

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110321\
 Data File : VY006615.D
 Acq On : 03 Nov 2021 20:39
 Operator : SY/MD
 Sample : M4436-01
 Misc : 5.01G/5ML/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S15-SP

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\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.516	110	114	117	rBV3	794	1307	1.21%	0.286%
2	2.595	123	127	131	rVB2	931	1656	1.53%	0.363%
3	2.668	136	139	145	rVB3	1221	1778	1.65%	0.389%
4	4.735	471	478	479	rBV4	1090	1987	1.84%	0.435%
5	5.771	643	648	654	rVB5	773	1246	1.15%	0.273%
6	7.728	959	969	974	rBV2	5690	13399	12.40%	2.934%
7	7.795	974	980	989	rVB	32106	71343	66.03%	15.620%
8	8.149	1030	1038	1048	rBV2	11089	24489	22.67%	5.362%
9	8.697	1119	1128	1140	rVB	43900	86703	80.25%	18.983%
10	10.185	1365	1372	1380	rBV	63949	108042	100.00%	23.655%
11	11.496	1581	1587	1595	rVB	37924	62298	57.66%	13.640%
12	12.483	1743	1749	1757	rBV3	17332	28183	26.09%	6.170%
13	13.056	1833	1843	1844	rBV4	980	2118	1.96%	0.464%
14	13.081	1844	1847	1854	rVB5	2303	3713	3.44%	0.813%
15	13.361	1887	1893	1895	rBV5	1412	2372	2.20%	0.519%
16	13.428	1898	1904	1910	rVB2	13541	21967	20.33%	4.809%
17	13.611	1931	1934	1936	rBV2	1020	1366	1.26%	0.299%
18	13.678	1941	1945	1950	rBV5	1359	2318	2.15%	0.508%
19	13.788	1957	1963	1967	rBV4	3351	5655	5.23%	1.238%
20	13.849	1969	1973	1978	rVB6	1489	2376	2.20%	0.520%
21	14.081	2007	2011	2015	rVV2	4409	5853	5.42%	1.281%
22	14.135	2015	2020	2024	rVB5	784	1451	1.34%	0.318%
23	14.373	2056	2059	2064	rBV5	874	1372	1.27%	0.300%
24	14.611	2094	2098	2101	rBV4	937	1319	1.22%	0.289%
25	16.166	2350	2353	2357	rBV4	821	1213	1.12%	0.266%
26	16.257	2362	2368	2369	rBV4	670	1218	1.13%	0.267%

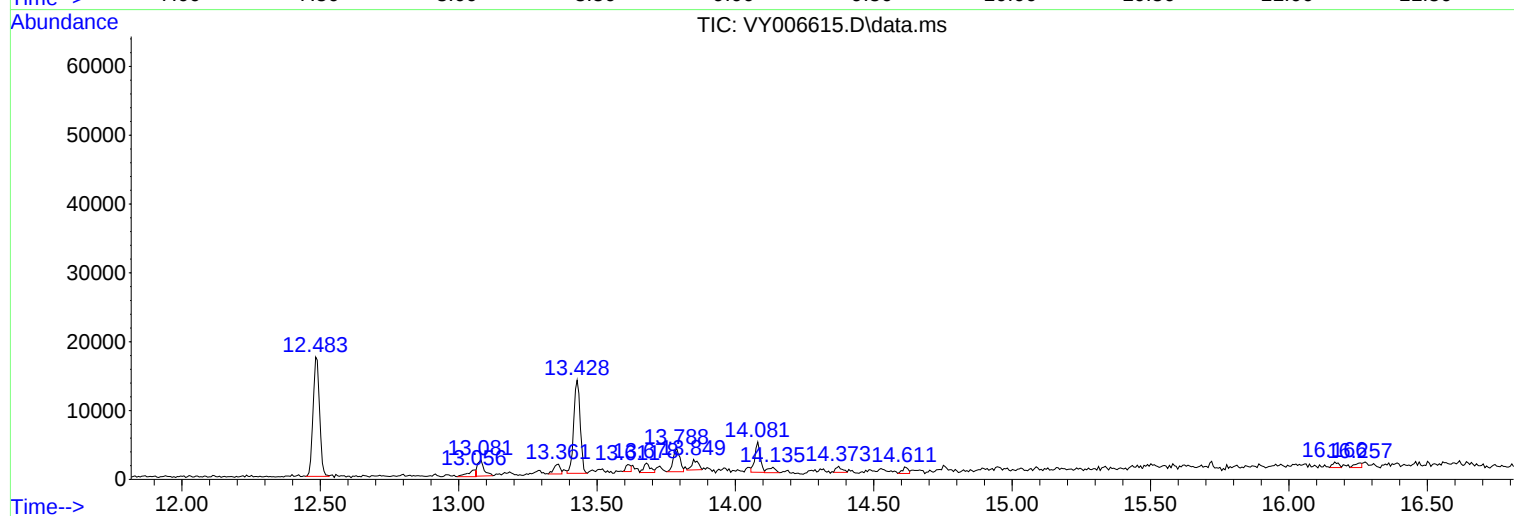
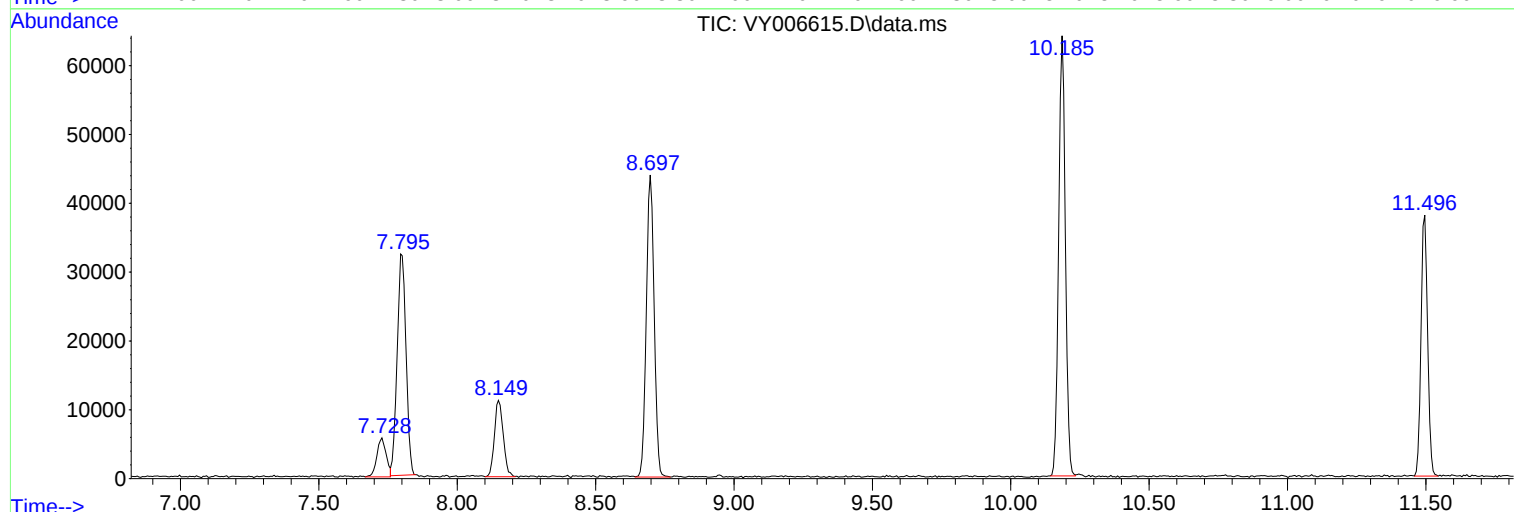
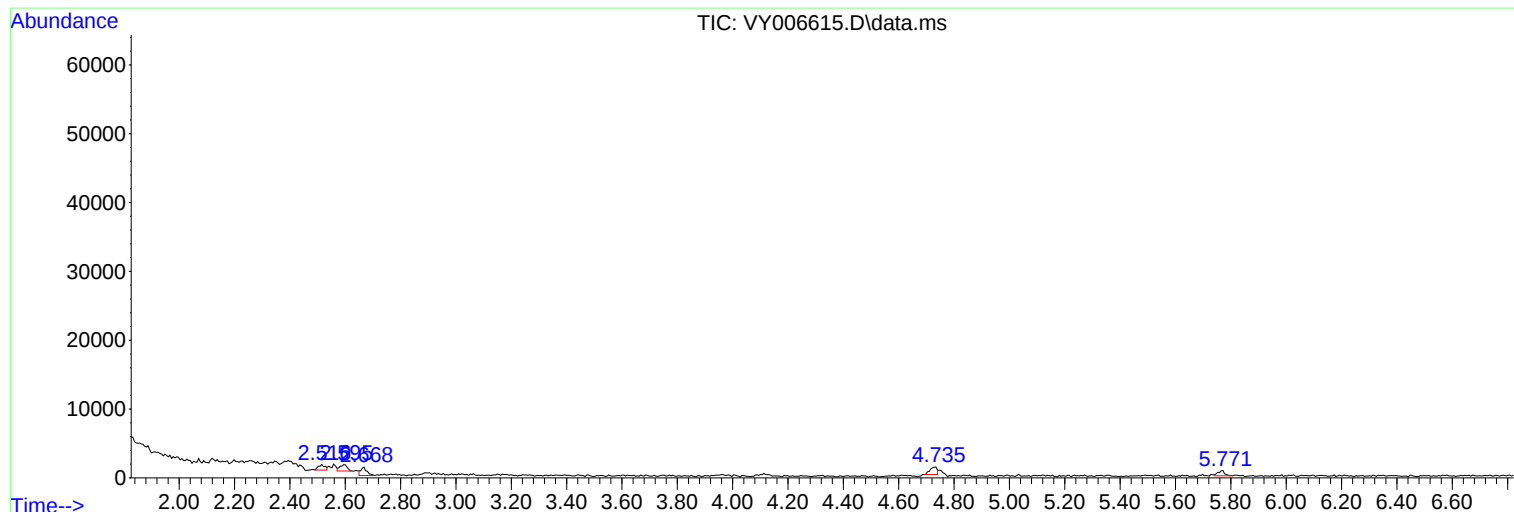
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S15-SP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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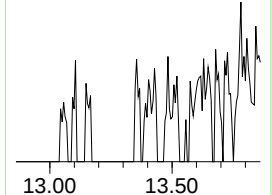
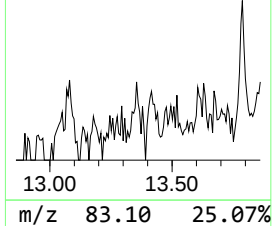
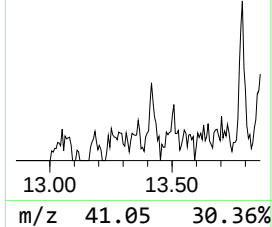
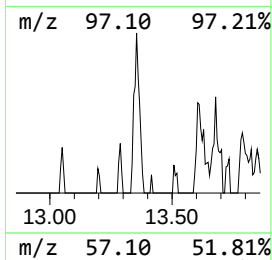
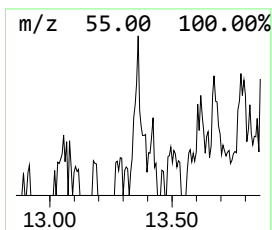
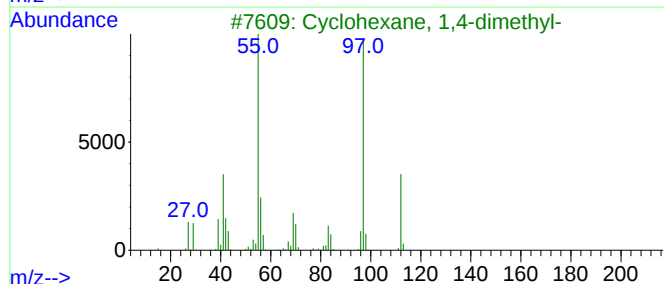
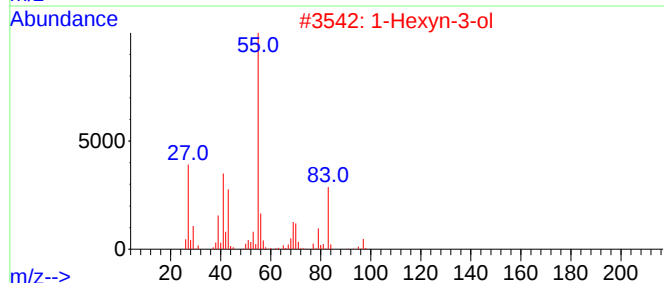
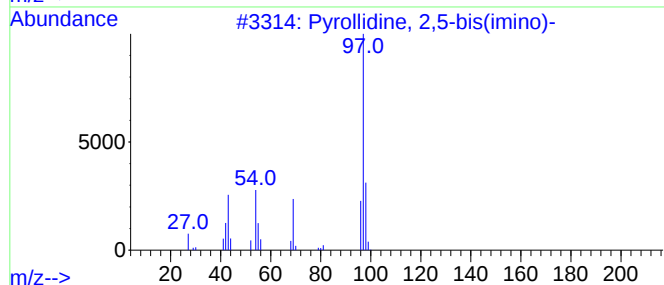
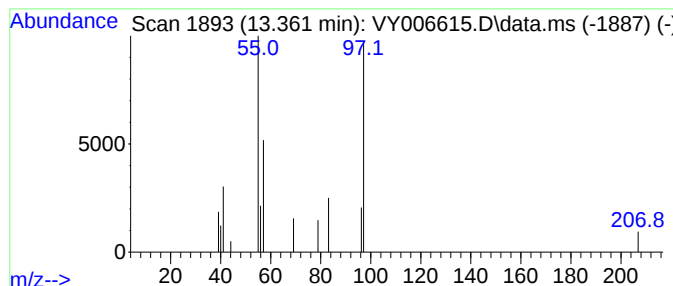
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown13.361 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.361	5.40 ug/l	2372	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrollidine, 2,5-bis(imino)-	97	C4H7N3	000503-84-4	38
2			1-Hexyn-3-ol	98	C6H10O	000105-31-7	17
3			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	9
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	9
5			Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	9



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Instrument :
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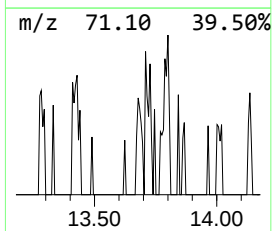
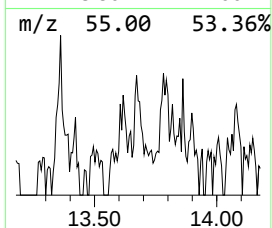
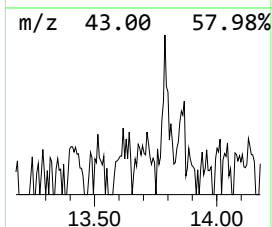
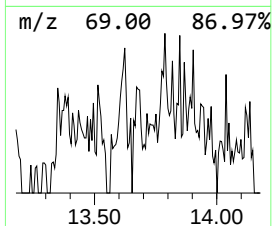
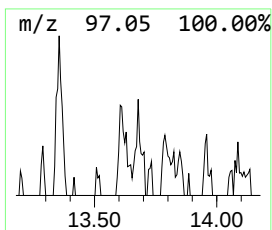
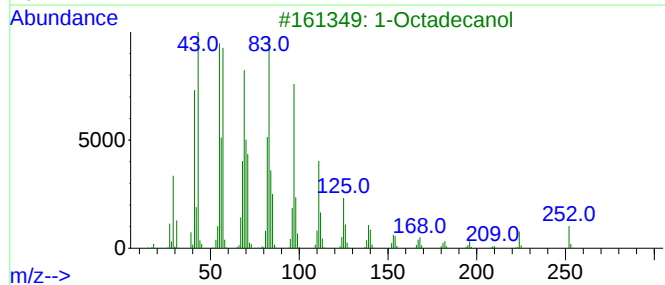
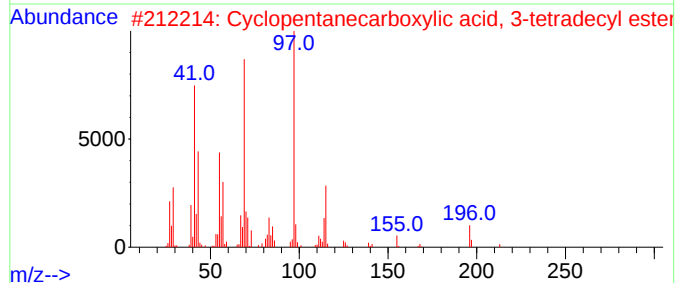
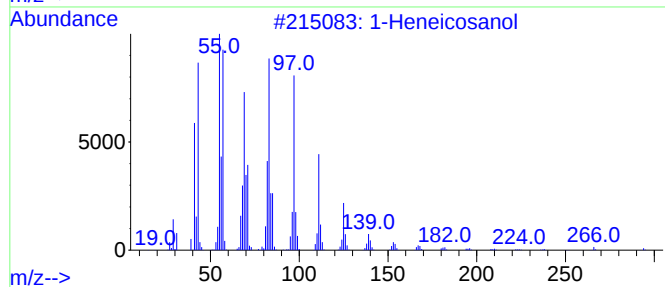
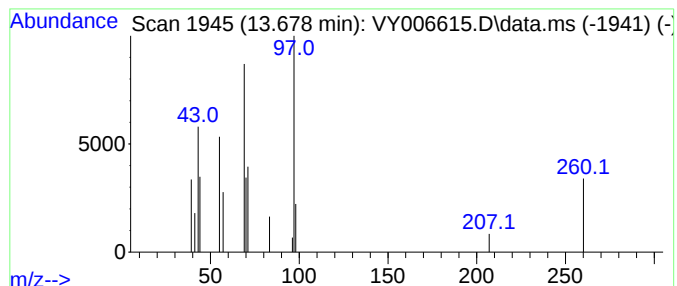
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.678	5.28 ug/l	2318	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	50
2			Cyclopentanecarboxylic acid, 3-t...	310	C20H38O2	1000280-58-8	40
3			1-Octadecanol	270	C18H38O	000112-92-5	36
4			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	36
5			Cyclohexadecane	224	C16H32	000295-65-8	36



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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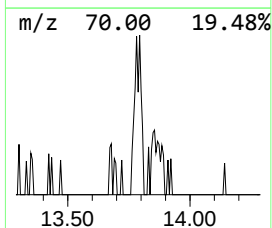
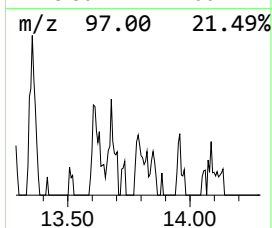
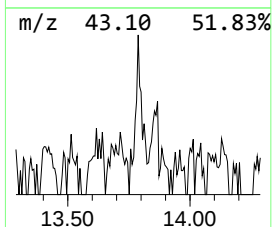
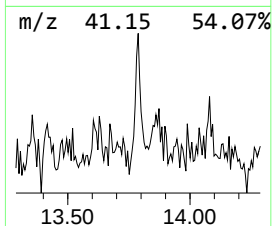
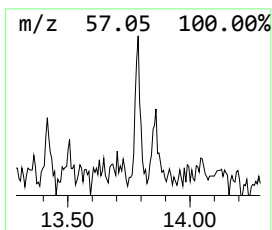
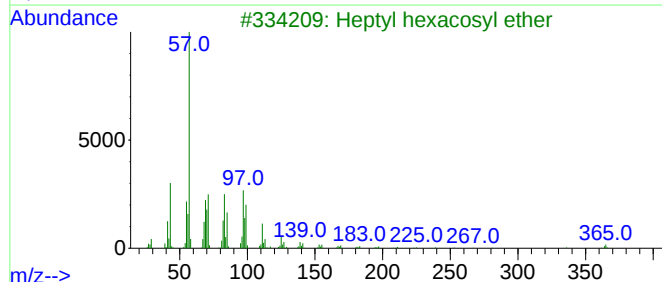
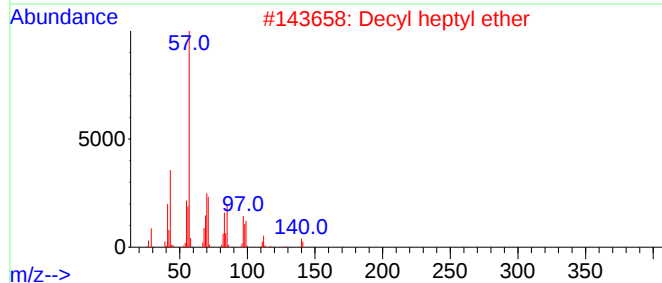
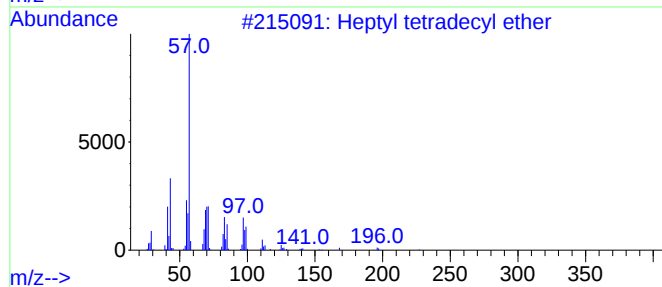
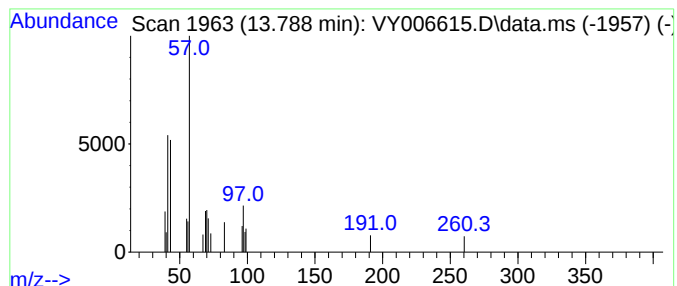
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptyl tetradecyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	12.87 ug/l	5655	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	53
2			Decyl heptyl ether	256	C17H36O	1000406-39-1	50
3			Heptyl hexacosyl ether	481	C33H68O	1000406-39-9	47
4			Dodecyl heptyl ether	284	C19H40O	1010406-39-2	47
5			Heptyl octadecyl ether	368	C25H52O	1000406-39-5	47



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Misc : 5.01G/5ML/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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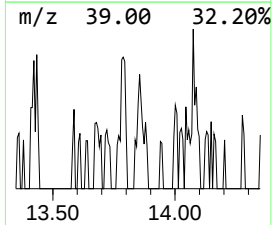
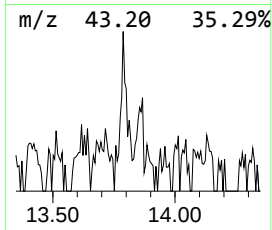
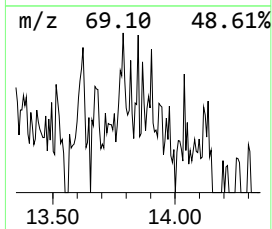
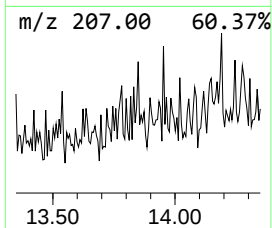
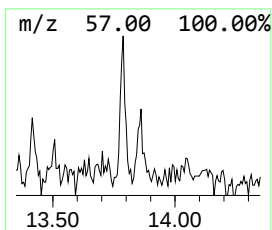
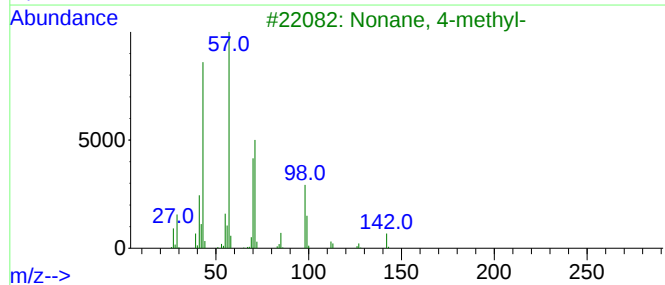
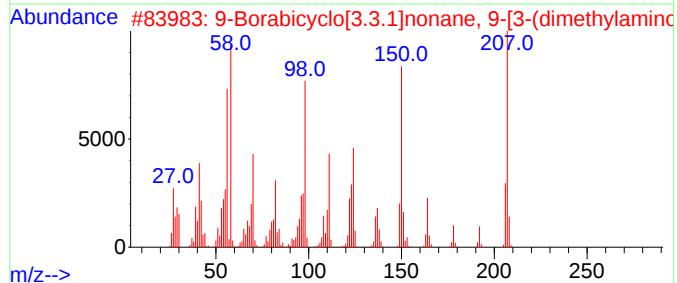
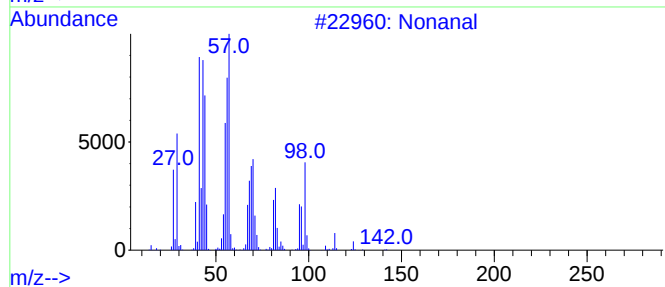
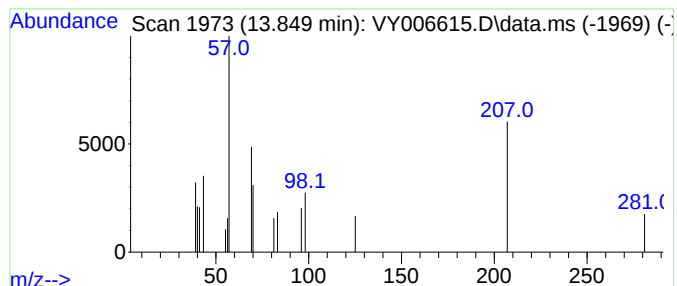
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.849 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.849	5.41 ug/l	2376	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	17
2			9-Borabicyclo[3.3.1]nonane, 9-[3...	207	C13H26BN	1000160-35-2	9
3			Nonane, 4-methyl-	142	C10H22	017301-94-9	9
4			2-Decen-1-ol, (E)-	156	C10H20O	018409-18-2	9
5			3,5,5-Trimethylhexyl acetate	186	C11H22O2	058430-94-7	9



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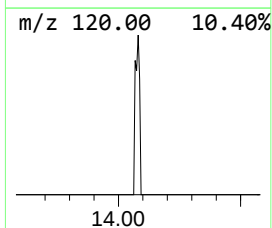
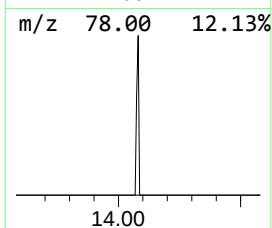
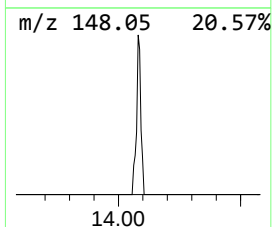
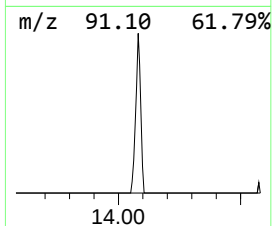
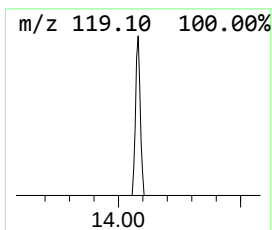
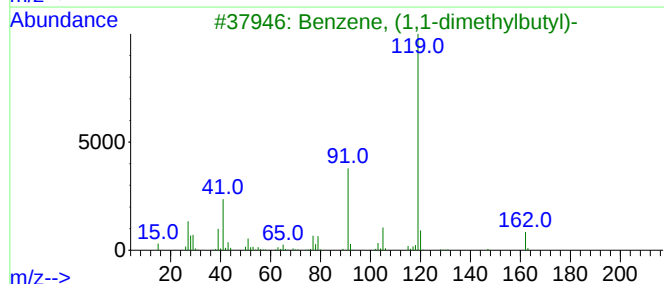
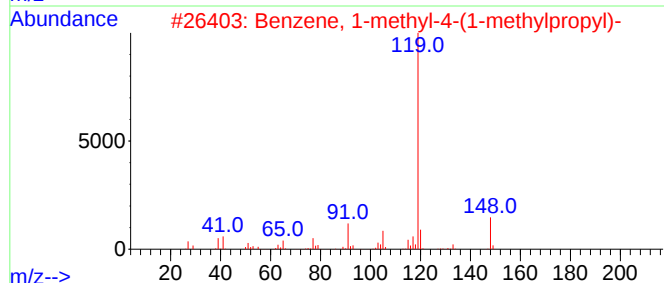
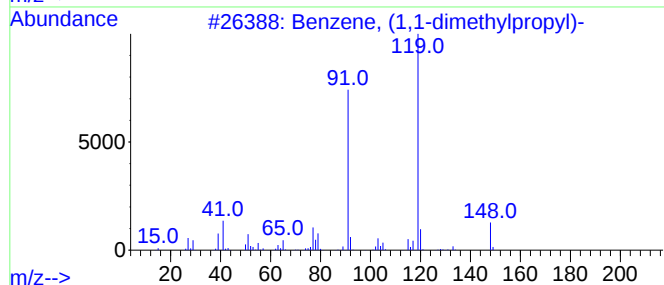
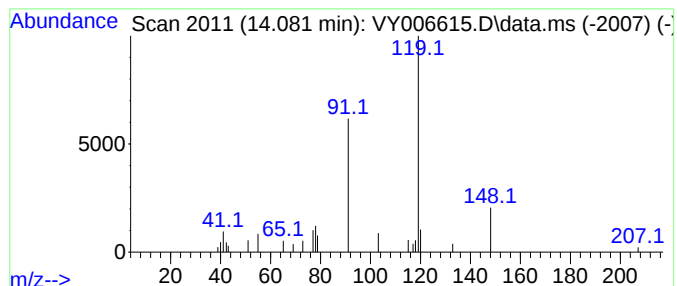
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1,1-dimethylpropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	13.32 ug/l	5853	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	64
3			Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	64
4			(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	64
5			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	59



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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
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1-Heneicosanol	13.678	5.3	ug/l	2318	4	13.428	21967	50.0
Heptyl tetradec...	13.788	12.9	ug/l	5655	4	13.428	21967	50.0
unknown13.849	13.849	5.4	ug/l	2376	4	13.428	21967	50.0
Benzene, (1,1-d...	14.081	13.3	ug/l	5853	4	13.428	21967	50.0