	1113660	50.0
dl-Menthol	13.591	11.3	ug/l	251222	4	12.024	1113660	50.0
unknown14.097	14.097	8.1	ug/l	180570	4	12.024	1113660	50.0