LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025442.D
Acq On : 02 Dec 2021 20:38
Operator : JC/MD
Sample : M4917-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

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\82X111721W.M
Title : SW846 8260

Signal : TIC: VX025442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	42	rBV	78090	125731	12.90%	2.153%
2	1.367	43	46	51	rVB	18770	19050	1.95%	0.326%
3	1.745	104	108	118	rVB	25326	37372	3.83%	0.640%
4	1.953	138	142	150	rVB3	7679	13451	1.38%	0.230%
5	2.215	181	185	196	rVB3	5986	10167	1.04%	0.174%
6	2.867	287	292	299	rVB3	8059	16007	1.64%	0.274%
7	2.965	299	308	323	rVV	274323	580457	59.55%	9.940%
8	3.117	323	333	344	rVB	61182	143874	14.76%	2.464%
9	3.763	427	439	448	rBV3	10460	30495	3.13%	0.522%
10	4.312	519	529	540	rVV5	9546	30138	3.09%	0.516%
11	5.391	695	706	716	rBV	64639	186365	19.12%	3.191%
12	5.556	723	733	754	rVB	104738	304838	31.28%	5.220%
13	5.964	788	800	805	rBV	65978	174486	17.90%	2.988%
14	6.043	805	813	829	rVB	371826	974691	100.00%	16.691%
15	6.238	836	845	856	rVB3	15298	45209	4.64%	0.774%
16	6.763	917	931	943	rBV	167154	403216	41.37%	6.905%
17	7.372	1023	1031	1041	rBV5	3880	10649	1.09%	0.182%
18	8.427	1199	1204	1210	rBV2	8484	14452	1.48%	0.247%
19	8.506	1210	1217	1225	rVB5	4965	9933	1.02%	0.170%
20	8.653	1233	1241	1249	rBV	342692	540154	55.42%	9.250%
21	8.957	1285	1291	1298	rVB	8005	13751	1.41%	0.235%
22	9.049	1301	1306	1311	rVB2	9192	13830	1.42%	0.237%
23	9.457	1365	1373	1378	rBV2	17740	29816	3.06%	0.511%
24	10.055	1465	1471	1489	rVB	348035	470648	48.29%	8.059%
25	10.195	1489	1494	1500	rBV	74322	95125	9.76%	1.629%
26	10.305	1507	1512	1518	rVB2	11201	15325	1.57%	0.262%
27	10.963	1614	1620	1625	rBV	28188	35166	3.61%	0.602%
28	11.085	1634	1640	1649	rBV	278193	359667	36.90%	6.159%
29	11.305	1671	1676	1686	rVB	51257	67472	6.92%	1.155%
30	11.756	1745	1750	1755	rVB	19896	24805	2.54%	0.425%
31	12.024	1789	1794	1801	rBV	353041	436406	44.77%	7.473%
32	12.243	1825	1830	1838	rBV	180795	226910	23.28%	3.886%
33	12.317	1838	1842	1849	rVB3	8727	15293	1.57%	0.262%
34	12.463	1862	1866	1872	rVB	15858	19213	1.97%	0.329%
35	12.615	1886	1891	1894	rBV	30667	36355	3.73%	0.623%
36	12.646	1894	1896	1901	rVV	11413	13128	1.35%	0.225%

LSC Area Percent Report

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Data File : VX025442.D
Acq On : 02 Dec 2021 20:38
Operator : JC/MD
Sample : M4917-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

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\82X111721W.M
Title : SW846 8260

37	12.701	1901	1905	1913	rVB	40093	50196	5.15%	0.860%
38	12.926	1935	1942	1945	rBV	35902	47096	4.83%	0.806%
39	12.963	1945	1948	1955	rVV	43050	51415	5.28%	0.880%
40	13.170	1979	1982	1992	rVB	17356	23731	2.43%	0.406%
41	13.298	1999	2003	2007	rVB2	26116	33347	3.42%	0.571%
42	13.548	2040	2044	2047	rVV	9050	14155	1.45%	0.242%
43	13.585	2047	2050	2056	rVV2	10409	20553	2.11%	0.352%
44	13.664	2061	2063	2071	rVB2	10790	16611	1.70%	0.284%
45	14.219	2149	2154	2161	rBV	8566	12949	1.33%	0.222%
46	14.780	2242	2246	2257	rBV	18830	25993	2.67%	0.445%

Sum of corrected areas: 5839691

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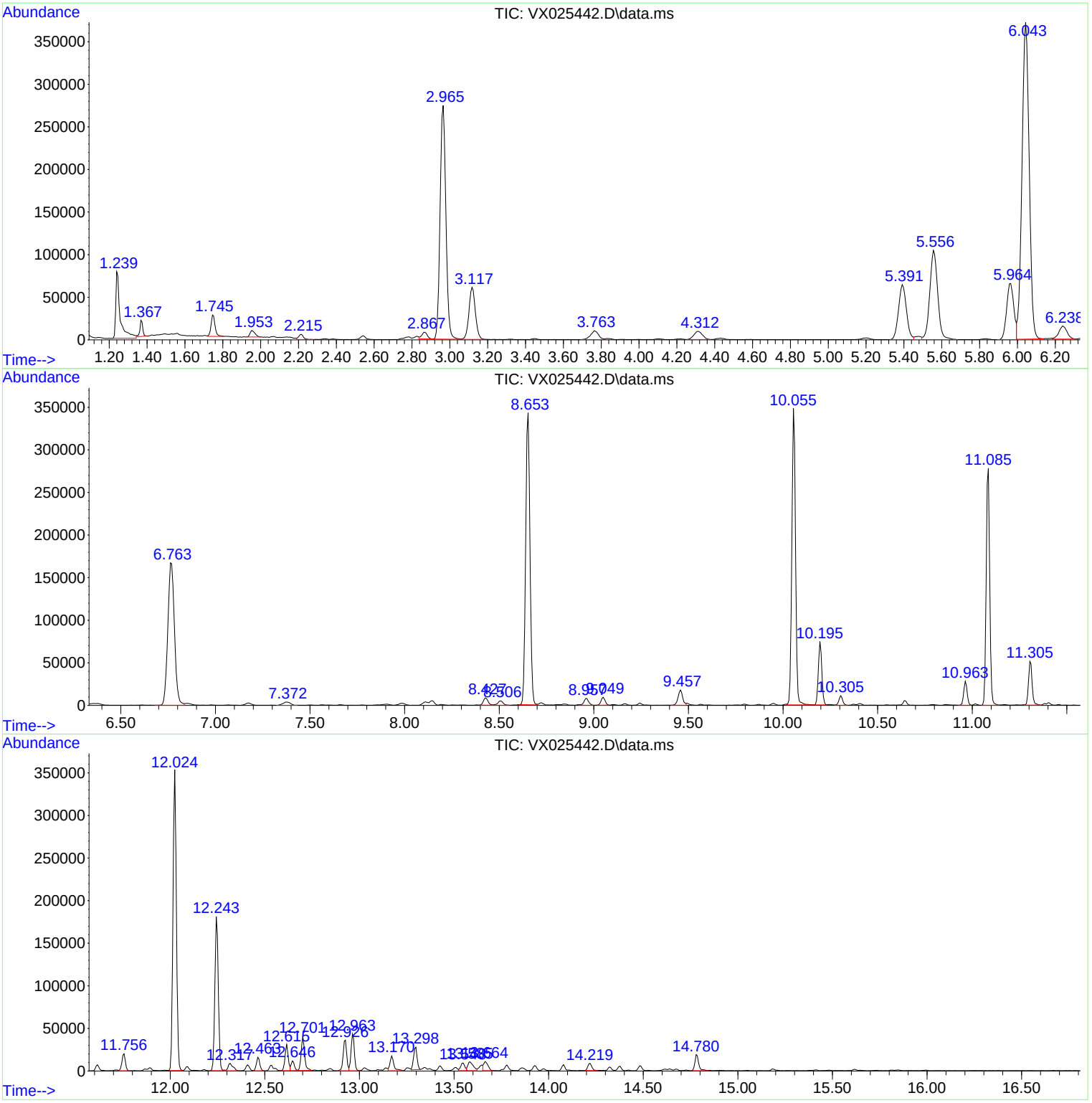
Instrument :
MSVOA_X
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025442.D
Acq On : 02 Dec 2021 20:38
Operator : JC/MD
Sample : M4917-12
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

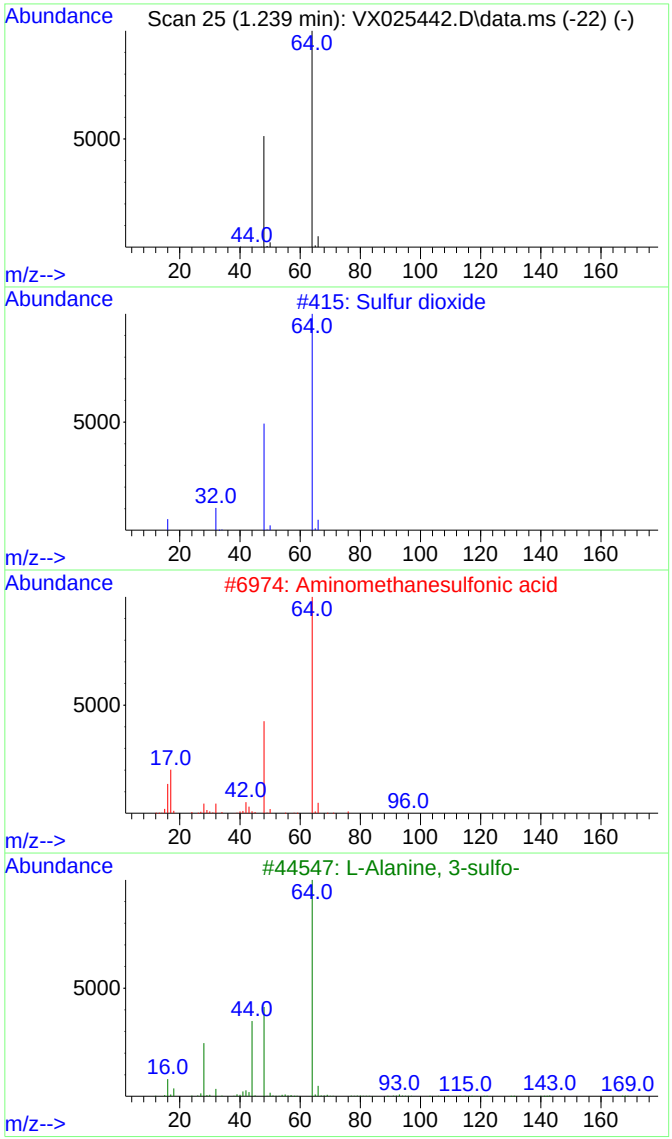
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

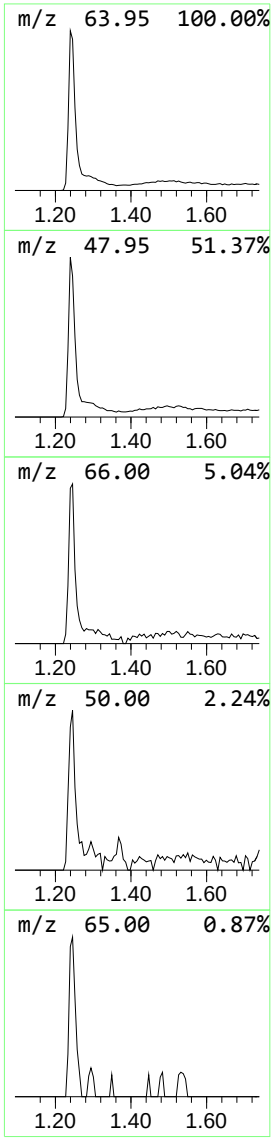
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	20.62 ug/l	125731	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\VX120221\
Data File : VX025442.D
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Operator : JC/MD
Sample : M4917-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

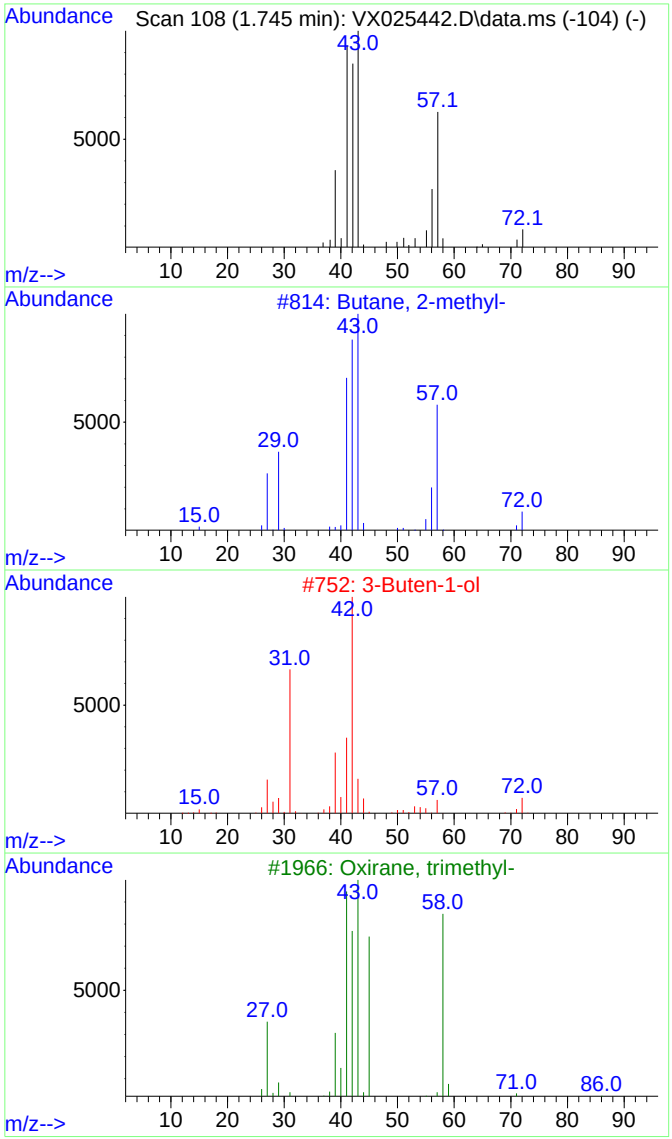
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

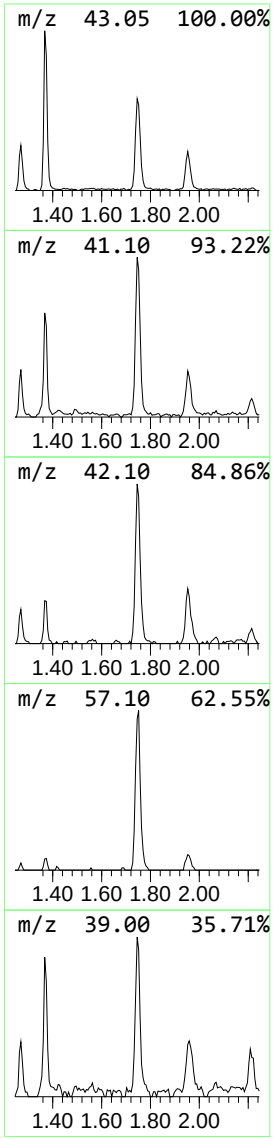
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	6.13 ug/l	37372	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	47
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4	Pentane	72	C5H12	000109-66-0	33
5	1-Butene	56	C4H8	000106-98-9	10





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Data File : VX025442.D
Acq On : 02 Dec 2021 20:38
Operator : JC/MD
Sample : M4917-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

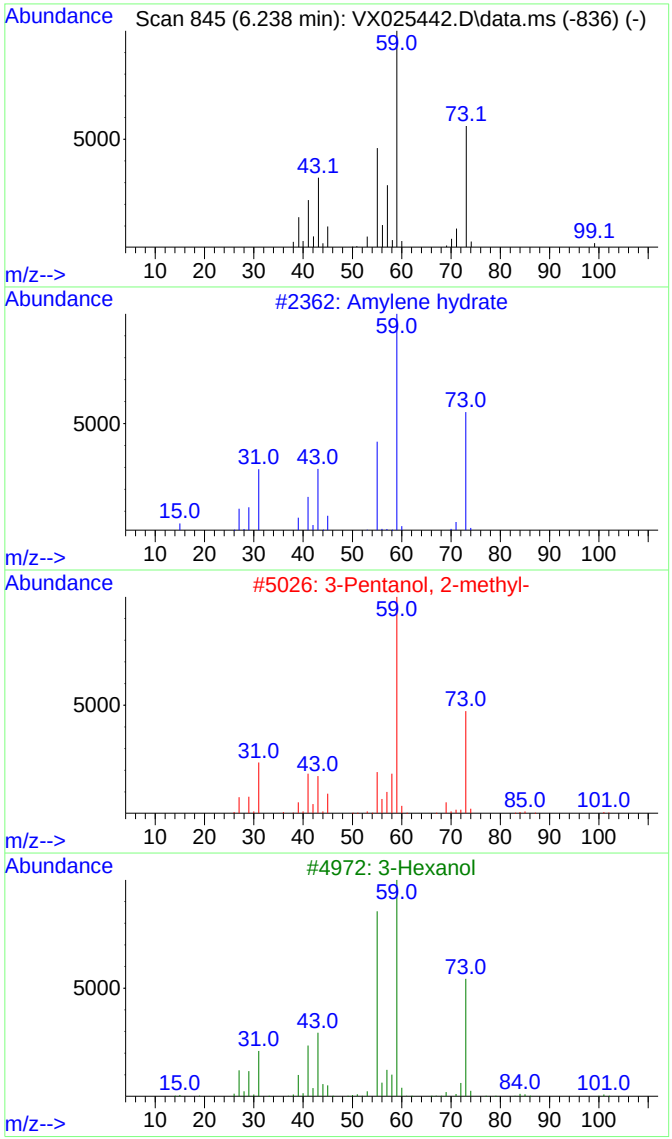
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

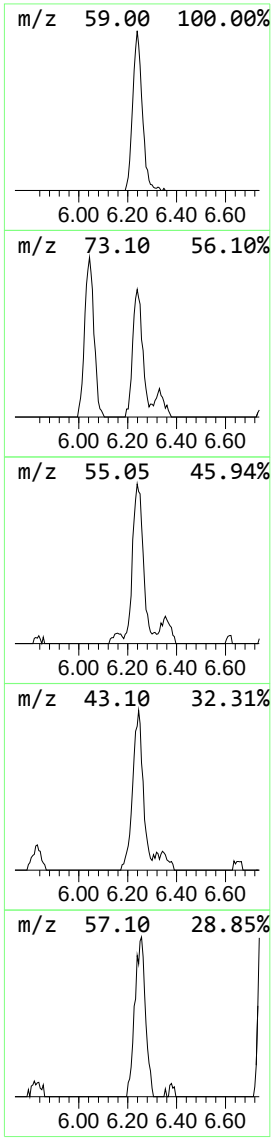
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Amylene hydrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.238	5.61 ug/l	45209	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	78
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
3	3-Hexanol	102	C6H14O	000623-37-0	38
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	36
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	36





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Sample : M4917-12
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

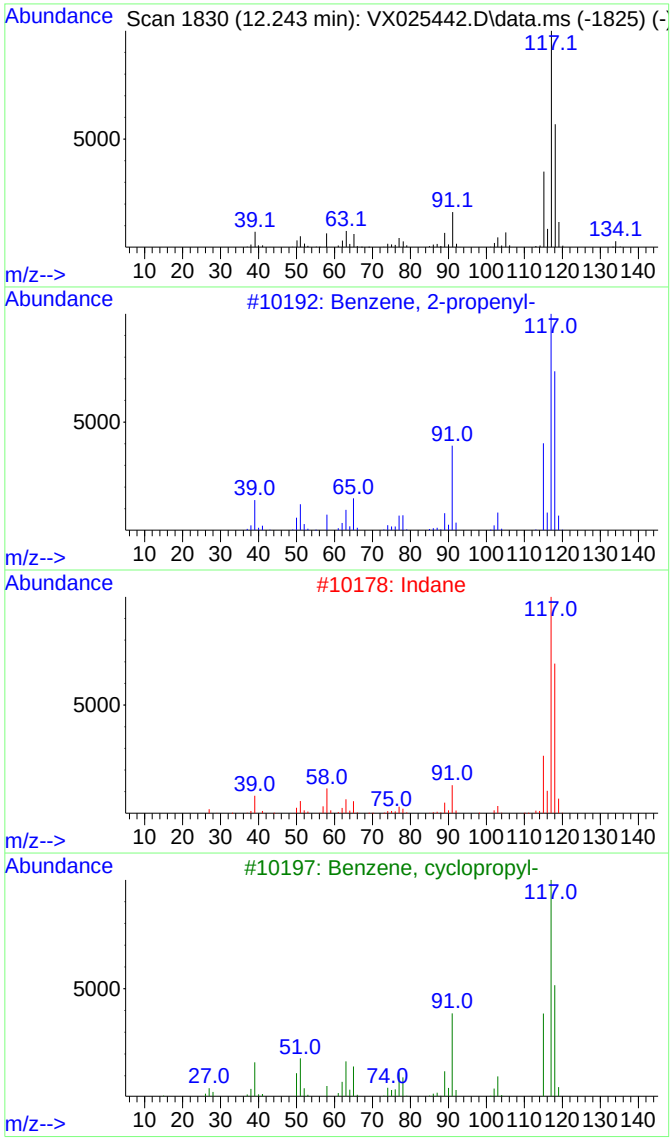
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

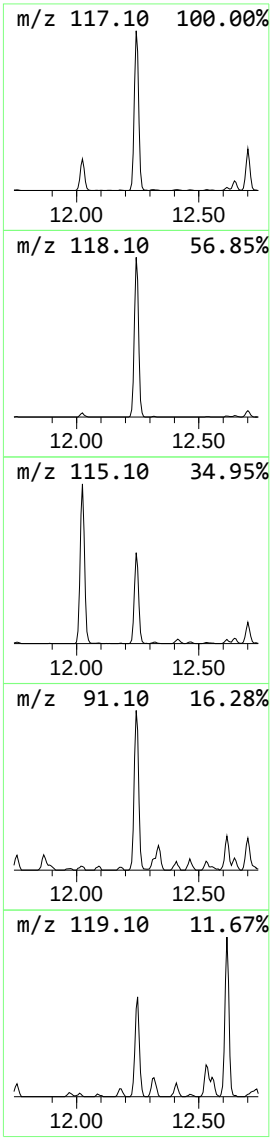
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	26.00 ug/l	226910	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
2	Indane	118	C9H10	000496-11-7	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50
5	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

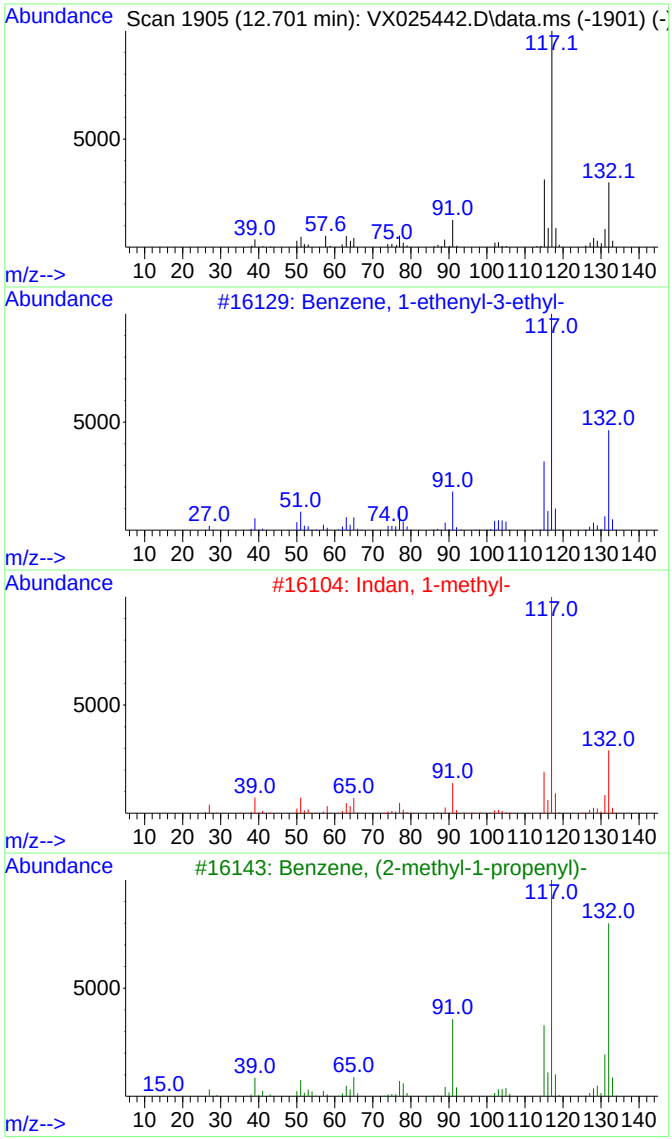
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

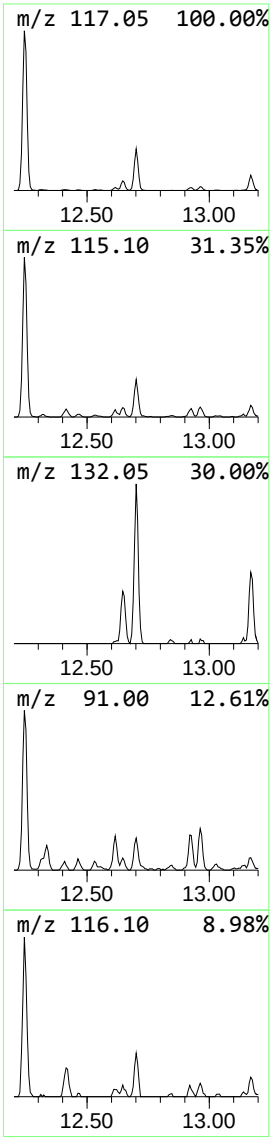
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	5.75 ug/l	50196	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	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	87





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

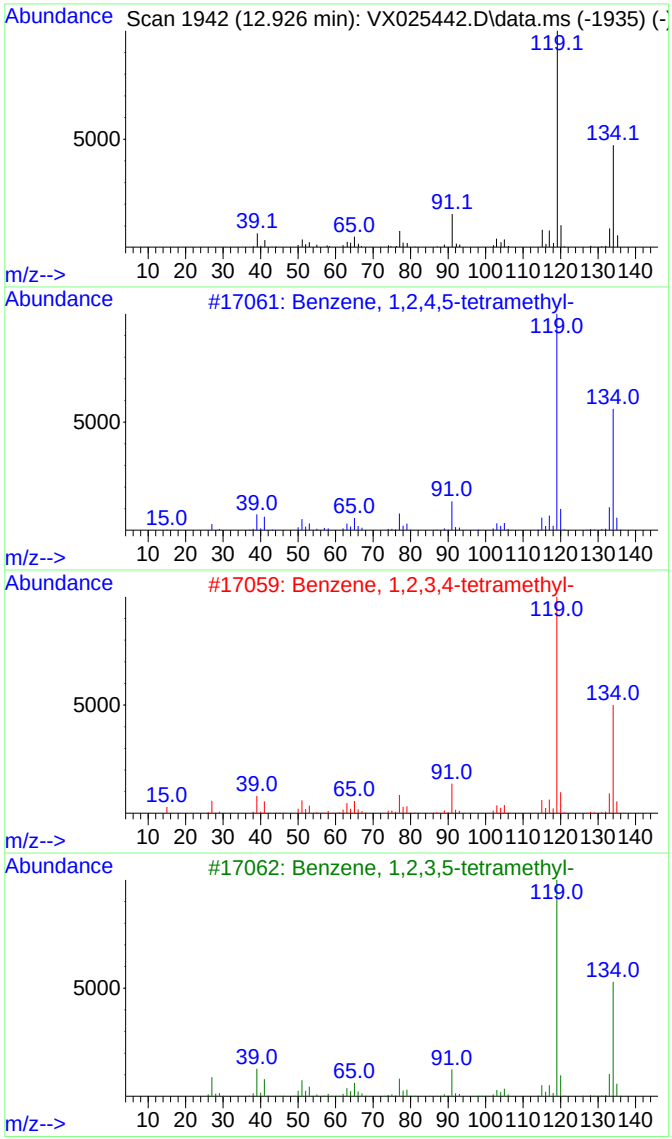
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

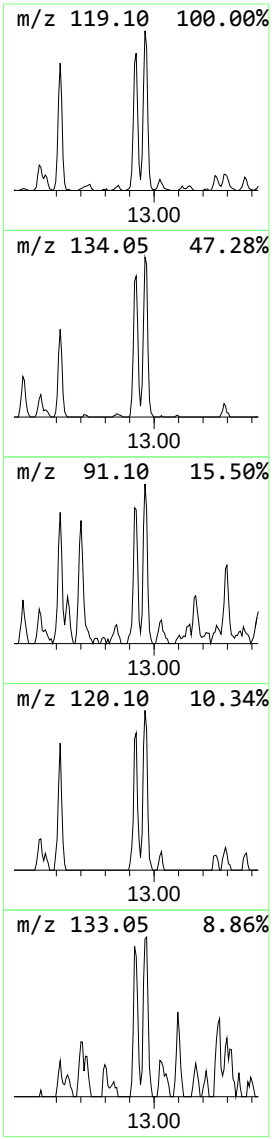
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.926	5.40 ug/l	47096	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

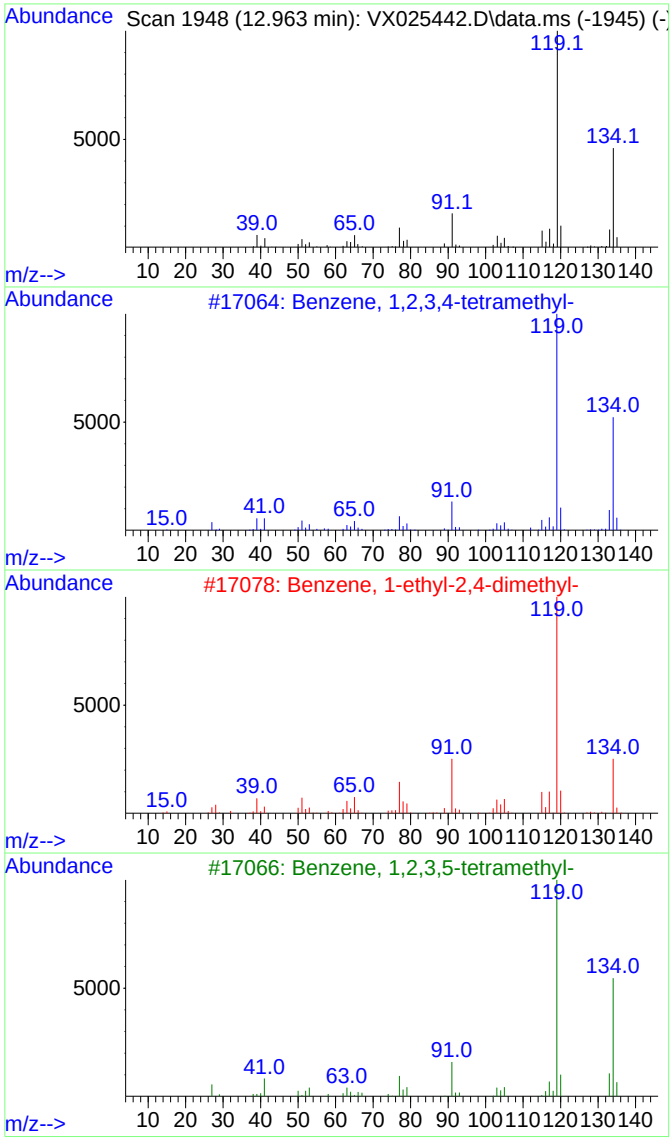
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

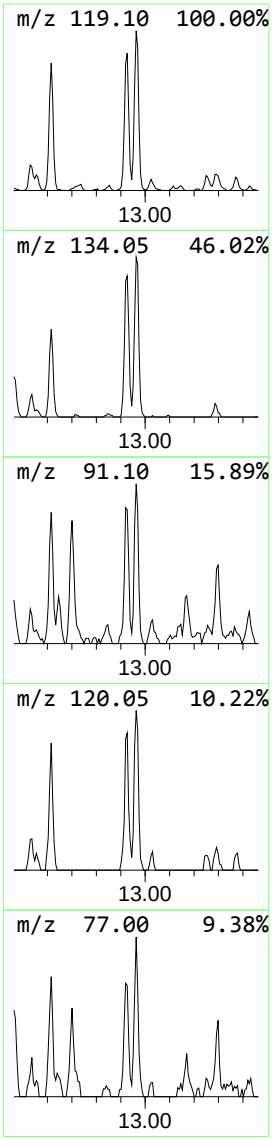
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	5.89 ug/l	51415	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	96
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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	1.239	20.6	ug/l	125731	1	5.556	304838	50.0
Butane, 2-methyl-	1.745	6.1	ug/l	37372	1	5.556	304838	50.0
Amylene hydrate	6.238	5.6	ug/l	45209	2	6.769	403216	50.0
Benzene, 2-prop...	12.243	26.0	ug/l	226910	4	12.024	436406	50.0
Benzene, 1-ethe...	12.701	5.8	ug/l	50196	4	12.024	436406	50.0
Benzene, 1,2,4,...	12.926	5.4	ug/l	47096	4	12.024	436406	50.0
Benzene, 1,2,3,...	12.963	5.9	ug/l	51415	4	12.024	436406	50.0