LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

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_N\methods\82N062724W.M
Title : SW846 8260

Signal : TIC: VN082764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.218	1058	1065	1075	rVB2	524988	1259196	5.08%	1.051%
2	8.324	1075	1083	1093	rVB	213304	517030	2.09%	0.432%
3	8.441	1093	1103	1113	rBV	878405	1985840	8.02%	1.658%
4	8.700	1136	1147	1154	rBV3	142251	393649	1.59%	0.329%
5	8.965	1183	1192	1206	rVB	376746	734922	2.97%	0.613%
6	9.100	1207	1215	1223	rBV	190866	394659	1.59%	0.329%
7	9.594	1285	1299	1304	rBV2	349066	895428	3.62%	0.747%
8	10.206	1397	1403	1416	rVB2	325057	800401	3.23%	0.668%
9	10.341	1416	1426	1439	rBV	328358	707930	2.86%	0.591%
10	10.570	1457	1465	1469	rBV	572549	1122820	4.53%	0.937%
11	10.629	1469	1475	1484	rVV	7158487	13142497	53.07%	10.970%
12	10.741	1488	1494	1502	rVB	776624	1341174	5.42%	1.120%
13	11.006	1530	1539	1548	rBV2	185170	445441	1.80%	0.372%
14	11.270	1574	1584	1592	rBV	159475	351198	1.42%	0.293%
15	11.353	1592	1598	1601	rVV3	160621	296568	1.20%	0.248%
16	11.417	1602	1609	1614	rVV2	199489	460773	1.86%	0.385%
17	11.641	1639	1647	1660	rVV3	598495	1507033	6.09%	1.258%
18	11.747	1660	1665	1672	rVB	433285	689210	2.78%	0.575%
19	11.865	1676	1685	1692	rBV	286955	546169	2.21%	0.456%
20	11.965	1694	1702	1712	rVV	3271367	5602309	22.62%	4.676%
21	12.070	1712	1720	1731	rVV	13304353	24766267	100.00%	20.673%
22	12.400	1764	1776	1784	rBV	5479832	9571411	38.65%	7.989%
23	12.700	1821	1827	1831	rBV	169347	298830	1.21%	0.249%
24	12.853	1847	1853	1862	rVB2	271075	669973	2.71%	0.559%
25	13.035	1878	1884	1889	rBV	455138	724714	2.93%	0.605%
26	13.100	1889	1895	1898	rBV	1578160	2640963	10.66%	2.204%
27	13.129	1898	1900	1903	rVV	723154	1097336	4.43%	0.916%
28	13.170	1903	1907	1914	rVB2	1052517	2001872	8.08%	1.671%
29	13.335	1927	1935	1942	rBV	737967	1401323	5.66%	1.170%
30	13.482	1954	1960	1966	rBV	3857672	6042364	24.40%	5.044%
31	13.617	1973	1983	1985	rBV2	99755	259192	1.05%	0.216%
32	13.676	1989	1993	1997	rVB2	183090	282723	1.14%	0.236%
33	13.823	2014	2018	2031	rVB2	1241128	2586024	10.44%	2.159%
34	13.953	2033	2040	2041	rBV	351208	500317	2.02%	0.418%
35	13.988	2041	2046	2049	rBV2	1104561	1987812	8.03%	1.659%
36	14.106	2062	2066	2072	rBV	633978	975448	3.94%	0.814%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
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Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
163

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_N\methods\82N062724W.M
Title : SW846 8260

37	14.182	2075	2079	2085	rVV	358407	635983	2.57%	0.531%
38	14.247	2085	2090	2092	rVV	712710	1158578	4.68%	0.967%
39	14.276	2092	2095	2099	rVV	723256	1062610	4.29%	0.887%
40	14.329	2099	2104	2111	rVB	1270080	2007261	8.10%	1.676%
41	14.441	2118	2123	2129	rVB3	604903	1063702	4.29%	0.888%
42	14.535	2132	2139	2143	rBV	920835	1651260	6.67%	1.378%
43	14.576	2143	2146	2151	rVB2	363033	511238	2.06%	0.427%
44	14.653	2151	2159	2162	rBV	874198	1602810	6.47%	1.338%
45	14.694	2162	2166	2170	rVB	1132085	1518730	6.13%	1.268%
46	14.735	2170	2173	2176	rVB	380755	457412	1.85%	0.382%
47	14.776	2176	2180	2187	rVB2	283101	538910	2.18%	0.450%
48	14.876	2193	2197	2201	rBV2	293212	400019	1.62%	0.334%
49	14.929	2201	2206	2210	rBV2	794464	1531265	6.18%	1.278%
50	15.053	2218	2227	2232	rBV4	1258225	3364993	13.59%	2.809%
51	15.100	2232	2235	2244	rVV	319071	581719	2.35%	0.486%
52	15.211	2245	2254	2261	rVV3	231898	570882	2.31%	0.477%
53	15.317	2261	2272	2285	rVV3	744194	2384490	9.63%	1.990%
54	15.441	2285	2293	2300	rVB4	562306	1368805	5.53%	1.143%
55	15.641	2313	2327	2333	rBV	1107314	2409474	9.73%	2.011%
56	15.747	2339	2345	2350	rBV2	320031	597392	2.41%	0.499%
57	15.805	2350	2355	2370	rVB5	242465	905324	3.66%	0.756%
58	15.947	2370	2379	2386	rBV2	390645	874587	3.53%	0.730%
59	16.123	2402	2409	2413	rBV3	147164	361276	1.46%	0.302%
60	16.252	2426	2431	2437	rVB	171268	321768	1.30%	0.269%
61	16.341	2438	2446	2462	rVB3	211429	706595	2.85%	0.590%
62	16.482	2463	2470	2478	rBV3	142165	403837	1.63%	0.337%
63	16.782	2513	2521	2522	rBV	1140561	1808500	7.30%	1.510%

Sum of corrected areas: 119800236

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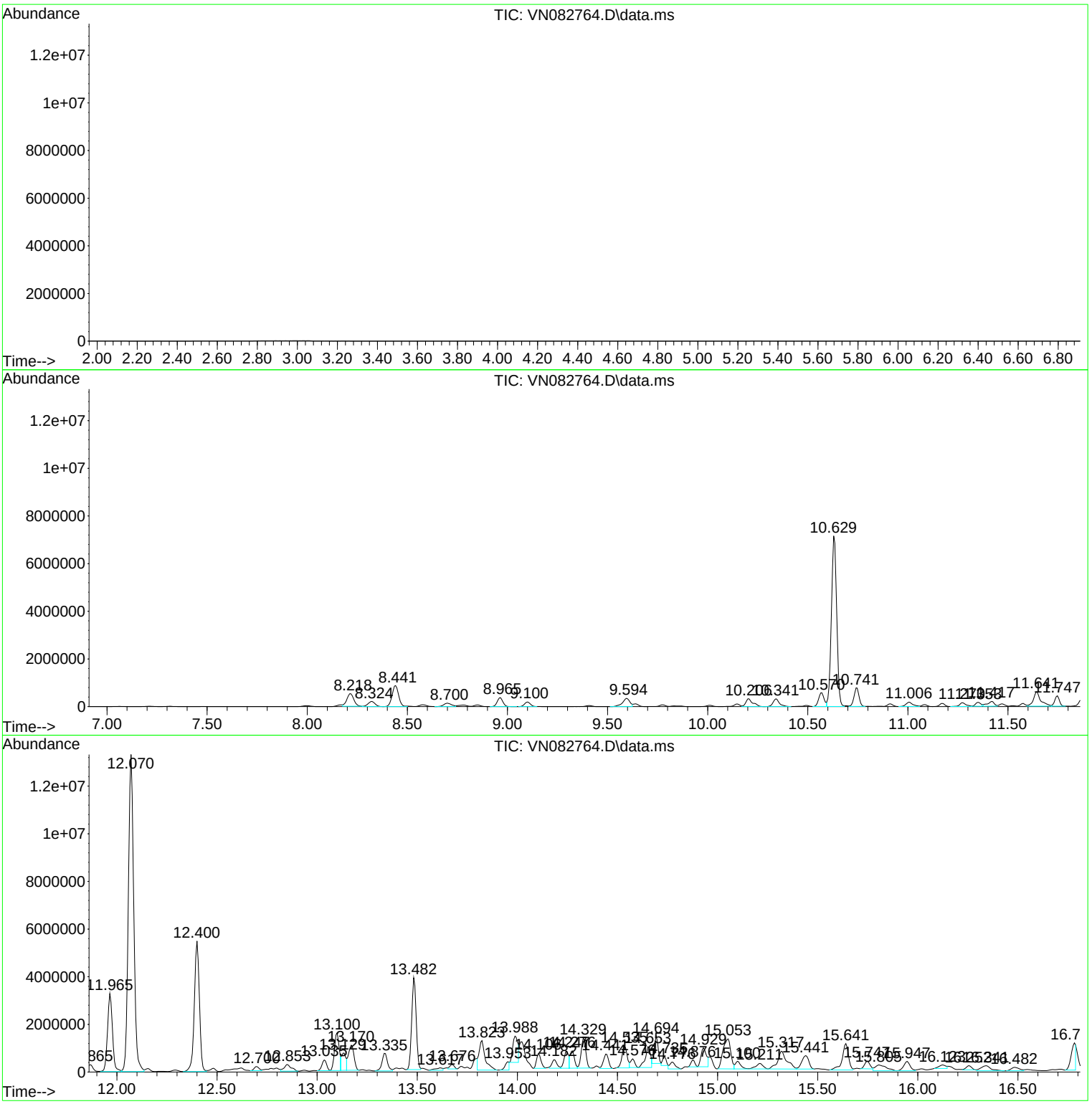
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
163

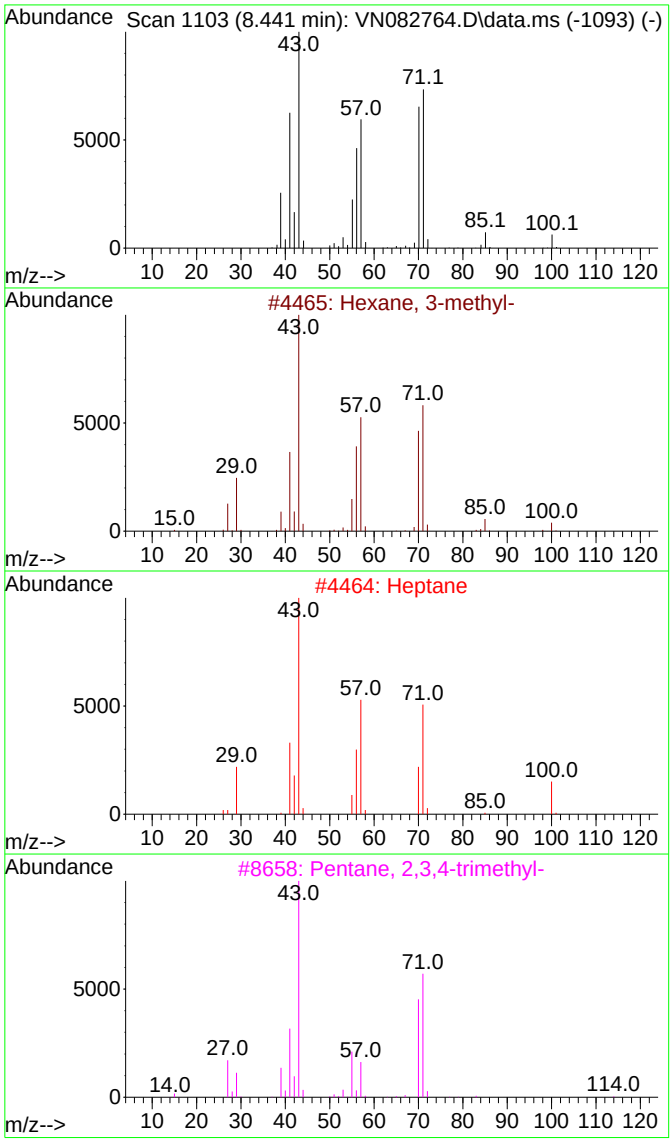
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

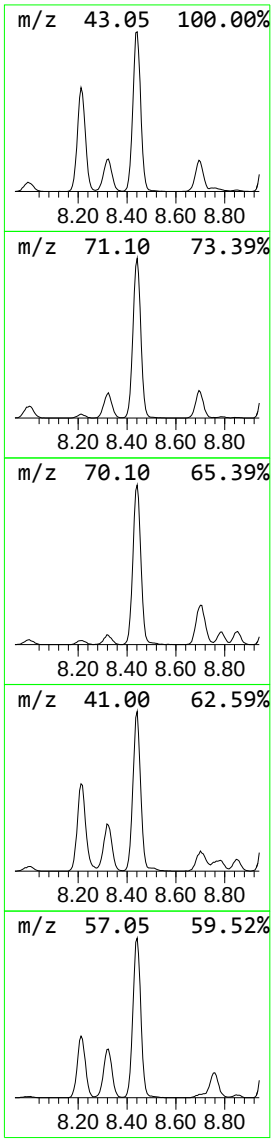
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	78.85 ug/l	1985840	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

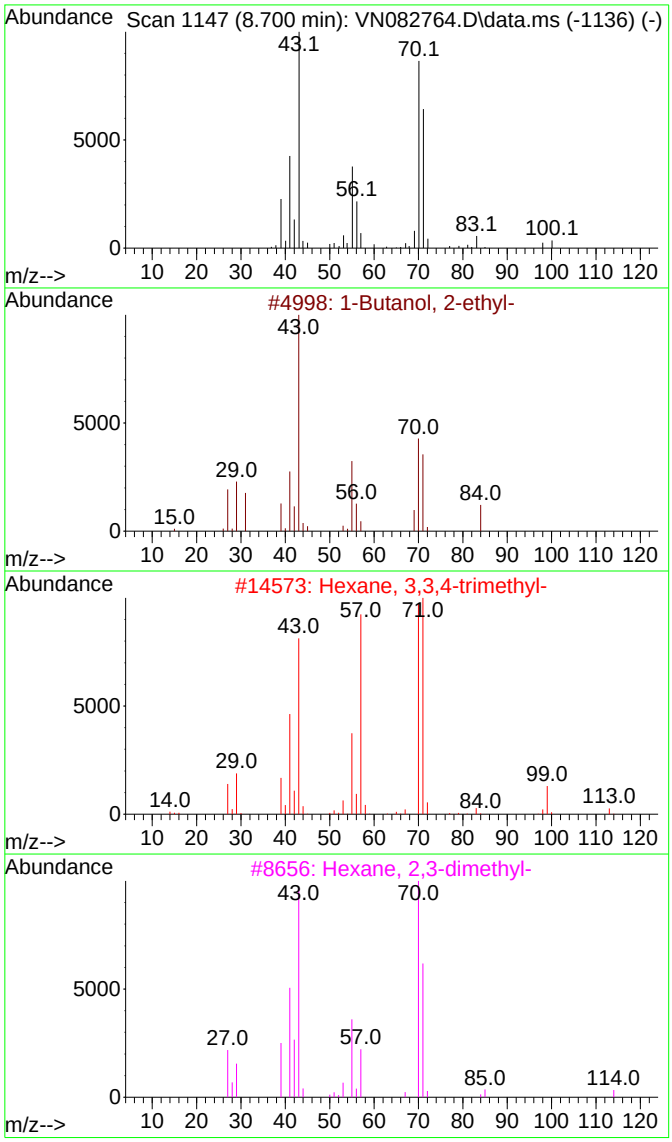
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

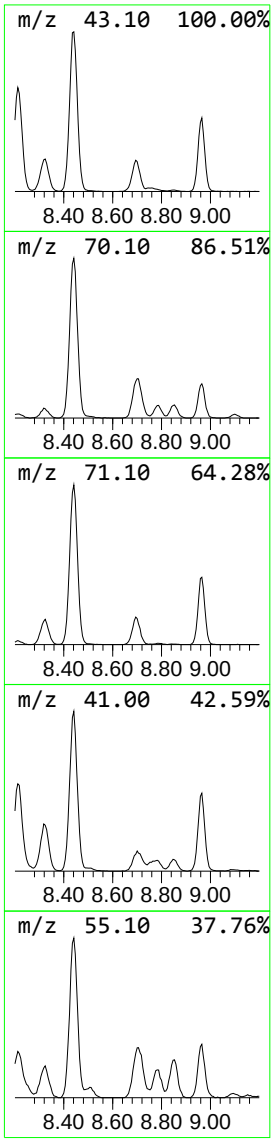
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Butanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.700	49.87 ug/l	393649	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
2	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	59
4	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	50
5	1-Butanol, 3-methyl-, acetate	130	C7H14O2	000123-92-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

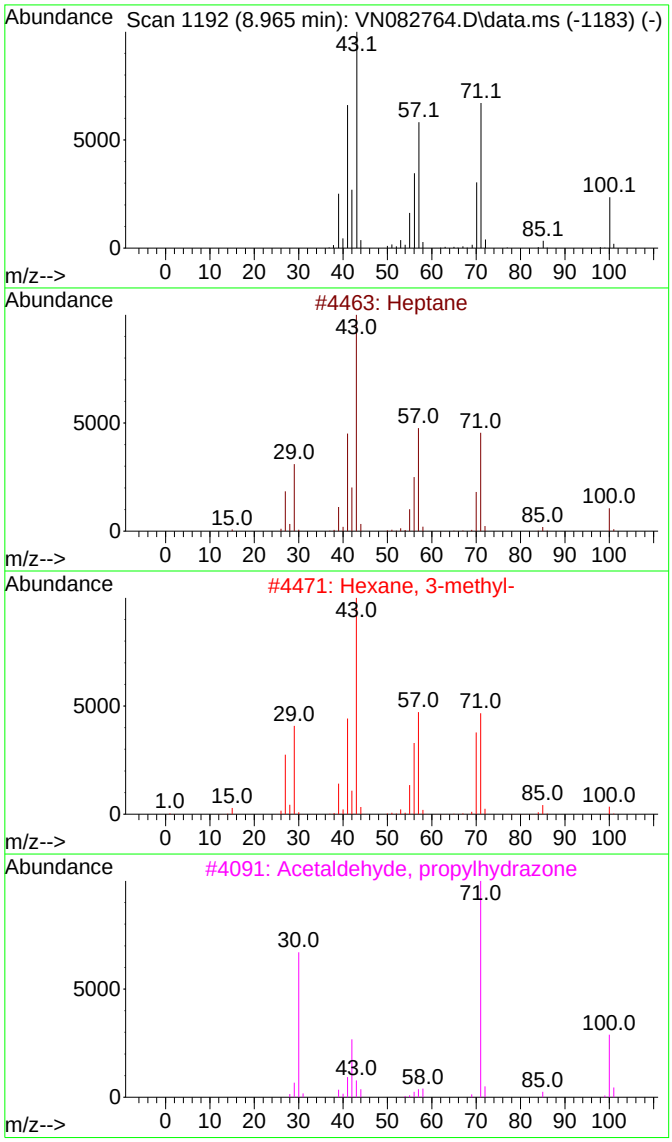
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

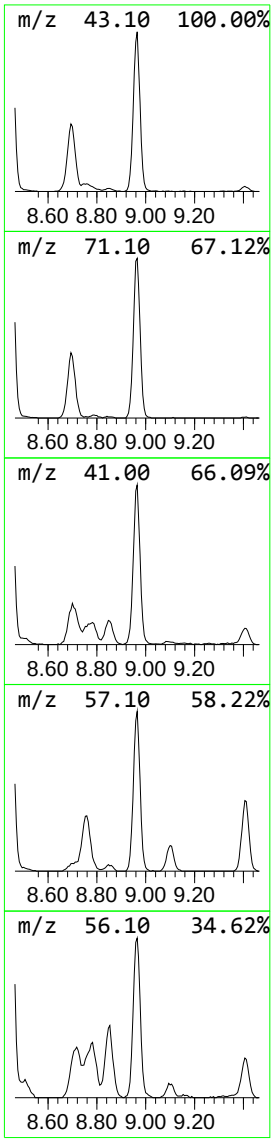
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	93.11 ug/l	734922	1,4-Difluorobenzene	9.100

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	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
4	3-Hexanone	100	C6H12O	000589-38-8	46
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

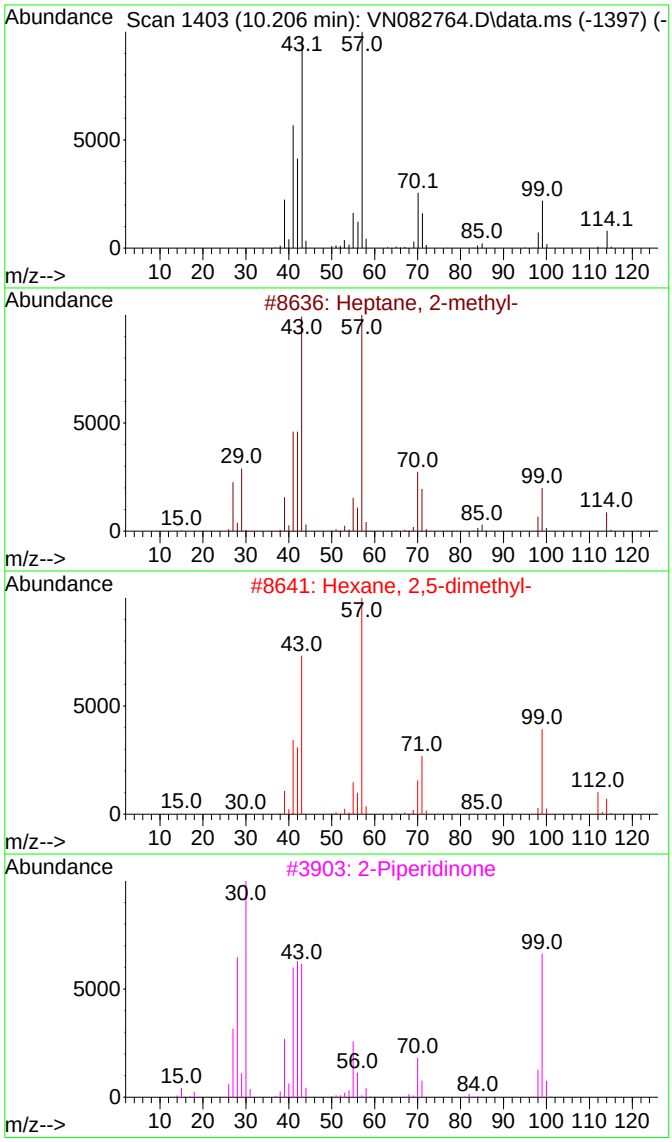
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

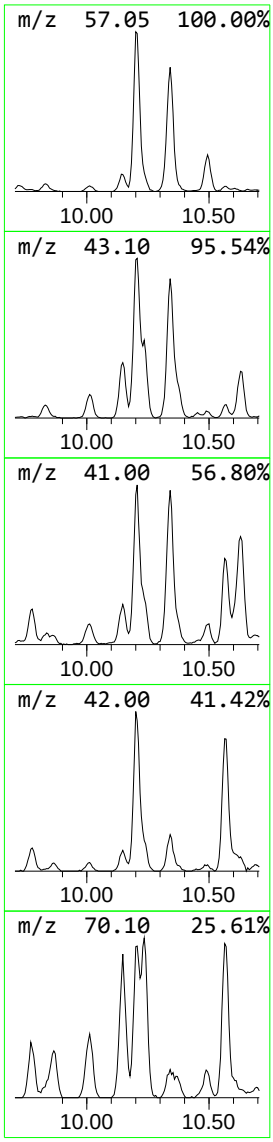
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.206	101.40 ug/l	800401	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	95
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	83
3	2-Piperidinone	99	C5H9NO	000675-20-7	59
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	38
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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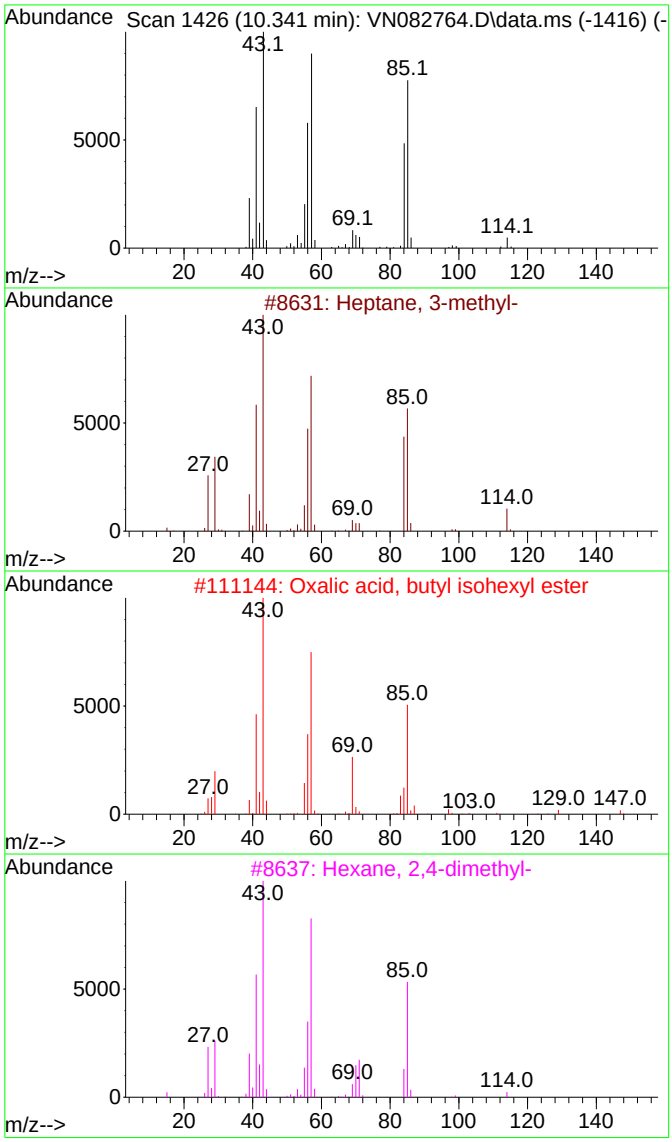
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

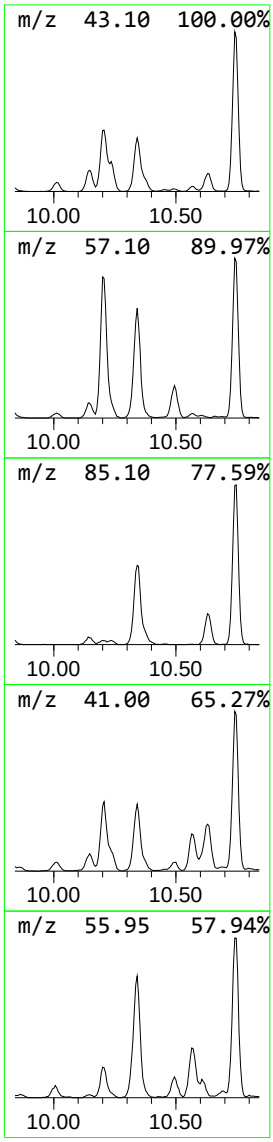
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.341	89.69 ug/l	707930	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	59
5	Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	53





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Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

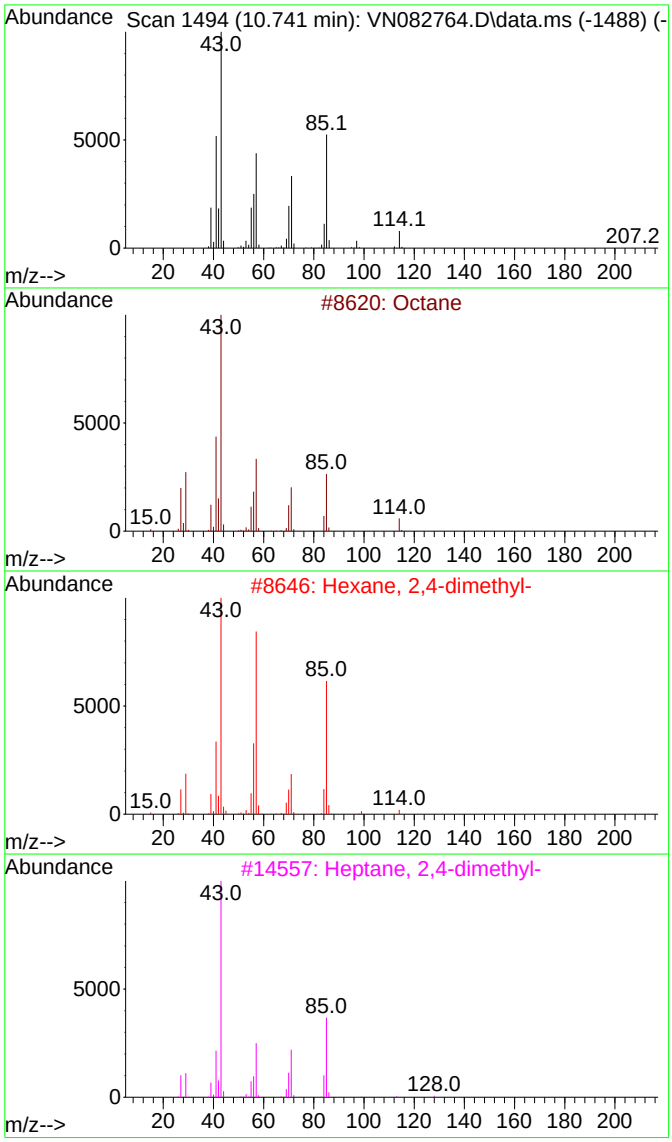
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

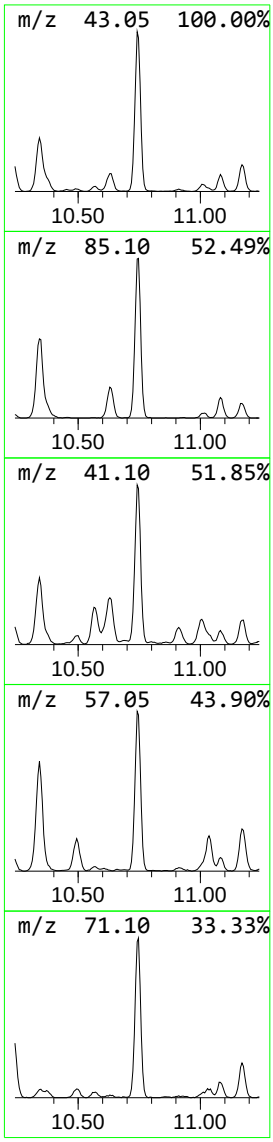
****

Peak Number 6 Octane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.741	122.78 ug/l	1341170	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	91
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
4	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	47
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

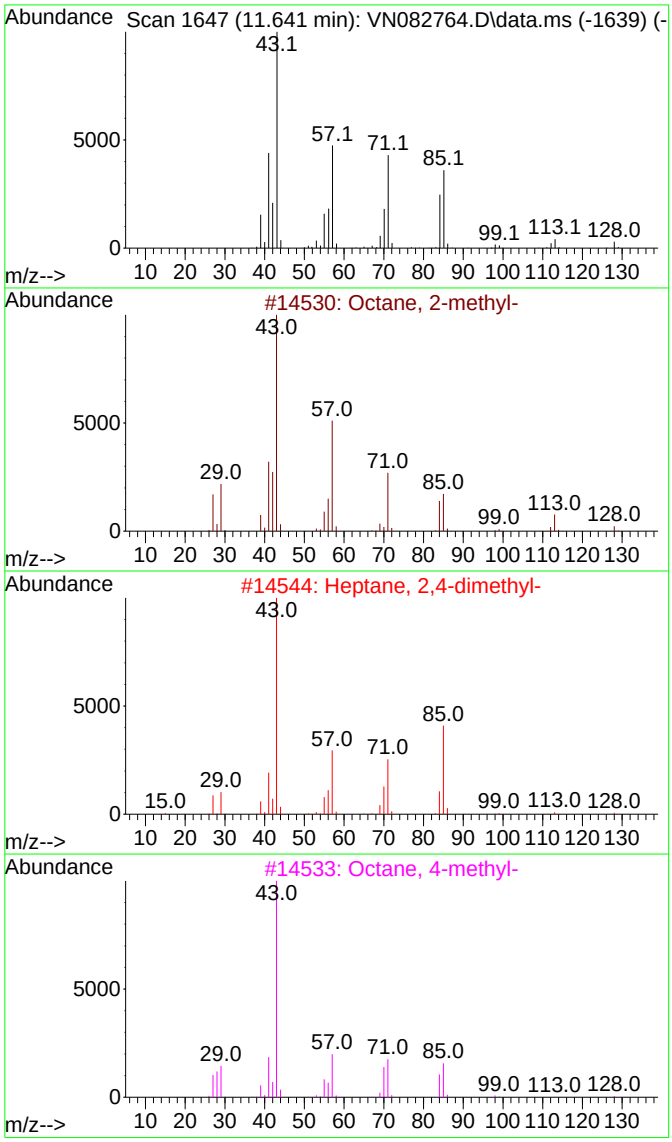
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

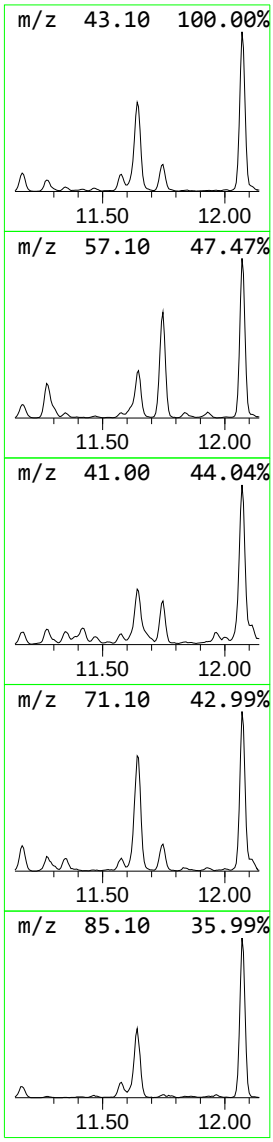
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Octane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	137.96 ug/l	1507030	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	80
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Octane, 4-methyl-	128	C9H20	002216-34-4	64
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Octane	114	C8H18	000111-65-9	53





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Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

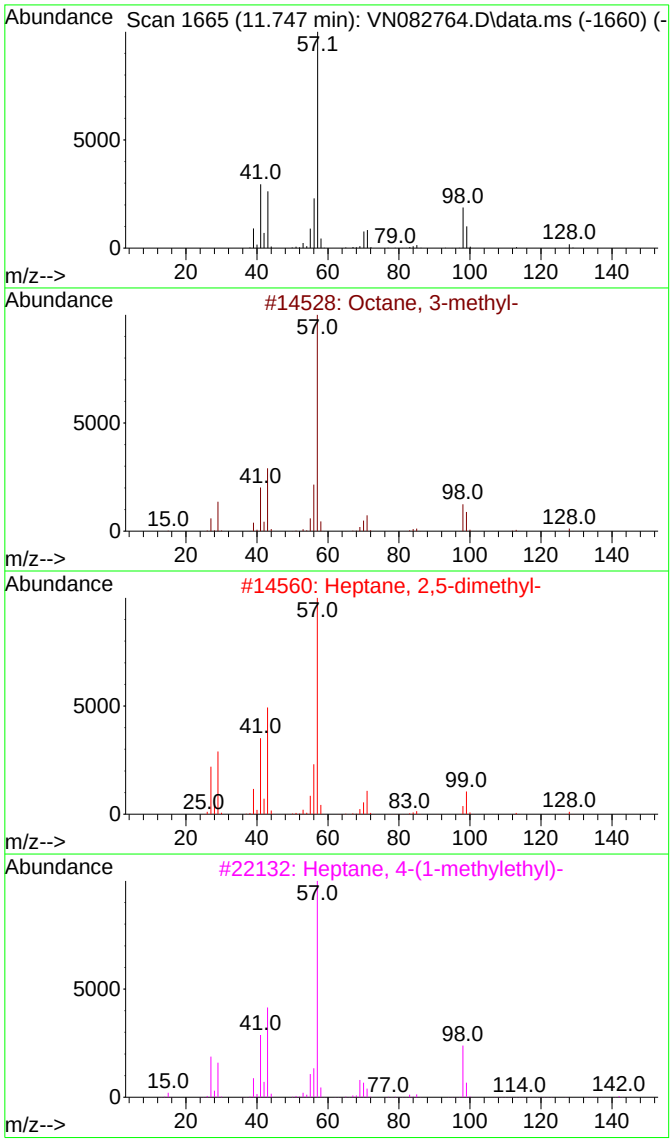
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

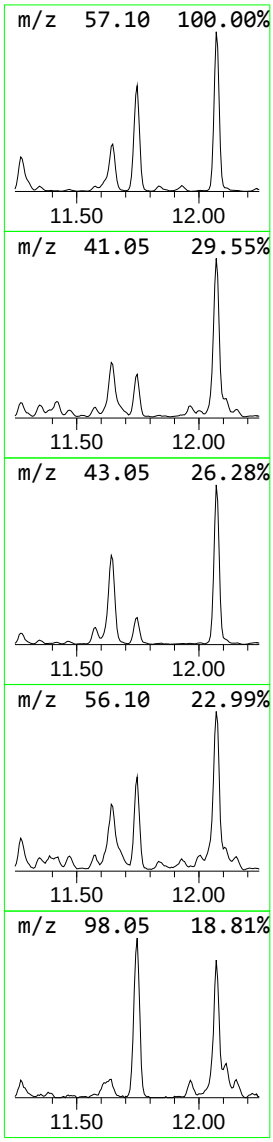
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Octane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.747	63.09 ug/l	689210	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	87
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	72
4	Undecane, 6-methyl-	170	C12H26	017302-33-9	64
5	Heptane, 4-propyl-	142	C10H22	003178-29-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
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Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

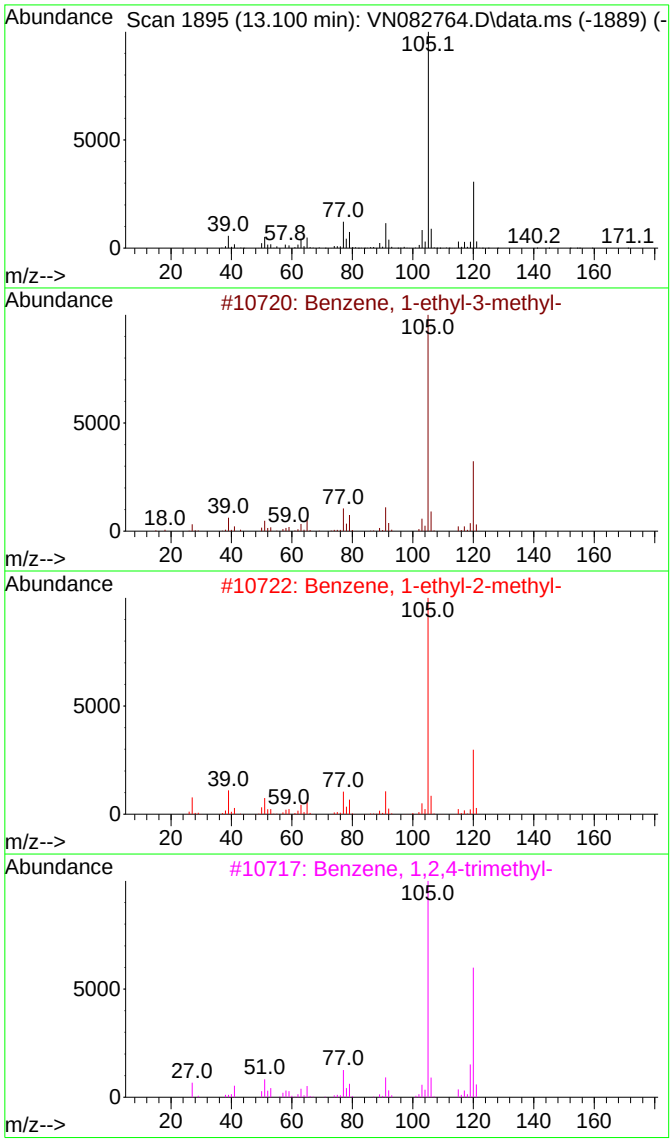
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

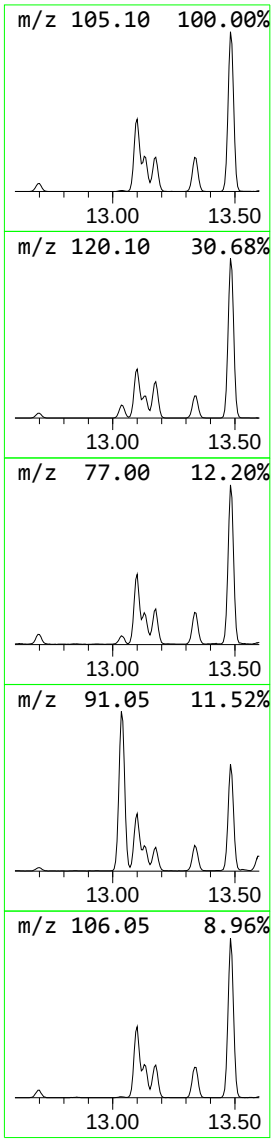
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	51.06 ug/l	2640960	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
Operator : JC\MD
Sample : P3110-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
163

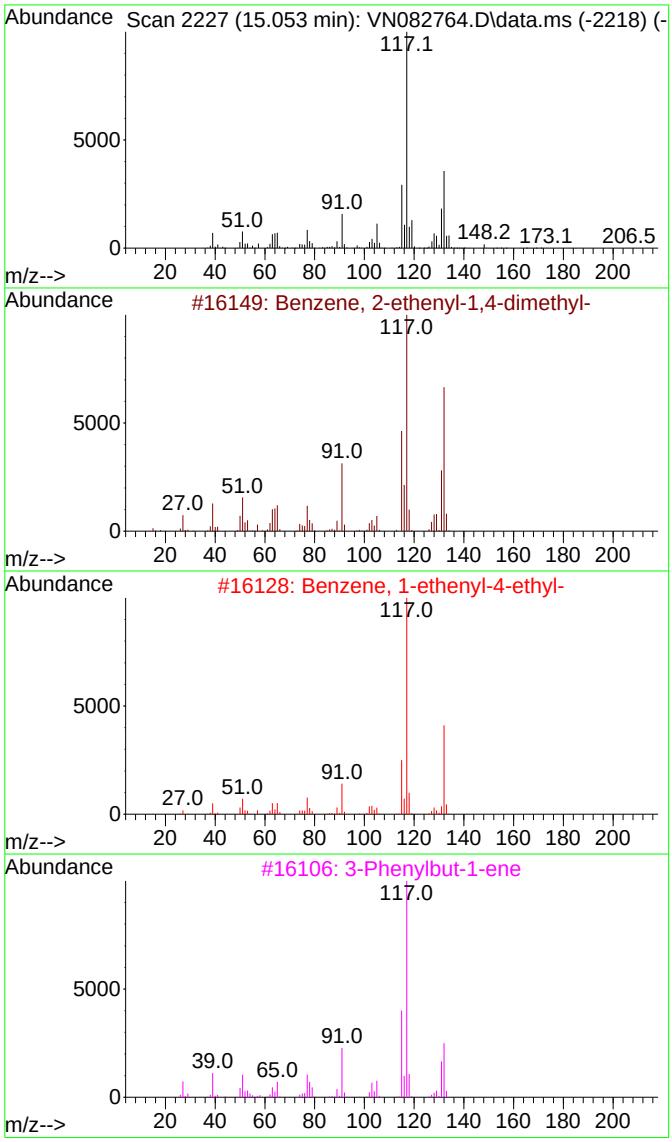
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

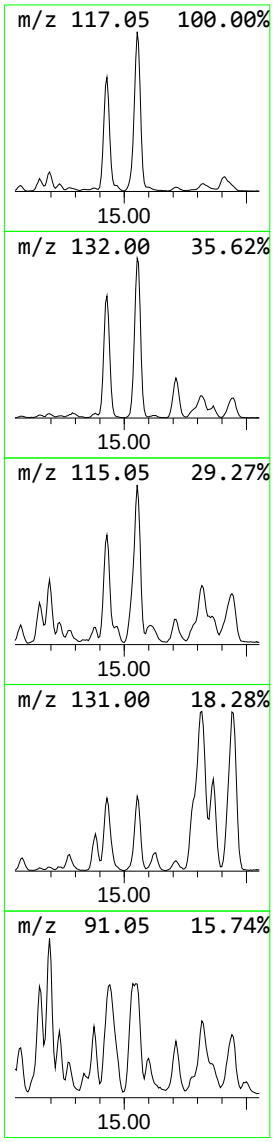
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	65.06 ug/l	3364990	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082764.D
Acq On : 01 Jul 2024 14:39
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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.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
Hexane, 3-methyl-	8.441	78.8	ug/l	1985840	1	8.224	1259200	50.0
1-Butanol, 2-et...	8.700	49.9	ug/l	393649	2	9.100	394659	50.0
Heptane	8.965	93.1	ug/l	734922	2	9.100	394659	50.0
Heptane, 2-methyl-	10.206	101.4	ug/l	800401	2	9.100	394659	50.0
Heptane, 3-methyl-	10.341	89.7	ug/l	707930	2	9.100	394659	50.0
Octane	10.741	122.8	ug/l	1341170	3	11.870	546169	50.0
Octane, 2-methyl-	11.641	138.0	ug/l	1507030	3	11.870	546169	50.0
Octane, 3-methyl-	11.747	63.1	ug/l	689210	3	11.870	546169	50.0
Benzene, 1-ethy...	13.100	51.1	ug/l	2640960	4	13.794	2586020	50.0
Benzene, 2-ethe...	15.053	65.1	ug/l	3364990	4	13.794	2586020	50.0