LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

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\82N062822W.M
Title : SW846 8260

Signal : TIC: VN073482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	193	204	226	rBV	1108895	2515399	1.38%	0.294%
2	3.457	258	267	284	rVB3	657858	1834861	1.00%	0.215%
3	3.928	338	347	363	rVB	842573	2239534	1.22%	0.262%
4	5.075	533	542	575	rVB5	879450	5270659	2.88%	0.617%
5	5.534	605	620	642	rBV	664584	2263683	1.24%	0.265%
6	6.822	829	839	851	rVB2	619093	1849676	1.01%	0.217%
7	7.069	870	881	890	rBV	2330501	6956460	3.80%	0.814%
8	7.769	992	1000	1010	rVB	778855	1906957	1.04%	0.223%
9	8.022	1033	1043	1051	rVV5	1384015	3990890	2.18%	0.467%
10	8.510	1114	1126	1132	rBV6	782784	2470733	1.35%	0.289%
11	8.898	1182	1192	1199	rBV2	1253140	3125560	1.71%	0.366%
12	9.392	1260	1276	1283	rBV2	1587949	4570908	2.50%	0.535%
13	10.380	1436	1444	1448	rBV	1043196	1982147	1.08%	0.232%
14	10.445	1448	1455	1468	rVV	13777924	26021032	14.23%	3.046%
15	11.786	1673	1683	1693	rBV2	35154537	67075312	36.69%	7.851%
16	11.904	1693	1703	1715	rVV3	72924050	182836959	100.00%	21.401%
17	12.227	1745	1758	1774	rBV2	43433088	84589470	46.26%	9.901%
18	12.516	1797	1807	1815	rBV	3102017	5218505	2.85%	0.611%
19	12.863	1858	1866	1871	rBV	9202817	15359988	8.40%	1.798%
20	12.927	1871	1877	1880	rVV	29620281	53830566	29.44%	6.301%
21	12.957	1880	1882	1886	rVV	15299963	21773397	11.91%	2.549%
22	13.004	1886	1890	1901	rVB	17488812	27409680	14.99%	3.208%
23	13.163	1909	1917	1926	rBV	15396279	25353556	13.87%	2.968%
24	13.310	1933	1942	1955	rBV2	47458306	89951412	49.20%	10.529%
25	13.498	1969	1974	1980	rBV	1289572	1987983	1.09%	0.233%
26	13.645	1988	1999	2008	rBV	19741698	34453986	18.84%	4.033%
27	13.815	2022	2028	2032	rBV2	17655090	30279239	16.56%	3.544%
28	14.004	2053	2060	2066	rVV2	2671649	4904813	2.68%	0.574%
29	14.068	2066	2071	2074	rVV	4184162	7049679	3.86%	0.825%
30	14.098	2074	2076	2081	rVV	3588867	4709461	2.58%	0.551%
31	14.157	2081	2086	2091	rVV	6203129	9428381	5.16%	1.104%
32	14.215	2091	2096	2100	rVV	1476425	2381464	1.30%	0.279%
33	14.268	2100	2105	2114	rVB2	4800556	8091317	4.43%	0.947%
34	14.398	2119	2127	2133	rVB	1781377	3018412	1.65%	0.353%
35	14.480	2133	2141	2144	rBV	3678621	6398566	3.50%	0.749%
36	14.515	2144	2147	2152	rVB	5069631	7190592	3.93%	0.842%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

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\82N062822W.M
Title : SW846 8260

37	14.745	2181	2186	2192	rBV	4417010	7114515	3.89%	0.833%
38	14.868	2198	2207	2213	rBV2	7263892	14946199	8.17%	1.749%
39	14.927	2213	2217	2226	rVB2	1094024	1977932	1.08%	0.232%
40	15.015	2226	2232	2240	rBV2	1730576	2998328	1.64%	0.351%
41	15.127	2240	2251	2255	rBV4	1143502	2853404	1.56%	0.334%
42	15.245	2263	2271	2278	rVB2	951649	2230518	1.22%	0.261%
43	15.433	2289	2303	2315	rBV	20157862	39570071	21.64%	4.632%
44	16.527	2481	2489	2503	rVB	6716957	14861893	8.13%	1.740%
45	16.733	2515	2524	2533	rBV	3345621	7501330	4.10%	0.878%

Sum of corrected areas: 854345427

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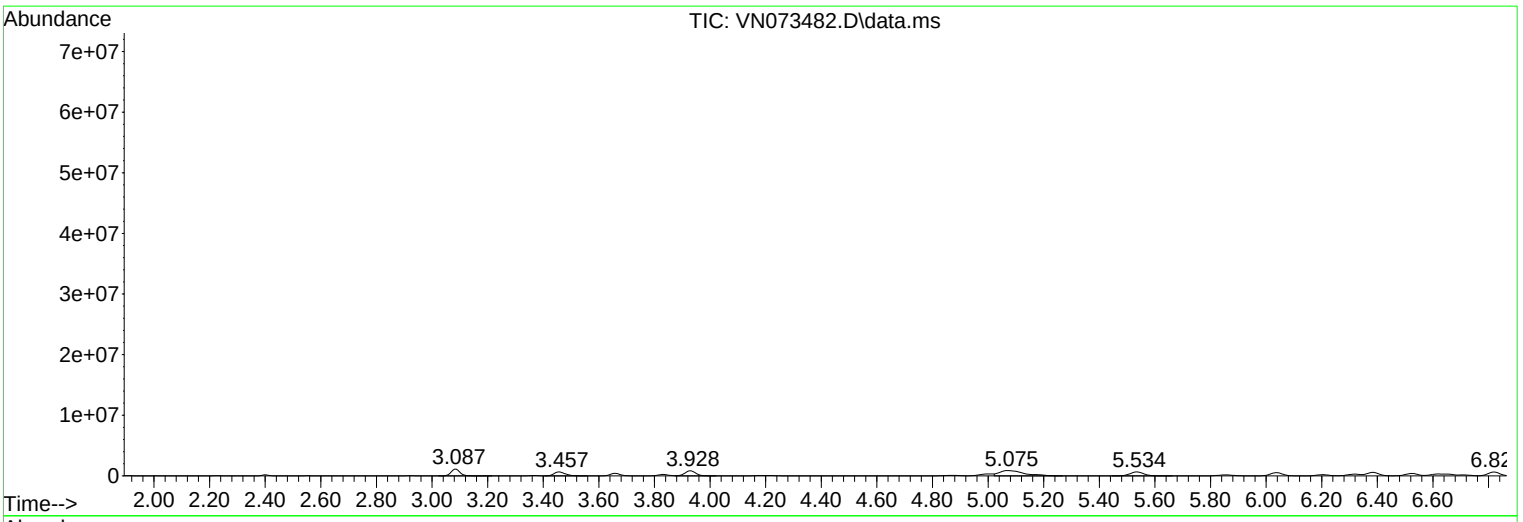
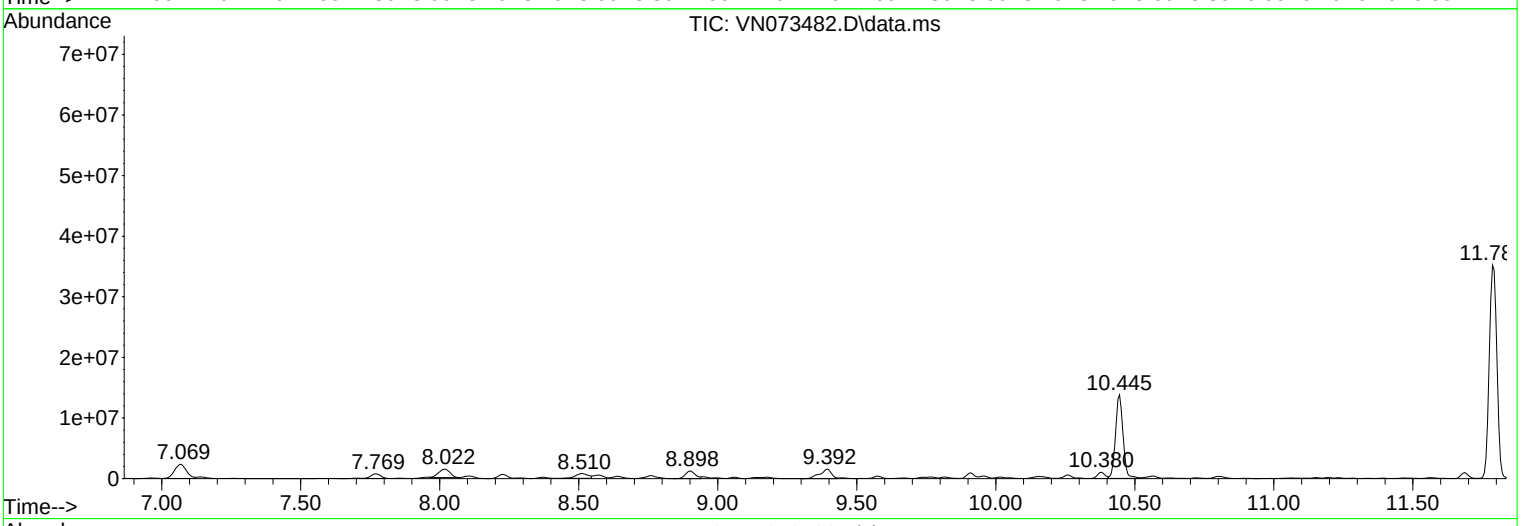
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

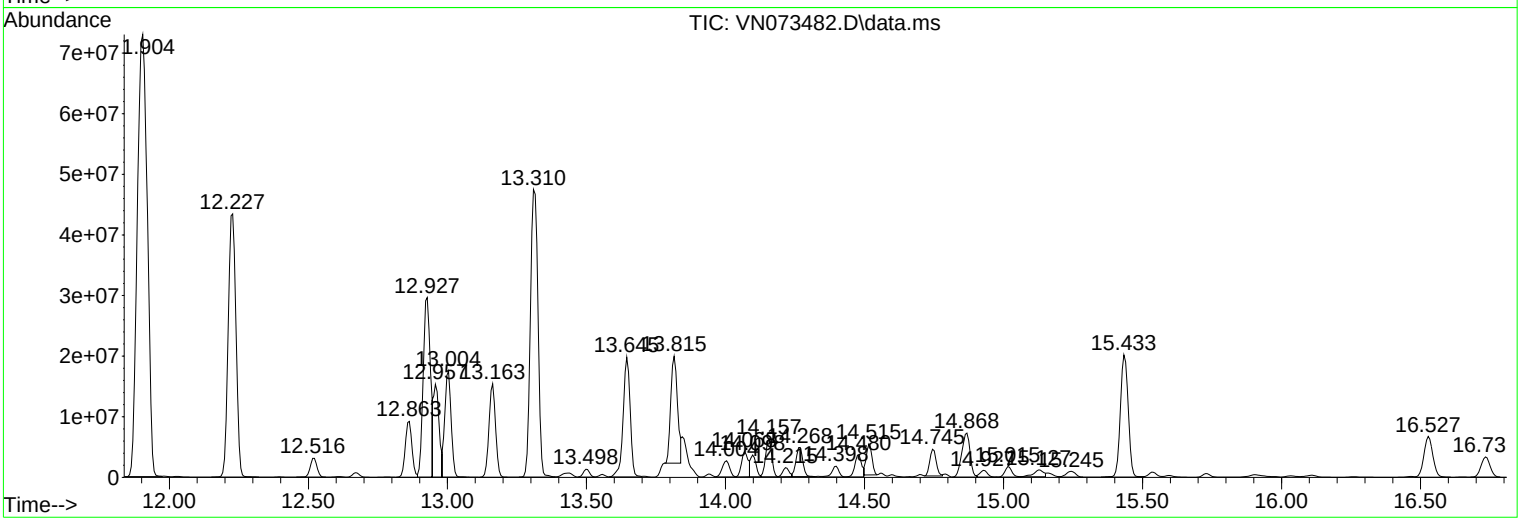
Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

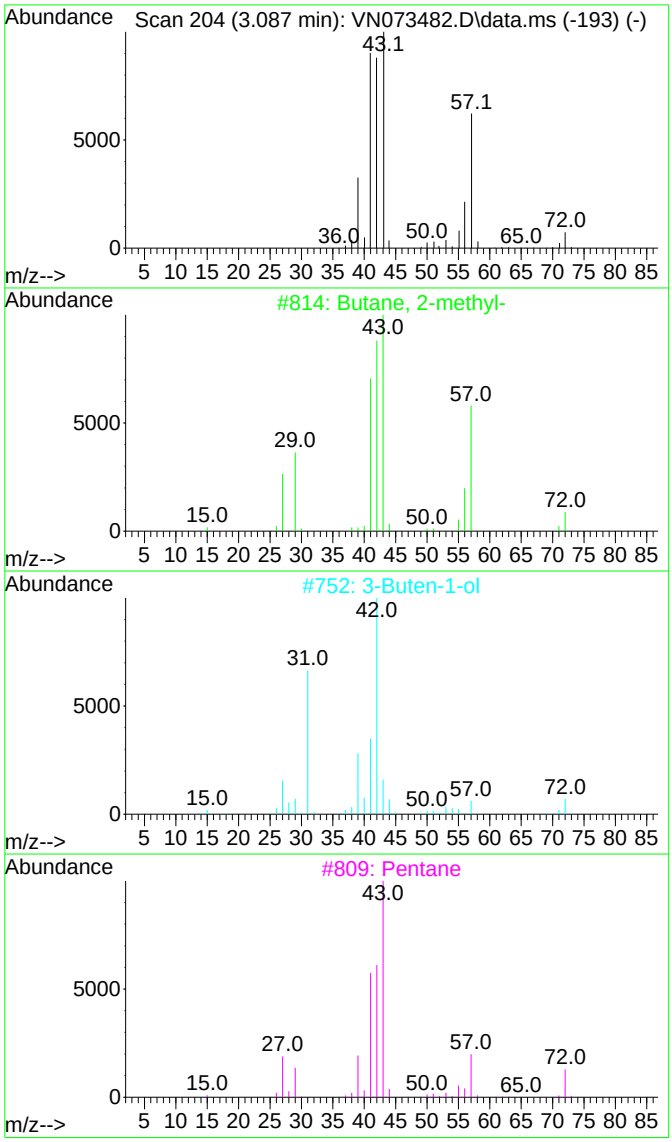
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

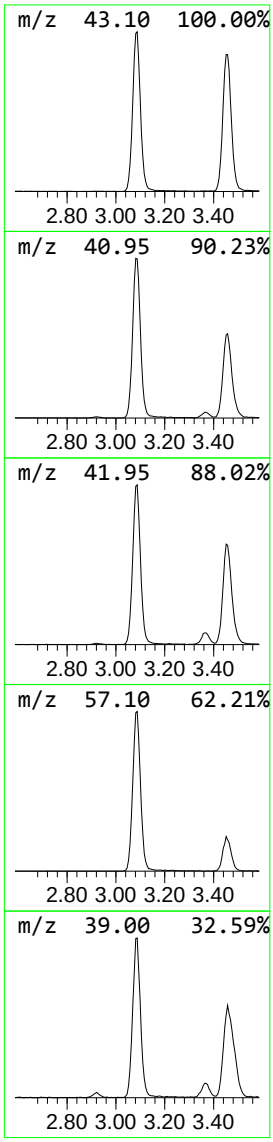
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	31.51 ug/l	2515400	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	42
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14
5	Azetidine	57	C3H7N	000503-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

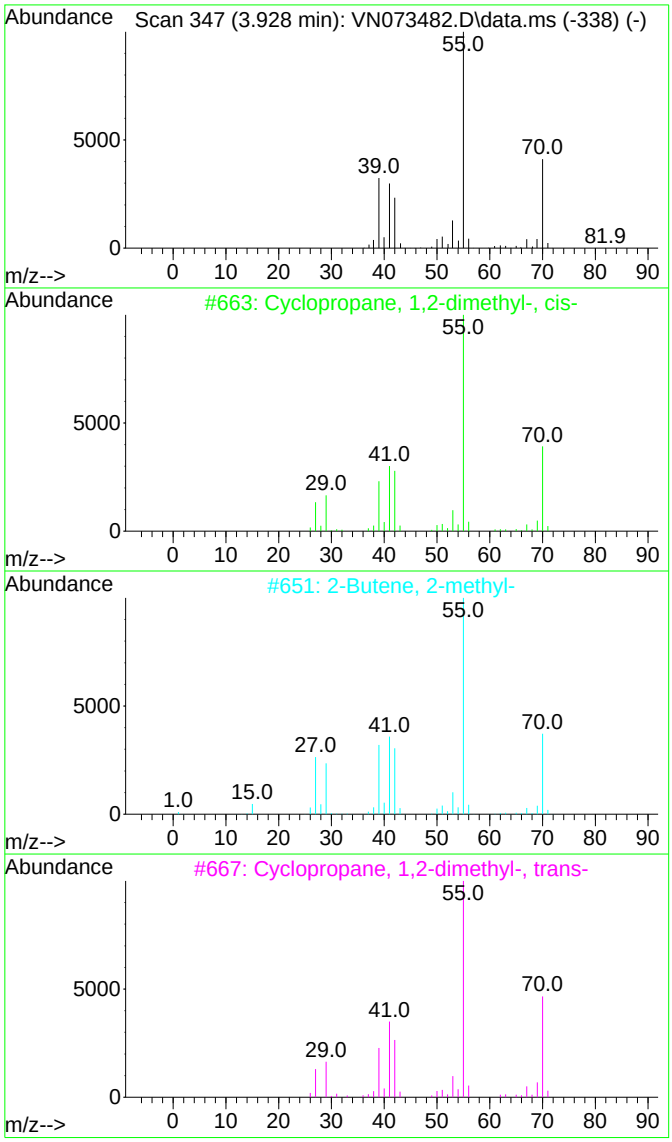
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

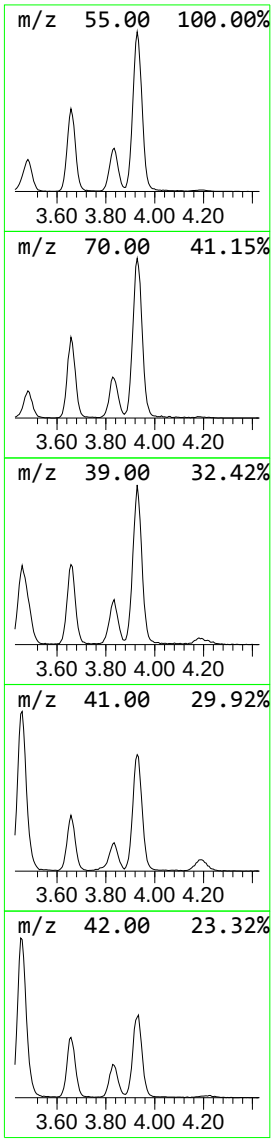
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopropane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	28.06 ug/l	2239530	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

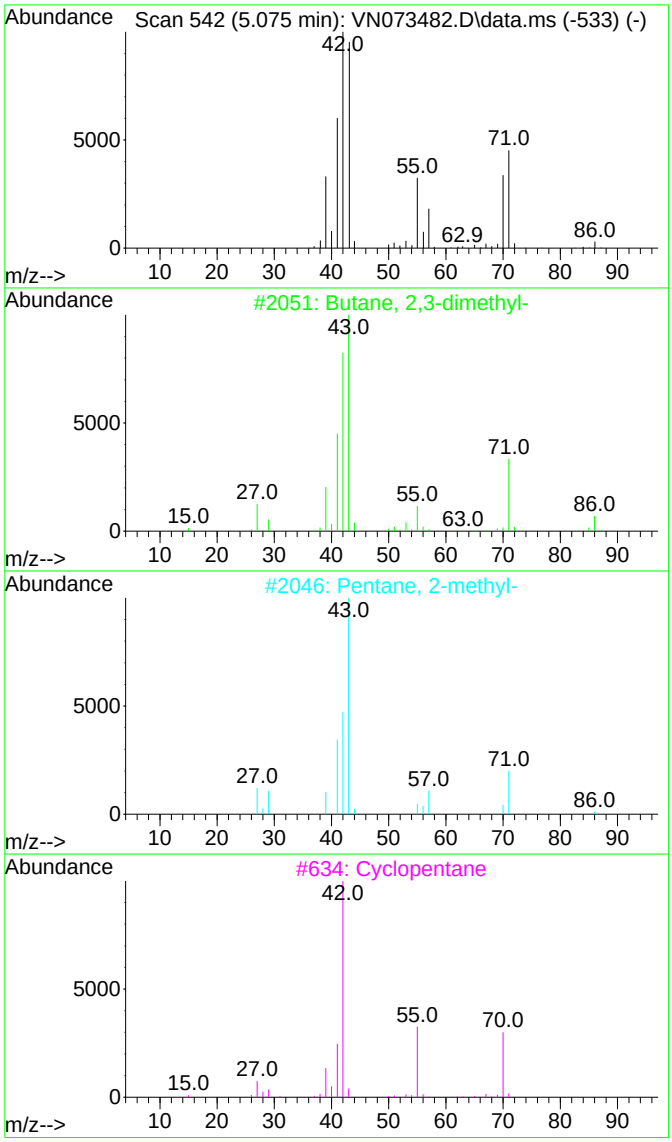
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

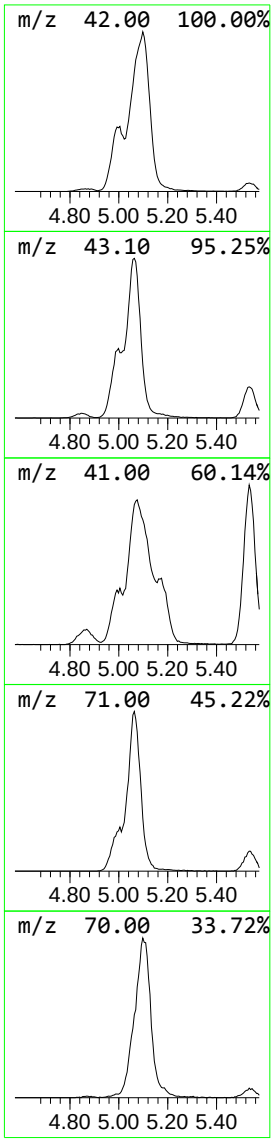
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	66.03 ug/l	5270660	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3	Cyclopentane	70	C5H10	000287-92-3	47
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	43
5	1-Pentene	70	C5H10	000109-67-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

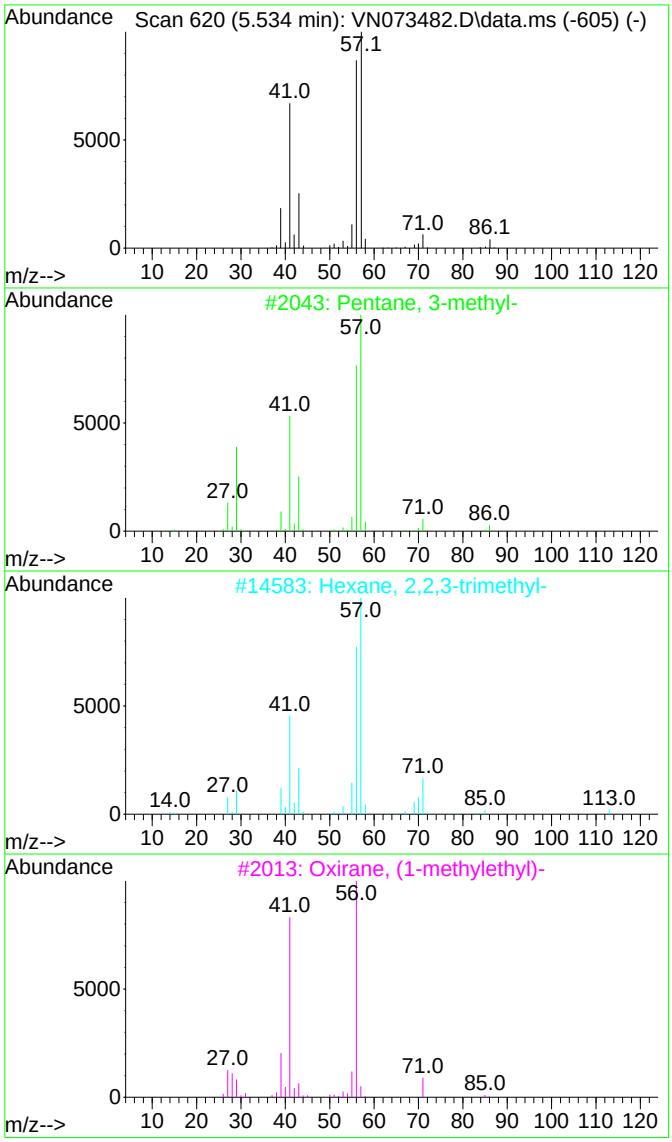
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

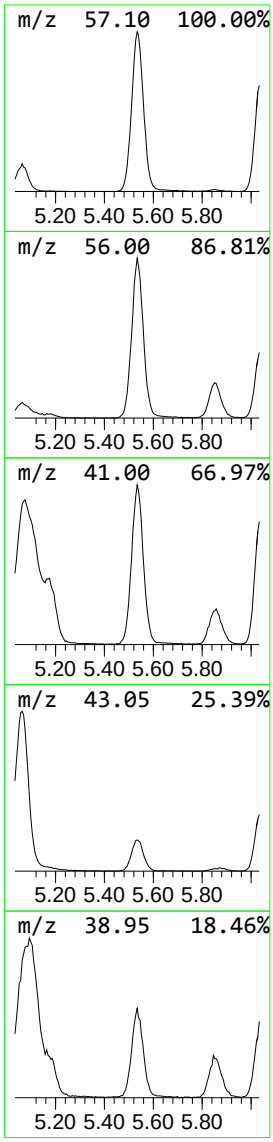
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.534	28.36 ug/l	2263680	Pentafluorobenzene	8.016

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	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

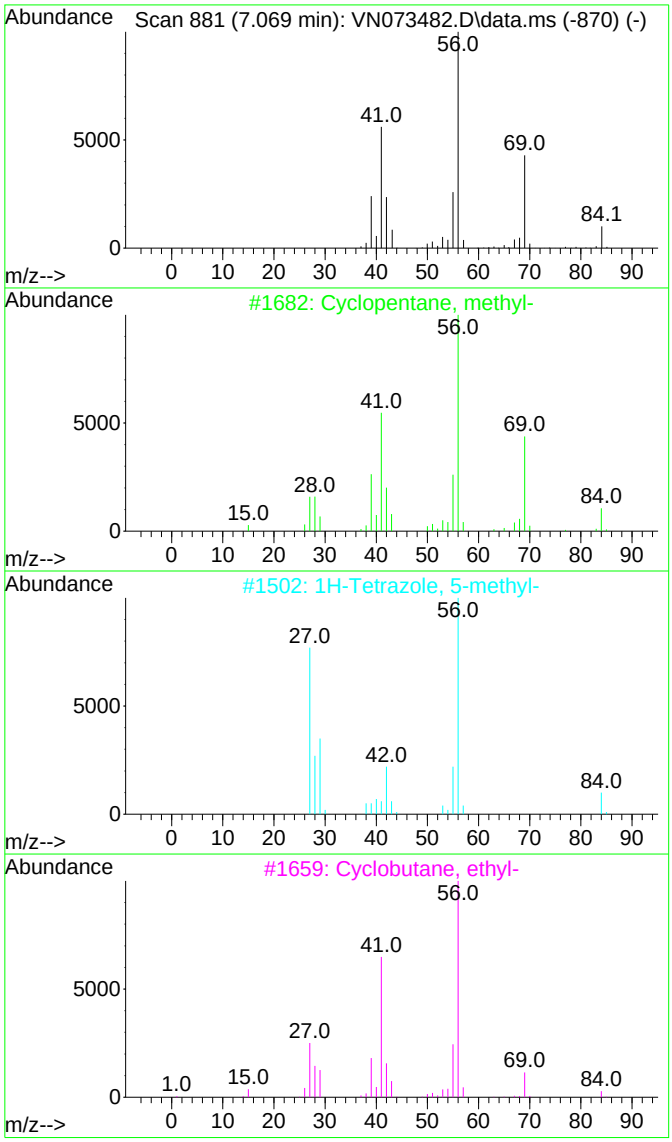
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

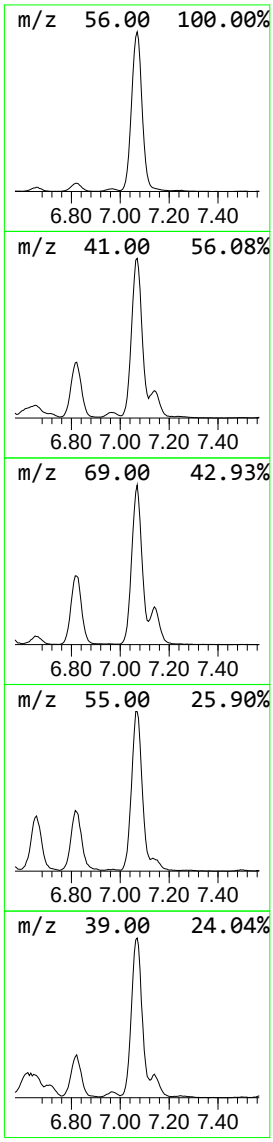
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	87.15 ug/l	6956460	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
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Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

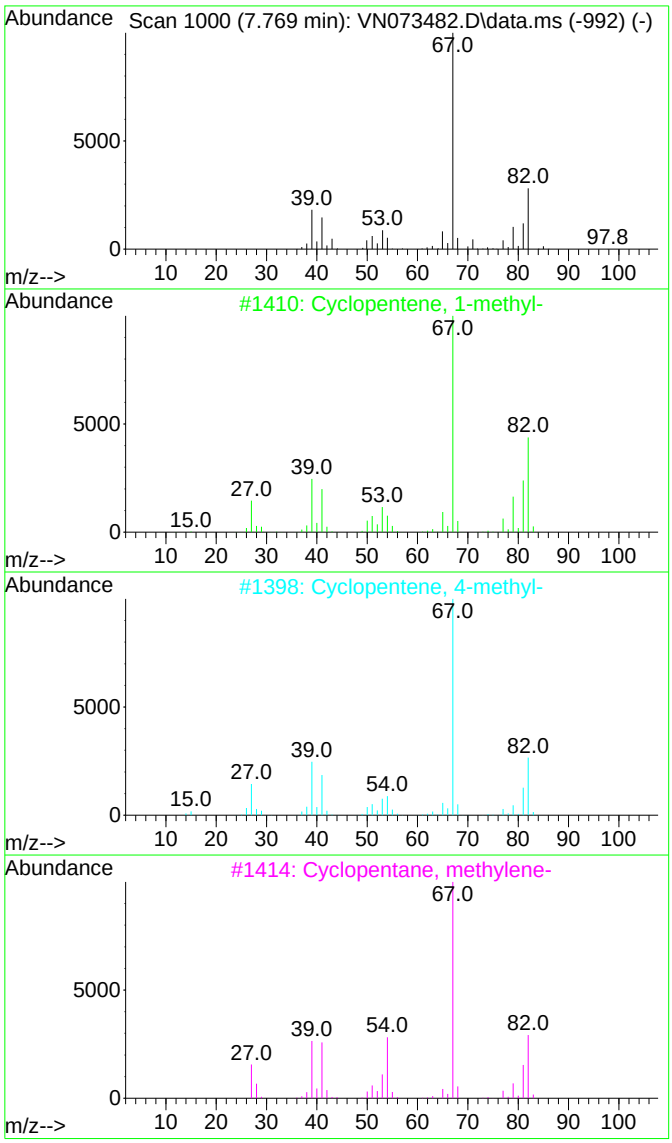
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

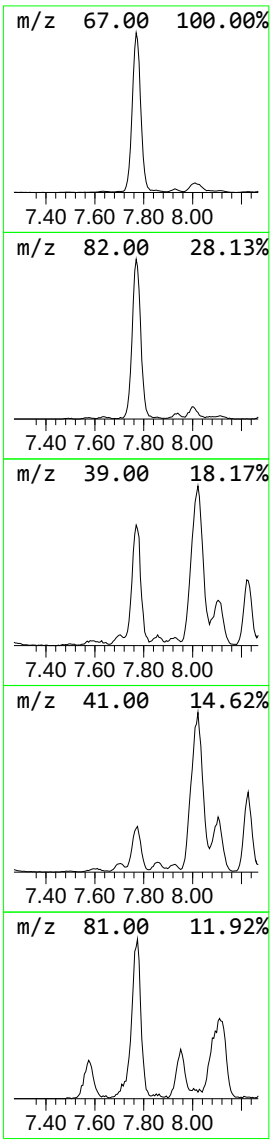
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.769	23.89 ug/l	1906960	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	87
2	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	83
3	Cyclopentane, methylene-	82	C6H10	001528-30-9	80
4	1,4-Hexadiene	82	C6H10	000592-45-0	80
5	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	80





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Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

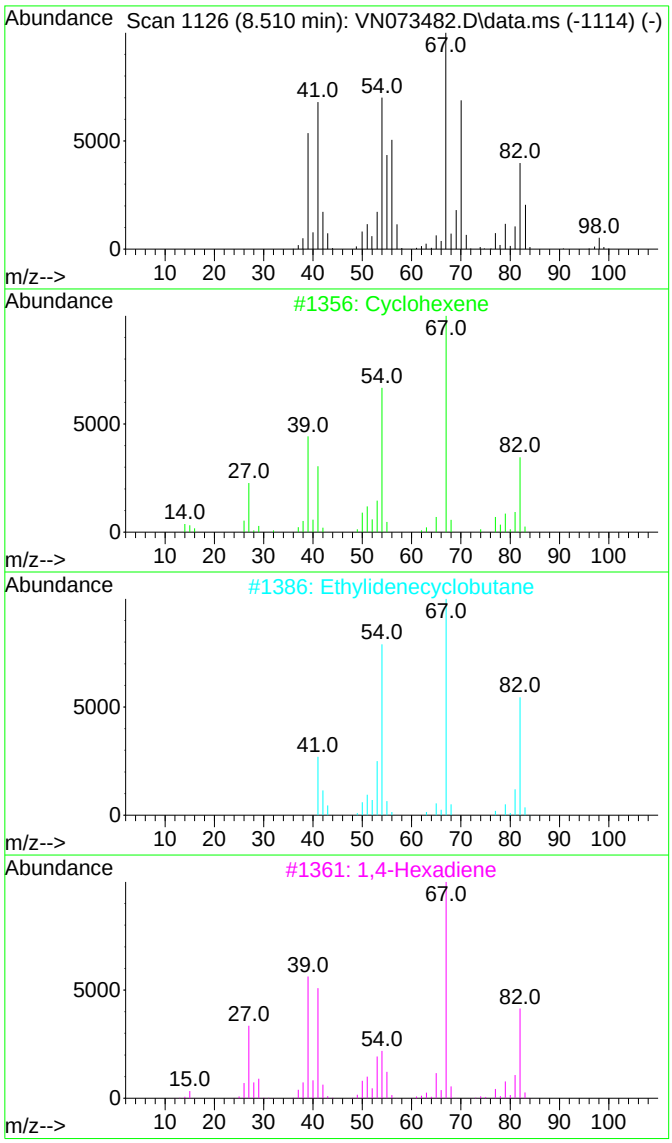
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

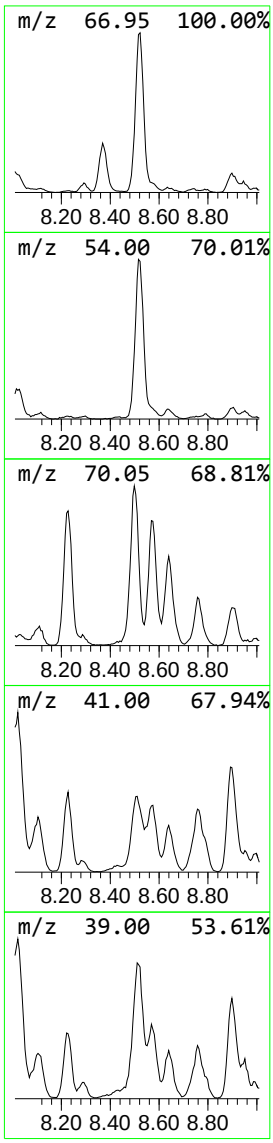
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethylidenecyclobutane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	39.52 ug/l	2470730	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	92
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	60
3	1,4-Hexadiene	82	C6H10	000592-45-0	55
4	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	55
5	1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
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Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

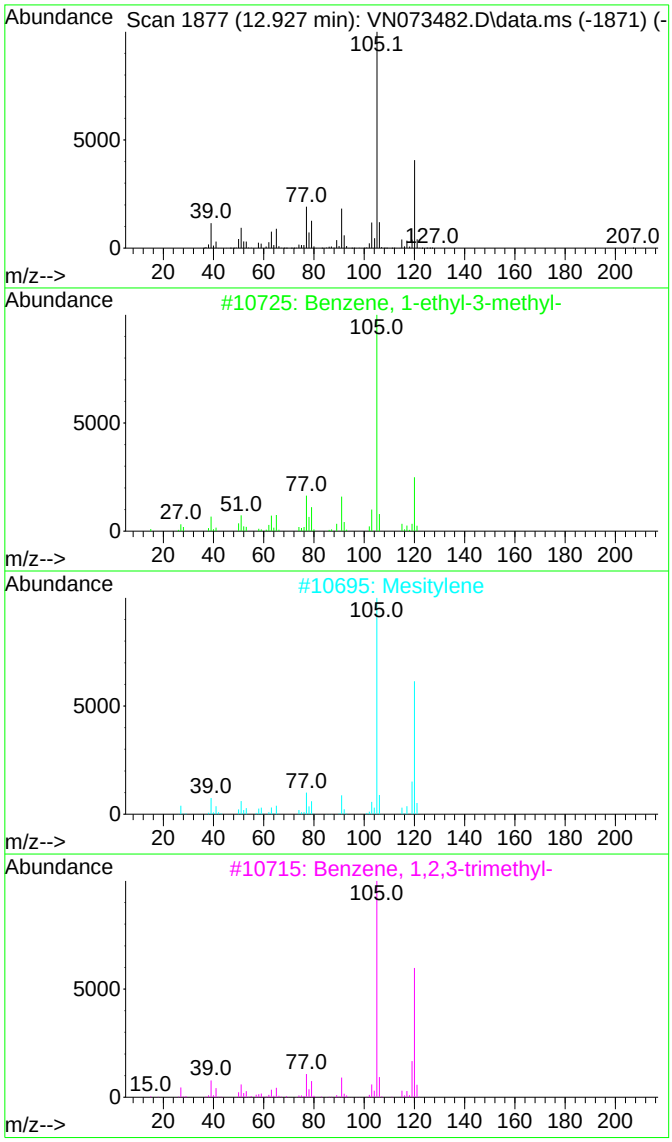
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

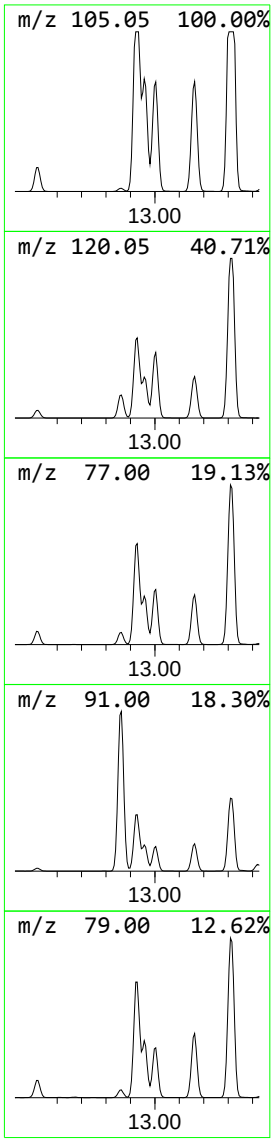
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	78.12 ug/l	53830600	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

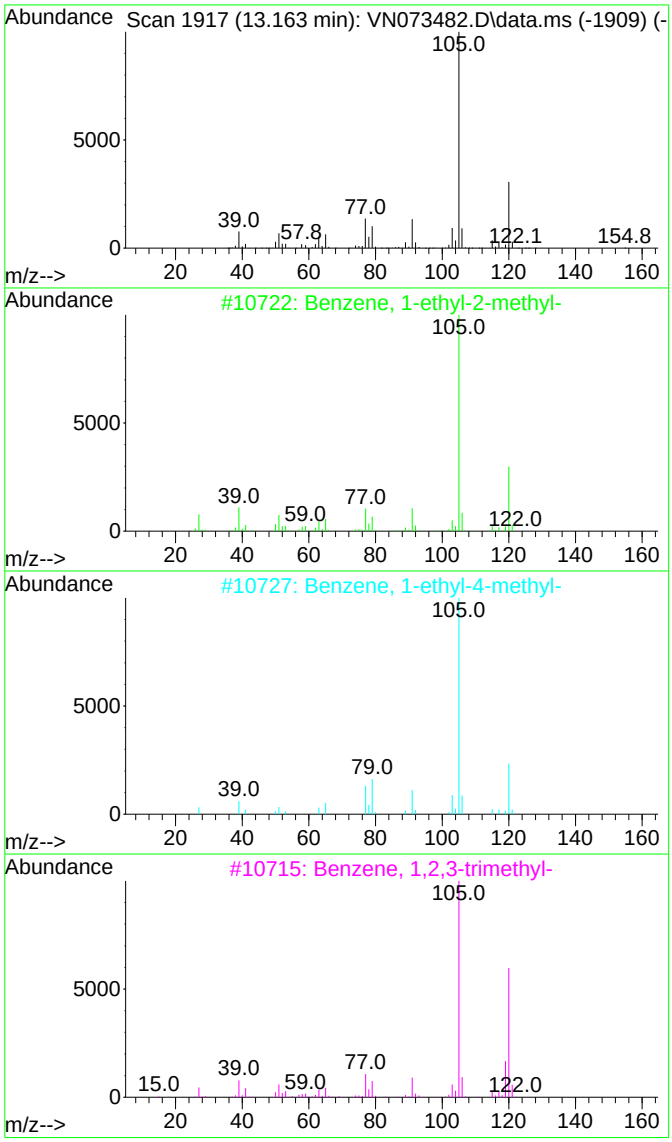
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

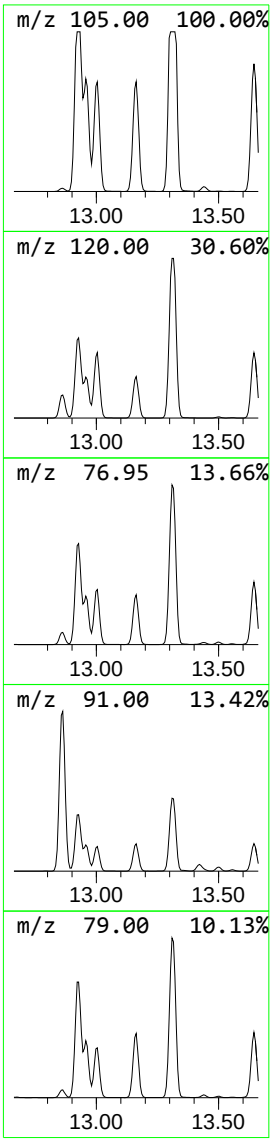
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	36.79 ug/l	25353600	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

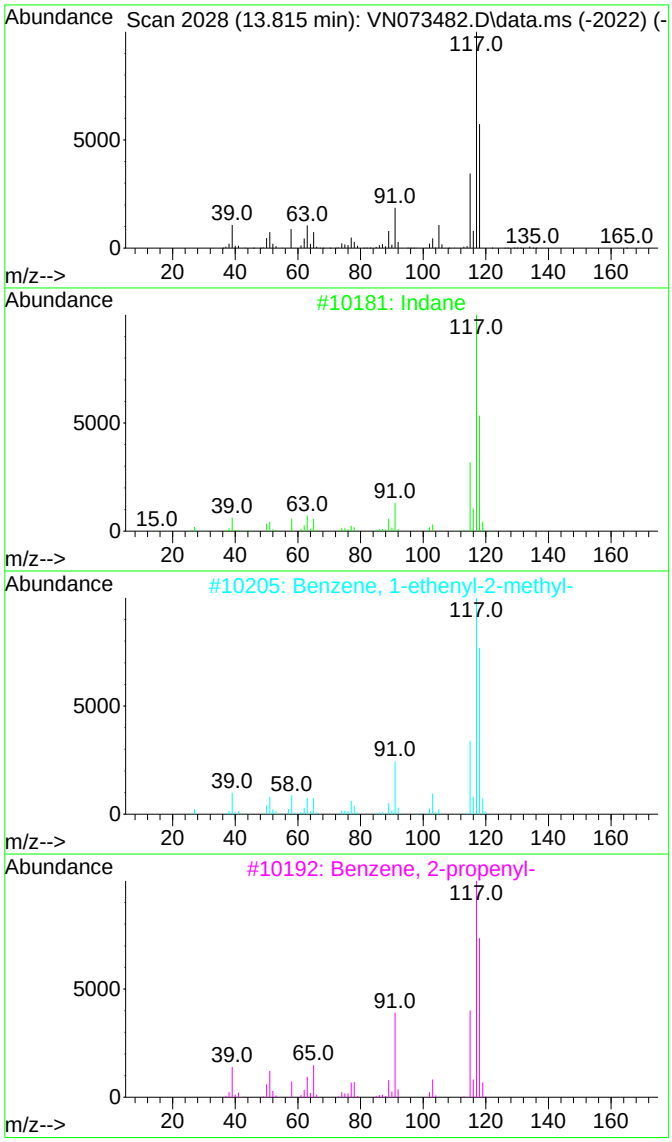
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

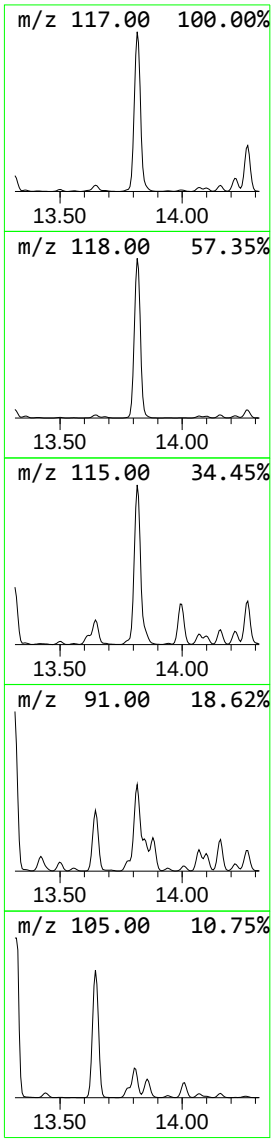
****

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	43.94 ug/l	30279200	1,4-Dichlorobenzene-d4	13.616

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	70
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4	1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071522\
Data File : VN073482.D
Acq On : 15 Jul 2022 13:42
Operator : JC\MD
Sample : N3726-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-ANOM

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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-	3.087	31.5	ug/l	2515400	1	8.016	3990890	50.0
Cyclopropane, 1...	3.928	28.1	ug/l	2239530	1	8.016	3990890	50.0
Butane, 2,3-dim...	5.075	66.0	ug/l	5270660	1	8.016	3990890	50.0
Pentane, 3-methyl-	5.534	28.4	ug/l	2263680	1	8.016	3990890	50.0
Cyclopentane, m...	7.069	87.2	ug/l	6956460	1	8.016	3990890	50.0
Cyclopentene, 1...	7.769	23.9	ug/l	1906960	1	8.016	3990890	50.0
Ethylidenecyclo...	8.510	39.5	ug/l	2470730	2	8.904	3125560	50.0
Benzene, 1-ethy...	12.927	78.1	ug/l	53830600	4	13.616	34454000	50.0
Benzene, 1-ethy...	13.163	36.8	ug/l	25353600	4	13.616	34454000	50.0
Indane	13.816	43.9	ug/l	30279200	4	13.616	34454000	50.0