LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 256

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_X\Method\82X081721W.M
Title : SW846 8260

Signal : TIC: VX024166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	39	rVB2	6496	14626	1.00%	0.135%
2	1.361	42	45	60	rBV	12343	23786	1.63%	0.219%
3	5.397	694	707	719	rBV	93044	272688	18.68%	2.512%
4	5.562	723	734	746	rVV2	157104	446904	30.62%	4.117%
5	5.964	787	800	815	rBV	103491	279868	19.17%	2.578%
6	6.769	921	932	950	rBV	248719	595584	40.80%	5.486%
7	8.653	1234	1241	1248	rBV	516982	815754	55.89%	7.514%
8	8.720	1248	1252	1260	rVB	15593	25563	1.75%	0.235%
9	10.055	1466	1471	1480	rVB	533988	728046	49.88%	6.706%
10	10.366	1517	1522	1529	rVB	17287	22522	1.54%	0.207%
11	10.860	1595	1603	1607	rBV4	9635	17462	1.20%	0.161%
12	11.085	1634	1640	1650	rVB	498129	665331	45.58%	6.129%
13	11.195	1650	1658	1661	rBV	29870	41759	2.86%	0.385%
14	11.384	1685	1689	1694	rBV	16041	27470	1.88%	0.253%
15	11.433	1694	1697	1699	rVV3	22247	30966	2.12%	0.285%
16	11.482	1701	1705	1711	rVB	353816	406283	27.83%	3.742%
17	11.634	1723	1730	1734	rBV5	21093	39778	2.73%	0.366%
18	11.689	1734	1739	1741	rBV3	22037	27266	1.87%	0.251%
19	11.719	1741	1744	1747	rBV	69721	72228	4.95%	0.665%
20	11.756	1747	1750	1753	rBV	53916	67516	4.63%	0.622%
21	11.841	1759	1764	1766	rBV	32146	42398	2.90%	0.391%
22	11.890	1766	1772	1777	rVV4	39809	86105	5.90%	0.793%
23	11.945	1777	1781	1784	rVV2	62425	91679	6.28%	0.844%
24	11.975	1784	1786	1789	rVV3	38468	51219	3.51%	0.472%
25	12.024	1789	1794	1800	rVV2	574681	852879	58.43%	7.856%
26	12.079	1800	1803	1805	rVV	102735	144979	9.93%	1.335%
27	12.103	1805	1807	1811	rVV	145878	158935	10.89%	1.464%
28	12.146	1811	1814	1816	rVV4	21538	32515	2.23%	0.300%
29	12.177	1816	1819	1826	rVB	128091	155615	10.66%	1.433%
30	12.268	1826	1834	1838	rBV3	39726	80262	5.50%	0.739%
31	12.317	1838	1842	1848	rVB3	84520	144333	9.89%	1.330%
32	12.427	1855	1860	1864	rBV	1389616	1459647	100.00%	13.445%
33	12.469	1864	1867	1873	rVB5	62271	107754	7.38%	0.993%
34	12.561	1873	1882	1883	rBV4	79019	162719	11.15%	1.499%
35	12.585	1883	1886	1889	rVV2	73245	122181	8.37%	1.125%
36	12.615	1889	1891	1893	rVV	40296	42170	2.89%	0.388%

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 256

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

37	12.640	1893	1895	1899	rVB2	36622	42567	2.92%	0.392%
38	12.689	1899	1903	1906	rBV2	63328	90595	6.21%	0.835%
39	12.731	1906	1910	1914	rVB3	33439	60177	4.12%	0.554%
40	12.798	1917	1921	1922	rBV4	24512	29857	2.05%	0.275%
41	12.823	1922	1925	1928	rVB	51340	57553	3.94%	0.530%
42	12.890	1931	1936	1943	rBV4	117053	283277	19.41%	2.609%
43	12.969	1943	1949	1956	rVV5	98160	249459	17.09%	2.298%
44	13.042	1957	1961	1964	rVB3	60632	66721	4.57%	0.615%
45	13.164	1975	1981	1985	rBV4	38490	64353	4.41%	0.593%
46	13.213	1986	1989	1992	rBV2	27983	32138	2.20%	0.296%
47	13.268	1992	1998	2001	rBV	244818	330444	22.64%	3.044%
48	13.384	2013	2017	2020	rVV2	19032	27799	1.90%	0.256%
49	13.426	2020	2024	2033	rVB3	60488	122732	8.41%	1.131%
50	13.506	2033	2037	2040	rBV3	15863	23853	1.63%	0.220%
51	13.585	2046	2050	2056	rBV3	24237	41477	2.84%	0.382%
52	13.676	2061	2065	2068	rBV3	17303	30424	2.08%	0.280%
53	13.737	2071	2075	2079	rBV6	24037	35708	2.45%	0.329%
54	13.841	2088	2092	2100	rVB6	24149	54991	3.77%	0.507%
55	13.932	2100	2107	2111	rBV6	16761	40934	2.80%	0.377%
56	14.042	2121	2125	2128	rVB	62819	66531	4.56%	0.613%
57	14.079	2128	2131	2134	rBV2	14186	15731	1.08%	0.145%
58	14.231	2150	2156	2163	rVB4	30116	59771	4.09%	0.551%
59	14.323	2167	2171	2175	rBV4	11115	16671	1.14%	0.154%
60	14.438	2183	2190	2194	rBV2	48469	70554	4.83%	0.650%
61	14.481	2194	2197	2200	rBV4	17861	28880	1.98%	0.266%
62	14.566	2206	2211	2216	rBV6	13421	24474	1.68%	0.225%
63	14.615	2216	2219	2221	rVV2	36967	46244	3.17%	0.426%
64	14.640	2221	2223	2226	rVV	43257	49047	3.36%	0.452%
65	14.676	2226	2229	2234	rVB5	14147	20644	1.41%	0.190%
66	14.755	2239	2242	2245	rVV	52405	60755	4.16%	0.560%
67	14.786	2245	2247	2251	rVB3	20721	23322	1.60%	0.215%
68	15.097	2295	2298	2303	rBV7	9872	18537	1.27%	0.171%
69	15.188	2308	2313	2315	rVV3	24391	35777	2.45%	0.330%
70	15.213	2315	2317	2321	rVV	28717	34569	2.37%	0.318%
71	15.280	2325	2328	2331	rVB4	13198	16799	1.15%	0.155%
72	15.493	2357	2363	2368	rBV3	47219	76214	5.22%	0.702%
73	15.566	2370	2375	2380	rVV2	31999	52633	3.61%	0.485%
74	15.615	2380	2383	2386	rVV5	12504	18152	1.24%	0.167%
75	16.109	2457	2464	2468	rBV10	13025	37897	2.60%	0.349%
76	16.377	2504	2508	2514	rVB2	22611	41033	2.81%	0.378%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

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_X\Method\82X081721W.M
Title : SW846 8260

Sum of corrected areas: 10856084

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
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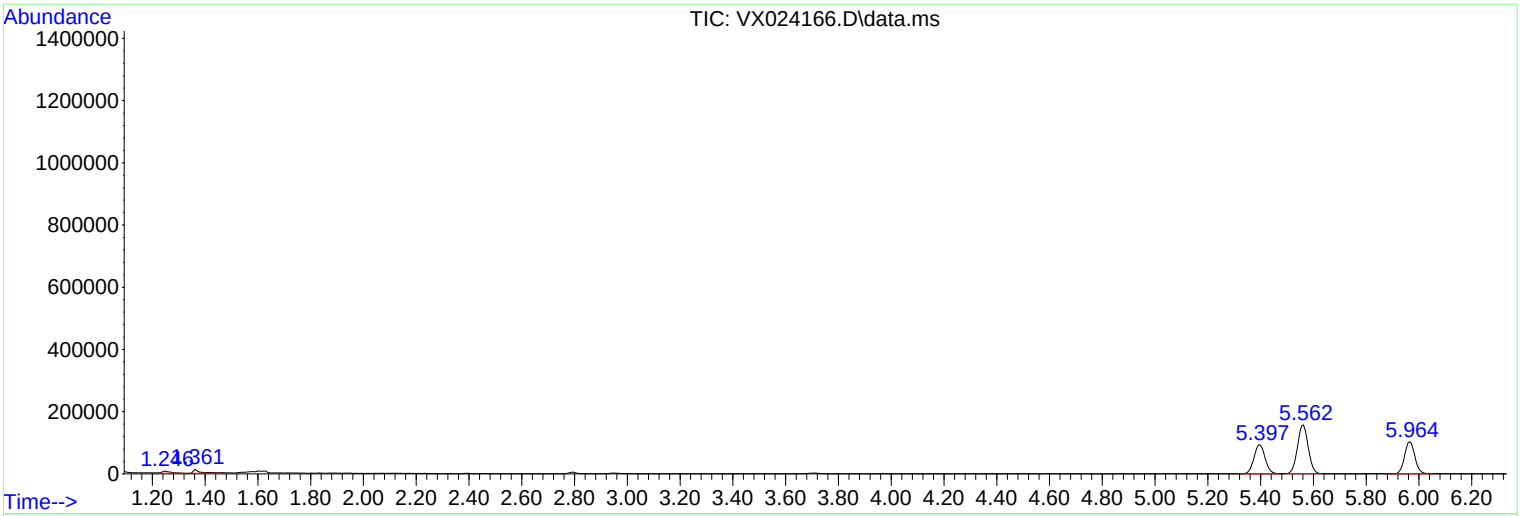
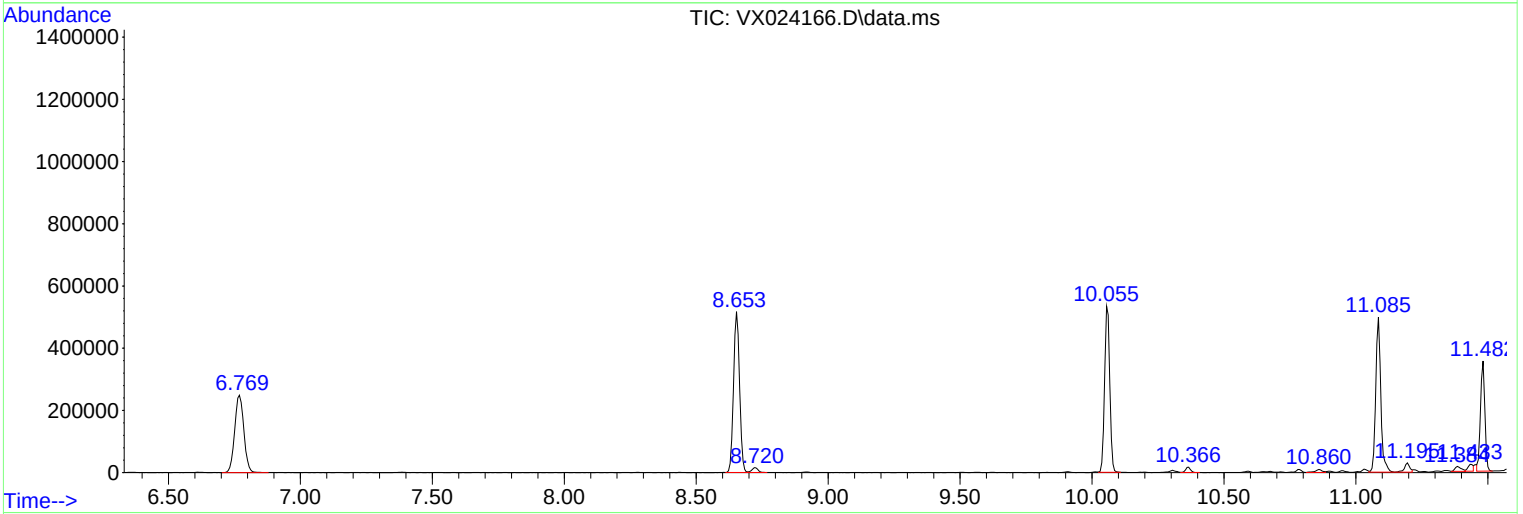
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

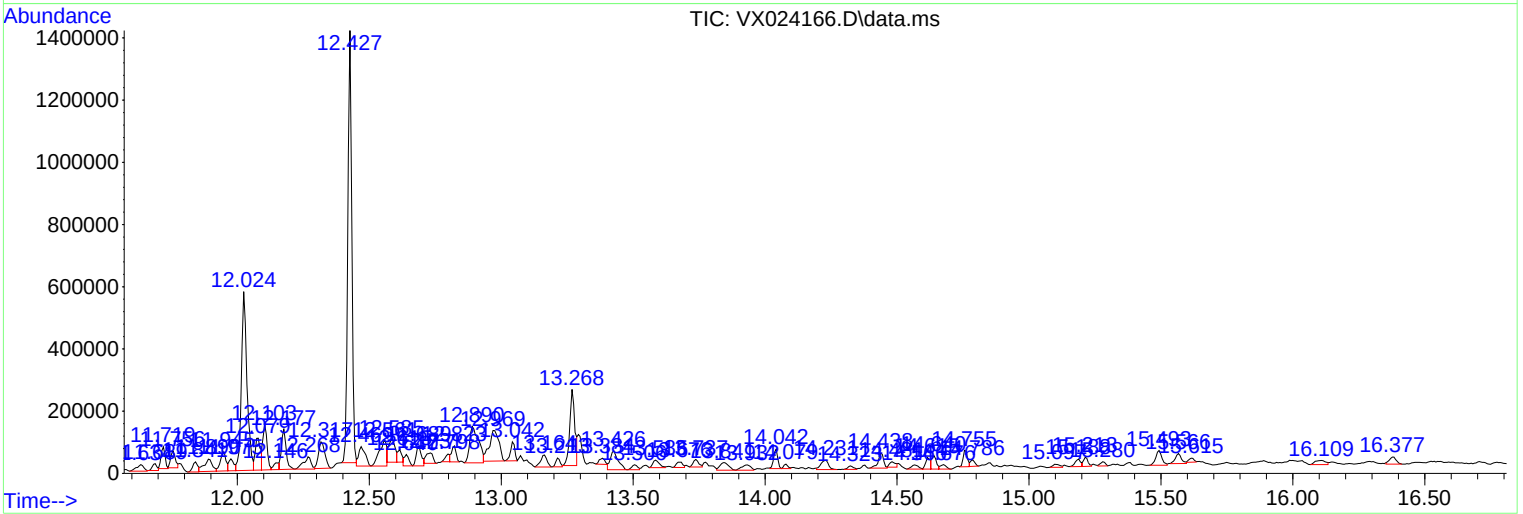
Instrument :
MSVOA_X
ClientSampleId :
256

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

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







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Instrument :
MSVOA_X
ClientSampleId :
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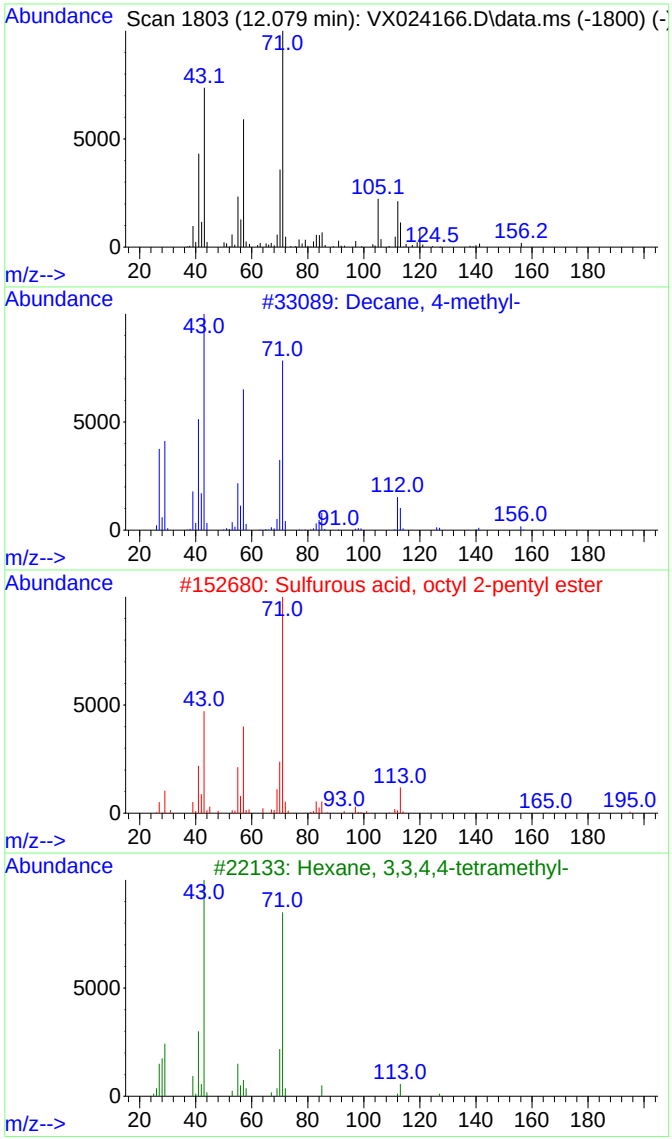
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

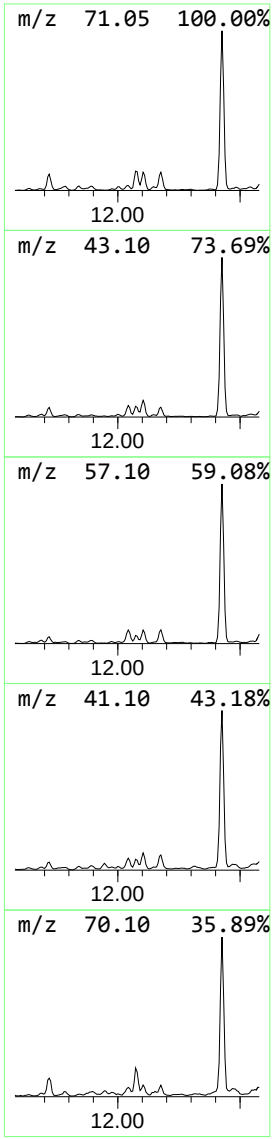
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Decane, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.079	8.50 ug/l	144979	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 4-methyl-	156	C11H24	002847-72-5	62
2	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	53
3	Hexane, 3,3,4,4-tetramethyl-	142	C10H22	005171-84-6	50
4	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	50
5	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	50





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Operator : JC/MD
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

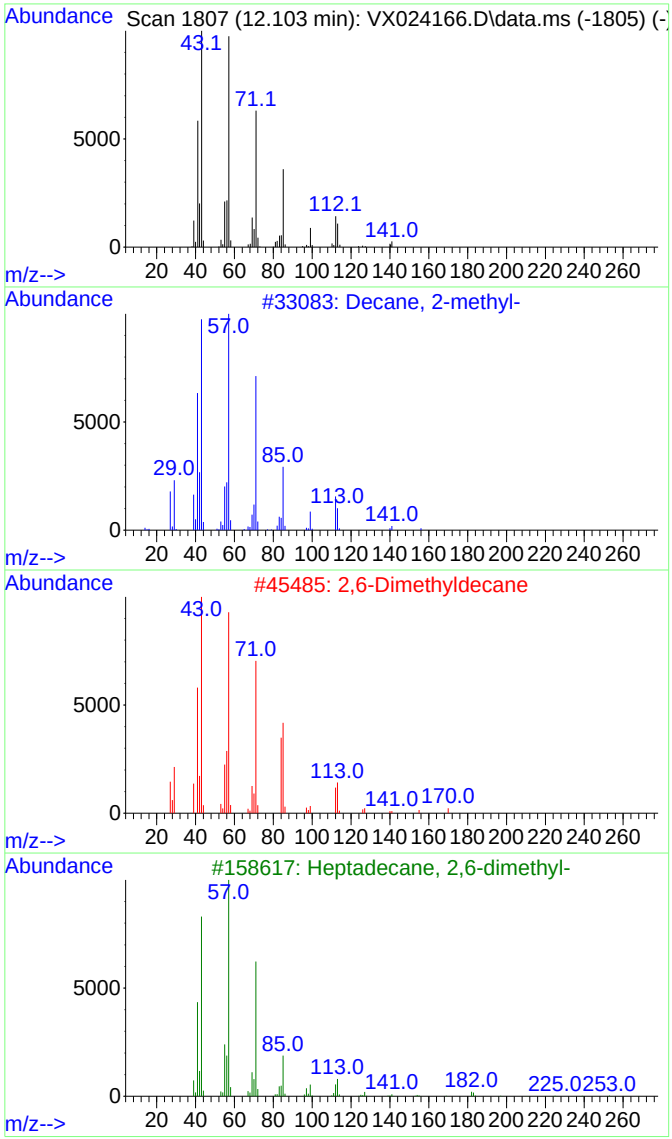
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

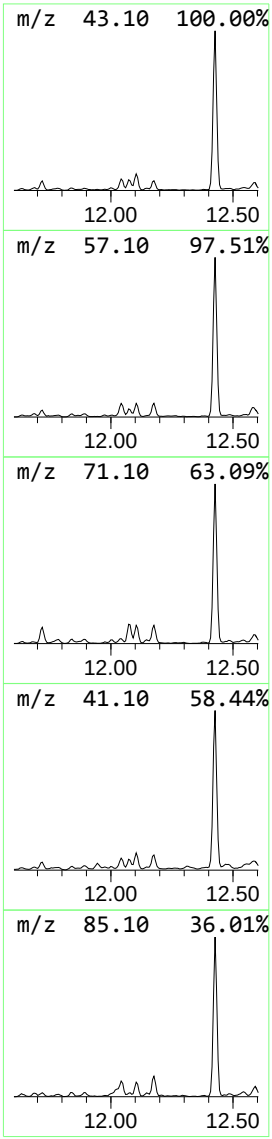
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Decane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	9.32 ug/l	158935	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	90
2	2,6-Dimethyldecane	170	C12H26	013150-81-7	80
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	64
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	64
5	Hexadecane	226	C16H34	000544-76-3	53





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Data File : VX024166.D
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

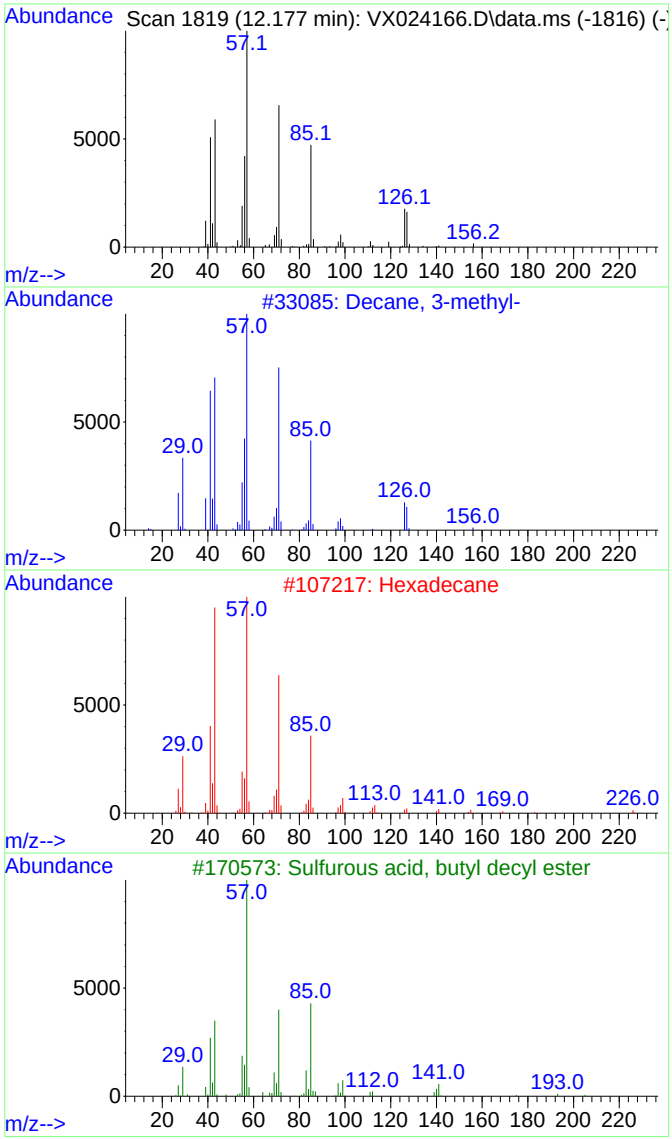
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

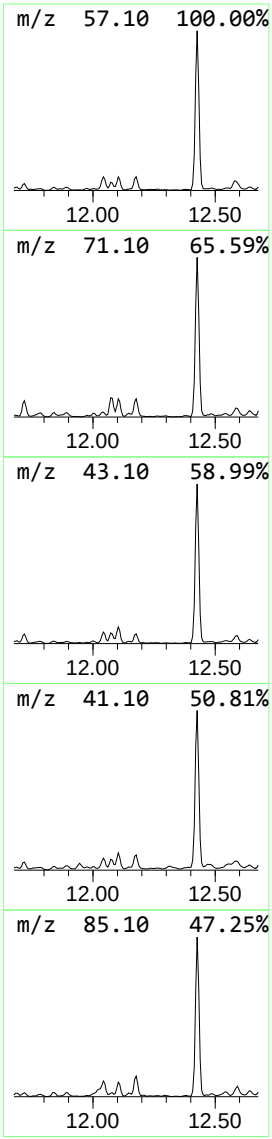
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Decane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.177	9.12 ug/l	155615	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	91
2	Hexadecane	226	C16H34	000544-76-3	53
3	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	53
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	53
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	50





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Instrument :
MSVOA_X
ClientSampleId :
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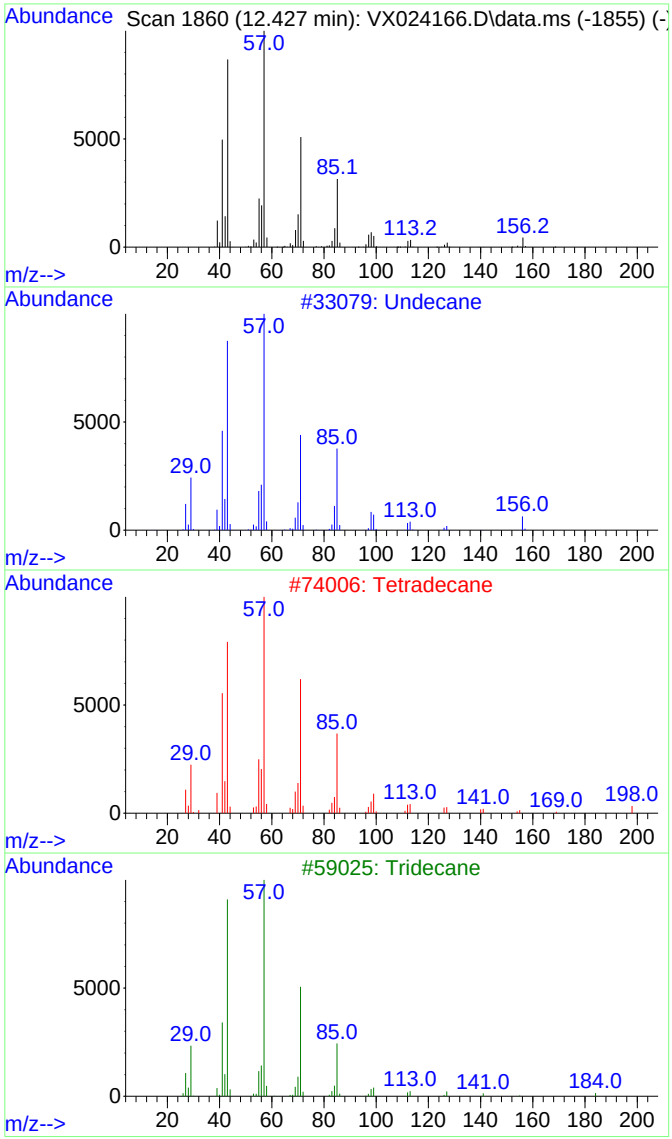
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

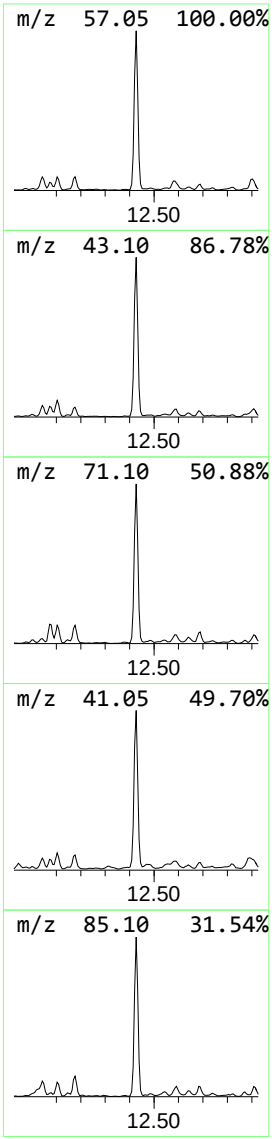
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	85.57 ug/l	1459650	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane	184	C13H28	000629-50-5	80
4	Hexadecane	226	C16H34	000544-76-3	72
5	Nonadecane	268	C19H40	000629-92-5	59





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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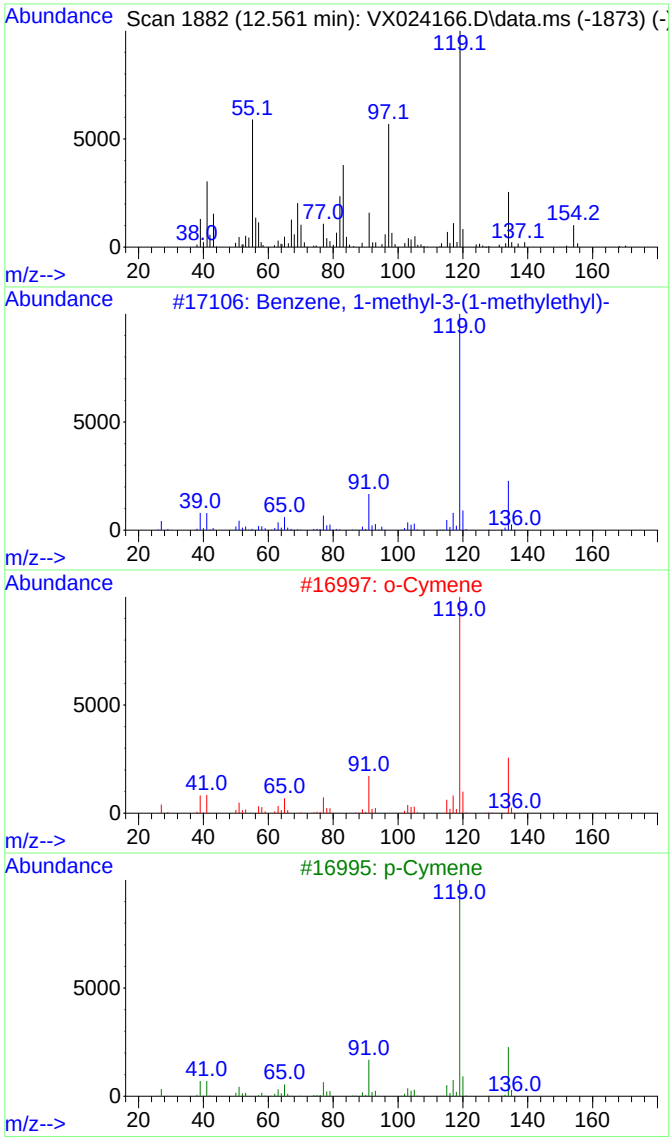
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

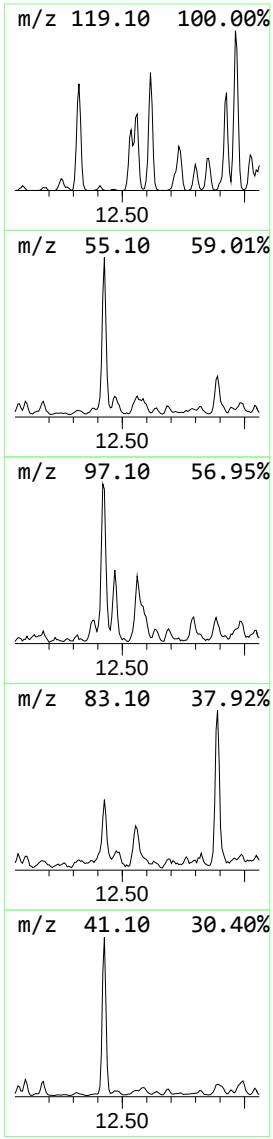
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-methyl-3-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.561	9.54 ug/l	162719	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
2	o-Cymene	134	C10H14	000527-84-4	91
3	p-Cymene	134	C10H14	000099-87-6	90
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	90
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	87





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Instrument :
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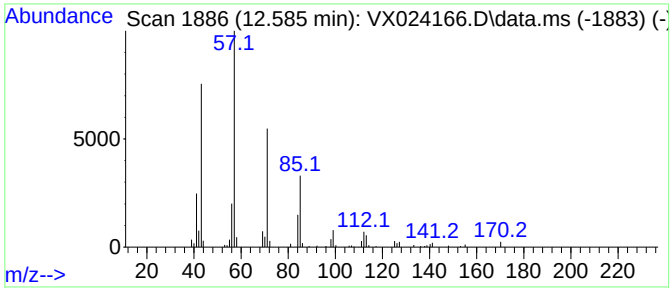
Quant Title : SW846 8260

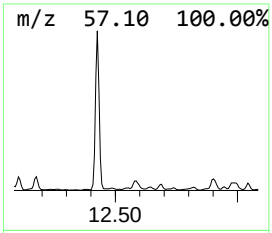
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

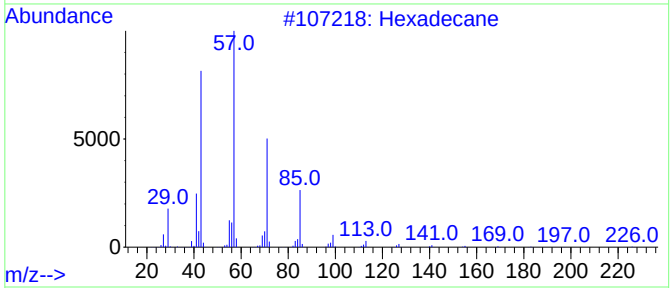
****
Peak Number 6 Hexadecane Concentration Rank 10

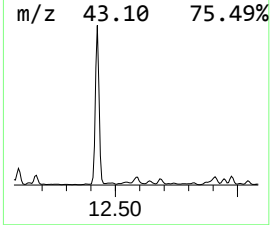
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	7.16 ug/l	122181	1,4-Dichlorobenzene-d4	12.024

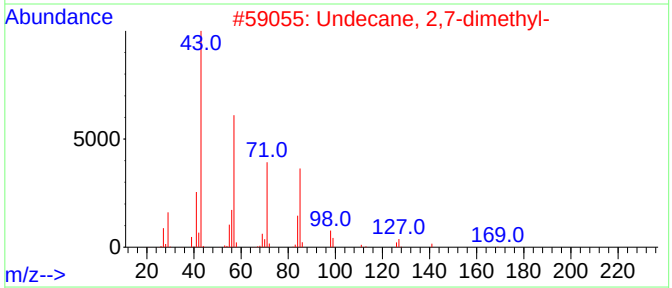
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	80
2	Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	72
3	Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	64
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58
5	Triacontane	422	C30H62	000638-68-6	53

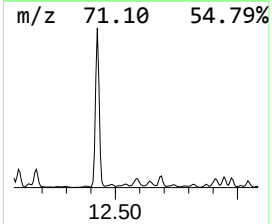


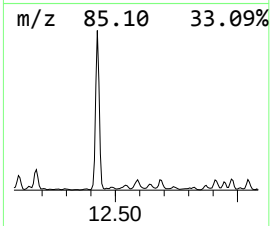


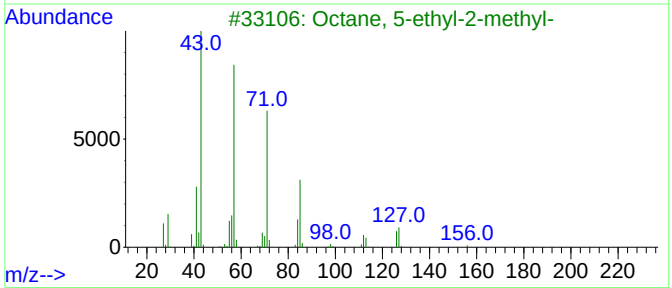


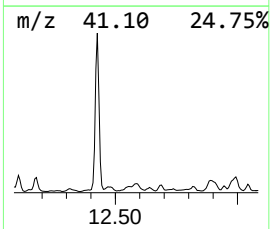












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

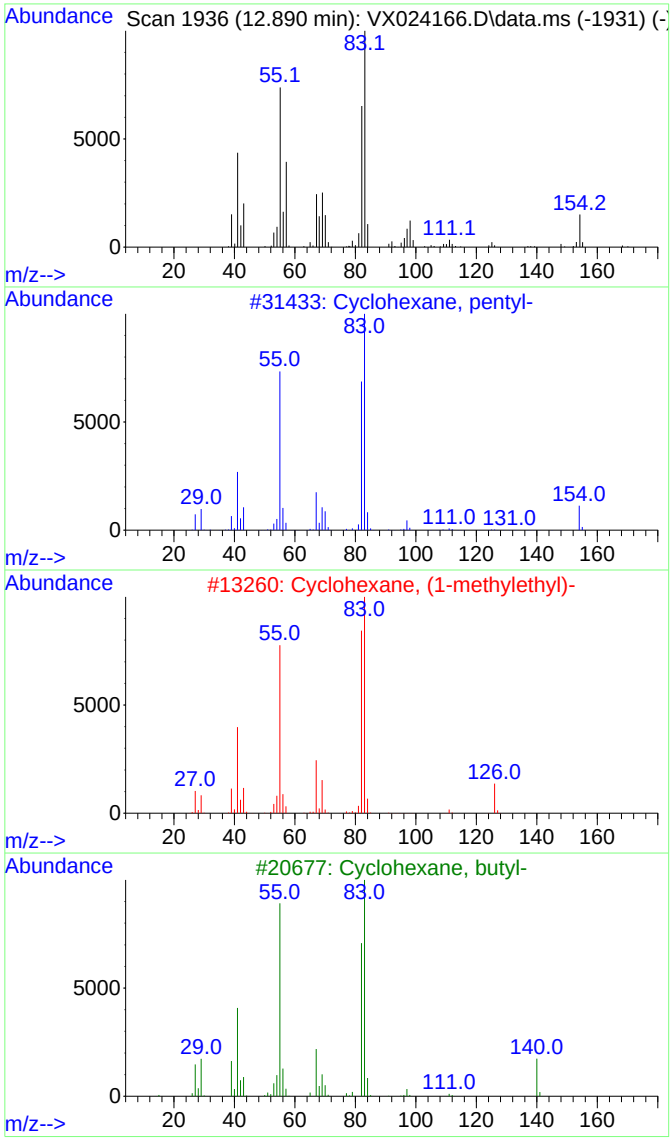
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

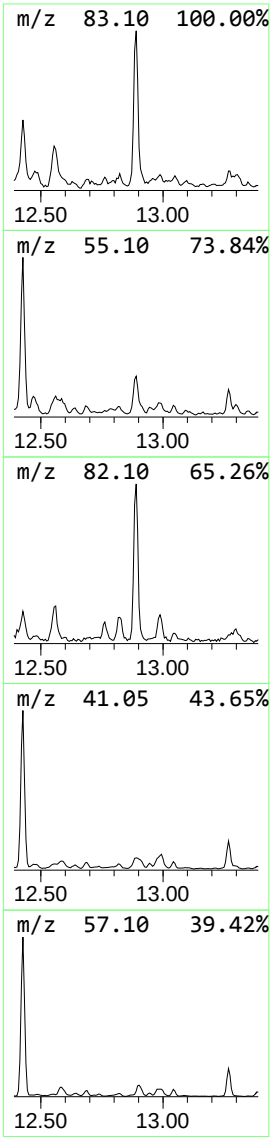
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexane, pentyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	16.61 ug/l	283277	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	90
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72
3	Cyclohexane, butyl-	140	C10H20	001678-93-9	72
4	Cyclohexane, octyl-	196	C14H28	001795-15-9	72
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

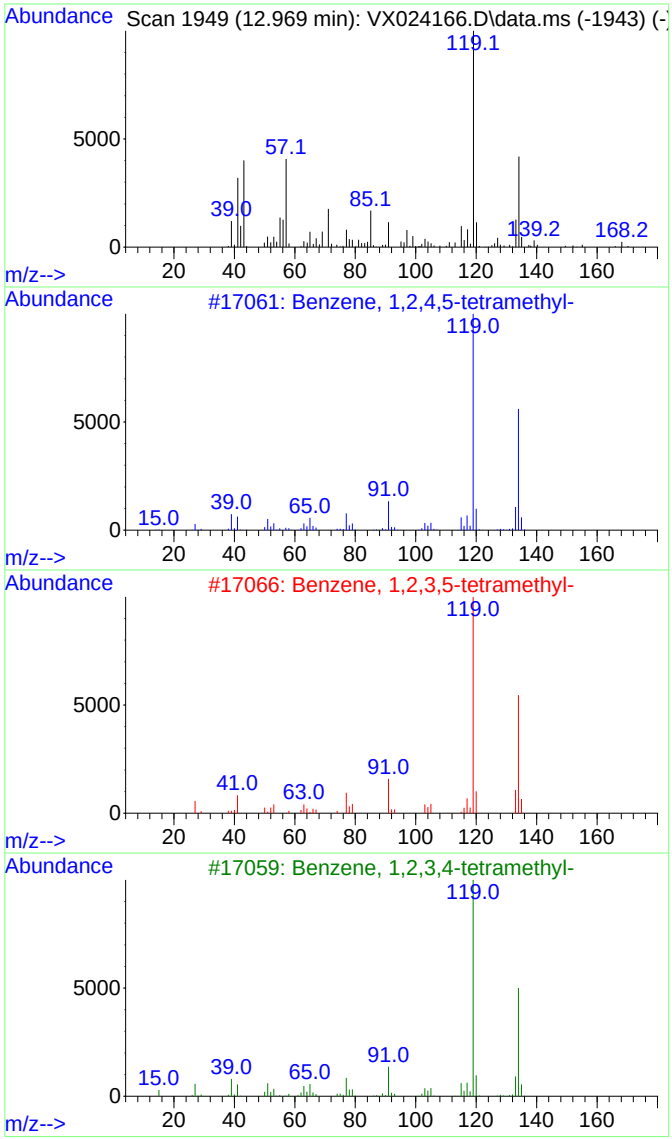
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

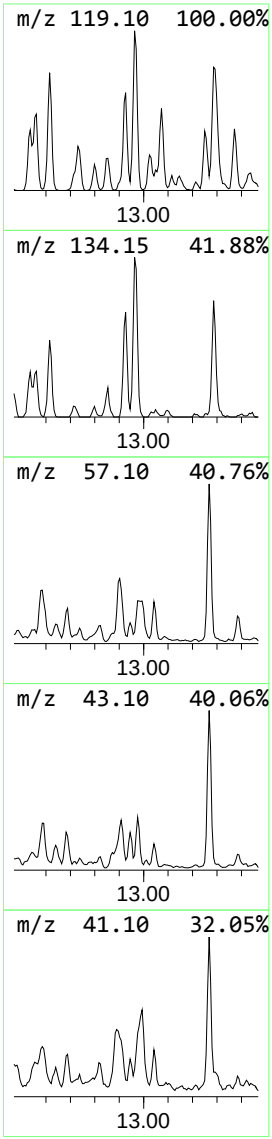
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	14.62 ug/l	249459	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	90
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	90
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

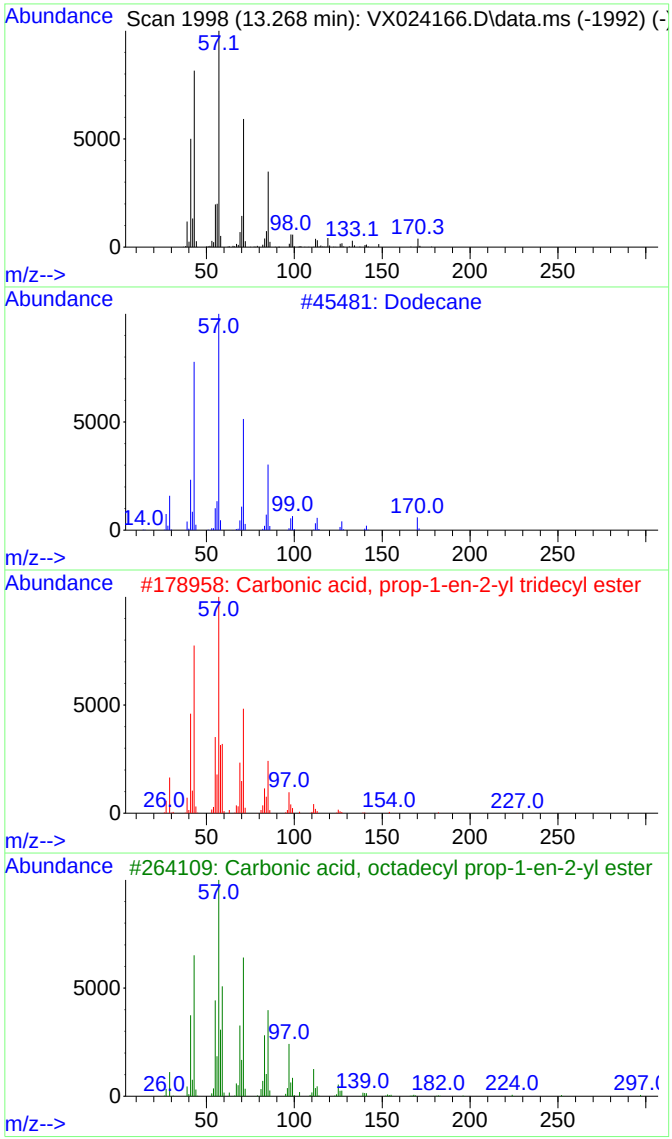
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

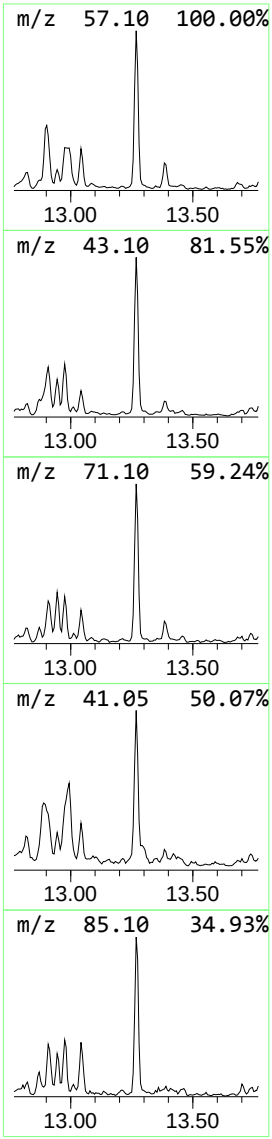
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	19.37 ug/l	330444	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	91
2	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	86
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
256

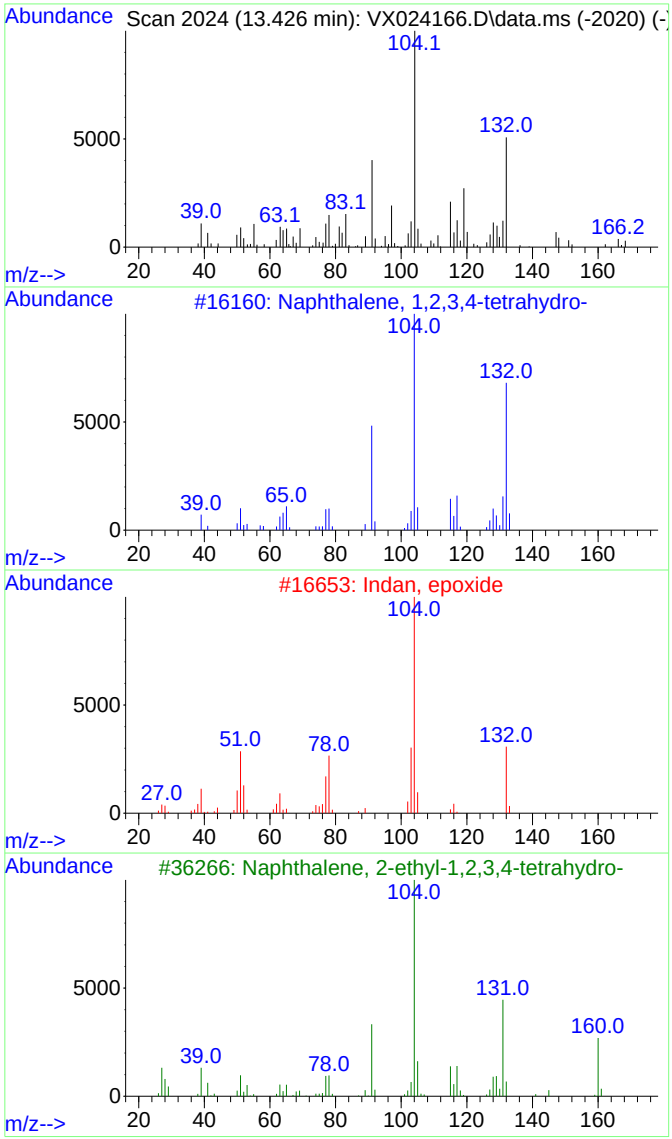
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

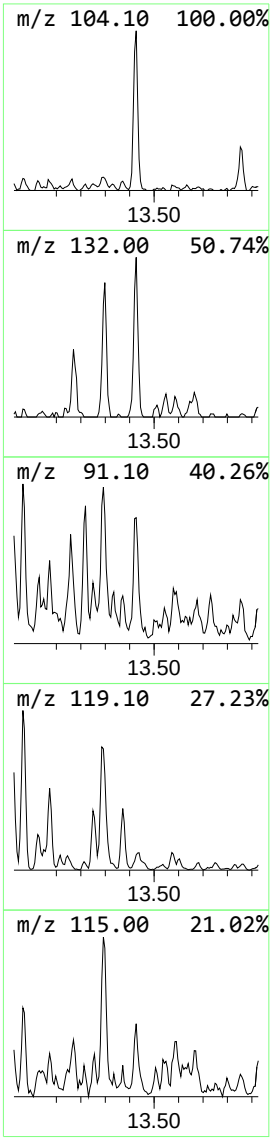
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	7.20 ug/l	122732	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2	Indan, epoxide	132	C9H8O	000768-22-9	50
3	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	43
4	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	38
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091021\
Data File : VX024166.D
Acq On : 10 Sep 2021 15:22
Operator : JC/MD
Sample : M3689-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 256

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Decane, 4-methyl-	12.079	8.5	ug/l	144979	4	12.024	852879	50.0
Decane, 2-methyl-	12.103	9.3	ug/l	158935	4	12.024	852879	50.0
Decane, 3-methyl-	12.177	9.1	ug/l	155615	4	12.024	852879	50.0
Undecane	12.427	85.6	ug/l	1459650	4	12.024	852879	50.0
Benzene, 1-meth...	12.561	9.5	ug/l	162719	4	12.024	852879	50.0
Hexadecane	12.585	7.2	ug/l	122181	4	12.024	852879	50.0
Cyclohexane, pe...	12.890	16.6	ug/l	283277	4	12.024	852879	50.0
Benzene, 1,2,4,...	12.969	14.6	ug/l	249459	4	12.024	852879	50.0
Dodecane	13.268	19.4	ug/l	330444	4	12.024	852879	50.0
Naphthalene, 1,...	13.426	7.2	ug/l	122732	4	12.024	852879	50.0