

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
 Data File : VD078990.D
 Acq On : 22 May 2024 20:12
 Operator : RP/MD
 Sample : P2511-01
 Misc : 5.06G/5ml/MSVOA_D/SOIL/B
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 510-C

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\82D051324S.M
 Title : SW846 8260

Signal : TIC: VD078990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	19	26	34	rBV	240863	396390	5.23%	1.878%
2	4.022	403	414	425	rBV	39460	110587	1.46%	0.524%
3	7.804	1045	1057	1061	rBV	89018	217285	2.87%	1.030%
4	7.869	1061	1068	1076	rVV3	176778	499266	6.58%	2.366%
5	7.957	1076	1083	1094	rVB4	32870	87722	1.16%	0.416%
6	8.087	1094	1105	1120	rBV2	140926	334211	4.41%	1.584%
7	8.228	1120	1129	1139	rVB	67221	149069	1.97%	0.706%
8	8.634	1190	1198	1208	rBV	154928	304019	4.01%	1.441%
9	8.775	1214	1222	1231	rBV	216955	434299	5.73%	2.058%
10	10.269	1467	1476	1481	rBV	325156	572477	7.55%	2.713%
11	10.334	1481	1487	1499	rVB	1283069	2227364	29.37%	10.555%
12	11.581	1691	1699	1705	rBV	271968	458936	6.05%	2.175%
13	11.792	1726	1735	1745	rBV2	103890	223675	2.95%	1.060%
14	12.116	1779	1790	1798	rBV2	42490	90344	1.19%	0.428%
15	12.428	1835	1843	1850	rBV	133905	238905	3.15%	1.132%
16	12.569	1862	1867	1873	rBV	188335	299264	3.95%	1.418%
17	12.892	1913	1922	1930	rBV4	165808	295921	3.90%	1.402%
18	13.128	1958	1962	1970	rVB2	45558	76487	1.01%	0.362%
19	13.428	2006	2013	2021	rBV	5197685	7583889	100.00%	35.939%
20	13.516	2021	2028	2033	rVV	279898	464392	6.12%	2.201%
21	13.586	2033	2040	2042	rVV3	76873	136293	1.80%	0.646%
22	13.610	2042	2044	2049	rVB	94771	119568	1.58%	0.567%
23	13.839	2077	2083	2088	rBV	670167	962050	12.69%	4.559%
24	13.963	2098	2104	2107	rBV5	103218	182406	2.41%	0.864%
25	14.051	2116	2119	2124	rVB4	66815	89678	1.18%	0.425%
26	14.098	2124	2127	2134	rVB2	76284	122187	1.61%	0.579%
27	14.357	2161	2171	2175	rBV8	134973	388722	5.13%	1.842%
28	14.398	2175	2178	2185	rVB4	94674	136873	1.80%	0.649%
29	14.469	2185	2190	2193	rBV2	97316	160776	2.12%	0.762%
30	14.510	2193	2197	2204	rVB	326203	453165	5.98%	2.147%
31	14.692	2223	2228	2236	rBV	354645	515905	6.80%	2.445%
32	14.769	2236	2241	2244	rVV5	51806	93819	1.24%	0.445%
33	14.816	2244	2249	2250	rVV	109792	166448	2.19%	0.789%
34	14.839	2250	2253	2258	rVB2	171283	249071	3.28%	1.180%
35	15.039	2283	2287	2296	rVB4	81790	203273	2.68%	0.963%
36	15.122	2296	2301	2302	rBV2	70631	90590	1.19%	0.429%

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Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	15.181	2308	2311	2315	rVB2	71992	92922	1.23%	0.440%
38	15.239	2315	2321	2324	rVV7	37556	89330	1.18%	0.423%
39	15.298	2326	2331	2334	rVV4	87535	193199	2.55%	0.916%
40	15.345	2334	2339	2351	rVB2	343531	702929	9.27%	3.331%
41	15.528	2365	2370	2377	rVB	107320	168457	2.22%	0.798%
42	15.698	2393	2399	2409	rBV2	309889	532038	7.02%	2.521%
43	16.263	2489	2495	2505	rVB2	49945	105494	1.39%	0.500%
44	16.686	2561	2567	2572	rBV3	42619	82553	1.09%	0.391%

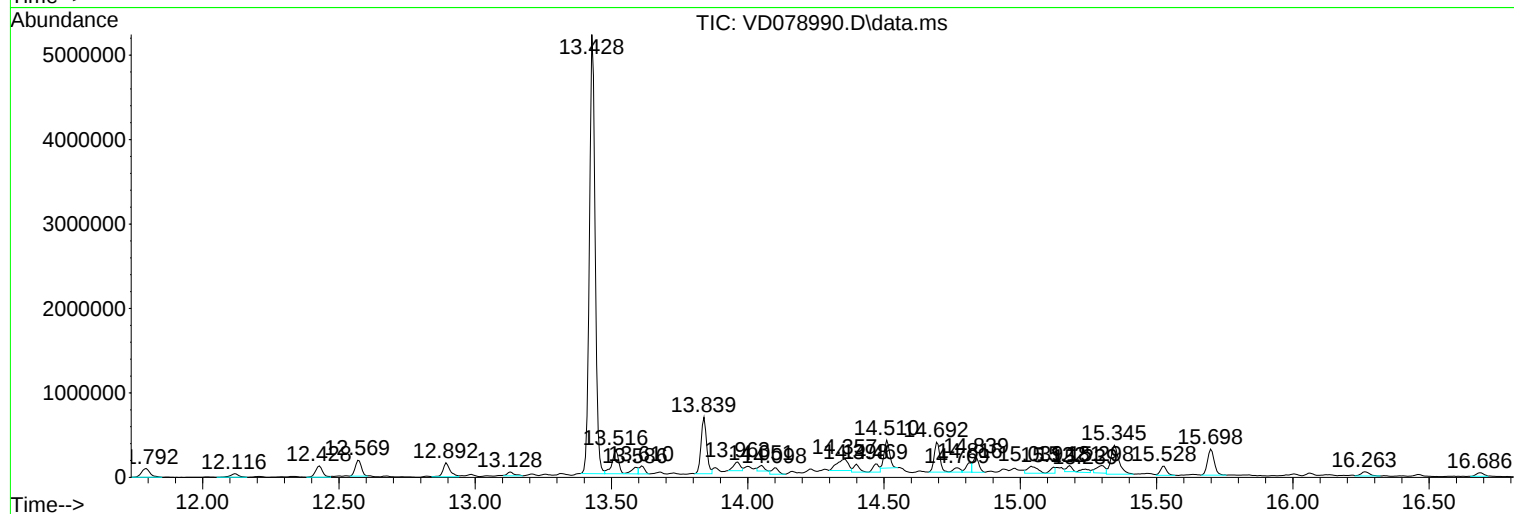
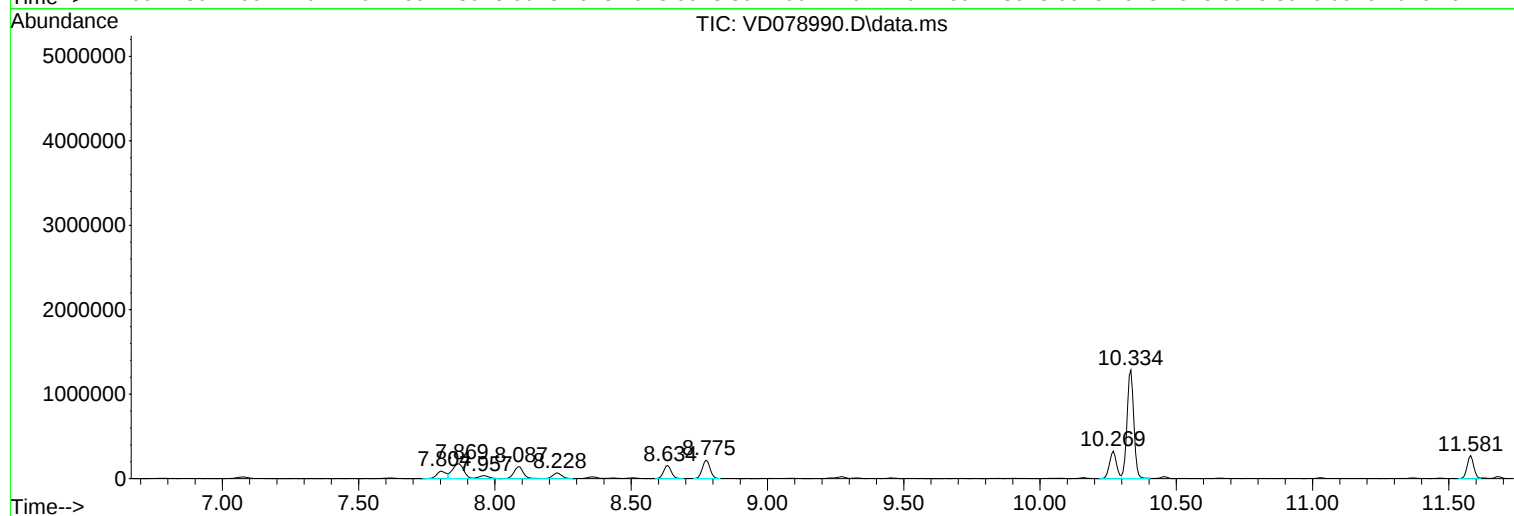
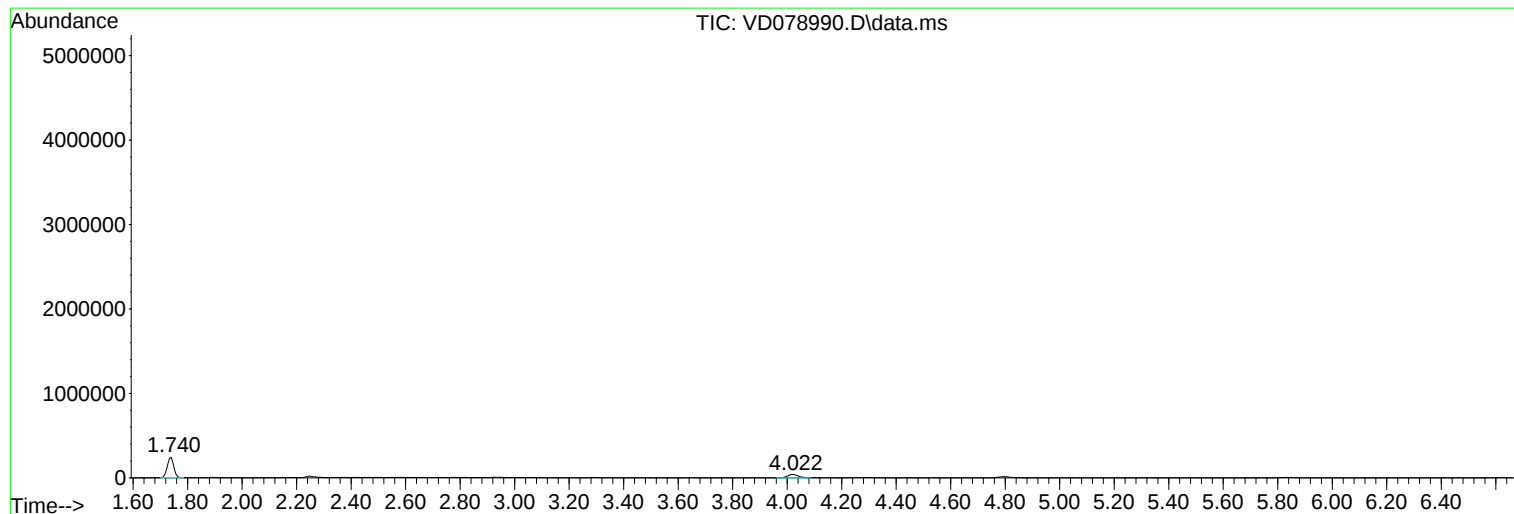
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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



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Misc : 5.06G/5ml/MSVOA_D/SOIL/B
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Instrument :
MSVOA_D
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510-C

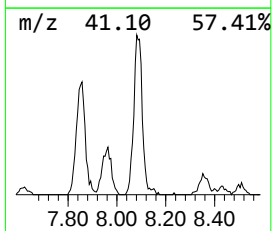
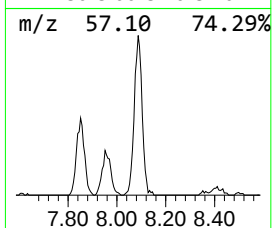
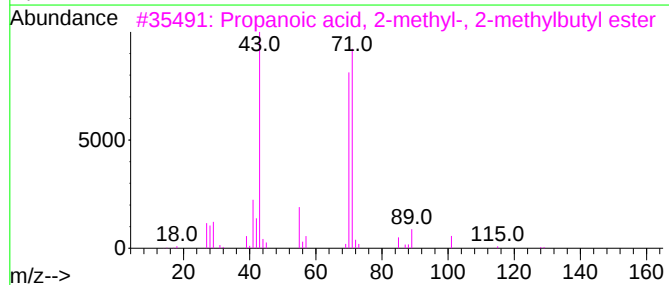
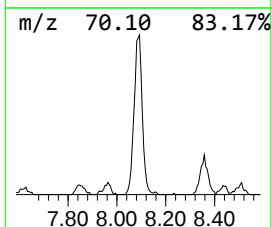
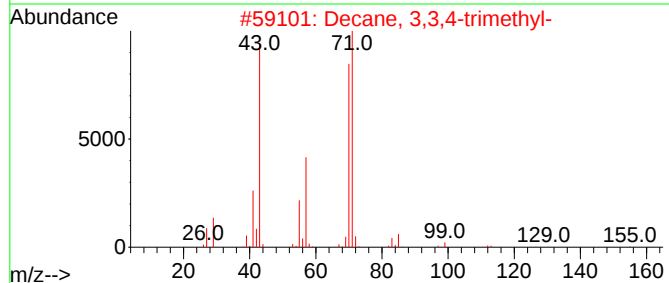
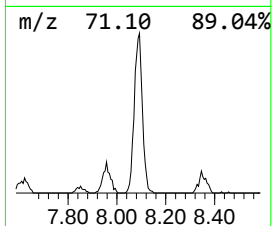
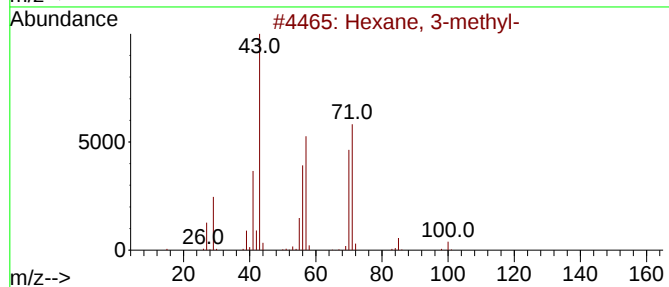
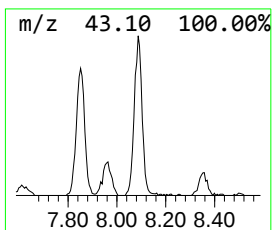
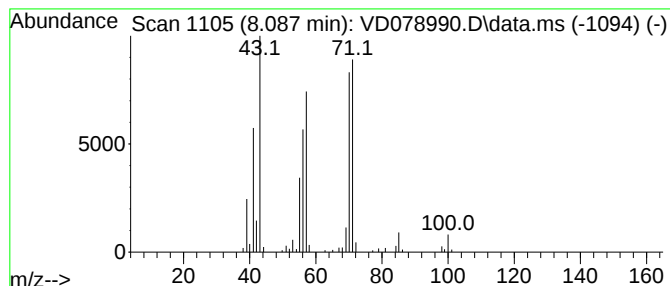
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	33.47 ug/l	334211	Pentafluorobenzene	7.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
3			Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	59



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Instrument :
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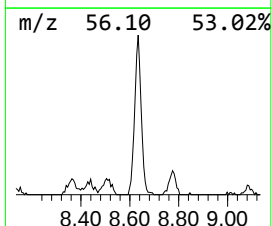
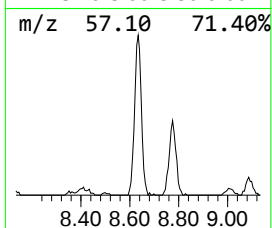
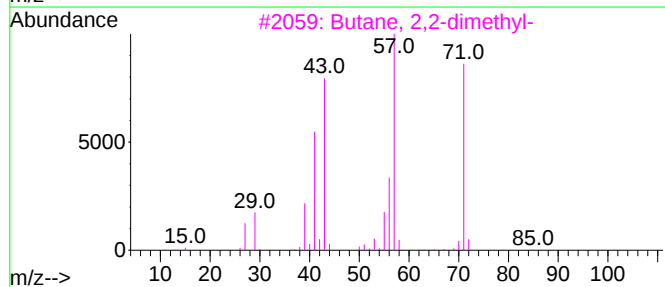
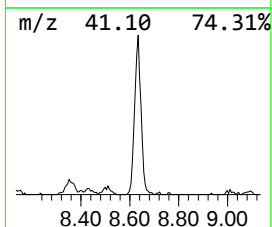
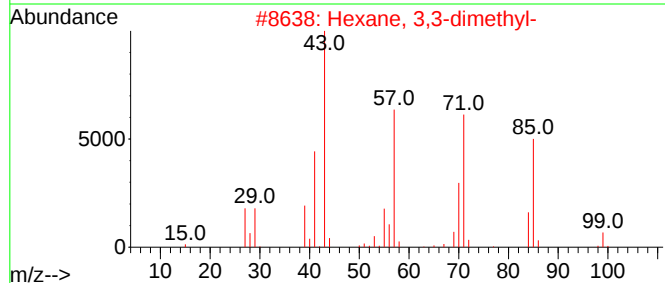
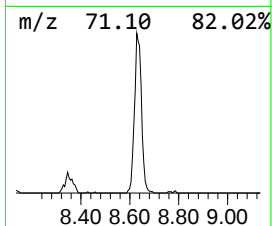
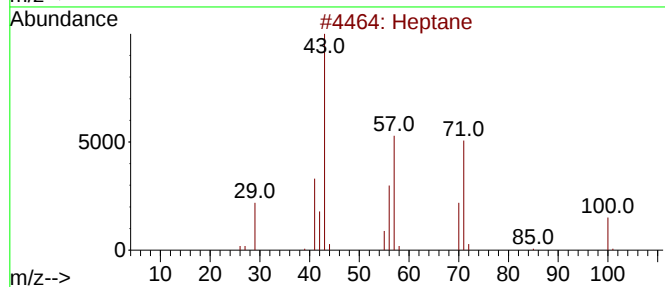
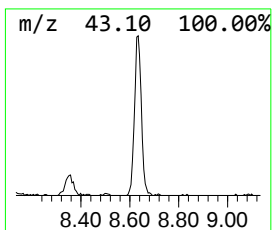
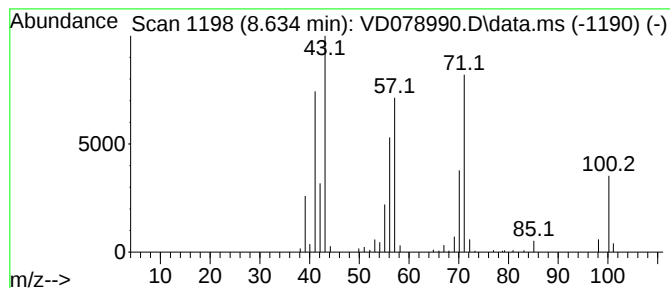
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.634	35.00 ug/l	304019	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	80
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
4			Oxirane, butyl-	100	C6H12O	001436-34-6	43
5			3-Hexanone	100	C6H12O	000589-38-8	38



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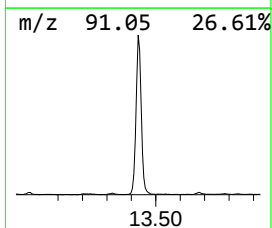
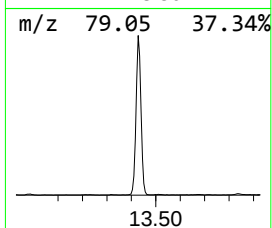
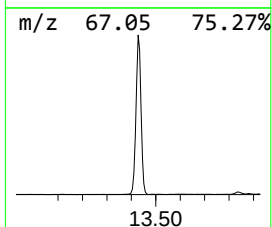
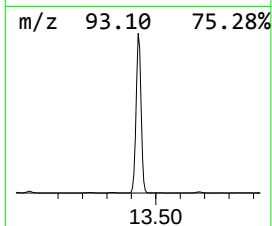
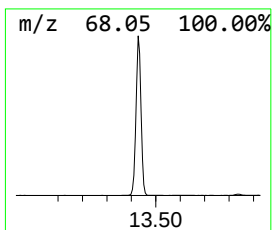
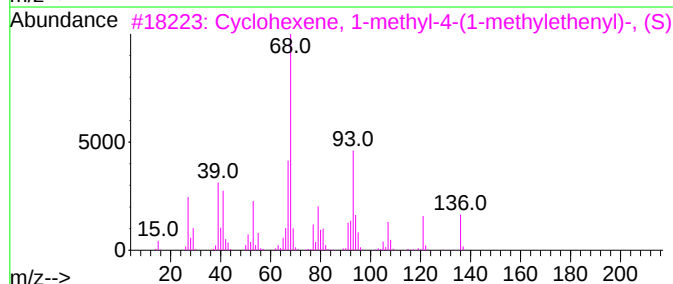
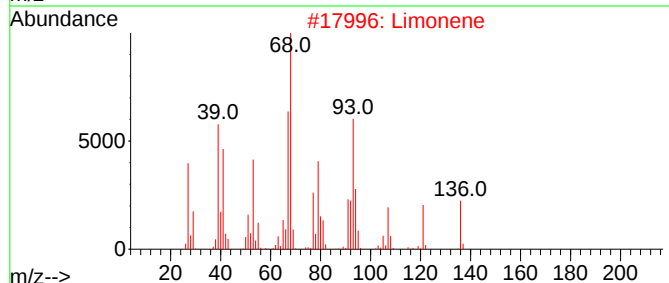
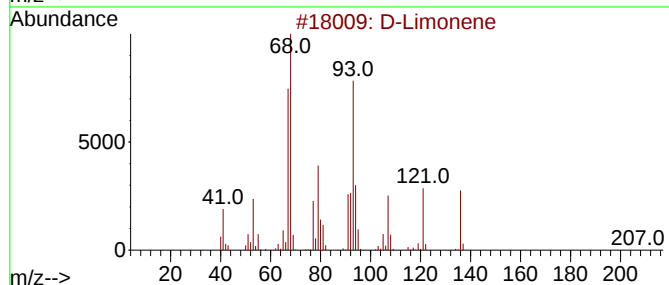
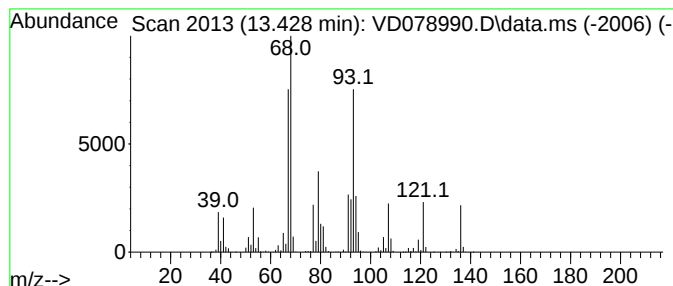
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 4 D-Limonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.428	816.54 ug/l	7583890	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	99
2			Limonene	136	C10H16	000138-86-3	94
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	76
4			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	62
5			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	53



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ClientSampleId :
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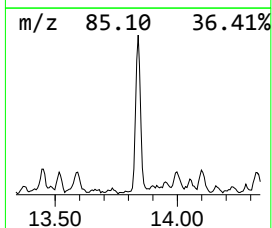
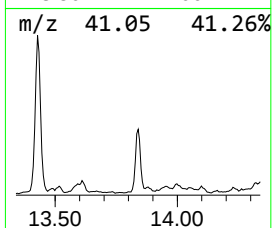
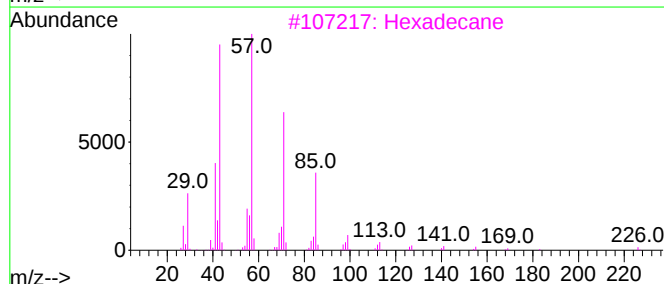
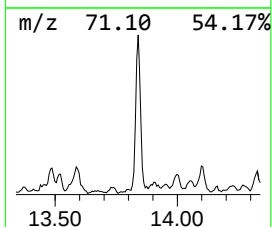
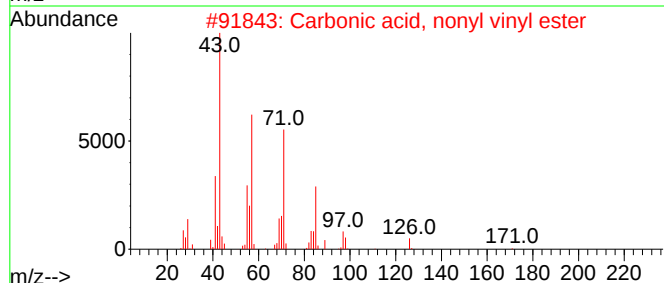
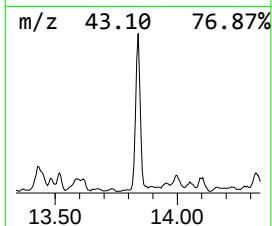
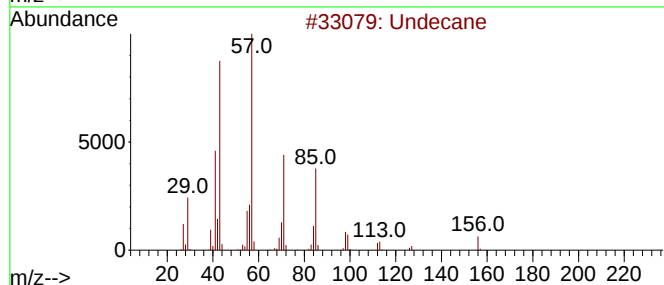
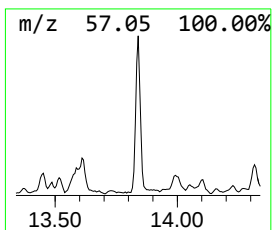
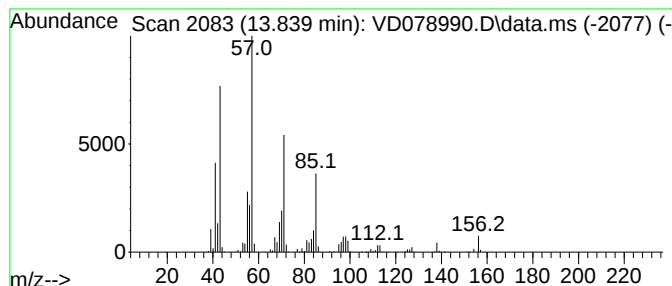
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 5 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	103.58 ug/l	962050	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	93
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64
3			Hexadecane	226	C16H34	000544-76-3	59
4			1-Decene, 4-methyl-	154	C11H22	013151-29-6	53
5			Allyl n-octyl ether	170	C11H22O	003295-97-4	47



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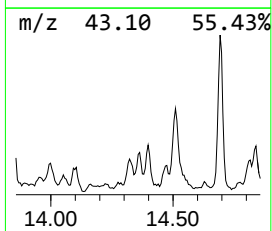
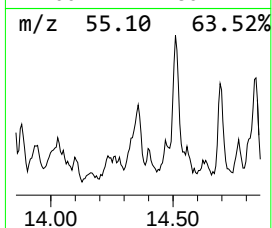
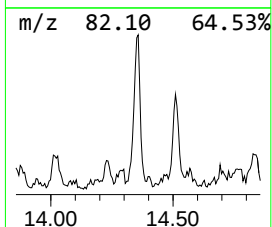
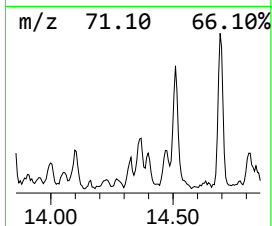
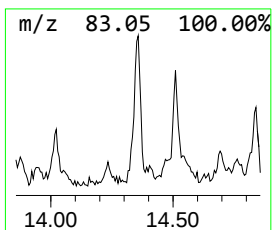
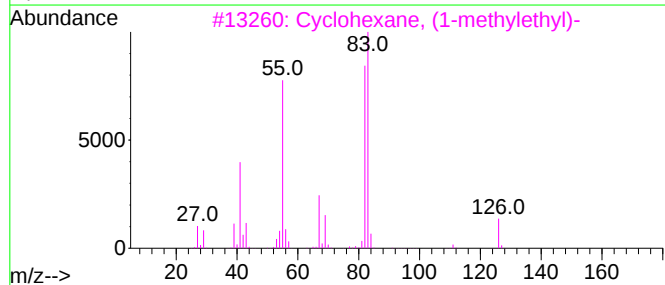
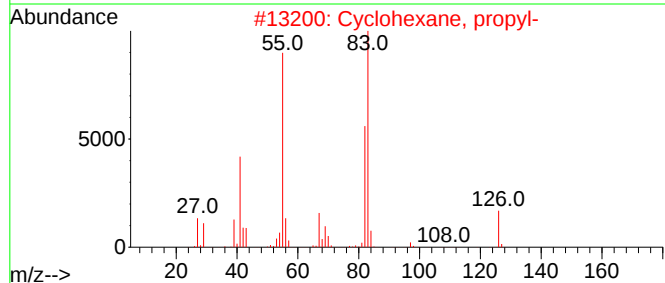
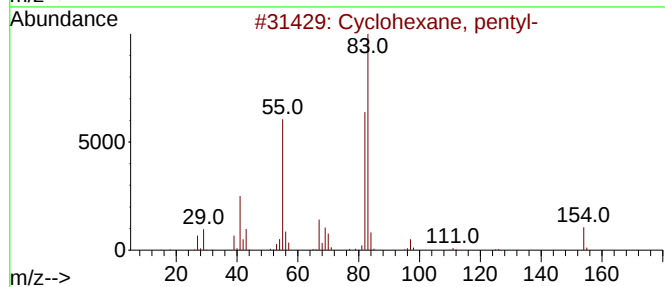
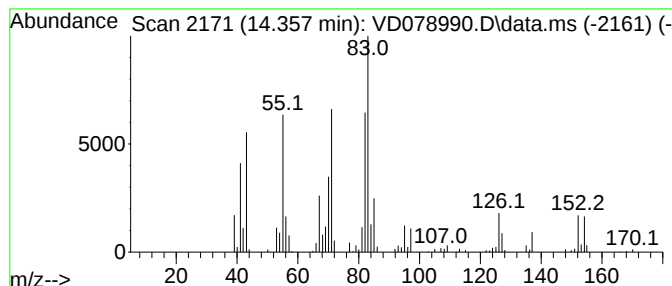
Instrument :
MSVOA_D
ClientSampleId :
510-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown14.357 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.357	41.85 ug/l	388722	1,4-Dichlorobenzene-d4			13.516
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-		154	C11H22	004292-92-6	49
2	Cyclohexane, propyl-		126	C9H18	001678-92-8	46
3	Cyclohexane, (1-methylethyl)-		126	C9H18	000696-29-7	46
4	Cyclohexane, hexyl-		168	C12H24	004292-75-5	38
5	Cyclohexane, octyl-		196	C14H28	001795-15-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
Data File : VD078990.D
Acq On : 22 May 2024 20:12
Operator : RP/MD
Sample : P2511-01
Misc : 5.06G/5ml/MSVOA_D/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

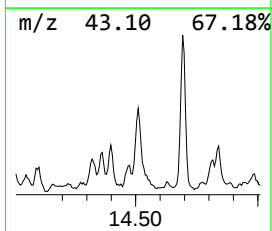
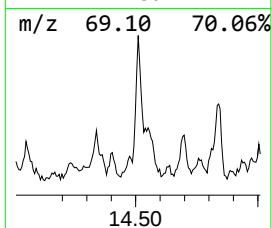
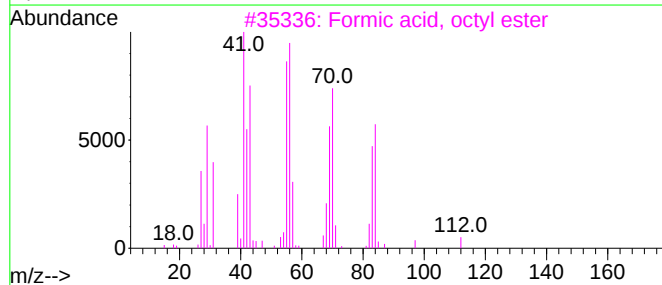
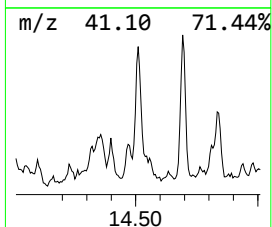
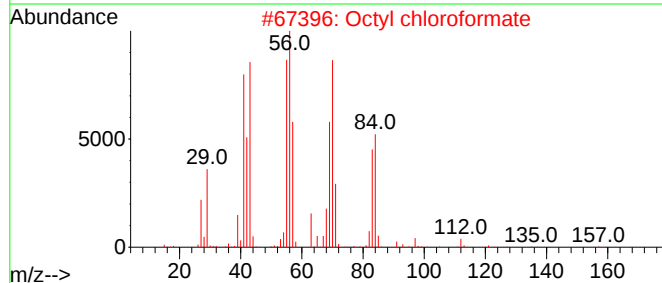
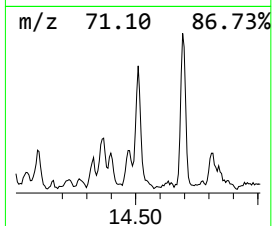
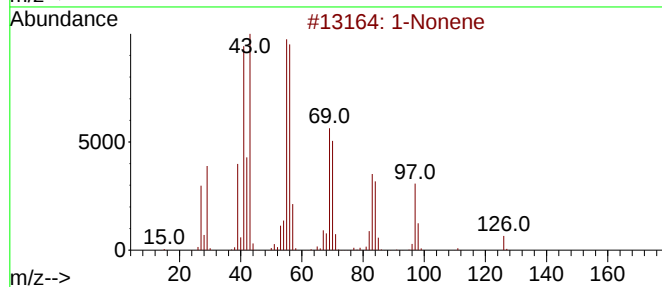
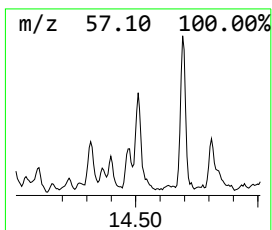
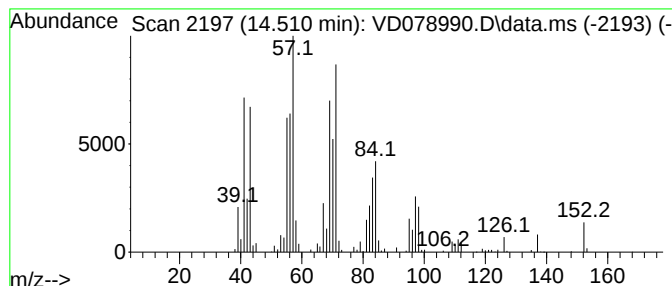
Instrument :
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ClientSampleId :
510-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 7 1-Nonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.510	48.79 ug/l	453165	1,4-Dichlorobenzene-d4			13.516
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Nonene		126	C9H18	000124-11-8	50
2	Octyl chloroformate		192	C9H17ClO2	007452-59-7	43
3	Formic acid, octyl ester		158	C9H18O2	000112-32-3	38
4	1-Undecanol		172	C11H24O	000112-42-5	35
5	1-Heptanol, 4-methyl-		130	C8H18O	000817-91-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
Data File : VD078990.D
Acq On : 22 May 2024 20:12
Operator : RP/MD
Sample : P2511-01
Misc : 5.06G/5ml/MSVOA_D/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
510-C

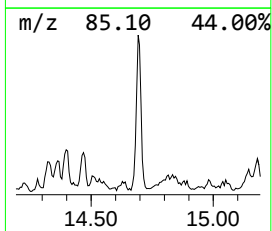
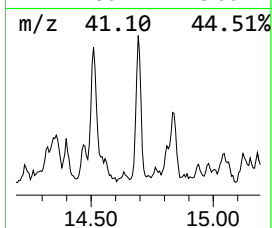
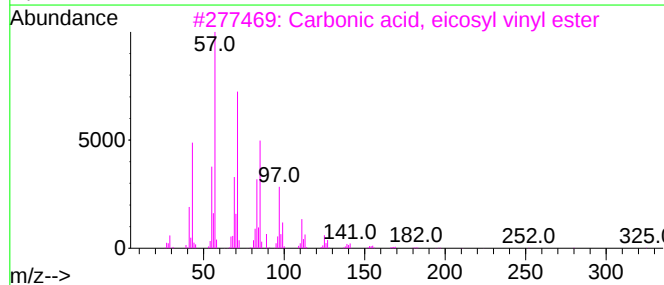
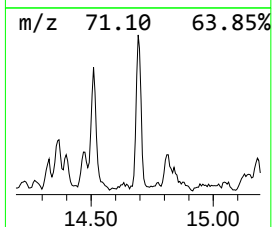
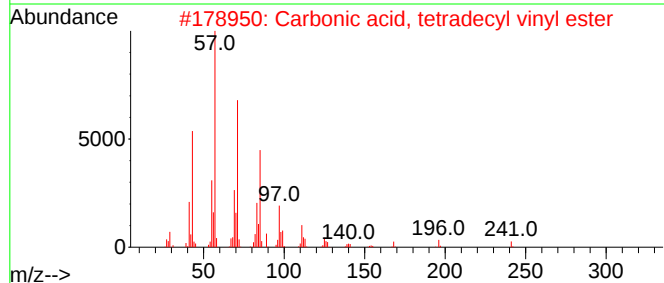
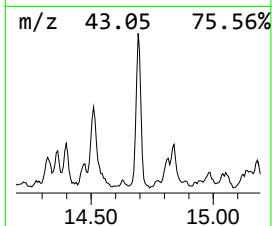
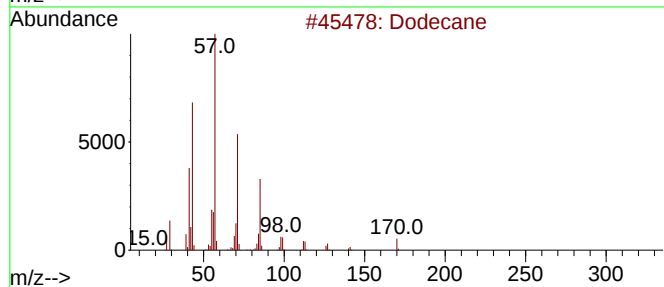
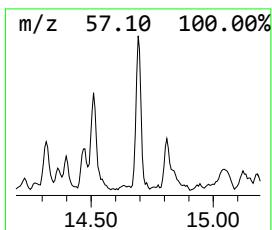
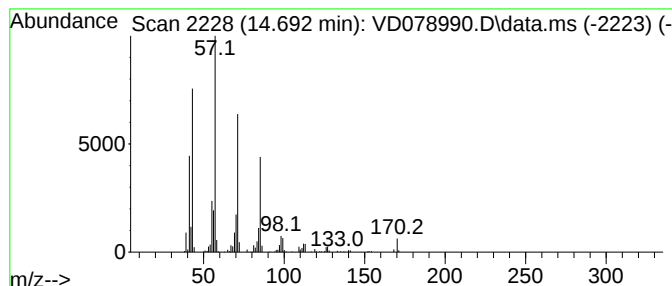
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	55.55 ug/l	515905	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	83
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	78
4			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	64
5			Tridecane	184	C13H28	000629-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
Data File : VD078990.D
Acq On : 22 May 2024 20:12
Operator : RP/MD
Sample : P2511-01
Misc : 5.06G/5ml/MSVOA_D/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
510-C

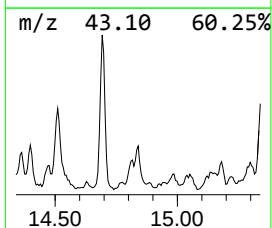
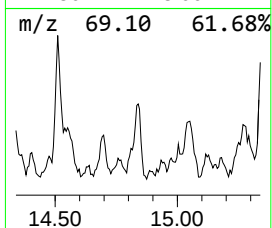
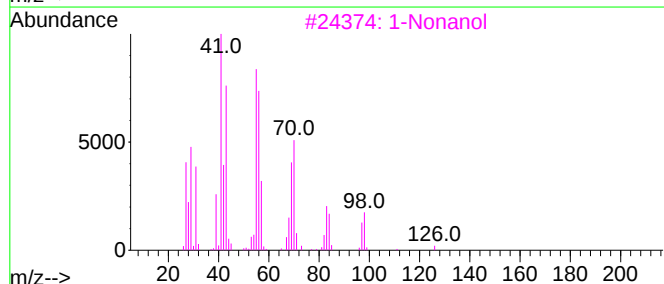
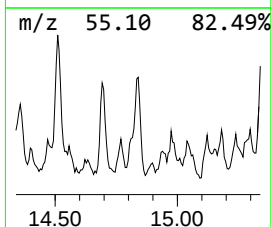
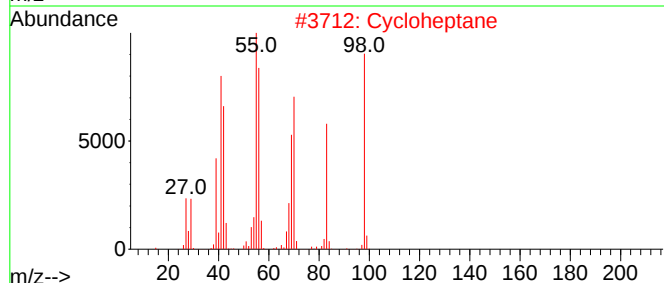
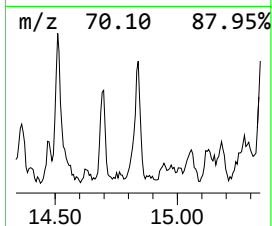
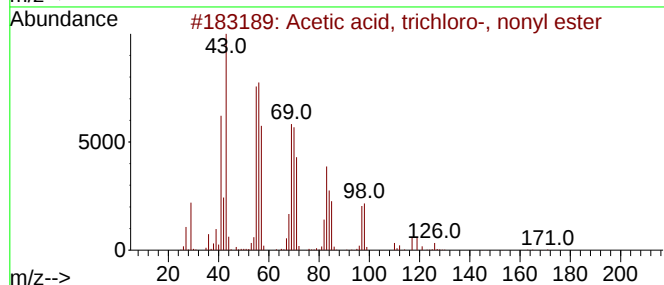
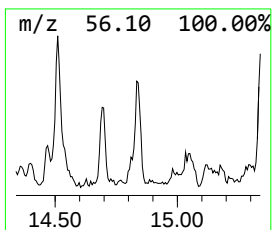
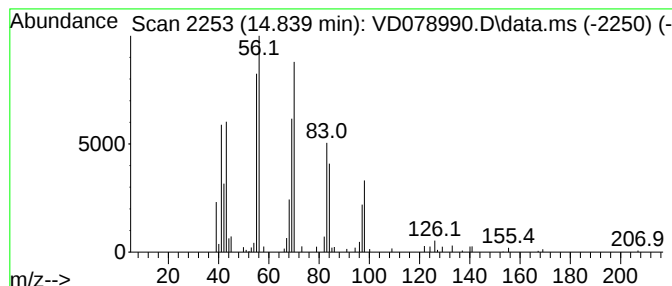
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Quant Title : SW846 8260

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

Peak Number 9 Acetic acid, trichloro-, no... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	26.82 ug/l	249071	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	83
2			Cycloheptane	98	C7H14	000291-64-5	81
3			1-Nonanol	144	C9H20O	000143-08-8	72
4			Chloroacetic acid, nonyl ester	220	C11H21ClO2	005451-96-7	72
5			1-Decene	140	C10H20	000872-05-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
Data File : VD078990.D
Acq On : 22 May 2024 20:12
Operator : RP/MD
Sample : P2511-01
Misc : 5.06G/5ml/MSVOA_D/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

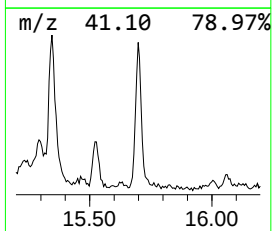
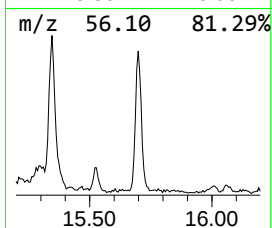
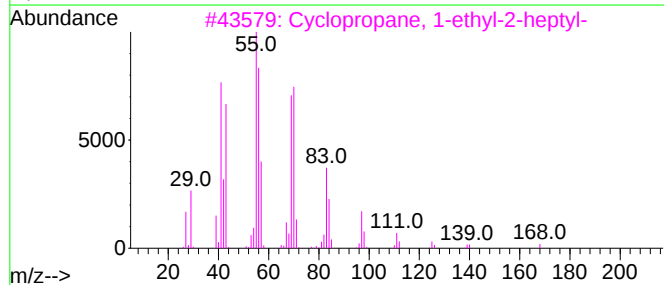
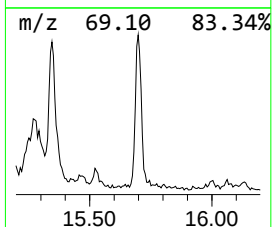
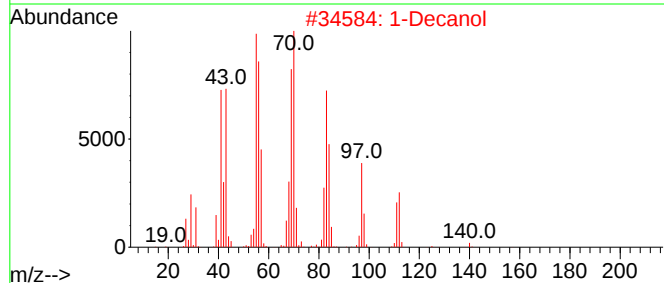
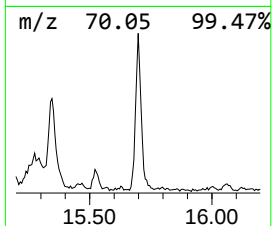
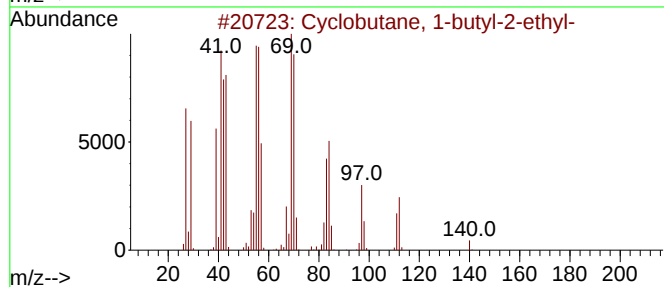
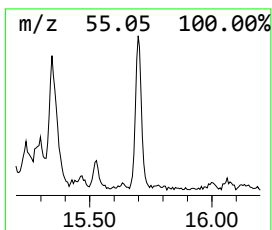
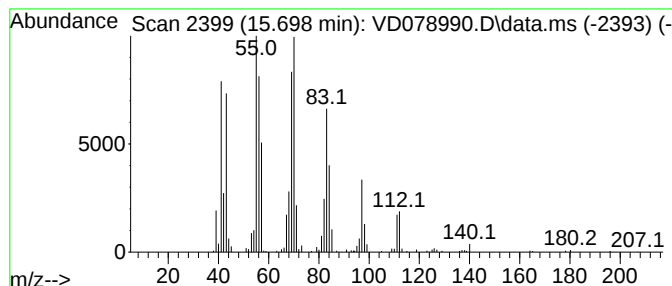
Instrument :
MSVOA_D
ClientSampleId :
510-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclobutane, 1-butyl-2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.698	57.28 ug/l	532038	1,4-Dichlorobenzene-d4			13.516
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclobutane, 1-butyl-2-ethyl-		140	C10H20	1010150-67-3	95
2	1-Decanol		158	C10H22O	000112-30-1	91
3	Cyclopropane, 1-ethyl-2-heptyl-		168	C12H24	074663-86-8	90
4	1-Undecene		154	C11H22	000821-95-4	90
5	Cyclooctane		112	C8H16	000292-64-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052224\
Data File : VD078990.D
Acq On : 22 May 2024 20:12
Operator : RP/MD
Sample : P2511-01
Misc : 5.06G/5ml/MSVOA_D/SOIL/B
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
510-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051324S.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
Hexane, 3-methyl-	8.087	33.5	ug/l	334211	1	7.869	499266	50.0
Heptane	8.634	35.0	ug/l	304019	2	8.775	434299	50.0
D-Limonene	13.428	816.5	ug/l	7583890	4	13.516	464392	50.0
Undecane	13.839	103.6	ug/l	962050	4	13.516	464392	50.0
unknown14.357	14.357	41.9	ug/l	388722	4	13.516	464392	50.0
1-Nonene	14.510	48.8	ug/l	453165	4	13.516	464392	50.0
Dodecane	14.692	55.5	ug/l	515905	4	13.516	464392	50.0
Acetic acid, tr...	14.839	26.8	ug/l	249071	4	13.516	464392	50.0
Cyclobutane, 1-...	15.698	57.3	ug/l	532038	4	13.516	464392	50.0