

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112421\
 Data File : VX025338.D
 Acq On : 24 Nov 2021 19:42
 Operator : JC/MD
 Sample : M4838-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 211123015-01-VOA

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: VX025338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	25	27	37	rVB	14366	22755	1.02%	0.285%
2	2.392	207	214	234	rBV2	27630	75528	3.37%	0.946%
3	2.959	296	307	326	rBV	748702	1629979	72.75%	20.423%
4	4.580	556	573	586	rBV	706106	2240409	100.00%	28.072%
5	5.007	631	643	661	rBV	135957	422112	18.84%	5.289%
6	5.385	693	705	719	rBV	70296	206579	9.22%	2.588%
7	5.556	721	733	745	rVV	124669	356527	15.91%	4.467%
8	5.958	787	799	810	rBV2	72513	197719	8.83%	2.477%
9	6.233	836	844	854	rVB3	19008	52498	2.34%	0.658%
10	6.763	921	931	942	rBV	189424	453714	20.25%	5.685%
11	8.574	1220	1228	1234	rVB2	18446	37415	1.67%	0.469%
12	8.653	1234	1241	1248	rBV	393650	623206	27.82%	7.809%
13	10.055	1460	1471	1478	rBV	399565	549693	24.54%	6.888%
14	10.305	1507	1512	1517	rVB2	15927	25438	1.14%	0.319%
15	11.079	1634	1639	1647	rBV	311679	412162	18.40%	5.164%
16	12.024	1788	1794	1801	rVB	393781	520907	23.25%	6.527%
17	13.475	2027	2032	2035	rBV	48509	66249	2.96%	0.830%
18	13.512	2035	2038	2045	rVB2	23981	32050	1.43%	0.402%
19	13.774	2077	2081	2086	rVB2	17269	24634	1.10%	0.309%
20	13.926	2101	2106	2113	rBV3	16044	31389	1.40%	0.393%

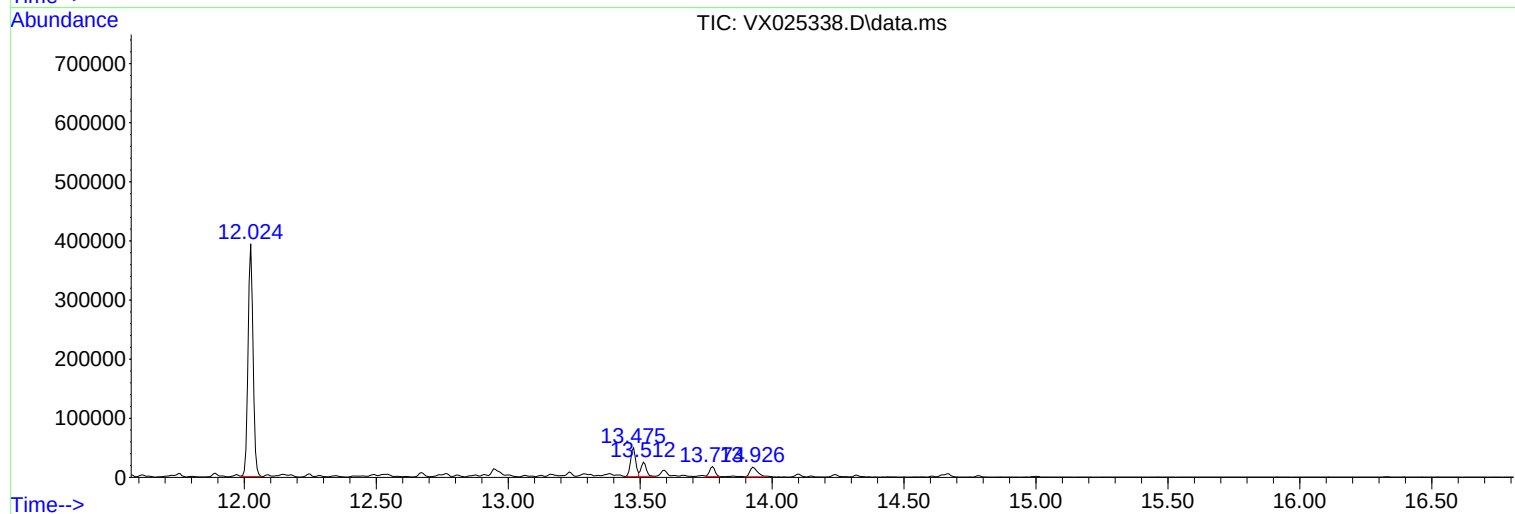
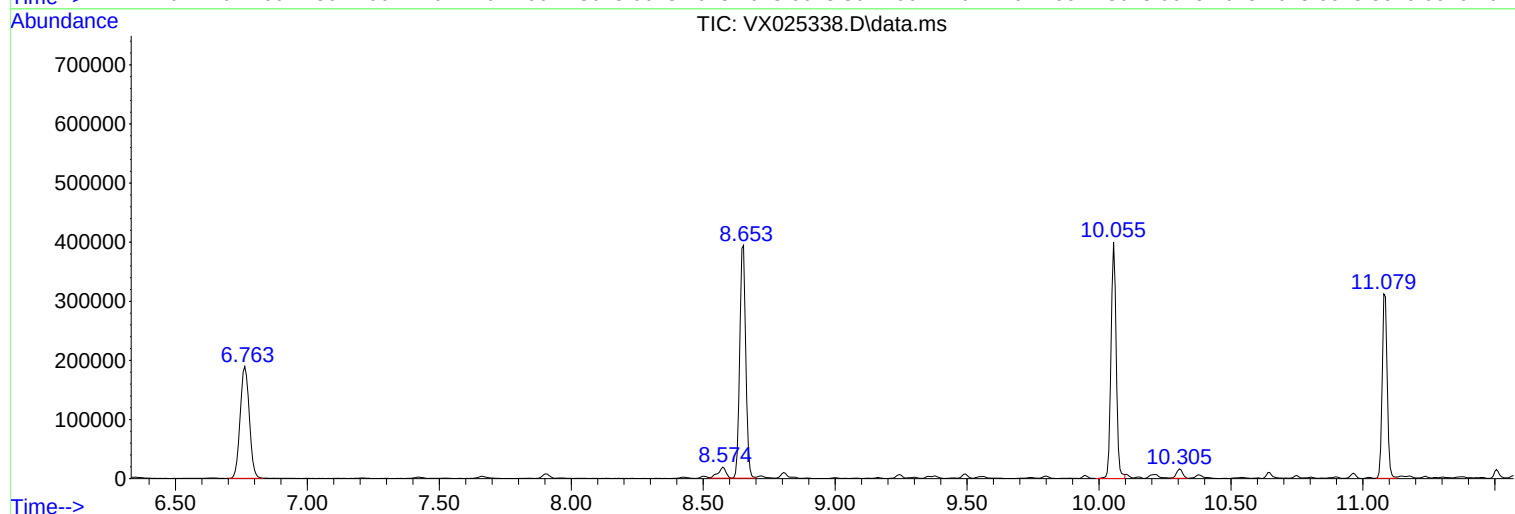
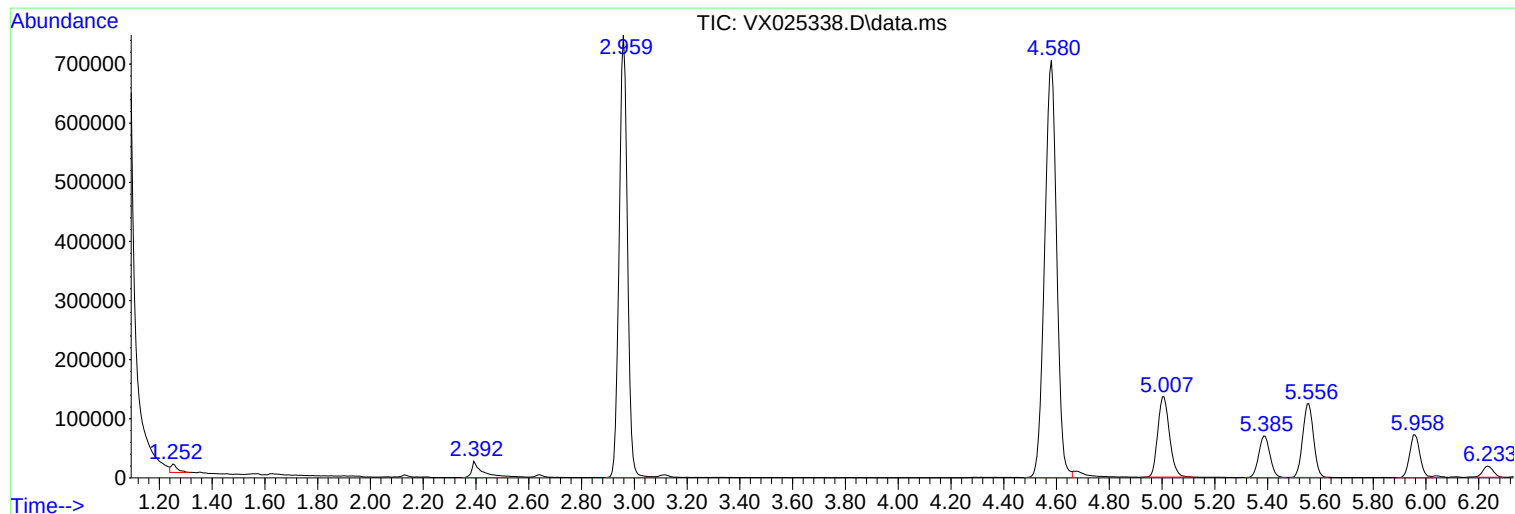
Sum of corrected areas: 7980963

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Quant Title : SW846 8260

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



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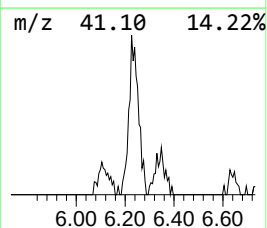
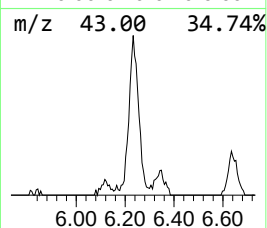
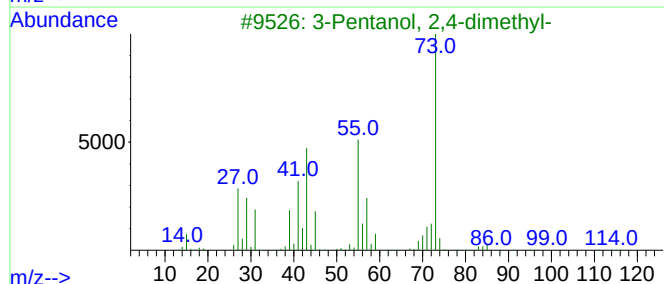
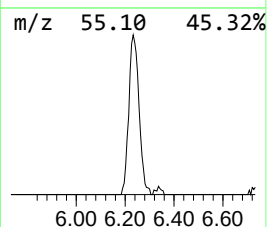
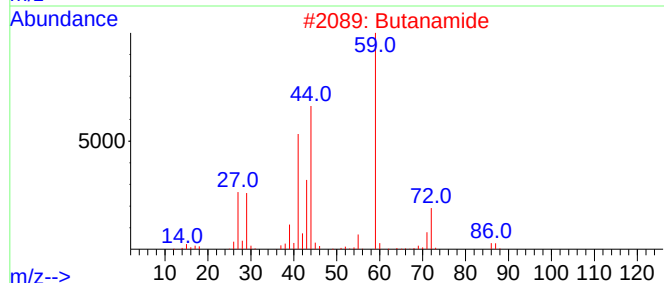
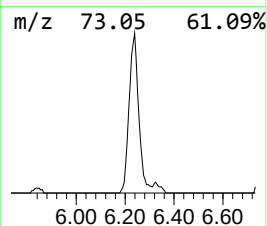
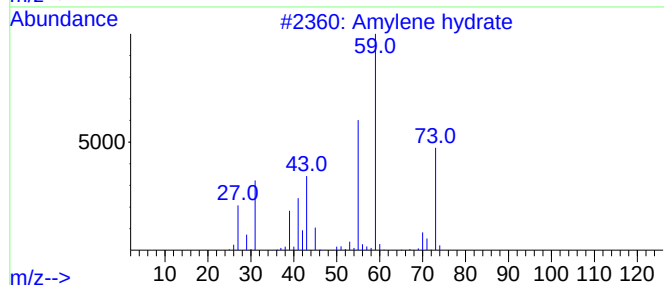
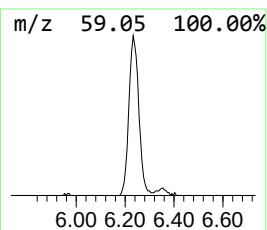
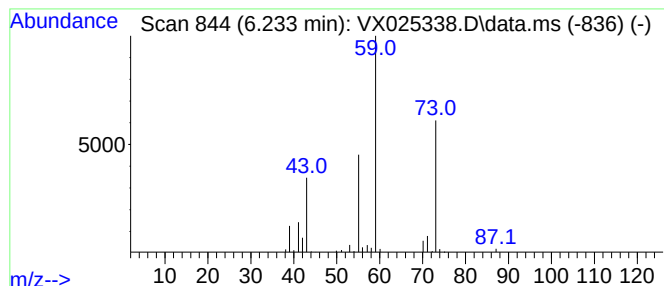
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Amylene hydrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	5.79 ug/l	52498	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			Butanamide	87	C4H9NO	000541-35-5	45
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4			Butanal, oxime	87	C4H9NO	000110-69-0	5
5			Formamide, N-formyl-N-methyl-	87	C3H5NO2	018197-25-6	5



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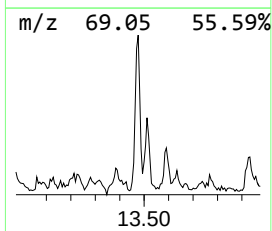
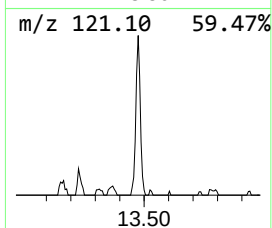
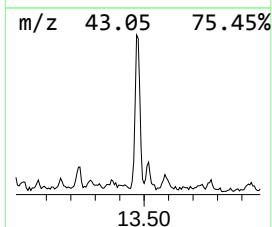
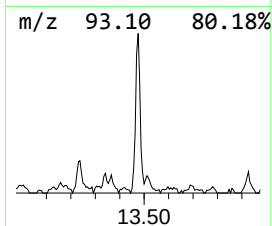
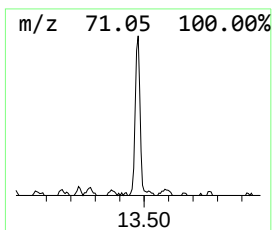
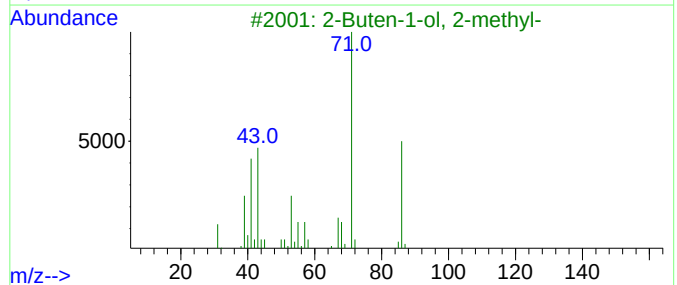
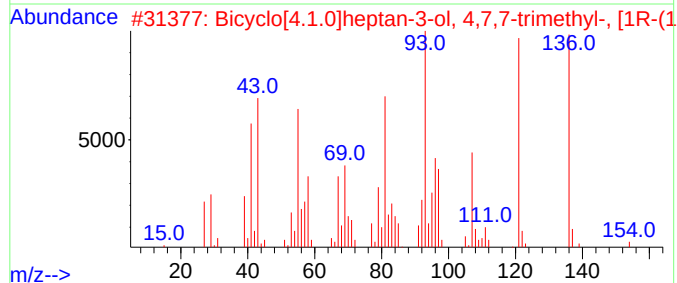
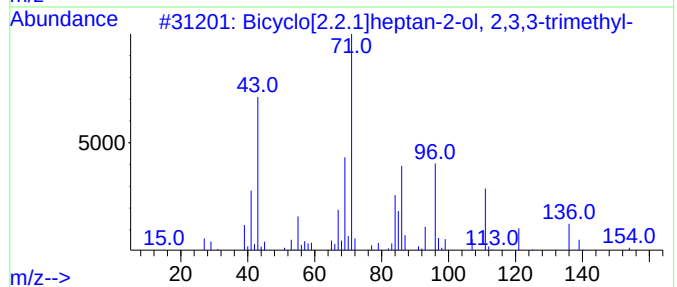
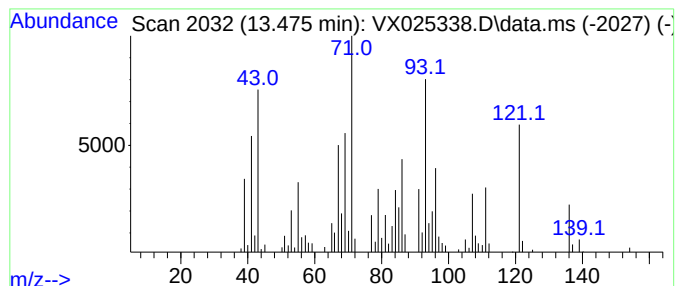
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Peak Number 3 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	6.36 ug/l	66249	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	64
2			Bicyclo[4.1.0]heptan-3-ol, 4,7,7...	154	C10H18O	004017-88-3	45
3			2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	38
4			2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	25
5			Bicyclo[4.1.0]heptane, 7-(1-meth...	136	C10H16	053282-47-6	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.233	5.8	ug/l	52498	2	6.763	453714	50.0
Bicyclo[2.2.1]h...	13.475	6.4	ug/l	66249	4	12.024	520907	50.0