LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075271.D
Acq On : 14 Nov 2022 17:38
Operator : JC\MD
Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

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\82N102622W.M
Title : SW846 8260

Signal : TIC: VN075271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	36	40	48	rVB4	6716	16592	1.75%	0.090%
2	3.112	179	180	189	rVB6	19769	29724	3.13%	0.161%
3	5.506	574	587	595	rBV3	3216	12039	1.27%	0.065%
4	8.000	1003	1011	1021	rVB3	9785	23714	2.50%	0.129%
5	8.165	1030	1039	1042	rBV	126249	268223	28.24%	1.455%
6	8.218	1042	1048	1058	rVV2	362635	875841	92.22%	4.752%
7	8.324	1058	1066	1076	rVB2	60424	143378	15.10%	0.778%
8	8.441	1076	1086	1095	rBV	284503	639545	67.34%	3.470%
9	8.577	1101	1109	1120	rVB2	137204	306868	32.31%	1.665%
10	8.700	1120	1130	1138	rBV3	44918	115589	12.17%	0.627%
11	8.782	1138	1144	1150	rVV6	15921	41339	4.35%	0.224%
12	8.847	1150	1155	1167	rVV3	18083	44119	4.65%	0.239%
13	8.965	1167	1175	1185	rVB	387957	742468	78.17%	4.029%
14	9.100	1190	1198	1206	rBV	341544	679685	71.56%	3.688%
15	9.406	1239	1250	1258	rVB	31235	68144	7.17%	0.370%
16	9.594	1270	1282	1286	rBV2	86284	223742	23.56%	1.214%
17	9.641	1286	1290	1298	rVB	46908	90845	9.57%	0.493%
18	9.771	1307	1312	1318	rBV4	24482	45324	4.77%	0.246%
19	10.200	1380	1385	1398	rVB5	7745	17959	1.89%	0.097%
20	10.341	1401	1409	1421	rVB3	6295	14658	1.54%	0.080%
21	10.565	1439	1447	1454	rBV	520448	949756	100.00%	5.153%
22	10.629	1454	1458	1465	rVB	45012	78218	8.24%	0.424%
23	10.741	1471	1477	1485	rVB2	21072	40941	4.31%	0.222%
24	10.912	1501	1506	1512	rVB3	6334	11649	1.23%	0.063%
25	11.000	1515	1521	1530	rBV4	9244	19688	2.07%	0.107%
26	11.171	1543	1550	1556	rVB3	10057	17332	1.82%	0.094%
27	11.271	1563	1567	1576	rVB4	7265	14490	1.53%	0.079%
28	11.347	1576	1580	1584	rBV4	8132	14564	1.53%	0.079%
29	11.418	1588	1592	1596	rVV2	16707	28489	3.00%	0.155%
30	11.465	1596	1600	1607	rVB2	21513	41586	4.38%	0.226%
31	11.571	1613	1618	1622	rBV2	15201	23339	2.46%	0.127%
32	11.641	1622	1630	1634	rBV3	30615	68506	7.21%	0.372%
33	11.676	1634	1636	1642	rVB	19244	27104	2.85%	0.147%
34	11.741	1642	1647	1653	rVB	34858	54635	5.75%	0.296%
35	11.865	1661	1668	1680	rVB	436192	772462	81.33%	4.191%
36	11.965	1680	1685	1688	rBV	21216	34188	3.60%	0.185%

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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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Peak separation: 5

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Title : SW846 8260

37	12.000	1688	1691	1694	rBV2	11098	13989	1.47%	0.076%
38	12.071	1694	1703	1707	rBV2	138417	255970	26.95%	1.389%
39	12.106	1707	1709	1713	rVB	30043	36591	3.85%	0.199%
40	12.153	1713	1717	1722	rVB5	32748	58842	6.20%	0.319%
41	12.212	1722	1727	1734	rBV5	9607	22562	2.38%	0.122%
42	12.294	1734	1741	1746	rVB6	15321	31759	3.34%	0.172%
43	12.371	1746	1754	1756	rBV3	76513	143773	15.14%	0.780%
44	12.482	1767	1773	1778	rVB	78684	137045	14.43%	0.744%
45	12.594	1778	1792	1804	rBV7	96747	441191	46.45%	2.394%
46	12.700	1805	1810	1813	rVV6	32089	74260	7.82%	0.403%
47	12.741	1813	1817	1819	rVV3	47891	85380	8.99%	0.463%
48	12.770	1819	1822	1824	rVV	64870	91061	9.59%	0.494%
49	12.794	1824	1826	1830	rVB	57526	65800	6.93%	0.357%
50	12.847	1830	1835	1844	rBV2	339100	660482	69.54%	3.584%
51	12.935	1844	1850	1854	rBV4	35944	56104	5.91%	0.304%
52	12.976	1854	1857	1860	rVB2	11153	14730	1.55%	0.080%
53	13.023	1860	1865	1870	rVB4	63653	123211	12.97%	0.669%
54	13.094	1870	1877	1881	rBV4	68478	154324	16.25%	0.837%
55	13.159	1881	1888	1896	rBV4	287621	669368	70.48%	3.632%
56	13.223	1896	1899	1905	rVB3	83345	133232	14.03%	0.723%
57	13.312	1905	1914	1918	rBV4	80351	180709	19.03%	0.980%
58	13.359	1918	1922	1924	rBV2	58058	81188	8.55%	0.441%
59	13.394	1924	1928	1936	rVB3	151714	276703	29.13%	1.501%
60	13.523	1947	1950	1954	rVB2	40239	49833	5.25%	0.270%
61	13.576	1955	1959	1962	rVV4	56534	79509	8.37%	0.431%
62	13.612	1963	1965	1969	rVB4	45412	54758	5.77%	0.297%
63	13.676	1970	1976	1980	rBV4	184097	393181	41.40%	2.133%
64	13.717	1980	1983	1987	rVV3	100887	147491	15.53%	0.800%
65	13.788	1990	1995	2004	rVB	466544	812721	85.57%	4.410%
66	13.859	2004	2007	2013	rVB5	76008	109711	11.55%	0.595%
67	13.935	2013	2020	2024	rBV5	79234	200221	21.08%	1.086%
68	13.982	2024	2028	2032	rBV2	84928	125790	13.24%	0.683%
69	14.023	2032	2035	2039	rVB2	53977	74759	7.87%	0.406%
70	14.112	2045	2050	2056	rBV3	345073	760864	80.11%	4.128%
71	14.212	2065	2067	2072	rVB4	68444	85641	9.02%	0.465%
72	14.264	2072	2076	2080	rBV4	63062	127214	13.39%	0.690%
73	14.435	2100	2105	2111	rBV4	204446	401574	42.28%	2.179%
74	14.506	2113	2117	2123	rVV6	109227	227847	23.99%	1.236%
75	14.570	2124	2128	2132	rVV7	78428	157754	16.61%	0.856%
76	14.623	2132	2137	2146	rVB4	409376	729469	76.81%	3.958%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Title : SW846 8260

77	14.735	2152	2156	2159	rBV2	141313	206244	21.72%	1.119%
78	14.794	2159	2166	2170	rVB4	187739	364908	38.42%	1.980%
79	14.847	2170	2175	2179	rBV4	137017	283504	29.85%	1.538%
80	15.053	2203	2210	2215	rBV6	152563	419662	44.19%	2.277%
81	15.106	2215	2219	2228	rVB6	202320	416624	43.87%	2.261%
82	15.176	2228	2231	2234	rBV5	45408	66045	6.95%	0.358%
83	15.317	2251	2255	2261	rBV6	128175	228629	24.07%	1.241%
84	15.441	2270	2276	2281	rVB3	121601	256271	26.98%	1.390%
85	15.600	2299	2303	2311	rVB7	102036	238528	25.11%	1.294%
86	15.694	2312	2319	2324	rBV4	98239	264800	27.88%	1.437%
87	15.947	2354	2362	2363	rBV7	66081	161959	17.05%	0.879%
88	16.111	2386	2390	2394	rBV6	36018	66283	6.98%	0.360%
89	16.164	2395	2399	2408	rVB6	110772	221251	23.30%	1.200%
90	16.711	2486	2492	2499	rVB2	133908	292231	30.77%	1.586%

Sum of corrected areas: 18430293

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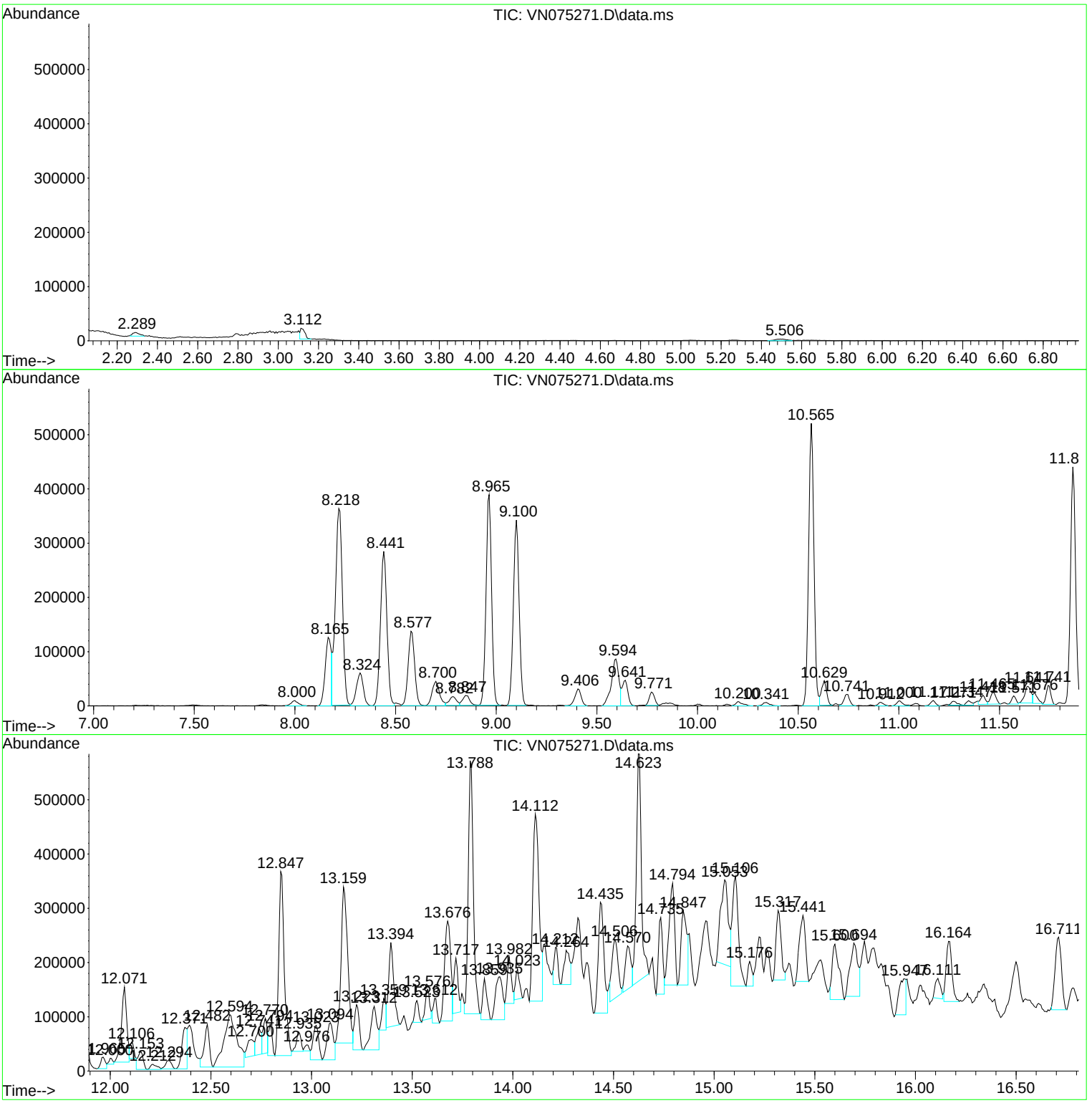
Instrument :
MSVOA_N
ClientSampleId :
31604

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

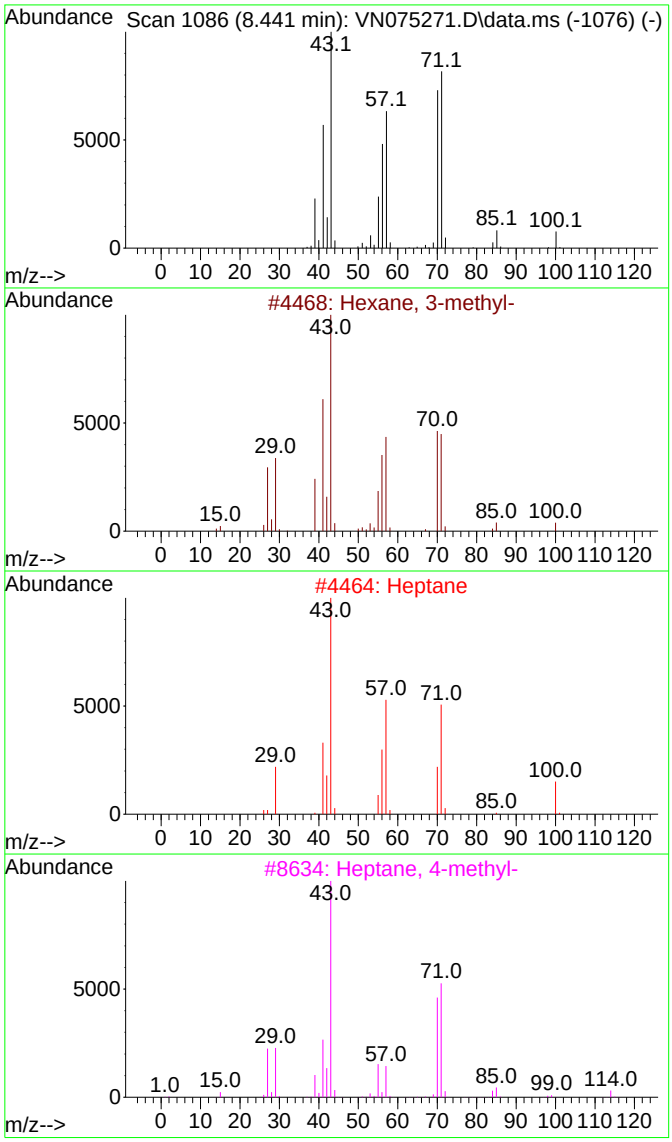
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

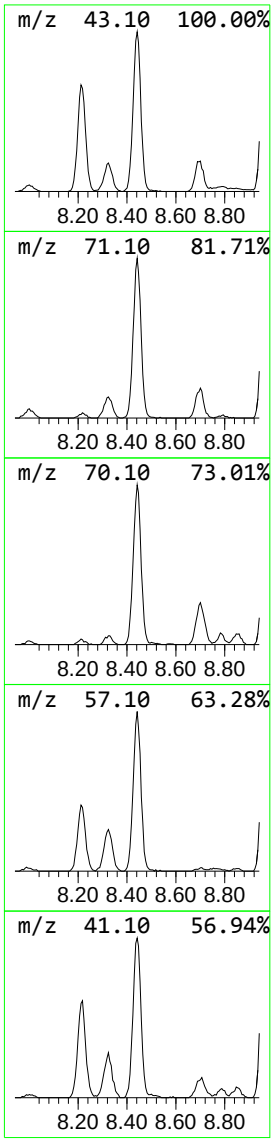
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	36.51 ug/l	639545	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2	Heptane	100	C7H16	000142-82-5	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
31604

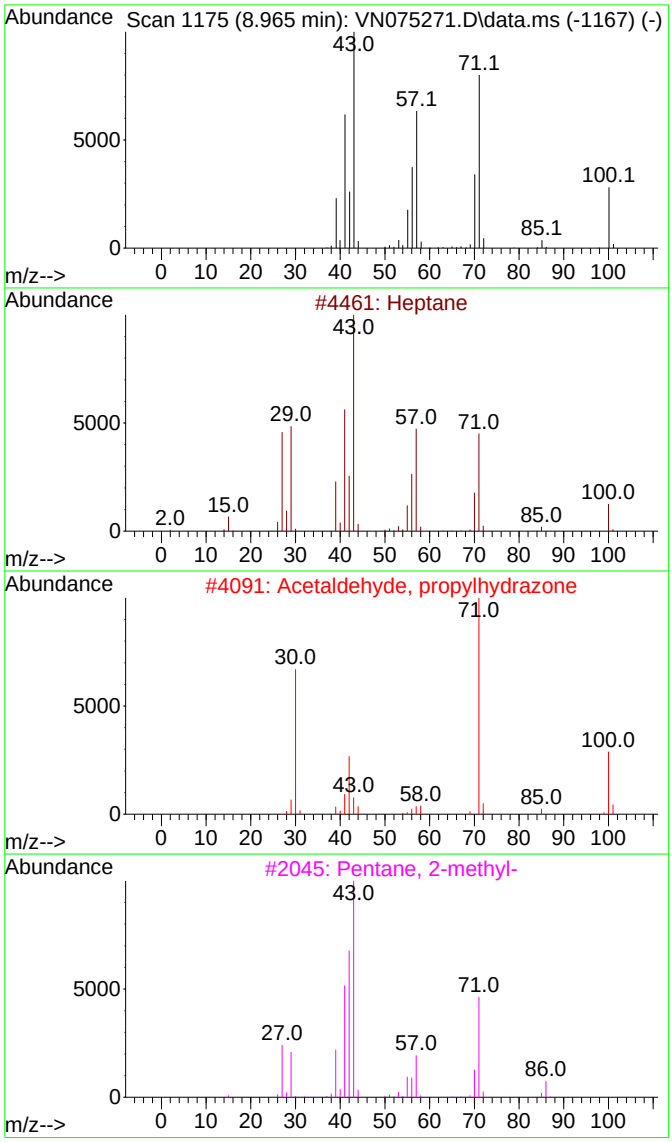
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

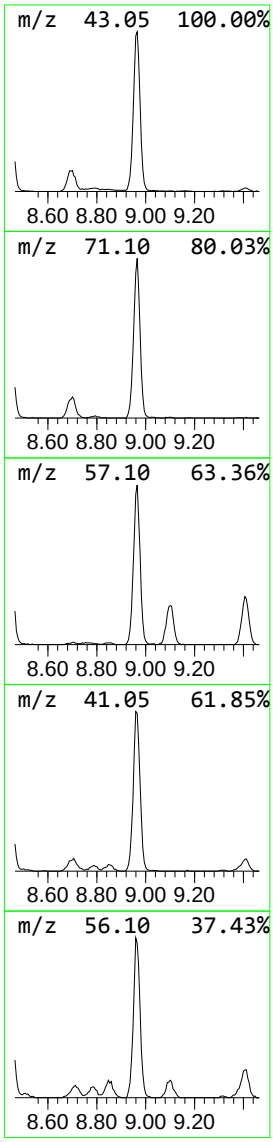
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	54.62 ug/l	742468	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	58
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	50
5	3-Hexanone	100	C6H12O	000589-38-8	46





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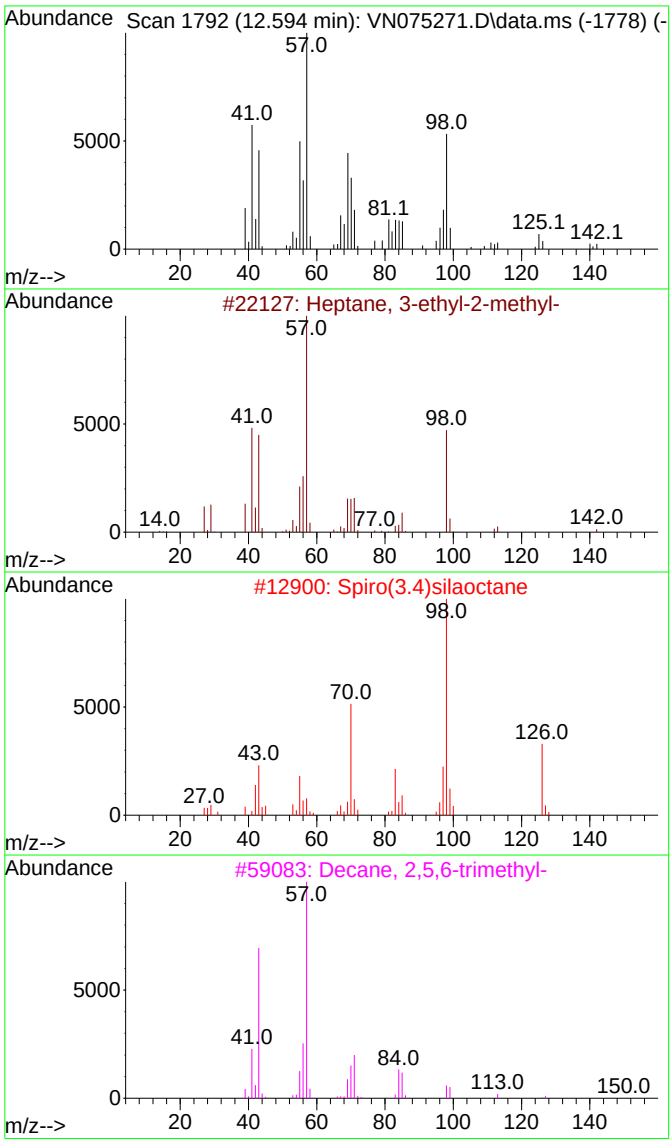
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

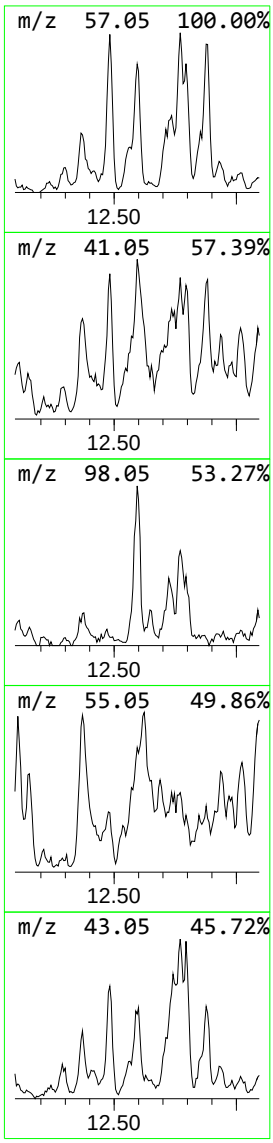
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane, 3-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.594	28.56 ug/l	441191	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	70
2	Spiro(3.4)silaoctane	126	C7H14Si	1000433-94-6	47
3	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	43
4	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	43
5	2-Hexene, 3-methyl-, (Z)-	98	C7H14	010574-36-4	43





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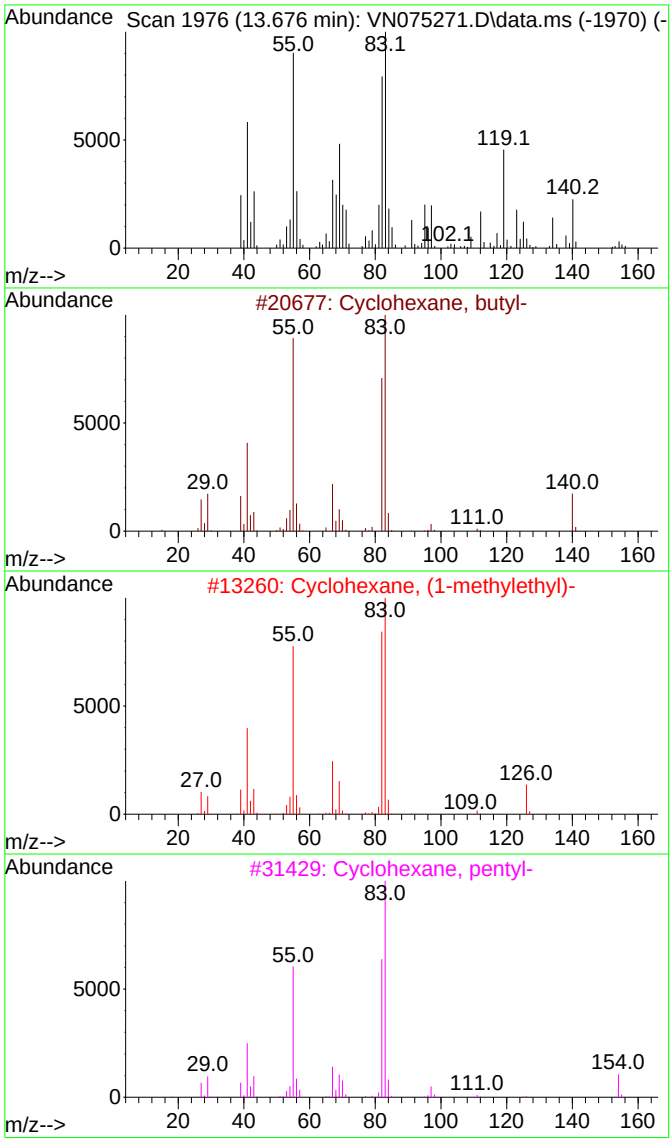
Quant Title : SW846 8260

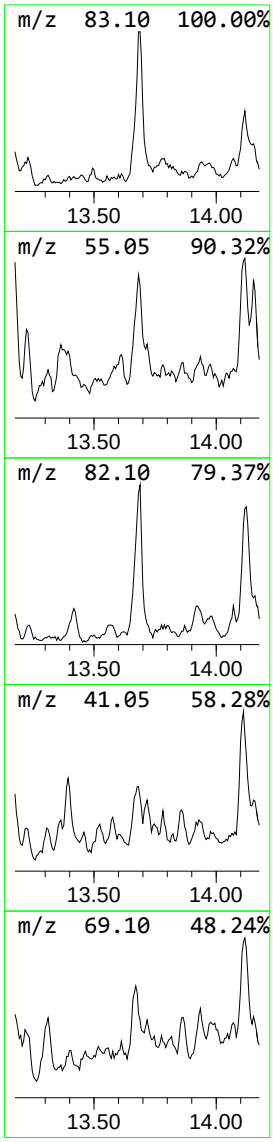
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	24.19 ug/l	393181	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	53
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43
3	Cyclohexane, pentyl-	154	C11H22	004292-92-6	43
4	2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	38
5	1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	30





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Instrument :
MSVOA_N
ClientSampleId :
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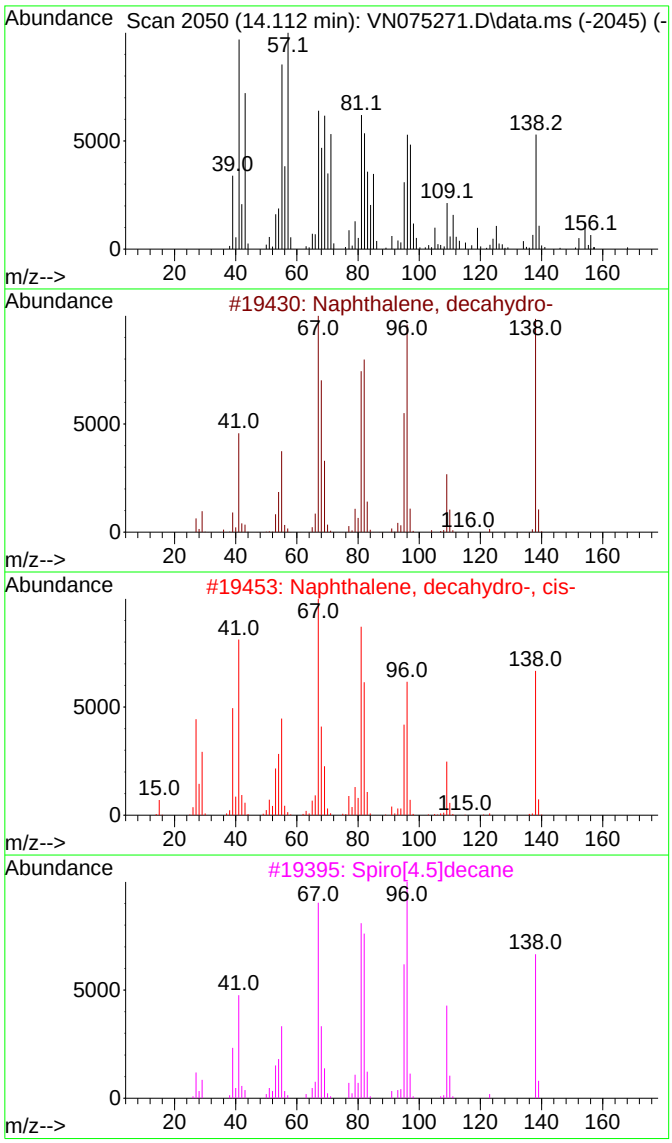
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

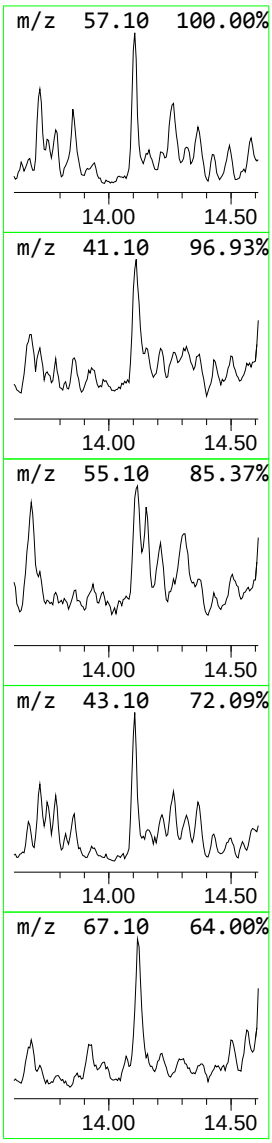
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, decahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.112	46.81 ug/l	760864	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	95
3	Spiro[4.5]decane	138	C10H18	000176-63-6	90
4	9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	64
5	2,2-Dimethyl-3-vinylcyclopentanone	138	C9H14O	1000427-24-5	46





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Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

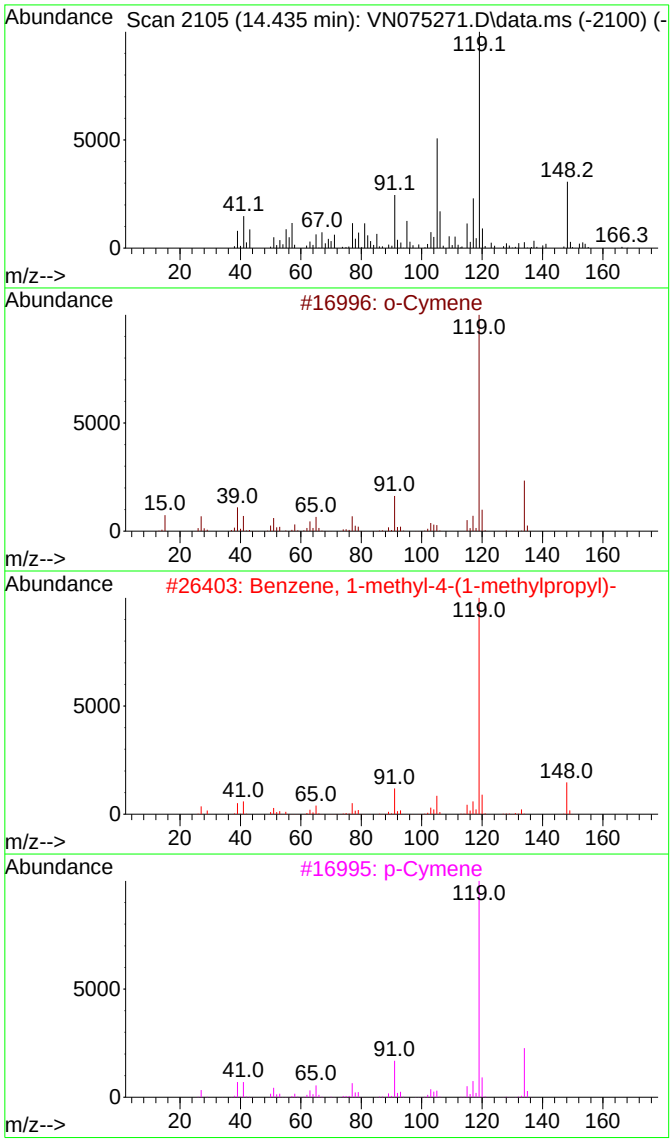
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

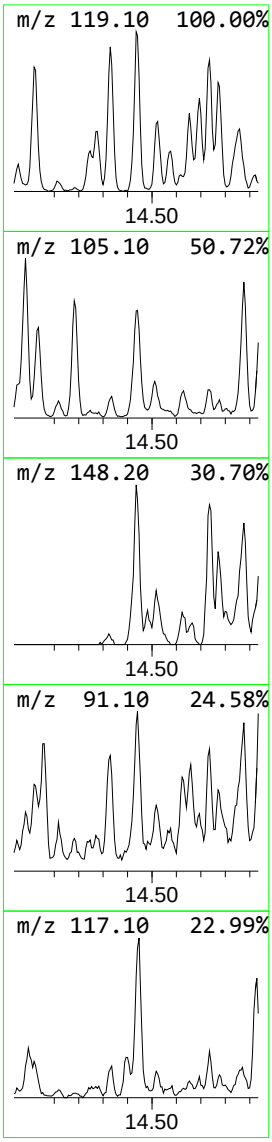
****

Peak Number 6 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.435	24.71 ug/l	401574	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	60
2	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	58
3	p-Cymene	134	C10H14	000099-87-6	53
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	52
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	52





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Data File : VN075271.D
Acq On : 14 Nov 2022 17:38
Operator : JC\MD
Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

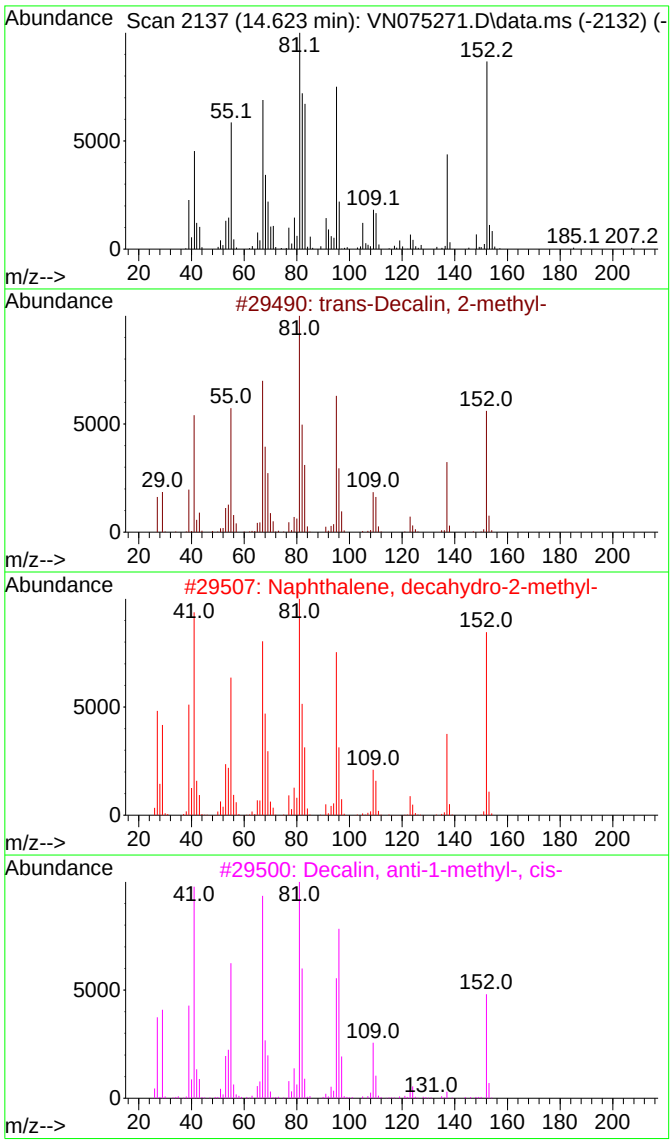
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

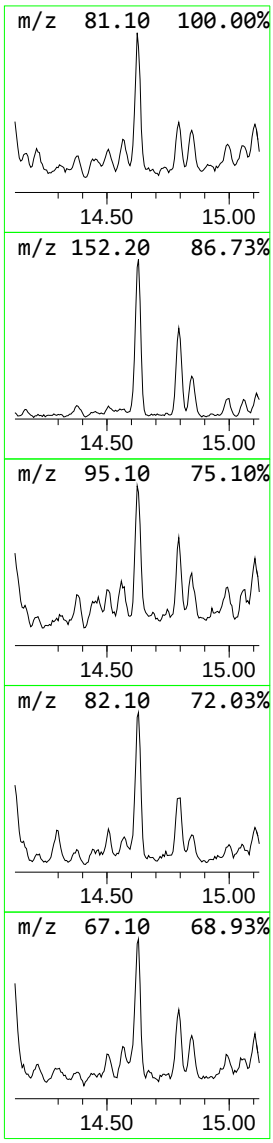
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 trans-Decalin, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.623	44.88 ug/l	729469	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	90
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	86
3	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	76
4	Pulegone	152	C10H16O	000089-82-7	52
5	Furan, 2-hexyl-	152	C10H16O	003777-70-6	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075271.D
Acq On : 14 Nov 2022 17:38
Operator : JC\MD
Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

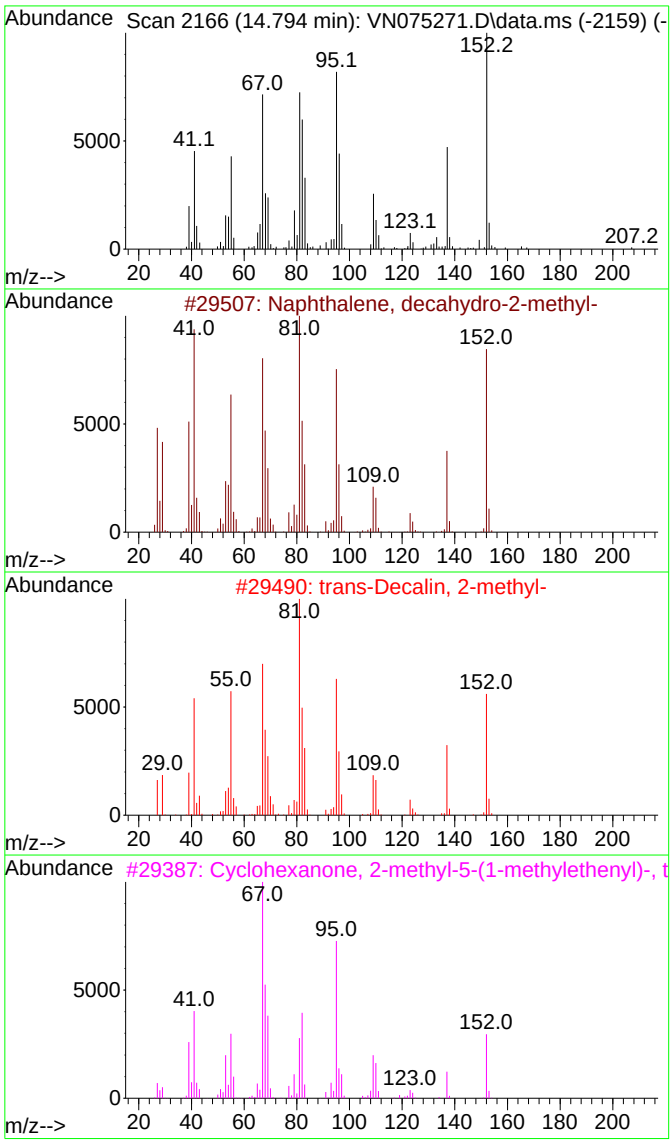
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

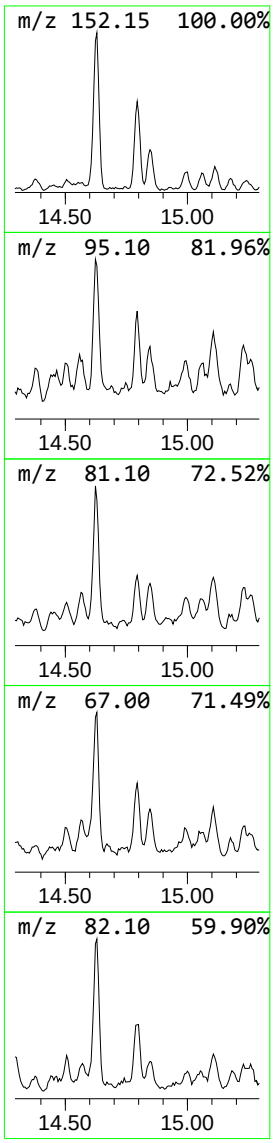
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, decahydro-2-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	22.45 ug/l	364908	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	87
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	80
3	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	68
4	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	64
5	Pulegone	152	C10H16O	000089-82-7	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075271.D
Acq On : 14 Nov 2022 17:38
Operator : JC\MD
Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

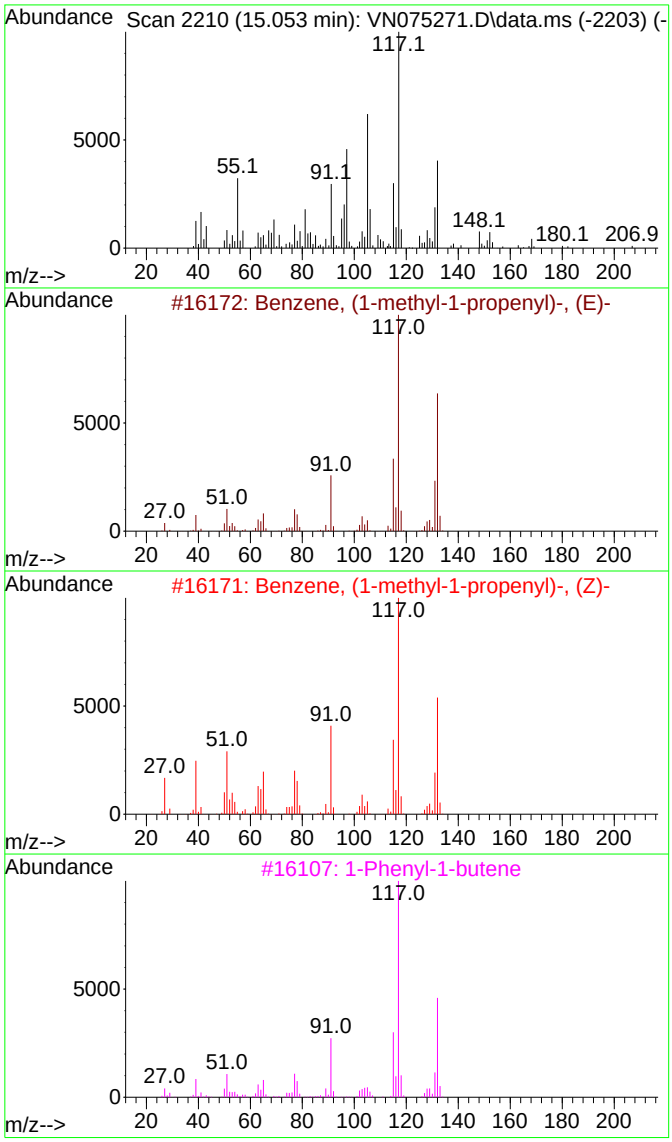
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

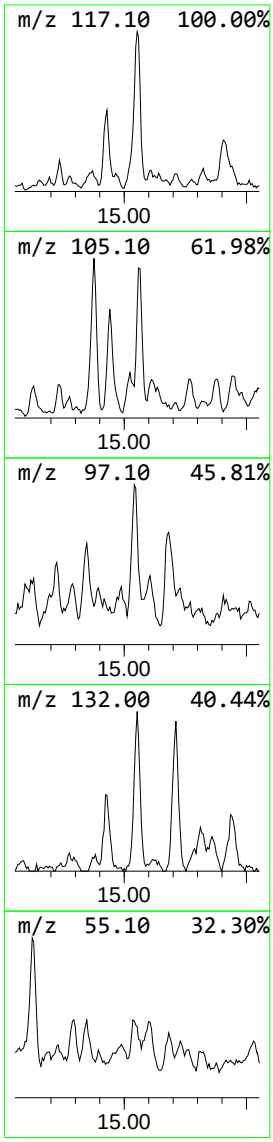
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-propen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	25.82 ug/l	419662	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	64
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	64
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075271.D
Acq On : 14 Nov 2022 17:38
Operator : JC\MD
Sample : N5572-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31604

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

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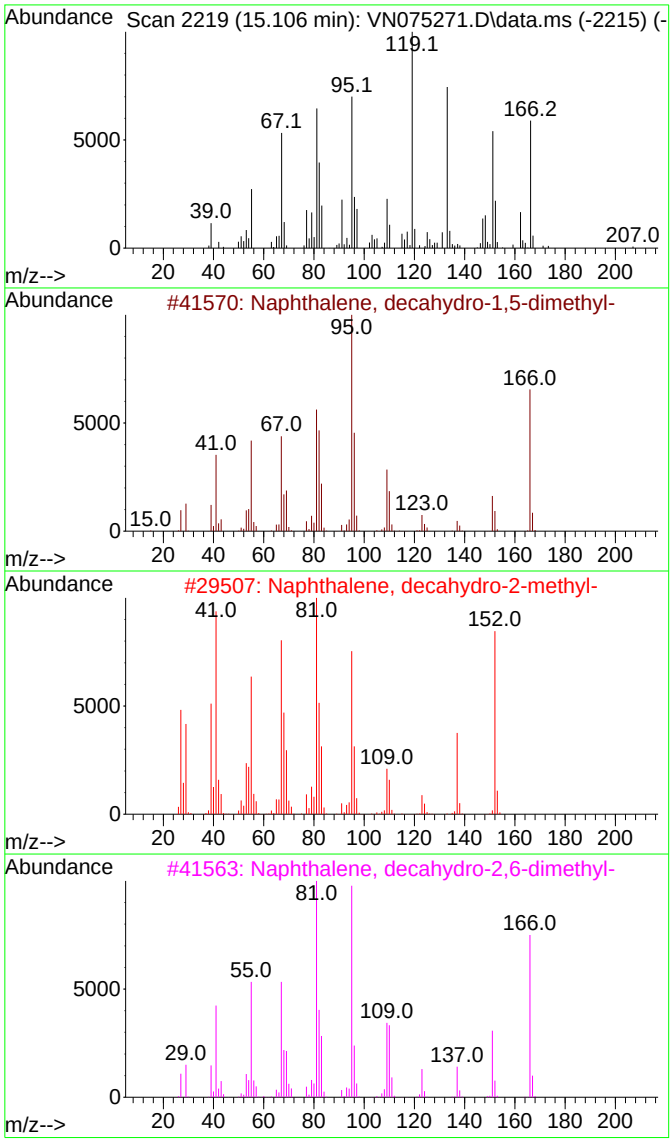
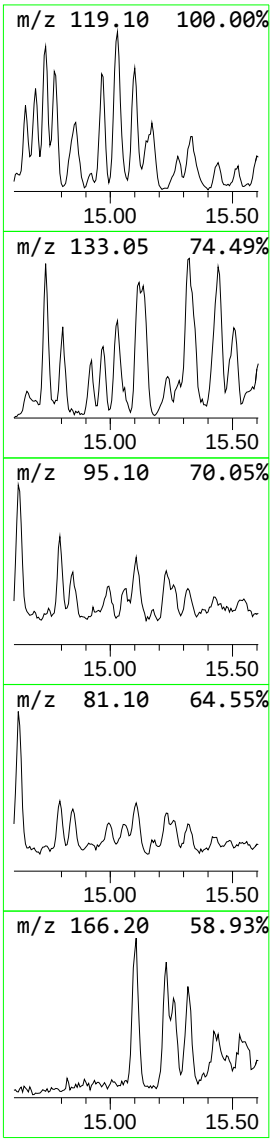
Peak Number 10 unknown15.106 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	25.63 ug/l	416624	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	46
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	42
3	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	30
4	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	003277-26-7	25
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	25





Tentatively Identified Compound (LSC) summary

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Data File : VN075271.D
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Operator : JC\MD
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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
Hexane, 3-methyl-	8.441	36.5	ug/l	639545	1	8.224	875841	50.0
Heptane	8.965	54.6	ug/l	742468	2	9.100	679685	50.0
Heptane, 3-ethy...	12.594	28.6	ug/l	441191	3	11.865	772462	50.0
Cyclohexane, bu...	13.676	24.2	ug/l	393181	4	13.794	812721	50.0
Naphthalene, de...	14.112	46.8	ug/l	760864	4	13.794	812721	50.0
o-Cymene	14.435	24.7	ug/l	401574	4	13.794	812721	50.0
trans-Decalin, ...	14.623	44.9	ug/l	729469	4	13.794	812721	50.0
Naphthalene, de...	14.794	22.4	ug/l	364908	4	13.794	812721	50.0
Benzene, (1-met...	15.053	25.8	ug/l	419662	4	13.794	812721	50.0
unknown15.106	15.106	25.6	ug/l	416624	4	13.794	812721	50.0