

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
 Data File : VD068787.D
 Acq On : 08 Apr 2021 14:16
 Operator : VA/SY
 Sample : M1979-14
 Misc : 5.52G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 S-14

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\82D040721S.M

Title : SW846 8260

Signal : TIC: VD068787.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.973	504	519	538	rBV7	37261	173578	7.16%	0.817%
2	5.497	596	608	621	rBV3	29600	101224	4.18%	0.476%
3	5.997	682	693	702	rBV6	11903	36181	1.49%	0.170%
4	6.932	841	852	863	rBV3	38843	116500	4.81%	0.548%
5	7.920	1009	1020	1025	rBV	301710	747062	30.83%	3.516%
6	7.985	1025	1031	1039	rVV	557981	1244389	51.35%	5.857%
7	8.067	1039	1045	1056	rVB2	80896	204212	8.43%	0.961%
8	8.332	1079	1090	1101	rVB	226997	521163	21.51%	2.453%
9	8.508	1101	1120	1131	rVV	342646	964895	39.82%	4.541%
10	8.603	1131	1136	1144	rVB7	12512	31381	1.29%	0.148%
11	8.867	1168	1181	1192	rBV	829217	1681241	69.38%	7.913%
12	9.326	1250	1259	1260	rBV6	22881	42191	1.74%	0.199%
13	9.355	1260	1264	1269	rVV5	38653	85762	3.54%	0.404%
14	9.408	1269	1273	1281	rVV3	37463	77366	3.19%	0.364%
15	9.491	1282	1287	1291	rVV2	14985	25547	1.05%	0.120%
16	9.632	1302	1311	1318	rVB7	18814	45004	1.86%	0.212%
17	9.779	1328	1336	1347	rBV	194833	398475	16.44%	1.875%
18	9.914	1349	1359	1365	rBV2	144848	300398	12.40%	1.414%
19	10.097	1385	1390	1395	rBV5	17781	34287	1.41%	0.161%
20	10.267	1413	1419	1424	rBV	127002	226840	9.36%	1.068%
21	10.338	1424	1431	1445	rVB	1309515	2423381	100.00%	11.406%
22	10.720	1491	1496	1502	rBV	73730	139708	5.77%	0.658%
23	10.785	1502	1507	1515	rVV6	52311	112897	4.66%	0.531%
24	10.873	1517	1522	1528	rVB8	17428	35181	1.45%	0.166%
25	10.955	1528	1536	1543	rBV3	37088	76007	3.14%	0.358%
26	11.055	1548	1553	1555	rBV	40806	69443	2.87%	0.327%
27	11.244	1579	1585	1590	rBV5	34202	60932	2.51%	0.287%
28	11.449	1616	1620	1629	rVB4	36587	83577	3.45%	0.393%
29	11.561	1635	1639	1644	rBV6	17698	29177	1.20%	0.137%
30	11.644	1644	1653	1662	rVV	1273246	2300985	94.95%	10.830%
31	11.708	1662	1664	1669	rVB2	42135	62887	2.60%	0.296%
32	11.838	1681	1686	1689	rBV6	19027	36603	1.51%	0.172%
33	11.891	1690	1695	1700	rVB3	57189	101716	4.20%	0.479%
34	12.085	1724	1728	1732	rBV3	25714	37737	1.56%	0.178%
35	12.155	1732	1740	1745	rBV7	49057	123374	5.09%	0.581%
36	12.202	1745	1748	1752	rBV5	29928	39758	1.64%	0.187%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
 Data File : VD068787.D
 Acq On : 08 Apr 2021 14:16
 Operator : VA/SY
 Sample : M1979-14
 Misc : 5.52G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 S-14

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\82D040721S.M
 Title : SW846 8260

37	12.267	1753	1759	1764	rVB	112825	221677	9.15%	1.043%
38	12.344	1767	1772	1775	rBV4	63052	117679	4.86%	0.554%
39	12.632	1810	1821	1827	rBV2	1109700	2253415	92.99%	10.606%
40	12.714	1828	1835	1840	rVV7	85970	216196	8.92%	1.018%
41	12.767	1840	1844	1856	rVB5	119198	357695	14.76%	1.683%
42	12.873	1857	1862	1867	rBV5	27322	62972	2.60%	0.296%
43	12.979	1870	1880	1891	rBV8	76017	255435	10.54%	1.202%
44	13.096	1896	1900	1904	rVV4	55837	98975	4.08%	0.466%
45	13.149	1904	1909	1911	rVV4	51225	91613	3.78%	0.431%
46	13.185	1911	1915	1916	rVV	89802	131979	5.45%	0.621%
47	13.208	1916	1919	1928	rVV	152166	335366	13.84%	1.578%
48	13.308	1932	1936	1942	rVV2	115190	219885	9.07%	1.035%
49	13.361	1942	1945	1948	rVV4	39764	67590	2.79%	0.318%
50	13.426	1948	1956	1965	rVV2	153033	390164	16.10%	1.836%
51	13.496	1965	1968	1972	rVV6	32433	57238	2.36%	0.269%
52	13.573	1972	1981	1986	rVV	1302434	2207185	91.08%	10.388%
53	13.620	1986	1989	1999	rVB	192019	405075	16.72%	1.906%
54	13.785	2013	2017	2024	rBV2	56644	97918	4.04%	0.461%
55	13.890	2032	2035	2040	rBV6	47138	69790	2.88%	0.328%
56	14.049	2057	2062	2067	rBV5	37280	65449	2.70%	0.308%
57	14.102	2067	2071	2075	rBV4	39566	68203	2.81%	0.321%
58	14.214	2086	2090	2094	rBV5	41879	65560	2.71%	0.309%
59	14.279	2097	2101	2108	rVB7	52503	104148	4.30%	0.490%
60	14.402	2118	2122	2126	rBV6	39720	74715	3.08%	0.352%
61	14.543	2138	2146	2153	rBV8	61762	210055	8.67%	0.989%
62	14.826	2189	2194	2197	rBV6	29668	55767	2.30%	0.262%
63	14.861	2197	2200	2209	rVB5	59208	121066	5.00%	0.570%
64	15.361	2280	2285	2288	rBV7	15944	33366	1.38%	0.157%

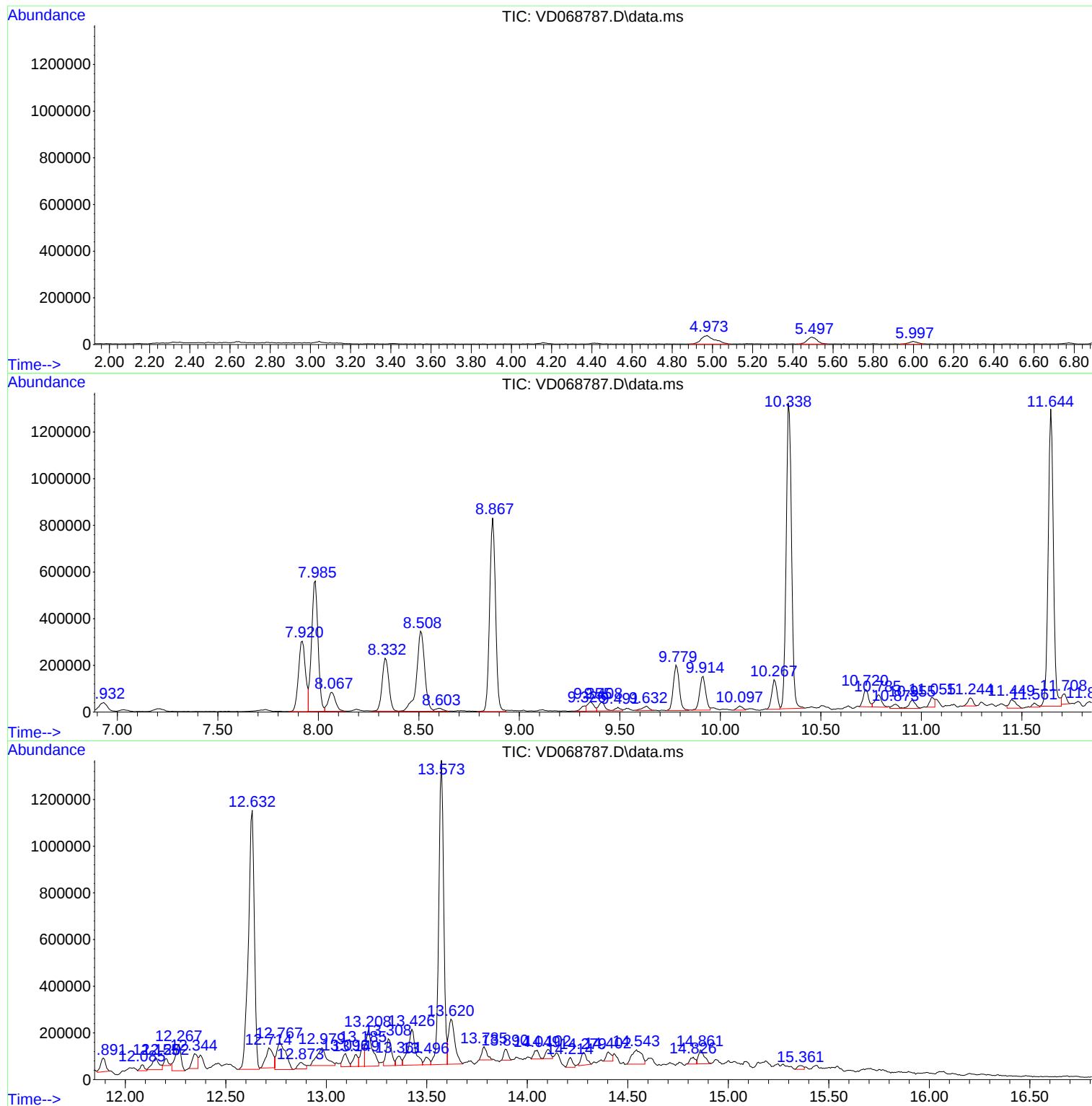
Sum of corrected areas: 21247235

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

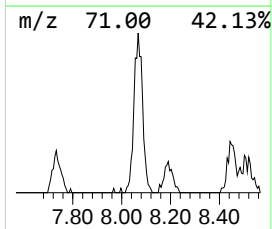
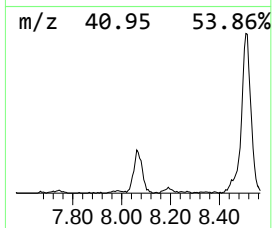
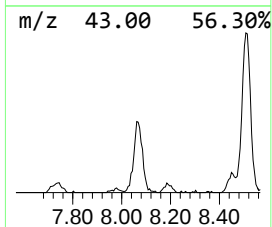
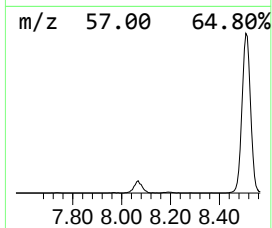
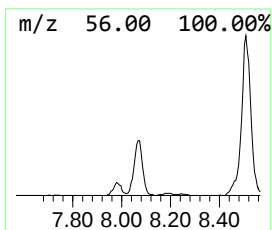
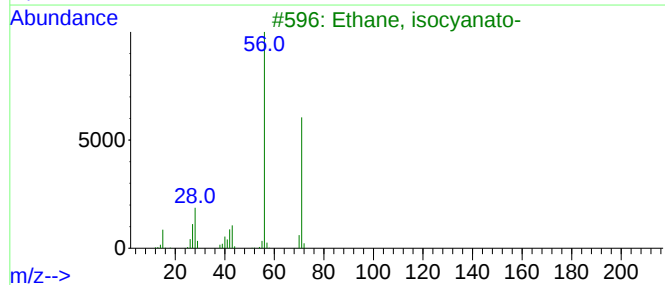
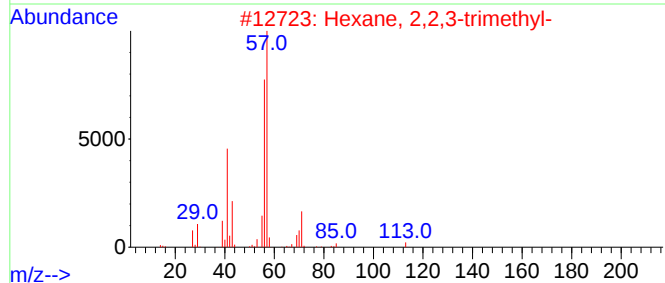
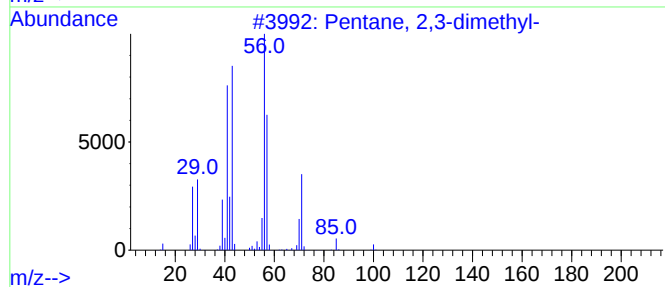
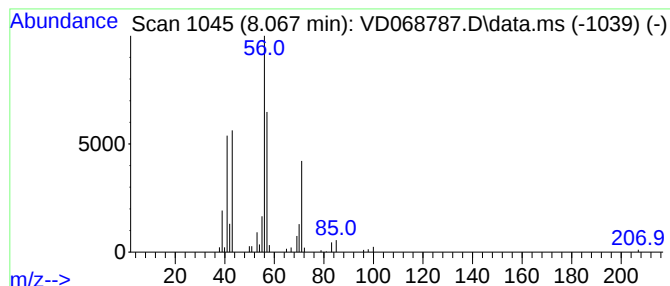
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.067	8.21 ug/l	204212	Pentafluorobenzene	7.985

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Ethane, isocyanato-	71	C3H5NO	000109-90-0	64
4			2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	50
5			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

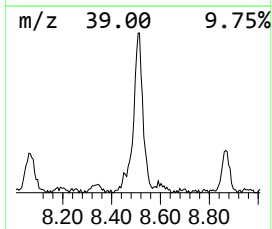
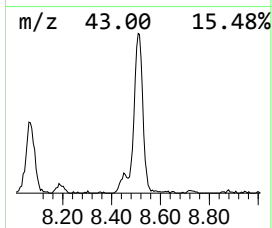
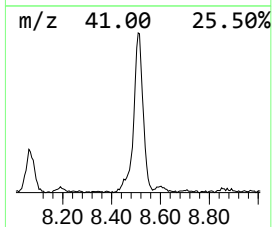
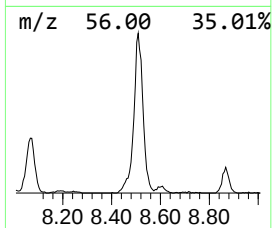
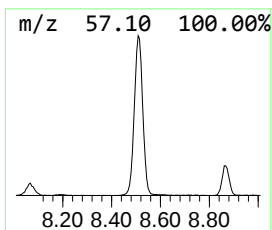
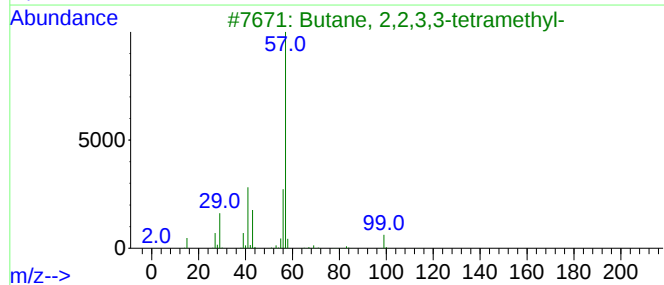
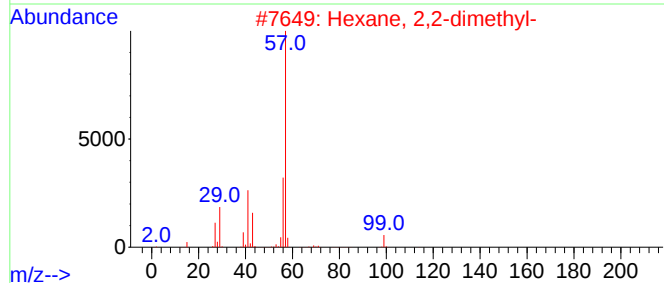
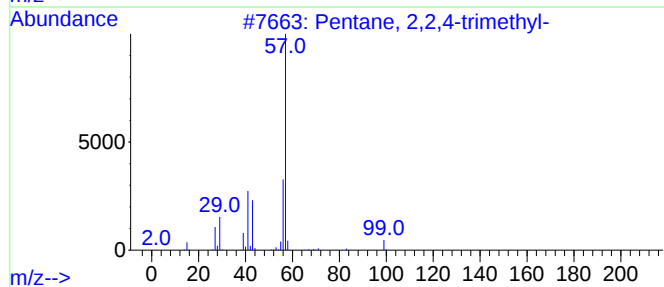
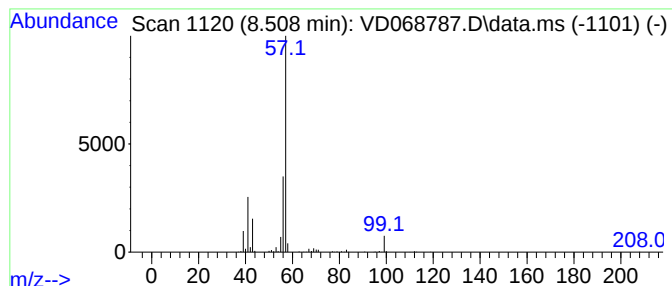
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.508	28.70 ug/l	964895	1,4-Difluorobenzene	8.867

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampled :
S-14

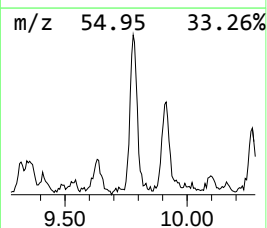
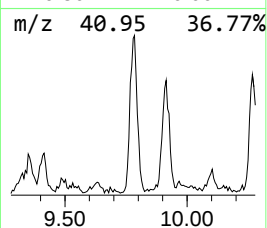
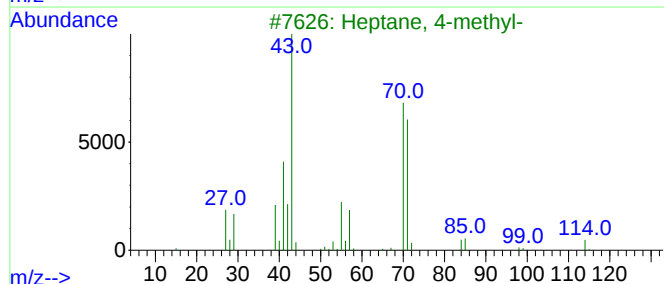
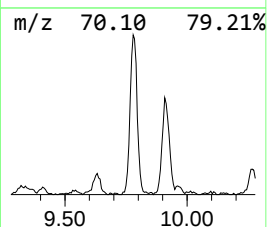
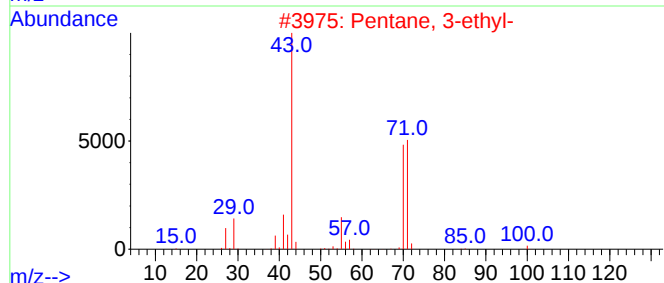
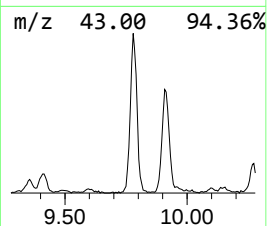
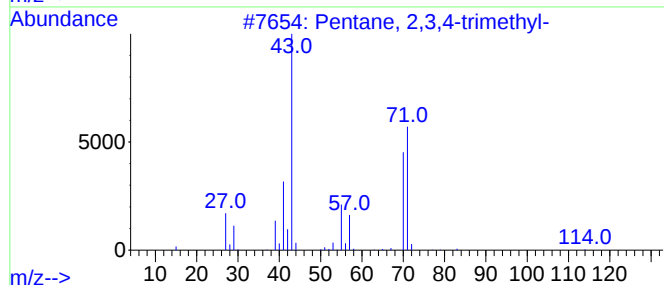
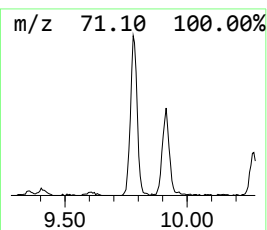
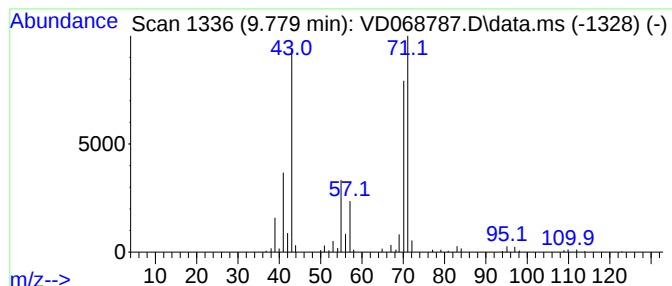
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.779	11.85 ug/l	398475	1,4-Difluorobenzene	8.867

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5			1-Butanol, 3-methyl-, carbonate ...	202	C11H22O3	002050-95-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampled :
S-14

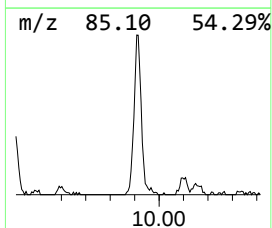
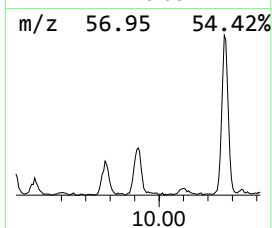
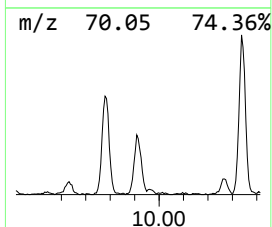
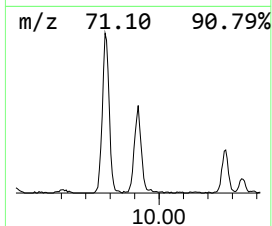
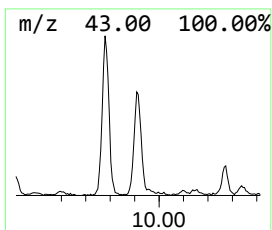
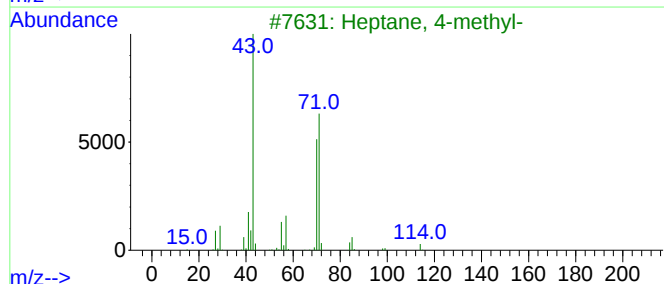
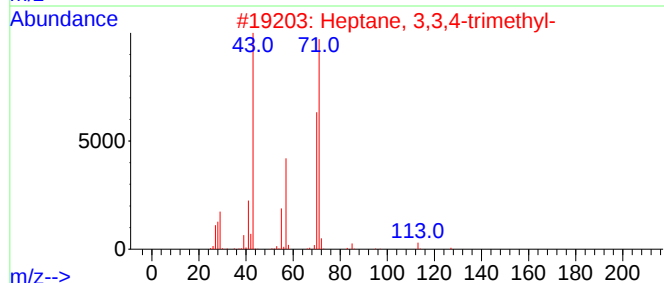
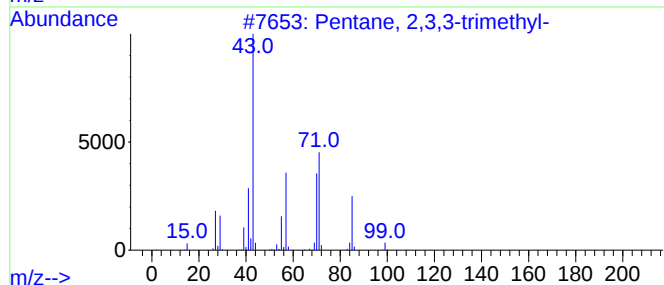
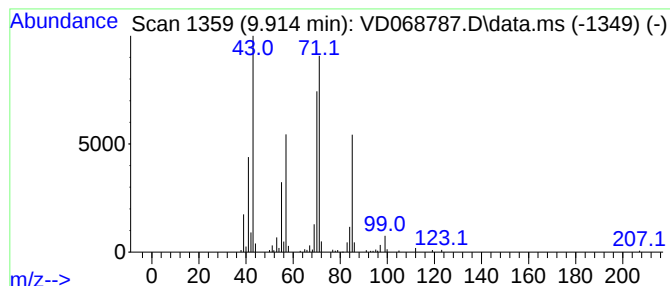
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.914	8.93 ug/l	300398	1,4-Difluorobenzene	8.867

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	58
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

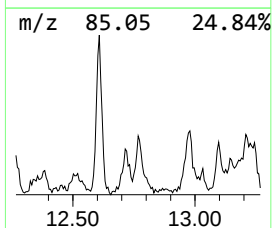
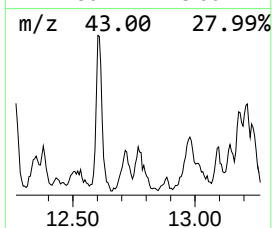
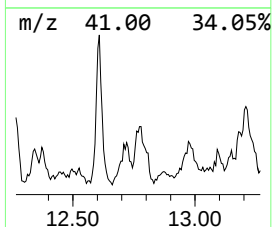
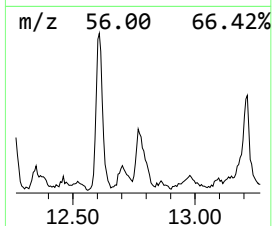
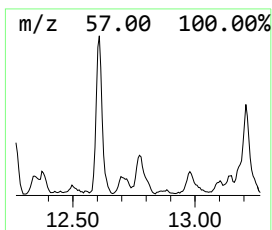
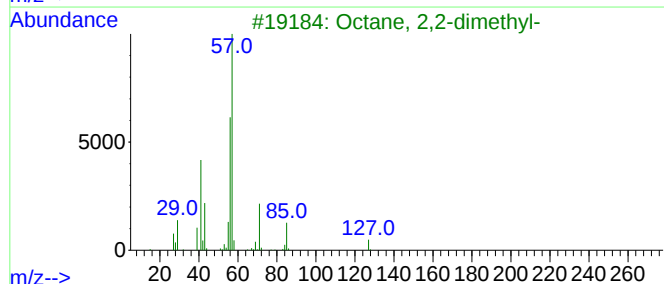
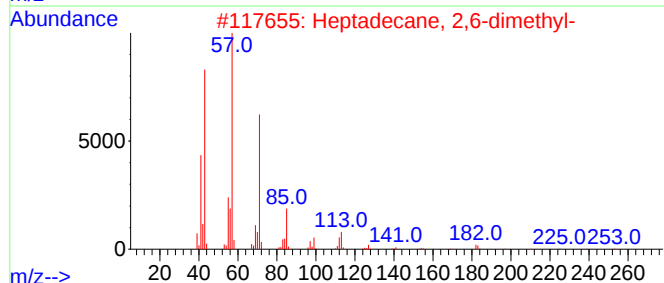
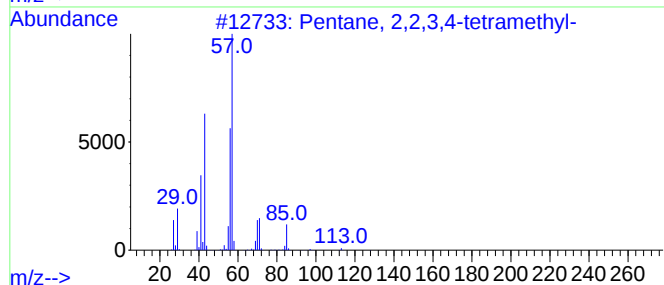
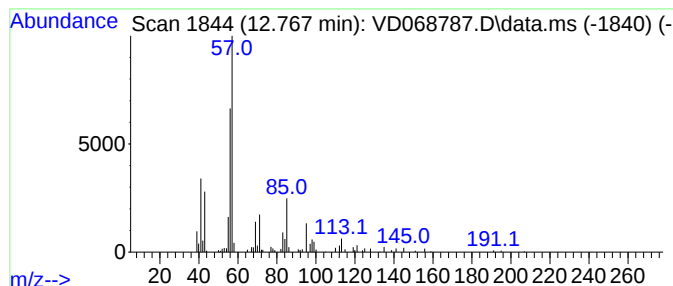
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown12.767 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.767	8.10 ug/l	357695	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	47
2			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	47
3			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	47
4			Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	47
5			Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

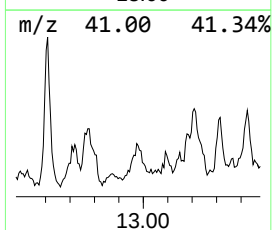
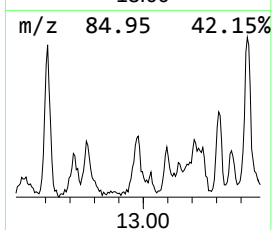
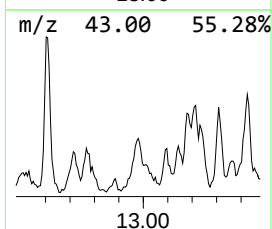
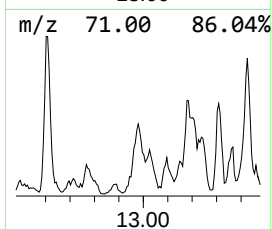
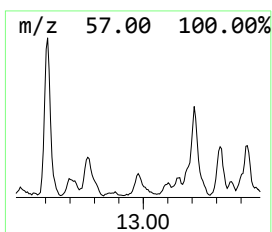
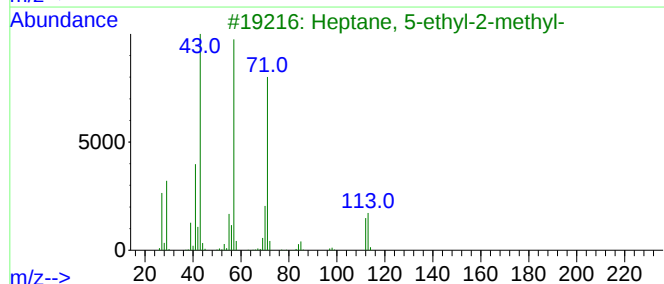
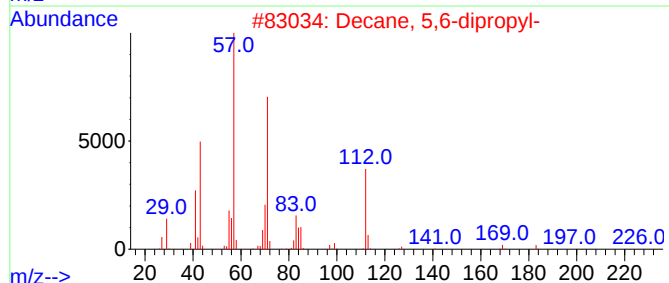
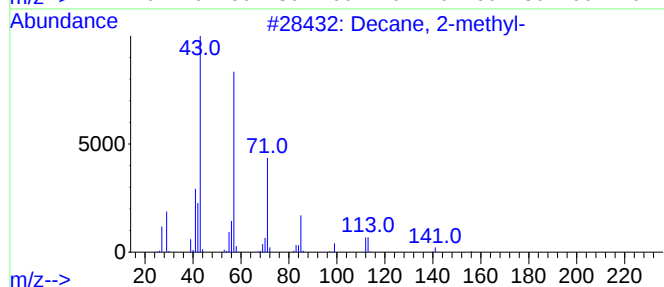
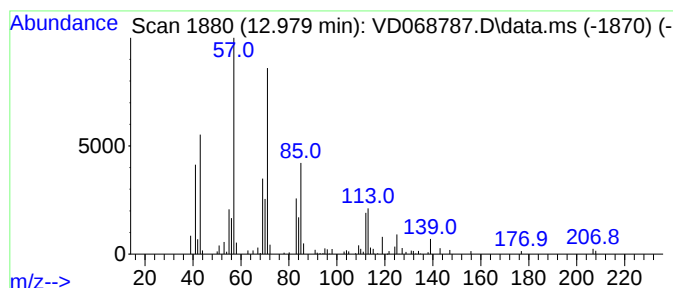
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 7 Decane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.979	5.79 ug/l	255435	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	72
2			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	53
3			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	53
4			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	53
5			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

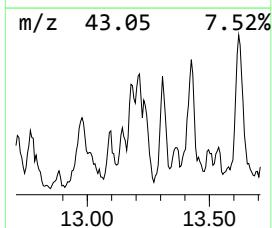
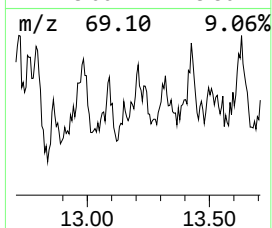
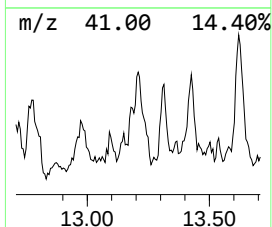
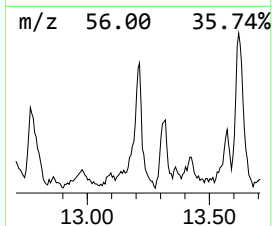
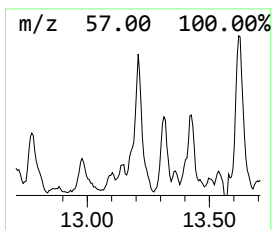
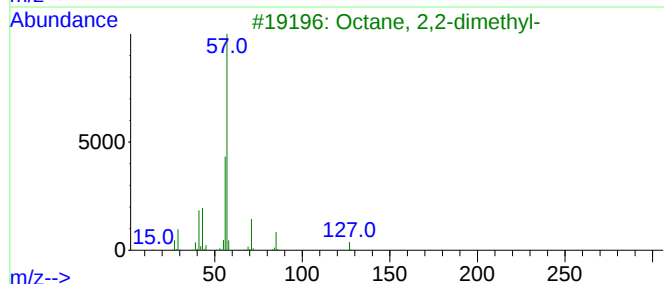
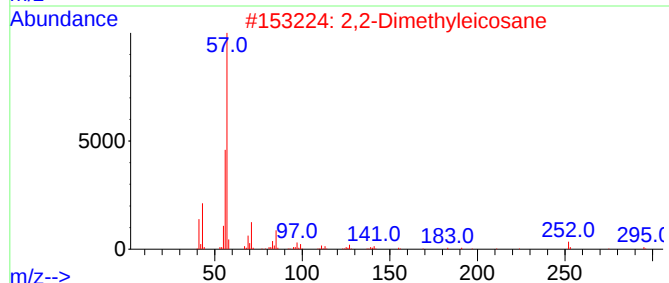
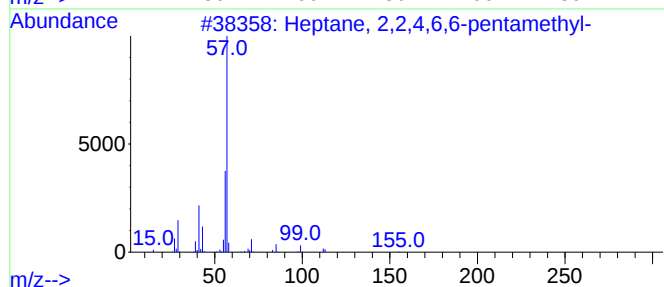
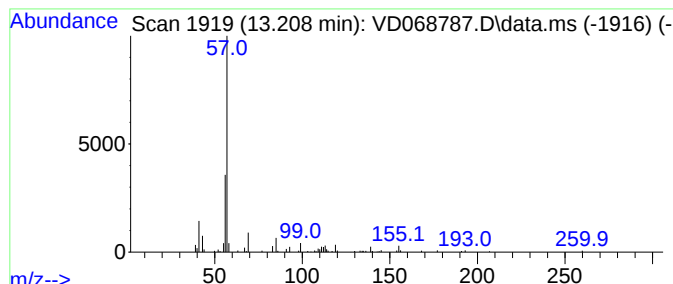
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 8 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	7.60 ug/l	335366	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
2			2,2-Dimethyleicosane	310	C22H46	1000360-43-4	50
3			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	40
4			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	38
5			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

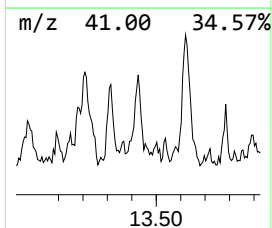
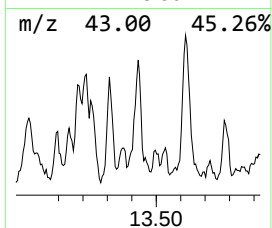
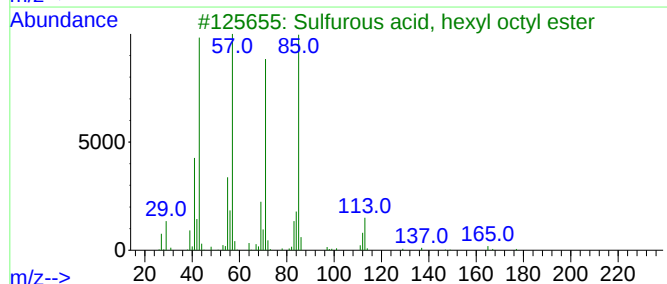
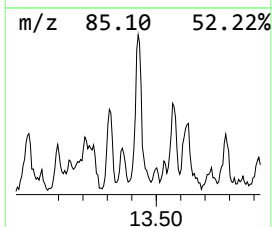
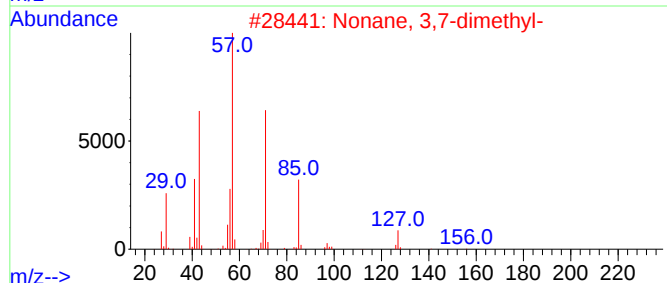
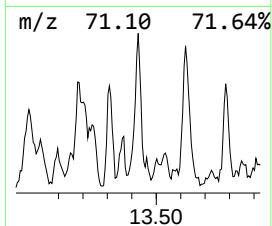
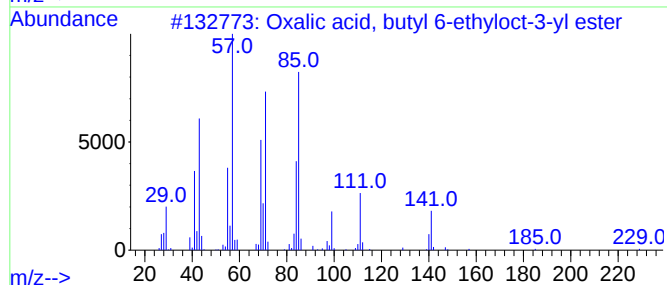
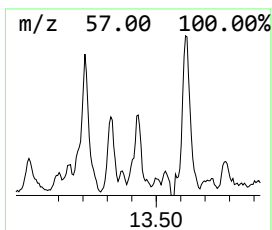
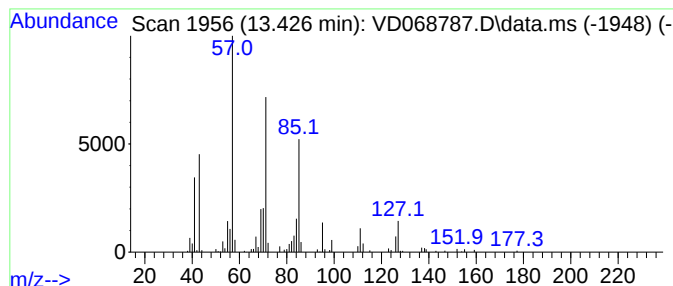
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.M
Quant Title : SW846 8260

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

Peak Number 9 Oxalic acid, butyl 6-ethylo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	8.84 ug/l	390164	1,4-Dichlorobenzene-d4	13.573

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, butyl 6-ethyloct-3-...	286	C16H30O4	1000309-34-2	59
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	53
3			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	50
4			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	47
5			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD040821\
Data File : VD068787.D
Acq On : 08 Apr 2021 14:16
Operator : VA/SY
Sample : M1979-14
Misc : 5.52G/5.00ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
S-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D040721S.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
Pentane, 2,3-di...	8.067	8.2	ug/l	204212	1	7.985	1244390	50.0
Pentane, 2,2,4-...	8.508	28.7	ug/l	964895	2	8.867	1681240	50.0
Pentane, 2,3,4-...	9.779	11.9	ug/l	398475	2	8.867	1681240	50.0
Pentane, 2,3,3-...	9.914	8.9	ug/l	300398	2	8.867	1681240	50.0
unknown12.767	12.767	8.1	ug/l	357695	4	13.573	2207190	50.0
Decane, 2-methyl-	12.979	5.8	ug/l	255435	4	13.573	2207190	50.0
Heptane, 2,2,4,...	13.208	7.6	ug/l	335366	4	13.573	2207190	50.0
Oxalic acid, bu...	13.426	8.8	ug/l	390164	4	13.573	2207190	50.0