

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
 Data File : VX028249.D
 Acq On : 21 Apr 2022 18:19
 Operator : JC/MD
 Sample : N2459-20
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4922B

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028249.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	20	26	30	rBV	13831	27887	1.13%	0.152%
2	1.557	69	77	83	rBV4	32678	75232	3.04%	0.410%
3	2.050	153	158	166	rVB	52403	79201	3.20%	0.432%
4	2.374	206	211	215	rBV	21523	36581	1.48%	0.199%
5	2.422	215	219	230	rVV	70053	115524	4.67%	0.629%
6	2.532	230	237	246	rVB	23505	45838	1.85%	0.250%
7	4.562	563	570	584	rVB2	10138	28744	1.16%	0.157%
8	5.391	694	706	721	rBV2	307267	890506	36.00%	4.852%
9	5.556	721	733	752	rVB	416759	1189574	48.10%	6.482%
10	5.958	786	799	816	rBV	316206	818175	33.08%	4.458%
11	6.763	921	931	950	rBV	642147	1535654	62.09%	8.368%
12	7.214	999	1005	1014	rBV3	10512	26754	1.08%	0.146%
13	8.574	1222	1228	1234	rBV	22636	39262	1.59%	0.214%
14	8.653	1234	1241	1249	rVV	1575912	2473340	100.00%	13.477%
15	10.055	1465	1471	1482	rBV	1421399	1896386	76.67%	10.333%
16	11.079	1630	1639	1651	rBV	1315489	1738654	70.30%	9.474%
17	11.756	1744	1750	1757	rBV2	17908	24873	1.01%	0.136%
18	11.890	1767	1772	1781	rBV2	110272	233659	9.45%	1.273%
19	12.024	1789	1794	1801	rVB	1543704	1883689	76.16%	10.264%
20	12.104	1801	1807	1812	rBV2	90926	123092	4.98%	0.671%
21	12.219	1821	1826	1831	rBV	142276	222639	9.00%	1.213%
22	12.286	1831	1837	1839	rBV3	109057	204220	8.26%	1.113%
23	12.360	1847	1849	1863	rVB6	30739	81252	3.29%	0.443%
24	12.768	1912	1916	1918	rBV2	21923	30688	1.24%	0.167%
25	12.860	1924	1931	1937	rBV2	89971	150692	6.09%	0.821%
26	12.969	1945	1949	1957	rBV6	24046	46289	1.87%	0.252%
27	13.073	1961	1966	1967	rBV3	25456	35039	1.42%	0.191%
28	13.103	1967	1971	1972	rVV	103386	128390	5.19%	0.700%
29	13.128	1972	1975	1986	rVV2	262110	582429	23.55%	3.174%
30	13.219	1986	1990	2001	rVV	358753	559999	22.64%	3.051%
31	13.420	2019	2023	2035	rBV	1043020	1561461	63.13%	8.508%
32	13.750	2071	2077	2089	rVB2	34805	89103	3.60%	0.486%
33	13.890	2097	2100	2112	rVB4	39581	81547	3.30%	0.444%
34	14.195	2145	2150	2168	rBV	584136	1180706	47.74%	6.434%
35	14.573	2208	2212	2217	rBV4	30317	52759	2.13%	0.287%
36	14.920	2264	2269	2279	rBV3	30634	62063	2.51%	0.338%

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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\82X041922W.M
Title : SW846 8260

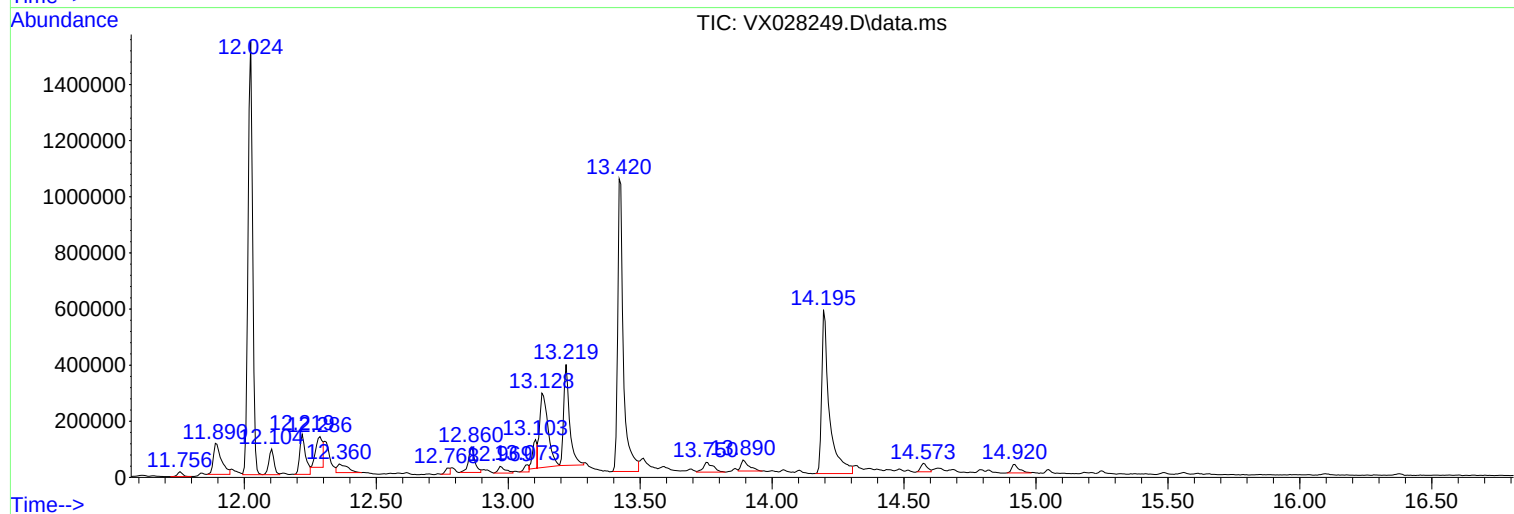
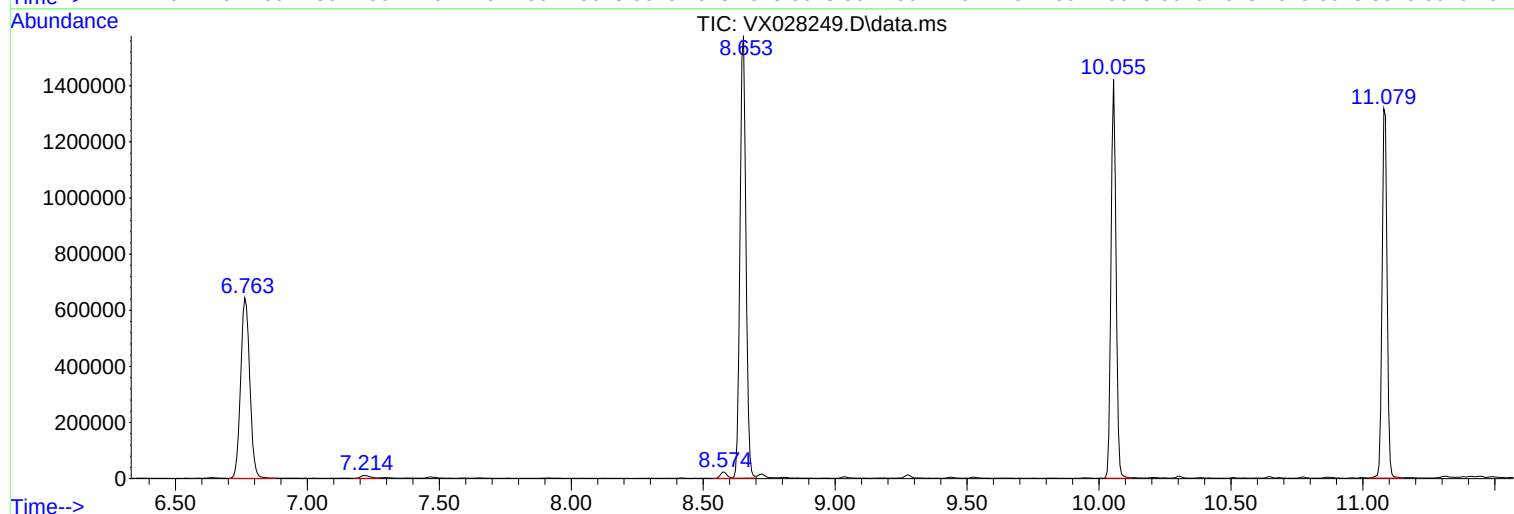
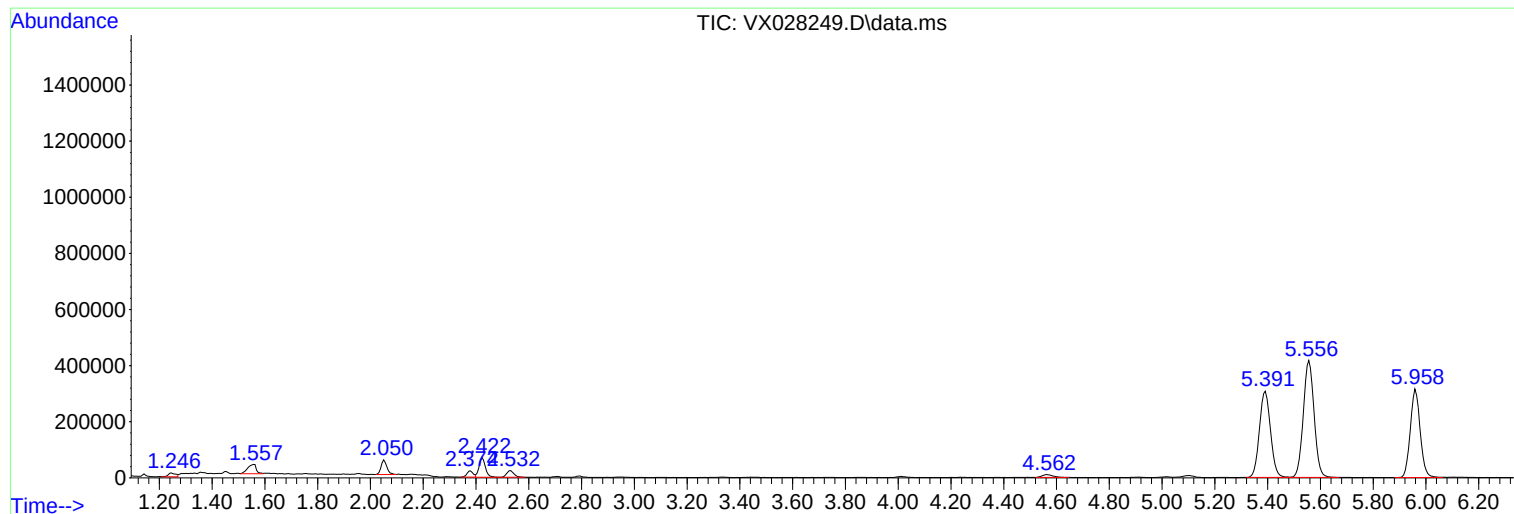
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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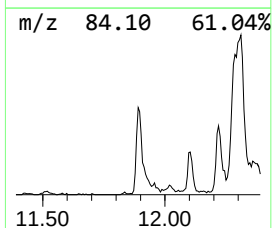
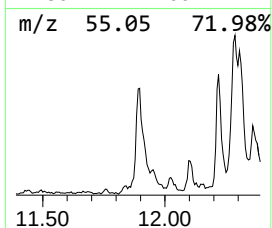
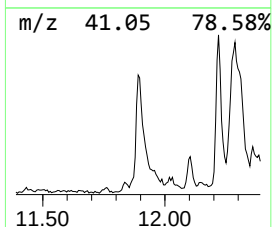
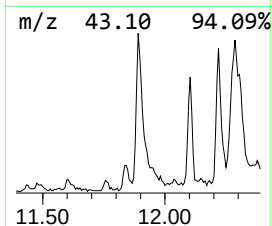
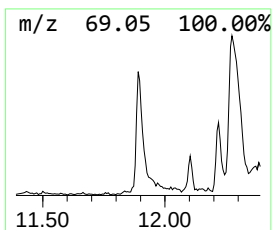
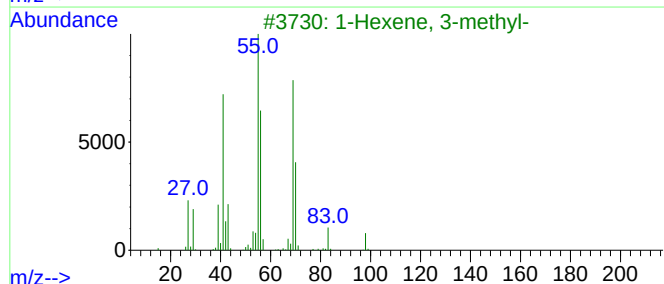
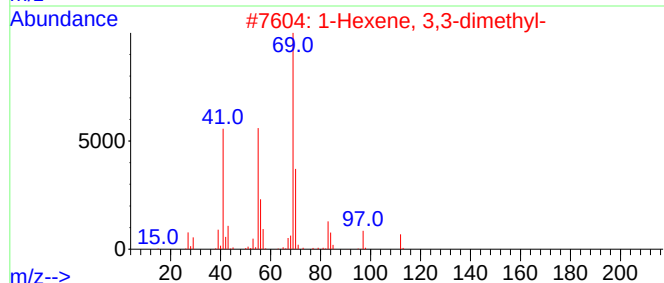
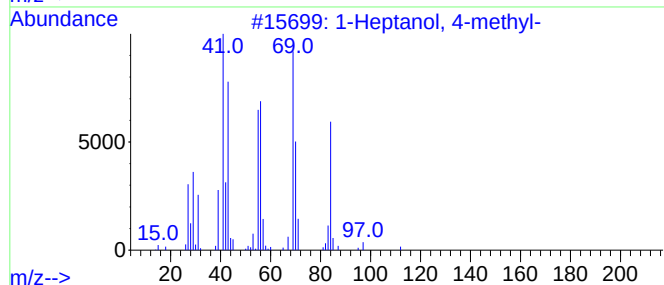
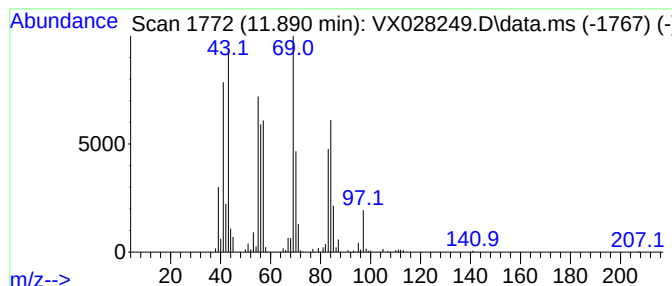
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Heptanol, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.890	6.20 ug/l	233659	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
2			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	43
3			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	43
4			Pentane, 3-methylene-	84	C6H12	000760-21-4	43
5			1-Undecanol	172	C11H24O	000112-42-5	38



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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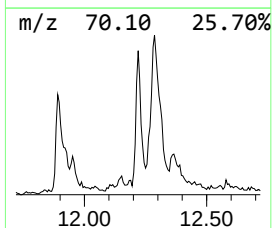
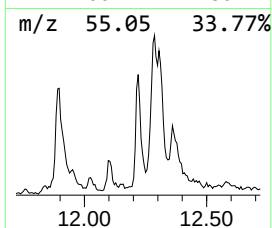
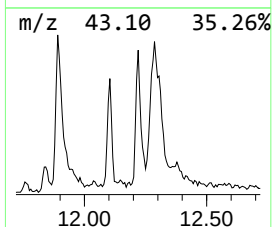
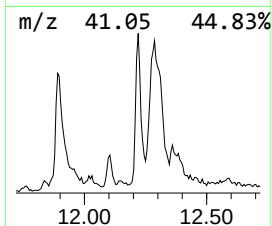
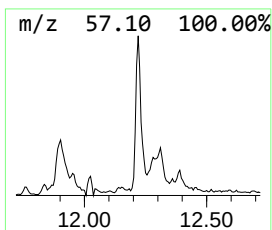
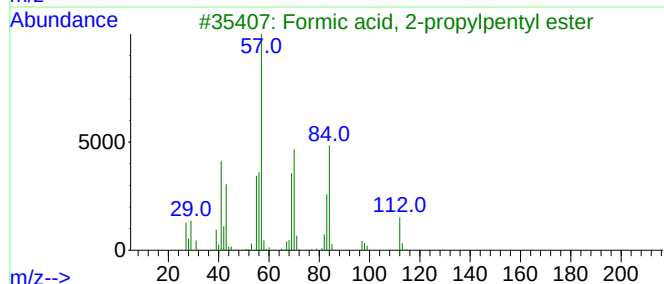
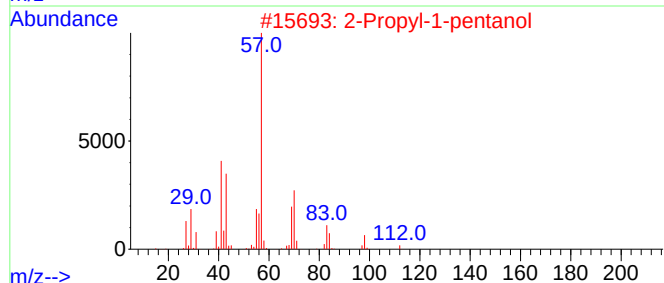
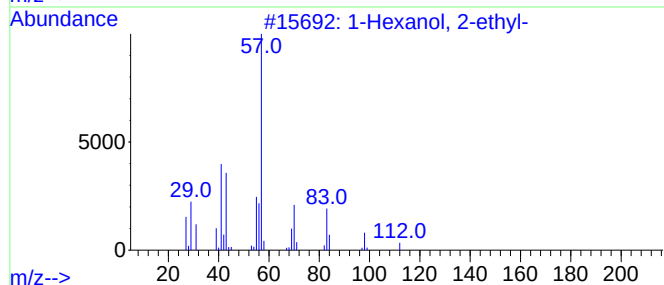
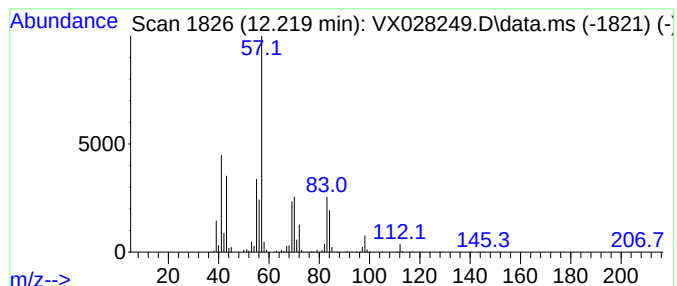
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	5.91 ug/l	222639	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
3			Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	47
4			2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	45
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43



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Instrument :
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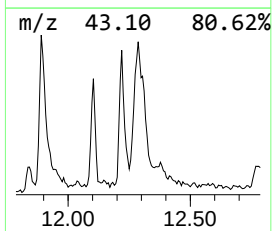
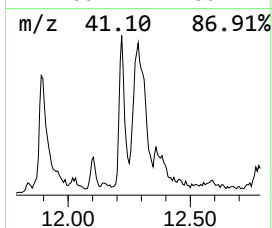
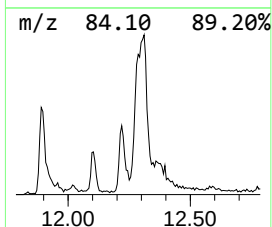
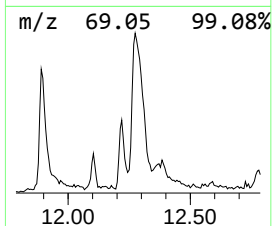
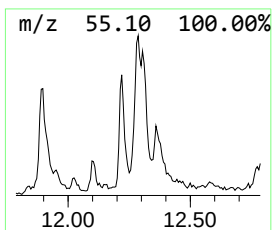
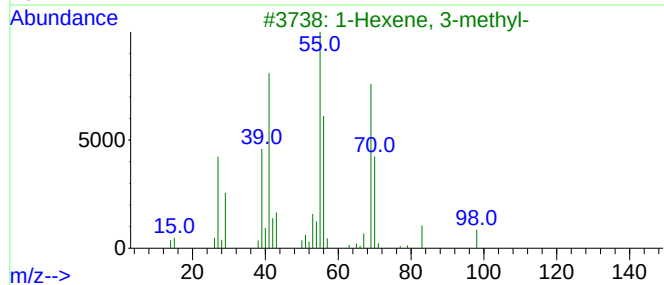
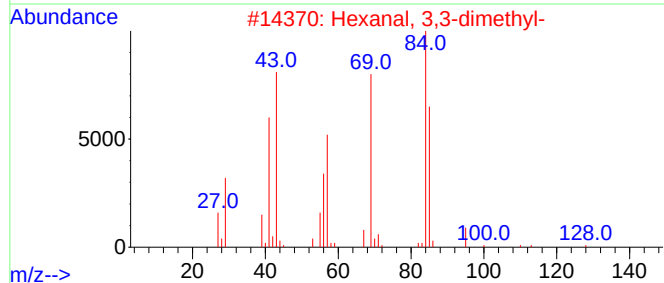
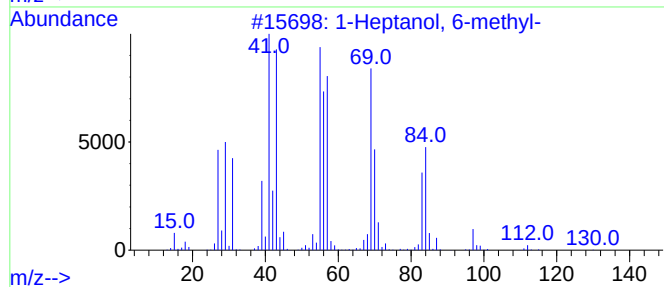
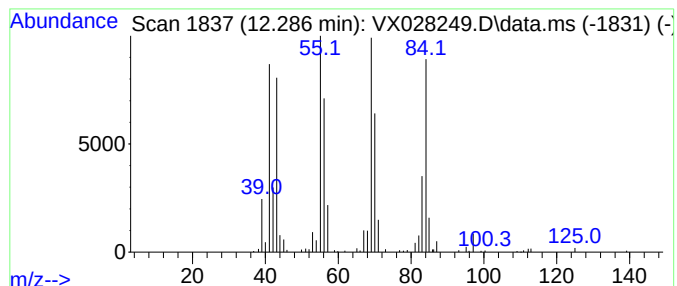
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Heptanol, 6-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.287	5.42 ug/l	204220	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	72
2			Hexanal, 3,3-dimethyl-	128	C8H16O	055320-57-5	50
3			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	47
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47
5			3-Octene, (E)-	112	C8H16	014919-01-8	38



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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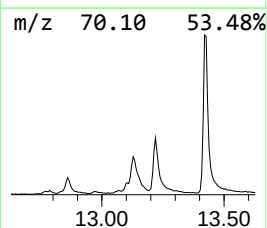
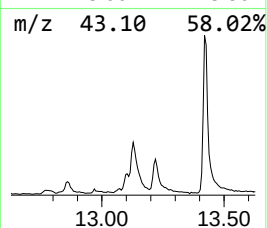
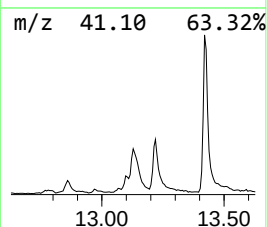
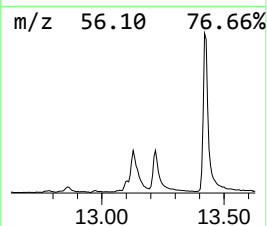
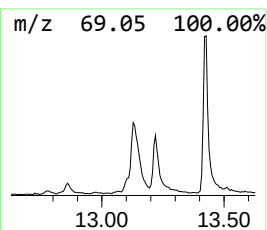
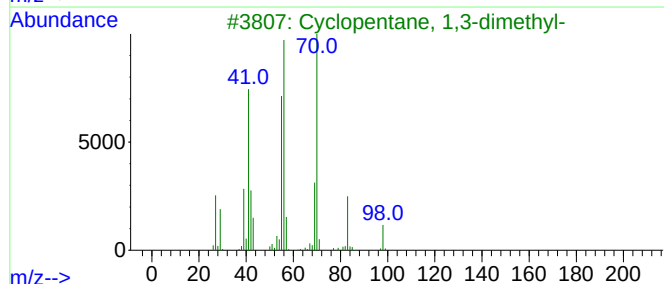
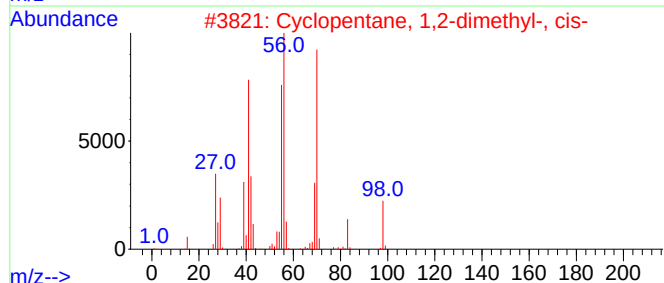
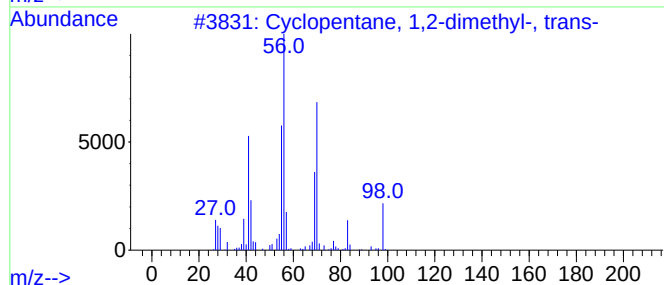
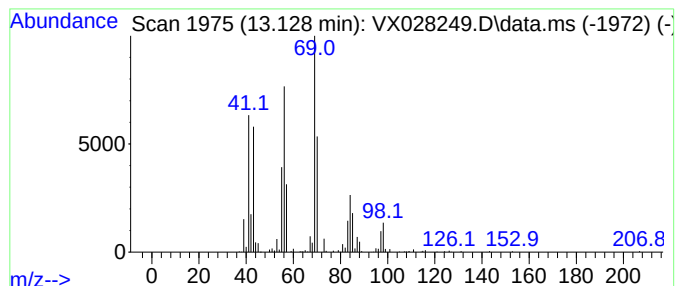
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.128 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	15.46 ug/l	582429	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	49
2			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	49
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	46
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	46
5			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	46



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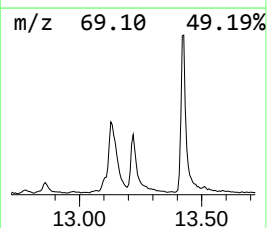
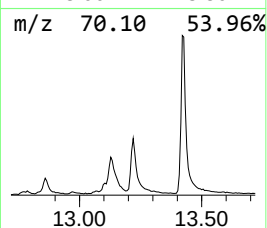
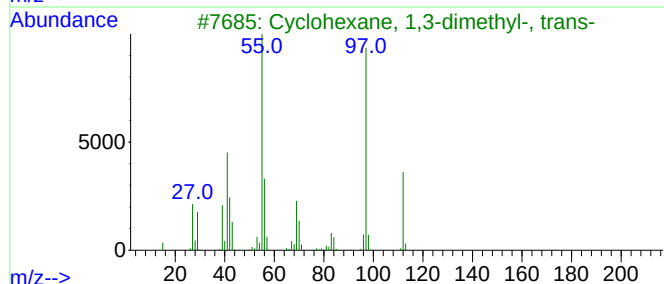
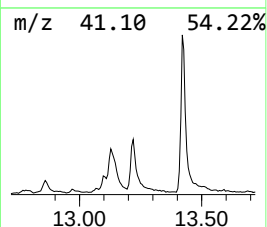
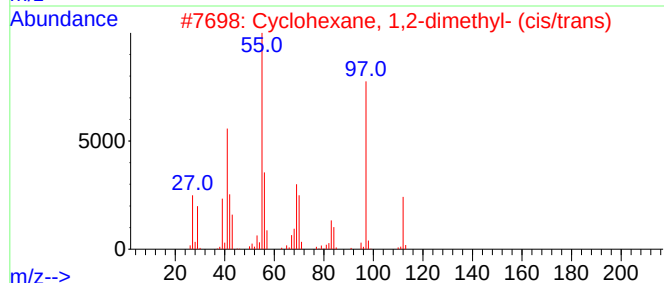
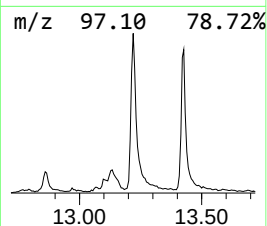
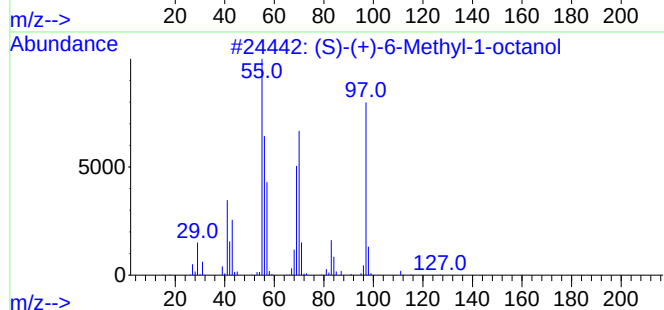
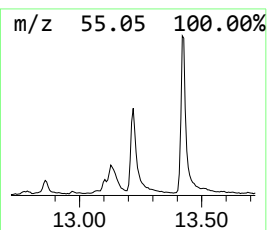
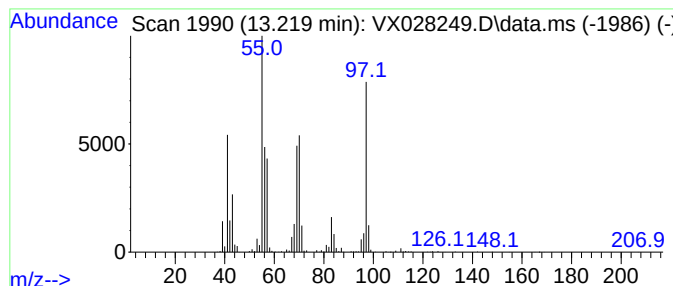
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 5 (S)-(+)-6-Methyl-1-octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	14.86 ug/l	559999	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	64
3			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	59
4			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	58
5			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028249.D
Acq On : 21 Apr 2022 18:19
Operator : JC/MD
Sample : N2459-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4922B

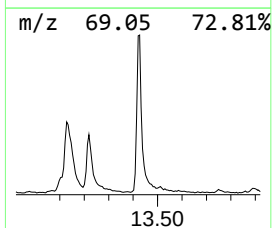
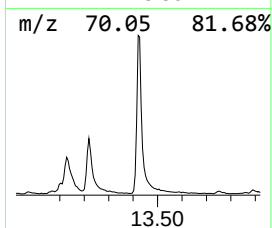
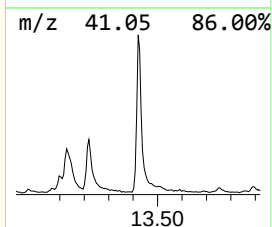
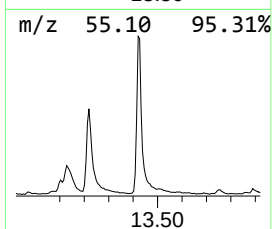
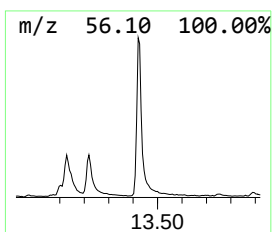
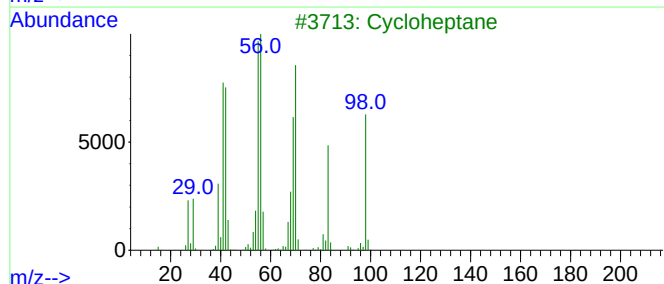
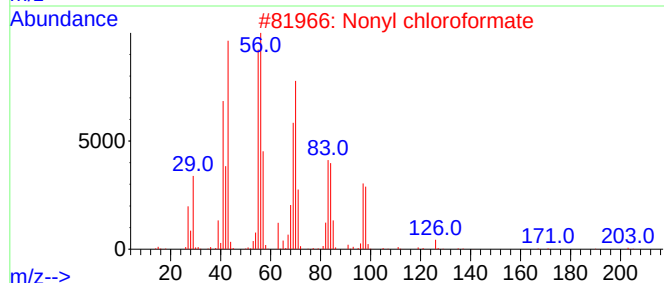
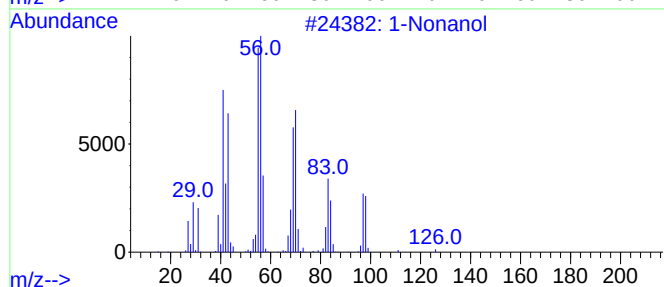
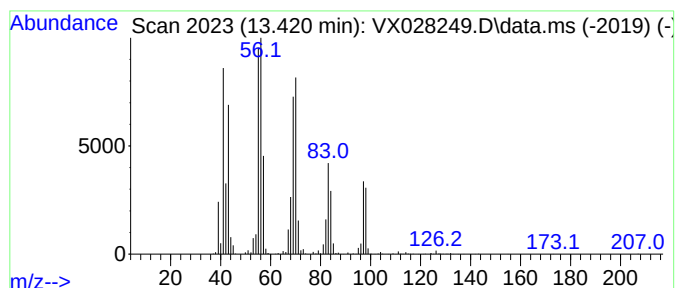
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Quant Title : SW846 8260

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

Peak Number 6 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	41.45 ug/l	1561460	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Nonyl chloroformate	206	C10H19ClO2	057045-82-6	80
3			Cycloheptane	98	C7H14	000291-64-5	74
4			1-Nonene	126	C9H18	000124-11-8	74
5			Isopropylcyclobutane	98	C7H14	000872-56-0	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028249.D
Acq On : 21 Apr 2022 18:19
Operator : JC/MD
Sample : N2459-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

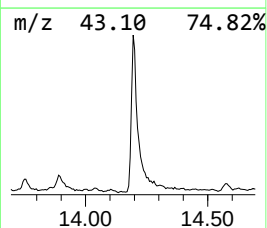
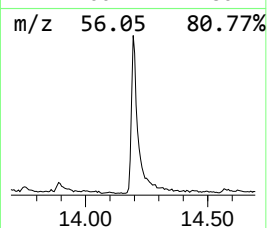
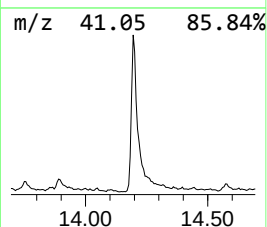
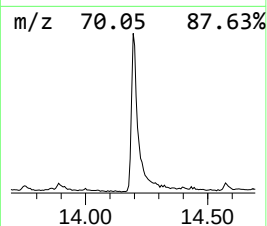
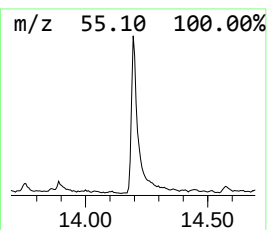
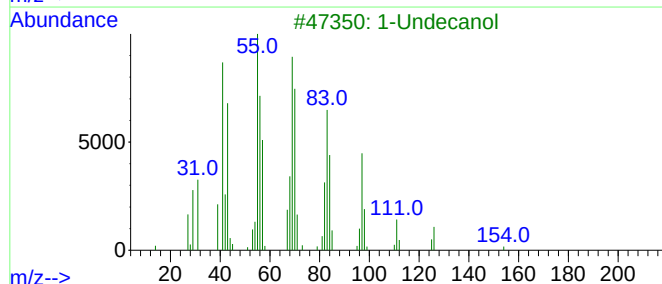
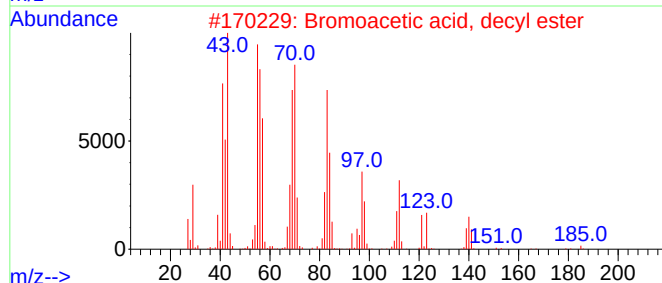
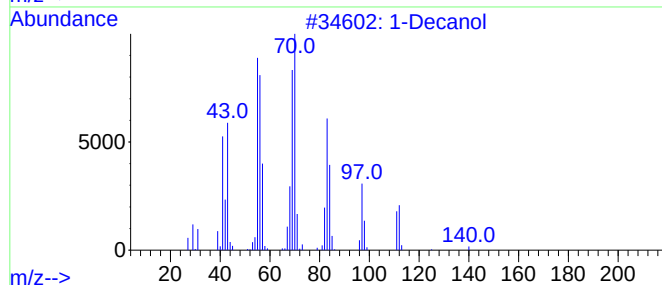
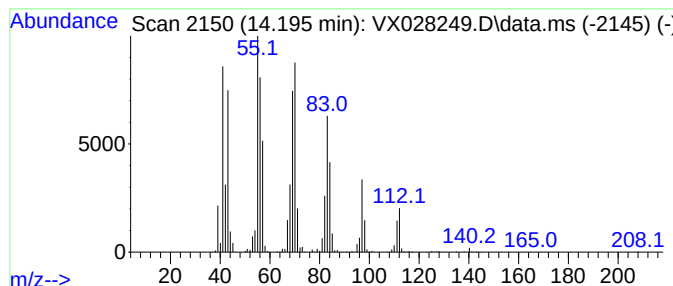
Instrument :
MSVOA_X
ClientSampleId :
4922B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.195	31.34 ug/l	1180710	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	91
3	1-Undecanol	172	C11H24O	000112-42-5	91
4	1-Dodecanol	186	C12H26O	000112-53-8	87
5	Cyclooctane	112	C8H16	000292-64-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028249.D
Acq On : 21 Apr 2022 18:19
Operator : JC/MD
Sample : N2459-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4922B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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
1-Heptanol, 4-m...	11.890	6.2	ug/l	233659	4	12.024	1883690	50.0
1-Hexanol, 2-et...	12.219	5.9	ug/l	222639	4	12.024	1883690	50.0
1-Heptanol, 6-m...	12.287	5.4	ug/l	204220	4	12.024	1883690	50.0
unknown13.128	13.128	15.5	ug/l	582429	4	12.024	1883690	50.0
(S)-(+)-6-Methy...	13.219	14.9	ug/l	559999	4	12.024	1883690	50.0
1-Nonanol	13.420	41.5	ug/l	1561460	4	12.024	1883690	50.0
1-Decanol	14.195	31.3	ug/l	1180710	4	12.024	1883690	50.0