LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N061722W.M
Title : SW846 8260

Signal : TIC: VN072961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	55	62	82	rBV	287526	1427283	2.48%	0.369%
2	8.016	1036	1042	1051	rVB	446932	1056728	1.83%	0.273%
3	8.545	1113	1132	1143	rVV	325911	962680	1.67%	0.249%
4	8.898	1183	1192	1204	rBV	611303	1328945	2.31%	0.343%
5	9.816	1341	1348	1357	rVB	413133	828848	1.44%	0.214%
6	9.945	1365	1370	1377	rVB	547203	1099893	1.91%	0.284%
7	10.133	1394	1402	1415	rBV3	262300	634930	1.10%	0.164%
8	10.375	1436	1443	1449	rBV	874227	1626322	2.82%	0.420%
9	11.063	1554	1560	1571	rVB	556369	1008797	1.75%	0.261%
10	11.680	1657	1665	1672	rBV	912669	1592051	2.76%	0.411%
11	11.780	1673	1682	1692	rVV	23450283	42447798	73.65%	10.967%
12	11.892	1692	1701	1718	rVB	22647251	48098739	83.45%	12.427%
13	12.216	1745	1756	1764	rBV	1868270	3124151	5.42%	0.807%
14	12.516	1800	1807	1814	rBV	1529703	2474509	4.29%	0.639%
15	12.663	1826	1832	1841	rVB	730567	1241637	2.15%	0.321%
16	12.857	1857	1865	1870	rBV	5867775	9663872	16.77%	2.497%
17	12.916	1870	1875	1878	rVV	8011862	13312965	23.10%	3.440%
18	12.951	1878	1881	1885	rVV	7795553	12140418	21.06%	3.137%
19	12.992	1885	1888	1896	rVB	7839479	12079646	20.96%	3.121%
20	13.157	1908	1916	1925	rBV	5485460	9135473	15.85%	2.360%
21	13.304	1930	1941	1948	rBV	32038133	57637171	100.00%	14.892%
22	13.427	1955	1962	1968	rVB3	370928	948576	1.65%	0.245%
23	13.639	1987	1998	2014	rVB	11696551	21005371	36.44%	5.427%
24	13.774	2014	2021	2022	rBV	2779230	3894432	6.76%	1.006%
25	13.810	2022	2027	2031	rVV	10593371	20143212	34.95%	5.204%
26	13.845	2031	2033	2043	rVB3	4391922	7386149	12.81%	1.908%
27	13.933	2043	2048	2053	rBV	471368	769813	1.34%	0.199%
28	13.998	2053	2059	2065	rVV2	2022654	3746768	6.50%	0.968%
29	14.063	2065	2070	2073	rVV	3303188	5559593	9.65%	1.436%
30	14.092	2073	2075	2080	rVV	2789335	3653444	6.34%	0.944%
31	14.151	2080	2085	2091	rVV	6267151	9551676	16.57%	2.468%
32	14.210	2091	2095	2099	rVV	724433	1202861	2.09%	0.311%
33	14.263	2099	2104	2113	rVB2	2888550	4839616	8.40%	1.250%
34	14.392	2120	2126	2131	rVB	1247756	1933853	3.36%	0.500%
35	14.469	2131	2139	2143	rBV	3460453	5911657	10.26%	1.527%
36	14.510	2143	2146	2151	rVV	4361275	6651318	11.54%	1.718%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N061722W.M
Title : SW846 8260

37	14.557	2151	2154	2157	rVV	830378	1124927	1.95%	0.291%
38	14.739	2180	2185	2190	rVV	3386992	5572918	9.67%	1.440%
39	14.786	2190	2193	2197	rVB2	661685	911662	1.58%	0.236%
40	14.857	2197	2205	2211	rBV2	5623857	11838803	20.54%	3.059%
41	14.921	2211	2216	2225	rVB2	1022561	2001448	3.47%	0.517%
42	15.010	2225	2231	2239	rBV2	1022856	1870979	3.25%	0.483%
43	15.121	2239	2250	2262	rVV2	1398860	4346818	7.54%	1.123%
44	15.239	2262	2270	2277	rVB3	1020493	2417653	4.19%	0.625%
45	15.427	2288	2302	2312	rBV	10819117	21097062	36.60%	5.451%
46	15.527	2313	2319	2325	rVV3	1232852	2516986	4.37%	0.650%
47	15.592	2325	2330	2344	rVB	376925	879051	1.53%	0.227%
48	15.721	2345	2352	2361	rBV	673353	1325417	2.30%	0.342%
49	15.898	2370	2382	2391	rBV2	401238	1387835	2.41%	0.359%
50	16.104	2409	2417	2423	rVB2	262497	619041	1.07%	0.160%
51	16.521	2481	2488	2503	rVB	2483137	5605684	9.73%	1.448%
52	16.727	2514	2523	2533	rVB	1475868	3407669	5.91%	0.880%

Sum of corrected areas: 387045148

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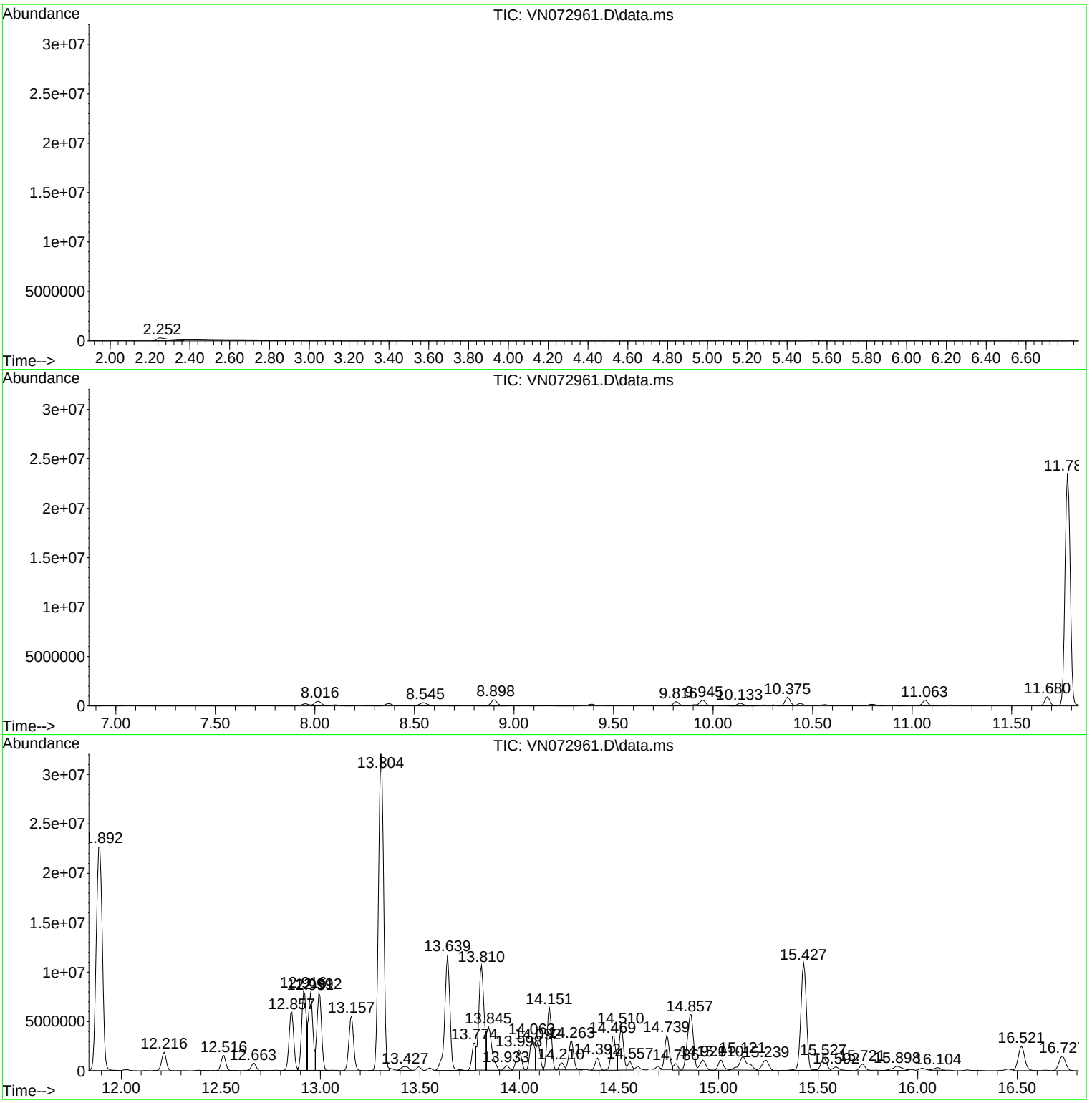
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
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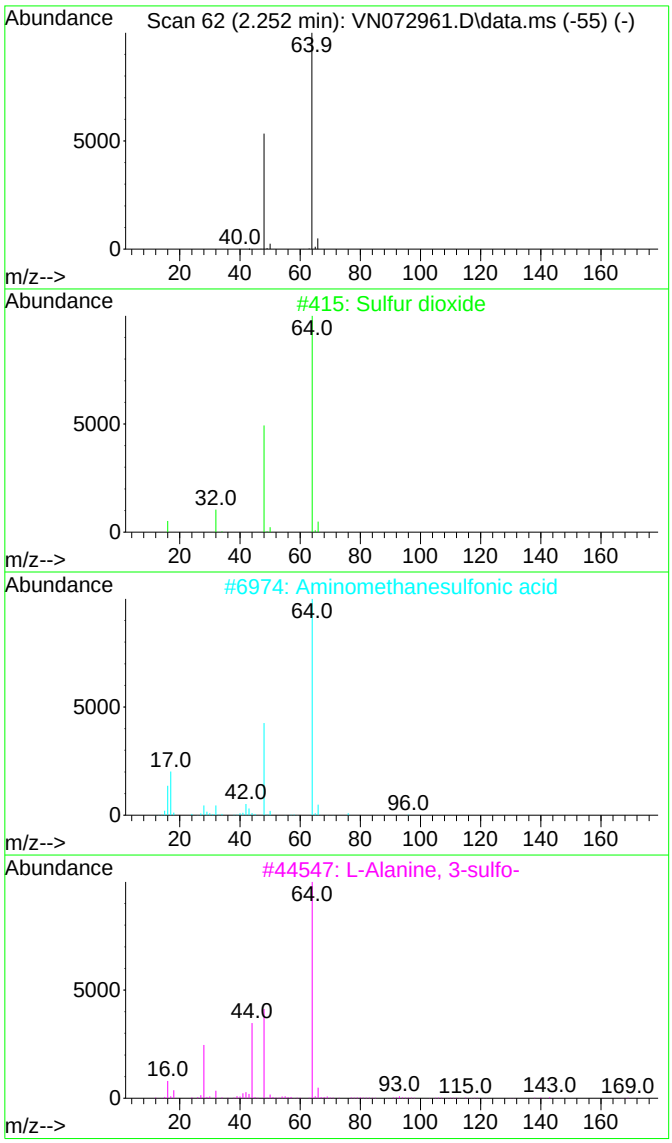
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

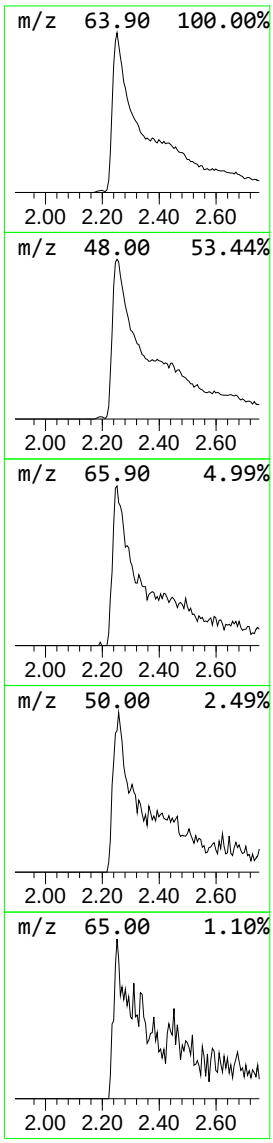
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	67.53 ug/l	1427280	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

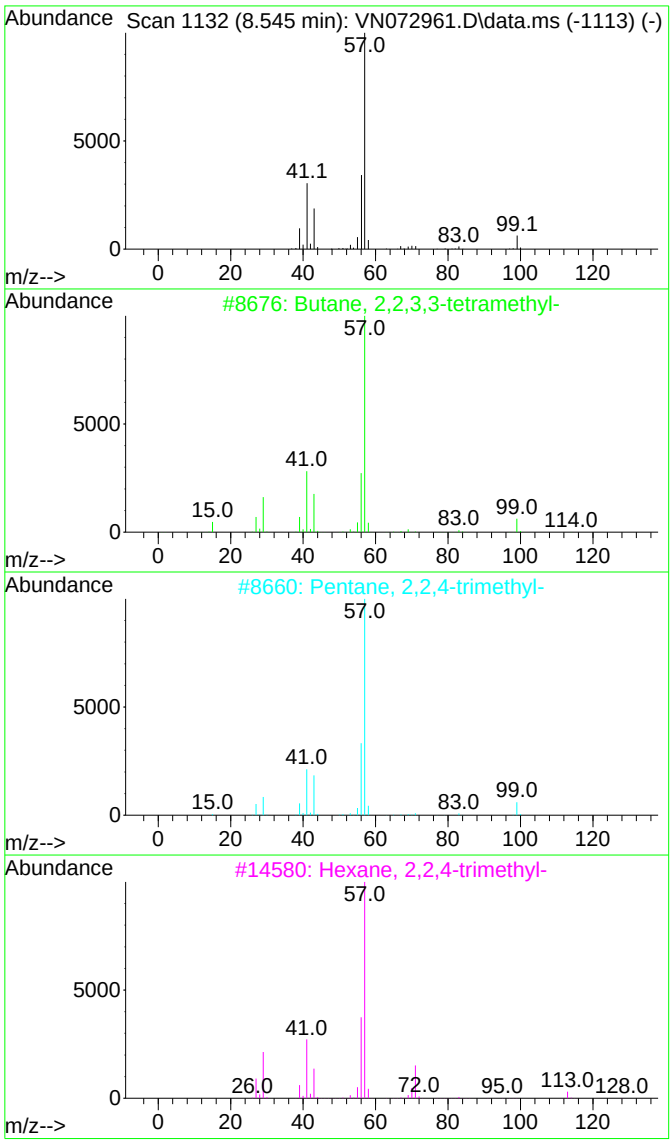
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

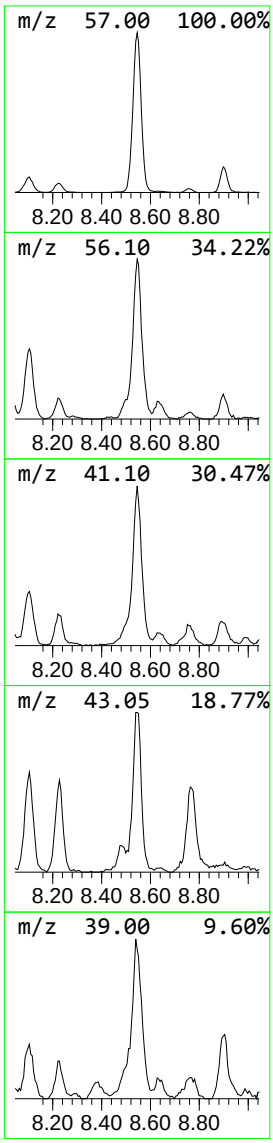
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	36.22 ug/l	962680	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

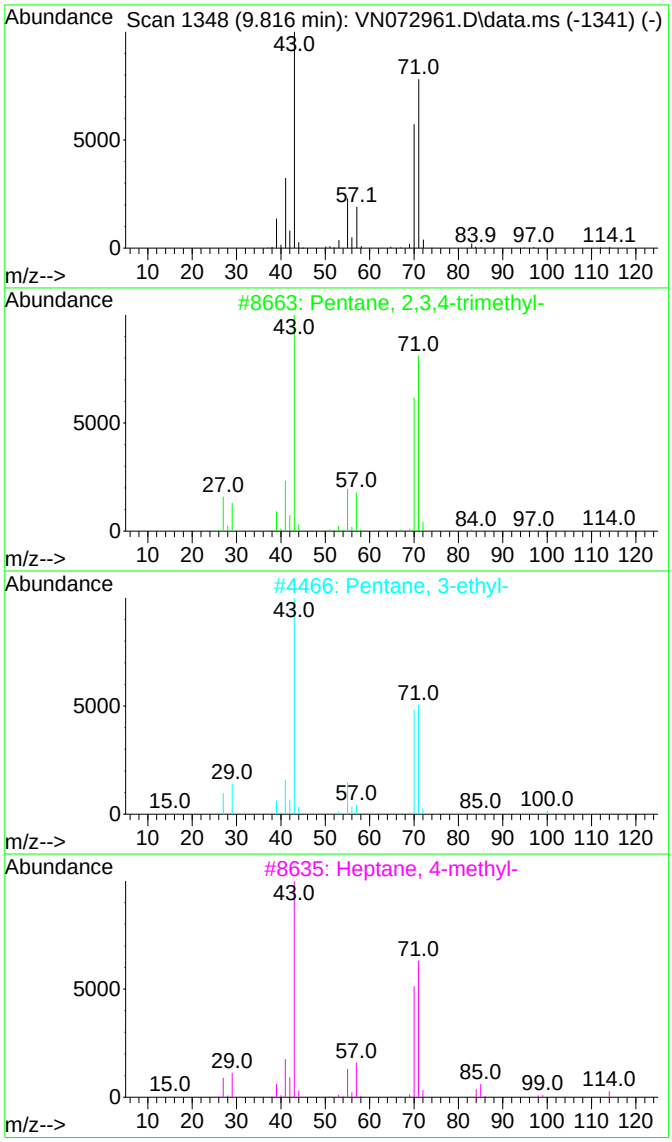
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

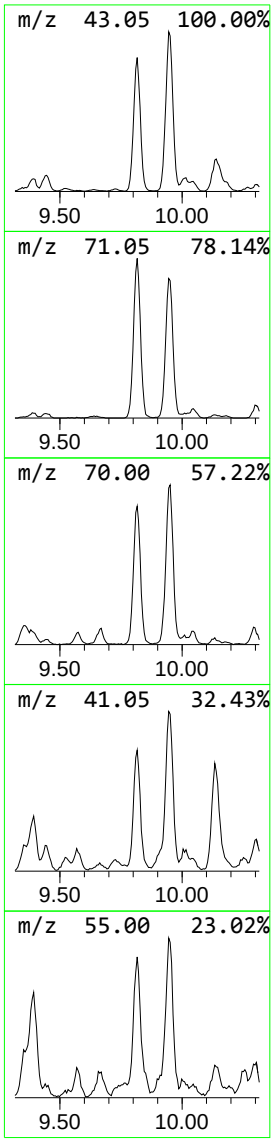
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	31.18 ug/l	828848	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

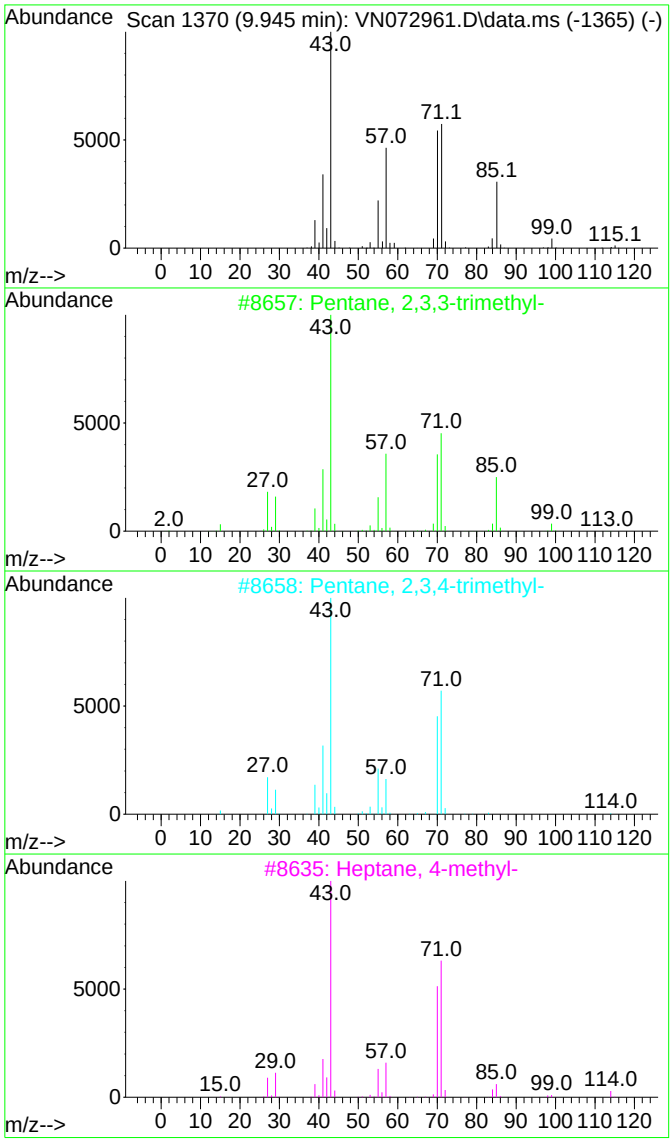
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

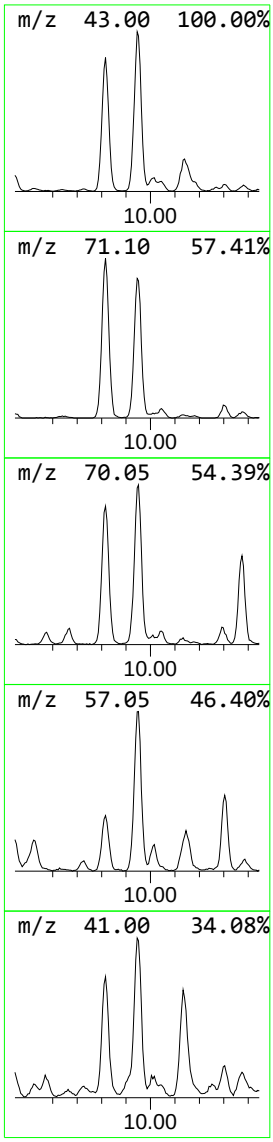
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	41.38 ug/l	1099890	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	80
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	74
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
5	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	59





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

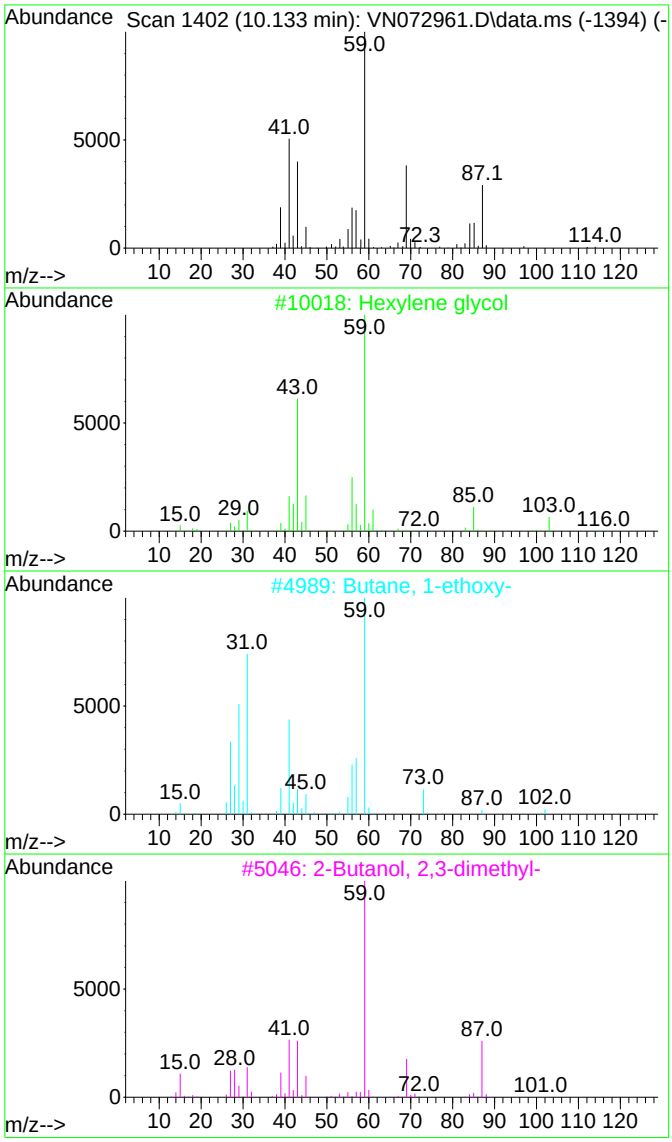
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

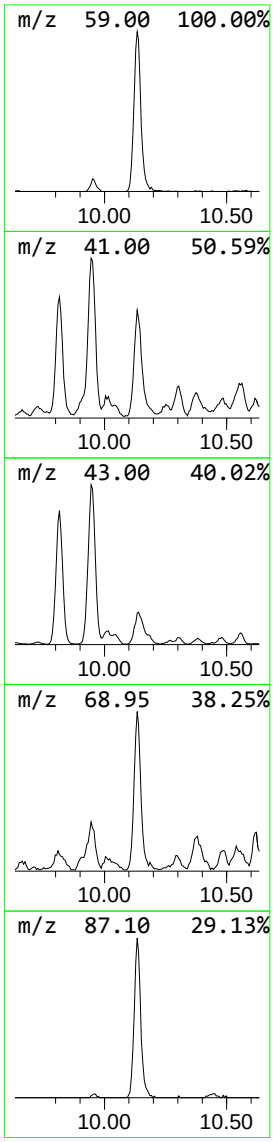
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	23.89 ug/l	634930	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	59
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	53
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	50
4	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	47
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	47





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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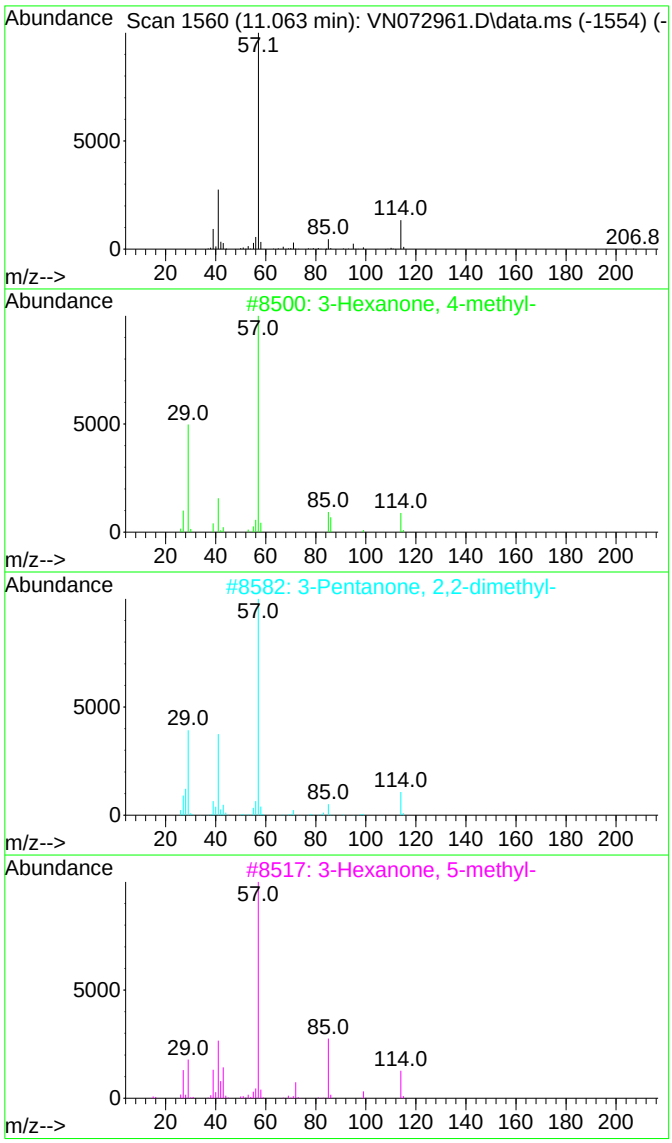
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

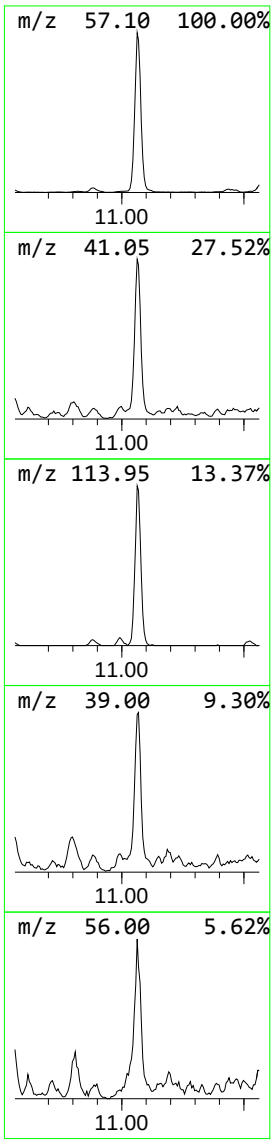
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.063	31.68 ug/l	1008800	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	50
2	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	47
3	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	47
4	Aluminum, triethyl-	114	C6H15Al	000097-93-8	38
5	3,4-Hexanedione	114	C6H10O2	004437-51-8	38





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

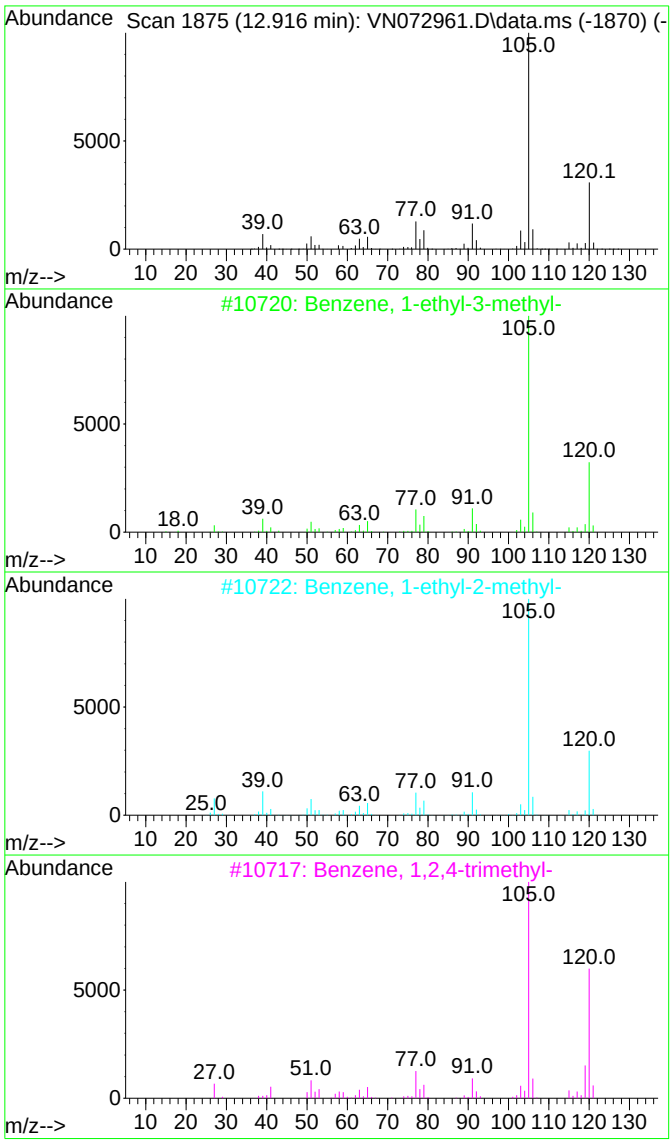
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

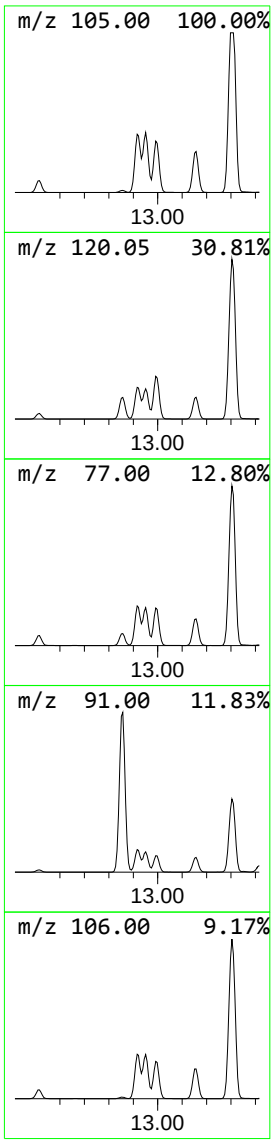
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	31.69 ug/l	13313000	1,4-Dichlorobenzene-d4	13.610

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





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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MW-14

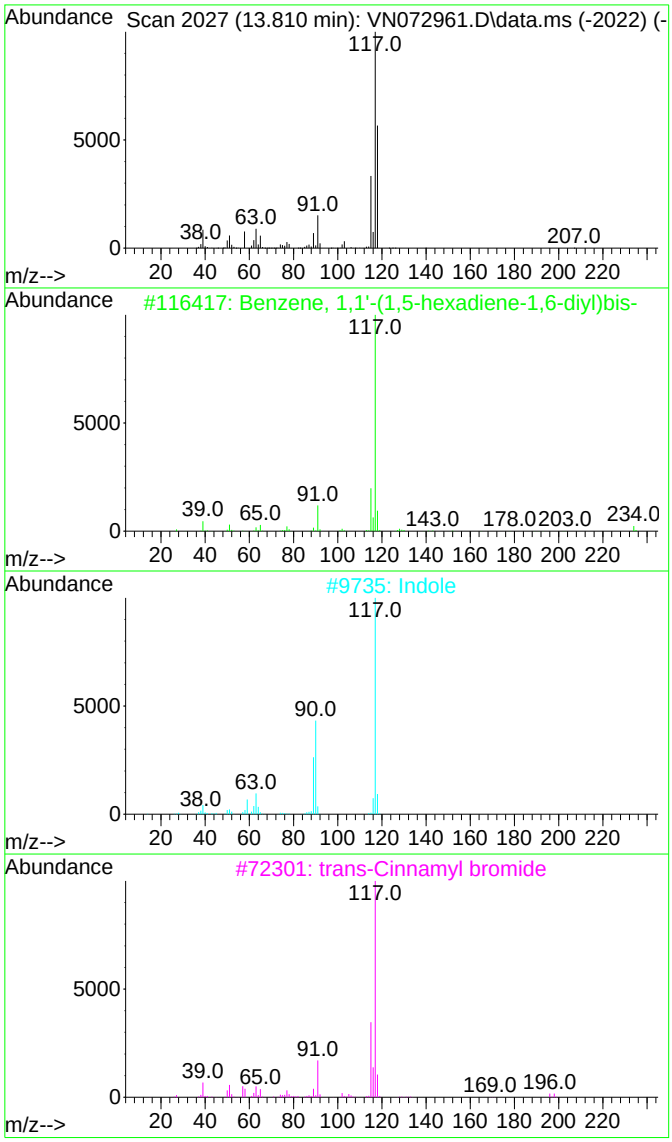
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

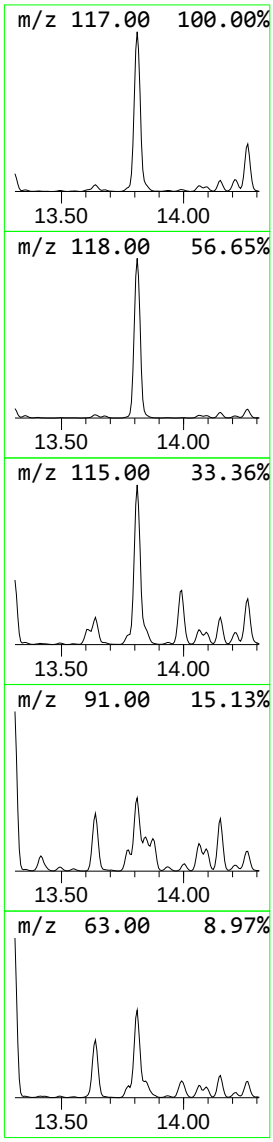
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	47.95 ug/l	20143200	1,4-Dichlorobenzene-d4	13.610

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	Indole	117	C8H7N	000120-72-9	49
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5	4-Ethynylaniline	117	C8H7N	014235-81-5	43





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Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

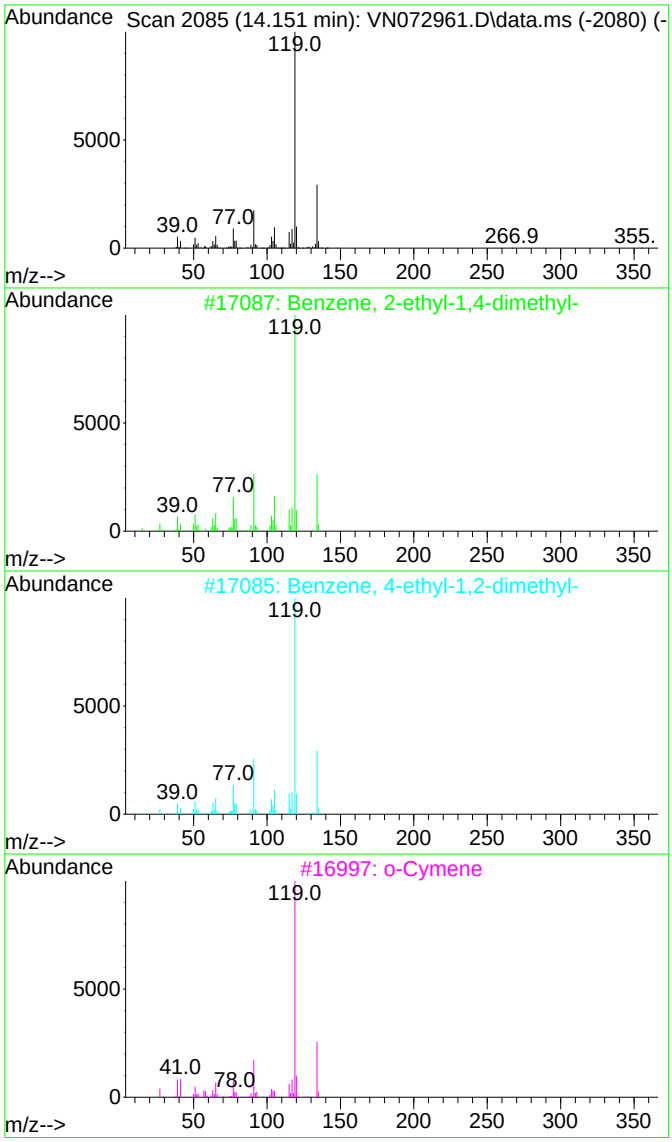
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

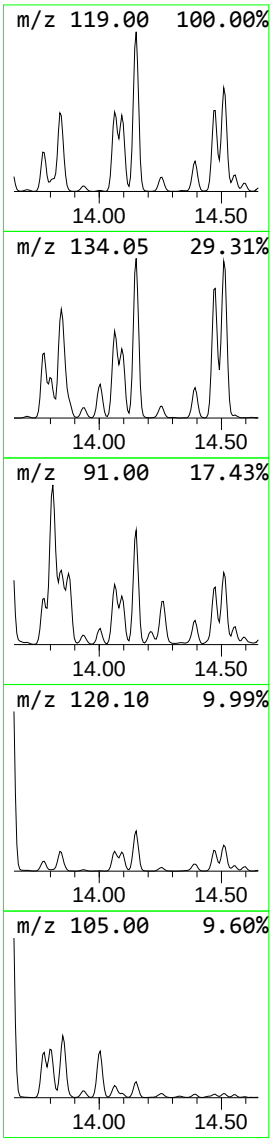
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	22.74 ug/l	9551680	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

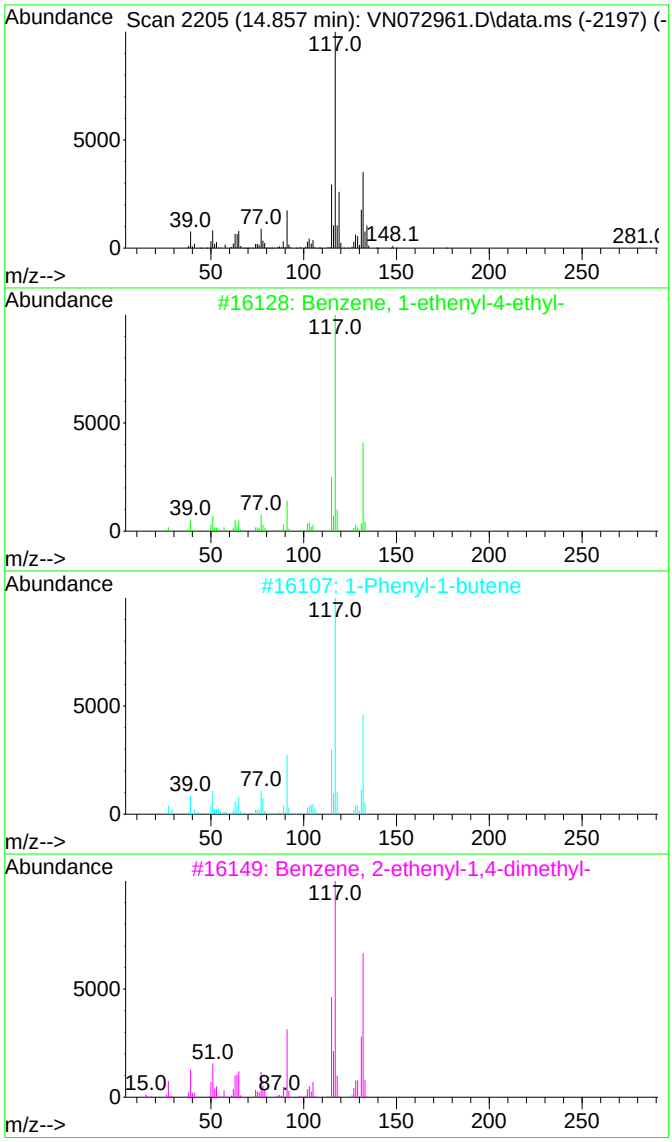
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

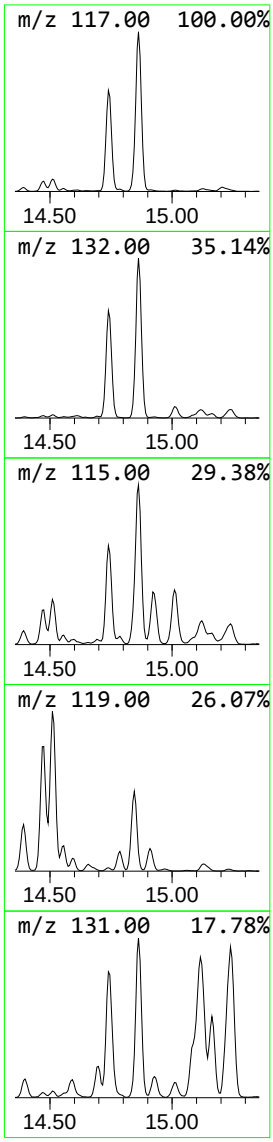
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	28.18 ug/l	11838800	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072961.D
Acq On : 20 Jun 2022 15:04
Operator : JC\MD
Sample : N3357-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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
Sulfur dioxide	2.252	67.5	ug/l	1427280	1	8.016	1056730	50.0
Butane, 2,2,3,3...	8.545	36.2	ug/l	962680	2	8.898	1328950	50.0
Pentane, 2,3,4-...	9.816	31.2	ug/l	828848	2	8.898	1328950	50.0
Pentane, 2,3,3-...	9.945	41.4	ug/l	1099890	2	8.898	1328950	50.0
Hexylene glycol	10.134	23.9	ug/l	634930	2	8.898	1328950	50.0
3-Hexanone, 4-m...	11.063	31.7	ug/l	1008800	3	11.680	1592050	50.0
Benzene, 1-ethy...	12.916	31.7	ug/l	13313000	4	13.610	21005400	50.0
Benzene, 1,1'-(...	13.810	47.9	ug/l	20143200	4	13.610	21005400	50.0
Benzene, 2-ethy...	14.151	22.7	ug/l	9551680	4	13.610	21005400	50.0
Benzene, 1-ethe...	14.857	28.2	ug/l	11838800	4	13.610	21005400	50.0