

Data Path : W:\HPCHEM1\MSVOA_H\DATA\XH092215\
 Data File : XH057106.D
 Acq On : 22 Sep 2015 15:59
 Operator : SY/FY
 Sample : I.BLK
 Misc : 12.84g/5mL//100uL/5mL/MSVOA_H/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_H
 ClientSampleId :
 I.BLK

Integration Parameters: rteint.p

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.001
 Stop Thrs : 0

Filtering: 9
 Min Area: 250 Area counts
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 1

Method : W:\HPCHEM1\MSVOA_H\METHODS\82H091715W.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	3.975	331	338	341	rBV	71749	257712	8.64%	0.701%
2	4.060	341	346	364	rVB2	469203	1621462	54.35%	4.409%
3	4.797	409	416	432	rBV2	663552	2706178	90.71%	7.359%
4	5.544	481	487	503	rBV	632651	1746969	58.56%	4.750%
5	7.499	668	673	688	rBV	780742	1944940	65.19%	5.289%
6	8.213	737	741	746	rVB2	12413	34624	1.16%	0.094%
7	9.591	868	872	878	rBV2	36291	90364	3.03%	0.246%
8	9.707	878	883	894	rVV	569402	1391034	46.63%	3.782%
9	10.611	963	969	973	rBV3	26589	52048	1.74%	0.142%
10	11.062	1010	1012	1014	rVV2	20635	41068	1.38%	0.112%
11	11.104	1014	1016	1020	rVV3	26234	40500	1.36%	0.110%
12	11.210	1020	1026	1030	rVB3	29492	64835	2.17%	0.176%
13	11.347	1035	1039	1051	rBV	509138	1006949	33.75%	2.738%
14	11.495	1051	1053	1056	rVV2	19811	39658	1.33%	0.108%
15	11.833	1081	1085	1088	rBV2	17271	29883	1.00%	0.081%
16	11.896	1088	1091	1092	rVV2	18773	35138	1.18%	0.096%
17	11.938	1092	1095	1099	rVB	105241	163218	5.47%	0.444%
18	12.012	1099	1102	1106	rVB2	21566	44993	1.51%	0.122%
19	12.085	1106	1109	1112	rBV2	38427	78223	2.62%	0.213%
20	12.137	1112	1114	1118	rVB4	55227	98461	3.30%	0.268%
21	12.316	1128	1131	1133	rBV	55317	88961	2.98%	0.242%
22	12.358	1133	1135	1137	rVV	58741	82130	2.75%	0.223%
23	12.390	1137	1138	1141	rVB	81150	99836	3.35%	0.271%
24	12.475	1143	1146	1154	rVB	403108	795029	26.65%	2.162%
25	12.717	1165	1169	1171	rBV2	37173	66592	2.23%	0.181%
26	12.780	1171	1175	1178	rVB4	35396	89768	3.01%	0.244%
27	12.864	1178	1183	1185	rBV4	44162	95263	3.19%	0.259%
28	12.949	1188	1191	1194	rVB2	67431	110232	3.69%	0.300%
29	13.002	1194	1196	1198	rBV3	23645	43550	1.46%	0.118%
30	13.055	1198	1201	1202	rBV2	44081	57527	1.93%	0.156%
31	13.118	1205	1207	1212	rBV5	33580	71988	2.41%	0.196%
32	13.224	1214	1217	1219	rBV2	64002	110453	3.70%	0.300%
33	13.277	1219	1222	1223	rVV2	56305	87964	2.95%	0.239%
34	13.309	1223	1225	1228	rVB3	60626	100341	3.36%	0.273%

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35	13.414	1233	1235	1238	rVB	72356	99257	3.33%	0.270%
36	13.467	1238	1240	1243	rBV3	21955	35285	1.18%	0.096%
37	13.594	1247	1252	1254	rBV6	27980	69684	2.34%	0.189%
38	13.657	1254	1258	1261	rBV5	56421	158822	5.32%	0.432%
39	13.773	1266	1269	1273	rBV2	243320	424728	14.24%	1.155%
40	13.847	1273	1276	1278	rVB3	49141	92071	3.09%	0.250%
41	13.890	1278	1280	1282	rVB3	19641	33363	1.12%	0.091%
42	13.996	1286	1290	1293	rBV4	37288	95495	3.20%	0.260%
43	14.080	1293	1298	1302	rVB5	137839	380381	12.75%	1.034%
44	14.144	1302	1304	1305	rBV2	35095	51712	1.73%	0.141%
45	14.229	1310	1312	1315	rVB	254791	315738	10.58%	0.859%
46	14.282	1315	1317	1320	rVB4	58770	85673	2.87%	0.233%
47	14.376	1322	1326	1329	rBV	1287835	1970344	66.04%	5.358%
48	14.451	1329	1333	1334	rBV3	71811	125986	4.22%	0.343%
49	14.483	1334	1336	1338	rVV2	93560	153702	5.15%	0.418%
50	14.534	1339	1341	1343	rVB	149532	186046	6.24%	0.506%
51	14.651	1349	1352	1356	rVV3	142732	280111	9.39%	0.762%
52	14.736	1356	1360	1363	rVV3	194937	597473	20.03%	1.625%
53	14.790	1363	1365	1367	rVV2	318540	643034	21.55%	1.749%
54	14.822	1367	1368	1370	rVV	324824	444829	14.91%	1.210%
55	14.927	1374	1378	1381	rVV2	848996	1885225	63.19%	5.126%
56	15.021	1384	1387	1389	rVV2	431803	994615	33.34%	2.705%
57	15.085	1390	1393	1395	rVV4	565325	1356451	45.47%	3.688%
58	15.127	1395	1397	1398	rVV2	436157	719112	24.10%	1.955%
59	15.191	1398	1403	1405	rVV	1392486	2983402	100.00%	8.112%
60	15.245	1405	1408	1410	rVV2	472443	1273168	42.68%	3.462%
61	15.309	1411	1414	1417	rVV	1013108	2186874	73.30%	5.946%
62	15.404	1420	1423	1427	rVV5	259474	1033445	34.64%	2.810%
63	15.467	1427	1429	1431	rVV	396581	787101	26.38%	2.140%
64	15.542	1434	1436	1440	rVV2	319953	904734	30.33%	2.460%
65	15.616	1440	1443	1446	rVV4	194816	559013	18.74%	1.520%
66	15.712	1448	1452	1457	rVV3	330236	992150	33.26%	2.698%
67	15.829	1461	1463	1466	rVV3	97864	251377	8.43%	0.684%
68	15.881	1466	1468	1471	rVV	104973	232093	7.78%	0.631%
69	15.945	1471	1474	1477	rVV4	89575	258272	8.66%	0.702%
70	15.997	1477	1479	1487	rVV3	209272	454968	15.25%	1.237%
71	16.110	1487	1490	1498	rVB3	88467	272427	9.13%	0.741%

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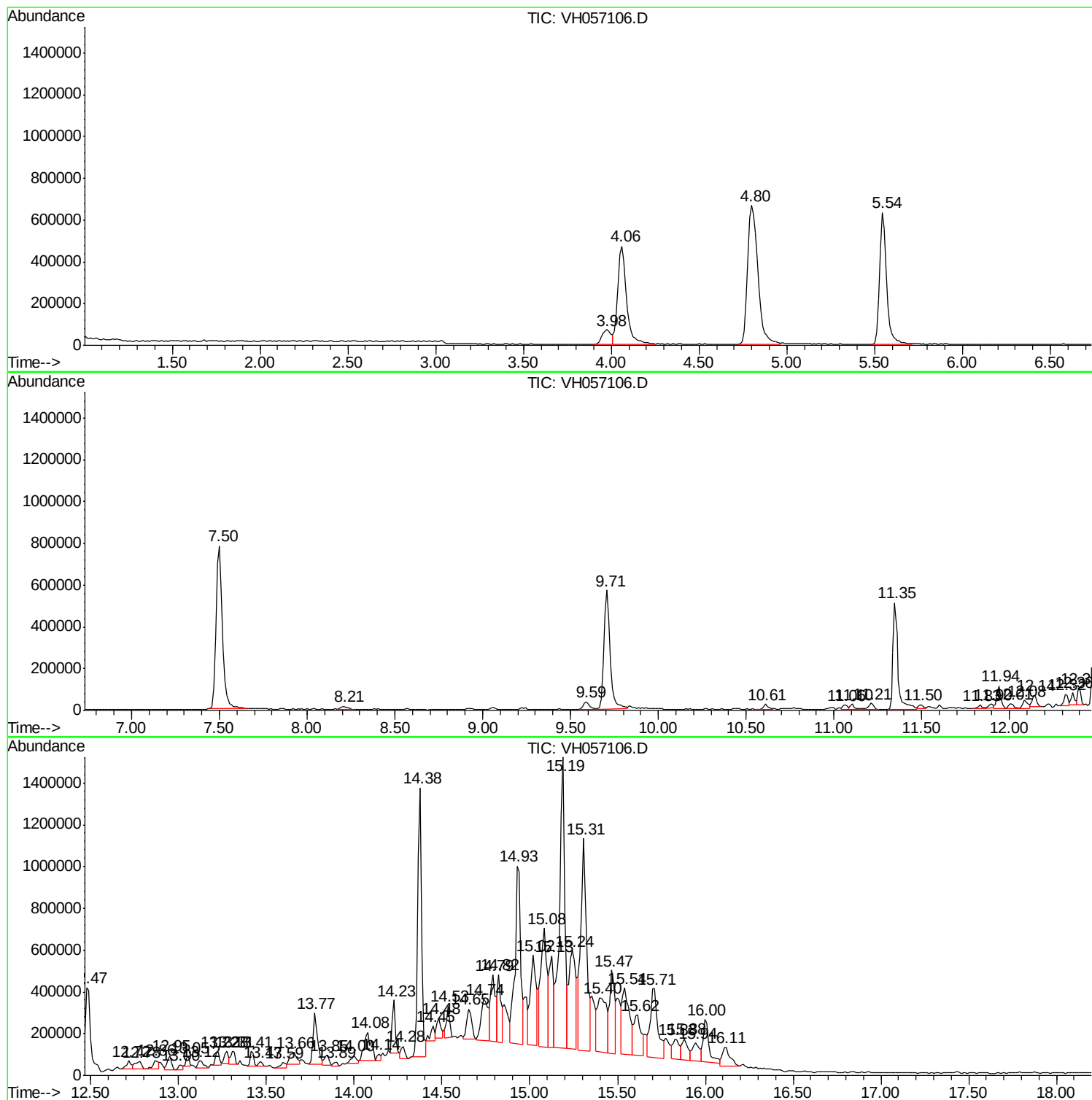
Sum of corrected areas: 36776052

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Quant Method : W:\HPCHEM1\MSVOA_H\METHODS\82H091715W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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TIC Integration Parameters: LSCINT.P

Peak Number 1 Dodecane, 2,7,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	118.56 ug/l	1885230	1,4-Dichlorobenzene-d4	12.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dodecane, 2,7,10-trimethyl-	212 C15H32	074645-98-0 91
2		Nonane, 3,7-dimethyl-	156 C11H24	017302-32-8 87
3		Dodecane, 2,6,10-trimethyl-	212 C15H32	003891-98-3 80
4		Dodecane, 2,6,11-trimethyl-	212 C15H32	031295-56-4 78
5		Nonane, 3-methyl-5-propyl-	184 C13H28	031081-18-2 64

Peak Number 2 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	62.55 ug/l	994615	1,4-Dichlorobenzene-d4	12.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,2,3,4-tetrahydro-	160 C12H16	004175-54-6 95
2		Benzene, 1,3,5-trimethyl-2-(1-methyl-2-propenyl)-	160 C12H16	014679-13-1 83
3		Benzene, 4-(2-butenyl)-1,2-dimethyl-	160 C12H16	054340-86-2 76
4		Naphthalene, 1,2,3,4-tetrahydro-	160 C12H16	013065-07-1 70
5		Benzene, 1-(1-methylethenyl)-3-(1-methylethenyl)-	160 C12H16	001129-29-9 64

Peak Number 3 unknown15.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	85.31 ug/l	1356450	1,4-Dichlorobenzene-d4	12.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decane, 6-ethyl-2-methyl-	184 C13H28	062108-21-8 27
2		Tridecane	184 C13H28	000629-50-5 27
3		Hydroxylamine, O-decyl-	173 C10H23NO	029812-79-1 22
4		Tetradecane	198 C14H30	000629-59-4 22
5		Decane, 1-iodo-	268 C10H21I	002050-77-3 22

Peak Number 4 unknown15.24 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
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15.24	80.07 ug/l	1273170	1,4-Dichlorobenzene-d4	12.49			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Quinololinol, 2-methyl-	159	C10H9NO	000826-81-3	25
2			Disiloxane, 1-ethenyl-1,1,3,3-te...	200	C9H20OSi2	055967-53-8	25
3			Bicyclo[4.2.0]oct-5-ene-2,3-dica...	206	C12H14O3	022467-69-2	11
4			1H-Imidazole, 4,5-dihydro-2-(phe...	160	C10H12N2	000059-98-3	10
5			2,3,4-Trifluorobenzoic acid, 4-p...	386	C22H33F3O2	1000280-62-3	10

 Peak Number 5 unknown15.40 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.40	64.99 ug/l	1033450	1,4-Dichlorobenzene-d4	12.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-3,4,...	174	C12H14O	035322-84-0	49	
2	1H-Indene, 2,3-dihydro-1,1,5,6-t...	174	C13H18	000942-43-8	46	
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	46	
4	Benzene, 1,2,3,4-tetramethyl-4-(...	174	C13H18	061142-76-5	45	
5	1(3H)-Isobenzofuranone, 3-propyl...	174	C11H10O2	017369-59-4	38	

 Peak Number 6 Decane, 5-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.47	49.50 ug/l	787101	1,4-Dichlorobenzene-d4	12.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 5-propyl-		184	C13H28	017312-62-8	90
2	Hexadecane, 7,9-dimethyl-		254	C18H38	021164-95-4	86
3	Dodecane, 4-methyl-		184	C13H28	006117-97-1	80
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80
5	Heptacosane		380	C27H56	000593-49-7	80

 Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.71	62.40 ug/l	992150	1,4-Dichlorobenzene-d4	12.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	91
2	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	43
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40
4	1-(P-FLUOROPHENYL)-4-PIPERIDONE	193	C11H12FNO	1000238-56-7	38
5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecane, 2,7,10-...	14.93	118.6	ug/l	1885230	4	12.49	795029	50.0
Naphthalene, 1,2,...	15.02	62.5	ug/l	994615	4	12.49	795029	50.0
unknown15.08	15.08	85.3	ug/l	1356450	4	12.49	795029	50.0
unknown15.24	15.24	80.1	ug/l	1273170	4	12.49	795029	50.0
unknown15.40	15.40	65.0	ug/l	1033450	4	12.49	795029	50.0
Decane, 5-propyl-	15.47	49.5	ug/l	787101	4	12.49	795029	50.0
Decahydro-4,4,8,9...	15.71	62.4	ug/l	992150	4	12.49	795029	50.0