

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112724\
 Data File : VY020467.D
 Acq On : 27 Nov 2024 17:48
 Operator : SY/MD
 Sample : P5045-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SU-04-11222024

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_Y\methods\82Y111924S.M
 Title : SW846 8260

Signal : TIC: VY020466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.890	837	848	858	rBV	3747	12156	11.16%	2.009%
2	7.640	962	971	977	rBV2	13612	34384	31.55%	5.683%
3	7.713	977	983	994	rVB	31255	70573	64.76%	11.664%
4	8.067	1031	1041	1051	rBV2	11345	28407	26.07%	4.695%
5	8.616	1123	1131	1141	rBV	42657	85178	78.17%	14.077%
6	10.109	1369	1376	1387	rBV	62328	108969	100.00%	18.009%
7	10.512	1437	1442	1450	rVB4	3121	5477	5.03%	0.905%
8	10.859	1494	1499	1502	rBV4	653	1324	1.22%	0.219%
9	11.249	1559	1563	1568	rVB3	652	1332	1.22%	0.220%
10	11.420	1585	1591	1600	rBV	48291	81570	74.86%	13.481%
11	11.713	1635	1639	1643	rBV5	827	1482	1.36%	0.245%
12	12.237	1720	1725	1726	rBV3	1421	2053	1.88%	0.339%
13	12.273	1727	1731	1734	rVV5	1611	3116	2.86%	0.515%
14	12.408	1748	1753	1760	rVB3	32280	55011	50.48%	9.092%
15	12.651	1789	1793	1796	rBV5	829	1491	1.37%	0.246%
16	12.731	1801	1806	1812	rVB7	1434	3071	2.82%	0.508%
17	13.353	1901	1908	1915	rBV	29541	46492	42.67%	7.684%
18	13.676	1955	1961	1965	rBV4	3688	6750	6.19%	1.116%
19	13.718	1965	1968	1971	rVB3	1224	1618	1.48%	0.267%
20	13.761	1971	1975	1976	rBV3	1026	1355	1.24%	0.224%
21	13.895	1994	1997	2001	rVB5	787	1136	1.04%	0.188%
22	14.182	2036	2044	2050	rVB9	2682	6980	6.41%	1.154%
23	14.230	2050	2052	2057	rBV4	934	1666	1.53%	0.275%
24	14.340	2067	2070	2074	rVV6	1367	1723	1.58%	0.285%
25	14.401	2076	2080	2085	rVB6	1462	2478	2.27%	0.410%
26	14.535	2097	2102	2107	rBV4	4369	7182	6.59%	1.187%
27	14.608	2109	2114	2116	rVV5	1315	2136	1.96%	0.353%
28	14.657	2116	2122	2126	rVB8	2477	4758	4.37%	0.786%
29	14.767	2136	2140	2143	rBV4	973	1661	1.52%	0.275%
30	15.060	2185	2188	2192	rVB4	2439	3157	2.90%	0.522%
31	15.127	2194	2199	2200	rBV5	1936	2703	2.48%	0.447%
32	15.291	2223	2226	2231	rBV6	582	1345	1.23%	0.222%
33	15.346	2231	2235	2241	rVB7	4388	7581	6.96%	1.253%
34	15.401	2241	2244	2246	rBV3	829	1108	1.02%	0.183%
35	15.462	2251	2254	2256	rVB4	1114	1121	1.03%	0.185%
36	15.828	2310	2314	2319	rVB4	1265	1649	1.51%	0.273%

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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

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Title : SW846 8260

37	16.059	2348	2352	2355	rBV6	804	1136	1.04%	0.188%
38	16.254	2379	2384	2391	rBV6	2324	3742	3.43%	0.618%

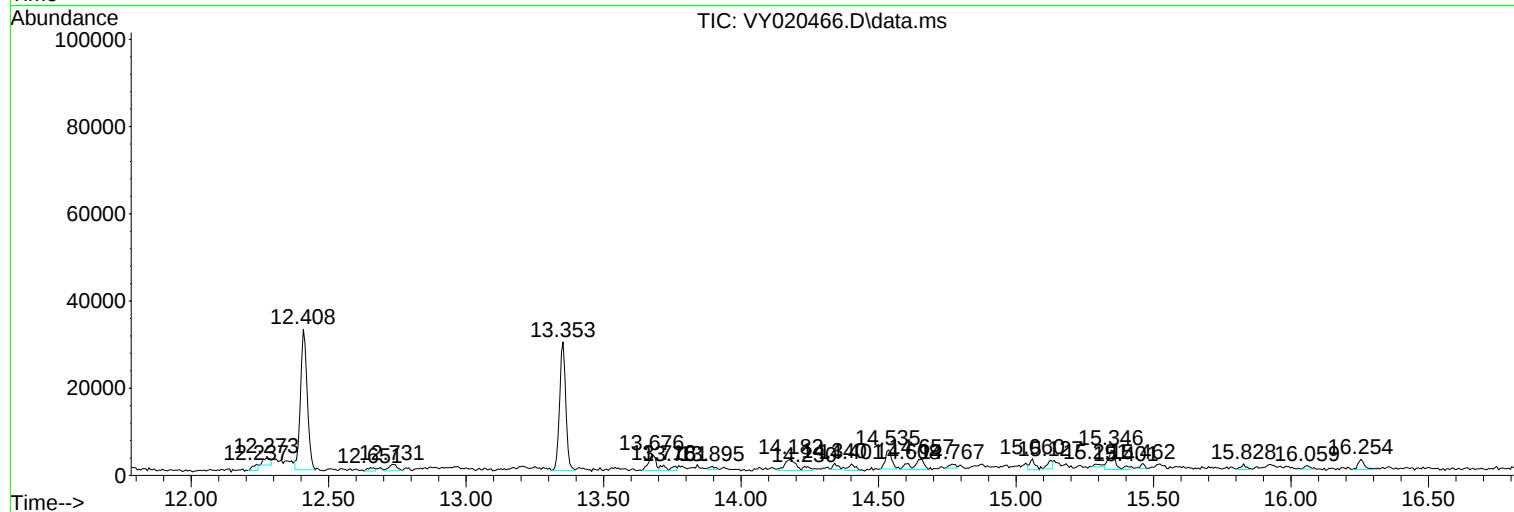
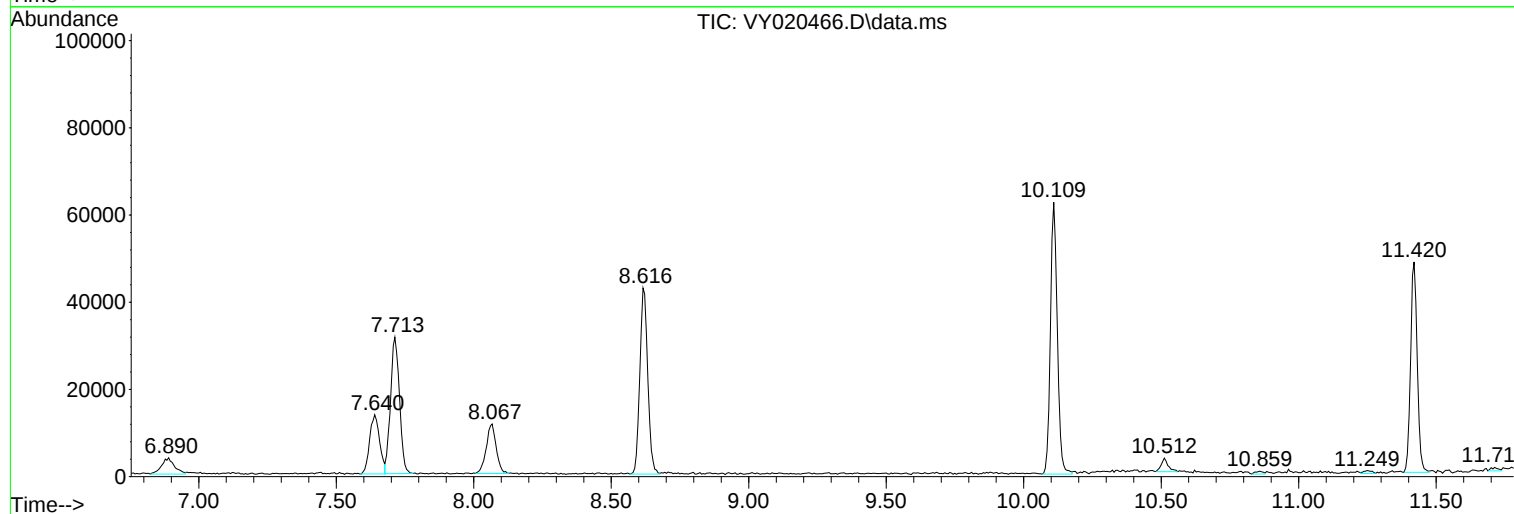
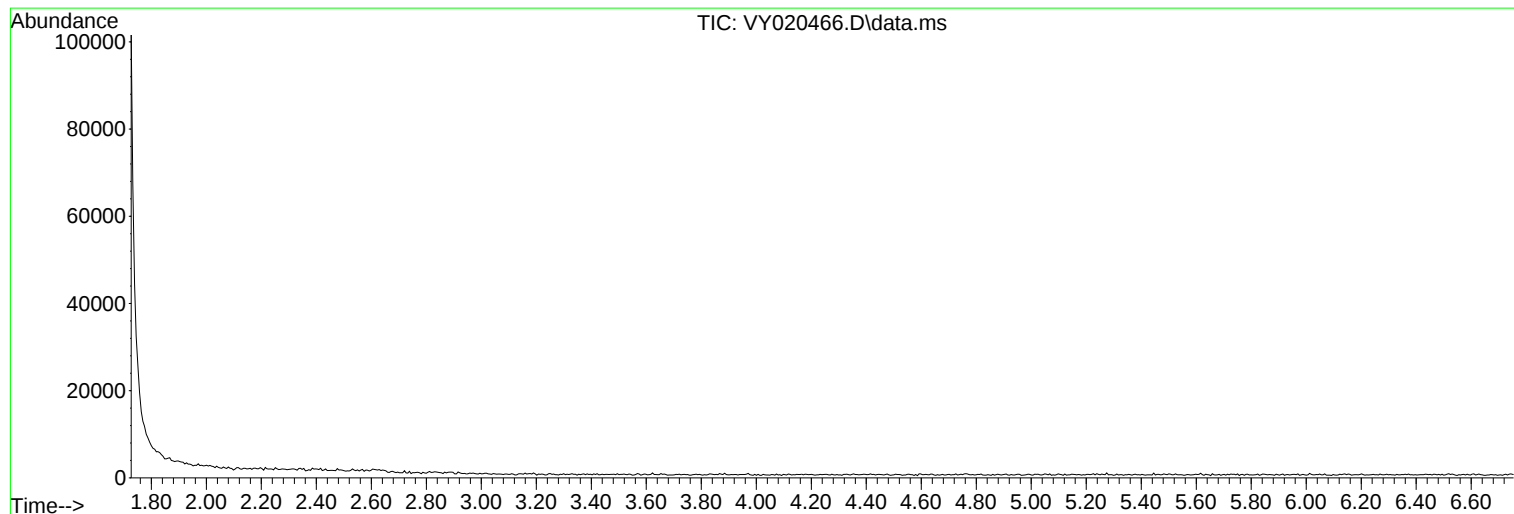
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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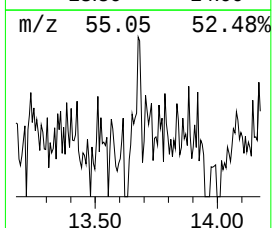
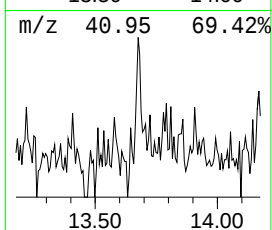
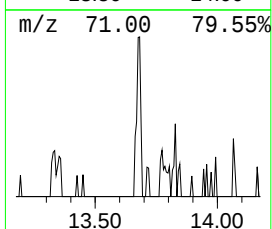
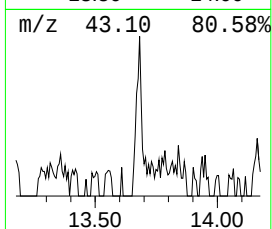
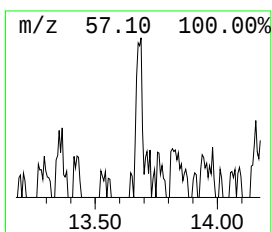
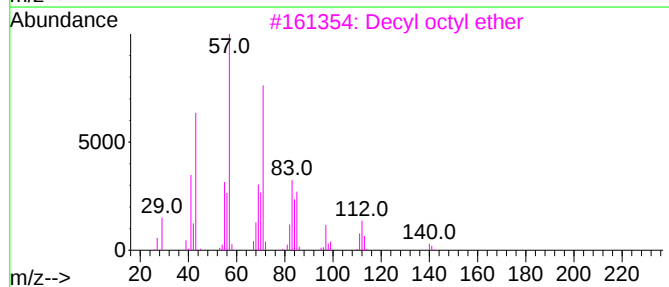
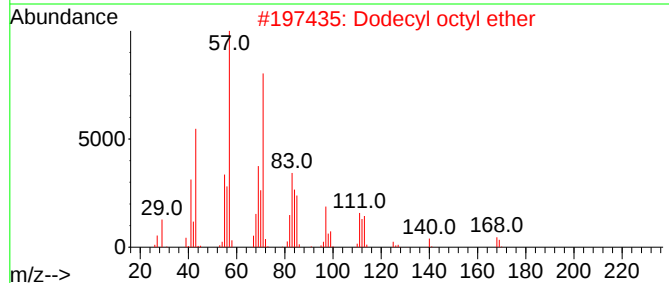
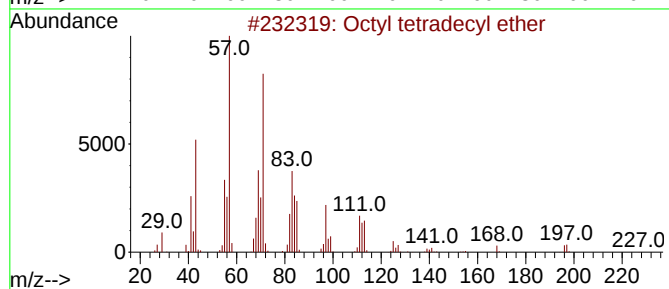
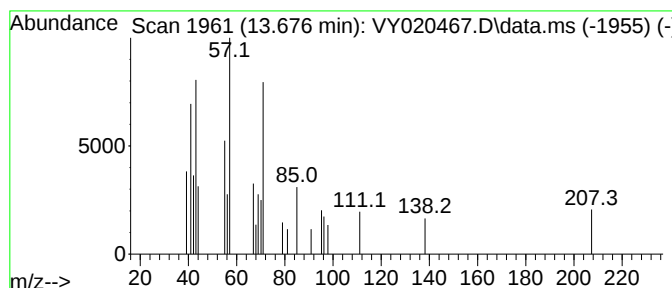
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Octyl tetradecyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	7.26 ug/l	6750	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octyl tetradecyl ether	326	C22H46O	1000406-38-5	50
2			Dodecyl octyl ether	298	C20H42O	1000406-38-4	47
3			Decyl octyl ether	270	C18H38O	1000406-38-3	43
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	43
5			Undecane	156	C11H24	001120-21-4	43



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Instrument :
MSVOA_Y
ClientSampleId :
SU-04-11222024

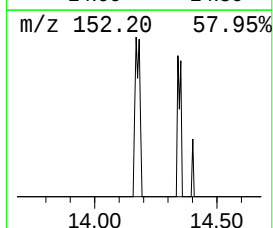
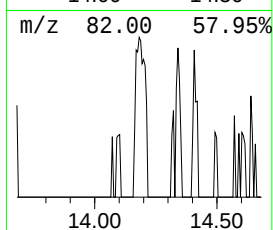
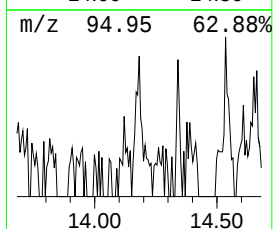
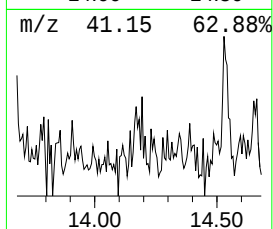
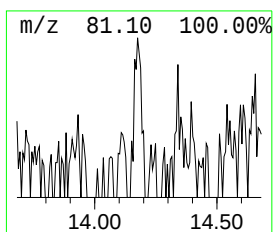
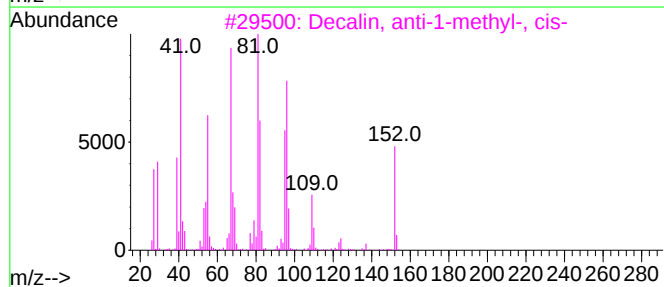
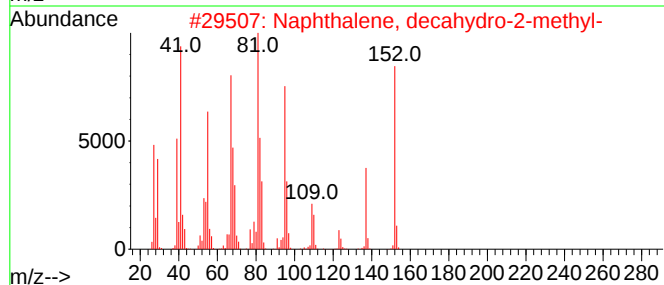
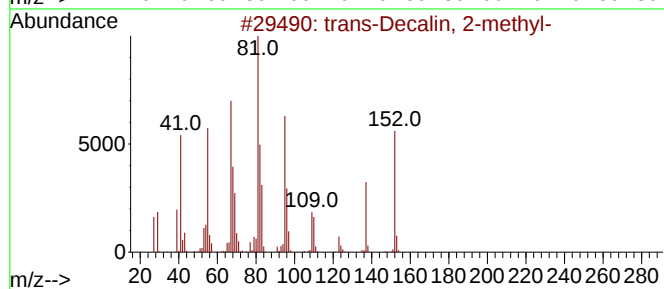
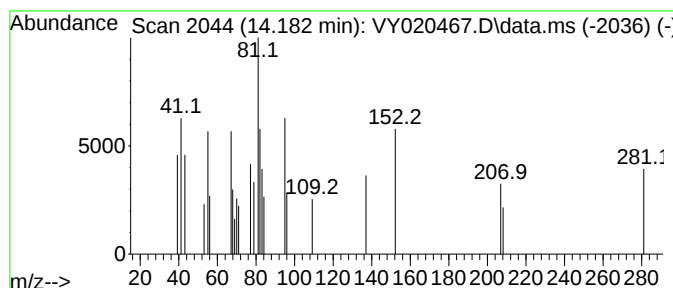
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-Decalin, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	7.51 ug/l	6980	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	83
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	64
3			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	55
4			Benzofuran, octahydro-6-methyl-3...	152	C10H16O	077954-13-3	49
5			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	42



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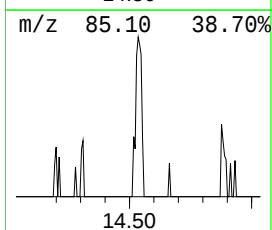
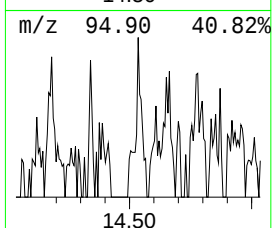
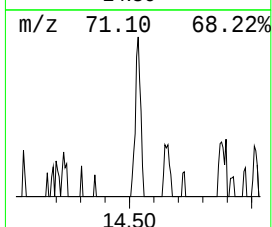
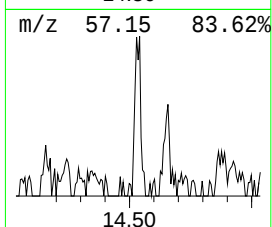
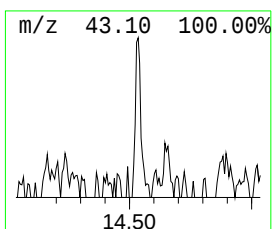
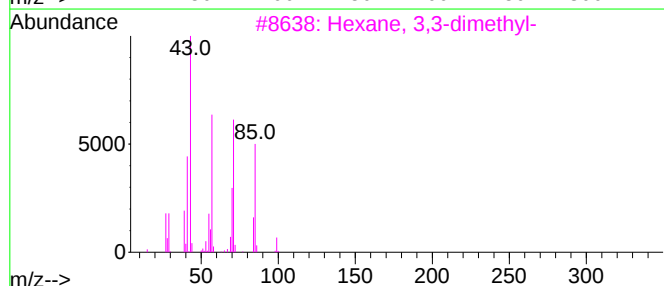
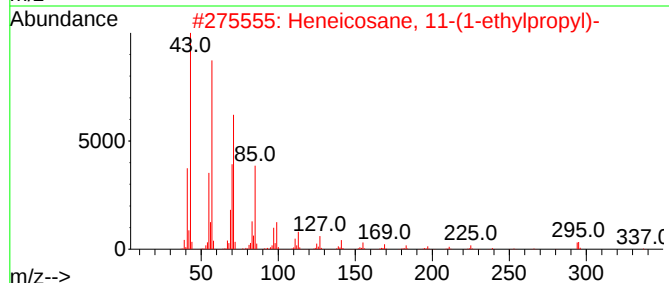
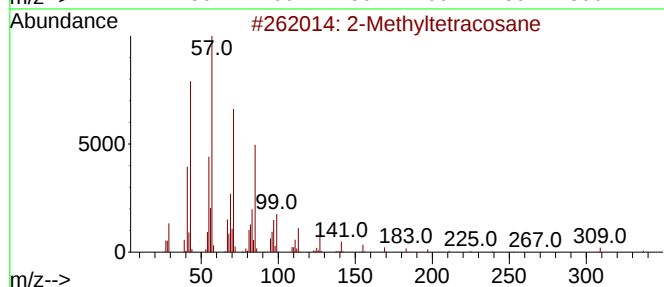
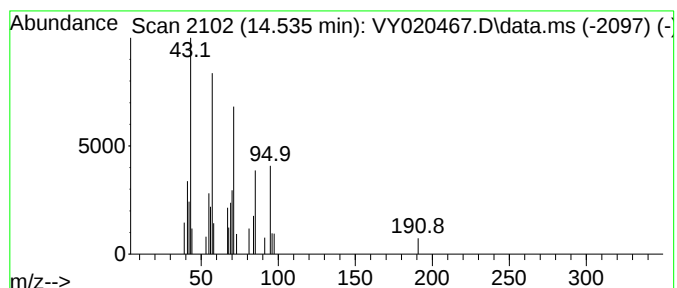
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Methyltetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.535	7.72 ug/l	7182	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyltetracosane	352	C25H52	001560-78-7	50
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	47
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
4			Hydroxylamine, 0-decyl-	173	C10H23NO	029812-79-1	47
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47



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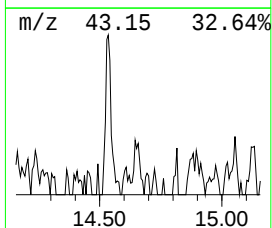
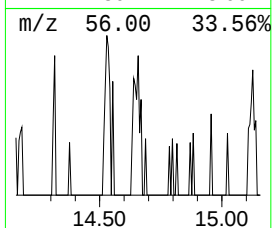
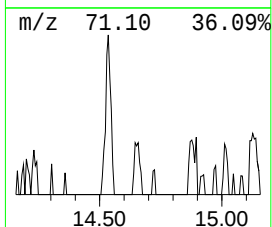
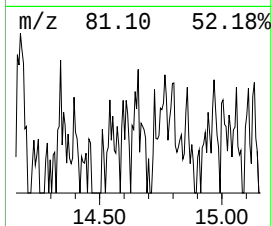
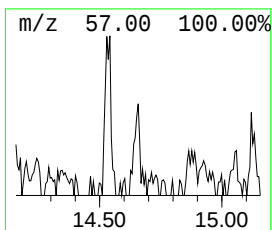
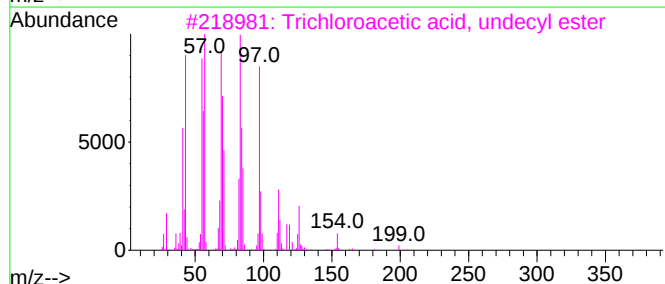
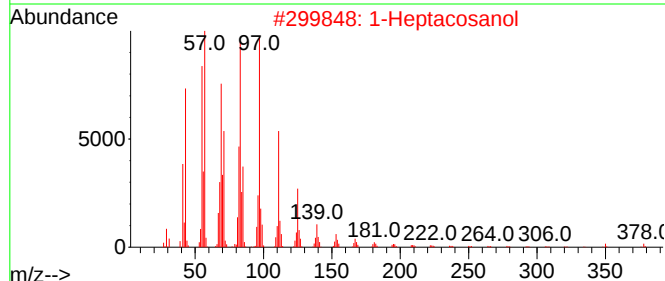
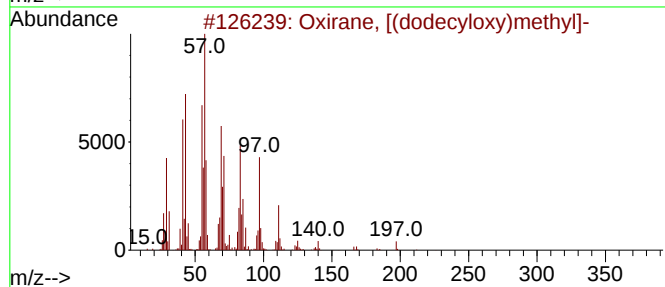
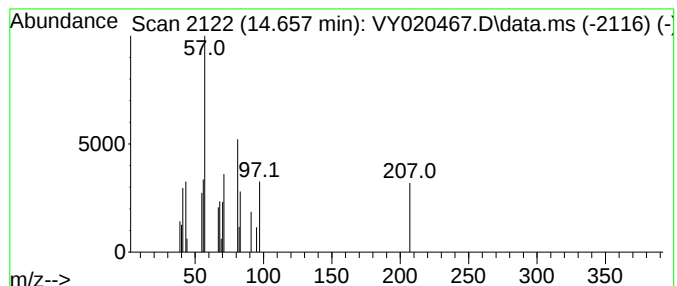
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.657 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	5.12 ug/l	4758	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	37
2			1-Heptacosanol	396	C27H56O	002004-39-9	33
3			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	25
4			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	25
5			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	23



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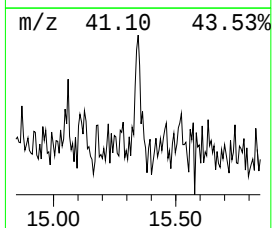
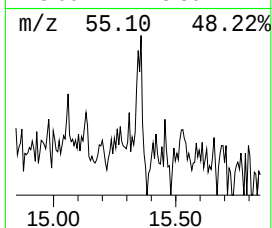
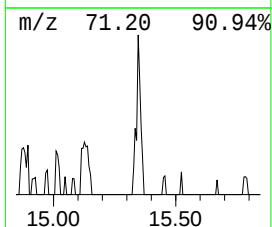
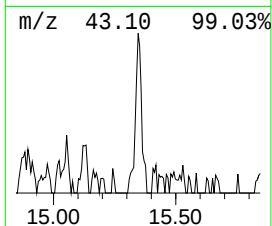
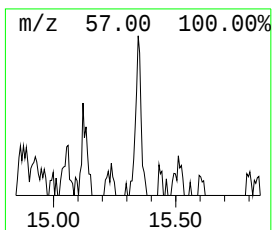
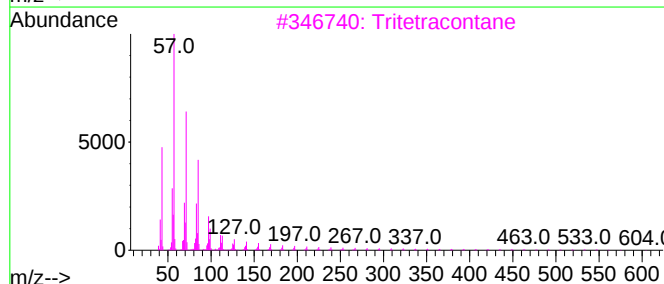
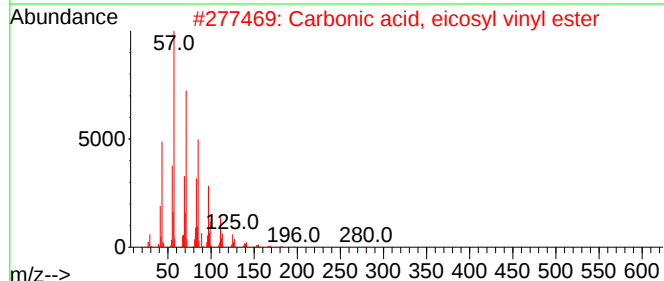
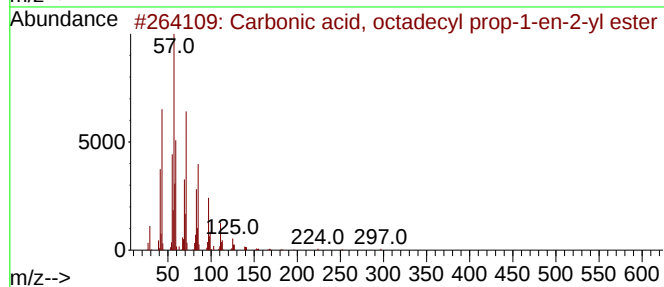
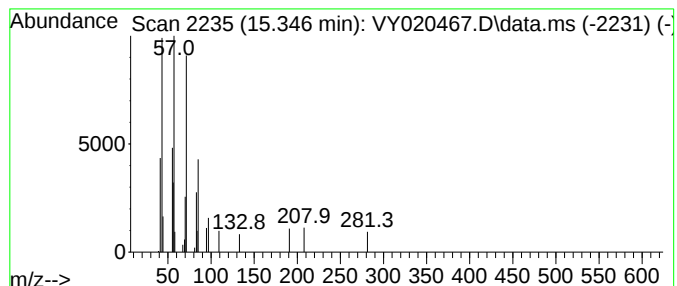
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Carbonic acid, octadecyl pr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.346	8.15 ug/l	7581	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	59
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	59
3			Tritetracontane	605	C43H88	007098-21-7	59
4			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	59
5			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112724\
Data File : VY020467.D
Acq On : 27 Nov 2024 17:48
Operator : SY/MD
Sample : P5045-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SU-04-11222024

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.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
Octyl tetradecy...	13.676	7.3	ug/l	6750	4	13.352	46492	50.0
trans-Decalin, ...	14.182	7.5	ug/l	6980	4	13.352	46492	50.0
2-Methyltetraco...	14.535	7.7	ug/l	7182	4	13.352	46492	50.0
unknown14.657	14.657	5.1	ug/l	4758	4	13.352	46492	50.0
Carbonic acid, ...	15.346	8.2	ug/l	7581	4	13.352	46492	50.0