LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025436.D
Acq On : 02 Dec 2021 18:17
Operator : JC/MD
Sample : M4917-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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: VX025436.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	41	rBV	154619	225833	44.38%	4.190%
2	1.368	43	46	52	rVB	9672	11016	2.16%	0.204%
3	1.752	104	109	115	rVB	47208	67735	13.31%	1.257%
4	1.953	138	142	150	rVB3	10959	17462	3.43%	0.324%
5	2.215	180	185	196	rVB3	8179	15583	3.06%	0.289%
6	2.386	209	213	220	rVB	3149	5387	1.06%	0.100%
7	2.544	228	239	248	rVB	2838	5596	1.10%	0.104%
8	2.776	267	277	282	rBV2	7299	18743	3.68%	0.348%
9	2.831	282	286	288	rVV2	7393	13898	2.73%	0.258%
10	2.867	288	292	301	rVV	16336	33453	6.57%	0.621%
11	2.965	301	308	319	rVV	23412	51659	10.15%	0.959%
12	3.117	322	333	345	rVB3	33204	84906	16.69%	1.575%
13	3.770	426	440	446	rBV4	5291	19991	3.93%	0.371%
14	3.843	446	452	458	rVB4	2714	6530	1.28%	0.121%
15	4.306	518	528	541	rBV3	37905	112081	22.03%	2.080%
16	4.428	541	548	558	rVB4	3767	10436	2.05%	0.194%
17	5.202	665	675	684	rVB2	4370	12507	2.46%	0.232%
18	5.391	695	706	713	rBV	61379	177822	34.95%	3.299%
19	5.477	713	720	726	rVV2	33494	104740	20.58%	1.943%
20	5.556	726	733	757	rVB	97942	286688	56.34%	5.319%
21	5.964	790	800	806	rBV	63223	168285	33.07%	3.123%
22	6.044	806	813	827	rVB	82955	217548	42.75%	4.037%
23	6.245	841	846	856	rVB7	5089	15723	3.09%	0.292%
24	6.355	856	864	873	rVB7	3438	11671	2.29%	0.217%
25	6.763	922	931	943	rBV	156707	382673	75.20%	7.100%
26	6.854	943	946	956	rVB5	4839	10466	2.06%	0.194%
27	7.178	991	999	1007	rVB	7187	15471	3.04%	0.287%
28	7.379	1023	1032	1044	rBV5	11492	30911	6.07%	0.574%
29	7.860	1105	1111	1113	rBV3	3593	6949	1.37%	0.129%
30	7.885	1113	1115	1122	rVB3	4450	7122	1.40%	0.132%
31	7.982	1122	1131	1140	rVB5	2197	6273	1.23%	0.116%
32	8.110	1144	1152	1153	rBV2	4183	6401	1.26%	0.119%
33	8.147	1153	1158	1163	rVB	12622	21877	4.30%	0.406%
34	8.427	1199	1204	1210	rBV	4839	7989	1.57%	0.148%
35	8.507	1210	1217	1224	rVB	15561	26235	5.16%	0.487%
36	8.653	1230	1241	1247	rBV	323738	508843	100.00%	9.442%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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	8.720	1247	1252	1266	rVB	37964	60728	11.93%	1.127%
38	8.958	1286	1291	1299	rVB	13204	22732	4.47%	0.422%
39	9.049	1299	1306	1312	rBV	13360	20553	4.04%	0.381%
40	9.165	1318	1325	1334	rVB2	5749	9464	1.86%	0.176%
41	9.458	1364	1373	1377	rBV4	9999	19204	3.77%	0.356%
42	9.951	1449	1454	1461	rVB4	3009	5805	1.14%	0.108%
43	10.055	1465	1471	1486	rVV	324417	436591	85.80%	8.101%
44	10.195	1490	1494	1500	rVB	42932	54384	10.69%	1.009%
45	10.305	1508	1512	1518	rVB2	6058	8822	1.73%	0.164%
46	10.963	1615	1620	1626	rBV	67230	86059	16.91%	1.597%
47	11.085	1634	1640	1650	rBV	249920	326112	64.09%	6.051%
48	11.305	1671	1676	1684	rVB	58656	75618	14.86%	1.403%
49	11.616	1722	1727	1734	rVB	18994	22980	4.52%	0.426%
50	11.756	1746	1750	1755	rVB	8088	9836	1.93%	0.183%
51	11.866	1764	1768	1770	rBV	7955	10101	1.99%	0.187%
52	11.890	1770	1772	1777	rVB	8501	10572	2.08%	0.196%
53	12.024	1789	1794	1802	rBV	320084	396513	77.92%	7.357%
54	12.091	1802	1805	1809	rVB	7386	8756	1.72%	0.162%
55	12.183	1814	1820	1824	rBV	3984	5151	1.01%	0.096%
56	12.244	1824	1830	1837	rBV	205443	265522	52.18%	4.927%
57	12.317	1837	1842	1848	rVB3	9413	14689	2.89%	0.273%
58	12.408	1850	1857	1862	rBV2	12614	15652	3.08%	0.290%
59	12.463	1862	1866	1872	rBV	26449	32538	6.39%	0.604%
60	12.536	1873	1878	1885	rVB	5001	6541	1.29%	0.121%
61	12.616	1885	1891	1893	rBV	7407	10284	2.02%	0.191%
62	12.646	1893	1896	1900	rVV	23174	27902	5.48%	0.518%
63	12.701	1900	1905	1912	rVB	109323	138083	27.14%	2.562%
64	12.847	1925	1929	1934	rVB	14051	18905	3.72%	0.351%
65	12.927	1934	1942	1945	rBV	52534	70777	13.91%	1.313%
66	12.963	1945	1948	1955	rVV	42735	51306	10.08%	0.952%
67	13.036	1955	1960	1964	rVB3	4831	6969	1.37%	0.129%
68	13.140	1973	1977	1979	rBV2	6829	7519	1.48%	0.140%
69	13.170	1979	1982	1985	rVV	18707	20588	4.05%	0.382%
70	13.256	1992	1996	1998	rBV2	4692	5850	1.15%	0.109%
71	13.298	1998	2003	2007	rVV	60554	78555	15.44%	1.458%
72	13.347	2007	2011	2014	rBV3	7846	11987	2.36%	0.222%
73	13.426	2020	2024	2028	rVB2	28450	35316	6.94%	0.655%
74	13.506	2033	2037	2040	rVV3	4710	6912	1.36%	0.128%
75	13.548	2040	2044	2047	rVV	12967	19862	3.90%	0.369%
76	13.579	2047	2049	2057	rVV4	17110	37008	7.27%	0.687%

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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

77	13.640	2057	2059	2061	rVV	9497	12221	2.40%	0.227%
78	13.664	2061	2063	2070	rVB2	12078	17848	3.51%	0.331%
79	13.780	2074	2082	2090	rBV	30747	43705	8.59%	0.811%
80	13.859	2090	2095	2100	rBV3	5444	9488	1.86%	0.176%
81	13.926	2100	2106	2110	rVV3	8524	12179	2.39%	0.226%
82	14.079	2127	2131	2134	rBV	6439	7631	1.50%	0.142%
83	14.213	2149	2153	2164	rBV3	20925	33637	6.61%	0.624%
84	14.323	2167	2171	2176	rVV	5818	7685	1.51%	0.143%
85	14.377	2176	2180	2184	rVB	6293	7973	1.57%	0.148%
86	14.487	2193	2198	2203	rBV5	3856	5290	1.04%	0.098%
87	14.780	2242	2246	2256	rVB	19449	26794	5.27%	0.497%
88	15.121	2298	2302	2309	rBV3	4486	5705	1.12%	0.106%

Sum of corrected areas: 5389405

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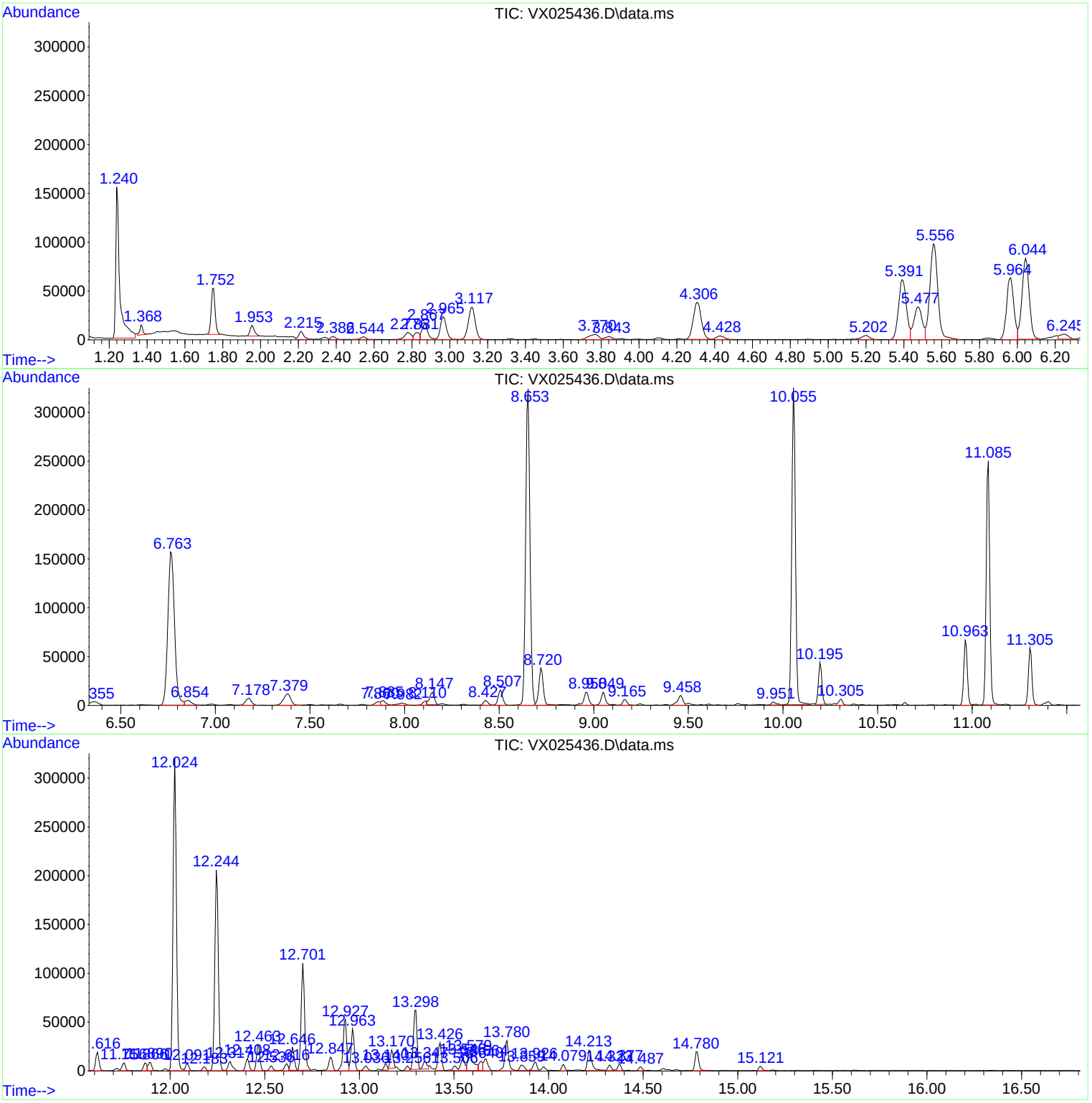
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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



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

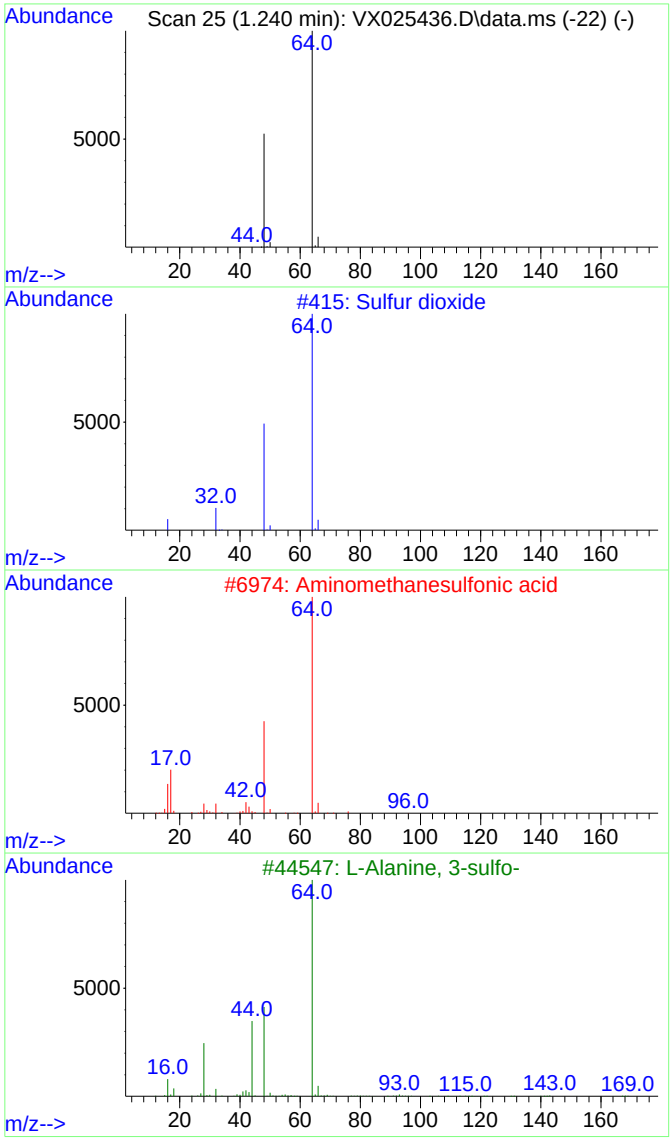
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

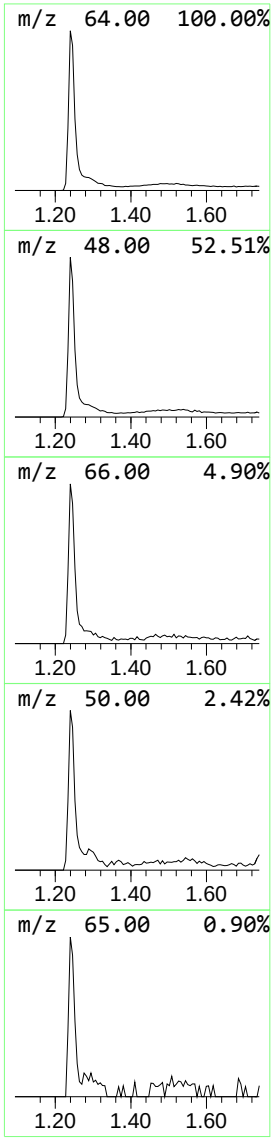
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	39.39 ug/l	225833	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





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Data File : VX025436.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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

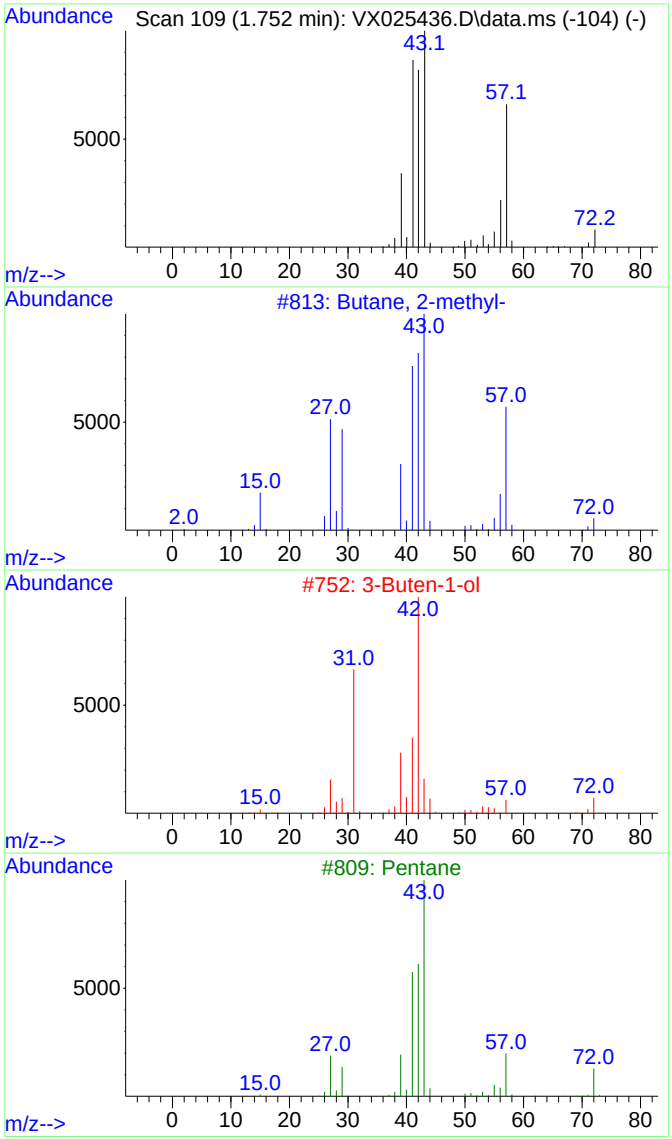
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

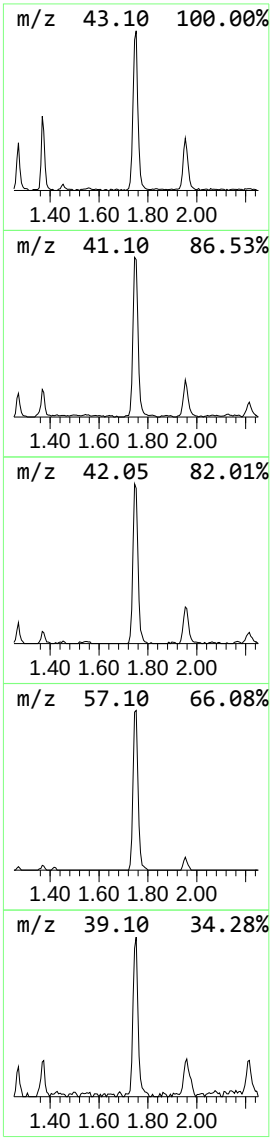
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	11.81 ug/l	67735	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





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ALS Vial : 22 Sample Multiplier: 1

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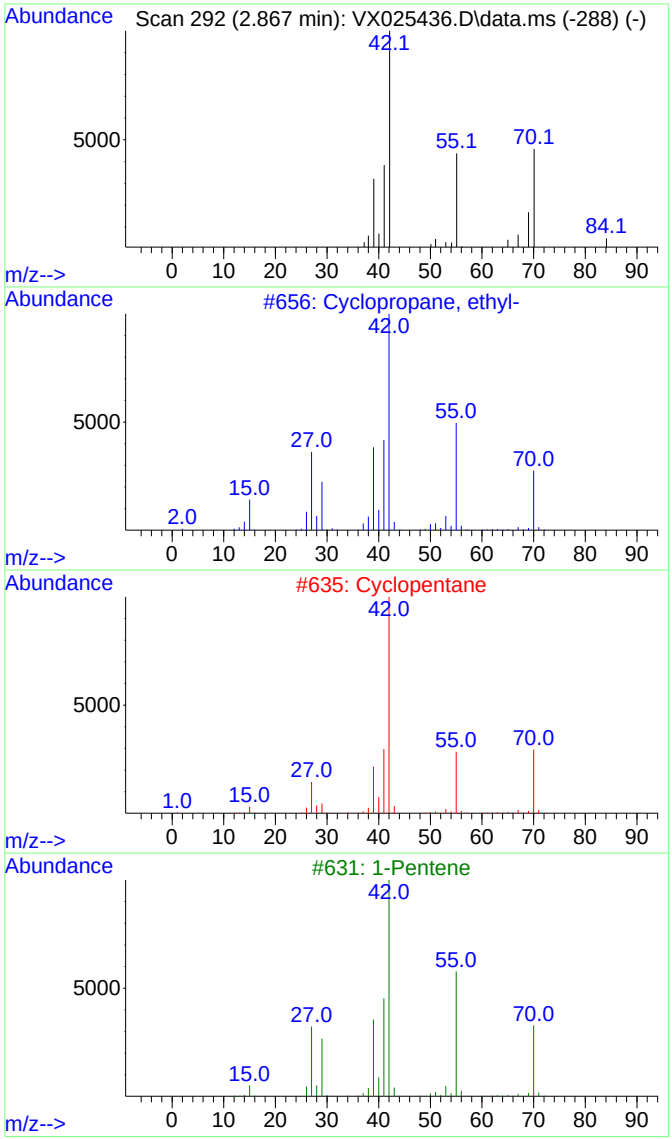
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

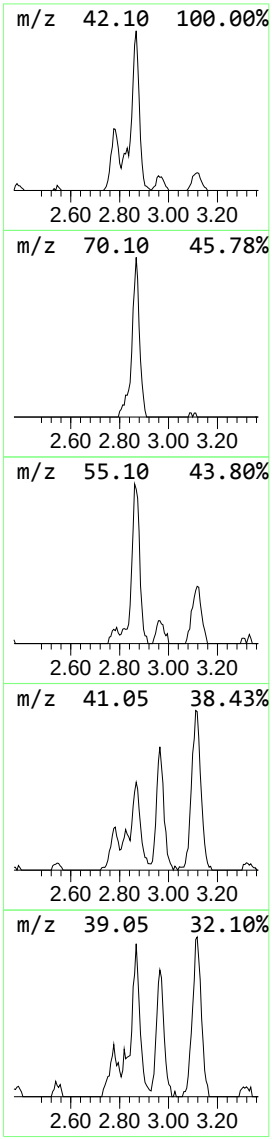
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.83 ug/l	33453	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
2	Cyclopentane	70	C5H10	000287-92-3	56
3	1-Pentene	70	C5H10	000109-67-1	50
4	3-Buten-1-ol	72	C4H8O	000627-27-0	25
5	1-Pentanol	88	C5H12O	000071-41-0	9





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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

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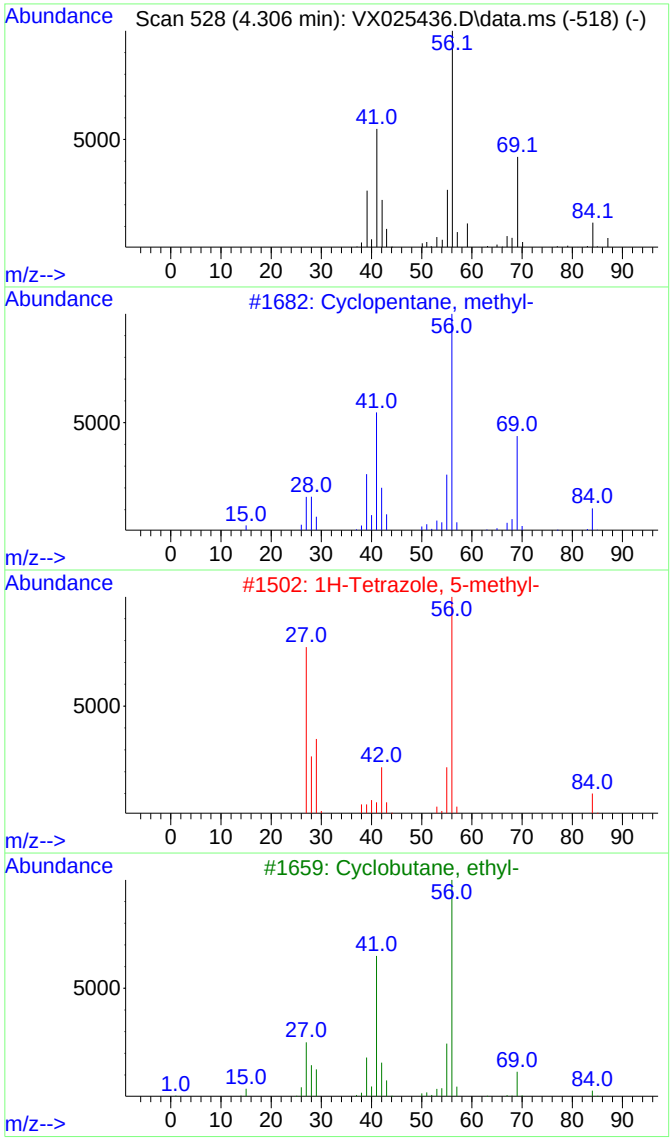
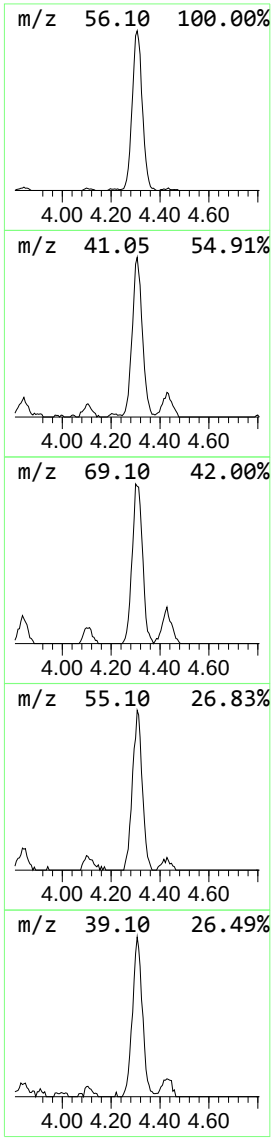
Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	19.55 ug/l	112081	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	93
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclohexane	84	C6H12	000110-82-7	50
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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

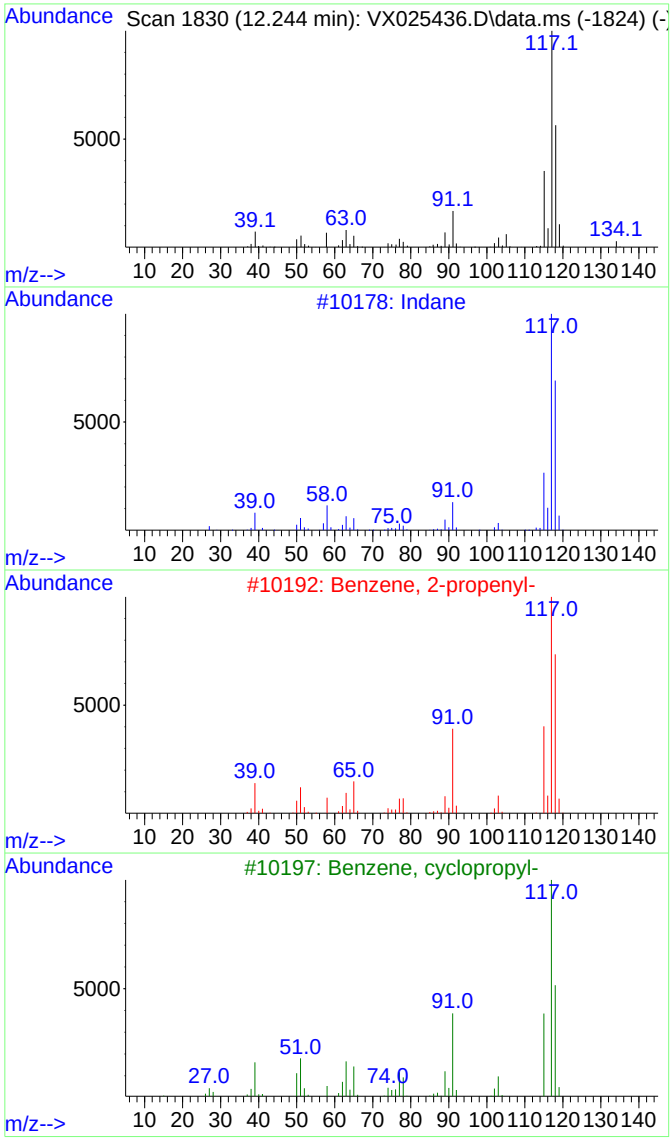
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

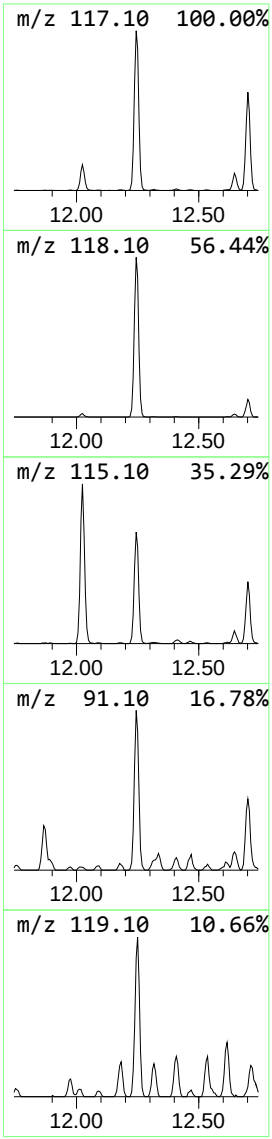
****

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	33.48 ug/l	265522	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	83
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64





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Data File : VX025436.D
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

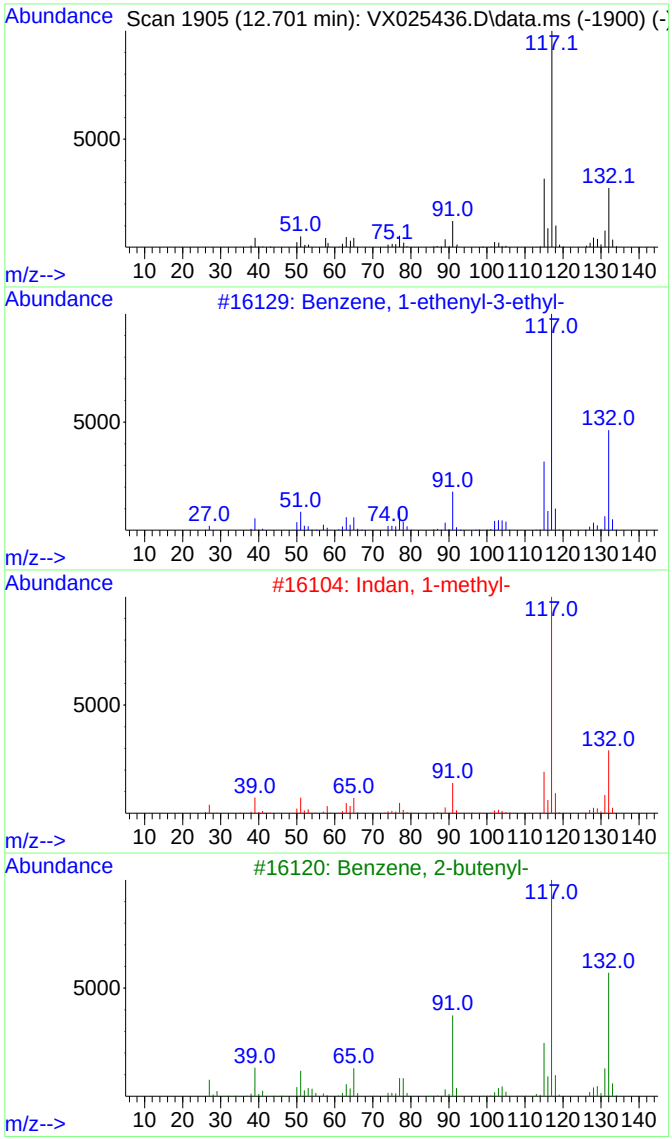
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

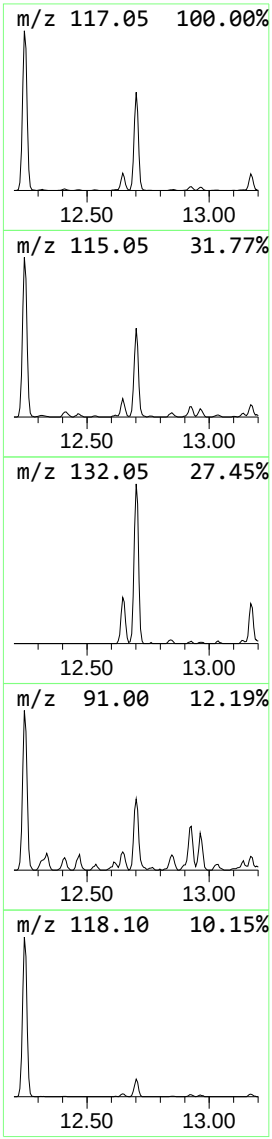
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	17.41 ug/l	138083	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-butenyl-	132	C10H12	001560-06-1	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025436.D
Acq On : 02 Dec 2021 18:17
Operator : JC/MD
Sample : M4917-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

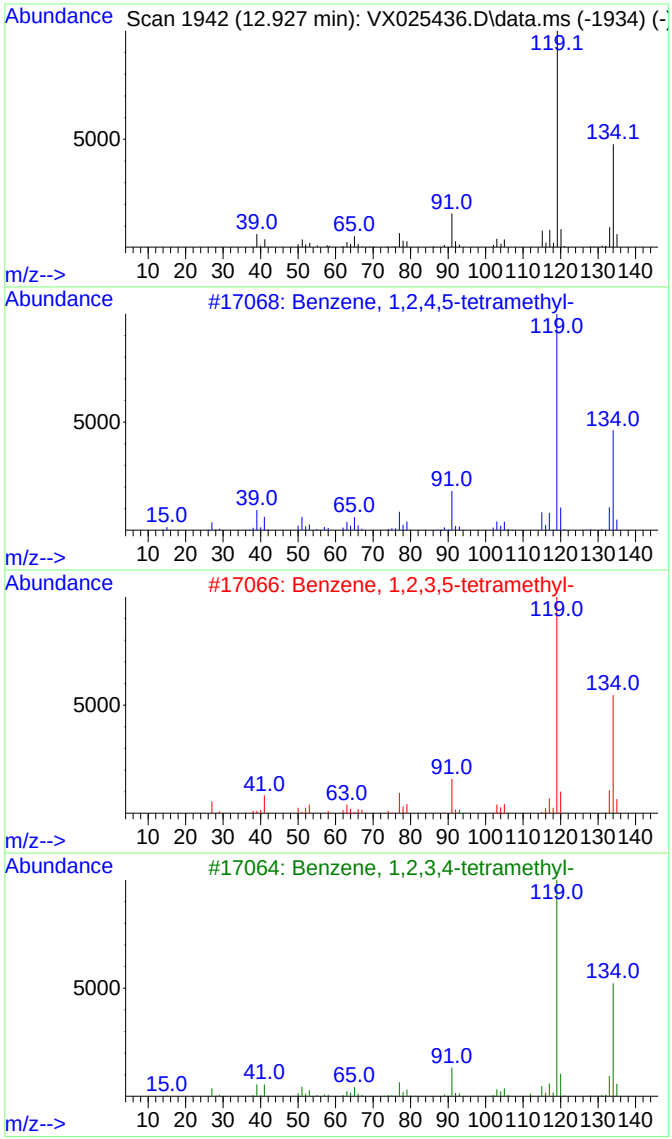
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

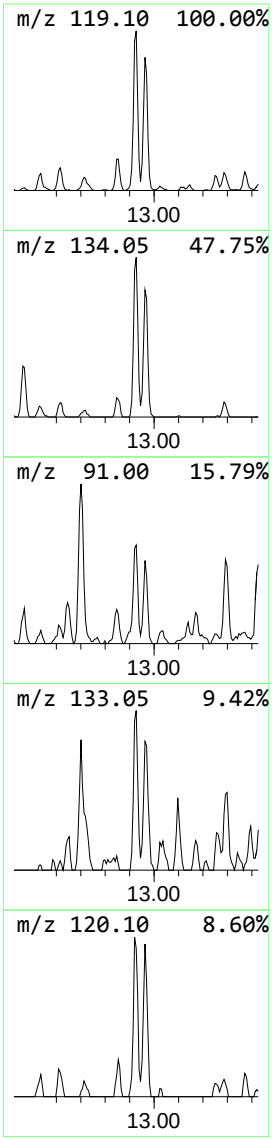
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	8.92 ug/l	70777	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, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025436.D
Acq On : 02 Dec 2021 18:17
Operator : JC/MD
Sample : M4917-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

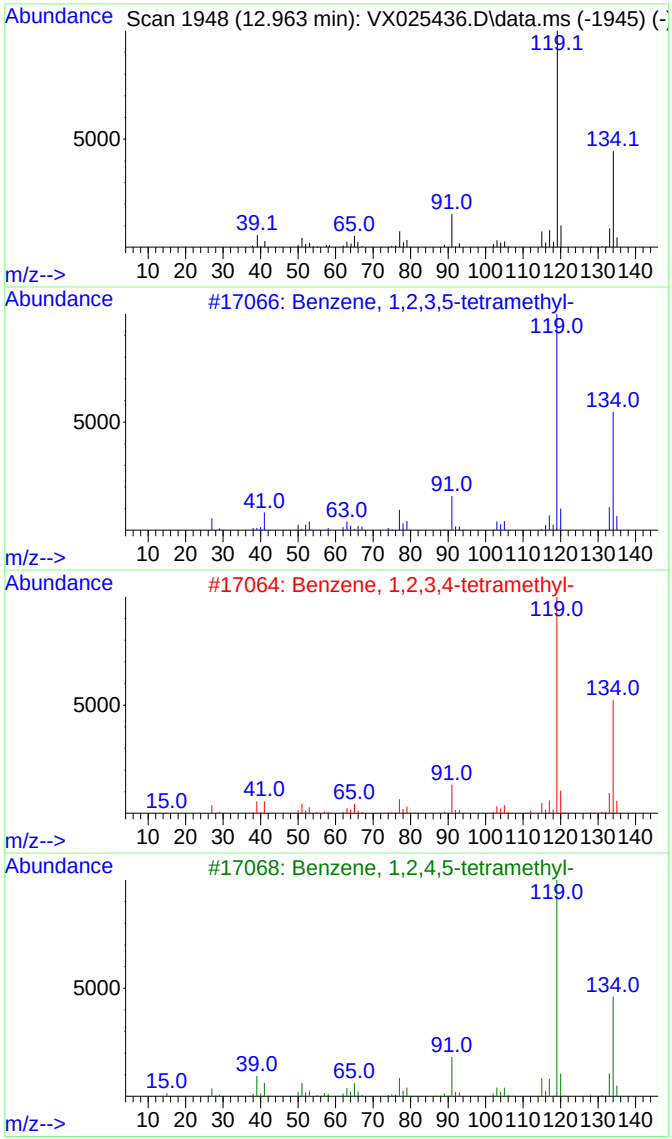
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

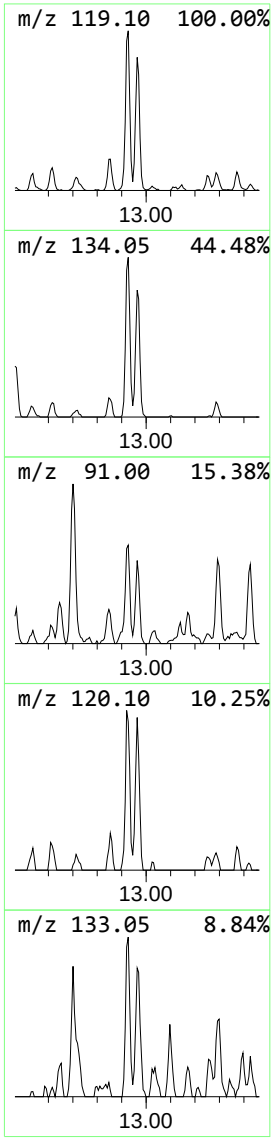
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	6.47 ug/l	51306	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025436.D
Acq On : 02 Dec 2021 18:17
Operator : JC/MD
Sample : M4917-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

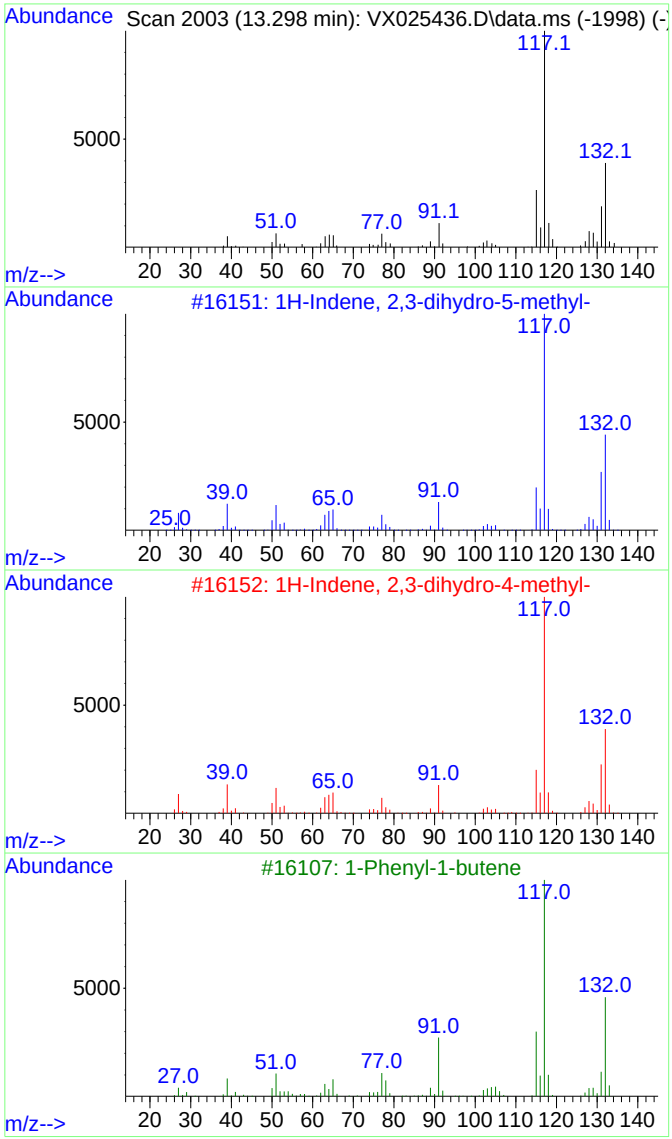
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

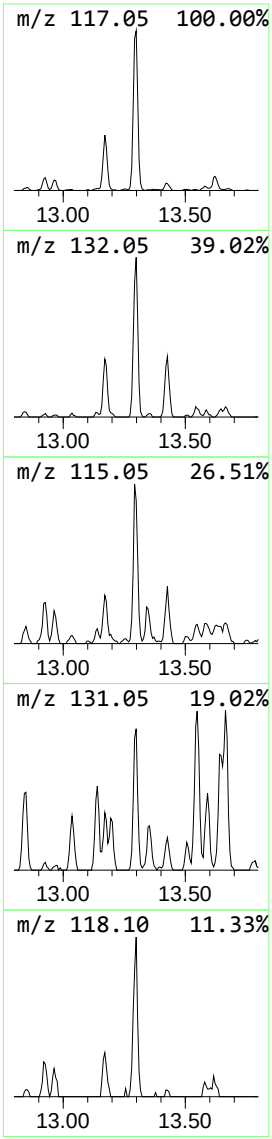
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	9.91 ug/l	78555	1,4-Dichlorobenzene-d4	12.024

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025436.D
Acq On : 02 Dec 2021 18:17
Operator : JC/MD
Sample : M4917-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP120121

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	1.240	39.4	ug/l	225833	1	5.556	286688	50.0
Butane, 2-methyl-	1.752	11.8	ug/l	67735	1	5.556	286688	50.0
Cyclopropane, e...	2.867	5.8	ug/l	33453	1	5.556	286688	50.0
Cyclopentane, m...	4.306	19.6	ug/l	112081	1	5.556	286688	50.0
Indane	12.244	33.5	ug/l	265522	4	12.024	396513	50.0
Benzene, 1-ethe...	12.701	17.4	ug/l	138083	4	12.024	396513	50.0
Benzene, 1,2,4,...	12.927	8.9	ug/l	70777	4	12.024	396513	50.0
Benzene, 1,2,3,...	12.963	6.5	ug/l	51306	4	12.024	396513	50.0
1H-Indene, 2,3-...	13.298	9.9	ug/l	78555	4	12.024	396513	50.0