

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX042518\
 Data File : VX001117.D
 Acq On : 25 Apr 2018 13:50
 Operator : JC/MD
 Sample : J2495-03ME
 Misc : 5.22g/5mL/100uL/5mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RS-RO-1-7-BME

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.069	75	79	93	rBV	435047	518093	7.36%	3.734%
2	5.513	796	808	820	rBV	127160	364907	5.19%	2.630%
3	5.665	822	833	847	rBV	207153	590423	8.39%	4.255%
4	6.074	887	900	917	rBV	149394	390247	5.55%	2.812%
5	6.866	1017	1030	1047	rBV	288997	711155	10.11%	5.125%
6	8.720	1326	1334	1350	rBV	715320	1139182	16.19%	8.209%
7	10.122	1557	1564	1577	rBV	570915	835471	11.87%	6.021%
8	11.146	1726	1732	1744	rBV	643263	823019	11.70%	5.931%
9	12.085	1880	1886	1897	rVB	789001	948294	13.48%	6.834%
10	15.499	2442	2446	2451	rVB	51630	72662	1.03%	0.524%
11	15.828	2497	2500	2504	rVB3	58288	85366	1.21%	0.615%
12	15.962	2517	2522	2533	rVB2	200527	361165	5.13%	2.603%
13	16.188	2552	2559	2572	rVB	4249536	7036872	100.00%	50.709%

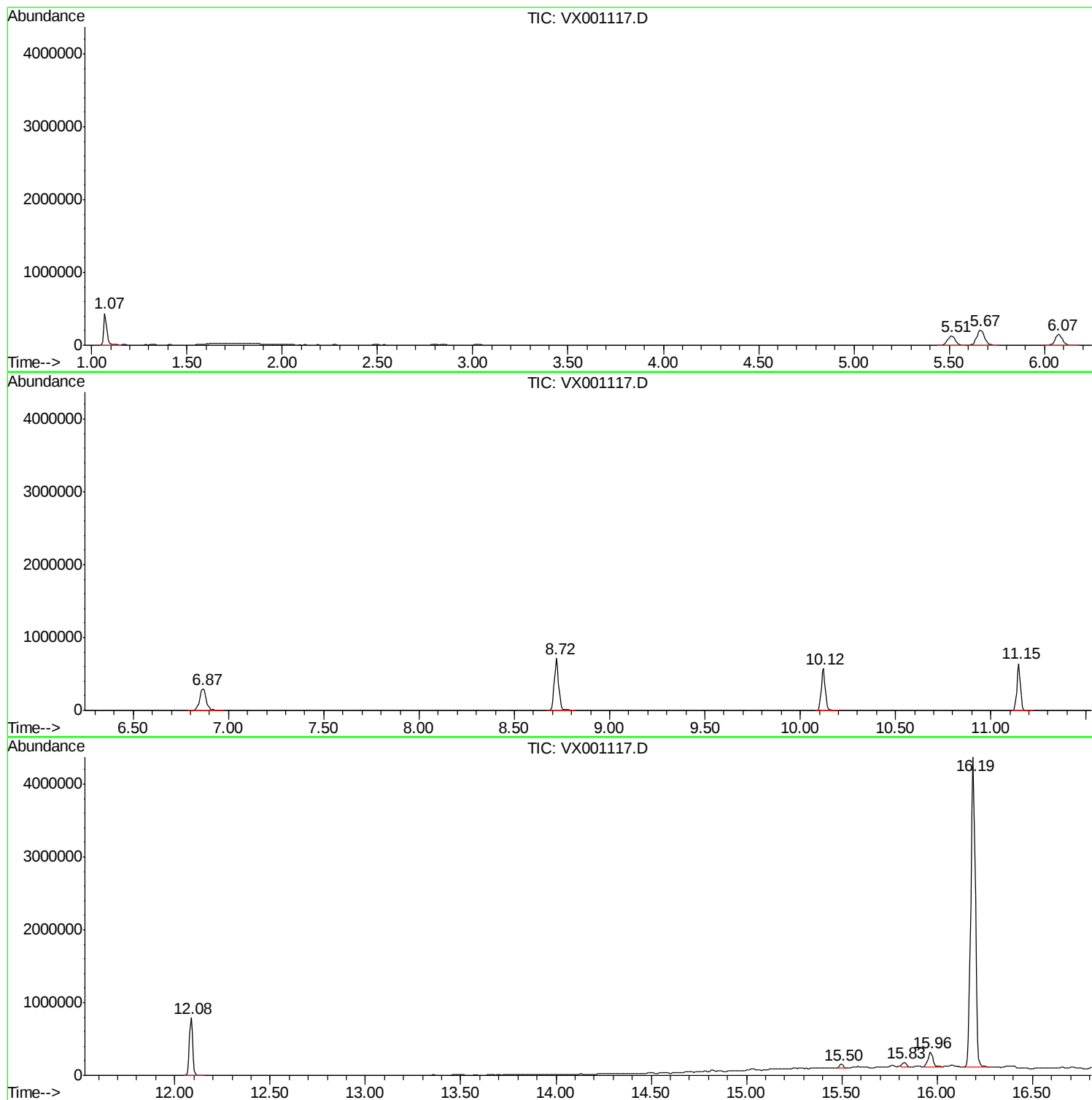
Sum of corrected areas: 13876856

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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

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



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 Peak Number 1 unknown15.96 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	19.04 ug/l	361165	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Neoisolongifolene	204	C15H24	1000156-12-4	42
2		Epizonarene	204	C15H24	041702-63-0	42
3		Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	41
4		4(3H)-Quinazolinone, 7-amino-3-e...	189	C10H11N3O	1000338-19-9	38
5		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	38

 Peak Number 2 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	371.03 ug/l	7036870	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2		Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	83
3		Phenol, 4,6-di(1,1-dimethylethyl)-	220	C15H24O	000616-55-7	81
4		Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	72
5		4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	64

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown15.96	15.96	19.0	ug/l	361165	4	12.08	948294	50.0
Butylated Hydroxy...	16.19	371.0	ug/l	7036870	4	12.08	948294	50.0