LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

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\82N083022W.M
Title : SW846 8260

Signal : TIC: VN074263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	78	87	97	rBV	654629	1121822	3.75%	0.530%
2	3.087	194	204	217	rBV	984275	2232532	7.45%	1.055%
3	3.457	258	267	282	rVB3	319185	919255	3.07%	0.434%
4	3.657	292	301	313	rBV2	286098	693946	2.32%	0.328%
5	3.834	319	331	339	rBV	188802	486649	1.62%	0.230%
6	3.928	339	347	364	rVB2	344738	921331	3.08%	0.435%
7	4.881	490	509	519	rBV2	255771	849280	2.84%	0.401%
8	5.104	534	547	567	rVV3	370316	1705390	5.69%	0.806%
9	5.287	567	578	594	rVB	332903	1179045	3.94%	0.557%
10	5.540	606	621	637	rBV3	211895	747930	2.50%	0.353%
11	6.387	758	765	778	rVV6	130466	473471	1.58%	0.224%
12	6.622	796	805	814	rVV4	111429	453914	1.52%	0.214%
13	7.069	868	881	891	rBV	617568	1883048	6.29%	0.889%
14	7.957	1021	1032	1036	rBV2	176794	448004	1.50%	0.212%
15	8.022	1036	1043	1052	rVV2	699205	1825265	6.09%	0.862%
16	8.392	1093	1106	1116	rBV	14450733	29949162	100.00%	14.147%
17	8.522	1123	1128	1134	rVB3	201413	426029	1.42%	0.201%
18	8.904	1184	1193	1206	rBV	584450	1332906	4.45%	0.630%
19	9.392	1261	1276	1284	rBV3	330348	921789	3.08%	0.435%
20	9.910	1356	1364	1368	rBV3	227805	442981	1.48%	0.209%
21	10.381	1435	1444	1449	rBV	763512	1455141	4.86%	0.687%
22	10.445	1449	1455	1461	rVV	1346589	2350762	7.85%	1.110%
23	10.581	1469	1478	1484	rVB2	165959	312080	1.04%	0.147%
24	11.680	1658	1665	1674	rBV	826409	1524689	5.09%	0.720%
25	11.786	1675	1683	1693	rVV	15505620	23119725	77.20%	10.921%
26	11.898	1693	1702	1713	rVV	14473970	25947331	86.64%	12.257%
27	12.222	1744	1757	1767	rBV	9372424	14346877	47.90%	6.777%
28	12.516	1801	1807	1815	rVB	902379	1482075	4.95%	0.700%
29	12.669	1824	1833	1843	rBV	698542	1199540	4.01%	0.567%
30	12.857	1857	1865	1871	rBV	2191634	3526597	11.78%	1.666%
31	12.922	1871	1876	1879	rVV	2936050	4818990	16.09%	2.276%
32	12.957	1879	1882	1885	rVV	2666527	3829878	12.79%	1.809%
33	12.998	1885	1889	1897	rVB	2254984	3528642	11.78%	1.667%
34	13.157	1909	1916	1927	rBV	3011042	4884775	16.31%	2.307%
35	13.304	1931	1941	1949	rBV	13497247	21585140	72.07%	10.196%
36	13.645	1987	1999	2008	rBV	5019019	8792073	29.36%	4.153%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

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\82N083022W.M
Title : SW846 8260

37	13.774	2015	2021	2022	rBV	480267	562015	1.88%	0.265%
38	13.816	2022	2028	2044	rVB	5302405	10004495	33.40%	4.726%
39	14.004	2053	2060	2066	rVV2	528617	972683	3.25%	0.459%
40	14.069	2066	2071	2074	rVV	620595	1062276	3.55%	0.502%
41	14.098	2074	2076	2081	rVV	492181	615618	2.06%	0.291%
42	14.157	2081	2086	2091	rVV	1209693	1866089	6.23%	0.881%
43	14.216	2091	2096	2100	rVV2	273603	455295	1.52%	0.215%
44	14.263	2100	2104	2113	rVB2	1057989	1725726	5.76%	0.815%
45	14.398	2121	2127	2133	rVB2	341068	537321	1.79%	0.254%
46	14.474	2133	2140	2144	rBV	760481	1295354	4.33%	0.612%
47	14.516	2144	2147	2152	rVB	876038	1239652	4.14%	0.586%
48	14.745	2181	2186	2191	rBV	877056	1332671	4.45%	0.630%
49	14.863	2198	2206	2213	rBV3	1740174	3697672	12.35%	1.747%
50	14.927	2213	2217	2224	rVV5	168486	323290	1.08%	0.153%
51	15.016	2225	2232	2239	rVV	549116	968070	3.23%	0.457%
52	15.127	2241	2251	2255	rVV2	274088	721504	2.41%	0.341%
53	15.239	2263	2270	2278	rVB5	261331	626110	2.09%	0.296%
54	15.433	2295	2303	2310	rBV	3851951	6853094	22.88%	3.237%
55	15.539	2315	2321	2327	rVV4	158822	363551	1.21%	0.172%
56	16.527	2481	2489	2505	rVB	1169781	2588907	8.64%	1.223%
57	16.733	2515	2524	2533	rBV	952858	2169821	7.25%	1.025%

Sum of corrected areas: 211699278

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Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
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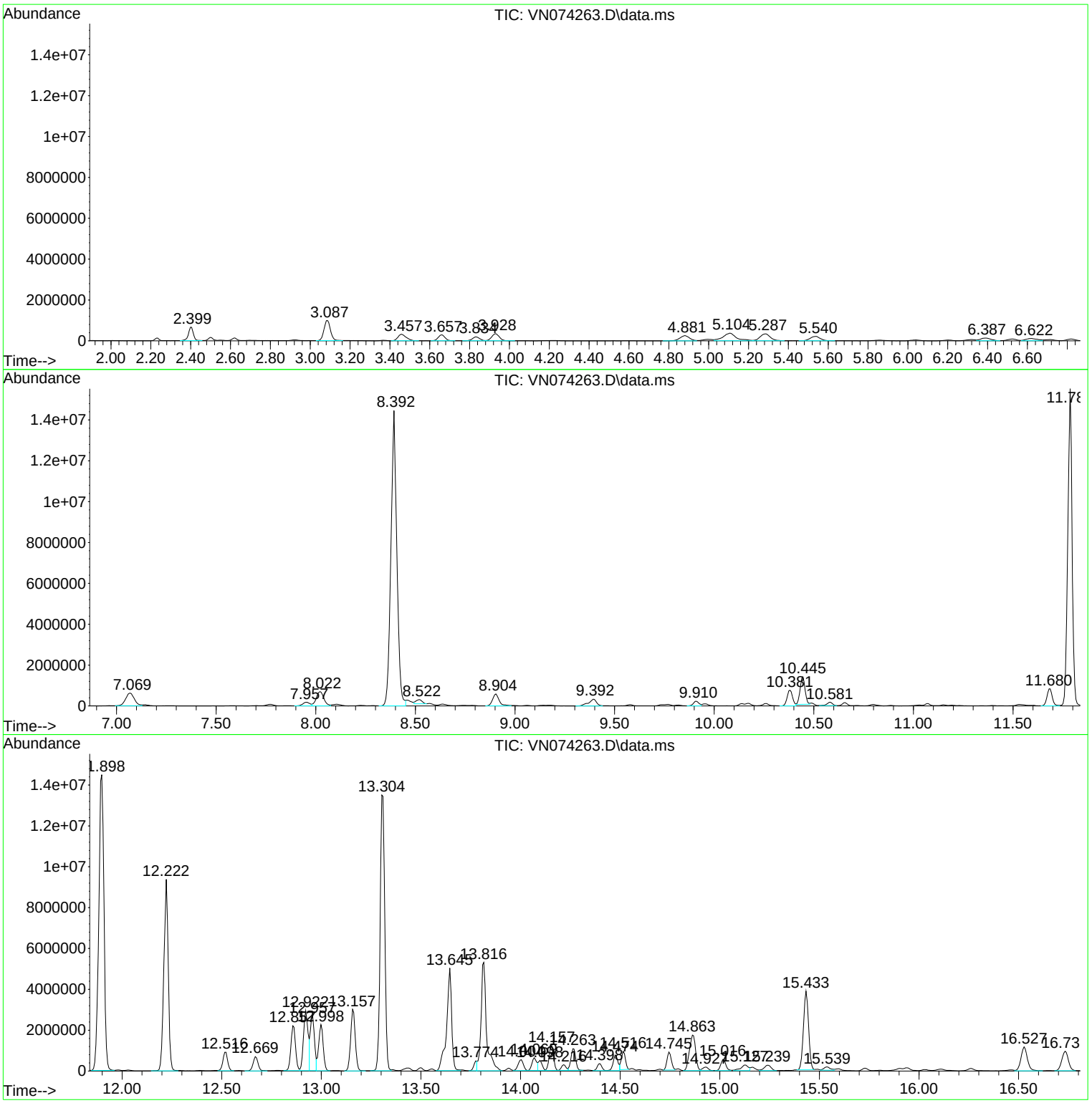
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

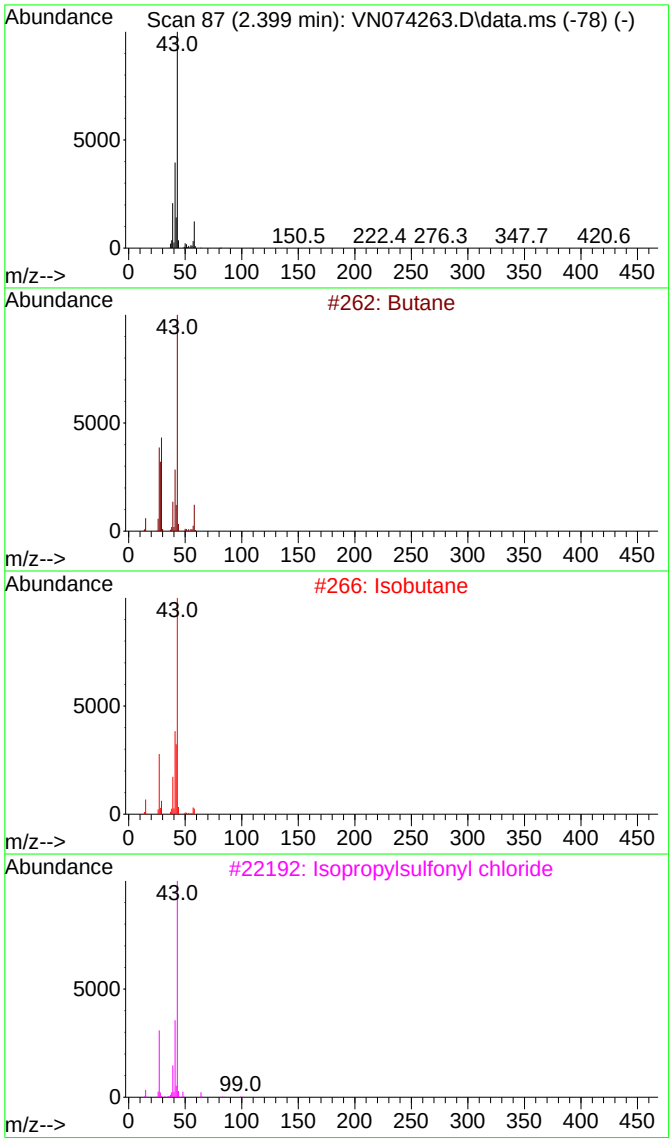
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

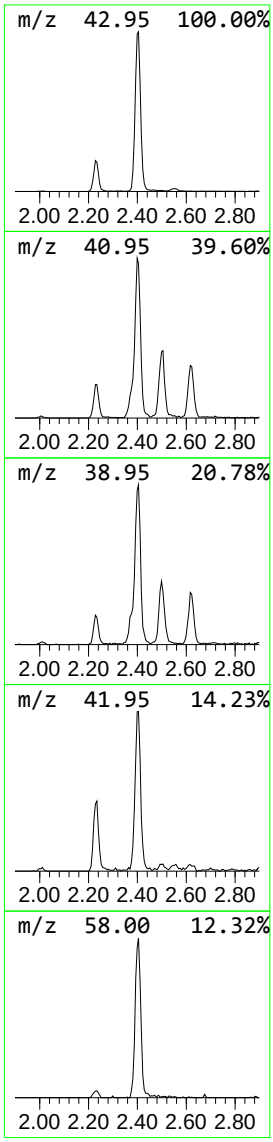
****

Peak Number 1 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	30.73 ug/l	1121820	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

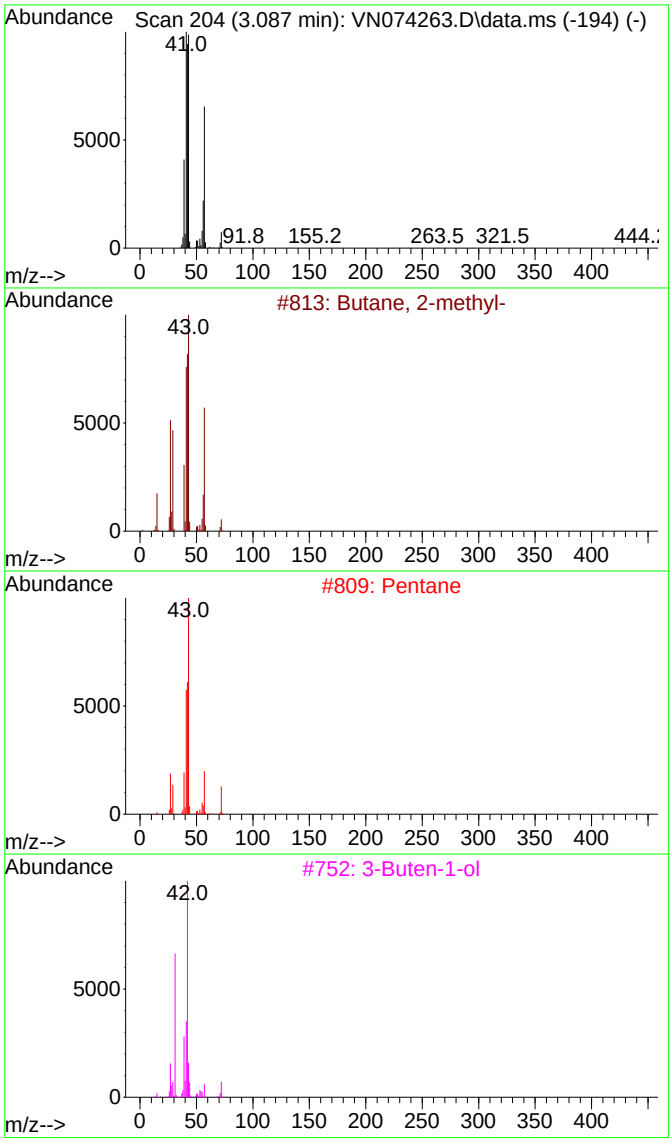
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

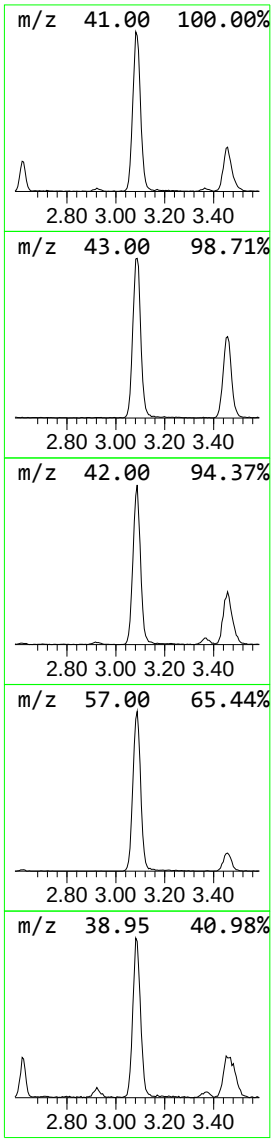
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	61.16 ug/l	2232530	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	35
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

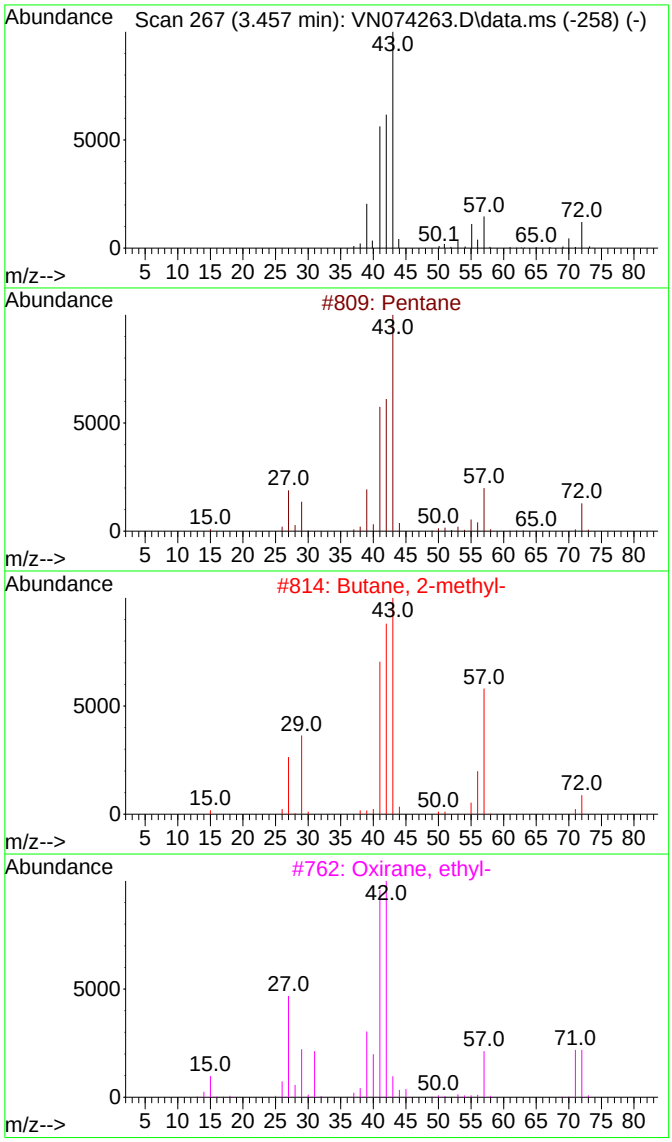
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

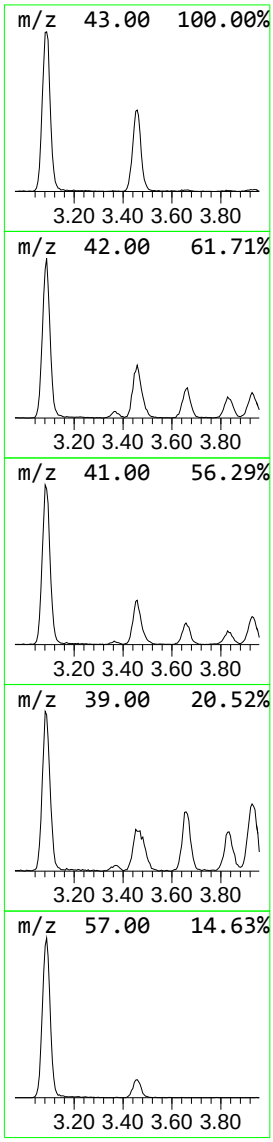
****

Peak Number 3 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	25.18 ug/l	919255	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Butane, 2-methyl-	72	C5H12	000078-78-4	45
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

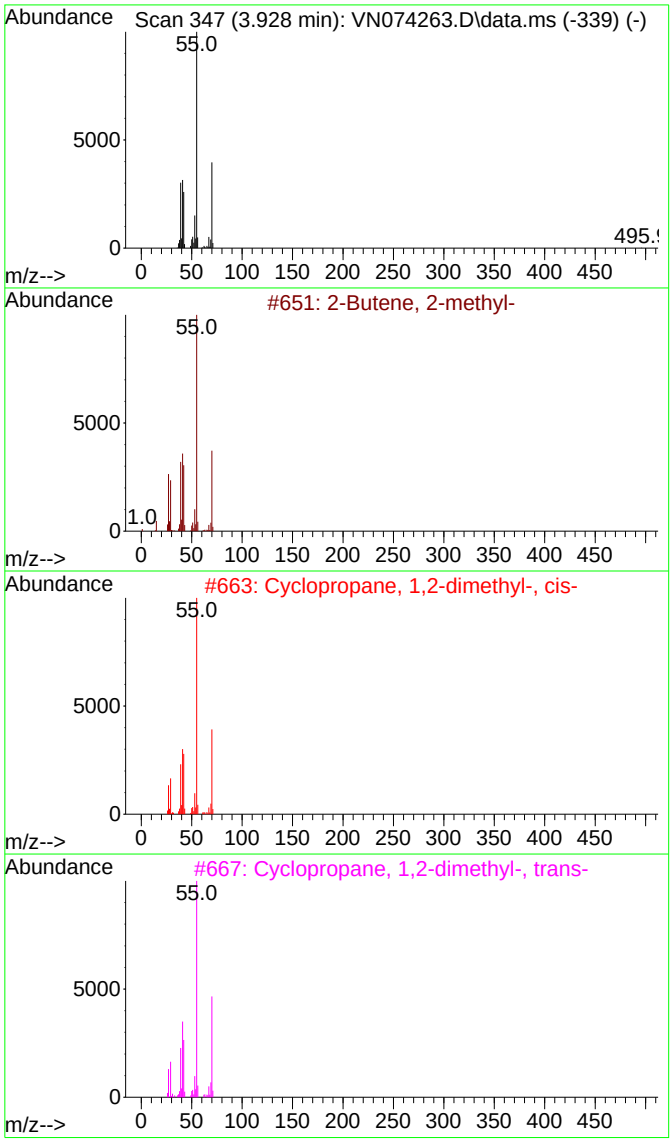
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

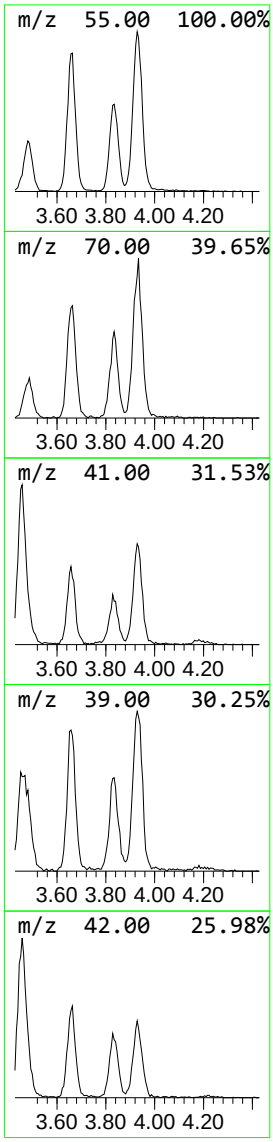
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	25.24 ug/l	921331	Pentafluorobenzene	8.016

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	91
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
4	2-Pentene, (E)-	70	C5H10	000646-04-8	87
5	2-Methyl-1-butene	70	C5H10	000563-46-2	86





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Data File : VN074263.D
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Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

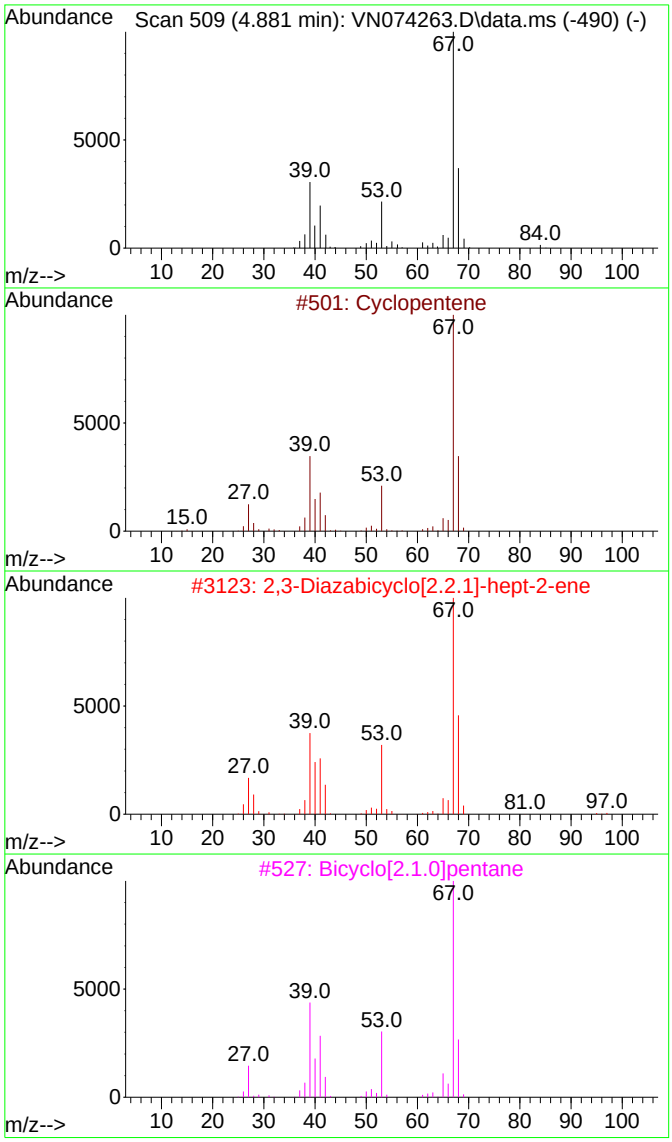
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

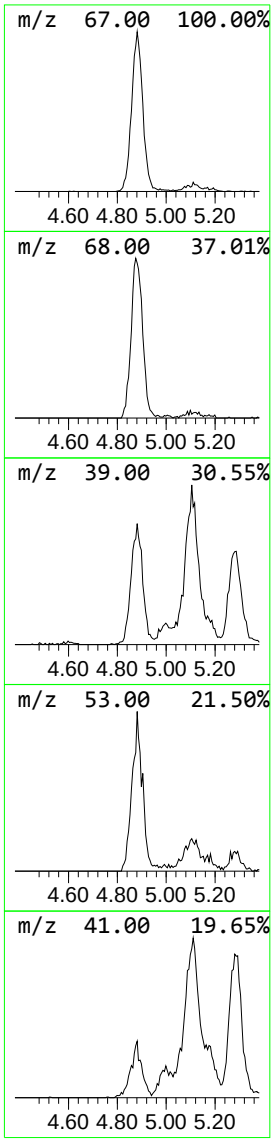
****

Peak Number 5 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	23.26 ug/l	849280	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	64
3	Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	59
4	1,4-Pentadiene	68	C5H8	000591-93-5	50
5	Isoprene	68	C5H8	000078-79-5	50





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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

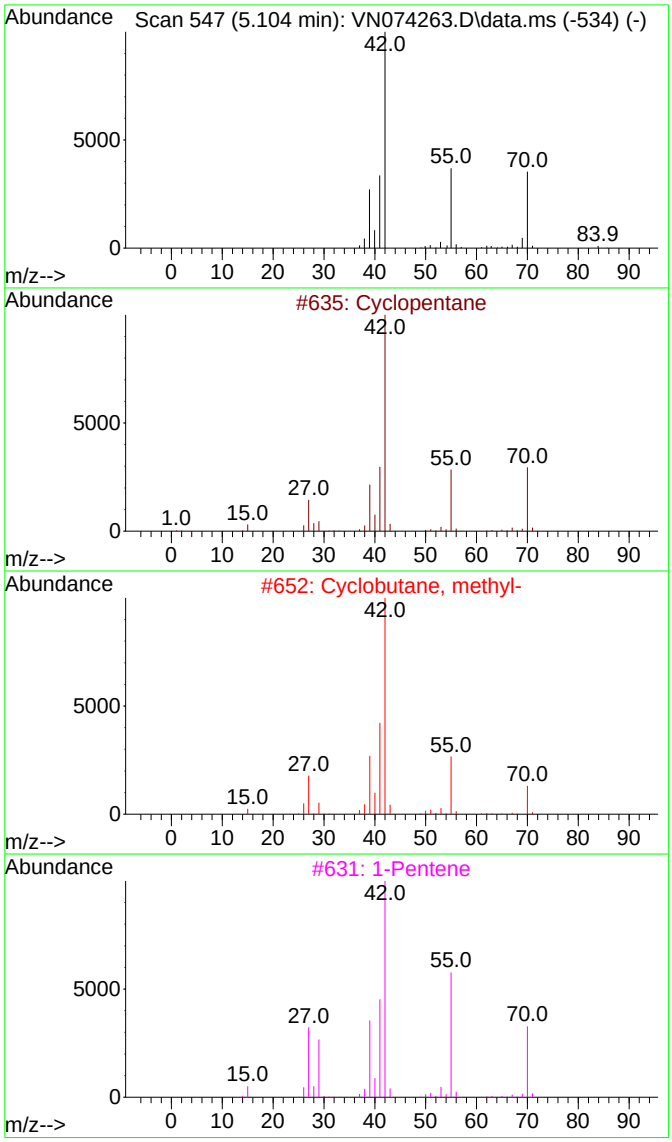
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

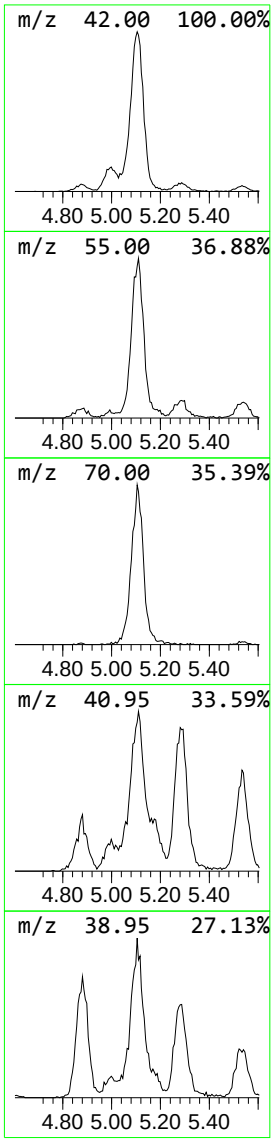
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	46.72 ug/l	1705390	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	56
3	1-Pentene	70	C5H10	000109-67-1	56
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	40
5	Cyclobutanone	70	C4H6O	001191-95-3	9





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Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

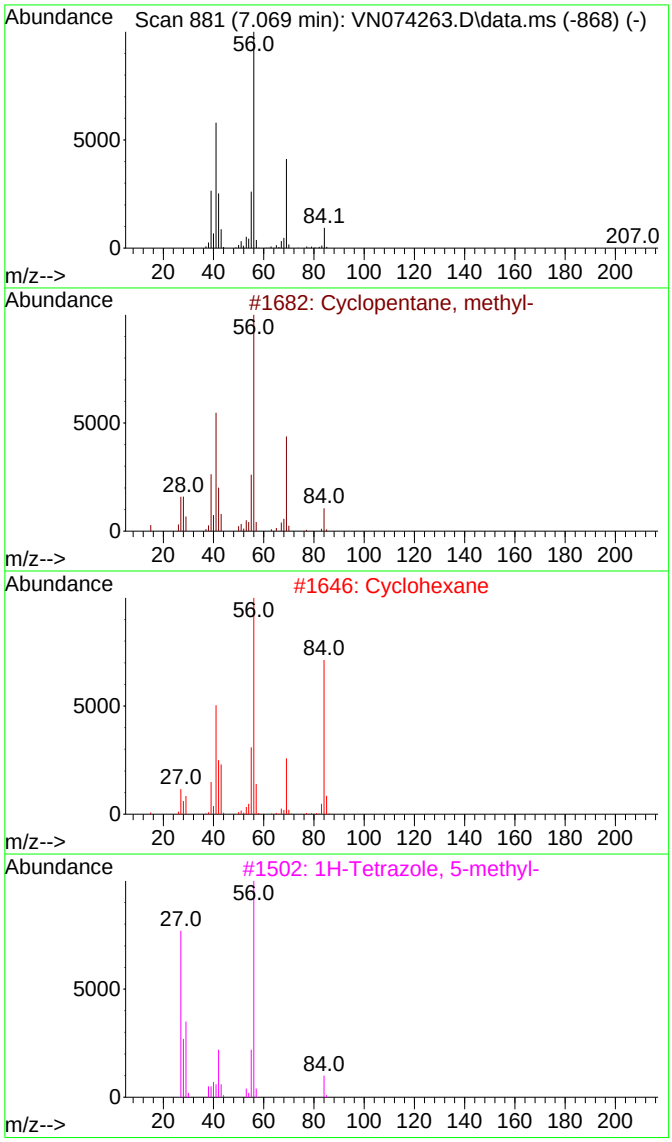
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

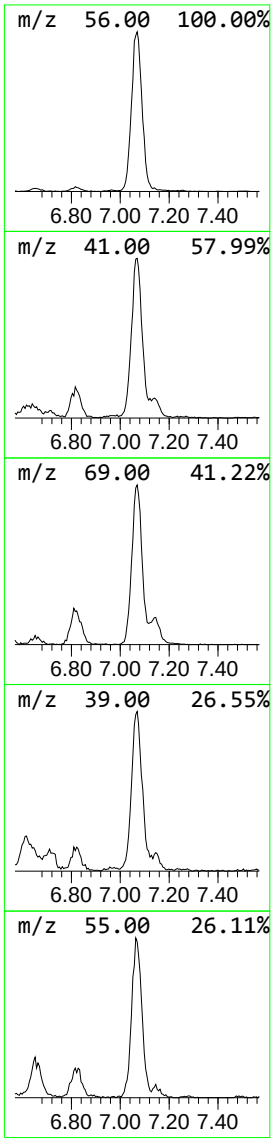
****

Peak Number 7 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	51.58 ug/l	1883050	Pentafluorobenzene	8.016

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	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	Cyclobutane	56	C4H8	000287-23-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

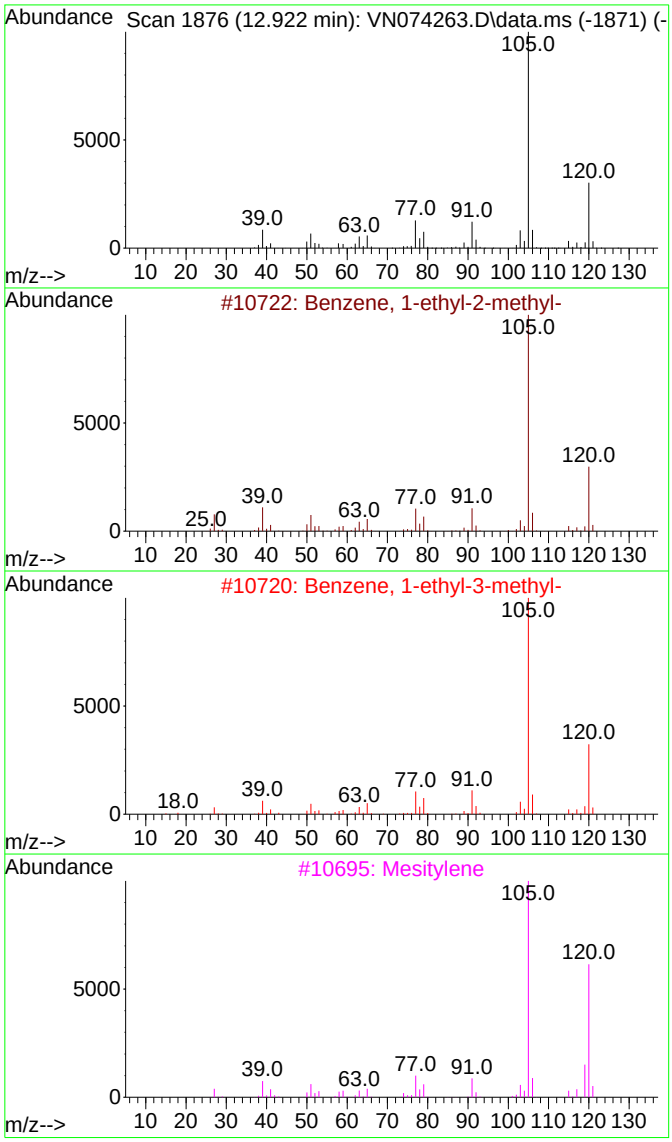
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

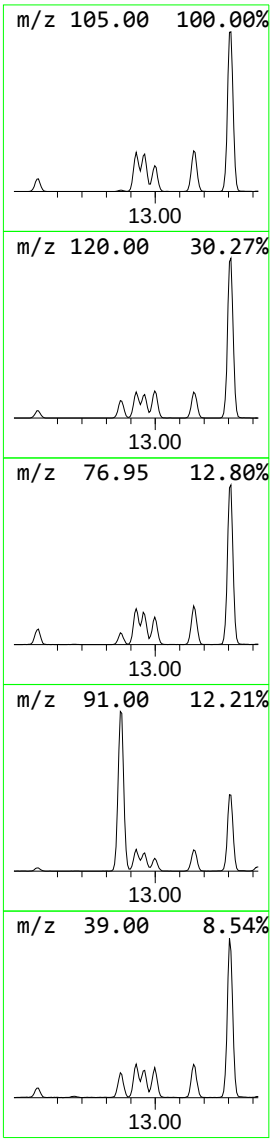
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	27.41 ug/l	4818990	1,4-Dichlorobenzene-d4	13.610

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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

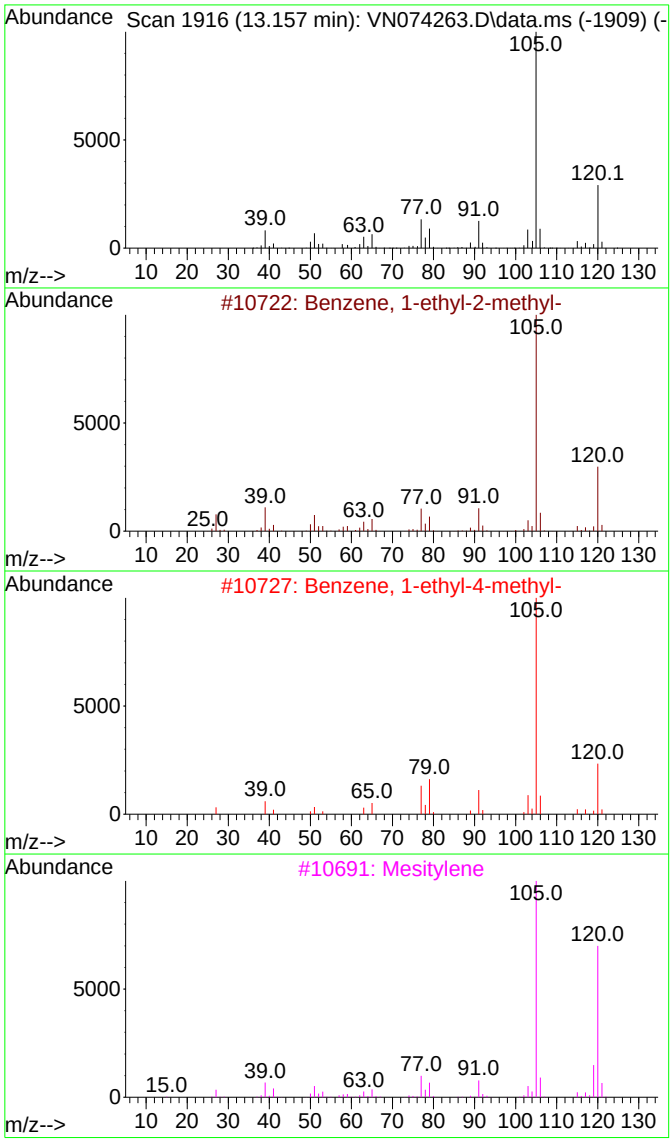
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

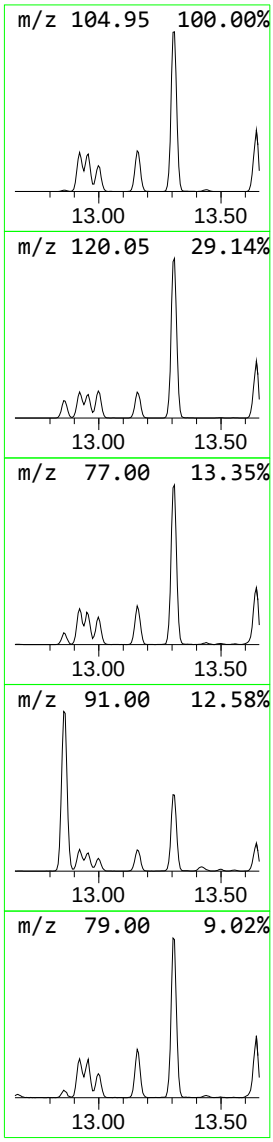
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	27.78 ug/l	4884780	1,4-Dichlorobenzene-d4	13.610

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

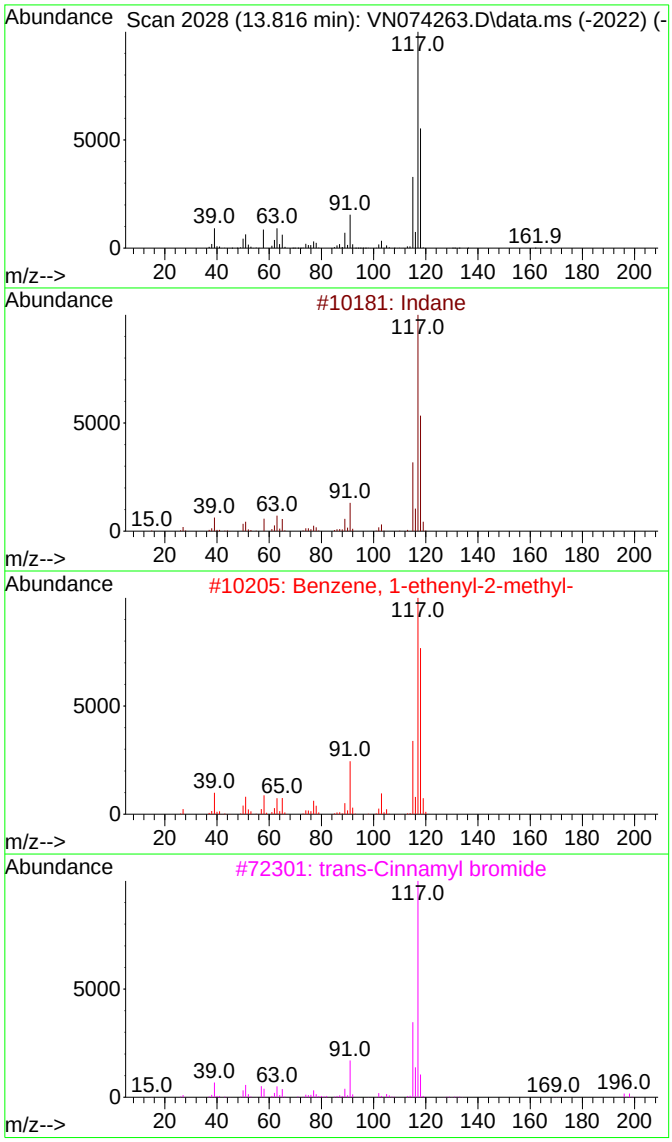
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

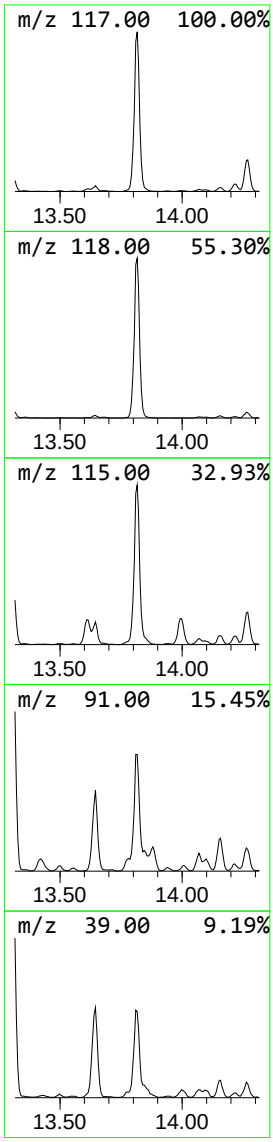
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	56.90 ug/l	10004500	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074263.D
Acq On : 02 Sep 2022 00:28
Operator : JC\MD
Sample : N4376-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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	2.399	30.7	ug/l	1121820	1	8.016	1825270	50.0
Butane, 2-methyl-	3.087	61.2	ug/l	2232530	1	8.016	1825270	50.0
Pentane	3.457	25.2	ug/l	919255	1	8.016	1825270	50.0
2-Butene, 2-met...	3.928	25.2	ug/l	921331	1	8.016	1825270	50.0
Cyclopentene	4.881	23.3	ug/l	849280	1	8.016	1825270	50.0
Cyclopentane	5.104	46.7	ug/l	1705390	1	8.016	1825270	50.0
Cyclopentane, m...	7.069	51.6	ug/l	1883050	1	8.016	1825270	50.0
Benzene, 1-ethy...	12.922	27.4	ug/l	4818990	4	13.610	8792070	50.0
Benzene, 1-ethy...	13.157	27.8	ug/l	4884780	4	13.610	8792070	50.0
Indane	13.816	56.9	ug/l	10004500	4	13.610	8792070	50.0