LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040822\
Data File : VN071921.D
Acq On : 08 Apr 2022 17:56
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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: VN071921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	35	46	63	rBV2	252466	898902	5.43%	0.629%
2	2.440	70	77	87	rVB	521060	804013	4.86%	0.562%
3	3.134	185	195	215	rVB	2733538	6160271	37.23%	4.309%
4	3.516	249	260	280	rBV3	1045117	2971853	17.96%	2.079%
5	3.722	285	295	309	rVB2	173164	429818	2.60%	0.301%
6	3.899	309	325	332	rBV	111576	322551	1.95%	0.226%
7	3.999	332	342	362	rVB	665244	1826711	11.04%	1.278%
8	4.257	372	386	404	rVB	107216	380868	2.30%	0.266%
9	4.957	488	505	515	rBV2	166030	604162	3.65%	0.423%
10	5.081	515	526	530	rBV	377832	1180218	7.13%	0.826%
11	5.169	532	541	542	rBV2	425810	1031718	6.23%	0.722%
12	5.622	602	618	637	rBV	569773	1980596	11.97%	1.385%
13	5.934	656	671	685	rVB2	110440	361903	2.19%	0.253%
14	6.122	690	703	716	rBV2	153279	468541	2.83%	0.328%
15	6.287	719	731	741	rBV2	109850	346428	2.09%	0.242%
16	6.469	753	762	774	rVB	266495	826457	4.99%	0.578%
17	6.604	774	785	794	rBV2	313971	972430	5.88%	0.680%
18	6.698	794	801	811	rVV	190891	635016	3.84%	0.444%
19	6.792	811	817	826	rVV2	86999	257571	1.56%	0.180%
20	6.904	826	836	851	rVB	321052	947318	5.72%	0.663%
21	7.045	851	860	866	rBV2	96400	272485	1.65%	0.191%
22	7.145	866	877	886	rVV	1957420	5831773	35.24%	4.079%
23	7.222	886	890	901	rVB	338279	805396	4.87%	0.563%
24	7.839	985	995	1005	rBV	1194992	2919048	17.64%	2.042%
25	8.016	1015	1025	1030	rBV	428158	1098007	6.64%	0.768%
26	8.087	1030	1037	1045	rVV2	1530338	3847525	23.25%	2.691%
27	8.175	1045	1052	1064	rVB2	467359	1247464	7.54%	0.873%
28	8.292	1064	1072	1078	rBV	154156	357184	2.16%	0.250%
29	8.457	1089	1100	1109	rBV2	2402007	6112277	36.94%	4.276%
30	8.581	1111	1121	1128	rBV3	426696	1341766	8.11%	0.939%
31	8.704	1136	1142	1152	rVB2	182332	453370	2.74%	0.317%
32	8.798	1152	1158	1176	rVB5	82106	289126	1.75%	0.202%
33	8.963	1176	1186	1199	rBV	1600344	3802750	22.98%	2.660%
34	9.198	1218	1226	1228	rBV	146164	273421	1.65%	0.191%
35	9.239	1228	1233	1251	rVB	459344	976373	5.90%	0.683%
36	9.457	1253	1270	1277	rBV2	608578	1864566	11.27%	1.304%

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Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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	9.639	1295	1301	1307	rVB	110559	214707	1.30%	0.150%
38	9.798	1321	1328	1331	rBV4	146573	314567	1.90%	0.220%
39	9.881	1337	1342	1350	rVB2	191048	391231	2.36%	0.274%
40	9.969	1350	1357	1362	rBV	835012	1647660	9.96%	1.153%
41	10.010	1362	1364	1378	rVB3	284215	554698	3.35%	0.388%
42	10.198	1390	1396	1409	rBV5	74980	244923	1.48%	0.171%
43	10.316	1409	1416	1423	rBV	518942	999383	6.04%	0.699%
44	10.439	1429	1437	1443	rBV	2040787	3834953	23.17%	2.683%
45	10.498	1443	1447	1460	rVV	510627	1082169	6.54%	0.757%
46	10.633	1460	1470	1477	rVV3	259777	605389	3.66%	0.423%
47	10.710	1477	1483	1490	rVB3	177760	351892	2.13%	0.246%
48	10.857	1501	1508	1517	rVV3	265511	577515	3.49%	0.404%
49	11.128	1548	1554	1559	rBV	123998	215821	1.30%	0.151%
50	11.645	1634	1642	1649	rBV6	77043	169314	1.02%	0.118%
51	11.739	1650	1658	1665	rBV	2002984	3511738	21.22%	2.457%
52	11.957	1684	1695	1706	rBV	9332462	16548456	100.00%	11.576%
53	12.274	1738	1749	1759	rBV	2991199	5025264	30.37%	3.515%
54	12.727	1816	1826	1835	rBV	1541757	2631616	15.90%	1.841%
55	12.980	1861	1869	1870	rBV	470776	674692	4.08%	0.472%
56	13.010	1870	1874	1878	rVV	1979495	3326782	20.10%	2.327%
57	13.057	1878	1882	1894	rVB	2425667	3838887	23.20%	2.685%
58	13.216	1901	1909	1918	rBV	3528793	5720674	34.57%	4.002%
59	13.363	1928	1934	1940	rBV	161740	261900	1.58%	0.183%
60	13.557	1960	1967	1972	rBV	101962	166906	1.01%	0.117%
61	13.698	1980	1991	2000	rBV2	5435168	11520651	69.62%	8.059%
62	13.833	2008	2014	2016	rBV	569111	877666	5.30%	0.614%
63	13.874	2016	2021	2037	rVB	3924678	7527956	45.49%	5.266%
64	13.998	2037	2042	2047	rBV	144616	212446	1.28%	0.149%
65	14.063	2047	2053	2059	rBV2	395246	640739	3.87%	0.448%
66	14.127	2059	2064	2066	rVV	154449	237026	1.43%	0.166%
67	14.151	2066	2068	2073	rVV	132348	195324	1.18%	0.137%
68	14.210	2073	2078	2085	rVV	1149116	1768974	10.69%	1.237%
69	14.321	2092	2097	2107	rVB2	990669	1654768	10.00%	1.158%
70	14.457	2113	2120	2126	rBV2	291721	482032	2.91%	0.337%
71	14.533	2126	2133	2137	rBV	865083	1436254	8.68%	1.005%
72	14.574	2137	2140	2145	rVB	685735	978155	5.91%	0.684%
73	14.804	2174	2179	2185	rBV	785488	1200091	7.25%	0.839%
74	14.927	2191	2200	2206	rBV2	1475491	3001090	18.14%	2.099%
75	14.992	2206	2211	2219	rVB3	119844	232899	1.41%	0.163%
76	15.080	2219	2226	2234	rBV3	198913	367489	2.22%	0.257%

LSC Area Percent Report

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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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	15.192	2234	2245	2250	rBV2	172857	448825	2.71%	0.314%
78	15.310	2257	2265	2277	rVB2	167247	417567	2.52%	0.292%
79	15.498	2283	2297	2310	rBV	981345	1944151	11.75%	1.360%

Sum of corrected areas: 142955116

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Sample : N2308-03
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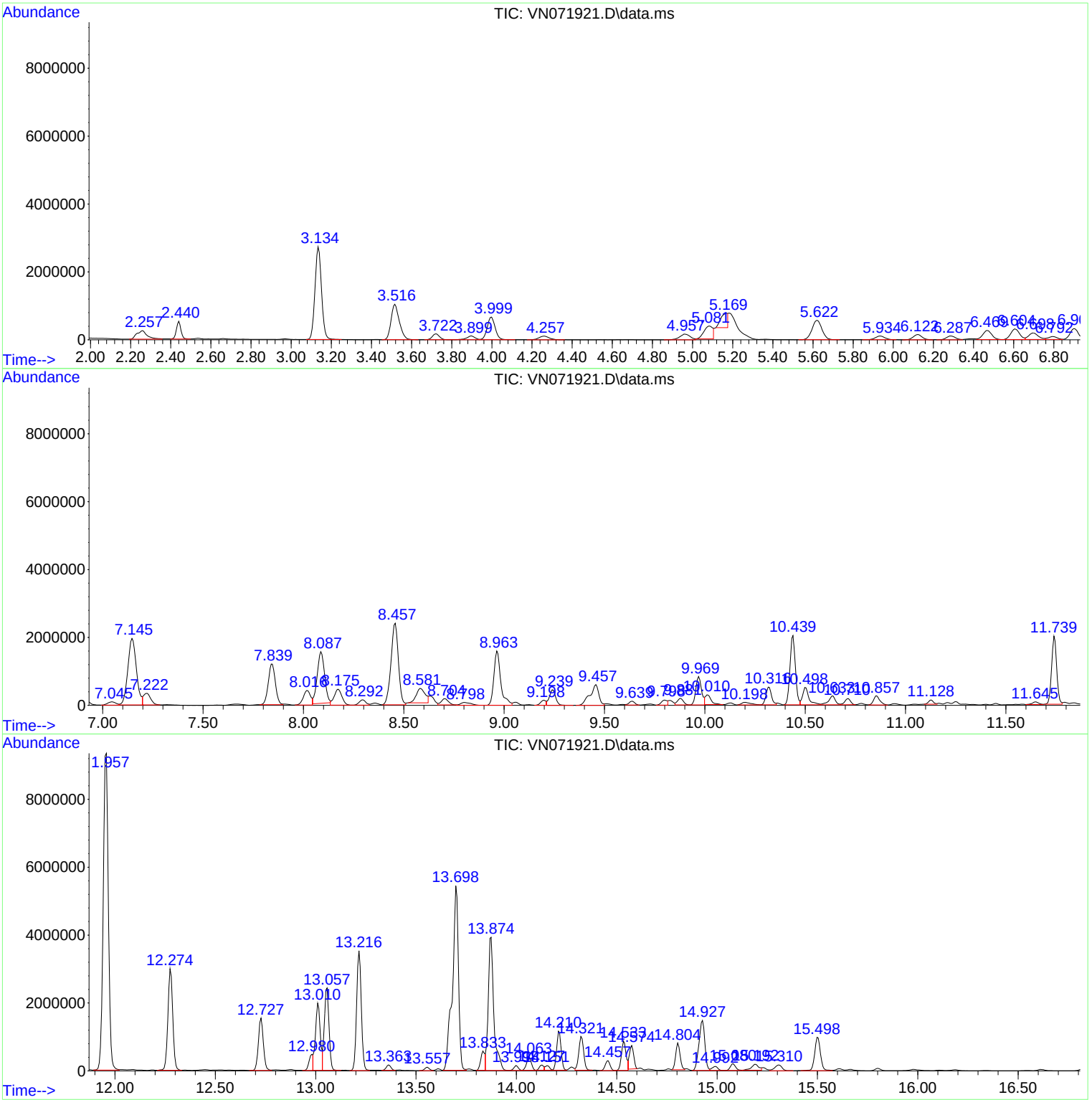
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040822\
Data File : VN071921.D
Acq On : 08 Apr 2022 17:56
Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
INF0422

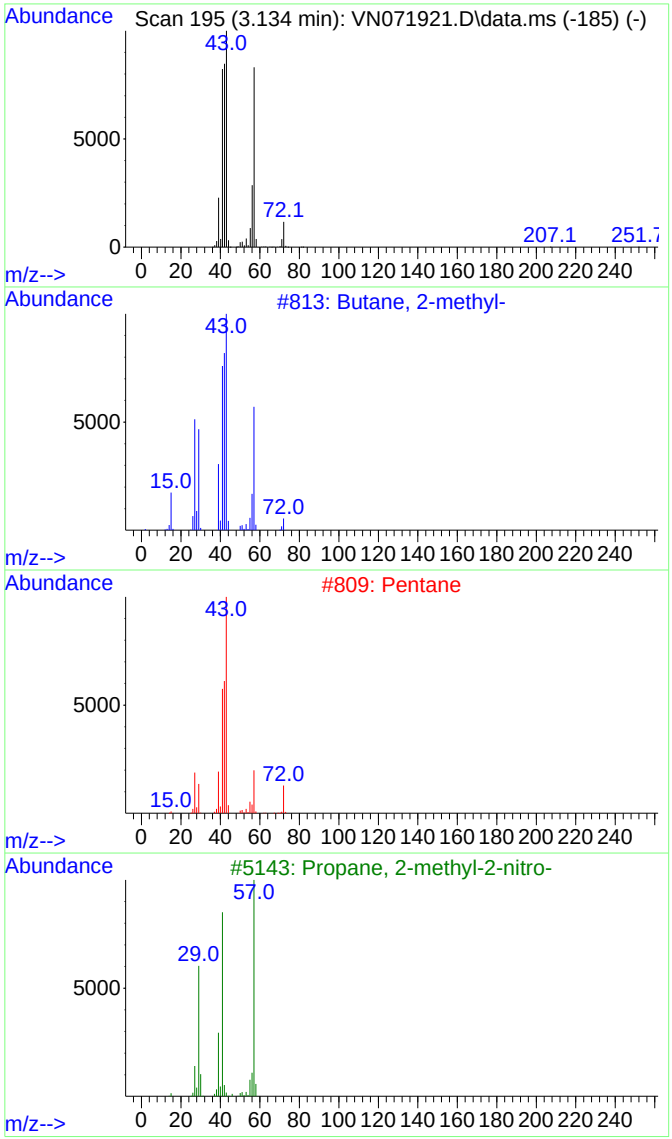
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

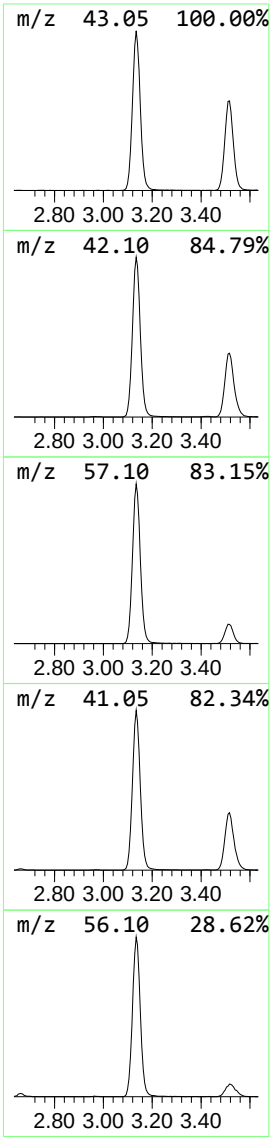
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	80.06 ug/l	6160270	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	38
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
4	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12
5	1-Butene	56	C4H8	000106-98-9	10





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

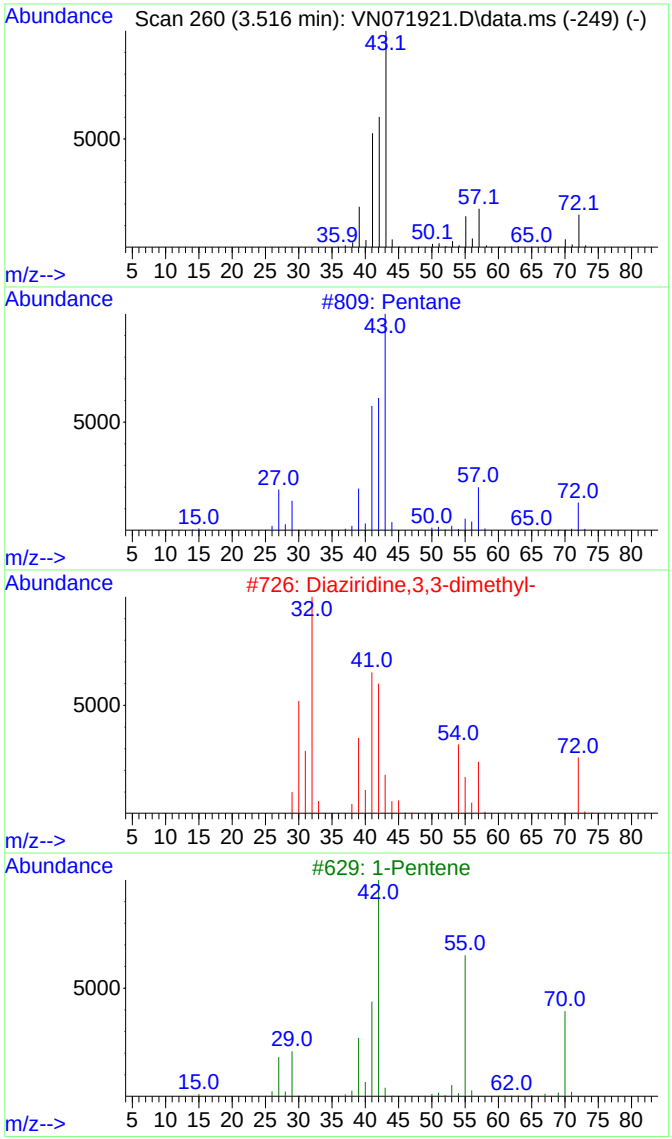
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

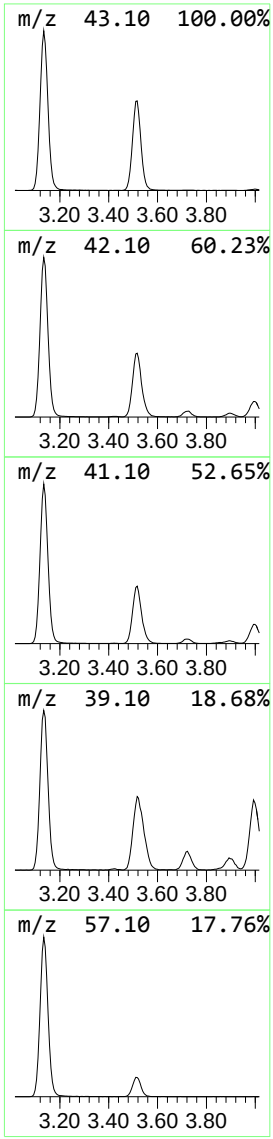
****

Peak Number 2 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	38.62 ug/l	2971850	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
3	1-Pentene	70	C5H10	000109-67-1	17
4	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12
5	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040822\
Data File : VN071921.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

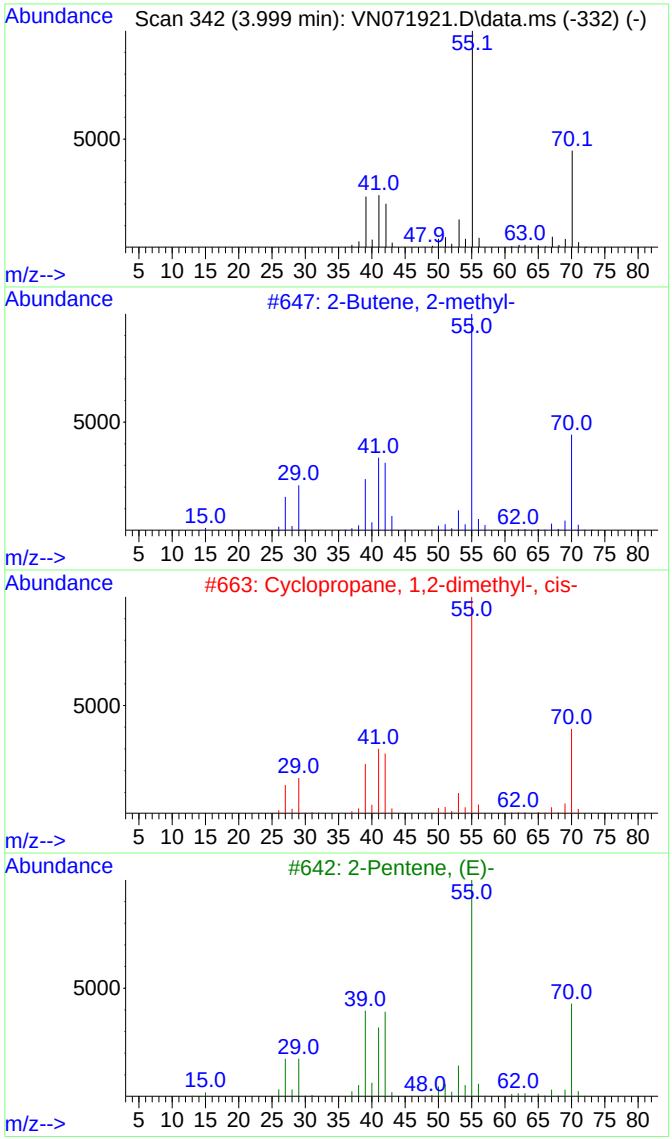
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

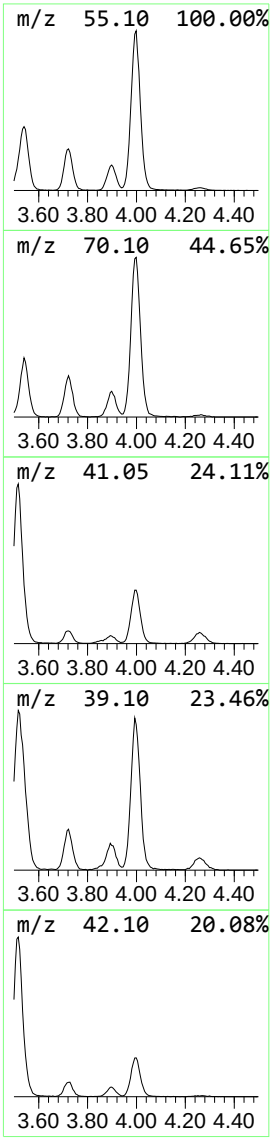
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.999	23.74 ug/l	1826710	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
3	2-Pentene, (E)-	70	C5H10	000646-04-8	86
4	2-Methyl-1-butene	70	C5H10	000563-46-2	83
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80





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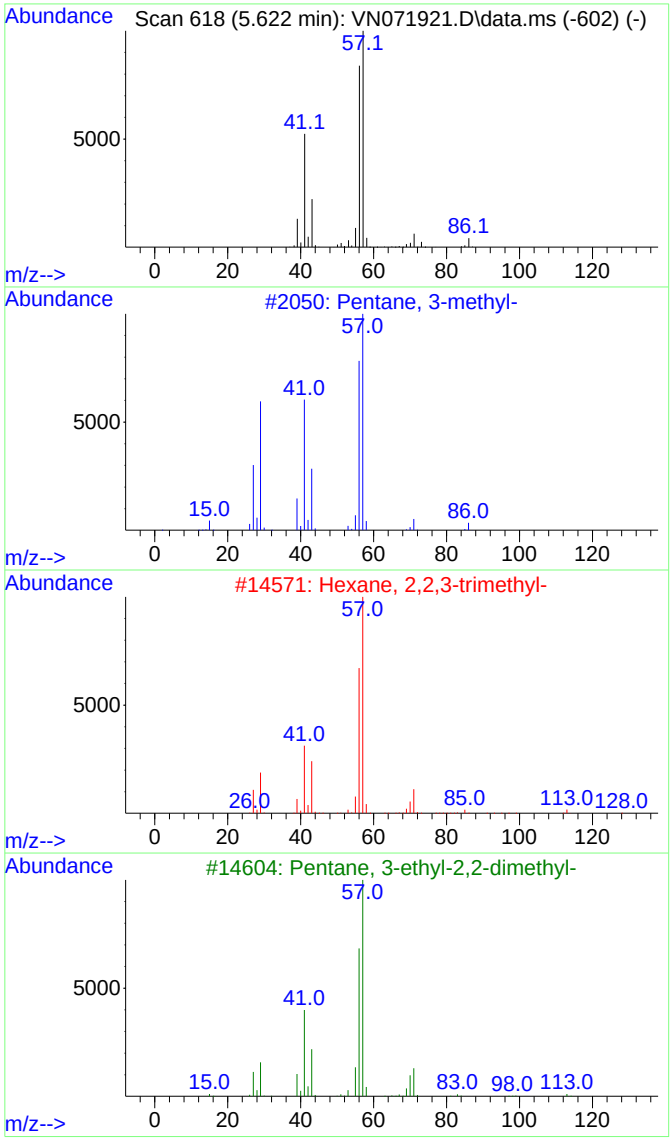
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

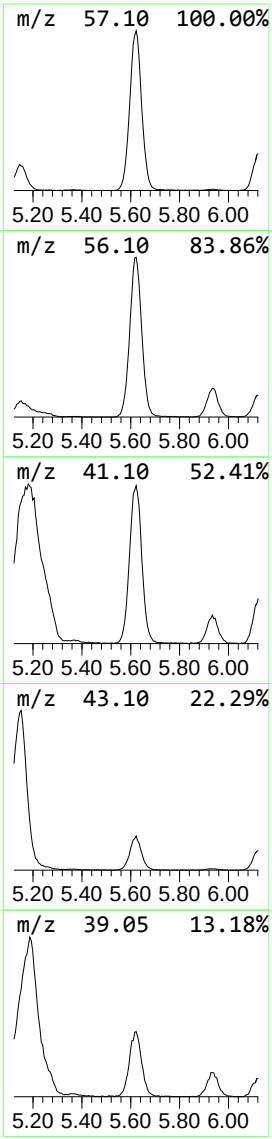
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	25.74 ug/l	1980600	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
4	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
5	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	38





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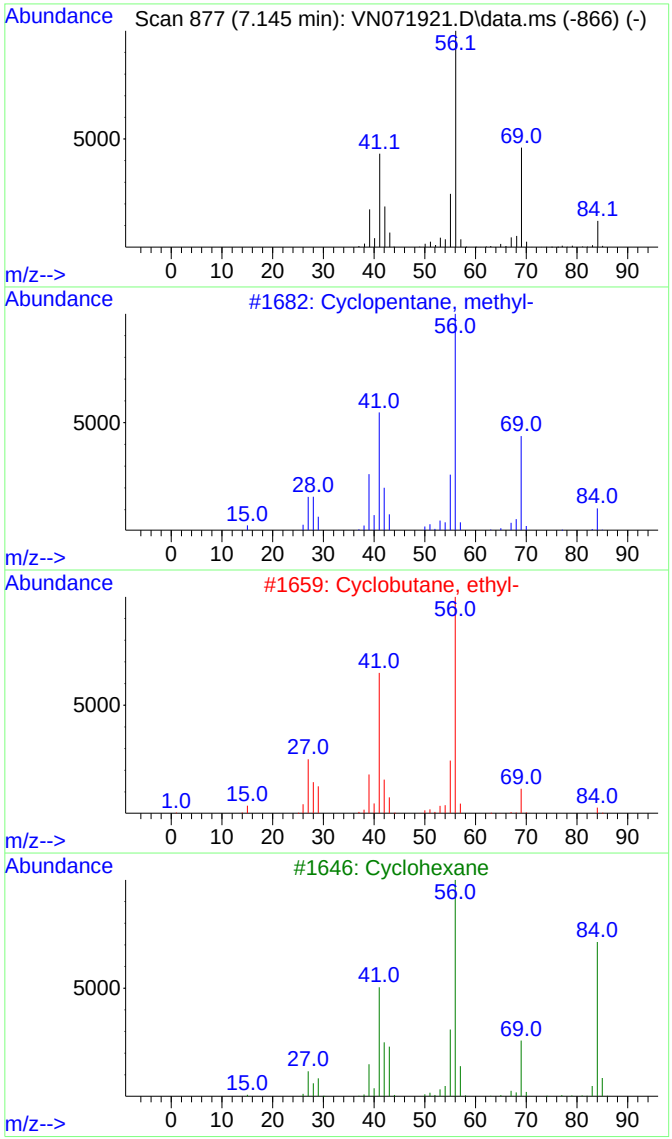
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

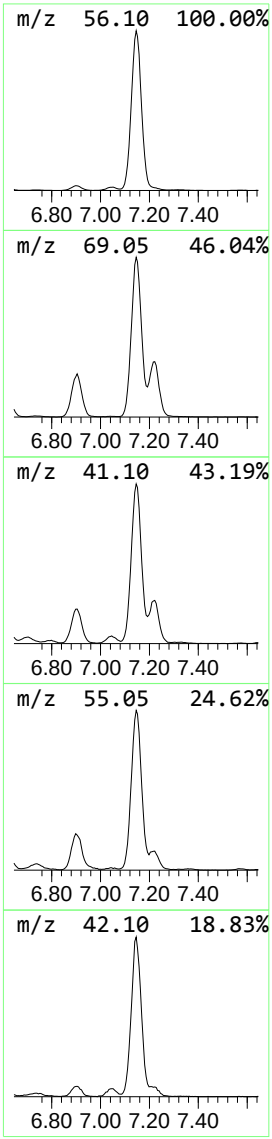
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	75.79 ug/l	5831770	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	Cyclohexane	84	C6H12	000110-82-7	64
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	52
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





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Data File : VN071921.D
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Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

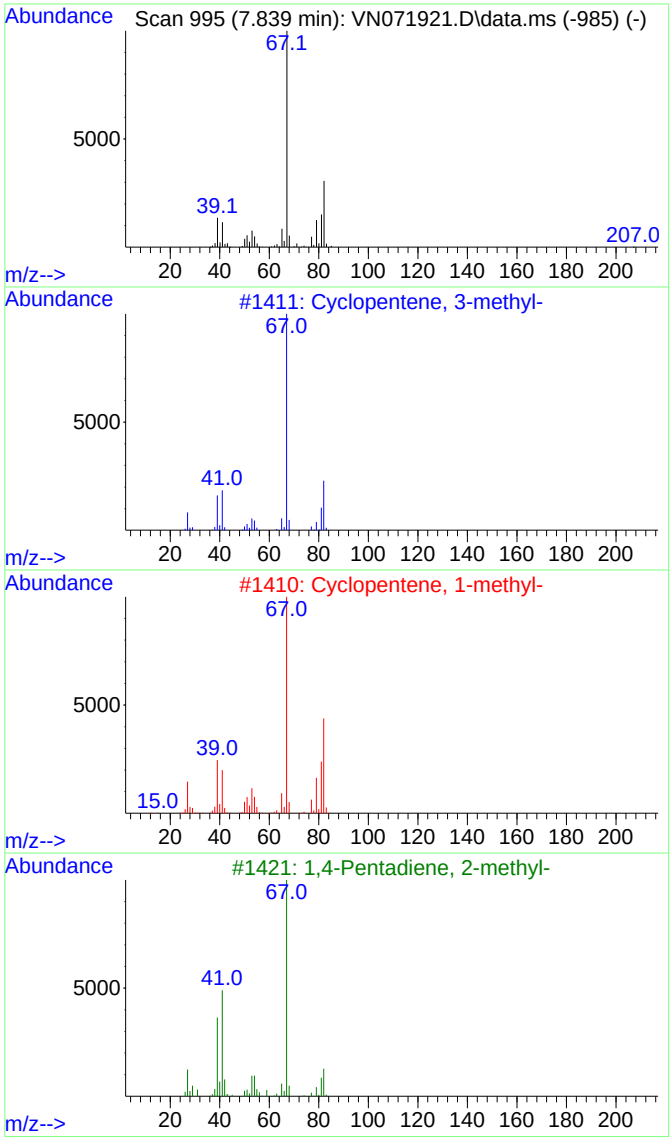
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

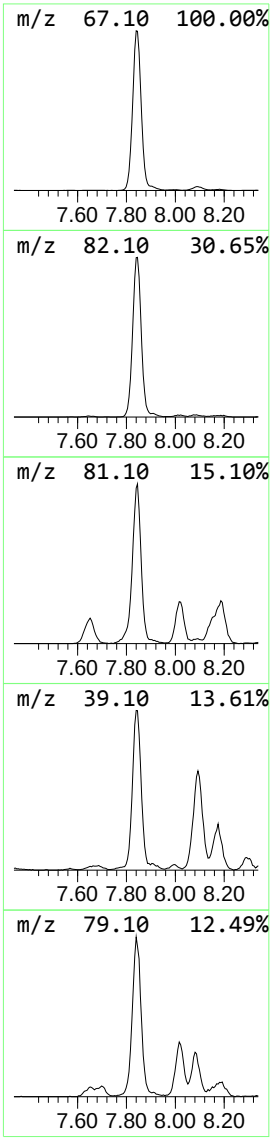
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentene, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.839	37.93 ug/l	2919050	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	90
2	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
3	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	90
4	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	87
5	1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	80





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Data File : VN071921.D
Acq On : 08 Apr 2022 17:56
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

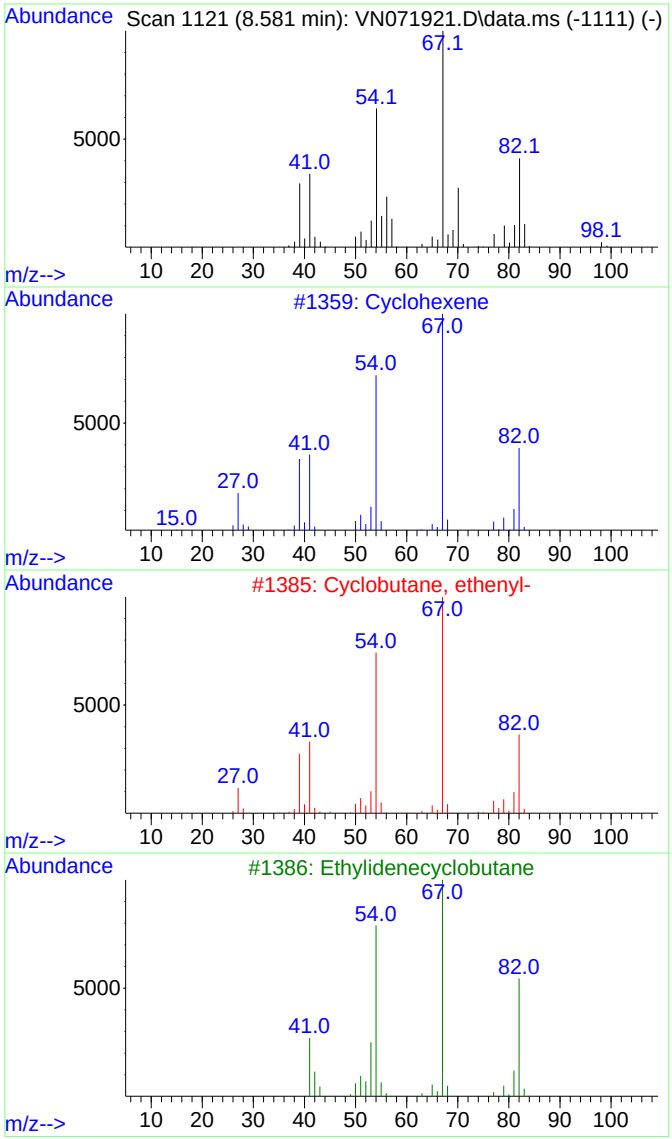
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

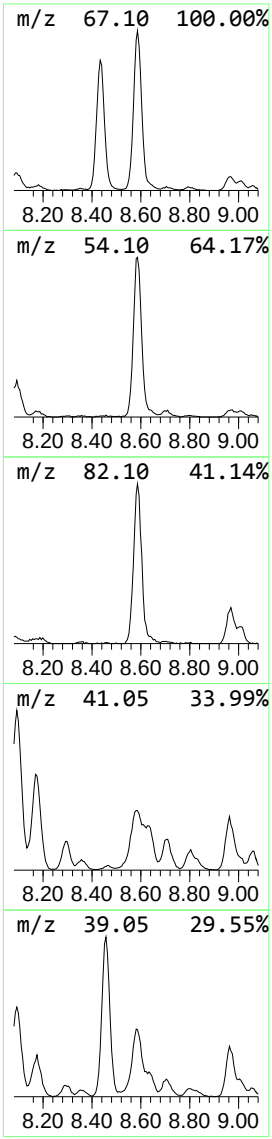
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclobutane, ethenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	17.64 ug/l	1341770	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	70
2	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	70
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	64
4	1,4-Hexadiene	82	C6H10	000592-45-0	60
5	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	55





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

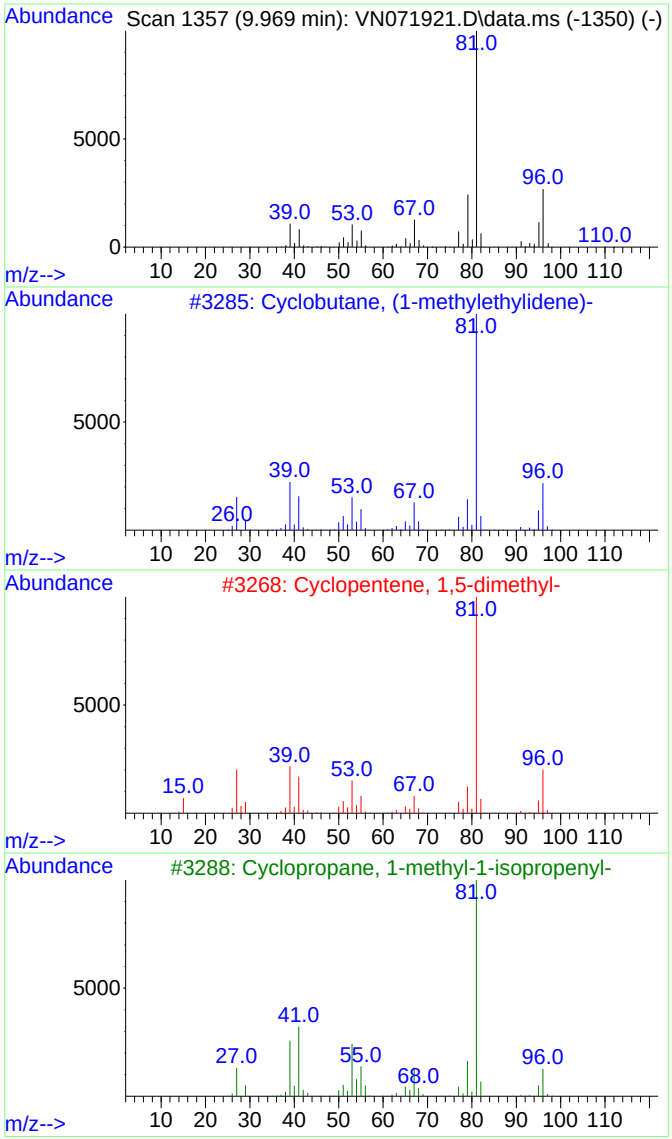
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

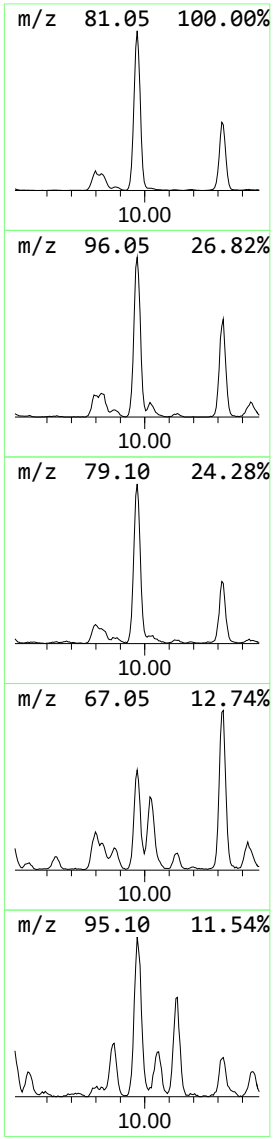
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclobutane, (1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.969	21.66 ug/l	1647660	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	87
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	87
3	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	86
4	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	72
5	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	64





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Data File : VN071921.D
Acq On : 08 Apr 2022 17:56
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

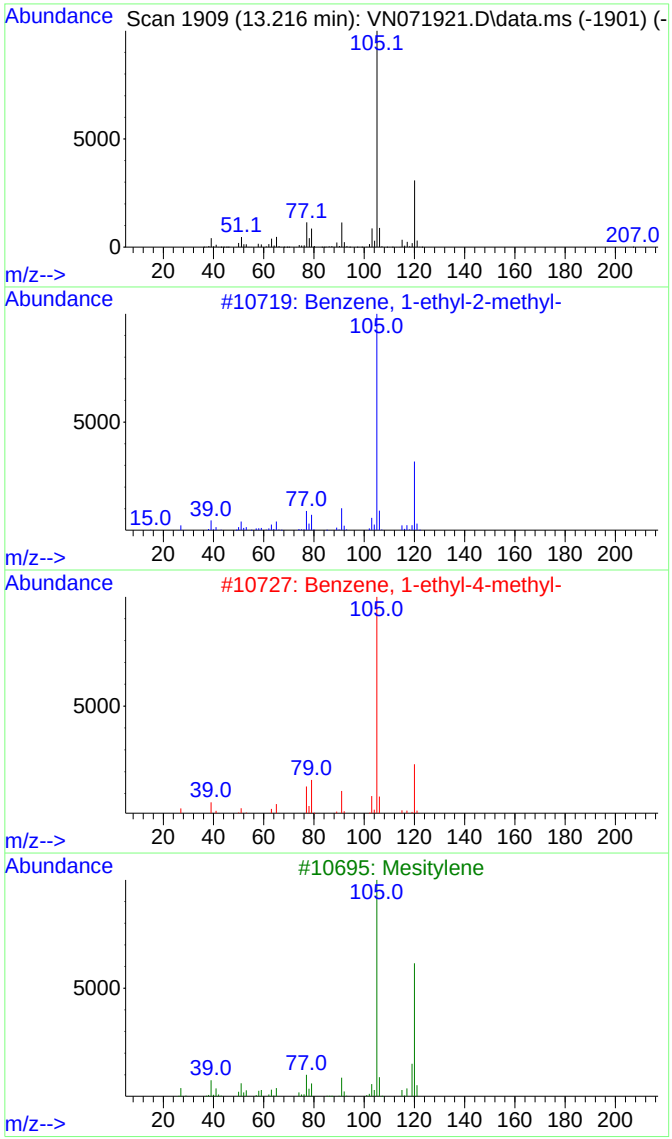
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

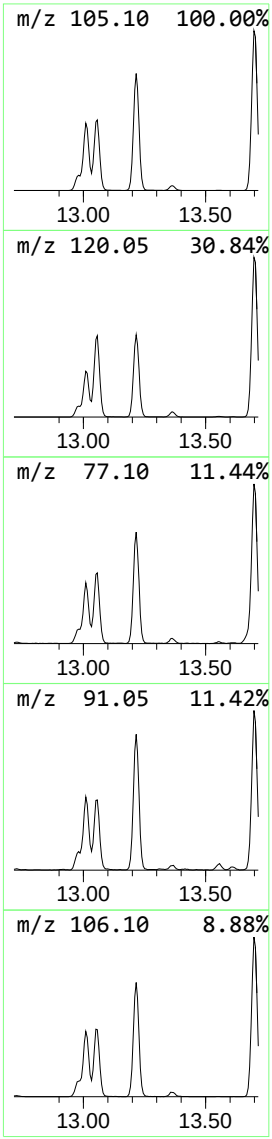
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	24.83 ug/l	5720670	1,4-Dichlorobenzene-d4	13.669

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-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Sample : N2308-03
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

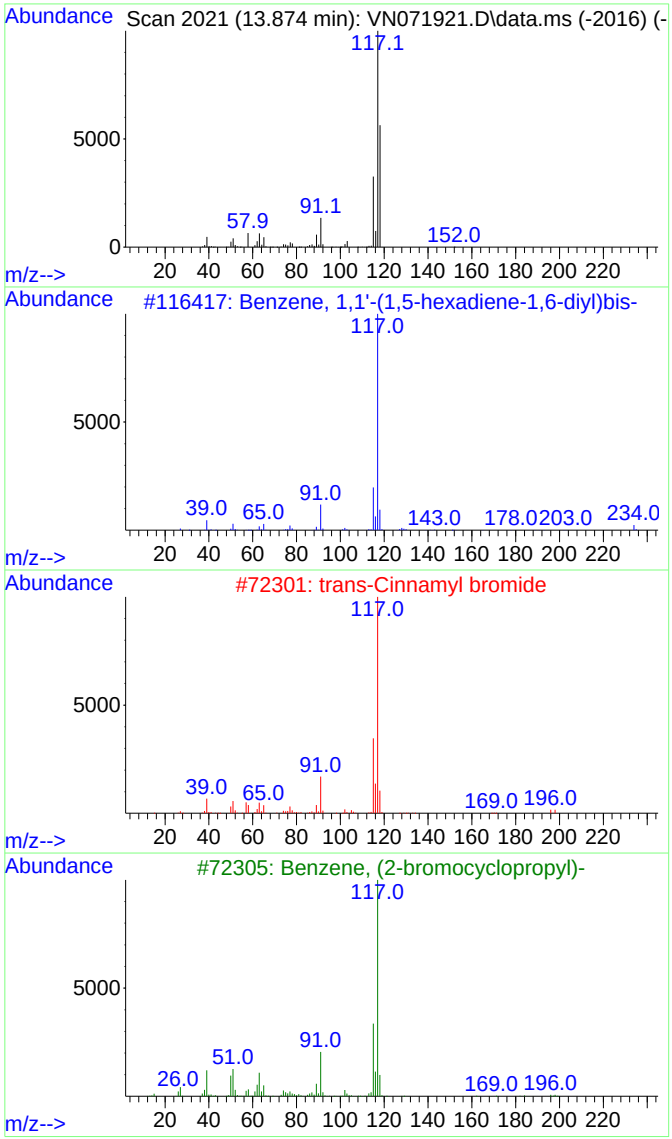
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

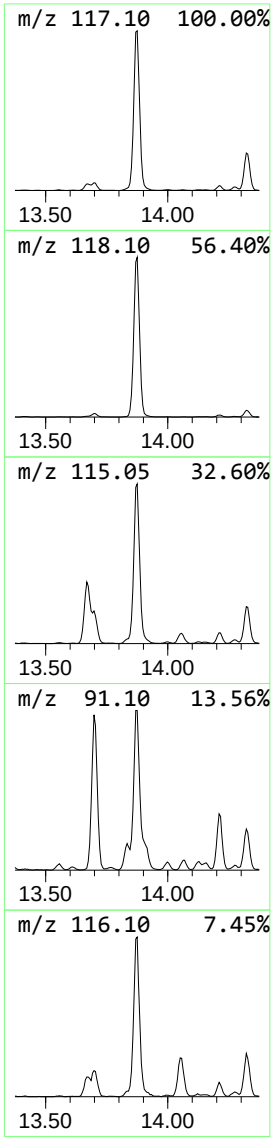
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	32.67 ug/l	7527960	1,4-Dichlorobenzene-d4	13.669

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	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
3	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
4	m-Aminophenylacetylene	117	C8H7N	054060-30-9	37
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	36





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040822\
Data File : VN071921.D
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Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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	80.1	ug/l	6160270	1	8.081	3847530	50.0
Pentane	3.516	38.6	ug/l	2971850	1	8.081	3847530	50.0
2-Butene, 2-met...	3.999	23.7	ug/l	1826710	1	8.081	3847530	50.0
Pentane, 3-methyl-	5.622	25.7	ug/l	1980600	1	8.081	3847530	50.0
Cyclopentane, m...	7.145	75.8	ug/l	5831770	1	8.081	3847530	50.0
Cyclopentene, 3...	7.839	37.9	ug/l	2919050	1	8.081	3847530	50.0
Cyclobutane, et...	8.581	17.6	ug/l	1341770	2	8.963	3802750	50.0
Cyclobutane, (1...	9.969	21.7	ug/l	1647660	2	8.963	3802750	50.0
Benzene, 1-ethy...	13.216	24.8	ug/l	5720670	4	13.669	11520700	50.0
Benzene, 1,1'-(...	13.874	32.7	ug/l	7527960	4	13.669	11520700	50.0