

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
 Data File : VY016390.D
 Acq On : 16 Nov 2023 15:17
 Operator : SY/MD
 Sample : 05418-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 STONE-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_Y\methods\82Y110823S.M
 Title : SW846 8260

Signal : TIC: VY016390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.710	464	474	490	rVB3	18744	57620	10.61%	1.210%
2	5.753	633	645	655	rBV2	8092	24858	4.58%	0.522%
3	7.716	957	967	973	rBV	73174	176714	32.53%	3.712%
4	7.789	973	979	988	rVB	120319	275682	50.75%	5.791%
5	8.002	1008	1014	1023	rBV3	3437	7901	1.45%	0.166%
6	8.143	1023	1037	1052	rVB2	77698	194931	35.89%	4.094%
7	8.551	1096	1104	1111	rVB	11539	22422	4.13%	0.471%
8	8.691	1118	1127	1137	rBV	193970	377707	69.54%	7.934%
9	9.185	1196	1208	1213	rBV3	9018	17115	3.15%	0.359%
10	9.758	1296	1302	1307	rBV4	3239	6694	1.23%	0.141%
11	9.819	1307	1312	1316	rBV2	18726	34329	6.32%	0.721%
12	9.959	1326	1335	1346	rBV2	22558	47136	8.68%	0.990%
13	10.179	1364	1371	1387	rBV	305999	543180	100.00%	11.409%
14	10.374	1392	1403	1409	rBV	50277	81939	15.09%	1.721%
15	10.526	1421	1428	1432	rBV4	3305	5776	1.06%	0.121%
16	10.581	1432	1437	1441	rBV2	6743	11836	2.18%	0.249%
17	10.715	1454	1459	1464	rVB	6200	9658	1.78%	0.203%
18	10.801	1466	1473	1481	rVB3	7570	13686	2.52%	0.287%
19	10.904	1483	1490	1495	rBV2	11599	21643	3.98%	0.455%
20	10.971	1495	1501	1507	rVV7	7151	20082	3.70%	0.422%
21	11.038	1508	1512	1516	rVV2	5455	9470	1.74%	0.199%
22	11.093	1517	1521	1525	rVB3	4062	6273	1.15%	0.132%
23	11.209	1535	1540	1543	rBV2	6056	10162	1.87%	0.213%
24	11.282	1543	1552	1563	rVV4	49477	117134	21.56%	2.460%
25	11.380	1563	1568	1578	rVB	39000	65227	12.01%	1.370%
26	11.496	1578	1587	1598	rBV	288308	482325	88.80%	10.131%
27	11.715	1614	1623	1631	rBV3	80196	145152	26.72%	3.049%
28	11.935	1654	1659	1664	rBV2	7020	11384	2.10%	0.239%
29	12.008	1664	1671	1678	rBV6	13208	36201	6.66%	0.760%
30	12.124	1686	1690	1695	rVB2	10386	15659	2.88%	0.329%
31	12.197	1695	1702	1706	rBV4	5862	13688	2.52%	0.288%
32	12.245	1706	1710	1715	rVB3	5142	9875	1.82%	0.207%
33	12.361	1721	1729	1730	rBV4	9352	15886	2.92%	0.334%
34	12.386	1730	1733	1734	rVV2	12578	16710	3.08%	0.351%
35	12.416	1734	1738	1740	rVV	22354	38497	7.09%	0.809%
36	12.441	1740	1742	1744	rVV	23394	26635	4.90%	0.559%

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37	12.483	1744	1749	1754	rVV	246648	402586	74.12%	8.456%
38	12.526	1754	1756	1761	rVV	23828	28794	5.30%	0.605%
39	12.739	1784	1791	1794	rBV2	7967	14190	2.61%	0.298%
40	12.806	1794	1802	1808	rVV2	73201	120353	22.16%	2.528%
41	12.867	1808	1812	1817	rVB5	4823	8413	1.55%	0.177%
42	12.959	1822	1827	1831	rBV4	7362	14860	2.74%	0.312%
43	13.007	1831	1835	1838	rVV4	6778	13052	2.40%	0.274%
44	13.044	1838	1841	1847	rVV2	8116	12564	2.31%	0.264%
45	13.123	1847	1854	1858	rVB2	15961	27168	5.00%	0.571%
46	13.172	1858	1862	1868	rBV4	8060	14505	2.67%	0.305%
47	13.325	1878	1887	1890	rBV7	10555	22725	4.18%	0.477%
48	13.367	1890	1894	1897	rVV3	21489	34541	6.36%	0.726%
49	13.428	1897	1904	1913	rVV	312593	500910	92.22%	10.521%
50	13.507	1913	1917	1924	rVB2	14189	20722	3.81%	0.435%
51	13.629	1932	1937	1939	rBV2	4372	6437	1.19%	0.135%
52	13.672	1940	1944	1952	rVB4	5648	12795	2.36%	0.269%
53	13.757	1952	1958	1962	rBV	54977	80265	14.78%	1.686%
54	13.916	1980	1984	1989	rBV7	5200	7456	1.37%	0.157%
55	13.971	1989	1993	1998	rVB3	11238	17696	3.26%	0.372%
56	14.013	1998	2000	2006	rVB5	4593	7359	1.35%	0.155%
57	14.080	2006	2011	2016	rBV4	7957	11606	2.14%	0.244%
58	14.141	2016	2021	2027	rBV8	4880	10499	1.93%	0.221%
59	14.245	2032	2038	2039	rBV4	9012	13604	2.50%	0.286%
60	14.312	2047	2049	2057	rVB5	9275	18045	3.32%	0.379%
61	14.385	2057	2061	2064	rVV3	10532	14302	2.63%	0.300%
62	14.422	2064	2067	2071	rVB5	6238	8504	1.57%	0.179%
63	14.611	2094	2098	2104	rVB	45717	64430	11.86%	1.353%
64	14.684	2104	2110	2114	rBV6	14496	29304	5.39%	0.616%
65	14.733	2114	2118	2124	rVB2	17106	27007	4.97%	0.567%
66	14.843	2132	2136	2146	rVB6	8006	16048	2.95%	0.337%
67	14.946	2148	2153	2156	rVB6	6203	9155	1.69%	0.192%
68	15.056	2165	2171	2175	rBV6	6587	13746	2.53%	0.289%
69	15.141	2181	2185	2191	rVB8	9556	17681	3.26%	0.371%
70	15.214	2192	2197	2206	rBV4	15084	32416	5.97%	0.681%
71	15.300	2206	2211	2212	rBV5	5897	8866	1.63%	0.186%
72	15.440	2229	2234	2241	rVB	35779	56311	10.37%	1.183%
73	15.696	2271	2276	2277	rBV4	6146	8113	1.49%	0.170%
74	15.733	2279	2282	2289	rVB9	11290	21336	3.93%	0.448%
75	15.940	2313	2316	2320	rBV6	5217	10164	1.87%	0.213%
76	16.367	2382	2386	2390	rBV2	16105	31145	5.73%	0.654%

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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_Y\methods\82Y110823S.M
Title : SW846 8260

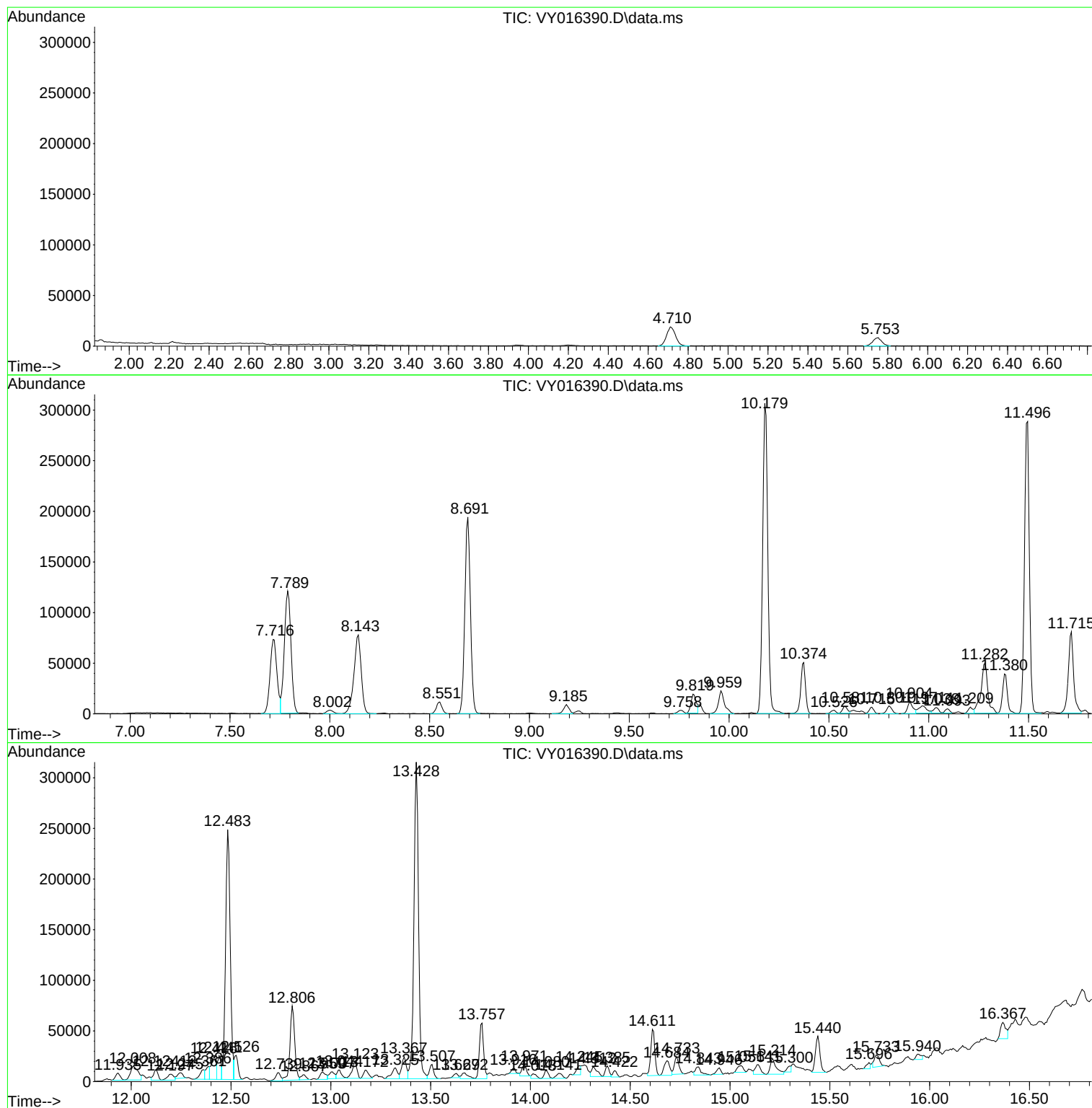
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Instrument :
MSVOA_Y
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110823S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
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Sample : 05418-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
STONE-1

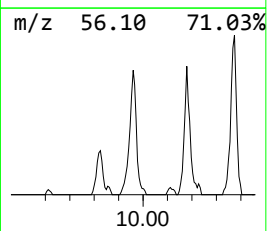
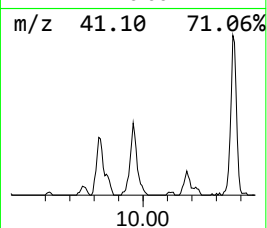
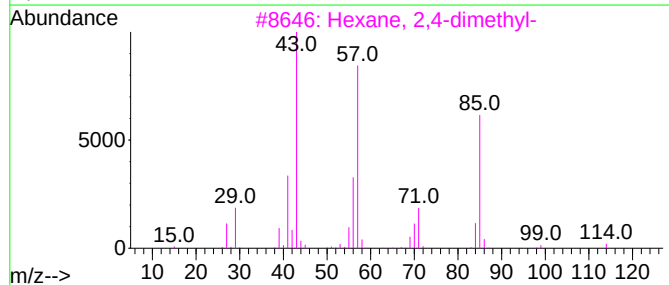
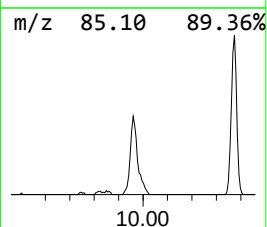
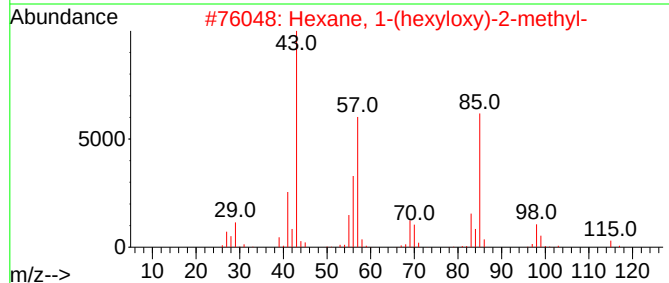
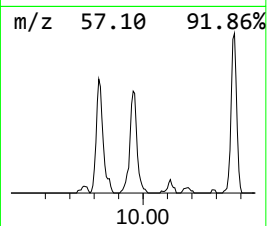
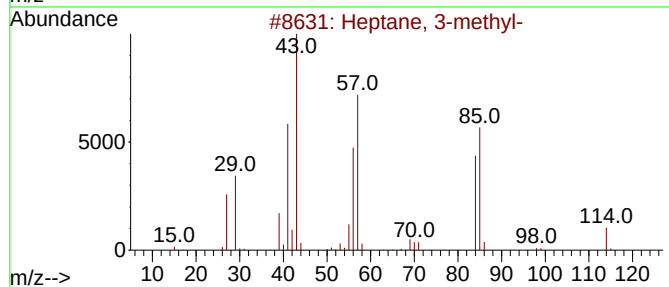
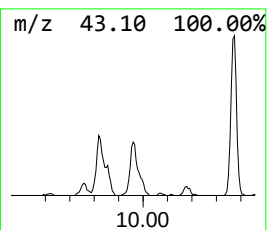
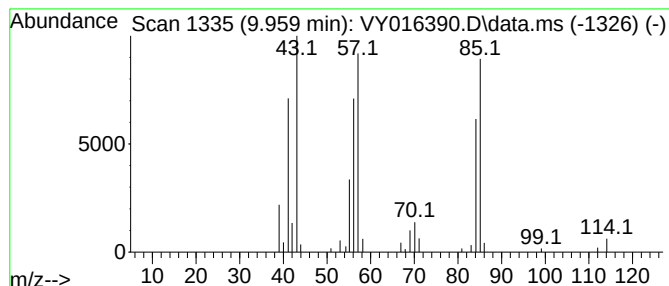
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110823S.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.959	6.24 ug/l	47136	1,4-Difluorobenzene	8.691

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2		Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	64
3		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
4		Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	50
5		Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	50



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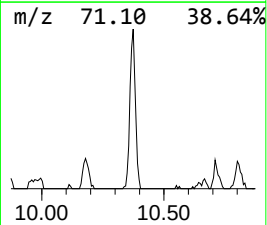
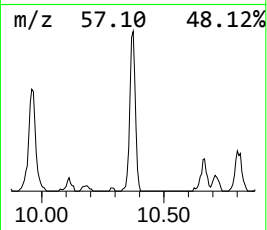
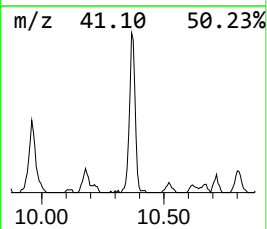
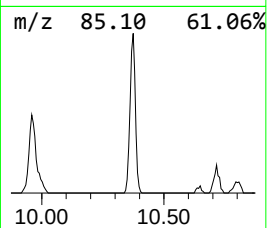
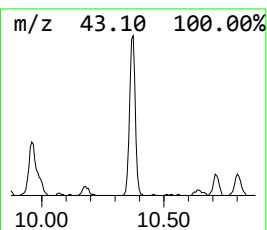
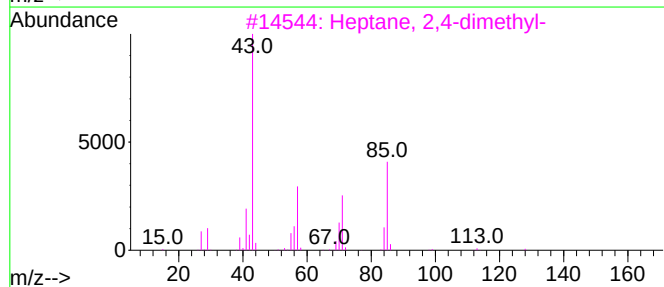
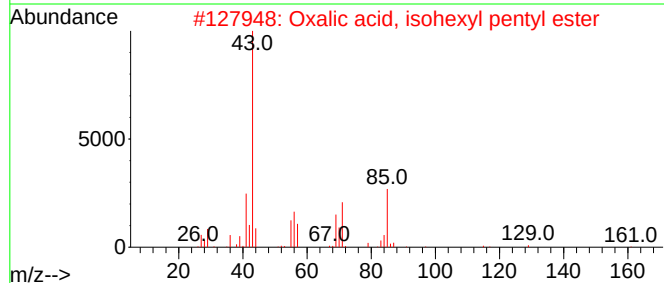
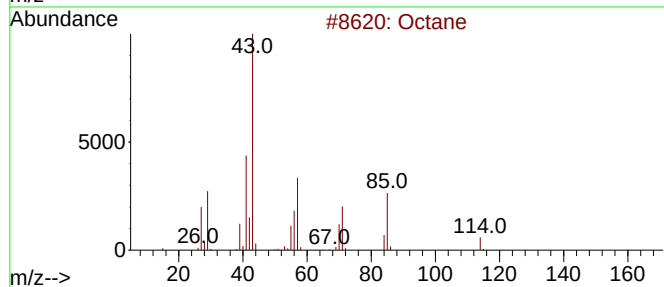
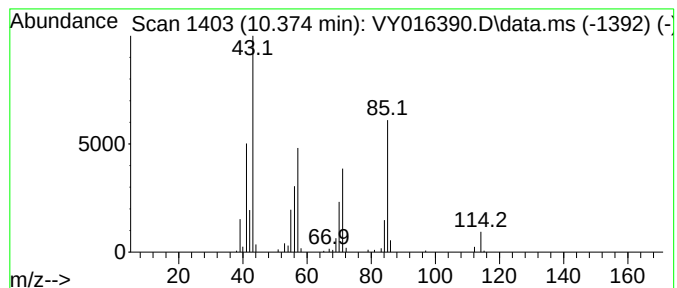
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110823S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	8.49 ug/l	81939	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	91
2			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	78
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	53
5			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	53



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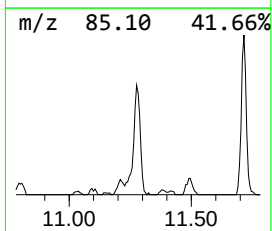
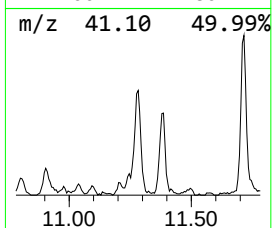
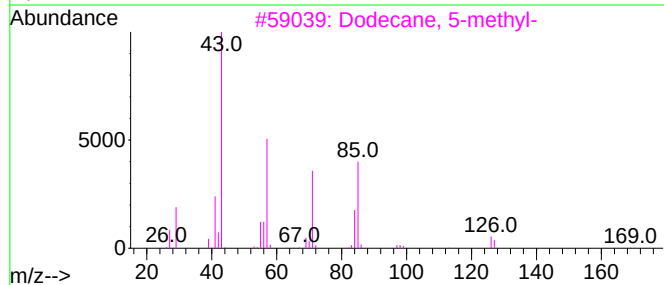
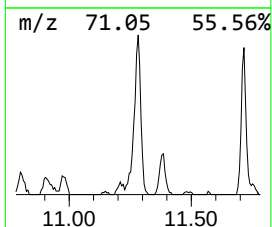
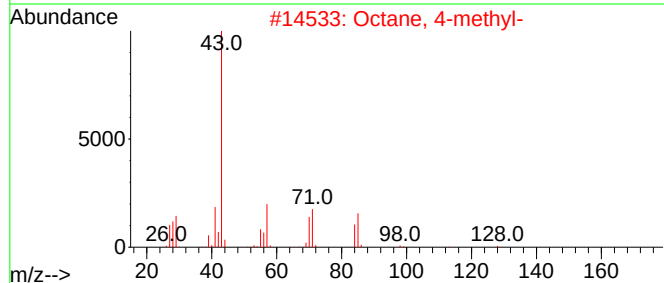
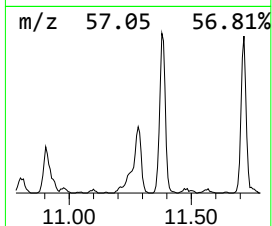
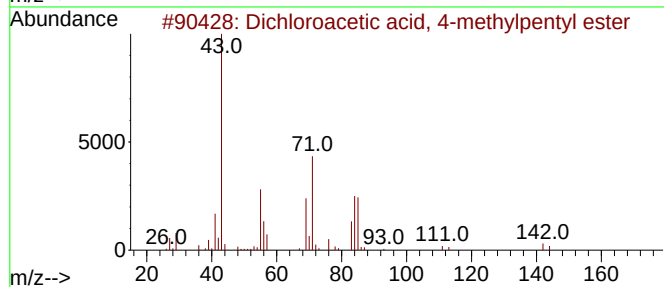
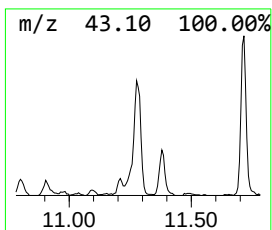
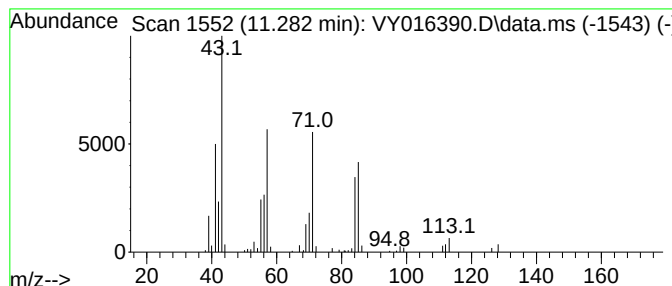
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Quant Title : SW846 8260

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

Peak Number 3 Dichloroacetic acid, 4-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	12.14 ug/l	117134	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	53
2			Octane, 4-methyl-	128	C9H20	002216-34-4	52
3			Dodecane, 5-methyl-	184	C13H28	017453-93-9	50
4			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	49
5			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	47



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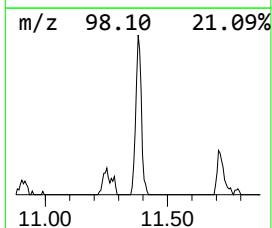
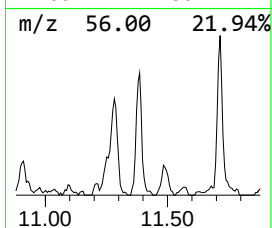
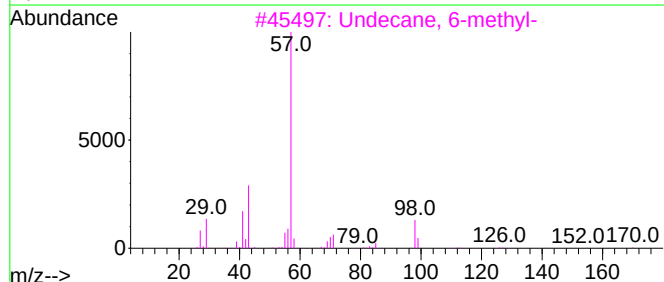
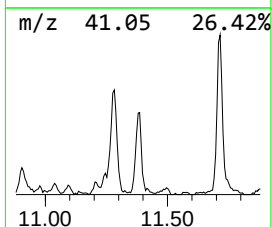
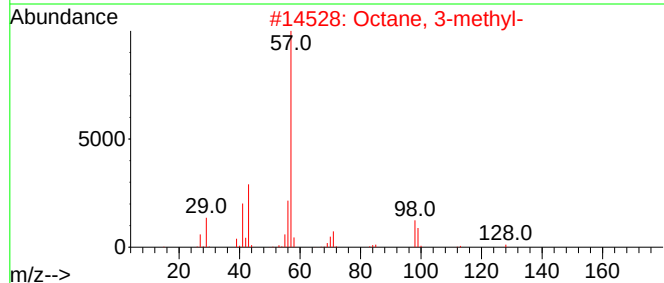
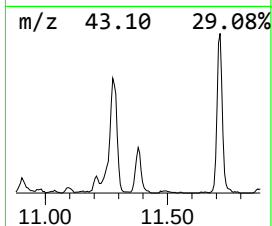
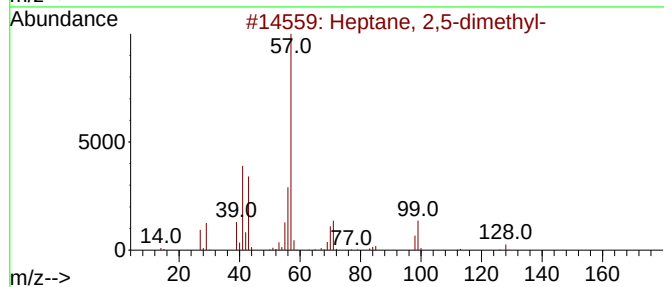
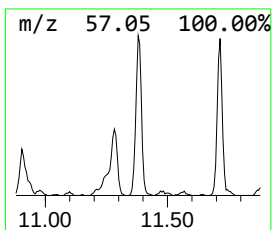
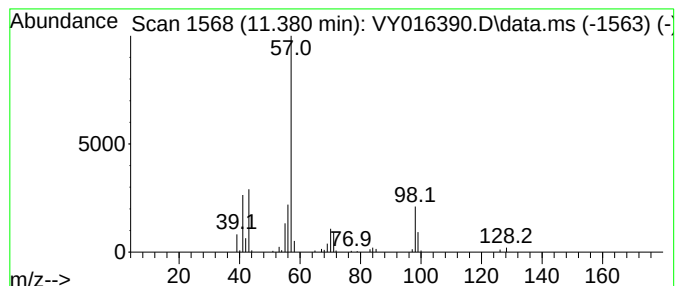
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Quant Title : SW846 8260

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

Peak Number 4 Heptane, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	6.76 ug/l	65227	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	81
2			Octane, 3-methyl-	128	C9H20	002216-33-3	74
3			Undecane, 6-methyl-	170	C12H26	017302-33-9	59
4			Heptane, 4-propyl-	142	C10H22	003178-29-8	59
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
Data File : VY016390.D
Acq On : 16 Nov 2023 15:17
Operator : SY/MD
Sample : 05418-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
STONE-1

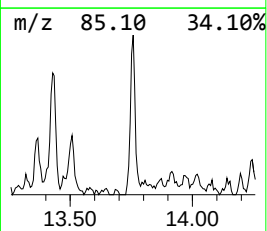
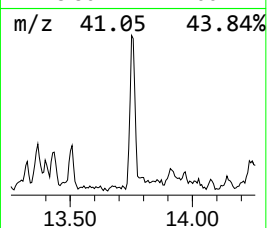
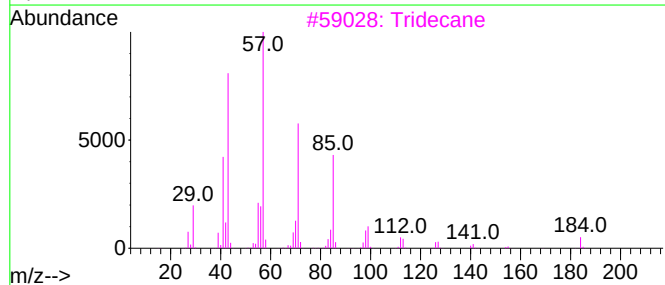
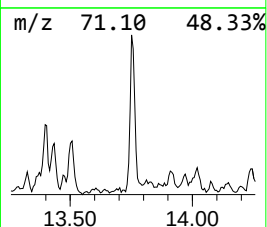
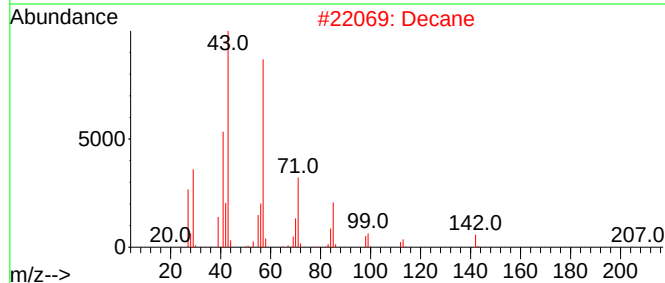
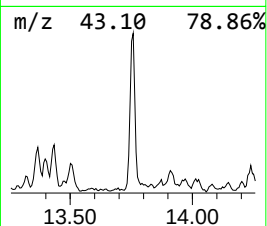
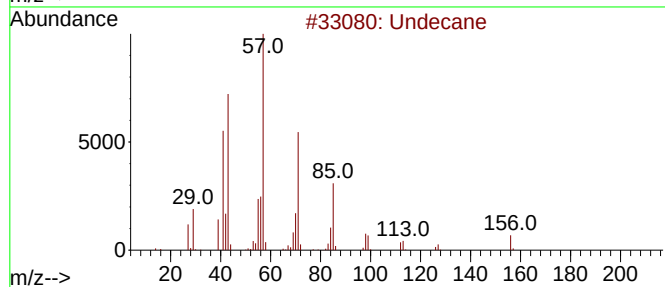
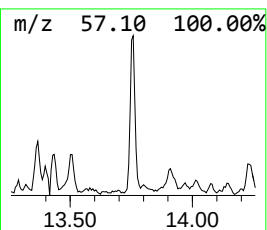
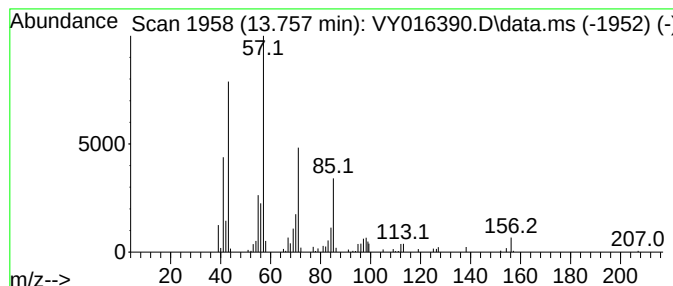
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Quant Title : SW846 8260

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

Peak Number 5 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	8.01 ug/l	80265	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	96
2			Decane	142	C10H22	000124-18-5	90
3			Tridecane	184	C13H28	000629-50-5	90
4			Tetradecane	198	C14H30	000629-59-4	80
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
Data File : VY016390.D
Acq On : 16 Nov 2023 15:17
Operator : SY/MD
Sample : 05418-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
STONE-1

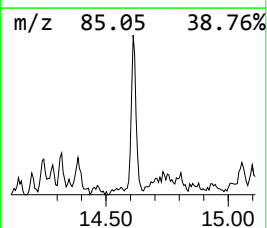
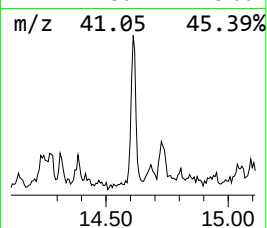
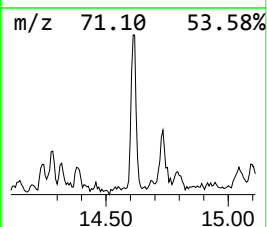
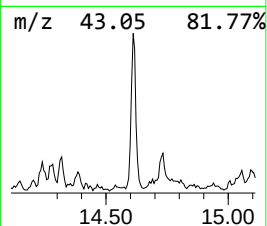
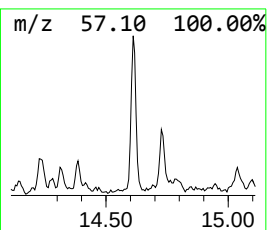
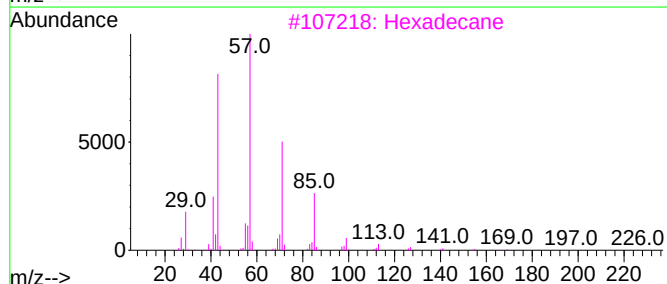
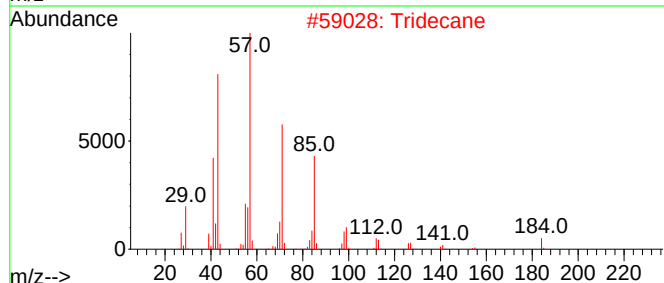
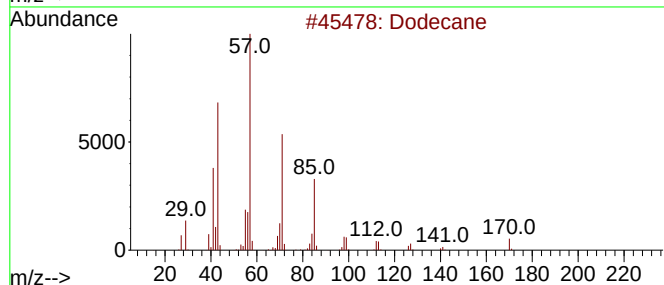
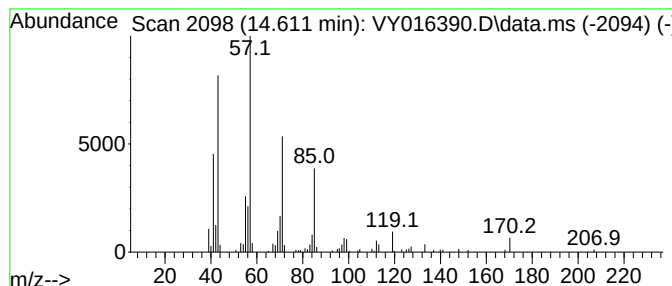
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	6.43 ug/l	64430	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	92
2			Tridecane	184	C13H28	000629-50-5	80
3			Hexadecane	226	C16H34	000544-76-3	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
Data File : VY016390.D
Acq On : 16 Nov 2023 15:17
Operator : SY/MD
Sample : 05418-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
STONE-1

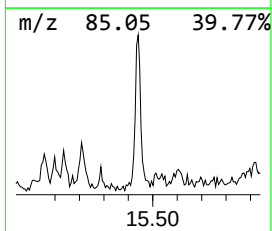
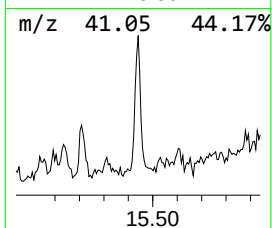
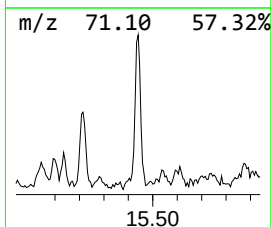
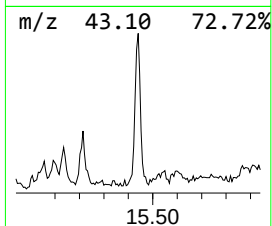
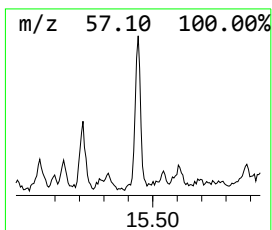
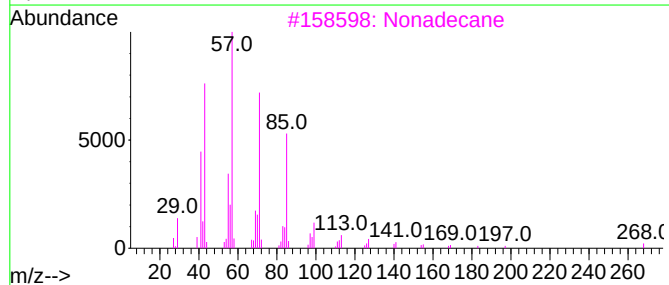
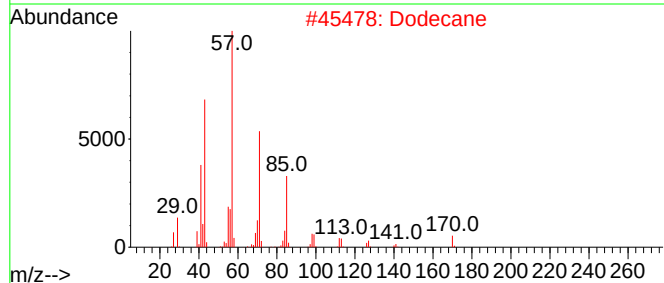
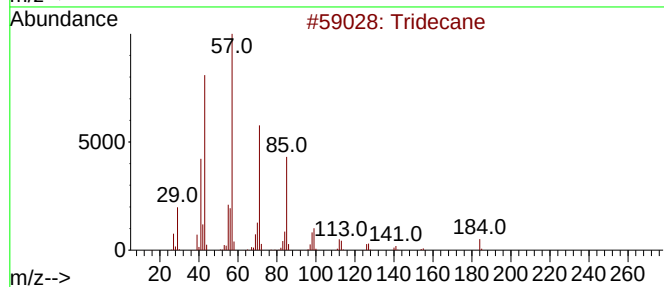
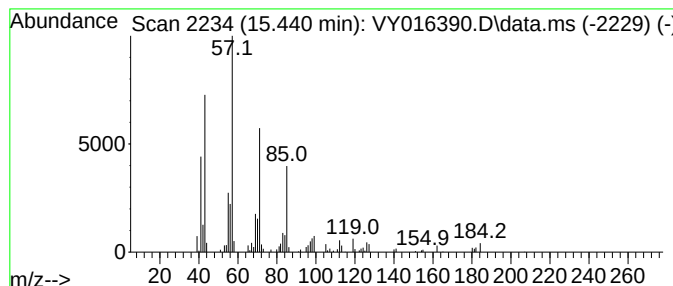
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.440	5.62 ug/l	56311	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	86
3			Nonadecane	268	C19H40	000629-92-5	83
4			Tetradecane	198	C14H30	000629-59-4	74
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111623\
Data File : VY016390.D
Acq On : 16 Nov 2023 15:17
Operator : SY/MD
Sample : 05418-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
STONE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y110823S.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
Heptane, 3-methyl-	9.959	6.2	ug/l	47136	2	8.691	377707	50.0
Octane	10.374	8.5	ug/l	81939	3	11.496	482325	50.0
Dichloroacetic ...	11.282	12.1	ug/l	117134	3	11.496	482325	50.0
Heptane, 2,5-di...	11.380	6.8	ug/l	65227	3	11.496	482325	50.0
Undecane	13.757	8.0	ug/l	80265	4	13.428	500910	50.0
Dodecane	14.611	6.4	ug/l	64430	4	13.428	500910	50.0
Tridecane	15.440	5.6	ug/l	56311	4	13.428	500910	50.0