

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103124\
 Data File : VX043649.D
 Acq On : 31 Oct 2024 14:27
 Operator : JC/MD
 Sample : P4646-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 241030069-01-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\82X102824W.M
 Title : SW846 8260

Signal : TIC: VX043649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	25	27	40	rVB	89898	145534	3.64%	0.862%
2	2.386	207	213	228	rBV	189620	367898	9.21%	2.179%
3	2.995	293	313	328	rBV	772846	2576325	64.47%	15.261%
4	4.611	562	578	625	rBV	934284	3996399	100.00%	23.673%
5	5.007	633	643	667	rVB	348645	1139599	28.52%	6.751%
6	5.385	694	705	720	rVB	60648	185305	4.64%	1.098%
7	5.544	722	731	745	rBV	98223	282500	7.07%	1.673%
8	5.952	789	798	806	rBV2	74012	197804	4.95%	1.172%
9	6.038	806	812	820	rVV3	16154	43308	1.08%	0.257%
10	6.147	820	830	841	rVB3	17773	59580	1.49%	0.353%
11	6.257	841	848	858	rBV3	19235	56762	1.42%	0.336%
12	6.757	921	930	943	rBV	161354	399775	10.00%	2.368%
13	8.647	1234	1240	1247	rVV	335038	536517	13.43%	3.178%
14	8.714	1247	1251	1261	rVB2	28697	53482	1.34%	0.317%
15	9.378	1353	1360	1367	rBV	66077	104143	2.61%	0.617%
16	9.488	1374	1378	1385	rVB	26824	42317	1.06%	0.251%
17	10.055	1460	1471	1484	rBV	340452	579460	14.50%	3.433%
18	10.189	1490	1493	1505	rBV2	60062	111785	2.80%	0.662%
19	10.299	1506	1511	1520	rVV	89130	137062	3.43%	0.812%
20	10.640	1562	1567	1573	rBV	58998	83335	2.09%	0.494%
21	11.079	1634	1639	1645	rBV	275659	375311	9.39%	2.223%
22	11.506	1704	1709	1715	rVV	45888	63053	1.58%	0.374%
23	11.750	1745	1749	1754	rVB	36472	49623	1.24%	0.294%
24	11.884	1767	1771	1780	rVB	57489	77963	1.95%	0.462%
25	12.018	1787	1793	1801	rBV	352642	510985	12.79%	3.027%
26	12.097	1801	1806	1810	rBV2	54675	91837	2.30%	0.544%
27	12.140	1810	1813	1822	rVB6	18656	42296	1.06%	0.251%
28	12.244	1822	1830	1834	rBV2	39275	75676	1.89%	0.448%
29	12.762	1906	1915	1920	rBV	111178	168658	4.22%	0.999%
30	12.902	1927	1938	1944	rBV	730239	964756	24.14%	5.715%
31	12.963	1944	1948	1958	rVB4	49468	91889	2.30%	0.544%
32	13.213	1985	1989	1995	rVB6	37052	69745	1.75%	0.413%
33	13.286	1995	2001	2005	rBV3	31798	46859	1.17%	0.278%
34	13.335	2005	2009	2012	rBV2	62757	84570	2.12%	0.501%
35	13.475	2027	2032	2034	rBV2	159507	240697	6.02%	1.426%
36	13.506	2034	2037	2045	rVB	1025842	1375271	34.41%	8.147%

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 Title : SW846 8260

37	13.591	2045	2051	2060	rBV2	202444	314821	7.88%	1.865%
38	13.731	2070	2074	2077	rBV2	81751	101893	2.55%	0.604%
39	13.774	2077	2081	2089	rVB	379719	469238	11.74%	2.780%
40	13.932	2100	2107	2113	rVB5	45575	102111	2.56%	0.605%
41	14.097	2127	2134	2146	rBV2	139792	218752	5.47%	1.296%
42	14.634	2219	2222	2234	rVB	42074	79946	2.00%	0.474%
43	14.780	2239	2246	2252	rVB2	38143	60476	1.51%	0.358%
44	16.213	2475	2481	2494	rBV3	26145	63478	1.59%	0.376%
45	16.328	2494	2500	2506	rVB	23506	42584	1.07%	0.252%

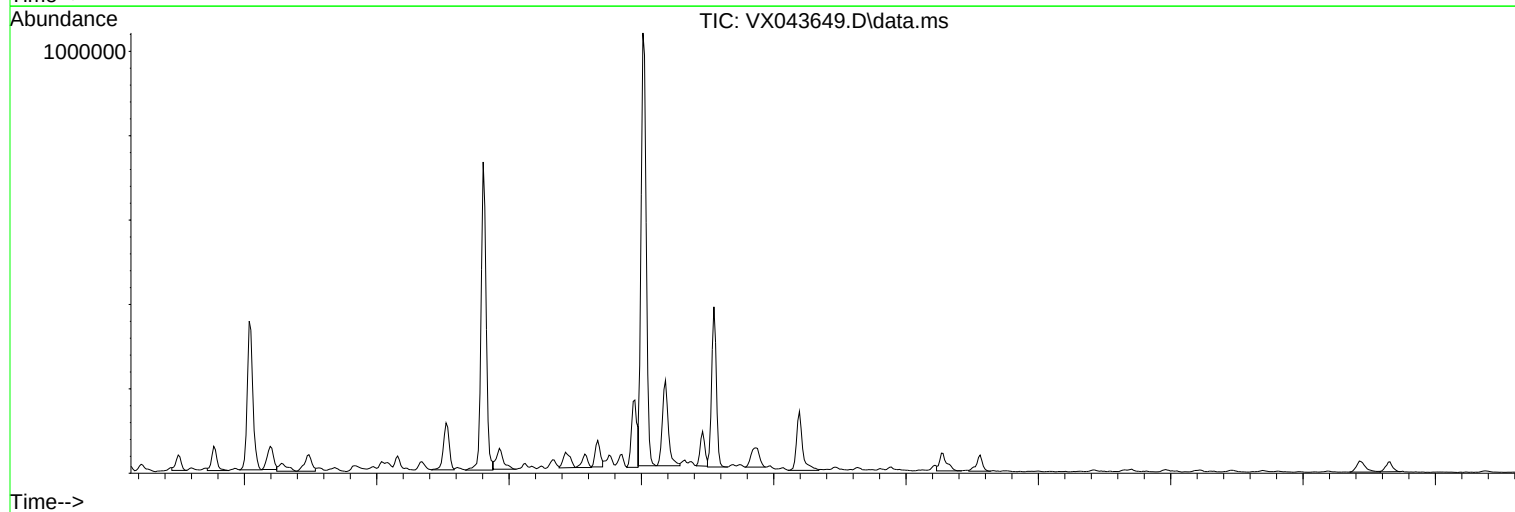
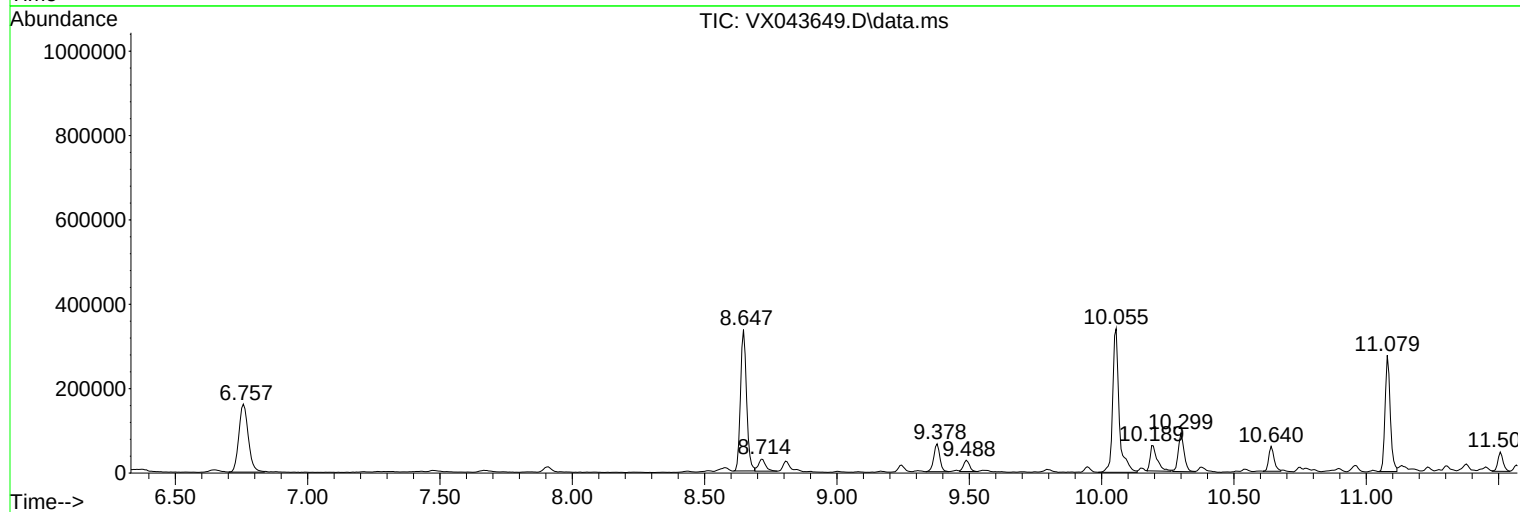
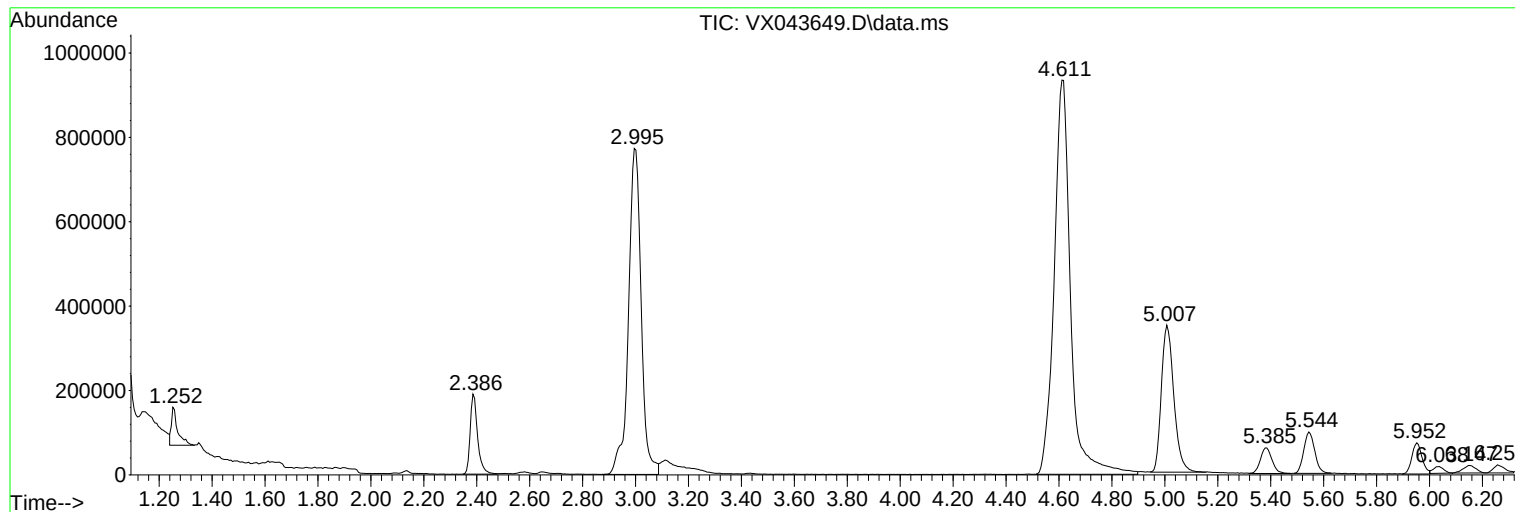
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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



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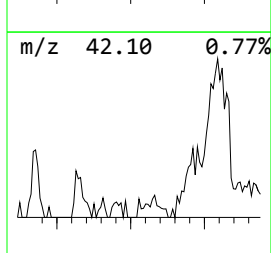
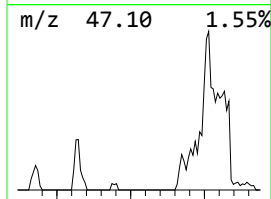
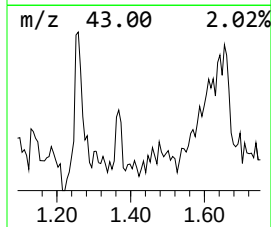
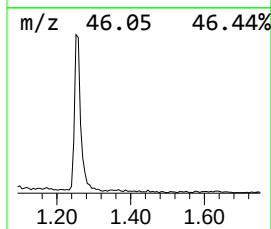
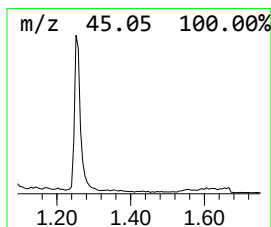
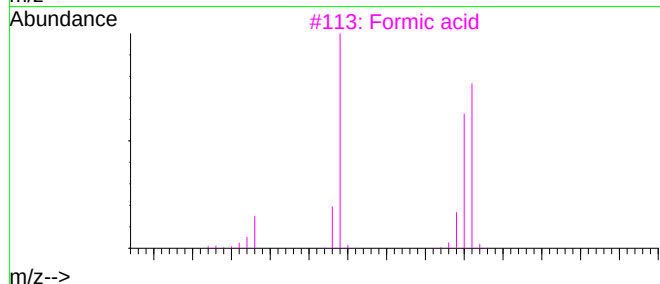
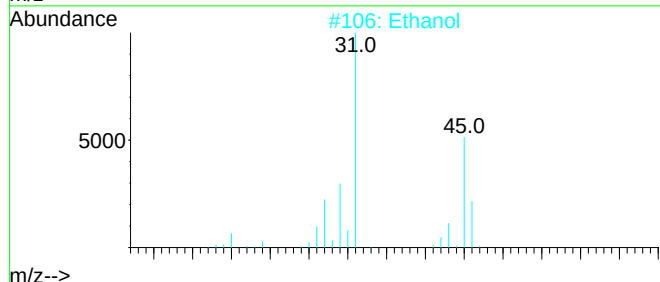
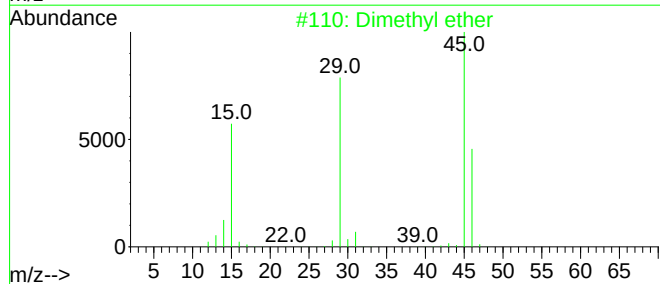
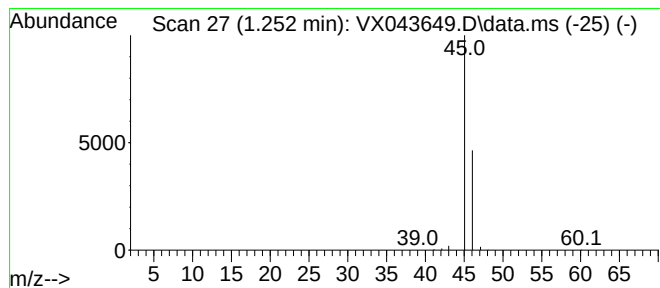
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	25.76 ug/l	145534	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	74
2	Ethanol	46	C2H6O	000064-17-5	7
3	Formic acid	46	CH2O2	000064-18-6	5
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3



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Instrument :
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ClientSampleId :
241030069-01-VOA

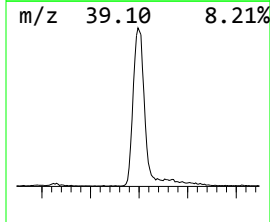
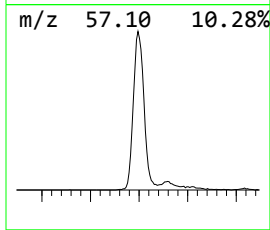
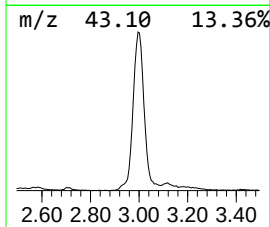
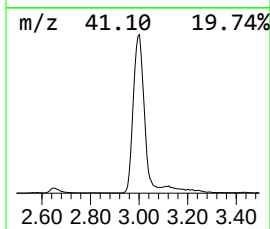
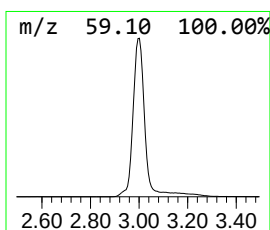
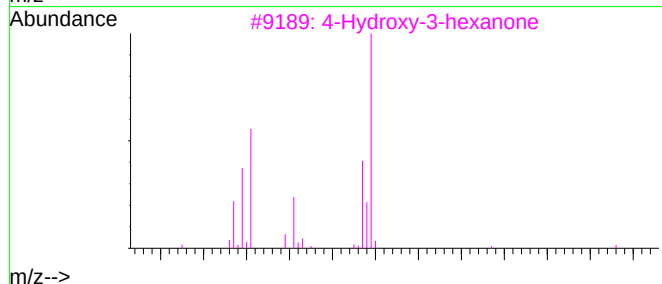
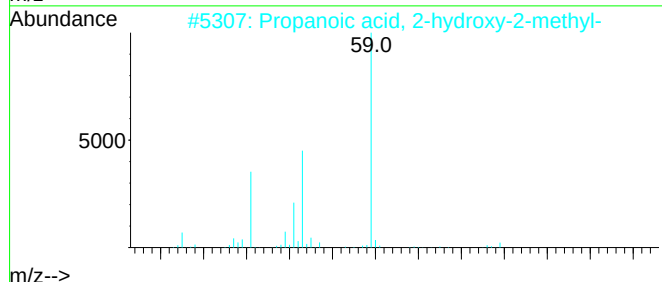
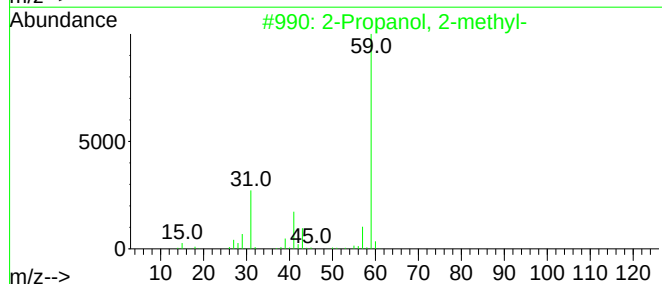
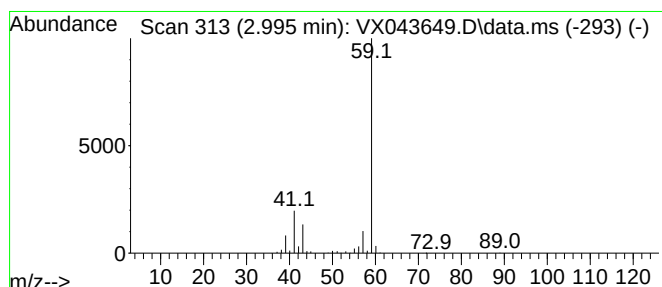
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Propanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.995	455.99 ug/l	2576330	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	83
2	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Guanidine	59	CH5N3	000113-00-8	4



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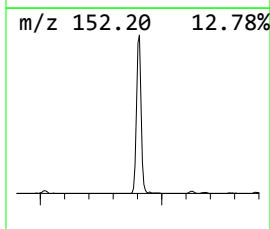
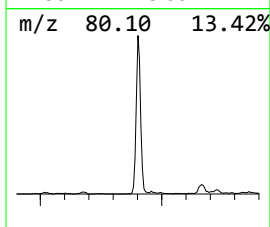
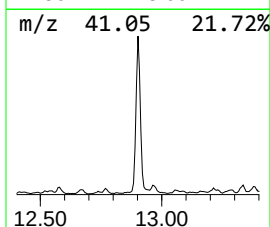
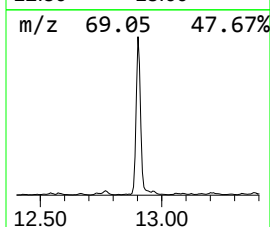
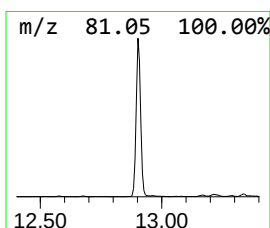
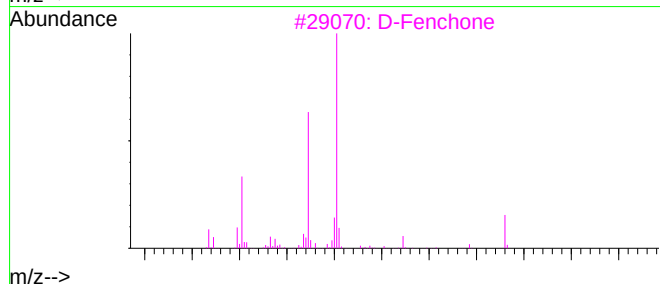
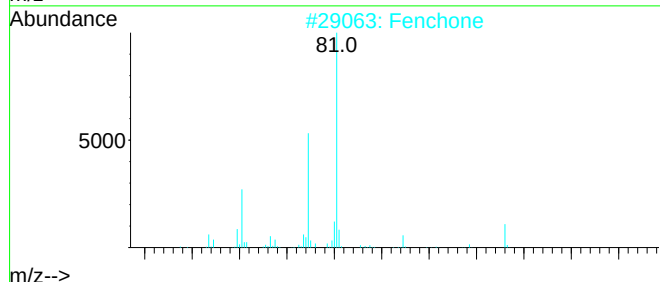
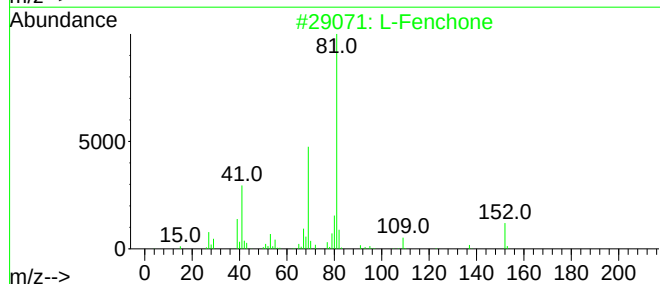
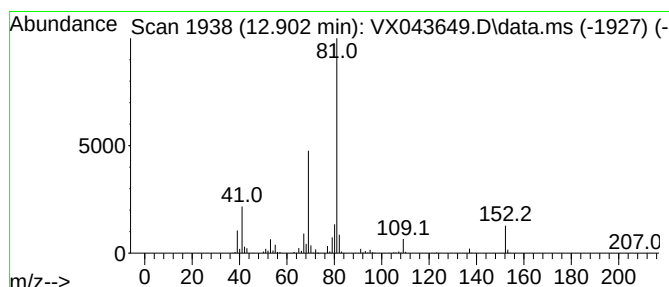
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 L-Fenchone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	94.40 ug/l	964756	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Fenchone	152	C10H16O	007787-20-4	95
2	Fenchone	152	C10H16O	001195-79-5	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



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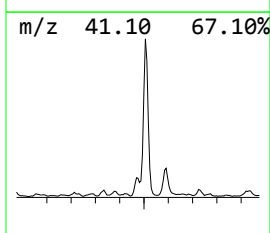
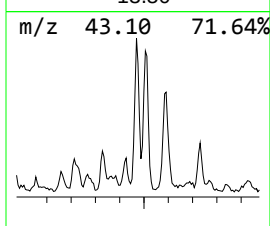
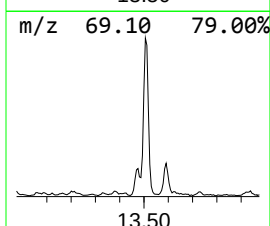
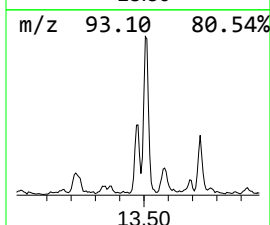
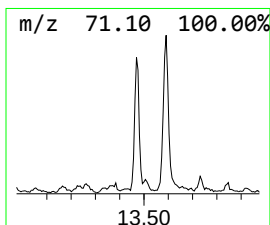
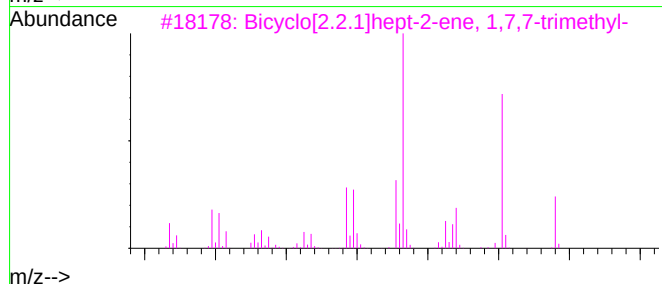
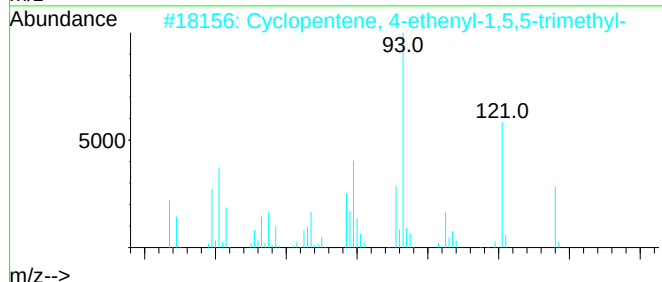
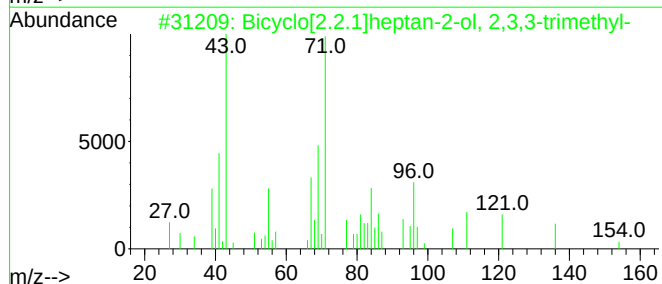
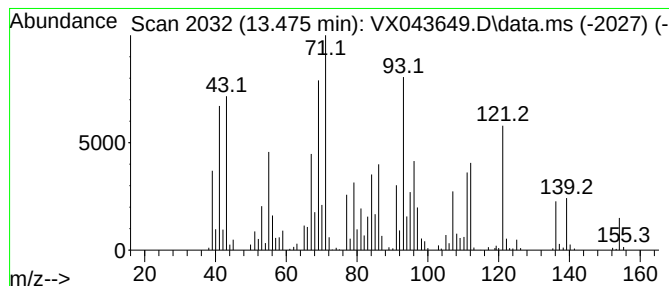
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.475 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	23.55 ug/l	240697	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	30
2	Cyclopentene, 4-ethenyl-1,5,5-tr...	136	C10H16	001727-69-1	25
3	Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	25
4	Terpinen-4-ol	154	C10H18O	000562-74-3	18
5	2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	18



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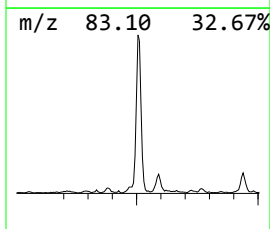
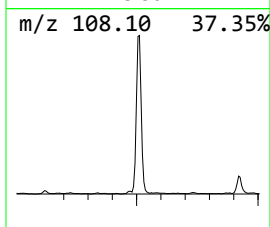
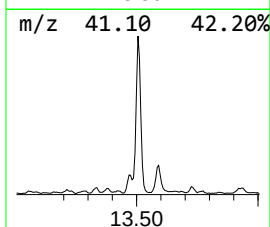
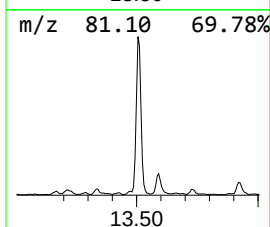
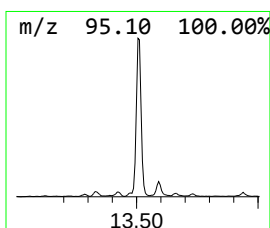
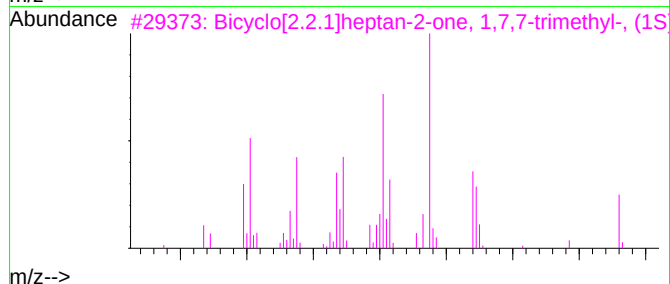
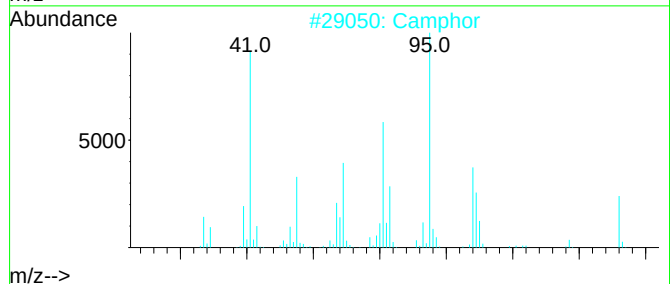
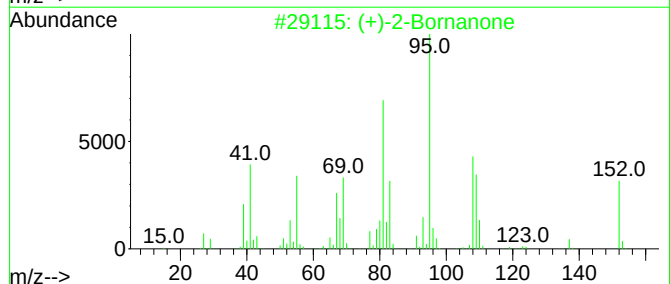
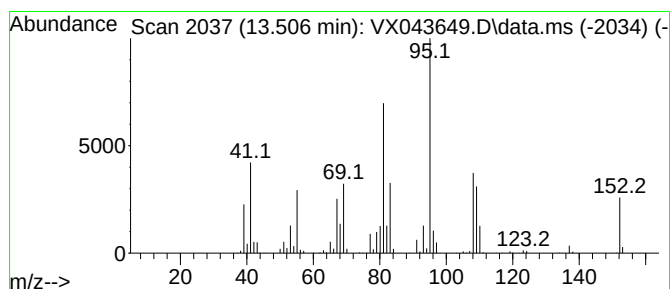
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Quant Title : SW846 8260

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

Peak Number 7 (+)-2-Bornanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	134.57 ug/l	1375270	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	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103124\
Data File : VX043649.D
Acq On : 31 Oct 2024 14:27
Operator : JC/MD
Sample : P4646-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

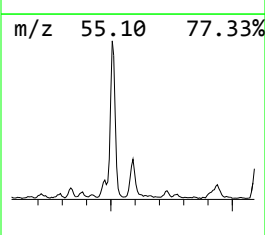
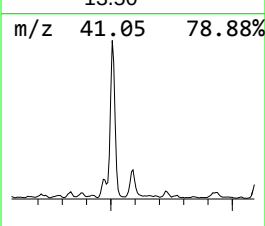
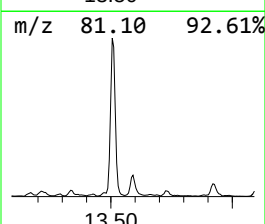
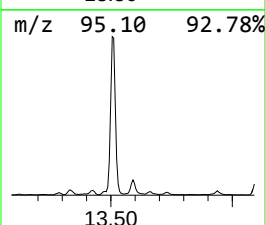
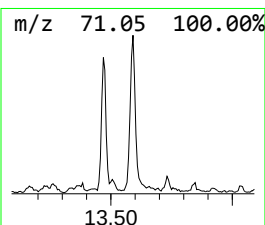
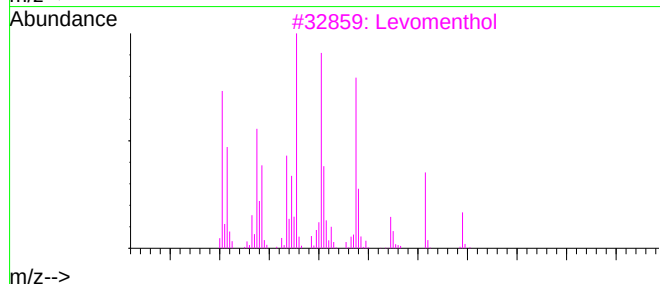
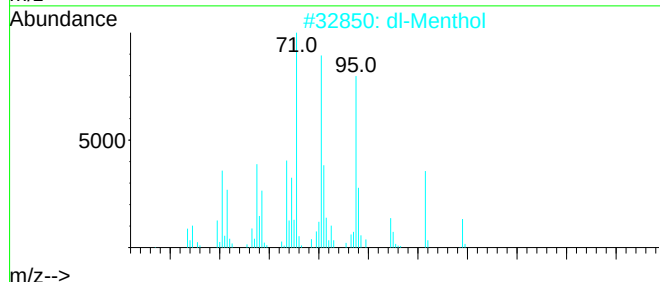
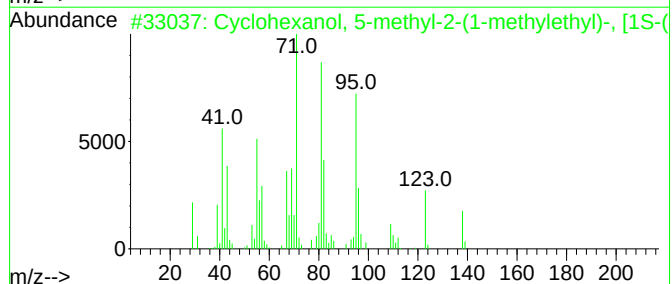
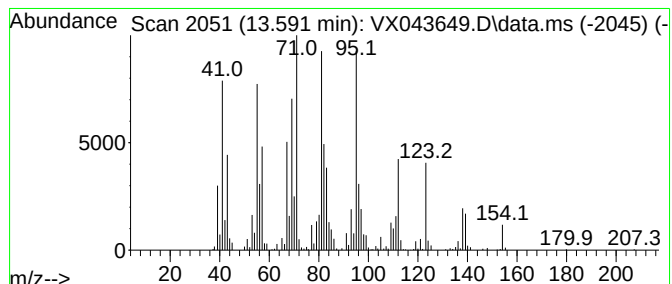
Instrument :
MSVOA_X
ClientSampleId :
241030069-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.591	30.81 ug/l	314821	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	74
2	dl-Menthol	156	C10H20O	000089-78-1	68
3	Levomenthol	156	C10H20O	002216-51-5	68
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	64
5	d-Menthol	156	C10H20O	015356-60-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103124\
Data File : VX043649.D
Acq On : 31 Oct 2024 14:27
Operator : JC/MD
Sample : P4646-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241030069-01-VOA

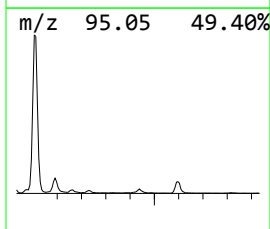
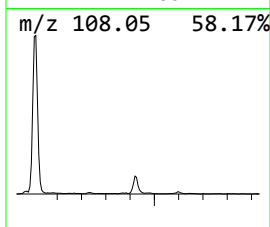
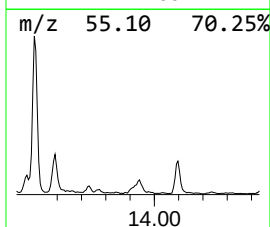
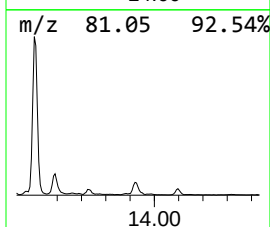
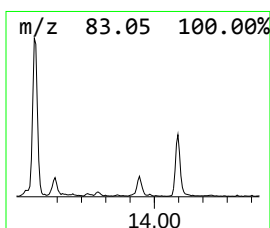
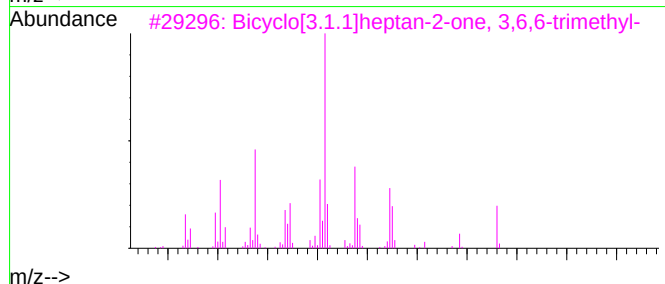
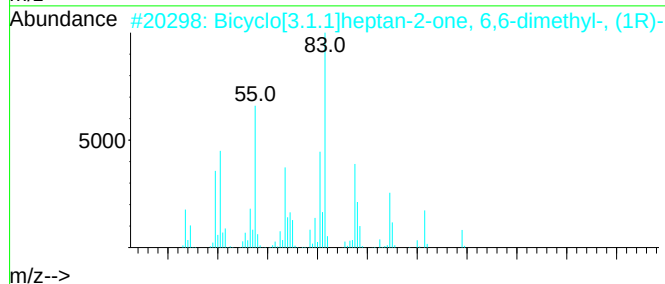
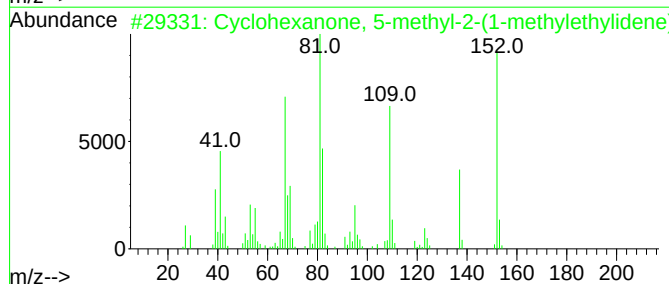
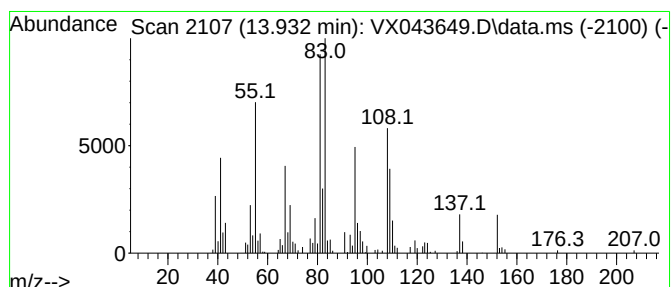
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.932 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.932	9.99 ug/l	102111	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	49
2	Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	46
3	Bicyclo[3.1.1]heptan-2-one, 3,6-...	152	C10H16O	016022-08-5	38
4	Spiro[3.4]octan-1-one, 5-methyl-...	138	C9H14O	065147-55-9	38
5	Cyclohexene, 1-pentyl-	152	C11H20	015232-85-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103124\
Data File : VX043649.D
Acq On : 31 Oct 2024 14:27
Operator : JC/MD
Sample : P4646-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241030069-01-VOA

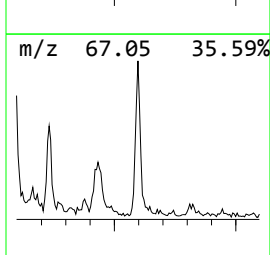
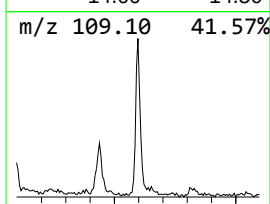
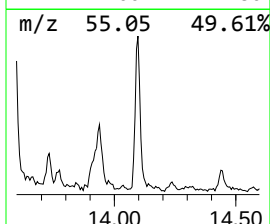
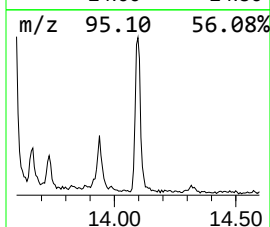
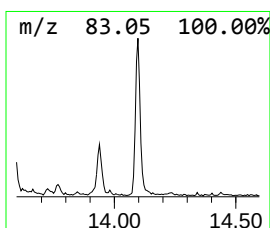
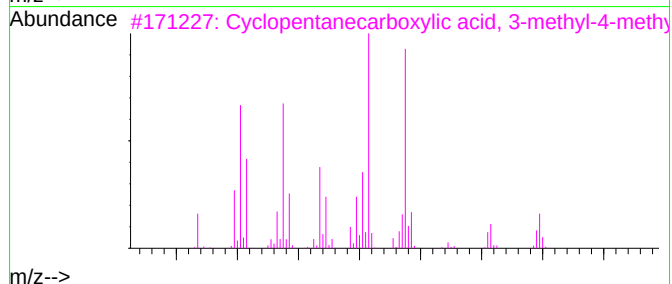
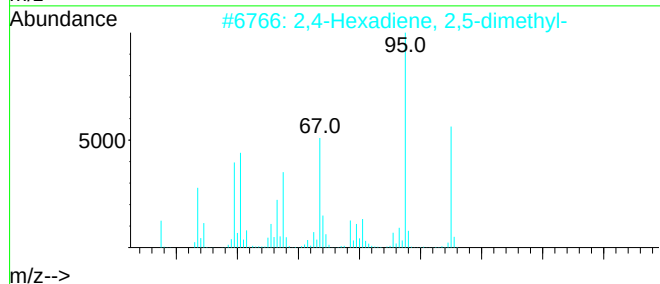
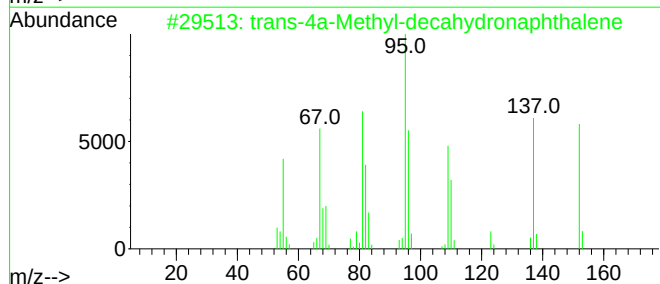
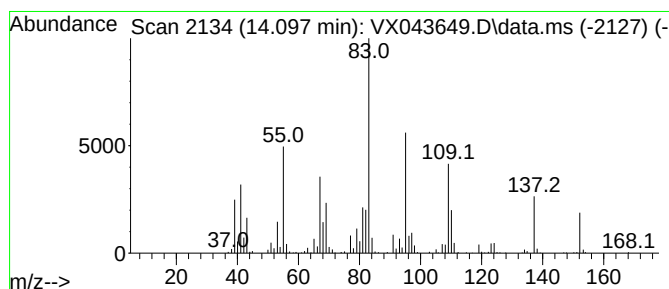
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown14.097 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	21.40 ug/l	218752	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
2	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	35
3	Cyclopentanecarboxylic acid, 3-m...	278	C18H30O2	1000152-25-8	22
4	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	20
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103124\
Data File : VX043649.D
Acq On : 31 Oct 2024 14:27
Operator : JC/MD
Sample : P4646-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
241030069-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102824W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.252	25.8	ug/l	145534	1	5.544	282500	50.0
2-Propanol, 2-m...	2.995	456.0	ug/l	2576330	1	5.544	282500	50.0
L-Fenchone	12.902	94.4	ug/l	964756	4	12.024	510985	50.0
unknown13.475	13.475	23.6	ug/l	240697	4	12.024	510985	50.0
(+)-2-Bornanone	13.506	134.6	ug/l	1375270	4	12.024	510985	50.0
Cyclohexanol, 5...	13.591	30.8	ug/l	314821	4	12.024	510985	50.0
unknown13.932	13.932	10.0	ug/l	102111	4	12.024	510985	50.0
unknown14.097	14.097	21.4	ug/l	218752	4	12.024	510985	50.0