LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060922\
Data File : VN072754.D
Acq On : 10 Jun 2022 01:37
Operator : JC\MD
Sample : N3202-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

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\82N060822W.M
Title : SW846 8260

Signal : TIC: VN072754.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	185	193	206	rVB	93840	216699	5.19%	1.154%
2	5.081	514	526	530	rBV4	21639	74265	1.78%	0.395%
3	5.175	531	542	554	rVB3	37073	181743	4.36%	0.968%
4	5.363	564	574	585	rBV2	15342	53190	1.27%	0.283%
5	5.610	602	616	635	rBV2	114103	406758	9.75%	2.166%
6	6.463	750	761	774	rVB5	15534	48970	1.17%	0.261%
7	6.604	774	785	793	rBV7	13887	45343	1.09%	0.241%
8	6.692	793	800	809	rVV4	13806	42833	1.03%	0.228%
9	7.140	866	876	886	rBV2	85955	245317	5.88%	1.306%
10	8.016	1015	1025	1031	rBV	258374	632722	15.16%	3.369%
11	8.081	1031	1036	1045	rVV2	292595	695036	16.66%	3.701%
12	8.175	1046	1052	1062	rVB4	26865	70749	1.70%	0.377%
13	8.445	1087	1098	1109	rBV3	488526	1485339	35.60%	7.909%
14	8.587	1116	1122	1137	rVB5	48175	193445	4.64%	1.030%
15	8.963	1177	1186	1199	rBV	416148	872753	20.92%	4.647%
16	9.457	1257	1270	1276	rBV6	24567	77688	1.86%	0.414%
17	9.881	1337	1342	1351	rVB	24079	47787	1.15%	0.254%
18	9.969	1351	1357	1360	rBV	26180	49212	1.18%	0.262%
19	10.016	1360	1365	1373	rVB2	45441	94974	2.28%	0.506%
20	10.198	1389	1396	1398	rBV3	34411	63067	1.51%	0.336%
21	10.233	1399	1402	1411	rVB3	36418	60060	1.44%	0.320%
22	10.328	1411	1418	1423	rBV5	22591	47017	1.13%	0.250%
23	10.439	1429	1437	1443	rBV	959764	1781924	42.70%	9.489%
24	10.504	1443	1448	1452	rVV	92696	180992	4.34%	0.964%
25	10.545	1452	1455	1462	rVB3	38854	70443	1.69%	0.375%
26	11.610	1626	1636	1648	rVB5	18479	59049	1.42%	0.314%
27	11.739	1648	1658	1668	rBV	598693	1105639	26.50%	5.887%
28	11.839	1668	1675	1686	rVV	2467812	4172698	100.00%	22.219%
29	11.951	1686	1694	1706	rVB	265591	512620	12.29%	2.730%
30	12.274	1739	1749	1758	rBV	172097	304852	7.31%	1.623%
31	12.574	1794	1800	1806	rVB	128461	212476	5.09%	1.131%
32	12.727	1818	1826	1838	rBV	718508	1217134	29.17%	6.481%
33	12.916	1850	1858	1865	rBV	207042	340975	8.17%	1.816%
34	13.010	1870	1874	1878	rVV	42095	74451	1.78%	0.396%
35	13.051	1878	1881	1888	rVB2	27565	44517	1.07%	0.237%
36	13.216	1902	1909	1917	rBV	139484	228270	5.47%	1.216%

LSC Area Percent Report

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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

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\82N060822W.M
Title : SW846 8260

37	13.363	1924	1934	1940	rVB	67666	116667	2.80%	0.621%
38	13.669	1979	1986	2001	rBV2	516091	1074951	25.76%	5.724%
39	13.833	2008	2014	2016	rBV2	56586	80911	1.94%	0.431%
40	13.874	2016	2021	2026	rVB	283252	469525	11.25%	2.500%
41	14.057	2046	2052	2059	rVB	37769	65034	1.56%	0.346%
42	14.210	2073	2078	2084	rBV	79803	132398	3.17%	0.705%
43	14.321	2092	2097	2106	rVB2	51709	90996	2.18%	0.485%
44	14.533	2124	2133	2140	rBV	39061	70282	1.68%	0.374%
45	14.804	2174	2179	2184	rBV2	27458	46133	1.11%	0.246%
46	14.927	2191	2200	2206	rBV2	52270	92597	2.22%	0.493%
47	15.080	2220	2226	2233	rVB3	23696	43689	1.05%	0.233%
48	15.504	2290	2298	2309	rVB	245696	485618	11.64%	2.586%

Sum of corrected areas: 18779808

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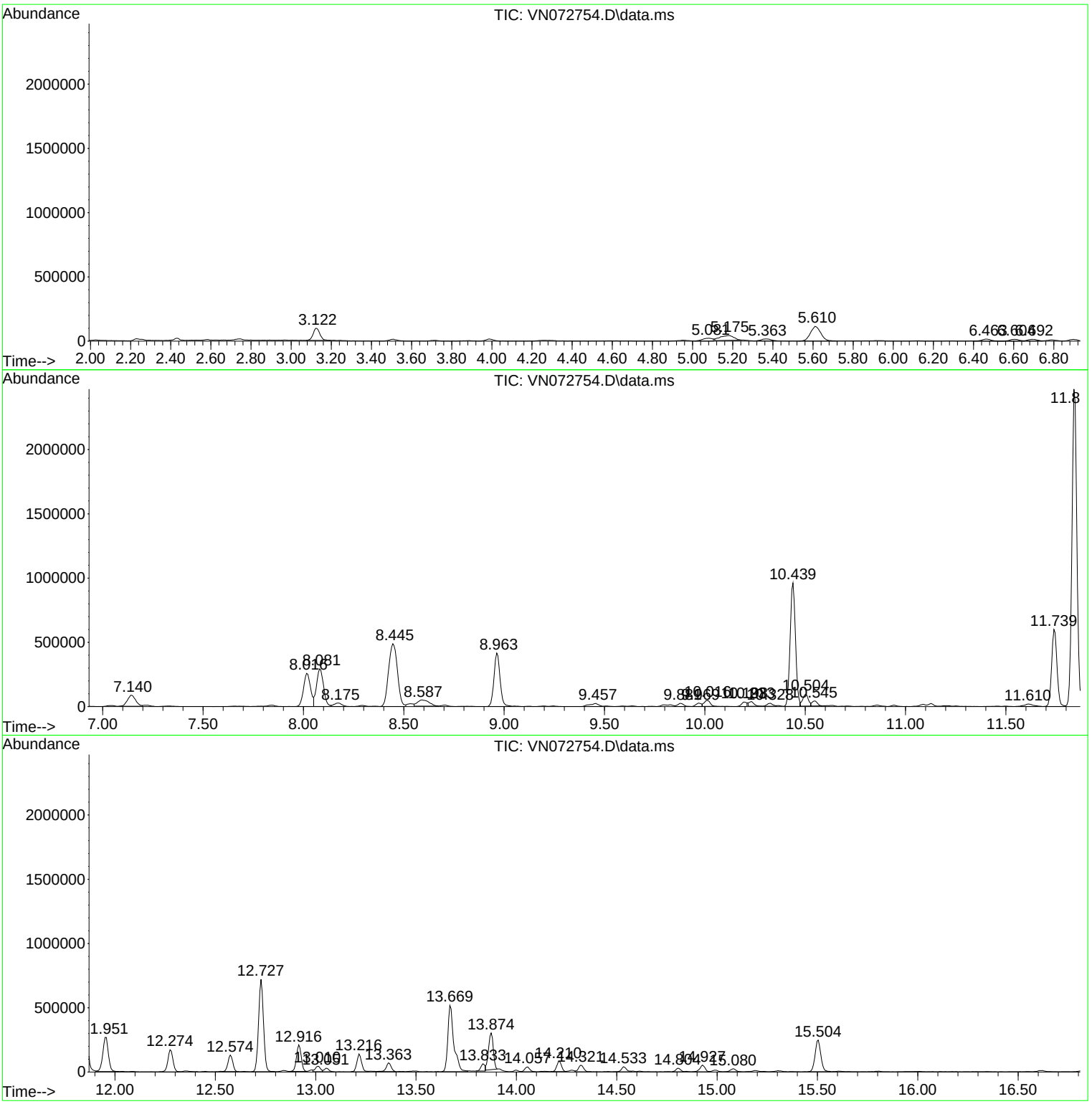
MSVOA_N
ClientSampleId :
MW-16

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

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



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Data File : VN072754.D
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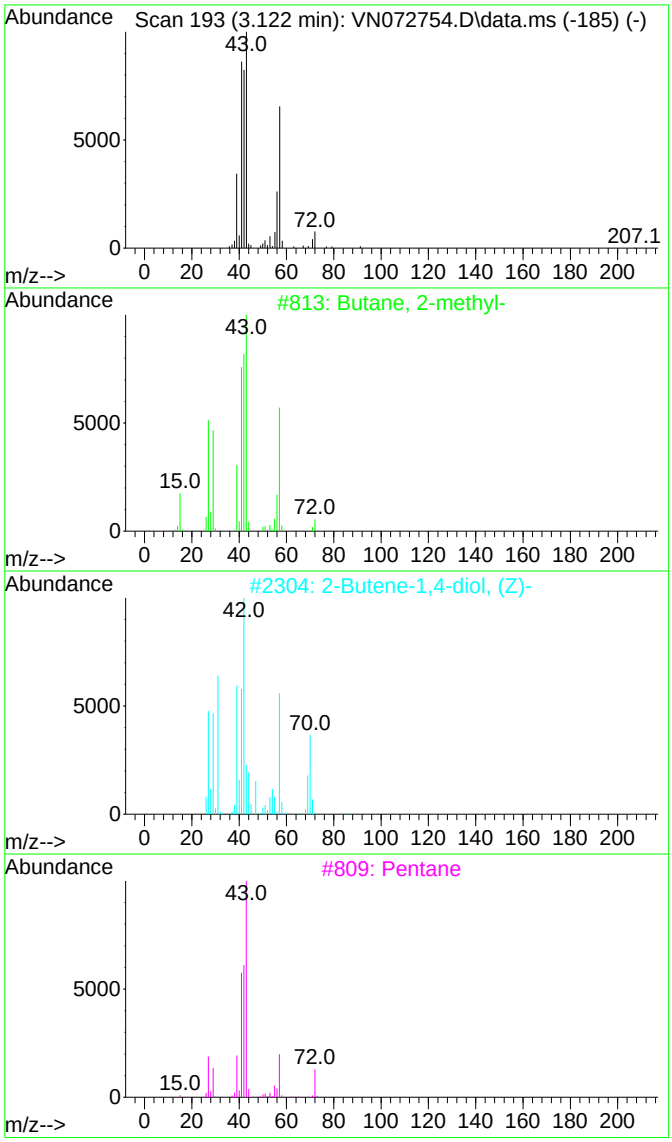
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

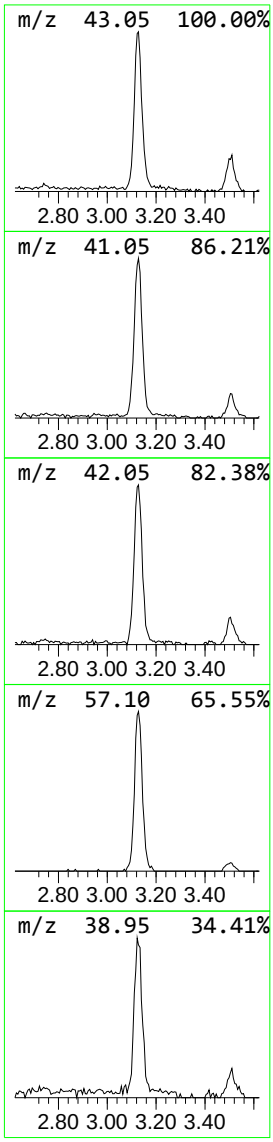
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	15.59 ug/l	216699	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	37
3	Pentane	72	C5H12	000109-66-0	36
4	3-Buten-1-ol	72	C4H8O	000627-27-0	28
5	1-Butene	56	C4H8	000106-98-9	18





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Data File : VN072754.D
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Operator : JC\MD
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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

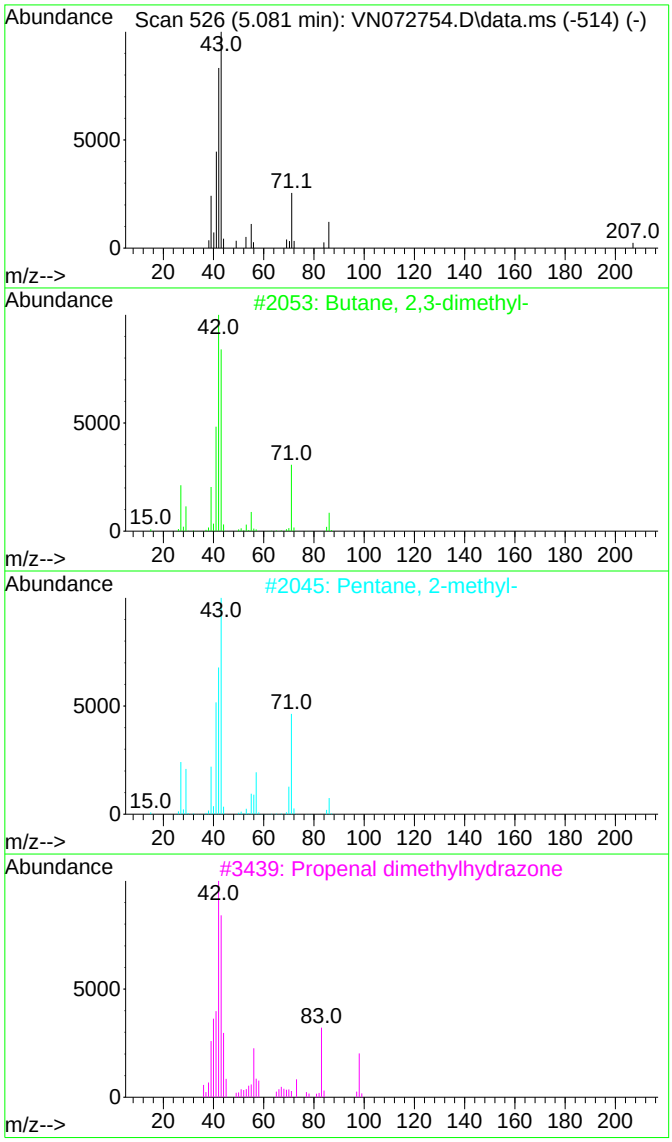
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

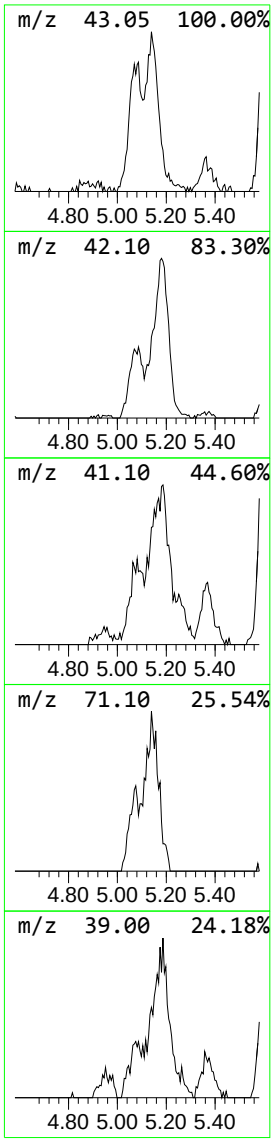
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	5.34 ug/l	74265	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	45
3	Propenal dimethylhydrazone	98	C5H10N2	025368-52-9	36
4	Tetrahydrofuran	72	C4H8O	000109-99-9	33
5	1-Pentene	70	C5H10	000109-67-1	25





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Operator : JC\MD
Sample : N3202-04
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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

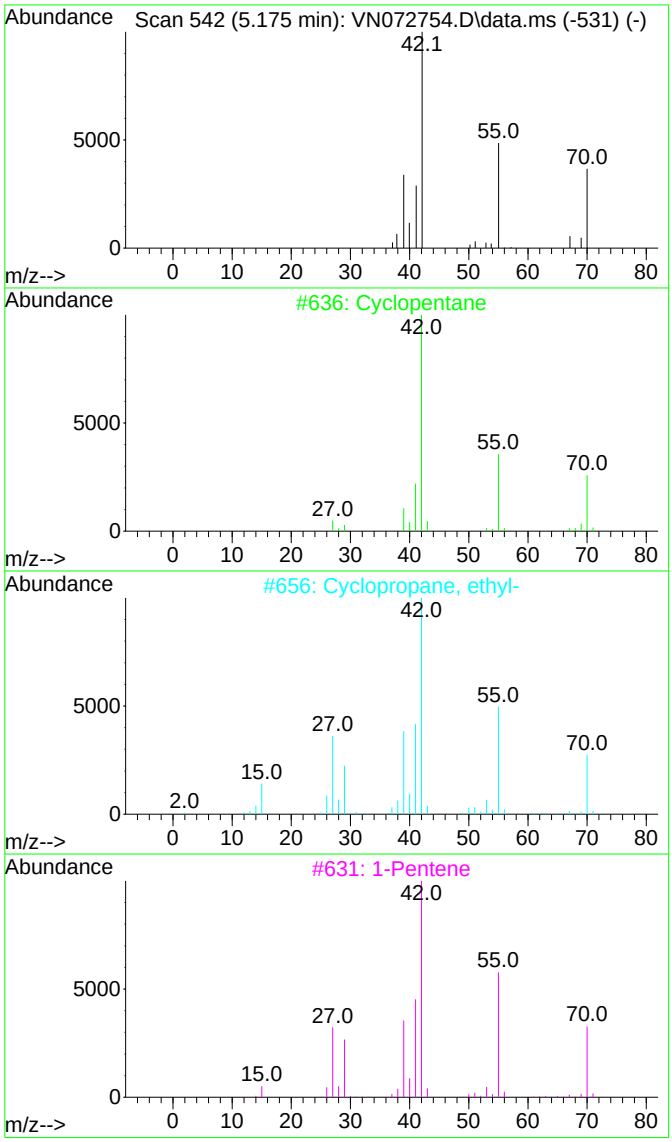
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

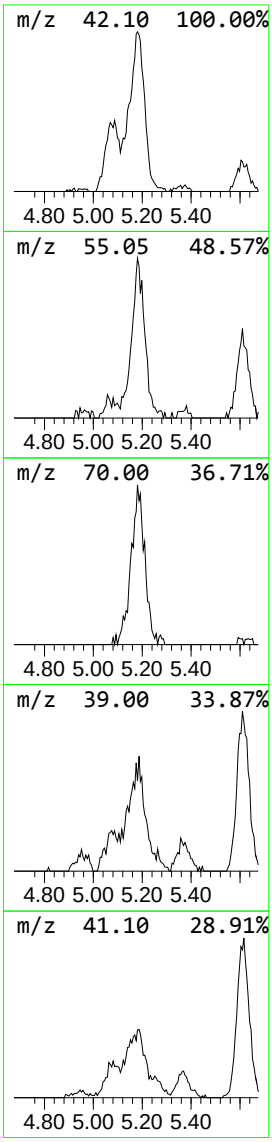
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	13.07 ug/l	181743	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	72
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
3	1-Pentene	70	C5H10	000109-67-1	72
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	56
5	Cyclobutanone	70	C4H6O	001191-95-3	9





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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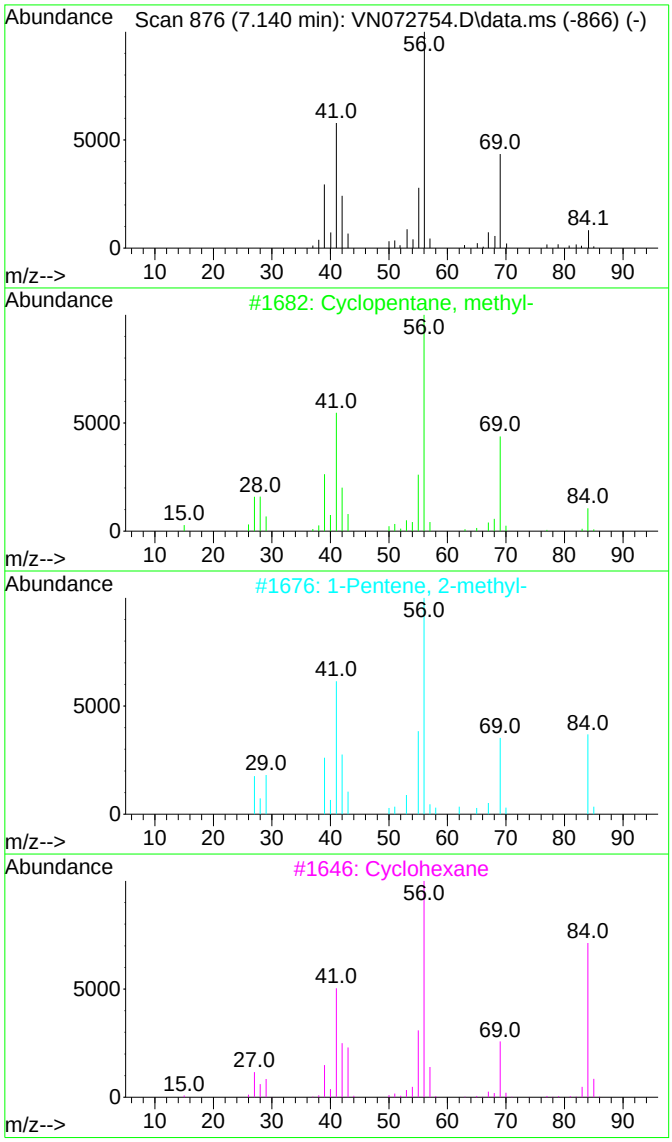
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

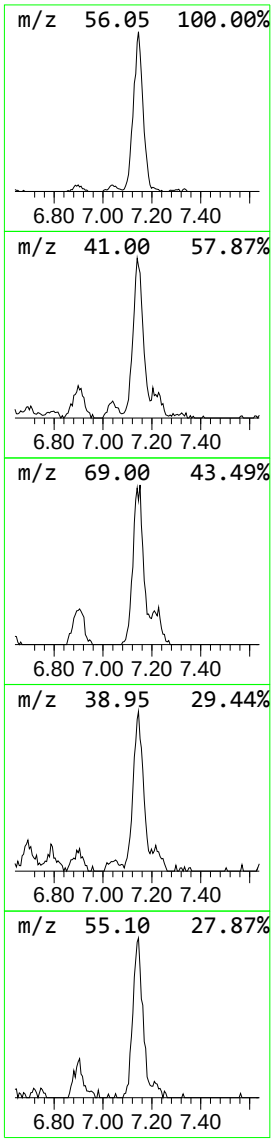
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.140	17.65 ug/l	245317	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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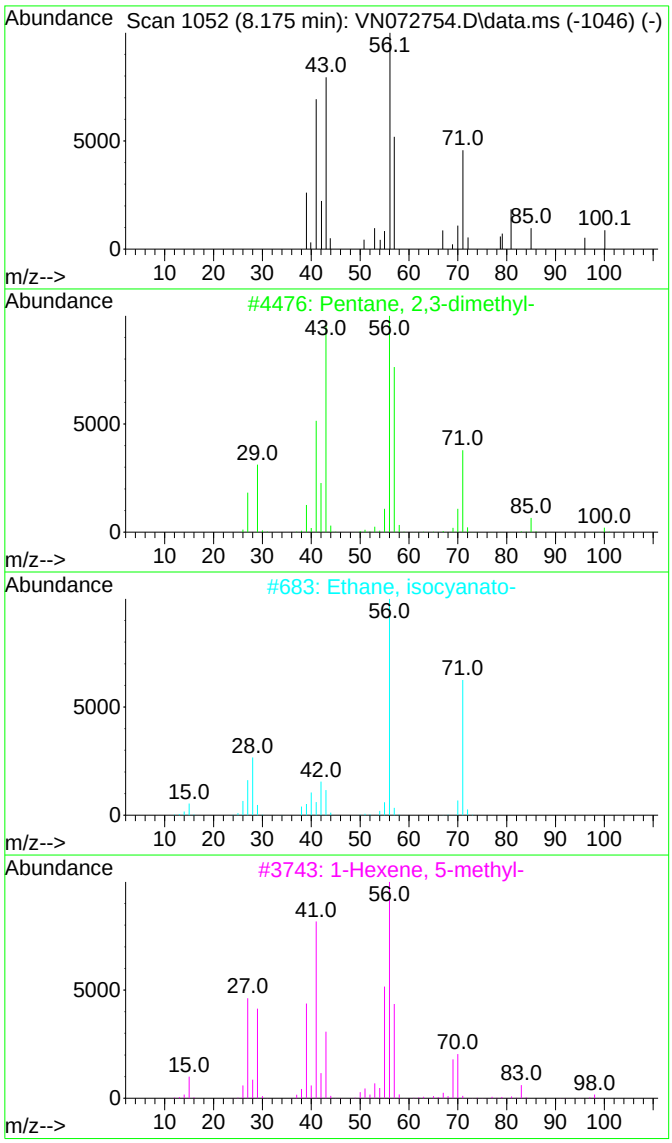
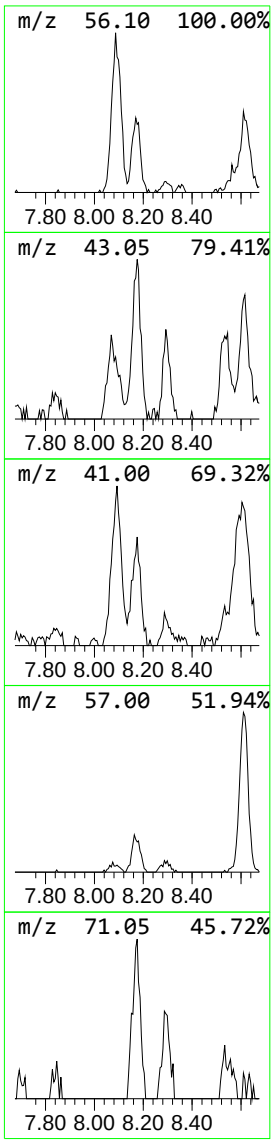
****
Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	5.09 ug/l	70749	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	56
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	42
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	38
4	Pentane, 1-bromo-3,4-dimethyl-	178	C7H15Br	006570-92-9	38
5	Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	002144-41-4	35





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ClientSampleId :
MW-16

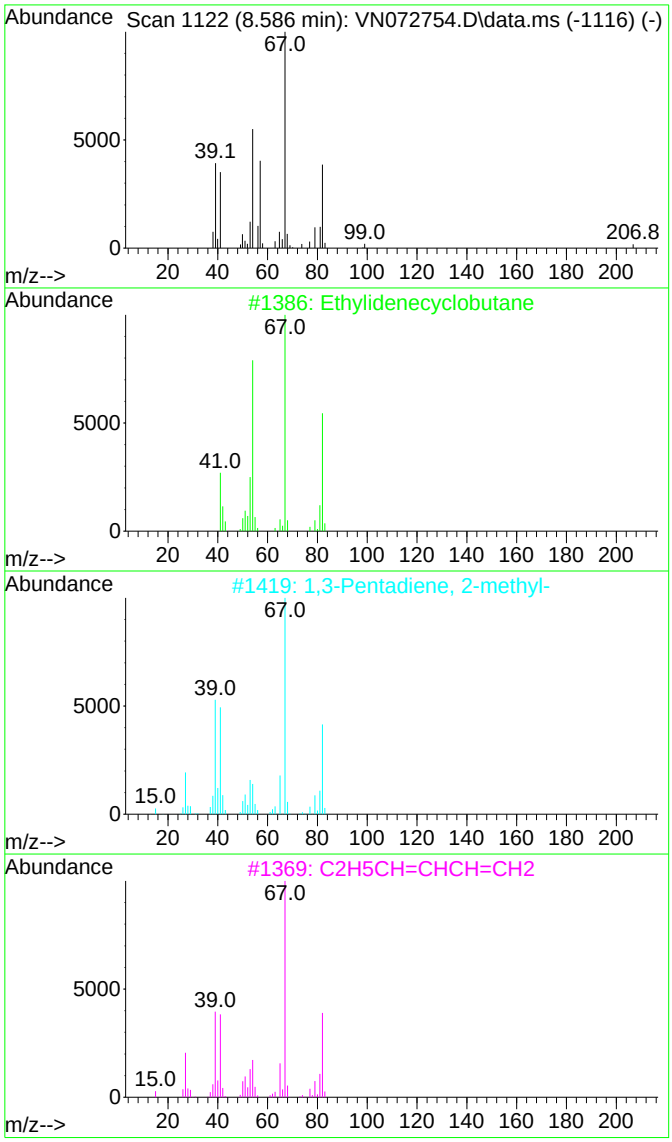
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

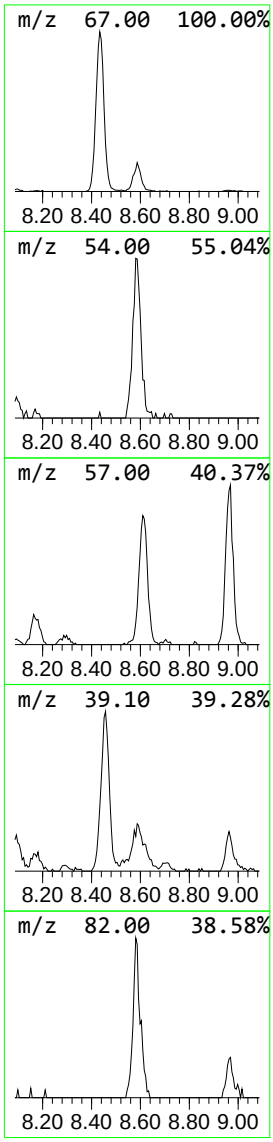
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethylidenecyclobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.586	11.08 ug/l	193445	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylidenecyclobutane	82	C6H10	001528-21-8	80
2	1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	64
3	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	64
4	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	58
5	Cyclohexene	82	C6H10	000110-83-8	58





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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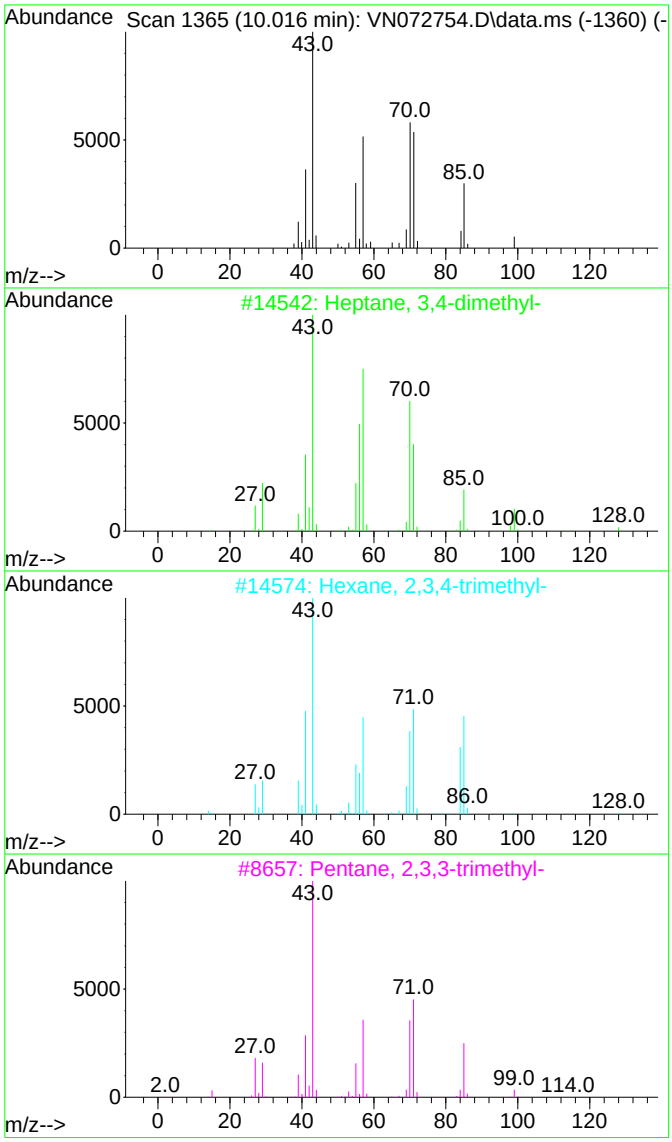
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

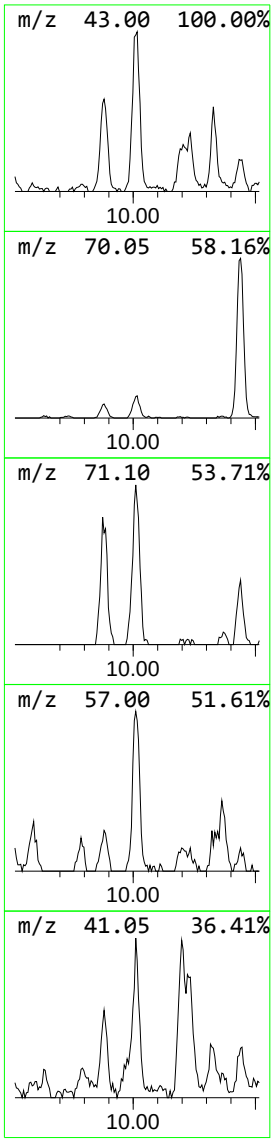
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptane, 3,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	5.44 ug/l	94974	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	72
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

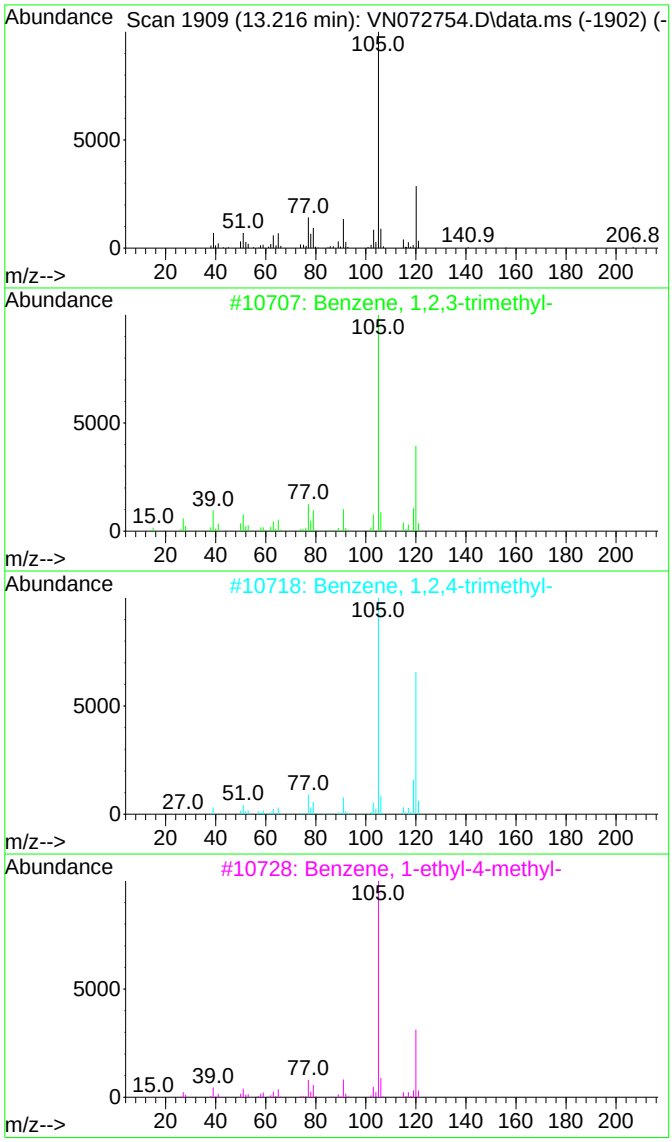
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

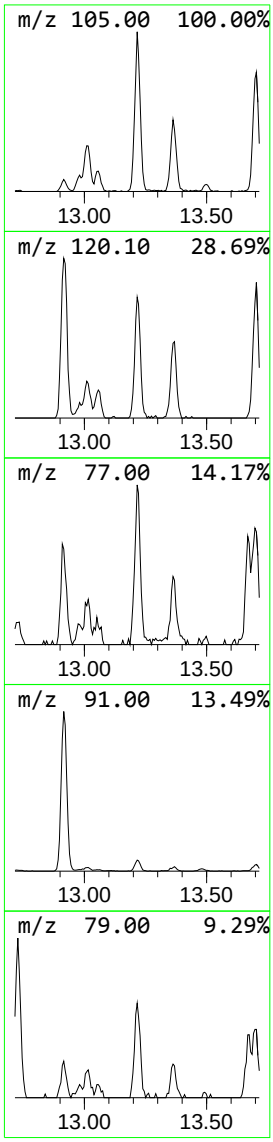
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	10.62 ug/l	228270	1,4-Dichlorobenzene-d4	13.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Data File : VN072754.D
Acq On : 10 Jun 2022 01:37
Operator : JC\MD
Sample : N3202-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

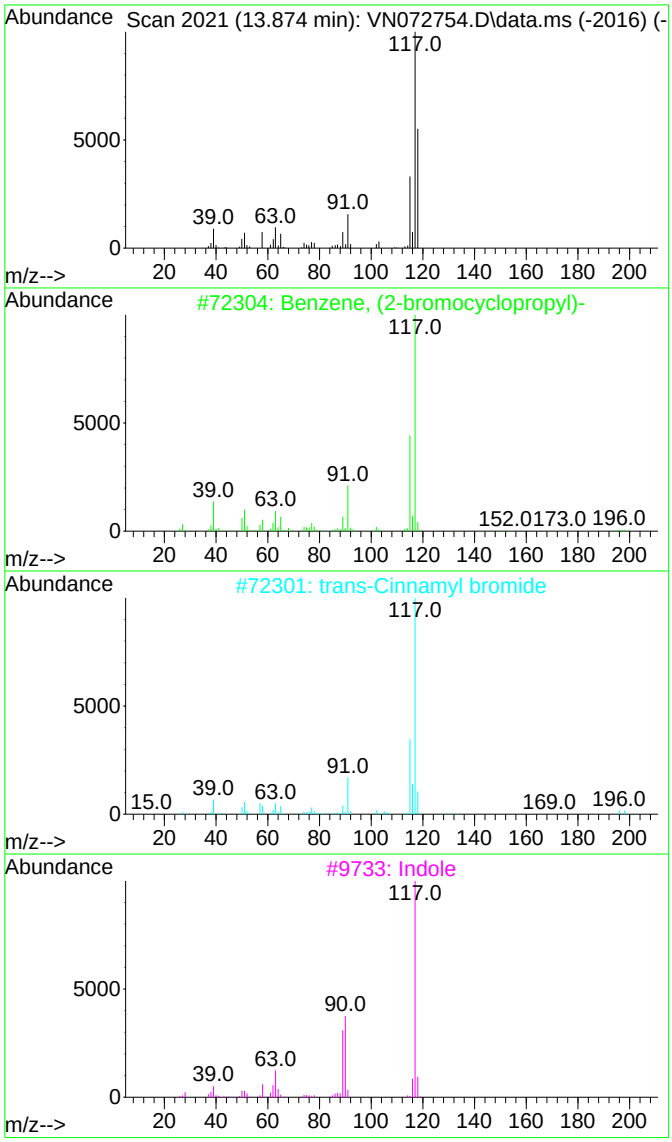
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

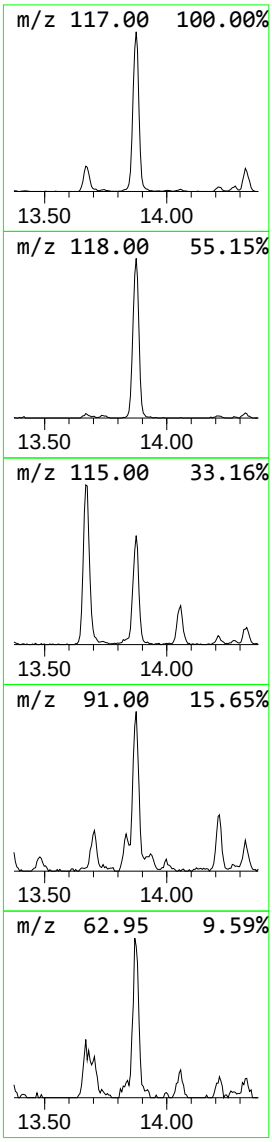
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (2-bromocyclopropyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	21.84 ug/l	469525	1,4-Dichlorobenzene-d4	13.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	64
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
3	Indole	117	C8H7N	000120-72-9	49
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	40
5	5H-1-Pyrindine	117	C8H7N	000270-91-7	38





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Data File : VN072754.D
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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

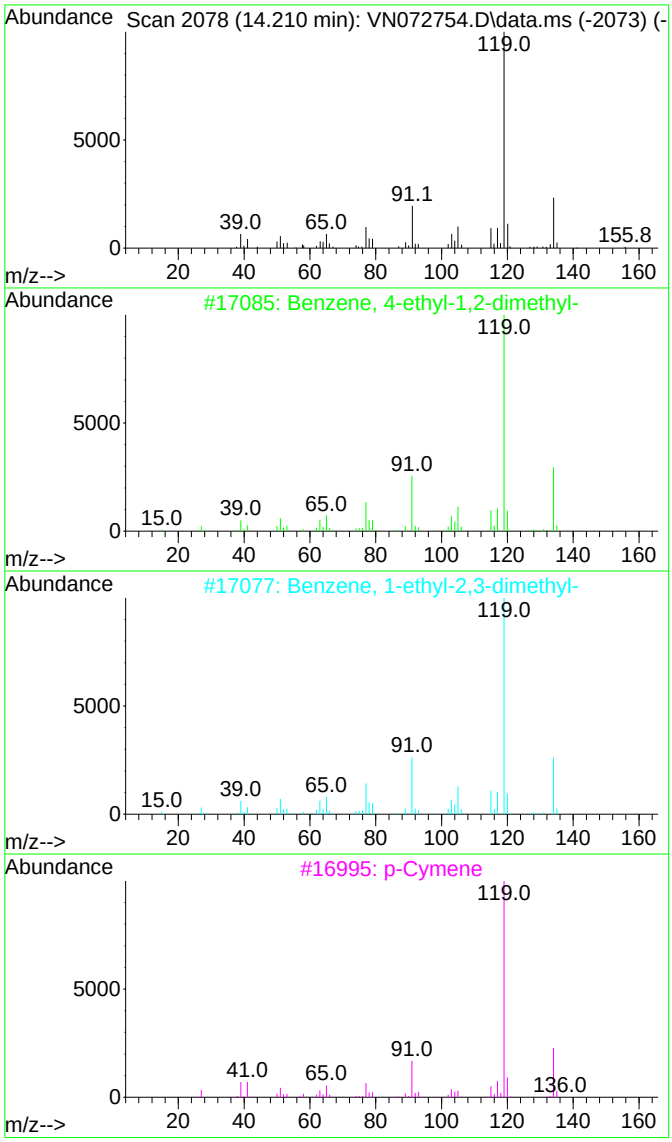
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

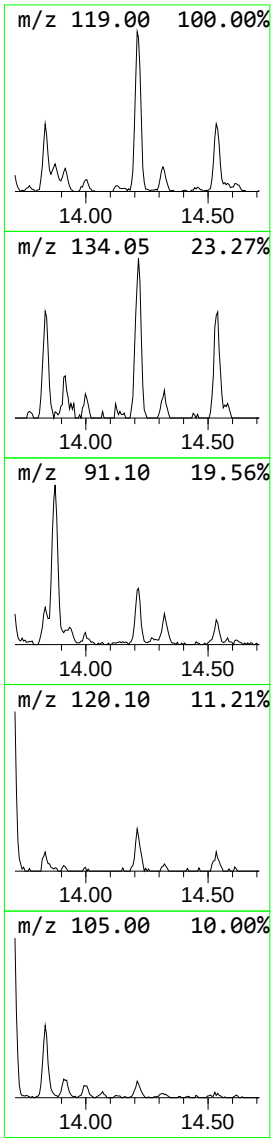
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	6.16 ug/l	132398	1,4-Dichlorobenzene-d4	13.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	p-Cymene	134	C10H14	000099-87-6	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060922\
Data File : VN072754.D
Acq On : 10 Jun 2022 01:37
Operator : JC\MD
Sample : N3202-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

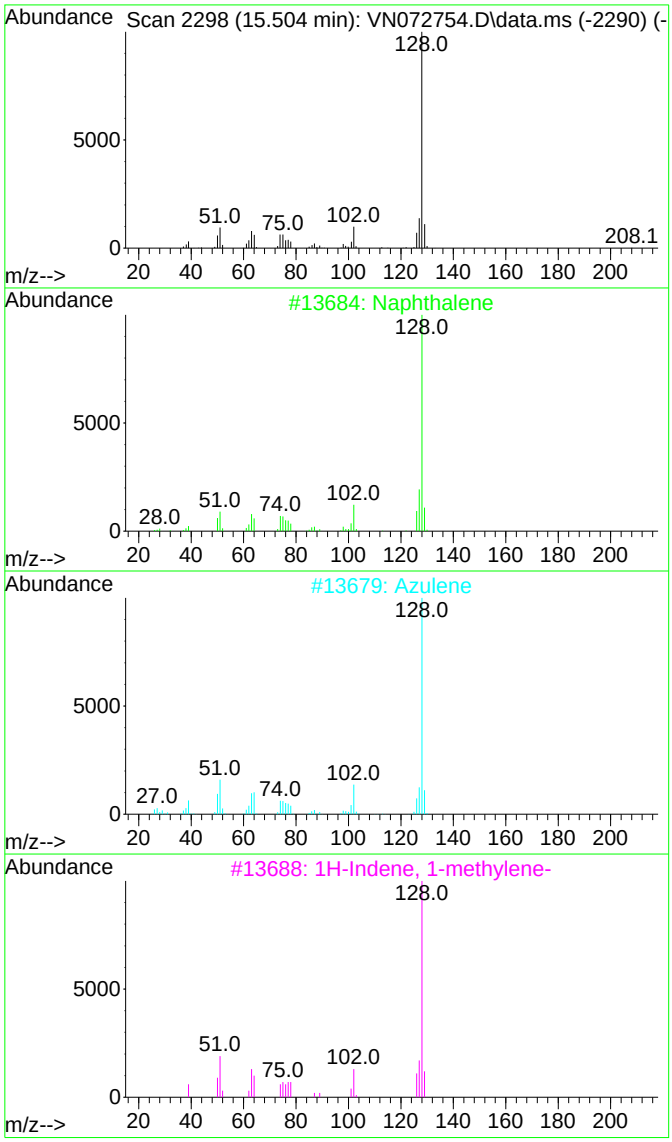
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

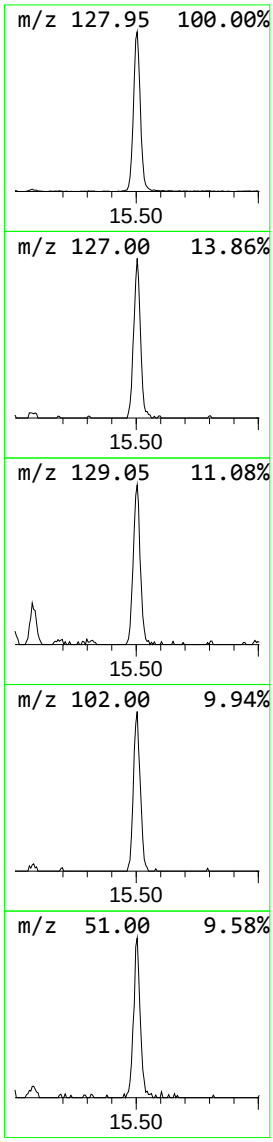
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1H-Indene, 1-methylene- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	22.59 ug/l	485618	1,4-Dichlorobenzene-d4	13.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
3	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	90
4	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
5	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	72





Tentatively Identified Compound (LSC) summary

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Data File : VN072754.D
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ClientSampleId :
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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
Butane, 2-methyl-	3.122	15.6	ug/l	216699	1	8.081	695036	50.0
Butane, 2,3-dim...	5.081	5.3	ug/l	74265	1	8.081	695036	50.0
Cyclopentane	5.175	13.1	ug/l	181743	1	8.081	695036	50.0
Cyclopentane, m...	7.140	17.6	ug/l	245317	1	8.081	695036	50.0
Pentane, 2,3-di...	8.175	5.1	ug/l	70749	1	8.081	695036	50.0
Ethylidenecyclo...	8.586	11.1	ug/l	193445	2	8.963	872753	50.0
Heptane, 3,4-di...	10.016	5.4	ug/l	94974	2	8.963	872753	50.0
Benzene, 1,2,3-...	13.216	10.6	ug/l	228270	4	13.674	1074950	50.0
Benzene, (2-bro...	13.874	21.8	ug/l	469525	4	13.674	1074950	50.0
Benzene, 4-ethy...	14.210	6.2	ug/l	132398	4	13.674	1074950	50.0
1H-Indene, 1-me...	15.504	22.6	ug/l	485618	4	13.674	1074950	50.0