

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061318\
 Data File : VX002545.D
 Acq On : 14 Jun 2018 08:27
 Operator : JC/MD
 Sample : J3383-04
 Misc : 7.06g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-11R

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\82X060418W.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	1.069	75	79	92	rBV	957930	1211095	74.29%	6.811%
2	1.264	108	111	118	rVB3	15961	23536	1.44%	0.132%
3	1.666	157	177	179	rBV9	29789	142167	8.72%	0.799%
4	1.947	218	223	230	rVB	24064	36011	2.21%	0.203%
5	2.812	360	365	367	rBV2	13602	23330	1.43%	0.131%
6	2.861	367	373	384	rVB	64797	140953	8.65%	0.793%
7	3.020	391	399	410	rBV	44628	115060	7.06%	0.647%
8	3.142	412	419	430	rVB	49212	116069	7.12%	0.653%
9	3.495	469	477	489	rVB	73949	167190	10.26%	0.940%
10	3.794	519	526	533	rVB	10244	24854	1.52%	0.140%
11	4.282	598	606	613	rVV2	7959	20971	1.29%	0.118%
12	4.379	613	622	635	rVB	41905	124183	7.62%	0.698%
13	4.873	692	703	715	rVB	5651	21709	1.33%	0.122%
14	5.281	766	770	780	rVB6	6132	18885	1.16%	0.106%
15	5.507	790	807	815	rBV	178532	554409	34.01%	3.118%
16	5.659	825	832	851	rVB	298335	894570	54.87%	5.031%
17	5.915	861	874	888	rVB2	61129	189846	11.64%	1.068%
18	6.068	889	899	914	rBV	208128	543546	33.34%	3.057%
19	6.251	914	929	938	rVV3	21654	80487	4.94%	0.453%
20	6.348	938	945	953	rVV3	23181	65918	4.04%	0.371%
21	6.446	953	961	974	rVB2	26397	80254	4.92%	0.451%
22	6.696	989	1002	1013	rBV2	88299	219865	13.49%	1.236%
23	6.860	1019	1029	1038	rBV	423766	1024685	62.85%	5.762%
24	7.251	1084	1093	1100	rBV4	13489	33076	2.03%	0.186%
25	7.458	1114	1127	1138	rBV2	146253	350608	21.51%	1.972%
26	7.574	1138	1146	1150	rBV2	12466	26514	1.63%	0.149%
27	7.635	1150	1156	1165	rVB	16859	35623	2.19%	0.200%
28	7.732	1165	1172	1180	rVB	19686	38095	2.34%	0.214%
29	7.842	1183	1190	1198	rVB3	15739	35801	2.20%	0.201%
30	7.958	1198	1209	1215	rBV9	5610	20908	1.28%	0.118%
31	8.171	1235	1244	1247	rBV4	12815	28144	1.73%	0.158%
32	8.214	1247	1251	1254	rVV	23241	41113	2.52%	0.231%
33	8.257	1254	1258	1263	rVV5	20162	42598	2.61%	0.240%
34	8.342	1267	1272	1275	rVV	49106	85756	5.26%	0.482%

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Integrator: RTE
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 Title : SW846 8260

35	8.378	1275	1278	1285	rVB2	29240	48506	2.98%	0.273%
36	8.500	1293	1298	1306	rBV	50077	94516	5.80%	0.532%
37	8.574	1306	1310	1319	rVB3	15939	32718	2.01%	0.184%
38	8.671	1319	1326	1328	rBV3	32286	61198	3.75%	0.344%
39	8.720	1328	1334	1343	rVB	1006975	1630296	100.00%	9.168%
40	8.836	1348	1353	1358	rBV3	14317	22505	1.38%	0.127%
41	8.976	1370	1376	1382	rBV3	50118	86155	5.28%	0.484%
42	9.043	1382	1387	1399	rVB4	18950	44364	2.72%	0.249%
43	9.226	1412	1417	1421	rBV	19412	28818	1.77%	0.162%
44	9.555	1468	1471	1478	rVB4	18253	37937	2.33%	0.213%
45	9.622	1478	1482	1486	rVB2	16872	24419	1.50%	0.137%
46	9.964	1534	1538	1548	rVB2	33227	50377	3.09%	0.283%
47	10.067	1548	1555	1558	rBV	29329	41693	2.56%	0.234%
48	10.116	1558	1563	1572	rVV	899281	1222244	74.97%	6.873%
49	10.256	1581	1586	1591	rVB	161850	204910	12.57%	1.152%
50	10.366	1592	1604	1609	rVV	165113	232032	14.23%	1.305%
51	10.421	1609	1613	1621	rVB6	10694	21788	1.34%	0.123%
52	11.024	1706	1712	1716	rBV	27065	39441	2.42%	0.222%
53	11.146	1726	1732	1743	rVB	966704	1307788	80.22%	7.354%
54	11.366	1763	1768	1775	rVB	108391	135205	8.29%	0.760%
55	11.457	1776	1783	1788	rVV	168088	228071	13.99%	1.283%
56	11.512	1788	1792	1801	rVB	118974	157234	9.64%	0.884%
57	11.671	1814	1818	1827	rBV	33102	49841	3.06%	0.280%
58	11.811	1836	1841	1847	rBV	565176	691256	42.40%	3.887%
59	12.085	1880	1886	1892	rVV	1240394	1544545	94.74%	8.686%
60	12.146	1892	1896	1901	rVB	119678	153515	9.42%	0.863%
61	12.305	1917	1922	1929	rBV	121397	161015	9.88%	0.905%
62	12.378	1929	1934	1942	rVB3	121144	210281	12.90%	1.183%
63	12.463	1945	1948	1953	rBV5	11028	19409	1.19%	0.109%
64	12.524	1954	1958	1963	rVB	41117	49981	3.07%	0.281%
65	12.591	1964	1969	1971	rBV	83677	105874	6.49%	0.595%
66	12.615	1971	1973	1978	rVB	68013	70869	4.35%	0.399%
67	12.670	1978	1982	1986	rBV	132481	164710	10.10%	0.926%
68	12.707	1986	1988	1991	rVB	20692	21231	1.30%	0.119%
69	12.762	1993	1997	2005	rBV3	57523	109248	6.70%	0.614%
70	12.908	2018	2021	2025	rBV	28951	33513	2.06%	0.188%
71	12.981	2029	2033	2037	rVV	82829	103591	6.35%	0.583%

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72	13.024	2037	2040	2046	rVB	118344	146704	9.00%	0.825%
73	13.085	2047	2050	2051	rBV	21481	22077	1.35%	0.124%
74	13.231	2070	2074	2078	rVB	70684	88911	5.45%	0.500%
75	13.274	2078	2081	2084	rVB2	21821	25853	1.59%	0.145%
76	13.317	2084	2088	2090	rBV2	30292	43055	2.64%	0.242%
77	13.353	2090	2094	2099	rVB2	115263	155872	9.56%	0.877%
78	13.432	2104	2107	2111	rVB2	24875	32800	2.01%	0.184%
79	13.487	2112	2116	2120	rBV4	22130	35433	2.17%	0.199%
80	13.567	2126	2129	2132	rBV3	19272	25526	1.57%	0.144%
81	13.603	2132	2135	2138	rVV	41183	55926	3.43%	0.315%
82	13.646	2138	2142	2147	rVV4	41760	74108	4.55%	0.417%
83	13.725	2149	2155	2162	rVV3	51042	116903	7.17%	0.657%
84	13.841	2170	2174	2179	rVB	68002	90847	5.57%	0.511%
85	13.908	2180	2185	2186	rBV5	20006	34449	2.11%	0.194%
86	13.987	2195	2198	2203	rVV3	25643	35600	2.18%	0.200%
87	14.140	2219	2223	2229	rBV3	46982	71829	4.41%	0.404%
88	14.280	2242	2246	2256	rVB4	49421	104245	6.39%	0.586%
89	14.383	2260	2263	2269	rVV4	29384	49542	3.04%	0.279%
90	14.432	2269	2271	2275	rVB2	24966	29172	1.79%	0.164%
91	14.554	2285	2291	2294	rBV7	17559	41842	2.57%	0.235%
92	14.676	2307	2311	2312	rBV3	28401	34681	2.13%	0.195%
93	14.700	2312	2315	2324	rVB	144634	203570	12.49%	1.145%
94	14.810	2326	2333	2336	rBV5	36970	94028	5.77%	0.529%
95	14.847	2336	2339	2343	rVB	47208	62823	3.85%	0.353%
96	15.280	2402	2410	2417	rBV6	32591	73503	4.51%	0.413%
97	15.353	2418	2422	2427	rBV7	11754	28864	1.77%	0.162%
98	15.554	2451	2455	2468	rVB6	48534	120198	7.37%	0.676%
99	15.694	2474	2478	2481	rBV2	27525	45065	2.76%	0.253%
100	16.182	2554	2558	2564	rBV9	10500	20006	1.23%	0.113%

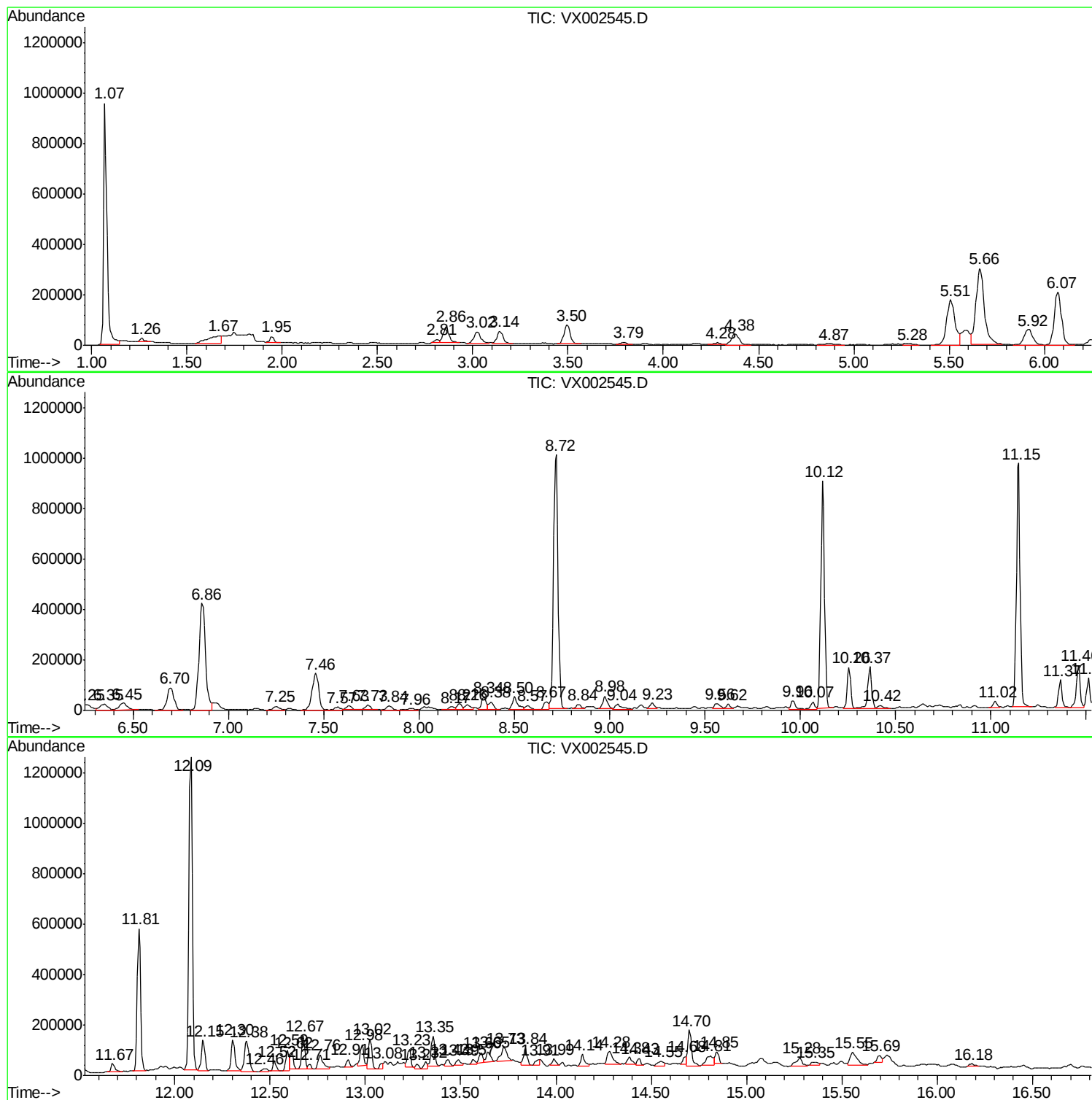
Sum of corrected areas: 17782355

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



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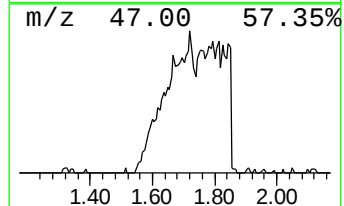
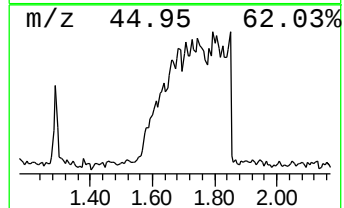
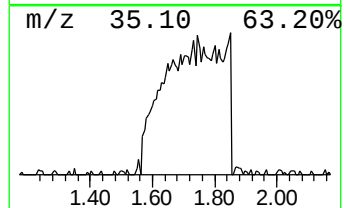
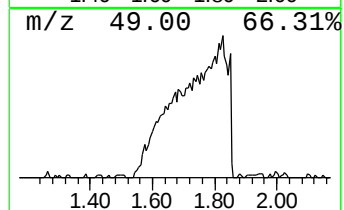
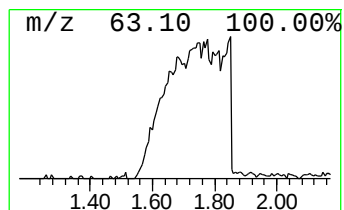
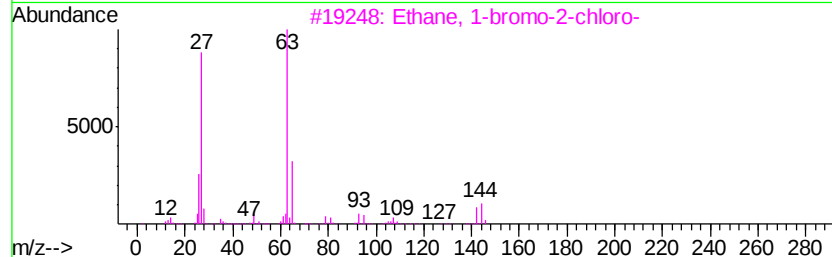
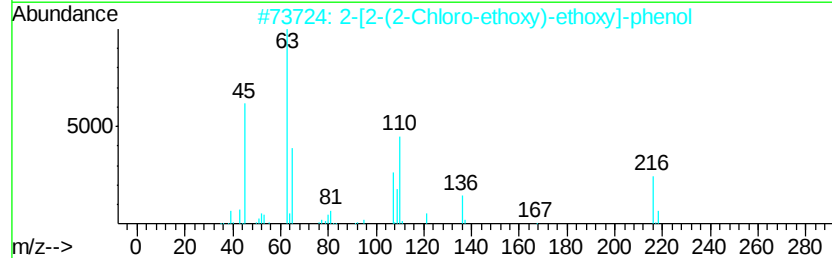
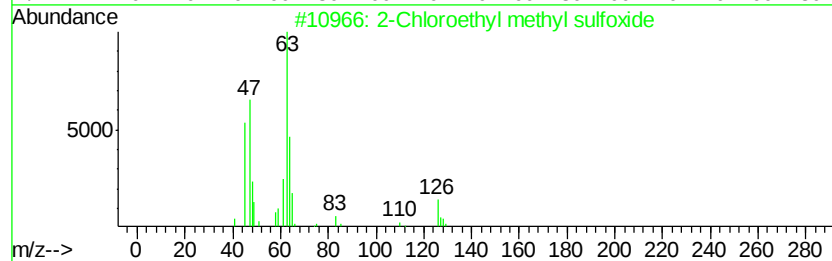
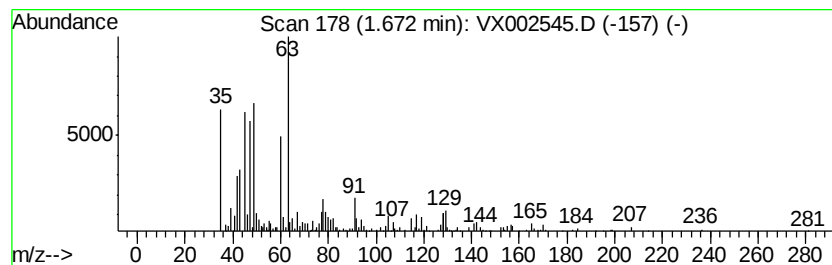
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown1.67 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	7.95 ug/l	142167	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	38
2		2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	37
3		Ethane, 1-bromo-2-chloro-	142	C2H4BrCl	000107-04-0	27
4		Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	25
5		Carbonfluoridodithioic acid, tri...	164	C2F4S2	000371-73-3	17



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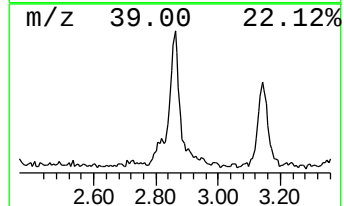
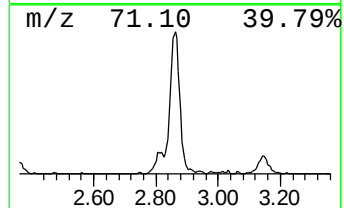
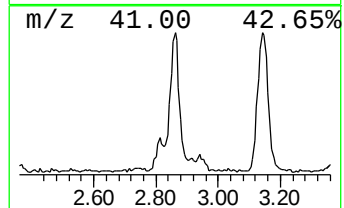
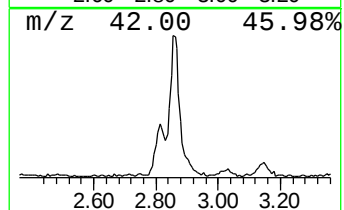
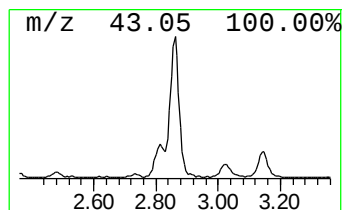
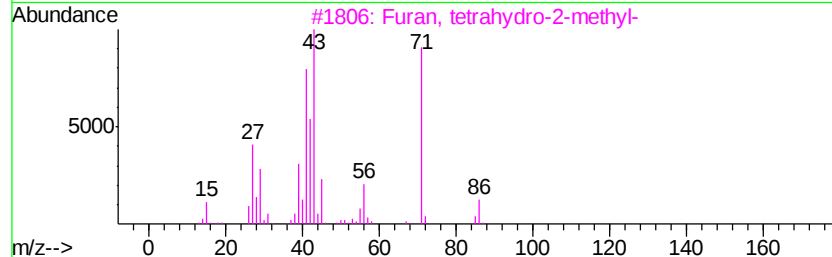
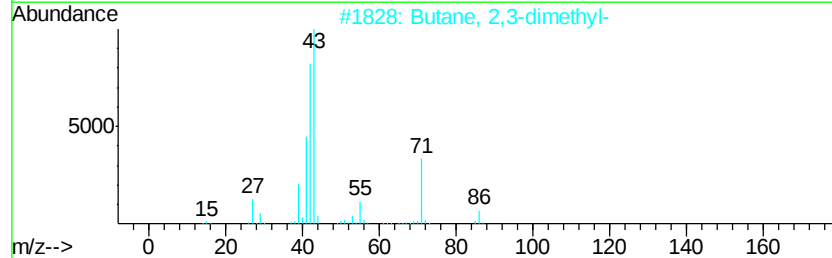
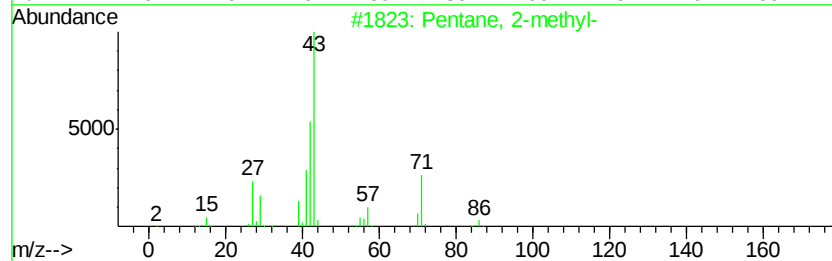
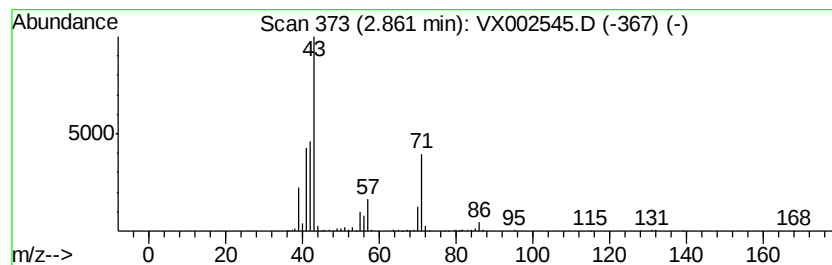
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	7.88 ug/l	140953	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
3		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38
4		Pentane	72	C5H12	000109-66-0	35
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28



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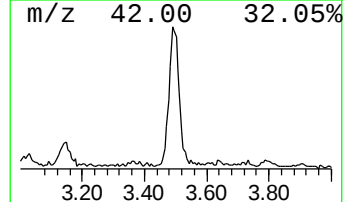
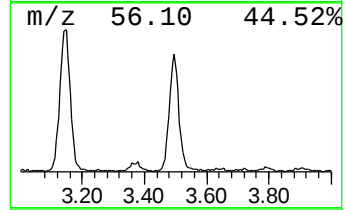
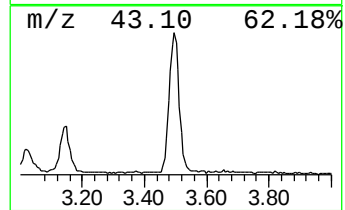
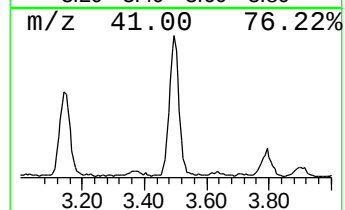
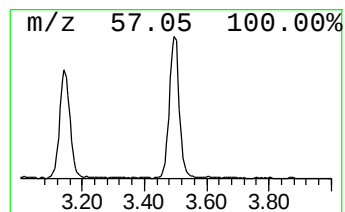
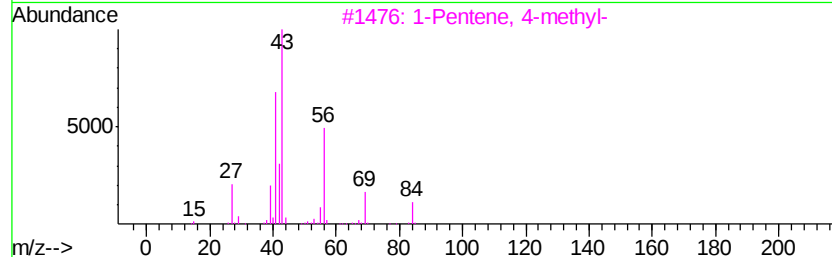
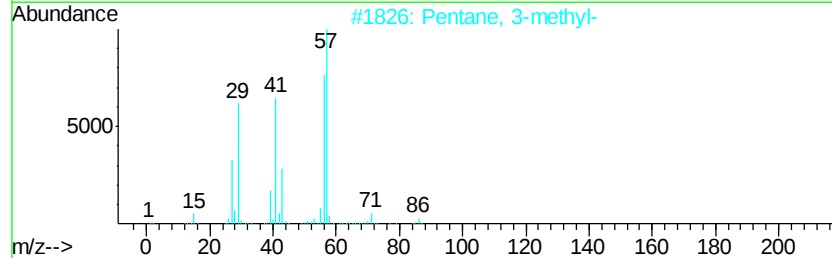
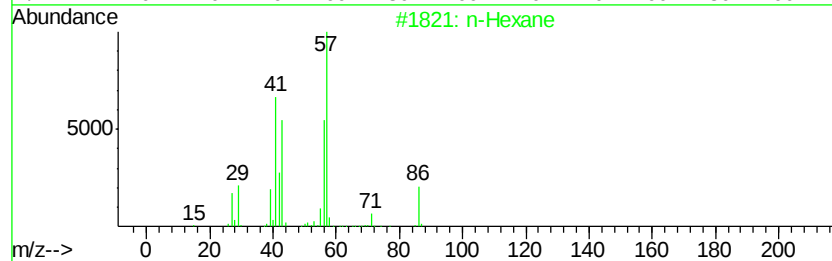
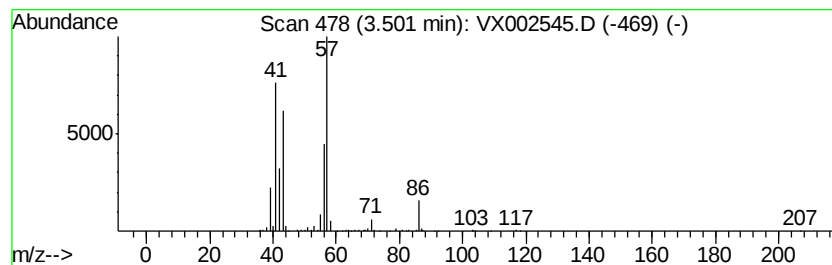
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Quant Title : SW846 8260

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

Peak Number 4 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	9.34 ug/l	167190	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	91
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	42
3		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4		Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-11R

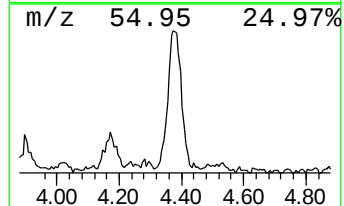
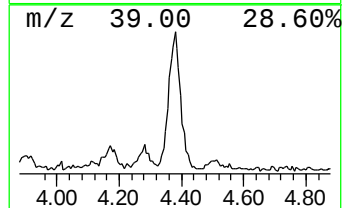
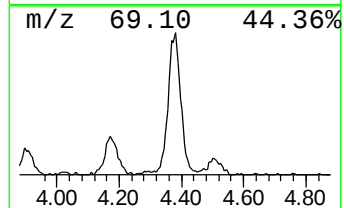
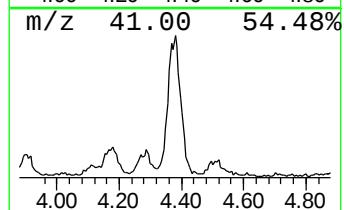
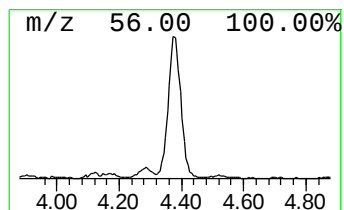
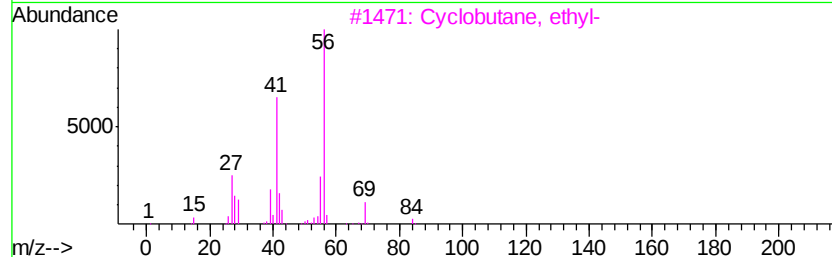
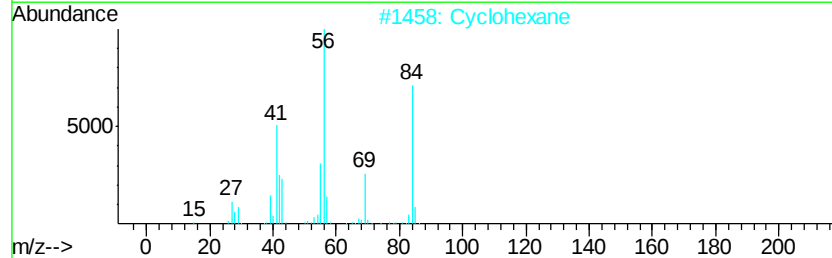
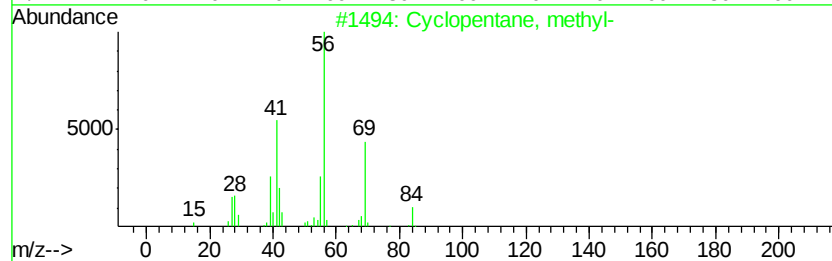
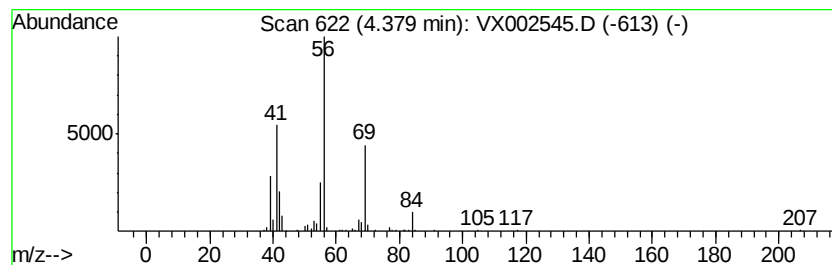
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	6.94 ug/l	124183	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclohexane	84	C6H12	000110-82-7	83
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06µ/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-11R

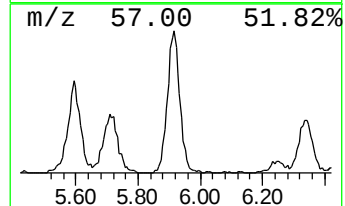
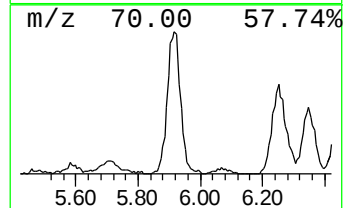
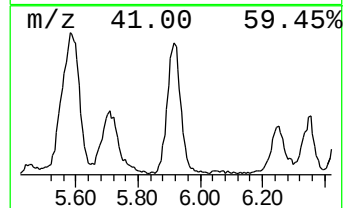
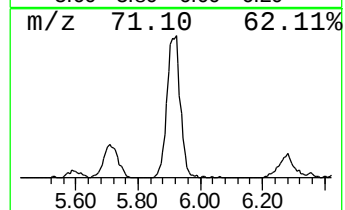
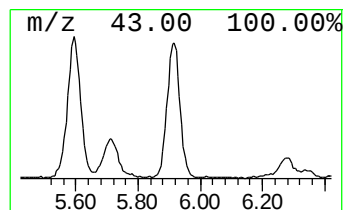
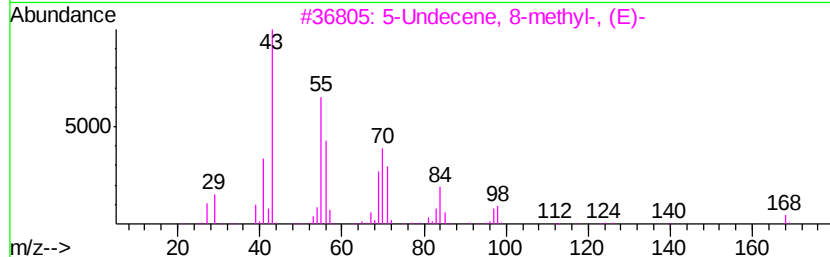
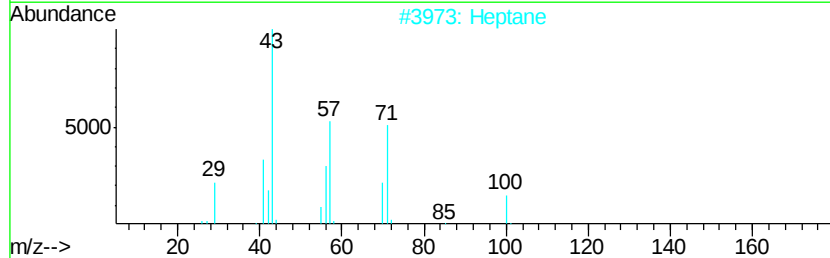
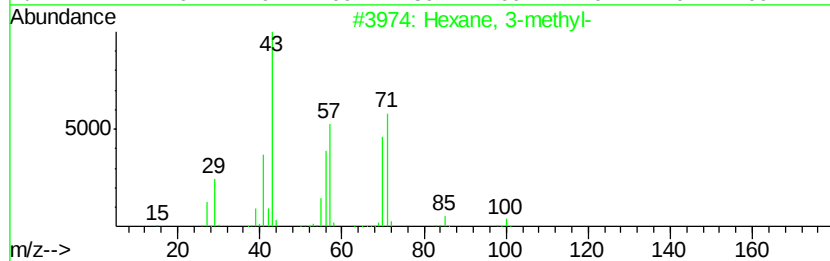
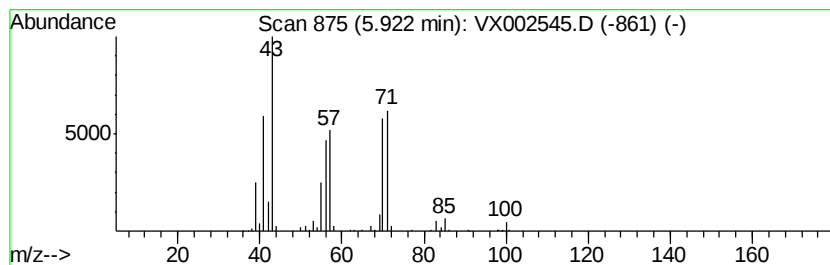
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	10.61 ug/l	189846	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2		Heptane	100	C7H16	000142-82-5	72
3		5-Undecene, 8-methyl-, (E)-	168	C12H24	039546-85-5	53
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-11R

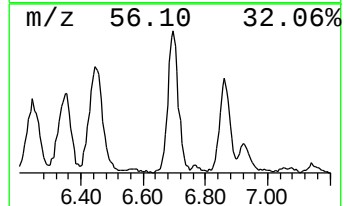
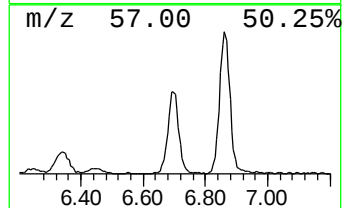
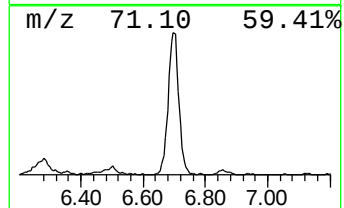
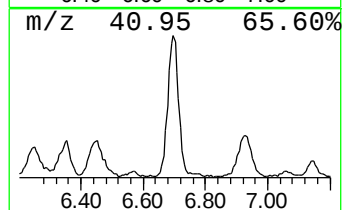
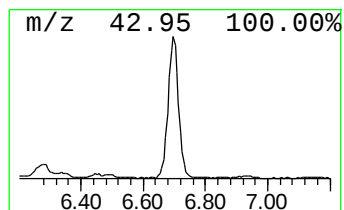
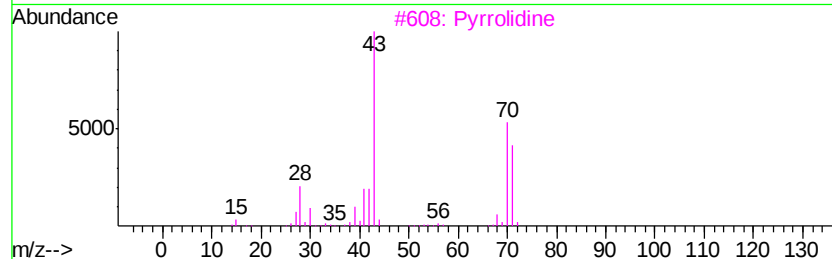
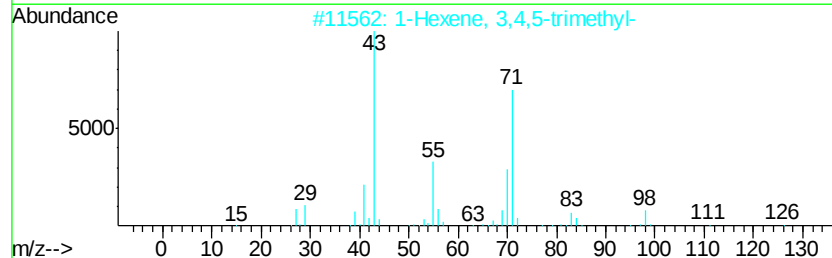
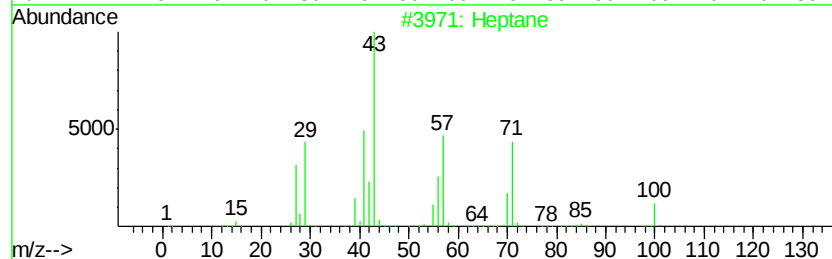
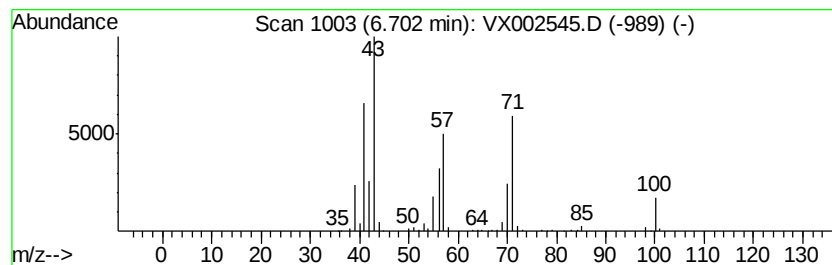
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Quant Title : SW846 8260

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

Peak Number 7 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	10.73 ug/l	219865	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	50
3		Pyrrolidine	71	C4H9N	000123-75-1	43
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	42
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
B-11R

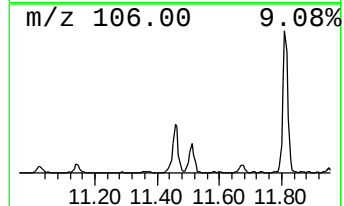
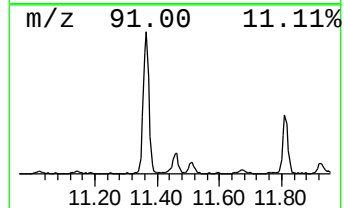
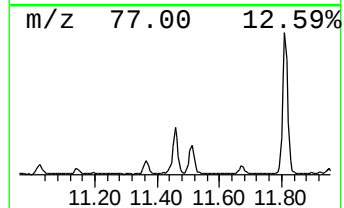
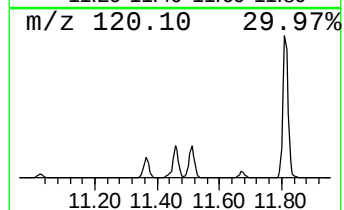
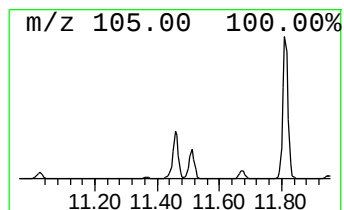
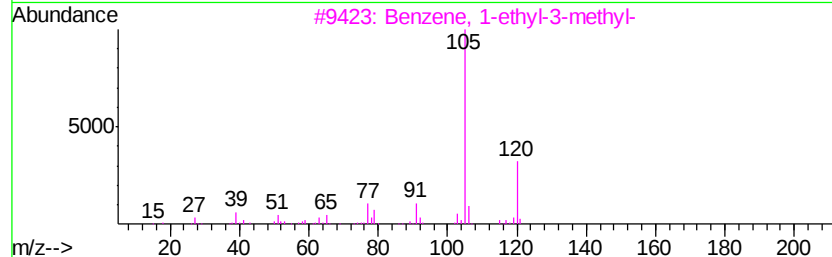
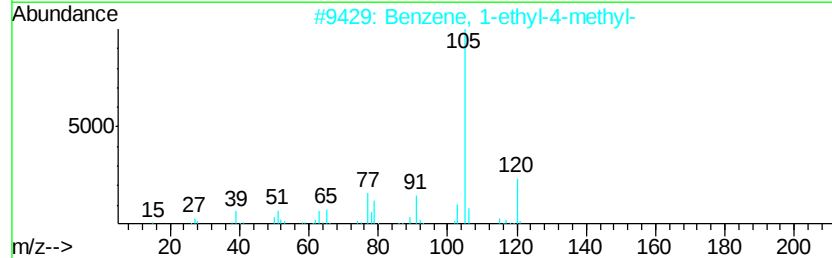
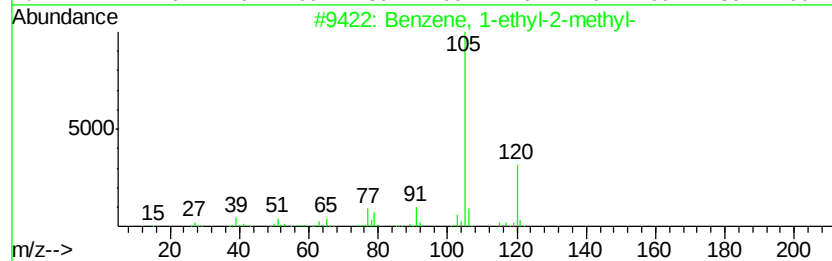
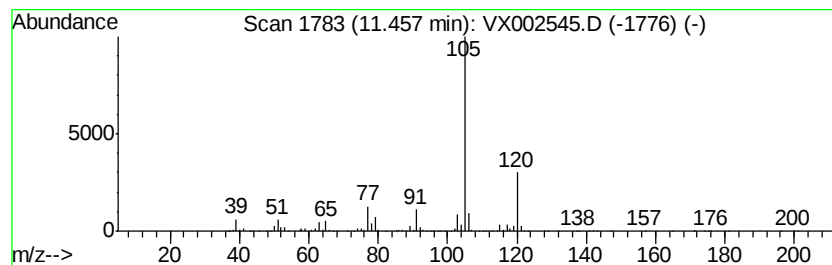
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	7.38 ug/l	228071	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06µ/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

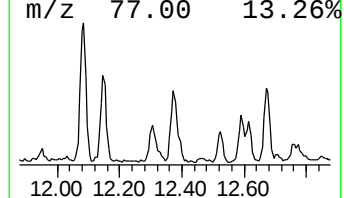
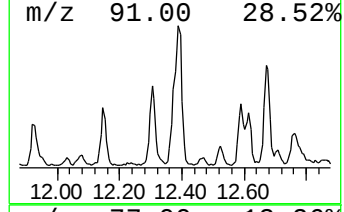
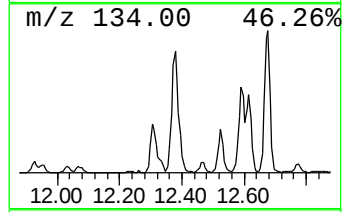
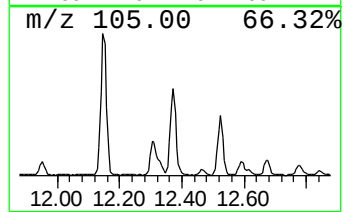
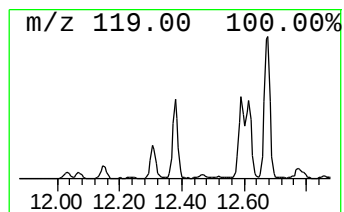
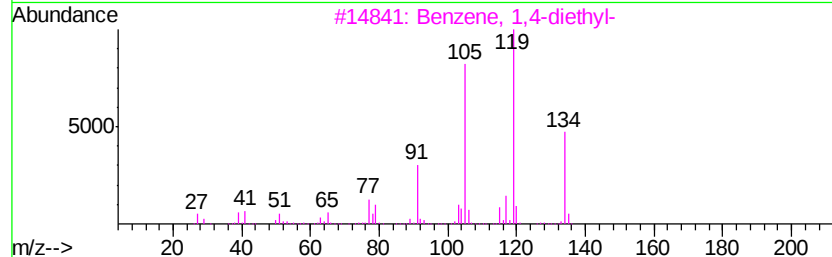
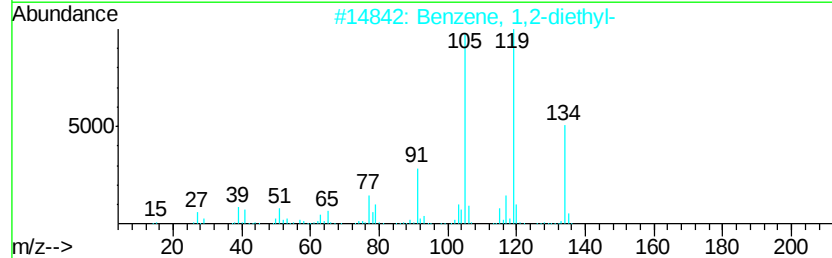
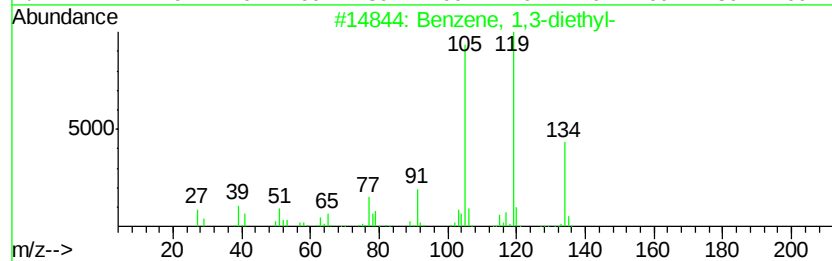
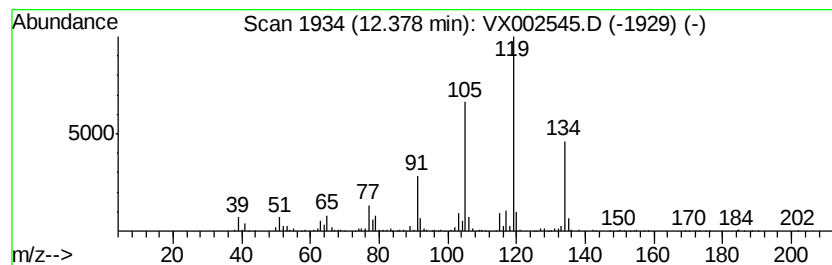
Instrument :
MSVOA_X
ClientSampled :
B-11R

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,3-diethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	6.81 ug/l	210281	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1,3-diethyl-	134 C10H14	000141-93-5 96
2		Benzene, 1,2-diethyl-	134 C10H14	000135-01-3 96
3		Benzene, 1,4-diethyl-	134 C10H14	000105-05-5 96
4		Benzene, 1,2,3,4-tetramethyl-	134 C10H14	000488-23-3 94
5		Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06µ/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

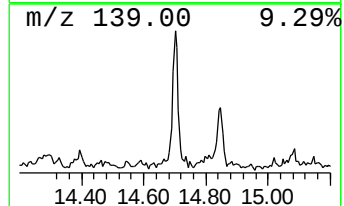
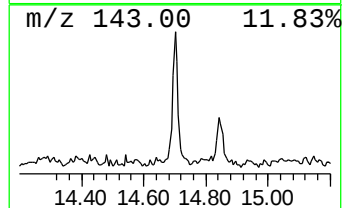
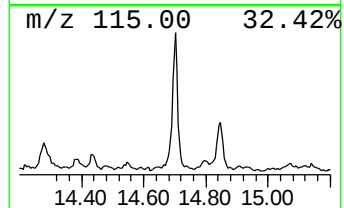
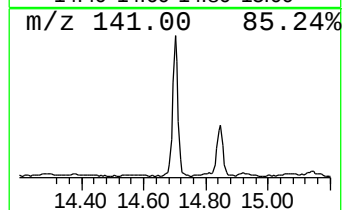
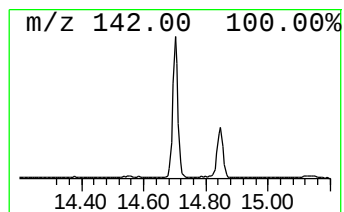
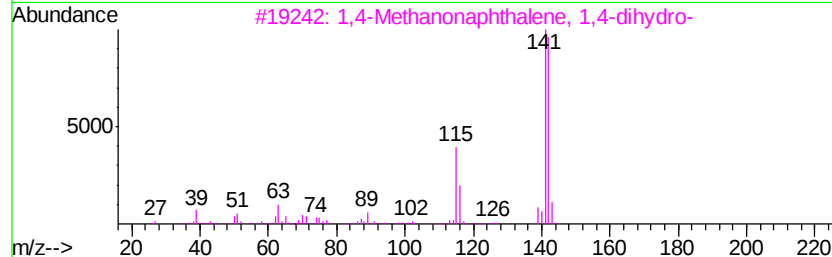
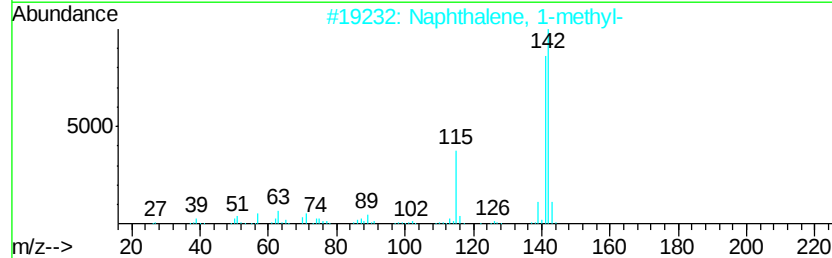
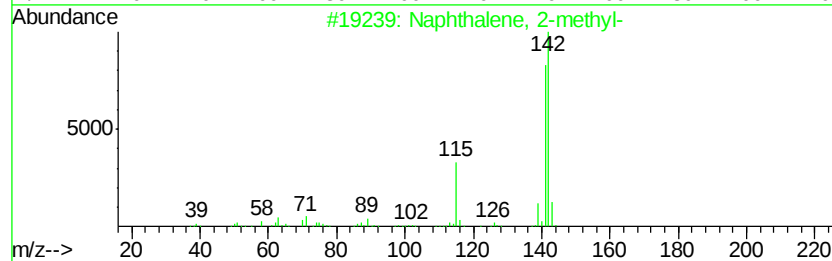
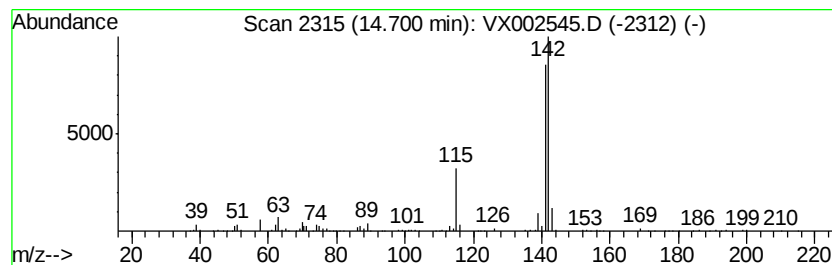
Instrument :
MSVOA_X
ClientSampleId :
B-11R

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.70	6.59 ug/l	203570	1,4-Dichlorobenzene-d4	12.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX061318\
Data File : VX002545.D
Acq On : 14 Jun 2018 08:27
Operator : JC/MD
Sample : J3383-04
Misc : 7.06g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-11R

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane, 2-methyl-	2.86	7.9	ug/l	140953	1	5.67	894570	50.0
n-Hexane	3.50	9.3	ug/l	167190	1	5.67	894570	50.0
Cyclopentane, met...	4.38	6.9	ug/l	124183	1	5.67	894570	50.0
Hexane, 3-methyl-	5.92	10.6	ug/l	189846	1	5.67	894570	50.0
Heptane	6.70	10.7	ug/l	219865	2	6.86	1024690	50.0
Benzene, 1-ethyl-...	11.46	7.4	ug/l	228071	4	12.09	1544550	50.0
Benzene, 1,3-diet...	12.38	6.8	ug/l	210281	4	12.09	1544550	50.0
Naphthalene, 1-me...	14.70	6.6	ug/l	203570	4	12.09	1544550	50.0