LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-23

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_X\Method\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	40	rBV	289802	505861	37.65%	4.425%
2	1.368	43	46	50	rVB	27587	29202	2.17%	0.255%
3	1.752	103	109	118	rVB	66398	93133	6.93%	0.815%
4	2.215	179	185	191	rVB2	9001	16229	1.21%	0.142%
5	2.337	199	205	211	rBV	14164	29012	2.16%	0.254%
6	2.550	230	240	250	rBV2	9138	25063	1.87%	0.219%
7	2.782	268	278	284	rBV	38800	90409	6.73%	0.791%
8	2.867	287	292	302	rVV	30452	61963	4.61%	0.542%
9	2.965	302	308	319	rVV2	7357	17936	1.33%	0.157%
10	3.105	323	331	345	rVB3	23713	58135	4.33%	0.509%
11	4.306	519	528	538	rVB2	19434	55820	4.15%	0.488%
12	4.434	538	549	556	rBV5	5116	14686	1.09%	0.128%
13	5.391	693	706	716	rBV	151072	442021	32.90%	3.867%
14	5.556	723	733	758	rVB	286626	832438	61.95%	7.282%
15	5.958	788	799	807	rBV	165180	430139	32.01%	3.763%
16	6.044	807	813	824	rVV	54624	144195	10.73%	1.261%
17	6.159	824	832	837	rVV5	6242	18396	1.37%	0.161%
18	6.251	841	847	858	rVV5	16718	51660	3.84%	0.452%
19	6.367	858	866	874	rVB9	5107	14051	1.05%	0.123%
20	6.763	922	931	945	rBV	427425	1018260	75.78%	8.907%
21	7.360	1021	1029	1039	rBV5	5905	16858	1.25%	0.147%
22	8.110	1145	1152	1154	rBV	16211	28736	2.14%	0.251%
23	8.147	1154	1158	1163	rVB	25230	42286	3.15%	0.370%
24	8.427	1197	1204	1211	rBV	13752	23785	1.77%	0.208%
25	8.507	1211	1217	1227	rVB3	19554	34614	2.58%	0.303%
26	8.653	1234	1241	1250	rBV	839030	1322738	98.45%	11.571%
27	8.842	1265	1272	1282	rVB2	18104	31889	2.37%	0.279%
28	8.958	1288	1291	1300	rVB3	11793	20283	1.51%	0.177%
29	9.049	1300	1306	1312	rBV3	11400	20185	1.50%	0.177%
30	9.165	1320	1325	1333	rVB	26465	41582	3.09%	0.364%
31	9.458	1364	1373	1378	rBV	28785	53643	3.99%	0.469%
32	10.055	1460	1471	1477	rBV	855265	1149390	85.54%	10.054%
33	10.147	1483	1486	1492	rVB5	11089	18455	1.37%	0.161%
34	10.963	1614	1620	1625	rVB	36984	48144	3.58%	0.421%
35	11.085	1634	1640	1649	rVB	645779	850291	63.28%	7.438%
36	11.305	1673	1676	1685	rVB	28115	38872	2.89%	0.340%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

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_X\Method\82X061822W.M
Title : SW846 8260

37	11.616	1723	1727	1736	rVB	20363	27628	2.06%	0.242%
38	11.890	1764	1772	1779	rBV4	8140	17826	1.33%	0.156%
39	12.024	1788	1794	1801	rBV	861781	1051138	78.23%	9.195%
40	12.177	1815	1819	1823	rVB	14520	18035	1.34%	0.158%
41	12.244	1823	1830	1837	rVV	1083287	1343626	100.00%	11.754%
42	12.317	1837	1842	1850	rVV	65496	81658	6.08%	0.714%
43	12.408	1853	1857	1862	rVB	25756	32252	2.40%	0.282%
44	12.646	1892	1896	1900	rVB	137439	160477	11.94%	1.404%
45	12.701	1900	1905	1912	rVB	361008	456004	33.94%	3.989%
46	12.841	1922	1928	1934	rVB	12973	17208	1.28%	0.151%
47	12.926	1934	1942	1946	rBV	74683	101483	7.55%	0.888%
48	13.170	1978	1982	1992	rVB	119008	155589	11.58%	1.361%
49	13.292	1998	2002	2007	rBV2	20381	29614	2.20%	0.259%
50	13.347	2007	2011	2016	rVV2	20107	26252	1.95%	0.230%
51	13.426	2020	2024	2031	rVB	41311	53278	3.97%	0.466%
52	13.542	2039	2043	2047	rVV2	22638	27771	2.07%	0.243%
53	13.585	2047	2050	2054	rVV2	10605	13861	1.03%	0.121%
54	13.640	2054	2059	2061	rVV2	27281	40860	3.04%	0.357%
55	13.664	2061	2063	2071	rVB	49669	53329	3.97%	0.467%
56	13.926	2101	2106	2110	rBV2	12662	16392	1.22%	0.143%
57	14.597	2211	2216	2222	rBV	11828	17022	1.27%	0.149%

Sum of corrected areas: 11431663

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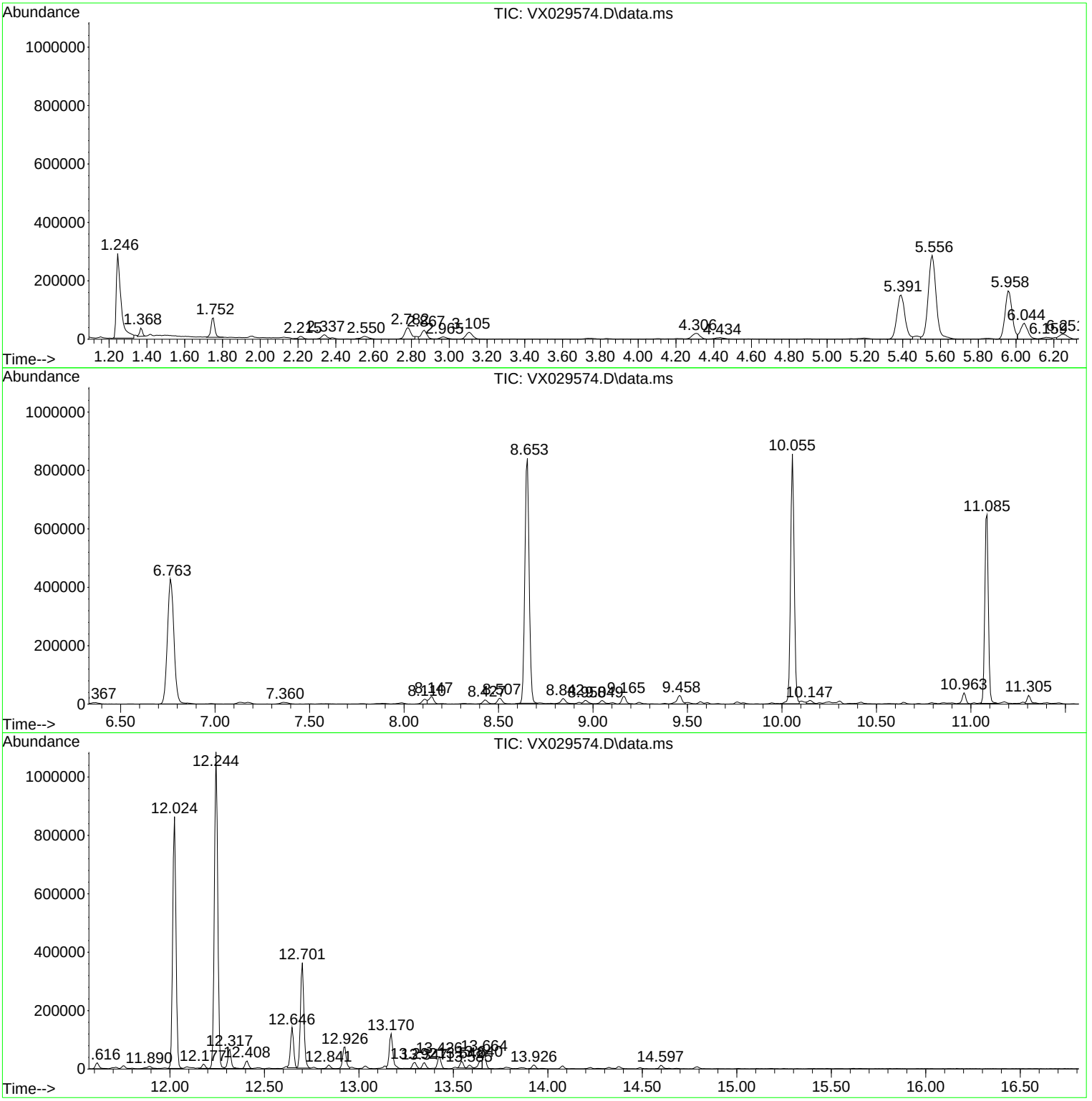
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
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MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

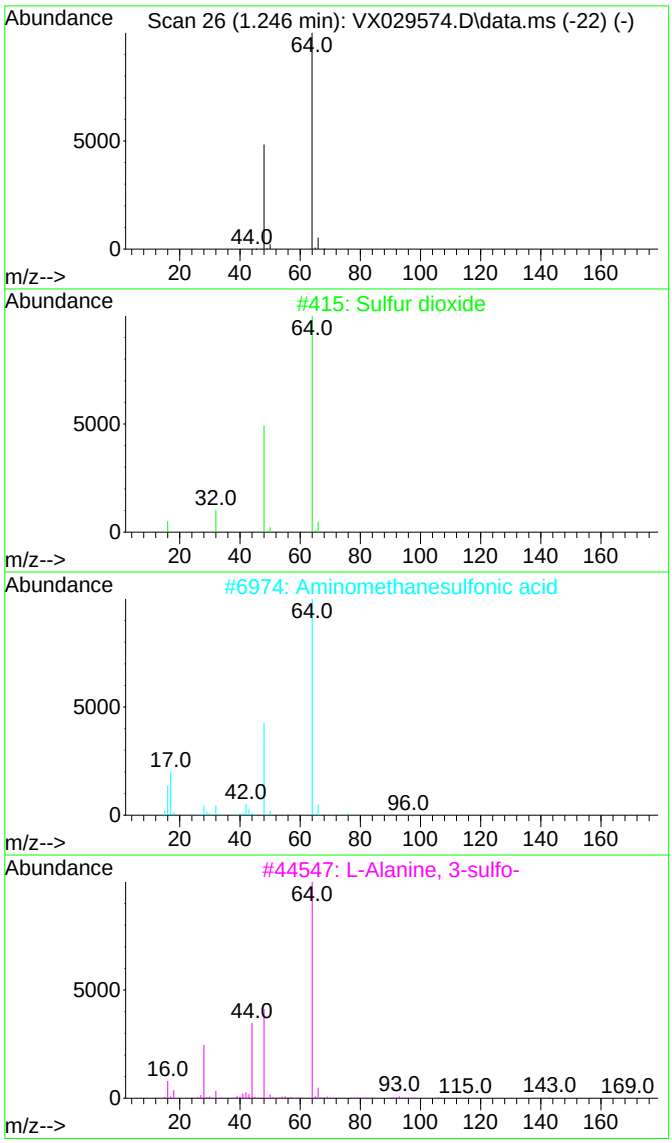
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

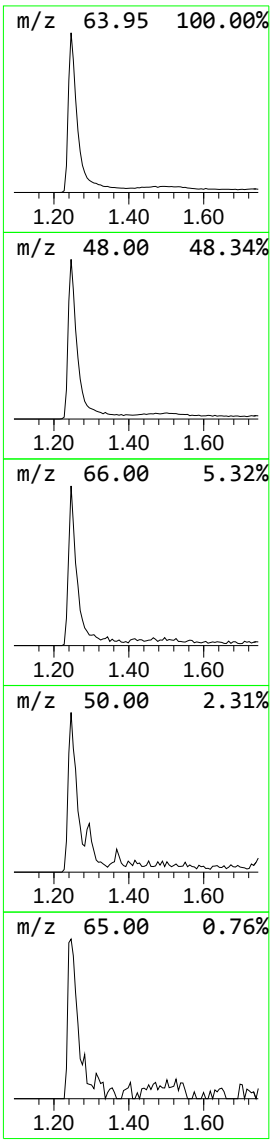
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	30.38 ug/l	505861	Pentafluorobenzene	5.556

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	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

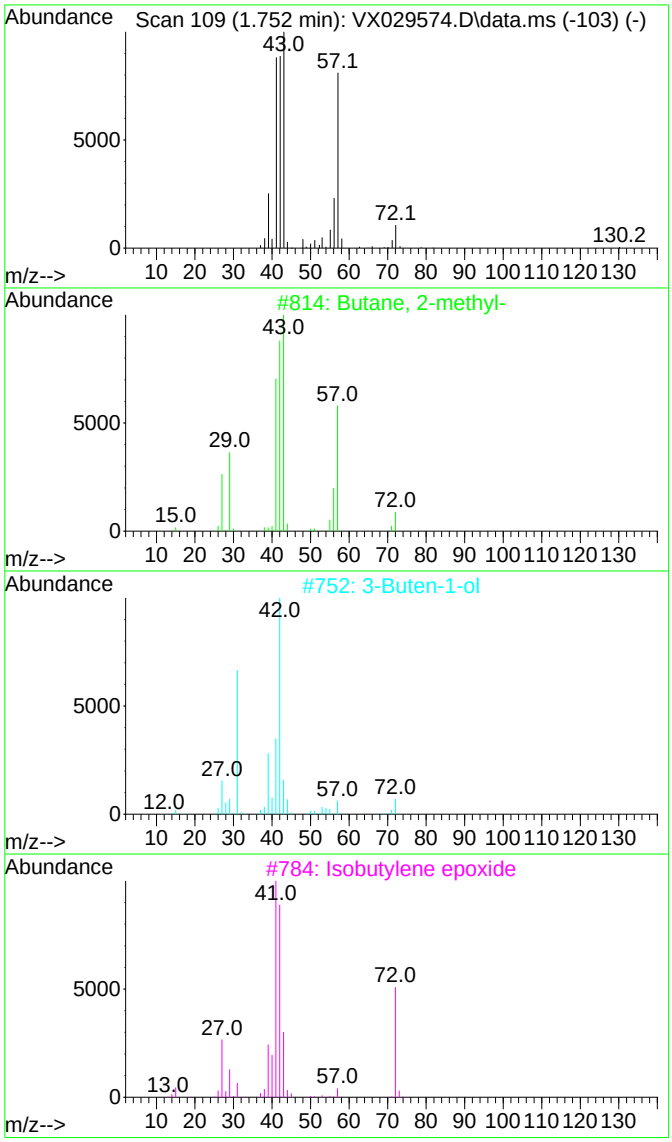
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

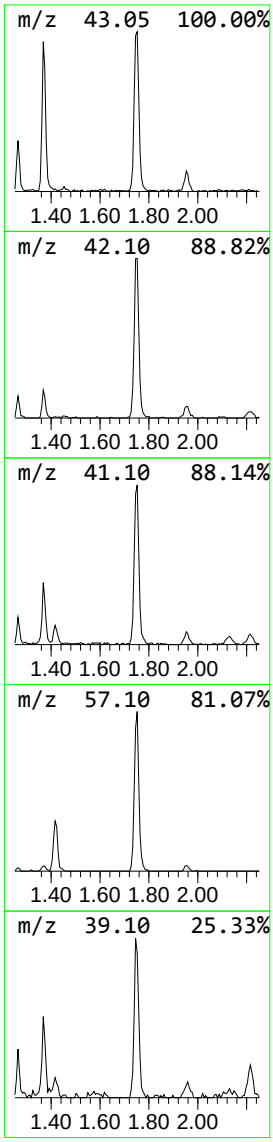
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.59 ug/l	93133	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Isobutylene epoxide	72	C4H8O	000558-30-5	38
4	Pentane	72	C5H12	000109-66-0	33
5	1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	16





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Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

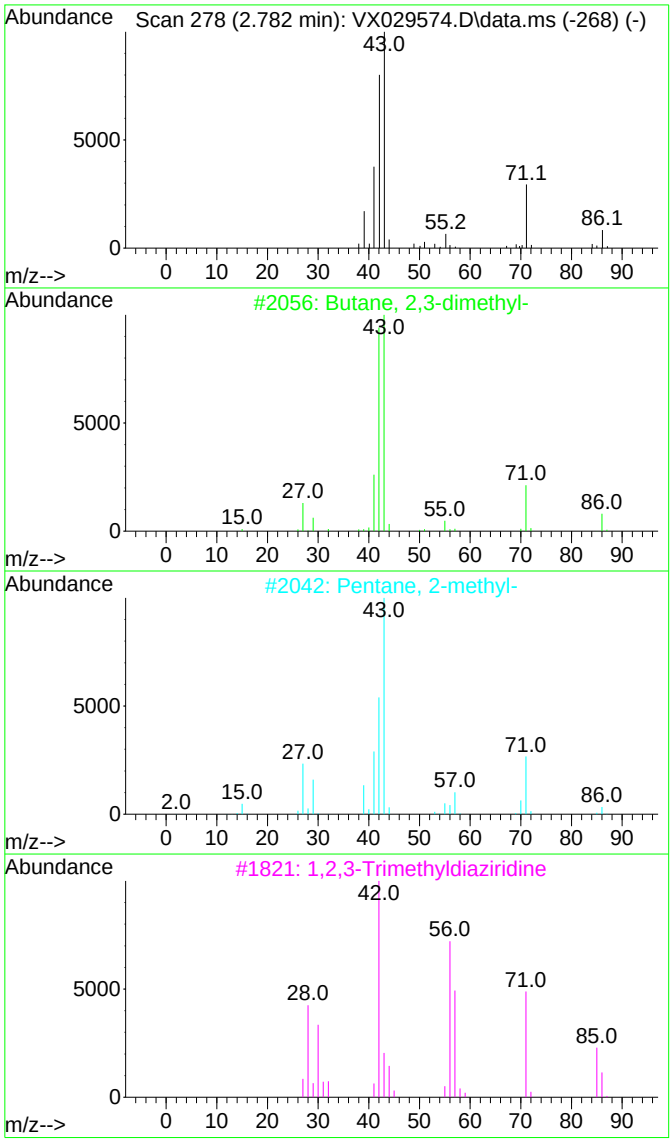
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

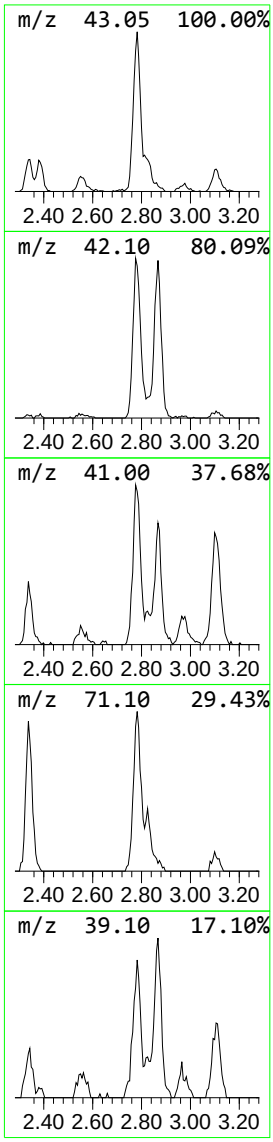
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	5.43 ug/l	90409	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	38
4	Pentane	72	C5H12	000109-66-0	38
5	Pyrrolidine	71	C4H9N	000123-75-1	27





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Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

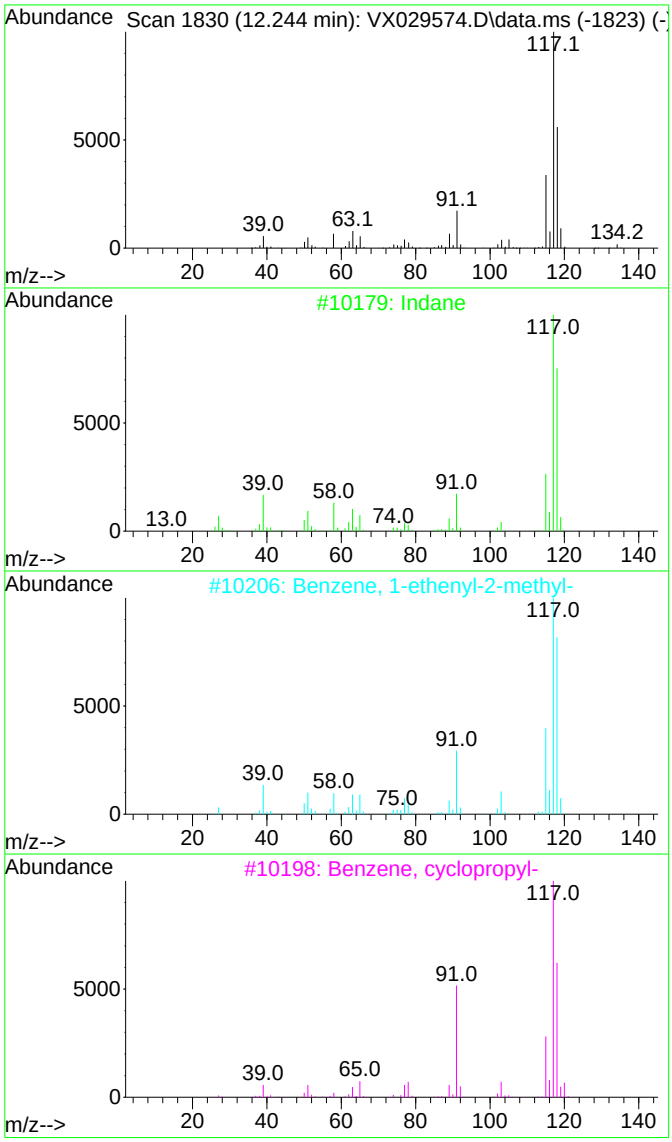
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

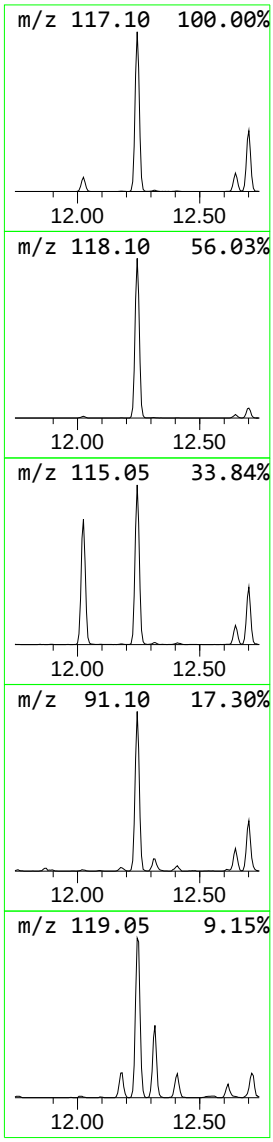
****

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	63.91 ug/l	1343630	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4	Deltacyclene	118	C9H10	007785-10-6	64
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

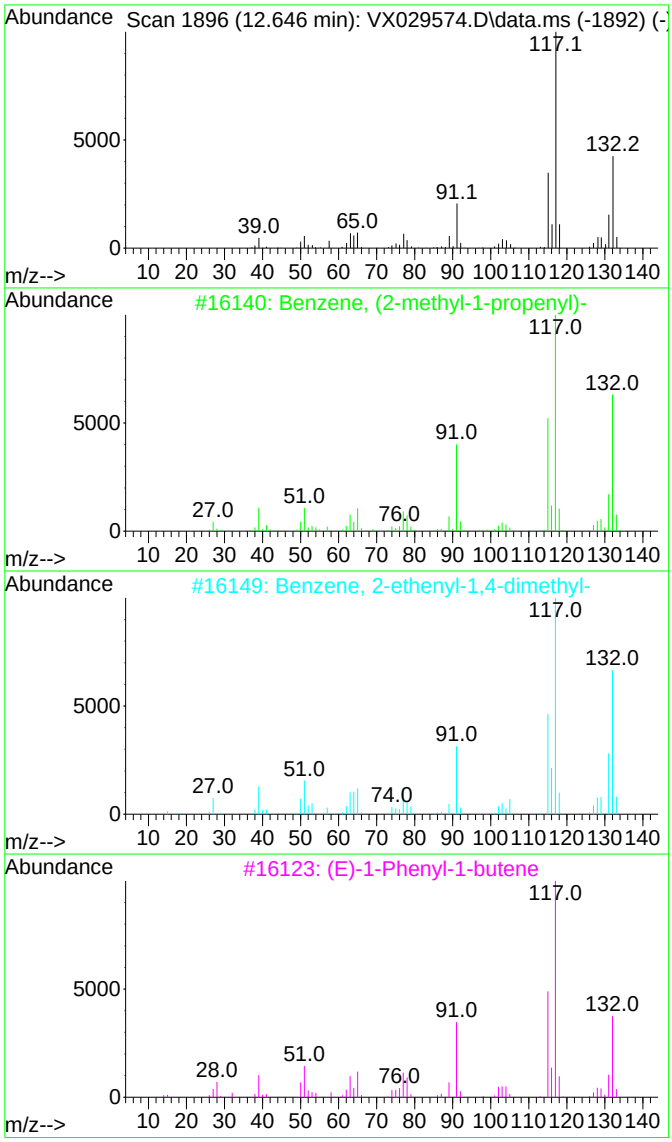
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

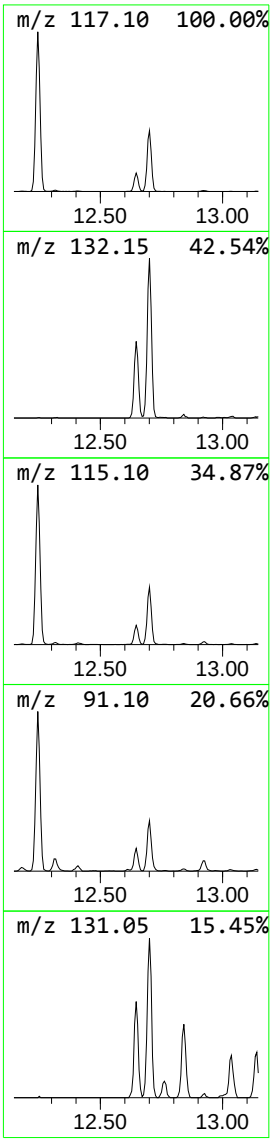
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.646	7.63 ug/l	160477	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	95
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
3	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	94
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	94





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

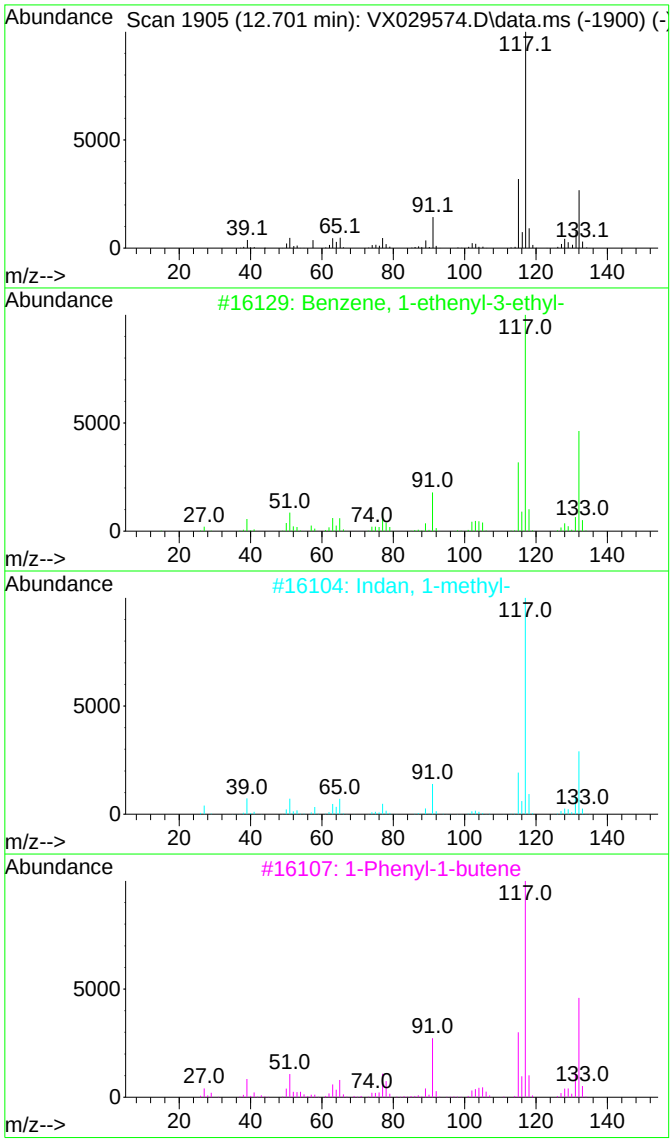
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

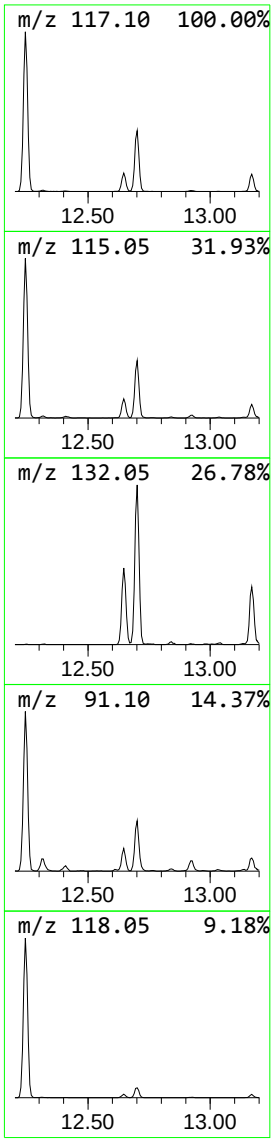
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	21.69 ug/l	456004	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	90
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

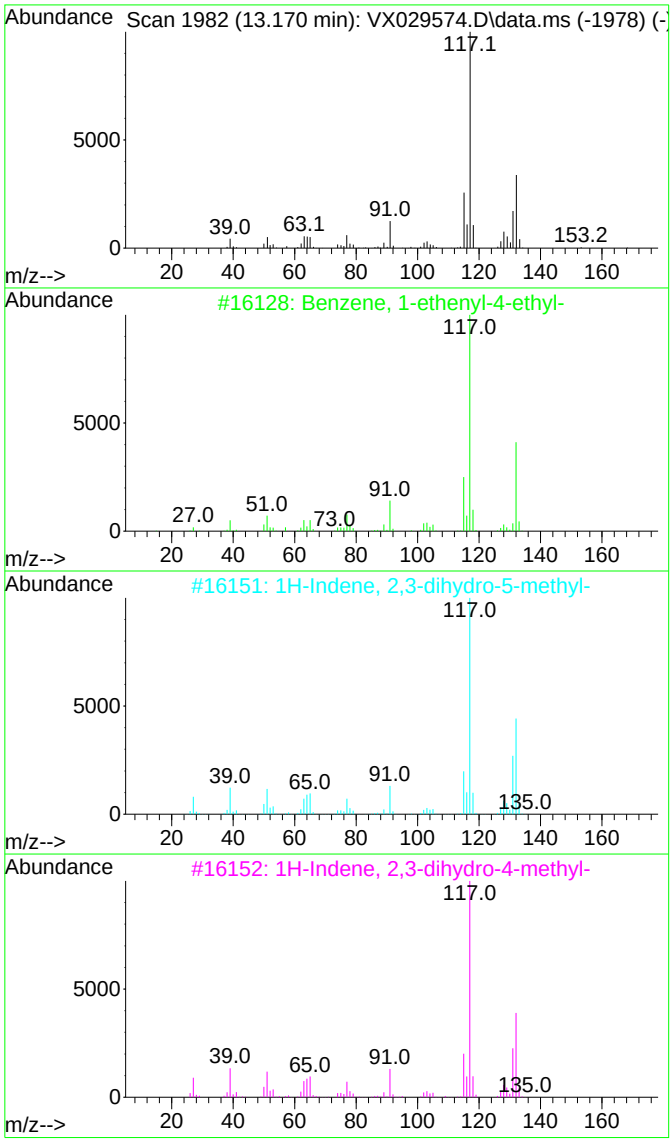
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

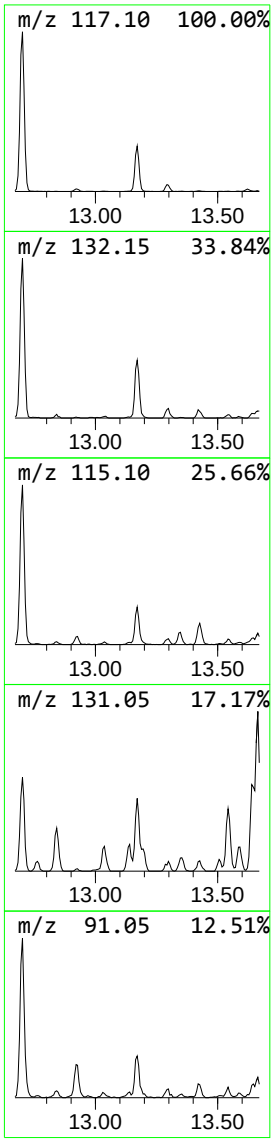
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	7.40 ug/l	155589	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4	Indan, 1-methyl-	132	C10H12	000767-58-8	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029574.D
Acq On : 18 Jun 2022 16:59
Operator : JC/MD
Sample : N3325-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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	1.246	30.4	ug/l	505861	1	5.556	832438	50.0
Butane, 2-methyl-	1.752	5.6	ug/l	93133	1	5.556	832438	50.0
Butane, 2,3-dim...	2.782	5.4	ug/l	90409	1	5.556	832438	50.0
Indane	12.244	63.9	ug/l	1343630	4	12.024	1051140	50.0
Benzene, (2-met...	12.646	7.6	ug/l	160477	4	12.024	1051140	50.0
Benzene, 1-ethe...	12.701	21.7	ug/l	456004	4	12.024	1051140	50.0
Benzene, 1-ethe...	13.170	7.4	ug/l	155589	4	12.024	1051140	50.0