

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\
 Data File : VX018827.D
 Acq On : 07 Oct 2020 21:56
 Operator : JC/SP
 Sample : L4286-01
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AR3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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\SOMXTR100220WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	9	12	21	rVB	71662	61477	11.02%	1.283%
2	1.282	27	32	35	rBV2	14233	14165	2.54%	0.296%
3	1.312	35	37	41	rVV2	6395	6095	1.09%	0.127%
4	1.392	45	50	57	rBV	75273	86980	15.60%	1.815%
5	1.696	96	100	107	rVB	47852	56408	10.12%	1.177%
6	1.776	110	113	117	rBV3	8649	12965	2.32%	0.270%
7	1.983	144	147	151	rVB2	8338	10685	1.92%	0.223%
8	2.343	199	206	213	rBV	98794	156293	28.03%	3.261%
9	2.446	216	223	235	rVB2	11811	36210	6.49%	0.755%
10	2.641	249	255	256	rBV4	3705	5659	1.01%	0.118%
11	2.867	289	292	298	rVB6	4063	7548	1.35%	0.157%
12	3.160	331	340	351	rBV	47857	116366	20.87%	2.428%
13	3.501	389	396	404	rVB3	11988	27847	4.99%	0.581%
14	4.543	553	567	580	rBV	63056	227952	40.88%	4.755%
15	5.141	652	665	679	rBV2	74831	231872	41.58%	4.837%
16	6.043	799	813	825	rBV2	168975	500574	89.76%	10.443%
17	6.830	933	942	957	rBV2	143600	350973	62.94%	7.322%
18	7.165	992	997	1001	rBV6	4337	5877	1.05%	0.123%
19	7.366	1015	1030	1044	rBV	109521	250158	44.86%	5.219%
20	7.653	1070	1077	1085	rVB4	15430	32918	5.90%	0.687%
21	8.372	1189	1195	1203	rBV2	64238	108964	19.54%	2.273%
22	8.463	1203	1210	1215	rVV2	2255	5620	1.01%	0.117%
23	8.531	1215	1221	1227	rVB4	5712	9770	1.75%	0.204%
24	8.695	1242	1248	1255	rBV	247715	382792	68.64%	7.986%
25	8.762	1256	1259	1267	rVB2	7866	13021	2.33%	0.272%
26	8.994	1292	1297	1304	rVB	46467	71455	12.81%	1.491%
27	9.427	1362	1368	1382	rBV	400349	557660	100.00%	11.634%
28	9.975	1453	1458	1466	rVB2	13482	20736	3.72%	0.433%
29	10.097	1471	1478	1484	rBV	308016	418455	75.04%	8.730%
30	10.335	1513	1517	1522	rBV4	4974	8122	1.46%	0.169%
31	10.664	1564	1571	1578	rBV2	16281	27611	4.95%	0.576%
32	11.231	1658	1664	1671	rVB	121735	158464	28.42%	3.306%
33	11.841	1760	1764	1769	rVB7	3541	5621	1.01%	0.117%
34	12.060	1795	1800	1807	rBV	308231	385742	69.17%	8.047%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMXTR100220WMA.M
Title : TRACE VOA SOM01.0

35	12.256	1828	1832	1839	rbV5	8410	15092	2.71%	0.315%
36	12.359	1843	1849	1855	rbV	288450	375257	67.29%	7.828%
37	12.896	1933	1937	1941	rbV4	8553	12125	2.17%	0.253%
38	13.731	2070	2074	2080	rbV7	3823	7635	1.37%	0.159%
39	13.895	2097	2101	2107	rbV7	4326	10332	1.85%	0.216%

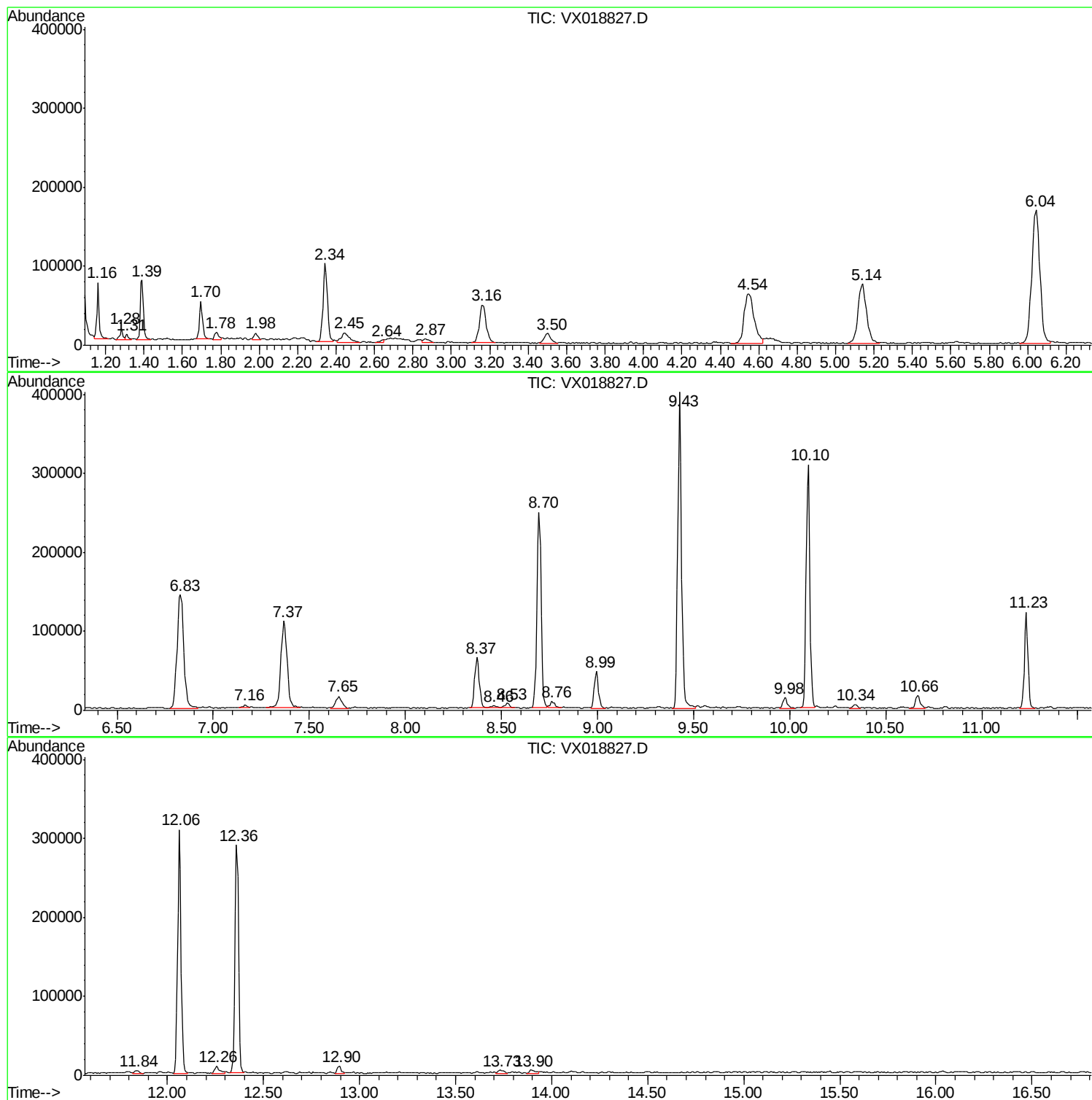
Sum of corrected areas: 4793496

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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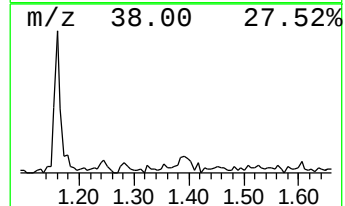
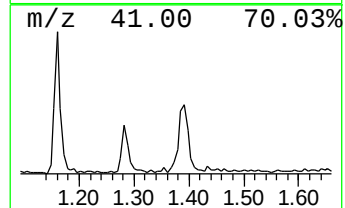
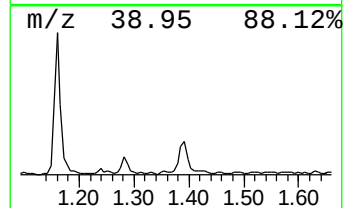
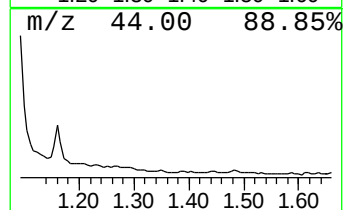
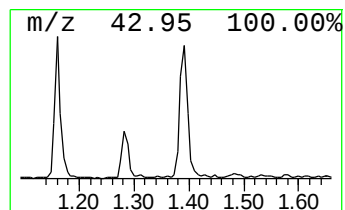
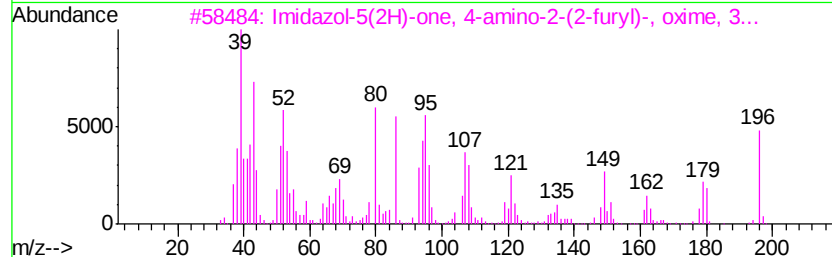
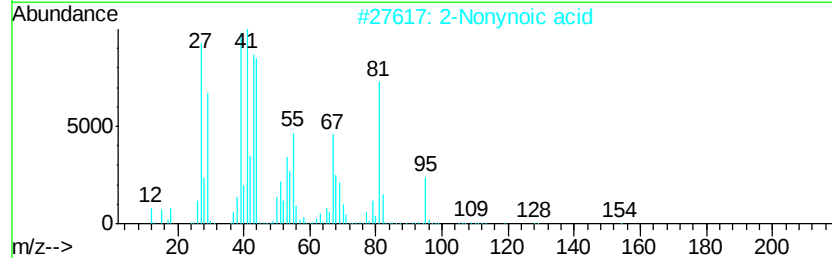
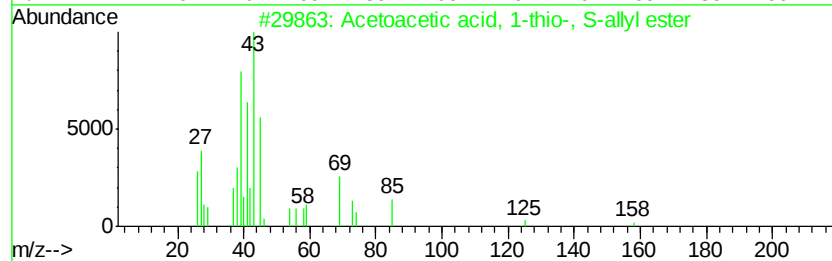
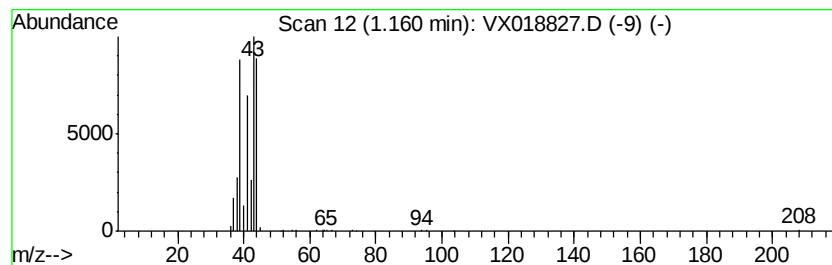
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetoacetic acid, 1-thio-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.16	0.88 ug/L	61477	1,4-Difluorobenzene	6.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	64
2		2-Nonynoic acid	154	C9H14O2	001846-70-4	59
3		Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	50
4		2-Butenal, (E)-	70	C4H6O	000123-73-9	39
5		1-Propyne, 3-bromo-	118	C3H3Br	000106-96-7	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetoacetic acid,...	1.16	0.9	ug/L	61477	1	6.83	350973	5.0