LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	60	rBV	238103	456365	22.97%	2.944%
2	2.693	133	137	141	rBV2	41083	86974	4.38%	0.561%
3	4.187	381	391	392	rBV3	12663	29802	1.50%	0.192%
4	4.210	393	395	404	rVB6	12181	33039	1.66%	0.213%
5	4.998	517	529	540	rBV3	34560	139745	7.03%	0.901%
6	5.239	561	570	573	rBV5	11807	35343	1.78%	0.228%
7	5.528	608	619	620	rBV4	17438	33948	1.71%	0.219%
8	5.545	620	622	632	rVB5	16316	30401	1.53%	0.196%
9	6.969	856	864	870	rBV5	10269	26340	1.33%	0.170%
10	7.233	896	909	925	rBV2	58953	174878	8.80%	1.128%
11	7.951	1020	1031	1036	rBV	267362	660161	33.22%	4.259%
12	8.016	1036	1042	1051	rVV	418678	966378	48.64%	6.234%
13	8.098	1051	1056	1065	rVB4	38683	99753	5.02%	0.644%
14	8.228	1070	1078	1084	rBV6	12867	34392	1.73%	0.222%
15	8.369	1092	1102	1113	rVV	306899	718572	36.16%	4.635%
16	8.492	1116	1123	1124	rVV6	18898	32395	1.63%	0.209%
17	8.545	1124	1132	1143	rVV2	173555	467361	23.52%	3.015%
18	8.639	1143	1148	1156	rVB6	22171	49506	2.49%	0.319%
19	8.904	1182	1193	1201	rBV	703560	1428838	71.91%	9.217%
20	9.357	1262	1270	1276	rBV4	45716	103029	5.19%	0.665%
21	9.527	1292	1299	1305	rVV3	22941	50237	2.53%	0.324%
22	9.674	1314	1324	1330	rVB4	19130	45811	2.31%	0.296%
23	9.816	1342	1348	1358	rVB2	159456	313642	15.79%	2.023%
24	9.951	1358	1371	1378	rBV	299463	614047	30.90%	3.961%
25	10.139	1396	1403	1409	rBV8	15809	37917	1.91%	0.245%
26	10.304	1427	1431	1435	rVV5	18361	33234	1.67%	0.214%
27	10.380	1437	1444	1459	rVV	1097471	1986956	100.00%	12.818%
28	10.551	1465	1473	1474	rBV5	17221	26354	1.33%	0.170%
29	10.574	1474	1477	1484	rVB6	24335	41964	2.11%	0.271%
30	10.810	1508	1517	1524	rVB5	39240	102686	5.17%	0.662%
31	11.198	1579	1583	1587	rVB6	17248	27051	1.36%	0.175%
32	11.686	1659	1666	1677	rBV	1089409	1877197	94.48%	12.110%
33	12.521	1803	1808	1815	rBV8	11940	26509	1.33%	0.171%
34	12.674	1826	1834	1844	rBV	842882	1429544	71.95%	9.222%
35	12.863	1863	1866	1872	rVB2	14609	20898	1.05%	0.135%
36	13.427	1955	1962	1970	rVB3	56961	135984	6.84%	0.877%

LSC Area Percent Report

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Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

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\82N091522W.M
Title : SW846 8260

37	13.615	1987	1994	2007	rBV	1031846	1712568	86.19%	11.048%
38	13.780	2015	2022	2031	rVV	125294	208095	10.47%	1.342%
39	13.868	2031	2037	2038	rVV4	14933	27268	1.37%	0.176%
40	13.886	2038	2040	2044	rVV3	20197	23476	1.18%	0.151%
41	13.945	2044	2050	2056	rVB5	27240	50549	2.54%	0.326%
42	14.092	2067	2075	2080	rBV4	25912	57163	2.88%	0.369%
43	14.157	2080	2086	2093	rVV	115075	177488	8.93%	1.145%
44	14.221	2093	2097	2100	rVV3	11648	21358	1.07%	0.138%
45	14.268	2100	2105	2111	rVV2	66017	116736	5.88%	0.753%
46	14.345	2114	2118	2125	rVV6	28557	49176	2.47%	0.317%
47	14.404	2125	2128	2132	rVV4	16646	24265	1.22%	0.157%
48	14.480	2132	2141	2150	rVB	180668	306220	15.41%	1.975%
49	14.751	2183	2187	2192	rBV5	31602	53976	2.72%	0.348%
50	14.874	2200	2208	2213	rBV5	37061	84051	4.23%	0.542%
51	15.127	2244	2251	2256	rBV6	42493	88575	4.46%	0.571%
52	15.245	2264	2271	2277	rVB5	41898	100653	5.07%	0.649%
53	16.033	2401	2405	2412	rBV5	11635	22744	1.14%	0.147%

Sum of corrected areas: 15501612

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Sample : N4549-11
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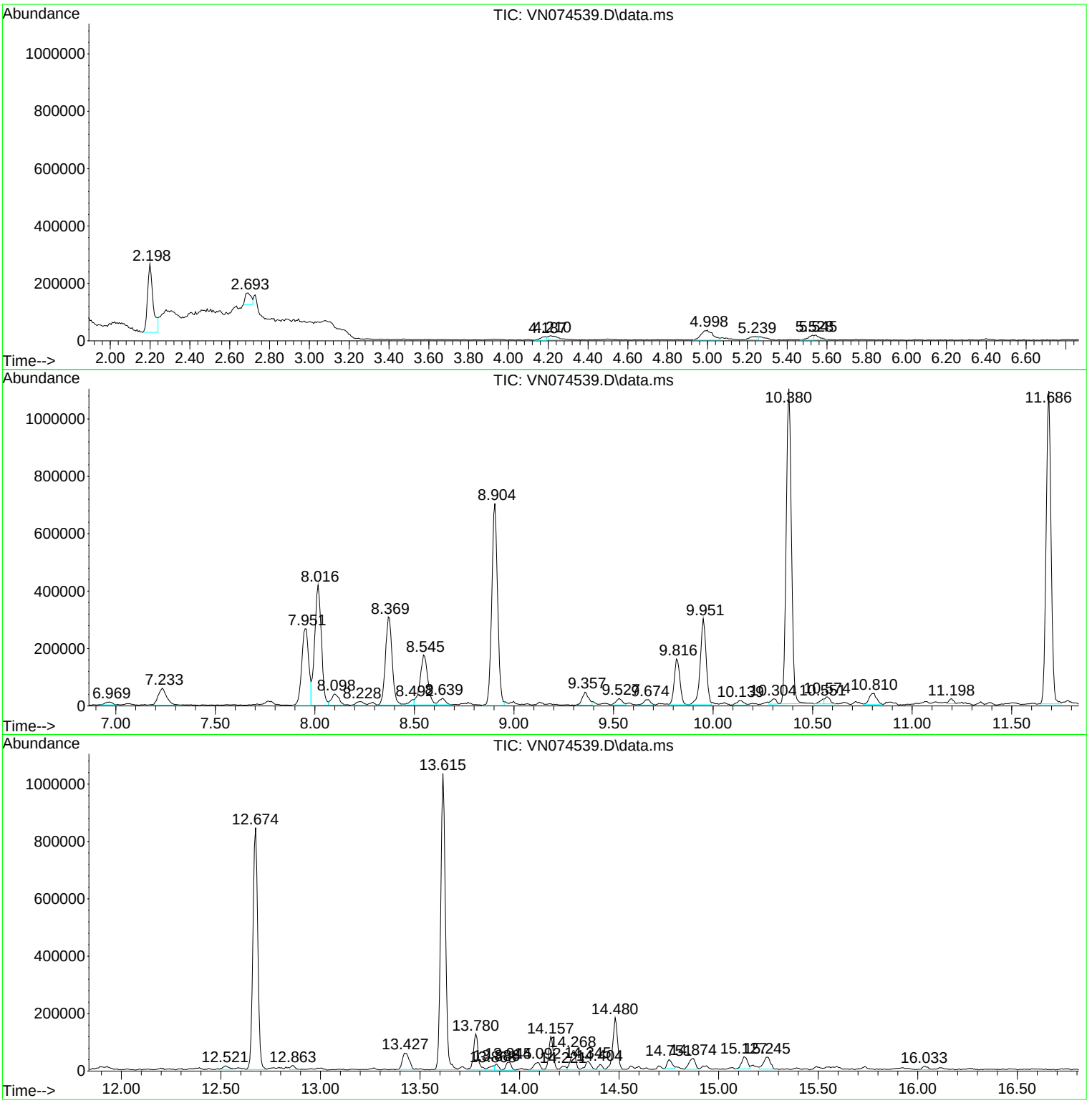
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

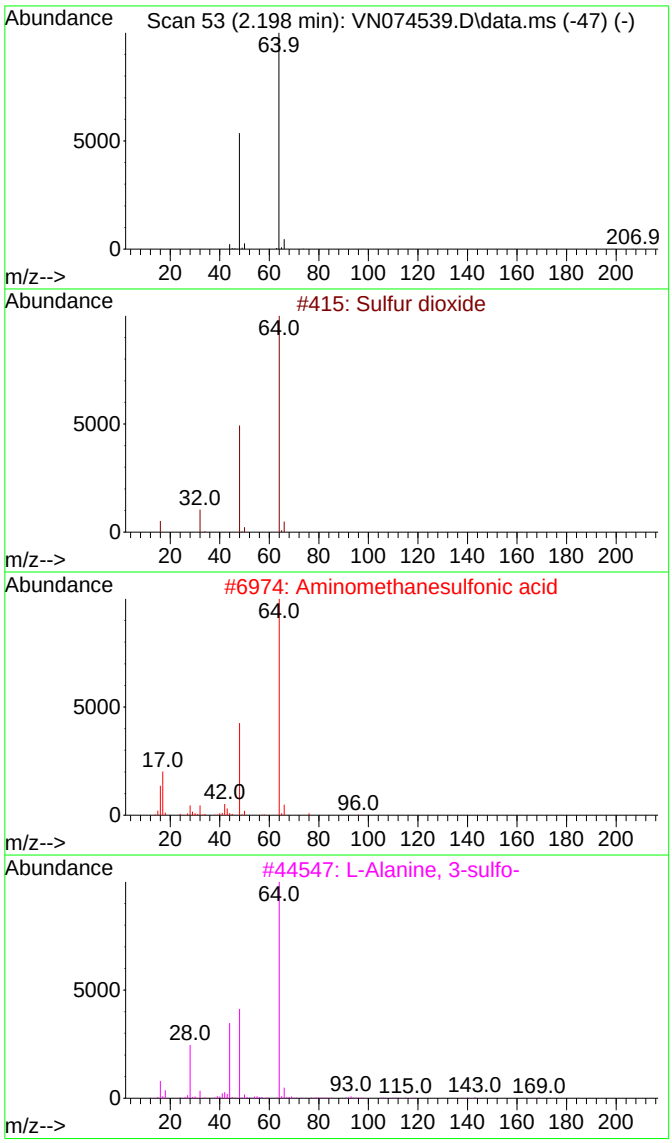
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

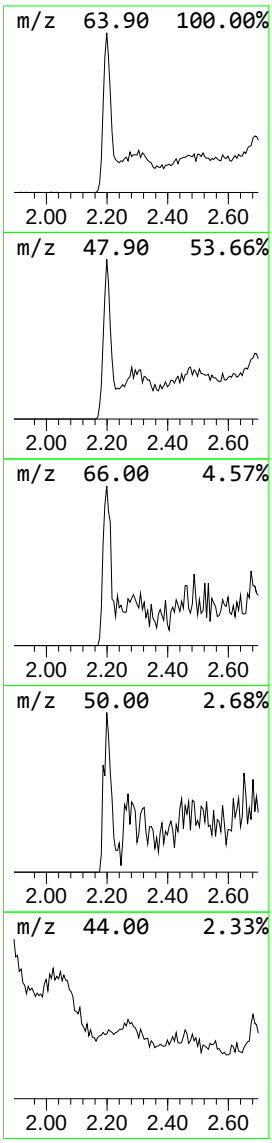
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.198	23.61 ug/l	456365	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	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

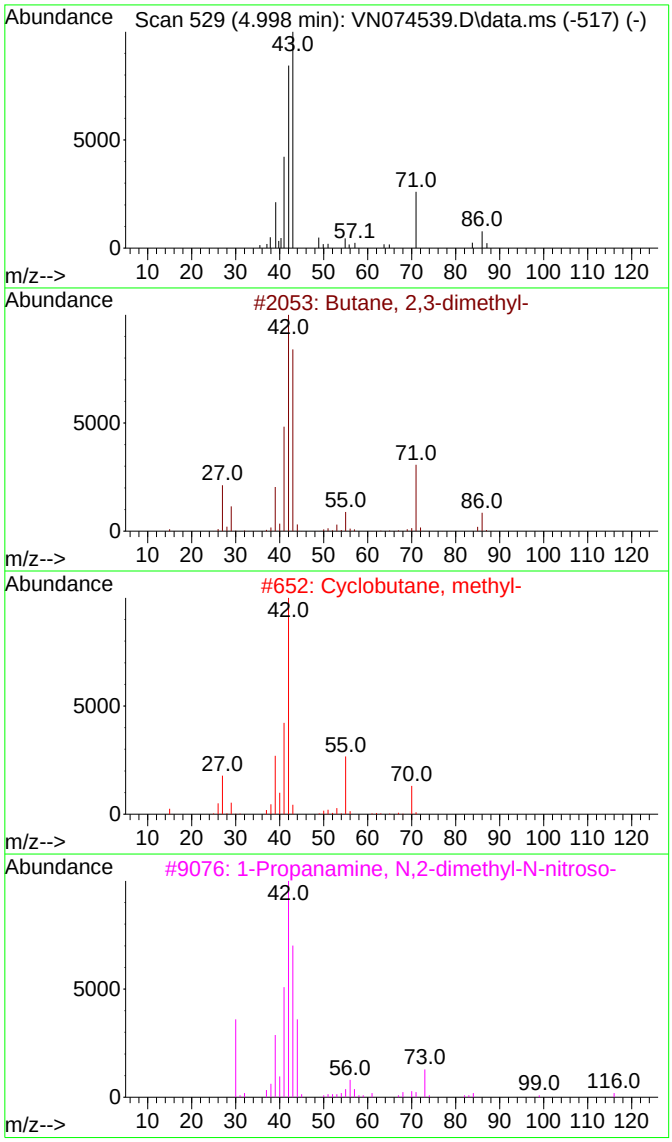
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

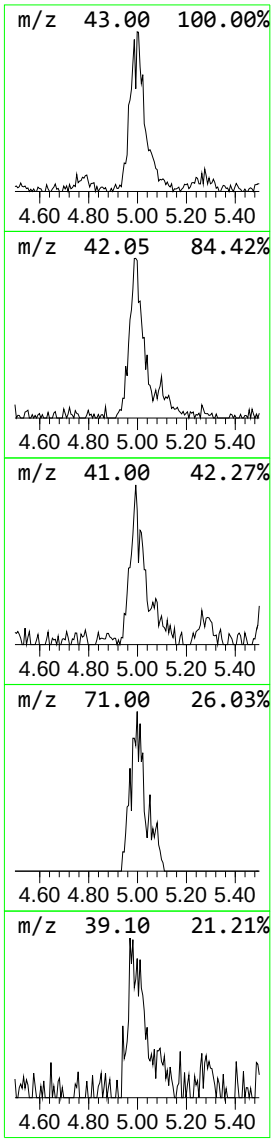
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	7.23 ug/l	139745	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
3	1-Propanamine, N,2-dimethyl-N-ni...	116	C5H12N2O	034419-76-6	33
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

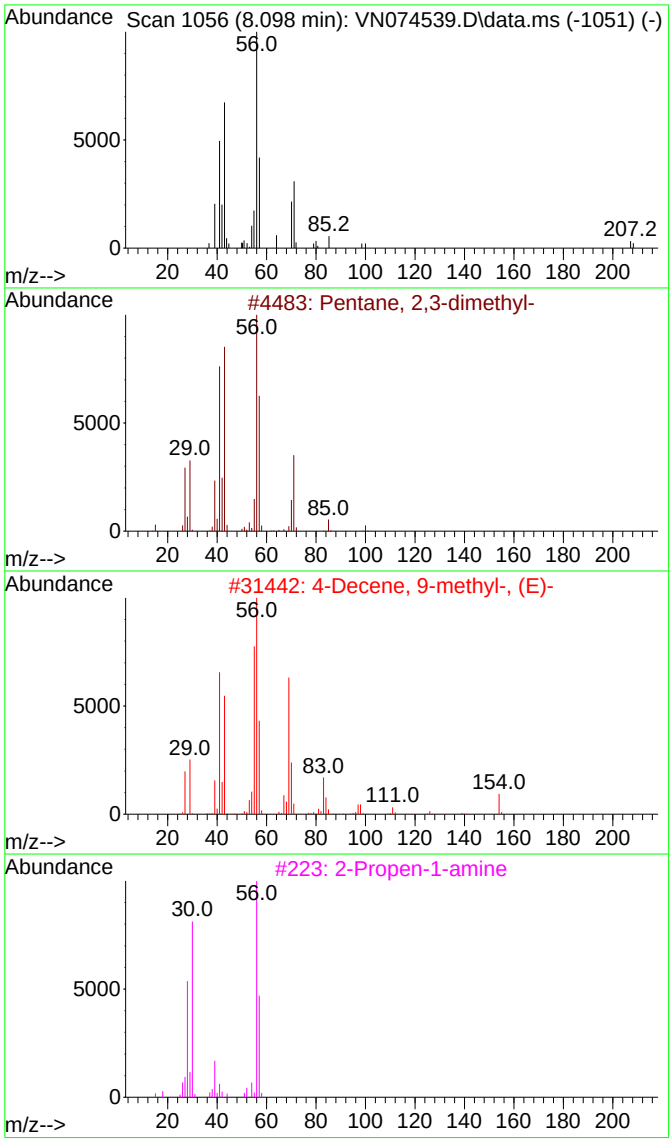
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

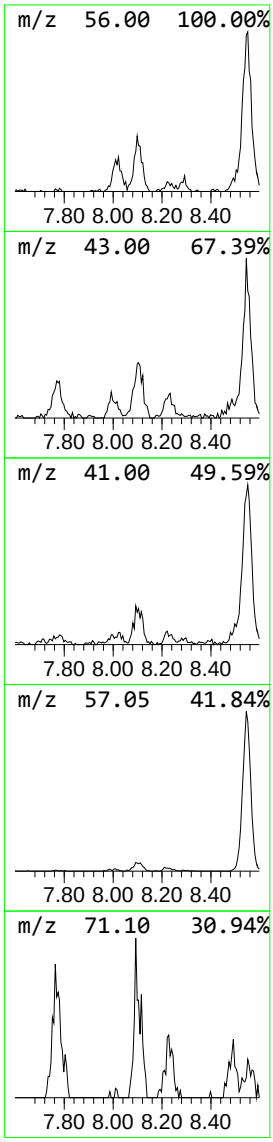
****

Peak Number 3 unknown8.098 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	5.16 ug/l	99753	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	49
2	4-Decene, 9-methyl-, (E)-	154	C11H22	062338-49-2	39
3	2-Propen-1-amine	57	C3H7N	000107-11-9	37
4	4-Undecene, 10-methyl-, (E)-	168	C12H24	074630-60-7	36
5	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
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Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

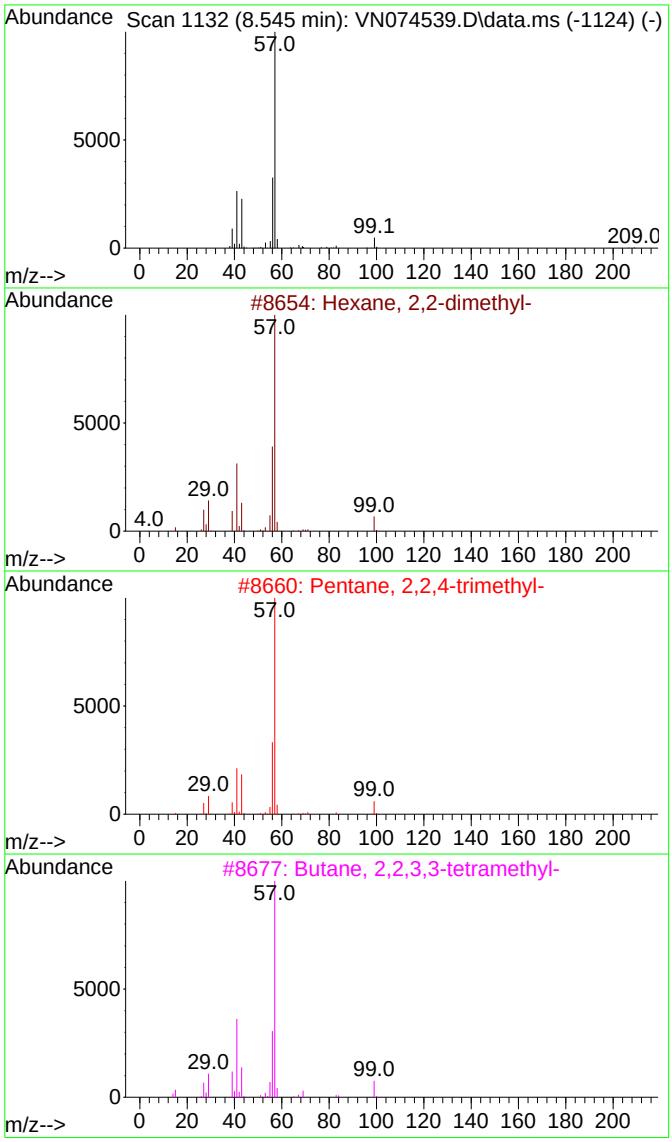
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

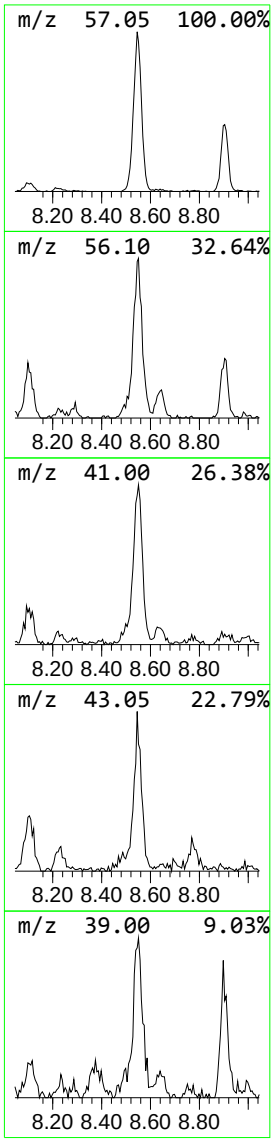
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	16.35 ug/l	467361	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	56
4	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

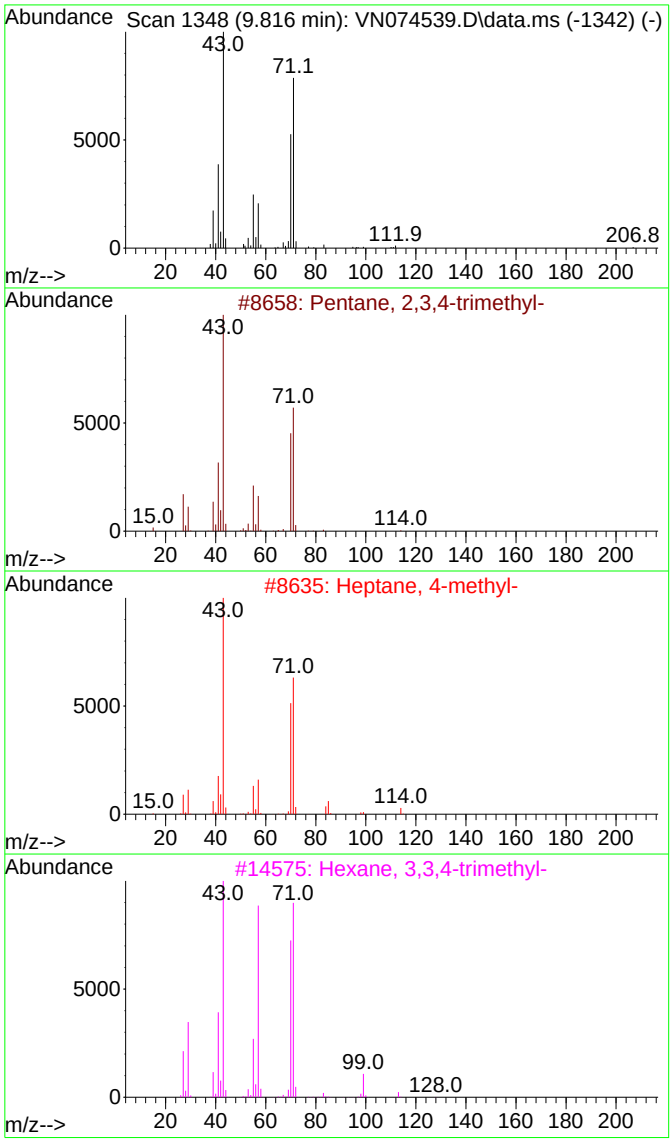
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

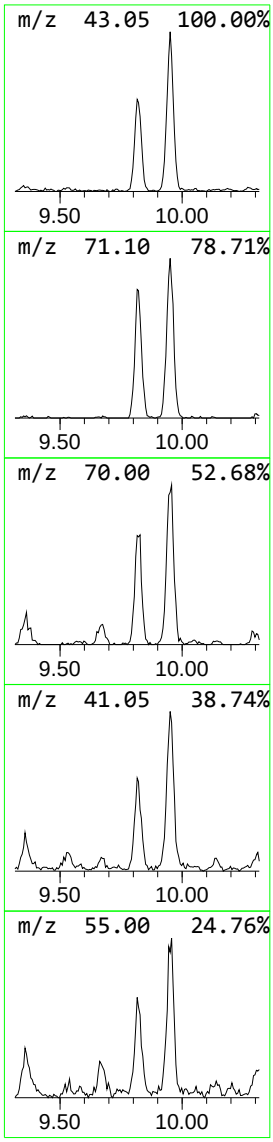
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	10.98 ug/l	313642	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64





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MSVOA_N
ClientSampleId :
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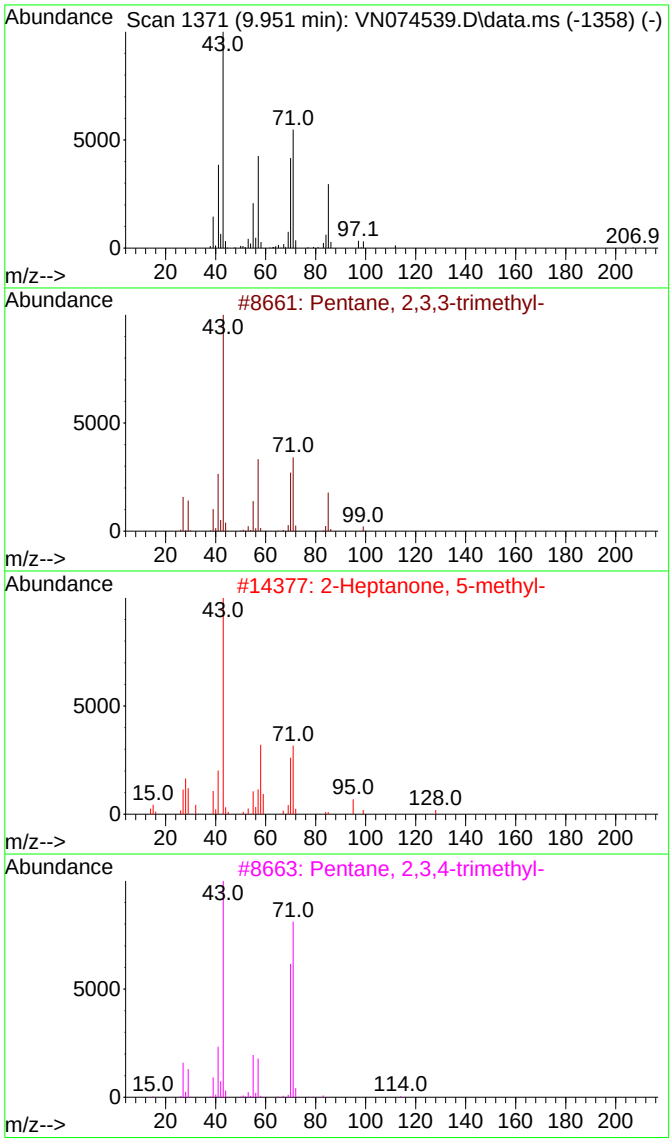
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

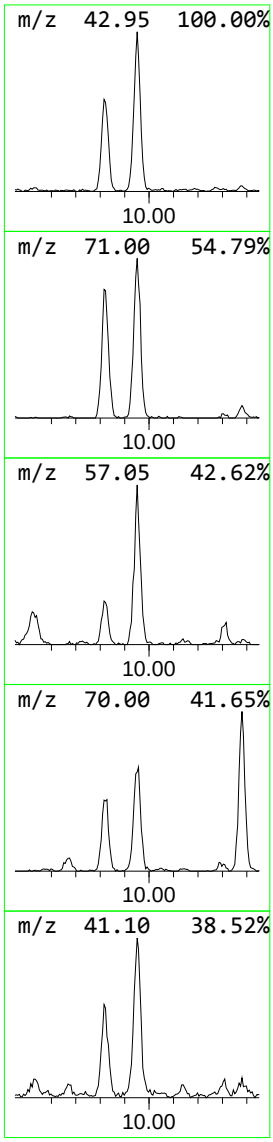
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	21.49 ug/l	614047	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2	2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	59
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4	Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





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Data File : VN074539.D
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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

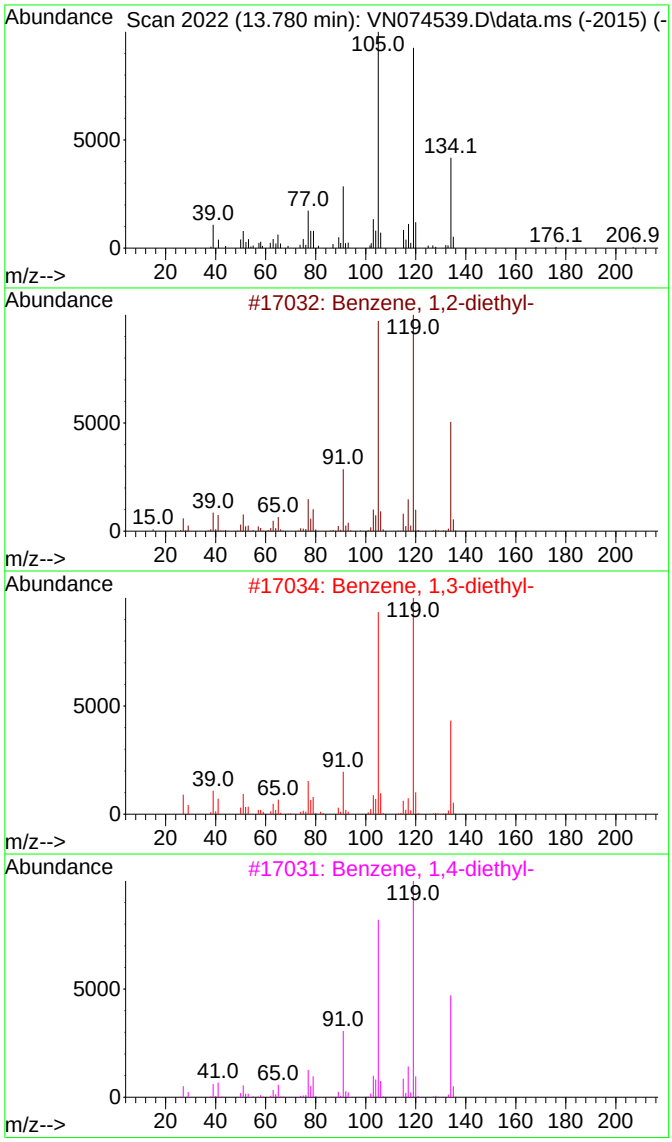
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

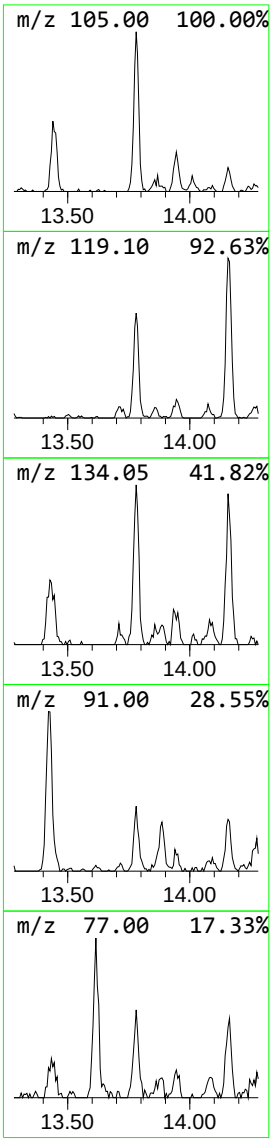
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	6.08 ug/l	208095	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

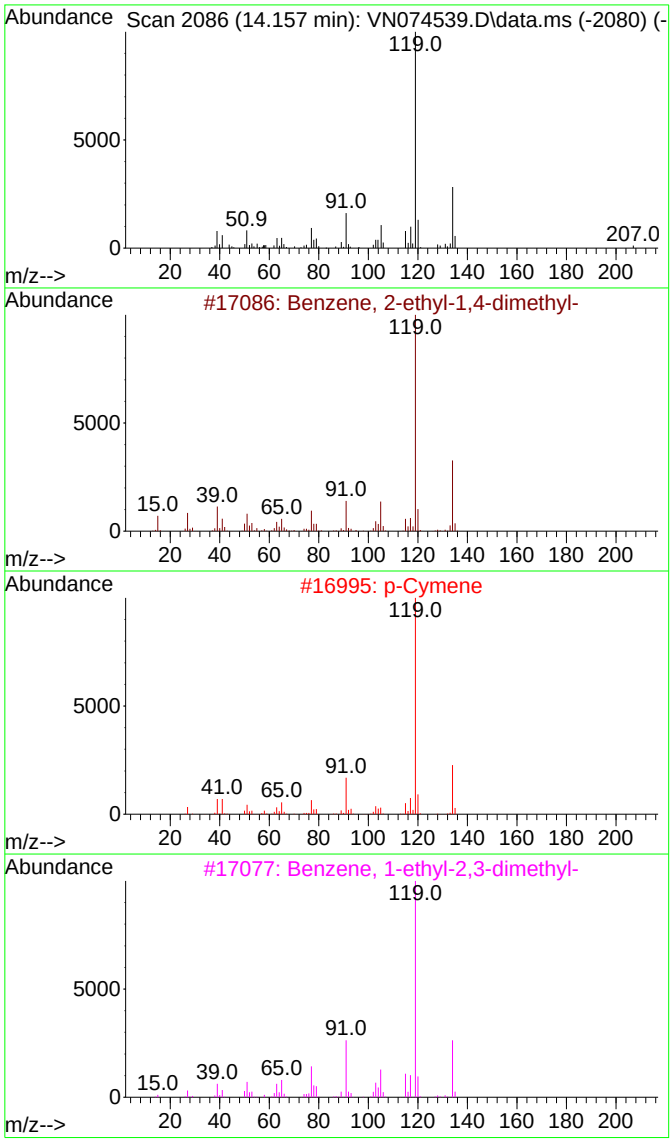
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

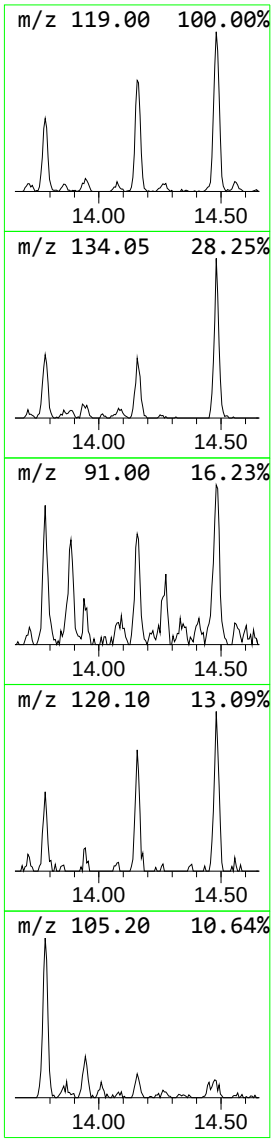
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.156	5.18 ug/l	177488	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	p-Cymene	134	C10H14	000099-87-6	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

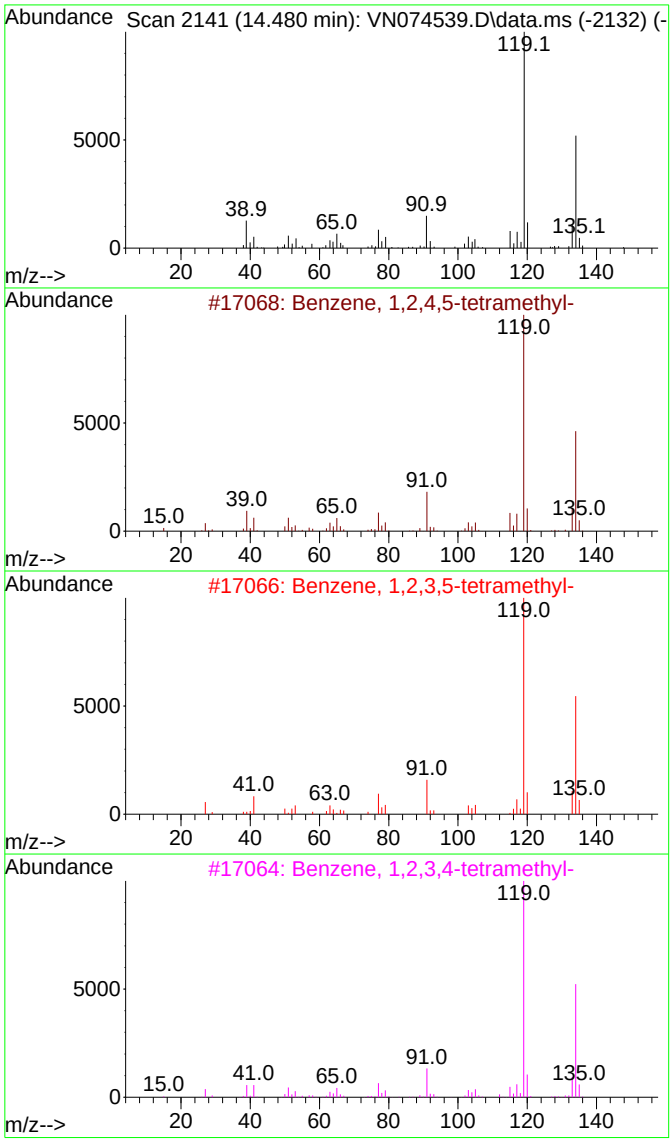
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

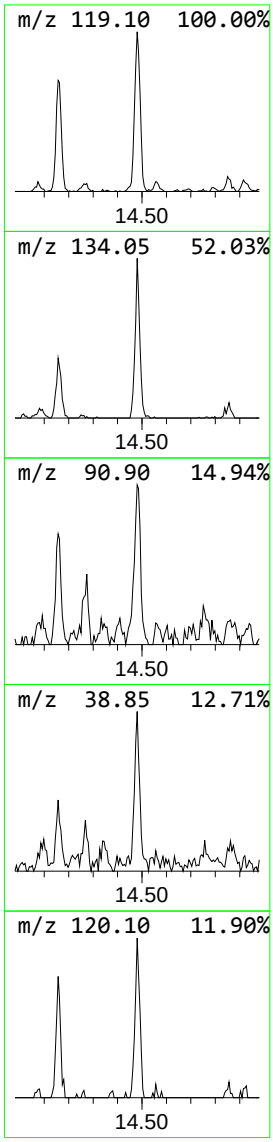
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	8.94 ug/l	306220	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074539.D
Acq On : 17 Sep 2022 03:44
Operator : JC\MD
Sample : N4549-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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	2.198	23.6	ug/l	456365	1	8.016	966378	50.0
Butane, 2,3-dim...	4.998	7.2	ug/l	139745	1	8.016	966378	50.0
unknown8.098	8.098	5.2	ug/l	99753	1	8.016	966378	50.0
Hexane, 2,2-dim...	8.545	16.4	ug/l	467361	2	8.904	1428840	50.0
Pentane, 2,3,4-...	9.816	11.0	ug/l	313642	2	8.904	1428840	50.0
Pentane, 2,3,3-...	9.951	21.5	ug/l	614047	2	8.904	1428840	50.0
Benzene, 1,2-di...	13.780	6.1	ug/l	208095	4	13.615	1712570	50.0
Benzene, 2-ethy...	14.156	5.2	ug/l	177488	4	13.615	1712570	50.0
Benzene, 1,2,4,...	14.480	8.9	ug/l	306220	4	13.615	1712570	50.0