LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

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: VN074543.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	61	rBV2	254475	575968	30.13%	3.611%
2	2.404	83	88	92	rBV3	56352	96421	5.04%	0.604%
3	2.687	131	136	141	rBV	69040	151380	7.92%	0.949%
4	3.075	199	202	203	rBV2	24194	25513	1.33%	0.160%
5	3.175	217	219	230	rVB3	33099	61303	3.21%	0.384%
6	4.181	379	390	398	rBV6	38752	135167	7.07%	0.847%
7	4.998	511	529	542	rBV3	141594	526073	27.52%	3.298%
8	5.522	610	618	619	rBV4	17948	31494	1.65%	0.197%
9	7.233	897	909	919	rBV5	22586	72891	3.81%	0.457%
10	7.769	991	1000	1008	rVB5	16334	46751	2.45%	0.293%
11	7.951	1022	1031	1036	rBV	258596	613815	32.11%	3.848%
12	8.016	1036	1042	1053	rVB	410068	916817	47.96%	5.747%
13	8.369	1093	1102	1115	rVV2	302241	685242	35.85%	4.296%
14	8.545	1120	1132	1143	rBV	423525	1023732	53.56%	6.418%
15	8.904	1184	1193	1203	rBV	666891	1364759	71.40%	8.555%
16	9.386	1265	1275	1282	rVB6	37540	98280	5.14%	0.616%
17	9.527	1294	1299	1306	rVB3	25910	51059	2.67%	0.320%
18	9.669	1314	1323	1330	rBV4	23456	51693	2.70%	0.324%
19	9.822	1340	1349	1357	rVB	226319	440841	23.06%	2.764%
20	9.951	1362	1371	1382	rBV2	272260	573556	30.00%	3.595%
21	10.133	1398	1402	1409	rVB8	11261	21954	1.15%	0.138%
22	10.310	1421	1432	1436	rBV4	26322	59260	3.10%	0.371%
23	10.380	1436	1444	1454	rBV	1091503	1911552	100.00%	11.983%
24	10.586	1470	1479	1484	rVB2	110606	197363	10.32%	1.237%
25	10.657	1484	1491	1498	rVB2	110541	192515	10.07%	1.207%
26	10.798	1508	1515	1521	rBV2	34376	64338	3.37%	0.403%
27	11.686	1656	1666	1673	rBV	1051031	1828522	95.66%	11.463%
28	11.927	1701	1707	1716	rVB	11316	31222	1.63%	0.196%
29	12.674	1827	1834	1844	rBV	840111	1402738	73.38%	8.793%
30	13.263	1927	1934	1945	rVB5	16363	33914	1.77%	0.213%
31	13.421	1955	1961	1967	rBV	50358	83164	4.35%	0.521%
32	13.615	1987	1994	2009	rBV	1050115	1728280	90.41%	10.834%
33	13.780	2018	2022	2027	rBV6	22684	38051	1.99%	0.239%
34	14.092	2069	2075	2081	rVV3	44171	80235	4.20%	0.503%
35	14.157	2081	2086	2092	rVB10	13071	23335	1.22%	0.146%
36	14.268	2100	2105	2110	rBV5	24045	43034	2.25%	0.270%

LSC Area Percent Report

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Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

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	14.345	2110	2118	2124	rVV6	46050	99985	5.23%	0.627%
38	14.409	2124	2129	2133	rVV	48468	80657	4.22%	0.506%
39	14.480	2133	2141	2150	rVB2	94998	181685	9.50%	1.139%
40	14.751	2182	2187	2195	rVV5	32263	62660	3.28%	0.393%
41	14.868	2198	2207	2214	rVV6	18873	53871	2.82%	0.338%
42	15.127	2245	2251	2256	rBV8	19858	41281	2.16%	0.259%
43	15.245	2266	2271	2275	rVB4	14509	27758	1.45%	0.174%
44	15.398	2292	2297	2302	rVB4	11912	19366	1.01%	0.121%
45	16.033	2400	2405	2411	rBV4	35668	71985	3.77%	0.451%
46	16.733	2517	2524	2525	rBV6	19347	30694	1.61%	0.192%

Sum of corrected areas: 15952174

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Sample : N4549-15
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Instrument :
MSVOA_N
ClientSampleId :
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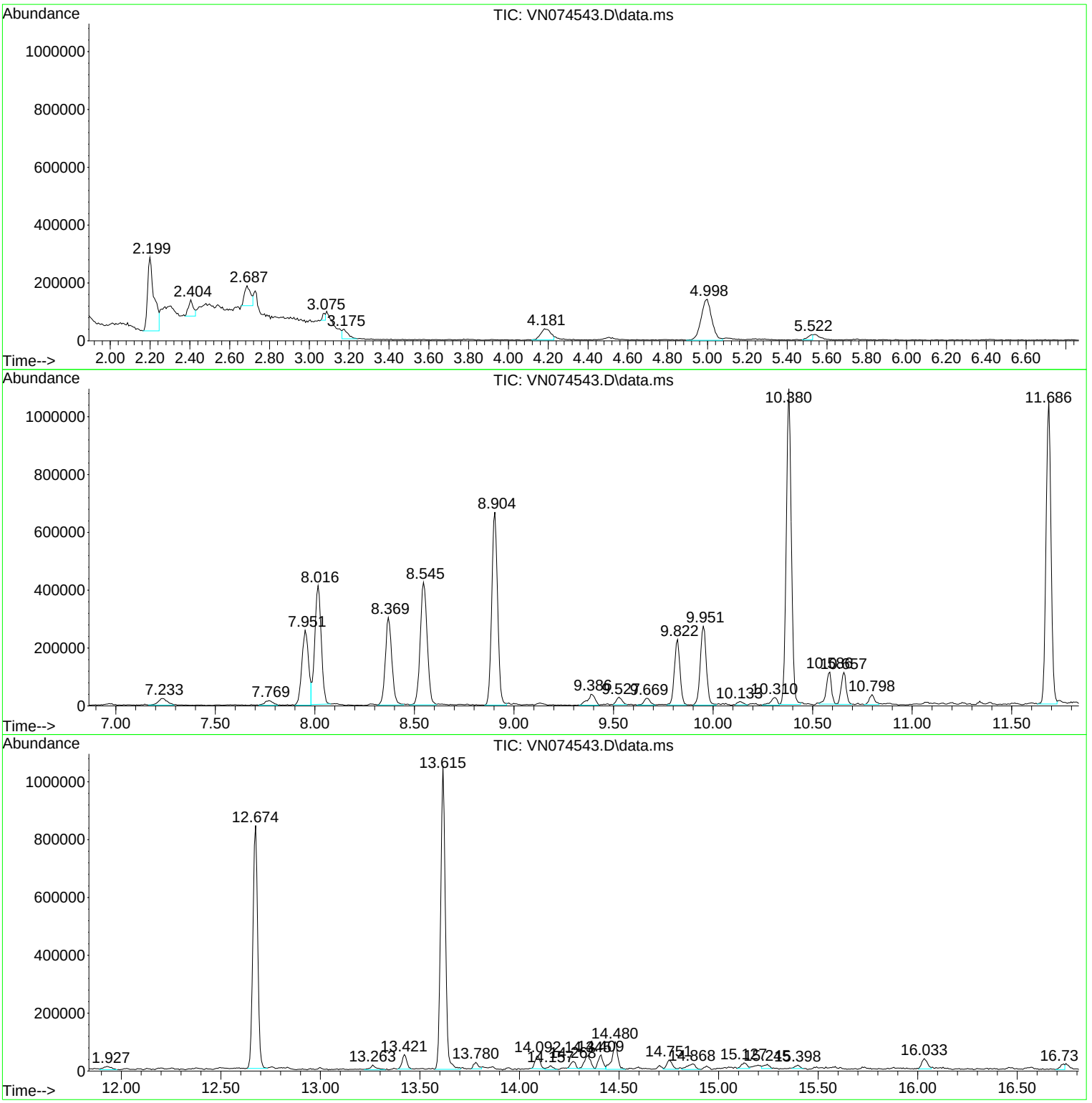
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

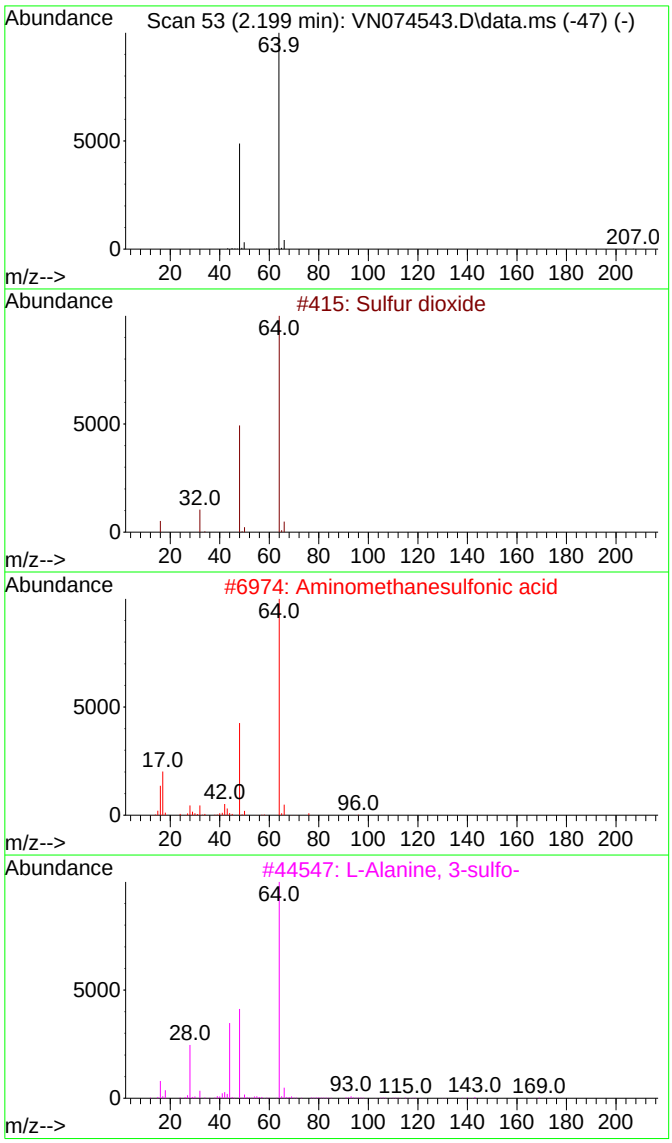
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

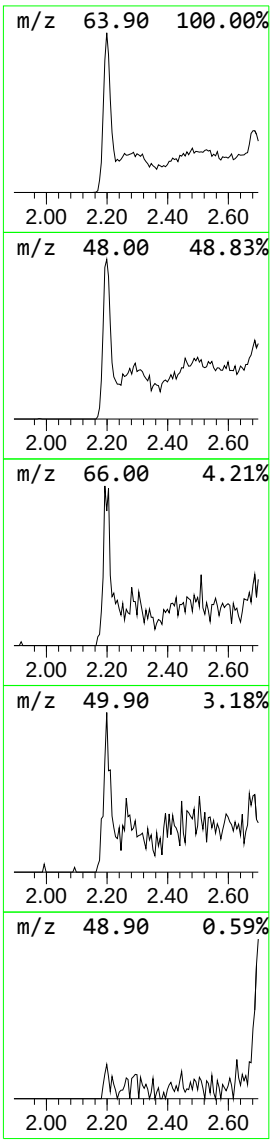
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	31.41 ug/l	575968	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
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\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

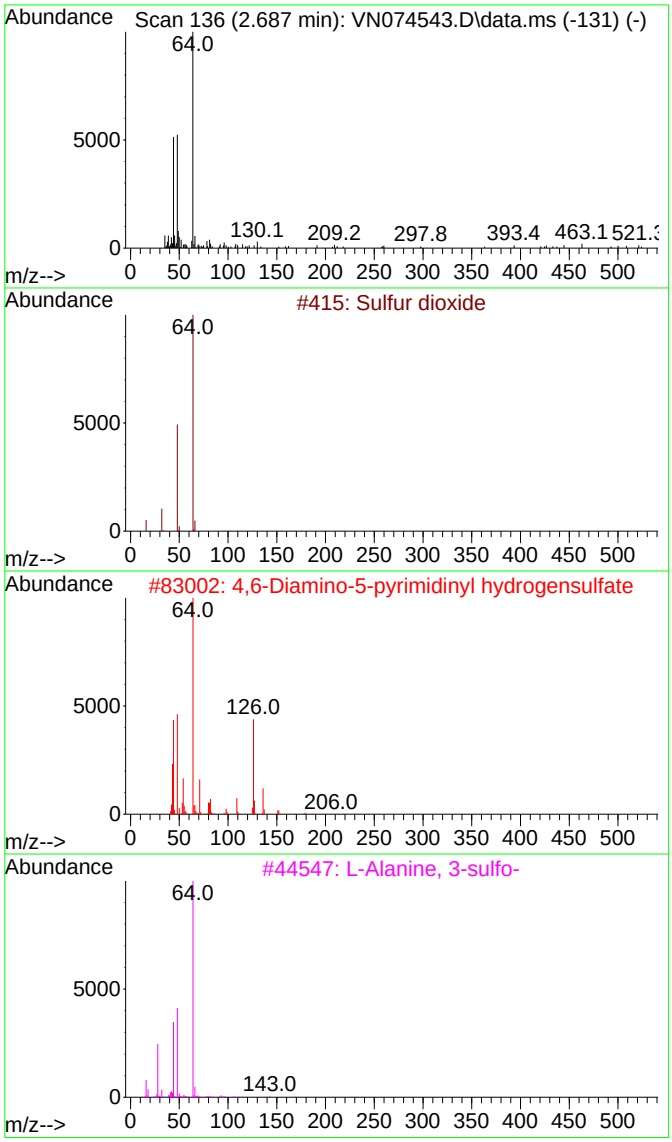
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

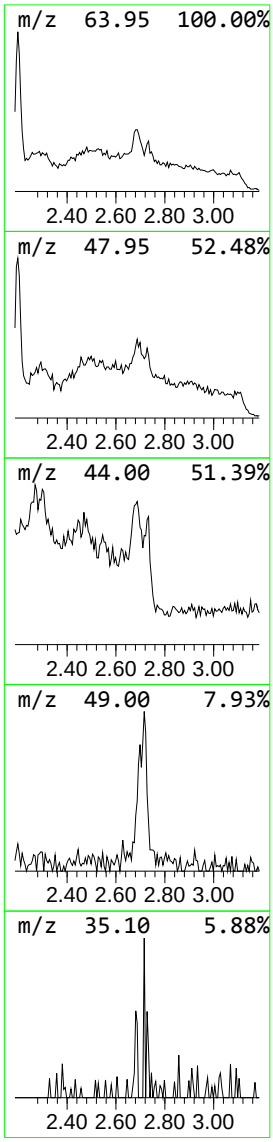
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4,6-Diamino-5-pyrimidinyl h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	8.26 ug/l	151380	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	80
2	4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	74
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	72
5	2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

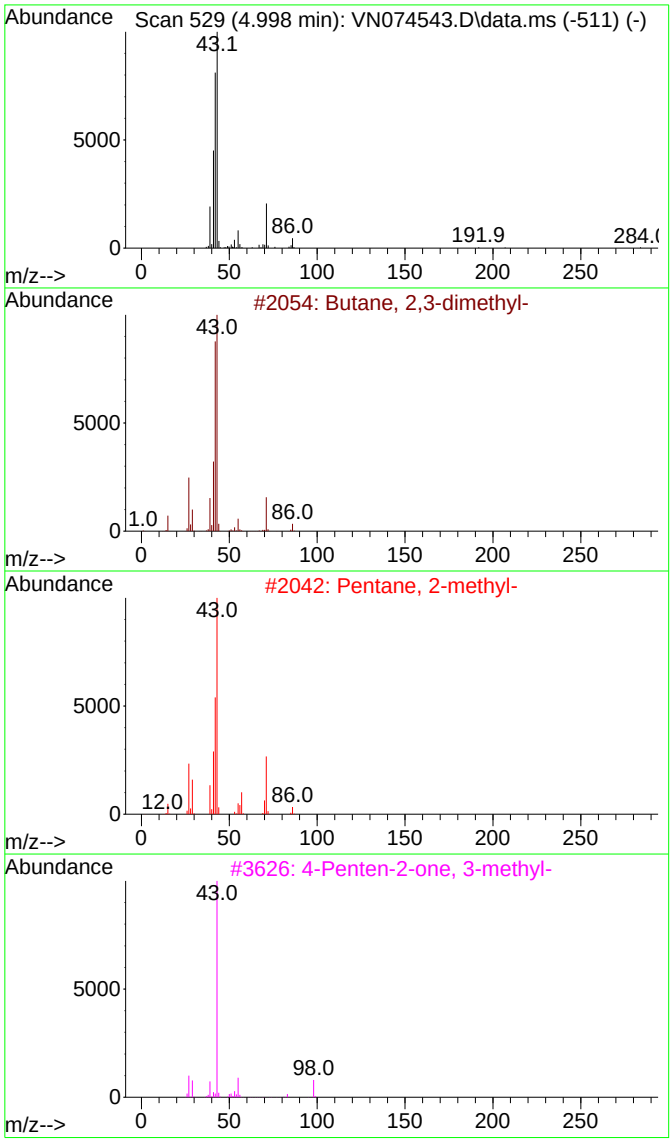
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

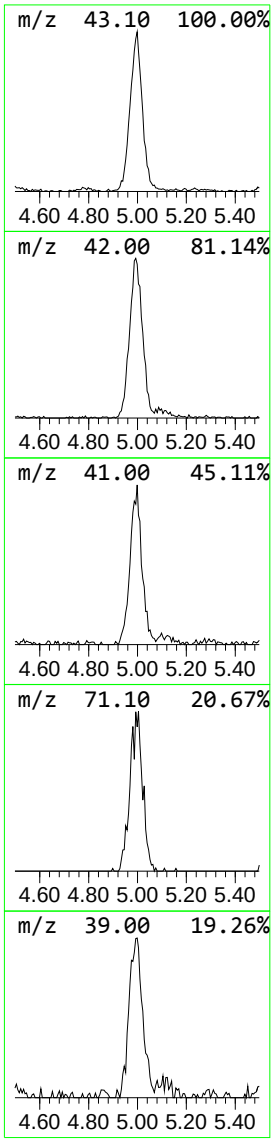
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	28.69 ug/l	526073	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	Pentane	72	C5H12	000109-66-0	9
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

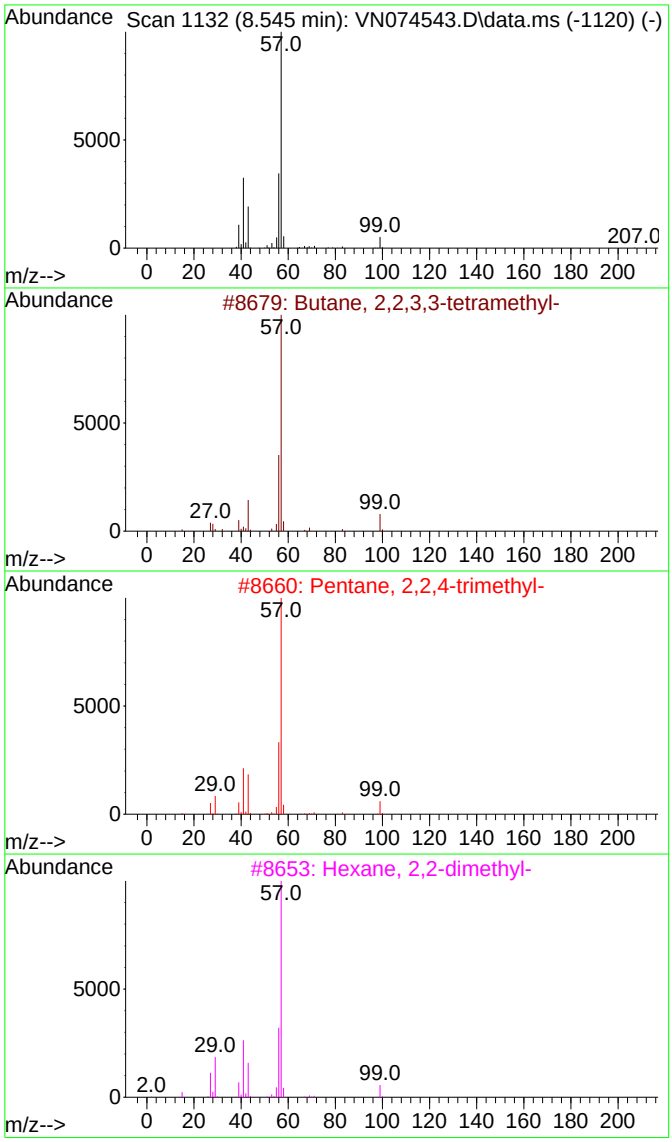
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

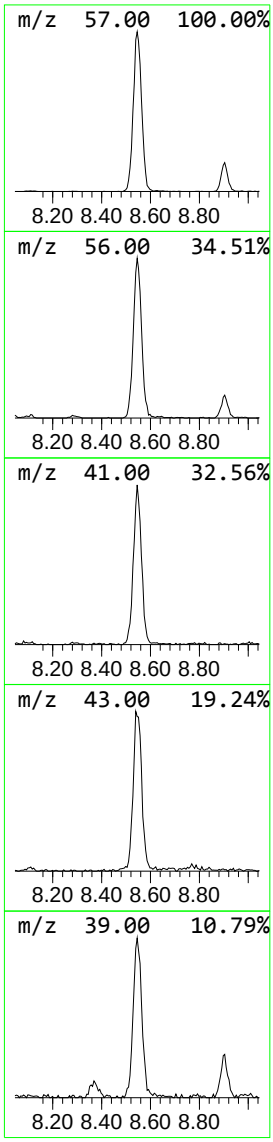
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	37.51 ug/l	1023730	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
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Operator : JC\MD
Sample : N4549-15
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ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

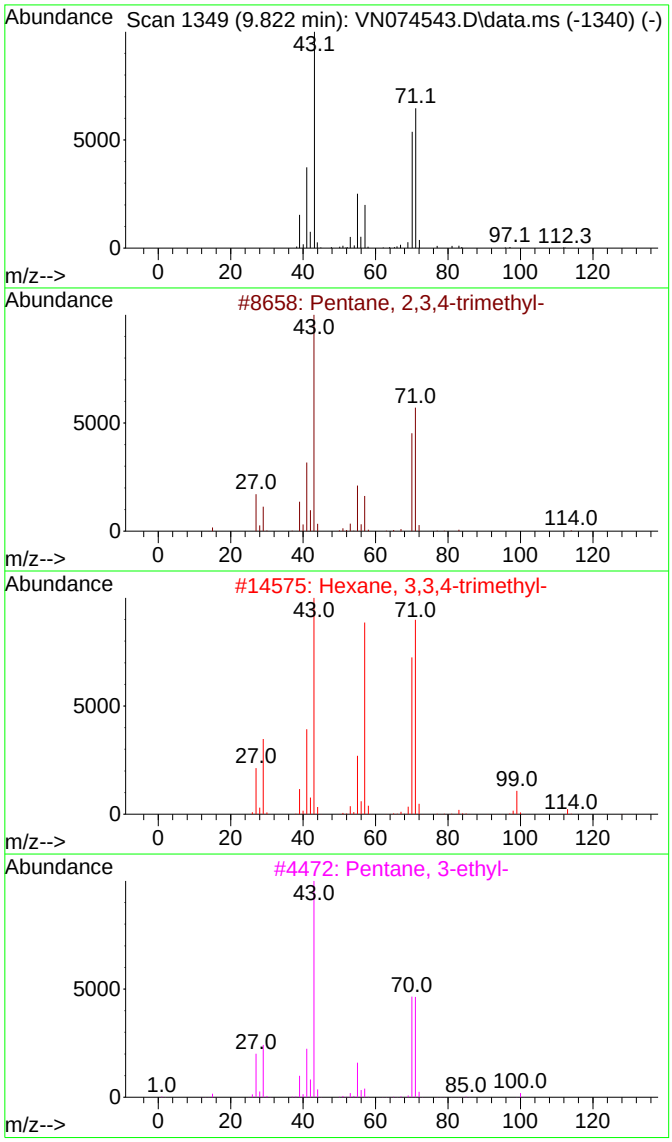
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

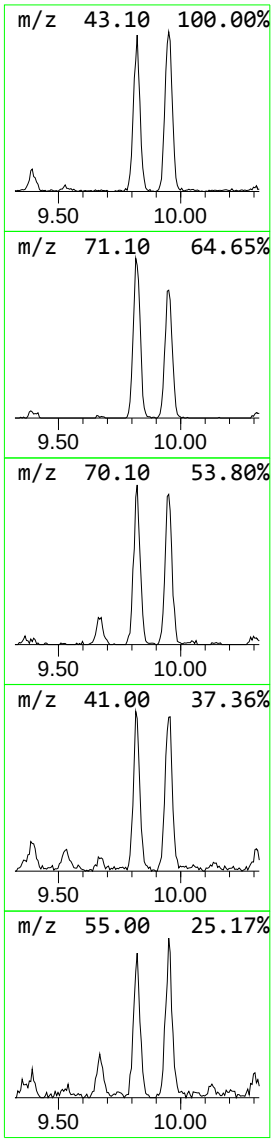
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.822	16.15 ug/l	440841	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	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Diisoamyl ether	158	C10H22O	000544-01-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
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Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

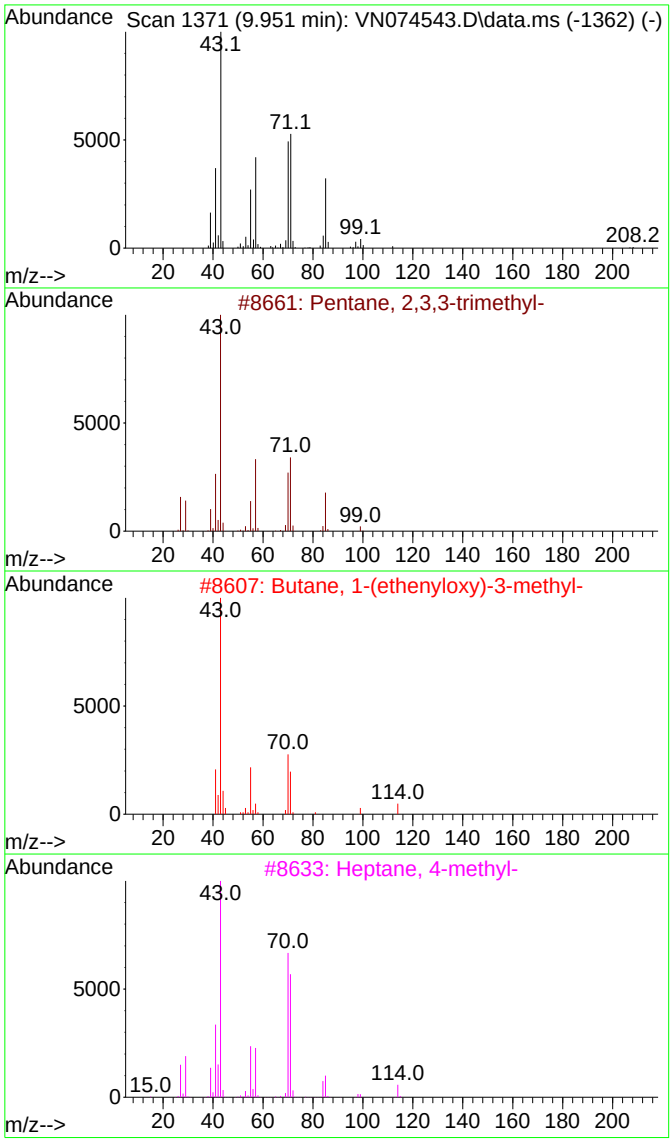
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

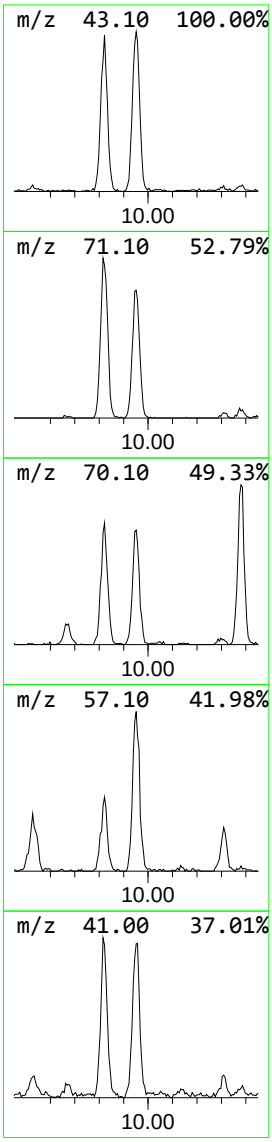
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	21.01 ug/l	573556	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	83
2	Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	59
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	58





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ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

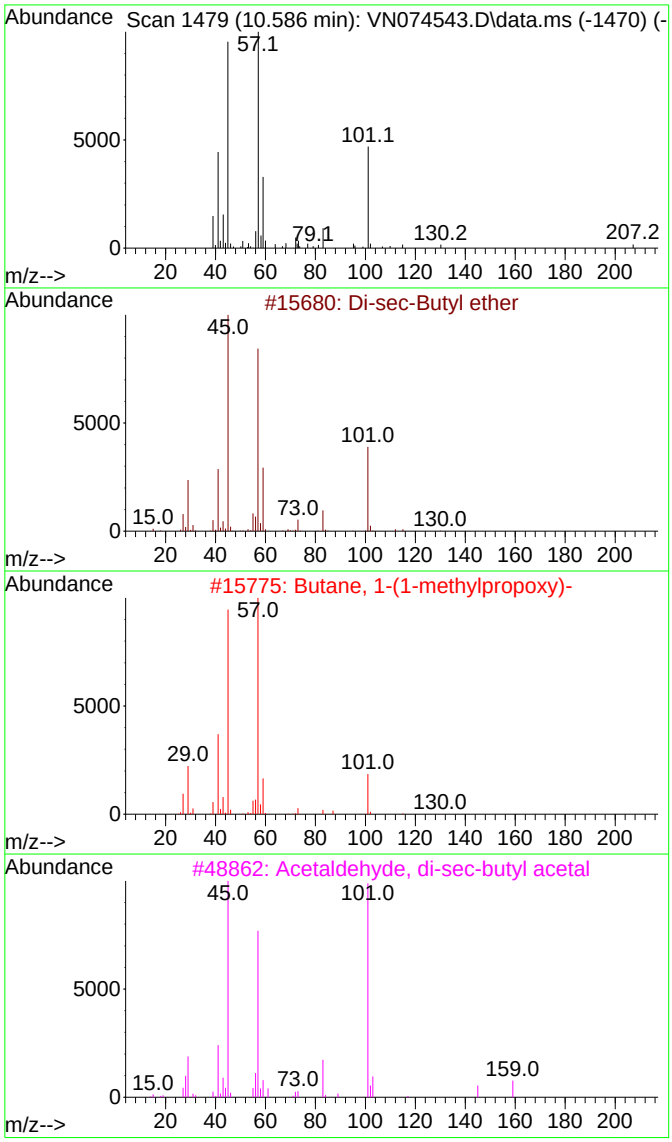
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

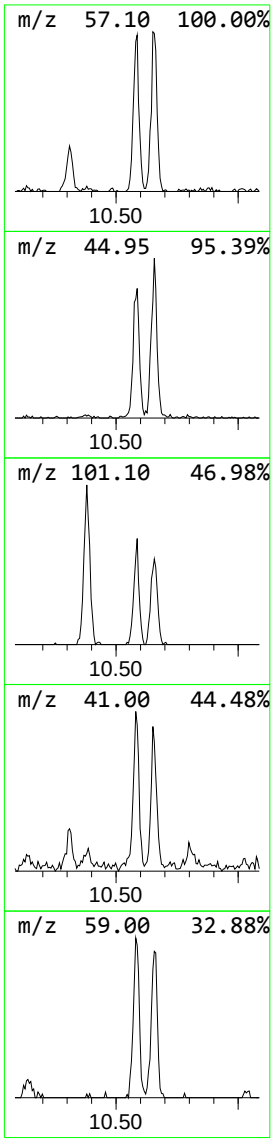
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	5.40 ug/l	197363	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	78
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	72
3	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	50
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	45
5	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

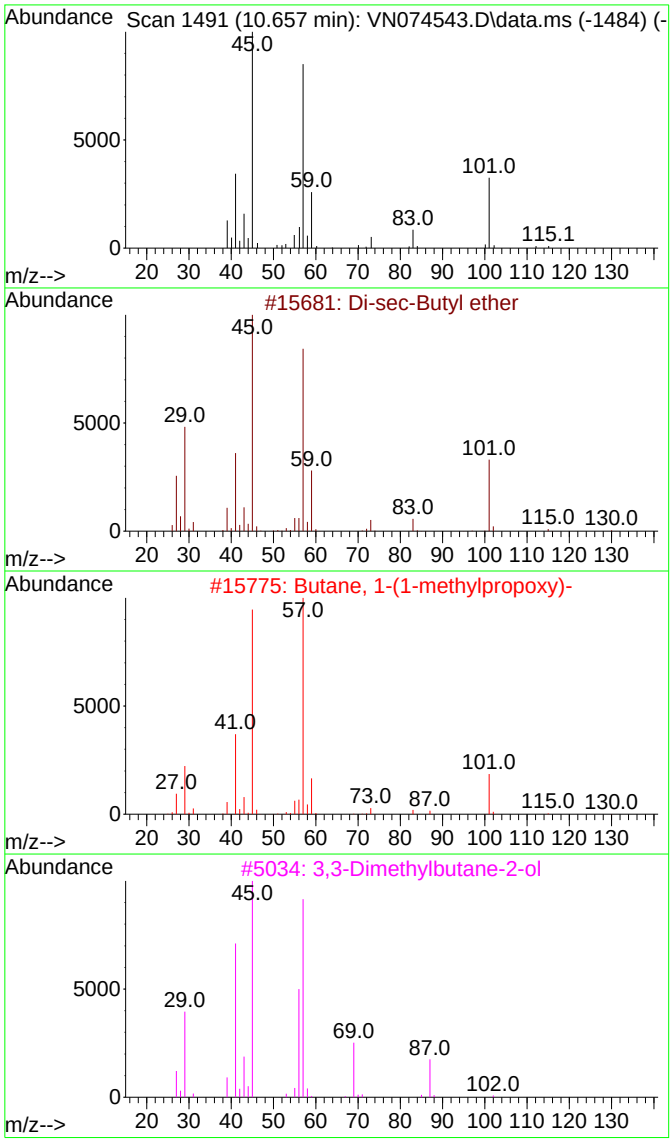
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

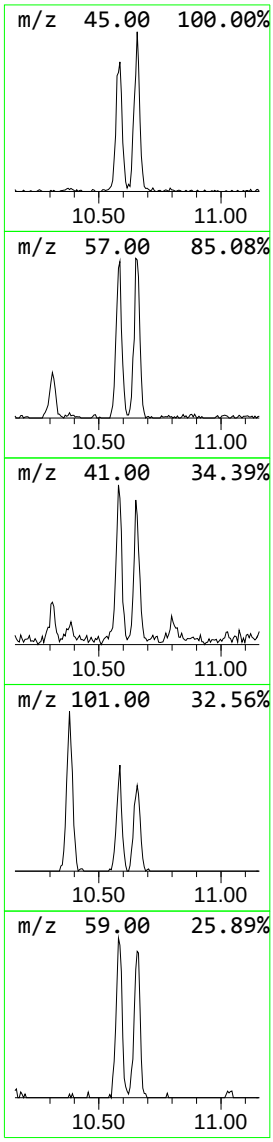
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butane, 1-(1-methylpropoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	5.26 ug/l	192515	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	40
5	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

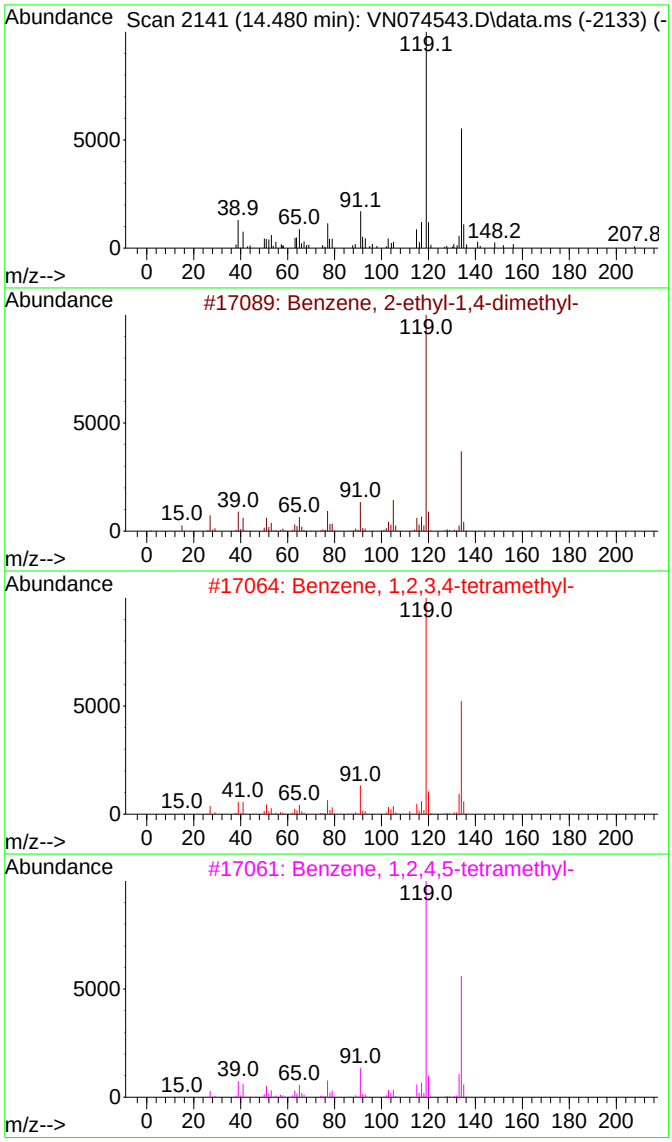
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

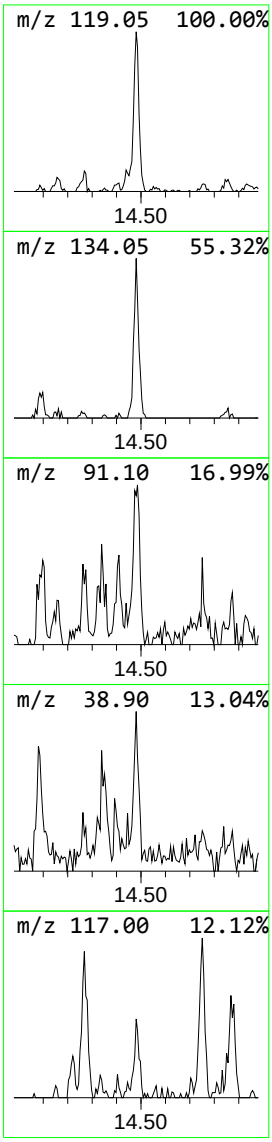
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	5.26 ug/l	181685	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	94
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074543.D
Acq On : 17 Sep 2022 05:21
Operator : JC\MD
Sample : N4549-15
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-59

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	2.199	31.4	ug/l	575968	1	8.016	916817	50.0
4,6-Diamino-5-p...	2.687	8.3	ug/l	151380	1	8.016	916817	50.0
Butane, 2,3-dim...	4.998	28.7	ug/l	526073	1	8.016	916817	50.0
Butane, 2,2,3,3...	8.545	37.5	ug/l	1023730	2	8.904	1364760	50.0
Pentane, 2,3,4-...	9.822	16.1	ug/l	440841	2	8.904	1364760	50.0
Pentane, 2,3,3-...	9.951	21.0	ug/l	573556	2	8.904	1364760	50.0
Di-sec-Butyl ether	10.586	5.4	ug/l	197363	3	11.686	1828520	50.0
Butane, 1-(1-me...	10.657	5.3	ug/l	192515	3	11.686	1828520	50.0
Benzene, 2-ethy...	14.480	5.3	ug/l	181685	4	13.615	1728280	50.0