LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	137	148	150	rBV6	51664	145901	5.84%	0.388%
2	2.865	152	155	158	rVV5	17787	35747	1.43%	0.095%
3	2.971	171	173	176	rBV4	21013	27624	1.11%	0.073%
4	8.159	1045	1055	1060	rBV	298686	748535	29.95%	1.992%
5	8.218	1060	1065	1075	rVV	710730	1571821	62.88%	4.182%
6	8.318	1077	1082	1092	rVB4	30497	71447	2.86%	0.190%
7	8.441	1092	1103	1111	rBV2	174527	394789	15.79%	1.050%
8	8.577	1118	1126	1133	rBV	325674	729053	29.17%	1.940%
9	8.647	1133	1138	1140	rVV3	37405	80808	3.23%	0.215%
10	8.700	1143	1147	1156	rVV8	60267	205821	8.23%	0.548%
11	8.783	1156	1161	1167	rVV6	36436	106966	4.28%	0.285%
12	8.847	1169	1172	1179	rVB5	22134	44958	1.80%	0.120%
13	8.965	1184	1192	1200	rVB	321663	622787	24.91%	1.657%
14	9.100	1205	1215	1232	rVV	835858	1715248	68.62%	4.564%
15	9.600	1285	1300	1314	rBV2	133495	353707	14.15%	0.941%
16	9.777	1323	1330	1337	rBV	41409	76855	3.07%	0.204%
17	9.865	1339	1345	1353	rVB6	14673	34090	1.36%	0.091%
18	10.200	1397	1402	1412	rVV3	64464	147424	5.90%	0.392%
19	10.341	1416	1426	1437	rBV2	53923	113784	4.55%	0.303%
20	10.565	1456	1464	1470	rBV	1295470	2411998	96.49%	6.417%
21	10.630	1470	1475	1481	rVV	143209	309351	12.38%	0.823%
22	10.694	1481	1486	1489	rVV3	36113	72486	2.90%	0.193%
23	10.741	1489	1494	1504	rVB2	229701	433700	17.35%	1.154%
24	10.906	1517	1522	1530	rVB3	48920	98428	3.94%	0.262%
25	11.000	1530	1538	1548	rBV4	69731	156095	6.24%	0.415%
26	11.088	1548	1553	1559	rVB6	27965	51747	2.07%	0.138%
27	11.171	1559	1567	1573	rBV3	52595	87903	3.52%	0.234%
28	11.235	1573	1578	1580	rBV3	20498	31704	1.27%	0.084%
29	11.271	1580	1584	1592	rVB5	32934	62763	2.51%	0.167%
30	11.347	1592	1597	1601	rBV2	50112	89386	3.58%	0.238%
31	11.418	1601	1609	1614	rBV	143818	268192	10.73%	0.714%
32	11.471	1614	1618	1624	rVB3	62433	123936	4.96%	0.330%
33	11.571	1631	1635	1640	rBV2	59142	91625	3.67%	0.244%
34	11.641	1640	1647	1659	rVB3	184943	472729	18.91%	1.258%
35	11.747	1659	1665	1670	rVB	173136	274141	10.97%	0.729%
36	11.800	1670	1674	1678	rBV4	15462	30408	1.22%	0.081%

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1276

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
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Title : SW846 8260

37	11.865	1678	1685	1696	rVB	1026380	1858004	74.33%	4.943%
38	11.965	1696	1702	1708	rBV	317089	551105	22.05%	1.466%
39	12.071	1711	1720	1726	rBV	1371819	2499675	100.00%	6.651%
40	12.153	1731	1734	1740	rVB2	126873	209922	8.40%	0.559%
41	12.206	1740	1743	1752	rVB9	14543	27141	1.09%	0.072%
42	12.288	1752	1757	1763	rBV5	35983	66591	2.66%	0.177%
43	12.400	1763	1776	1784	rBV2	517710	1271968	50.89%	3.384%
44	12.482	1785	1790	1795	rVB	150590	245256	9.81%	0.653%
45	12.541	1795	1800	1801	rBV3	48517	72161	2.89%	0.192%
46	12.618	1801	1813	1822	rVB7	154392	536194	21.45%	1.427%
47	12.694	1822	1826	1831	rBV2	95459	171656	6.87%	0.457%
48	12.741	1831	1834	1835	rVV2	52103	60106	2.40%	0.160%
49	12.771	1835	1839	1841	rVV2	132452	195670	7.83%	0.521%
50	12.794	1841	1843	1847	rVB2	145444	182695	7.31%	0.486%
51	12.853	1847	1853	1863	rVB2	881778	1665944	66.65%	4.432%
52	12.935	1863	1867	1872	rBV6	41278	70132	2.81%	0.187%
53	13.035	1878	1884	1889	rBV	314521	522514	20.90%	1.390%
54	13.100	1889	1895	1898	rBV	810409	1332123	53.29%	3.544%
55	13.165	1898	1906	1913	rVB3	906297	2327122	93.10%	6.191%
56	13.229	1913	1917	1922	rVB3	97856	150602	6.02%	0.401%
57	13.335	1923	1935	1941	rBV	331470	747505	29.90%	1.989%
58	13.394	1941	1945	1954	rVB4	130504	258180	10.33%	0.687%
59	13.482	1954	1960	1971	rVB	913709	1505228	60.22%	4.005%
60	13.576	1972	1976	1979	rBV6	38894	63082	2.52%	0.168%
61	13.618	1979	1983	1987	rVB	89303	137950	5.52%	0.367%
62	13.676	1987	1993	1998	rBV3	198566	400541	16.02%	1.066%
63	13.718	1998	2000	2004	rVV3	59426	83934	3.36%	0.223%
64	13.794	2007	2013	2022	rBV2	1114947	2204481	88.19%	5.865%
65	13.988	2041	2046	2050	rBV2	388077	680004	27.20%	1.809%
66	14.106	2062	2066	2076	rBV5	412825	766092	30.65%	2.038%
67	14.182	2076	2079	2083	rVB	104359	140391	5.62%	0.374%
68	14.247	2086	2090	2092	rBV	104357	146161	5.85%	0.389%
69	14.276	2092	2095	2099	rVB	134571	188046	7.52%	0.500%
70	14.329	2099	2104	2111	rVB	215703	318101	12.73%	0.846%
71	14.394	2112	2115	2118	rBV2	29638	30622	1.23%	0.081%
72	14.447	2118	2124	2129	rVB4	216891	389776	15.59%	1.037%
73	14.512	2131	2135	2140	rVB7	31245	60582	2.42%	0.161%
74	14.576	2140	2146	2150	rBV5	85358	169402	6.78%	0.451%
75	14.629	2150	2155	2158	rBV2	116138	192326	7.69%	0.512%
76	14.659	2158	2160	2163	rVB3	58780	55106	2.20%	0.147%

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Integrator: RTE
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Title : SW846 8260

77	14.694	2163	2166	2170	rVB	93751	120947	4.84%	0.322%
78	14.735	2170	2173	2177	rBV3	78056	94233	3.77%	0.251%
79	14.776	2177	2180	2187	rVB7	53235	123358	4.93%	0.328%
80	14.876	2187	2197	2201	rBV5	82431	196770	7.87%	0.524%
81	14.929	2201	2206	2209	rBV2	171619	320323	12.81%	0.852%
82	15.053	2218	2227	2233	rBV4	245591	610668	24.43%	1.625%
83	15.212	2245	2254	2262	rBV2	180683	332069	13.28%	0.883%
84	15.276	2262	2265	2267	rBV4	25412	35283	1.41%	0.094%
85	15.323	2268	2273	2276	rVV5	46556	82037	3.28%	0.218%
86	15.441	2287	2293	2300	rVB4	62624	146150	5.85%	0.389%
87	15.600	2314	2320	2322	rBV7	21888	38189	1.53%	0.102%
88	15.700	2332	2337	2341	rBV3	41906	76354	3.05%	0.203%
89	15.753	2342	2346	2349	rBV6	19250	30934	1.24%	0.082%
90	15.947	2371	2379	2383	rBV4	39440	95760	3.83%	0.255%
91	16.106	2401	2406	2409	rBV7	15088	34695	1.39%	0.092%
92	16.164	2411	2416	2427	rVB4	71937	168835	6.75%	0.449%
93	16.341	2441	2446	2453	rVB6	15700	34689	1.39%	0.092%
94	16.500	2463	2473	2479	rBV8	38519	124434	4.98%	0.331%
95	16.717	2500	2510	2517	rBV5	32694	72377	2.90%	0.193%

Sum of corrected areas: 37586153

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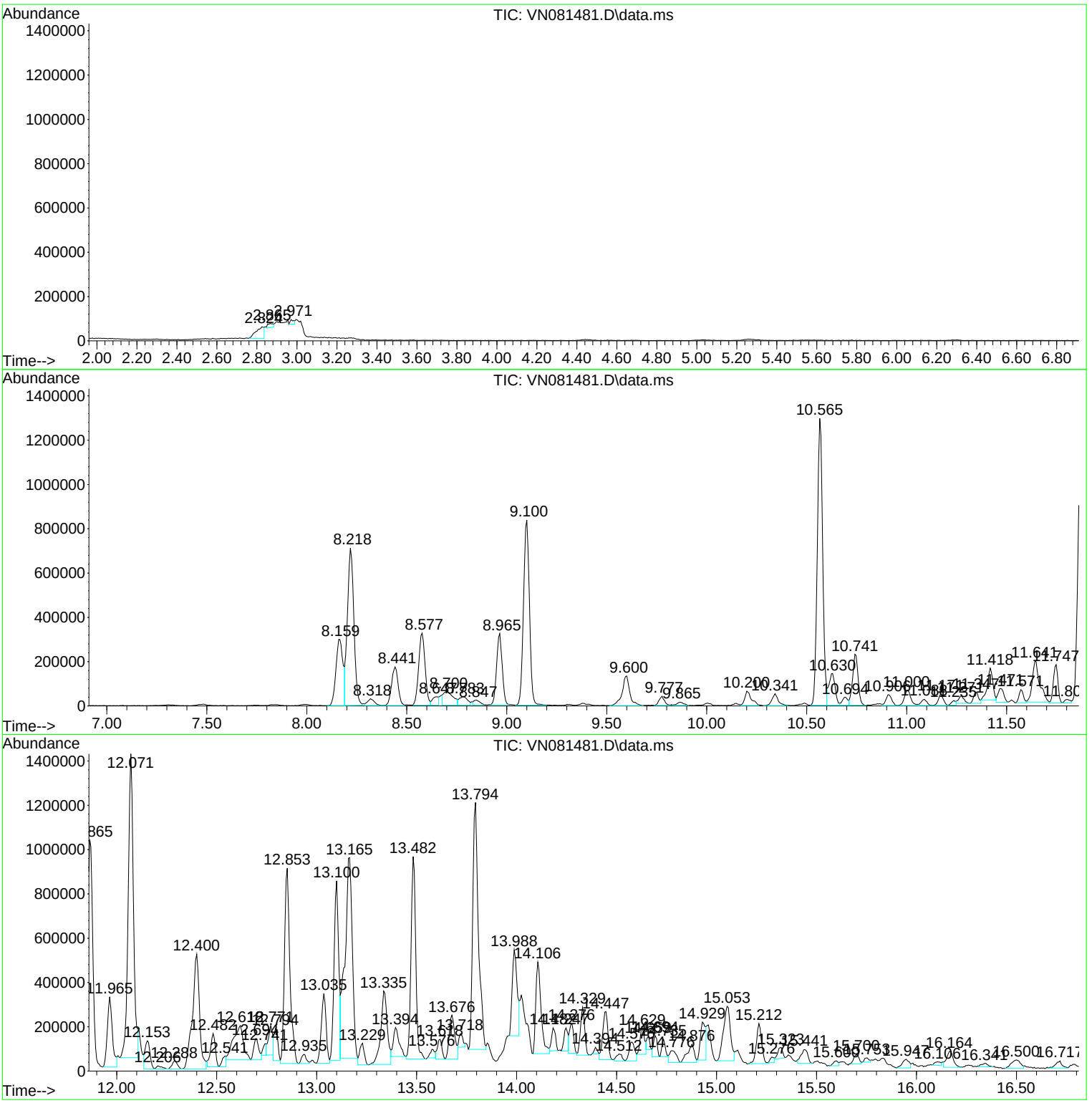
Instrument :
MSVOA_N
ClientSampleId :
1276

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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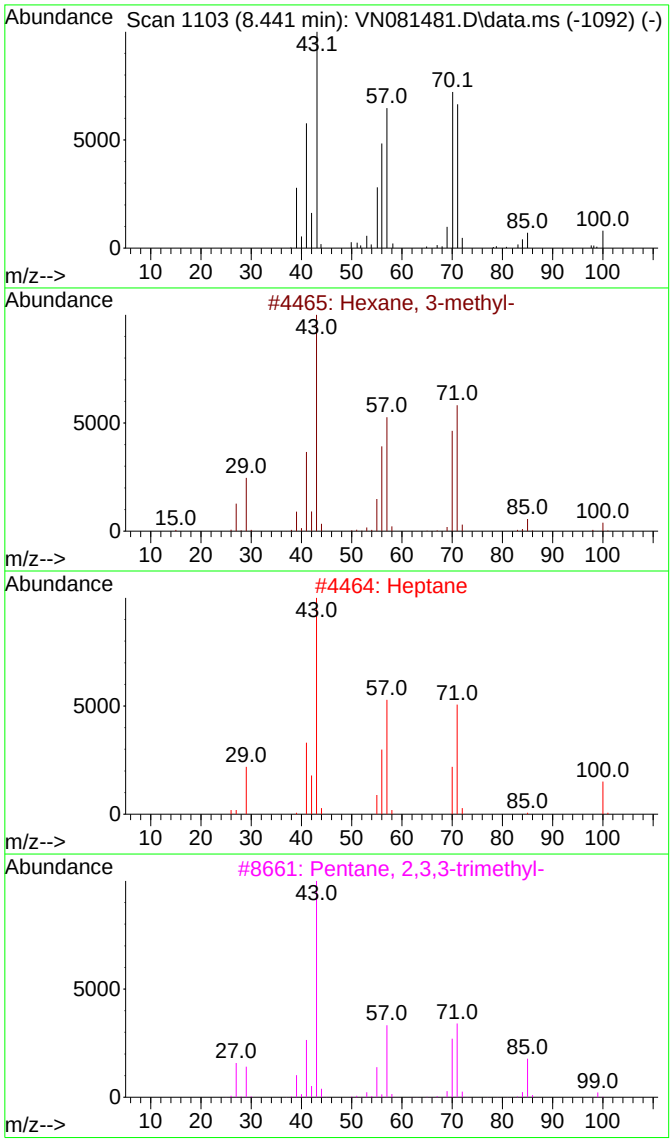
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

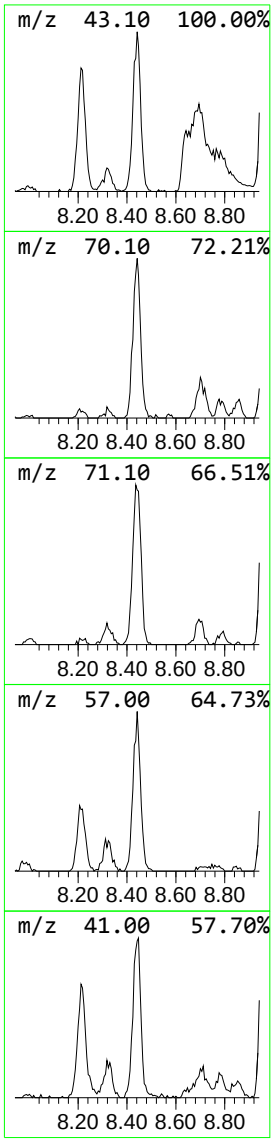
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	12.56 ug/l	394789	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	86
2	Heptane	100	C7H16	000142-82-5	64
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
4	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	53
5	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

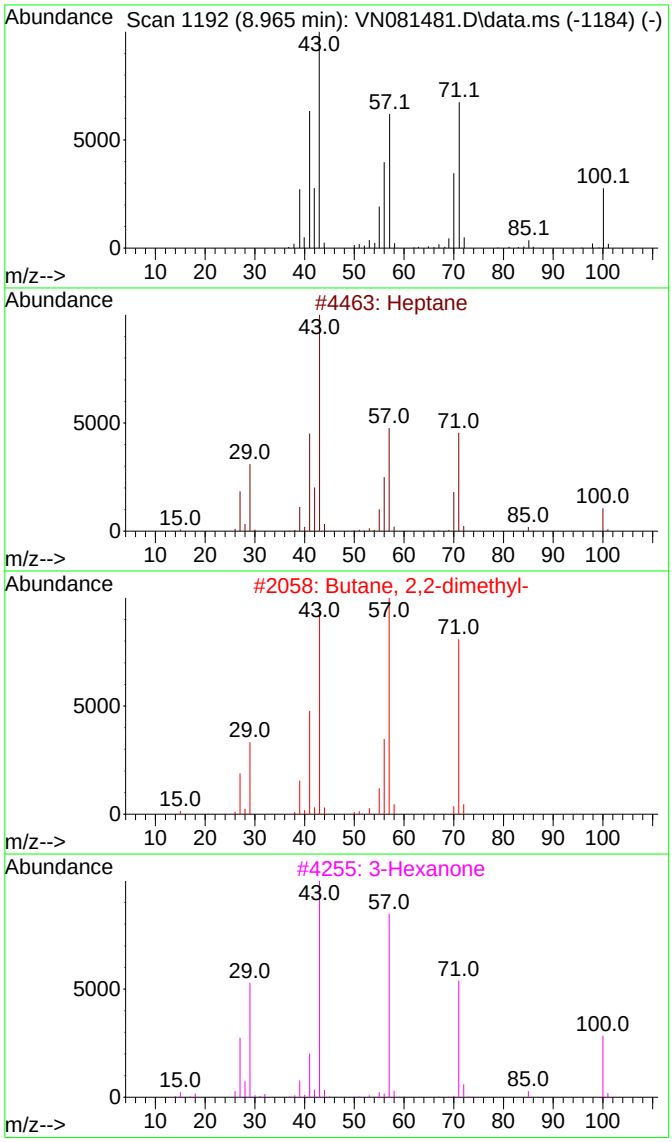
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

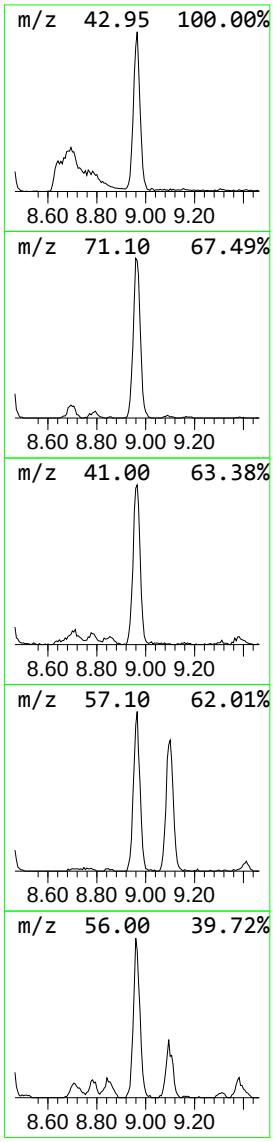
****

Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	18.15 ug/l	622787	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	83
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
3	3-Hexanone	100	C6H12O	000589-38-8	46
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38





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Quant Title : SW846 8260

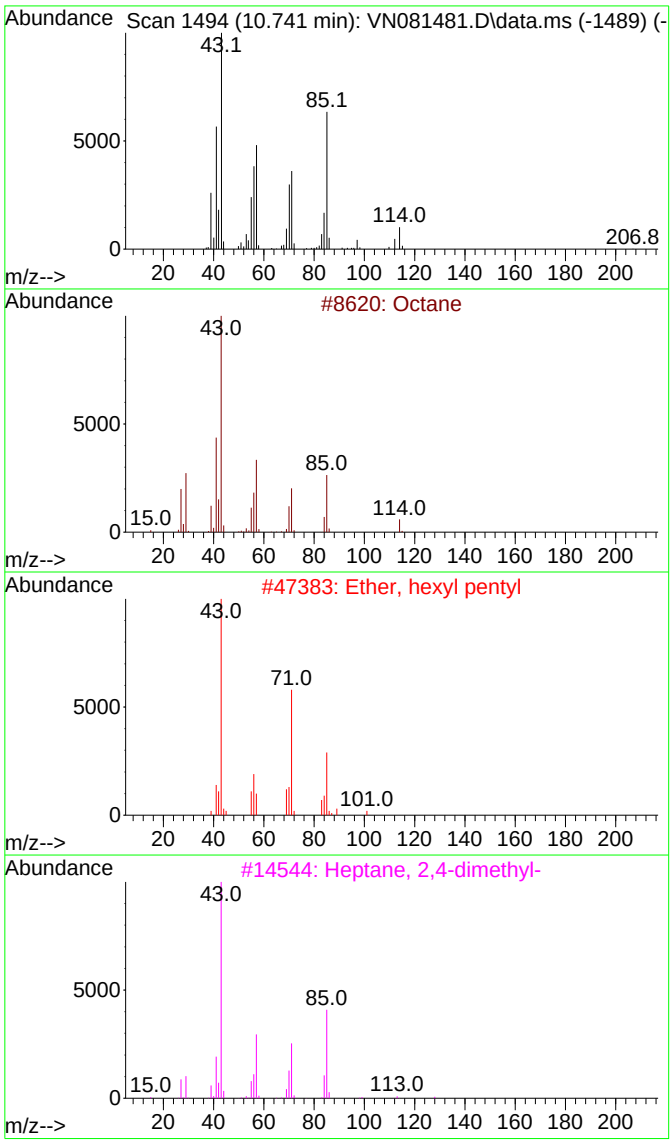
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

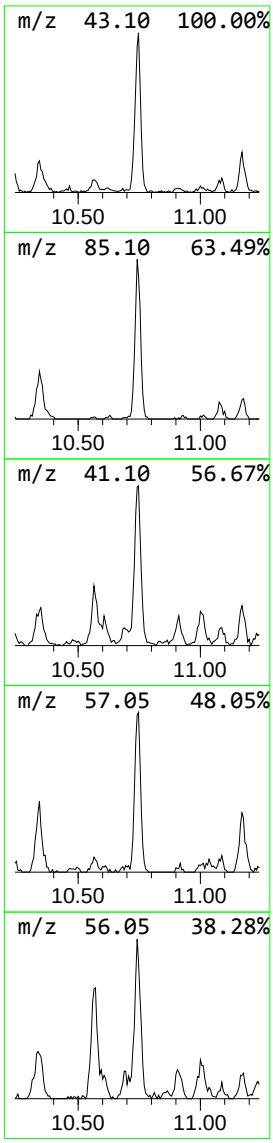
****

Peak Number 3 Octane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.741	11.67 ug/l	433700	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	86
2	Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47
4	Hexane, 1-propoxy-	144	C9H20O	053685-78-2	47
5	Carbonic acid, dihexyl ester	230	C13H26O3	007523-15-1	38





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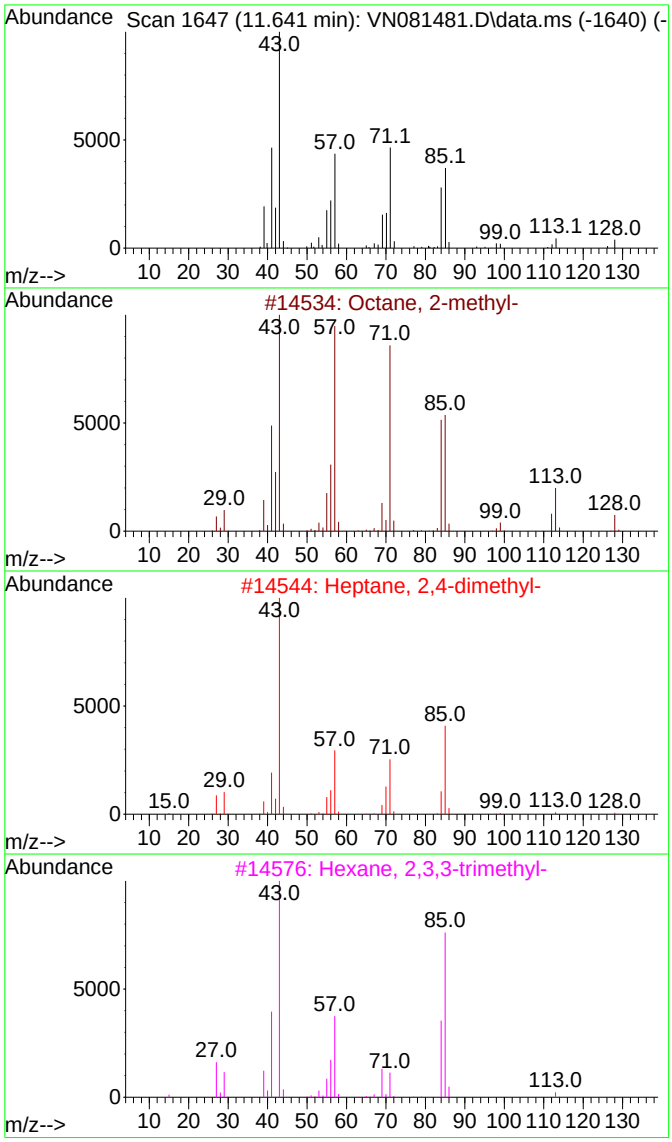
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

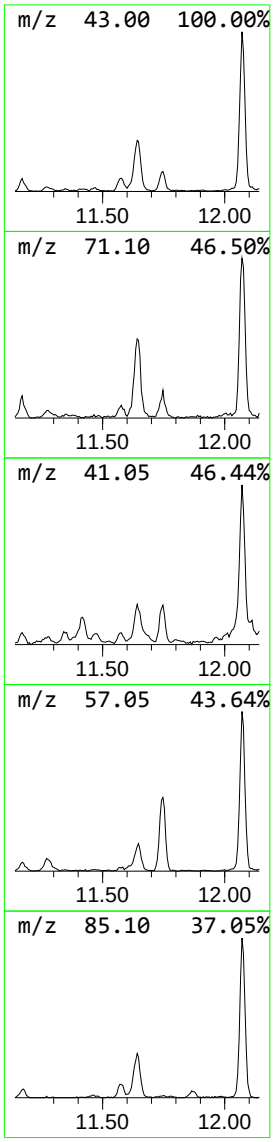
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	12.72 ug/l	472729	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	68
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
3	Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	58
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
5	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	53





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Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

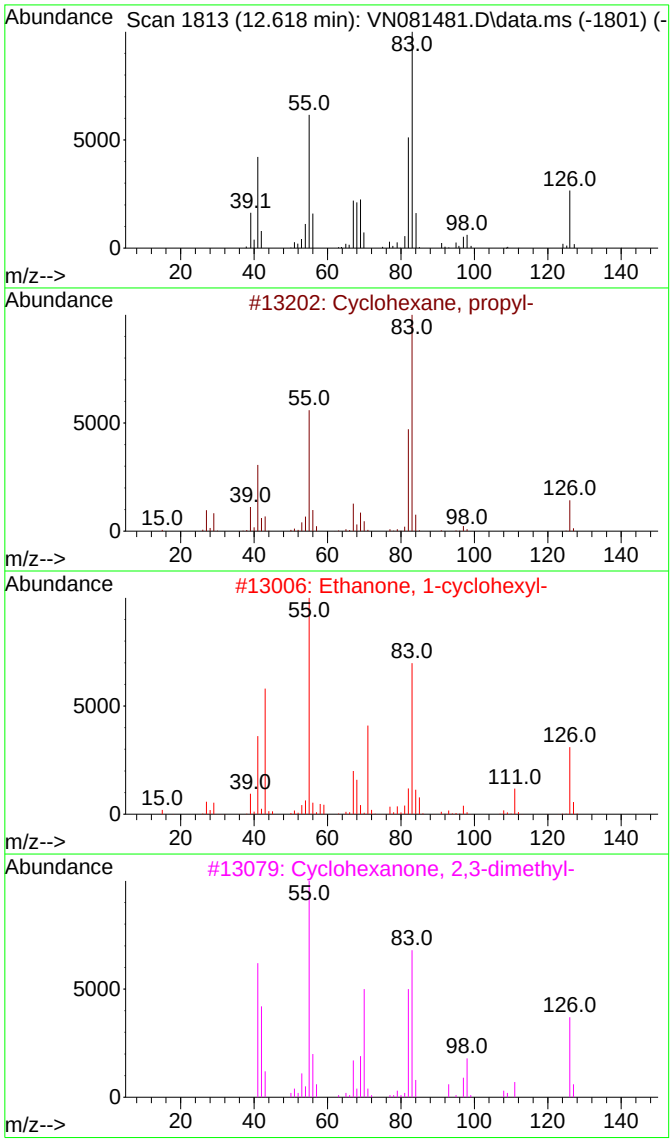
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

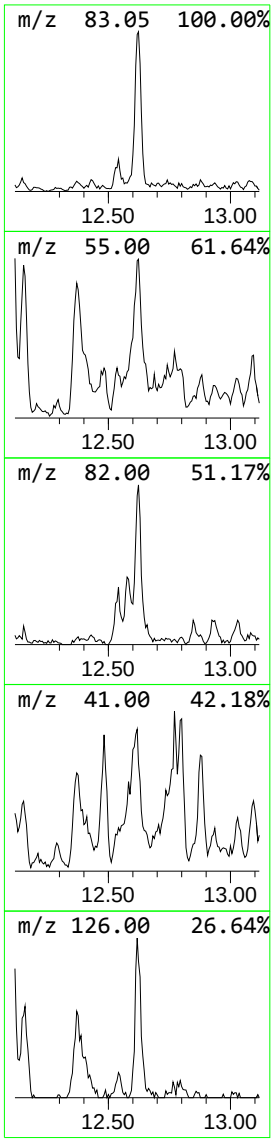
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.618	14.43 ug/l	536194	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	64
3	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	64
4	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	53
5	2-Pyrazoline, 1-methyl-4-propyl-	126	C7H14N2	033063-77-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

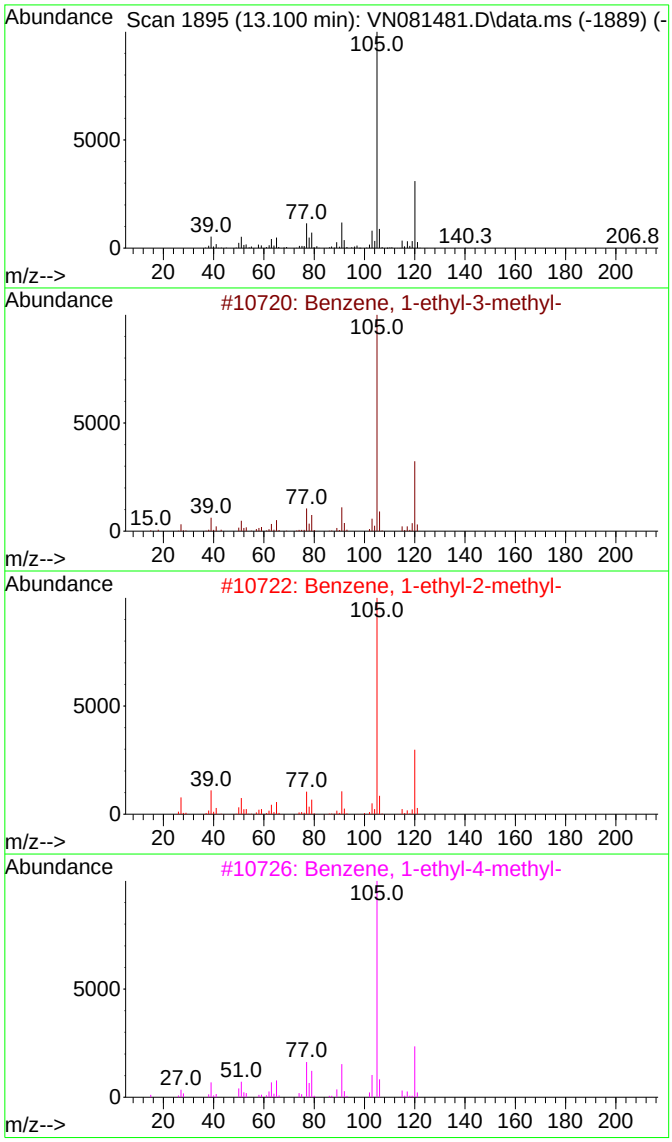
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

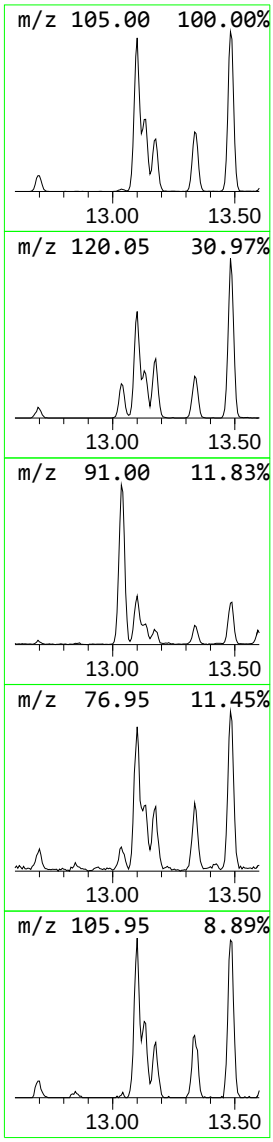
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	30.21 ug/l	1332120	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	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

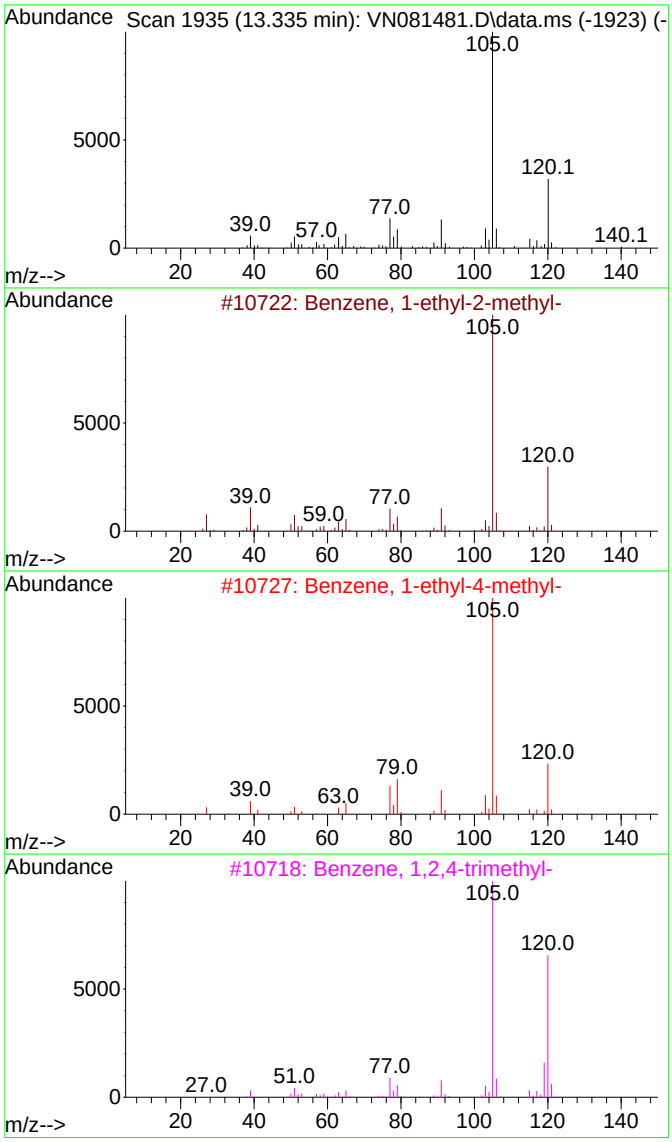
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

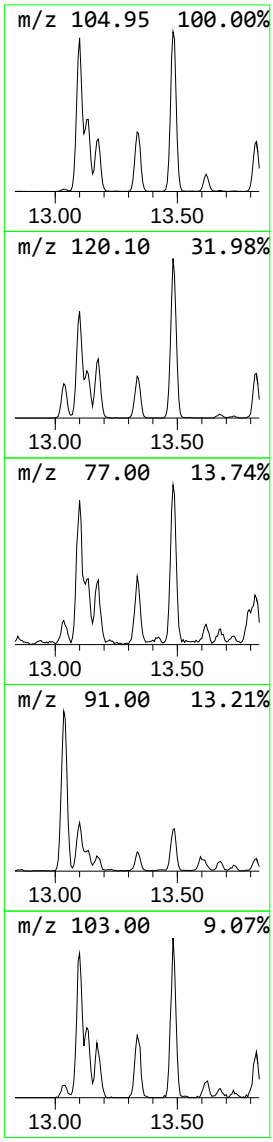
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	16.95 ug/l	747505	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

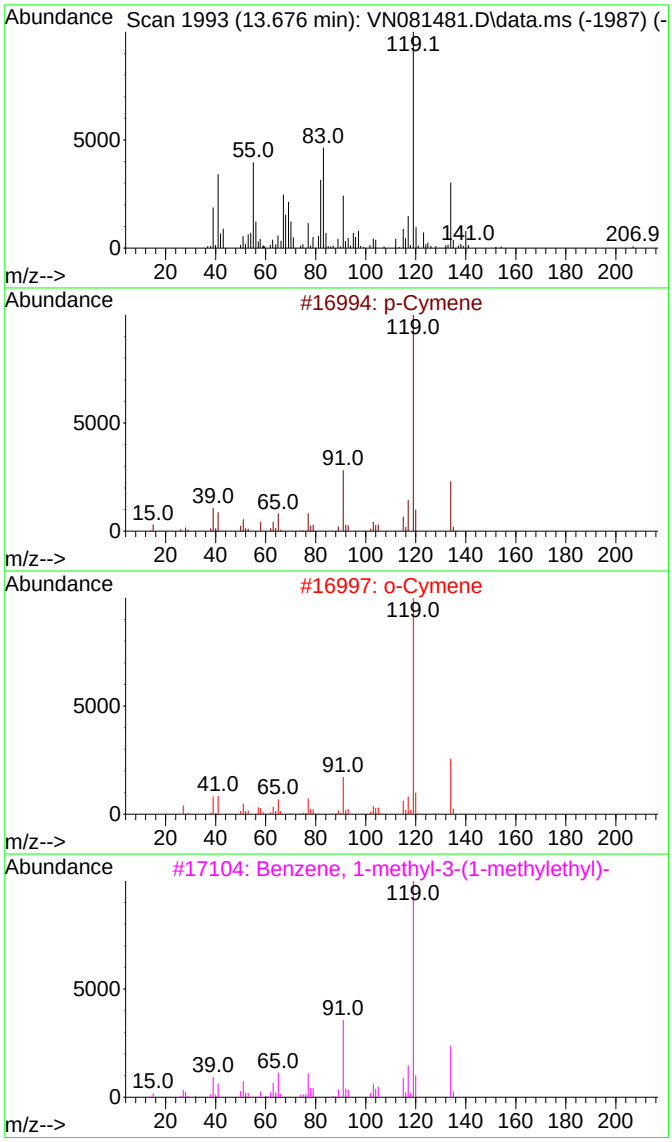
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

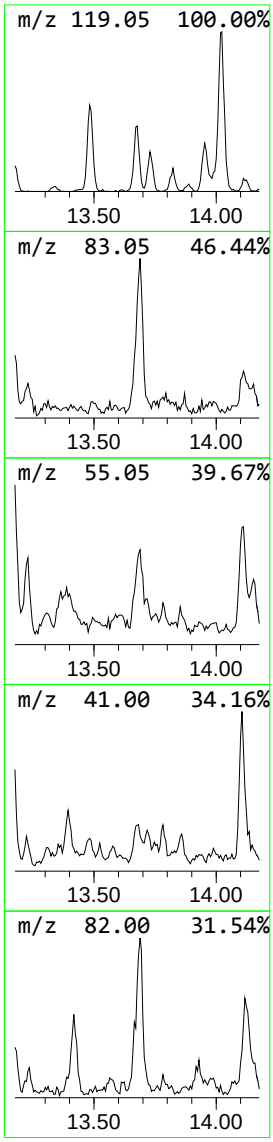
****

Peak Number 8 p-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	9.08 ug/l	400541	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	55
2	o-Cymene	134	C10H14	000527-84-4	55
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	55
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	55
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	55





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Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

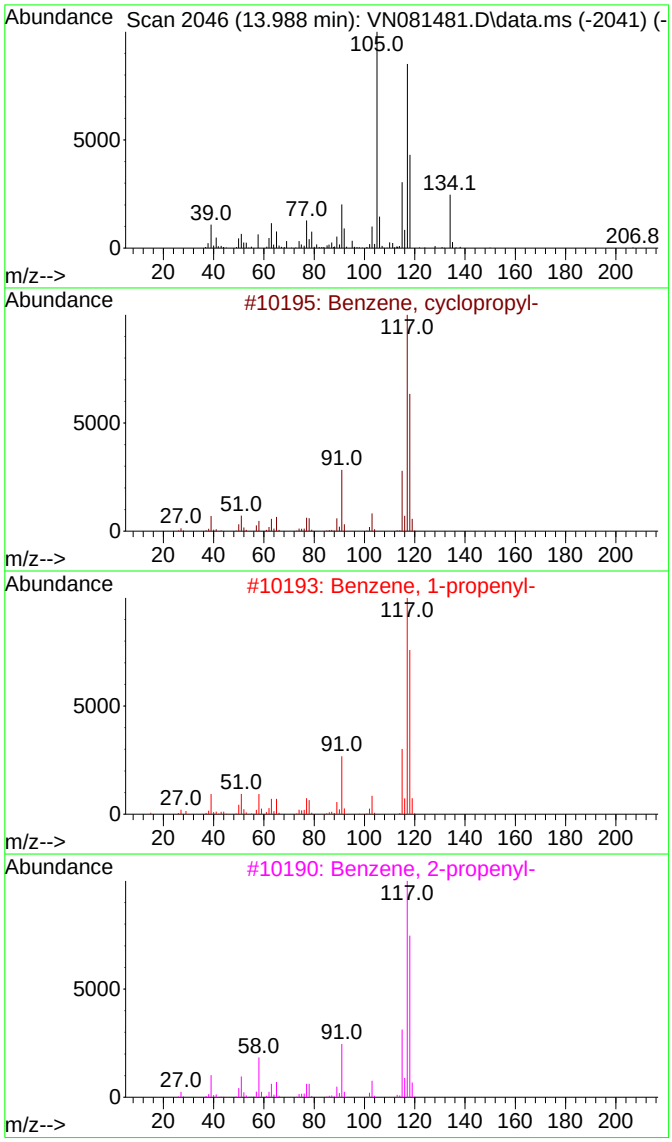
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

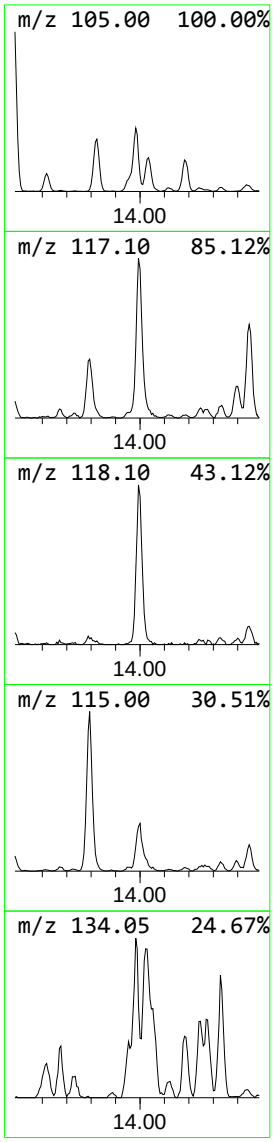
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	15.42 ug/l	680004	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4	Indane	118	C9H10	000496-11-7	60
5	Deltacyclene	118	C9H10	007785-10-6	52





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Data File : VN081481.D
Acq On : 19 Mar 2024 19:20
Operator : JC\MD
Sample : P1772-02
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1276

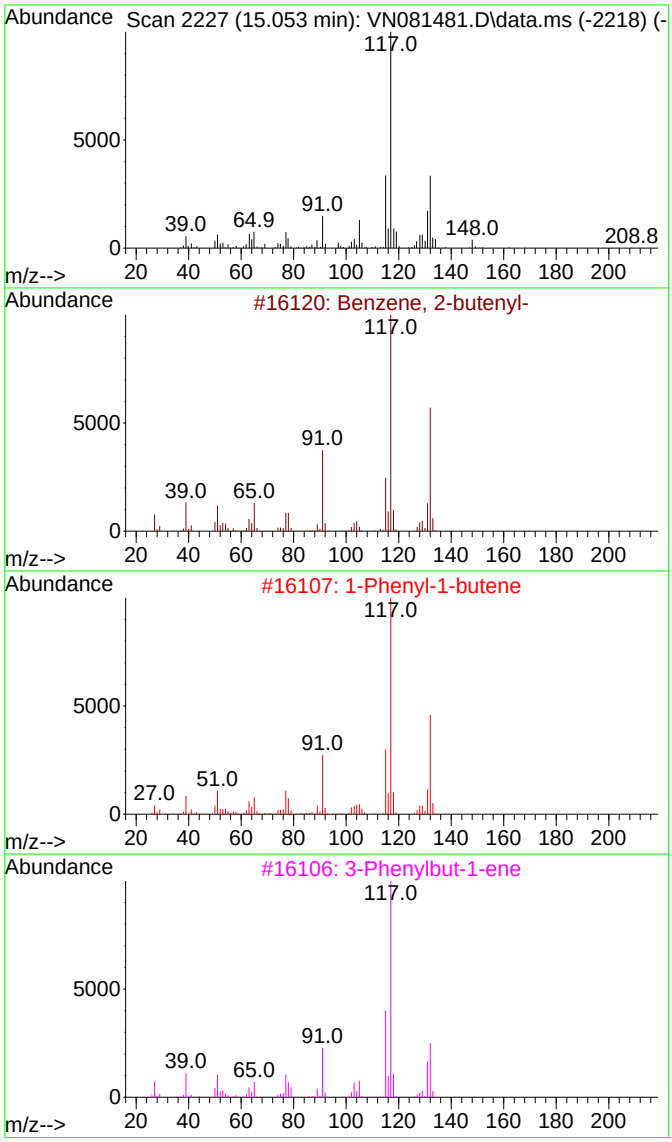
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

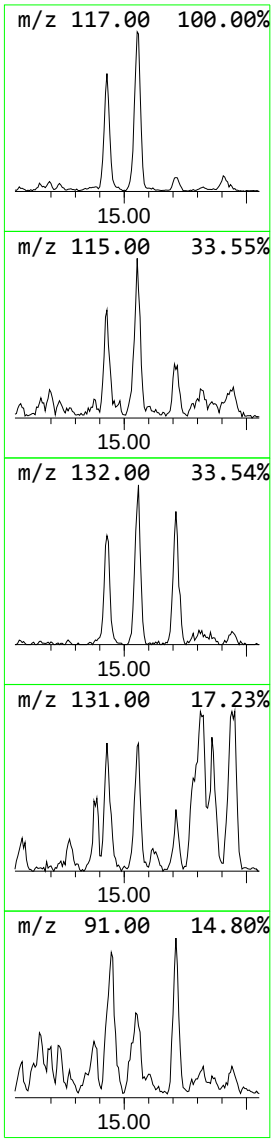
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-butenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	13.85 ug/l	610668	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	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\VN031924\
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Instrument :
MSVOA_N
ClientSampleId :
1276

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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	12.6	ug/l	394789	1	8.218	1571820	50.0
Heptane	8.965	18.1	ug/l	622787	2	9.100	1715250	50.0
Octane	10.741	11.7	ug/l	433700	3	11.865	1858000	50.0
Octane, 2-methyl-	11.641	12.7	ug/l	472729	3	11.865	1858000	50.0
Cyclohexane, pr...	12.618	14.4	ug/l	536194	3	11.865	1858000	50.0
Benzene, 1-ethy...	13.100	30.2	ug/l	1332120	4	13.794	2204480	50.0
Benzene, 1-ethy...	13.335	16.9	ug/l	747505	4	13.794	2204480	50.0
p-Cymene	13.676	9.1	ug/l	400541	4	13.794	2204480	50.0
Benzene, cyclop...	13.988	15.4	ug/l	680004	4	13.794	2204480	50.0
Benzene, 2-bute...	15.053	13.9	ug/l	610668	4	13.794	2204480	50.0