

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX110918\
 Data File : VX005887.D
 Acq On : 10 Nov 2018 03:31
 Operator : JC/MD
 Sample : J5889-13
 Misc : 16.55µ/5mL/100µL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BOTTOM-D

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.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	1.666	63	84	87	rBV3	13292	49492	8.57%	1.215%
2	5.507	702	714	727	rBV	67675	204785	35.45%	5.028%
3	5.659	727	739	755	rVV	130033	370553	64.14%	9.099%
4	6.068	795	806	826	rBV	79808	217509	37.65%	5.341%
5	6.860	926	936	947	rBV2	181638	458402	79.35%	11.256%
6	8.714	1233	1240	1265	rVB	356324	577688	100.00%	14.184%
7	10.116	1464	1470	1487	rBV	358923	497356	86.09%	12.212%
8	10.360	1505	1510	1516	rBV	5037	7039	1.22%	0.173%
9	11.140	1632	1638	1653	rVB	312755	396929	68.71%	9.746%
10	11.439	1682	1687	1689	rBV	9395	14338	2.48%	0.352%
11	11.811	1743	1748	1754	rVB	29169	35348	6.12%	0.868%
12	12.079	1787	1792	1799	rBV	415731	520921	90.17%	12.791%
13	12.146	1799	1803	1807	rVB	9071	11192	1.94%	0.275%
14	12.304	1824	1829	1830	rBV	10711	13229	2.29%	0.325%
15	12.323	1830	1832	1836	rVB	9677	10964	1.90%	0.269%
16	12.371	1836	1840	1846	rVB3	11579	20518	3.55%	0.504%
17	12.475	1851	1857	1861	rBV2	9691	13064	2.26%	0.321%
18	12.591	1871	1876	1877	rBV	5729	7418	1.28%	0.182%
19	12.609	1877	1879	1885	rVV	7483	8660	1.50%	0.213%
20	12.670	1885	1889	1893	rVB	18036	20875	3.61%	0.513%
21	12.981	1935	1940	1943	rBV	6935	8673	1.50%	0.213%
22	13.018	1943	1946	1953	rVB	9684	13605	2.36%	0.334%
23	13.225	1975	1980	1984	rBV3	8043	9855	1.71%	0.242%
24	13.322	1990	1996	1998	rBV	11241	14984	2.59%	0.368%
25	13.347	1998	2000	2005	rVB2	10927	13911	2.41%	0.342%
26	13.402	2005	2009	2012	rBV	5731	7465	1.29%	0.183%
27	13.481	2017	2022	2030	rVB2	8652	14541	2.52%	0.357%
28	13.835	2075	2080	2087	rVB	244323	302280	52.33%	7.422%
29	13.902	2087	2091	2098	rVB3	4490	7372	1.28%	0.181%
30	14.097	2118	2123	2126	rBV	13993	17072	2.96%	0.419%
31	14.560	2190	2199	2206	rBV9	2081	6287	1.09%	0.154%
32	14.694	2213	2221	2232	rBV	65598	92669	16.04%	2.275%
33	14.810	2232	2240	2242	rBV	14405	18617	3.22%	0.457%
34	14.840	2242	2245	2251	rVB	29944	37960	6.57%	0.932%

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Stop Thrs : 0 Peak Location: TOP

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35	15.273	2306	2316	2322	rBV3	7614	14546	2.52%	0.357%
36	15.493	2348	2352	2357	rVB4	4781	6901	1.19%	0.169%
37	15.560	2357	2363	2367	rBV3	8343	13505	2.34%	0.332%
38	15.688	2379	2384	2388	rBV2	4236	7112	1.23%	0.175%
39	15.822	2400	2406	2413	rVB7	4503	9039	1.56%	0.222%

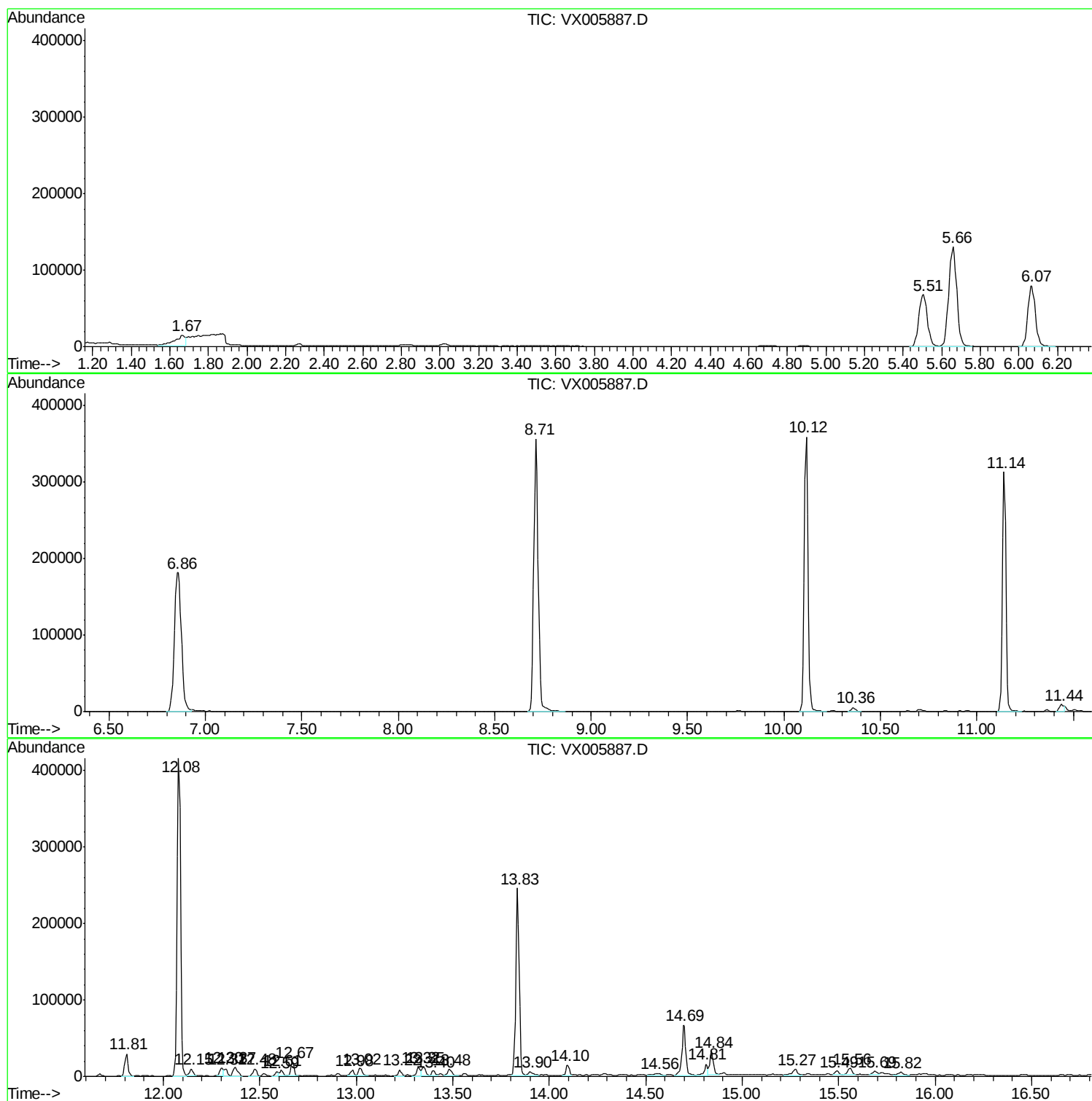
Sum of corrected areas: 4072674

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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



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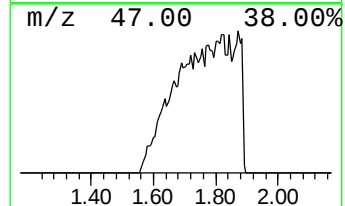
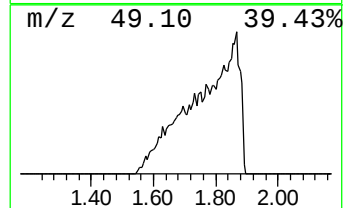
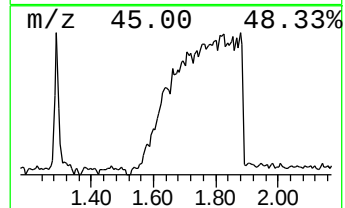
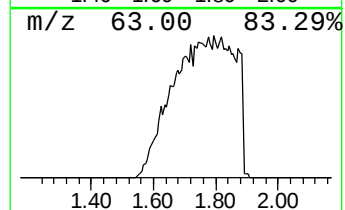
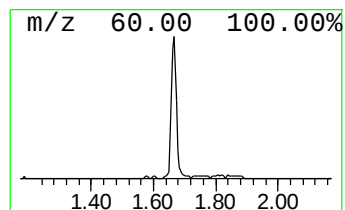
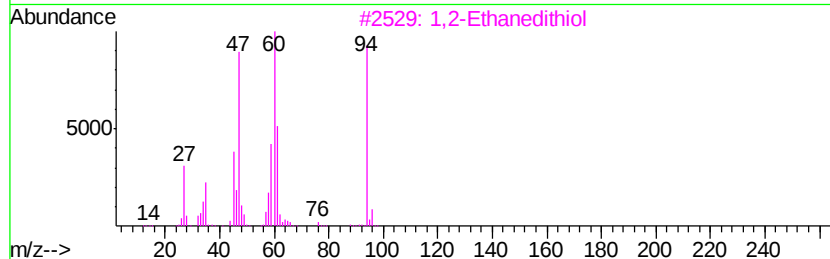
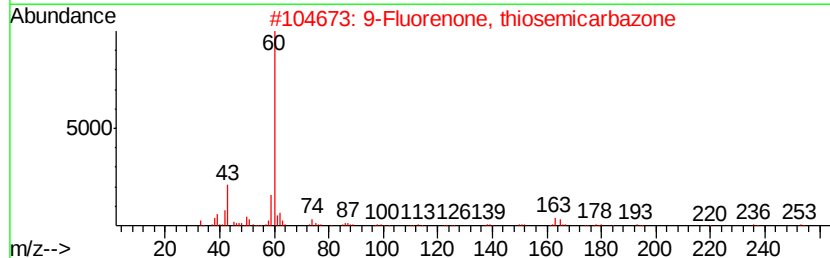
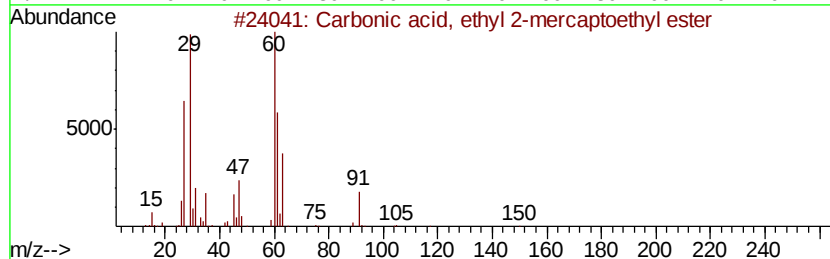
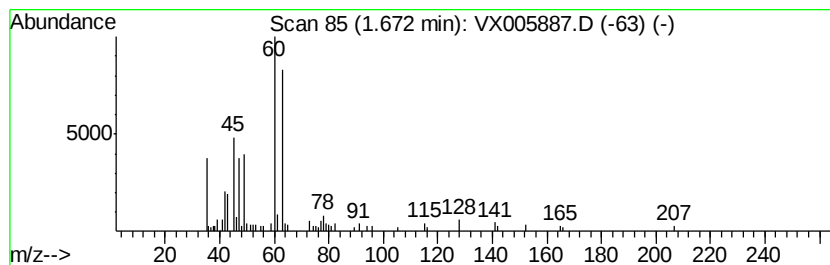
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Peak Number 1 unknown1.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	6.68 ug/l	49492	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, ethyl 2-mercaptoe...	150	C5H10O3S	005628-96-6	28
2		9-Fluorenone, thiosemicarbazone	253	C14H11N3S	1000293-93-5	9
3		1,2-Ethanedithiol	94	C2H6S2	000540-63-6	9
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9
5		Rhamnose	164	C6H12O5	003615-41-6	9



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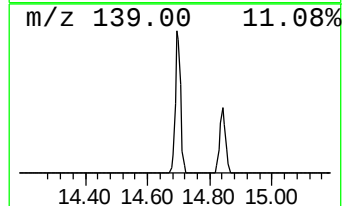
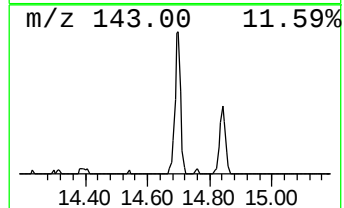
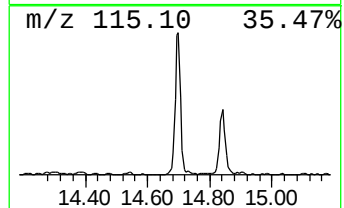
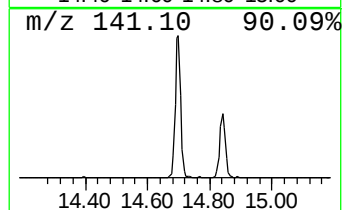
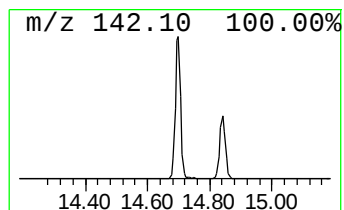
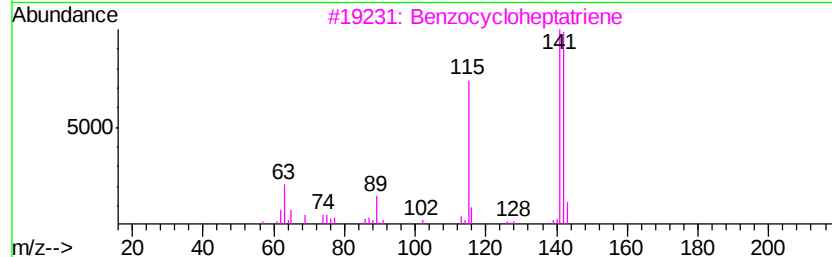
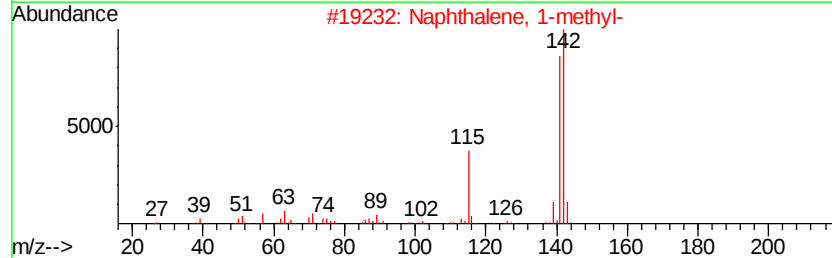
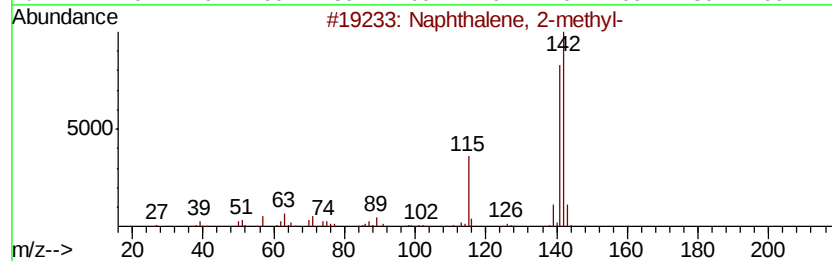
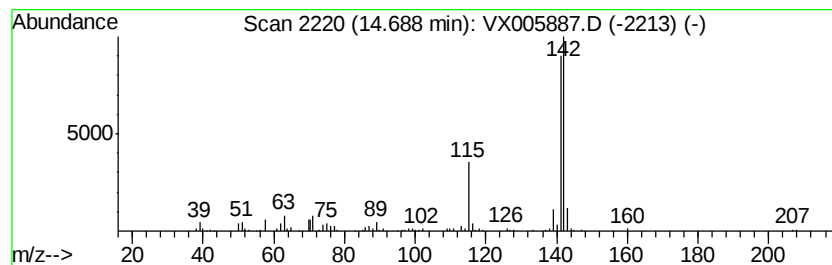
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Peak Number 2 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	8.89 ug/l	92669	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	94
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.67	1.67	6.7	ug/l	49492	1	5.66	370553	50.0
Naphthalene, 1-me...	14.69	8.9	ug/l	92669	4	12.08	520921	50.0