LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

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\82N052422W.M
Title : SW846 8260

Signal : TIC: VN072611.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.434	65	76	86	rBV	251069	422823	3.74%	0.465%
2	3.116	181	192	213	rVB	285076	675361	5.97%	0.743%
3	3.504	249	258	277	rVB4	115356	393731	3.48%	0.433%
4	3.710	281	293	308	rBV	138720	344710	3.05%	0.379%
5	3.887	313	323	331	rVV	81965	210653	1.86%	0.232%
6	3.987	331	340	356	rVB2	177711	494439	4.37%	0.544%
7	4.957	489	505	516	rBV2	96039	332609	2.94%	0.366%
8	5.187	530	544	563	rVV3	164865	807355	7.13%	0.889%
9	5.357	563	573	593	rVB	130485	452177	3.99%	0.498%
10	5.610	604	616	631	rBV	107535	374735	3.31%	0.412%
11	6.398	739	750	755	rVV2	34842	121187	1.07%	0.133%
12	6.463	755	761	775	rVV5	85963	289596	2.56%	0.319%
13	6.604	775	785	792	rVV3	53622	170152	1.50%	0.187%
14	6.698	792	801	813	rVV3	56546	248912	2.20%	0.274%
15	6.898	825	835	850	rVB2	60426	174541	1.54%	0.192%
16	7.145	865	877	886	rBV	289320	849929	7.51%	0.936%
17	7.839	987	995	1003	rVB2	56987	139416	1.23%	0.153%
18	8.016	1016	1025	1030	rBV2	101032	248736	2.20%	0.274%
19	8.086	1030	1037	1046	rVV3	363203	962751	8.50%	1.060%
20	8.169	1046	1051	1062	rVB2	42681	119831	1.06%	0.132%
21	8.457	1088	1100	1110	rBV	4930175	11207492	99.01%	12.336%
22	8.580	1116	1121	1128	rVB2	102721	205997	1.82%	0.227%
23	8.963	1176	1186	1199	rBV	345734	796521	7.04%	0.877%
24	9.457	1254	1270	1279	rBV3	144476	407466	3.60%	0.449%
25	9.969	1350	1357	1362	rBV	183768	355983	3.14%	0.392%
26	10.016	1362	1365	1372	rVB3	73648	124071	1.10%	0.137%
27	10.198	1388	1396	1399	rBV	65359	139057	1.23%	0.153%
28	10.316	1410	1416	1424	rVV2	97926	182188	1.61%	0.201%
29	10.439	1429	1437	1442	rBV	678376	1249553	11.04%	1.375%
30	10.498	1442	1447	1454	rVV	578840	997715	8.81%	1.098%
31	10.639	1461	1471	1477	rVV2	94153	186935	1.65%	0.206%
32	10.710	1477	1483	1490	rVB	76842	134823	1.19%	0.148%
33	11.739	1650	1658	1667	rBV	541725	934796	8.26%	1.029%
34	11.839	1667	1675	1685	rVV	5503887	9160929	80.93%	10.084%
35	11.951	1685	1694	1705	rVB	5417056	9661913	85.35%	10.635%
36	12.274	1737	1749	1760	rBV	2875102	4800935	42.41%	5.284%

LSC Area Percent Report

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Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

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\82N052422W.M
Title : SW846 8260

37	12.574	1793	1800	1808	rVB	456888	692952	6.12%	0.763%
38	12.727	1819	1826	1834	rBV	413800	691121	6.11%	0.761%
39	12.915	1849	1858	1863	rBV	931628	1483219	13.10%	1.633%
40	12.974	1863	1868	1871	rVV	1320009	1951263	17.24%	2.148%
41	13.010	1871	1874	1878	rVV	1208824	2001430	17.68%	2.203%
42	13.057	1878	1882	1890	rVB	1064086	1614561	14.26%	1.777%
43	13.215	1901	1909	1919	rBV	1460783	2440380	21.56%	2.686%
44	13.362	1924	1934	1948	rVV	7061042	11320047	100.00%	12.460%
45	13.492	1948	1956	1962	rVV3	76480	185917	1.64%	0.205%
46	13.551	1962	1966	1972	rVV	73768	114840	1.01%	0.126%
47	13.698	1980	1991	2000	rBV2	2123455	4433608	39.17%	4.880%
48	13.833	2007	2014	2015	rBV	239098	325529	2.88%	0.358%
49	13.868	2015	2020	2037	rVB	2467536	4796983	42.38%	5.280%
50	14.057	2046	2052	2058	rVB2	240203	451025	3.98%	0.496%
51	14.127	2058	2064	2066	rBV	284347	454108	4.01%	0.500%
52	14.151	2066	2068	2073	rVV	239655	330826	2.92%	0.364%
53	14.209	2073	2078	2084	rVV	635749	926691	8.19%	1.020%
54	14.274	2084	2089	2092	rVV	153910	238935	2.11%	0.263%
55	14.321	2092	2097	2107	rVB2	467433	786476	6.95%	0.866%
56	14.451	2114	2119	2125	rVB2	153206	230711	2.04%	0.254%
57	14.533	2125	2133	2136	rBV	353556	573926	5.07%	0.632%
58	14.574	2136	2140	2145	rVB	427067	608724	5.38%	0.670%
59	14.804	2174	2179	2184	rBV	403082	619052	5.47%	0.681%
60	14.921	2191	2199	2206	rBV3	750099	1563411	13.81%	1.721%
61	14.986	2206	2210	2219	rVB4	58654	114903	1.02%	0.126%
62	15.074	2219	2225	2234	rBV	167377	301540	2.66%	0.332%
63	15.186	2234	2244	2248	rBV3	88326	216651	1.91%	0.238%
64	15.304	2257	2264	2274	rVB2	90000	211799	1.87%	0.233%
65	15.498	2289	2297	2304	rBV	1075339	1978370	17.48%	2.178%
66	16.609	2478	2486	2502	rVB	349722	811481	7.17%	0.893%

Sum of corrected areas: 90850497

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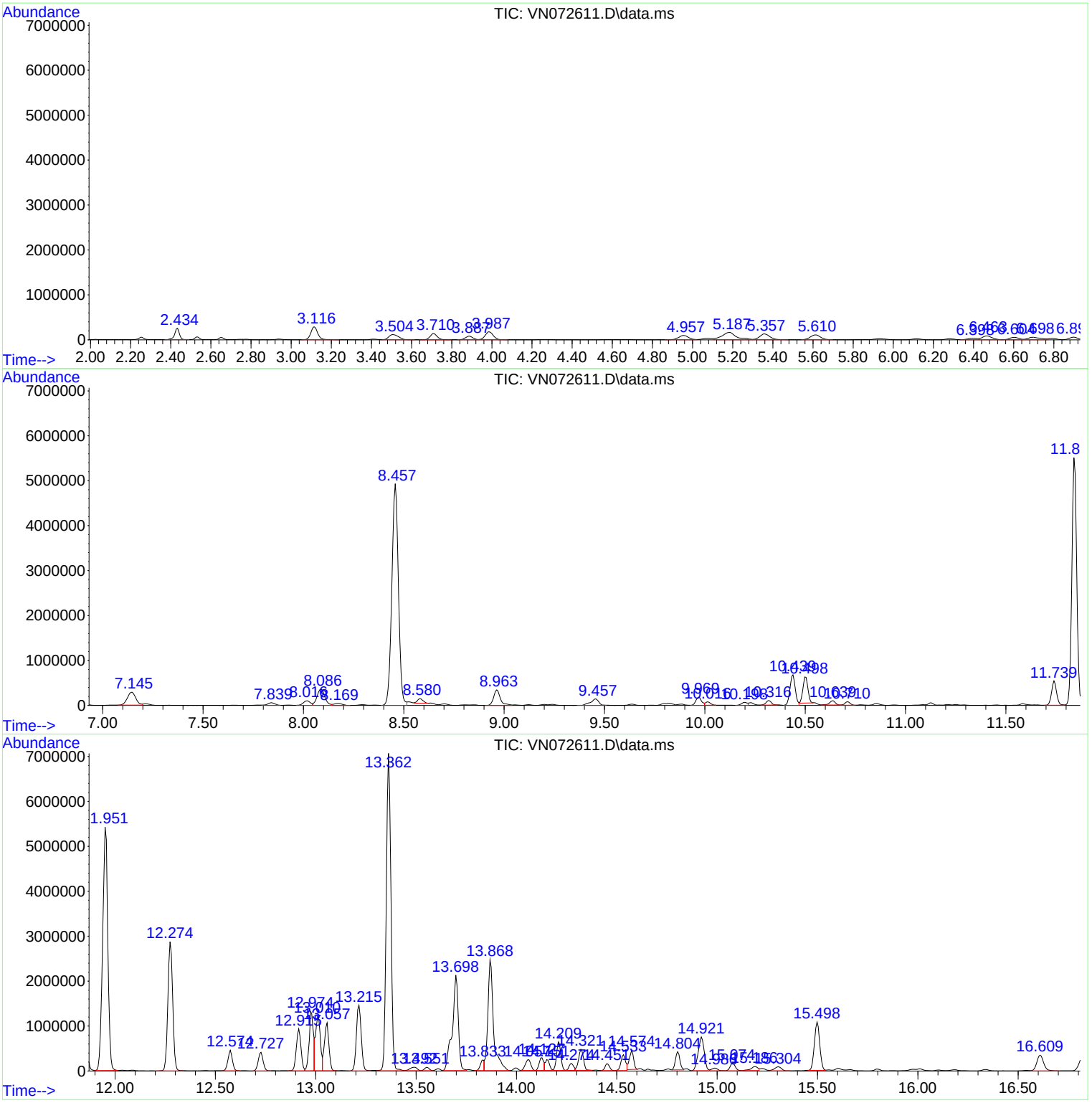
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

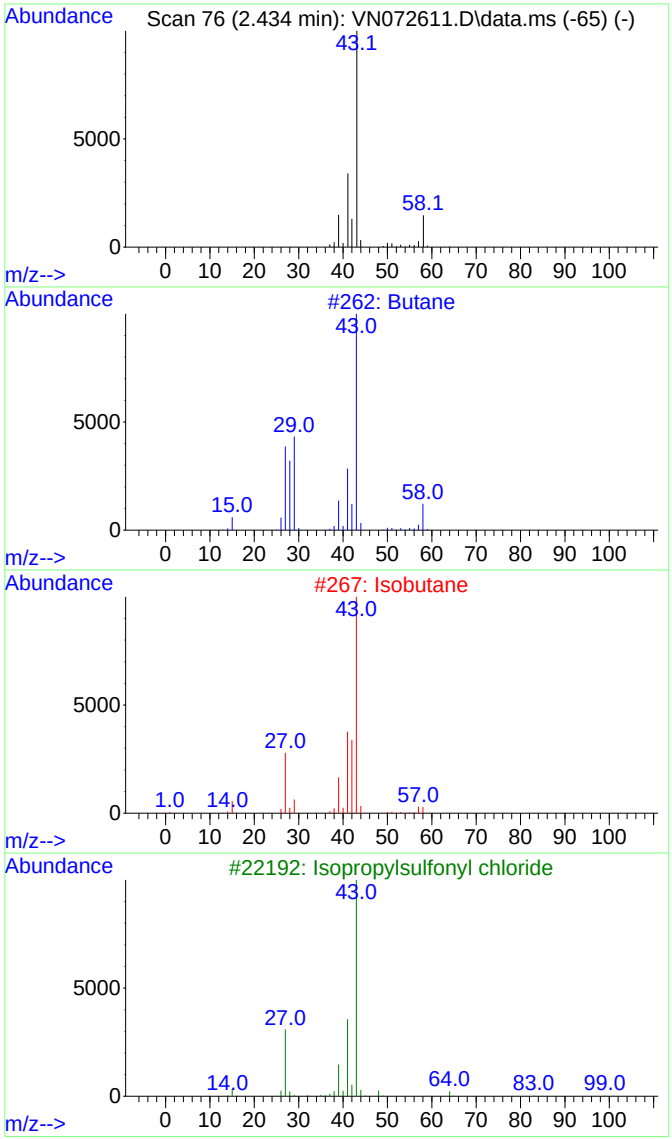
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

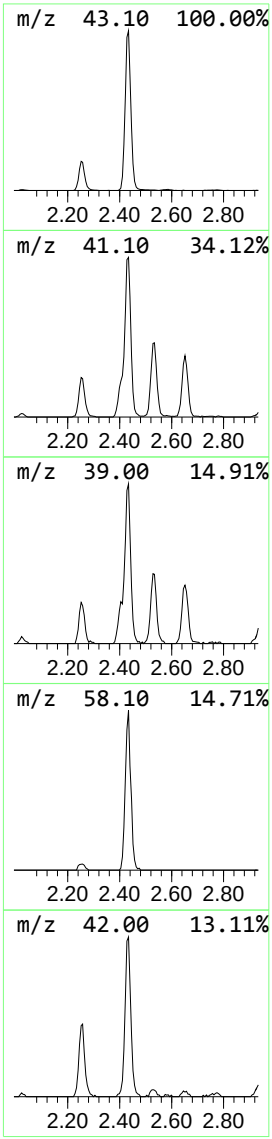
****

Peak Number 1 Butane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	21.96 ug/l	422823	Pentafluorobenzene	8.080

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	Acetone	58	C3H6O	000067-64-1	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

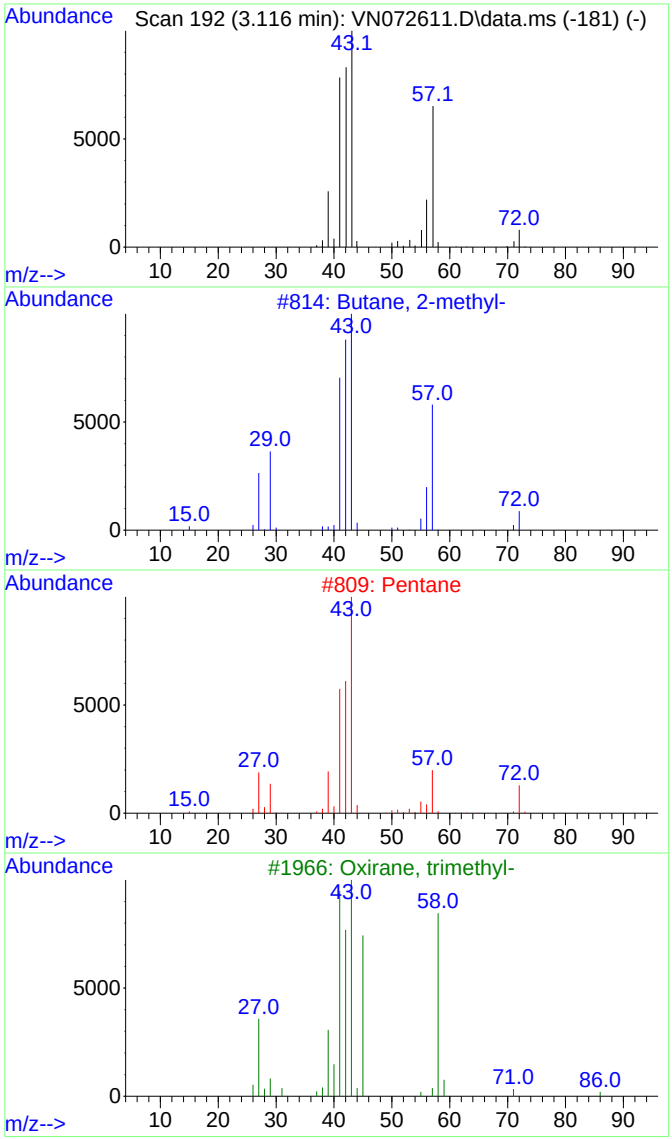
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

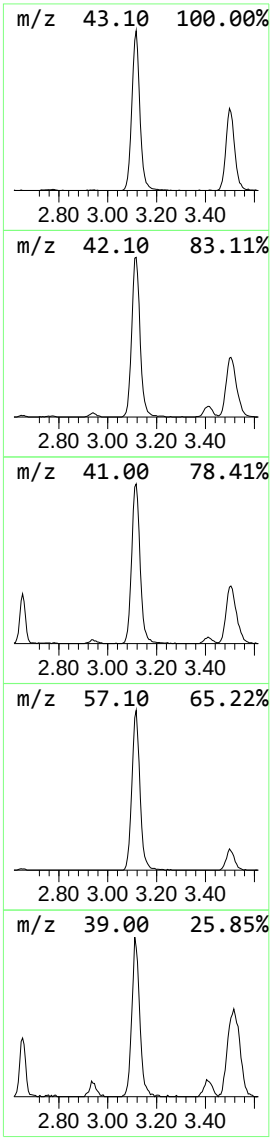
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	35.07 ug/l	675361	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	50
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	38
4	3-Buten-1-ol	72	C4H8O	000627-27-0	28
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

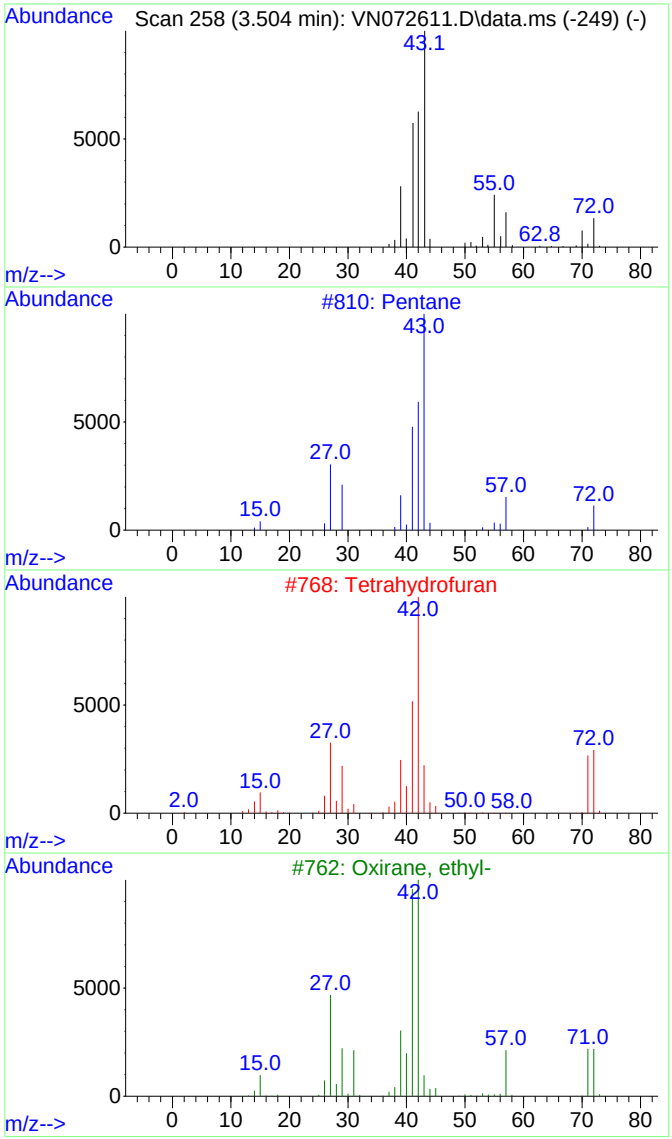
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

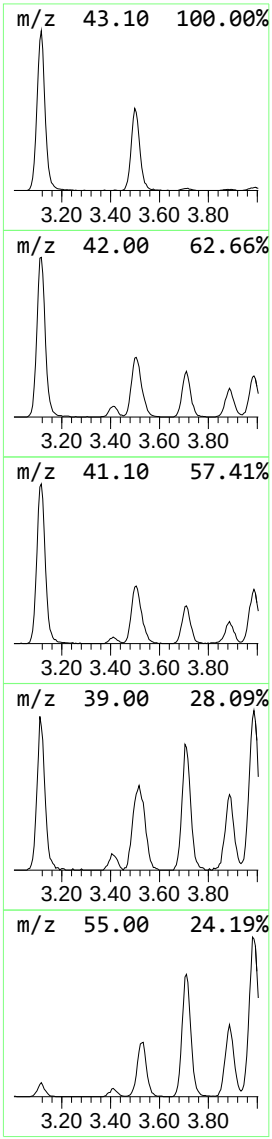
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.504	20.45 ug/l	393731	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Tetrahydrofuran	72	C4H8O	000109-99-9	38
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	37
5	1-Pentene	70	C5H10	000109-67-1	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

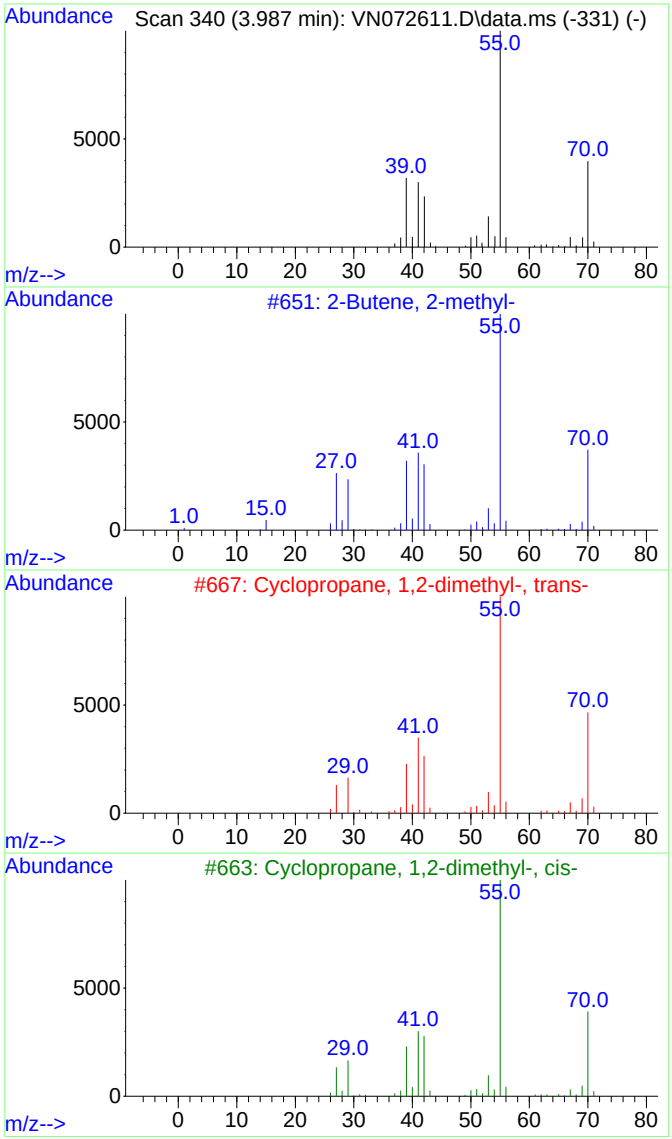
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

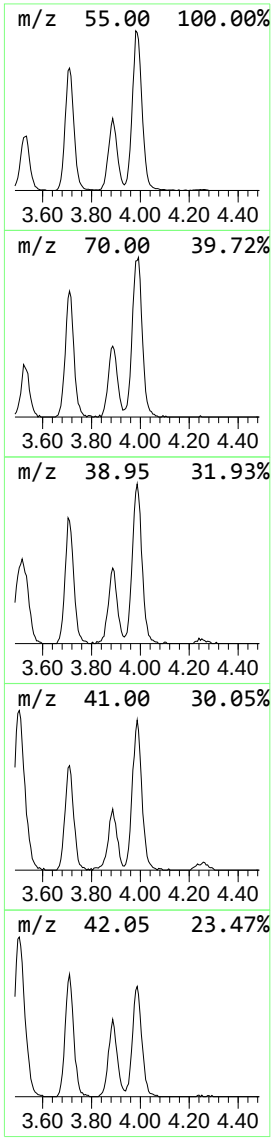
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.987	25.68 ug/l	494439	Pentafluorobenzene	8.080

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-, trans-	70	C5H10	002402-06-4	91
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
4	2-Pentene, (E)-	70	C5H10	000646-04-8	87
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
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Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

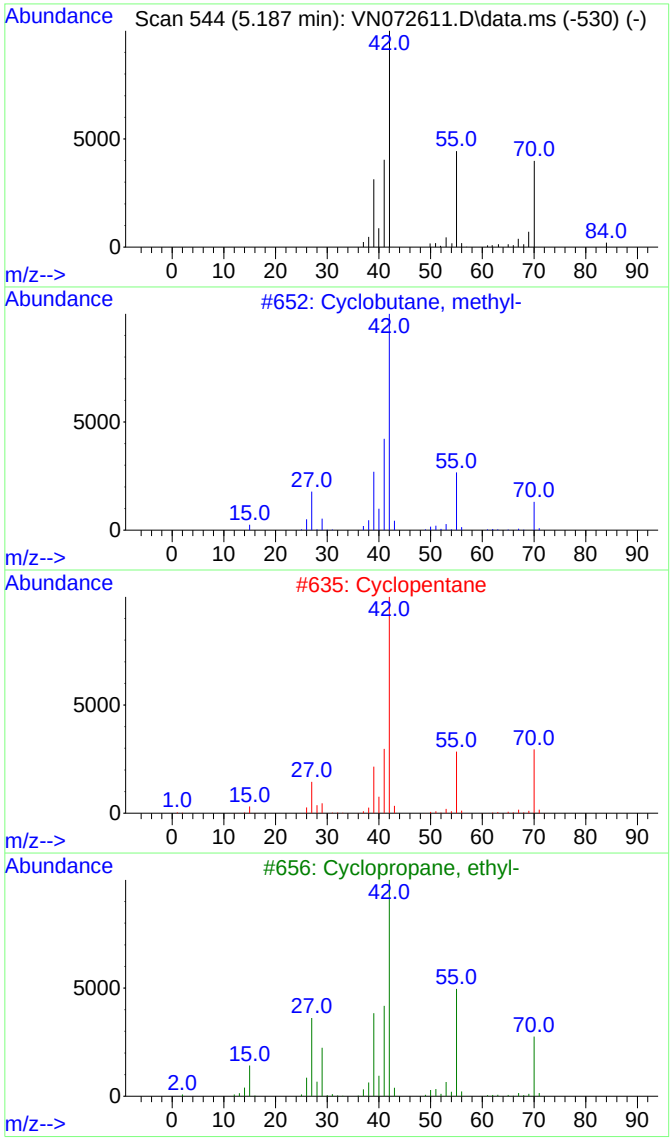
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

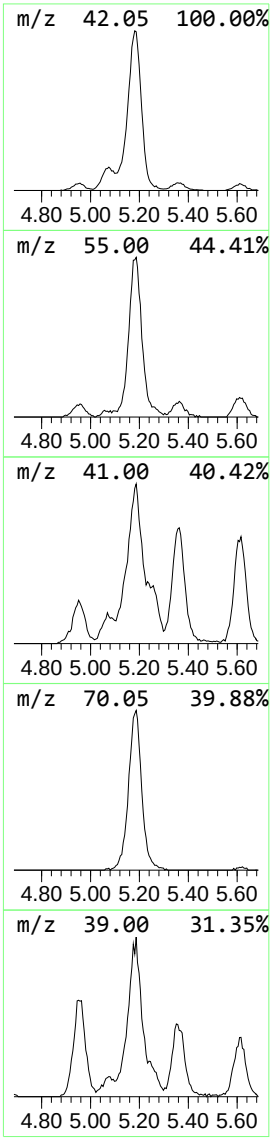
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclobutane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	41.93 ug/l	807355	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2	Cyclopentane	70	C5H10	000287-92-3	78
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
4	1-Pentene	70	C5H10	000109-67-1	72
5	1-Pentanol	88	C5H12O	000071-41-0	40





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ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

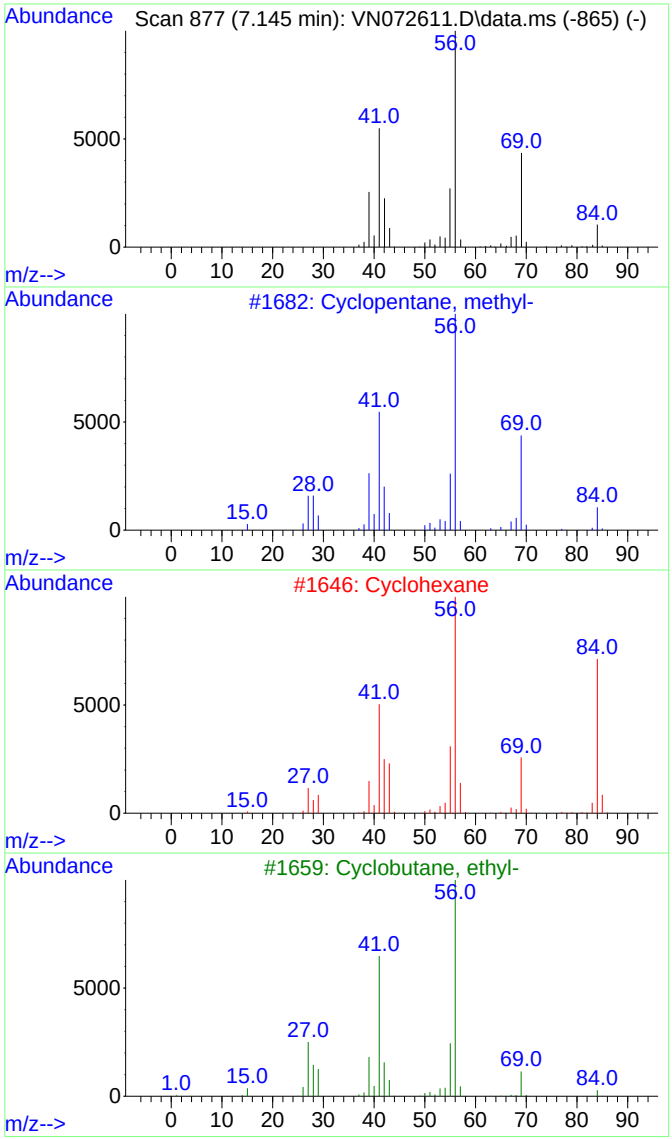
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

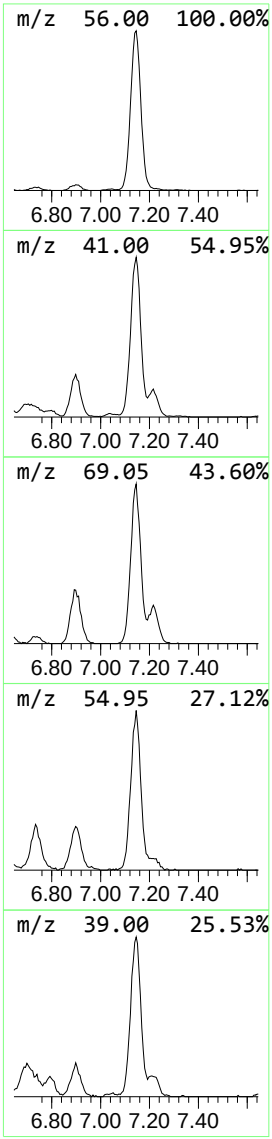
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	44.14 ug/l	849929	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

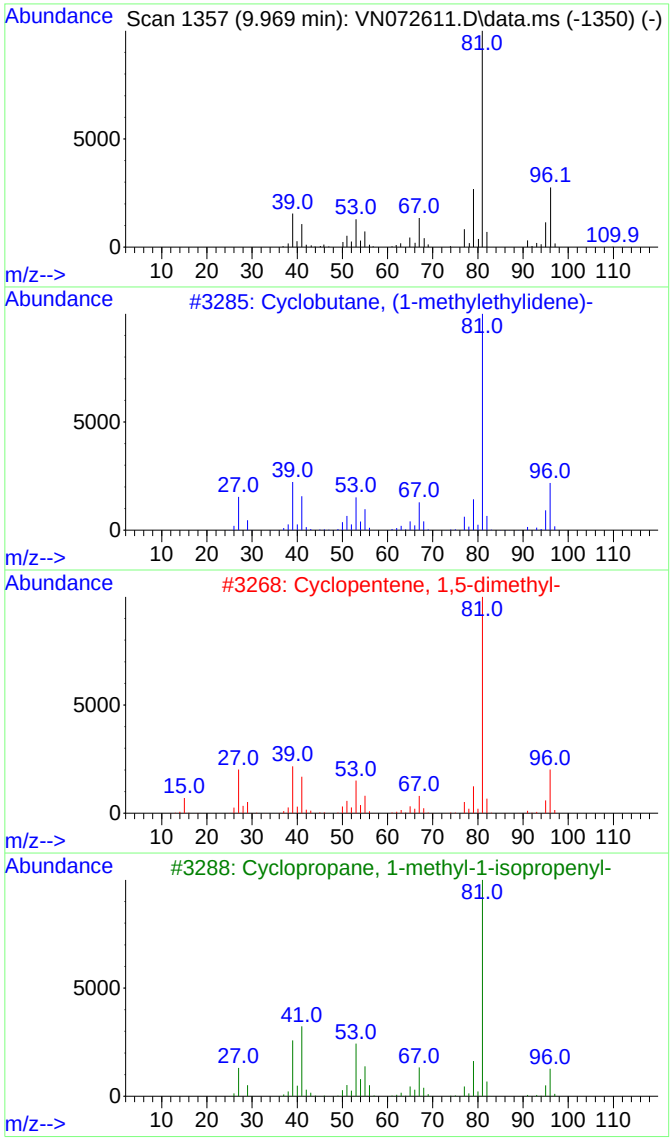
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

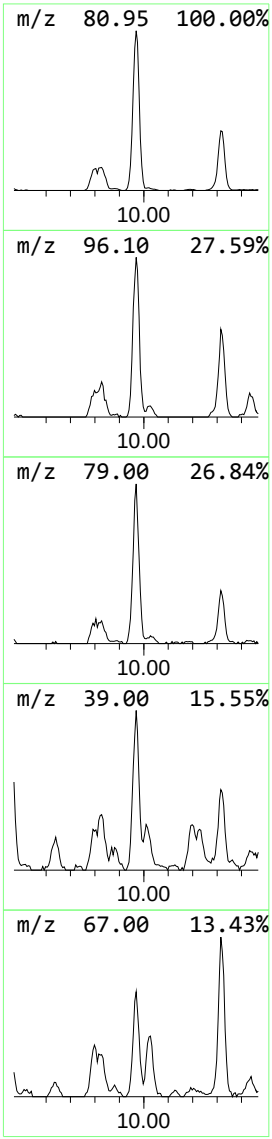
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclobutane, (1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.969	22.35 ug/l	355983	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	87
3	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	86
4	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

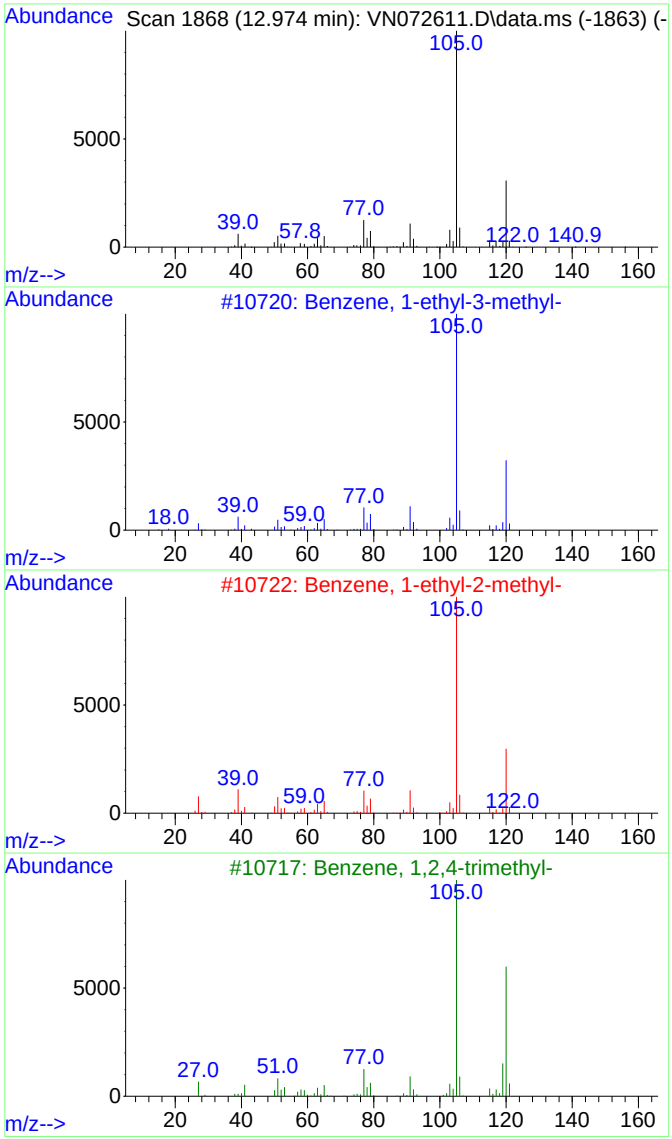
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

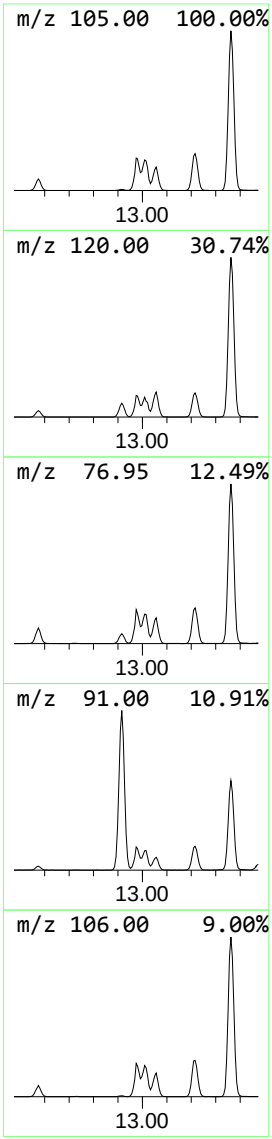
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.974	22.01 ug/l	1951260	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

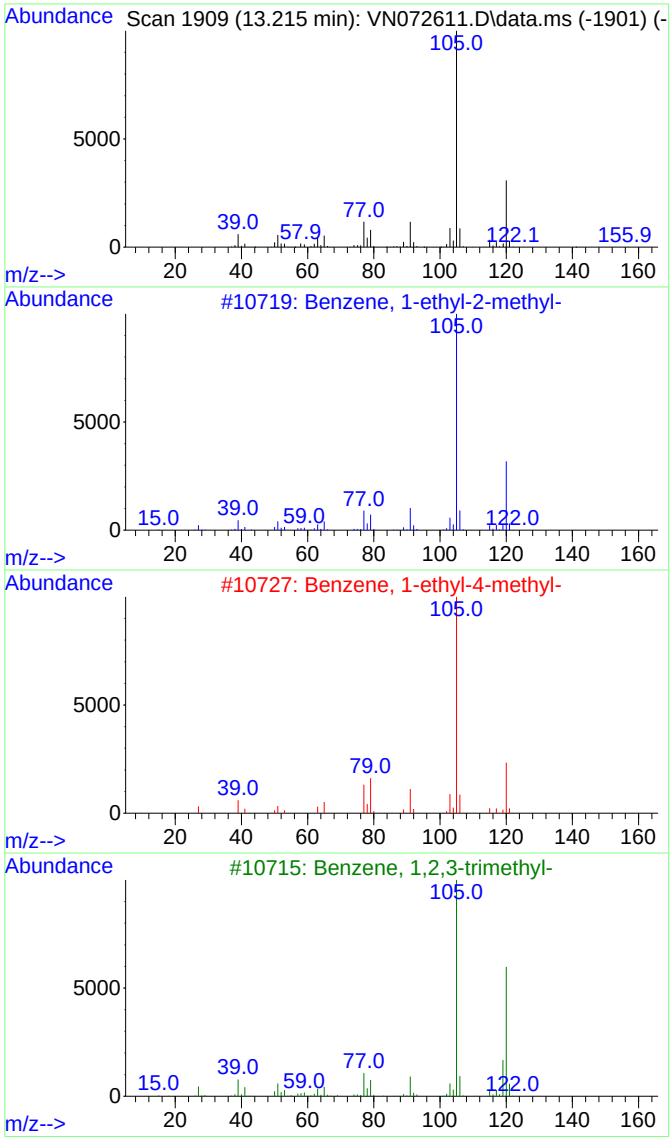
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

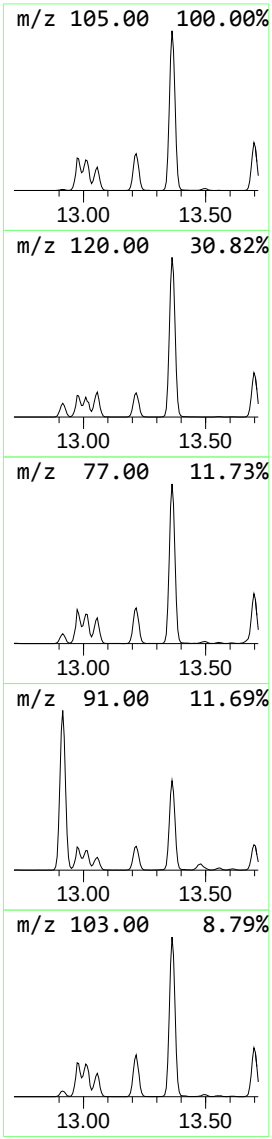
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	27.52 ug/l	2440380	1,4-Dichlorobenzene-d4	13.668

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

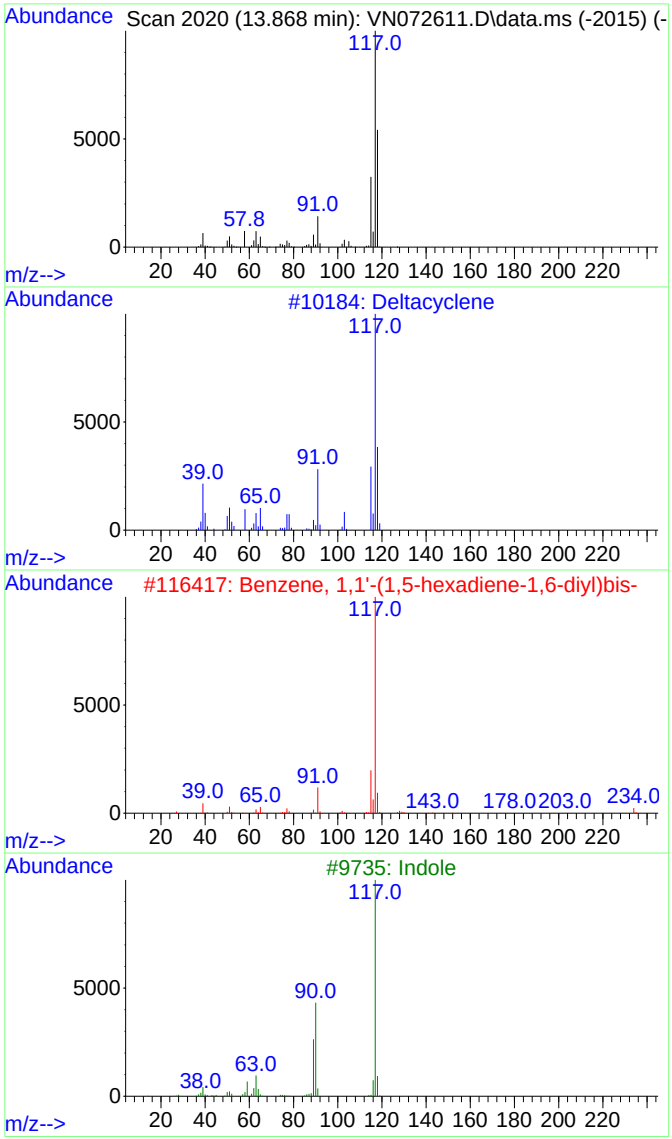
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

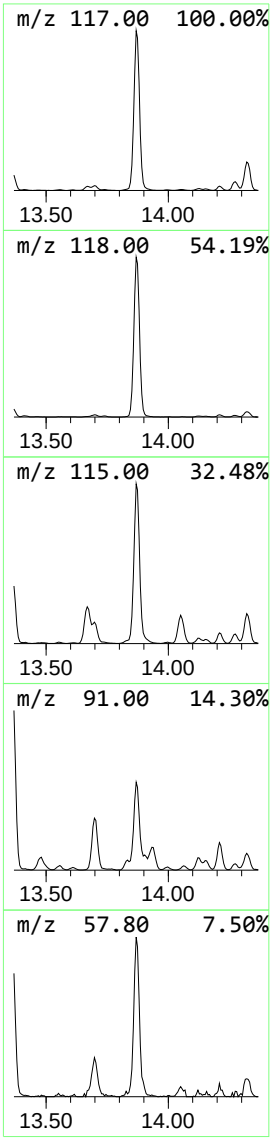
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	54.10 ug/l	4796980	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	64
2	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
3	Indole	117	C8H7N	000120-72-9	46
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072611.D
Acq On : 25 May 2022 01:20
Operator : JC\MD
Sample : N2968-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP-051922

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.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	2.434	22.0	ug/l	422823	1	8.080	962751	50.0
Butane, 2-methyl-	3.116	35.1	ug/l	675361	1	8.080	962751	50.0
Pentane	3.504	20.4	ug/l	393731	1	8.080	962751	50.0
2-Butene, 2-met...	3.987	25.7	ug/l	494439	1	8.080	962751	50.0
Cyclobutane, me...	5.187	41.9	ug/l	807355	1	8.080	962751	50.0
Cyclopentane, m...	7.145	44.1	ug/l	849929	1	8.080	962751	50.0
Cyclobutane, (1...	9.969	22.4	ug/l	355983	2	8.963	796521	50.0
Benzene, 1-ethy...	12.974	22.0	ug/l	1951260	4	13.668	4433610	50.0
Benzene, 1-ethy...	13.215	27.5	ug/l	2440380	4	13.668	4433610	50.0
Benzene, 1,1'-(...	13.868	54.1	ug/l	4796980	4	13.668	4433610	50.0