LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

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\82X061518W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	89	rBV	1059147	1379704	77.74%	9.451%
2	1.148	89	92	95	rBV	59425	70749	3.99%	0.485%
3	1.270	109	112	114	rBV	62016	74241	4.18%	0.509%
4	1.319	114	120	144	rVV	497764	1774771	100.00%	12.157%
5	1.489	144	148	154	rVB	97050	127200	7.17%	0.871%
6	1.581	160	163	176	rVB3	46630	96647	5.45%	0.662%
7	2.355	285	290	300	rVB	29683	49844	2.81%	0.341%
8	2.447	300	305	315	rBV	94967	160786	9.06%	1.101%
9	2.575	321	326	330	rBV	16019	28898	1.63%	0.198%
10	2.629	330	335	337	rBV	14969	25929	1.46%	0.178%
11	3.026	397	400	407	rVB4	11542	21240	1.20%	0.145%
12	4.355	611	618	630	rVB2	19120	57049	3.21%	0.391%
13	4.714	670	677	684	rBV	15654	46582	2.62%	0.319%
14	4.788	684	689	702	rVB	9961	32017	1.80%	0.219%
15	5.507	796	807	823	rBV2	152375	443335	24.98%	3.037%
16	5.665	823	833	848	rVB	228843	641322	36.14%	4.393%
17	6.074	889	900	908	rBV	163559	424703	23.93%	2.909%
18	6.147	909	912	921	rVB2	14400	31305	1.76%	0.214%
19	6.489	954	968	976	rVB10	5988	19396	1.09%	0.133%
20	6.867	1020	1030	1046	rBV	329176	764209	43.06%	5.235%
21	7.458	1120	1127	1135	rVB6	7337	19125	1.08%	0.131%
22	7.561	1139	1144	1153	rVV2	18861	37099	2.09%	0.254%
23	7.671	1156	1162	1169	rVB2	15310	28800	1.62%	0.197%
24	8.659	1317	1324	1328	rBV2	37740	68609	3.87%	0.470%
25	8.720	1328	1334	1342	rVB	780654	1228544	69.22%	8.416%
26	8.915	1358	1366	1374	rVB3	26714	56715	3.20%	0.388%
27	9.043	1382	1387	1395	rBV4	12391	27810	1.57%	0.190%
28	9.500	1457	1462	1468	rBV	12959	24302	1.37%	0.166%
29	9.586	1469	1476	1480	rVV4	29183	49560	2.79%	0.339%
30	9.646	1480	1486	1489	rVV	41742	63204	3.56%	0.433%
31	9.683	1489	1492	1496	rVB	14735	20860	1.18%	0.143%
32	9.823	1508	1515	1521	rBV4	12741	27988	1.58%	0.192%
33	10.116	1558	1563	1571	rVB	700545	926593	52.21%	6.347%
34	10.256	1580	1586	1591	rBV3	11591	23908	1.35%	0.164%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

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\82X061518W.M
Title : SW846 8260

35	10.366	1601	1604	1609	rVB4	15054	26827	1.51%	0.184%
36	10.646	1642	1650	1656	rBV5	18787	45249	2.55%	0.310%
37	10.835	1674	1681	1686	rBV3	34787	59033	3.33%	0.404%
38	10.915	1690	1694	1698	rVV2	26145	39918	2.25%	0.273%
39	11.140	1726	1731	1736	rBV	747253	914918	51.55%	6.267%
40	11.183	1736	1738	1742	rVB3	14730	18204	1.03%	0.125%
41	11.280	1750	1754	1760	rVB3	27083	39761	2.24%	0.272%
42	11.396	1770	1773	1777	rBV3	11533	19206	1.08%	0.132%
43	11.451	1777	1782	1786	rVB4	14416	24277	1.37%	0.166%
44	11.671	1813	1818	1826	rBV4	33043	69473	3.91%	0.476%
45	11.768	1827	1834	1837	rBV5	34759	71443	4.03%	0.489%
46	11.805	1837	1840	1843	rBV2	35776	54154	3.05%	0.371%
47	11.902	1851	1856	1858	rBV3	19602	33573	1.89%	0.230%
48	11.945	1859	1863	1868	rVV2	92013	159834	9.01%	1.095%
49	11.988	1868	1870	1874	rVV	37250	57992	3.27%	0.397%
50	12.030	1874	1877	1880	rVV4	21076	30395	1.71%	0.208%
51	12.079	1880	1885	1892	rVV	831977	1126113	63.45%	7.714%
52	12.152	1893	1897	1900	rVV2	53341	95955	5.41%	0.657%
53	12.207	1904	1906	1913	rVV2	52202	72899	4.11%	0.499%
54	12.274	1913	1917	1918	rVV	31805	35112	1.98%	0.241%
55	12.305	1918	1922	1927	rVV	117728	165628	9.33%	1.135%
56	12.372	1927	1933	1940	rVV7	66168	127616	7.19%	0.874%
57	12.524	1955	1958	1964	rVB3	30306	57914	3.26%	0.397%
58	12.615	1967	1973	1974	rBV5	22189	38088	2.15%	0.261%
59	12.640	1974	1977	1980	rVB3	17073	25097	1.41%	0.172%
60	12.743	1988	1994	1997	rBV6	23055	45127	2.54%	0.309%
61	12.780	1998	2000	2005	rVB4	22418	30718	1.73%	0.210%
62	12.878	2012	2016	2023	rVB3	70467	124493	7.01%	0.853%
63	12.963	2024	2030	2031	rBV5	25333	45881	2.59%	0.314%
64	13.024	2036	2040	2041	rVV3	28839	35454	2.00%	0.243%
65	13.048	2041	2044	2047	rVV	51460	66764	3.76%	0.457%
66	13.085	2047	2050	2057	rVB2	30320	58891	3.32%	0.403%
67	13.152	2057	2061	2066	rBV4	26798	50419	2.84%	0.345%
68	13.201	2066	2069	2075	rVB4	33894	50274	2.83%	0.344%
69	13.268	2076	2080	2083	rBV5	24255	32573	1.84%	0.223%
70	13.310	2083	2087	2090	rBV3	21771	32277	1.82%	0.221%
71	13.353	2090	2094	2099	rVV4	62470	93445	5.27%	0.640%

LSC Area Percent Report

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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Title : SW846 8260

72	13.408	2099	2103	2105	rVV3	20275	29766	1.68%	0.204%
73	13.445	2105	2109	2111	rVV2	70999	104517	5.89%	0.716%
74	13.481	2112	2115	2124	rVB7	69325	173989	9.80%	1.192%
75	13.652	2138	2143	2147	rBV6	29765	73648	4.15%	0.504%
76	13.737	2153	2157	2159	rBV2	19771	22135	1.25%	0.152%
77	13.762	2159	2161	2165	rVB4	19244	20427	1.15%	0.140%
78	13.810	2166	2169	2171	rBV2	23974	29023	1.64%	0.199%
79	13.841	2171	2174	2176	rBV	45688	54678	3.08%	0.375%
80	13.902	2181	2184	2191	rVB3	106658	152072	8.57%	1.042%
81	13.987	2191	2198	2203	rVB9	42608	103446	5.83%	0.709%
82	14.048	2205	2208	2216	rVB9	20988	48673	2.74%	0.333%
83	14.134	2218	2222	2225	rBV3	29684	44049	2.48%	0.302%
84	14.164	2225	2227	2230	rVB3	24021	24146	1.36%	0.165%
85	14.274	2242	2245	2250	rVB4	47635	67565	3.81%	0.463%
86	14.383	2260	2263	2267	rVB2	26281	32635	1.84%	0.224%
87	14.432	2269	2271	2275	rVB	29435	34120	1.92%	0.234%
88	14.481	2276	2279	2285	rVB4	33611	51772	2.92%	0.355%
89	14.548	2286	2290	2293	rBV2	34385	53903	3.04%	0.369%
90	14.676	2307	2311	2317	rVB3	77803	105567	5.95%	0.723%
91	14.737	2318	2321	2324	rVB2	28905	36728	2.07%	0.252%
92	14.786	2325	2329	2332	rBV2	33733	48331	2.72%	0.331%
93	14.853	2336	2340	2344	rVV3	49236	85391	4.81%	0.585%
94	14.914	2347	2350	2353	rVB4	24370	30312	1.71%	0.208%
95	15.249	2401	2405	2408	rBV3	31855	53316	3.00%	0.365%
96	15.280	2408	2410	2414	rVB	43757	49322	2.78%	0.338%
97	15.450	2435	2438	2441	rBV5	14827	20027	1.13%	0.137%
98	15.493	2441	2445	2449	rVV4	17921	26057	1.47%	0.178%
99	15.822	2496	2499	2505	rVB5	15662	28322	1.60%	0.194%
100	15.932	2514	2517	2531	rVB4	18451	46544	2.62%	0.319%

Sum of corrected areas: 14598520

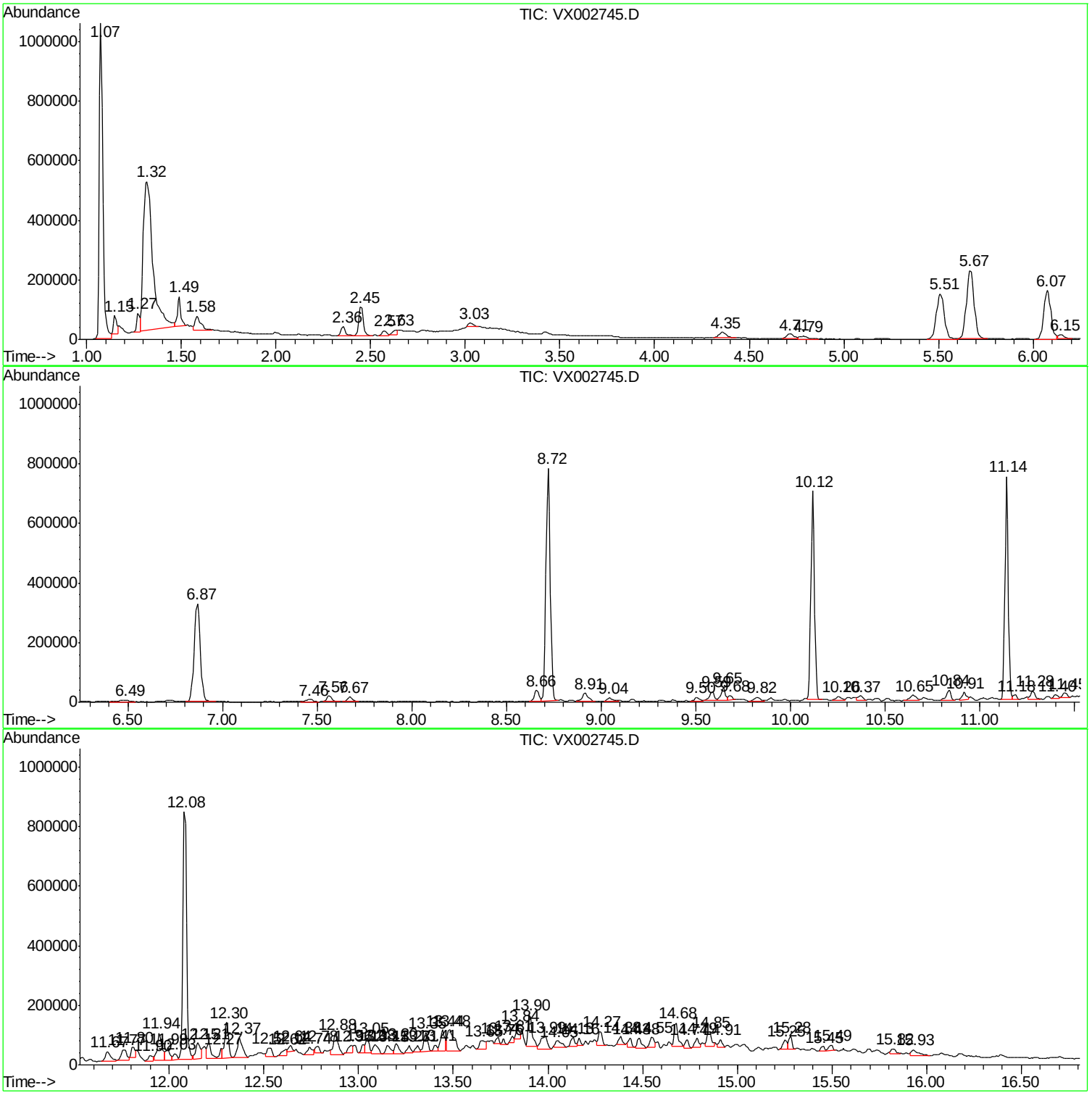
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002745.D
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

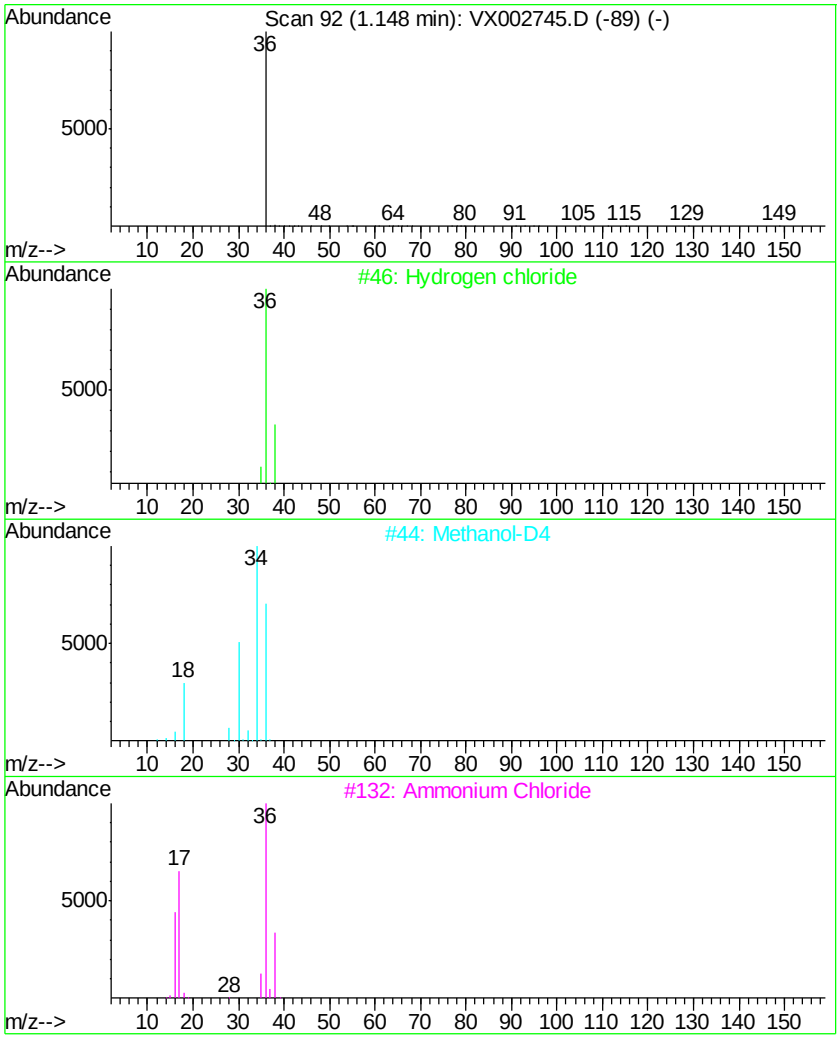
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

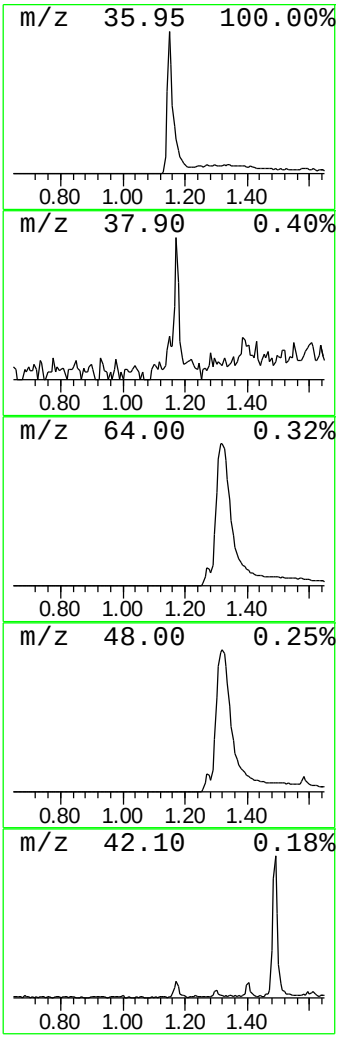
****

Peak Number 2 unknown1.15 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.15	5.52 ug/l	70749	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen chloride	36	ClH	007647-01-0	2
2	Methanol-D4	36	CD4O	000811-98-3	2
3	Ammonium Chloride	53	ClH4N	012125-02-9	1
4	2-Chloroethylamine	79	C2H6ClN	000689-98-5	1
5	Hydrogen sulfide	34	H2S	007783-06-4	1





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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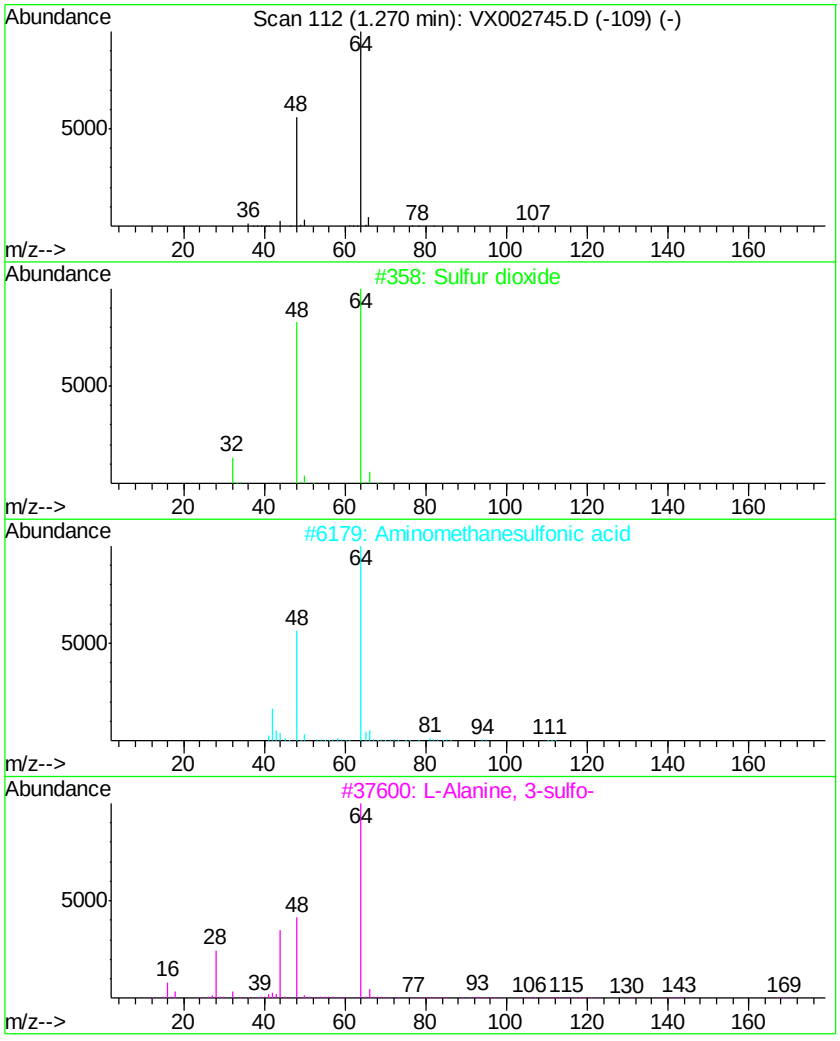
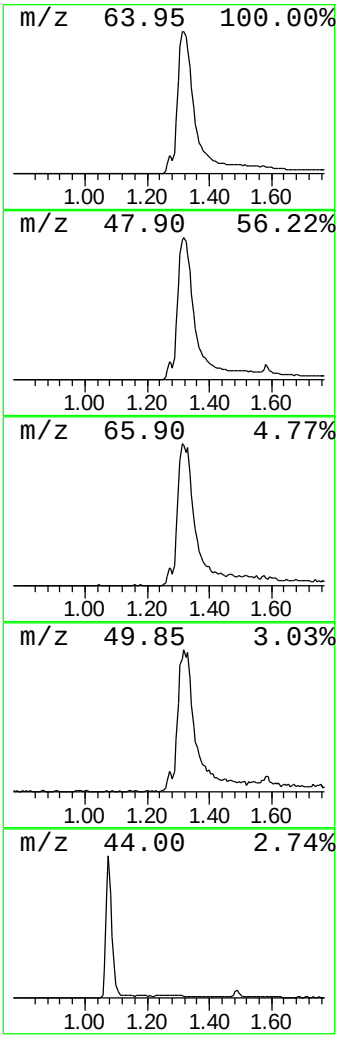
Peak Number 3 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	5.79 ug/l	74241	Pentafluorobenzene	5.67

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	64
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





Library Search Compound Report

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Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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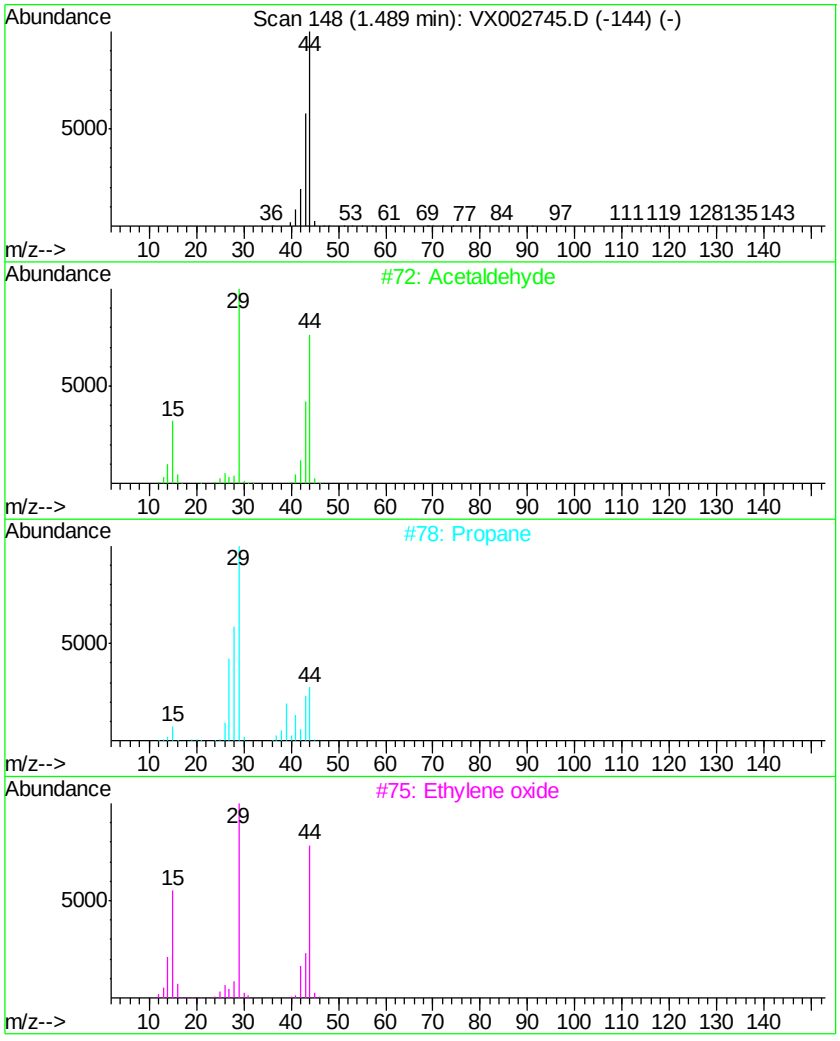
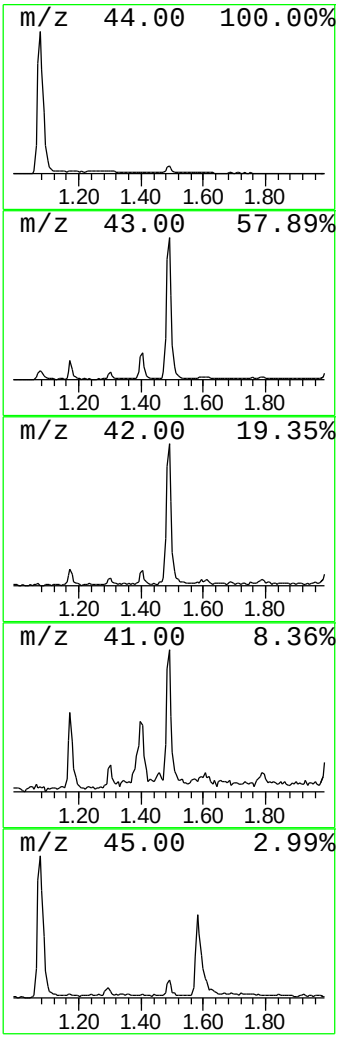
Peak Number 5 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	9.92 ug/l	127200	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	1-Propanol, 2-amino-, (.+/-.)-	75	C3H9NO	006168-72-5	4





Library Search Compound Report

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Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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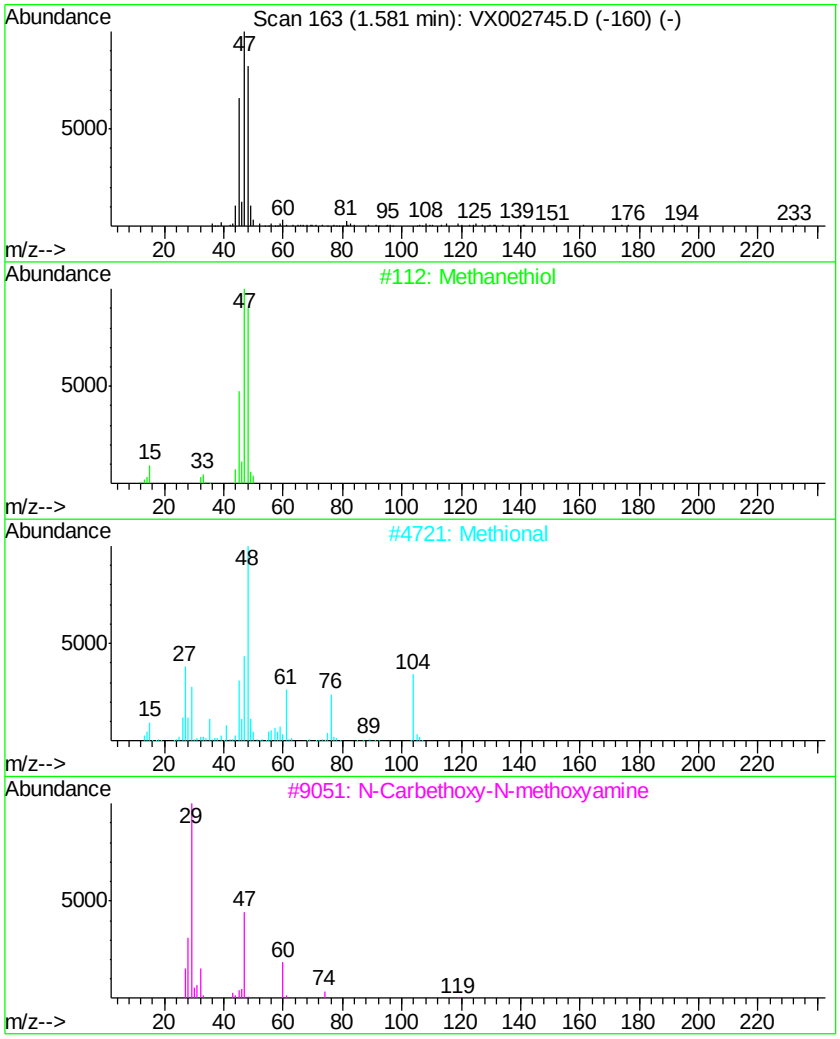
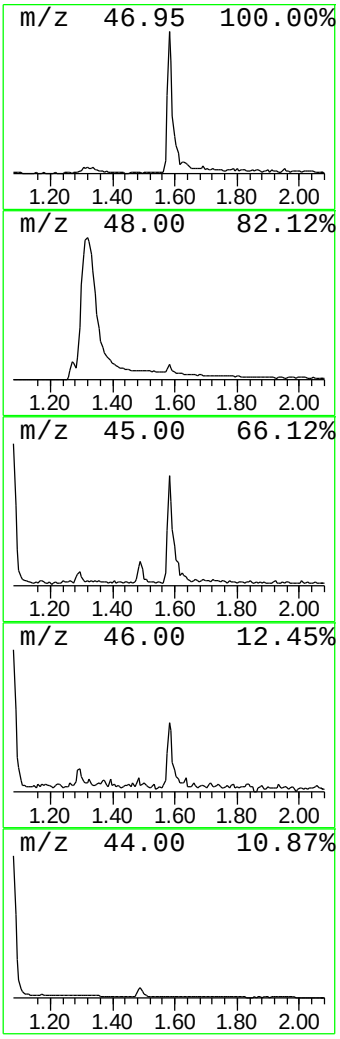
Peak Number 6 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.58	7.53 ug/l	96647	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methional	104	C4H8OS	003268-49-3	9
3	N-Carbethoxy-N-methoxyamine	119	C4H9NO3	003871-28-1	7
4	Propanamide, 2-hydroxy-	89	C3H7NO2	002043-43-8	7
5	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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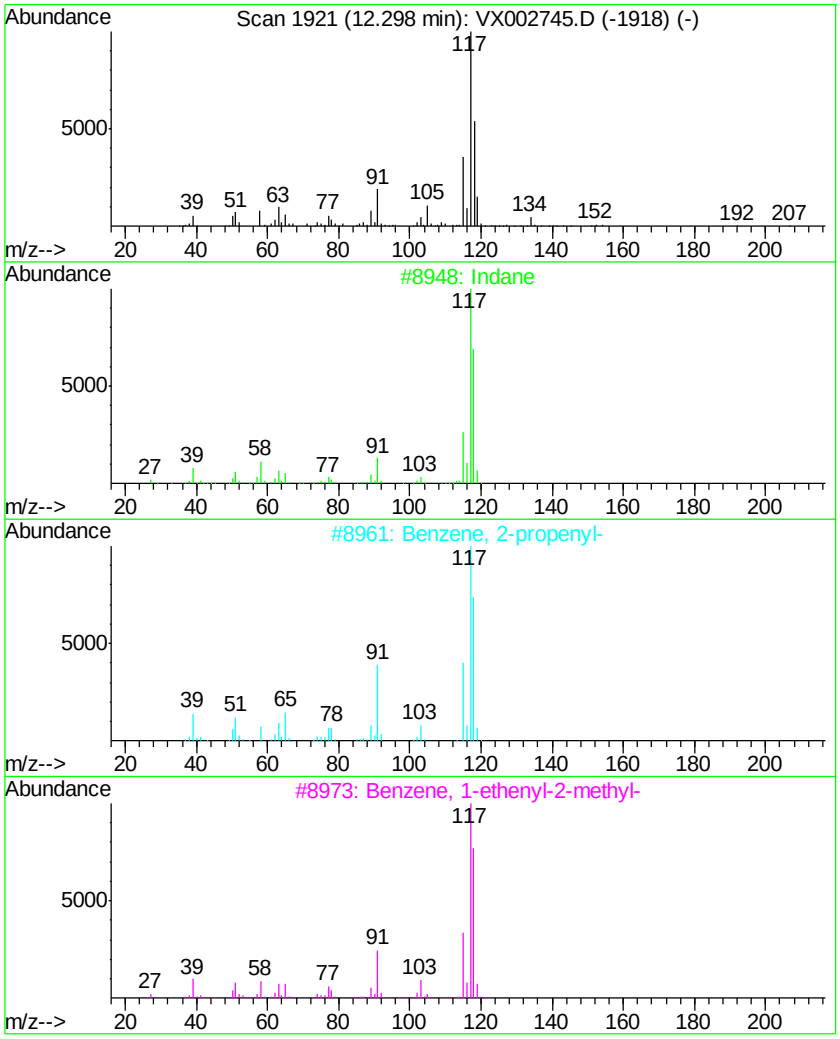
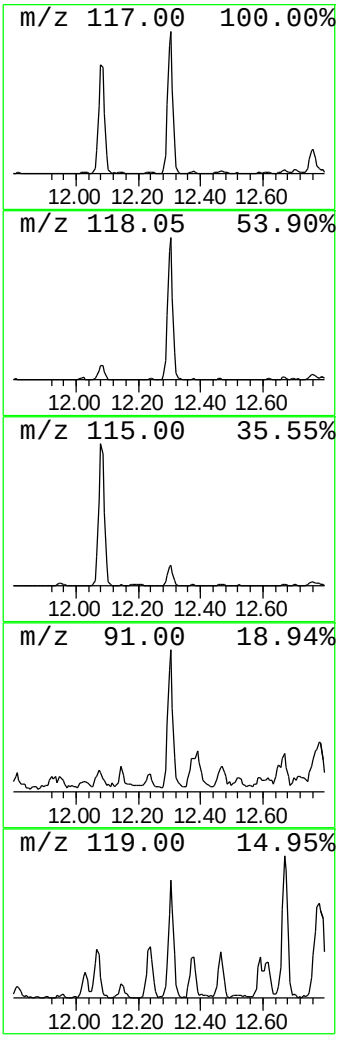
Peak Number 7 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	7.35 ug/l	165628	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	62
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	62
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58





Library Search Compound Report

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Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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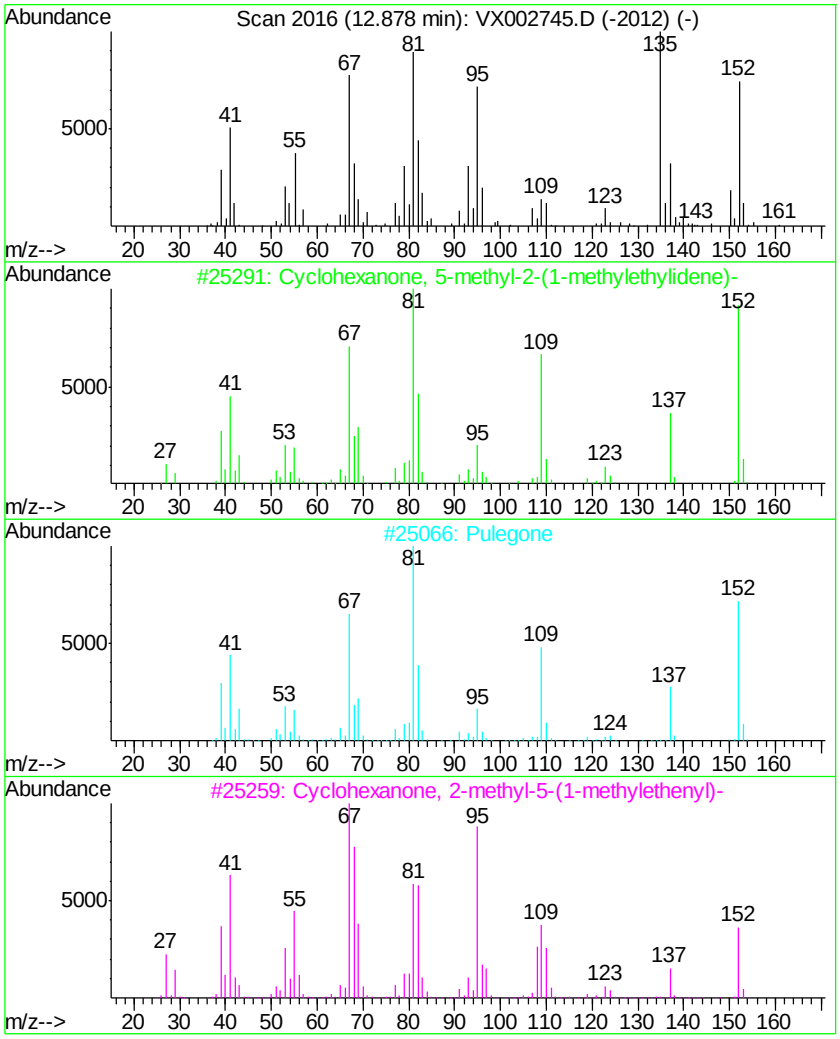
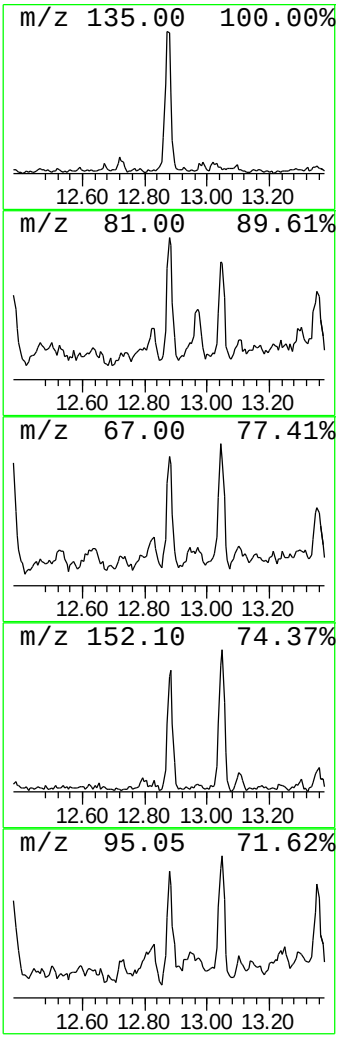
Peak Number 8 Cyclohexanone, 5-methyl-2-(... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	5.53 ug/l	124493	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	86
2	Pulegone	152	C10H16O	000089-82-7	70
3	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	60
4	Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	58
5	Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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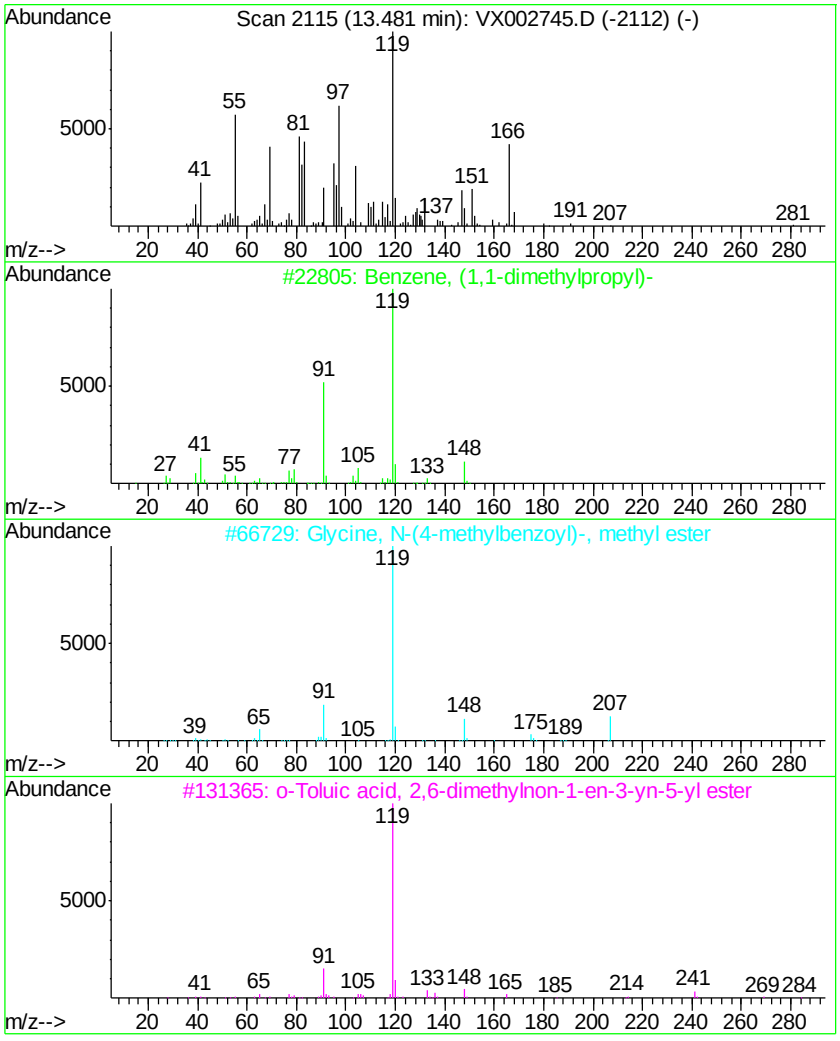
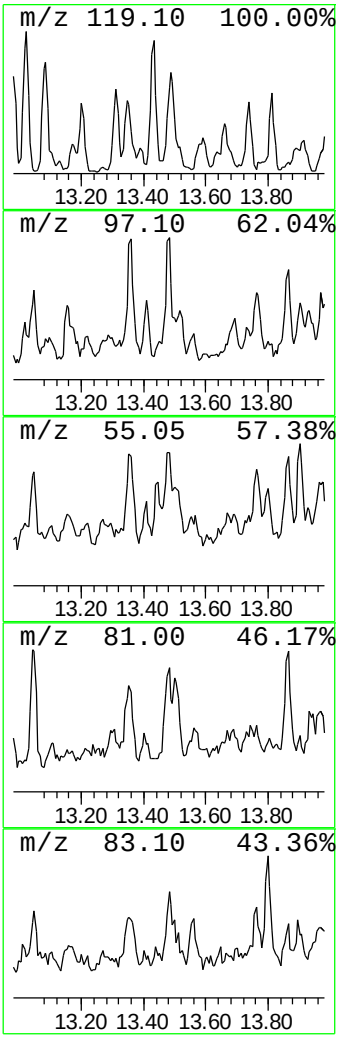
Peak Number 9 unknown13.48 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	7.73 ug/l	173989	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	14
2	Glycine, N-(4-methylbenzoyl)-, m...	207	C11H13NO3	001208-23-7	14
3	o-Toluic acid, 2,6-dimethylnon-1...	284	C19H24O2	1000292-51-6	14
4	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	14
5	.alpha.-Bromomesitylene	198	C9H11Br	027129-86-8	10





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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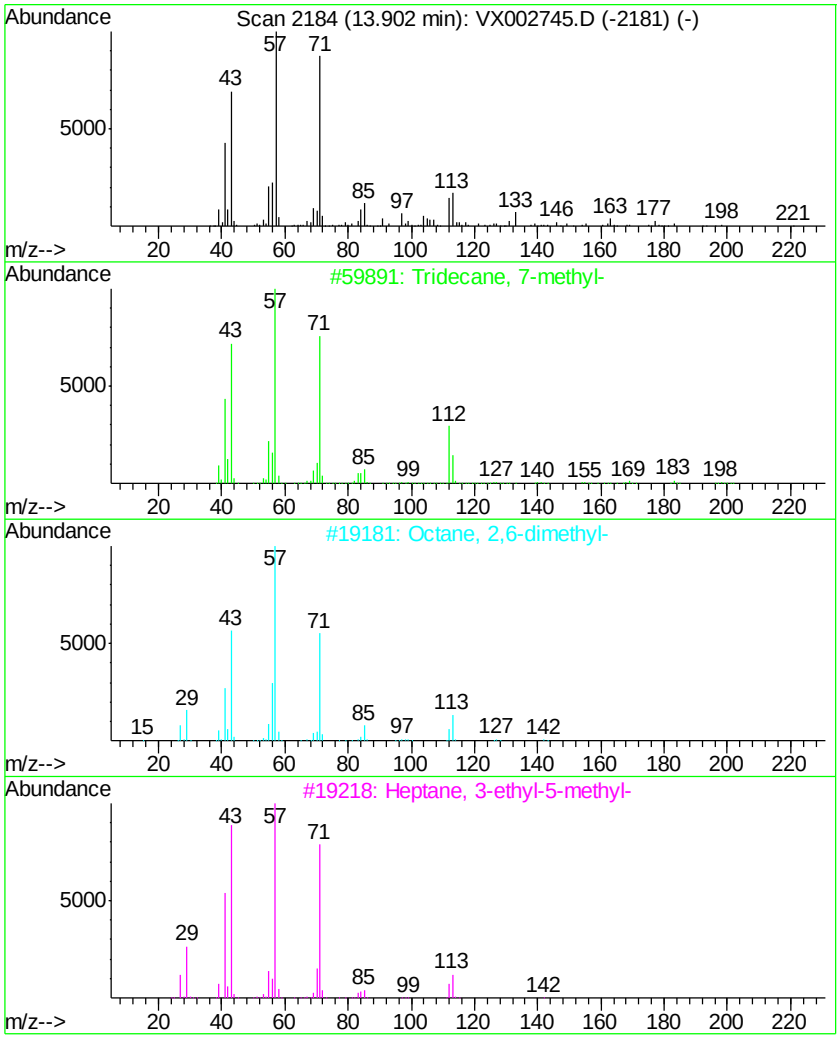
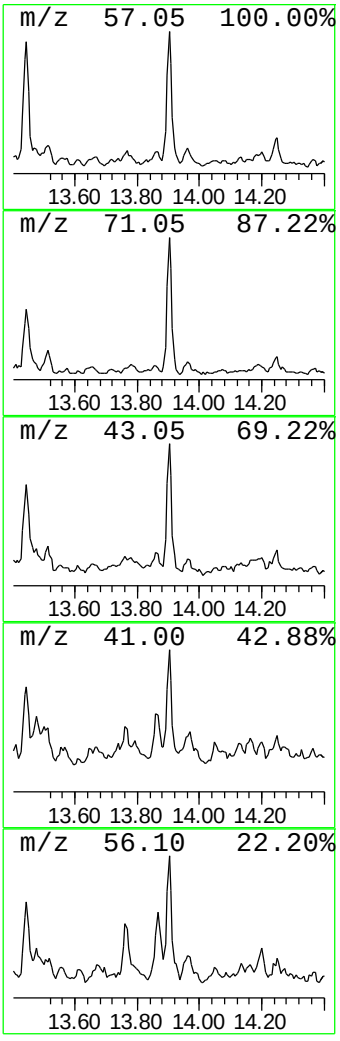
Peak Number 10 Tridecane, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.75 ug/l	152072	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	87
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	86
3	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	72
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002745.D
Acq On : 20 Jun 2018 16:47
Operator : JC/MD
Sample : J3596-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.15	1.15	5.5	ug/l	70749	1	5.67	641322	50.0
Sulfur dioxide	1.27	5.8	ug/l	74241	1	5.67	641322	50.0
Acetaldehyde	1.49	9.9	ug/l	127200	1	5.67	641322	50.0
Methanethiol	1.58	7.5	ug/l	96647	1	5.67	641322	50.0
Indane	12.30	7.3	ug/l	165628	4	12.08	1126110	50.0
Cyclohexanone, 5-...	12.88	5.5	ug/l	124493	4	12.08	1126110	50.0
unknown13.48	13.48	7.7	ug/l	173989	4	12.08	1126110	50.0
Tridecane, 7-methyl-	13.90	6.8	ug/l	152072	4	12.08	1126110	50.0