

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061618\
 Data File : VN049315.D
 Acq On : 16 Jun 2018 17:46
 Operator : MD\SY
 Sample : J3564-01
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-15

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	1.658	3	21	48	rBV	8672675	13106500	100.00%	22.564%
2	2.027	129	136	140	rBV	113761	158048	1.21%	0.272%
3	7.593	1847	1867	1878	rBV2	1063353	2675746	20.42%	4.607%
4	7.667	1878	1890	1921	rVB	1587003	3813896	29.10%	6.566%
5	8.030	1985	2003	2033	rBV	1059210	2527111	19.28%	4.351%
6	8.233	2040	2066	2068	rBV4	113260	332482	2.54%	0.572%
7	8.587	2160	2176	2217	rBV	2269502	4880505	37.24%	8.402%
8	10.095	2629	2645	2684	rBV	4102391	7797378	59.49%	13.424%
9	11.410	3039	3054	3073	rBV	2900778	5193591	39.63%	8.941%
10	12.120	3268	3275	3294	rVB8	77142	133604	1.02%	0.230%
11	12.403	3350	3363	3379	rBV	2283887	4017934	30.66%	6.917%
12	12.564	3405	3413	3428	rVB5	127285	259070	1.98%	0.446%
13	13.162	3590	3599	3610	rBV3	154282	350365	2.67%	0.603%
14	13.345	3645	3656	3670	rVB	2178155	3655412	27.89%	6.293%
15	13.445	3680	3687	3695	rBV	186987	283224	2.16%	0.488%
16	13.664	3746	3755	3768	rVB6	352347	670306	5.11%	1.154%
17	13.998	3848	3859	3868	rBV2	620272	1088097	8.30%	1.873%
18	14.133	3891	3901	3908	rBV	490306	840402	6.41%	1.447%
19	14.175	3908	3914	3918	rVV4	390586	633034	4.83%	1.090%
20	14.213	3919	3926	3941	rVB2	964372	1738996	13.27%	2.994%
21	14.332	3956	3963	3970	rBV5	271613	430055	3.28%	0.740%
22	14.535	4021	4026	4034	rVB3	105940	139557	1.06%	0.240%
23	14.654	4055	4063	4073	rVB6	290277	594398	4.54%	1.023%
24	14.853	4118	4125	4133	rVB2	481633	664924	5.07%	1.145%
25	15.117	4202	4207	4216	rVB3	315587	436795	3.33%	0.752%
26	15.191	4221	4230	4239	rBV	632675	1085723	8.28%	1.869%
27	16.352	4586	4591	4604	rVB5	288552	578785	4.42%	0.996%

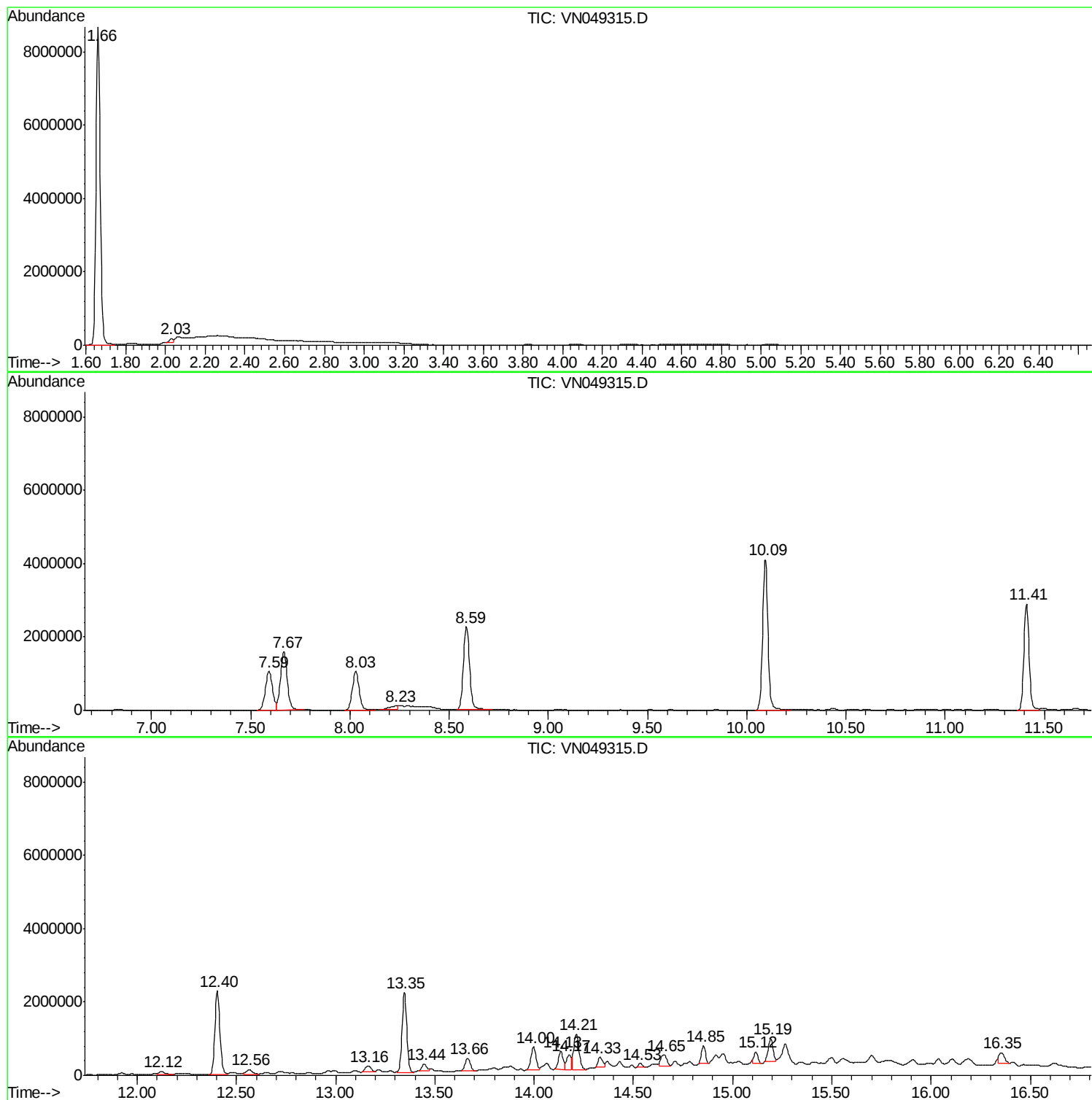
Sum of corrected areas: 58085938

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Quant Title : SW846 8260

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



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Peak Number 1 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	14.88 ug/l	1088100	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4 87
2		Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0 87
3		Benzene, 1-methyl-2-(2-propenyl)-	132 C10H12	001587-04-8 87
4		Benzene, 2-butenyl-	132 C10H12	001560-06-1 86
5		Benzene, (2-methyl-1-propenyl)-	132 C10H12	000768-49-0 86

Peak Number 2 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	11.50 ug/l	840402	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Indene, 2,3-dihydro-4,7-dimet...	146 C11H14	006682-71-9 91
2		1H-Indene, 2,3-dihydro-1,1-dimet...	146 C11H14	004912-92-9 90
3		1H-Indene, 2,3-dihydro-1,3-dimet...	146 C11H14	004175-53-5 90
4		2,2-Dimethylindene, 2,3-dihydro-	146 C11H14	020836-11-7 87
5		Cyclopropane, 1-chloro-1-methyl-...	166 C10H11Cl	1000161-07-9 72

Peak Number 3 unknown14.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	8.66 ug/l	633034	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2-Ethyl[1,3]dithiane	148 C6H12S2	006007-23-4 35
2		1-Ethanone, 1-(5,6-dimethyl-3H-t...	194 C9H10N2OS	1000337-12-5 35
3		4-Methylbenzamide, N-(4-methoxyb...	268 C16H16N2O2	051771-24-5 22
4		1,3,8-p-Menthatriene	134 C10H14	018368-95-1 16
5		1,3,5-Cycloheptatriene, 3,7,7-tr...	134 C10H14	003479-89-8 12

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
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14.21	23.79 ug/l	1739000	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, 1,2,3,5-tetramethyl-	134 C10H14	000527-53-7 95
3		o-Cymene	134 C10H14	000527-84-4 91
4		1,3-Cyclopentadiene, 1,2,3,4-tet...	134 C10H14	076089-59-3 91
5		Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2 91

 Peak Number 5 unknown14.65 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	8.13 ug/l	594398	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-methyl-4-(1-methylpro...	148 C11H16	001595-16-0 43
2		Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9 38
3		Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14	000934-74-7 38
4		o-Cymene	134 C10H14	000527-84-4 38
5		Benzene, (1,1-dimethylpropyl)-	148 C11H16	002049-95-8 35

 Peak Number 6 unknown14.85 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	9.10 ug/l	664924	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, pentamethyl-	148 C11H16	000700-12-9 49
2		Benzene, 1,3-dimethyl-5-(1-methy...	148 C11H16	004706-90-5 46
3		Benzene, 1,4-dimethyl-2-(1-methy...	148 C11H16	004132-72-3 46
4		Phenol, 2-(2-methyl-2-propenyl)-	148 C10H12O	020944-88-1 46
5		Benzene, 2,4-dimethyl-1-(1-methy...	148 C11H16	004706-89-2 46

 Peak Number 7 Sulfurous acid, 2-ethylhexy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	5.97 ug/l	436795	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual

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1 Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	80
2 Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
3 Tridecane, 7-methyl-	198	C14H30	026730-14-3	74
4 Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	72
5 Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	14.85 ug/l	1085720	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	94
2		2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	62
3		Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	62
4		Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	35
5		[2.2]Paracyclophane	208	C16H16	001633-22-3	35

Peak Number 9 1-Naphthalenemethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	7.92 ug/l	578785	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Naphthalenemethanol	158	C11H10O	004780-79-4	53
2		1,4-Ethanonaphthalene, 1,2,3,4-t...	158	C12H14	004175-52-4	50
3		Naphthalene, 1,2-dihydro-2-methyl-	144	C11H12	021564-79-4	47
4		1-(2-Methyl-allyl)-1,2,3,4-tetra...	202	C14H18O	1000192-52-9	42
5		Hexa-2,4-dienylbenzene	158	C12H14	079482-86-3	42

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-etheny...	14.00	14.9	ug/l	1088100	4	13.35	3655410	50.0
1H-Indene, 2,3-di...	14.13	11.5	ug/l	840402	4	13.35	3655410	50.0
unknown14.17	14.17	8.7	ug/l	633034	4	13.35	3655410	50.0
Benzene, 1,2,4,5-...	14.21	23.8	ug/l	1739000	4	13.35	3655410	50.0
unknown14.65	14.65	8.1	ug/l	594398	4	13.35	3655410	50.0
unknown14.85	14.85	9.1	ug/l	664924	4	13.35	3655410	50.0
Sulfurous acid, 2...	15.12	6.0	ug/l	436795	4	13.35	3655410	50.0
Naphthalene, 1,2,...	15.19	14.9	ug/l	1085720	4	13.35	3655410	50.0
1-Naphthalenemeth...	16.35	7.9	ug/l	578785	4	13.35	3655410	50.0