LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080559.D
Acq On : 20 Dec 2023 20:04
Operator : JC\MD
Sample : 05896-04
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1108

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\82N121223W.M
Title : SW846 8260

Signal : TIC: VN080559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.424	409	420	439	rBV	308094	948131	16.31%	1.447%
2	8.165	1046	1056	1059	rBV	191304	421652	7.26%	0.643%
3	8.218	1059	1065	1077	rVV3	534221	1389672	23.91%	2.121%
4	8.324	1077	1083	1093	rVB2	75860	180628	3.11%	0.276%
5	8.441	1093	1103	1112	rBV	345987	777323	13.38%	1.186%
6	8.576	1118	1126	1137	rVB2	182030	411400	7.08%	0.628%
7	8.700	1139	1147	1156	rBV4	49676	135680	2.33%	0.207%
8	8.853	1167	1173	1182	rVB4	29340	64872	1.12%	0.099%
9	8.965	1182	1192	1204	rBV	479417	937970	16.14%	1.431%
10	9.100	1206	1215	1225	rBV	512999	1035698	17.82%	1.580%
11	9.594	1283	1299	1305	rBV2	161184	422931	7.28%	0.645%
12	9.776	1323	1330	1336	rBV2	40146	78001	1.34%	0.119%
13	10.206	1397	1403	1416	rVB3	71003	172584	2.97%	0.263%
14	10.341	1418	1426	1438	rBV2	60984	138804	2.39%	0.212%
15	10.565	1457	1464	1469	rBV	834406	1580766	27.20%	2.412%
16	10.629	1469	1475	1483	rVB	3176119	5811757	100.00%	8.868%
17	10.747	1489	1495	1503	rVB	240010	450126	7.75%	0.687%
18	10.912	1518	1523	1531	rVB2	64295	118251	2.03%	0.180%
19	11.006	1532	1539	1547	rBV	92911	190684	3.28%	0.291%
20	11.170	1560	1567	1573	rBV2	57688	105957	1.82%	0.162%
21	11.270	1580	1584	1592	rVB	44716	91326	1.57%	0.139%
22	11.347	1592	1597	1601	rBV3	61507	113919	1.96%	0.174%
23	11.417	1601	1609	1614	rVV	167389	380391	6.55%	0.580%
24	11.470	1614	1618	1624	rVB	142537	260963	4.49%	0.398%
25	11.576	1630	1636	1640	rBV3	81236	126027	2.17%	0.192%
26	11.641	1640	1647	1651	rBV3	187713	395120	6.80%	0.603%
27	11.747	1660	1665	1671	rVB	201086	300793	5.18%	0.459%
28	11.870	1679	1686	1696	rVB	733882	1327241	22.84%	2.025%
29	11.964	1696	1702	1706	rBV	220523	386759	6.65%	0.590%
30	12.070	1711	1720	1725	rBV	1038226	1960220	33.73%	2.991%
31	12.153	1731	1734	1740	rVB2	184899	303683	5.23%	0.463%
32	12.288	1752	1757	1763	rVB5	45340	93655	1.61%	0.143%
33	12.400	1764	1776	1784	rBV2	459418	1428724	24.58%	2.180%
34	12.482	1784	1790	1795	rVB3	149967	278205	4.79%	0.425%
35	12.541	1795	1800	1802	rBV3	86622	153136	2.63%	0.234%
36	12.617	1802	1813	1822	rVB7	240928	882456	15.18%	1.347%

LSC Area Percent Report

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Integrator: RTE
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Peak separation: 5

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Title : SW846 8260

37	12.694	1822	1826	1831	rBV2	108259	175866	3.03%	0.268%
38	12.770	1836	1839	1841	rBV2	64863	59605	1.03%	0.091%
39	12.853	1847	1853	1862	rVB2	592762	1118101	19.24%	1.706%
40	12.935	1864	1867	1871	rVB4	76433	109433	1.88%	0.167%
41	13.035	1877	1884	1889	rVB3	309521	595275	10.24%	0.908%
42	13.100	1889	1895	1898	rBV	725155	1231684	21.19%	1.879%
43	13.164	1898	1906	1913	rVV5	1002822	2668757	45.92%	4.072%
44	13.229	1913	1917	1921	rVB2	139680	207703	3.57%	0.317%
45	13.335	1928	1935	1942	rBV2	315845	700529	12.05%	1.069%
46	13.400	1943	1946	1954	rVB5	162514	398277	6.85%	0.608%
47	13.482	1954	1960	1969	rBV	1054422	1834093	31.56%	2.799%
48	13.617	1979	1983	1987	rVB3	179458	262034	4.51%	0.400%
49	13.676	1987	1993	1998	rBV3	460103	926801	15.95%	1.414%
50	13.723	1998	2001	2007	rVB3	132462	215064	3.70%	0.328%
51	13.794	2007	2013	2017	rBV	802272	1571678	27.04%	2.398%
52	13.947	2030	2039	2041	rBV5	214128	531316	9.14%	0.811%
53	13.988	2041	2046	2049	rVV2	534862	910269	15.66%	1.389%
54	14.023	2049	2052	2057	rVB3	276890	503119	8.66%	0.768%
55	14.111	2062	2067	2075	rVV4	773102	1711788	29.45%	2.612%
56	14.182	2076	2079	2084	rVV	271120	450095	7.74%	0.687%
57	14.247	2086	2090	2092	rVV	300991	477035	8.21%	0.728%
58	14.276	2092	2095	2099	rVV	342653	521256	8.97%	0.795%
59	14.329	2100	2104	2109	rVB	484619	738656	12.71%	1.127%
60	14.441	2118	2123	2129	rVB3	611674	1042313	17.93%	1.590%
61	14.576	2141	2146	2150	rBV4	297691	489218	8.42%	0.747%
62	14.629	2150	2155	2158	rBV	701003	1114866	19.18%	1.701%
63	14.694	2163	2166	2170	rVB	313963	388051	6.68%	0.592%
64	14.735	2170	2173	2177	rBV	366984	453241	7.80%	0.692%
65	14.794	2177	2183	2188	rVB4	420812	986257	16.97%	1.505%
66	14.852	2188	2193	2194	rBV3	279512	425143	7.32%	0.649%
67	14.876	2194	2197	2202	rVB2	457292	674911	11.61%	1.030%
68	14.941	2202	2208	2210	rBV5	662439	1434281	24.68%	2.189%
69	15.058	2218	2228	2233	rBV4	940425	2543723	43.77%	3.882%
70	15.105	2233	2236	2245	rVB4	373218	714413	12.29%	1.090%
71	15.211	2249	2254	2261	rVV	657276	1179878	20.30%	1.800%
72	15.323	2268	2273	2277	rBV3	371036	650448	11.19%	0.993%
73	15.447	2287	2294	2300	rVB4	557159	1257814	21.64%	1.919%
74	15.600	2315	2320	2323	rBV5	224968	442381	7.61%	0.675%
75	15.699	2331	2337	2341	rBV	505593	1000374	17.21%	1.526%
76	15.747	2341	2345	2349	rVV3	337377	574202	9.88%	0.876%

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Title : SW846 8260

77	15.947	2371	2379	2386	rBV3	441207	1113280	19.16%	1.699%
78	16.023	2389	2392	2397	rVB2	81642	144737	2.49%	0.221%
79	16.123	2404	2409	2411	rBV3	150493	281886	4.85%	0.430%
80	16.170	2411	2417	2426	rVB	927803	1952385	33.59%	2.979%
81	16.258	2428	2432	2438	rBV4	112600	184692	3.18%	0.282%
82	16.341	2439	2446	2460	rVB4	320420	1243714	21.40%	1.898%
83	16.499	2464	2473	2493	rVB3	516174	1619550	27.87%	2.471%
84	16.711	2499	2509	2516	rBV3	601167	1532047	26.36%	2.338%
85	16.782	2516	2521	2522	rBV3	217896	316116	5.44%	0.482%

Sum of corrected areas: 65533860

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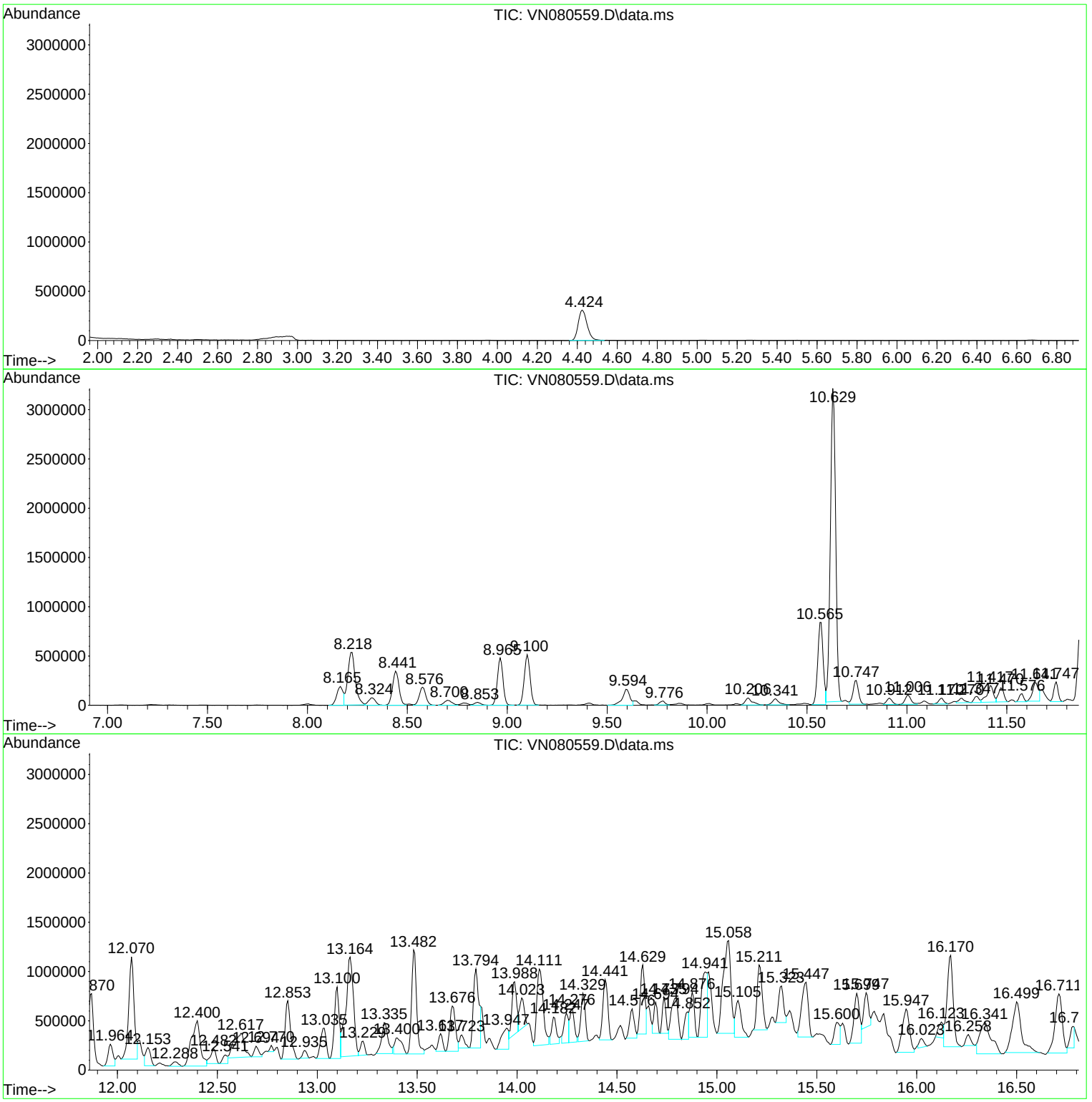
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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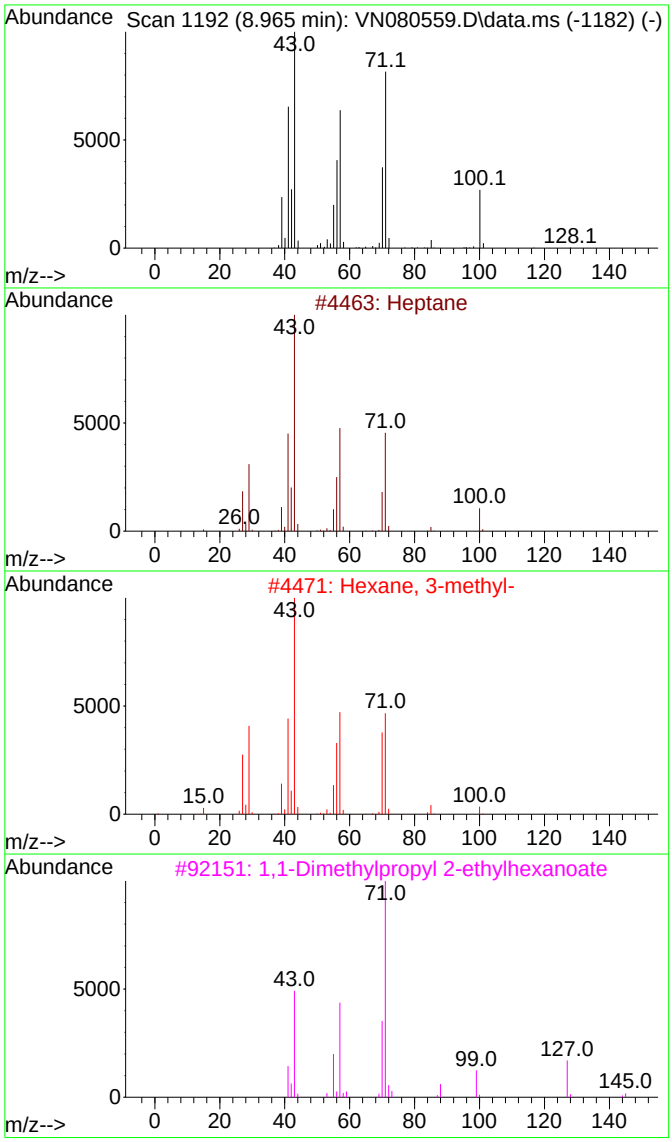
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

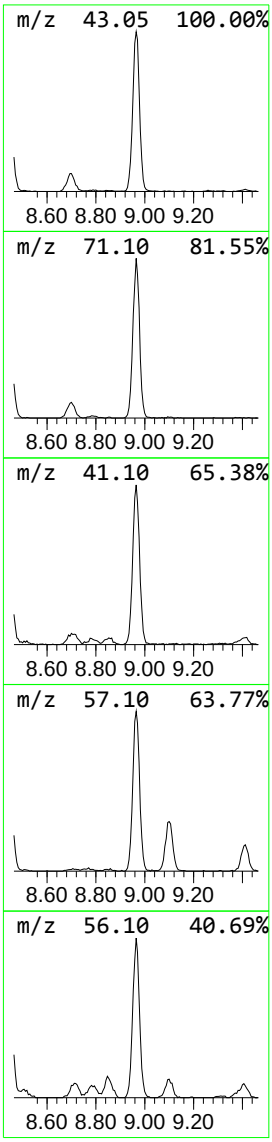
****

Peak Number 1 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	45.28 ug/l	937970	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	1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	50
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5	3-Hexanone, 4-ethyl-	128	C8H16O	006137-12-8	47





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Instrument :
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ClientSampleId :
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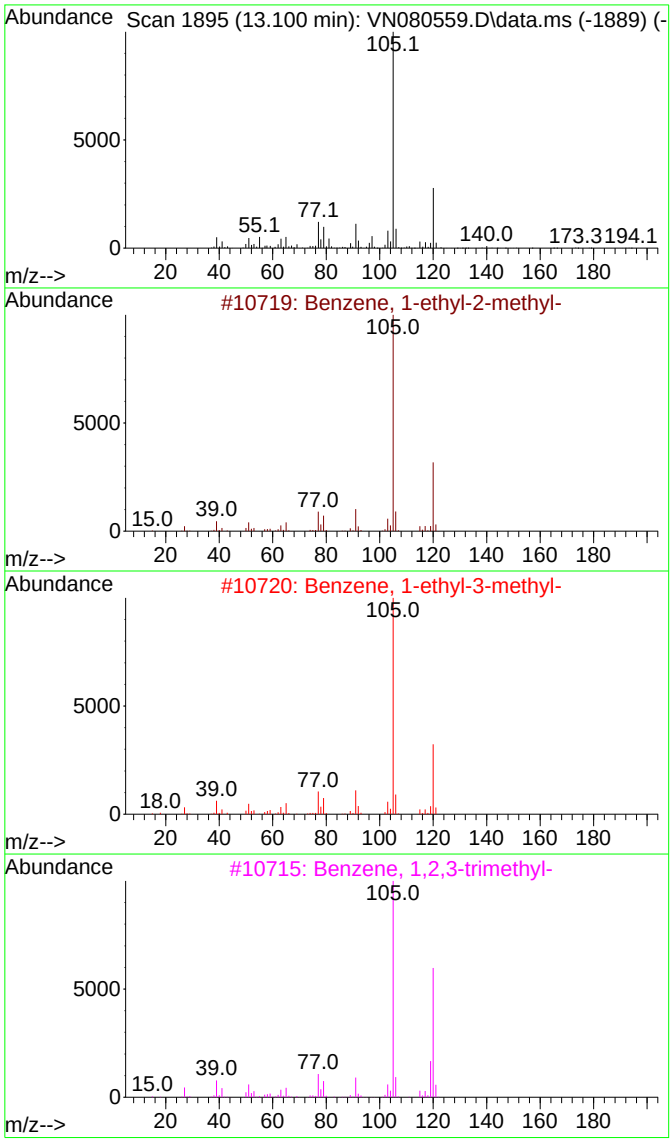
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

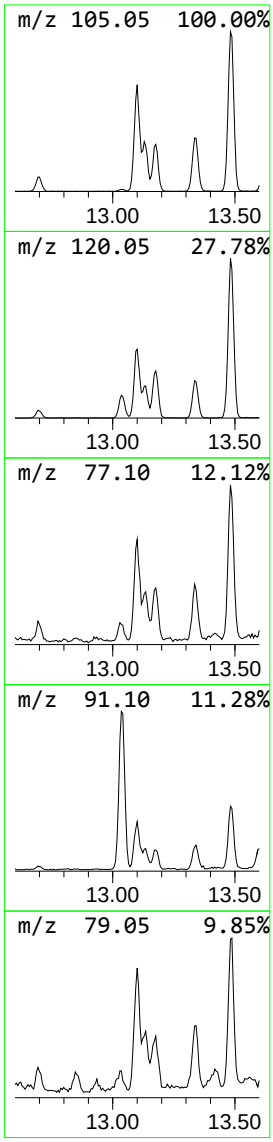
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	39.18 ug/l	1231680	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	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





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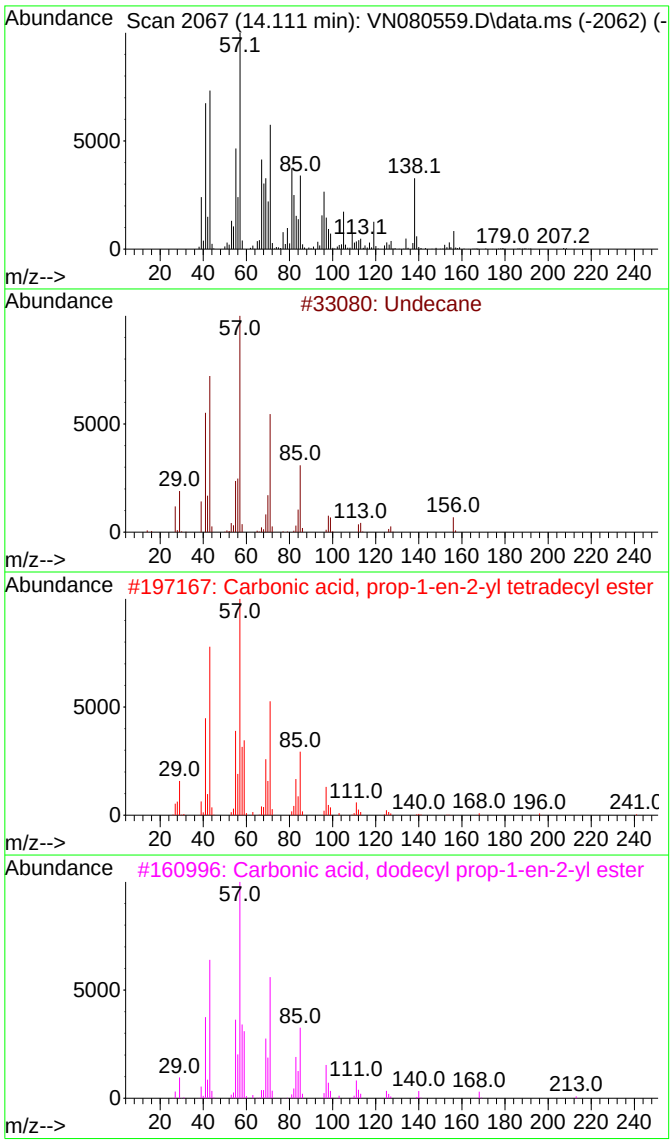
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

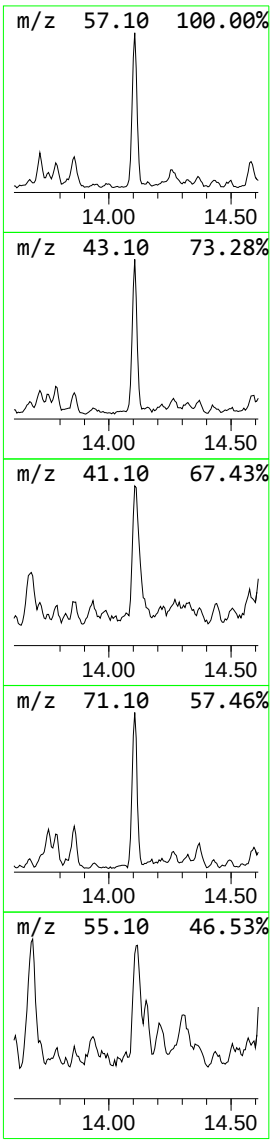
****

Peak Number 3 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	54.46 ug/l	1711790	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	83
2	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	38
3	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	30
4	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	30
5	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	30





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Quant Title : SW846 8260

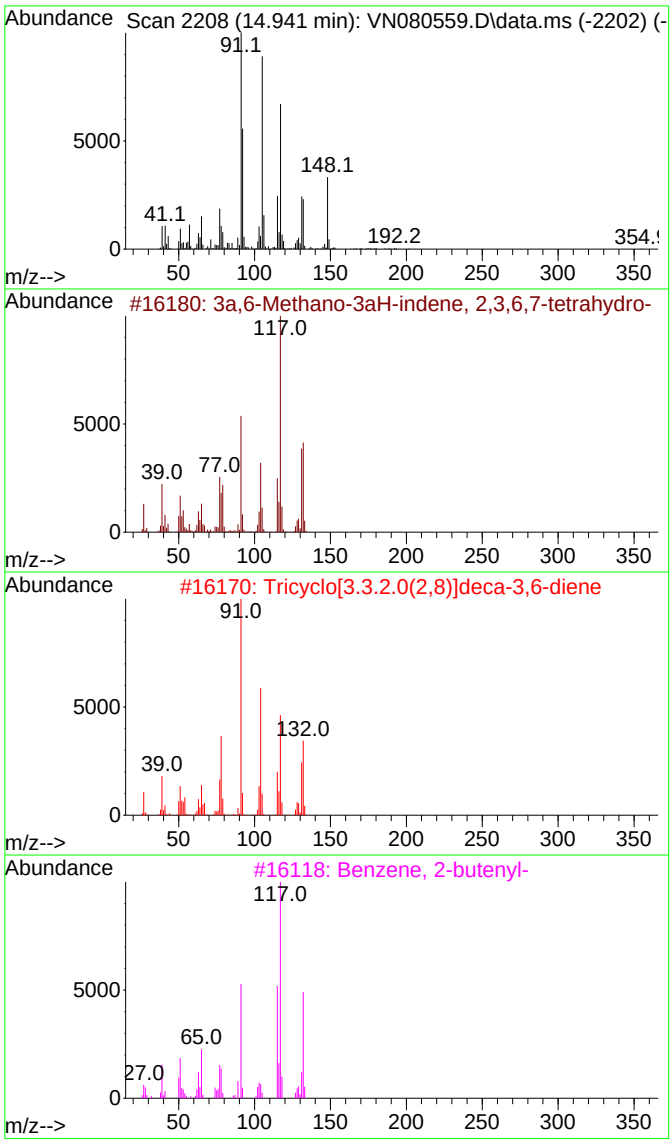
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

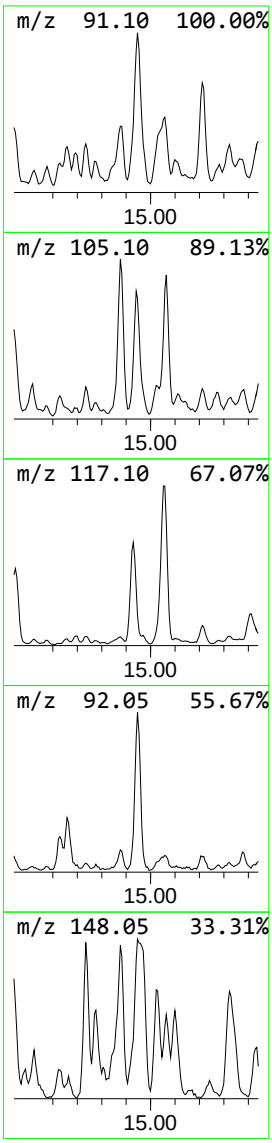
****

Peak Number 4 unknown14.941 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.941	45.63 ug/l	1434280	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3a,6-Methano-3aH-indene, 2,3,6,7...	132	C10H12	098640-29-0	45
2	Tricyclo[3.3.2.0(2,8)]deca-3,6-d...	132	C10H12	000768-46-7	43
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	42
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	41
5	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	38





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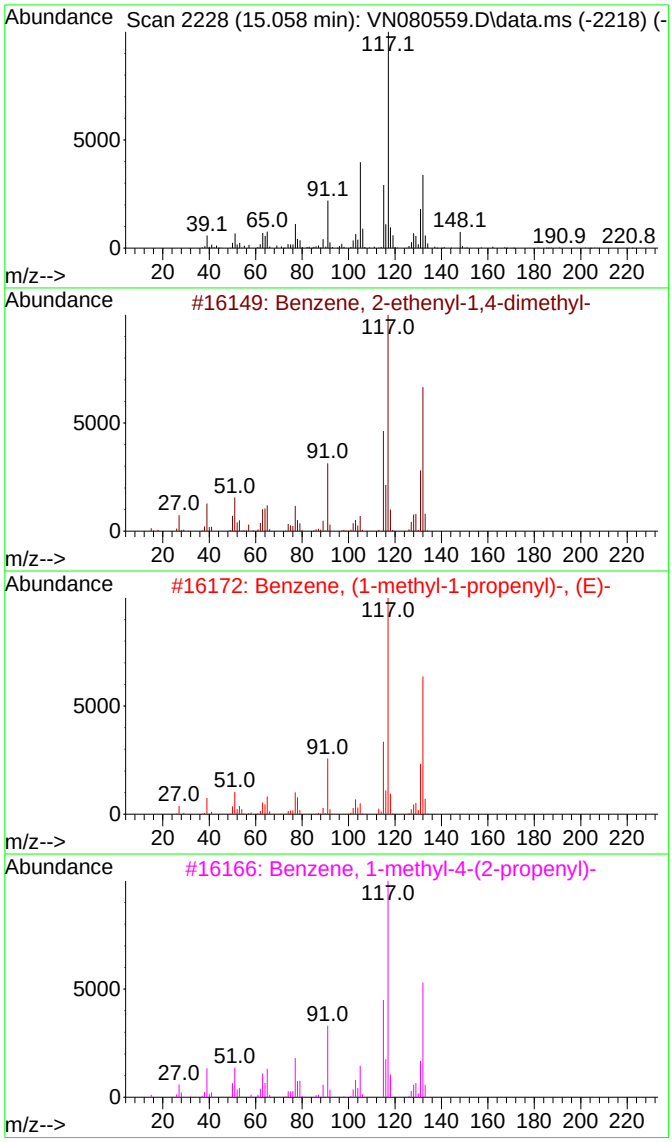
Quant Title : SW846 8260

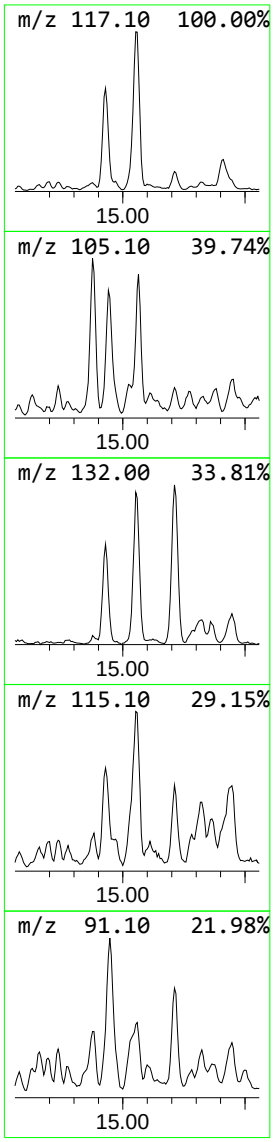
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.058	80.92 ug/l	2543720	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	93
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	93
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90





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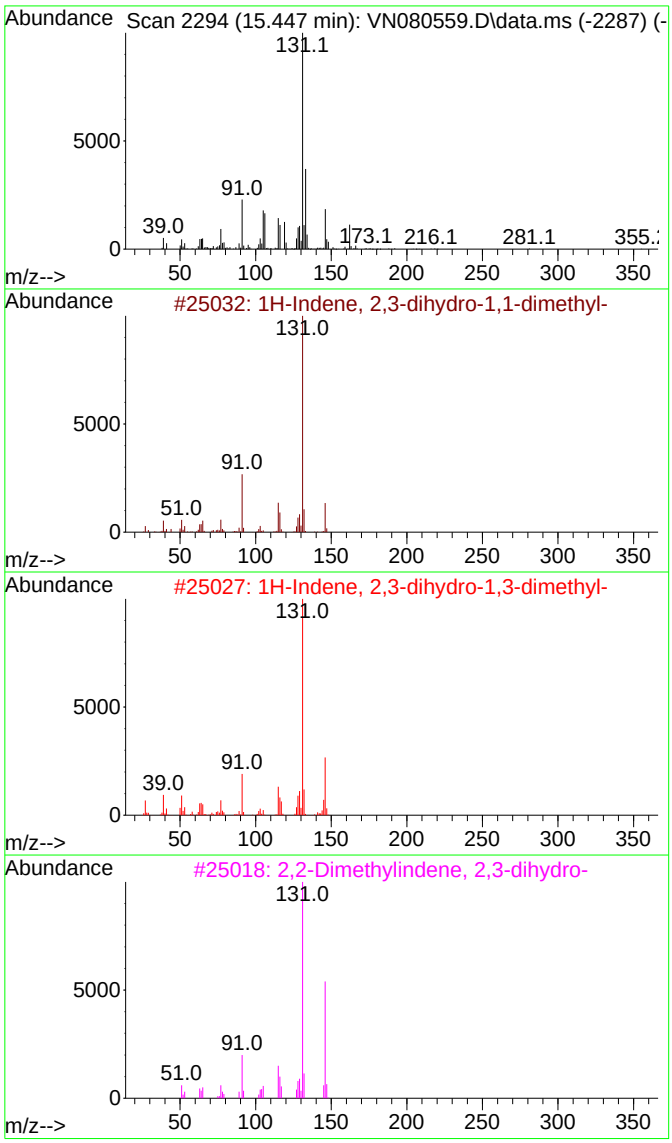
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

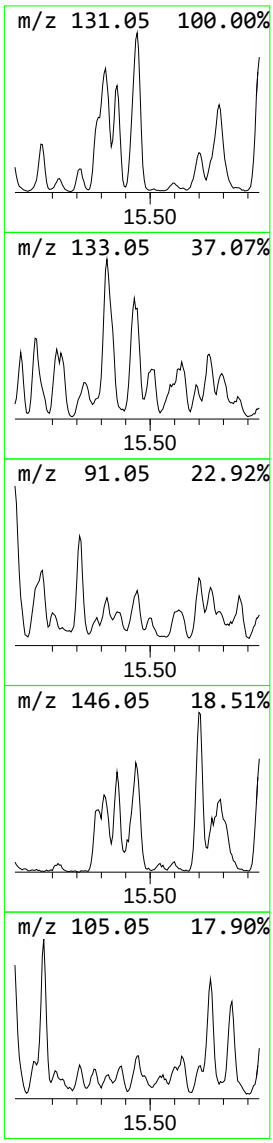
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.447	40.02 ug/l	1257810	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	70
2	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080559.D
Acq On : 20 Dec 2023 20:04
Operator : JC\MD
Sample : 05896-04
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1108

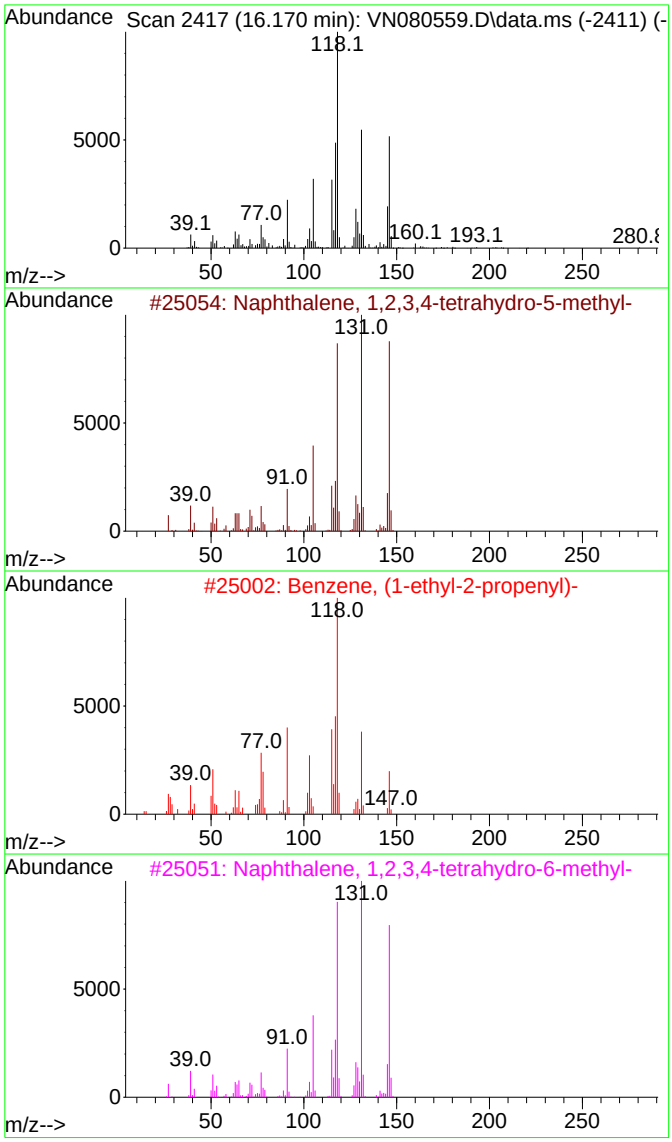
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

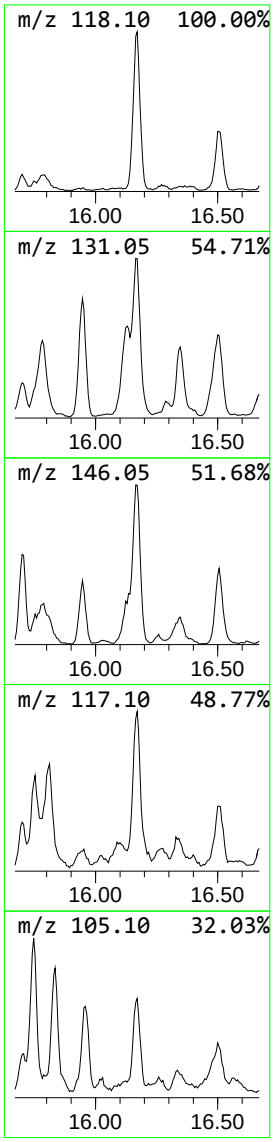
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	62.11 ug/l	1952390	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
2	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	60
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	52
5	5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080559.D
Acq On : 20 Dec 2023 20:04
Operator : JC\MD
Sample : 05896-04
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1108

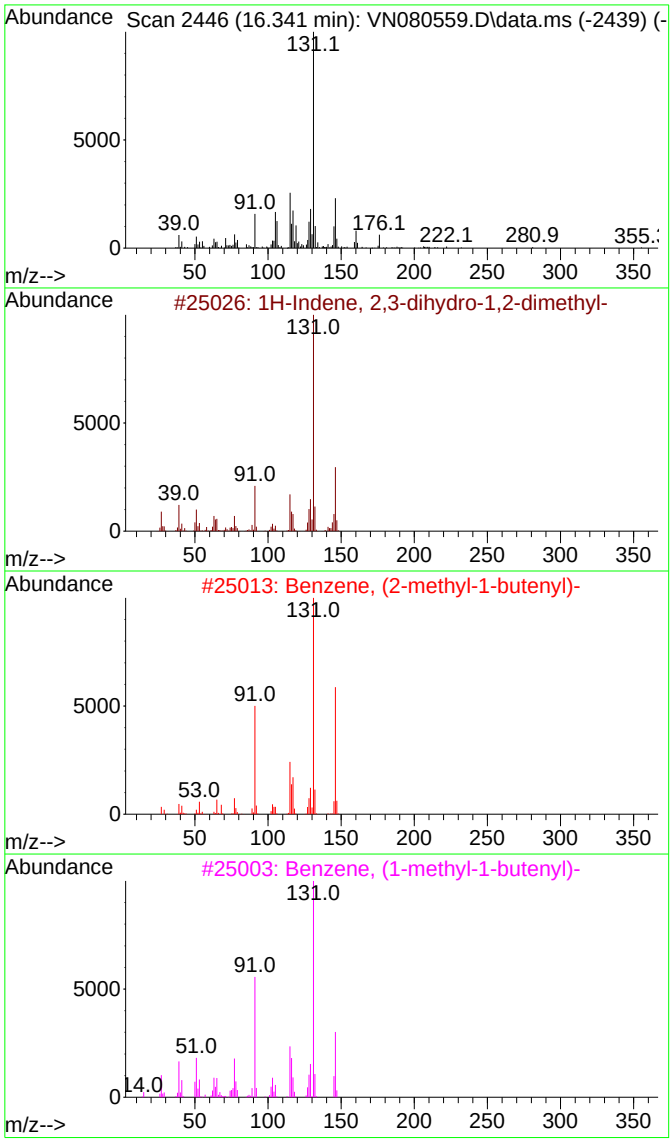
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

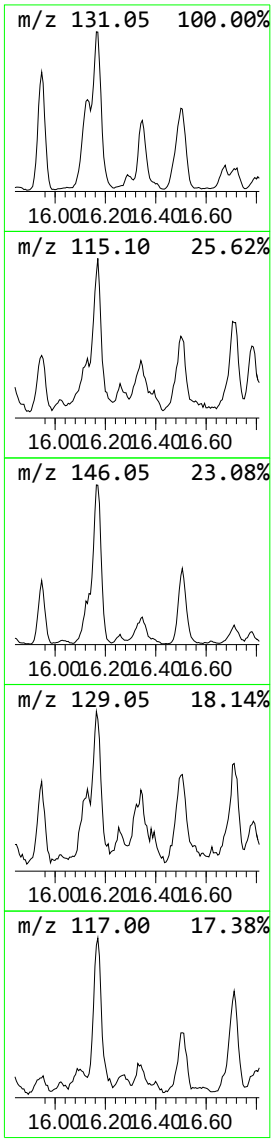
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.341	39.57 ug/l	1243710	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	94
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	90
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	87
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	87





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Data File : VN080559.D
Acq On : 20 Dec 2023 20:04
Operator : JC\MD
Sample : 05896-04
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1108

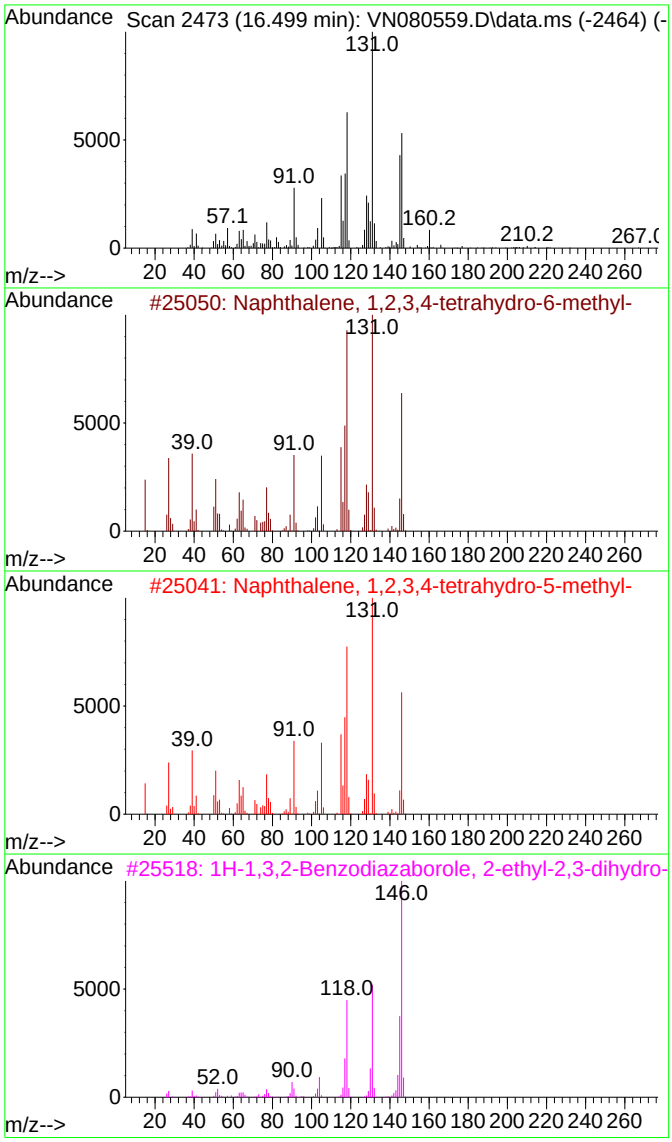
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

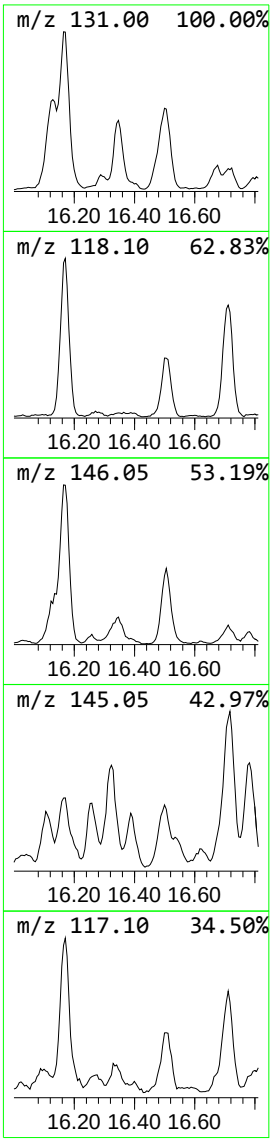
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.499	51.52 ug/l	1619550	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	89
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	89
3	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
4	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	64
5	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	55





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Acq On : 20 Dec 2023 20:04
Operator : JC\MD
Sample : 05896-04
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1108

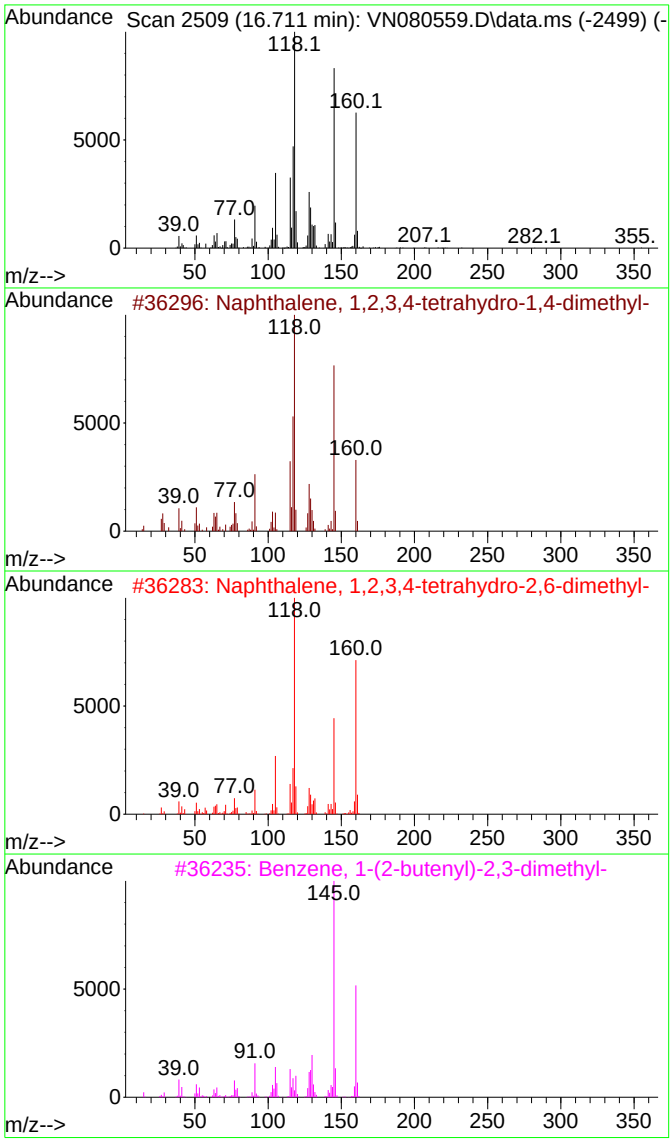
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

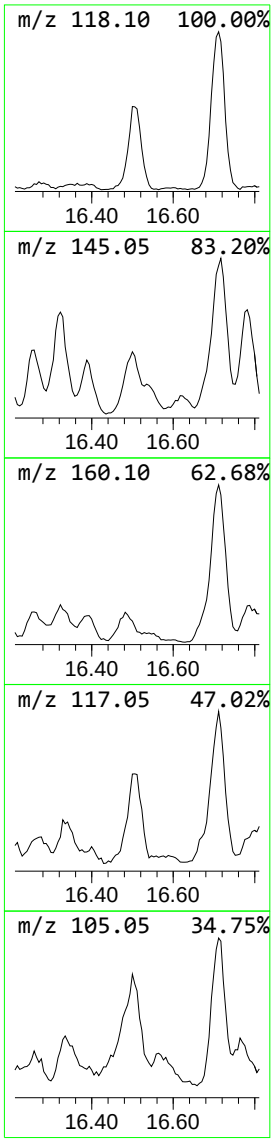
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.711	48.74 ug/l	1532050	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	90
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	70
5	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122023\
Data File : VN080559.D
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MSVOA_N
ClientSampleId :
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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	8.965	45.3	ug/l	937970	2	9.100	1035700	50.0
Benzene, 1-ethy...	13.100	39.2	ug/l	1231680	4	13.794	1571680	50.0
Undecane	14.111	54.5	ug/l	1711790	4	13.794	1571680	50.0
unknown14.941	14.941	45.6	ug/l	1434280	4	13.794	1571680	50.0
Benzene, 2-ethe...	15.058	80.9	ug/l	2543720	4	13.794	1571680	50.0
1H-Indene, 2,3-...	15.447	40.0	ug/l	1257810	4	13.794	1571680	50.0
Naphthalene, 1,...	16.170	62.1	ug/l	1952390	4	13.794	1571680	50.0
1H-Indene, 2,3-...	16.341	39.6	ug/l	1243710	4	13.794	1571680	50.0
Naphthalene, 1,...	16.499	51.5	ug/l	1619550	4	13.794	1571680	50.0
Naphthalene, 1,...	16.711	48.7	ug/l	1532050	4	13.794	1571680	50.0