

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD060718\
 Data File : VD057984.D
 Acq On : 7 Jun 2018 21:03
 Operator : JC/SY
 Sample : J3331-01
 Misc : 4.29g/5ml/MSVOA D/SOIL
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 CAS1-SB-02-1-2

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_D\METHOD\82D060618S.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	1.220	94	101	104	rBV	981187	2527601	62.61%	5.729%
2	1.279	104	107	130	rVB	1200598	4036968	100.00%	9.150%
3	2.608	237	242	252	rBV	37930	115198	2.85%	0.261%
4	3.071	285	289	298	rVB5	17769	50964	1.26%	0.116%
5	3.730	349	356	363	rBV2	28701	82881	2.05%	0.188%
6	4.616	438	446	455	rBV3	16941	51662	1.28%	0.117%
7	4.842	461	469	475	rBV2	26395	94229	2.33%	0.214%
8	5.541	532	540	544	rBV	426170	1125416	27.88%	2.551%
9	5.630	544	549	566	rVV	720051	2155510	53.39%	4.885%
10	6.004	581	587	599	rBV	424444	1147641	28.43%	2.601%
11	6.486	632	636	646	rVB2	23600	63827	1.58%	0.145%
12	6.683	650	656	671	rVV	954320	2460265	60.94%	5.576%
13	7.274	710	716	726	rBV2	24028	65010	1.61%	0.147%
14	8.692	855	860	868	rBV	984027	2293410	56.81%	5.198%
15	10.099	1000	1003	1009	rBV3	22962	54605	1.35%	0.124%
16	10.680	1057	1062	1070	rVB	1447121	2536609	62.83%	5.749%
17	10.848	1076	1079	1086	rVB	58371	112833	2.79%	0.256%
18	11.005	1086	1095	1101	rBV3	44793	171070	4.24%	0.388%
19	11.350	1126	1130	1132	rBV2	44859	92625	2.29%	0.210%
20	11.399	1132	1135	1138	rVB3	33940	66203	1.64%	0.150%
21	11.546	1145	1150	1151	rBV4	23364	42906	1.06%	0.097%
22	11.586	1151	1154	1157	rVV	53937	89999	2.23%	0.204%
23	11.665	1157	1162	1163	rVV4	50014	90612	2.24%	0.205%
24	11.694	1163	1165	1169	rVV	60512	112640	2.79%	0.255%
25	11.763	1169	1172	1175	rVB3	37019	66346	1.64%	0.150%
26	11.832	1175	1179	1185	rBV3	42321	124365	3.08%	0.282%
27	11.921	1185	1188	1192	rVV	1252609	1764916	43.72%	4.000%
28	12.078	1201	1204	1209	rVB2	166148	289037	7.16%	0.655%
29	12.196	1212	1216	1217	rBV2	54934	99287	2.46%	0.225%
30	12.255	1220	1222	1225	rBV2	71385	120645	2.99%	0.273%
31	12.304	1225	1227	1229	rBV3	50723	70980	1.76%	0.161%
32	12.344	1229	1231	1234	rVB2	75935	117758	2.92%	0.267%
33	12.403	1234	1237	1239	rVB2	50964	75515	1.87%	0.171%
34	12.462	1239	1243	1244	rBV2	49941	93879	2.33%	0.213%

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35	12.492	1244	1246	1250	rVB3	56913	102165	2.53%	0.232%
36	12.551	1250	1252	1254	rBV2	47929	70640	1.75%	0.160%
37	12.620	1254	1259	1260	rBV3	134655	267147	6.62%	0.605%
38	12.728	1267	1270	1272	rBV3	110620	241001	5.97%	0.546%
39	12.767	1272	1274	1277	rVV2	133126	219681	5.44%	0.498%
40	12.856	1277	1283	1285	rVV7	88546	271835	6.73%	0.616%
41	12.905	1285	1288	1291	rVV	1589728	2494425	61.79%	5.654%
42	13.023	1294	1300	1303	rVB5	117540	327078	8.10%	0.741%
43	13.092	1303	1307	1313	rVB5	194876	501034	12.41%	1.136%
44	13.190	1313	1317	1321	rBV4	456795	1034101	25.62%	2.344%
45	13.259	1321	1324	1325	rVV	107776	131123	3.25%	0.297%
46	13.299	1325	1328	1329	rVV2	93729	164442	4.07%	0.373%
47	13.328	1329	1331	1334	rVB2	182956	263192	6.52%	0.597%
48	13.437	1334	1342	1345	rVB6	181236	709004	17.56%	1.607%
49	13.486	1345	1347	1348	rVB2	43081	47399	1.17%	0.107%
50	13.525	1348	1351	1355	rBV6	280661	472125	11.70%	1.070%
51	13.584	1355	1357	1358	rBV2	78254	121059	3.00%	0.274%
52	13.614	1358	1360	1362	rVB2	117654	137011	3.39%	0.311%
53	13.673	1362	1366	1368	rBV3	518259	787369	19.50%	1.785%
54	13.732	1368	1372	1374	rVB4	155954	375400	9.30%	0.851%
55	13.771	1374	1376	1378	rBV2	179295	242381	6.00%	0.549%
56	13.811	1378	1380	1383	rBV2	512622	739539	18.32%	1.676%
57	13.870	1383	1386	1389	rBV3	89352	174502	4.32%	0.396%
58	13.958	1393	1395	1396	rBV	64922	84706	2.10%	0.192%
59	13.988	1396	1398	1400	rBV3	87704	109795	2.72%	0.249%
60	14.057	1400	1405	1407	rBV3	304404	552593	13.69%	1.252%
61	14.086	1407	1408	1410	rVV2	159947	194312	4.81%	0.440%
62	14.155	1413	1415	1416	rVV	124268	123397	3.06%	0.280%
63	14.195	1416	1419	1424	rVB3	378549	742462	18.39%	1.683%
64	14.313	1429	1431	1435	rBV4	173959	366111	9.07%	0.830%
65	14.431	1441	1443	1445	rBV3	186084	304625	7.55%	0.690%
66	14.460	1445	1446	1448	rVV2	138693	204737	5.07%	0.464%
67	14.510	1448	1451	1453	rVV	1972685	2432974	60.27%	5.514%
68	14.549	1453	1455	1458	rVV3	478459	746511	18.49%	1.692%
69	14.618	1458	1462	1465	rVV6	291125	597197	14.79%	1.354%
70	14.687	1467	1469	1471	rVV2	74696	76183	1.89%	0.173%
71	14.726	1471	1473	1474	rVB	70118	55906	1.38%	0.127%

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72	14.766	1474	1477	1478	rBV3	56991	94577	2.34%	0.214%
73	14.795	1478	1480	1483	rVB3	181007	311766	7.72%	0.707%
74	14.864	1483	1487	1491	rBV5	204795	538734	13.35%	1.221%
75	14.953	1494	1496	1499	rBV3	212415	339881	8.42%	0.770%
76	15.002	1499	1501	1502	rBV2	50143	65904	1.63%	0.149%
77	15.090	1507	1510	1513	rVV4	184168	289072	7.16%	0.655%
78	15.140	1513	1515	1517	rVV2	78934	105036	2.60%	0.238%
79	15.209	1520	1522	1524	rBV2	155810	193397	4.79%	0.438%
80	15.258	1524	1527	1530	rVB	884731	1262247	31.27%	2.861%
81	15.376	1536	1539	1543	rVB	1308278	1614066	39.98%	3.658%
82	15.553	1554	1557	1559	rVB4	55956	95634	2.37%	0.217%
83	15.602	1559	1562	1566	rVB6	38572	86769	2.15%	0.197%
84	15.760	1574	1578	1583	rVB3	33176	117657	2.91%	0.267%
85	16.035	1603	1606	1613	rVB3	23773	57606	1.43%	0.131%

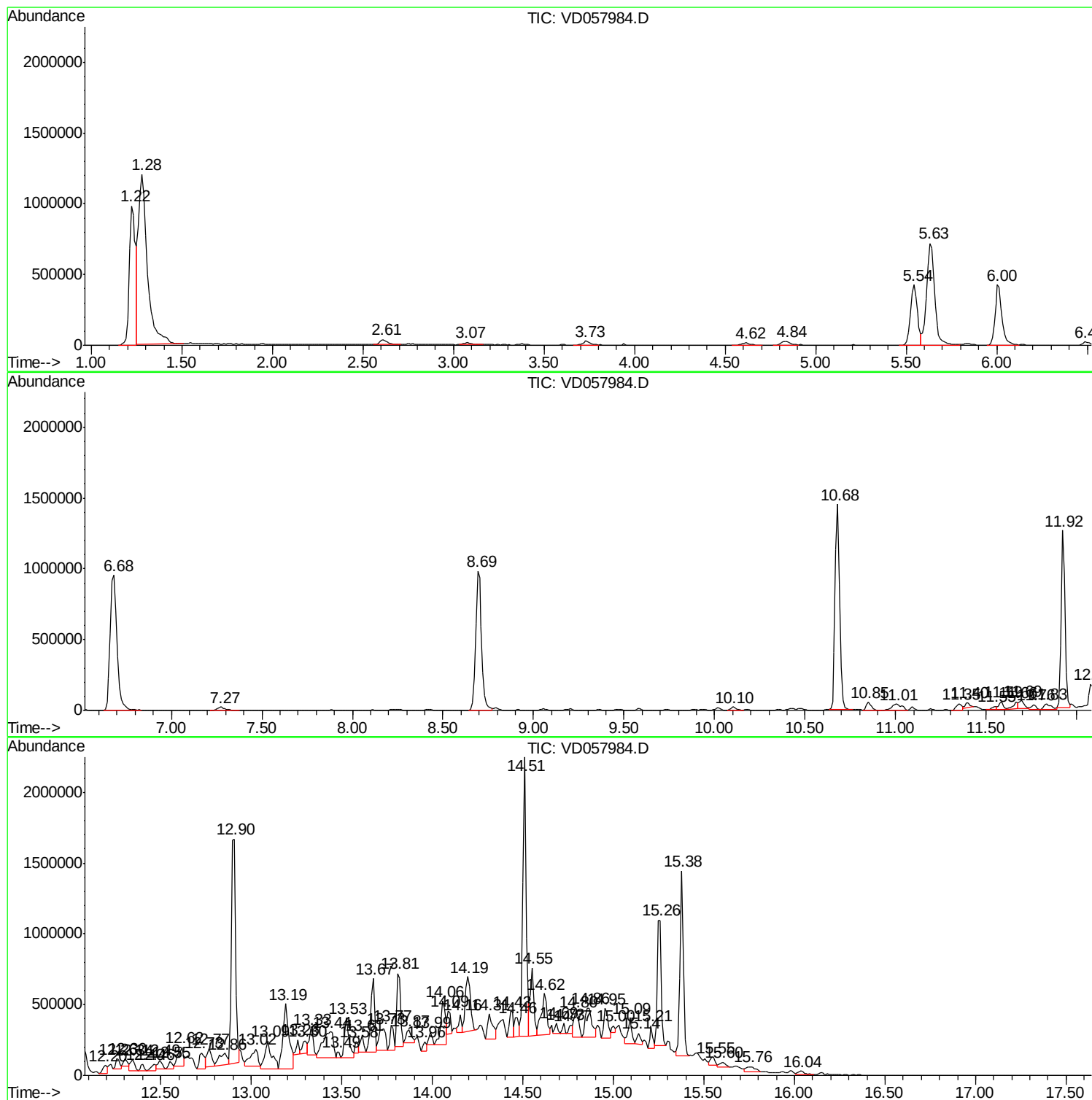
Sum of corrected areas: 44120920

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



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Peak Number 1 Naphthalene, decahydro-, tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	20.73 ug/l	1034100	1,4-Dichlorobenzene-d4	12.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, decahydro-, trans-	138 C10H18	000493-02-7 96
2		Naphthalene, decahydro-	138 C10H18	000091-17-8 95
3		Naphthalene, decahydro-, cis-	138 C10H18	000493-01-6 93
4		Spiro[4.5]decane	138 C10H18	000176-63-6 87
5		Cyclohexane, 1-methyl-3-(1-methy...	138 C10H18	024399-15-3 87

Peak Number 2 unknown13.44 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	14.21 ug/l	709004	1,4-Dichlorobenzene-d4	12.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentanecarboxylic acid, all...	154 C9H14O2	178905-33-4 46
2		Cyclohexane, 1-ethyl-2-propyl-	154 C11H22	062238-33-9 43
3		3-Hexene, 3-ethyl-2,5-dimethyl-	140 C10H20	062338-08-3 43
4		1-Pentyn-3-ol, 3,4-dimethyl-	112 C7H12O	001482-15-1 38
5		Cyclohexane, 1,1-dimethyl-2-propyl-	154 C11H22	081983-71-3 38

Peak Number 3 Cyclohexanone, 5-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	15.78 ug/l	787369	1,4-Dichlorobenzene-d4	12.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexanone, 5-methyl-2-(1-met...	152 C10H16O	000529-00-0 60
2		4,5-Nonadiene, 2-methyl-	138 C10H18	055956-32-6 55
3		Cyclohexanone, 5-methyl-2-(1-met...	152 C10H16O	015932-80-6 53
4		Cyclohexanone, 5-methyl-2-(1-met...	152 C10H16O	029606-79-9 52
5		1-Methyl-2-methylenecyclohexane	110 C8H14	002808-75-5 46

Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
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13.81	14.82 ug/l	739539	1,4-Dichlorobenzene-d4	12.90			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	99
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	99
3			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	74
4			Cyclohexene, 1-pentyl-	152	C11H20	015232-85-6	62
5			4,5-Nonadiene, 2-methyl-	138	C10H18	055956-32-6	62

 Peak Number 5 unknown14.19 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.19	14.88 ug/l	742462	1,4-Dichlorobenzene-d4	12.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	43
2		Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	38
3		Hexylidencyclohexane	166	C12H22	010201-62-4	25
4		3-Hexyne	82	C6H10	000928-49-4	25
5		Cyclohexane, ethenyl-	110	C8H14	000695-12-5	25

 Peak Number 6 unknown14.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.62	11.97 ug/l	597197	1,4-Dichlorobenzene-d4	12.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Hexadiene, 2-methyl-	96	C7H12	001119-14-8	25
2		1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	25
3		Ethanone, 1-(4-ethylphenyl)-	148	C10H12O	000937-30-4	25
4		7-Acetyl-3,3-dimethylbicyclo[4.1...	180	C11H16O2	1000185-00-8	14
5		1,3-Pentadiene, 2,3-dimethyl-	96	C7H12	001113-56-0	11

 Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.26	25.30 ug/l	1262250	1,4-Dichlorobenzene-d4	12.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, deca...	13.19	20.7	ug/l	1034100	4	12.90	2494430	50.0
unknown13.44	13.44	14.2	ug/l	709004	4	12.90	2494430	50.0
Cyclohexanone, 5-...	13.67	15.8	ug/l	787369	4	12.90	2494430	50.0
1-Methyldecahydro...	13.81	14.8	ug/l	739539	4	12.90	2494430	50.0
unknown14.19	14.19	14.9	ug/l	742462	4	12.90	2494430	50.0
unknown14.62	14.62	12.0	ug/l	597197	4	12.90	2494430	50.0
Naphthalene, 1-me...	15.26	25.3	ug/l	1262250	4	12.90	2494430	50.0