LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071767.D
Acq On : 01 Apr 2022 20:57
Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

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\82N033022W.M
Title : SW846 8260

Signal : TIC: VN071767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	36	46	61	rBV3	156253	381510	10.63%	0.880%
2	2.440	72	77	83	rVB	91485	135874	3.78%	0.314%
3	3.134	185	195	208	rBV	1235315	2780746	77.46%	6.417%
4	3.516	252	260	272	rVB4	31211	86048	2.40%	0.199%
5	3.999	331	342	355	rBV2	48181	130084	3.62%	0.300%
6	4.257	372	386	400	rBV2	243383	850971	23.70%	1.964%
7	5.081	508	526	537	rBV2	455279	1797673	50.07%	4.148%
8	5.622	601	618	632	rBV2	165195	566571	15.78%	1.307%
9	6.475	751	763	776	rBV5	19965	68327	1.90%	0.158%
10	6.610	776	786	796	rBV4	45844	141019	3.93%	0.325%
11	6.898	822	835	843	rBV4	55717	188999	5.26%	0.436%
12	7.046	850	860	869	rBV2	161526	477035	13.29%	1.101%
13	7.146	869	877	884	rVV	177370	534308	14.88%	1.233%
14	7.222	884	890	901	rVV	163958	457078	12.73%	1.055%
15	7.328	901	908	922	rVB7	23200	87517	2.44%	0.202%
16	7.663	956	965	977	rVB4	17614	62523	1.74%	0.144%
17	7.845	977	996	1009	rBV2	144033	406963	11.34%	0.939%
18	8.022	1013	1026	1031	rBV	401477	1017224	28.33%	2.347%
19	8.087	1031	1037	1044	rVV	816024	1875871	52.25%	4.329%
20	8.175	1044	1052	1063	rVB	492436	1259822	35.09%	2.907%
21	8.357	1076	1083	1088	rBV4	28343	63135	1.76%	0.146%
22	8.440	1088	1097	1109	rVV	412895	1011114	28.16%	2.333%
23	8.616	1109	1127	1136	rVV	673069	1882487	52.44%	4.344%
24	8.710	1136	1143	1152	rVB	121894	288625	8.04%	0.666%
25	8.963	1177	1186	1198	rBV	1214898	2710388	75.50%	6.255%
26	9.057	1198	1202	1211	rVB2	81002	174493	4.86%	0.403%
27	9.198	1218	1226	1229	rBV2	122368	242727	6.76%	0.560%
28	9.245	1229	1234	1242	rVB	173402	365579	10.18%	0.844%
29	9.422	1255	1264	1276	rBV5	193599	635599	17.70%	1.467%
30	9.516	1276	1280	1288	rVV4	51790	112461	3.13%	0.260%
31	9.592	1288	1293	1297	rVV	33726	66364	1.85%	0.153%
32	9.639	1297	1301	1307	rVV6	17891	42237	1.18%	0.097%
33	9.728	1307	1316	1323	rVB2	57785	142336	3.96%	0.328%
34	9.804	1323	1329	1332	rBV6	24989	57110	1.59%	0.132%
35	9.881	1335	1342	1351	rVB2	321363	666200	18.56%	1.537%
36	9.975	1351	1358	1359	rBV2	109766	169482	4.72%	0.391%

LSC Area Percent Report

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Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

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\82N033022W.M
Title : SW846 8260

37	10.010	1359	1364	1377	rVB	329647	800877	22.31%	1.848%
38	10.128	1377	1384	1389	rBV2	91971	184943	5.15%	0.427%
39	10.198	1389	1396	1402	rVB5	61242	130786	3.64%	0.302%
40	10.263	1402	1407	1411	rBV3	22411	39451	1.10%	0.091%
41	10.322	1411	1417	1421	rBV	141606	274329	7.64%	0.633%
42	10.363	1421	1424	1430	rVB3	92095	156860	4.37%	0.362%
43	10.439	1430	1437	1450	rBV	1871548	3590037	100.00%	8.285%
44	10.639	1457	1471	1477	rBV2	326573	758712	21.13%	1.751%
45	10.716	1477	1484	1490	rVV2	283061	539521	15.03%	1.245%
46	10.775	1490	1494	1500	rVV3	38682	65033	1.81%	0.150%
47	10.857	1500	1508	1517	rVV3	419200	881101	24.54%	2.033%
48	10.945	1518	1523	1531	rVB2	45684	95055	2.65%	0.219%
49	11.034	1531	1538	1542	rBV2	24926	53837	1.50%	0.124%
50	11.128	1547	1554	1558	rBV2	91377	171002	4.76%	0.395%
51	11.204	1564	1567	1571	rVB3	29697	42746	1.19%	0.099%
52	11.257	1571	1576	1581	rVB3	49092	81847	2.28%	0.189%
53	11.310	1581	1585	1588	rBV2	22758	39812	1.11%	0.092%
54	11.404	1595	1601	1604	rBV4	22838	43492	1.21%	0.100%
55	11.451	1604	1609	1617	rVB	62167	112154	3.12%	0.259%
56	11.563	1617	1628	1637	rVB8	22632	71632	2.00%	0.165%
57	11.657	1637	1644	1651	rBV7	26585	79222	2.21%	0.183%
58	11.739	1651	1658	1666	rBV	1770850	3136609	87.37%	7.238%
59	11.798	1666	1668	1671	rVV2	52436	70313	1.96%	0.162%
60	11.833	1671	1674	1679	rVB2	38288	63969	1.78%	0.148%
61	11.986	1697	1700	1707	rVB4	23955	46964	1.31%	0.108%
62	12.445	1766	1778	1788	rBV9	22158	84452	2.35%	0.195%
63	12.728	1819	1826	1836	rVV	1311300	2201204	61.31%	5.080%
64	13.216	1903	1909	1915	rVB	47130	80553	2.24%	0.186%
65	13.669	1979	1986	1999	rBV	1336303	2442902	68.05%	5.637%
66	13.769	1999	2003	2008	rVB	35347	52500	1.46%	0.121%
67	13.833	2008	2014	2016	rBV	184937	275383	7.67%	0.635%
68	13.874	2016	2021	2027	rVB	1257969	2007425	55.92%	4.632%
69	13.998	2037	2042	2048	rVB	175056	284499	7.92%	0.657%
70	14.063	2048	2053	2059	rVB	132299	210401	5.86%	0.486%
71	14.145	2061	2067	2073	rBV	130251	224252	6.25%	0.517%
72	14.216	2073	2079	2083	rBV	43375	63974	1.78%	0.148%
73	14.274	2083	2089	2092	rBV	35916	64568	1.80%	0.149%
74	14.327	2092	2098	2104	rVV	384397	651094	18.14%	1.503%
75	14.404	2104	2111	2116	rVV3	61464	129747	3.61%	0.299%
76	14.463	2116	2121	2126	rVV	57363	87664	2.44%	0.202%

LSC Area Percent Report

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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

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\82N033022W.M
Title : SW846 8260

77	14.533	2126	2133	2139	rVV2	105064	175154	4.88%	0.404%
78	14.651	2150	2153	2160	rVB	42475	64460	1.80%	0.149%
79	14.763	2164	2172	2176	rBV2	57340	97548	2.72%	0.225%
80	14.816	2176	2181	2192	rVB4	61358	124971	3.48%	0.288%
81	14.921	2192	2199	2206	rBV9	26547	62616	1.74%	0.144%
82	14.992	2206	2211	2217	rBV3	35038	61789	1.72%	0.143%
83	15.192	2239	2245	2249	rBV2	44864	83447	2.32%	0.193%
84	15.298	2254	2263	2272	rVB5	64329	182184	5.07%	0.420%
85	15.557	2301	2307	2314	rBV5	21721	39587	1.10%	0.091%
86	15.639	2314	2321	2331	rVB5	24038	56998	1.59%	0.132%
87	16.104	2394	2400	2408	rBV2	23573	57641	1.61%	0.133%

Sum of corrected areas: 43333817

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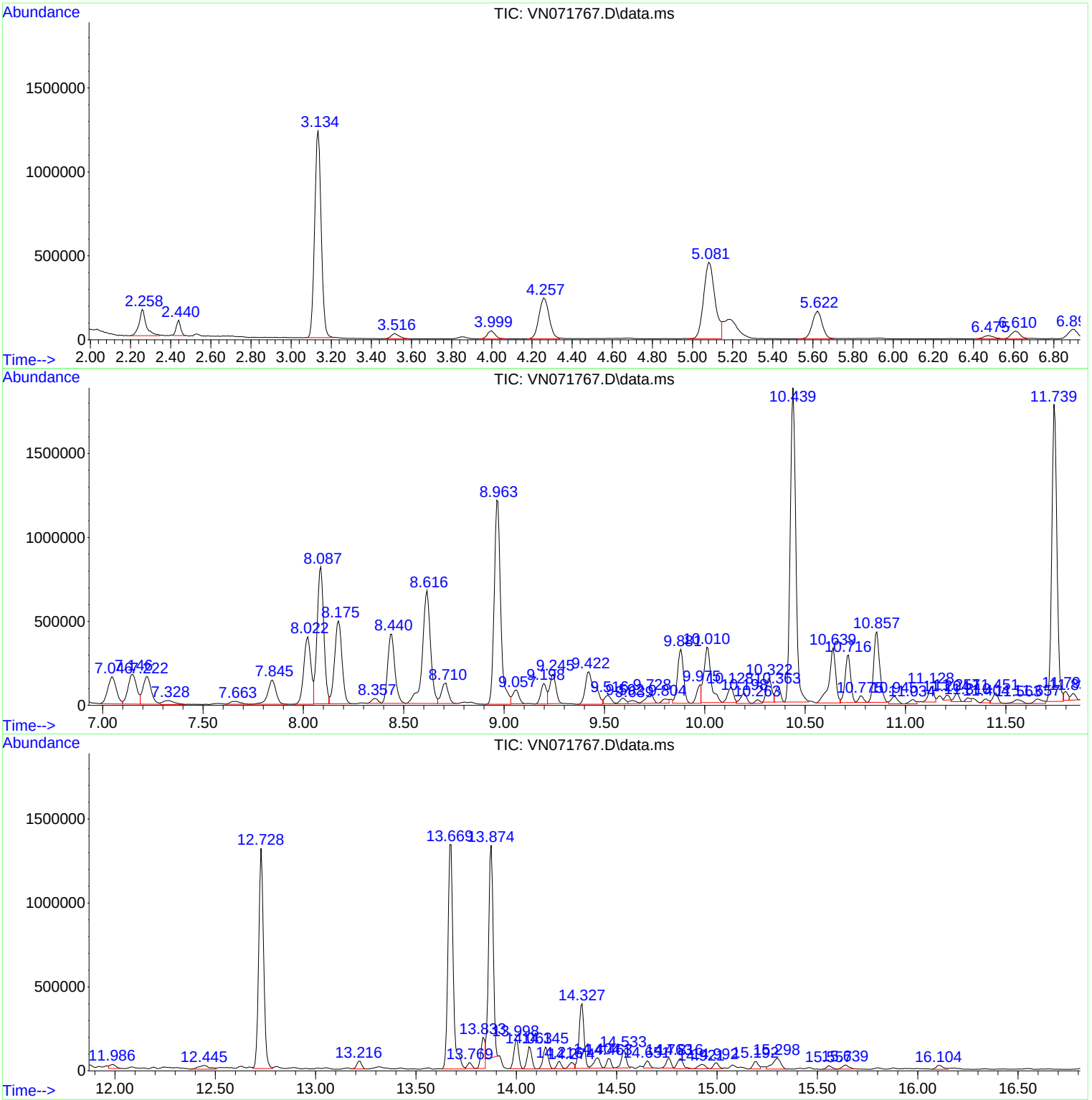
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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Operator : JC\MD
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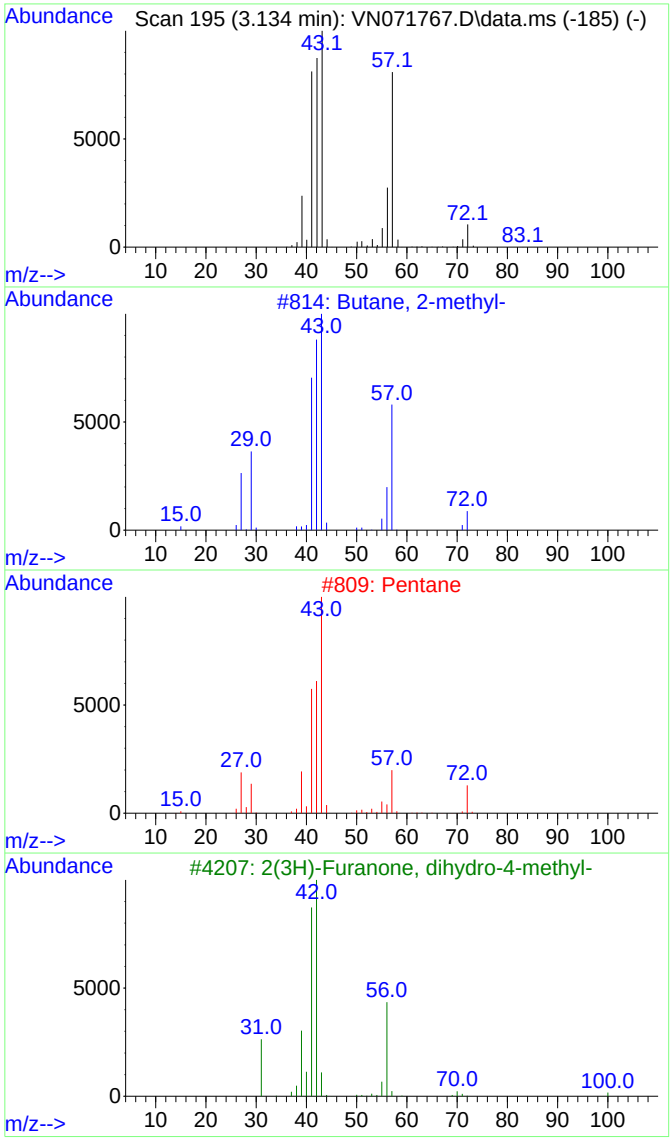
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

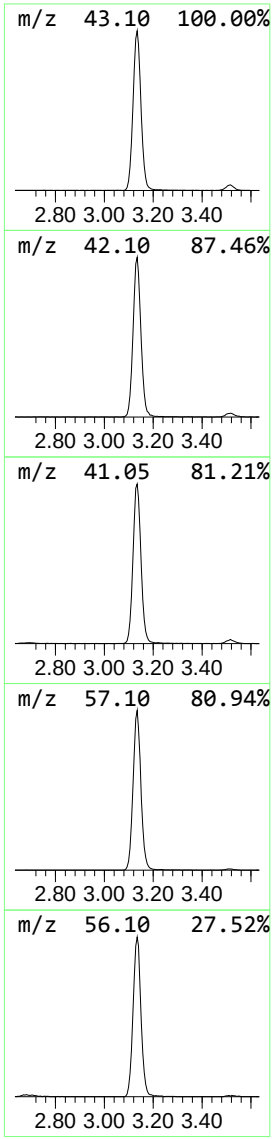
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	74.12 ug/l	2780750	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	38
3	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	17
5	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	17





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

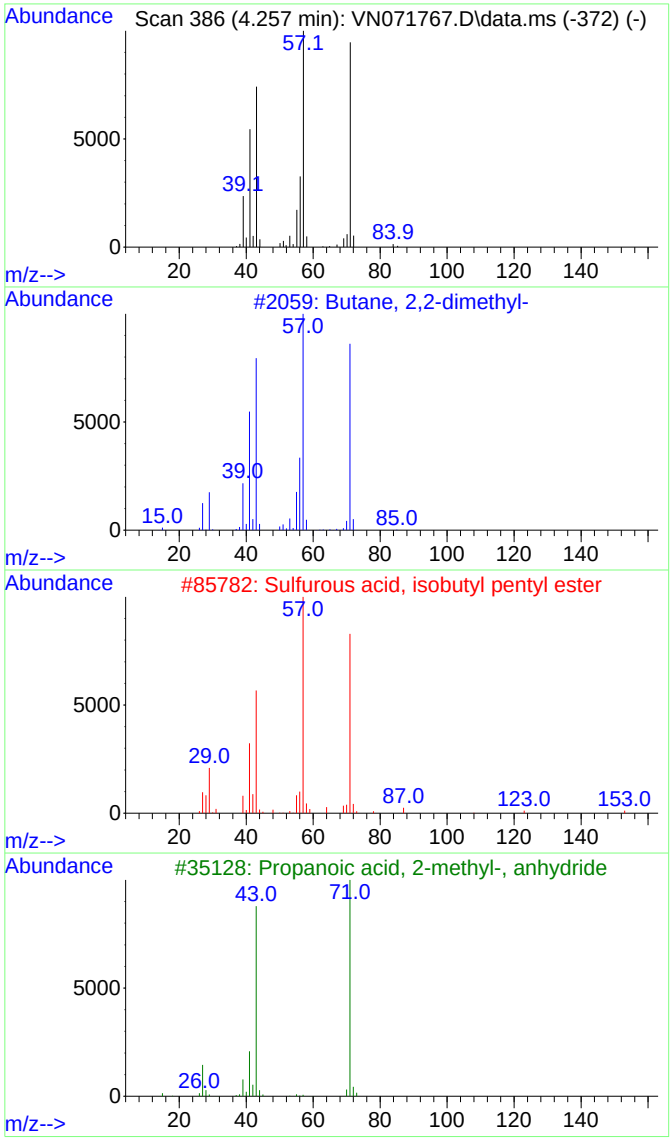
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

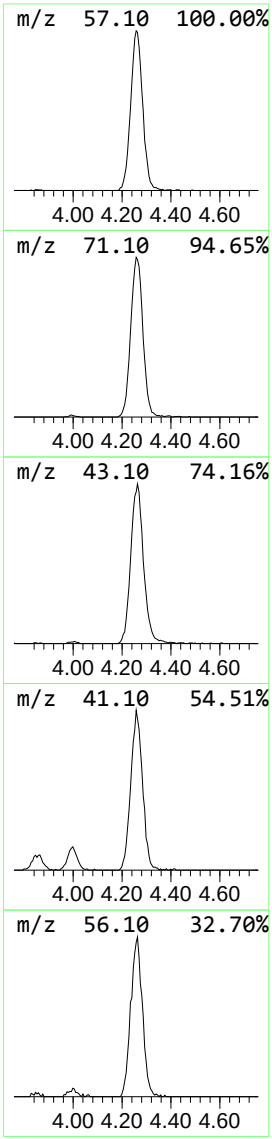
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	22.68 ug/l	850971	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	90
2	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	64
3	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	40
4	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	40
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	33





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

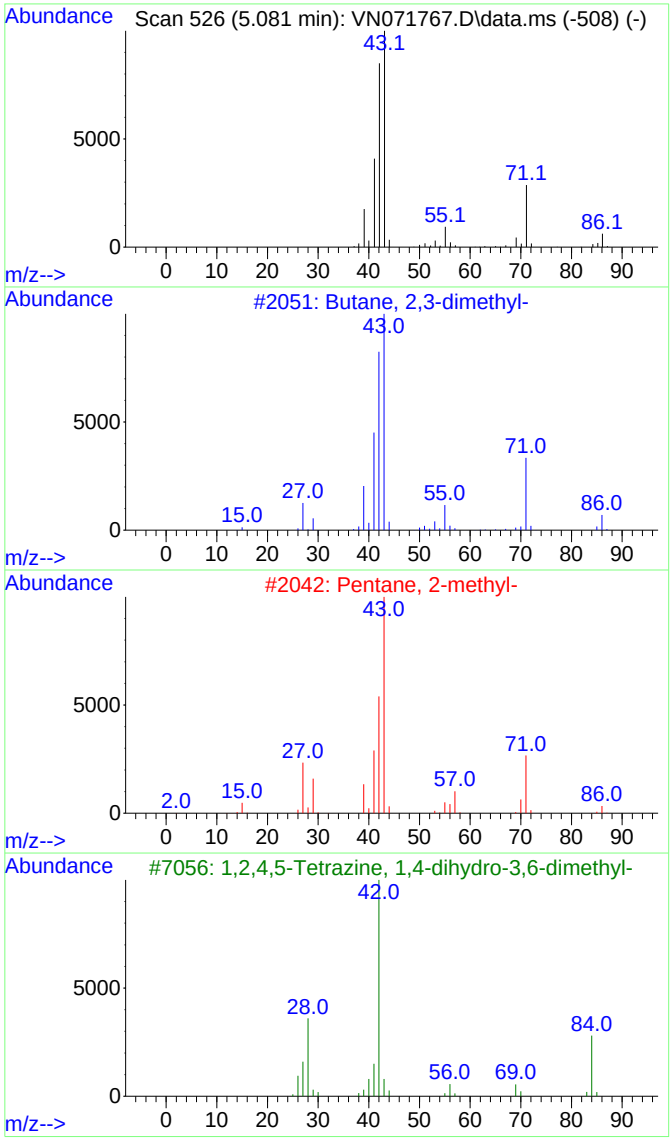
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

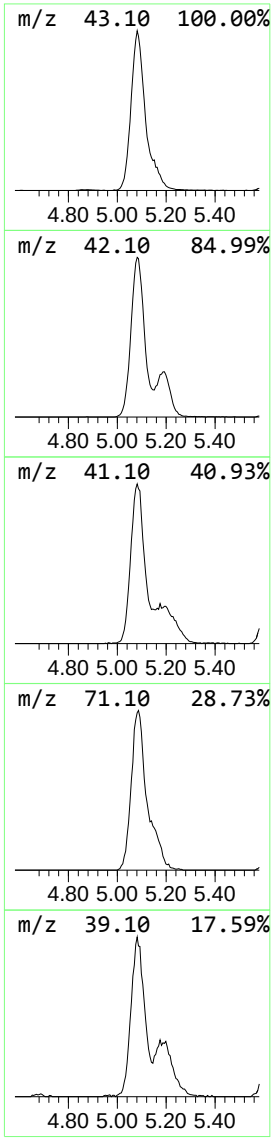
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	47.92 ug/l	1797670	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	1,2,4,5-Tetrazine, 1,4-dihydro-3...	112	C4H8N4	037454-64-1	28
4	C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	10
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	10





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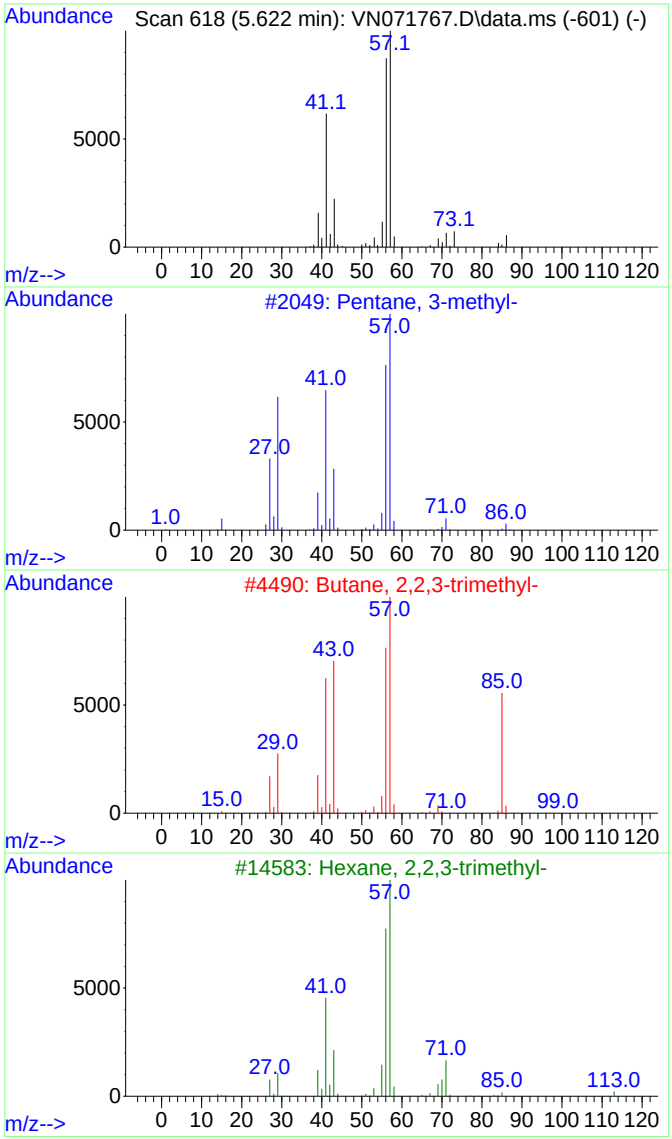
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

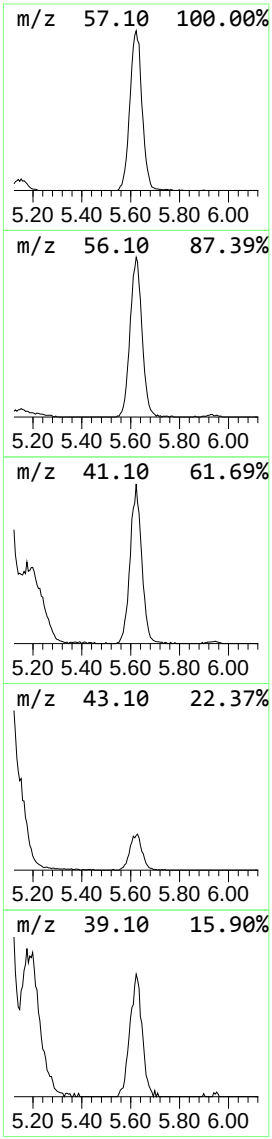
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	15.10 ug/l	566571	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
4	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	64
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

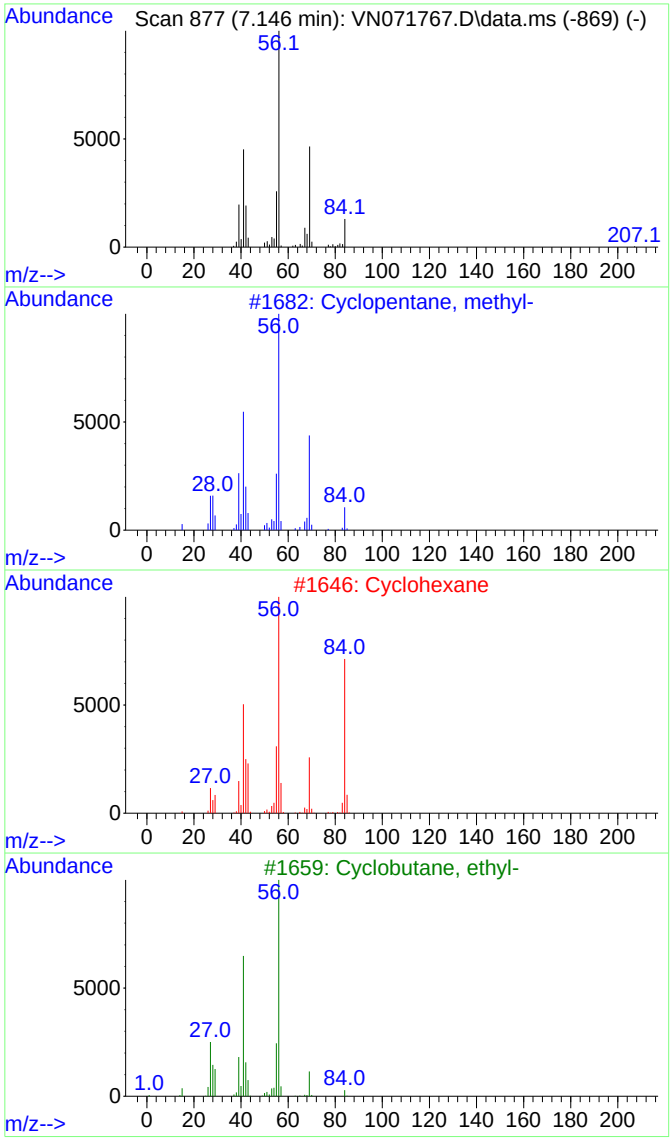
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

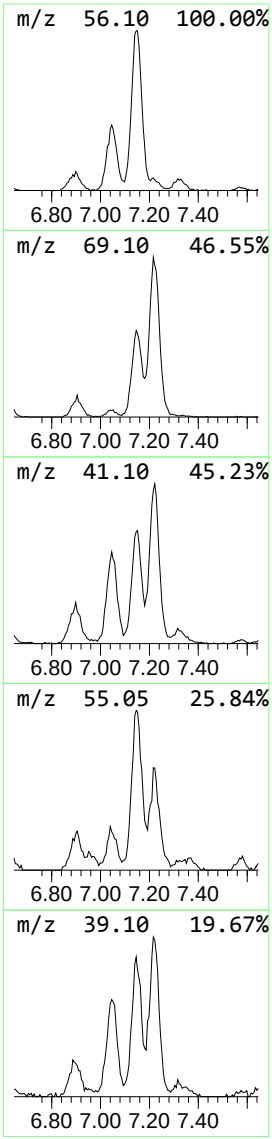
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.146	14.24 ug/l	534308	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	83
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	56





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ALS Vial : 26 Sample Multiplier: 1

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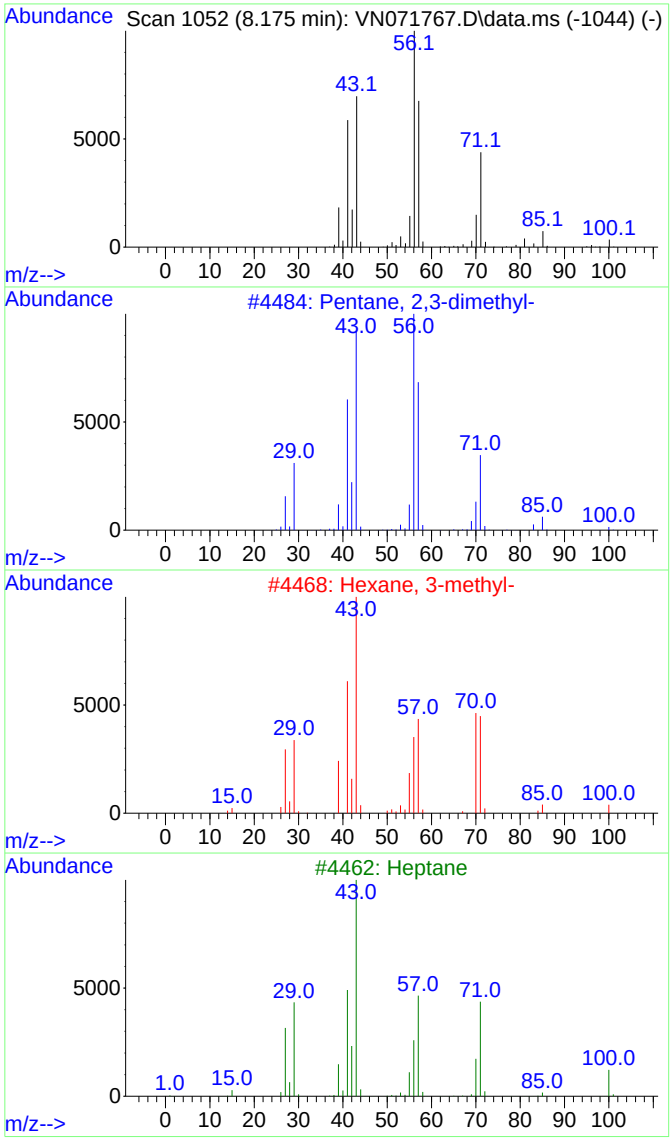
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

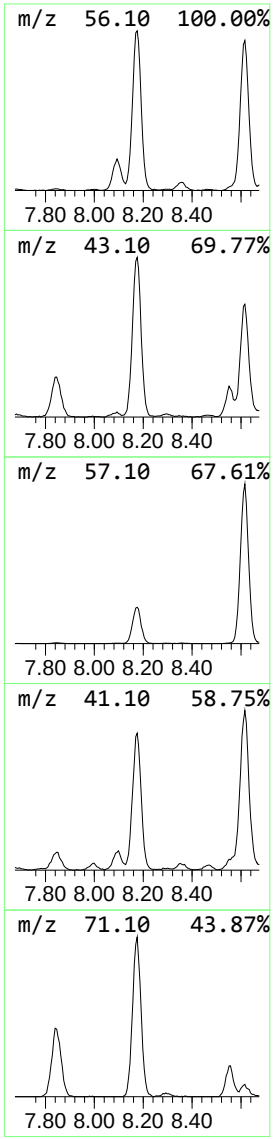
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	33.58 ug/l	1259820	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	43
3	Heptane	100	C7H16	000142-82-5	43
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42





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Data File : VN071767.D
Acq On : 01 Apr 2022 20:57
Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

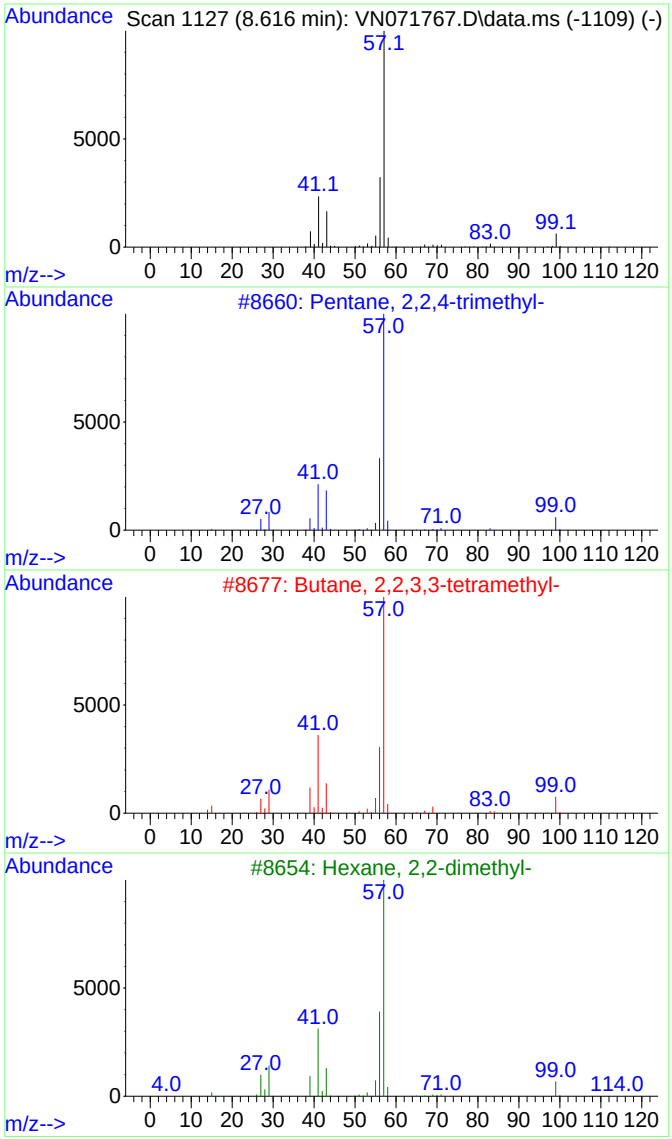
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

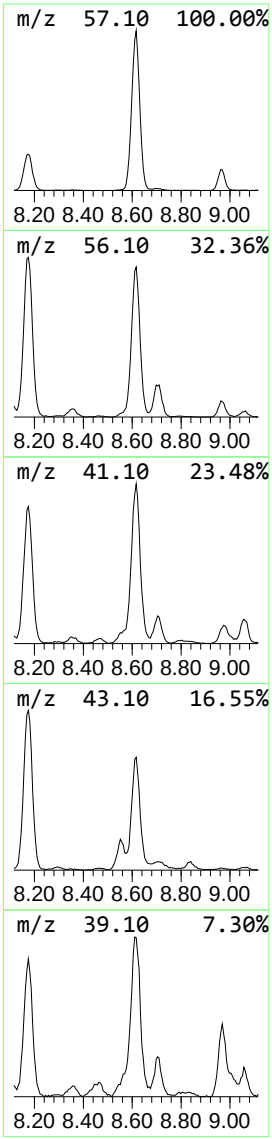
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 2,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	34.73 ug/l	1882490	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





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Data File : VN071767.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

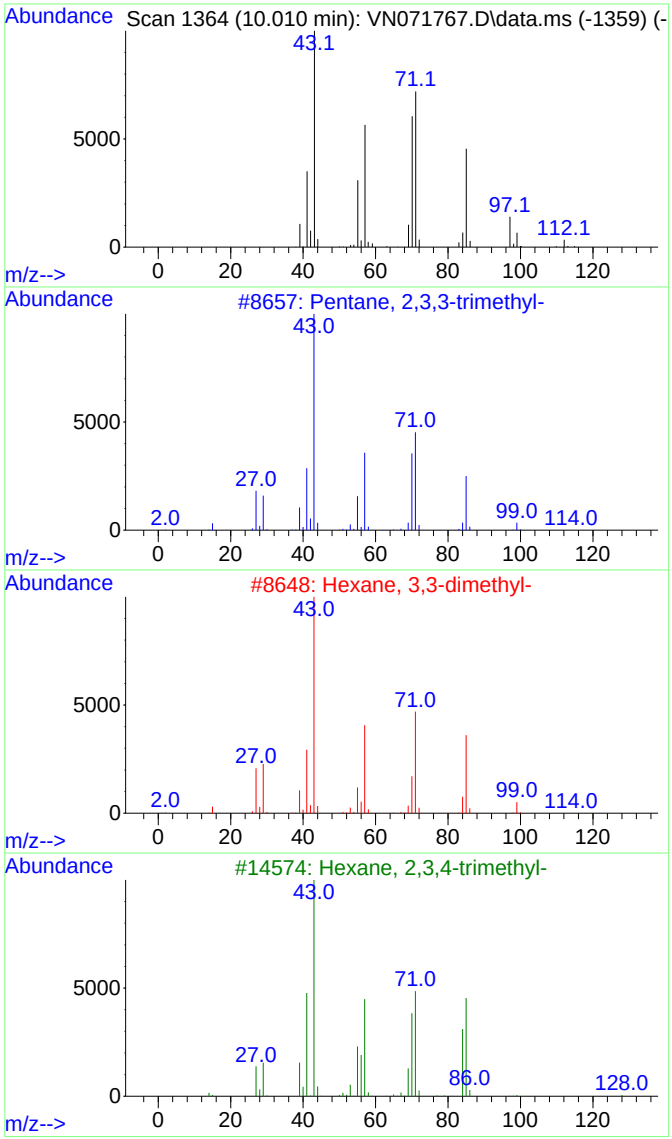
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

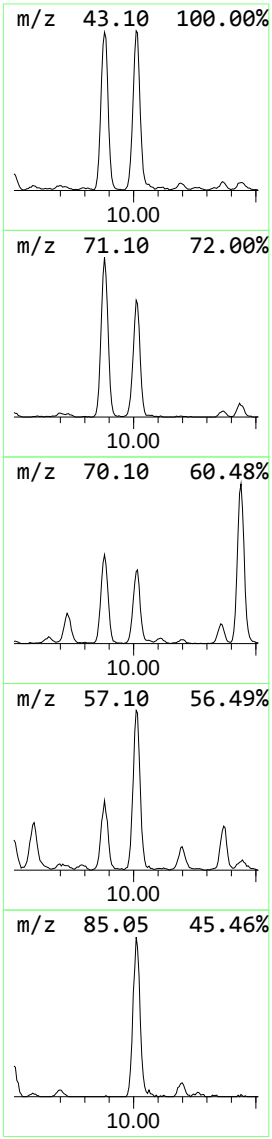
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	14.77 ug/l	800877	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	47
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	47





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Data File : VN071767.D
Acq On : 01 Apr 2022 20:57
Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

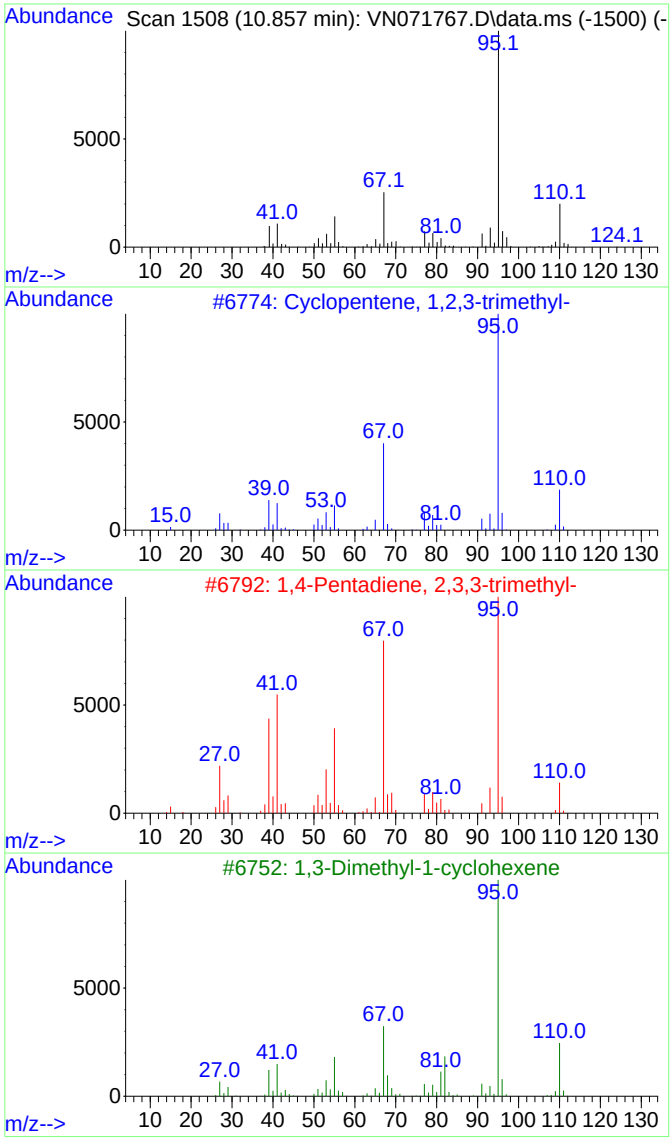
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

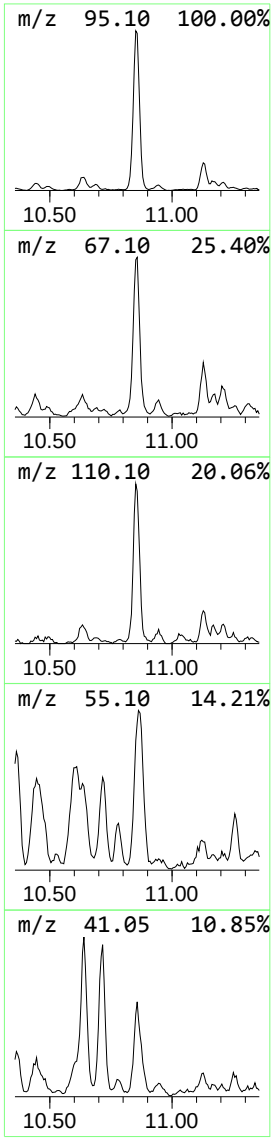
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.857	14.05 ug/l	881101	Chlorobenzene-d5	11.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	90
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	87
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	86
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	72
5	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	59





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Data File : VN071767.D
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Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

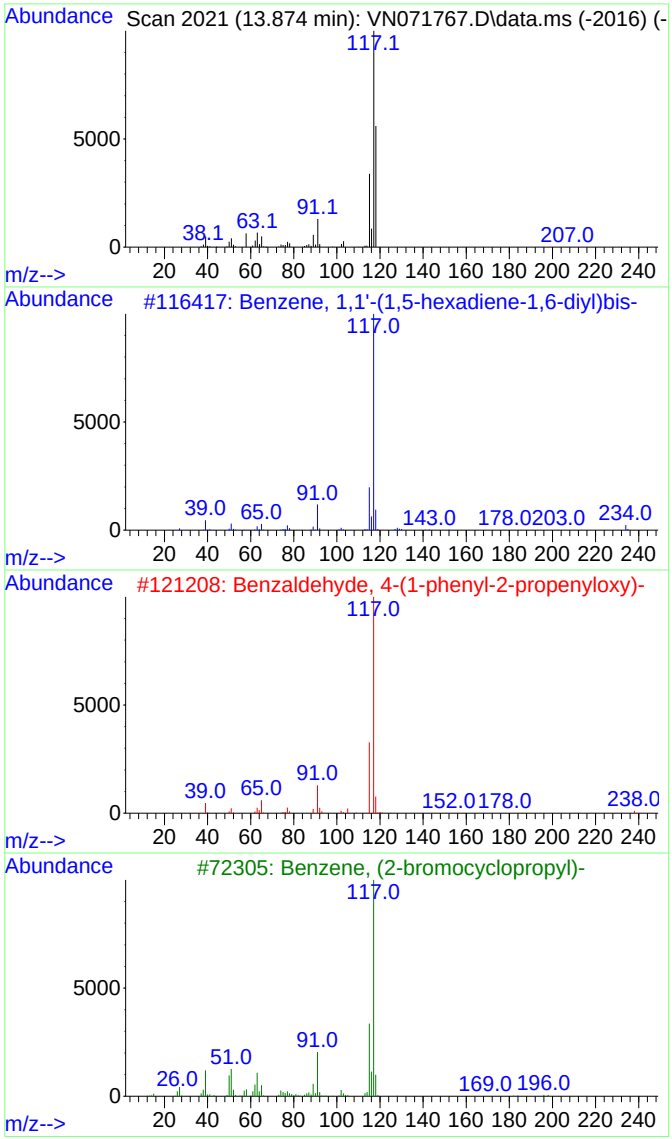
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

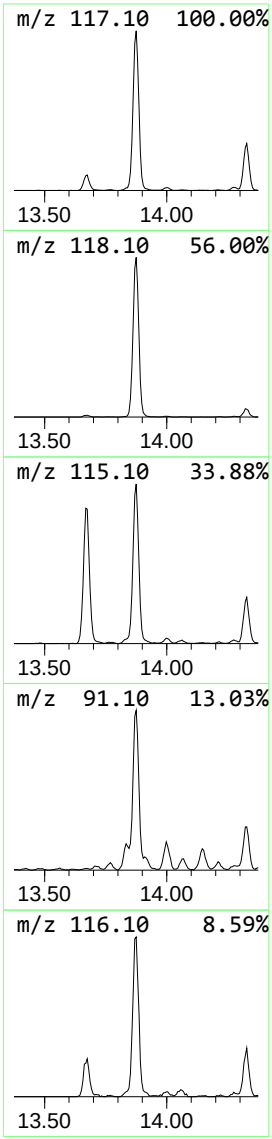
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	41.09 ug/l	2007430	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
3	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
4	Indole	117	C8H7N	000120-72-9	43
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071767.D
Acq On : 01 Apr 2022 20:57
Operator : JC\MD
Sample : N2090-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP032322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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
Butane, 2-methyl-	3.134	74.1	ug/l	2780750	1	8.087	1875870	50.0
Butane, 2,2-dim...	4.257	22.7	ug/l	850971	1	8.087	1875870	50.0
Butane, 2,3-dim...	5.081	47.9	ug/l	1797670	1	8.087	1875870	50.0
Pentane, 3-methyl-	5.622	15.1	ug/l	566571	1	8.087	1875870	50.0
Cyclopentane, m...	7.146	14.2	ug/l	534308	1	8.087	1875870	50.0
Pentane, 2,3-di...	8.175	33.6	ug/l	1259820	1	8.087	1875870	50.0
Pentane, 2,2,4-...	8.616	34.7	ug/l	1882490	2	8.963	2710390	50.0
Pentane, 2,3,3-...	10.010	14.8	ug/l	800877	2	8.963	2710390	50.0
Cyclopentene, 1...	10.857	14.1	ug/l	881101	3	11.739	3136610	50.0
Benzene, 1,1'-(...	13.874	41.1	ug/l	2007430	4	13.675	2442900	50.0