

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061918\
 Data File : VX002712.D
 Acq On : 19 Jun 2018 14:58
 Operator : JC/MD
 Sample : J3512-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FADW4710L

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\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	93	rBV	960585	1233552	100.00%	15.247%
2	2.453	301	306	313	rBV	7211	12824	1.04%	0.159%
3	2.623	329	334	342	rVB	11166	22607	1.83%	0.279%
4	5.172	741	752	768	rBV	58530	178241	14.45%	2.203%
5	5.507	793	807	821	rBV2	144441	410470	33.28%	5.074%
6	5.666	821	833	846	rVV	223218	619301	50.20%	7.655%
7	6.074	888	900	919	rBV	159574	415002	33.64%	5.130%
8	6.769	1005	1014	1020	rBV	8673	21881	1.77%	0.270%
9	6.867	1020	1030	1046	rVB	313050	736379	59.70%	9.102%
10	7.074	1057	1064	1074	rVB2	11927	26905	2.18%	0.333%
11	8.720	1327	1334	1343	rBV	773861	1186508	96.19%	14.666%
12	10.116	1557	1563	1577	rBV	666525	892676	72.37%	11.034%
13	11.140	1726	1731	1743	rVB	685496	843708	68.40%	10.428%
14	11.512	1788	1792	1799	rVB2	8484	16259	1.32%	0.201%
15	11.811	1837	1841	1847	rVB	11761	13959	1.13%	0.173%
16	11.994	1867	1871	1874	rBV2	11046	13742	1.11%	0.170%
17	12.079	1880	1885	1892	rVV	768208	991907	80.41%	12.260%
18	12.146	1892	1896	1901	rVB2	10590	14806	1.20%	0.183%
19	12.268	1912	1916	1919	rBV2	10828	15794	1.28%	0.195%
20	12.305	1919	1922	1930	rVV3	18582	29090	2.36%	0.360%
21	12.378	1930	1934	1945	rVB8	7645	19729	1.60%	0.244%
22	13.353	2083	2094	2100	rBV3	17789	34443	2.79%	0.426%
23	13.481	2109	2115	2124	rVB3	11604	22732	1.84%	0.281%
24	14.292	2241	2248	2253	rVB5	10904	20958	1.70%	0.259%
25	14.438	2267	2272	2277	rBV2	13947	20370	1.65%	0.252%
26	14.542	2285	2289	2293	rBV3	12290	17445	1.41%	0.216%
27	14.713	2313	2317	2322	rVV	77124	102671	8.32%	1.269%
28	14.762	2322	2325	2328	rVB	17865	20916	1.70%	0.259%
29	14.847	2336	2339	2346	rVB3	8833	12896	1.05%	0.159%
30	14.999	2359	2364	2373	rVB	51733	69093	5.60%	0.854%
31	15.688	2473	2477	2482	rBV4	6910	12646	1.03%	0.156%
32	16.170	2552	2556	2561	rVB	7287	12902	1.05%	0.159%
33	16.261	2567	2571	2577	rVB3	7006	12827	1.04%	0.159%
34	16.475	2602	2606	2613	rVB4	7835	15203	1.23%	0.188%

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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

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Title : SW846 8260

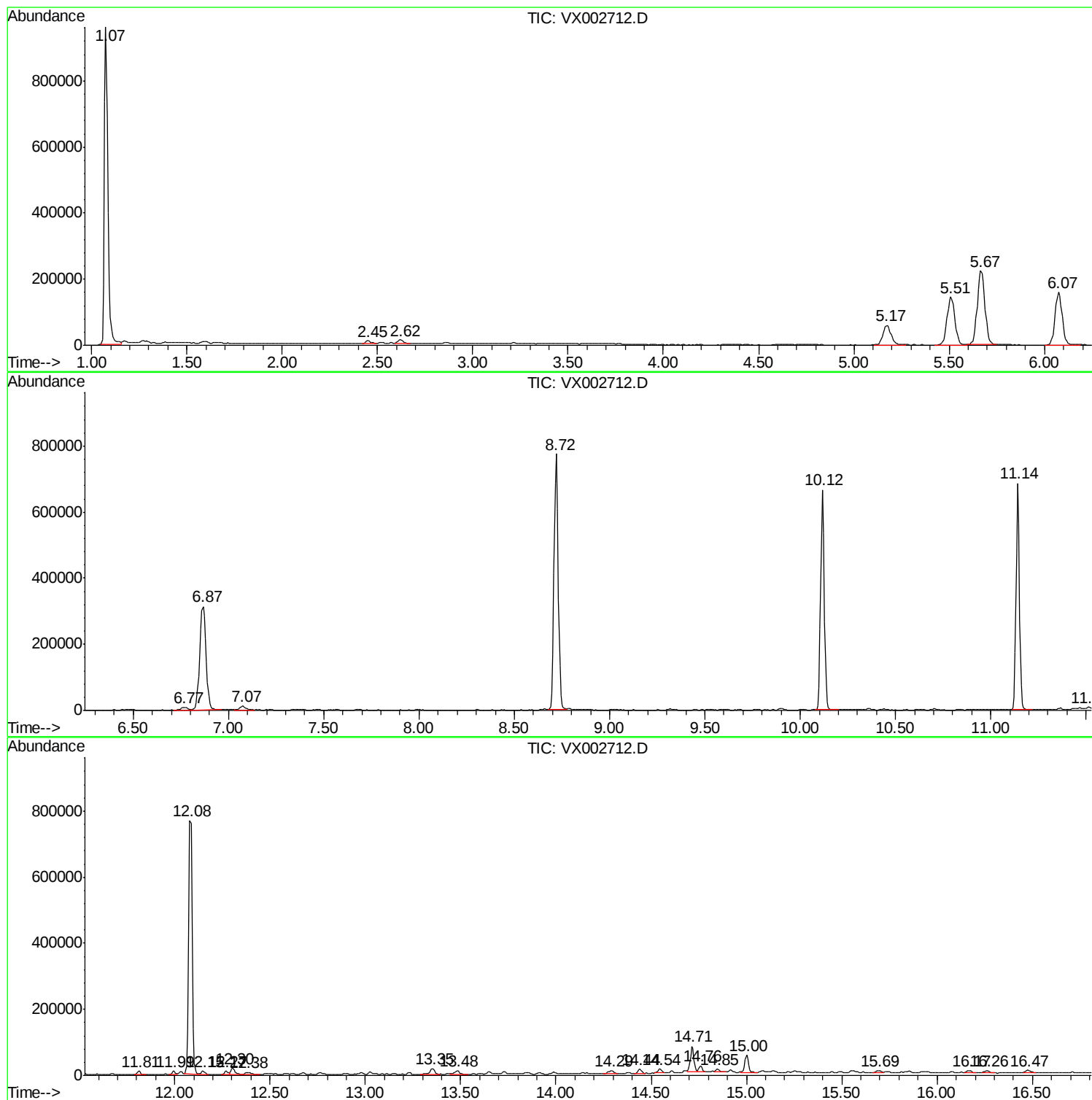
Sum of corrected areas: 8090442

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Quant Method : Z:\V0ASRV\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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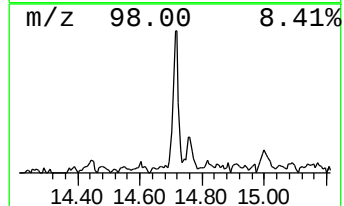
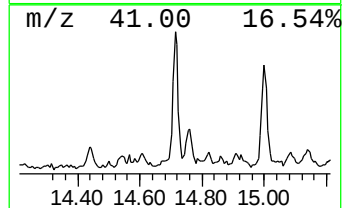
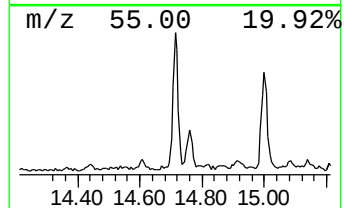
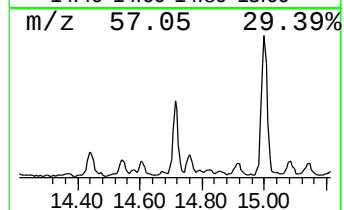
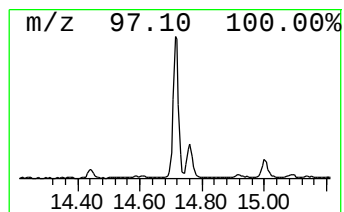
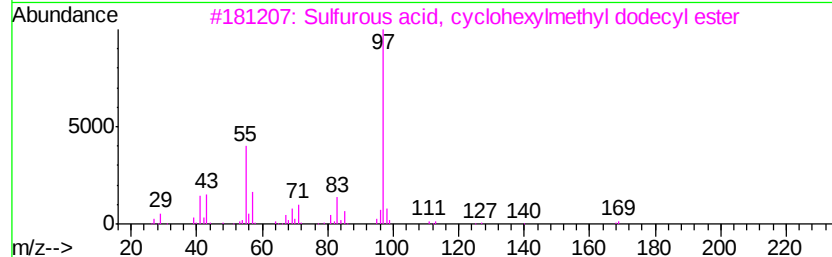
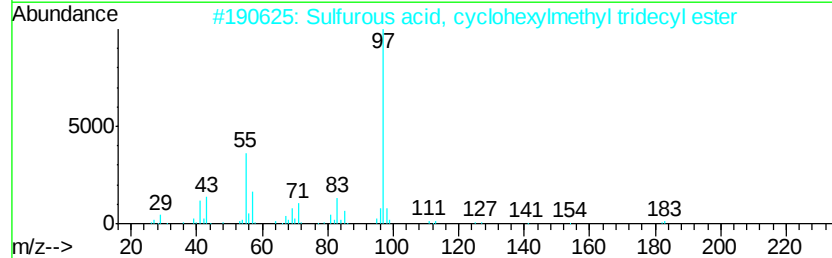
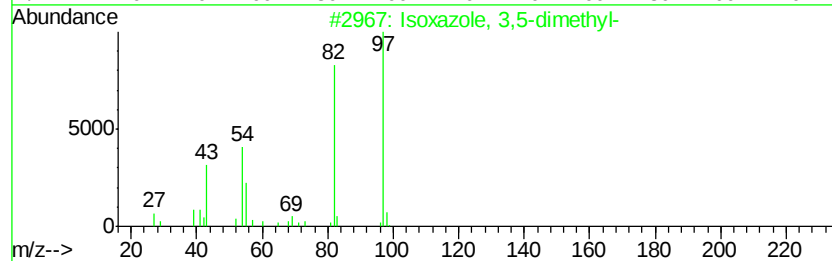
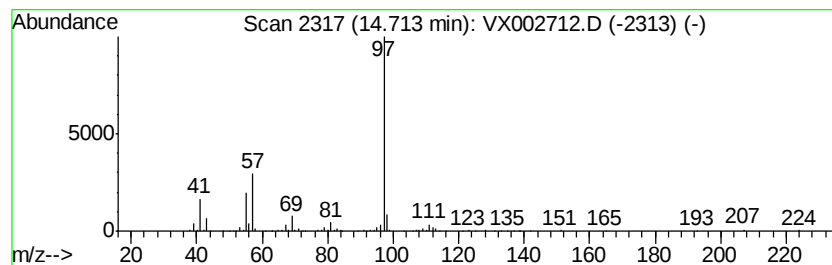
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ClientSampled :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isoxazole, 3,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.18 ug/l	102671	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Isoxazole, 3,5-dimethyl-	97 C5H7NO	000300-87-8 64
2		Sulfurous acid, cyclohexylmethyl...	360 C20H40O3S	1000309-22-1 56
3		Sulfurous acid, cyclohexylmethyl...	346 C19H38O3S	1000309-22-0 56
4		Sulfurous acid, cyclohexylmethyl...	388 C22H44O3S	1000309-22-3 56
5		Cycloheptane, bromo-	176 C7H13Br	002404-35-5 50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isoxazole, 3,5-di...	14.71	5.2	ug/l	102671	4	12.09	991907	50.0