LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

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\82Y102623S.M
Title : SW846 8260

Signal : TIC: VY016117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.906	169	178	194	rBV	244397	536608	1.07%	0.119%
2	4.771	463	484	512	rVB2	232661	1203967	2.39%	0.267%
3	5.247	542	562	579	rBV2	156654	566525	1.13%	0.126%
4	5.753	631	645	665	rBV	377169	1182503	2.35%	0.262%
5	6.801	807	817	836	rVB	422284	1327543	2.64%	0.294%
6	7.789	970	979	988	rVB4	1332414	3801278	7.56%	0.843%
7	8.008	1003	1015	1021	rBV	554494	1343843	2.67%	0.298%
8	8.167	1030	1041	1053	rVB	16097779	35895223	71.40%	7.959%
9	8.283	1053	1060	1066	rBV2	230766	524750	1.04%	0.116%
10	8.423	1077	1083	1093	rVB2	353161	850739	1.69%	0.189%
11	8.551	1095	1104	1117	rBV	1336532	2607294	5.19%	0.578%
12	8.691	1119	1127	1135	rBV	361055	737721	1.47%	0.164%
13	9.191	1193	1209	1215	rBV	3350314	7372197	14.66%	1.635%
14	9.825	1307	1313	1325	rVB2	1021778	2342051	4.66%	0.519%
15	9.965	1325	1336	1347	rBV	890828	2100681	4.18%	0.466%
16	10.069	1347	1353	1365	rBV3	218143	560476	1.11%	0.124%
17	10.179	1365	1371	1376	rBV2	1549252	3026122	6.02%	0.671%
18	10.252	1376	1383	1390	rVV	24600391	48157607	95.79%	10.677%
19	10.374	1394	1403	1410	rVB2	2374215	4326020	8.61%	0.959%
20	10.526	1418	1428	1434	rVB2	628031	1316316	2.62%	0.292%
21	10.618	1434	1443	1448	rBV3	354871	763014	1.52%	0.169%
22	10.807	1464	1474	1480	rBV	425710	764913	1.52%	0.170%
23	10.904	1484	1490	1498	rBV	380926	869706	1.73%	0.193%
24	11.038	1504	1512	1517	rVV	793327	1352592	2.69%	0.300%
25	11.093	1517	1521	1526	rVB	707455	1130348	2.25%	0.251%
26	11.209	1534	1540	1544	rBV2	415309	721976	1.44%	0.160%
27	11.282	1544	1552	1563	rVV4	1151013	2591950	5.16%	0.575%
28	11.386	1563	1569	1579	rVB	819720	1413115	2.81%	0.313%
29	11.496	1580	1587	1591	rBV	454171	790579	1.57%	0.175%
30	11.593	1596	1603	1612	rBV	4788452	7771180	15.46%	1.723%
31	11.703	1612	1621	1632	rVV	20120447	38388090	76.36%	8.511%
32	11.892	1647	1652	1656	rVV4	314462	679619	1.35%	0.151%
33	12.032	1664	1675	1683	rBV	12084410	21323594	42.42%	4.728%
34	12.123	1687	1690	1694	rVV	391571	537815	1.07%	0.119%
35	12.203	1694	1703	1706	rVV5	526652	1159901	2.31%	0.257%
36	12.245	1707	1710	1715	rVB3	466474	813546	1.62%	0.180%

LSC Area Percent Report

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ClientSampleId :
1079

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Title : SW846 8260

37	12.331	1720	1724	1728	rBV	526870	894195	1.78%	0.198%
38	12.416	1728	1738	1740	rBV5	543686	1446692	2.88%	0.321%
39	12.483	1746	1749	1753	rVV3	446581	677745	1.35%	0.150%
40	12.526	1753	1756	1760	rVB	393359	524131	1.04%	0.116%
41	12.672	1772	1780	1785	rVB2	900108	2089962	4.16%	0.463%
42	12.739	1785	1791	1794	rBV	3671401	5969246	11.87%	1.323%
43	12.770	1794	1796	1798	rVV	1275491	1514932	3.01%	0.336%
44	12.812	1798	1803	1809	rVB2	6808964	10575221	21.04%	2.345%
45	12.977	1817	1830	1837	rBV2	2480297	6606152	13.14%	1.465%
46	13.044	1837	1841	1844	rVV	765735	1238495	2.46%	0.275%
47	13.123	1848	1854	1859	rVV	9282929	14666948	29.18%	3.252%
48	13.172	1859	1862	1867	rVV	1190727	1630193	3.24%	0.361%
49	13.227	1867	1871	1879	rVB4	417827	1056646	2.10%	0.234%
50	13.318	1879	1886	1890	rBV2	992472	1819677	3.62%	0.403%
51	13.367	1890	1894	1897	rVV3	708101	1169609	2.33%	0.259%
52	13.459	1901	1909	1914	rVV	4856485	8250386	16.41%	1.829%
53	13.501	1914	1916	1923	rVB3	593508	784524	1.56%	0.174%
54	13.629	1933	1937	1940	rBV2	1309958	1905659	3.79%	0.423%
55	13.666	1940	1943	1951	rVB2	1993703	3184357	6.33%	0.706%
56	13.751	1952	1957	1962	rBV	3438756	5086923	10.12%	1.128%
57	13.812	1962	1967	1973	rVB	6887674	10970819	21.82%	2.432%
58	13.891	1975	1980	1981	rBV	877573	1249138	2.48%	0.277%
59	13.916	1982	1984	1989	rVB2	1200779	1560230	3.10%	0.346%
60	13.971	1989	1993	1998	rVB	1285447	1752102	3.49%	0.388%
61	14.019	1998	2001	2006	rVB3	416492	712367	1.42%	0.158%
62	14.080	2006	2011	2015	rBV	1646228	2474389	4.92%	0.549%
63	14.135	2015	2020	2028	rVB6	599305	1593470	3.17%	0.353%
64	14.221	2028	2034	2036	rBV2	815918	1503917	2.99%	0.333%
65	14.294	2037	2046	2050	rVV4	1333920	4250429	8.45%	0.942%
66	14.336	2050	2053	2057	rVB	2138412	2965496	5.90%	0.658%
67	14.385	2057	2061	2064	rBV2	1359224	1899569	3.78%	0.421%
68	14.422	2064	2067	2071	rVB2	924897	1145213	2.28%	0.254%
69	14.568	2087	2091	2094	rBV2	501749	870630	1.73%	0.193%
70	14.617	2094	2099	2103	rVB	4505829	6071386	12.08%	1.346%
71	14.678	2103	2109	2114	rBV3	3054850	6296771	12.53%	1.396%
72	14.739	2114	2119	2125	rVB3	2089428	4668037	9.29%	1.035%
73	14.836	2130	2135	2139	rVB	1780740	2761720	5.49%	0.612%
74	14.946	2149	2153	2157	rBV5	1053480	1598420	3.18%	0.354%
75	15.056	2166	2171	2176	rBV5	988082	1994463	3.97%	0.442%
76	15.141	2181	2185	2191	rVB5	1317770	2470556	4.91%	0.548%

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Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

77	15.239	2191	2201	2212	rBV2	24236381	50271933	100.00%	11.146%
78	15.342	2212	2218	2224	rBV2	1212798	2505864	4.98%	0.556%
79	15.440	2230	2234	2242	rVB	4070484	5996849	11.93%	1.330%
80	15.531	2243	2249	2256	rBV4	759276	2153671	4.28%	0.478%
81	15.696	2268	2276	2285	rBV7	625957	2164194	4.30%	0.480%
82	16.031	2325	2331	2336	rVB3	581624	1286541	2.56%	0.285%
83	16.159	2348	2352	2358	rVB	609205	999683	1.99%	0.222%
84	16.232	2359	2364	2367	rVV	461098	892446	1.78%	0.198%
85	16.293	2367	2374	2382	rVV	13572817	27865729	55.43%	6.178%
86	16.361	2382	2385	2390	rVB	755457	1232031	2.45%	0.273%
87	16.495	2399	2407	2419	rVB	11297331	23971247	47.68%	5.315%
88	16.598	2421	2424	2439	rVB8	291881	932482	1.85%	0.207%

Sum of corrected areas: 451024887

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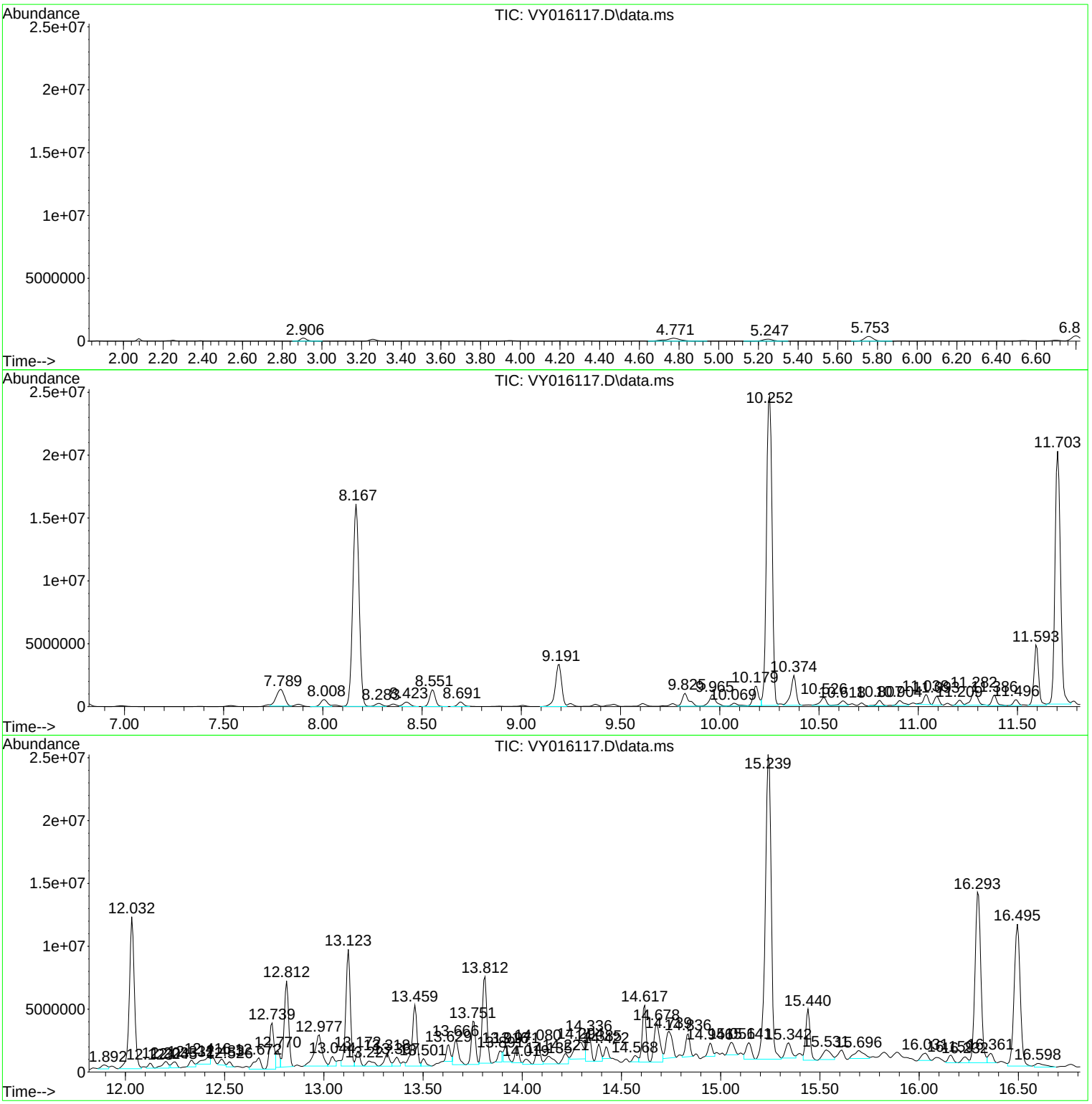
Instrument :
MSVOA_Y
ClientSampleId :
1079

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
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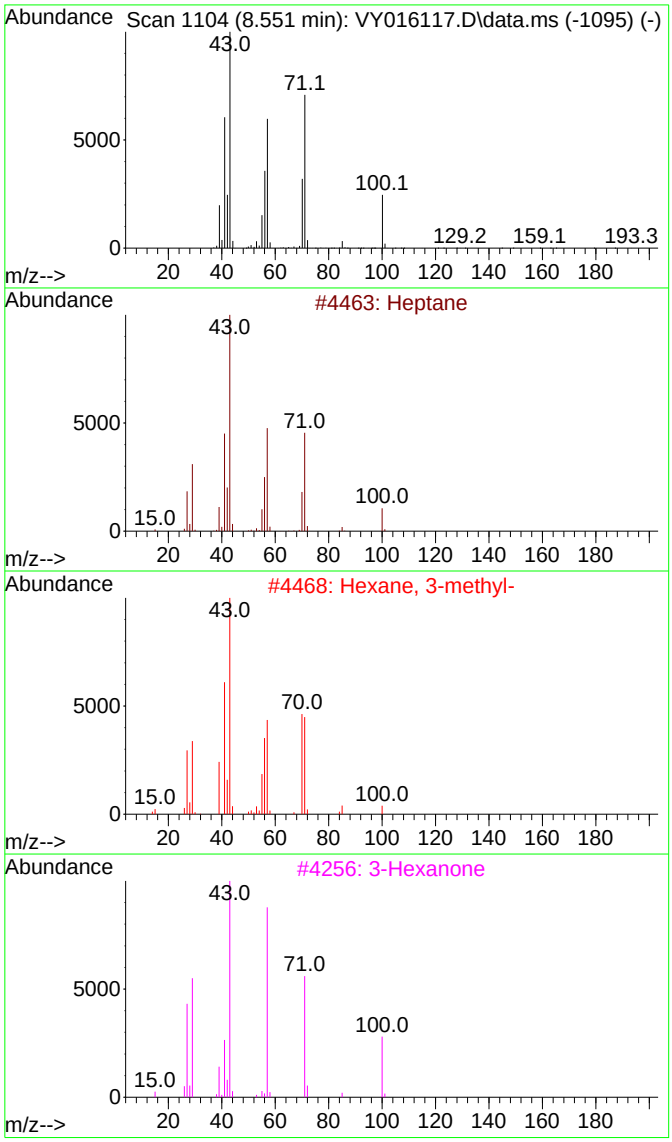
Quant Title : SW846 8260

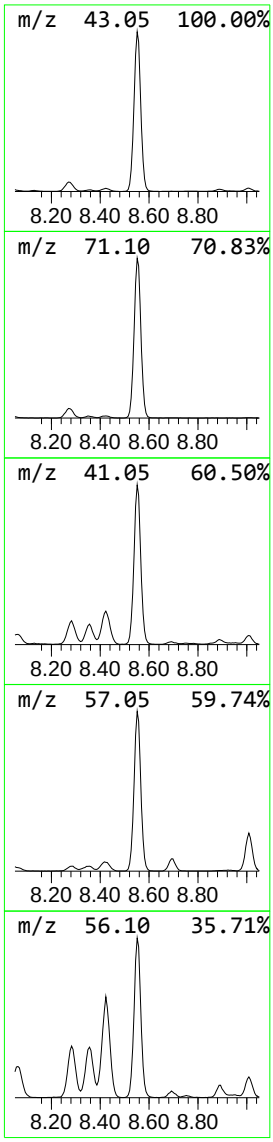
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	176.71 ug/l	2607290	1,4-Difluorobenzene	8.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3	3-Hexanone	100	C6H12O	000589-38-8	50
4	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	43





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Data File : VY016117.D
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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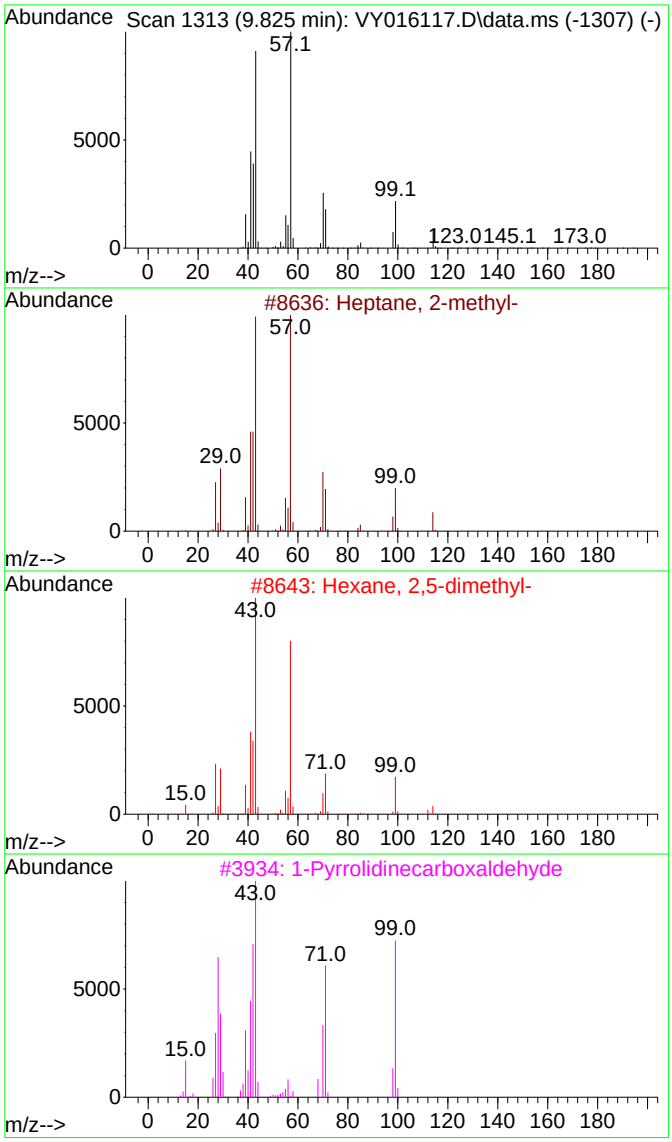
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

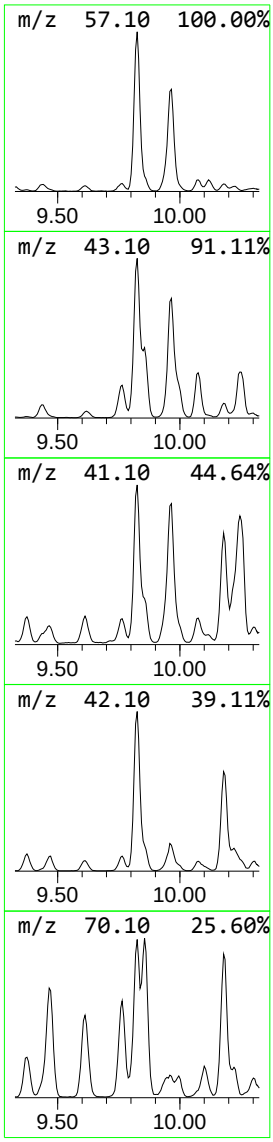
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Heptane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.825	158.74 ug/l	2342050	1,4-Difluorobenzene	8.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	97
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	58
3	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	38
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	38
5	Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	38





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Instrument :
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ClientSampleId :
1079

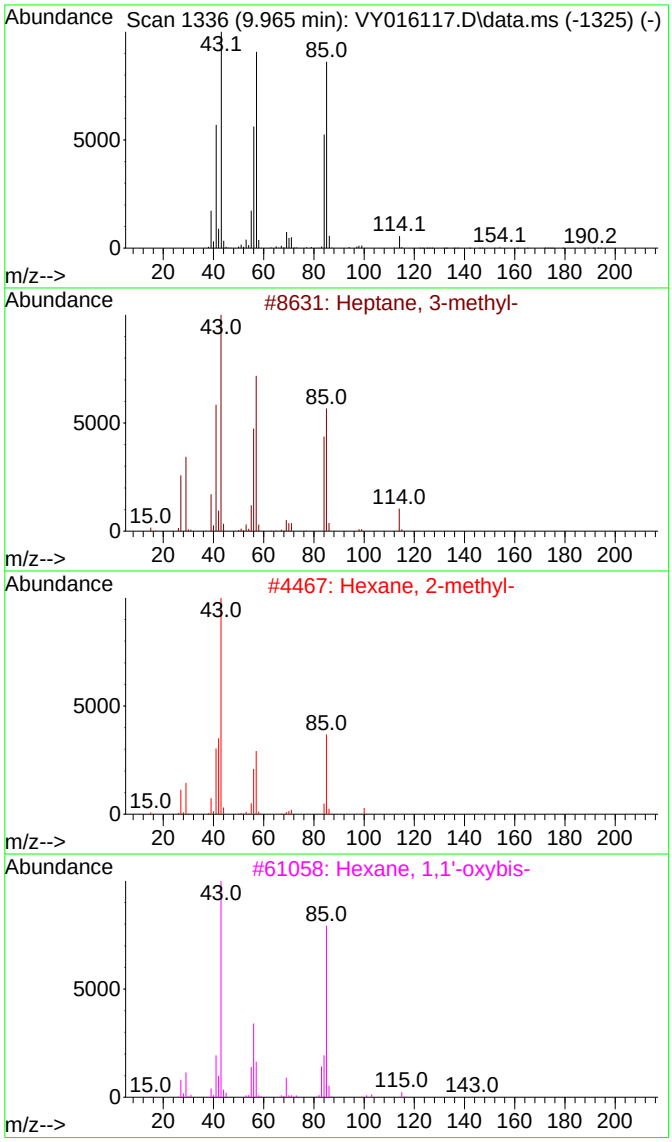
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

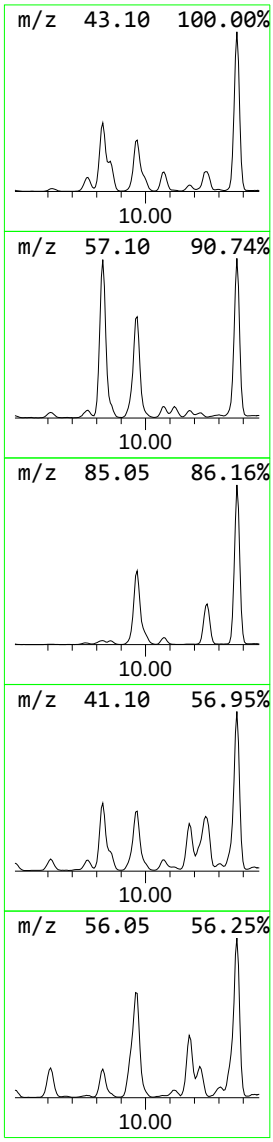
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.965	142.38 ug/l	2100680	1,4-Difluorobenzene	8.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	94
2	Hexane, 2-methyl-	100	C7H16	000591-76-4	64
3	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	59
4	Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	59
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53





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MSVOA_Y
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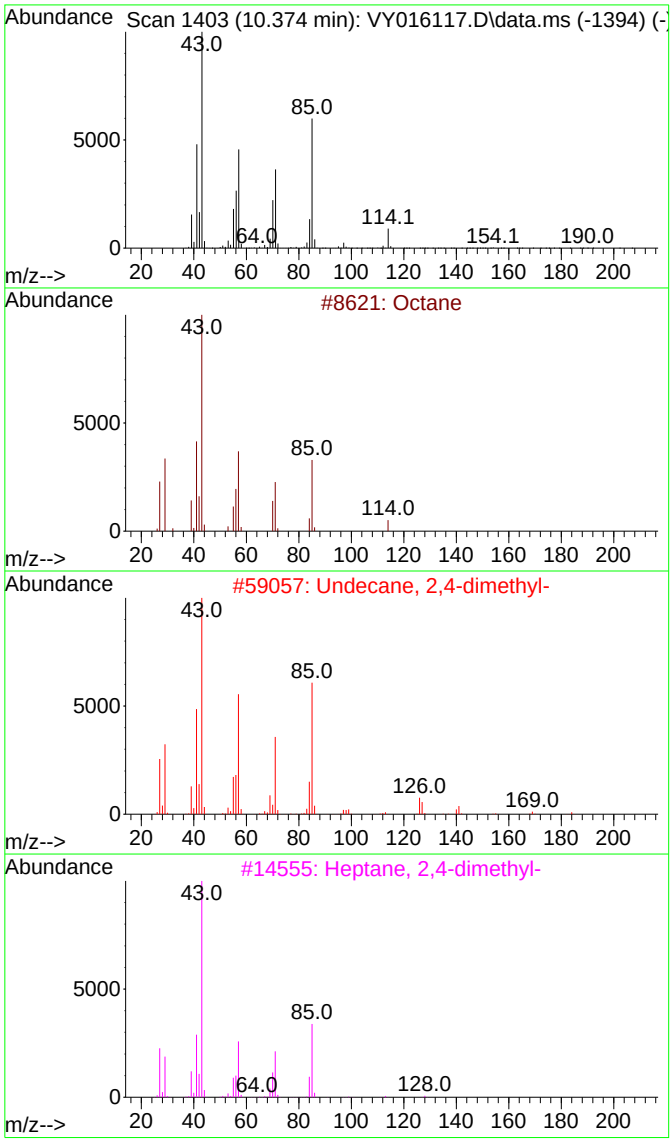
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

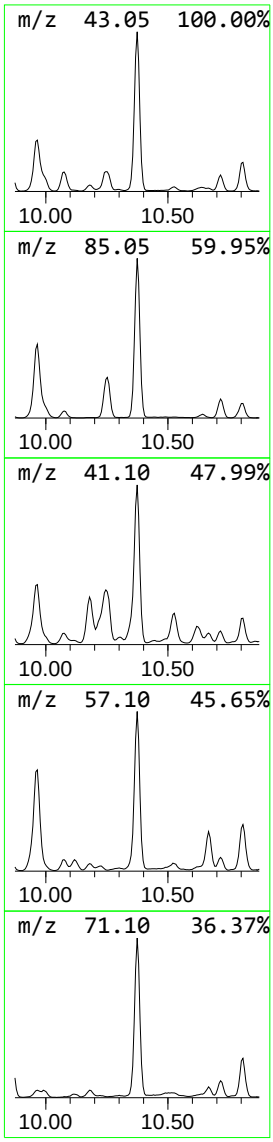
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	273.60 ug/l	4326020	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	94
2	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	59
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
4	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	58
5	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	50





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

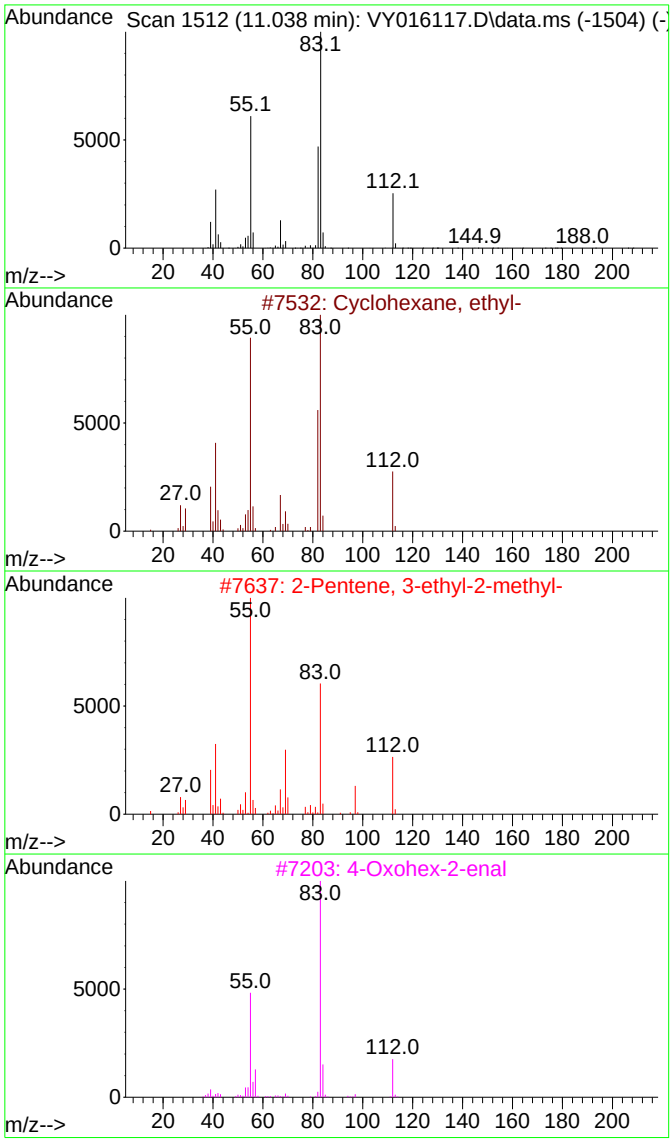
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

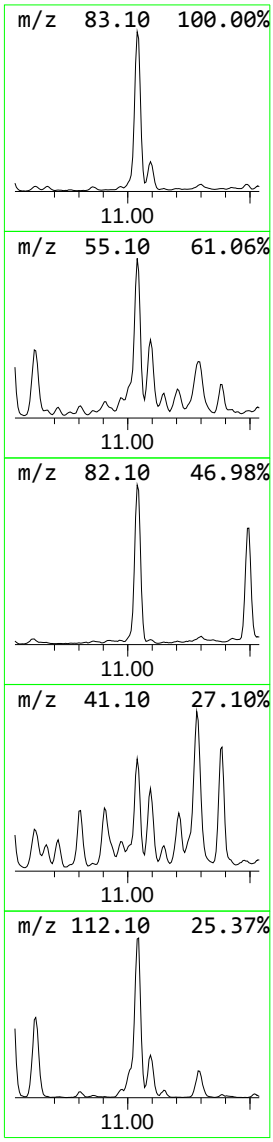
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.038	85.54 ug/l	1352590	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	91
2	2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	64
3	4-Oxohex-2-enal	112	C6H8O2	020697-55-6	58
4	3-Hexene, 2,2-dimethyl-, (Z)-	112	C8H16	000690-92-6	53
5	2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	53





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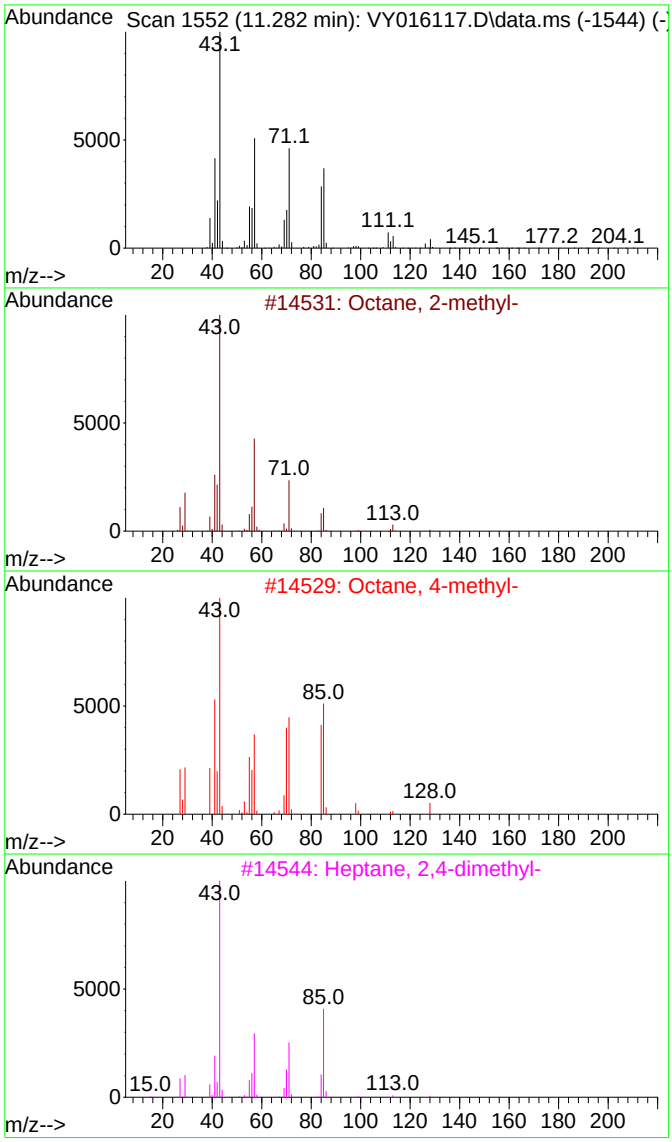
Quant Title : SW846 8260

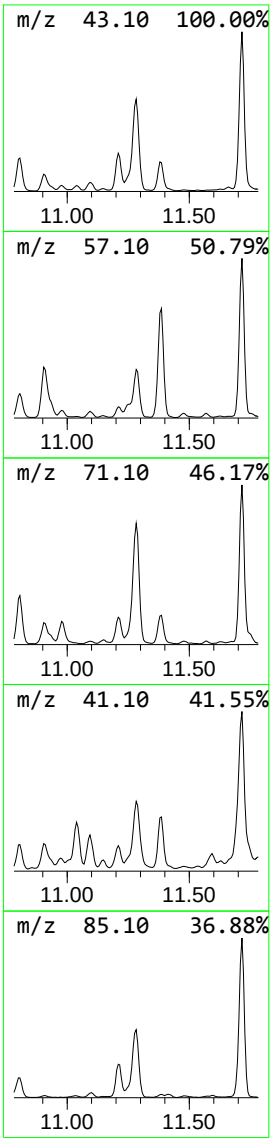
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	163.93 ug/l	2591950	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	64
2	Octane, 4-methyl-	128	C9H20	002216-34-4	52
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	50
5	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

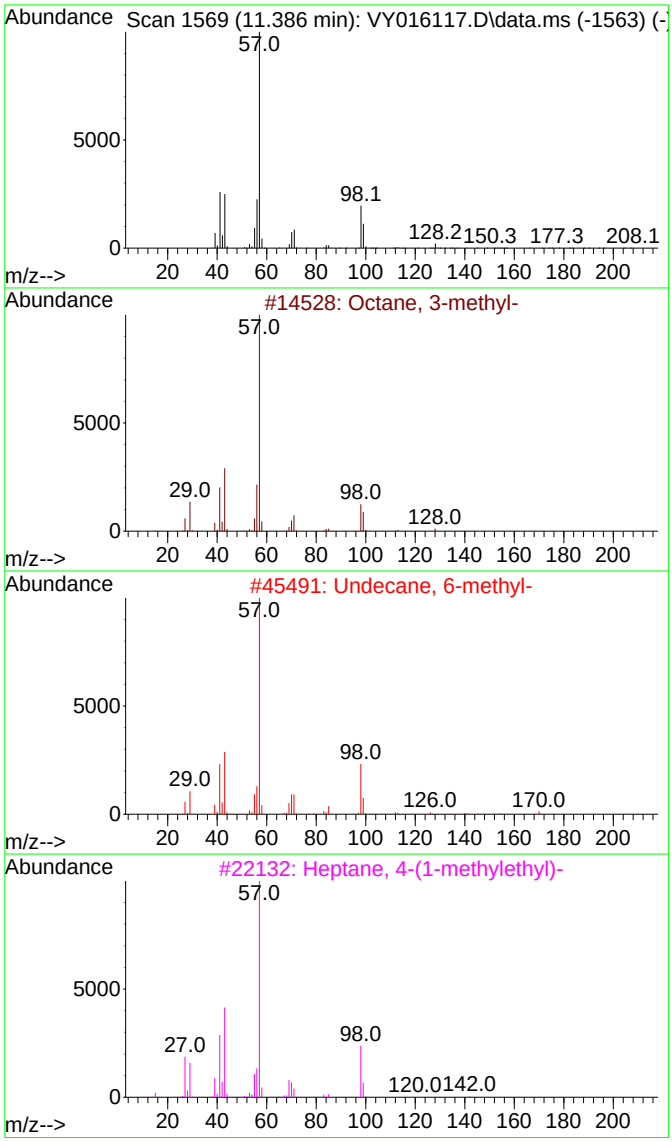
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

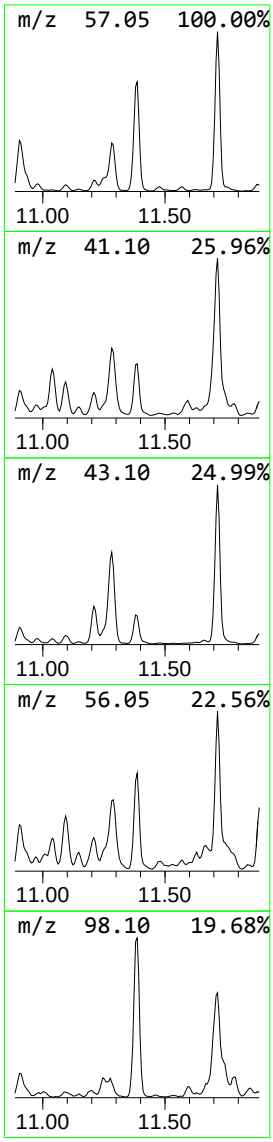
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Octane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.386	89.37 ug/l	1413120	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	87
2	Undecane, 6-methyl-	170	C12H26	017302-33-9	64
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	59
5	Heptane, 3-ethyl-	128	C9H20	015869-80-4	53





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Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

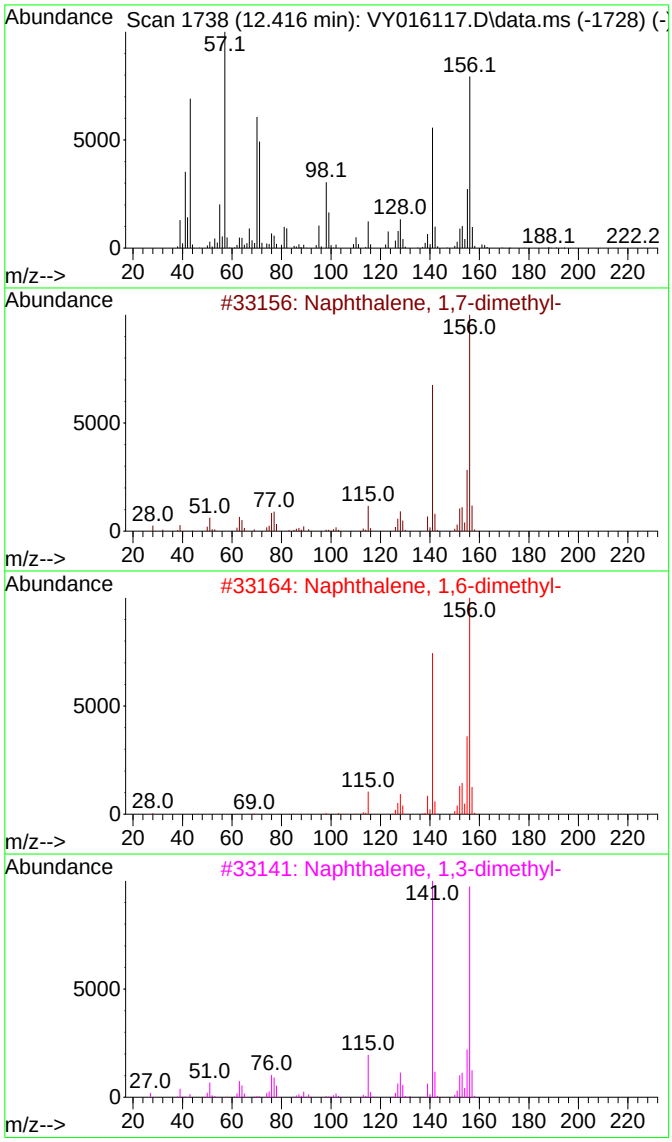
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

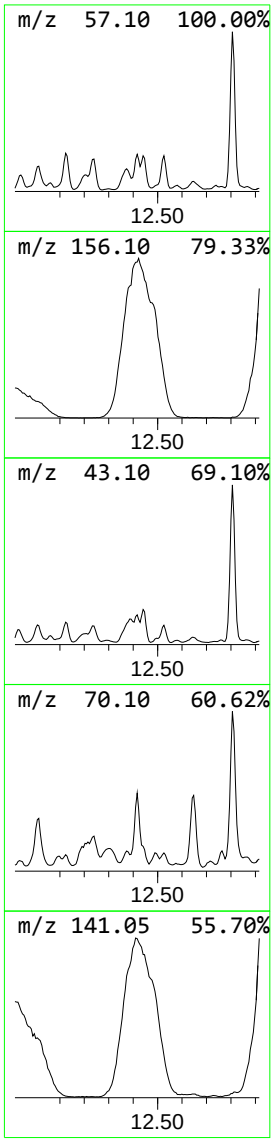
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,7-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	91.50 ug/l	1446690	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

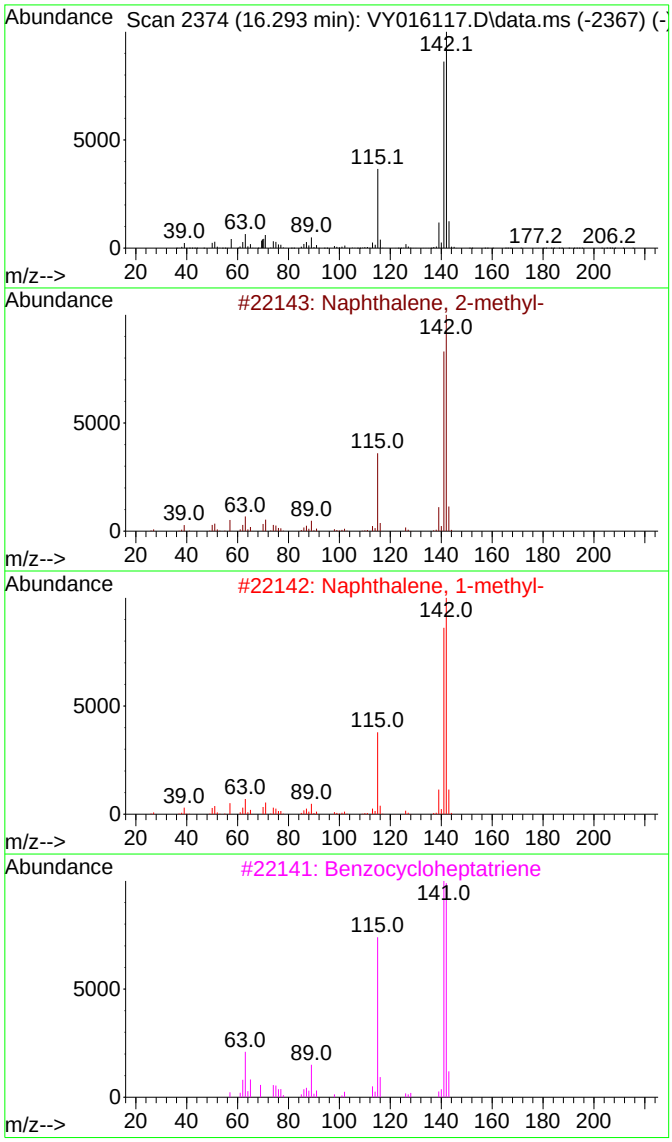
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

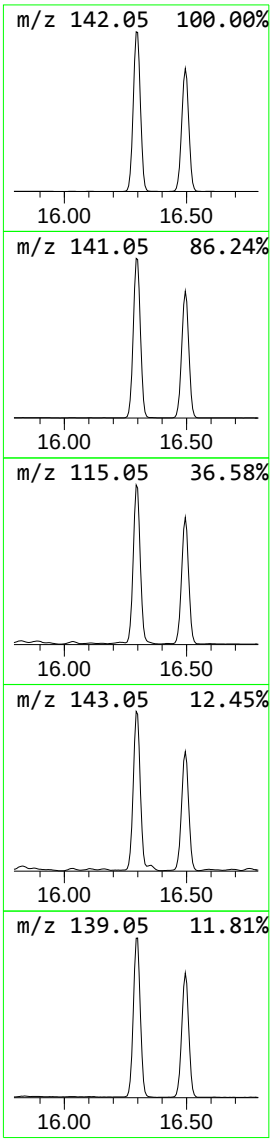
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.294	168.88 ug/l	27865700	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

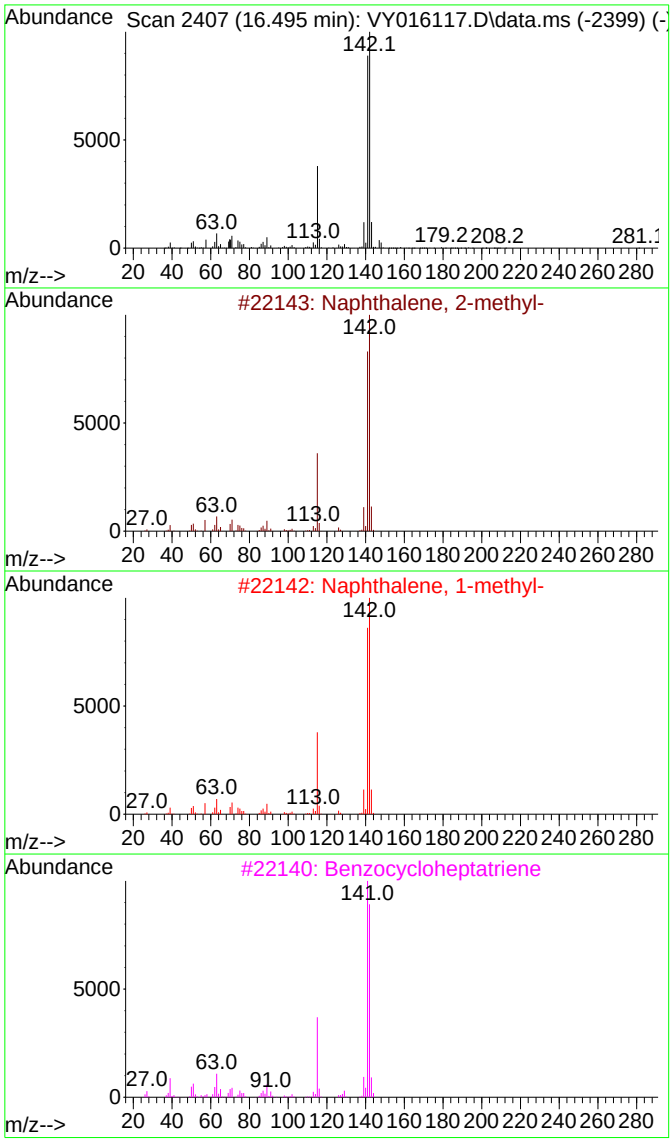
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.M
Quant Title : SW846 8260

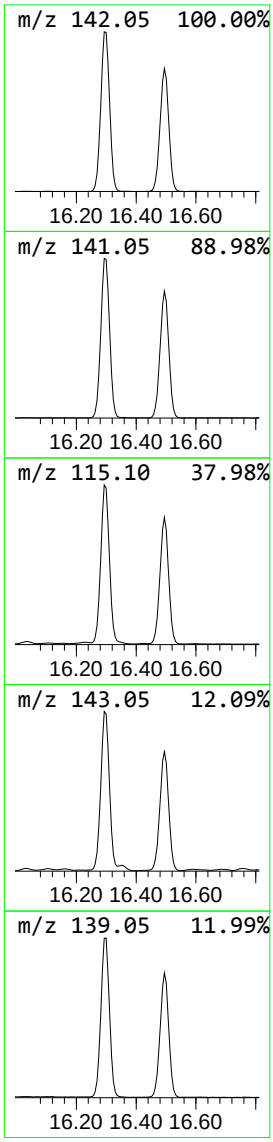
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.495	145.27 ug/l	23971200	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102723\
Data File : VY016117.D
Acq On : 27 Oct 2023 20:27
Operator : SY/MD
Sample : 05107-09
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1079

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102623S.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
Heptane	8.551	176.7	ug/l	2607290	2	8.697	737721	50.0
Heptane, 2-methyl-	9.825	158.7	ug/l	2342050	2	8.697	737721	50.0
Heptane, 3-methyl-	9.965	142.4	ug/l	2100680	2	8.697	737721	50.0
Octane	10.374	273.6	ug/l	4326020	3	11.496	790579	50.0
Cyclohexane, et...	11.038	85.5	ug/l	1352590	3	11.496	790579	50.0
Octane, 2-methyl-	11.282	163.9	ug/l	2591950	3	11.496	790579	50.0
Octane, 3-methyl-	11.386	89.4	ug/l	1413120	3	11.496	790579	50.0
Naphthalene, 1,...	12.416	91.5	ug/l	1446690	3	11.496	790579	50.0
Naphthalene, 2-...	16.294	168.9	ug/l	27865700	4	13.428	8250390	50.0
Naphthalene, 1-...	16.495	145.3	ug/l	23971200	4	13.428	8250390	50.0