

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
 Data File : VY009594.D
 Acq On : 19 Jul 2022 17:02
 Operator : KP/MD
 Sample : N3651-05
 Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 DUP-SED

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\82Y071822S.M

Title : SW846 8260

Signal : TIC: VY009594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.710	956	966	972	rBV	145252	351650	3.13%	0.687%
2	7.783	972	978	987	rVB	285466	641315	5.71%	1.254%
3	8.130	1027	1035	1046	rBV	139685	311248	2.77%	0.608%
4	8.319	1057	1066	1075	rBV	138780	335182	2.98%	0.655%
5	8.685	1117	1126	1135	rBV	457524	895026	7.97%	1.749%
6	9.612	1270	1278	1287	rBV	187274	369874	3.29%	0.723%
7	9.740	1292	1299	1309	rVV	177279	355271	3.16%	0.694%
8	10.106	1353	1359	1365	rBV	265870	471959	4.20%	0.923%
9	10.173	1365	1370	1380	rVB	595644	1033774	9.20%	2.021%
10	10.636	1440	1446	1455	rVB	113470	198024	1.76%	0.387%
11	11.410	1568	1573	1578	rVB	121569	184022	1.64%	0.360%
12	11.489	1578	1586	1590	rBV	935974	1670204	14.87%	3.265%
13	11.532	1590	1593	1595	rVV	161152	253893	2.26%	0.496%
14	11.563	1595	1598	1603	rVB	227046	338893	3.02%	0.662%
15	11.739	1623	1627	1636	rVB	258241	446292	3.97%	0.872%
16	11.892	1648	1652	1657	rVB2	92672	152406	1.36%	0.298%
17	12.105	1682	1687	1698	rVB	349536	653589	5.82%	1.278%
18	12.191	1698	1701	1713	rVB6	74502	206868	1.84%	0.404%
19	12.459	1739	1745	1755	rVB	6953184	11235391	100.00%	21.961%
20	12.569	1756	1763	1767	rBV2	234423	494902	4.40%	0.967%
21	12.623	1767	1772	1782	rVB	869963	1899694	16.91%	3.713%
22	12.733	1788	1790	1796	rVB3	99706	155046	1.38%	0.303%
23	12.837	1797	1807	1812	rBV3	980616	2164964	19.27%	4.232%
24	13.038	1835	1840	1841	rBV2	321757	482430	4.29%	0.943%
25	13.068	1841	1845	1851	rVB	1642414	2438549	21.70%	4.766%
26	13.172	1858	1862	1869	rVB	410283	671283	5.97%	1.312%
27	13.282	1872	1880	1888	rVV	3946250	6380526	56.79%	12.472%
28	13.349	1888	1891	1894	rVV	174857	244587	2.18%	0.478%
29	13.398	1894	1899	1900	rVV	469204	676192	6.02%	1.322%
30	13.422	1900	1903	1907	rVV	741495	1329222	11.83%	2.598%
31	13.477	1907	1912	1921	rVB	2666565	5951186	52.97%	11.632%
32	13.556	1922	1925	1927	rBV2	87347	117227	1.04%	0.229%
33	13.641	1933	1939	1950	rVB	813089	1493874	13.30%	2.920%
34	13.818	1964	1968	1975	rVB2	249241	527701	4.70%	1.031%
35	13.959	1986	1991	1993	rVV2	331008	606994	5.40%	1.186%
36	13.989	1994	1996	2006	rVB2	476626	995347	8.86%	1.946%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	14.074	2007	2010	2013	rVB	157216	184945	1.65%	0.361%
38	14.141	2017	2021	2029	rVB5	226152	588841	5.24%	1.151%
39	14.385	2055	2061	2069	rVV3	1007684	2315677	20.61%	4.526%
40	14.458	2070	2073	2079	rVB2	181314	292274	2.60%	0.571%
41	15.227	2195	2199	2204	rVB	285915	485049	4.32%	0.948%
42	15.891	2305	2308	2313	rVB2	113119	172710	1.54%	0.338%
43	16.763	2445	2451	2455	rBV4	180301	386408	3.44%	0.755%

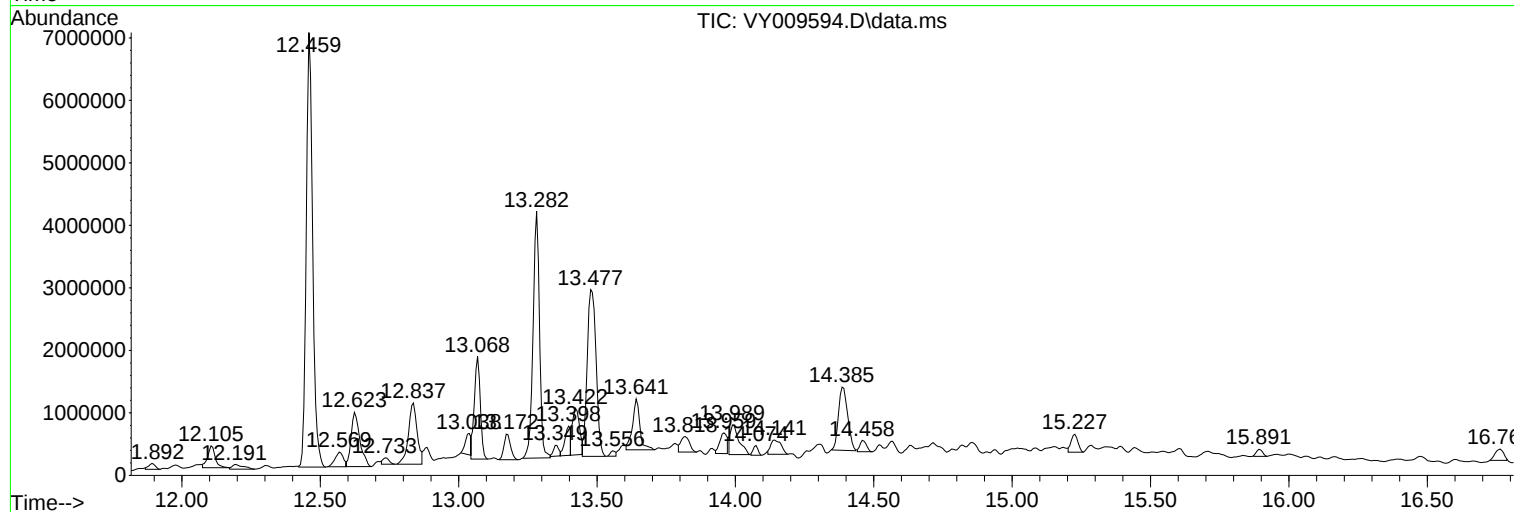
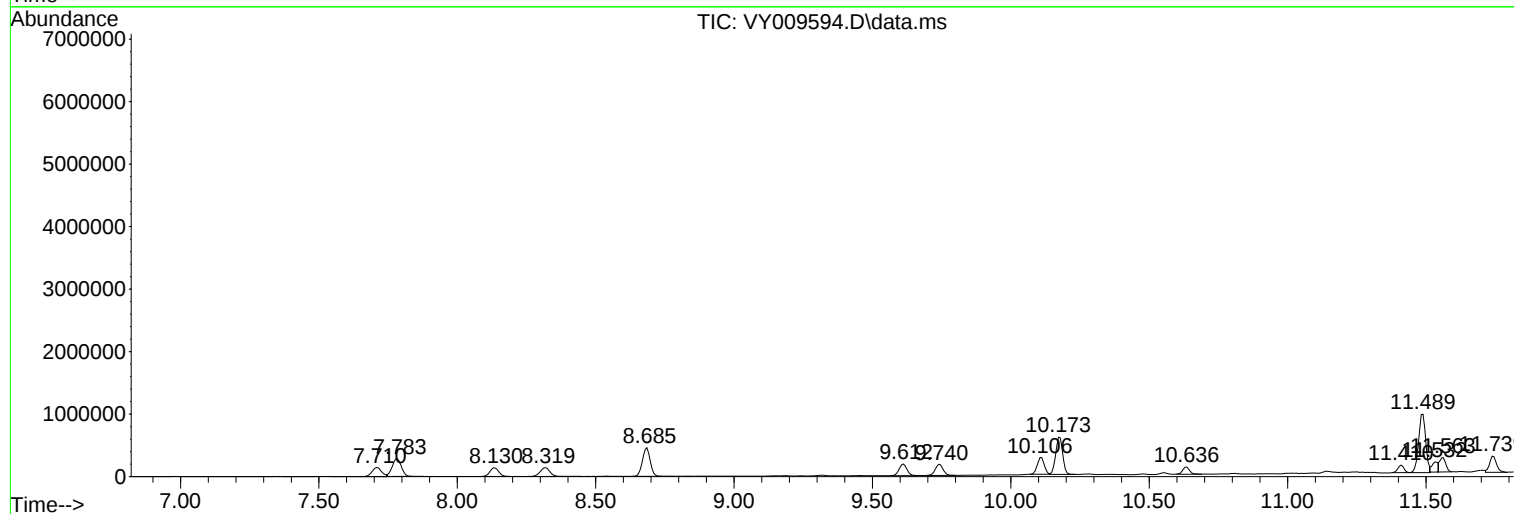
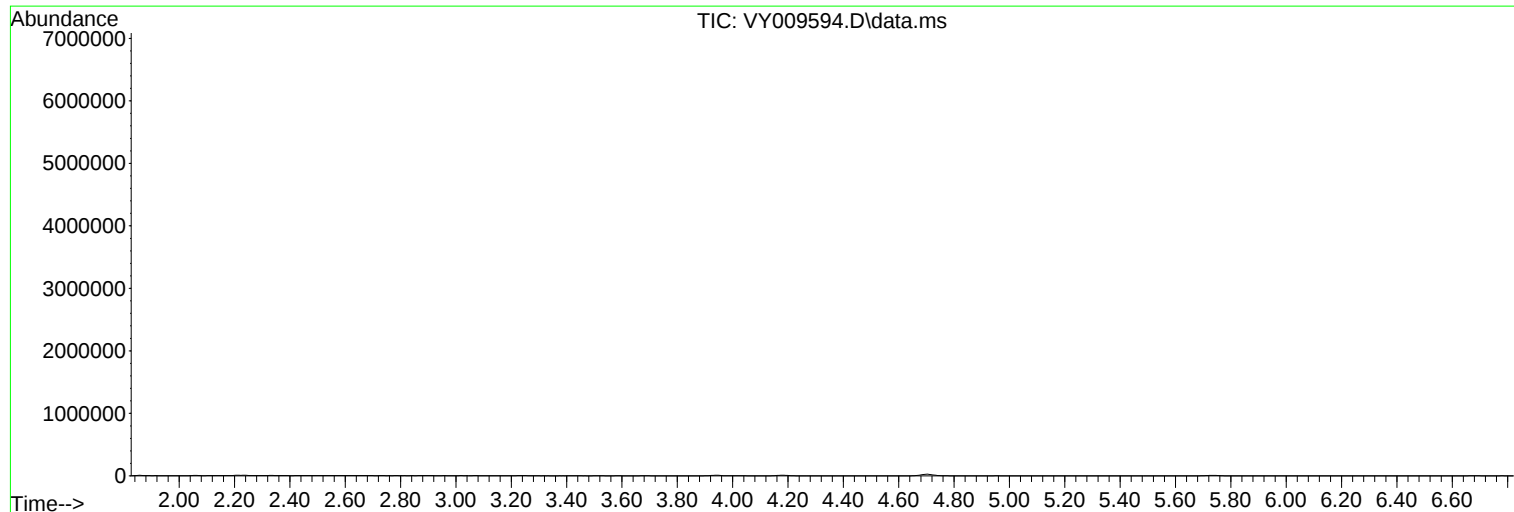
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DUP-SED

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

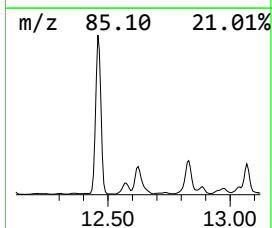
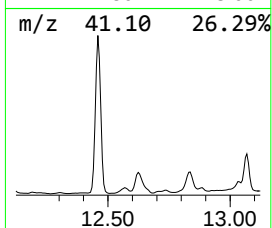
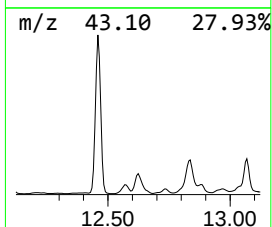
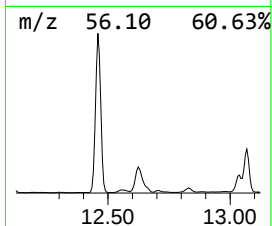
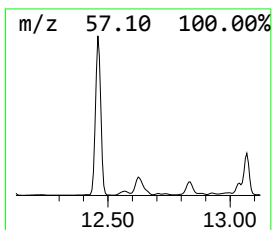
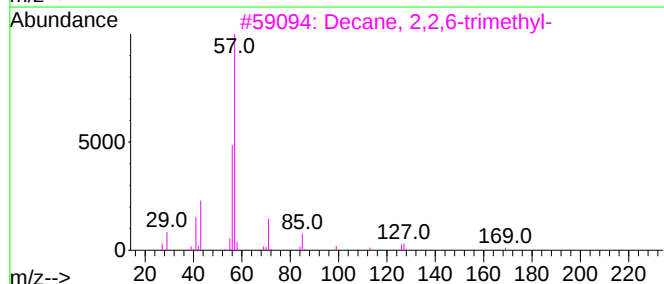
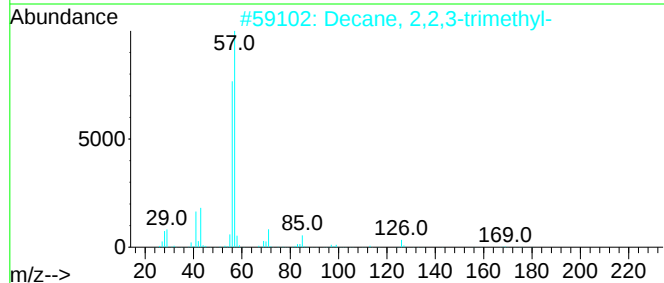
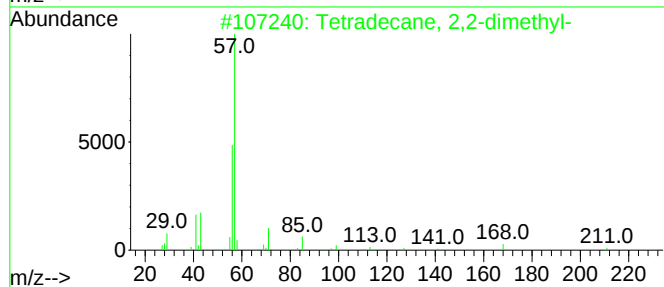
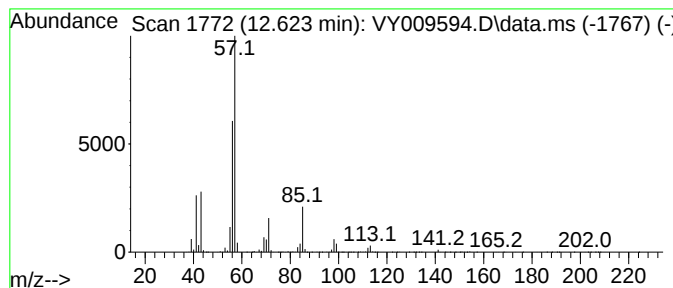
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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

Peak Number 1 Tetradecane, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.623	71.46 ug/l	1899690	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	64
2			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	59
3			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	59
4			2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	53
5			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50



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Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

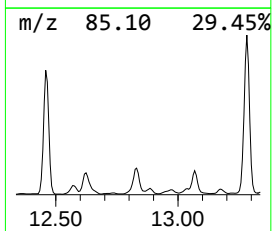
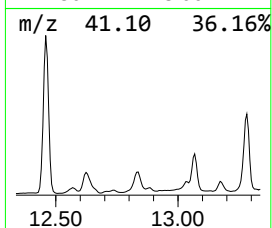
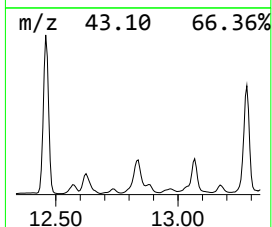
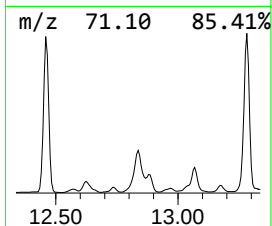
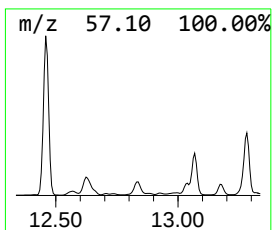
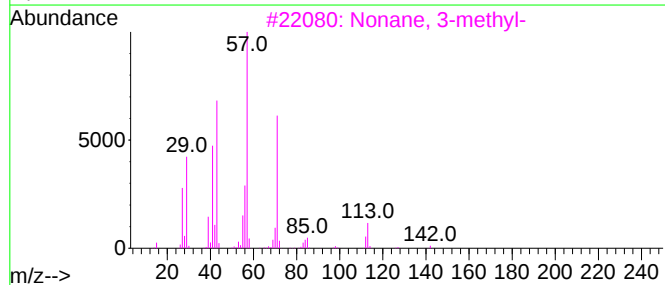
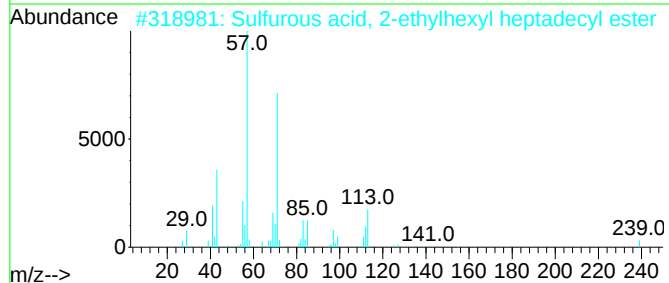
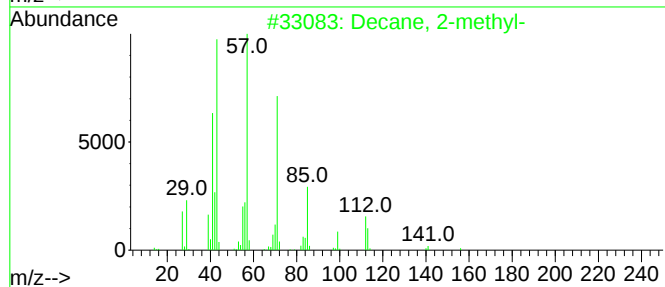
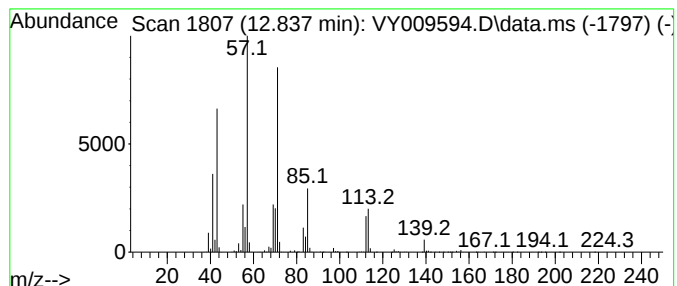
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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

Peak Number 2 Decane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	81.44 ug/l	2164960	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	72
2			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	72
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
4			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	52
5			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	50



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Misc : 6.08g/5.0mL/MSVOA_Y/soil
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

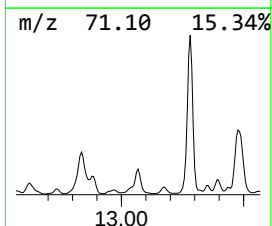
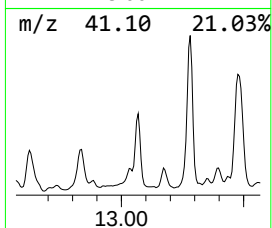
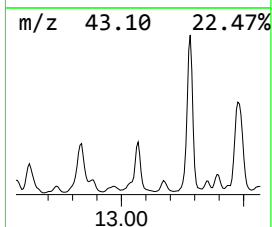
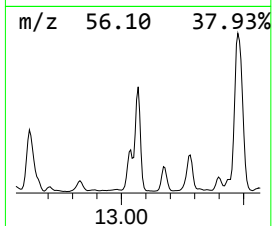
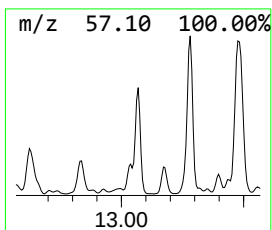
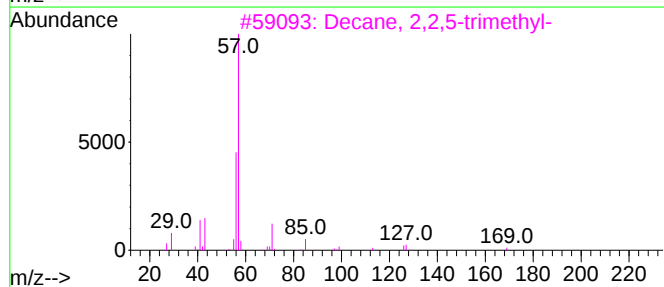
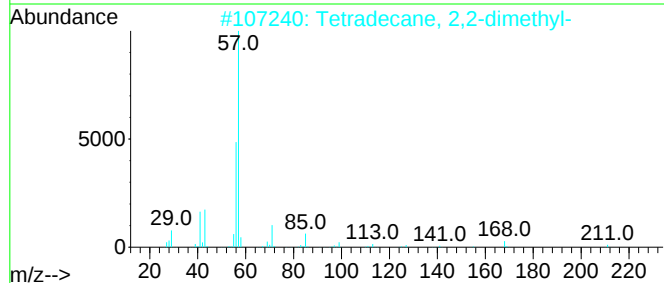
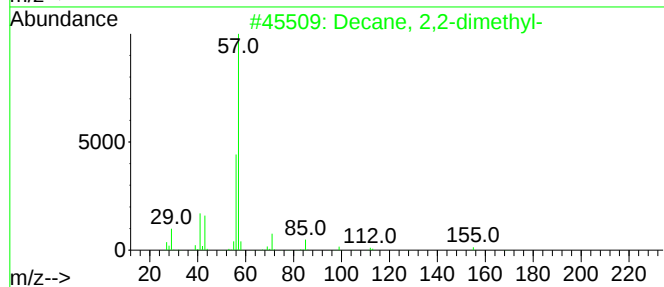
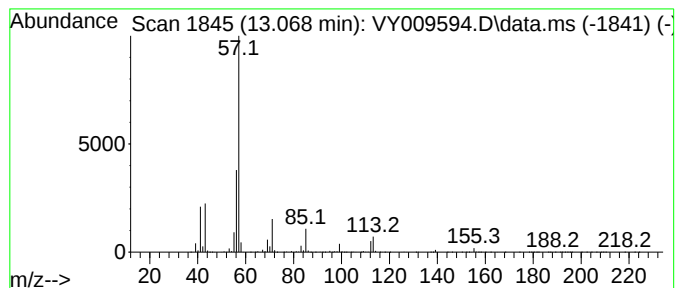
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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

Peak Number 3 Decane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.068	91.73 ug/l	2438550	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	72
2			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	64
3			Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	64
4			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	59
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	59



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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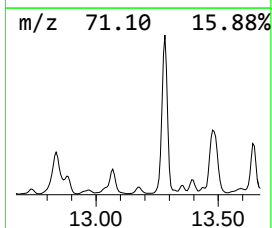
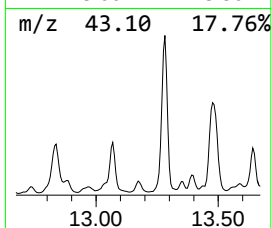
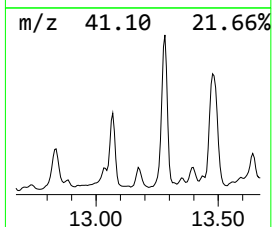
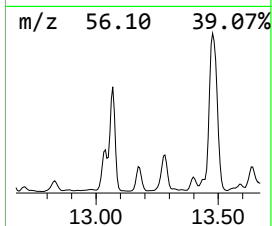
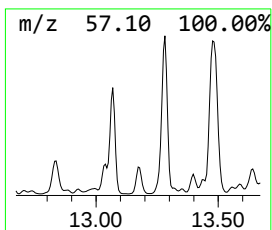
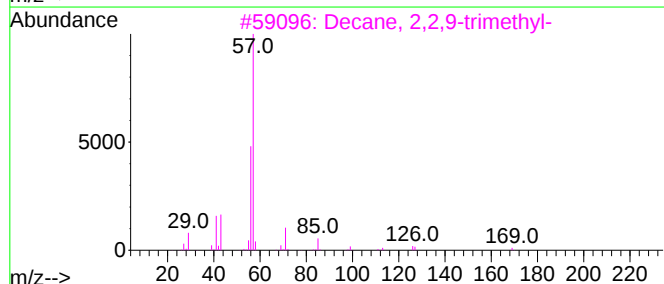
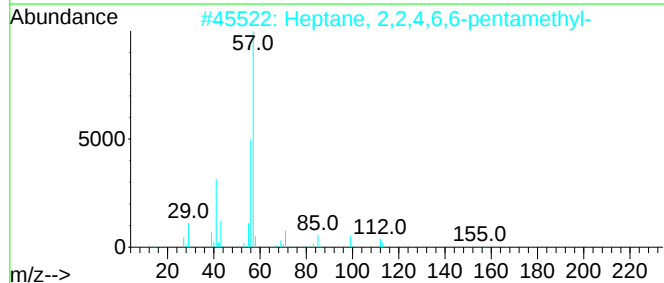
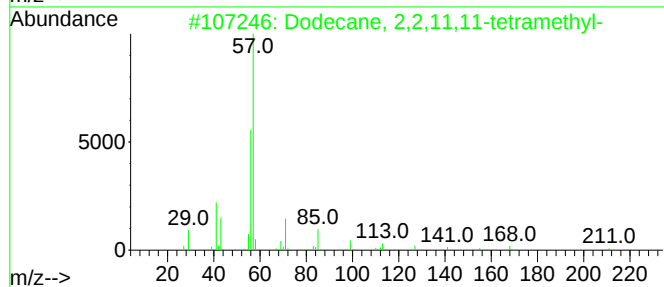
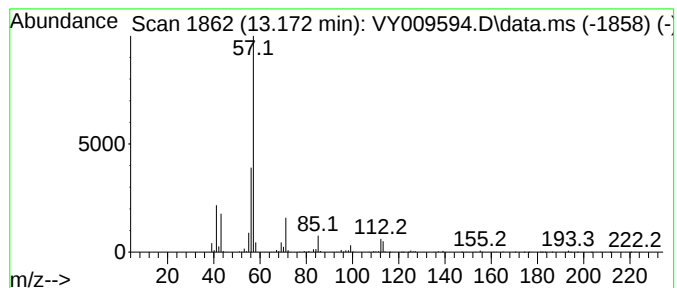
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.M
Quant Title : SW846 8260

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

Peak Number 4 Dodecane, 2,2,11,11-tetrame... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.172	25.25 ug/l	671283	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
3			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64



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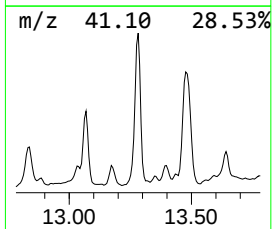
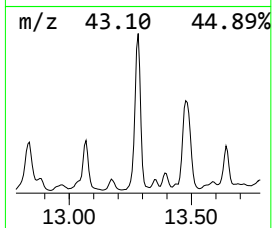
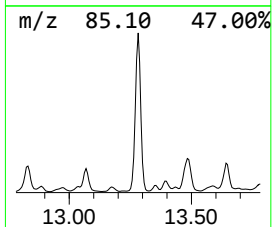
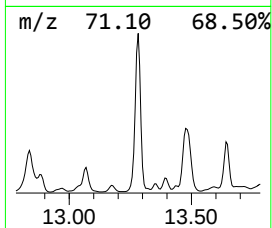
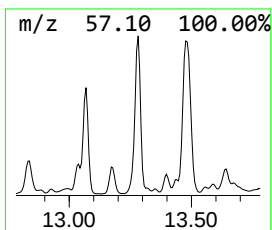
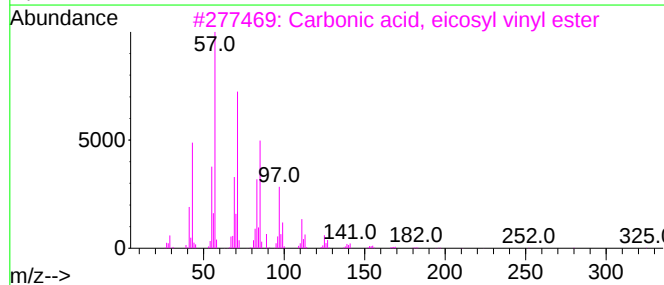
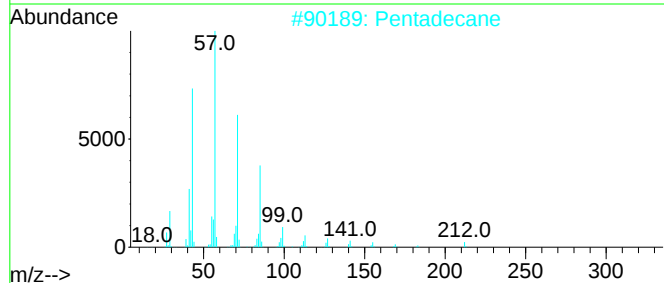
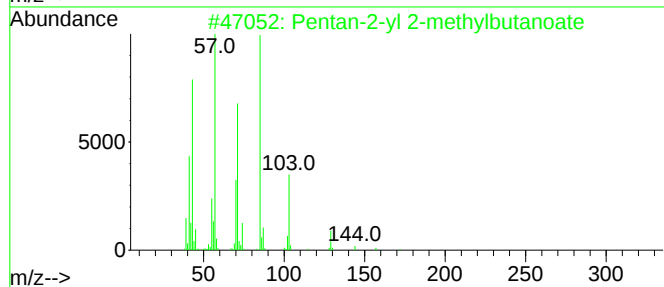
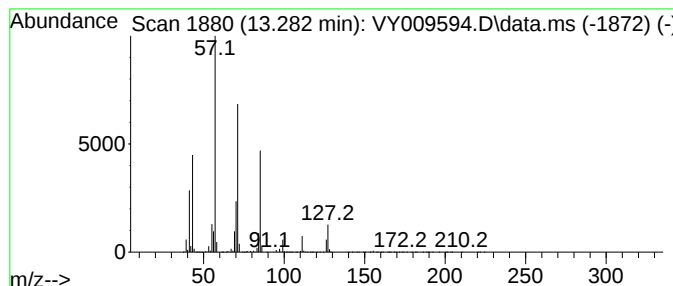
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Quant Title : SW846 8260

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

Peak Number 5 Pentan-2-yl 2-methylbutanoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	240.01 ug/l	6380530	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	64
2			Pentadecane	212	C15H32	000629-62-9	64
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	64
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

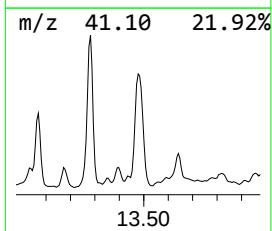
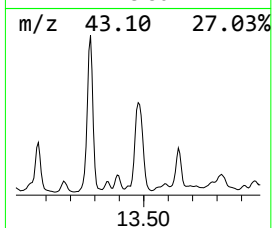
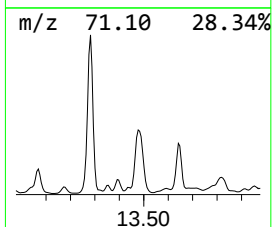
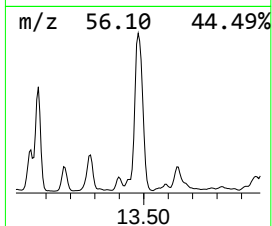
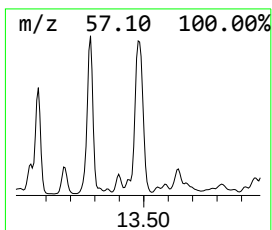
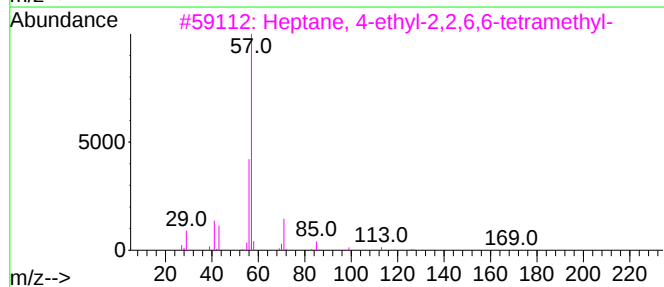
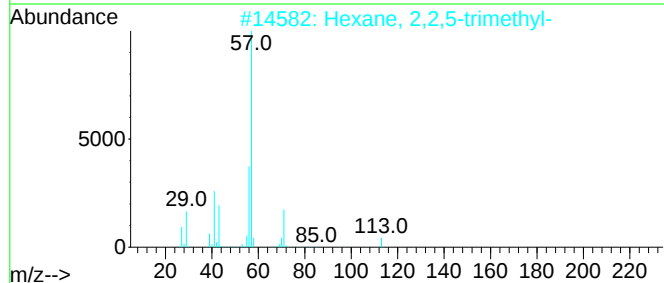
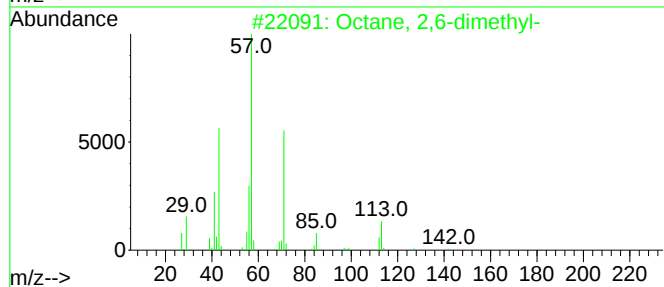
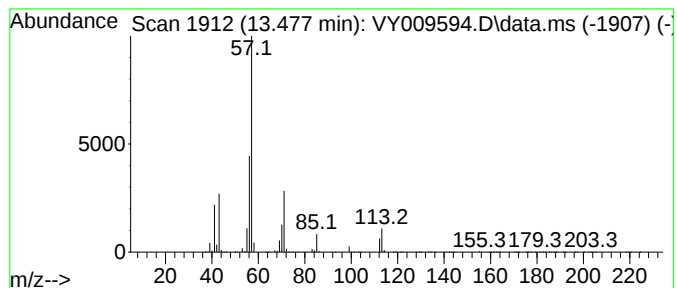
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	223.86 ug/l	5951190	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
2		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	72
3		Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	72
4		Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	59
5		Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

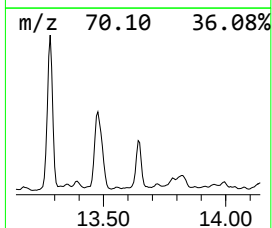
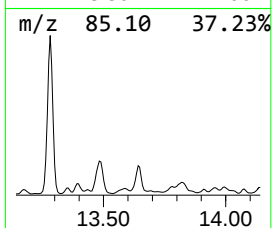
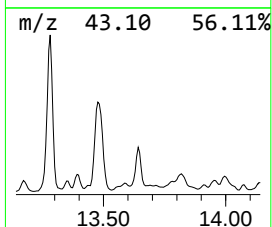
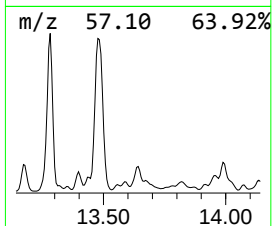
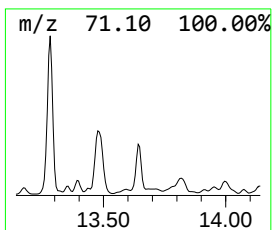
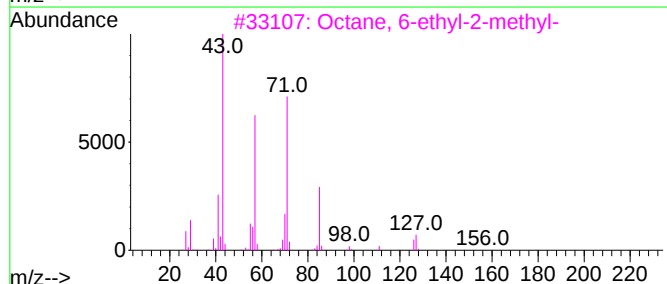
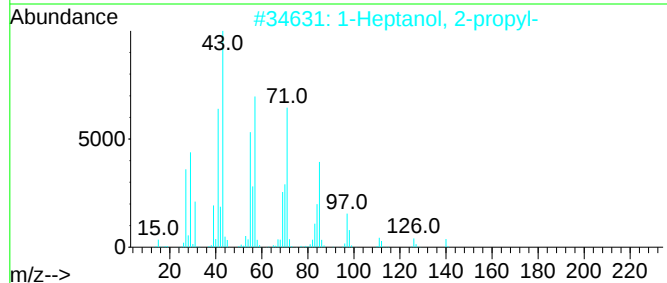
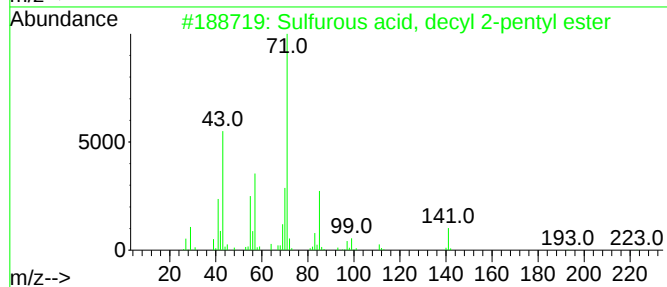
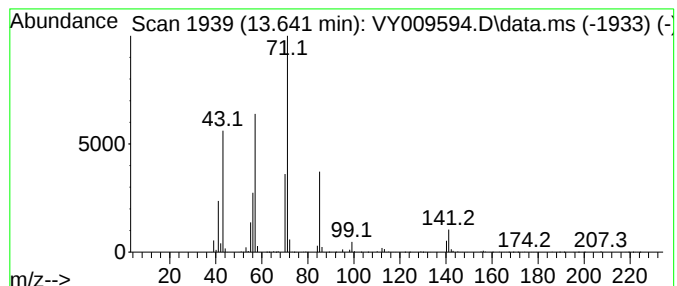
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Quant Title : SW846 8260

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

Peak Number 7 Sulfurous acid, decyl 2-pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.642	56.19 ug/l	1493870	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	72
2			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	64
3			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	59
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	59
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

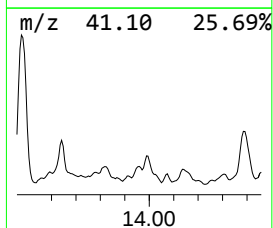
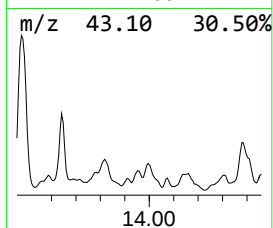
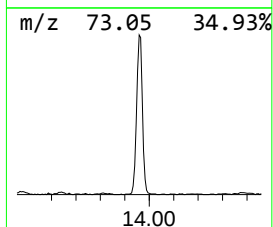
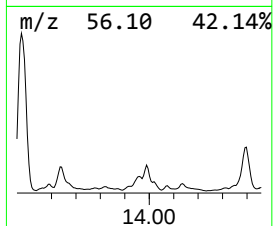
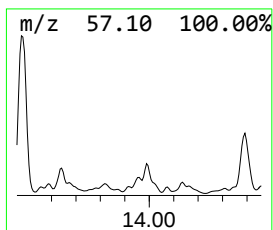
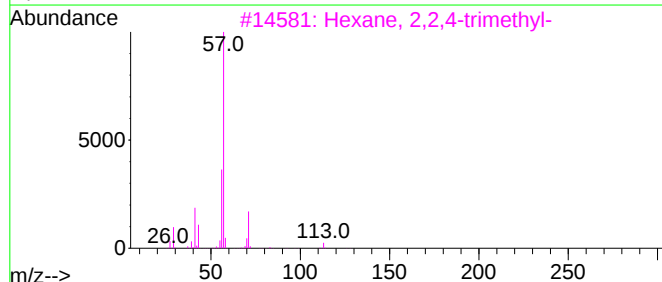
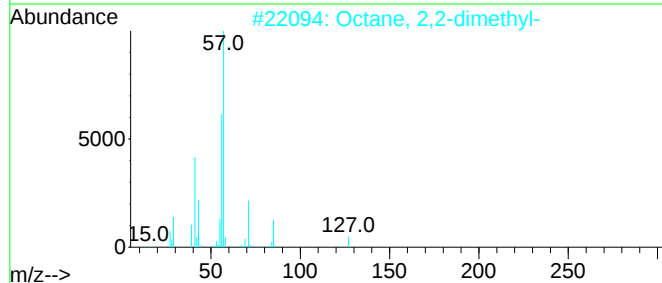
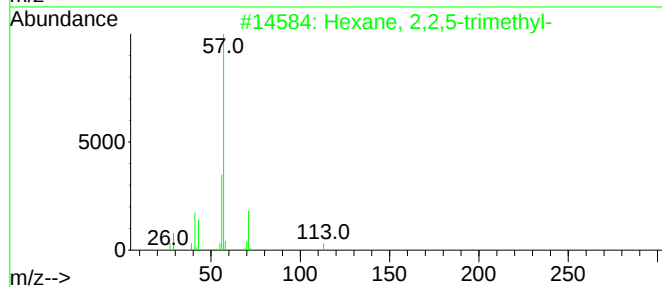
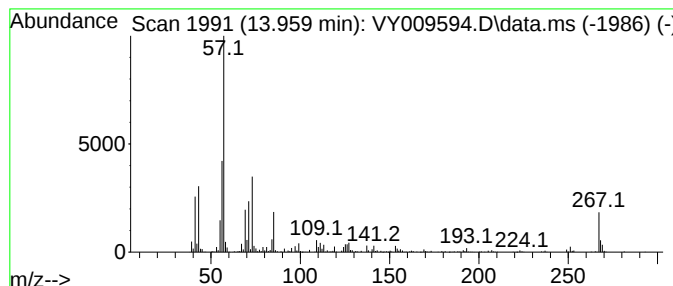
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.959 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	22.83 ug/l	606994	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	47
2			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	47
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	47
4			2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	38
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

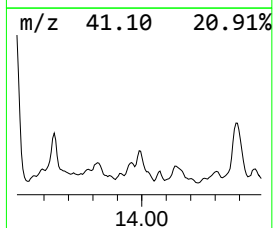
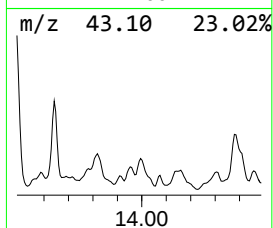
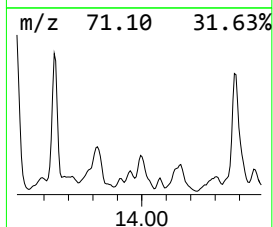
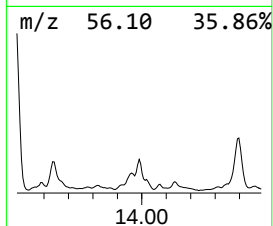
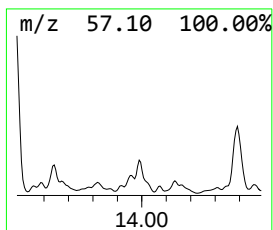
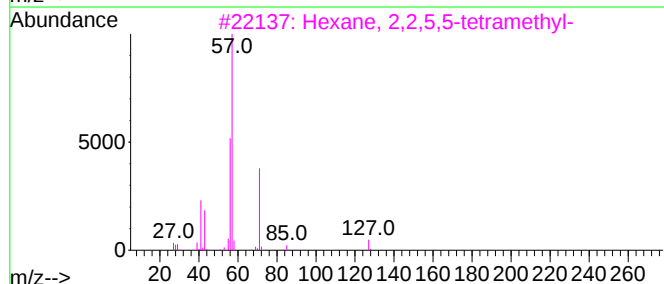
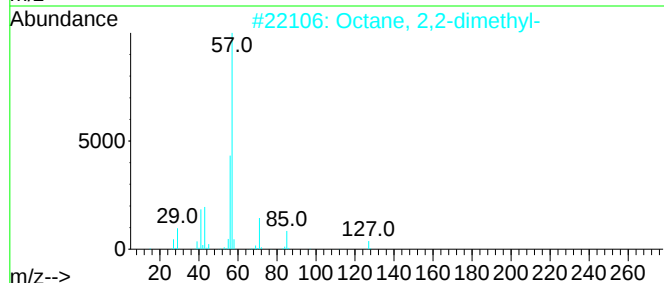
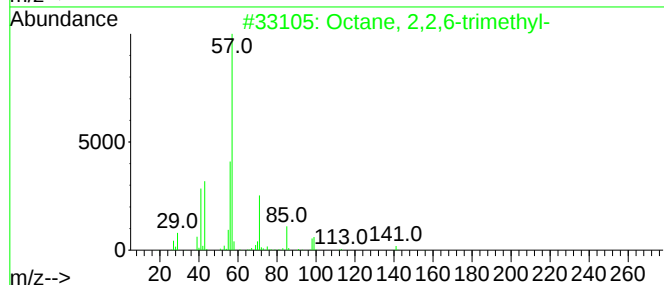
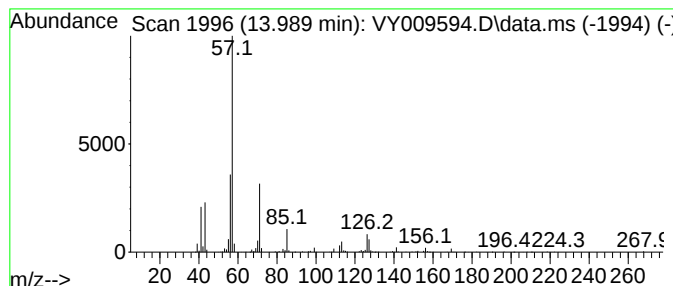
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 2,2,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.989	37.44 ug/l	995347	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
2			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	53
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
4			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	53
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/soil
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

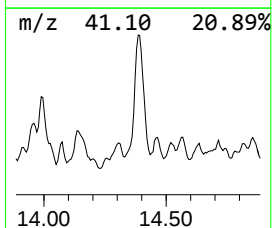
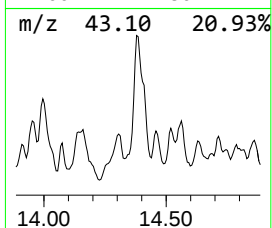
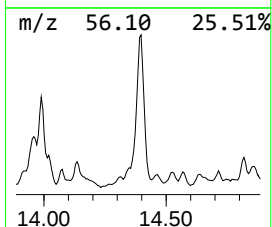
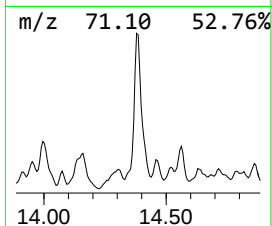
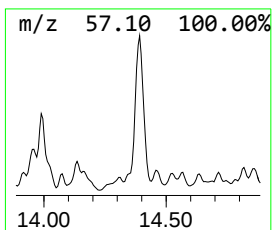
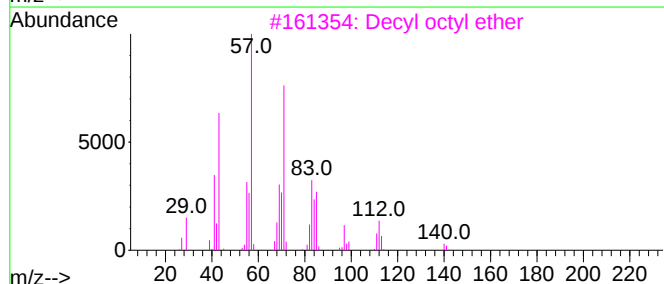
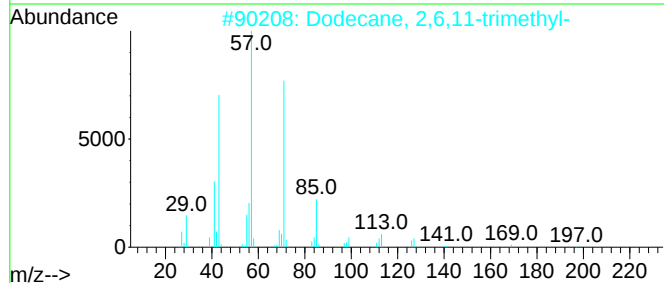
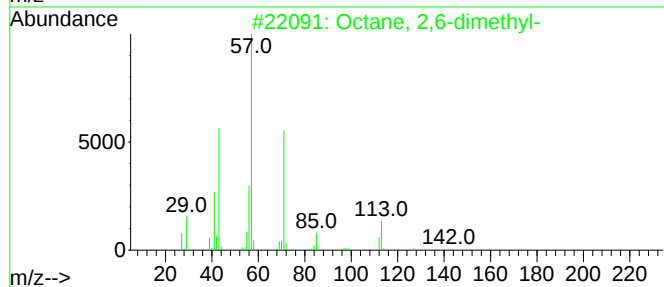
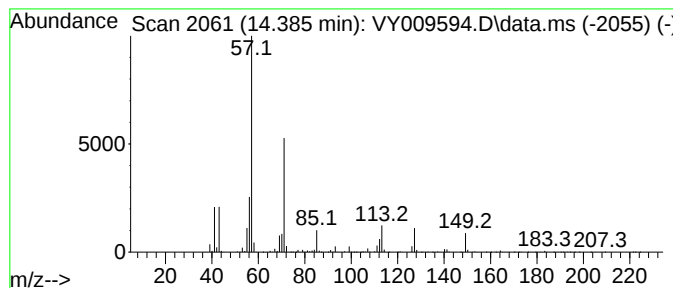
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Quant Title : SW846 8260

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

Peak Number 10 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.385	87.11 ug/l	2315680	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
3			Decyl octyl ether	270	C18H38O	1000406-38-3	59
4			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	59
5			Tridecane, 7-methyl-	198	C14H30	026730-14-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071922\
Data File : VY009594.D
Acq On : 19 Jul 2022 17:02
Operator : KP/MD
Sample : N3651-05
Misc : 6.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
DUP-SED

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071822S.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
Tetradecane, 2,...	12.623	71.5	ug/l	1899690	4	13.422	1329220	50.0
Decane, 2-methyl-	12.837	81.4	ug/l	2164960	4	13.422	1329220	50.0
Decane, 2,2-dim...	13.068	91.7	ug/l	2438550	4	13.422	1329220	50.0
Dodecane, 2,2,1...	13.172	25.3	ug/l	671283	4	13.422	1329220	50.0
Pentan-2-yl 2-m...	13.282	240.0	ug/l	6380530	4	13.422	1329220	50.0
Octane, 2,6-dim...	13.477	223.9	ug/l	5951190	4	13.422	1329220	50.0
Sulfurous acid,...	13.642	56.2	ug/l	1493870	4	13.422	1329220	50.0
unknown13.959	13.959	22.8	ug/l	606994	4	13.422	1329220	50.0
Octane, 2,2,6-t...	13.989	37.4	ug/l	995347	4	13.422	1329220	50.0
Dodecane, 2,6,1...	14.385	87.1	ug/l	2315680	4	13.422	1329220	50.0