

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061618\
 Data File : VN049318.D
 Acq On : 16 Jun 2018 19:03
 Operator : MD\SY
 Sample : J3564-04
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-14

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\82N061618W.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	3	22	51	rBV	11105336	16838707	61.11%	7.663%
2	1.989	114	124	128	rBV	281990	409491	1.49%	0.186%
3	2.027	128	136	154	rVB	1423885	2187764	7.94%	0.996%
4	6.831	1607	1630	1657	rBV2	475236	1506815	5.47%	0.686%
5	7.593	1845	1867	1877	rBV2	1229044	3068519	11.14%	1.396%
6	7.667	1878	1890	1937	rVB	2004084	5097606	18.50%	2.320%
7	8.030	1984	2003	2027	rBV	1243151	3011148	10.93%	1.370%
8	8.236	2030	2067	2080	rBV4	402587	1529045	5.55%	0.696%
9	8.587	2160	2176	2211	rBV	2553650	5641057	20.47%	2.567%
10	9.082	2306	2330	2357	rBV	546669	1263138	4.58%	0.575%
11	10.091	2627	2644	2680	rBV	4864118	9448393	34.29%	4.300%
12	10.953	2896	2912	2921	rBV2	181005	347100	1.26%	0.158%
13	11.410	3040	3054	3073	rBV	3466656	6293488	22.84%	2.864%
14	12.252	3305	3316	3328	rVB	1562380	2576455	9.35%	1.173%
15	12.403	3351	3363	3378	rBV	3237176	5418957	19.67%	2.466%
16	12.593	3406	3422	3434	rVB	2265354	3782231	13.73%	1.721%
17	13.172	3589	3602	3612	rBV2	957093	1952273	7.09%	0.888%
18	13.345	3644	3656	3671	rBV	3305405	5572429	20.22%	2.536%
19	13.445	3679	3687	3697	rBV	482525	780130	2.83%	0.355%
20	13.545	3699	3718	3728	rBV2	7171783	13816827	50.14%	6.288%
21	13.599	3728	3735	3737	rBV2	394896	478954	1.74%	0.218%
22	13.673	3747	3758	3768	rVB5	1138510	2103261	7.63%	0.957%
23	13.892	3815	3826	3835	rBV	5742447	8534708	30.97%	3.884%
24	13.950	3835	3844	3850	rVV	2565932	4092269	14.85%	1.862%
25	13.995	3850	3858	3870	rVB2	7198796	11768742	42.71%	5.356%
26	14.133	3889	3901	3909	rBV	1421199	2494629	9.05%	1.135%
27	14.210	3909	3925	3942	rVB	5147707	9679803	35.13%	4.405%
28	14.294	3943	3951	3957	rBV	590423	952394	3.46%	0.433%
29	14.329	3957	3962	3968	rVV3	528272	788956	2.86%	0.359%
30	14.368	3968	3974	3981	rVV	668726	1012844	3.68%	0.461%
31	14.429	3985	3993	4001	rVV3	881854	1591931	5.78%	0.724%
32	14.480	4002	4009	4018	rVV3	818252	1424811	5.17%	0.648%
33	14.532	4019	4025	4030	rVV3	410997	550054	2.00%	0.250%
34	14.586	4030	4042	4055	rVV4	13993081	27553940	100.00%	12.539%

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35	14.654	4056	4063	4073	rVB3	1013329	1803407	6.55%	0.821%
36	14.853	4108	4125	4130	rBV4	1455165	3023416	10.97%	1.376%
37	14.889	4131	4136	4146	rVV2	1730897	3047103	11.06%	1.387%
38	14.956	4148	4157	4169	rVB2	2703907	5909536	21.45%	2.689%
39	15.049	4179	4186	4193	rBV	533549	760176	2.76%	0.346%
40	15.094	4193	4200	4217	rVB4	771456	1740996	6.32%	0.792%
41	15.191	4220	4230	4239	rBV	2678495	4612576	16.74%	2.099%
42	15.265	4239	4253	4288	rVB4	2720784	8313538	30.17%	3.783%
43	15.419	4291	4301	4311	rBV3	384776	716851	2.60%	0.326%
44	15.487	4313	4322	4333	rBV3	718067	1339510	4.86%	0.610%
45	15.583	4342	4352	4353	rBV2	814671	1121571	4.07%	0.510%
46	15.615	4354	4362	4378	rVB	4661168	8554070	31.04%	3.893%
47	15.702	4381	4389	4399	rVB	548513	940247	3.41%	0.428%
48	15.773	4402	4411	4421	rBV5	384278	780793	2.83%	0.355%
49	15.918	4442	4456	4474	rBV	4130675	8205080	29.78%	3.734%
50	16.104	4504	4514	4526	rVV3	776182	1569434	5.70%	0.714%
51	16.172	4527	4535	4559	rVB5	493754	1751356	6.36%	0.797%
52	16.358	4580	4593	4605	rBV4	799307	1980069	7.19%	0.901%

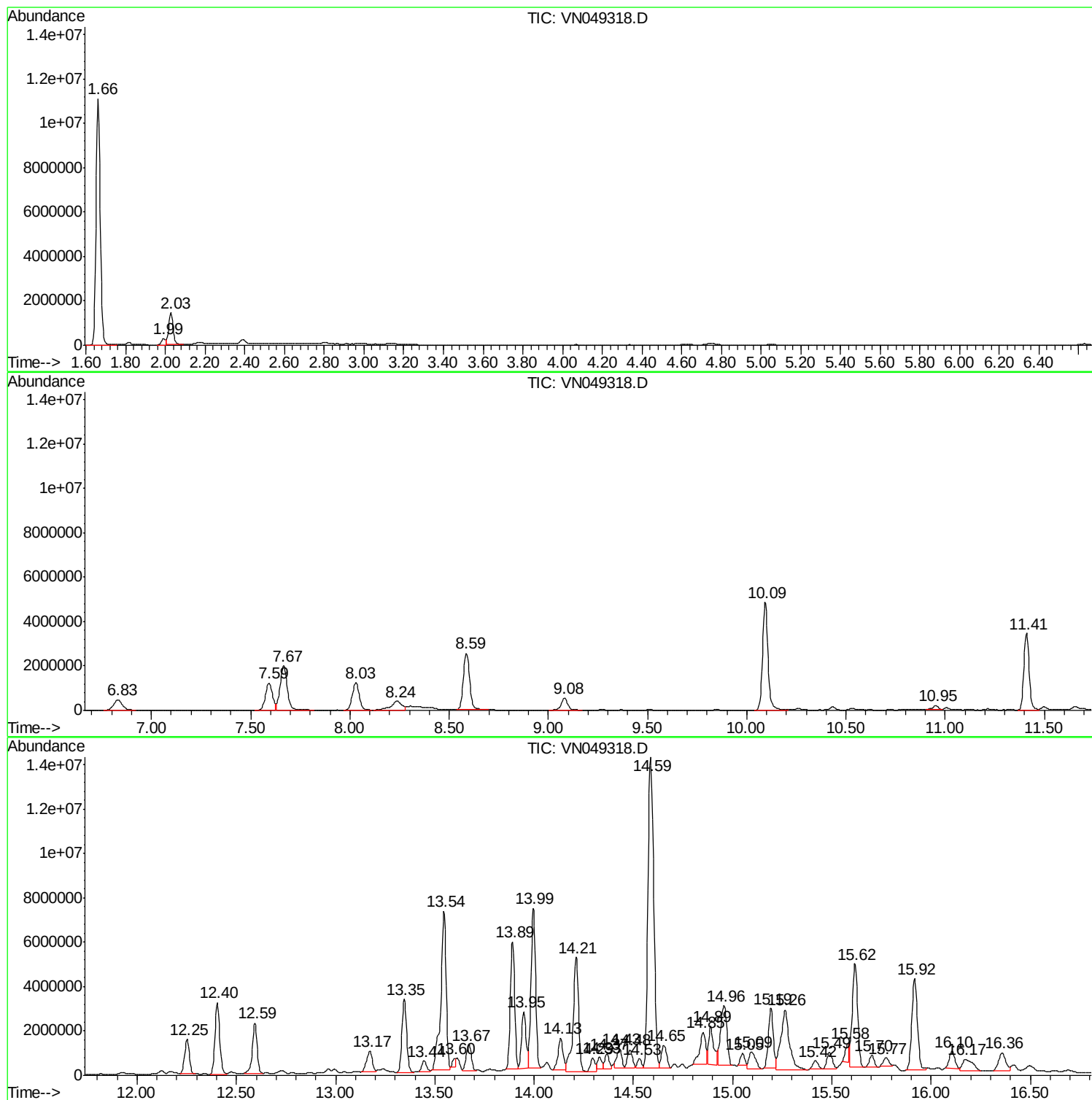
Sum of corrected areas: 219738598

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



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Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	123.98 ug/l	13816800	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane	118 C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118 C9H10	1000191-13-7	83
3	Deltacyclene	118 C9H10	007785-10-6	72
4	Benzene, 1-ethenyl-4-methyl-	118 C9H10	000622-97-9	64
5	Benzene, 1,1'-(1,5-hexadiene-1,6...	234 C18H18	004439-45-6	59

Peak Number 2 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	76.58 ug/l	8534710	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14	000874-41-9	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5	96
3	Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134 C10H14	002870-04-4	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2	95

Peak Number 3 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	105.60 ug/l	11768700	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Phenyl-1-butene	132 C10H12	000824-90-8	70
2	Benzene, (2-methyl-1-propenyl)-	132 C10H12	000768-49-0	70
3	Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0	64
4	Indan, 1-methyl-	132 C10H12	000767-58-8	64
5	Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4	62

Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
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14.21	86.85 ug/l	9679800	1,4-Dichlorobenzene-d4	13.35			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	94
5			p-Cymene	134	C10H14	000099-87-6	94

 Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	247.24 ug/l	27553900	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	87
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81

 Peak Number 6 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.96	53.02 ug/l	5909540	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	70
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70

 Peak Number 7 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.26	74.60 ug/l	8313540	1,4-Dichlorobenzene-d4	13.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1 Naphthalene, 1,2,3,4-tetrahydro-... 146 C11H14 001559-81-5 94
2 1H-Indene, 2,3-dihydro-1,3-dimet... 146 C11H14 004175-53-5 90
3 1H-Indene, 2,3-dihydro-4,7-dimet... 146 C11H14 006682-71-9 90
4 1H-Indene, 2,3-dihydro-1,6-dimet... 146 C11H14 017059-48-2 87
5 Benzene, (1,2-dimethyl-1-propenyl)- 146 C11H14 000769-57-3 86
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 Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	76.75 ug/l	8554070	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	87
3		1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	46
4		2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	43
5		1,5-Naphthyridin-4-ol	146	C8H6N2O	005423-54-1	38

 Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	73.62 ug/l	8205080	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3		1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	90
4		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
5		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Indane	13.54	124.0	ug/l	13816800	4	13.35	5572430	50.0
Benzene, 1-ethyl-...	13.89	76.6	ug/l	8534710	4	13.35	5572430	50.0
1-Phenyl-1-butene	13.99	105.6	ug/l	11768700	4	13.35	5572430	50.0
Benzene, 1,2,3,4-...	14.21	86.8	ug/l	9679800	4	13.35	5572430	50.0
Benzene, 1,2,4,5-...	14.59	247.2	ug/l	27553900	4	13.35	5572430	50.0
Bicyclo[4.2.0]oct...	14.96	53.0	ug/l	5909540	4	13.35	5572430	50.0
Naphthalene, 1,2,...	15.26	74.6	ug/l	8313540	4	13.35	5572430	50.0
Naphthalene, 1,2,...	15.62	76.8	ug/l	8554070	4	13.35	5572430	50.0
Naphthalene, 1,2,...	15.92	73.6	ug/l	8205080	4	13.35	5572430	50.0