

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061418\
 Data File : VN049228.D
 Acq On : 14 Jun 2018 15:24
 Operator : MD\SY
 Sample : J3435-02
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW8

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_N\METHODS\82N061318W.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	1.661	6	22	50	rBV	2036432	3055434	11.75%	1.843%
2	2.182	173	184	194	rBV	363673	529504	2.04%	0.319%
3	2.805	362	378	399	rBV	3564833	7200170	27.68%	4.343%
4	3.137	466	481	499	rBV	1303676	2764556	10.63%	1.667%
5	3.317	523	537	554	rVB	218398	508883	1.96%	0.307%
6	3.474	562	586	599	rBV2	127198	327423	1.26%	0.197%
7	3.561	599	613	635	rVB2	180909	438112	1.68%	0.264%
8	3.799	667	687	709	rBV3	183333	583466	2.24%	0.352%
9	4.426	860	882	895	rBV4	109108	353823	1.36%	0.213%
10	4.535	895	916	920	rBV2	461282	1245368	4.79%	0.751%
11	5.053	1051	1077	1108	rBV2	804830	2949807	11.34%	1.779%
12	5.571	1216	1238	1260	rBV3	210559	665387	2.56%	0.401%
13	5.860	1308	1328	1339	rBV	82164	272329	1.05%	0.164%
14	6.162	1408	1422	1442	rBV3	99966	375116	1.44%	0.226%
15	6.628	1546	1567	1612	rVB	1988930	6322232	24.31%	3.813%
16	7.593	1848	1867	1874	rBV2	486955	1183049	4.55%	0.714%
17	7.661	1875	1888	1904	rVV4	1809879	5140422	19.76%	3.100%
18	7.744	1905	1914	1939	rVB3	327569	909152	3.50%	0.548%
19	7.879	1939	1956	1966	rBV3	211529	524953	2.02%	0.317%
20	8.034	1988	2004	2027	rBV2	634423	1649011	6.34%	0.995%
21	8.165	2027	2045	2055	rBV5	423217	1307952	5.03%	0.789%
22	8.304	2080	2088	2104	rVB2	202456	445742	1.71%	0.269%
23	8.590	2160	2177	2203	rBV	1337912	3016402	11.60%	1.819%
24	9.082	2302	2330	2343	rBV4	614597	1848992	7.11%	1.115%
25	9.519	2457	2466	2484	rVB3	142496	293102	1.13%	0.177%
26	9.654	2502	2508	2524	rVB2	189935	384490	1.48%	0.232%
27	10.091	2630	2644	2655	rBV	2101317	4087445	15.72%	2.465%
28	10.159	2655	2665	2677	rVB	1368511	2547287	9.79%	1.536%
29	10.525	2766	2779	2794	rBV4	122983	281436	1.08%	0.170%
30	11.410	3038	3054	3072	rBV	2166386	3946930	15.17%	2.381%
31	11.513	3072	3086	3105	rVV	9458105	15806295	60.77%	9.533%
32	11.622	3105	3120	3144	rVB	13668249	26009474	100.00%	15.687%
33	11.950	3201	3222	3244	rVB	5547160	9215700	35.43%	5.558%
34	12.252	3303	3316	3334	rVB	967110	1595526	6.13%	0.962%

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35	12.403	3349	3363	3379	rBV	1752880	2979551	11.46%	1.797%
36	12.593	3409	3422	3432	rBV	1742278	2760175	10.61%	1.665%
37	12.657	3432	3442	3449	rBV	3570544	6001886	23.08%	3.620%
38	12.734	3459	3466	3479	rVB	1694766	2673935	10.28%	1.613%
39	12.892	3500	3515	3531	rBV	2449927	4001994	15.39%	2.414%
40	13.043	3548	3562	3576	rBV	8052726	12576194	48.35%	7.585%
41	13.172	3586	3602	3613	rBV4	186868	445620	1.71%	0.269%
42	13.345	3645	3656	3661	rBV	1958239	3207122	12.33%	1.934%
43	13.545	3697	3718	3727	rBV	3202234	6111830	23.50%	3.686%
44	13.590	3727	3732	3749	rVB4	682027	1278040	4.91%	0.771%
45	13.738	3766	3778	3789	rVB2	221310	450013	1.73%	0.271%
46	13.805	3789	3799	3805	rBV	608576	1011428	3.89%	0.610%
47	13.892	3816	3826	3835	rBV	968028	1438627	5.53%	0.868%
48	13.947	3835	3843	3850	rVV	374264	573050	2.20%	0.346%
49	13.998	3850	3859	3871	rVB	1427619	2302302	8.85%	1.389%
50	14.213	3910	3926	3931	rBV	587267	941678	3.62%	0.568%
51	14.252	3931	3938	3947	rVB	661589	997533	3.84%	0.602%
52	14.480	3999	4009	4019	rBV	931806	1446340	5.56%	0.872%
53	14.596	4031	4045	4057	rBV3	1779587	3286712	12.64%	1.982%
54	14.744	4081	4091	4100	rBV2	201324	321338	1.24%	0.194%
55	14.850	4107	4124	4131	rBV4	264240	637760	2.45%	0.385%
56	14.959	4147	4158	4176	rVB3	291301	663043	2.55%	0.400%
57	15.136	4193	4213	4226	rBV	1084759	1907490	7.33%	1.150%

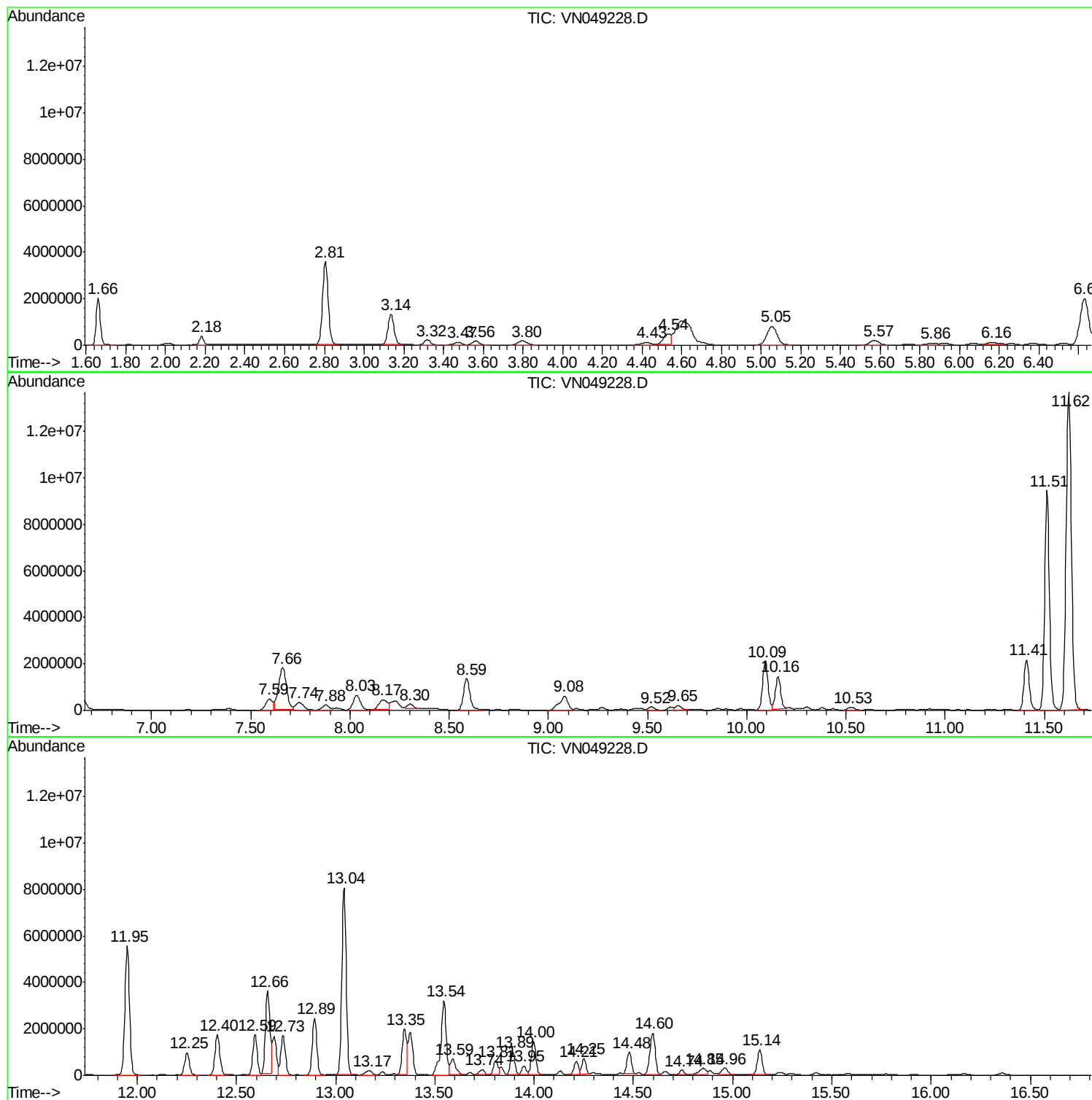
Sum of corrected areas: 165798631

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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	70.03 ug/l	7200170	Pentafluorobenzene	7.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4 94
2	Pentane	72	C5H12	000109-66-0 42
3	3-Buten-1-ol	72	C4H8O	000627-27-0 28
4	1-Butene	56	C4H8	000106-98-9 9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9 9

 Peak Number 2 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	26.89 ug/l	2764560	Pentafluorobenzene	7.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentane	72	C5H12	000109-66-0 91
2	Butane, 2-methyl-	72	C5H12	000078-78-4 42
3	Oxirane, ethyl-	72	C4H8O	000106-88-7 40
4	Cyclobutylamine	71	C4H9N	002516-34-9 9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2 7

 Peak Number 3 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	28.69 ug/l	2949810	Pentafluorobenzene	7.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0 91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2 78
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4 64
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8 45
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7 45

 Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
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6.63	61.50 ug/l	6322230	Pentafluorobenzene	7.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	45

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.66	93.57 ug/l	6001890	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.54	95.29 ug/l	6111830	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	92
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	76
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
5	Deltacyclene	118	C9H10	007785-10-6	62

Peak Number 7 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.00	35.89 ug/l	2302300	1,4-Dichlorobenzene-d4		13.35	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1 Indan, 1-methyl-	132	C10H12	000767-58-8	87
2 Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
3 3-Phenylbut-1-ene	132	C10H12	000934-10-1	83
4 Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83
5 Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	80

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	51.24 ug/l	3286710	1,4-Dichlorobenzene-d4	13.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5			Indan, 1-methyl-	132	C10H12	000767-58-8	87

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	2.81	70.0	ug/l	7200170	1	7.67	5140420	50.0
Pentane	3.14	26.9	ug/l	2764560	1	7.67	5140420	50.0
Pentane, 3-methyl-	5.05	28.7	ug/l	2949810	1	7.67	5140420	50.0
Cyclopentane, met...	6.63	61.5	ug/l	6322230	1	7.67	5140420	50.0
Benzene, 1-ethyl-...	12.66	93.6	ug/l	6001890	4	13.35	3207120	50.0
Indane	13.54	95.3	ug/l	6111830	4	13.35	3207120	50.0
Indan, 1-methyl-	14.00	35.9	ug/l	2302300	4	13.35	3207120	50.0
Benzene, 2-etheny...	14.60	51.2	ug/l	3286710	4	13.35	3207120	50.0