LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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\82X022322W.M
Title : SW846 8260

Signal : TIC: VX027253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	29	rBV	32497	46273	4.70%	1.019%
2	1.374	44	47	53	rVB	11644	11734	1.19%	0.258%
3	1.752	105	109	117	rVB	17235	23734	2.41%	0.523%
4	2.221	180	186	194	rVB	9647	15156	1.54%	0.334%
5	2.758	267	274	277	rBV	4965	10931	1.11%	0.241%
6	2.873	284	293	300	rVV	15510	34793	3.54%	0.766%
7	2.959	300	307	323	rVV	49730	109663	11.15%	2.415%
8	3.117	324	333	345	rVB	55850	130683	13.29%	2.878%
9	3.763	428	439	447	rBV4	9657	29976	3.05%	0.660%
10	4.318	520	530	542	rVV4	15594	47569	4.84%	1.048%
11	5.391	696	706	715	rBV2	50265	144799	14.72%	3.189%
12	5.477	715	720	725	rVV4	7923	21610	2.20%	0.476%
13	5.556	725	733	756	rVB	86038	252180	25.64%	5.555%
14	5.964	788	800	805	rBV2	52097	136324	13.86%	3.003%
15	6.044	805	813	829	rVV	375874	983670	100.00%	21.666%
16	6.239	831	845	855	rBV7	9444	39877	4.05%	0.878%
17	6.763	920	931	943	rBV	131465	319219	32.45%	7.031%
18	8.110	1145	1152	1156	rBV2	6943	15395	1.57%	0.339%
19	8.427	1198	1204	1210	rBV2	5609	9910	1.01%	0.218%
20	8.507	1210	1217	1226	rVB5	5794	11411	1.16%	0.251%
21	8.653	1226	1241	1248	rBV	271020	432909	44.01%	9.535%
22	8.958	1282	1291	1300	rVB2	12481	22527	2.29%	0.496%
23	9.049	1300	1306	1312	rBV	15067	22855	2.32%	0.503%
24	9.458	1365	1373	1378	rBV	19378	32241	3.28%	0.710%
25	10.055	1465	1471	1477	rBV	284423	374415	38.06%	8.247%
26	10.195	1489	1494	1499	rVB	50432	63252	6.43%	1.393%
27	10.305	1504	1512	1517	rVB	7827	11912	1.21%	0.262%
28	10.963	1614	1620	1626	rBV	19945	24991	2.54%	0.550%
29	11.079	1634	1639	1656	rBV	221448	292051	29.69%	6.433%
30	11.305	1672	1676	1684	rVB	16820	20450	2.08%	0.450%
31	11.616	1722	1727	1732	rBV	14631	17460	1.77%	0.385%
32	11.756	1745	1750	1757	rVB	29154	34623	3.52%	0.763%
33	12.024	1789	1794	1801	rVV	294707	362142	36.82%	7.977%
34	12.244	1825	1830	1838	rBV	97222	117820	11.98%	2.595%
35	12.463	1862	1866	1873	rVB	10734	12525	1.27%	0.276%
36	12.616	1885	1891	1893	rBV	11715	13873	1.41%	0.306%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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\82X022322W.M
Title : SW846 8260

37	12.646	1893	1896	1900	rVB	11507	13005	1.32%	0.286%
38	12.701	1900	1905	1913	rBV	41444	53426	5.43%	1.177%
39	12.847	1924	1929	1934	rVB2	7846	10750	1.09%	0.237%
40	12.920	1934	1941	1945	rBV	20618	27841	2.83%	0.613%
41	12.963	1945	1948	1954	rVV	22834	26819	2.73%	0.591%
42	13.170	1979	1982	1991	rVB2	9039	14072	1.43%	0.310%
43	13.292	1998	2002	2007	rVB2	36843	46510	4.73%	1.024%
44	13.426	2020	2024	2028	rVB	11106	14570	1.48%	0.321%
45	13.585	2046	2050	2056	rVV3	7570	15583	1.58%	0.343%
46	13.664	2061	2063	2069	rVB2	8905	12263	1.25%	0.270%
47	13.780	2075	2082	2091	rBV	11934	17348	1.76%	0.382%
48	14.213	2147	2153	2160	rBV4	6841	12384	1.26%	0.273%
49	14.780	2241	2246	2255	rBV	17248	24530	2.49%	0.540%

Sum of corrected areas: 4540054

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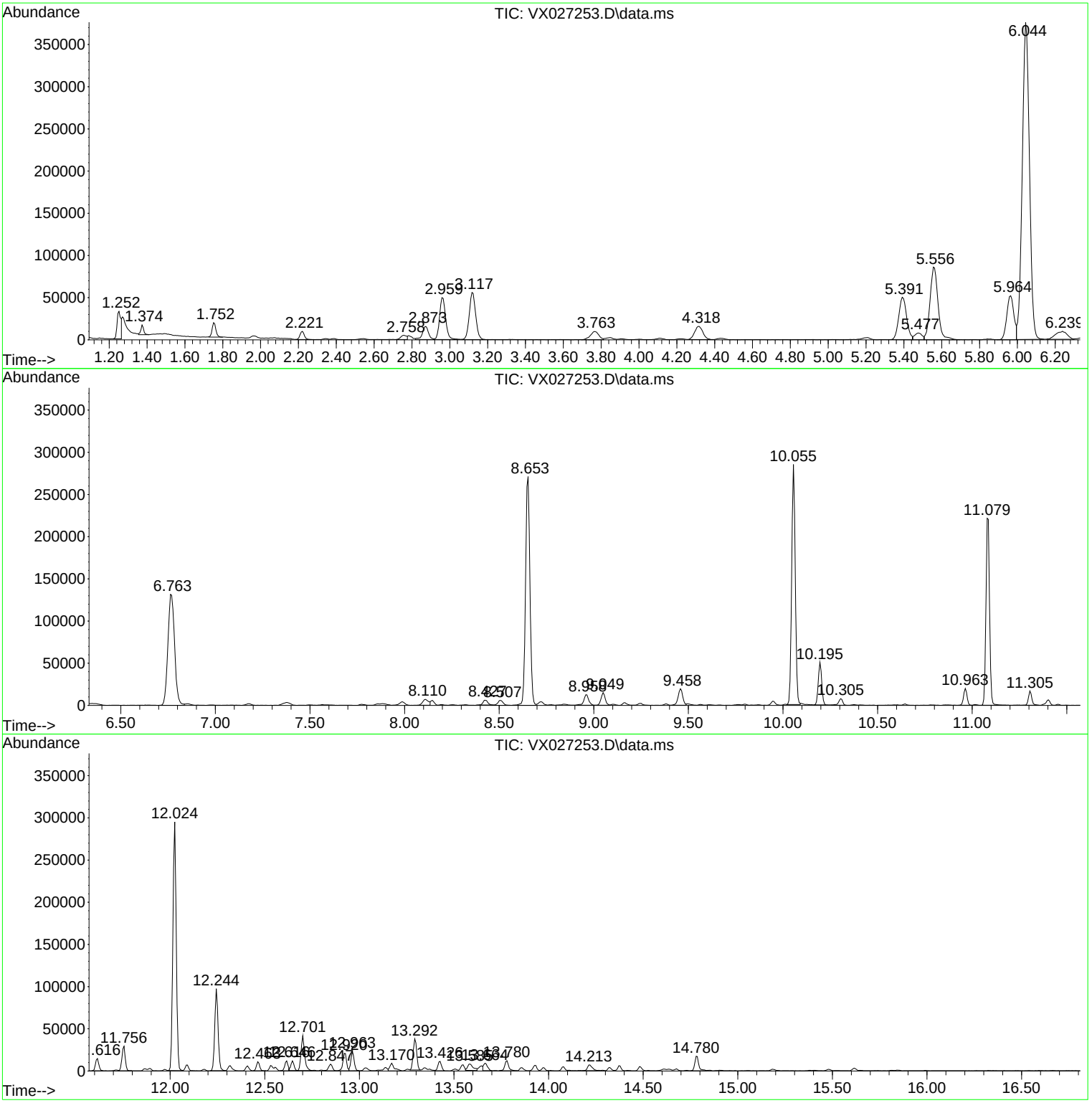
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

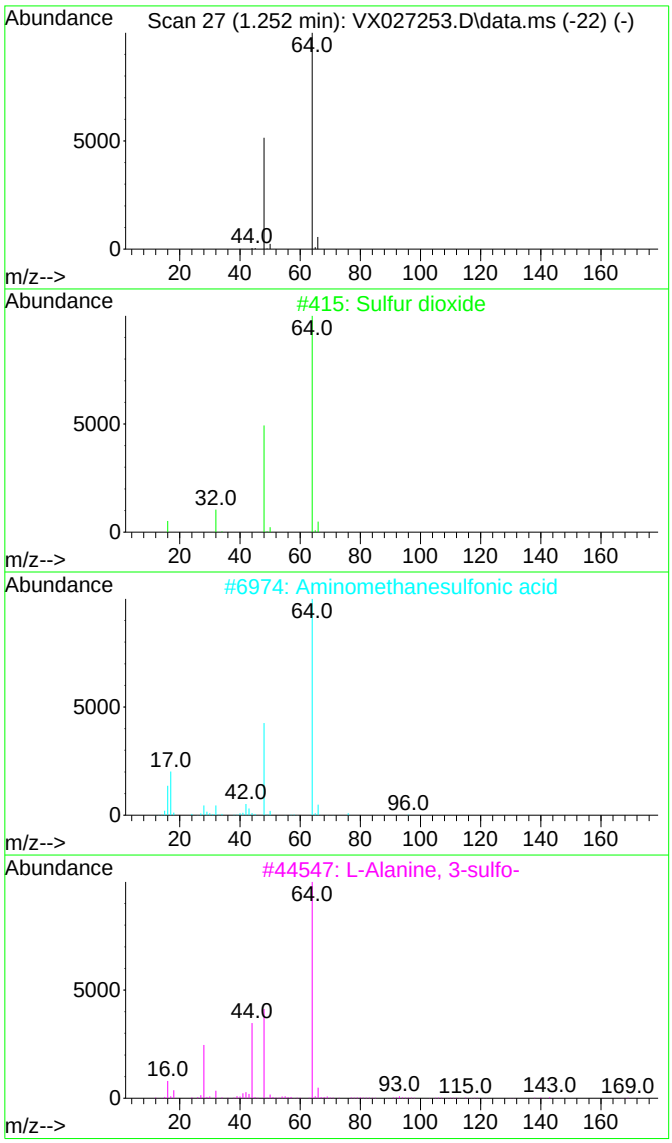
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

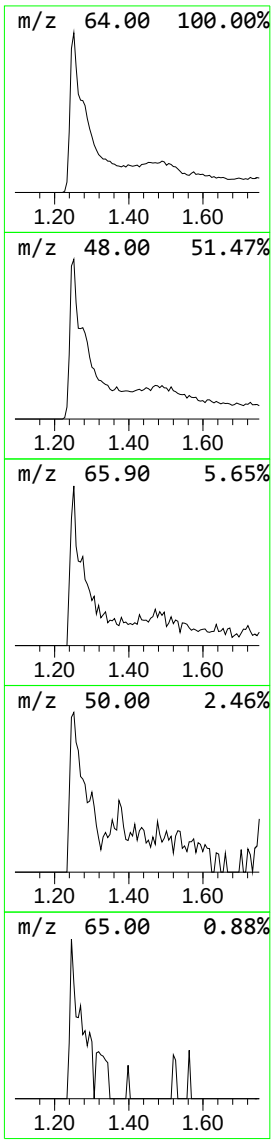
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	9.17 ug/l	46273	Pentafluorobenzene	5.562

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	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\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

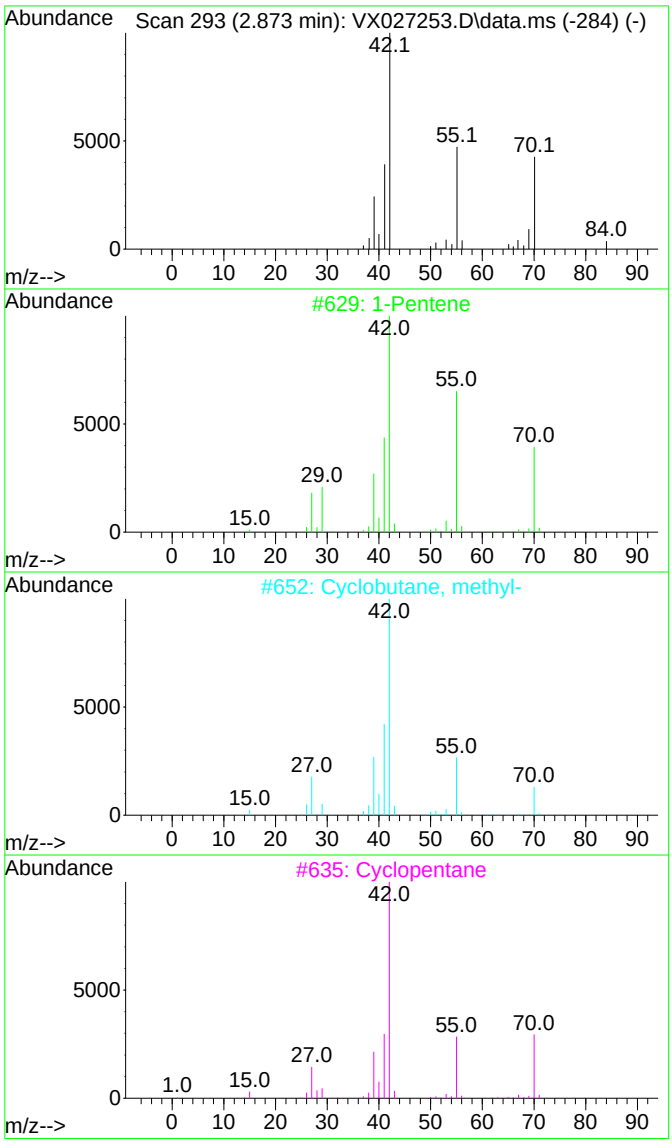
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

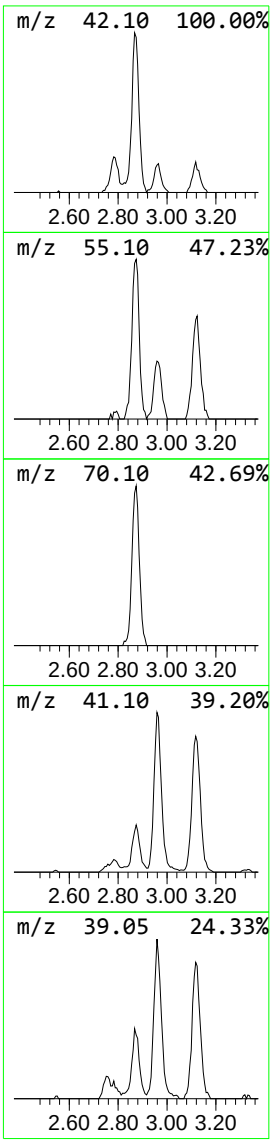
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Pentene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.873	6.90 ug/l	34793	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	Cyclopentane	70	C5H10	000287-92-3	72
4	3-Buten-1-ol	72	C4H8O	000627-27-0	37
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

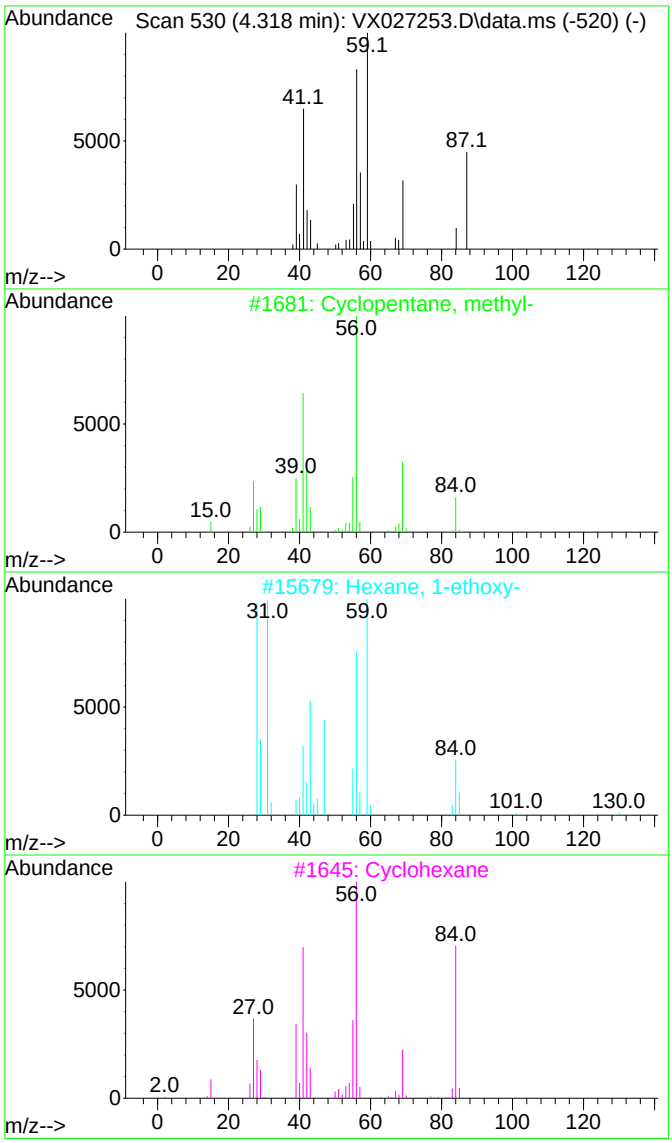
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

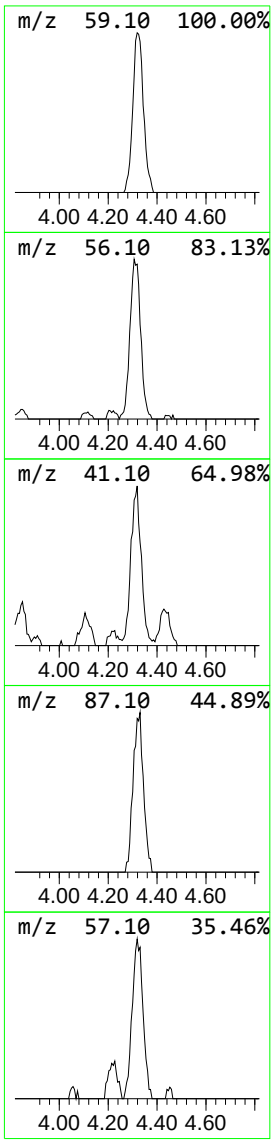
****

Peak Number 3 unknown4.318 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.318	9.43 ug/l	47569	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	38
2	Hexane, 1-ethoxy-	130	C8H18O	005756-43-4	36
3	Cyclohexane	84	C6H12	000110-82-7	35
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	27
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

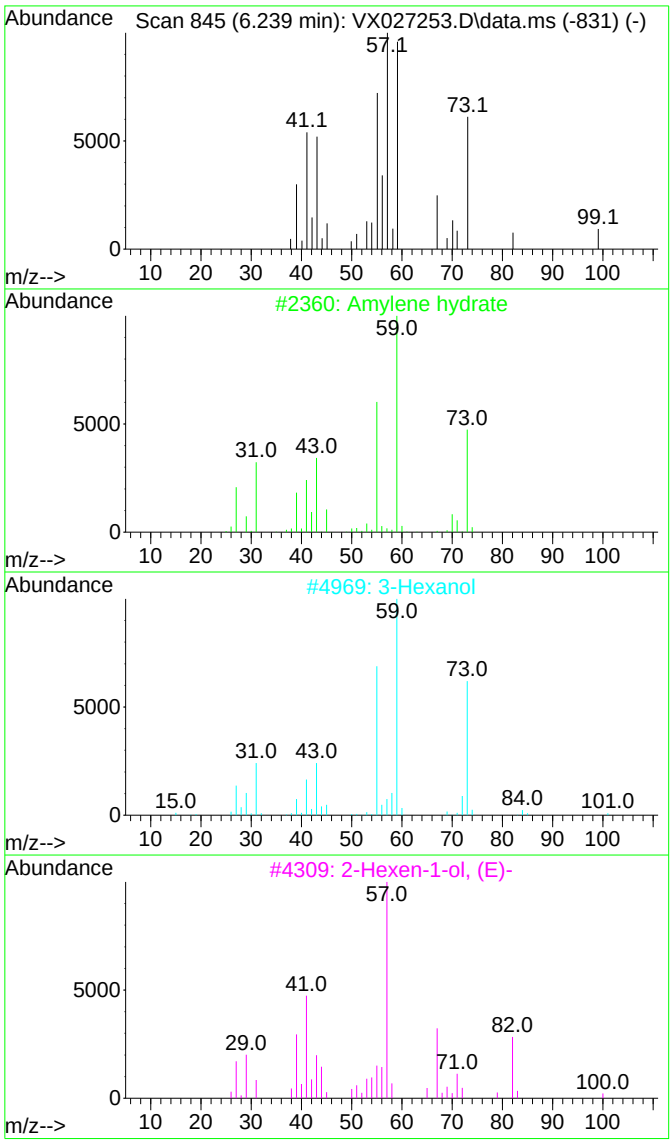
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

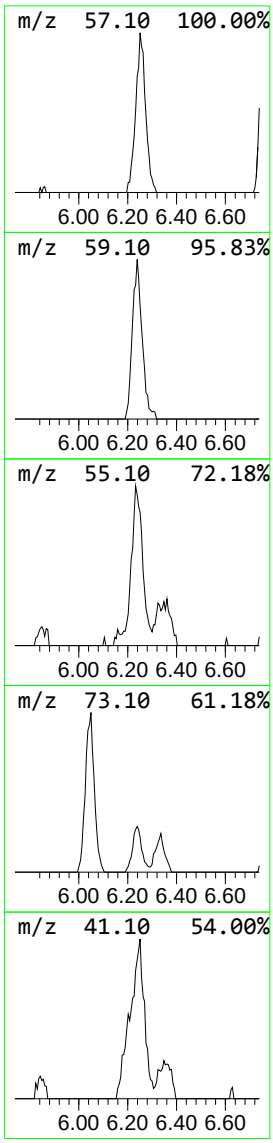
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown6.239 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	6.25 ug/l	39877	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	43
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	22
4	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	14
5	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

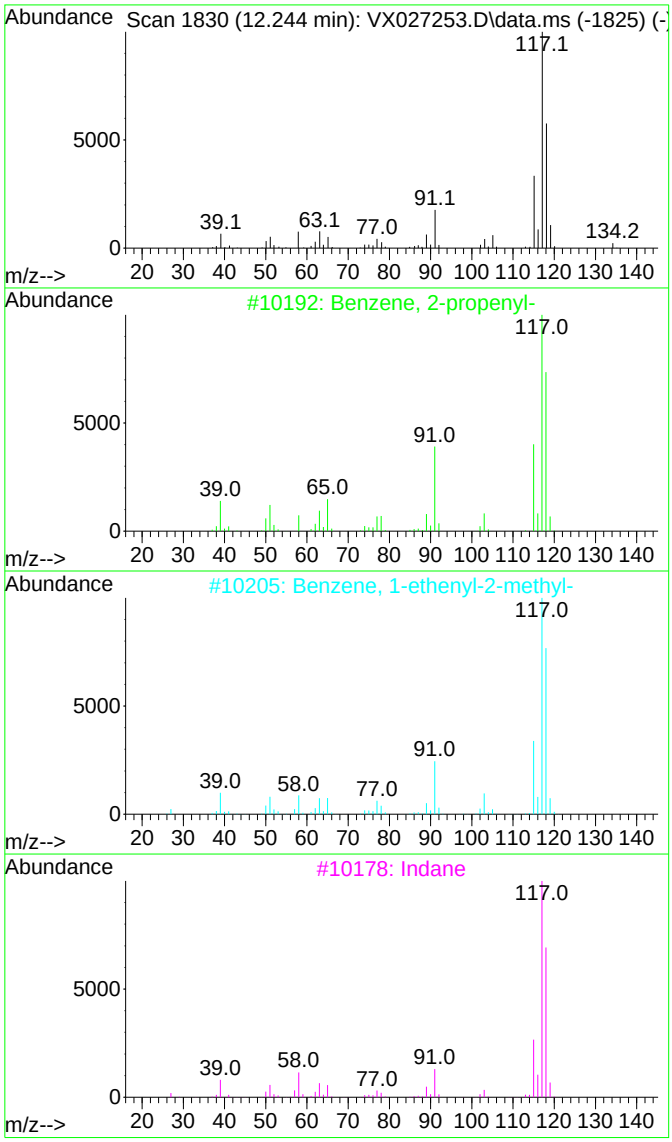
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

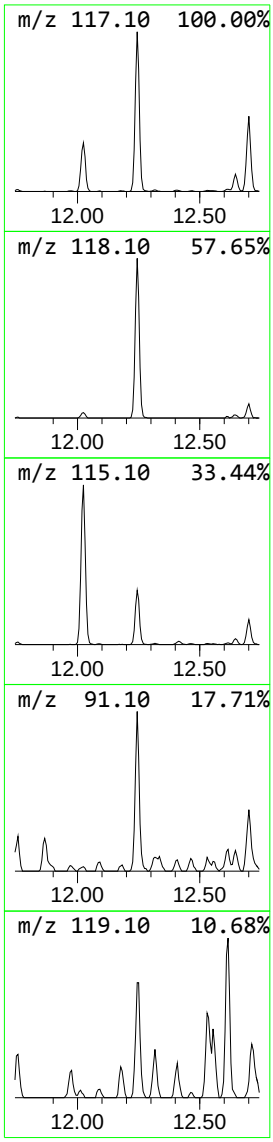
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	16.27 ug/l	117820	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3	Indane	118	C9H10	000496-11-7	81
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

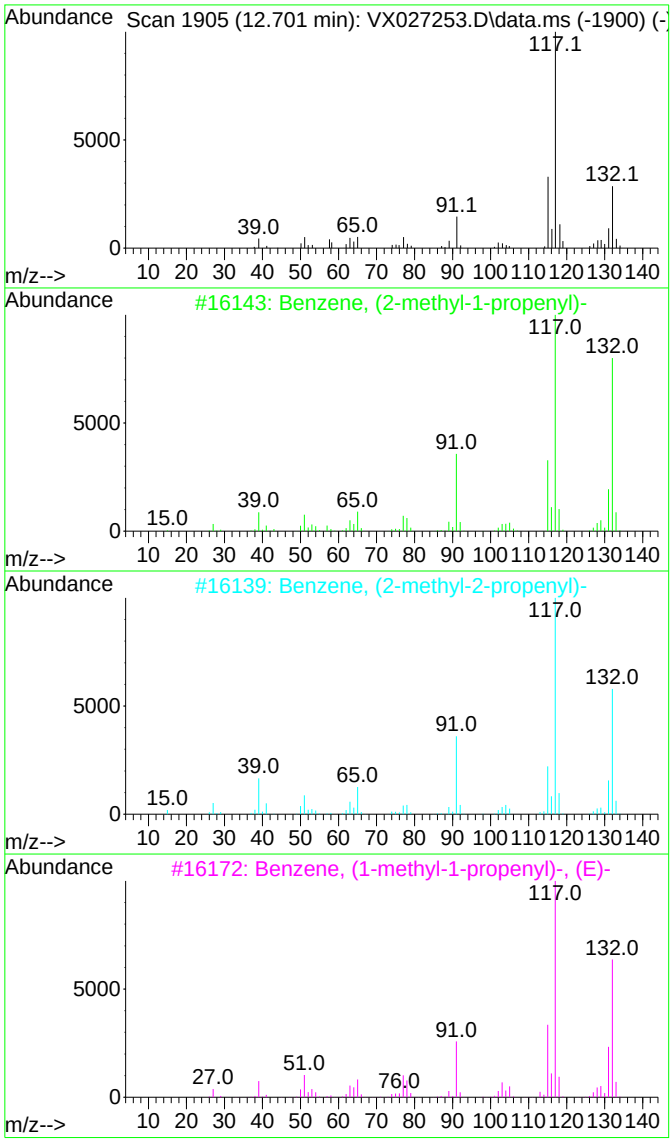
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

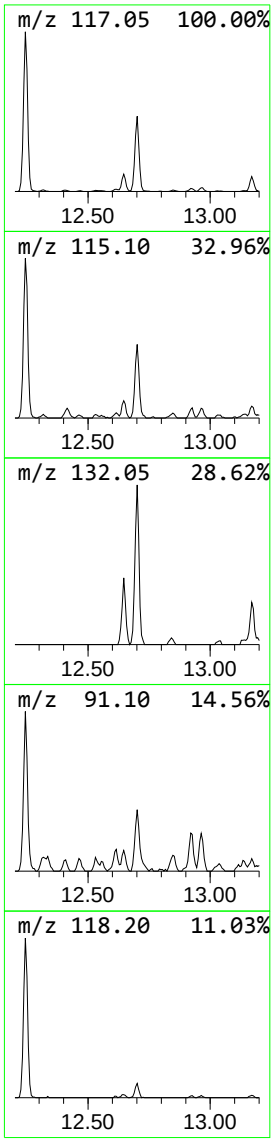
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	7.38 ug/l	53426	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	91
2	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	91
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
5	Indan, 1-methyl-	132	C10H12	000767-58-8	90





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

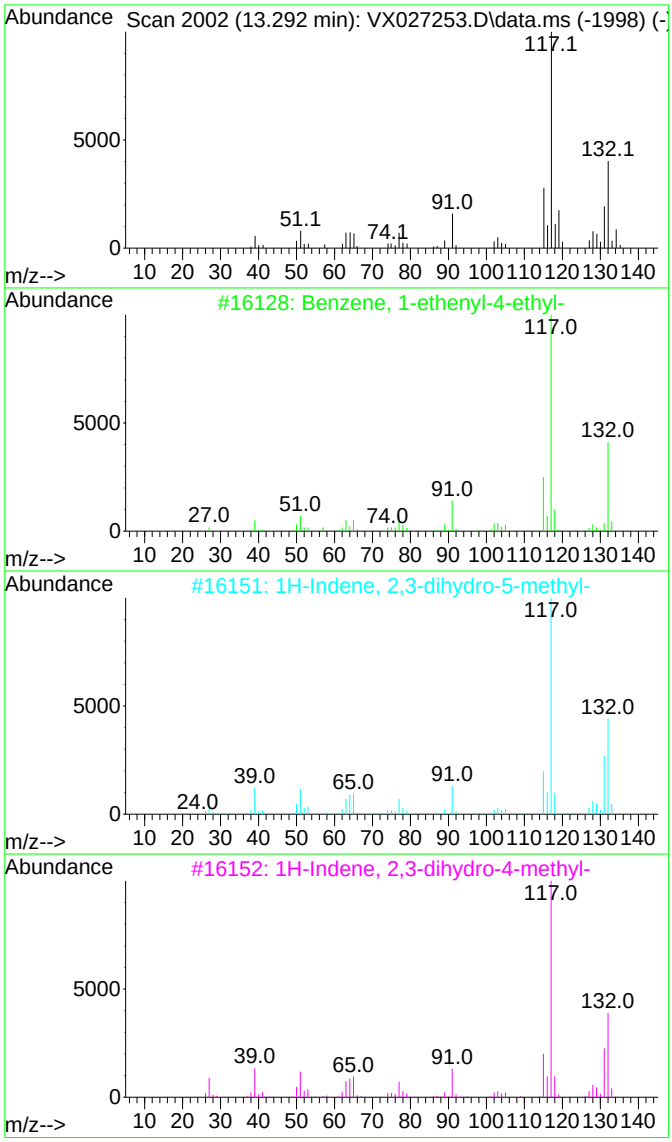
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

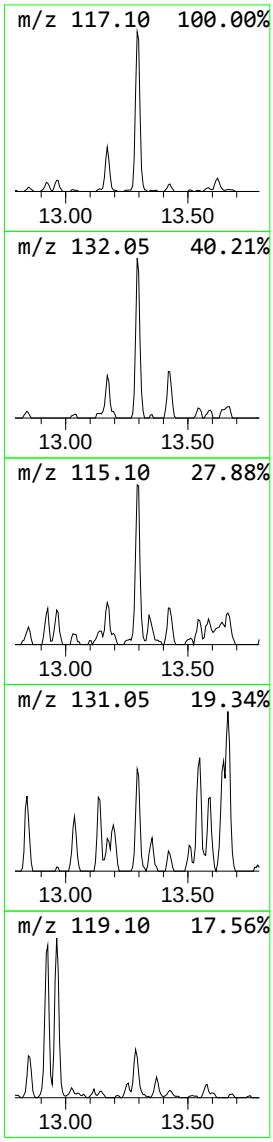
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.42 ug/l	46510	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	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027253.D
Acq On : 01 Mar 2022 17:03
Operator : JC/MD
Sample : N1688-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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	1.252	9.2	ug/l	46273	1	5.562	252180	50.0
1-Pentene	2.873	6.9	ug/l	34793	1	5.562	252180	50.0
unknown4.318	4.318	9.4	ug/l	47569	1	5.562	252180	50.0
unknown6.239	6.239	6.3	ug/l	39877	2	6.769	319219	50.0
Benzene, 2-prop...	12.244	16.3	ug/l	117820	4	12.024	362142	50.0
Benzene, (2-met...	12.701	7.4	ug/l	53426	4	12.024	362142	50.0
Benzene, 1-ethe...	13.292	6.4	ug/l	46510	4	12.024	362142	50.0