

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051122\
 Data File : VD072933.D
 Acq On : 11 May 2022 16:18
 Operator : VA/SY
 Sample : N2749-01
 Misc : 3.50G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 TP-1

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_D\Method\82D050222S.M
 Title : SW846 8260

Signal : TIC: VD072933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.150	372	379	392	rBV4	10234	29978	1.47%	0.190%
2	4.967	507	518	527	rBV4	25458	85447	4.20%	0.541%
3	5.179	543	554	565	rBV3	16417	58910	2.90%	0.373%
4	5.991	685	692	702	rVB4	11797	35999	1.77%	0.228%
5	7.185	886	895	907	rBV	34926	102728	5.05%	0.650%
6	7.908	1007	1018	1023	rBV2	278854	672158	33.06%	4.253%
7	7.973	1023	1029	1040	rVB	491382	1092162	53.72%	6.910%
8	8.320	1070	1088	1099	rBV3	268032	973354	47.88%	6.158%
9	8.855	1171	1179	1190	rBV	718600	1484176	73.00%	9.390%
10	9.896	1351	1356	1363	rVB7	10147	22160	1.09%	0.140%
11	10.332	1422	1430	1439	rBV	1165539	2033100	100.00%	12.863%
12	10.714	1488	1495	1503	rVB	111945	203426	10.01%	1.287%
13	11.079	1550	1557	1567	rBV	66572	116126	5.71%	0.735%
14	11.449	1614	1620	1626	rVB2	82441	134914	6.64%	0.854%
15	11.632	1643	1651	1662	rBV	1070038	1909562	93.92%	12.082%
16	12.620	1809	1819	1827	rBV2	1029609	1856547	91.32%	11.746%
17	12.702	1827	1833	1838	rVV5	18201	46133	2.27%	0.292%
18	12.767	1838	1844	1852	rVB2	50840	120334	5.92%	0.761%
19	12.943	1869	1874	1876	rBV4	35938	58587	2.88%	0.371%
20	12.967	1876	1878	1884	rVV3	44972	72885	3.58%	0.461%
21	13.014	1884	1886	1895	rVB5	14938	27439	1.35%	0.174%
22	13.202	1895	1918	1927	rBV	220438	486038	23.91%	3.075%
23	13.308	1929	1936	1944	rBV	118452	205566	10.11%	1.301%
24	13.414	1944	1954	1962	rVV	318991	608304	29.92%	3.849%
25	13.485	1963	1966	1969	rVV4	27454	43991	2.16%	0.278%
26	13.561	1969	1979	1984	rVV	1116409	1999195	98.33%	12.649%
27	13.614	1984	1988	1998	rVB	329351	670913	33.00%	4.245%
28	13.773	2008	2015	2022	rVV3	110697	207326	10.20%	1.312%
29	13.843	2023	2027	2031	rVV3	17615	30682	1.51%	0.194%
30	13.908	2031	2038	2041	rVV8	21150	49182	2.42%	0.311%
31	13.955	2043	2046	2052	rVB5	27649	46109	2.27%	0.292%
32	14.090	2063	2069	2083	rVB5	45820	136460	6.71%	0.863%
33	14.261	2093	2098	2103	rBV8	10427	21440	1.05%	0.136%
34	14.508	2135	2140	2145	rBV7	23453	42692	2.10%	0.270%
35	14.814	2185	2192	2194	rBV7	19247	38148	1.88%	0.241%
36	15.073	2230	2236	2241	rBV6	25149	50326	2.48%	0.318%

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Instrument :
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ClientSampleId :
TP-1

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_D\Method\82D050222S.M
Title : SW846 8260

37	15.349	2279	2283	2286	rBV5	17697	32695	1.61%	0.207%
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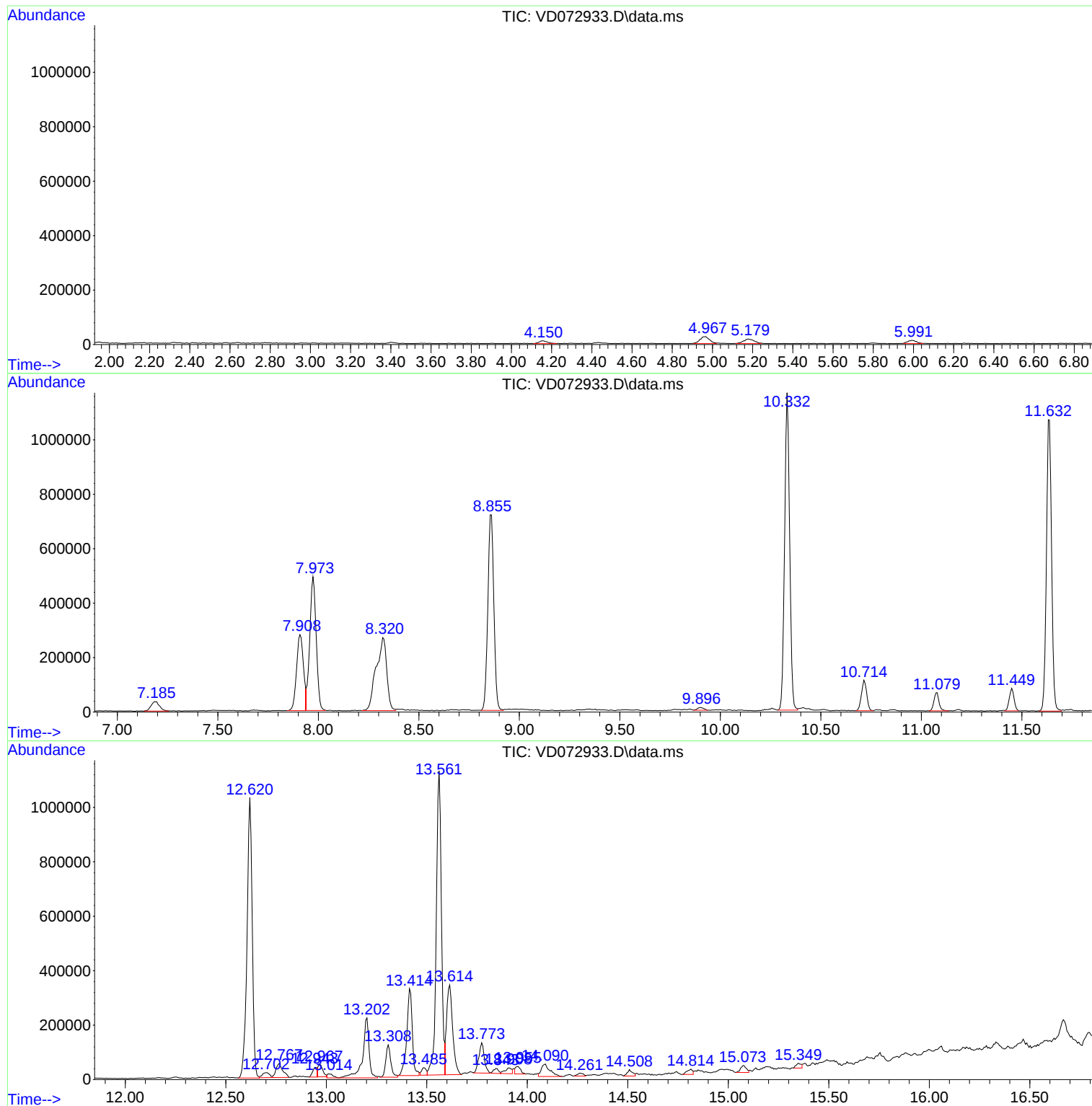
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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



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Instrument :
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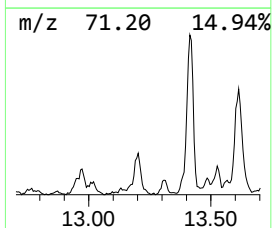
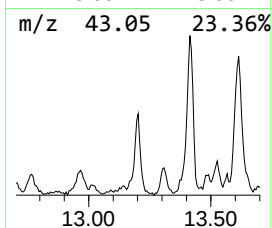
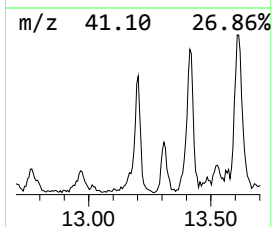
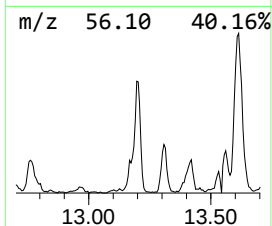
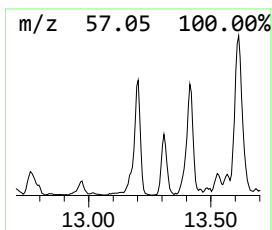
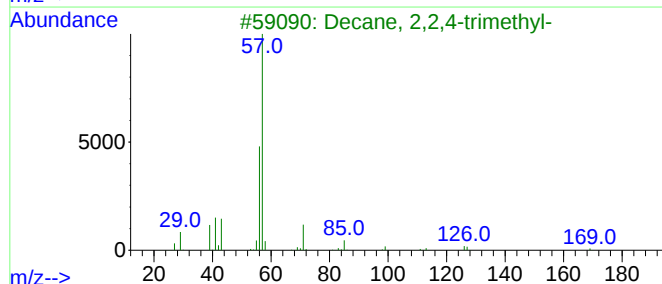
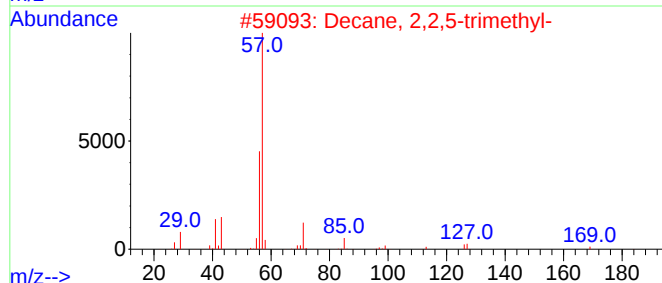
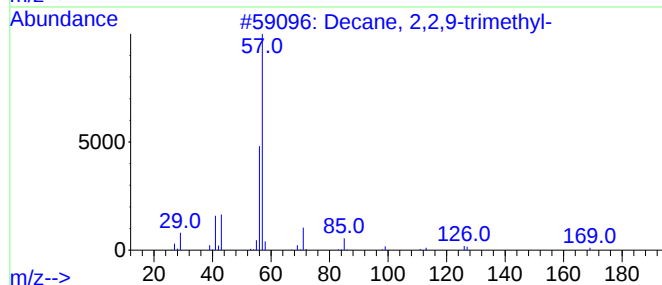
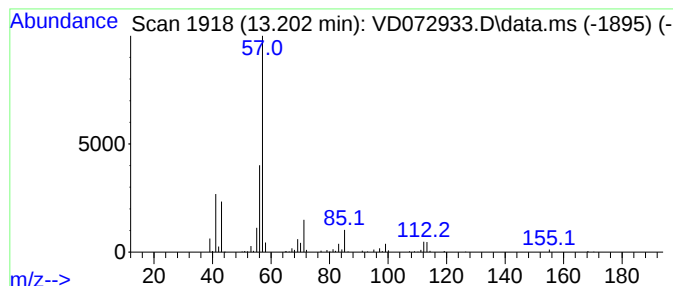
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 2 Decane, 2,2,9-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.202	12.16 ug/l	486038	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	72
2			Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	72
3			Decane, 2,2,4-trimethyl-	184	C13H28	062237-98-3	72
4			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64
5			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64



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Misc : 3.50G/5.00ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP-1

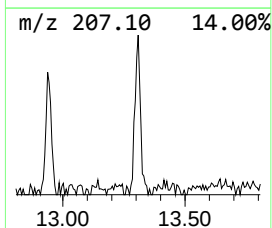
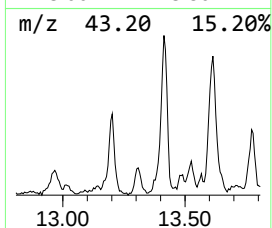
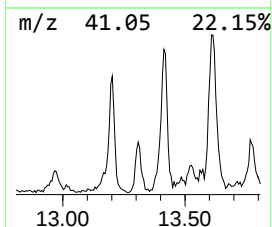
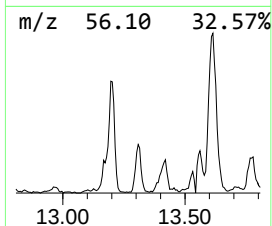
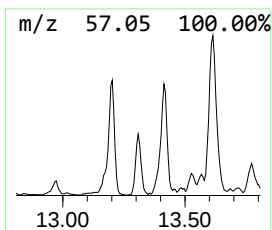
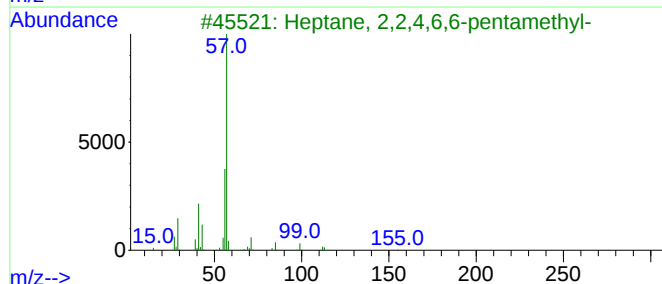
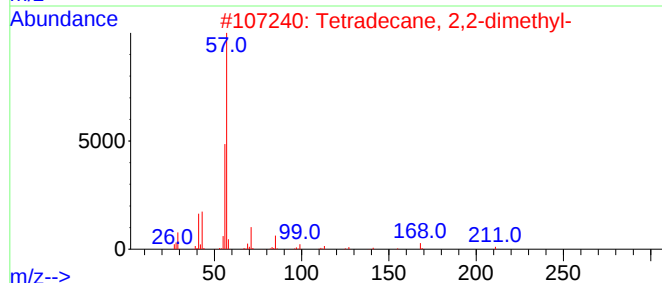
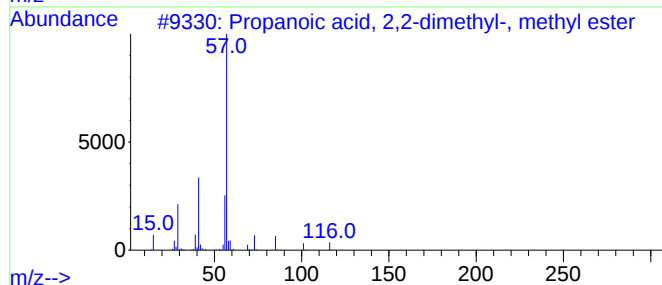
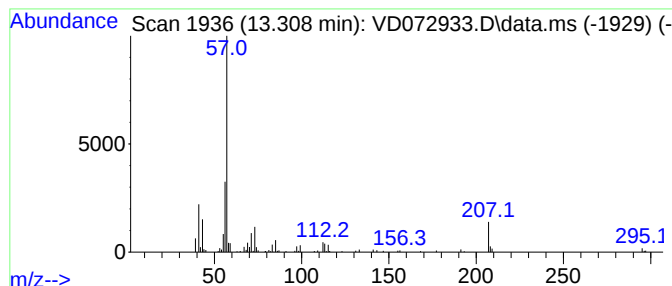
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 3 Propanoic acid, 2,2-dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.308	5.14 ug/l	205566	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	53
2			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	43
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	43
4			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	35
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	32



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Misc : 3.50G/5.00ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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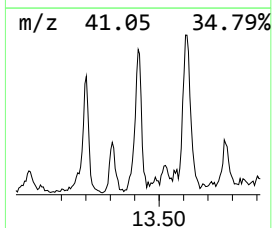
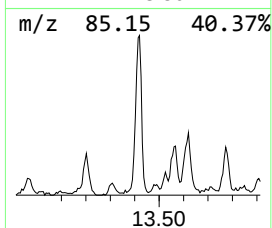
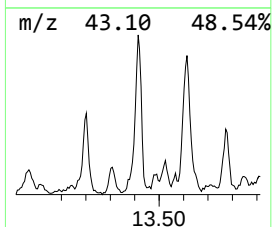
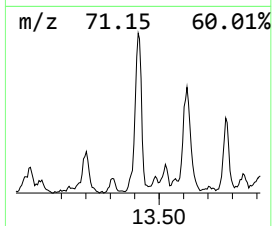
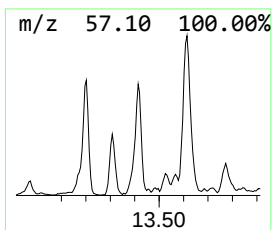
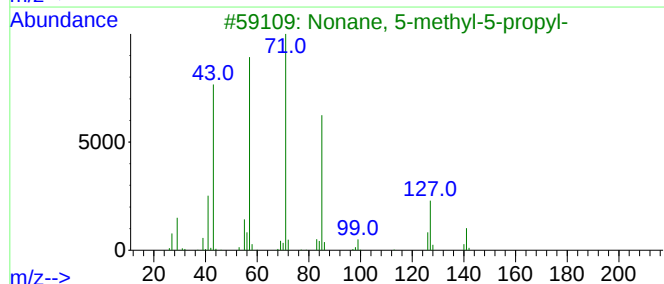
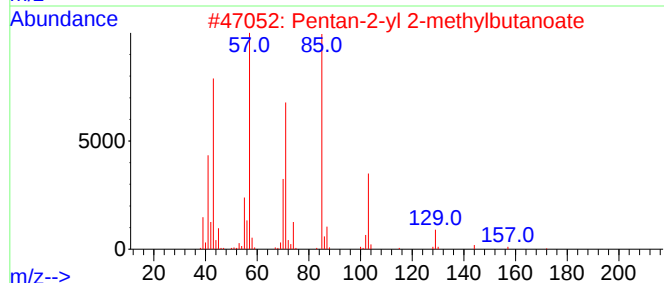
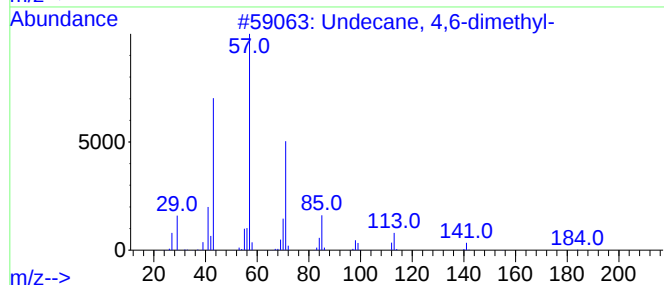
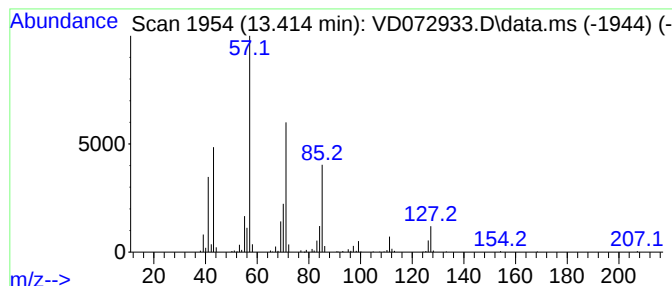
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane, 4,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	15.21 ug/l	608304	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
2			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
3			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50
4			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	50
5			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	50



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Misc : 3.50G/5.00ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1

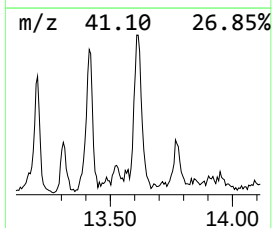
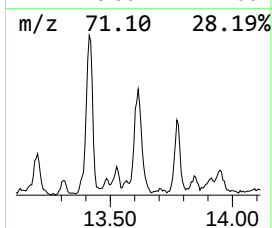
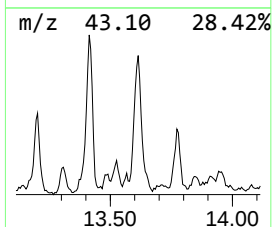
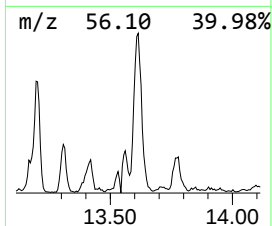
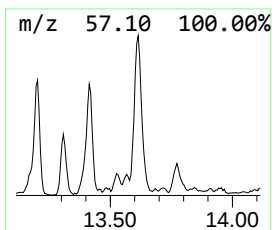
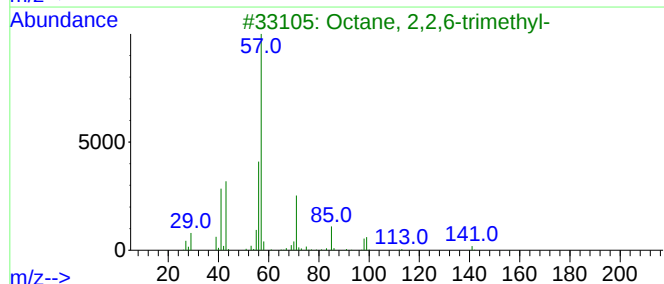
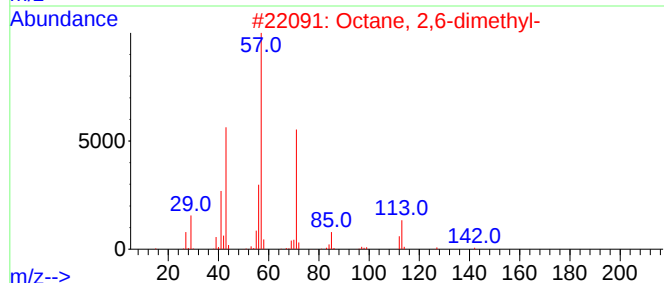
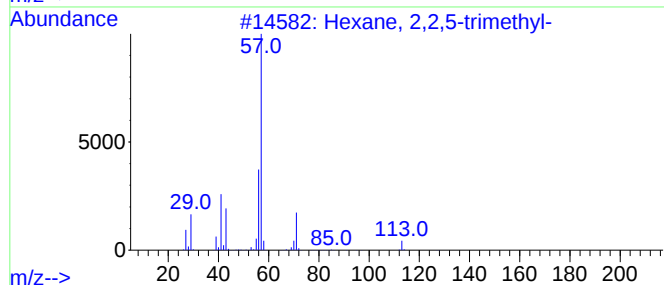
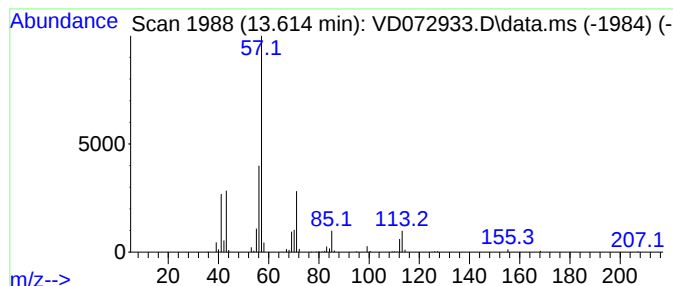
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,2,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.614	16.78 ug/l	670913	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
5			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP-1

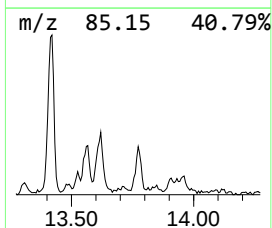
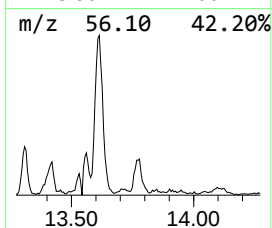
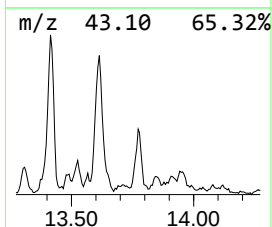
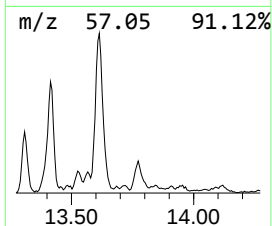
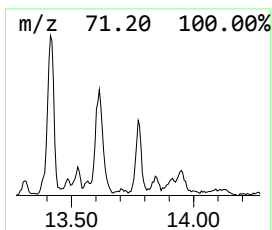
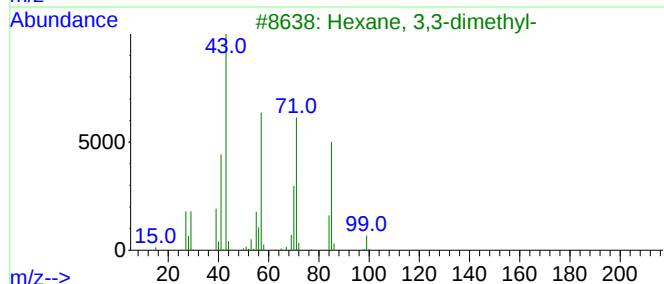
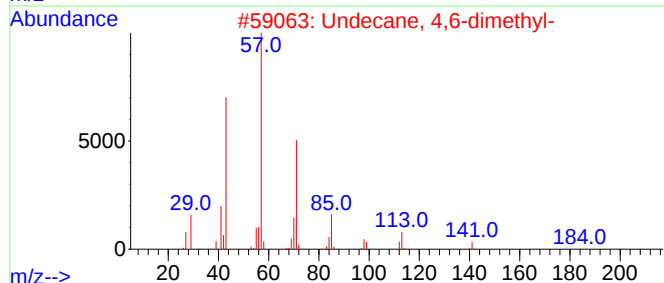
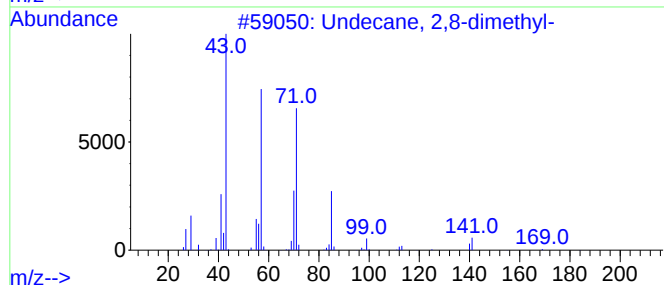
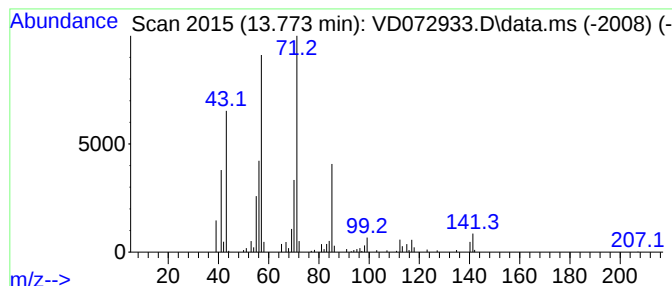
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.M
Quant Title : SW846 8260

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

Peak Number 6 Undecane, 2,8-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.773	5.19 ug/l	207326	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	64
2			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD051122\
Data File : VD072933.D
Acq On : 11 May 2022 16:18
Operator : VA/SY
Sample : N2749-01
Misc : 3.50G/5.00ml/MSVOA_D/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
TP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D050222S.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
Decane, 2,2,9-t...	13.202	12.2	ug/l	486038	4	13.561	1999200	50.0
Propanoic acid,...	13.308	5.1	ug/l	205566	4	13.561	1999200	50.0
Undecane, 4,6-d...	13.414	15.2	ug/l	608304	4	13.561	1999200	50.0
Hexane, 2,2,5-t...	13.614	16.8	ug/l	670913	4	13.561	1999200	50.0
Undecane, 2,8-d...	13.773	5.2	ug/l	207326	4	13.561	1999200	50.0