

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061418\
 Data File : VU024576.D
 Acq On : 15 Jun 2018 05:59
 Operator : MD/SY
 Sample : J3478-13
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 SS050MW612-180612

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_U\METHOD\82U061318W.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	1.089	138	155	176	rBV	1577399	1778921	100.00%	20.031%
2	1.407	249	254	261	rBV	18727	19942	1.12%	0.225%
3	2.323	532	539	550	rVB	12592	19700	1.11%	0.222%
4	2.841	687	700	712	rVB	10115	21751	1.22%	0.245%
5	4.198	1103	1122	1140	rBV	33921	111150	6.25%	1.252%
6	4.889	1321	1337	1354	rBV	178324	405995	22.82%	4.572%
7	4.989	1354	1368	1390	rVB	229023	509109	28.62%	5.733%
8	5.317	1453	1470	1491	rBV	171690	372134	20.92%	4.190%
9	5.892	1635	1649	1670	rBV	352559	696458	39.15%	7.842%
10	6.423	1801	1814	1837	rBV2	98741	198603	11.16%	2.236%
11	7.571	2156	2171	2191	rBV	647668	1162602	65.35%	13.091%
12	8.368	2408	2419	2439	rBV	57383	101606	5.71%	1.144%
13	8.468	2439	2450	2467	rVV2	57258	99651	5.60%	1.122%
14	9.095	2630	2645	2669	rBV	499983	865172	48.63%	9.742%
15	9.696	2823	2832	2848	rBV3	11653	25524	1.43%	0.287%
16	9.921	2891	2902	2926	rBV	208180	342462	19.25%	3.856%
17	10.059	2931	2945	2962	rVB3	8038	22075	1.24%	0.249%
18	10.310	3011	3023	3047	rBV	519857	851573	47.87%	9.589%
19	11.159	3281	3287	3299	rVB3	11515	17974	1.01%	0.202%
20	11.262	3310	3319	3340	rBV2	36256	66633	3.75%	0.750%
21	11.487	3376	3389	3407	rBV	661252	1047941	58.91%	11.800%
22	11.638	3427	3436	3447	rBV4	15641	27365	1.54%	0.308%
23	12.461	3683	3692	3710	rVB	78326	116575	6.55%	1.313%

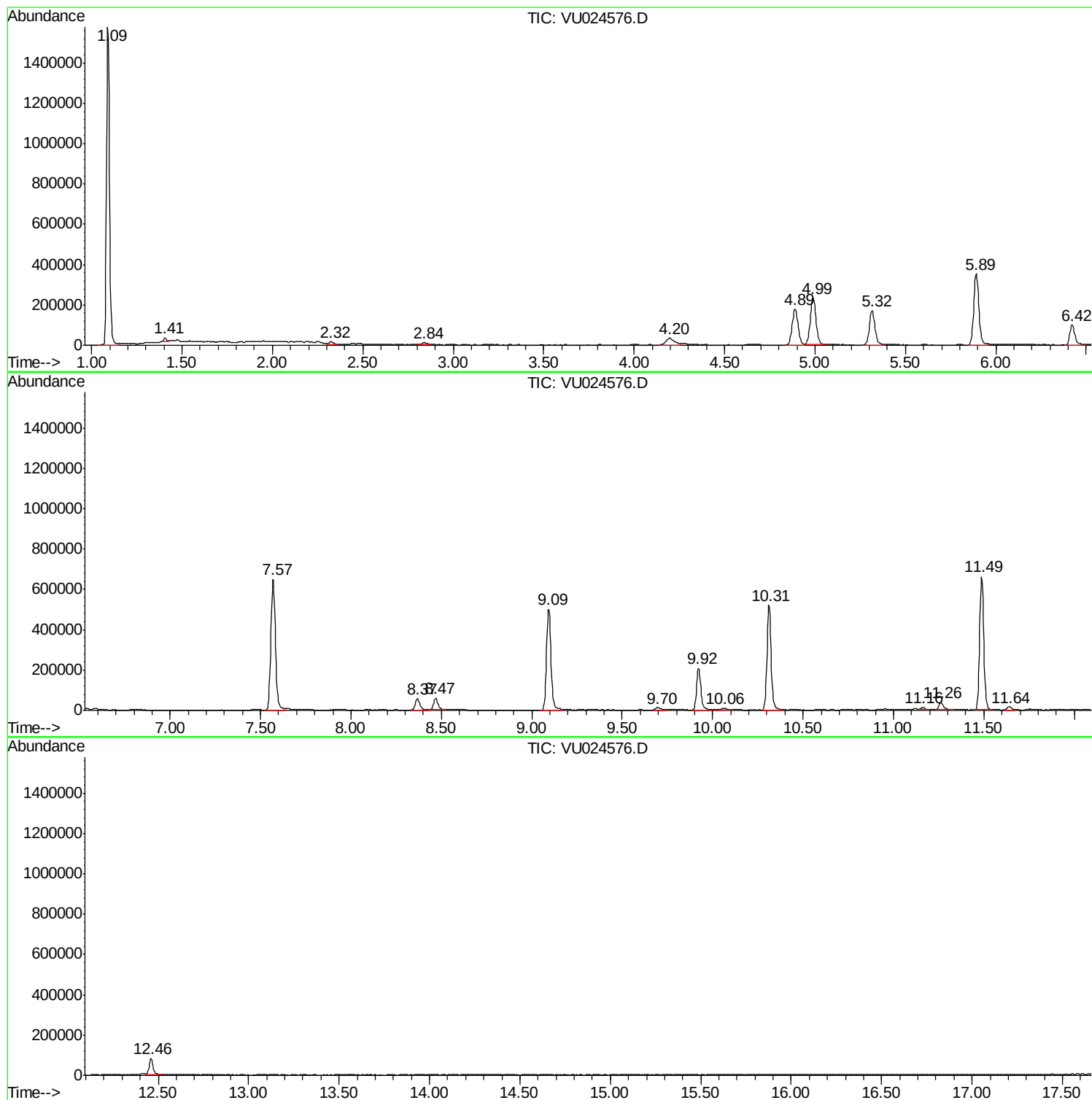
Sum of corrected areas: 8880916

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Quant Title : SW846 8260

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



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 Peak Number 1 2-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	14.26 ug/l	198603	1,4-Difluorobenzene	5.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Pentanone	86	C5H10O	000107-87-9 91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4 64
3	2,3-Butanedione	86	C4H6O2	000431-03-8 52
4	Butane	58	C4H10	000106-97-8 9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7 9

 Peak Number 2 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	5.76 ug/l	99651	Chlorobenzene-d5	9.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexanal	100	C6H12O	000066-25-1 86
2	Glutaraldehyde	100	C5H8O2	000111-30-8 32
3	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9 23
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8 12
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5 12

 Peak Number 3 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	19.79 ug/l	342462	Chlorobenzene-d5	9.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Heptanone	114	C7H14O	000110-43-0 91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3 90
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0 64
4	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1 52
5	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3 39

 Peak Number 4 2-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
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12.46	5.56 ug/l	116575	1,4-Dichlorobenzene-d4		11.49	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual

1		2-Nonanone	142	C9H18O	000821-55-6	95
2		2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	64
3		2-Heptanone	114	C7H14O	000110-43-0	64
4		2-Octanone	128	C8H16O	000111-13-7	64
5		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	59

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone	6.42	14.3	ug/l	198603	2	5.89	696458	50.0
Hexanal	8.47	5.8	ug/l	99651	3	9.09	865172	50.0
2-Heptanone	9.92	19.8	ug/l	342462	3	9.09	865172	50.0
2-Nonanone	12.46	5.6	ug/l	116575	4	11.49	1047940	50.0