

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
 Data File : VD079303.D
 Acq On : 01 Jul 2024 18:30
 Operator : RP/MD
 Sample : P3141-01
 Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 B-140-SB00

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\82D062824S.M
 Title : SW846 8260

Signal : TIC: VD079303.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	41	rVB	579832	940541	58.84%	5.796%
2	4.805	535	547	559	rVB3	40588	124417	7.78%	0.767%
3	5.840	711	723	732	rBV5	11035	34623	2.17%	0.213%
4	7.810	1047	1058	1063	rBV3	90345	226353	14.16%	1.395%
5	7.875	1063	1069	1081	rVB2	141606	308245	19.28%	1.899%
6	8.234	1120	1130	1139	rBV2	70934	170223	10.65%	1.049%
7	8.775	1213	1222	1235	rBV	216701	435511	27.25%	2.684%
8	10.269	1468	1476	1483	rBV	273817	495983	31.03%	3.056%
9	11.057	1604	1610	1614	rBV4	10383	18531	1.16%	0.114%
10	11.122	1618	1621	1626	rVB3	10291	16071	1.01%	0.099%
11	11.375	1654	1664	1674	rVB5	34030	101920	6.38%	0.628%
12	11.469	1674	1680	1690	rVB2	27264	48094	3.01%	0.296%
13	11.581	1690	1699	1707	rBV	269727	483307	30.24%	2.978%
14	11.716	1718	1722	1725	rVB4	13594	17056	1.07%	0.105%
15	11.798	1725	1736	1745	rVV5	145413	385570	24.12%	2.376%
16	11.869	1745	1748	1754	rVB2	26487	41638	2.60%	0.257%
17	12.022	1766	1774	1778	rVB4	19645	35216	2.20%	0.217%
18	12.093	1779	1786	1798	rBV6	84014	263031	16.46%	1.621%
19	12.210	1801	1806	1810	rVV	49912	75891	4.75%	0.468%
20	12.263	1810	1815	1816	rVV3	21186	32318	2.02%	0.199%
21	12.287	1816	1819	1822	rVV5	38293	63979	4.00%	0.394%
22	12.340	1823	1828	1837	rVV4	79939	192890	12.07%	1.189%
23	12.410	1837	1840	1843	rVV4	24792	38948	2.44%	0.240%
24	12.469	1843	1850	1851	rVV4	47959	88535	5.54%	0.546%
25	12.504	1852	1856	1858	rVV	78939	143373	8.97%	0.883%
26	12.528	1858	1860	1863	rVV	88712	108236	6.77%	0.667%
27	12.569	1863	1867	1871	rVV2	186539	305527	19.11%	1.883%
28	12.610	1871	1874	1879	rVV2	78897	126969	7.94%	0.782%
29	12.657	1879	1882	1886	rVB5	17716	28458	1.78%	0.175%
30	12.734	1892	1895	1903	rVB7	37367	76530	4.79%	0.472%
31	12.816	1903	1909	1913	rBV3	32833	66468	4.16%	0.410%
32	12.892	1913	1922	1928	rVV2	435340	741720	46.40%	4.571%
33	12.951	1928	1932	1937	rVV3	60475	100621	6.30%	0.620%
34	13.004	1937	1941	1943	rVV4	18702	27655	1.73%	0.170%
35	13.040	1943	1947	1951	rVV5	38769	62630	3.92%	0.386%
36	13.098	1951	1957	1959	rVV5	40074	87937	5.50%	0.542%

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 ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062824S.M
 Title : SW846 8260

37	13.128	1959	1962	1969	rVV5	72301	122685	7.68%	0.756%
38	13.187	1970	1972	1979	rVB8	13535	23835	1.49%	0.147%
39	13.257	1980	1984	1987	rBV4	23038	33109	2.07%	0.204%
40	13.339	1994	1998	2001	rVB3	18611	24877	1.56%	0.153%
41	13.410	2001	2010	2014	rBV4	74348	189751	11.87%	1.169%
42	13.451	2014	2017	2020	rVV3	65730	93272	5.84%	0.575%
43	13.516	2020	2028	2036	rVB2	240569	432460	27.06%	2.665%
44	13.587	2036	2040	2046	rBV4	45808	70036	4.38%	0.432%
45	13.787	2068	2074	2077	rBV	24528	45275	2.83%	0.279%
46	13.839	2077	2083	2088	rVV	338363	507460	31.75%	3.127%
47	13.881	2088	2090	2094	rVB4	25760	29646	1.85%	0.183%
48	13.939	2094	2100	2105	rBV5	24982	52322	3.27%	0.322%
49	13.998	2105	2110	2111	rBV3	18985	25446	1.59%	0.157%
50	14.104	2124	2128	2133	rVB5	30057	49631	3.10%	0.306%
51	14.157	2133	2137	2141	rBV5	17724	29000	1.81%	0.179%
52	14.228	2142	2149	2153	rBV9	34732	67089	4.20%	0.413%
53	14.287	2155	2159	2161	rVV3	37557	54987	3.44%	0.339%
54	14.351	2161	2170	2175	rVV8	121677	355011	22.21%	2.188%
55	14.398	2175	2178	2186	rVV3	71886	104911	6.56%	0.646%
56	14.469	2186	2190	2193	rVV	59808	89314	5.59%	0.550%
57	14.504	2193	2196	2201	rVV6	51002	80568	5.04%	0.496%
58	14.563	2202	2206	2212	rVB7	37115	71454	4.47%	0.440%
59	14.692	2223	2228	2236	rBV	570963	831928	52.05%	5.126%
60	14.769	2236	2241	2244	rVV4	68696	124852	7.81%	0.769%
61	14.810	2244	2248	2256	rVV	189407	337605	21.12%	2.080%
62	14.886	2256	2261	2265	rVV5	52464	89726	5.61%	0.553%
63	14.945	2265	2271	2279	rVV9	59870	174541	10.92%	1.076%
64	15.028	2282	2285	2290	rVB4	43899	71475	4.47%	0.440%
65	15.128	2292	2302	2307	rBV6	121590	342727	21.44%	2.112%
66	15.181	2307	2311	2314	rVV2	115664	196138	12.27%	1.209%
67	15.222	2314	2318	2325	rVV3	203297	384593	24.06%	2.370%
68	15.298	2325	2331	2337	rVB2	303636	517151	32.35%	3.187%
69	15.369	2337	2343	2349	rBV6	55964	132147	8.27%	0.814%
70	15.522	2364	2369	2377	rVB	1066168	1598426	100.00%	9.850%
71	15.639	2385	2389	2393	rVB5	59587	94713	5.93%	0.584%
72	15.975	2441	2446	2449	rBV3	70552	135039	8.45%	0.832%
73	16.057	2456	2460	2464	rBV2	76542	136863	8.56%	0.843%
74	16.104	2464	2468	2477	rVV5	113830	300226	18.78%	1.850%
75	16.186	2477	2482	2487	rVV3	113852	227027	14.20%	1.399%
76	16.251	2488	2493	2502	rVB2	135955	260017	16.27%	1.602%

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Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

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

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Title : SW846 8260

77	16.463	2522	2529	2542	rVV	508746	989986	61.94%	6.100%
78	16.569	2542	2547	2553	rVV5	44913	117332	7.34%	0.723%
79	16.633	2553	2558	2563	rVB8	43488	98458	6.16%	0.607%

Sum of corrected areas: 16228124

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

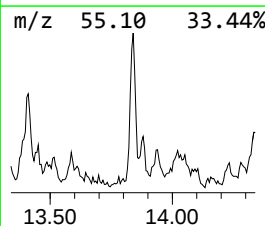
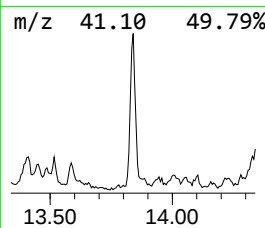
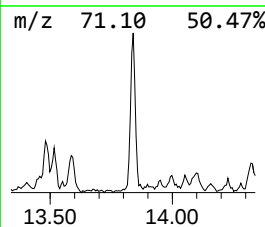
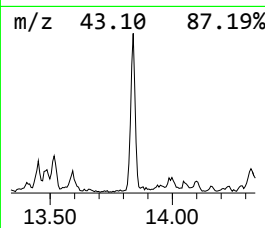
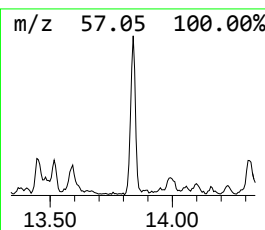
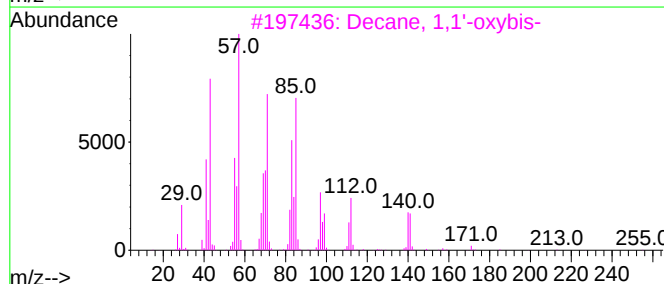
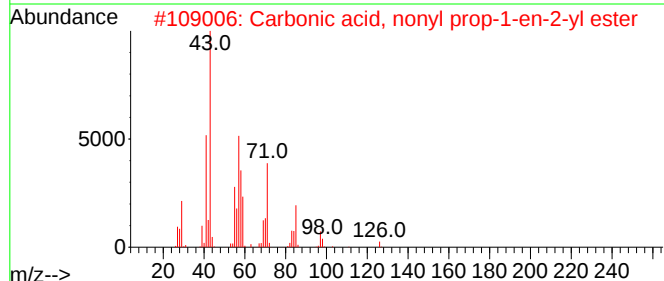
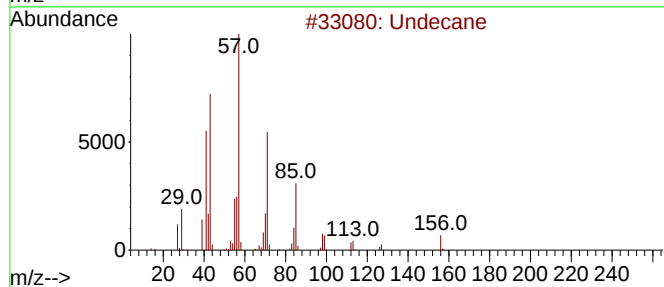
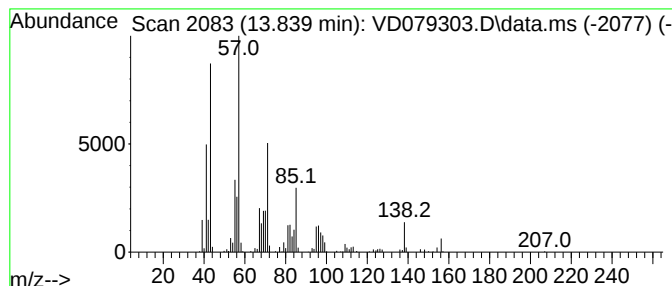
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062824S.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	58.67 ug/l	507460	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	60
2	Carbonic acid, nonyl prop-1-en-2...			228	C13H24O3	1000382-53-9	52
3	Decane, 1,1'-oxybis-			298	C20H42O	002456-28-2	50
4	Carbonic acid, nonyl vinyl ester			214	C12H22O3	1000383-25-6	50
5	1-Iodo-2-methylundecane			296	C12H25I	073105-67-6	43



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

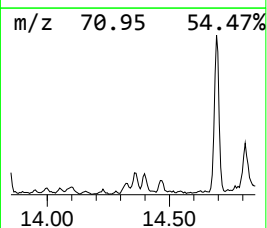
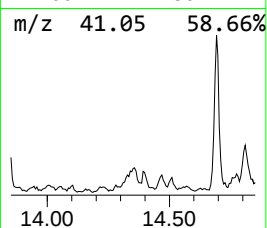
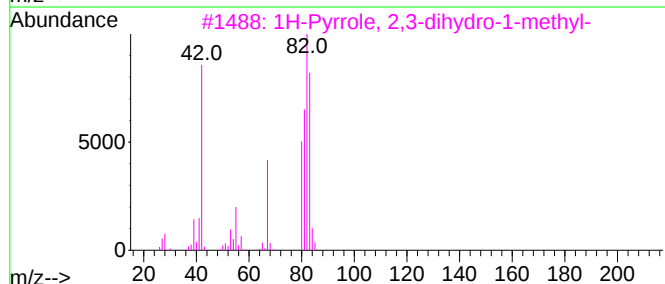
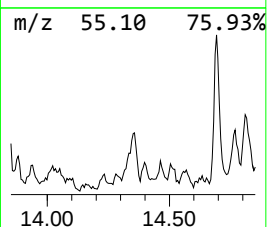
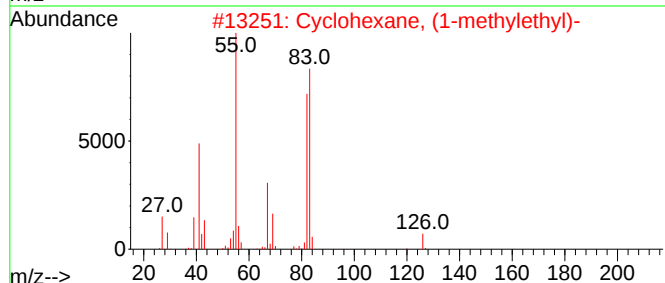
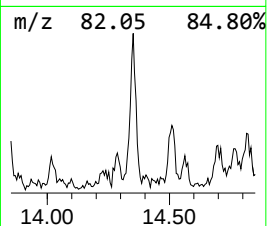
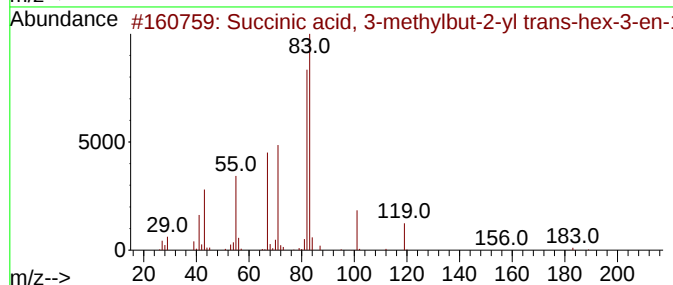
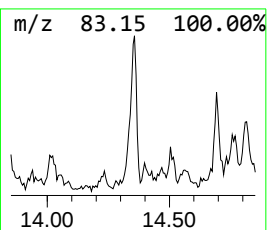
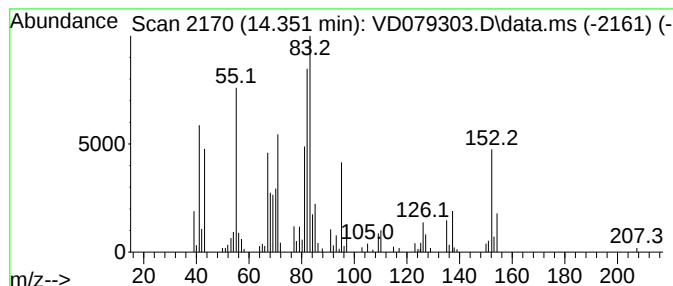
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062824S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.351 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	41.05 ug/l	355011	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 3-methylbut-2-yl ...	270	C15H26O4	1000391-11-1	47
2			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	45
3			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	43
4			Cyclohexane, pentyl-	154	C11H22	004292-92-6	38
5			Cyclohexane, butyl-	140	C10H20	001678-93-9	35



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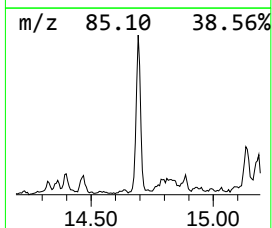
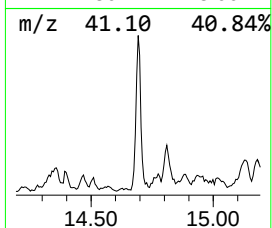
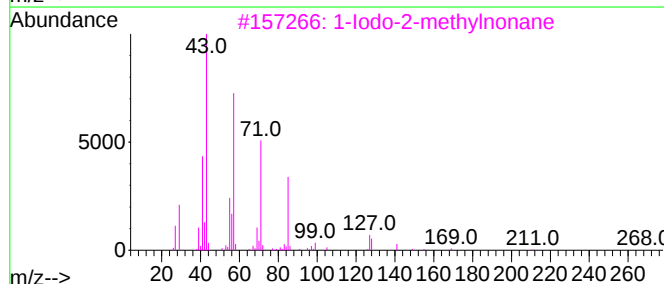
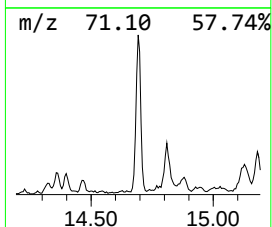
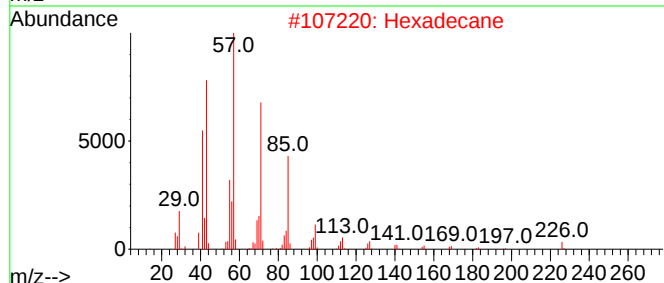
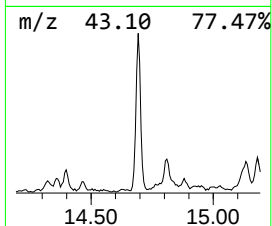
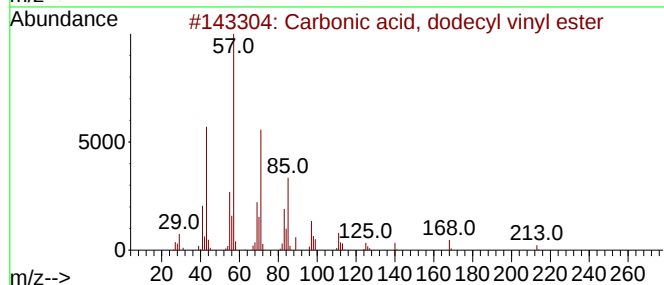
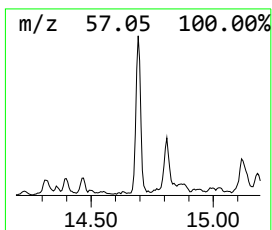
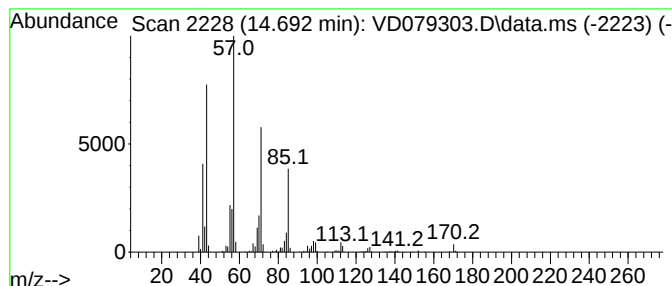
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062824S.M
Quant Title : SW846 8260

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

Peak Number 4 Carbonic acid, dodecyl vinyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	96.19 ug/l	831928	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	78
2			Hexadecane	226	C16H34	000544-76-3	78
3			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	72
4			Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
5			Tridecane, 2-methyl-	198	C14H30	001560-96-9	64



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Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

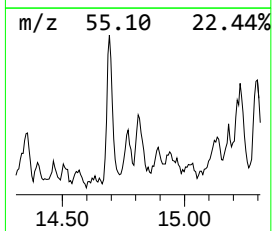
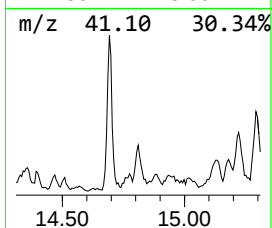
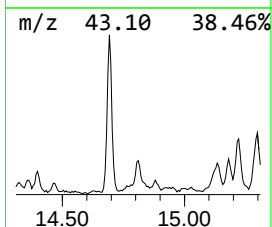
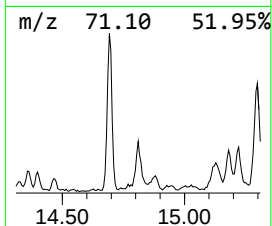
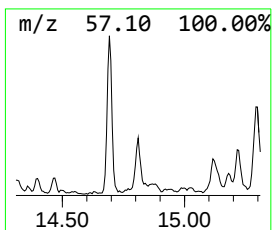
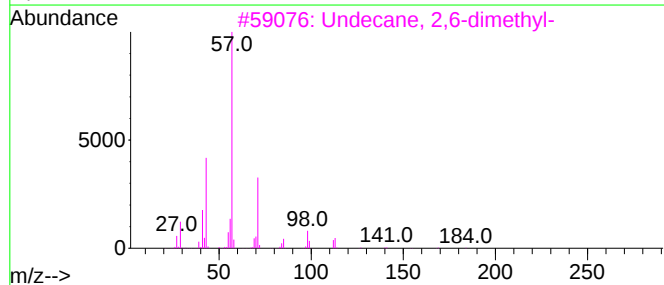
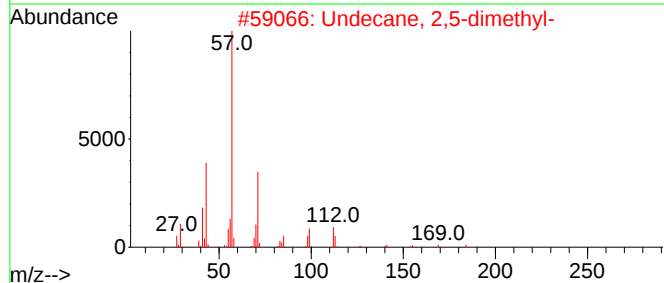
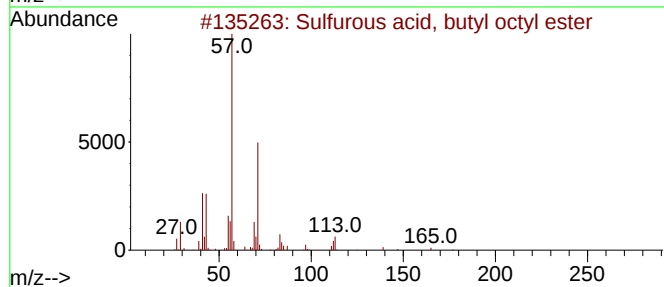
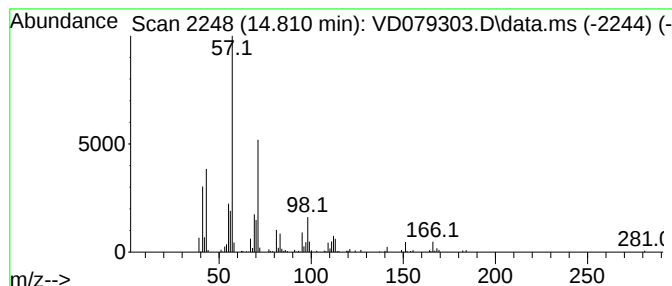
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Quant Title : SW846 8260

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

Peak Number 5 Sulfurous acid, butyl octyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	39.03 ug/l	337605	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	53
2			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	53
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	47
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

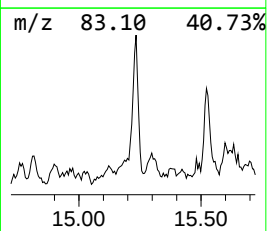
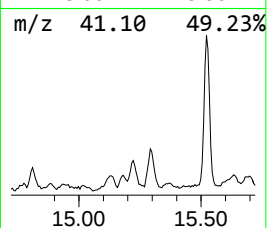
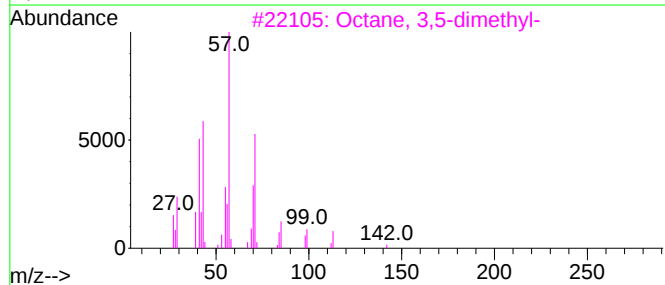
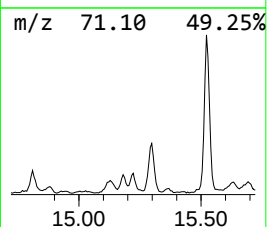
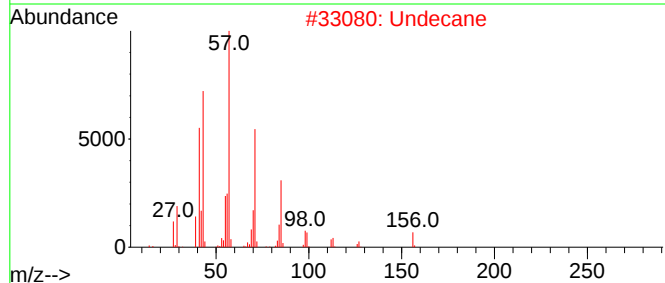
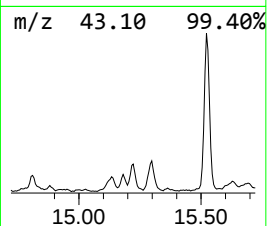
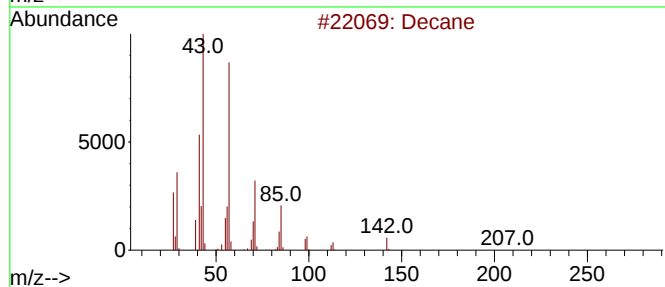
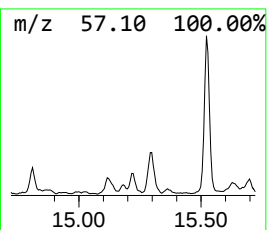
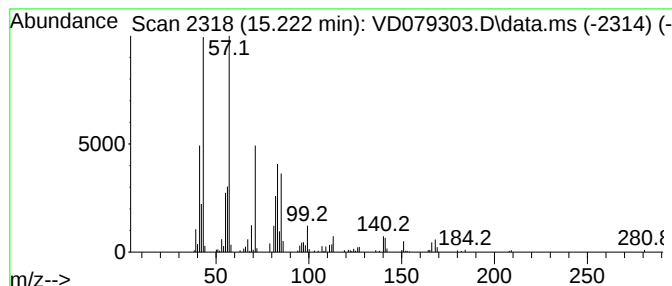
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Quant Title : SW846 8260

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

Peak Number 6 Decane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.222	44.47 ug/l	384593	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	58
2			Undecane	156	C11H24	001120-21-4	53
3			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	49
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

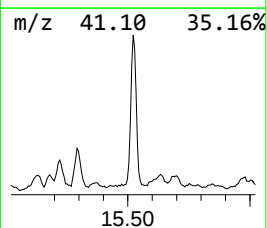
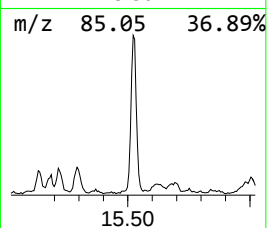
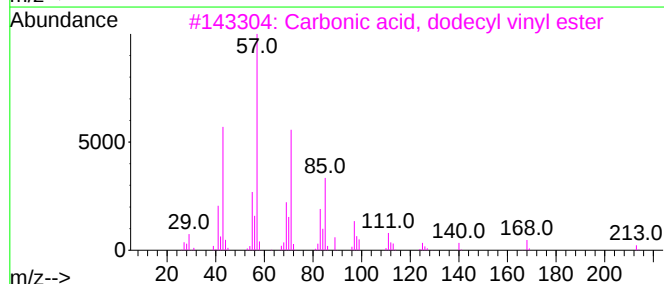
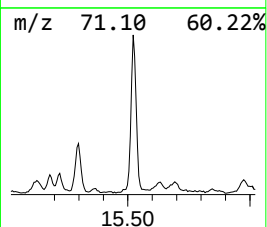
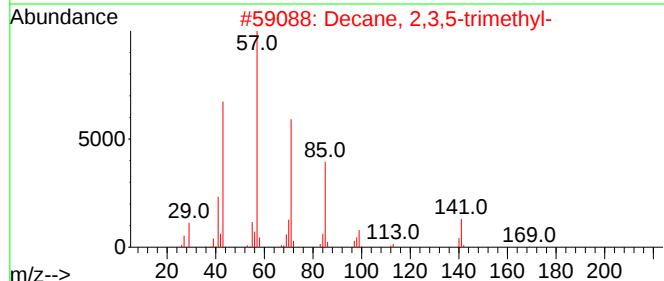
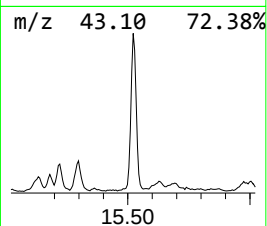
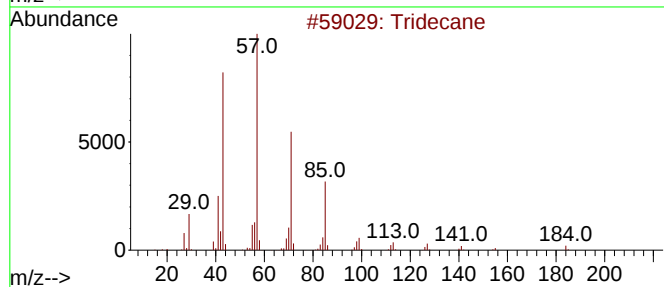
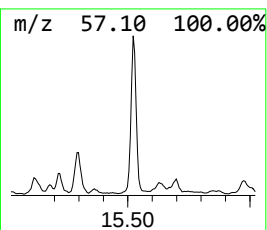
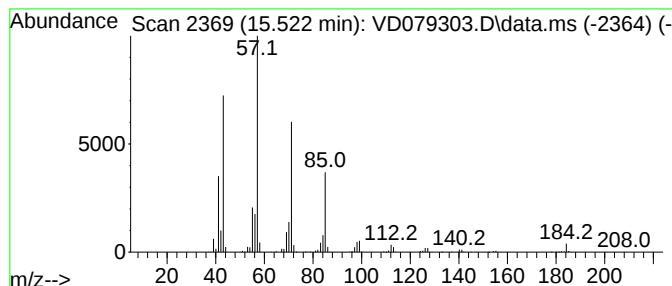
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.522	184.81 ug/l	1598430	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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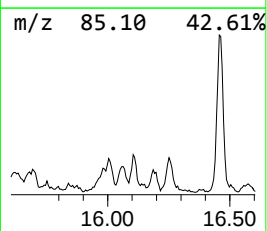
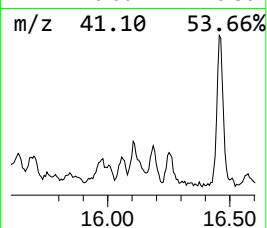
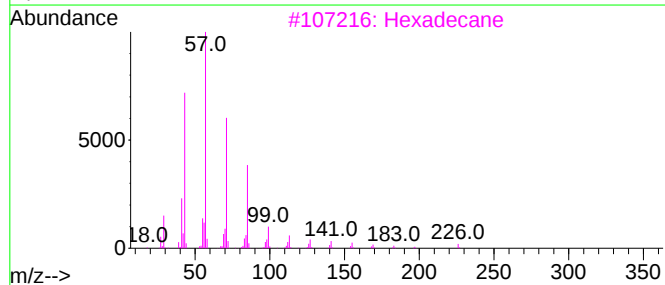
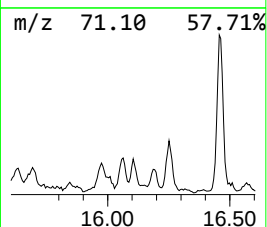
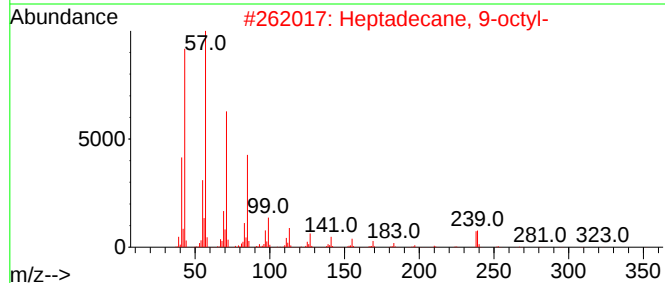
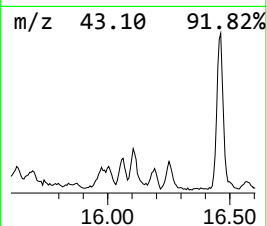
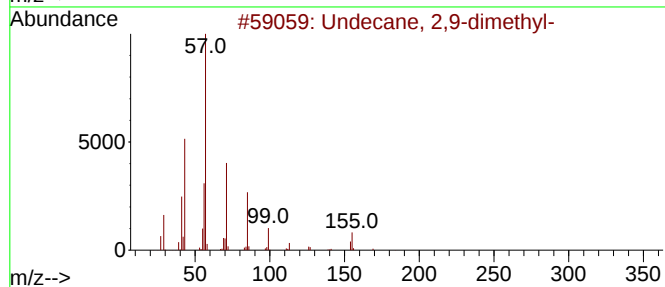
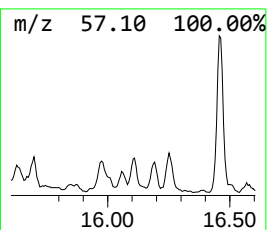
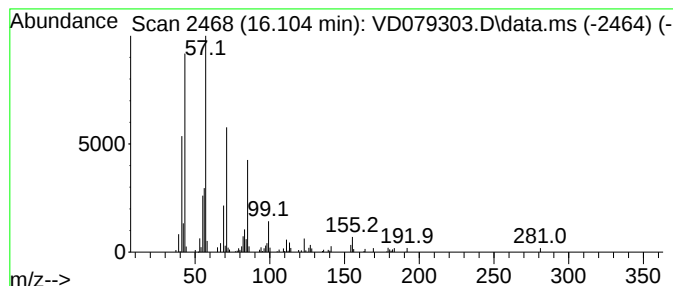
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Quant Title : SW846 8260

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

Peak Number 8 Undecane, 2,9-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	34.71 ug/l	300226	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	86
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
3			Hexadecane	226	C16H34	000544-76-3	72
4			Heptadecane	240	C17H36	000629-78-7	72
5			Undecane, 3-methyl-	170	C12H26	001002-43-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

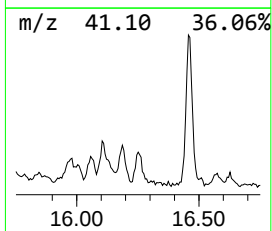
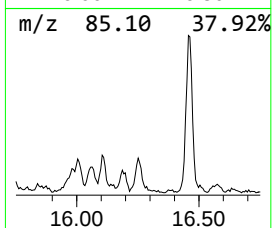
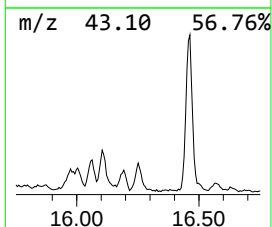
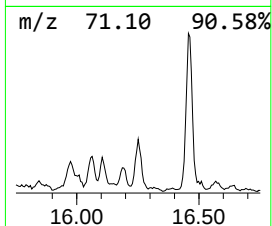
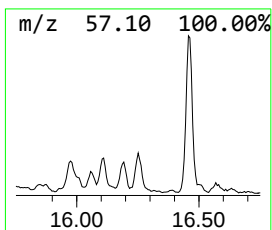
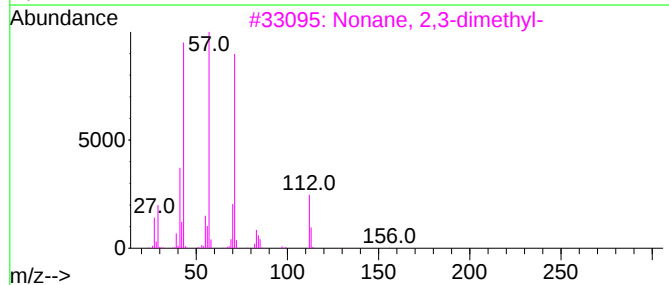
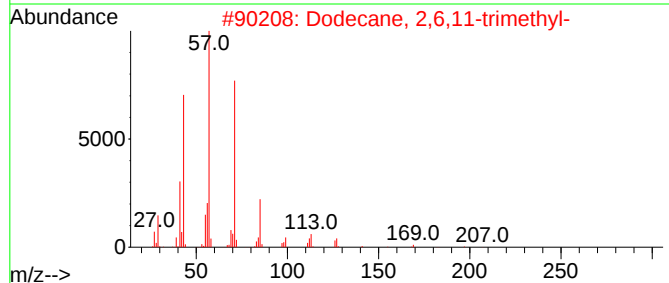
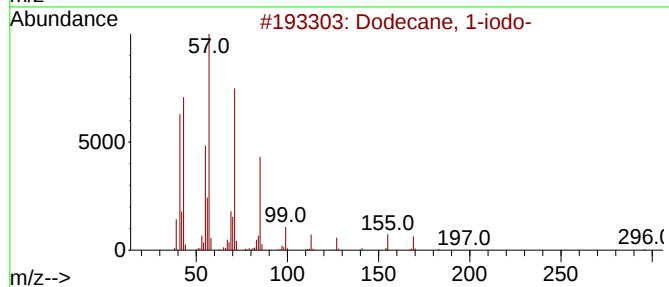
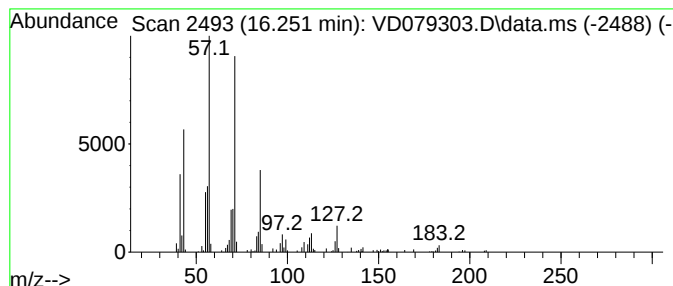
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.251	30.06 ug/l	260017	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
3			Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	59
4			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	59
5			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

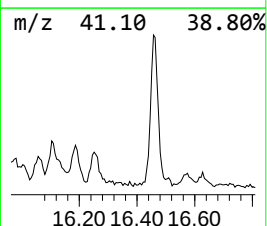
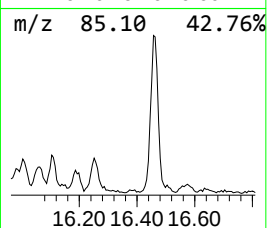
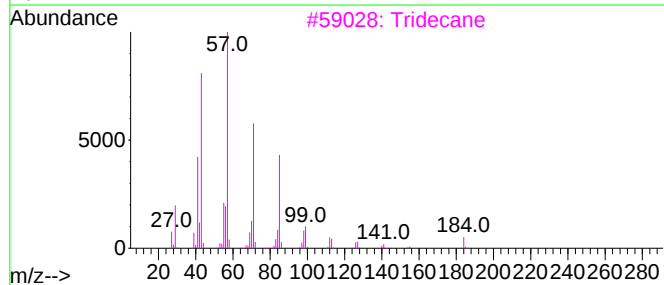
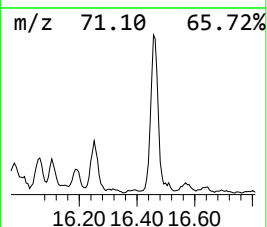
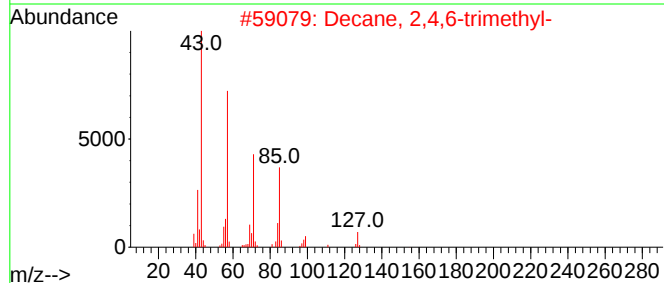
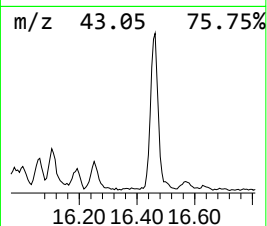
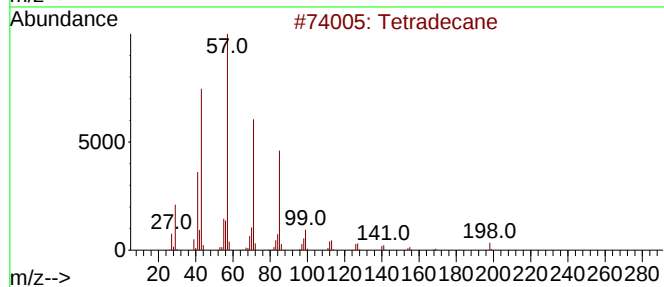
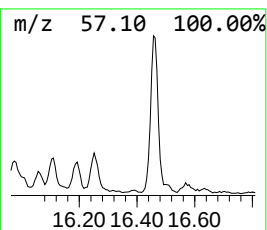
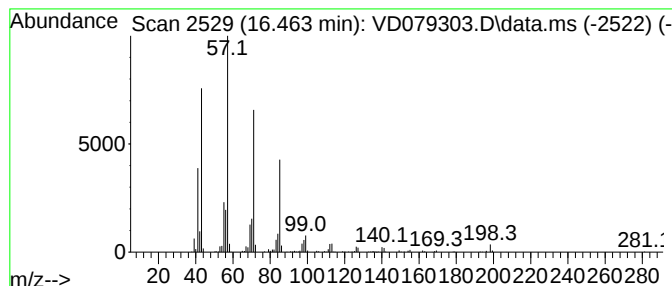
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.463	114.46 ug/l	989986	1,4-Dichlorobenzene-d4	13.516

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	93
2		Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	86
3		Tridecane	184	C13H28	000629-50-5	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Dodecane	170	C12H26	000112-40-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070124\
Data File : VD079303.D
Acq On : 01 Jul 2024 18:30
Operator : RP/MD
Sample : P3141-01
Misc : 7.62G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
B-140-SB00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D062824S.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
Undecane	13.839	58.7	ug/l	507460	4	13.516	432460	50.0
unknown14.351	14.351	41.0	ug/l	355011	4	13.516	432460	50.0
Carbonic acid, ...	14.692	96.2	ug/l	831928	4	13.516	432460	50.0
Sulfurous acid,...	14.810	39.0	ug/l	337605	4	13.516	432460	50.0
Decane	15.222	44.5	ug/l	384593	4	13.516	432460	50.0
Tridecane	15.522	184.8	ug/l	1598430	4	13.516	432460	50.0
Undecane, 2,9-d...	16.104	34.7	ug/l	300226	4	13.516	432460	50.0
Dodecane, 1-iodo-	16.251	30.1	ug/l	260017	4	13.516	432460	50.0
Tetradecane	16.463	114.5	ug/l	989986	4	13.516	432460	50.0