LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

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\82N061722W.M
Title : SW846 8260

Signal : TIC: VN072962.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	57	64	81	rBV2	133080	726575	1.22%	0.179%
2	8.016	1036	1042	1050	rVB	489399	1144380	1.92%	0.283%
3	8.369	1093	1102	1114	rBV2	244954	610078	1.02%	0.151%
4	8.545	1114	1132	1142	rVV	326158	955234	1.60%	0.236%
5	8.898	1183	1192	1204	rBV	669763	1432907	2.40%	0.354%
6	9.816	1341	1348	1357	rVB	420444	832158	1.39%	0.205%
7	9.945	1365	1370	1378	rVB	551824	1105857	1.85%	0.273%
8	10.133	1394	1402	1415	rBV3	279170	668127	1.12%	0.165%
9	10.375	1436	1443	1449	rBV	926794	1744758	2.92%	0.431%
10	11.063	1554	1560	1571	rVB	598753	1107041	1.85%	0.273%
11	11.680	1657	1665	1671	rBV	972300	1678552	2.81%	0.414%
12	11.780	1673	1682	1691	rVV	24157832	43835581	73.44%	10.823%
13	11.892	1692	1701	1718	rVB	22906820	49166985	82.37%	12.140%
14	12.216	1744	1756	1764	rBV	1971570	3335127	5.59%	0.823%
15	12.516	1800	1807	1813	rBV	1590602	2642079	4.43%	0.652%
16	12.663	1826	1832	1840	rBV	773183	1316578	2.21%	0.325%
17	12.857	1857	1865	1870	rBV	6239536	10108202	16.93%	2.496%
18	12.916	1870	1875	1878	rVV	8282829	13922897	23.32%	3.438%
19	12.951	1878	1881	1885	rVV	8129515	12838553	21.51%	3.170%
20	12.992	1885	1888	1896	rVB	8183933	12631084	21.16%	3.119%
21	13.157	1909	1916	1926	rVB	5762415	9665404	16.19%	2.386%
22	13.304	1932	1941	1948	rBV	33410995	59692666	100.00%	14.739%
23	13.427	1954	1962	1968	rBV3	390241	918986	1.54%	0.227%
24	13.492	1968	1973	1978	rBV	407798	642368	1.08%	0.159%
25	13.639	1987	1998	2014	rVB	12190703	22169945	37.14%	5.474%
26	13.774	2014	2021	2022	rBV	2938990	4144288	6.94%	1.023%
27	13.810	2022	2027	2031	rVV	11123493	21081044	35.32%	5.205%
28	13.845	2031	2033	2043	rVB3	4676889	7796625	13.06%	1.925%
29	13.933	2043	2048	2053	rBV	494814	814191	1.36%	0.201%
30	13.998	2053	2059	2065	rVV2	2045668	3770467	6.32%	0.931%
31	14.063	2065	2070	2073	rVV	3516977	5942539	9.96%	1.467%
32	14.092	2073	2075	2080	rVV	2910424	3867778	6.48%	0.955%
33	14.151	2080	2085	2091	rVV	6628294	10063232	16.86%	2.485%
34	14.210	2091	2095	2099	rVV	780341	1269066	2.13%	0.313%
35	14.263	2099	2104	2113	rVB2	3011362	5083448	8.52%	1.255%
36	14.392	2120	2126	2131	rVB	1343693	2078013	3.48%	0.513%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

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\82N061722W.M
Title : SW846 8260

37	14.474	2131	2140	2143	rBV	3637268	6254006	10.48%	1.544%
38	14.510	2143	2146	2151	rVV	4682679	7123997	11.93%	1.759%
39	14.557	2151	2154	2157	rVV	858527	1207257	2.02%	0.298%
40	14.592	2157	2160	2167	rVB	382807	600878	1.01%	0.148%
41	14.739	2180	2185	2190	rVV	3579060	5624033	9.42%	1.389%
42	14.786	2190	2193	2197	rVB	690594	964879	1.62%	0.238%
43	14.863	2197	2206	2211	rBV2	5997332	12590146	21.09%	3.109%
44	14.921	2211	2216	2225	rVB3	1002566	1986154	3.33%	0.490%
45	15.010	2225	2231	2239	rBV2	1037700	1857578	3.11%	0.459%
46	15.121	2239	2250	2255	rBV3	1454770	3583205	6.00%	0.885%
47	15.233	2262	2269	2278	rVB3	1073654	2581331	4.32%	0.637%
48	15.427	2288	2302	2311	rBV	11785179	22586433	37.84%	5.577%
49	15.527	2313	2319	2325	rVV3	1371586	2701540	4.53%	0.667%
50	15.586	2325	2329	2345	rVB	404265	948710	1.59%	0.234%
51	15.721	2345	2352	2361	rBV	694983	1420494	2.38%	0.351%
52	15.898	2370	2382	2391	rBV2	420660	1420274	2.38%	0.351%
53	16.098	2410	2416	2423	rVB3	291972	645430	1.08%	0.159%
54	16.521	2481	2488	2502	rVB	2760973	6343043	10.63%	1.566%
55	16.727	2514	2523	2533	rVB	1626838	3764634	6.31%	0.930%

Sum of corrected areas: 405006835

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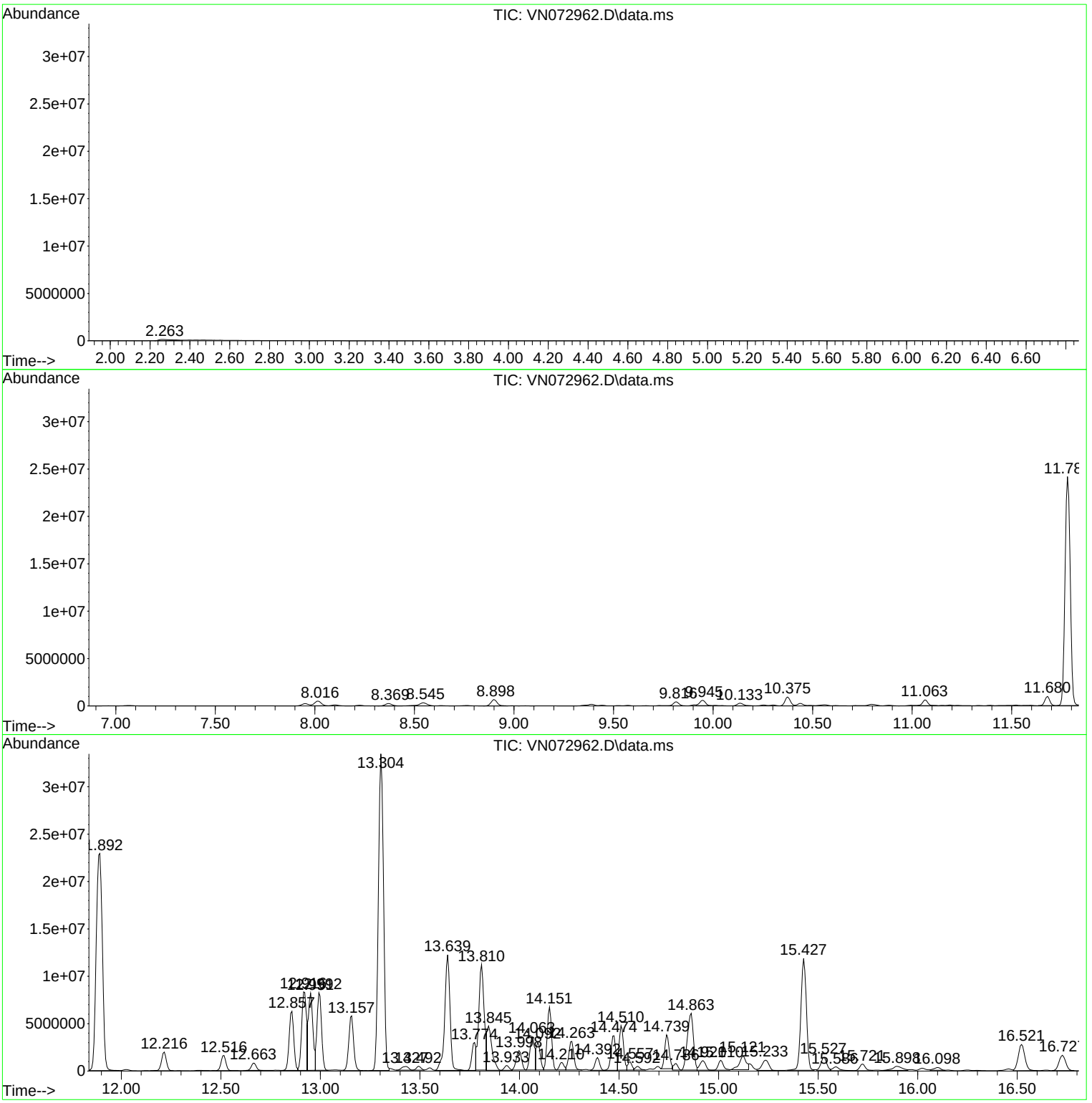
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

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



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Data File : VN072962.D
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Quant Title : SW846 8260

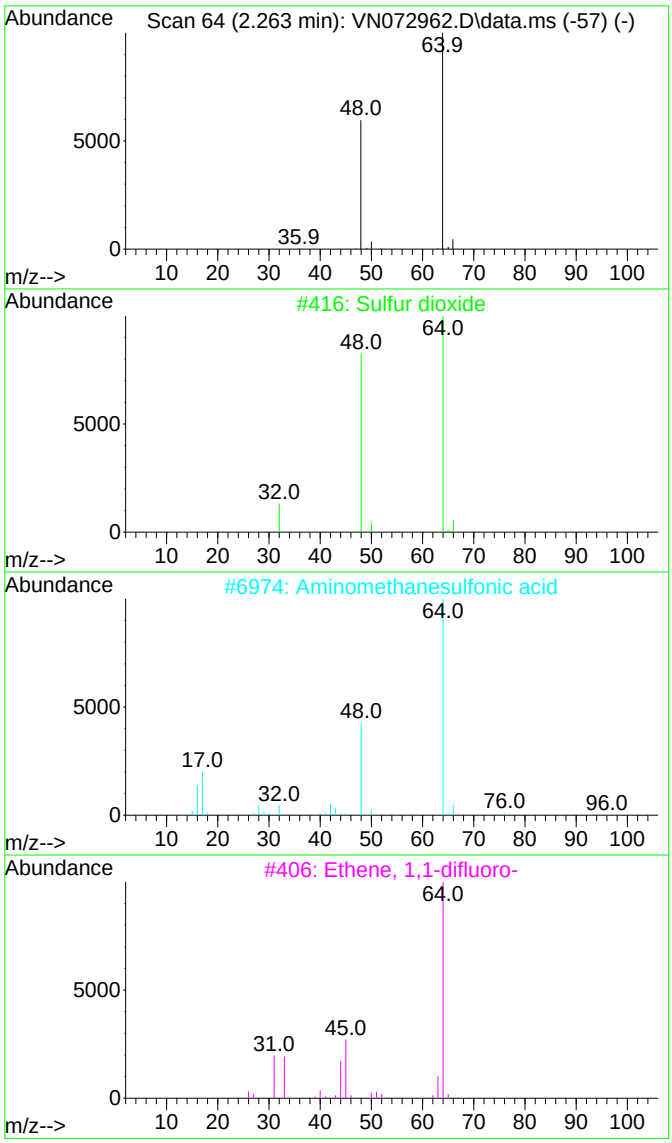
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

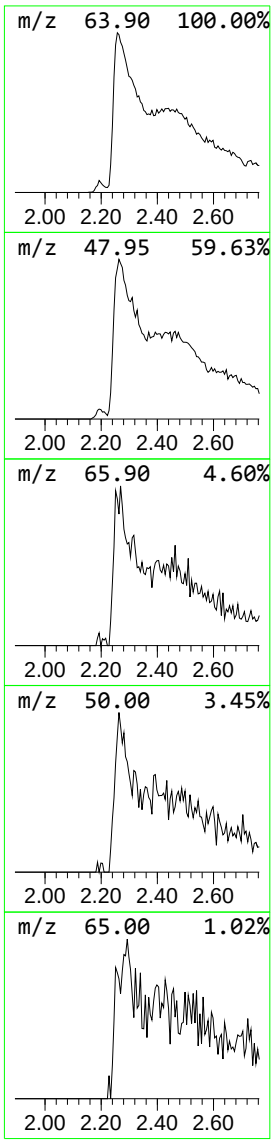
****

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	31.75 ug/l	726575	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	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3





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Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

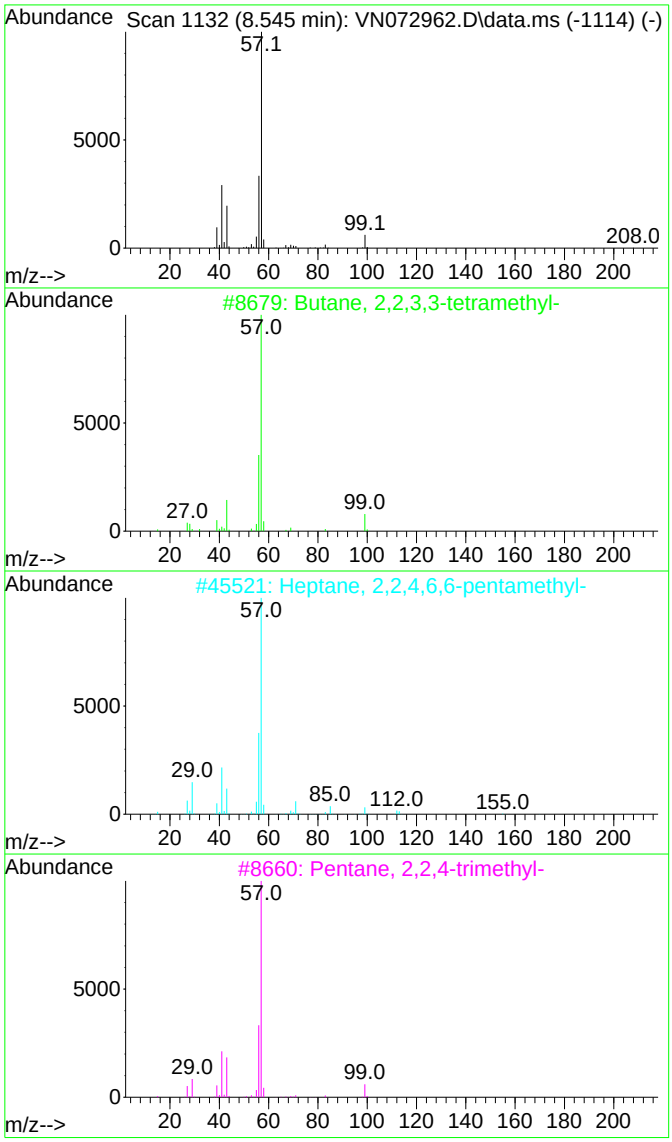
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

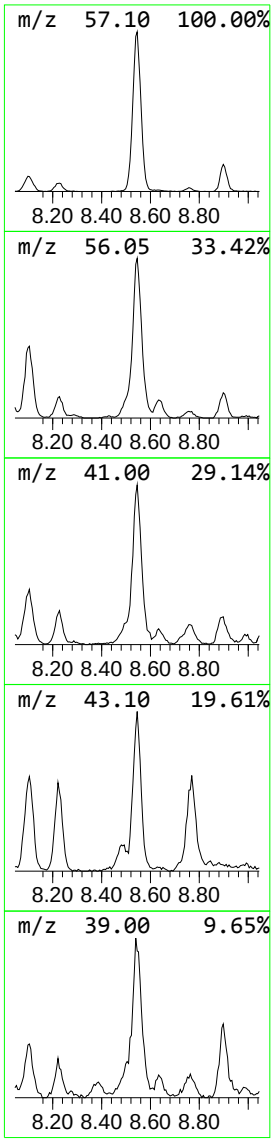
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	33.33 ug/l	955234	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	78
2	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

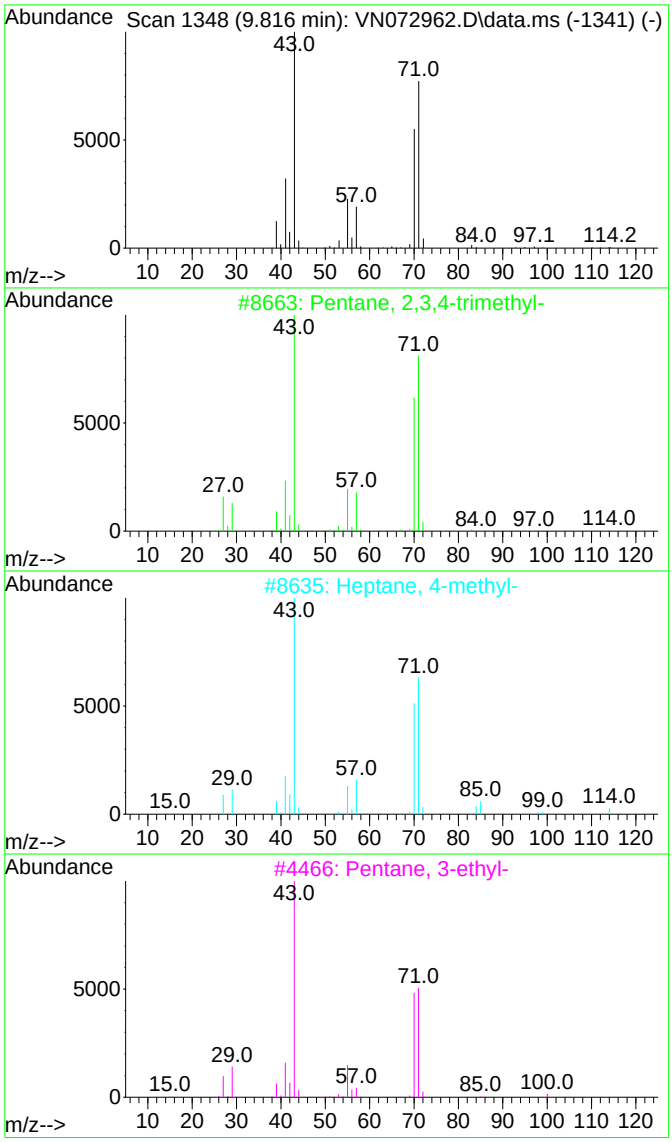
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

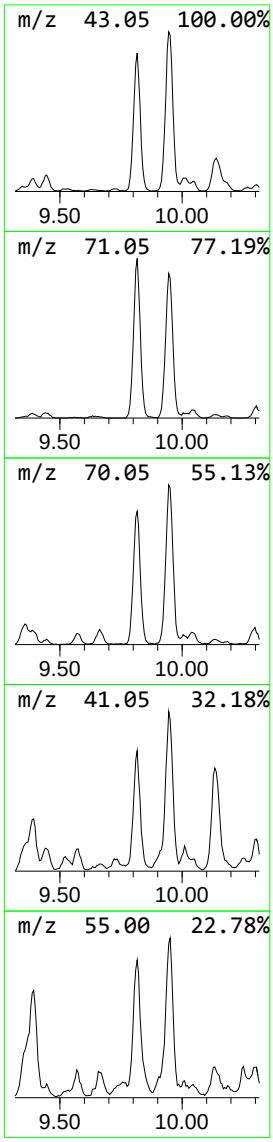
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	29.04 ug/l	832158	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	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

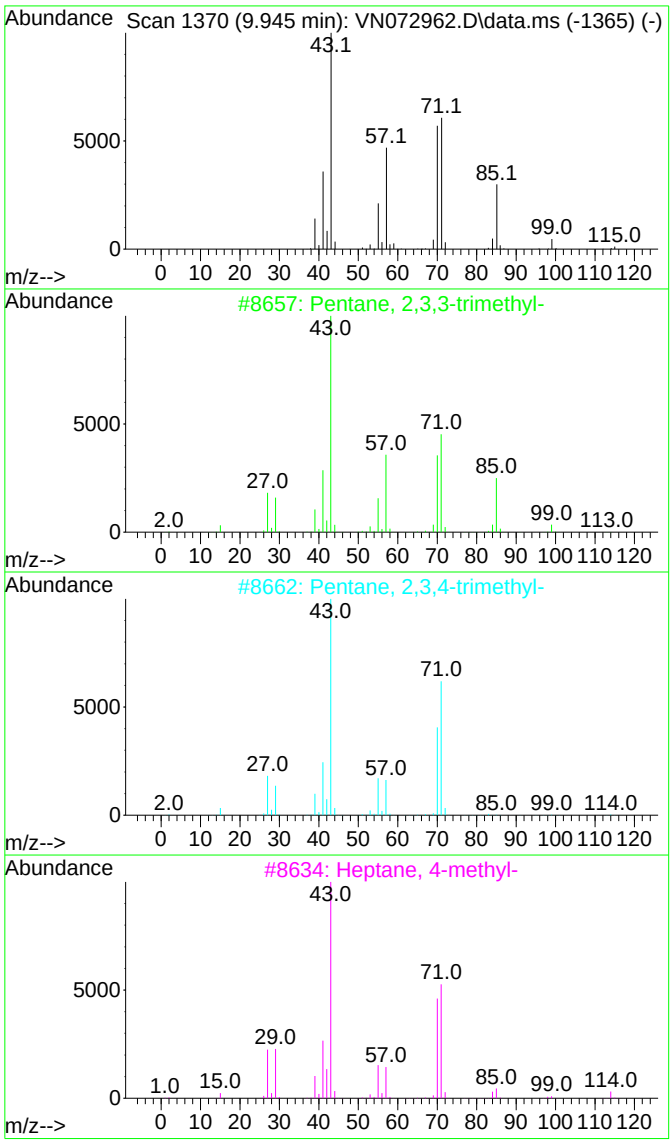
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

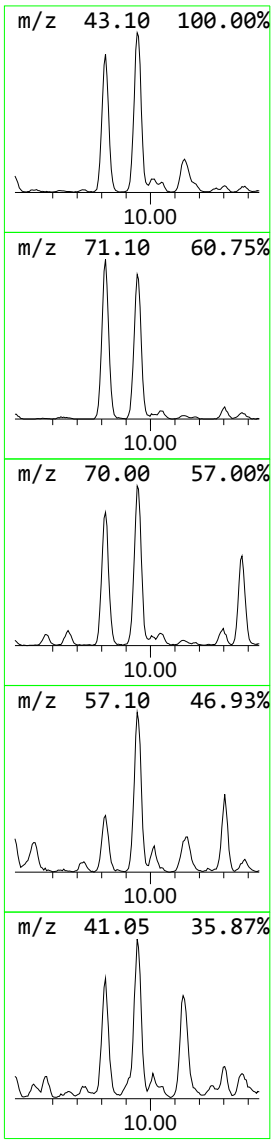
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	38.59 ug/l	1105860	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	83
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53





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Operator : JC\MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

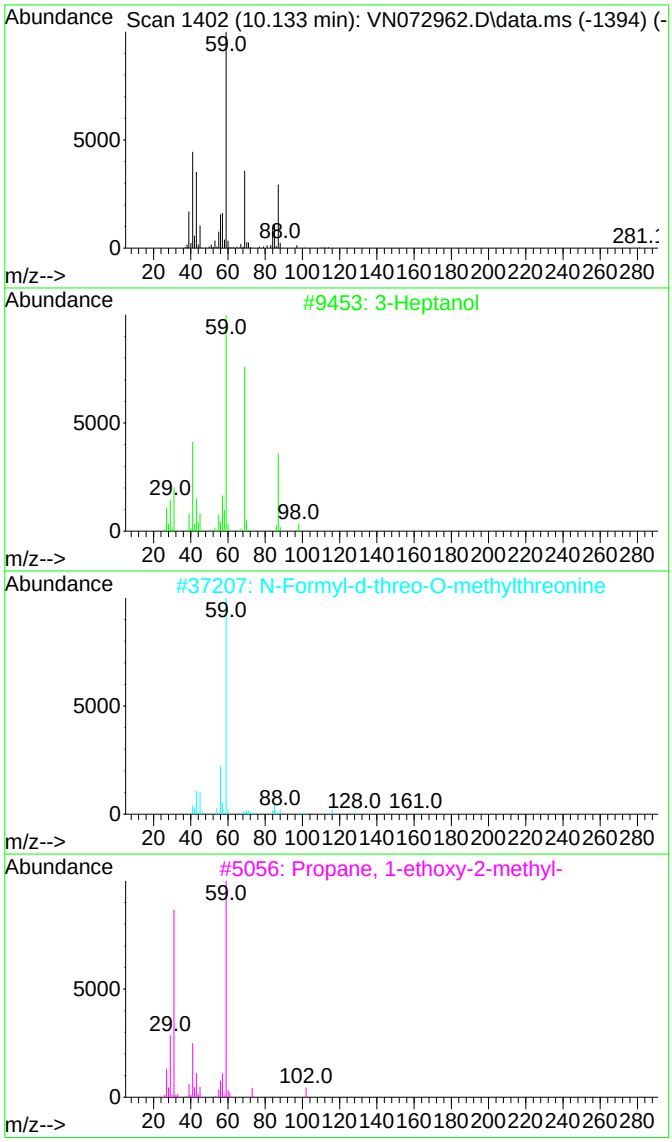
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

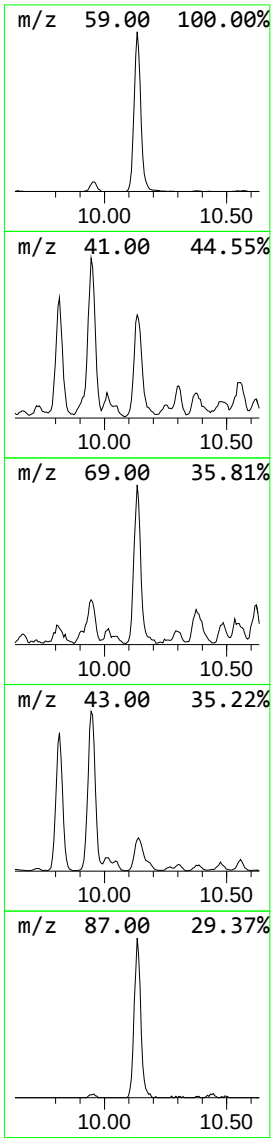
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	23.31 ug/l	668127	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol	116	C7H16O	000589-82-2	64
2	N-Formyl-d-threo-O-methylthreonine	161	C6H11NO4	1000214-69-5	59
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	53
4	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	50
5	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	49





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

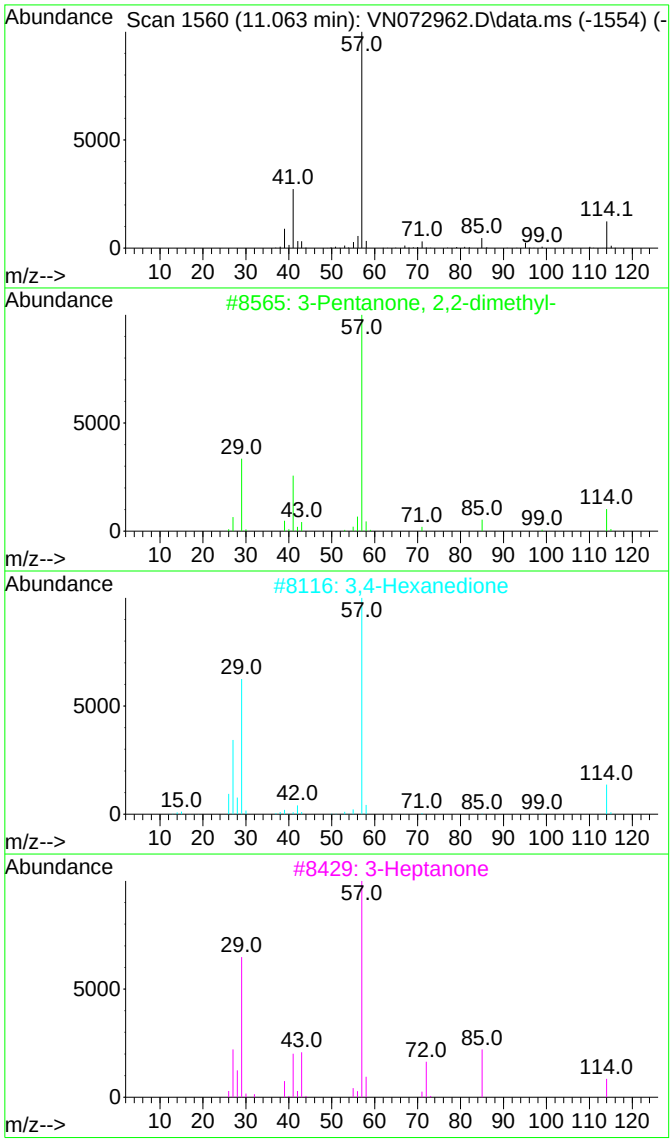
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

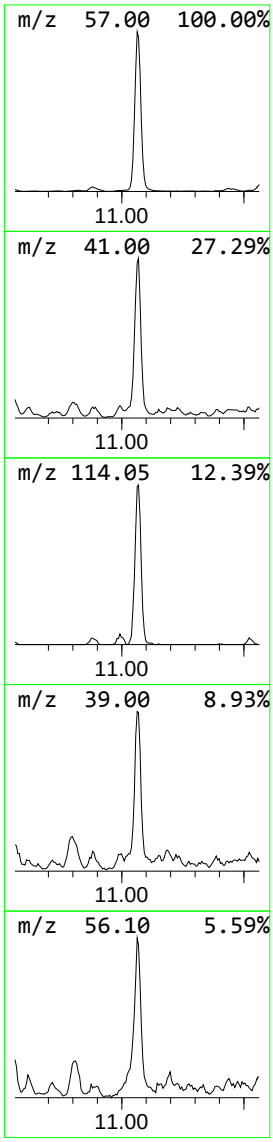
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.063	32.98 ug/l	1107040	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	64
2	3,4-Hexanedione	114	C6H10O2	004437-51-8	49
3	3-Heptanone	114	C7H14O	000106-35-4	47
4	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	47
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	47





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Data File : VN072962.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

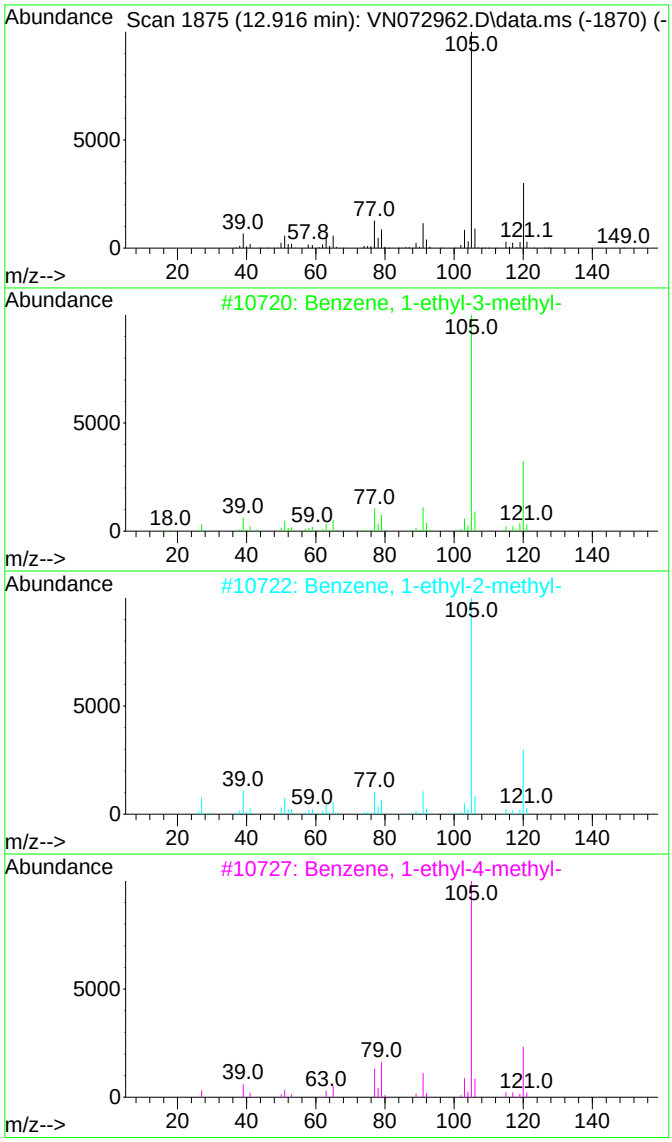
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

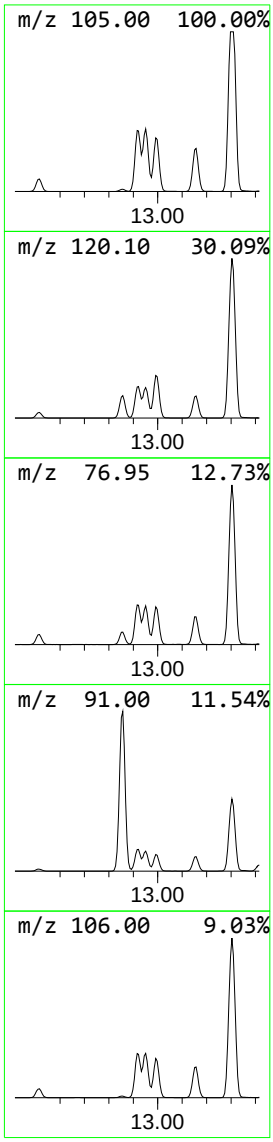
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	31.40 ug/l	13922900	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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
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ALS Vial : 18 Sample Multiplier: 1

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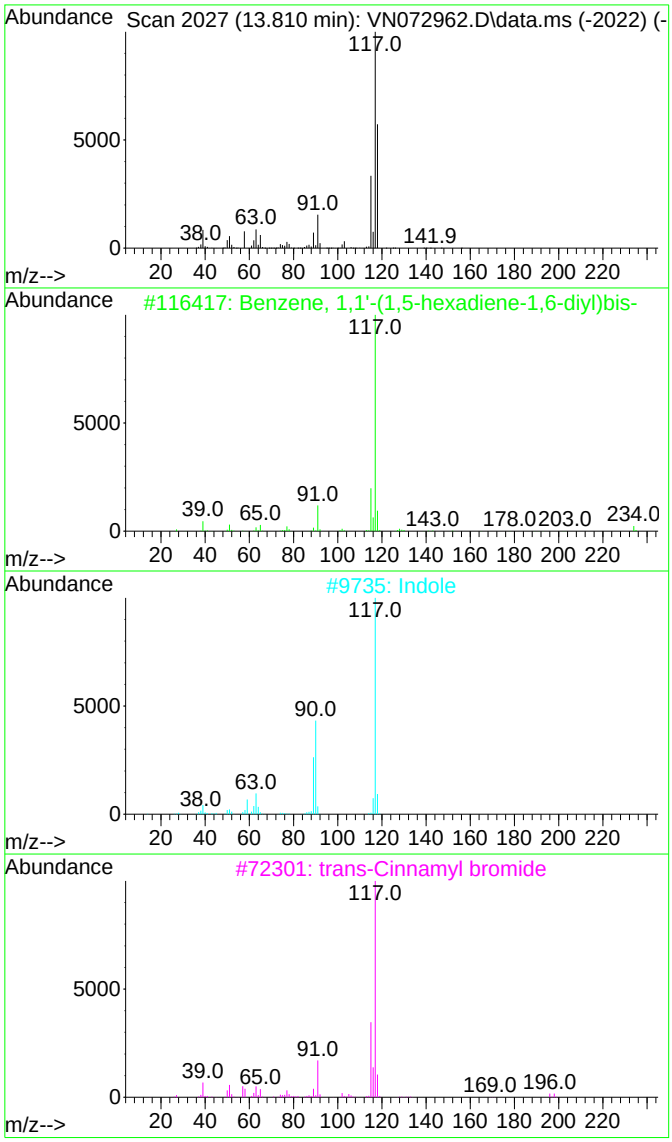
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

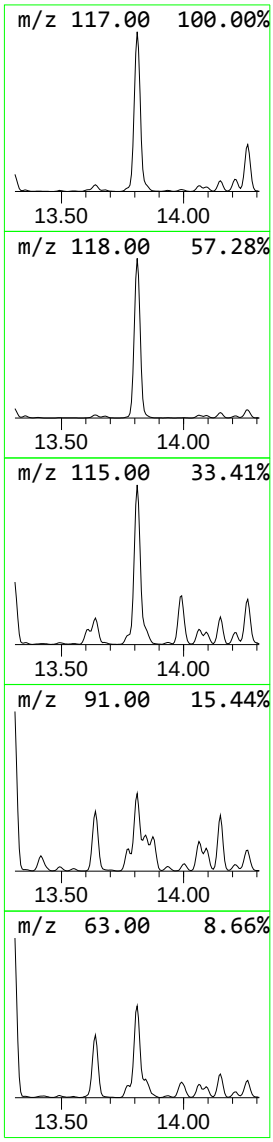
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	47.54 ug/l	21081000	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 : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

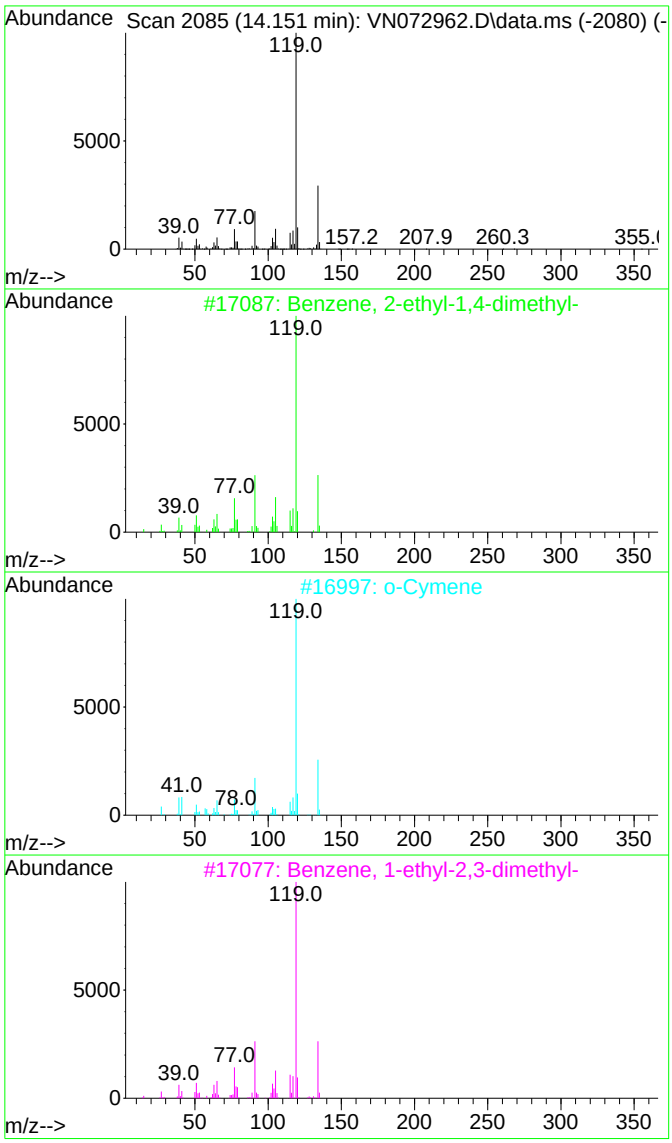
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

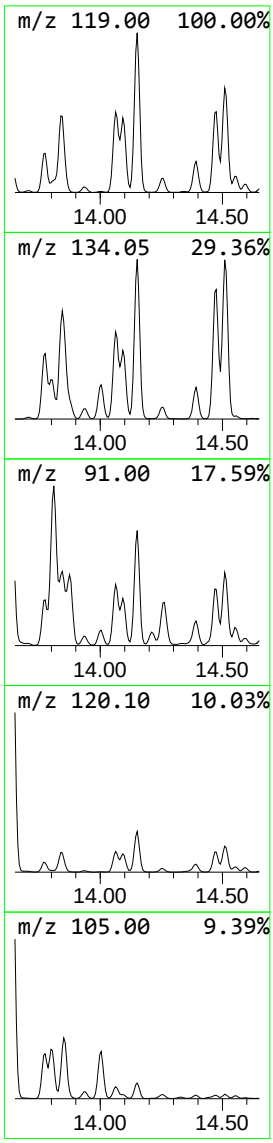
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	22.70 ug/l	10063200	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	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

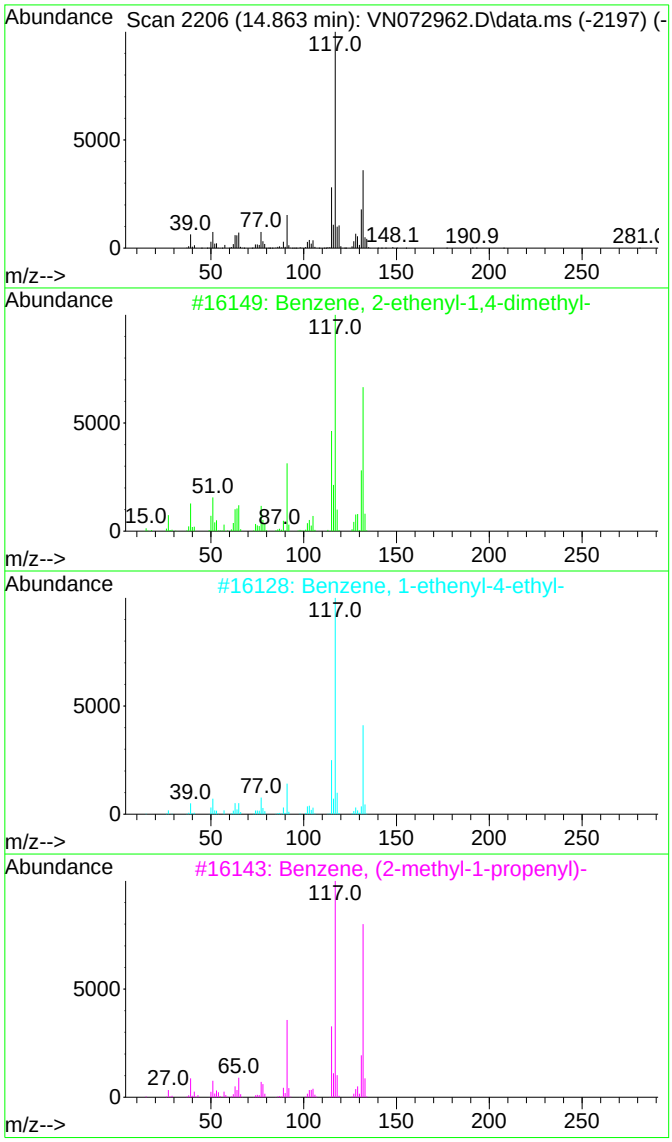
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

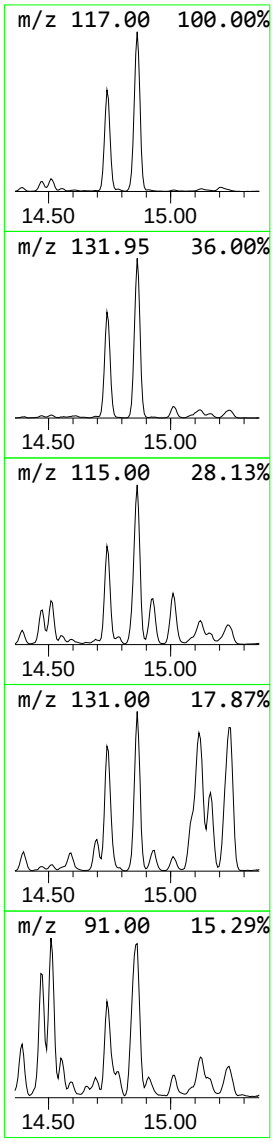
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	28.39 ug/l	12590100	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
Data File : VN072962.D
Acq On : 20 Jun 2022 15:28
Operator : JC\MD
Sample : N3357-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-44

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	2.263	31.8	ug/l	726575	1	8.016	1144380	50.0
Butane, 2,2,3,3...	8.545	33.3	ug/l	955234	2	8.898	1432910	50.0
Pentane, 2,3,4-...	9.816	29.0	ug/l	832158	2	8.898	1432910	50.0
Pentane, 2,3,3-...	9.945	38.6	ug/l	1105860	2	8.898	1432910	50.0
3-Heptanol	10.133	23.3	ug/l	668127	2	8.898	1432910	50.0
3-Pentanone, 2,...	11.063	33.0	ug/l	1107040	3	11.680	1678550	50.0
Benzene, 1-ethy...	12.916	31.4	ug/l	13922900	4	13.610	22169900	50.0
Benzene, 1,1'-(...	13.810	47.5	ug/l	21081000	4	13.610	22169900	50.0
Benzene, 2-ethy...	14.151	22.7	ug/l	10063200	4	13.610	22169900	50.0
Benzene, 2-ethe...	14.863	28.4	ug/l	12590100	4	13.610	22169900	50.0