

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091218\
 Data File : VU026687.D
 Acq On : 11 Sep 2018 18:35
 Operator : MD/SY
 Sample : J4803-11ME
 Misc : 4.89g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EP1-Q2-H6ME

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 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_U\METHOD\82U091218W.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	2.144	281	302	315	rBV	186601	401034	2.33%	0.199%
2	4.881	1136	1153	1170	rBV	98632	252146	1.46%	0.125%
3	4.977	1170	1183	1212	rVB2	133882	315684	1.83%	0.157%
4	5.308	1271	1286	1316	rBV2	103063	247770	1.44%	0.123%
5	5.884	1451	1465	1494	rBV	204046	439764	2.55%	0.218%
6	7.565	1967	1988	2008	rBV	405572	744846	4.32%	0.370%
7	8.906	2398	2405	2419	rVB	136238	220545	1.28%	0.110%
8	9.032	2432	2444	2453	rBV	183019	311220	1.80%	0.155%
9	9.096	2453	2464	2475	rVV	343578	594744	3.45%	0.295%
10	9.247	2500	2511	2525	rBV4	111192	220275	1.28%	0.109%
11	9.356	2525	2545	2552	rBV3	258073	596226	3.46%	0.296%
12	9.405	2552	2560	2568	rVV2	392614	622549	3.61%	0.309%
13	9.446	2568	2573	2598	rVB4	276433	619353	3.59%	0.308%
14	9.565	2598	2610	2623	rBV3	218923	418332	2.43%	0.208%
15	9.655	2627	2638	2643	rBV4	145884	250058	1.45%	0.124%
16	9.720	2644	2658	2668	rBV5	1251255	2470398	14.32%	1.227%
17	9.819	2677	2689	2697	rBV2	922780	1588979	9.21%	0.789%
18	9.871	2700	2705	2713	rVB2	569148	801651	4.65%	0.398%
19	9.954	2713	2731	2741	rBV	4514884	7684197	44.55%	3.816%
20	10.048	2741	2760	2768	rBV2	2614437	5714003	33.13%	2.838%
21	10.093	2768	2774	2786	rVB2	2394461	3902676	22.63%	1.938%
22	10.160	2786	2795	2806	rVB6	761819	1475583	8.56%	0.733%
23	10.228	2806	2816	2819	rBV4	884255	1352806	7.84%	0.672%
24	10.260	2820	2826	2835	rVV3	1921740	3139389	18.20%	1.559%
25	10.327	2836	2847	2856	rVB	3430265	5676002	32.91%	2.819%
26	10.379	2856	2863	2871	rVB6	772399	1211774	7.03%	0.602%
27	10.427	2871	2878	2882	rBV2	651442	919740	5.33%	0.457%
28	10.495	2884	2899	2909	rVB3	3054746	5613194	32.55%	2.788%
29	10.642	2935	2945	2955	rBV5	1387498	3069021	17.79%	1.524%
30	10.704	2957	2964	2972	rVV5	1619872	2787356	16.16%	1.384%
31	10.758	2972	2981	2991	rVV2	4577804	8157546	47.30%	4.051%
32	10.819	2992	3000	3010	rVB6	2419741	4809204	27.88%	2.388%
33	10.974	3043	3048	3053	rBV2	728184	981694	5.69%	0.488%
34	11.015	3055	3061	3070	rVB4	2342148	3479912	20.18%	1.728%

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35	11.080	3072	3081	3087	rBV4	2319866	3712257	21.52%	1.844%
36	11.128	3087	3096	3102	rBV	11363875	17247418	100.00%	8.565%
37	11.279	3132	3143	3150	rBV3	2798746	5294499	30.70%	2.629%
38	11.343	3158	3163	3173	rVB5	3786963	5914662	34.29%	2.937%
39	11.408	3173	3183	3190	rBV3	6524227	10401339	60.31%	5.166%
40	11.485	3202	3207	3214	rVB3	1553423	1817459	10.54%	0.903%
41	11.536	3216	3223	3230	rVV3	2287525	3210817	18.62%	1.595%
42	11.578	3230	3236	3243	rVB	2517716	3039307	17.62%	1.509%
43	11.675	3260	3266	3273	rVB3	1816960	2365420	13.71%	1.175%
44	11.790	3293	3302	3307	rBV4	2222498	3857644	22.37%	1.916%
45	11.871	3317	3327	3345	rVB6	6474776	16420477	95.21%	8.155%
46	12.070	3383	3389	3407	rVB5	3408910	7925643	45.95%	3.936%
47	12.157	3408	3416	3418	rBV	1916547	2522240	14.62%	1.253%
48	12.186	3419	3425	3433	rVB3	3961922	6018378	34.89%	2.989%
49	12.366	3473	3481	3487	rBV3	2613301	4519674	26.20%	2.245%
50	12.514	3515	3527	3534	rBV7	1994901	4774773	27.68%	2.371%
51	12.620	3550	3560	3565	rBV3	3693097	6063739	35.16%	3.011%
52	12.710	3579	3588	3605	rVB2	3522163	7630586	44.24%	3.790%
53	12.790	3605	3613	3620	rBV2	1718061	2723472	15.79%	1.353%
54	12.883	3638	3642	3651	rVB	606875	720512	4.18%	0.358%
55	12.967	3664	3668	3676	rVB2	874922	1068508	6.20%	0.531%
56	13.035	3683	3689	3697	rBV2	620397	895589	5.19%	0.445%
57	13.086	3698	3705	3710	rBV3	788194	1168267	6.77%	0.580%
58	13.125	3710	3717	3732	rVB2	2371498	4430838	25.69%	2.200%
59	13.240	3747	3753	3759	rBV	378695	471180	2.73%	0.234%
60	13.292	3760	3769	3777	rBV3	1301882	2185845	12.67%	1.086%
61	13.411	3798	3806	3814	rBV4	413620	659556	3.82%	0.328%
62	13.459	3815	3821	3828	rVB	295371	408350	2.37%	0.203%
63	13.510	3828	3837	3844	rBV4	810006	1375798	7.98%	0.683%
64	13.736	3899	3907	3917	rVB7	352705	664920	3.86%	0.330%
65	13.790	3917	3924	3934	rVB2	205175	302837	1.76%	0.150%
66	13.961	3969	3977	3989	rVB6	97497	188023	1.09%	0.093%
67	14.350	4084	4098	4110	rVB5	116150	271177	1.57%	0.135%

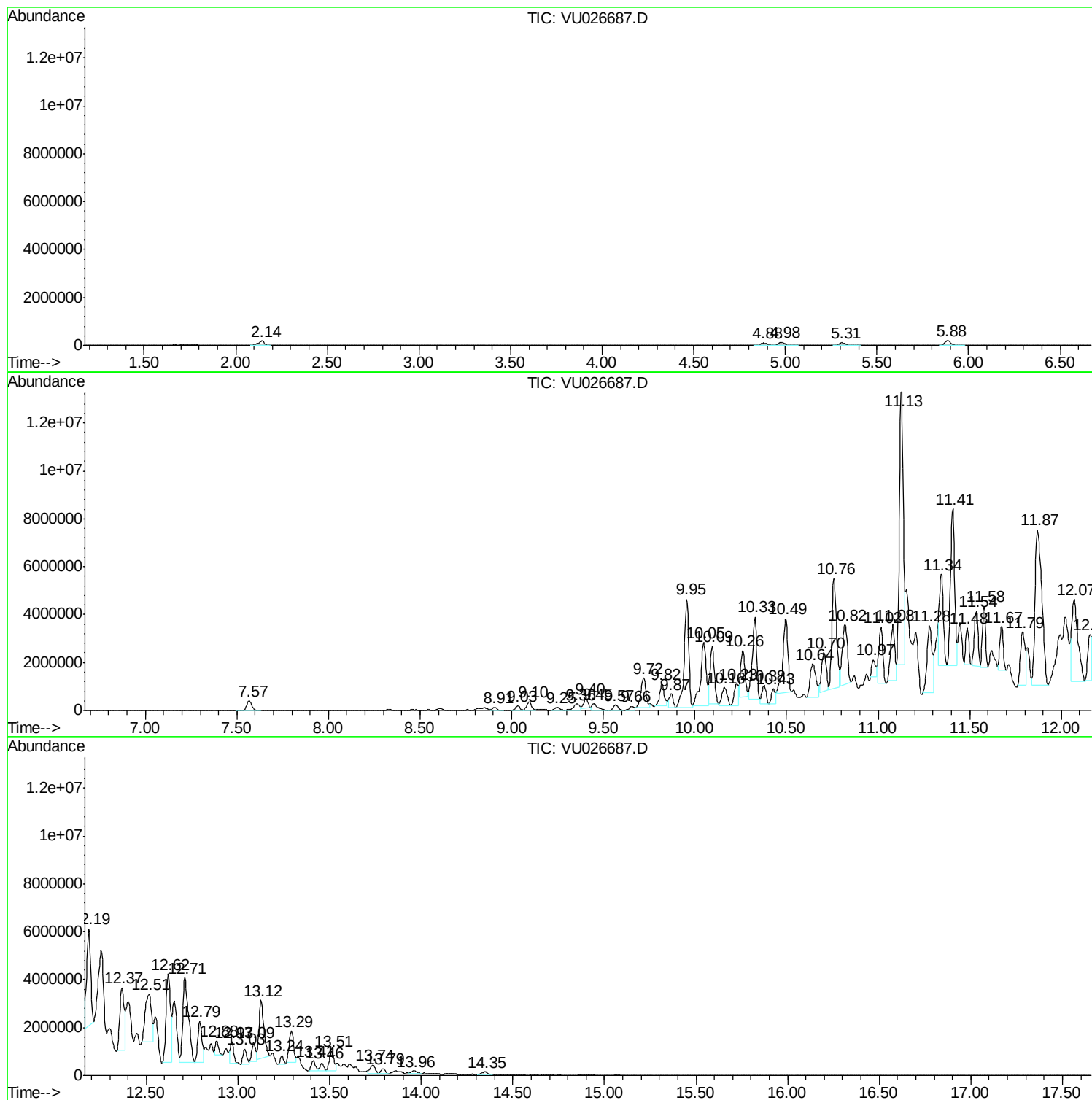
Sum of corrected areas: 201360875

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 1 unknown9.72 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	207.69 ug/l	2470400	Chlorobenzene-d5	9.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	46
3		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	43
4		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	38
5		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	38

 Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.95	646.01 ug/l	7684200	Chlorobenzene-d5	9.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	93
3		Nonane, 3-methyl-	142	C10H22	005911-04-6	87
4		Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	59
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59

 Peak Number 3 Cyclohexane, (1-methylethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	480.38 ug/l	5714000	Chlorobenzene-d5	9.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	60
2		Cyclohexane, propyl-	126	C9H18	001678-92-8	58
3		Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	47
4		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
5		Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	38

 Peak Number 4 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
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10.09	328.10 ug/l	3902680	Chlorobenzene-d5	9.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heptane, 3-ethyl-2-methyl-	142 C10H22	014676-29-0 72
2		Hexane, 3-ethyl-2,5-dimethyl-	142 C10H22	052897-04-8 53
3		Octane, 3-methyl-	128 C9H20	002216-33-3 43
4		Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9 43
5		Decane, 2,5-dimethyl-	170 C12H26	017312-50-4 40

 Peak Number 5 unknown10.26 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	263.93 ug/l	3139390	Chlorobenzene-d5	9.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9 47
2		Tridecane, 6-methyl-	198 C14H30	013287-21-3 47
3		Nonane, 4-methyl-	142 C10H22	017301-94-9 43
4		Undecane, 5-methyl-	170 C12H26	001632-70-8 43
5		1-Azacyclononan-2-one	141 C8H15NO	000935-30-8 43

 Peak Number 6 Cyclohexane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	286.15 ug/l	10401300	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, butyl-	140 C10H20	001678-93-9 87
2		Cyclohexane, octyl-	196 C14H28	001795-15-9 86
3		Cyclohexane, (1-methylethyl)-	126 C9H18	000696-29-7 74
4		Cyclohexane, 2-propenyl-	124 C9H16	002114-42-3 64
5		Cyclohexane, pentyl-	154 C11H22	004292-92-6 64

 Peak Number 7 Naphthalene, decahydro-, tr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	451.74 ug/l	16420500	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual

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1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	95
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	70
4	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	46
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	38

 Peak Number 8 unknown12.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	218.04 ug/l	7925640	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	47
2		Cyclopentanecarboxylic acid, 4-n...	235	C12H13NO4	1000307-58-0	43
3		1-Heptyne, 3-ethoxy-3,4-dimethyl-	168	C11H20O	054411-04-0	43
4		Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	38
5		Cyclohexane, 1-isopropyl-1-methyl-	140	C10H20	016580-26-0	35

 Peak Number 9 Cyclohexane, pentyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	166.82 ug/l	6063740	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, pentyl-	154	C11H22	004292-92-6	76
2		Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	62
3		Cyclohexane, butyl-	140	C10H20	001678-93-9	53
4		Cyclohexane, octyl-	196	C14H28	001795-15-9	53
5		Cyclohexane, propyl-	126	C9H18	001678-92-8	50

 Peak Number 10 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	209.93 ug/l	7630590	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95

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4 o-Cymene	134 C10H14	000527-84-4 94
5 Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14	000874-41-9 94

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.72	9.72	207.7	ug/l	2470400	3	9.10	594744	50.0
Octane, 2,6-dimet...	9.95	646.0	ug/l	7684200	3	9.10	594744	50.0
Cyclohexane, (1-m...	10.05	480.4	ug/l	5714000	3	9.10	594744	50.0
Heptane, 3-ethyl-...	10.09	328.1	ug/l	3902680	3	9.10	594744	50.0
unknown10.26	10.26	263.9	ug/l	3139390	3	9.10	594744	50.0
Cyclohexane, butyl-	11.41	286.1	ug/l	10401300	4	11.49	1817460	50.0
Naphthalene, deca...	11.87	451.7	ug/l	16420500	4	11.49	1817460	50.0
unknown12.07	12.07	218.0	ug/l	7925640	4	11.49	1817460	50.0
Cyclohexane, pentyl-	12.62	166.8	ug/l	6063740	4	11.49	1817460	50.0
Benzene, 1,2,3,5-...	12.71	209.9	ug/l	7630590	4	11.49	1817460	50.0