LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100423\
Data File : VN079418.D
Acq On : 04 Oct 2023 21:13
Operator : JC\MD
Sample : 04689-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-1

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\82N091123W.M
Title : SW846 8260

Signal : TIC: VN079418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	24	rBV2	8051	11677	1.51%	0.187%
2	2.112	24	27	35	rVB	9314	17072	2.21%	0.273%
3	2.330	53	64	77	rBV	189451	746392	96.49%	11.942%
4	2.801	142	144	146	rBV	9813	10869	1.41%	0.174%
5	4.718	464	470	481	rBV3	4122	10540	1.36%	0.169%
6	5.806	647	655	664	rBV3	4175	12252	1.58%	0.196%
7	7.441	925	933	940	rBV2	5240	13372	1.73%	0.214%
8	8.171	1047	1057	1062	rBV	127276	307648	39.77%	4.922%
9	8.230	1062	1067	1077	rVV	180702	401685	51.93%	6.427%
10	8.335	1078	1085	1091	rVB4	9266	22520	2.91%	0.360%
11	8.583	1117	1127	1137	rBV2	151015	425940	55.06%	6.815%
12	8.688	1137	1145	1146	rBV	14153	29188	3.77%	0.467%
13	8.765	1152	1158	1184	rVB4	70051	309487	40.01%	4.952%
14	9.106	1208	1216	1230	rVB	305504	628403	81.24%	10.054%
15	9.600	1289	1300	1304	rBV9	11697	34159	4.42%	0.547%
16	9.653	1304	1309	1316	rVB4	8998	18309	2.37%	0.293%
17	10.018	1364	1371	1380	rVB	43685	88282	11.41%	1.412%
18	10.153	1383	1394	1406	rBV	60201	126113	16.30%	2.018%
19	10.329	1418	1424	1430	rBV6	5078	12866	1.66%	0.206%
20	10.494	1447	1452	1458	rBV3	22863	40010	5.17%	0.640%
21	10.571	1458	1465	1476	rBV	417815	773524	100.00%	12.376%
22	10.988	1530	1536	1538	rBV4	8060	14197	1.84%	0.227%
23	11.300	1587	1589	1596	rVB4	5317	8386	1.08%	0.134%
24	11.871	1678	1686	1698	rBV	374401	683640	88.38%	10.938%
25	12.400	1767	1776	1782	rVB4	4056	9866	1.28%	0.158%
26	12.700	1822	1827	1832	rVB3	7206	10038	1.30%	0.161%
27	12.853	1843	1853	1861	rBV	273063	478314	61.84%	7.653%
28	13.035	1881	1884	1891	rVB3	5964	9968	1.29%	0.159%
29	13.341	1928	1936	1944	rBV	8656	15295	1.98%	0.245%
30	13.617	1974	1983	1991	rBV4	13627	34880	4.51%	0.558%
31	13.800	2006	2014	2024	rBV	244328	433748	56.07%	6.940%
32	13.953	2035	2040	2044	rBV	44288	73002	9.44%	1.168%
33	14.000	2044	2048	2051	rVV	28728	48080	6.22%	0.769%
34	14.035	2051	2054	2062	rVB3	18627	33170	4.29%	0.531%
35	14.123	2062	2069	2075	rVB	9124	14483	1.87%	0.232%
36	14.335	2100	2105	2110	rVB3	18091	30109	3.89%	0.482%

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Title : SW846 8260

37	14.400	2110	2116	2119	rBV4	9553	15778	2.04%	0.252%
38	14.447	2119	2124	2130	rVB2	29377	53245	6.88%	0.852%
39	14.541	2132	2140	2142	rBV6	5797	11433	1.48%	0.183%
40	14.659	2152	2160	2165	rBV	28318	49134	6.35%	0.786%
41	14.929	2201	2206	2217	rVB5	26105	51048	6.60%	0.817%
42	15.059	2217	2228	2235	rBV3	41746	83481	10.79%	1.336%
43	15.206	2249	2253	2261	rBV6	4056	7829	1.01%	0.125%
44	15.317	2266	2272	2278	rBV3	7546	16433	2.12%	0.263%
45	15.441	2285	2293	2300	rVB5	10581	24245	3.13%	0.388%

Sum of corrected areas: 6250110

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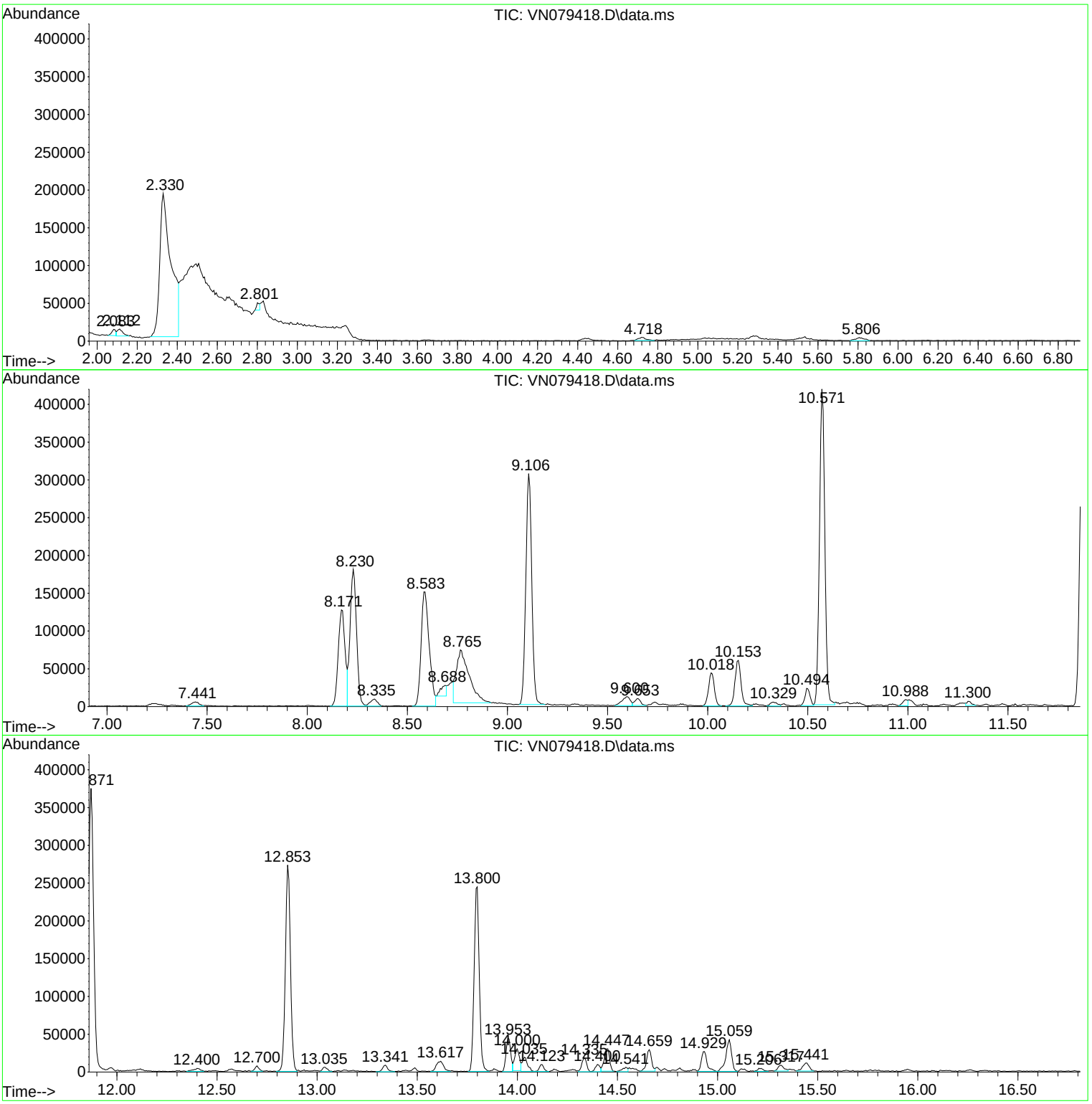
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

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



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Data File : VN079418.D
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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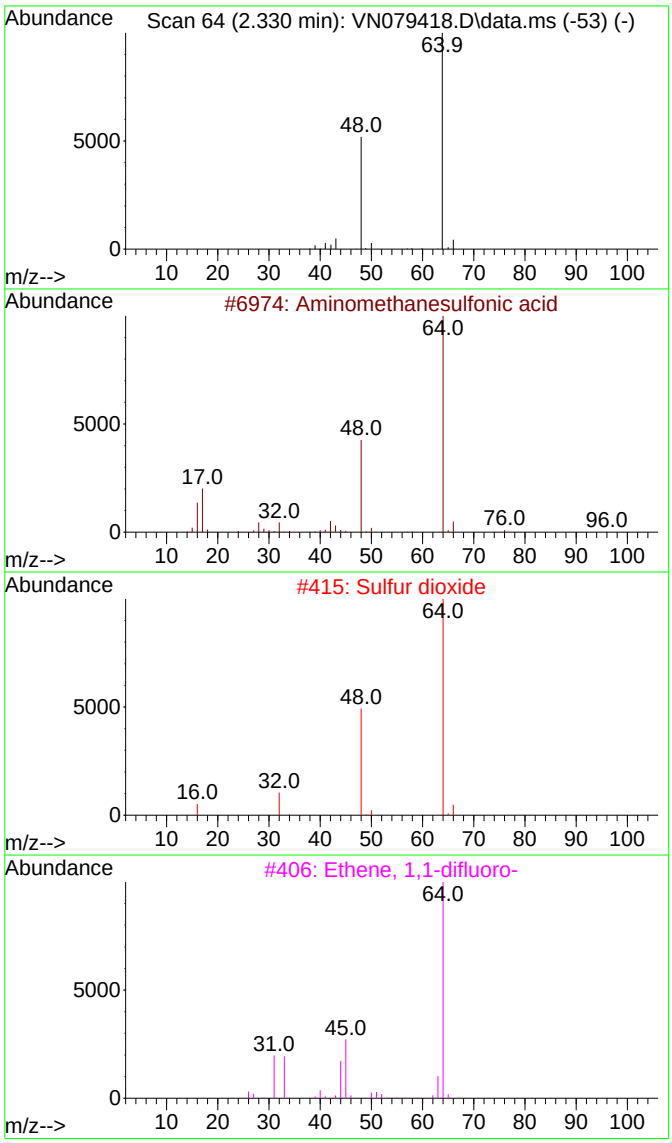
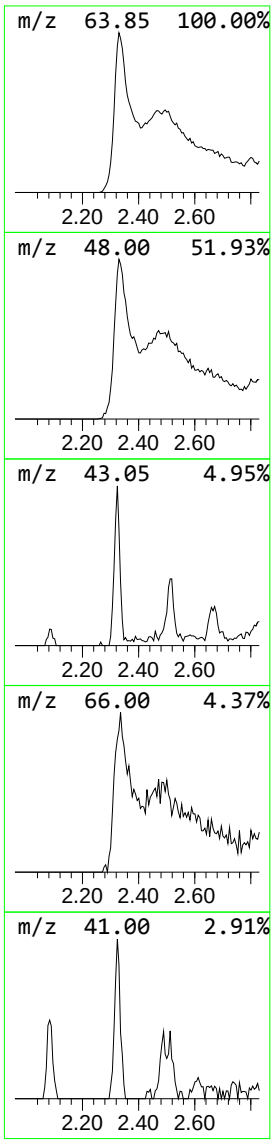
****
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.330	92.91 ug/l	746392	Pentafluorobenzene	8.230

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





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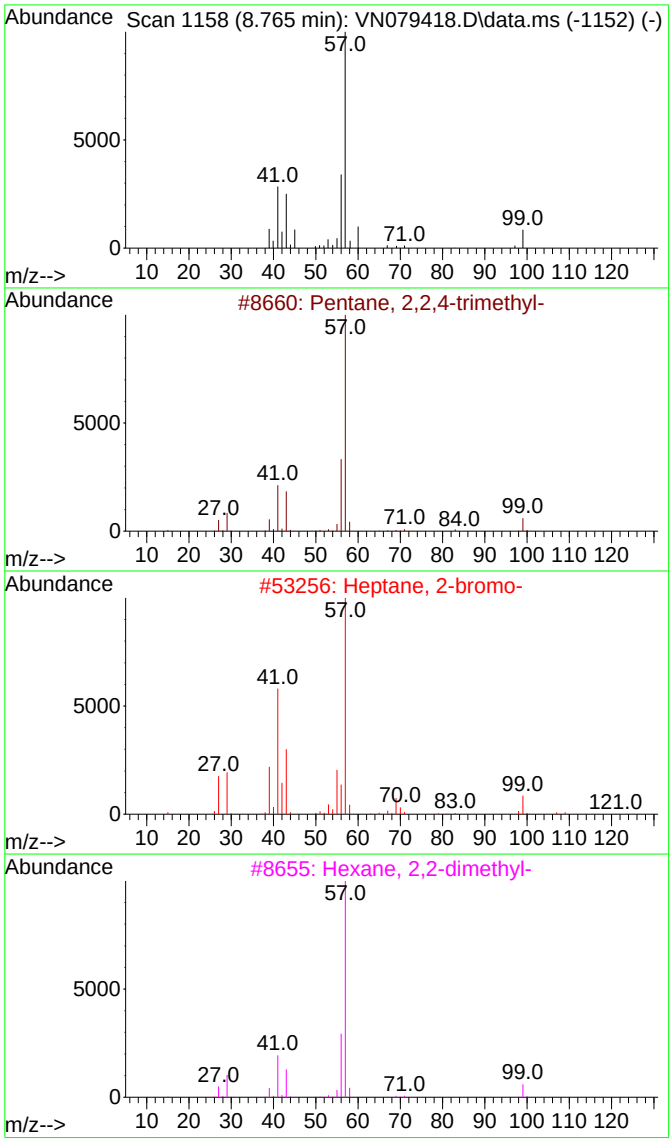
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

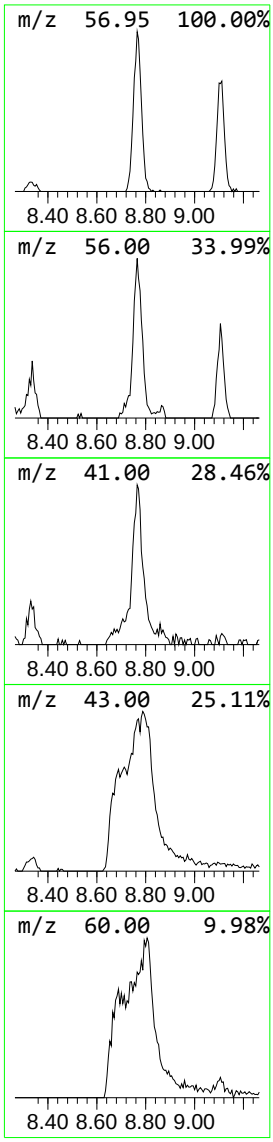
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	24.62 ug/l	309487	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	50
2	Heptane, 2-bromo-	178	C7H15Br	001974-04-5	43
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	40
4	Azetidine	57	C3H7N	000503-29-7	37
5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	33





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-1

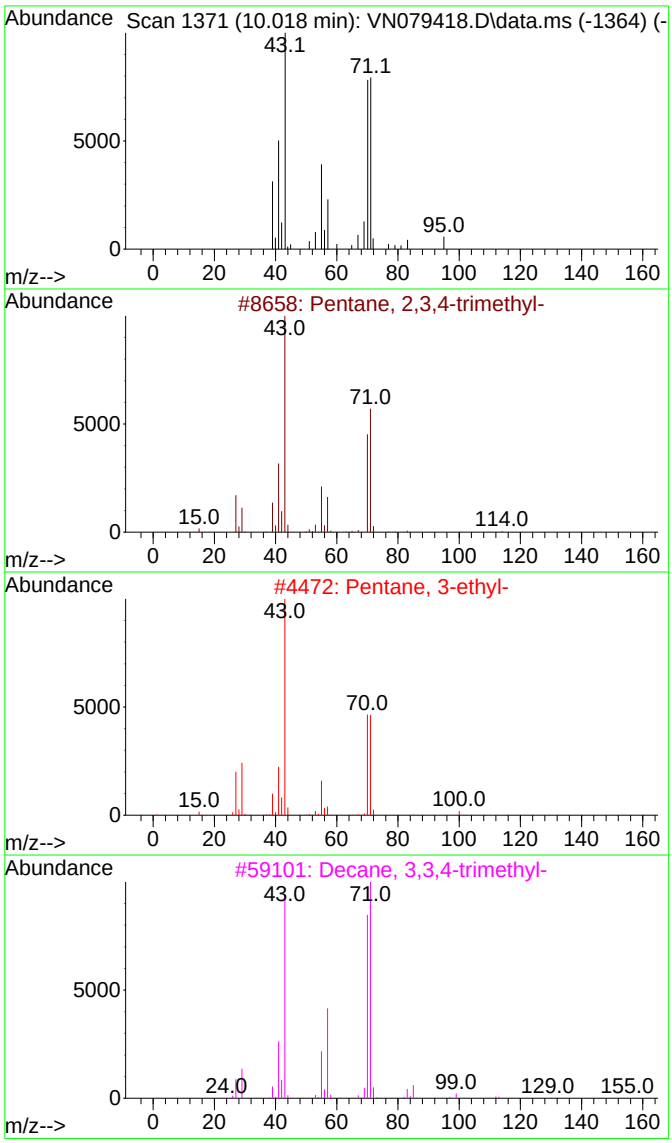
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

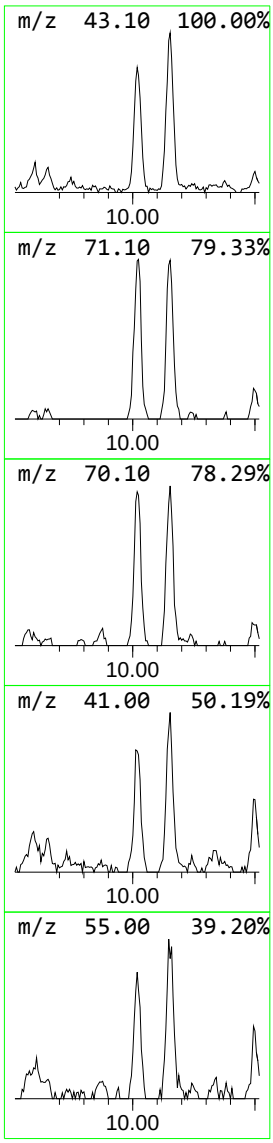
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.018	7.02 ug/l	88282	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
4	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	50
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	50





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Instrument :
MSVOA_N
ClientSampleId :
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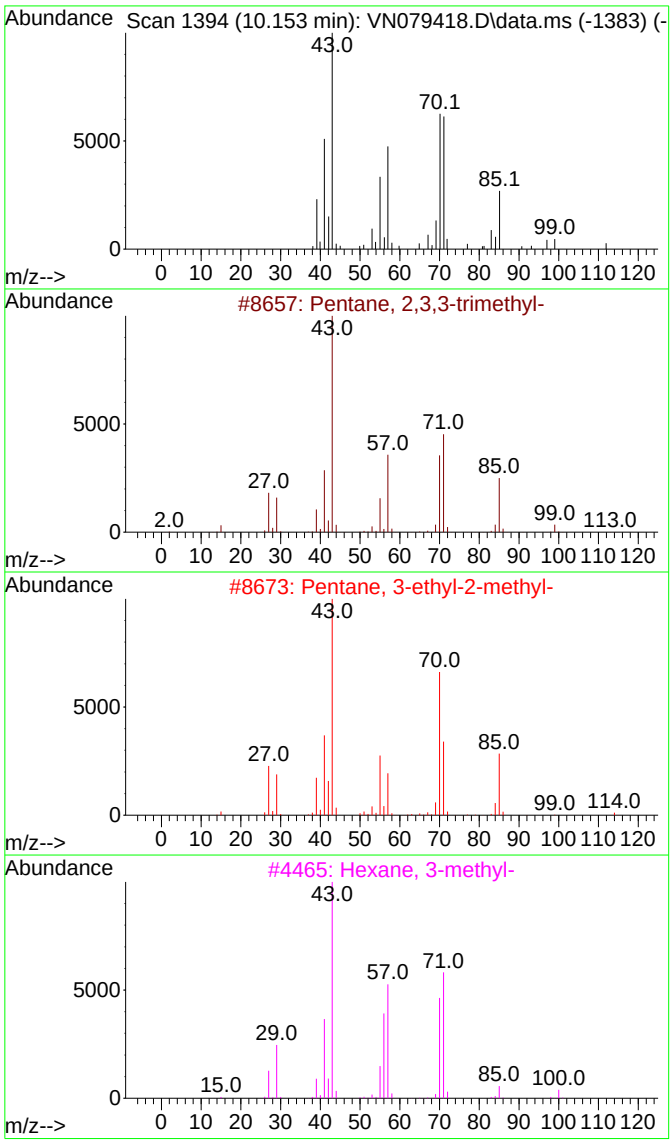
Quant Title : SW846 8260

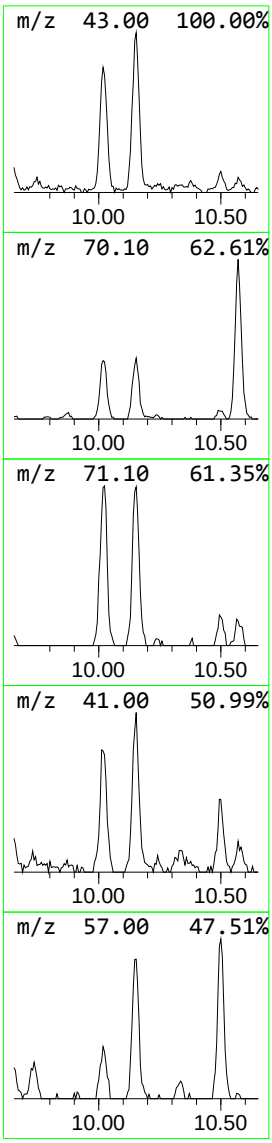
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	10.03 ug/l	126113	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	53
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4	Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	50
5	1-Heptene, 4-methyl-	112	C8H16	013151-05-8	50





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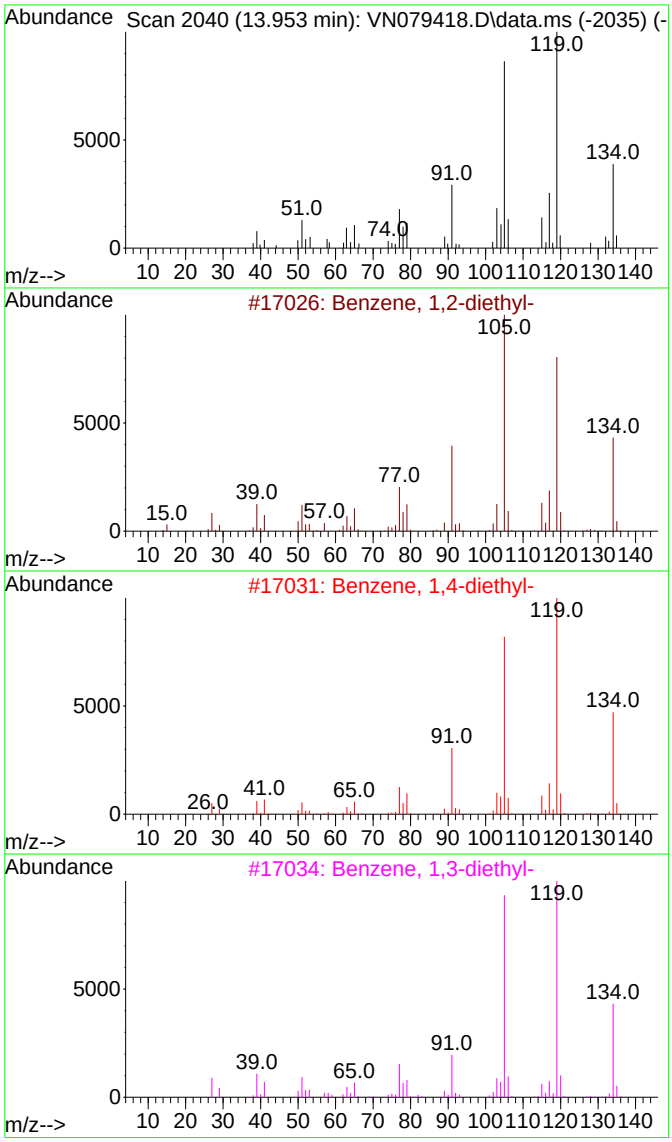
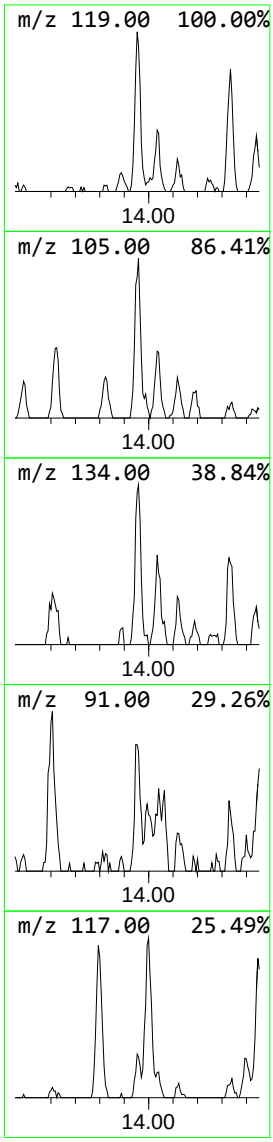
****
Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.953	8.42 ug/l	73002	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	91
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	90
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	64
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	58





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TIC Library : C:\Database\NIST20.L
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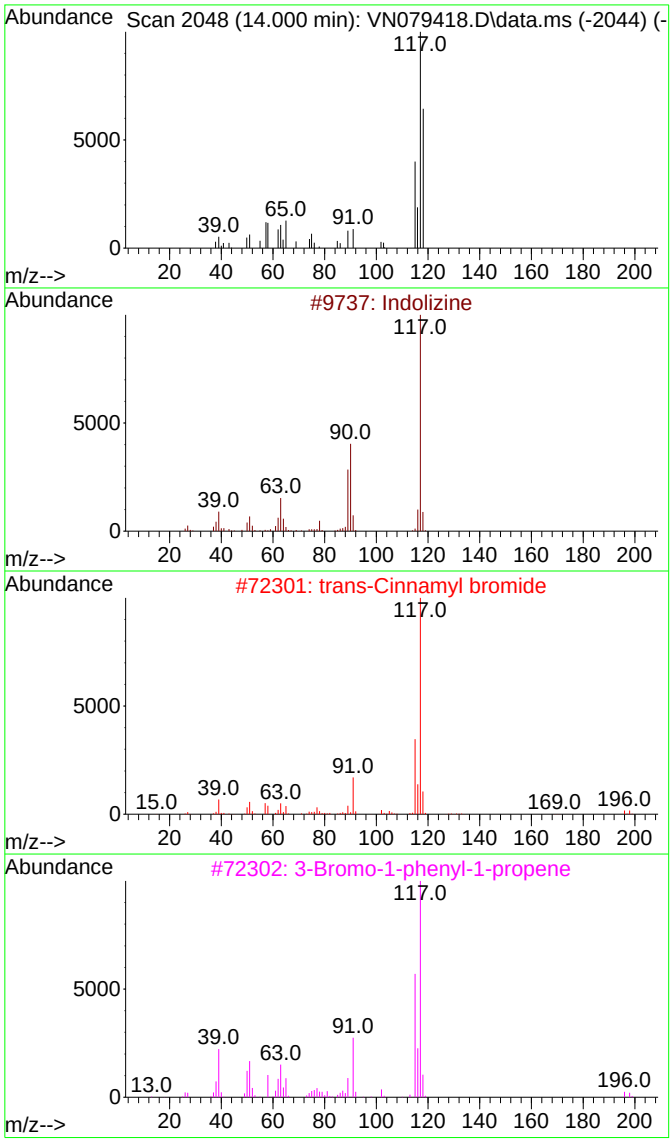
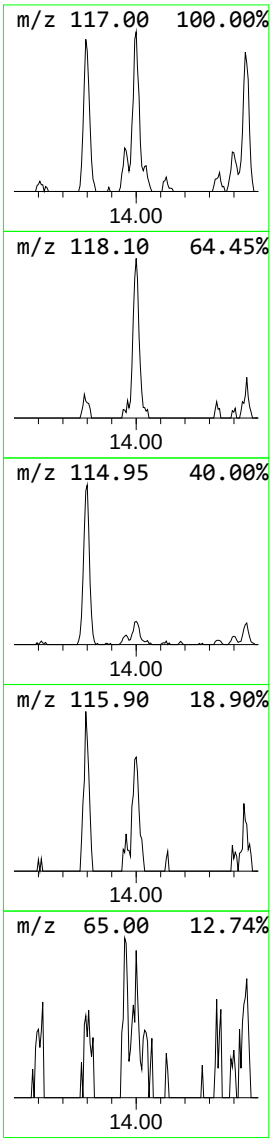
****
Peak Number 6 unknown14.000 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	5.54 ug/l	48080	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indolizine	117	C8H7N	000274-40-8	46
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
3	3-Bromo-1-phenyl-1-propene	196	C9H9Br	004392-24-9	45
4	4-Ethynylaniline	117	C8H7N	014235-81-5	43
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	38





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TIC Library : C:\Database\NIST20.L
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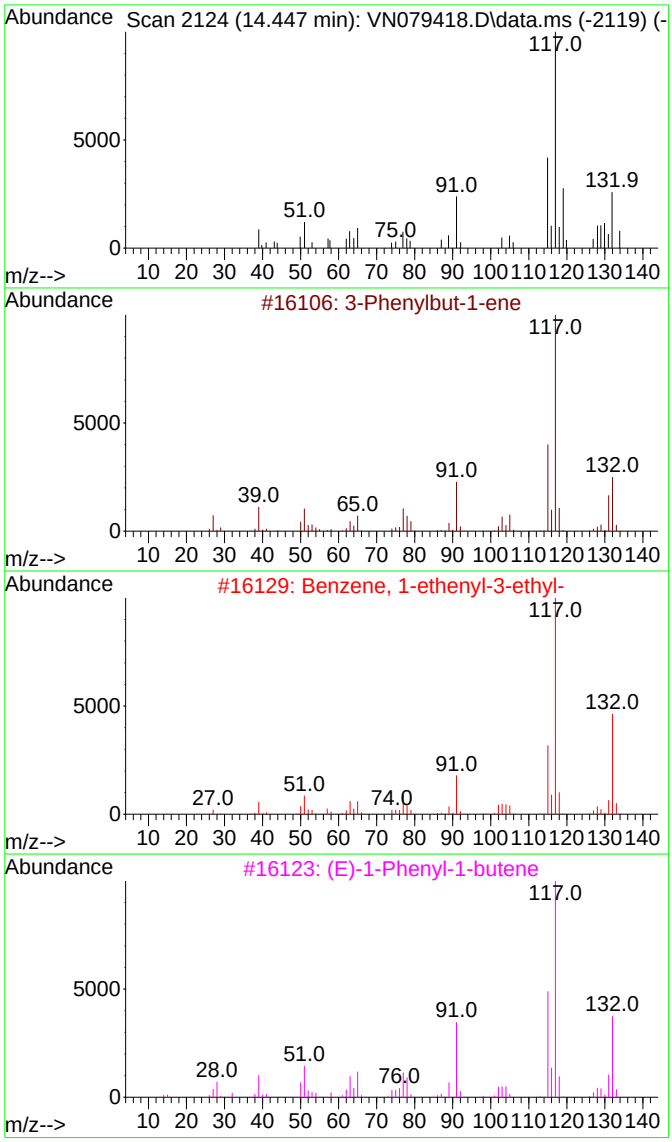
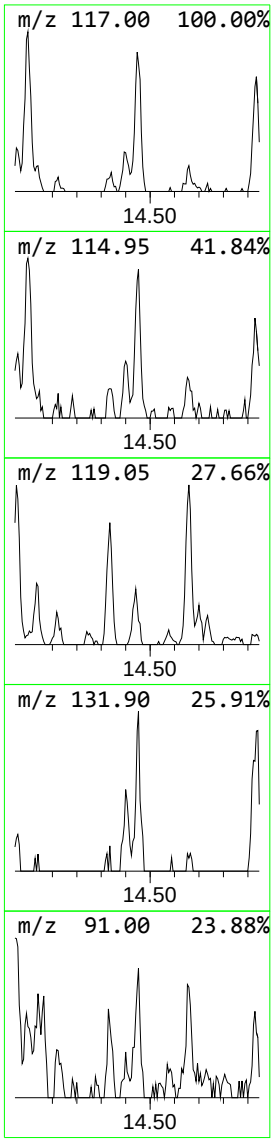
****
Peak Number 7 3-Phenylbut-1-ene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	6.14 ug/l	53245	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
3	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	76
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	68
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64





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Instrument :
MSVOA_N
ClientSampleId :
TW-1

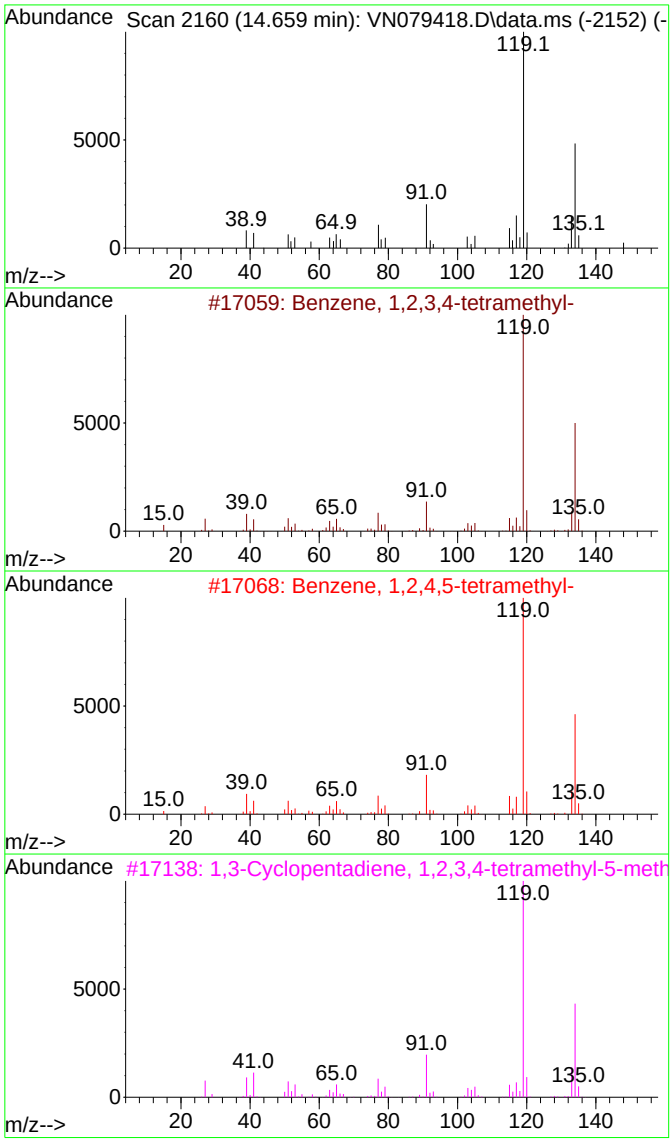
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

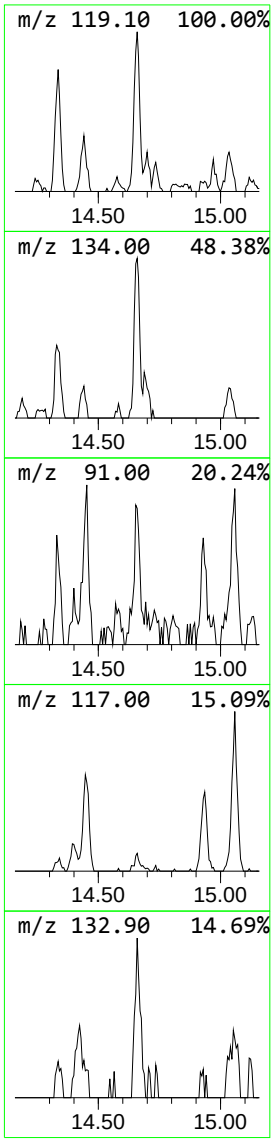
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	5.66 ug/l	49134	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
3	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	91
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100423\
Data File : VN079418.D
Acq On : 04 Oct 2023 21:13
Operator : JC\MD
Sample : 04689-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-1

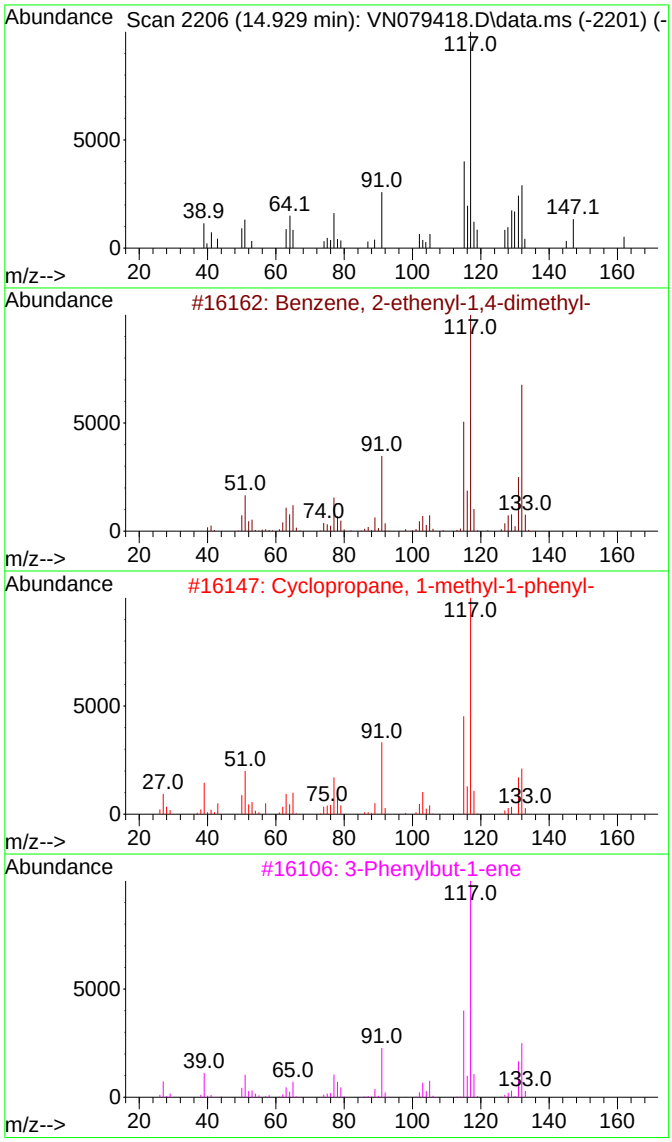
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

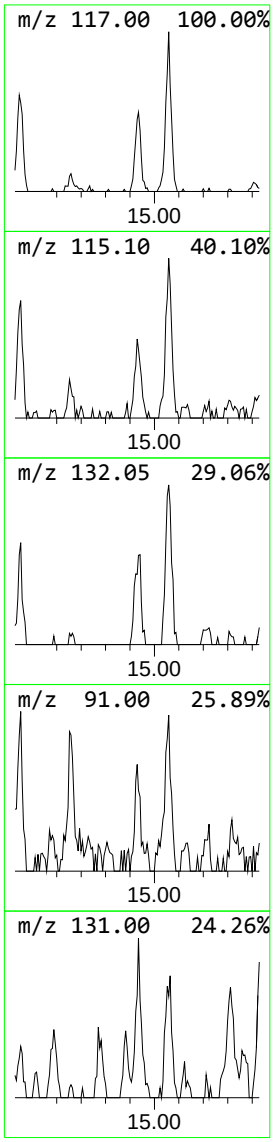
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	5.88 ug/l	51048	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	74
2	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	68
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	58
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	58
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100423\
Data File : VN079418.D
Acq On : 04 Oct 2023 21:13
Operator : JC\MD
Sample : 04689-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-1

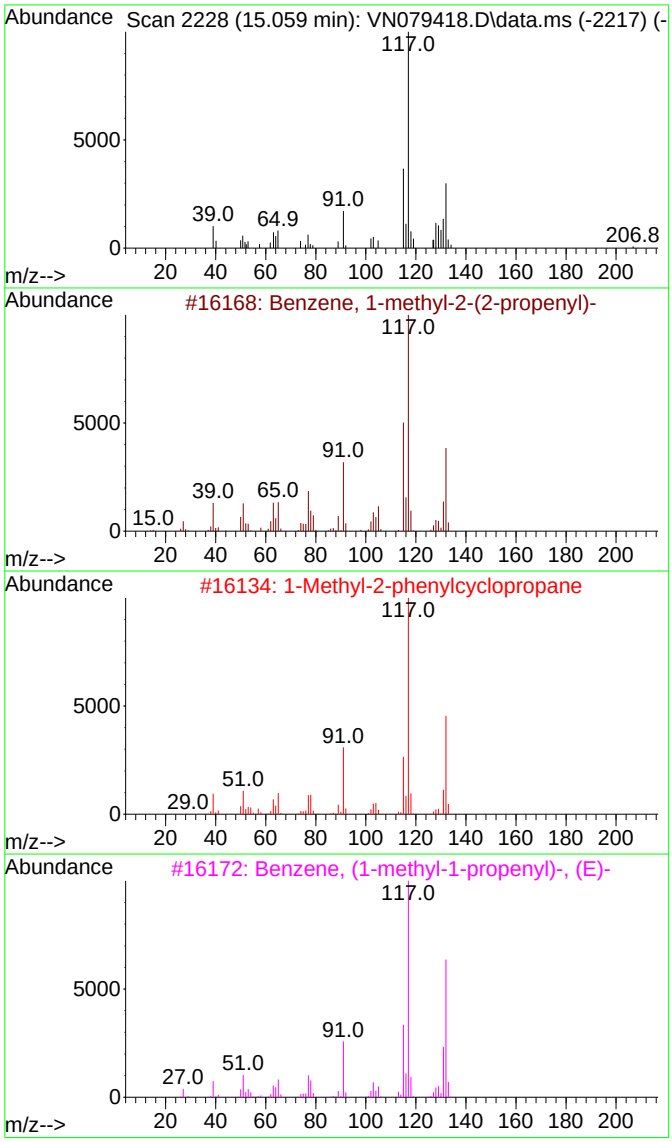
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.M
Quant Title : SW846 8260

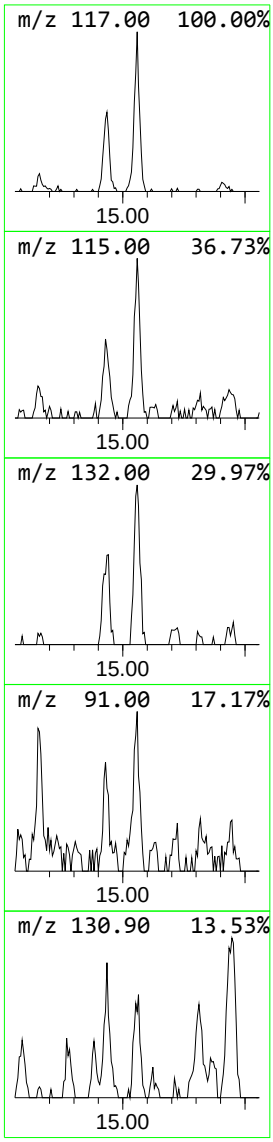
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-methyl-2-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	9.62 ug/l	83481	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100423\
Data File : VN079418.D
Acq On : 04 Oct 2023 21:13
Operator : JC\MD
Sample : 04689-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091123W.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
Aminomethanesul...	2.330	92.9	ug/l	746392	1	8.230	401685	50.0
Pentane, 2,2,4-...	8.765	24.6	ug/l	309487	2	9.106	628403	50.0
Pentane, 2,3,4-...	10.018	7.0	ug/l	88282	2	9.106	628403	50.0
Pentane, 2,3,3-...	10.153	10.0	ug/l	126113	2	9.106	628403	50.0
Benzene, 1,2-di...	13.953	8.4	ug/l	73002	4	13.800	433748	50.0
unknown14.000	14.000	5.5	ug/l	48080	4	13.800	433748	50.0
3-Phenylbut-1-ene	14.447	6.1	ug/l	53245	4	13.800	433748	50.0
Benzene, 1,2,3,...	14.659	5.7	ug/l	49134	4	13.800	433748	50.0
Benzene, 2-ethe...	14.929	5.9	ug/l	51048	4	13.800	433748	50.0
Benzene, 1-meth...	15.059	9.6	ug/l	83481	4	13.800	433748	50.0