

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
 Data File : VX029029.D
 Acq On : 27 May 2022 17:10
 Operator : JC/MD
 Sample : N2968-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-40

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX029029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.538	230	238	250	rBV	15487	32396	1.35%	0.230%
2	2.959	298	307	323	rVV	279305	620042	25.82%	4.396%
3	3.117	324	333	348	rVB	94065	224826	9.36%	1.594%
4	3.764	429	439	452	rBV	66981	182165	7.59%	1.292%
5	4.318	519	530	542	rBV4	25455	77735	3.24%	0.551%
6	5.391	694	706	717	rBV	207759	601057	25.03%	4.262%
7	5.556	722	733	751	rVB2	326072	936268	38.99%	6.639%
8	5.958	788	799	805	rBV	210042	553367	23.05%	3.924%
9	6.044	805	813	828	rVB	897976	2401039	100.00%	17.024%
10	6.239	834	845	855	rVB4	26397	82643	3.44%	0.586%
11	6.763	921	931	947	rBV	526250	1262177	52.57%	8.949%
12	8.427	1199	1204	1210	rBV	49985	84768	3.53%	0.601%
13	8.501	1210	1216	1226	rVB6	8167	24112	1.00%	0.171%
14	8.653	1234	1241	1248	rBV	1106752	1711163	71.27%	12.133%
15	8.720	1248	1252	1259	rVB2	17022	28929	1.20%	0.205%
16	8.958	1282	1291	1299	rBV	61636	104568	4.36%	0.741%
17	9.049	1299	1306	1312	rBV	82411	120341	5.01%	0.853%
18	9.244	1331	1338	1347	rBV	15380	25791	1.07%	0.183%
19	9.458	1365	1373	1386	rBV2	98528	175195	7.30%	1.242%
20	9.945	1448	1453	1460	rBV	31199	49954	2.08%	0.354%
21	10.055	1466	1471	1477	rBV	1170781	1545160	64.35%	10.956%
22	10.195	1490	1494	1501	rBV2	18052	36923	1.54%	0.262%
23	10.305	1505	1512	1519	rVB2	20285	33168	1.38%	0.235%
24	10.647	1564	1568	1573	rVB	29592	40658	1.69%	0.288%
25	10.964	1613	1620	1625	rBV	29084	42808	1.78%	0.304%
26	11.085	1634	1640	1651	rBV	951783	1246236	51.90%	8.836%
27	11.616	1722	1727	1734	rVB	31945	44435	1.85%	0.315%
28	11.756	1746	1750	1756	rVB	30040	37891	1.58%	0.269%
29	12.024	1788	1794	1800	rBV	1274327	1535196	63.94%	10.885%
30	12.091	1800	1805	1811	rVB	32866	44367	1.85%	0.315%
31	12.244	1823	1830	1836	rBV	62515	81880	3.41%	0.581%
32	12.701	1901	1905	1912	rVB2	33828	50030	2.08%	0.355%
33	13.292	1997	2002	2007	rVB2	27131	38068	1.59%	0.270%
34	13.683	2061	2066	2073	rVB3	14338	28162	1.17%	0.200%

Sum of corrected areas: 14103518

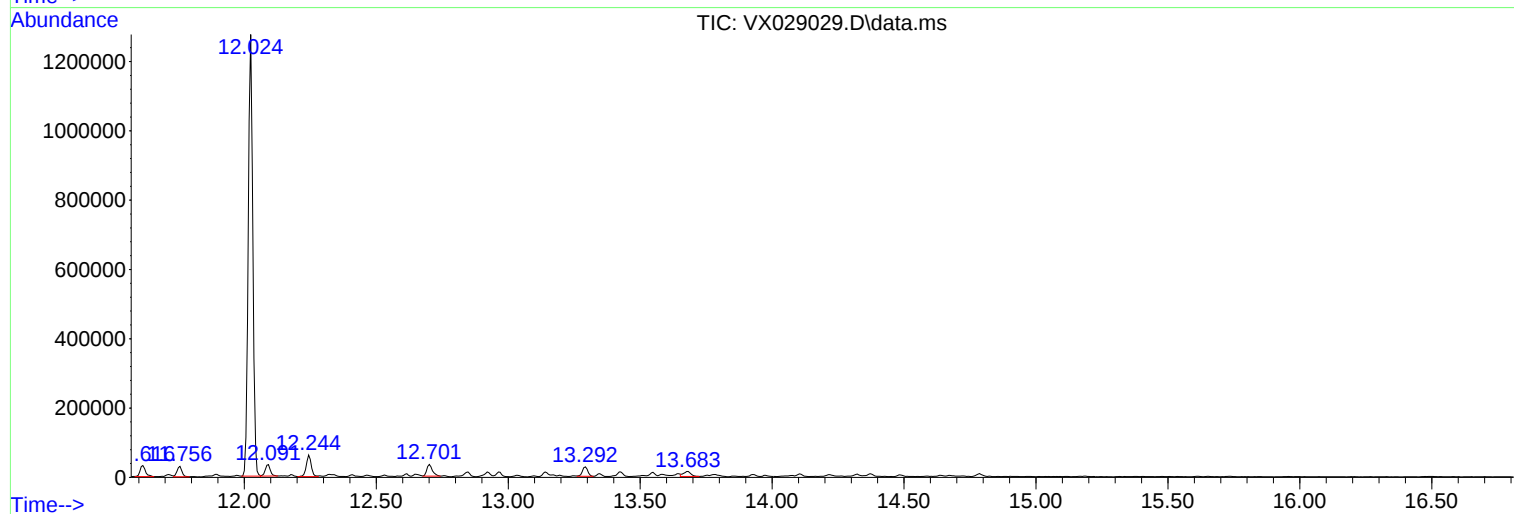
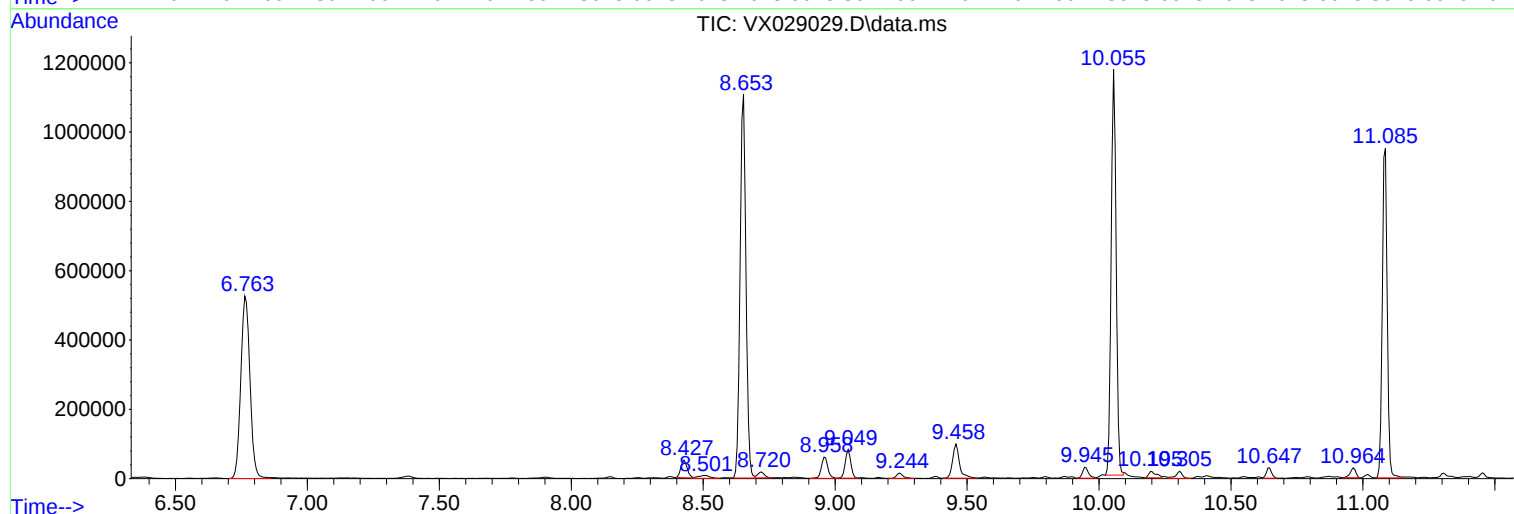
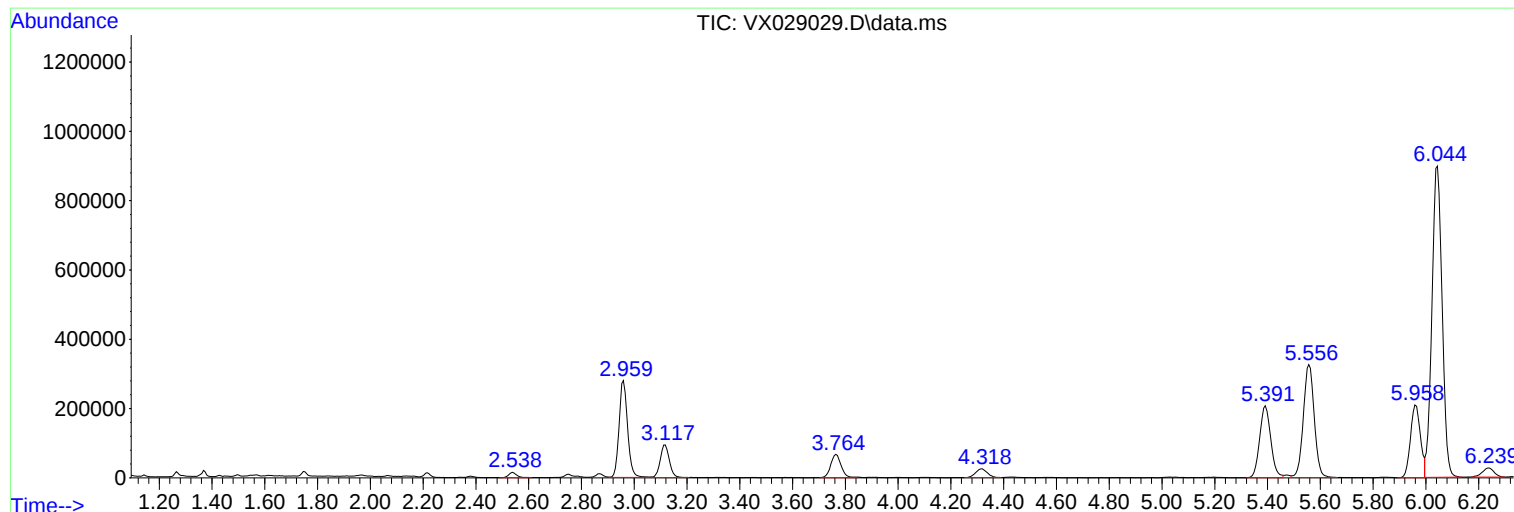
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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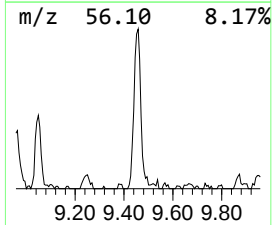
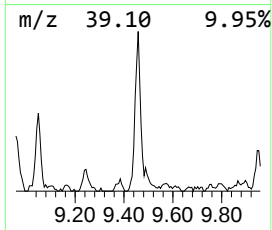
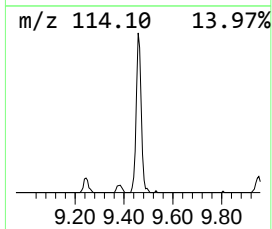
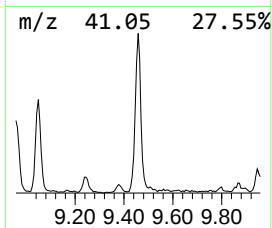
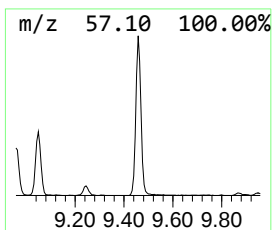
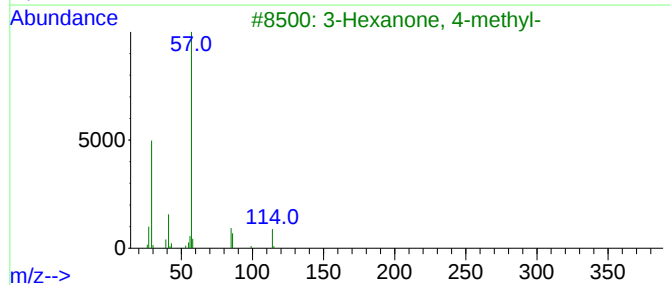
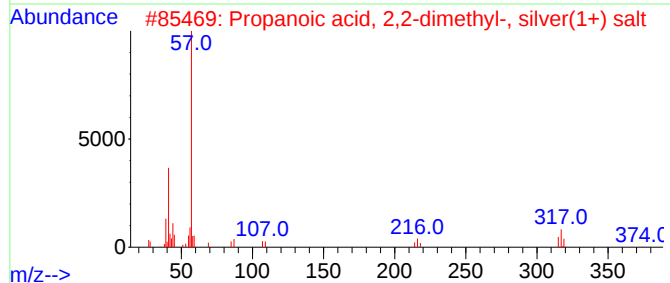
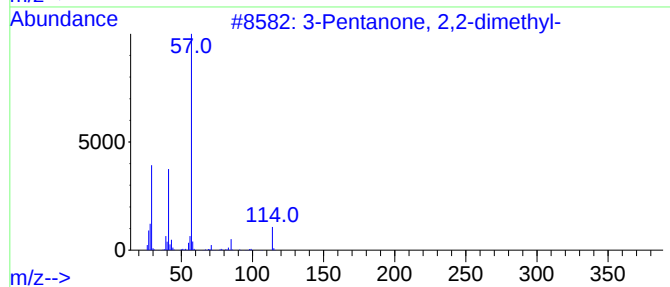
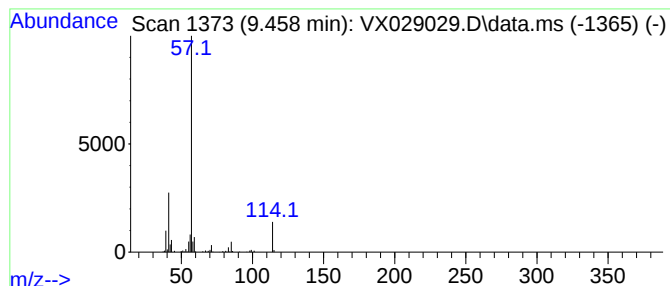
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Pentanone, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	5.67 ug/l	175195	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	80
2			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	53
3			3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	53
4			2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	53
5			3-Heptanone	114	C7H14O	000106-35-4	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone, 2,...	9.458	5.7	ug/l	175195	3	10.055	1545160	50.0