

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV090419\
 Data File : VV012577.D
 Acq On : 04 Sep 2019 19:44
 Operator : SY/MD
 Sample : K4685-12
 Misc : 25mL/MSVOA V/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFD81

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_V\METHOD\SOMVTR090219WMA.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	1.229	38	43	49	rVB3	9809	10093	1.97%	0.284%
2	1.319	63	71	81	rBV	59748	67858	13.28%	1.909%
3	1.476	109	120	129	rBV2	29455	48434	9.48%	1.362%
4	1.579	146	152	161	rVB	58900	67188	13.15%	1.890%
5	2.132	315	324	335	rBV	110369	155347	30.39%	4.370%
6	2.187	336	341	353	rVB5	12557	21054	4.12%	0.592%
7	2.306	370	378	388	rBV	16953	28885	5.65%	0.812%
8	3.936	869	885	915	rBV3	75363	237240	46.42%	6.673%
9	4.402	1016	1030	1053	rVB	58237	151262	29.60%	4.255%
10	5.093	1230	1245	1265	rBV4	136135	339343	66.39%	9.545%
11	5.663	1409	1422	1437	rBV	100194	203445	39.81%	5.723%
12	5.949	1504	1511	1522	rBV	6903	14396	2.82%	0.405%
13	6.119	1548	1564	1579	rBV3	84255	177140	34.66%	4.983%
14	7.029	1838	1847	1861	rVB2	34215	62701	12.27%	1.764%
15	7.360	1937	1950	1966	rBV2	121864	223331	43.70%	6.282%
16	7.663	2031	2044	2053	rBV3	23668	43473	8.51%	1.223%
17	8.016	2136	2154	2175	rBV	253570	444413	86.95%	12.500%
18	8.132	2175	2190	2221	rBV2	215390	511098	100.00%	14.376%
19	8.894	2416	2427	2451	rBV	157059	265278	51.90%	7.462%
20	10.260	2841	2852	2866	rBV	74526	119349	23.35%	3.357%
21	11.293	3162	3173	3192	rBV	98541	176561	34.55%	4.966%
22	11.669	3279	3290	3310	rBV	104706	187286	36.64%	5.268%

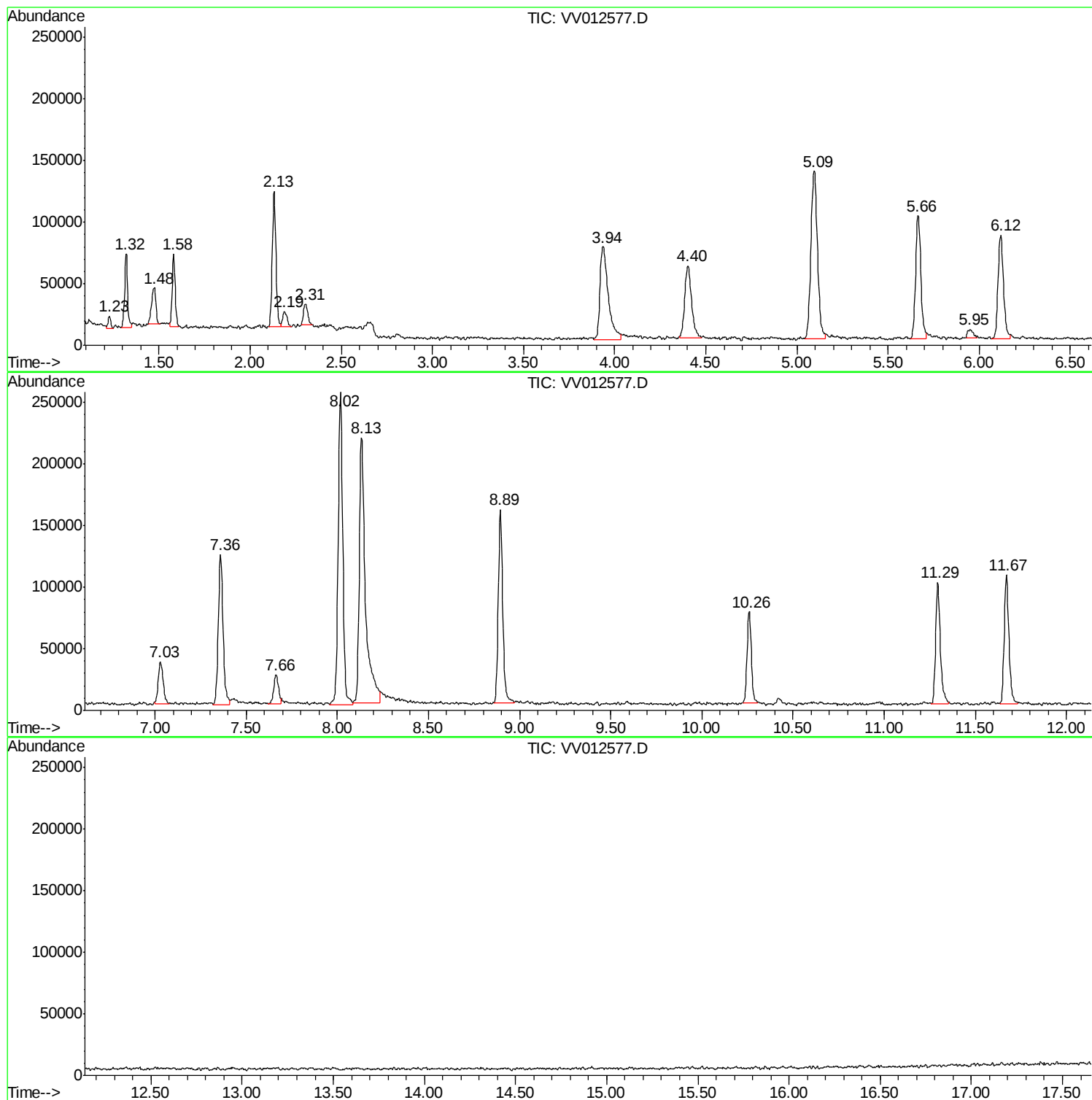
Sum of corrected areas: 3555175

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR090219WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	1.19 ug/L	48434	1,4-Difluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-[Tri-t-butoxysilyl]-2-mercapto...	323	C14H33N03SSi	1000252-63-8	12	
2	Acetic acid, hydroxy[(1-oxo-2-pr...	145	C5H7N04	006737-24-2	10	
3	Acetamide, 2-fluoro-	77	C2H4FNO	000640-19-7	10	
4	Methylpent-4-enylamine	99	C6H13N	005831-72-1	10	
5	2-Pentanamine	87	C5H13N	063493-28-7	9	

Peak Number 2 (2R,4R)-(-)-Pentanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	0.71 ug/L	28885	1,4-Difluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	50	
2	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	45	
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	45	
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39	
5	2,4-Pentanediol	104	C5H12O2	000625-69-4	39	

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.48	1.2	ug/L	48434	1	5.67	203445	5.0
(2R,4R)-(-)-Penta...	2.31	0.7	ug/L	28885	1	5.67	203445	5.0