

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
 Data File : VY004825.D
 Acq On : 18 May 2021 14:42
 Operator : SY/MD
 Sample : M2413-01RE
 Misc : 5.10G/5ML/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 124035

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\82Y051021S.M
 Title : SW846 8260

Signal : TIC: VY004825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.722	468	476	485	rBV4	5677	17410	3.34%	0.586%
2	7.728	958	969	974	rBV	46195	108993	20.90%	3.666%
3	7.795	974	980	990	rVB	82994	191796	36.79%	6.450%
4	8.149	1029	1038	1050	rVB2	41788	90954	17.44%	3.059%
5	8.697	1120	1128	1137	rBV	130734	254281	48.77%	8.552%
6	9.185	1196	1208	1215	rBV7	5275	12662	2.43%	0.426%
7	10.185	1362	1372	1379	rBV	212853	380967	73.07%	12.812%
8	11.489	1580	1586	1593	rVB	179632	299240	57.39%	10.064%
9	12.123	1683	1690	1693	rBV9	6425	15325	2.94%	0.515%
10	12.489	1743	1750	1758	rVB2	289355	521396	100.00%	17.535%
11	12.806	1798	1802	1807	rBV7	4689	8320	1.60%	0.280%
12	13.038	1838	1840	1843	rVB3	5998	6355	1.22%	0.214%
13	13.428	1897	1904	1913	rVB	165986	267486	51.30%	8.996%
14	13.751	1952	1957	1961	rBV3	16109	25942	4.98%	0.872%
15	13.794	1961	1964	1968	rVB6	6671	10279	1.97%	0.346%
16	13.965	1988	1992	1997	rVB3	23113	35983	6.90%	1.210%
17	14.013	1997	2000	2006	rVB7	6787	9833	1.89%	0.331%
18	14.074	2008	2010	2016	rVB6	5388	7397	1.42%	0.249%
19	14.141	2018	2021	2027	rVB8	5430	10047	1.93%	0.338%
20	14.269	2033	2042	2047	rBV9	15155	46135	8.85%	1.552%
21	14.312	2047	2049	2056	rVB4	13006	20342	3.90%	0.684%
22	14.385	2057	2061	2063	rBV2	9222	11174	2.14%	0.376%
23	14.422	2063	2067	2071	rVB5	6876	9681	1.86%	0.326%
24	14.611	2095	2098	2103	rVB2	15923	23002	4.41%	0.774%
25	14.684	2105	2110	2113	rVV6	12630	25211	4.84%	0.848%
26	14.727	2113	2117	2125	rVB2	41976	72719	13.95%	2.446%
27	14.849	2134	2137	2139	rBV4	4563	5888	1.13%	0.198%
28	14.946	2150	2153	2156	rVB4	7314	9508	1.82%	0.320%
29	15.050	2165	2170	2175	rBV7	13957	32526	6.24%	1.094%
30	15.141	2181	2185	2191	rVB5	21298	41328	7.93%	1.390%
31	15.214	2191	2197	2204	rBV	48451	90053	17.27%	3.029%
32	15.440	2230	2234	2241	rVB4	22179	40235	7.72%	1.353%
33	15.544	2242	2251	2255	rVV4	13791	41272	7.92%	1.388%
34	15.611	2257	2262	2267	rVB6	18852	36096	6.92%	1.214%
35	15.964	2317	2320	2324	rVB5	8517	11944	2.29%	0.402%
36	16.019	2325	2329	2335	rVV8	12087	26998	5.18%	0.908%

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Instrument :
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ClientSampleId :
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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_Y\methods\82Y051021S.M
Title : SW846 8260

37	16.086	2335	2340	2346	rVB4	15214	38235	7.33%	1.286%
38	16.159	2346	2352	2359	rBV2	32433	61268	11.75%	2.061%
39	16.360	2379	2385	2389	rBV4	15951	33814	6.49%	1.137%
40	16.476	2399	2404	2410	rBV10	10344	21354	4.10%	0.718%

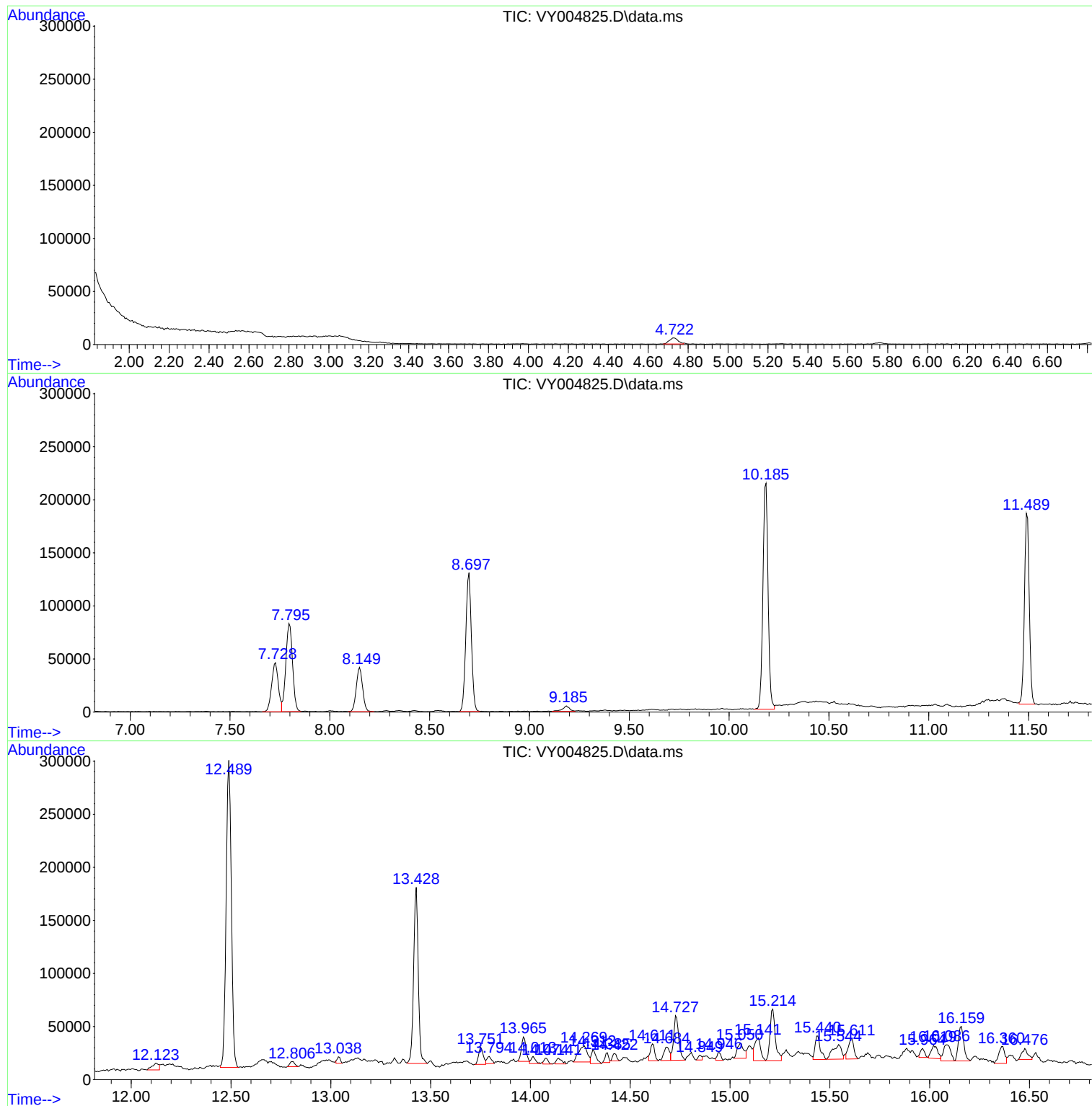
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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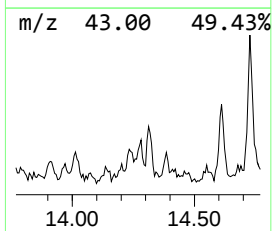
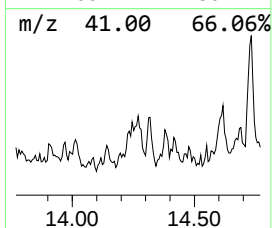
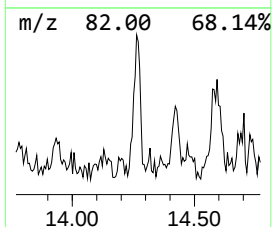
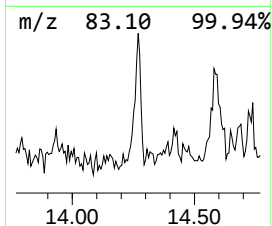
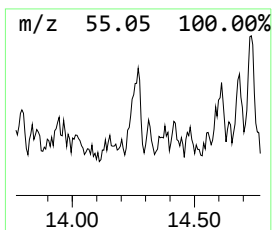
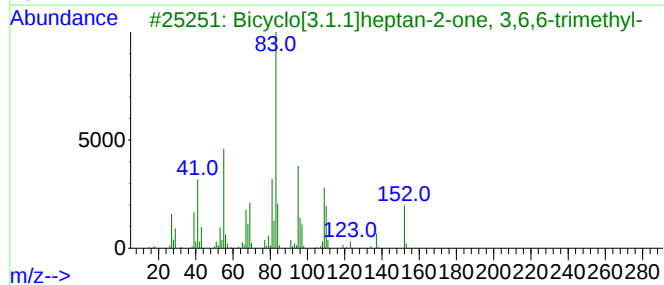
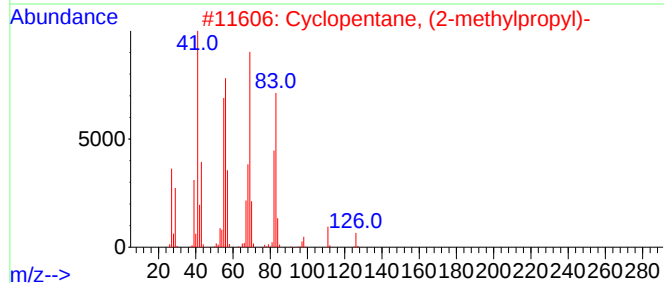
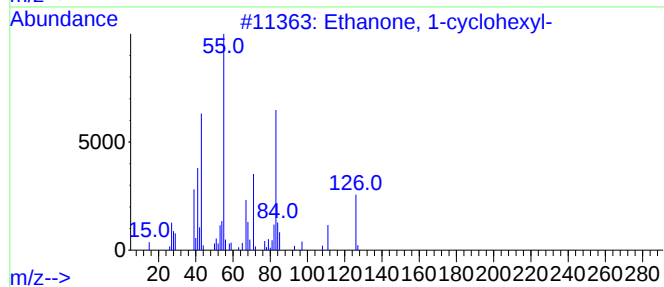
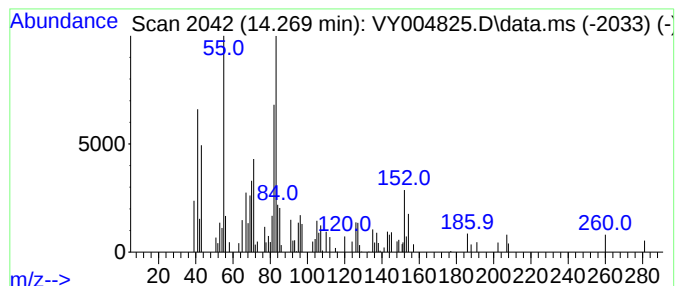
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanone, 1-cyclohexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	8.62 ug/l	46135	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	64
2			Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	46
3			Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	46
4			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43
5			1-Methylbicyclo[3.3.0]octane-3,7...	152	C9H12O2	021170-08-1	43



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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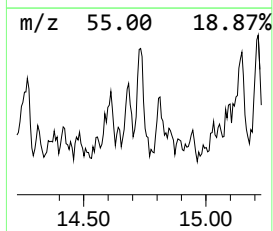
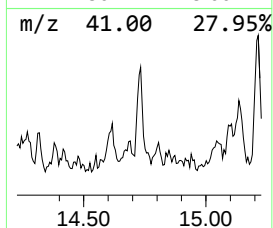
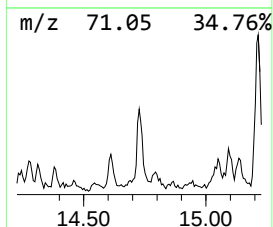
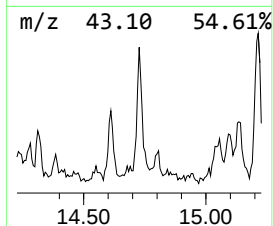
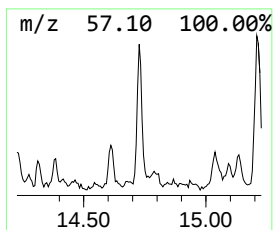
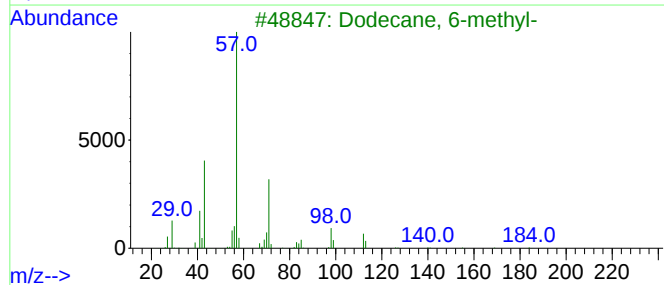
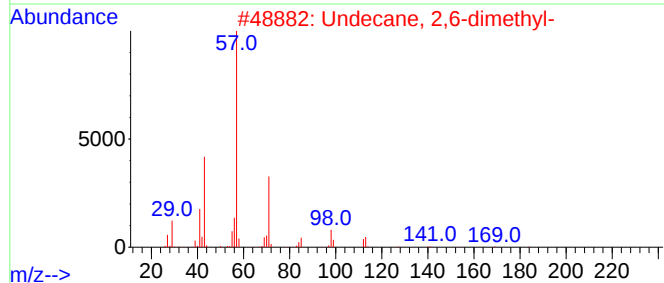
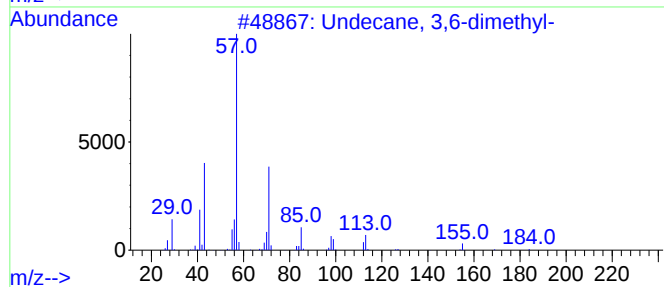
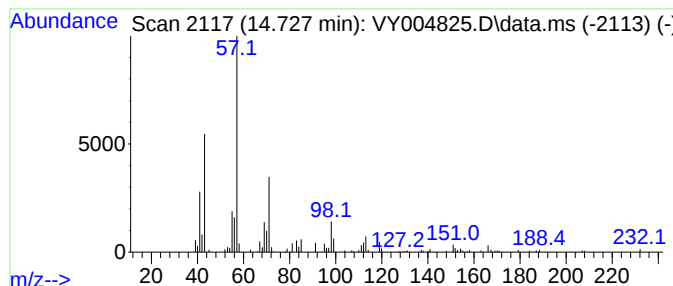
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
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Peak Number 3 Undecane, 3,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	13.59 ug/l	72719	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	76
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
3			Dodecane, 6-methyl-	184	C13H28	006044-71-9	70
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	50
5			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	49



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Misc : 5.10G/5ML/MSVOA_Y/SOIL
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Instrument :
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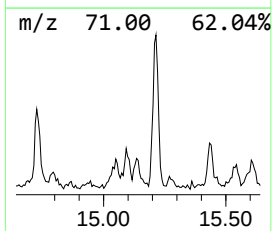
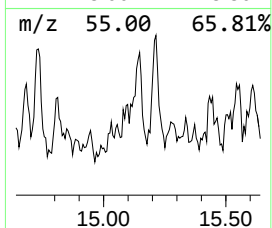
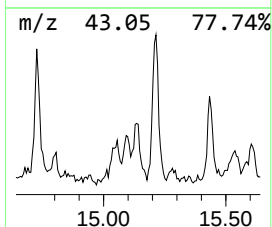
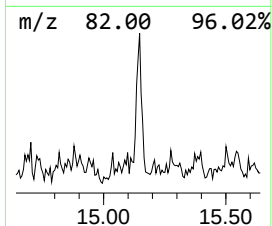
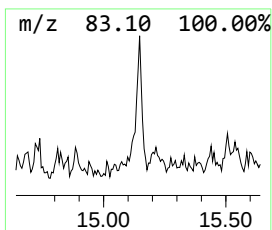
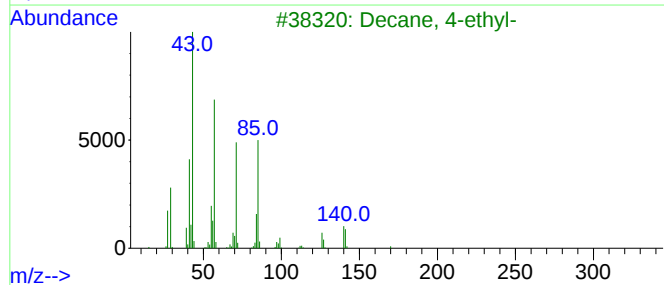
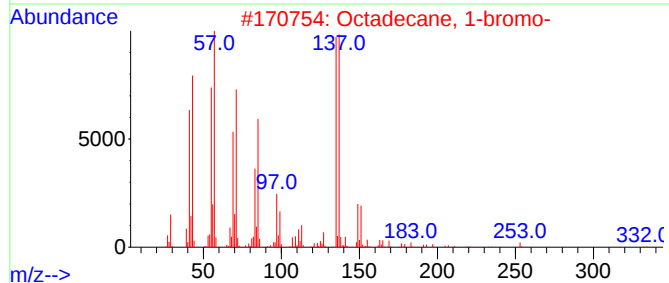
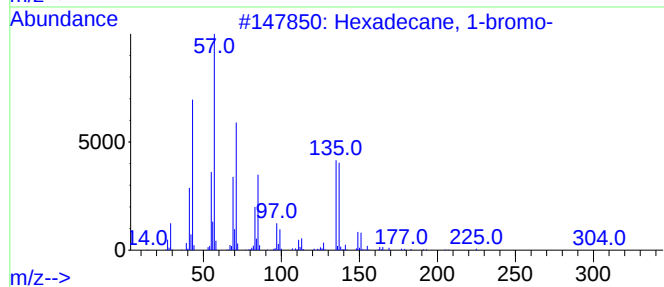
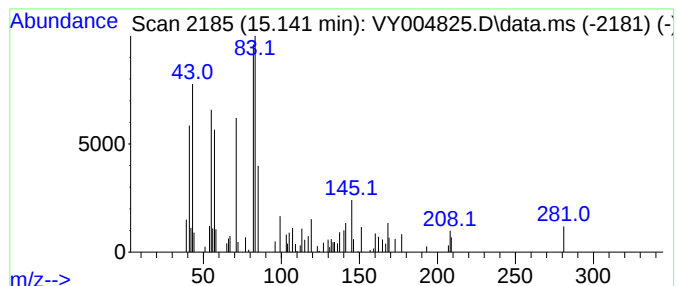
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.141 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.141	7.73 ug/l	41328	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	14
2		Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	14
3		Decane, 4-ethyl-	170	C12H26	001636-44-8	14
4		Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	14
5		1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	14



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Instrument :
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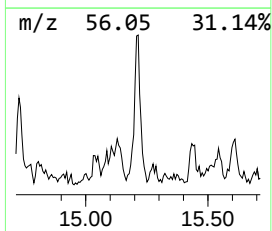
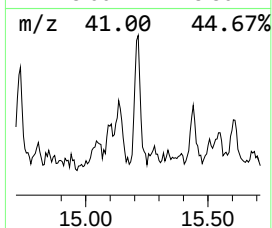
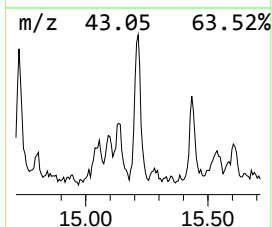
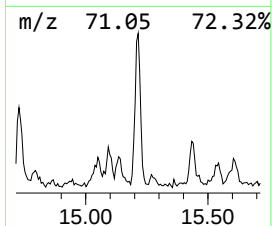
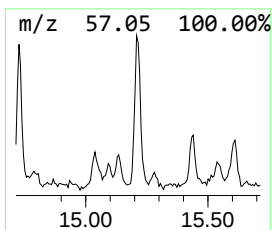
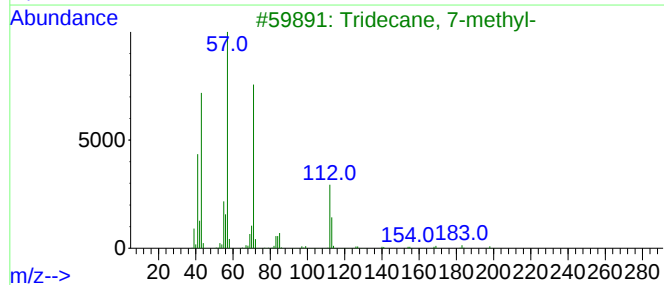
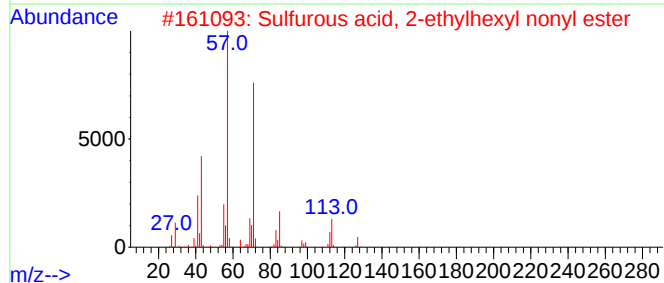
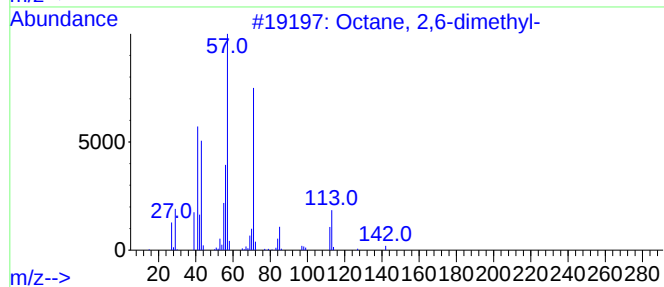
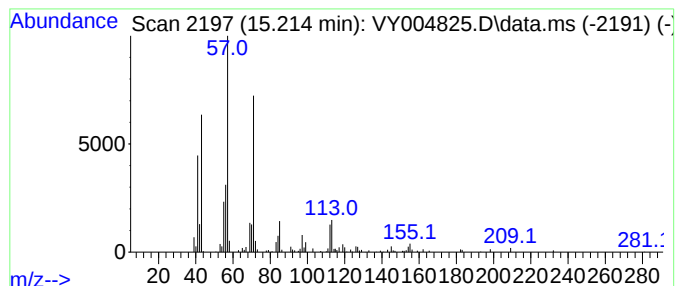
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.214	16.83 ug/l	90053	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	80
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	72
3			Tridecane, 7-methyl-	198	C14H30	026730-14-3	70
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64



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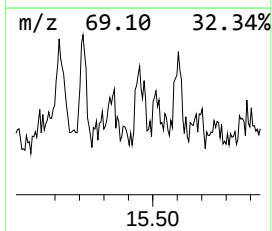
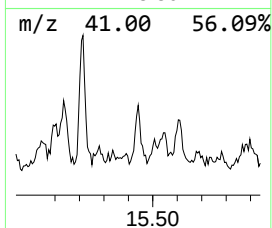
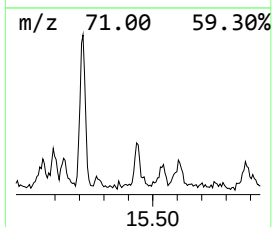
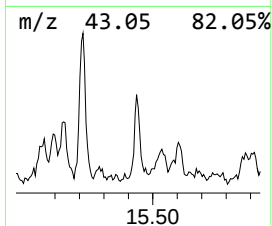
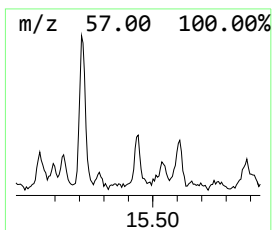
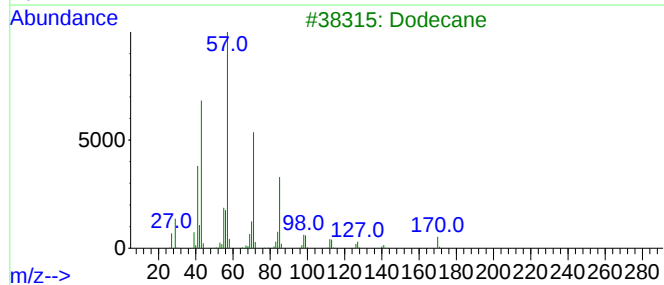
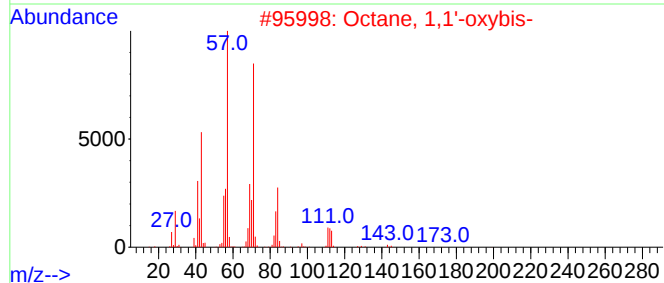
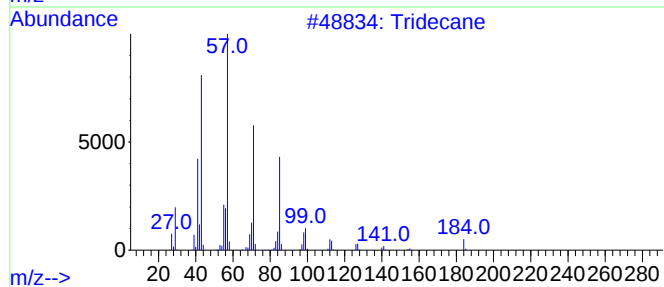
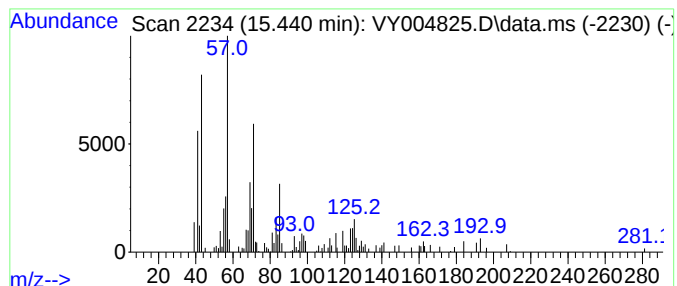
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.440	7.52 ug/l	40235	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	60
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	49
3			Dodecane	170	C12H26	000112-40-3	47
4			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	43
5			Pentadecane	212	C15H32	000629-62-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
Data File : VY004825.D
Acq On : 18 May 2021 14:42
Operator : SY/MD
Sample : M2413-01RE
Misc : 5.10G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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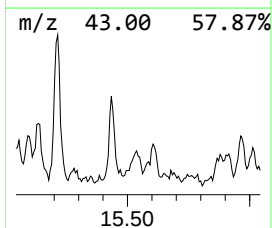
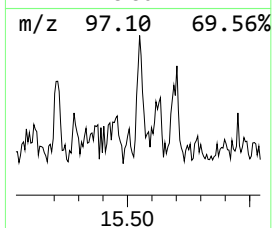
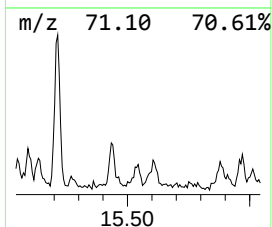
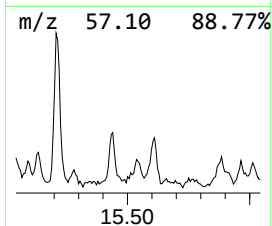
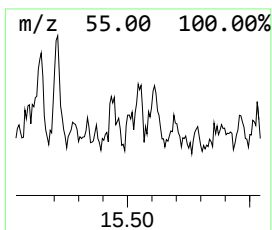
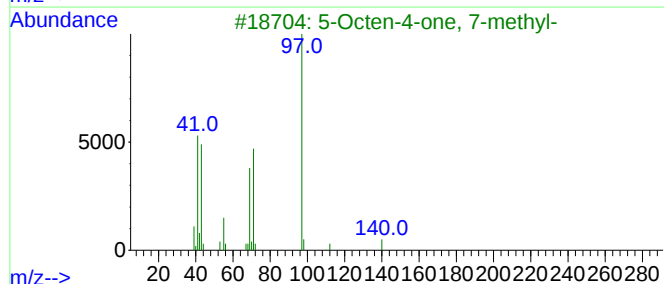
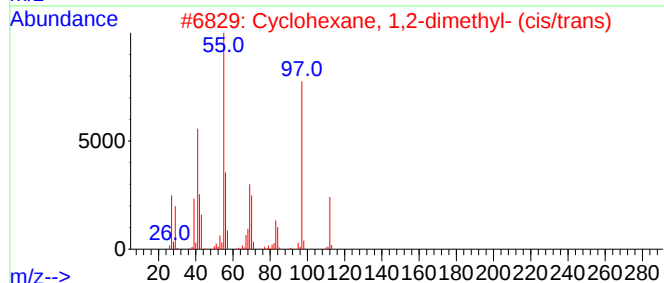
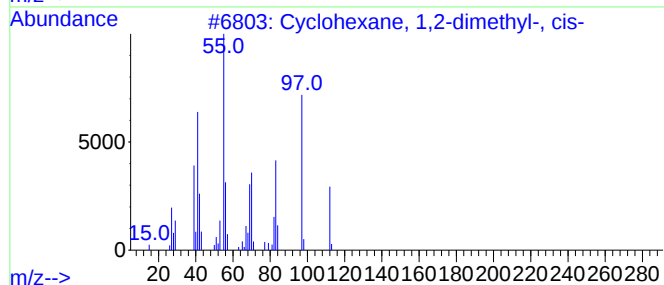
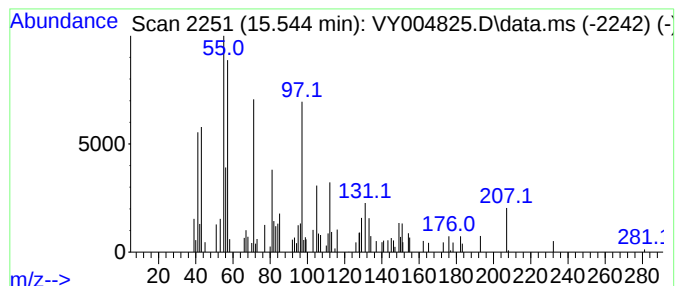
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown15.544 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.544	7.71 ug/l	41272	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	46
2			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	38
3			5-Octen-4-one, 7-methyl-	140	C9H16O	032064-78-1	27
4			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	25
5			Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
Data File : VY004825.D
Acq On : 18 May 2021 14:42
Operator : SY/MD
Sample : M2413-01RE
Misc : 5.10G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
124035

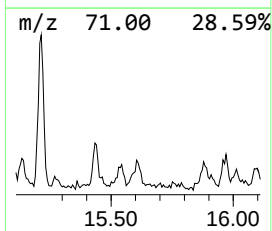
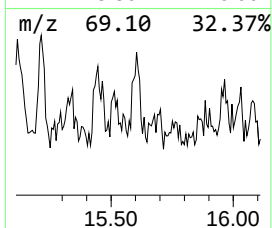
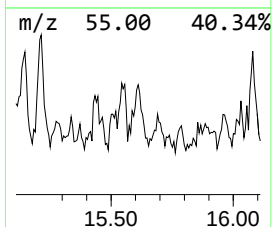
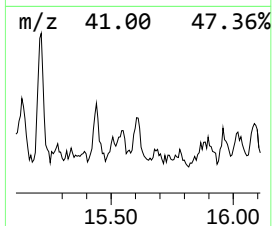
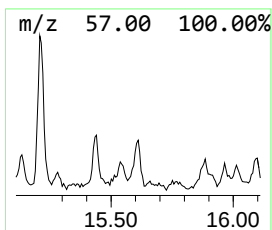
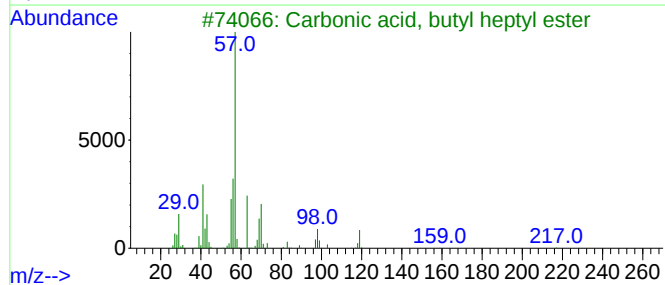
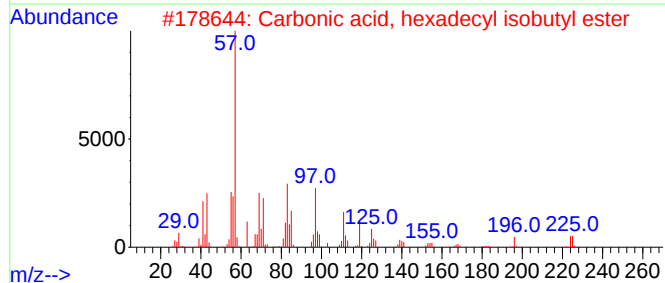
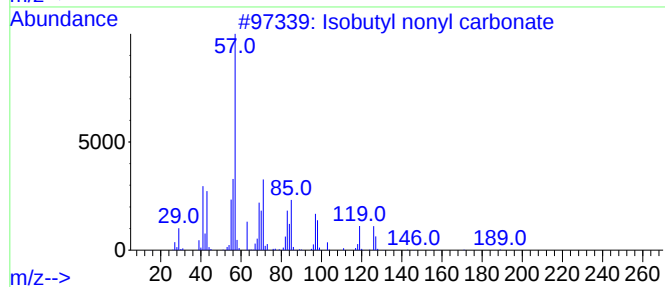
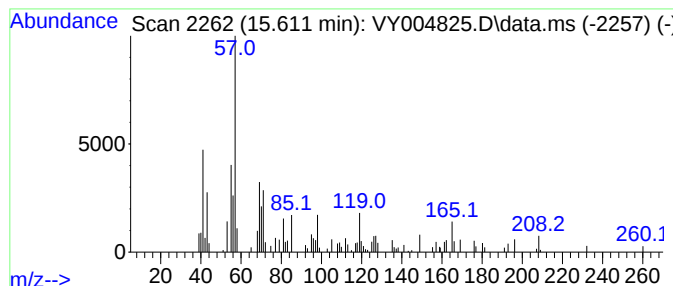
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Isobutyl nonyl carbonate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.611	6.75 ug/l	36096	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	53
2			Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1000314-61-3	53
3			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	47
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	47
5			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
Data File : VY004825.D
Acq On : 18 May 2021 14:42
Operator : SY/MD
Sample : M2413-01RE
Misc : 5.10G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
124035

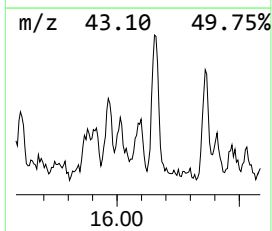
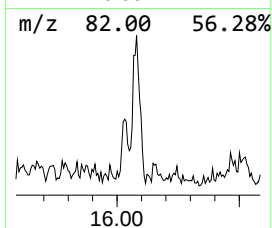
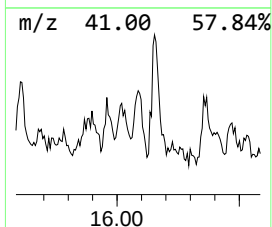
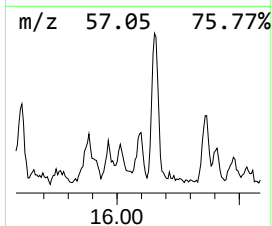
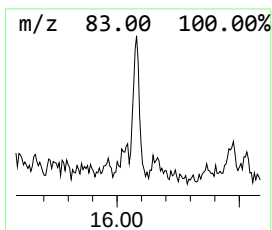
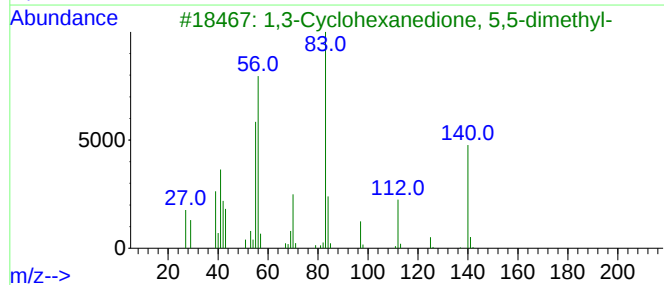
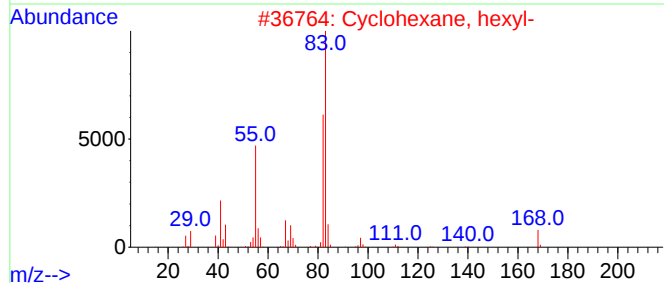
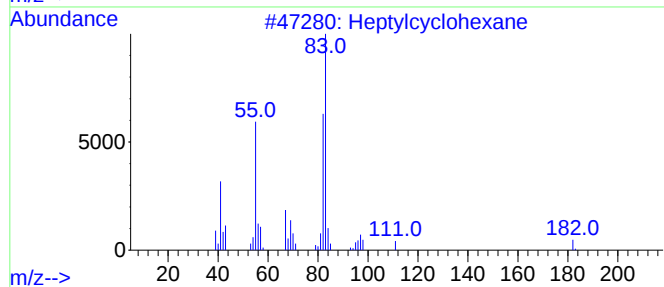
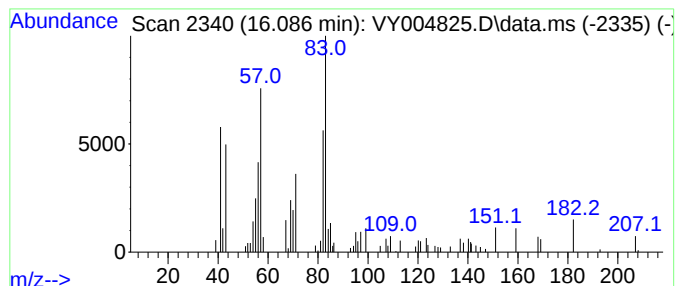
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptylcyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	7.15 ug/l	38235	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptylcyclohexane	182	C13H26	005617-41-4	50
2			Cyclohexane, hexyl-	168	C12H24	004292-75-5	43
3			1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	43
4			Cyclohexane, butyl-	140	C10H20	001678-93-9	43
5			Cyclohexane, propyl-	126	C9H18	001678-92-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
Data File : VY004825.D
Acq On : 18 May 2021 14:42
Operator : SY/MD
Sample : M2413-01RE
Misc : 5.10G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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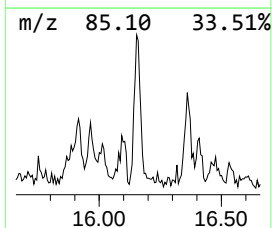
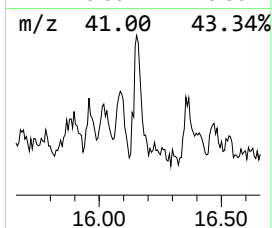
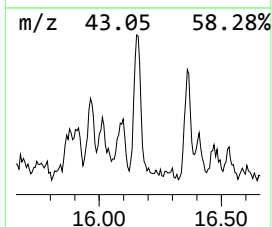
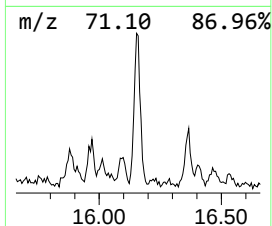
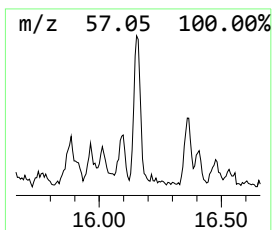
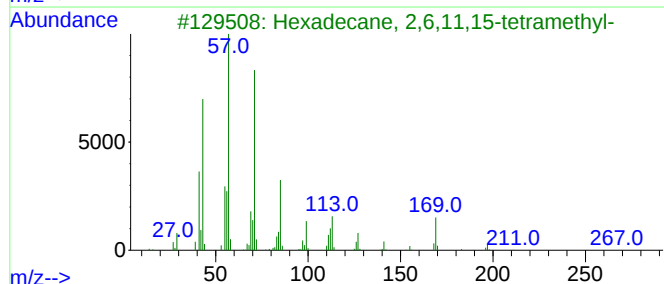
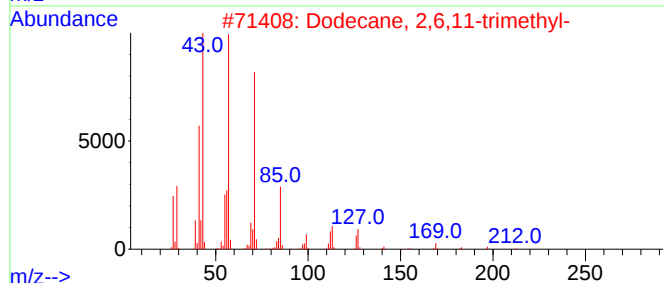
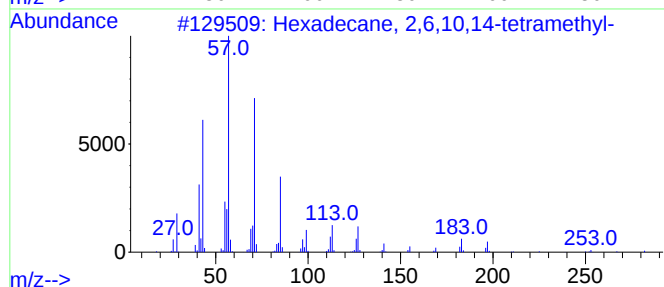
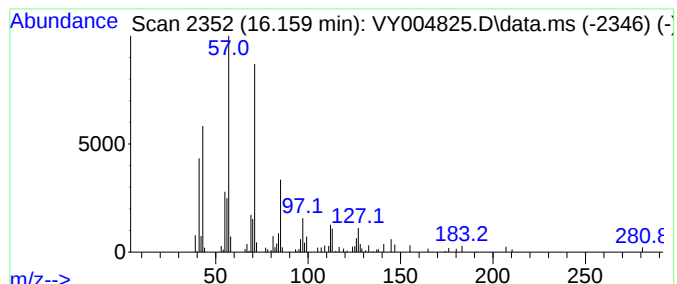
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.159	11.45 ug/l	61268	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	86
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
5			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051821\
Data File : VY004825.D
Acq On : 18 May 2021 14:42
Operator : SY/MD
Sample : M2413-01RE
Misc : 5.10G/5ML/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
124035

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051021S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Undecane, 3,6-d...	14.727	13.6	ug/l	72719	4	13.428	267486	50.0
unknown15.141	15.141	7.7	ug/l	41328	4	13.428	267486	50.0
Octane, 2,6-dim...	15.214	16.8	ug/l	90053	4	13.428	267486	50.0
Tridecane	15.440	7.5	ug/l	40235	4	13.428	267486	50.0
unknown15.544	15.544	7.7	ug/l	41272	4	13.428	267486	50.0
Isobutyl nonyl ...	15.611	6.8	ug/l	36096	4	13.428	267486	50.0
Heptylcyclohexane	16.086	7.2	ug/l	38235	4	13.428	267486	50.0
Hexadecane, 2,6...	16.159	11.4	ug/l	61268	4	13.428	267486	50.0