LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

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: VN074556.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	48	53	57	rBV	209360	381096	12.46%	1.315%
2	2.405	83	88	92	rBV	87640	135780	4.44%	0.468%
3	2.687	133	136	142	rVV2	44872	95781	3.13%	0.330%
4	3.081	194	203	216	rVB	1307744	3058027	100.00%	10.552%
5	3.458	260	267	277	rVB2	42474	109081	3.57%	0.376%
6	4.187	378	391	405	rBV3	171499	595164	19.46%	2.054%
7	4.993	515	528	539	rBV4	349205	1367433	44.72%	4.718%
8	5.240	561	570	578	rVB4	16901	51076	1.67%	0.176%
9	5.534	607	620	633	rBV2	86866	300478	9.83%	1.037%
10	6.522	780	788	793	rBV6	13740	35638	1.17%	0.123%
11	6.810	823	837	845	rBV6	28557	103111	3.37%	0.356%
12	6.957	852	862	871	rBV3	120085	358713	11.73%	1.238%
13	7.063	872	880	888	rBV2	102813	287537	9.40%	0.992%
14	7.240	901	910	919	rVB2	81356	225617	7.38%	0.778%
15	7.775	992	1001	1013	rVB4	60447	175143	5.73%	0.604%
16	7.951	1021	1031	1036	rBV	268992	642972	21.03%	2.219%
17	8.016	1036	1042	1050	rVV2	454410	1090822	35.67%	3.764%
18	8.104	1050	1057	1069	rVB2	268327	676511	22.12%	2.334%
19	8.292	1081	1089	1094	rVV5	16201	35841	1.17%	0.124%
20	8.375	1094	1103	1115	rVV2	342888	906068	29.63%	3.126%
21	8.487	1115	1122	1123	rVV	28742	42852	1.40%	0.148%
22	8.545	1124	1132	1142	rVV	450668	1138302	37.22%	3.928%
23	8.640	1142	1148	1157	rVB2	61307	140737	4.60%	0.486%
24	8.904	1183	1193	1204	rBV	712297	1517344	49.62%	5.235%
25	8.992	1204	1208	1216	rVB3	36562	74696	2.44%	0.258%
26	9.134	1224	1232	1237	rBV4	38959	91783	3.00%	0.317%
27	9.181	1237	1240	1247	rVB3	30962	57280	1.87%	0.198%
28	9.363	1263	1271	1282	rBV5	117314	370805	12.13%	1.279%
29	9.457	1283	1287	1294	rVV8	17054	37086	1.21%	0.128%
30	9.534	1294	1300	1304	rVV5	20514	40285	1.32%	0.139%
31	9.675	1314	1324	1330	rVB3	53274	126219	4.13%	0.436%
32	9.822	1342	1349	1358	rVB	204245	423468	13.85%	1.461%
33	9.951	1358	1371	1383	rBV3	253228	632687	20.69%	2.183%
34	10.069	1384	1391	1395	rVB8	21110	46575	1.52%	0.161%
35	10.134	1395	1402	1409	rVB4	47316	93486	3.06%	0.323%
36	10.263	1418	1424	1427	rBV4	50051	85964	2.81%	0.297%

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP090822

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

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Peak separation: 5

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Title : SW846 8260

37	10.304	1427	1431	1437	rVB5	50182	92543	3.03%	0.319%
38	10.381	1437	1444	1457	rBV	1128109	2073767	67.81%	7.155%
39	10.581	1464	1478	1485	rBV3	226115	507619	16.60%	1.752%
40	10.657	1485	1491	1497	rVV2	208791	358684	11.73%	1.238%
41	10.722	1497	1502	1507	rVV4	31532	58534	1.91%	0.202%
42	10.798	1508	1515	1525	rVV4	146192	344346	11.26%	1.188%
43	10.886	1525	1530	1541	rVB8	22703	54702	1.79%	0.189%
44	11.075	1549	1562	1566	rBV6	42605	106110	3.47%	0.366%
45	11.198	1578	1583	1589	rVB7	35768	67168	2.20%	0.232%
46	11.257	1589	1593	1596	rVV4	18670	31334	1.02%	0.108%
47	11.392	1611	1616	1621	rVB6	29078	53852	1.76%	0.186%
48	11.686	1659	1666	1673	rBV	1155773	1967986	64.35%	6.790%
49	11.933	1701	1708	1713	rVB	22827	50834	1.66%	0.175%
50	12.522	1799	1808	1814	rBV	249951	415527	13.59%	1.434%
51	12.675	1827	1834	1844	rVB	928746	1521871	49.77%	5.251%
52	12.863	1858	1866	1876	rVB	198878	341271	11.16%	1.178%
53	13.163	1911	1917	1922	rBV2	38556	68380	2.24%	0.236%
54	13.263	1924	1934	1938	rBV8	15453	36742	1.20%	0.127%
55	13.422	1955	1961	1970	rVB2	98596	176802	5.78%	0.610%
56	13.616	1987	1994	2007	rBV	1119642	1968499	64.37%	6.792%
57	13.816	2017	2028	2034	rBV	702615	1269988	41.53%	4.382%
58	13.945	2044	2050	2055	rVB3	88000	140580	4.60%	0.485%
59	14.010	2057	2061	2067	rVB2	26832	41831	1.37%	0.144%
60	14.092	2067	2075	2081	rBV2	148267	251688	8.23%	0.868%
61	14.222	2092	2097	2100	rBV5	20776	36483	1.19%	0.126%
62	14.269	2100	2105	2112	rVV	220136	371766	12.16%	1.283%
63	14.345	2112	2118	2124	rVV5	52172	116140	3.80%	0.401%
64	14.404	2124	2128	2134	rVV2	54438	90137	2.95%	0.311%
65	14.480	2134	2141	2147	rVB2	68400	124768	4.08%	0.431%
66	14.598	2157	2161	2168	rVB2	42733	66165	2.16%	0.228%
67	14.704	2171	2179	2183	rBV2	51715	84668	2.77%	0.292%
68	14.769	2183	2190	2195	rVB3	56500	101593	3.32%	0.351%
69	14.863	2199	2206	2214	rVB3	24291	61312	2.00%	0.212%
70	14.939	2214	2219	2225	rBV5	33536	54932	1.80%	0.190%
71	15.133	2247	2252	2257	rBV7	19195	34920	1.14%	0.120%
72	15.216	2257	2266	2267	rBV3	36335	60518	1.98%	0.209%
73	15.498	2307	2314	2319	rBV6	16637	35496	1.16%	0.122%
74	15.580	2323	2328	2338	rVB8	25982	61030	2.00%	0.211%
75	16.039	2399	2406	2413	rBV4	25487	59379	1.94%	0.205%
76	16.463	2473	2478	2487	rBV7	13552	31938	1.04%	0.110%

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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP090822

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

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Title : SW846 8260

77	16.745	2519	2526	2533	rBV8	14858	38515	1.26%	0.133%

Sum of corrected areas: 28981876

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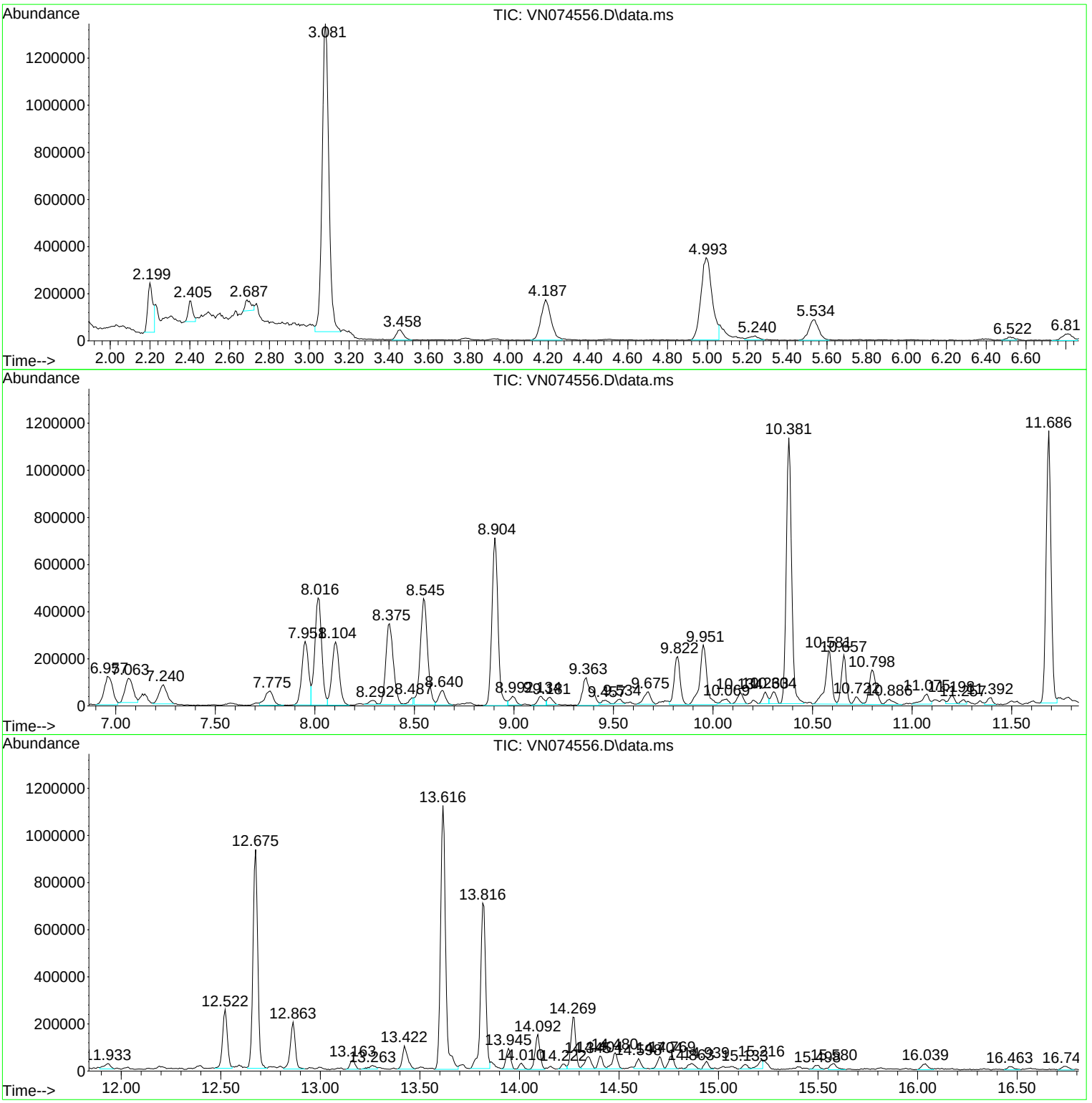
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

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



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Data File : VN074556.D
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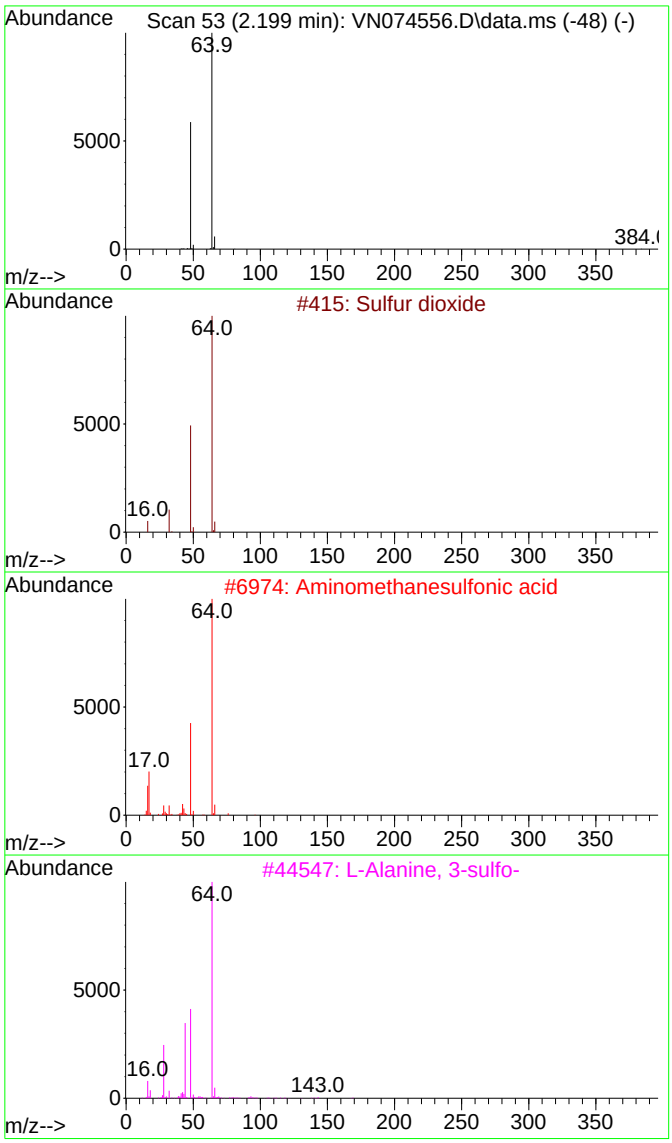
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

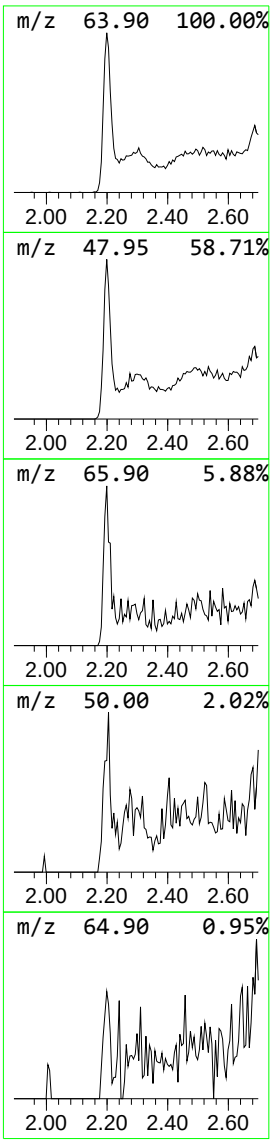
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	17.47 ug/l	381096	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	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

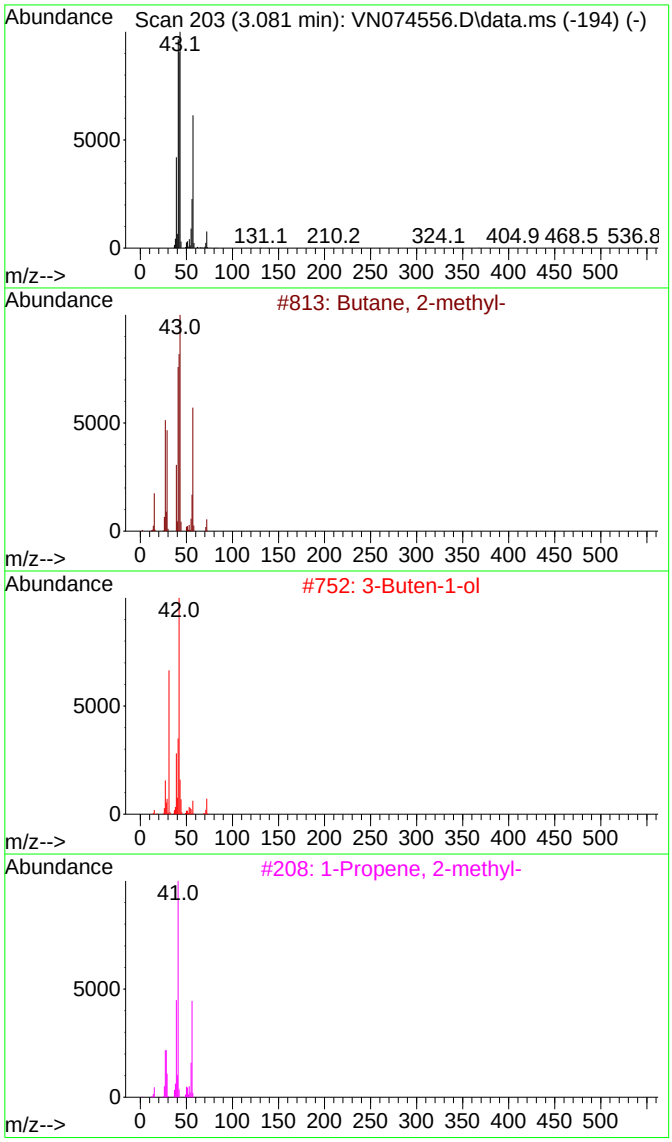
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

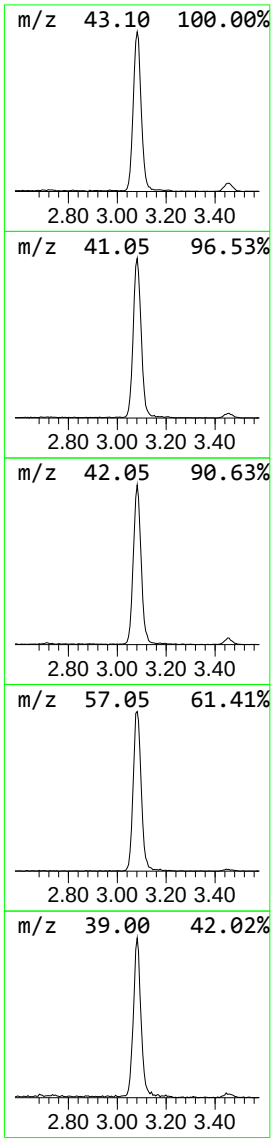
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	140.17 ug/l	3058030	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	35
4	Pentane	72	C5H12	000109-66-0	28
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
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Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

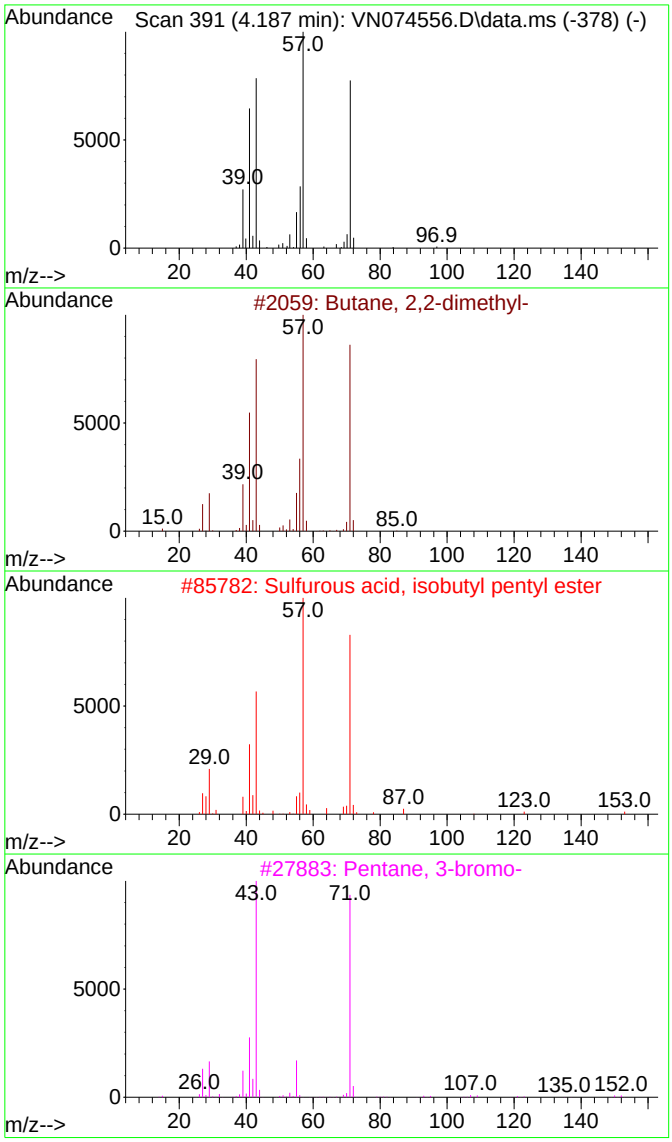
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

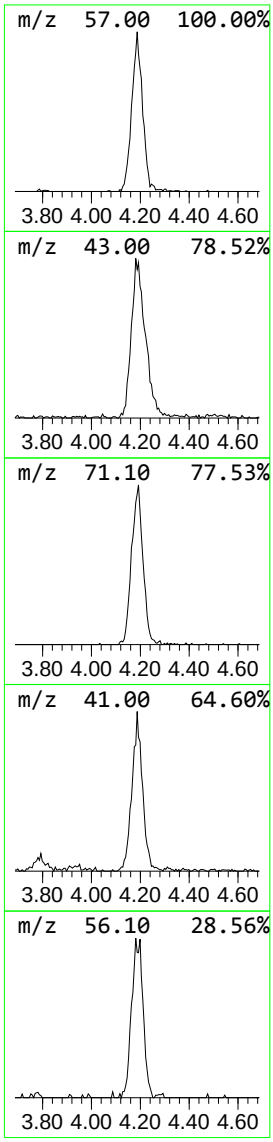
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.187	27.28 ug/l	595164	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	90
2	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	64
3	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	40
4	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	40
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





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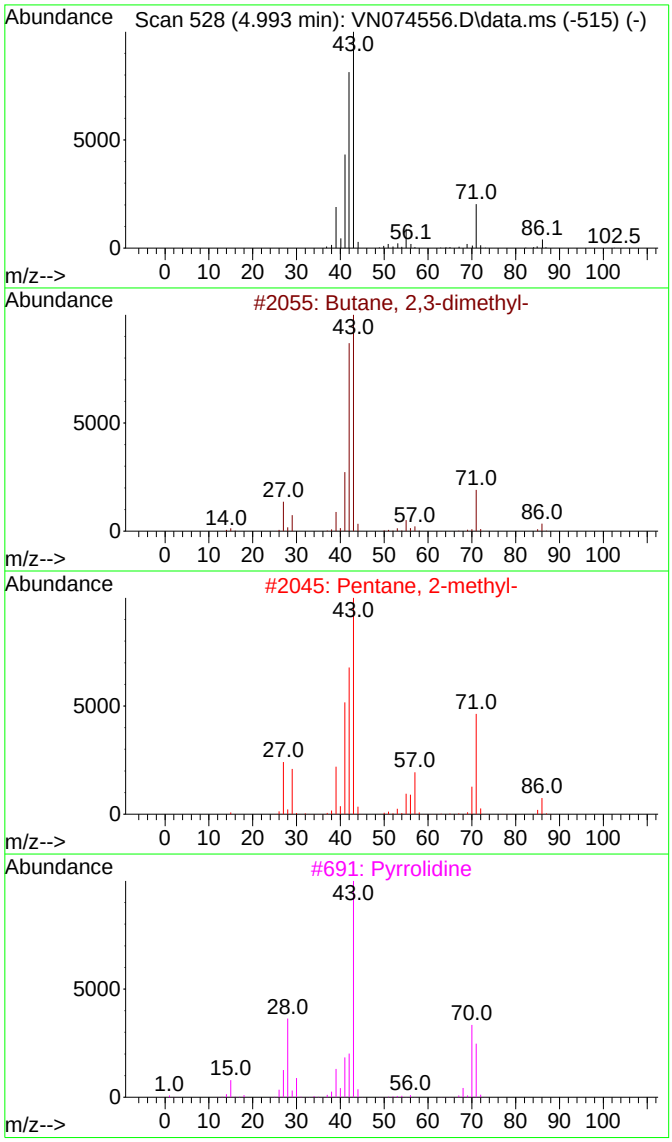
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

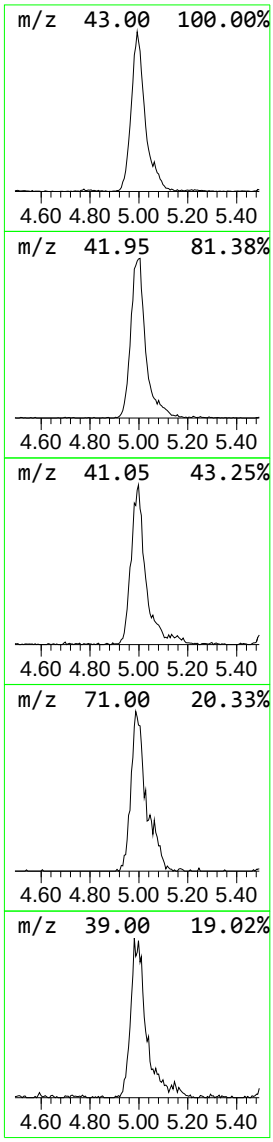
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	62.68 ug/l	1367430	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3	Pyrrolidine	71	C4H9N	000123-75-1	9
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	9





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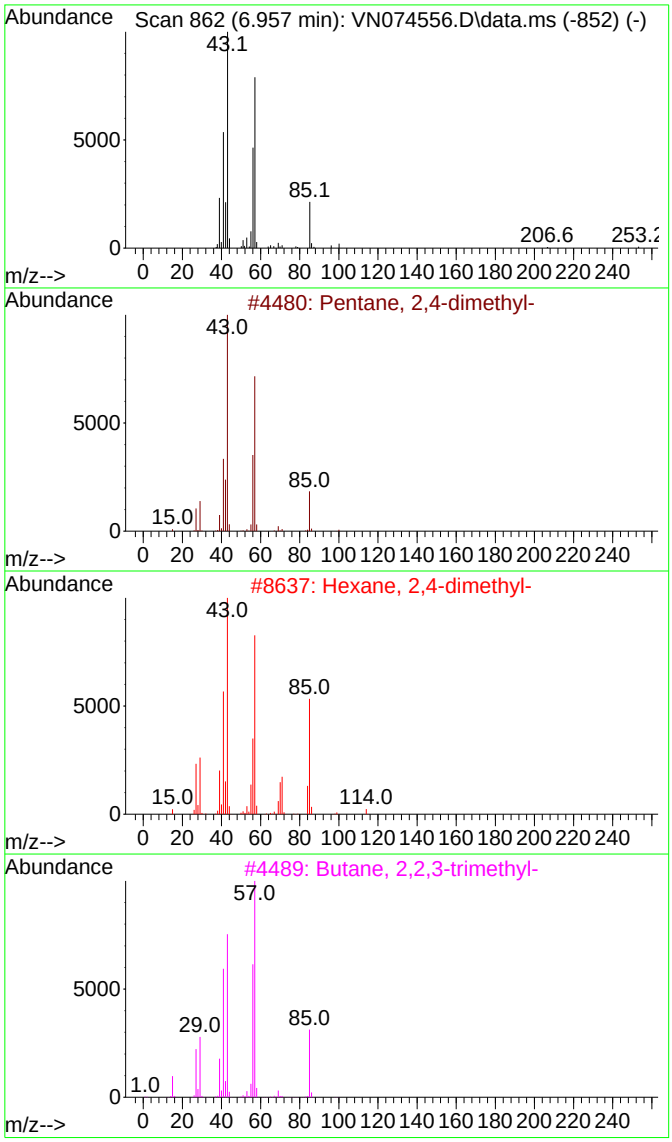
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

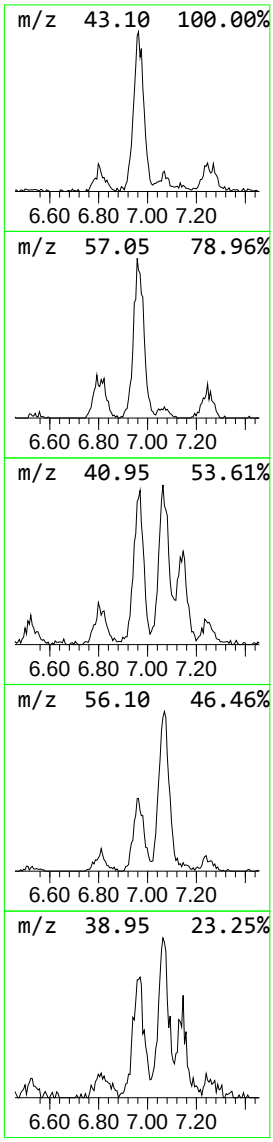
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.957	16.44 ug/l	358713	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	45
4	Nonane	128	C9H20	000111-84-2	45
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	43





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Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

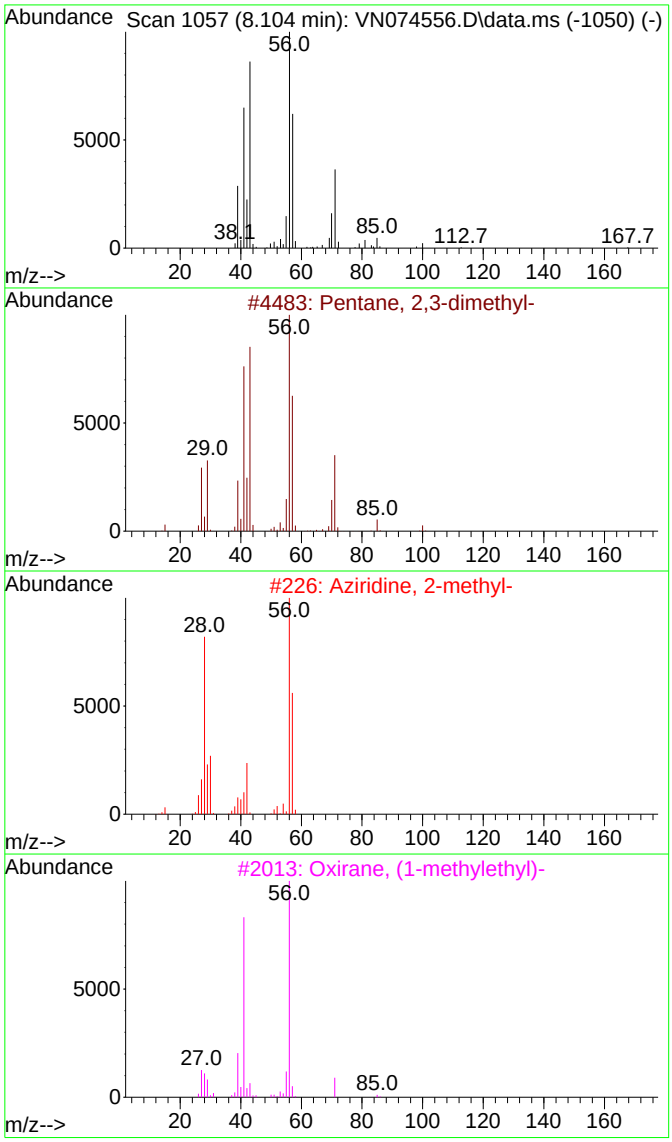
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

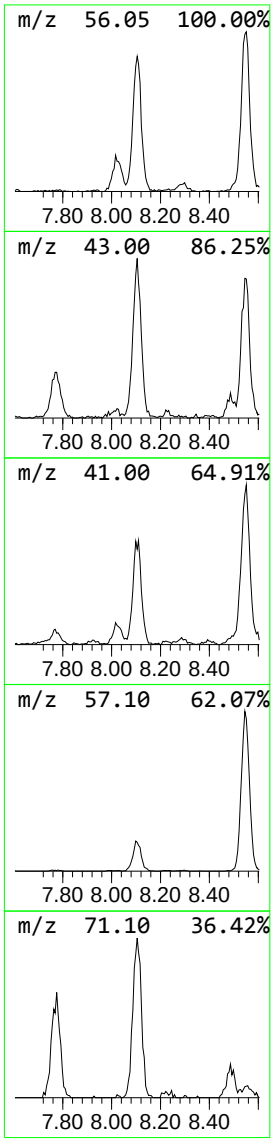
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	31.01 ug/l	676511	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	40
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

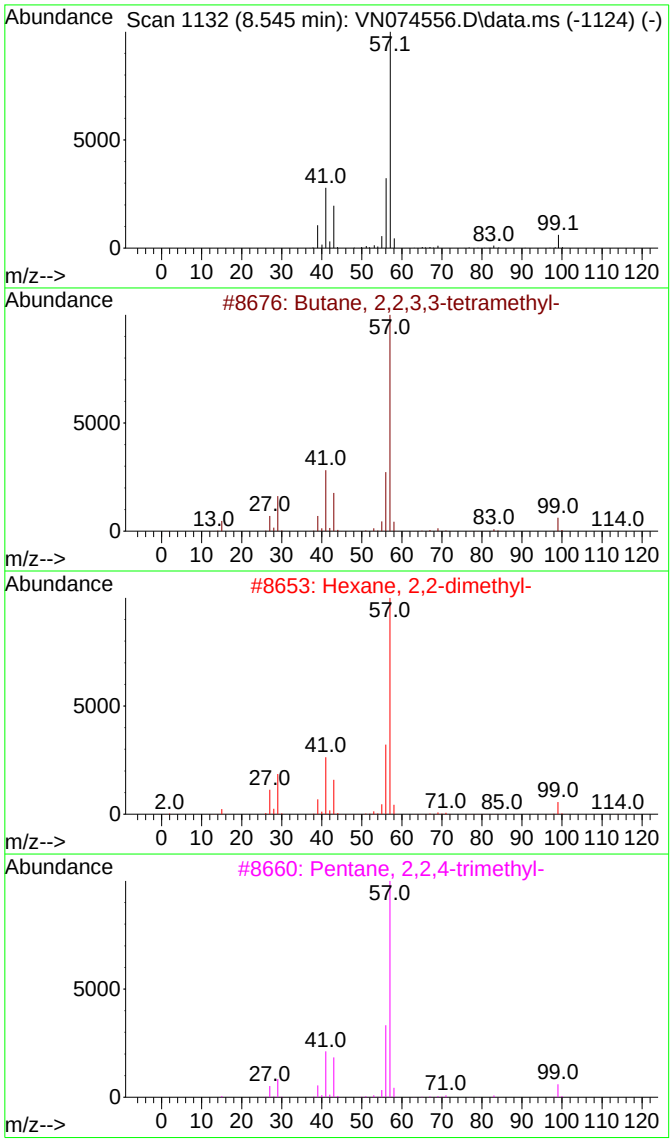
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

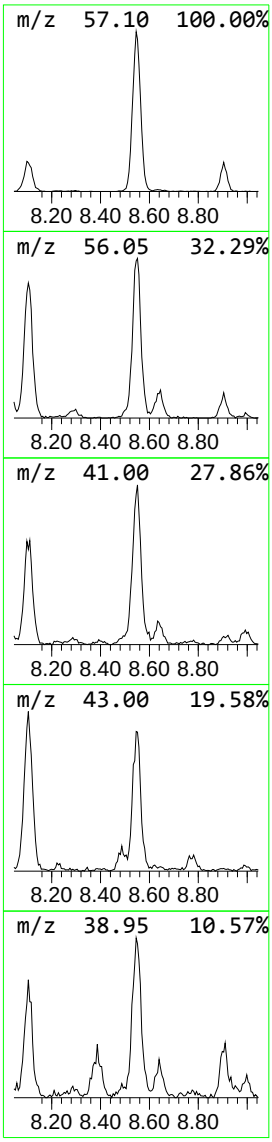
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	37.51 ug/l	1138300	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	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45





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Operator : JC\MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

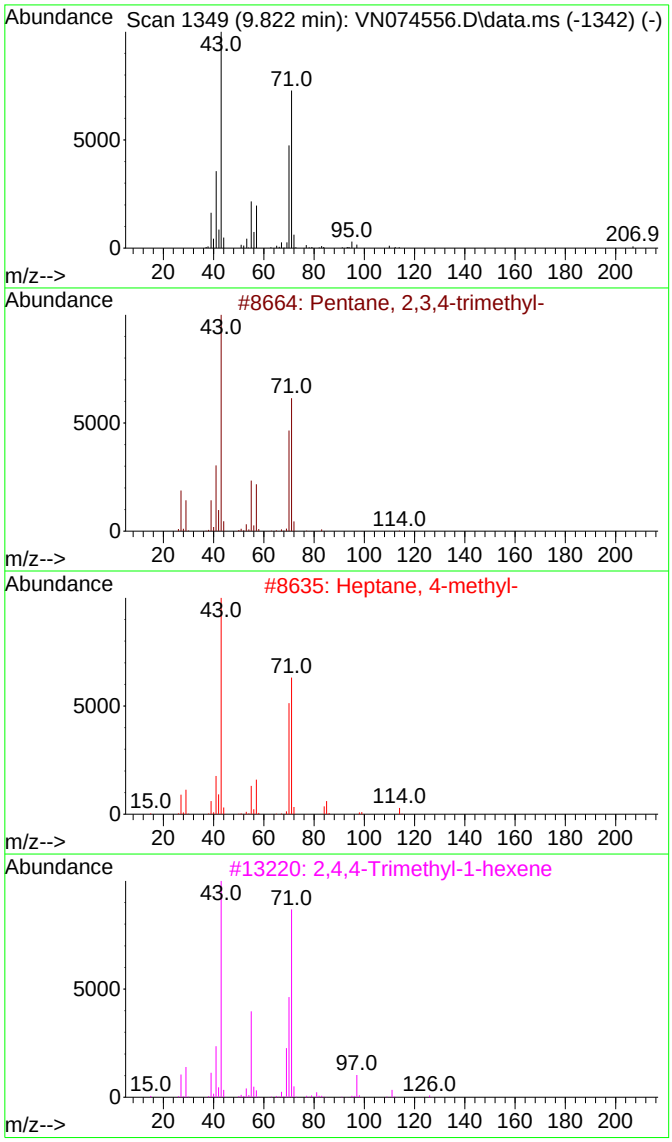
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

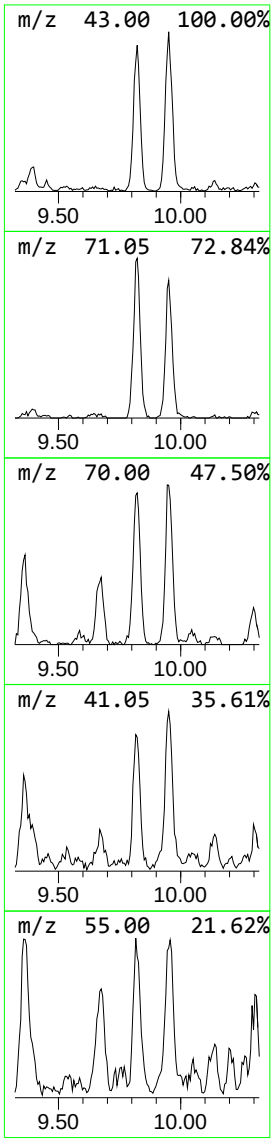
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.822	13.95 ug/l	423468	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	64
3	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	56
4	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	56
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

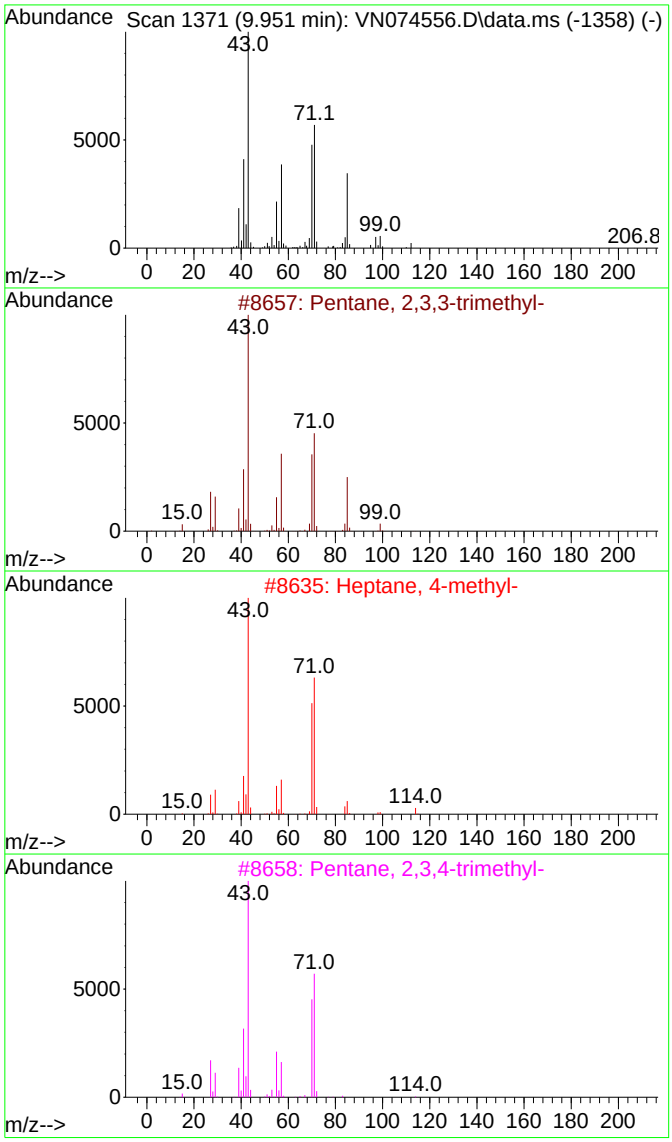
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

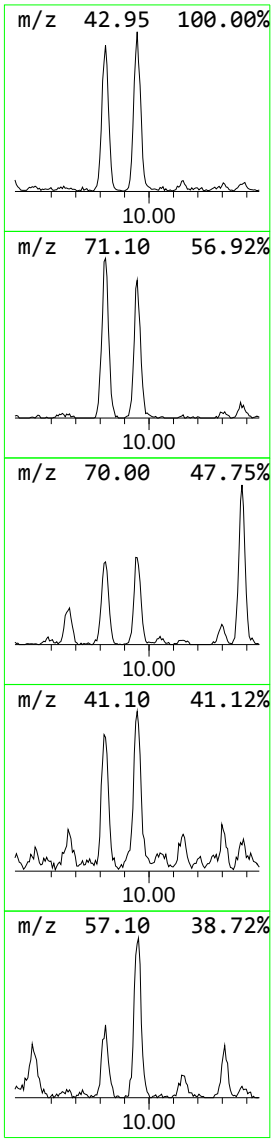
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.951	20.85 ug/l	632687	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	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	53





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Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
Operator : JC\MD
Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP090822

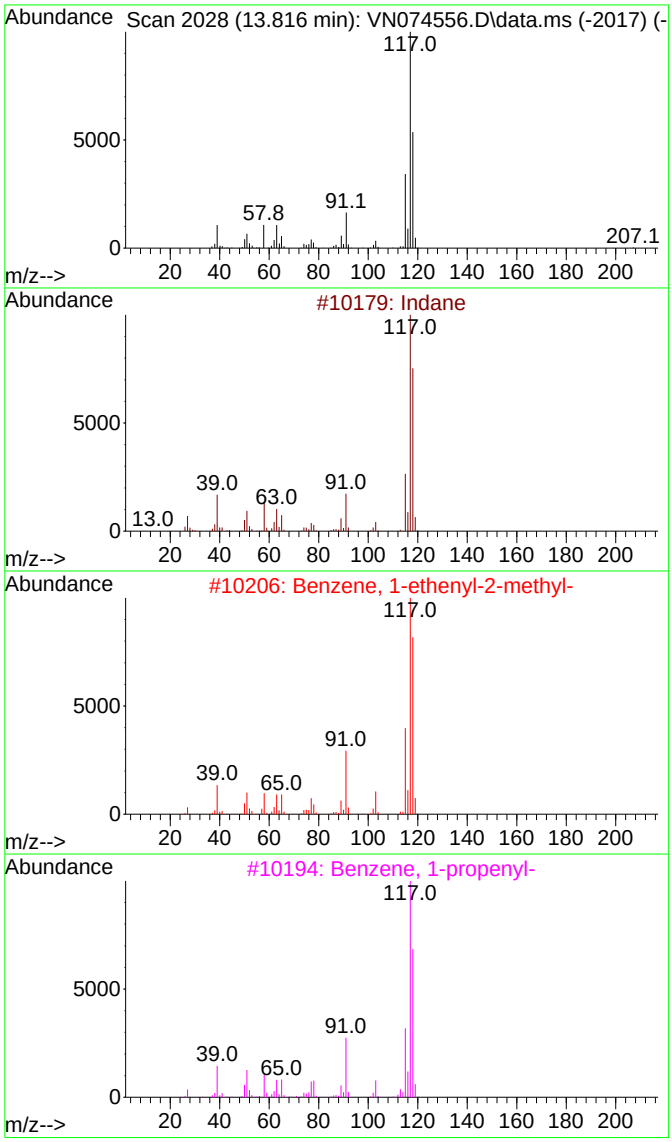
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

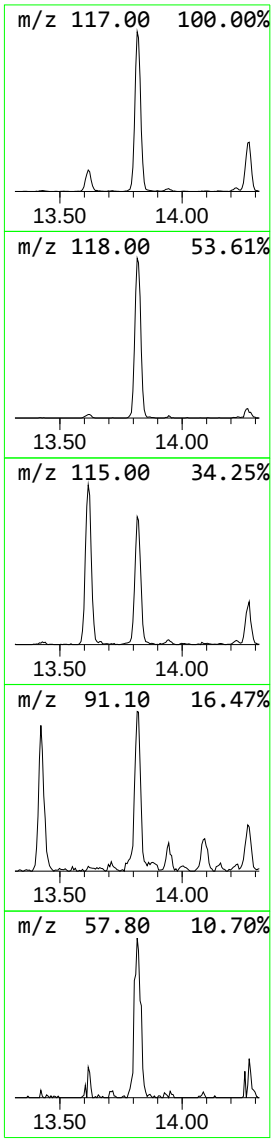
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	32.26 ug/l	1269990	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	96
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4	Deltacyclene	118	C9H10	007785-10-6	74
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074556.D
Acq On : 17 Sep 2022 15:16
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Sample : N4549-21
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

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MSVOA_N
ClientSampleId :
DUP090822

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	17.5	ug/l	381096	1	8.016	1090820	50.0
Butane, 2-methyl-	3.081	140.2	ug/l	3058030	1	8.016	1090820	50.0
Butane, 2,2-dim...	4.187	27.3	ug/l	595164	1	8.016	1090820	50.0
Butane, 2,3-dim...	4.993	62.7	ug/l	1367430	1	8.016	1090820	50.0
Pentane, 2,4-di...	6.957	16.4	ug/l	358713	1	8.016	1090820	50.0
Pentane, 2,3-di...	8.104	31.0	ug/l	676511	1	8.016	1090820	50.0
Butane, 2,2,3,3...	8.545	37.5	ug/l	1138300	2	8.904	1517340	50.0
Pentane, 2,3,4-...	9.822	13.9	ug/l	423468	2	8.904	1517340	50.0
Pentane, 2,3,3-...	9.951	20.9	ug/l	632687	2	8.904	1517340	50.0
Indane	13.816	32.3	ug/l	1269990	4	13.616	1968500	50.0