

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120321\
 Data File : VX025486.D
 Acq On : 03 Dec 2021 16:42
 Operator : JC/MD
 Sample : M4918-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	34	rBV	33262	53527	7.12%	1.273%
2	1.367	41	46	52	rVB2	6944	10031	1.33%	0.239%
3	2.215	180	185	194	rVB2	5819	9968	1.33%	0.237%
4	2.959	299	307	324	rVV	71614	154442	20.53%	3.674%
5	3.117	324	333	345	rVB	31327	72449	9.63%	1.723%
6	3.763	429	439	451	rBV2	21533	57936	7.70%	1.378%
7	4.312	519	529	541	rVB3	8299	26162	3.48%	0.622%
8	5.391	695	706	717	rBV2	61660	180139	23.95%	4.285%
9	5.556	723	733	750	rVB	100905	285789	37.99%	6.798%
10	5.958	789	799	805	rBV	65523	170709	22.69%	4.061%
11	6.043	805	813	829	rVV	283405	752261	100.00%	17.895%
12	6.232	833	844	855	rVB4	9384	27920	3.71%	0.664%
13	6.763	921	931	942	rBV	161723	382897	50.90%	9.108%
14	8.427	1199	1204	1211	rBV	18268	30636	4.07%	0.729%
15	8.653	1234	1241	1248	rBV	327965	519897	69.11%	12.367%
16	8.720	1248	1252	1259	rVB3	5510	9606	1.28%	0.229%
17	8.958	1285	1291	1299	rVB	21766	33709	4.48%	0.802%
18	9.049	1299	1306	1312	rBV	26390	40944	5.44%	0.974%
19	9.244	1332	1338	1345	rBV	5888	8847	1.18%	0.210%
20	9.457	1364	1373	1386	rVV	43109	71356	9.49%	1.697%
21	9.945	1448	1453	1460	rBV	9957	14979	1.99%	0.356%
22	10.055	1465	1471	1485	rVB	336925	462805	61.52%	11.009%
23	10.646	1564	1568	1573	rVB	6706	8856	1.18%	0.211%
24	10.963	1614	1620	1624	rBV	7530	10699	1.42%	0.255%
25	11.085	1634	1640	1651	rBV	266577	346186	46.02%	8.235%
26	11.756	1746	1750	1755	rVB	6340	8225	1.09%	0.196%
27	12.024	1789	1794	1800	rBV	337598	415925	55.29%	9.894%
28	12.091	1800	1805	1809	rVB	6597	8376	1.11%	0.199%
29	12.244	1823	1830	1835	rBV	12800	16788	2.23%	0.399%
30	12.701	1901	1905	1913	rVB2	8895	11687	1.55%	0.278%

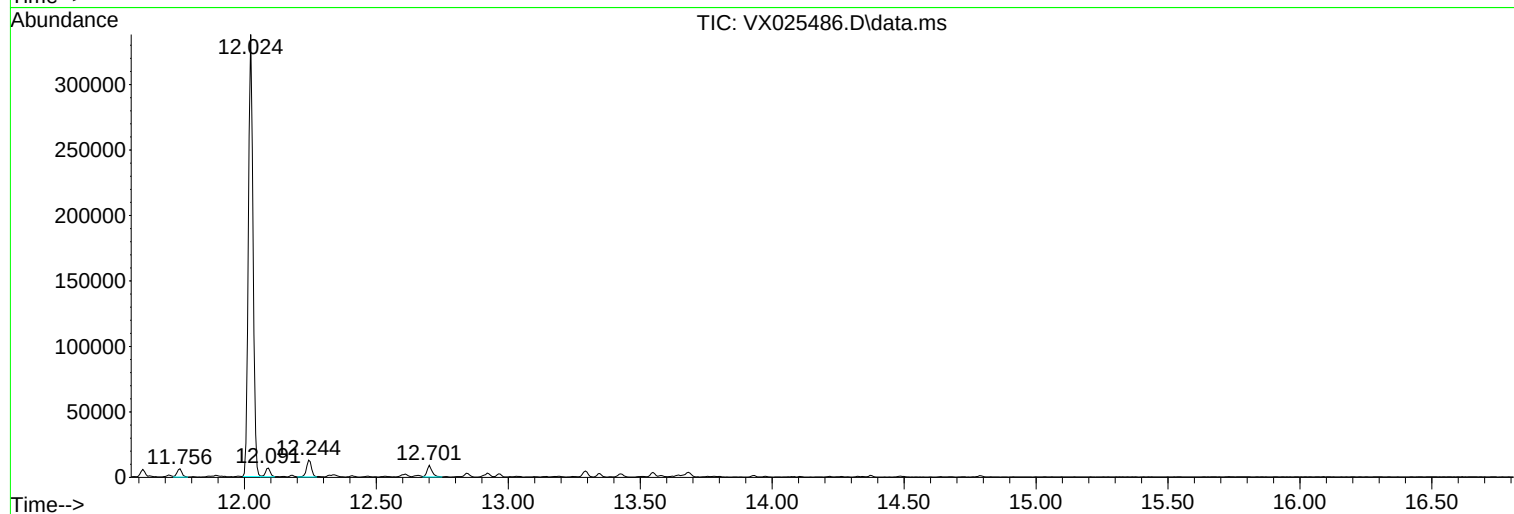
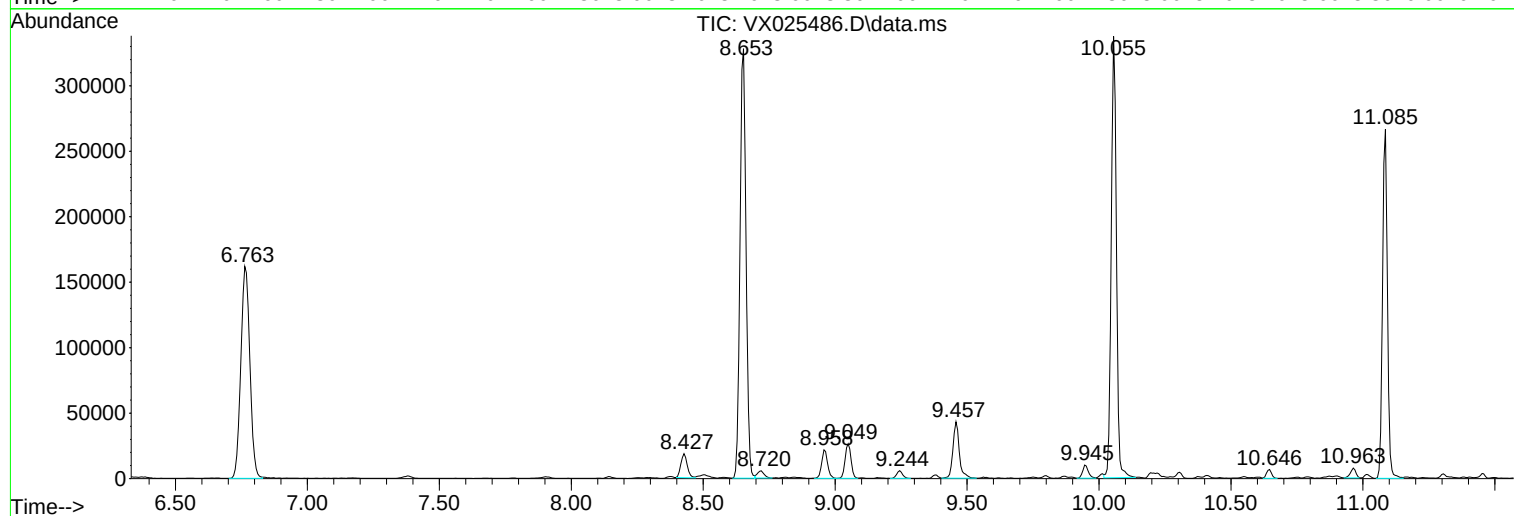
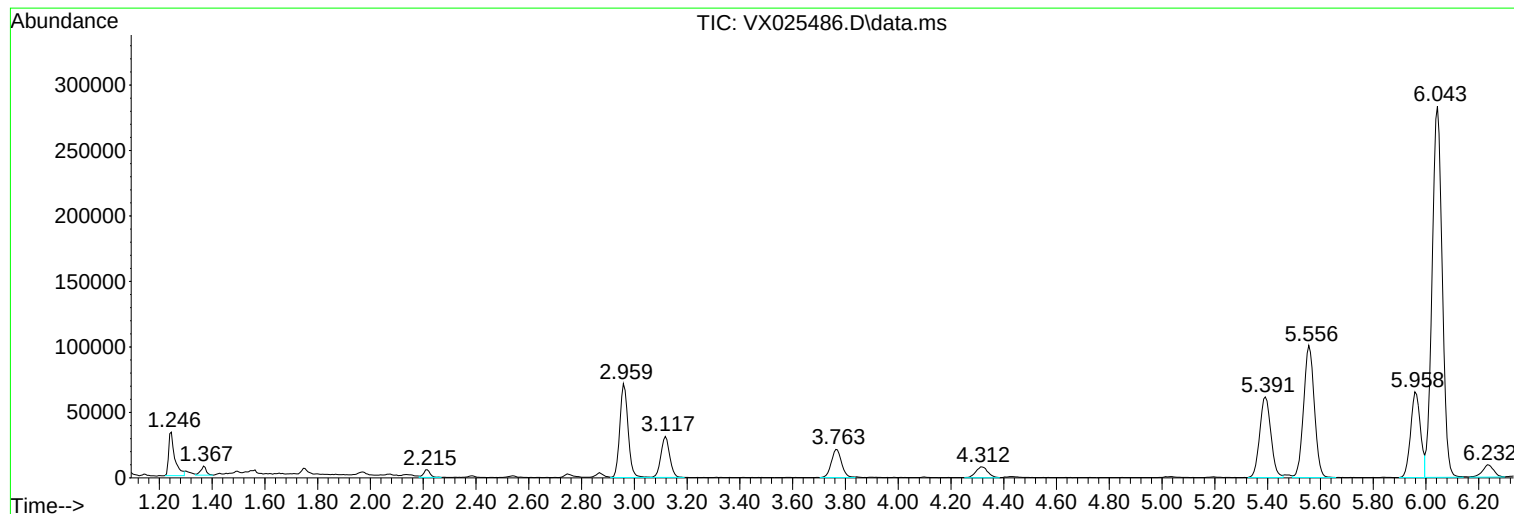
Sum of corrected areas: 4203751

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

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



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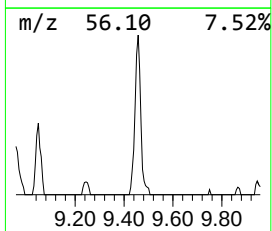
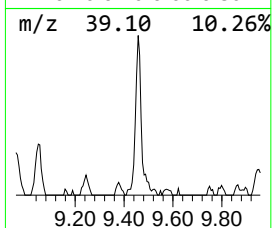
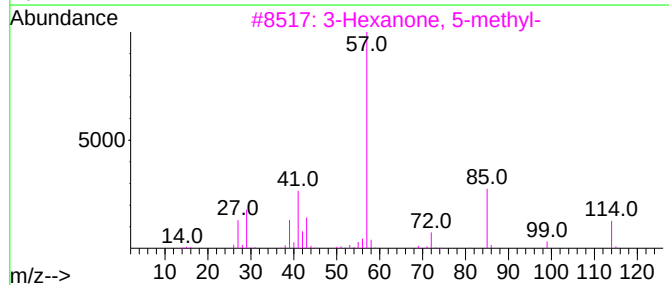
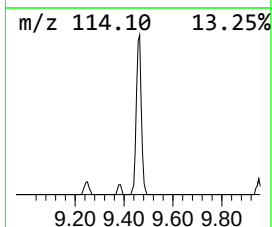
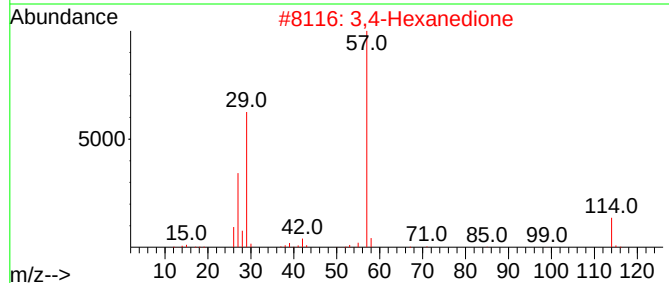
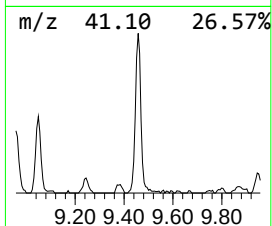
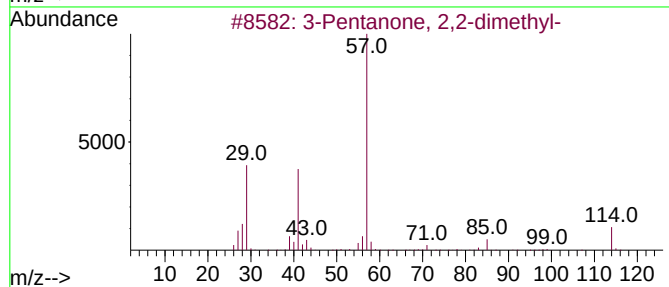
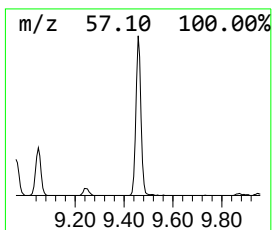
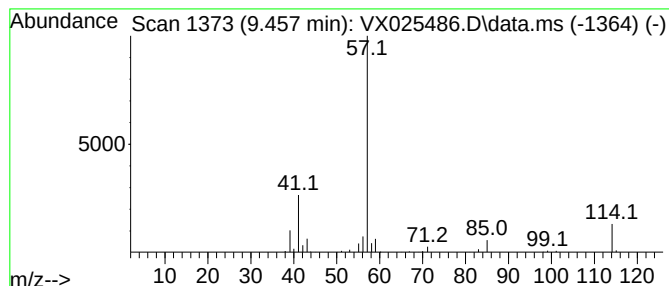
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	7.71 ug/l	71356	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	3,4-Hexanedione			114	C6H10O2	004437-51-8	58
3	3-Hexanone, 5-methyl-			114	C7H14O	000623-56-3	53
4	3-Hexanone, 4-methyl-			114	C7H14O	017042-16-9	53
5	3-Heptanone			114	C7H14O	000106-35-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone, 2,...	9.457	7.7	ug/l	71356	3	10.055	462805	50.0