

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061418\
 Data File : VN049223.D
 Acq On : 14 Jun 2018 13:15
 Operator : MD\SY
 Sample : J3435-06
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NW1

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	1.658	3	21	46	rBV	4025647	5887111	22.43%	4.201%
2	2.018	115	133	155	rBV	1834171	2960237	11.28%	2.112%
3	2.179	170	183	198	rBV	6483637	9218049	35.12%	6.577%
4	2.654	321	331	346	rVB	290275	539339	2.05%	0.385%
5	2.802	361	377	403	rBV	13214771	26247216	100.00%	18.728%
6	3.133	465	480	519	rVB	2130043	4880239	18.59%	3.482%
7	3.313	522	536	556	rVB	713810	1550202	5.91%	1.106%
8	3.471	562	585	597	rBV	283886	713253	2.72%	0.509%
9	3.558	597	612	637	rVB	821504	2007891	7.65%	1.433%
10	3.796	663	686	715	rVB5	235469	824055	3.14%	0.588%
11	4.423	855	881	896	rBV4	479289	1590140	6.06%	1.135%
12	4.532	897	915	919	rBV3	560075	1463396	5.58%	1.044%
13	5.053	1050	1077	1112	rBV2	1022399	3661519	13.95%	2.613%
14	5.567	1210	1237	1261	rBV3	85002	266808	1.02%	0.190%
15	6.069	1369	1393	1405	rBV4	134250	433476	1.65%	0.309%
16	6.159	1406	1421	1439	rVV3	315673	1032383	3.93%	0.737%
17	6.259	1440	1452	1470	rVV	154514	470726	1.79%	0.336%
18	6.628	1545	1567	1611	rVB	2604967	8271834	31.52%	5.902%
19	7.593	1848	1867	1873	rBV2	468905	1118981	4.26%	0.798%
20	7.657	1874	1887	1904	rVB2	2202466	6008825	22.89%	4.287%
21	7.876	1940	1955	1966	rBV	207086	508611	1.94%	0.363%
22	8.034	1987	2004	2024	rBV3	743965	1968569	7.50%	1.405%
23	8.172	2027	2047	2058	rBV7	627124	2113274	8.05%	1.508%
24	8.300	2079	2087	2108	rVB3	229778	546559	2.08%	0.390%
25	8.587	2159	2176	2198	rBV	1283940	2894278	11.03%	2.065%
26	9.082	2303	2330	2343	rBV	921821	2472441	9.42%	1.764%
27	10.091	2630	2644	2655	rBV	2058768	3867390	14.73%	2.759%
28	10.156	2656	2664	2677	rVB	786374	1440398	5.49%	1.028%
29	10.304	2702	2710	2723	rVB2	148284	284559	1.08%	0.203%
30	11.410	3040	3054	3073	rBV	2072341	3712456	14.14%	2.649%
31	11.513	3073	3086	3105	rVV	3662009	6189112	23.58%	4.416%
32	11.628	3109	3122	3141	rVB	1780291	3065229	11.68%	2.187%
33	11.950	3199	3222	3242	rBV	407995	735379	2.80%	0.525%
34	12.252	3303	3316	3328	rBV	696550	1136664	4.33%	0.811%

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35	12.403	3350	3363	3380	rBV	1634064	2818056	10.74%	2.011%
36	12.593	3410	3422	3434	rBV	787898	1247022	4.75%	0.890%
37	12.689	3434	3452	3462	rBV	617572	1078872	4.11%	0.770%
38	12.892	3501	3515	3531	rBV	1589232	2564905	9.77%	1.830%
39	13.043	3549	3562	3577	rVB	1978743	3138816	11.96%	2.240%
40	13.172	3585	3602	3612	rBV3	110089	265781	1.01%	0.190%
41	13.345	3644	3656	3679	rVB2	1847383	3726185	14.20%	2.659%
42	13.545	3697	3718	3728	rBV	1985201	3582765	13.65%	2.556%
43	13.593	3728	3733	3749	rVB4	202031	452973	1.73%	0.323%
44	13.731	3766	3776	3788	rVB2	157833	337491	1.29%	0.241%
45	13.805	3788	3799	3816	rBV	424077	841305	3.21%	0.600%
46	13.892	3816	3826	3836	rVV	557639	854651	3.26%	0.610%
47	13.998	3849	3859	3872	rVB	1057169	1709131	6.51%	1.220%
48	14.213	3910	3926	3931	rBV	425675	691164	2.63%	0.493%
49	14.252	3931	3938	3947	rVB	668533	1010389	3.85%	0.721%
50	14.477	3999	4008	4019	rBV	466843	722399	2.75%	0.515%
51	14.596	4031	4045	4057	rBV2	1163994	2120257	8.08%	1.513%
52	14.850	4107	4124	4131	rBV3	179398	421015	1.60%	0.300%
53	14.963	4147	4159	4171	rVB2	201142	428985	1.63%	0.306%
54	15.136	4199	4213	4227	rVB	1172284	2056948	7.84%	1.468%

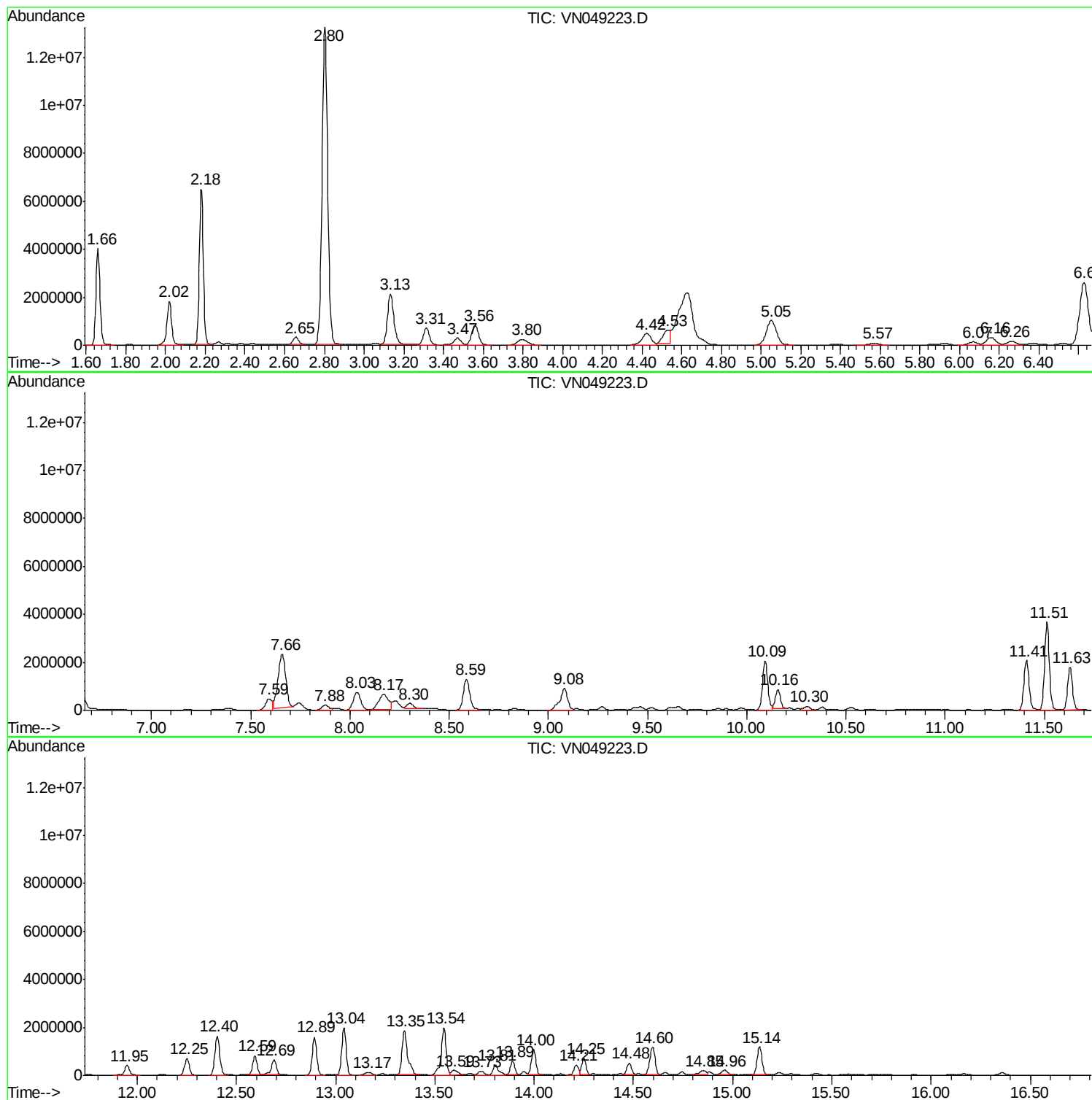
Sum of corrected areas: 140149709

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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 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	76.70 ug/l	9218050	Pentafluorobenzene	7.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane		58	C4H10	000106-97-8	80
2	Isobutane		58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride		142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-		89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-		58	C2H6N2	000503-28-6	5

 Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	218.41 ug/l	26247200	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	36
3	3-Buten-1-ol		72	C4H8O	000627-27-0	28
4	Methane, isocyanato-		57	C2H3NO	000624-83-9	9
5	1-Butene		56	C4H8	000106-98-9	9

 Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	40.61 ug/l	4880240	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	50
3	Diaziridine,3,3-dimethyl-		72	C3H8N2	004901-76-2	9
4	Oxirane, ethyl-		72	C4H8O	000106-88-7	9
5	Isobutyl nitrite		103	C4H9NO2	000542-56-3	9

 Peak Number 4 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
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5.05	30.47 ug/l	3661520	Pentafluorobenzene	7.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40

 Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.63	68.83 ug/l	8271830	Pentafluorobenzene	7.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56

 Peak Number 6 Ethylidenecyclobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.17	36.51 ug/l	2113270	1,4-Difluorobenzene	8.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylidenecyclobutane	82	C6H10	001528-21-8	70
2	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	64
3	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	62
4	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	60
5	Cyclohexene	82	C6H10	000110-83-8	60

 Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.89	34.42 ug/l	2564910	1,4-Dichlorobenzene-d4	13.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1 Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2 Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3 Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4 Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5 Mesitylene	120	C9H12	000108-67-8	91

 Peak Number 8 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	48.08 ug/l	3582770	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	93
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72

 Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	28.45 ug/l	2120260	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	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	2.18	76.7	ug/l	9218050	1	7.67	6008830	50.0
Butane, 2-methyl-	2.80	218.4	ug/l	26247200	1	7.67	6008830	50.0
Pentane	3.13	40.6	ug/l	4880240	1	7.67	6008830	50.0
Pentane, 3-methyl-	5.05	30.5	ug/l	3661520	1	7.67	6008830	50.0
Cyclopentane, met...	6.63	68.8	ug/l	8271830	1	7.67	6008830	50.0
Ethylidenecyclobu...	8.17	36.5	ug/l	2113270	2	8.59	2894280	50.0
Benzene, 1-ethyl-...	12.89	34.4	ug/l	2564910	4	13.35	3726190	50.0
Indane	13.54	48.1	ug/l	3582770	4	13.35	3726190	50.0
Benzene, 2-etheny...	14.60	28.4	ug/l	2120260	4	13.35	3726190	50.0