LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

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: VN082762.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.830	140	149	155	rVB5	7836	23859	4.61%	0.397%
2	3.801	305	314	323	rBV3	3819	10559	2.04%	0.176%
3	8.165	1046	1056	1061	rBV2	68917	166312	32.15%	2.766%
4	8.224	1061	1066	1078	rVV	120495	260476	50.36%	4.332%
5	8.330	1078	1084	1091	rVV3	4551	9930	1.92%	0.165%
6	8.447	1095	1104	1111	rVB2	16443	38037	7.35%	0.633%
7	8.577	1117	1126	1137	rBV	74516	170615	32.99%	2.837%
8	8.700	1137	1147	1153	rBV4	4928	14959	2.89%	0.249%
9	8.971	1186	1193	1201	rVB2	21520	44055	8.52%	0.733%
10	9.100	1207	1215	1228	rVB	172030	353118	68.27%	5.872%
11	9.600	1294	1300	1305	rVB4	5162	9522	1.84%	0.158%
12	10.341	1421	1426	1434	rBV4	2435	5315	1.03%	0.088%
13	10.565	1456	1464	1470	rBV	276728	517246	100.00%	8.602%
14	10.630	1470	1475	1484	rVB	266258	487651	94.28%	8.110%
15	10.747	1489	1495	1504	rVB3	8340	17368	3.36%	0.289%
16	11.000	1534	1538	1544	rBV5	3160	5385	1.04%	0.090%
17	11.171	1561	1567	1572	rBV5	3755	7428	1.44%	0.124%
18	11.347	1593	1597	1601	rBV5	3180	5200	1.01%	0.086%
19	11.424	1606	1610	1613	rVV4	5550	8653	1.67%	0.144%
20	11.477	1613	1619	1623	rVB2	5942	11536	2.23%	0.192%
21	11.577	1630	1636	1639	rBV3	5102	8993	1.74%	0.150%
22	11.647	1639	1648	1658	rVV5	16524	44271	8.56%	0.736%
23	11.747	1660	1665	1671	rVB	16559	25444	4.92%	0.423%
24	11.865	1678	1685	1695	rVB	261695	467621	90.41%	7.777%
25	11.965	1697	1702	1706	rBV2	11229	18886	3.65%	0.314%
26	12.071	1711	1720	1725	rBV2	83493	157990	30.54%	2.627%
27	12.159	1730	1735	1741	rVB5	10832	21618	4.18%	0.360%
28	12.294	1753	1758	1764	rVB6	4520	9397	1.82%	0.156%
29	12.400	1764	1776	1782	rBV3	33406	100046	19.34%	1.664%
30	12.482	1785	1790	1796	rVV2	22882	38954	7.53%	0.648%
31	12.547	1796	1801	1802	rVV5	6400	9627	1.86%	0.160%
32	12.594	1802	1809	1819	rVV6	17796	75687	14.63%	1.259%
33	12.706	1822	1828	1829	rVV6	12823	23451	4.53%	0.390%
34	12.741	1831	1834	1835	rVV2	17748	21574	4.17%	0.359%
35	12.771	1836	1839	1841	rVV2	26676	39554	7.65%	0.658%
36	12.794	1841	1843	1847	rVV2	24824	36580	7.07%	0.608%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
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Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

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	12.847	1847	1852	1863	rVV	212776	401628	77.65%	6.679%
38	12.935	1864	1867	1871	rVB6	7603	9872	1.91%	0.164%
39	13.035	1877	1884	1888	rBV3	24040	45583	8.81%	0.758%
40	13.094	1889	1894	1898	rVV	60173	106221	20.54%	1.766%
41	13.159	1900	1905	1913	rVV2	119562	253726	49.05%	4.220%
42	13.224	1913	1916	1920	rVB3	12600	17795	3.44%	0.296%
43	13.335	1926	1935	1941	rBV3	28522	76279	14.75%	1.269%
44	13.394	1941	1945	1952	rVB7	16961	29371	5.68%	0.488%
45	13.482	1953	1960	1971	rVB	98951	202548	39.16%	3.368%
46	13.576	1973	1976	1978	rBV3	5340	6167	1.19%	0.103%
47	13.618	1980	1983	1987	rBV4	7122	9915	1.92%	0.165%
48	13.671	1987	1992	1997	rBV6	31730	65131	12.59%	1.083%
49	13.718	1998	2000	2004	rVB4	12561	10830	2.09%	0.180%
50	13.794	2007	2013	2021	rVB2	271572	490136	94.76%	8.151%
51	13.859	2021	2024	2031	rVB3	22535	36105	6.98%	0.600%
52	13.947	2031	2039	2041	rBV9	13819	33826	6.54%	0.563%
53	13.988	2041	2046	2051	rBV3	37582	89798	17.36%	1.493%
54	14.106	2061	2066	2073	rBV	105758	186498	36.06%	3.102%
55	14.329	2100	2104	2108	rBV	18775	28198	5.45%	0.469%
56	14.441	2120	2123	2129	rVB4	26236	42288	8.18%	0.703%
57	14.512	2133	2135	2137	rBV3	6934	6951	1.34%	0.116%
58	14.629	2150	2155	2158	rBV6	34413	56762	10.97%	0.944%
59	14.729	2170	2172	2176	rBV4	12286	17009	3.29%	0.283%
60	14.929	2202	2206	2208	rBV4	18717	25546	4.94%	0.425%
61	15.035	2215	2224	2235	rVB5	61887	210480	40.69%	3.500%
62	15.212	2250	2254	2263	rVB3	31341	61862	11.96%	1.029%
63	15.317	2268	2272	2278	rVV9	10980	21809	4.22%	0.363%
64	15.447	2284	2294	2313	rVB9	39951	203872	39.41%	3.390%

Sum of corrected areas: 6013123

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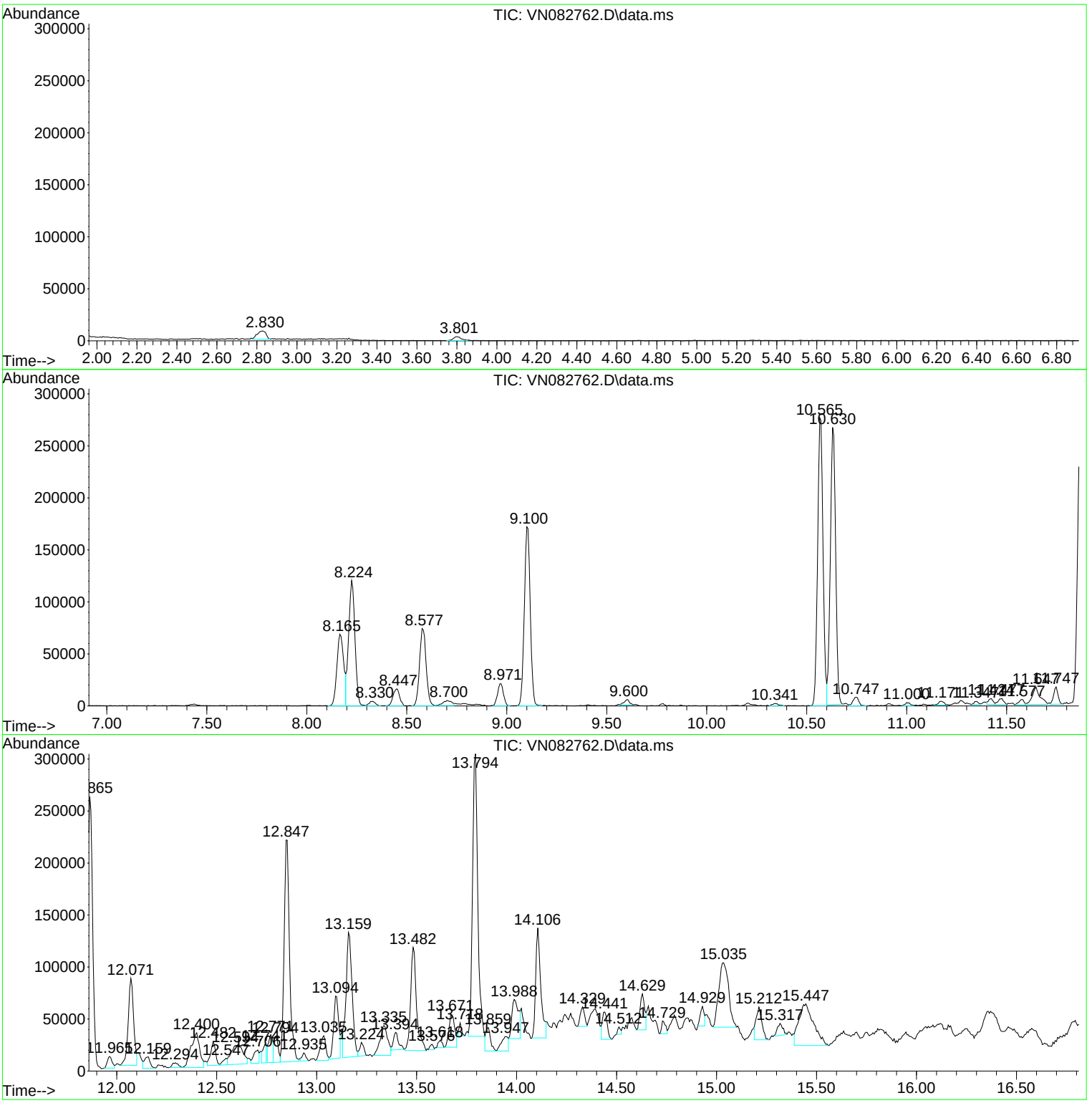
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

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



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Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
170

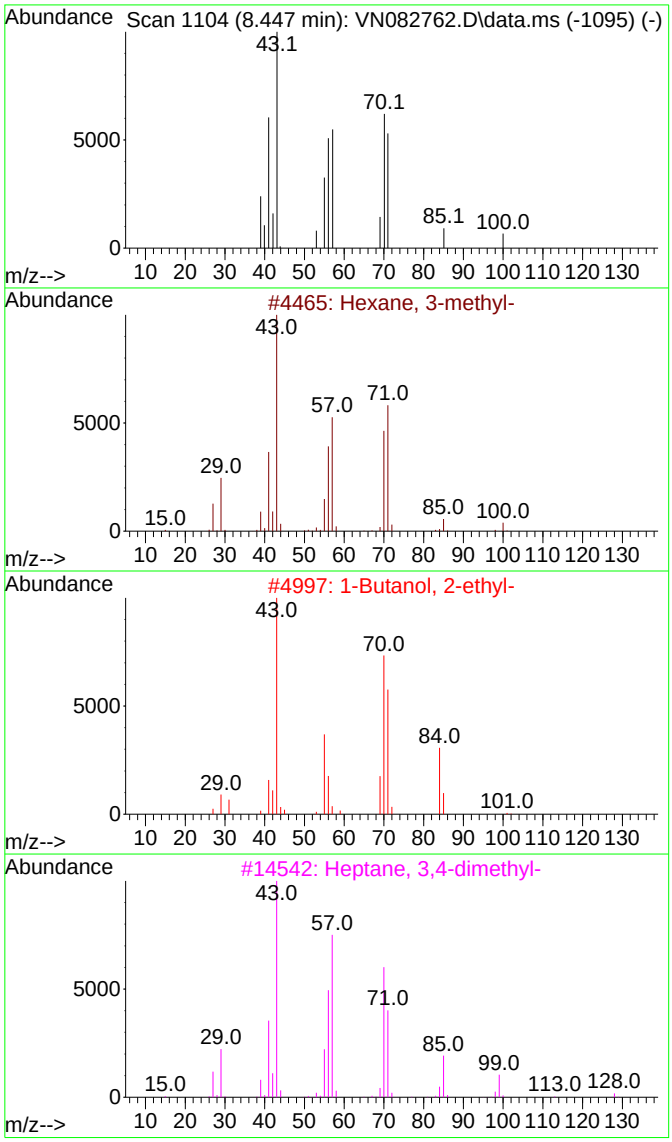
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

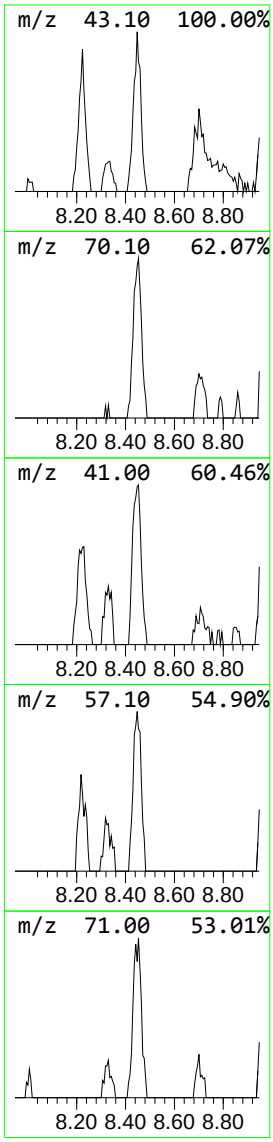
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.447	7.30 ug/l	38037	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	90
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	59
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	56
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	47





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Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

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

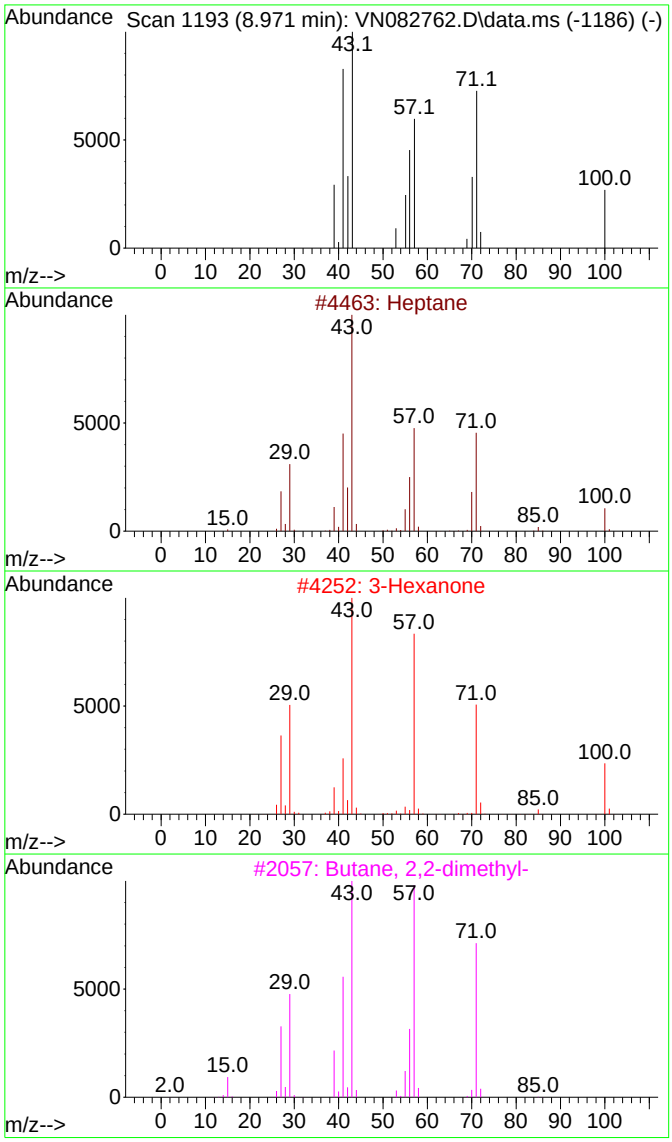
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

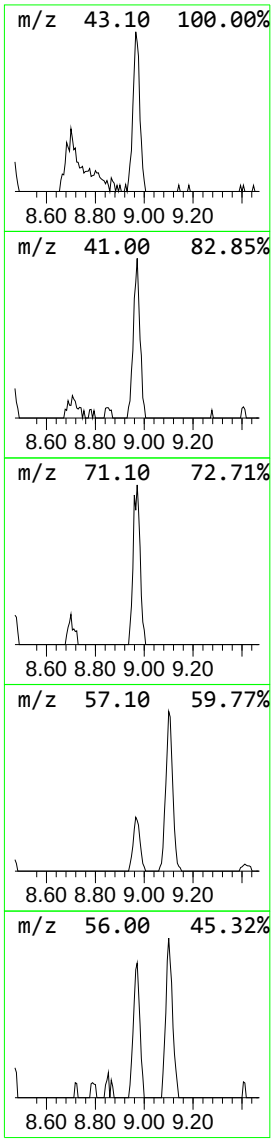
****

Peak Number 2 Heptane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	6.24 ug/l	44055	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	83
2	3-Hexanone	100	C6H12O	000589-38-8	32
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	28
4	1-Heptene	98	C7H14	000592-76-7	25
5	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

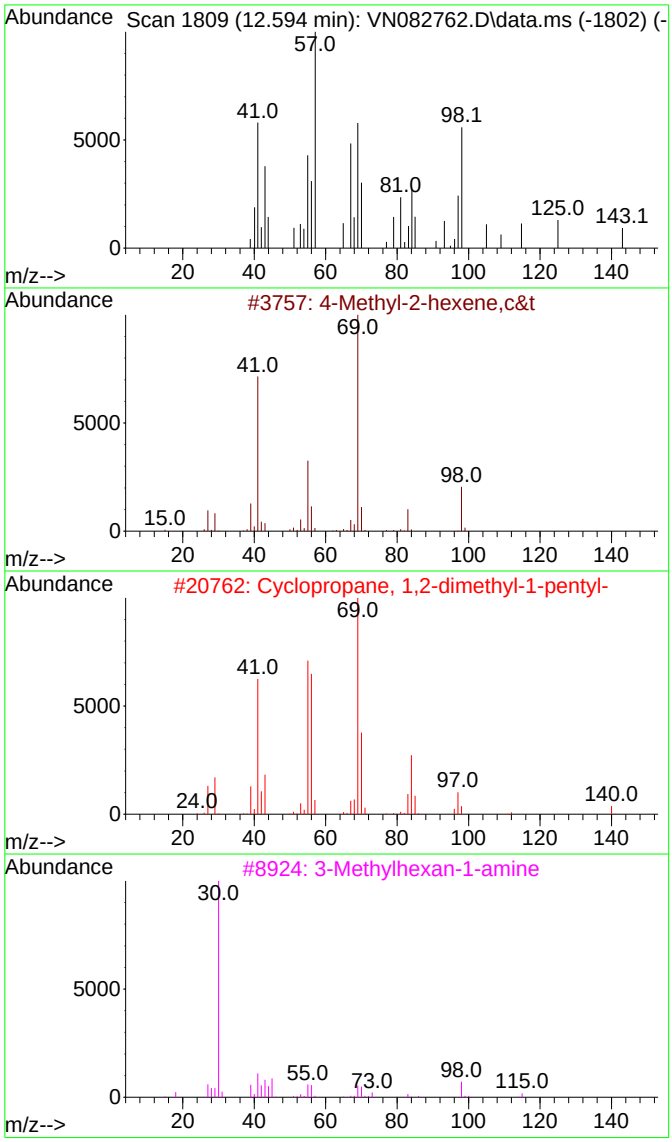
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

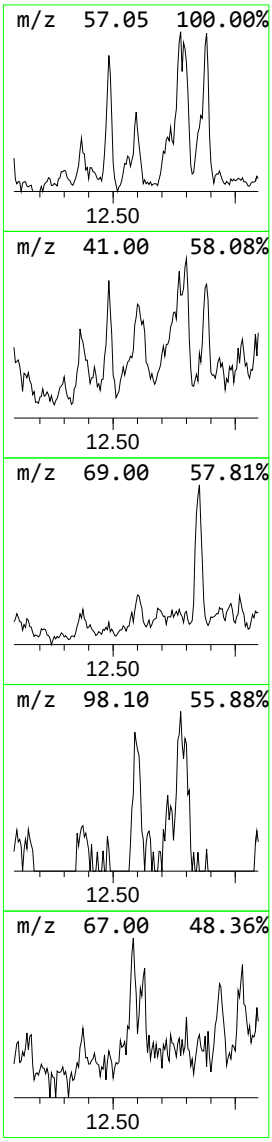
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown12.594 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.594	8.09 ug/l	75687	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-2-hexene,c&t	98	C7H14	003404-55-5	35
2	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	27
3	3-Methylhexan-1-amine	115	C7H17N	065530-93-0	22
4	N,N-Diallylformamide	125	C7H11NO	018889-09-3	14
5	3-Methyl-3-hexene	98	C7H14	003404-65-7	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
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Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

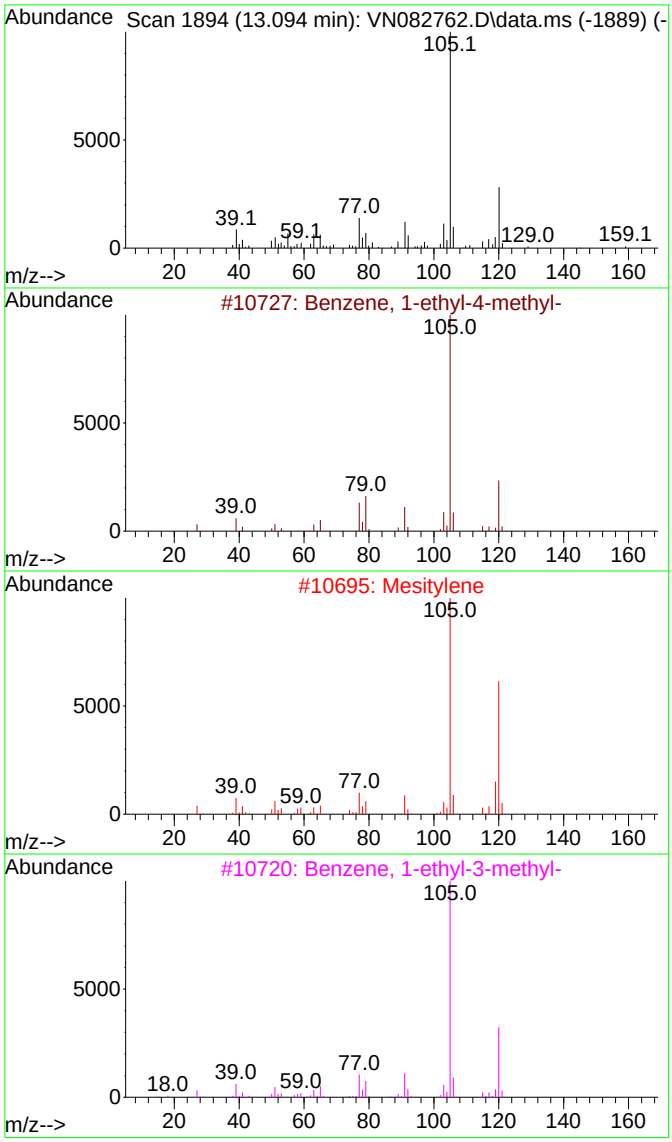
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

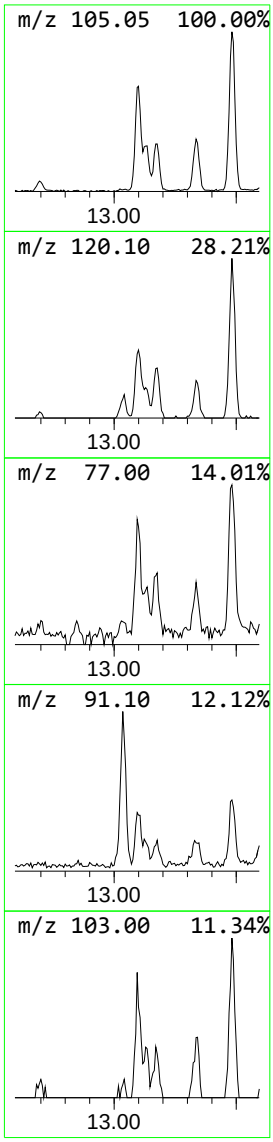
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	10.84 ug/l	106221	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	86
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

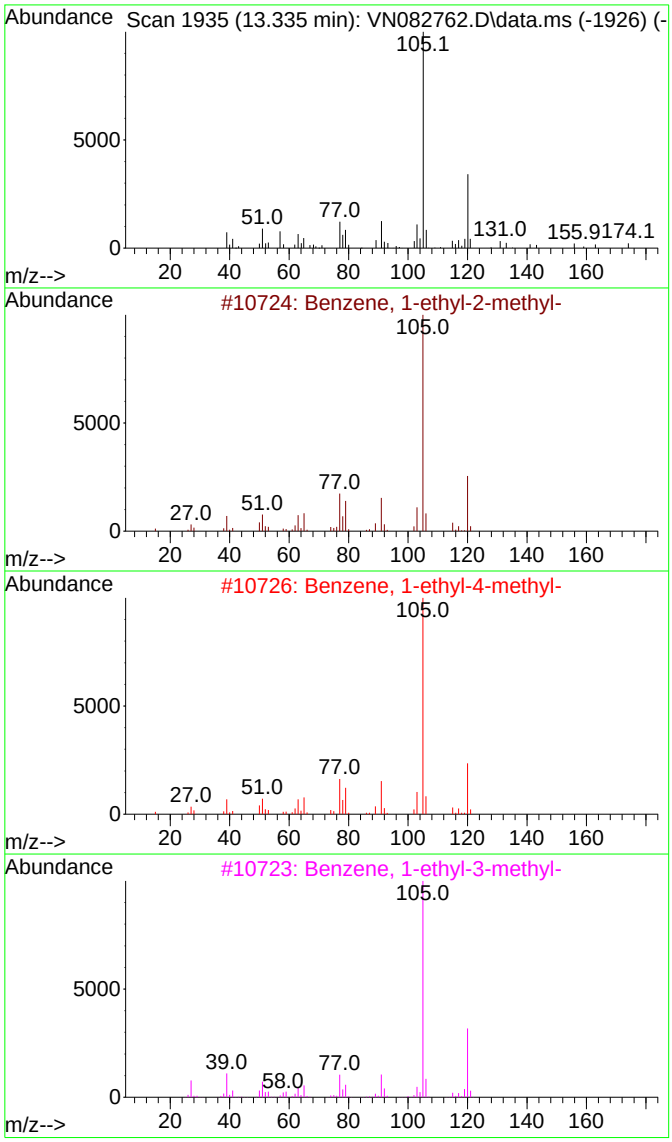
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

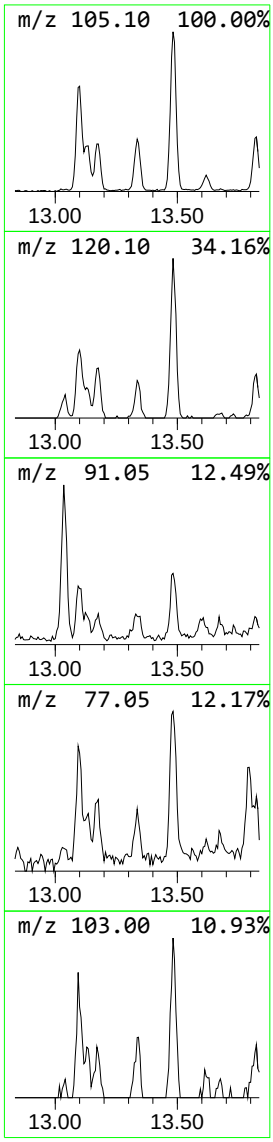
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	7.78 ug/l	76279	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	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5	Mesitylene	120	C9H12	000108-67-8	90





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Data File : VN082762.D
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Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 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

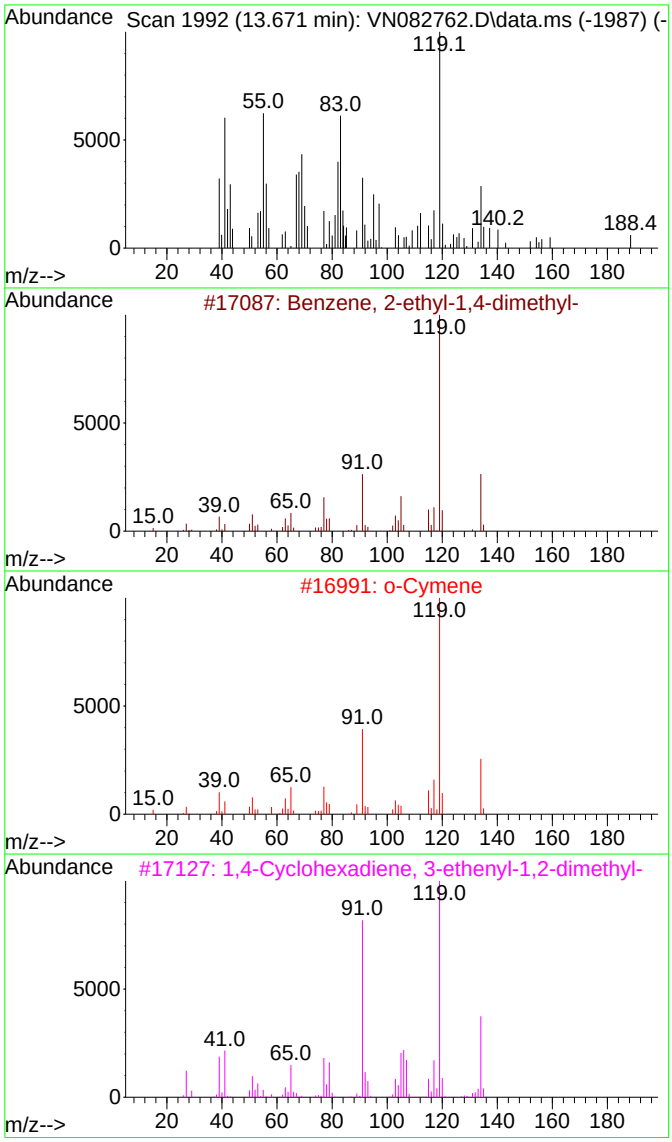
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

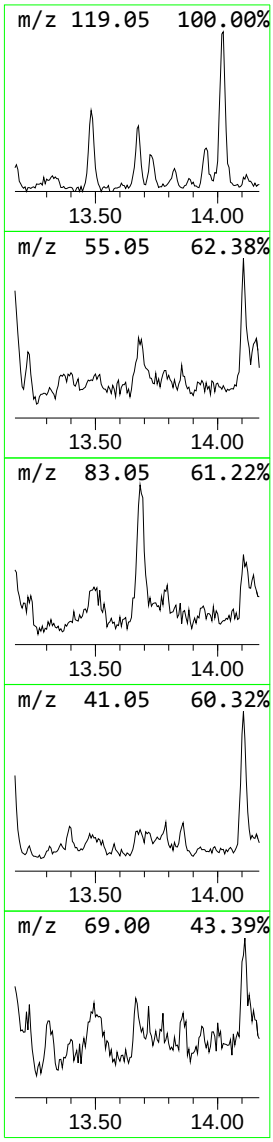
****

Peak Number 6 unknown13.671 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.671	6.64 ug/l	65131	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	38
2	o-Cymene	134	C10H14	000527-84-4	38
3	1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	38
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	38
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
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Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

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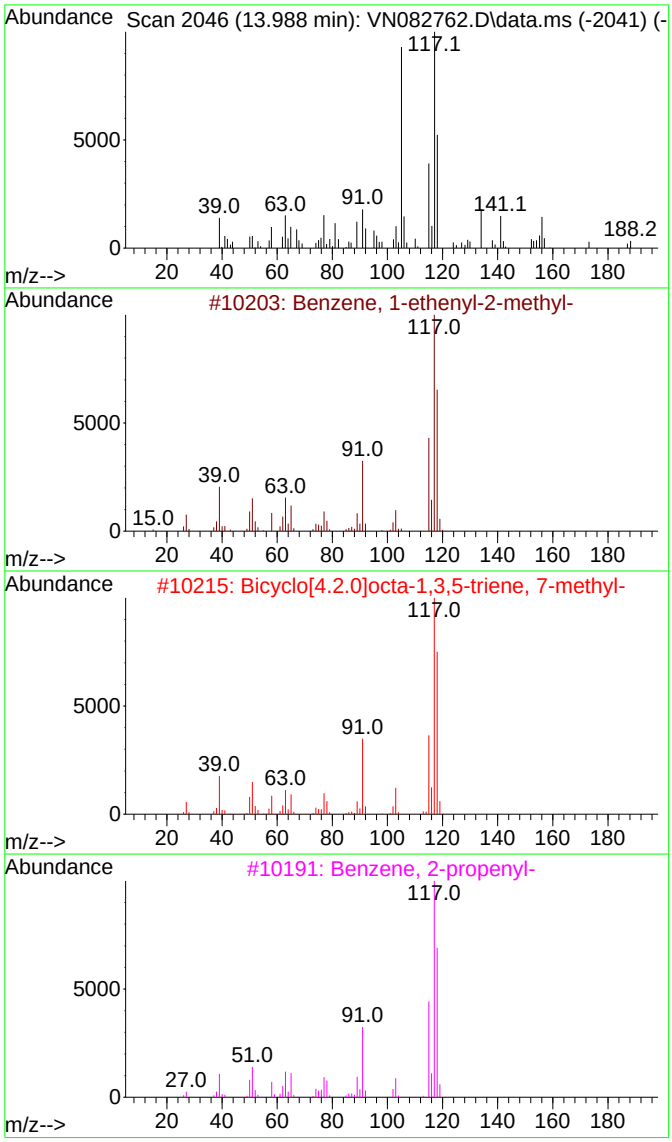
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

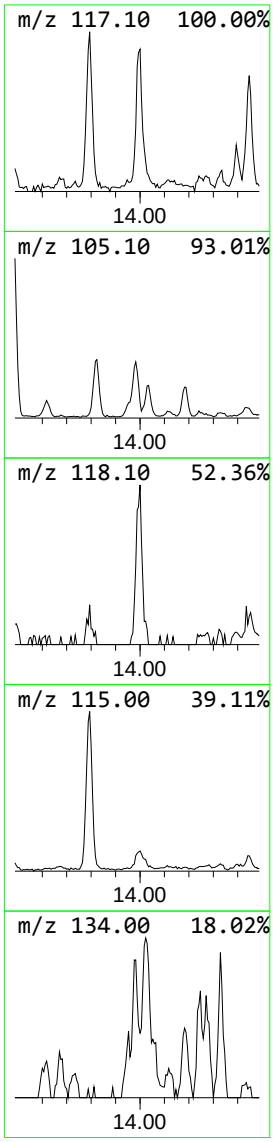
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	9.16 ug/l	89798	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	55
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
4	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

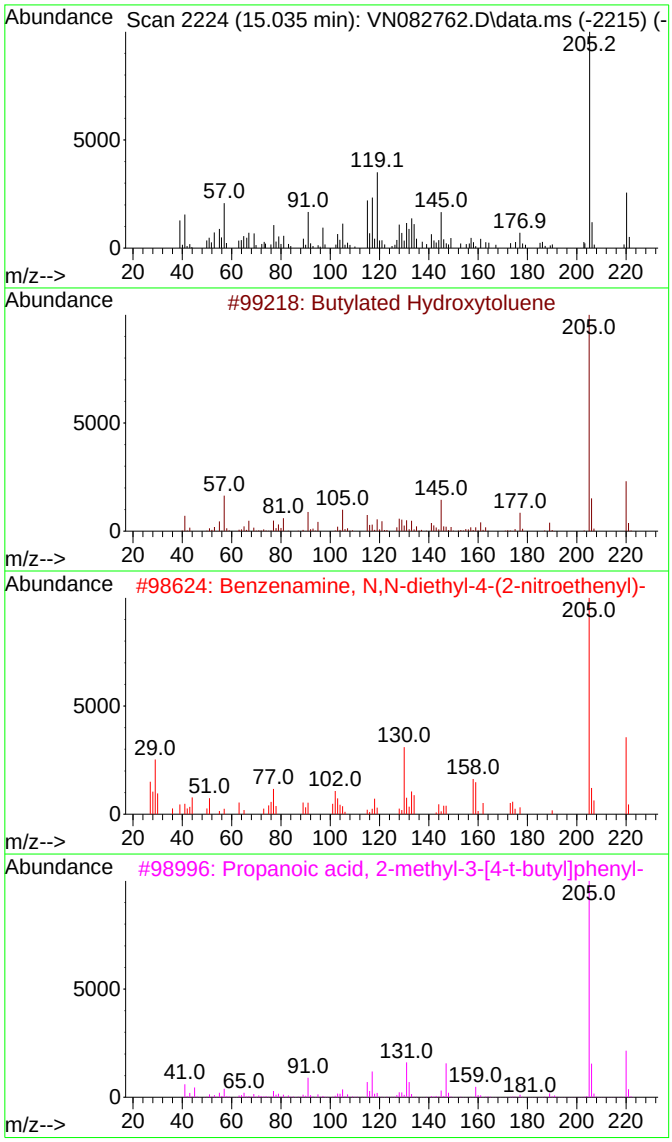
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

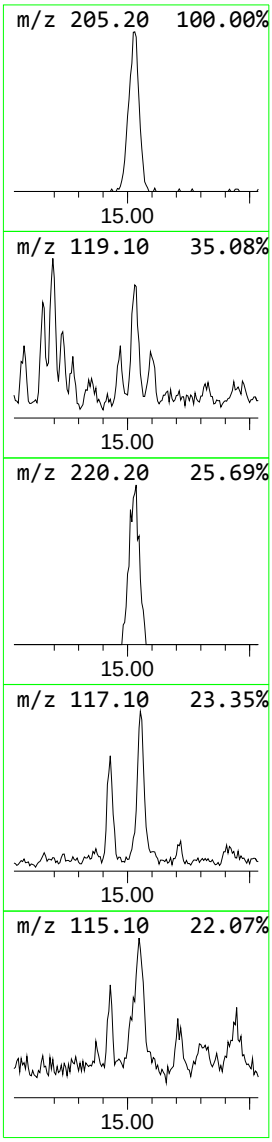
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	21.47 ug/l	210480	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	70
2	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	62
3	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	58
4	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	49
5	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

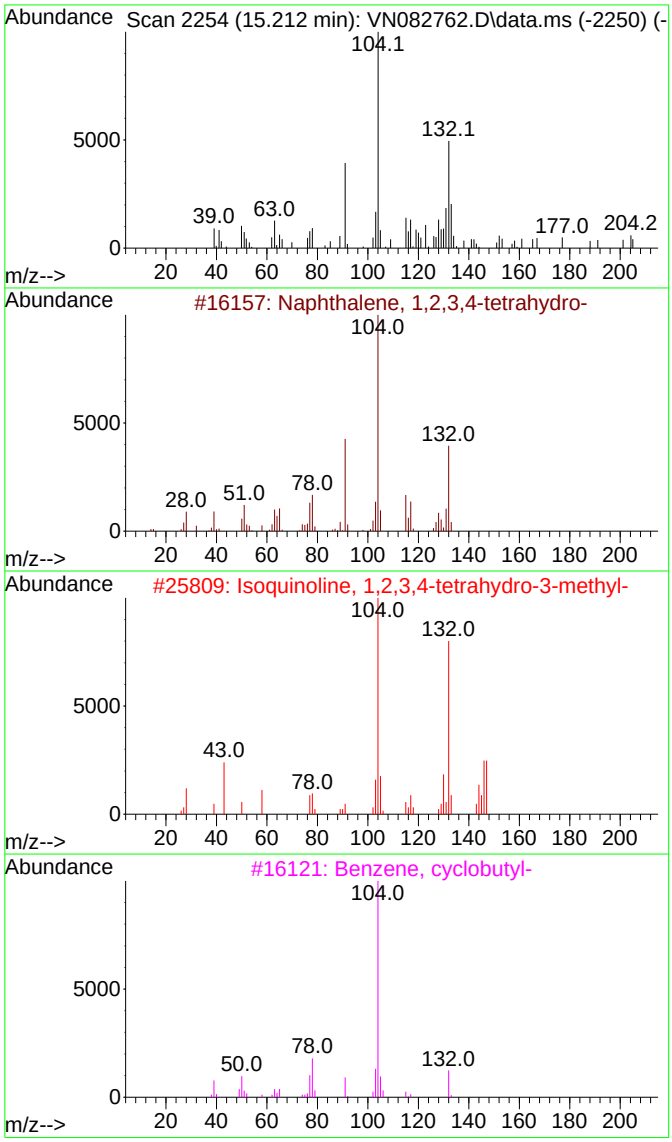
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

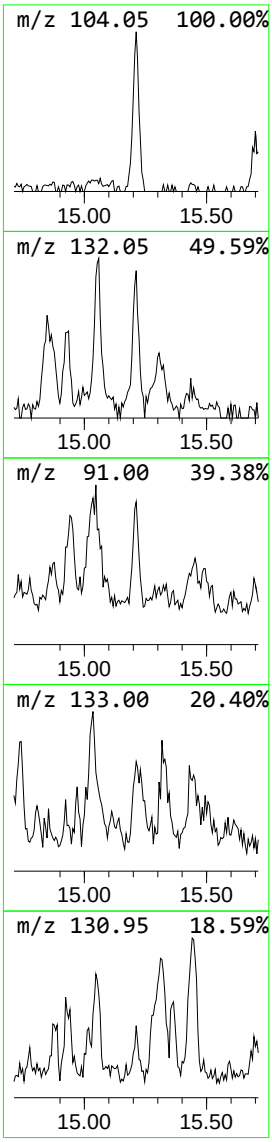
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	6.31 ug/l	61862	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	89
2	Isoquinoline, 1,2,3,4-tetrahydro...	147	C10H13N	029726-60-1	59
3	Benzene, cyclobutyl-	132	C10H12	004392-30-7	52
4	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	49
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

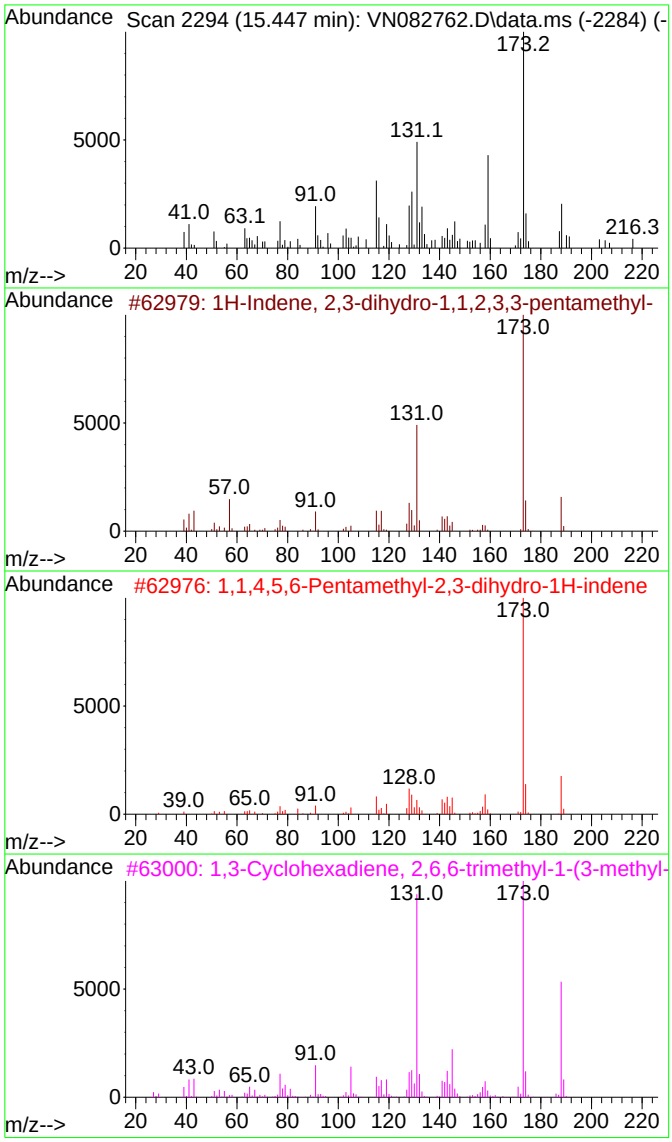
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

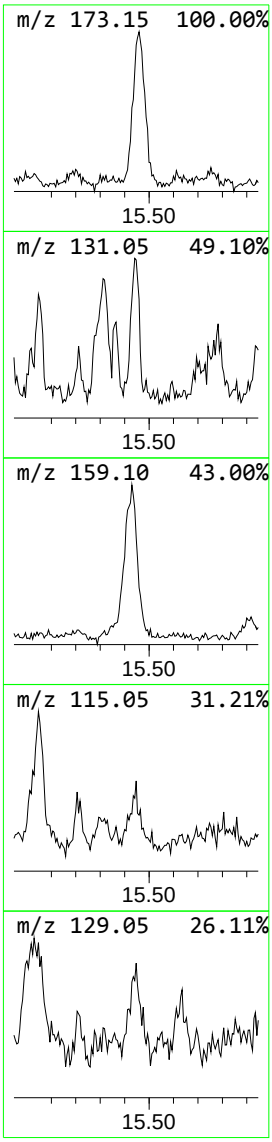
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.447	20.80 ug/l	203872	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,2,3,3...	188	C14H20	001203-17-4	50
2	1,1,4,5,6-Pentamethyl-2,3-dihydr...	188	C14H20	016204-67-4	50
3	1,3-Cyclohexadiene, 2,6,6-trimet...	188	C14H20	052260-01-2	49
4	1,1,5,6-Tetramethyl-1,2,3,4-tetr...	188	C14H20	031197-54-3	45
5	Benzene, 1-tert-butyl-4-cyclopro...	188	C14H20	058249-45-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082762.D
Acq On : 01 Jul 2024 13:51
Operator : JC\MD
Sample : P3110-03 20X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
170

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-	8.447	7.3	ug/l	38037	1	8.224	260476	50.0
Heptane	8.971	6.2	ug/l	44055	2	9.100	353118	50.0
unknown12.594	12.594	8.1	ug/l	75687	3	11.865	467621	50.0
Benzene, 1-ethy...	13.094	10.8	ug/l	106221	4	13.794	490136	50.0
Benzene, 1-ethy...	13.335	7.8	ug/l	76279	4	13.794	490136	50.0
unknown13.671	13.671	6.6	ug/l	65131	4	13.794	490136	50.0
Benzene, 1-ethe...	13.988	9.2	ug/l	89798	4	13.794	490136	50.0
Butylated Hydro...	15.035	21.5	ug/l	210480	4	13.794	490136	50.0
Naphthalene, 1,...	15.212	6.3	ug/l	61862	4	13.794	490136	50.0
1H-Indene, 2,3-...	15.447	20.8	ug/l	203872	4	13.794	490136	50.0