

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061418\
 Data File : VN049240.D
 Acq On : 14 Jun 2018 20:34
 Operator : MD\SY
 Sample : J3447-03
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 W-19

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	44	rBV	2739072	4020525	81.90%	7.078%
2	1.995	116	126	141	rBV2	47015	88361	1.80%	0.156%
3	3.796	663	686	710	rBV3	129858	420409	8.56%	0.740%
4	4.529	887	914	939	rBV2	302470	1081292	22.03%	1.904%
5	5.050	1054	1076	1101	rBV5	76455	279515	5.69%	0.492%
6	5.847	1308	1324	1341	rBV2	17121	54032	1.10%	0.095%
7	6.358	1460	1483	1498	rBV5	26647	92243	1.88%	0.162%
8	6.522	1518	1534	1554	rVB4	59737	185768	3.78%	0.327%
9	6.828	1611	1629	1648	rVB6	27507	98601	2.01%	0.174%
10	7.387	1791	1803	1826	rVB3	81575	254509	5.18%	0.448%
11	7.593	1846	1867	1878	rBV2	523865	1343860	27.37%	2.366%
12	7.667	1878	1890	1902	rVV	773469	1862521	37.94%	3.279%
13	7.744	1902	1914	1945	rVB	612361	1631748	33.24%	2.873%
14	7.934	1959	1973	1987	rVB2	92961	226558	4.62%	0.399%
15	8.030	1987	2003	2026	rBV	546339	1314083	26.77%	2.314%
16	8.156	2026	2042	2051	rBV3	274252	704952	14.36%	1.241%
17	8.587	2159	2176	2197	rBV	1384078	3028448	61.69%	5.332%
18	8.825	2236	2250	2268	rBV6	92304	227564	4.64%	0.401%
19	9.050	2301	2320	2342	rBV2	450700	1048074	21.35%	1.845%
20	9.159	2343	2354	2365	rVB7	39935	87428	1.78%	0.154%
21	9.227	2365	2375	2385	rBV5	32528	73462	1.50%	0.129%
22	9.365	2400	2418	2434	rBV	490969	1067937	21.75%	1.880%
23	9.516	2453	2465	2485	rVB5	159967	333720	6.80%	0.588%
24	9.654	2488	2508	2518	rBV5	143841	399722	8.14%	0.704%
25	9.706	2520	2524	2535	rVV4	53538	85278	1.74%	0.150%
26	9.767	2536	2543	2554	rVB8	28369	61575	1.25%	0.108%
27	9.844	2554	2567	2581	rBV2	440928	908418	18.50%	1.599%
28	9.918	2582	2590	2599	rBV5	27312	53593	1.09%	0.094%
29	10.008	2610	2618	2630	rVB4	113696	234292	4.77%	0.412%
30	10.091	2630	2644	2677	rBV	2438744	4909138	100.00%	8.643%
31	10.259	2682	2696	2719	rBV2	703247	1805713	36.78%	3.179%
32	10.365	2719	2729	2739	rBV3	82012	190758	3.89%	0.336%
33	10.435	2739	2751	2763	rVV	1416909	2568603	52.32%	4.522%
34	10.522	2764	2778	2793	rVV5	1140022	2471568	50.35%	4.351%

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35	10.593	2794	2800	2819	rVB7	114167	315950	6.44%	0.556%
36	10.680	2819	2827	2835	rBV8	29307	59529	1.21%	0.105%
37	10.738	2836	2845	2851	rBV6	45245	80878	1.65%	0.142%
38	10.792	2854	2862	2869	rBV2	153435	245564	5.00%	0.432%
39	10.837	2869	2876	2884	rVB2	116807	175998	3.59%	0.310%
40	10.918	2893	2901	2912	rVB2	460557	791257	16.12%	1.393%
41	11.005	2912	2928	2938	rVV6	143148	417749	8.51%	0.735%
42	11.066	2938	2947	2955	rVV5	160763	304046	6.19%	0.535%
43	11.114	2956	2962	2974	rVB7	124649	214331	4.37%	0.377%
44	11.217	2979	2994	3000	rBV5	181688	382661	7.79%	0.674%
45	11.323	3015	3027	3038	rBV3	236190	468940	9.55%	0.826%
46	11.410	3042	3054	3070	rVV	2212611	4026742	82.03%	7.089%
47	11.497	3072	3081	3092	rVV	496471	865977	17.64%	1.525%
48	11.593	3105	3111	3118	rBV10	53740	77340	1.58%	0.136%
49	11.654	3119	3130	3152	rVB7	293926	848880	17.29%	1.494%
50	11.751	3153	3160	3168	rBV4	54213	86228	1.76%	0.152%
51	11.815	3169	3180	3189	rBV	331814	546209	11.13%	0.962%
52	11.870	3190	3197	3204	rBV3	58351	96215	1.96%	0.169%
53	11.921	3204	3213	3221	rVV3	160839	298791	6.09%	0.526%
54	11.972	3222	3229	3254	rVB6	208181	602352	12.27%	1.060%
55	12.120	3254	3275	3291	rBV2	500243	1161062	23.65%	2.044%
56	12.201	3293	3300	3312	rVB7	107816	202716	4.13%	0.357%
57	12.262	3313	3319	3322	rBV3	46486	58254	1.19%	0.103%
58	12.310	3325	3334	3351	rVV10	150148	439505	8.95%	0.774%
59	12.403	3352	3363	3379	rVV	1712011	3240778	66.02%	5.706%
60	12.474	3379	3385	3398	rVB3	205559	369173	7.52%	0.650%
61	12.567	3408	3414	3436	rVB7	117166	229025	4.67%	0.403%
62	12.863	3498	3506	3517	rVB3	93582	158192	3.22%	0.279%
63	12.966	3529	3538	3554	rVB5	123769	292795	5.96%	0.515%
64	13.098	3571	3579	3589	rVB4	118093	202357	4.12%	0.356%
65	13.175	3589	3603	3612	rBV3	301310	607953	12.38%	1.070%
66	13.349	3646	3657	3666	rBV	1606753	2753871	56.10%	4.848%
67	13.596	3724	3734	3746	rBV2	86072	158361	3.23%	0.279%
68	13.670	3748	3757	3767	rVB6	64634	126003	2.57%	0.222%
69	13.815	3795	3802	3809	rBV2	46707	78668	1.60%	0.138%
70	13.927	3832	3837	3848	rVB	45810	71797	1.46%	0.126%
71	14.001	3850	3860	3865	rBV5	53323	94424	1.92%	0.166%

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72	14.043	3867	3873	3876	rBV3	54911	67261	1.37%	0.118%
73	14.136	3892	3902	3909	rBV	148729	227236	4.63%	0.400%
74	14.185	3910	3917	3925	rVV5	50621	115562	2.35%	0.203%
75	14.230	3927	3931	3944	rVB3	59343	90734	1.85%	0.160%
76	14.329	3948	3962	3973	rVB	286814	473215	9.64%	0.833%
77	14.435	3985	3995	4003	rBV	185749	284789	5.80%	0.501%
78	14.493	4003	4013	4022	rVV2	278039	438114	8.92%	0.771%
79	14.667	4058	4067	4078	rVB2	83033	133340	2.72%	0.235%
80	14.947	4133	4154	4168	rVB3	226266	486302	9.91%	0.856%
81	15.268	4241	4254	4274	rVB9	34556	118897	2.42%	0.209%

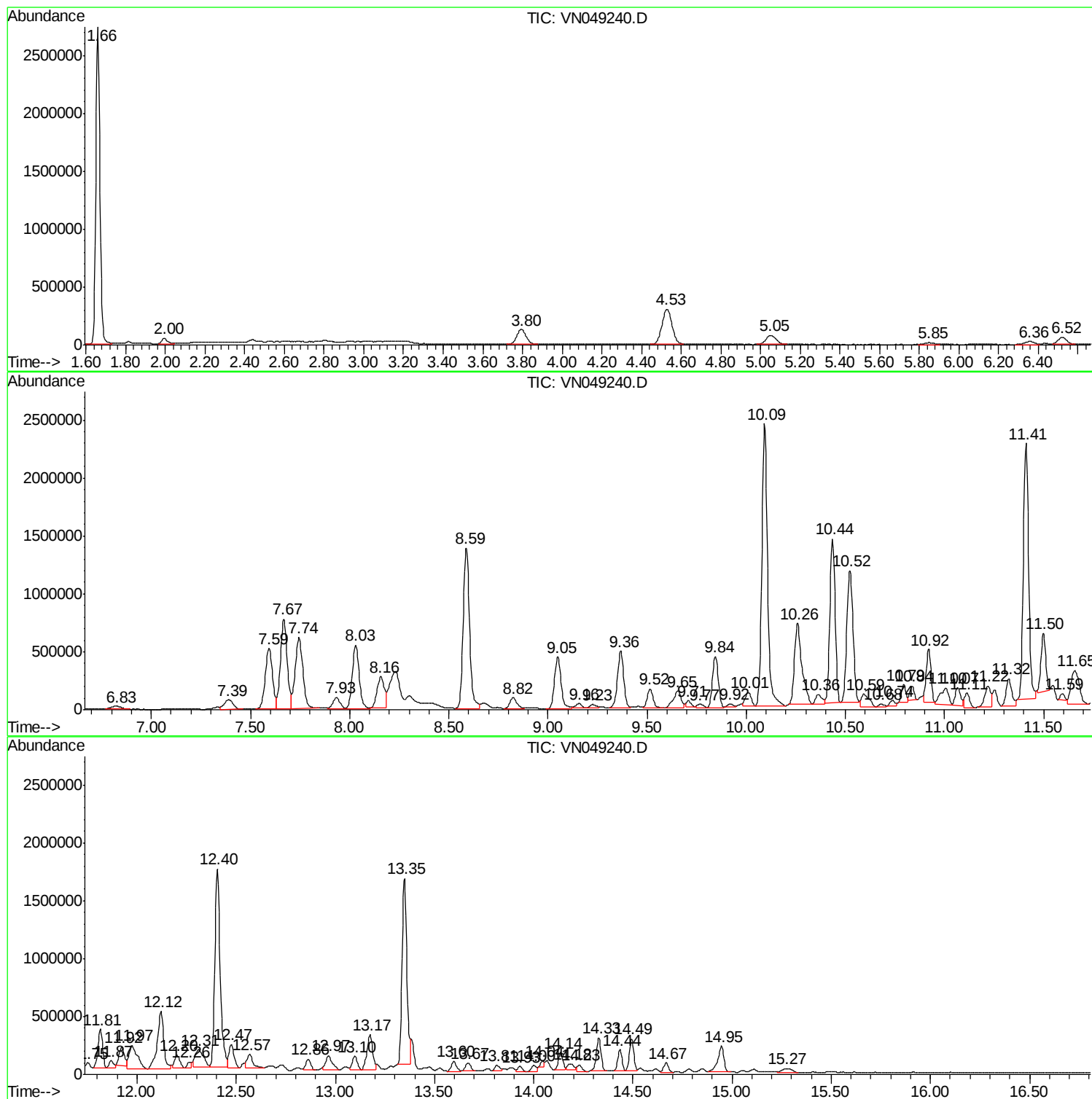
Sum of corrected areas: 56800289

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



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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	29.03 ug/l	1081290	Pentafluorobenzene	7.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8 86
2	Butane, 2-methyl-	72	C5H12	000078-78-4 38
3	1-Pentene	70	C5H10	000109-67-1 28
4	Pentane, 2-methyl-	86	C6H14	000107-83-5 17
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9 9

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	43.80 ug/l	1631750	Pentafluorobenzene	7.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3 94
2	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3 59
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8 47
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5 42
5	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1 40

Peak Number 3 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	17.30 ug/l	1048070	1,4-Difluorobenzene	8.59
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2 86
2	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9 64
3	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2 58
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9 43
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1 35

Peak Number 4 Cyclopentane, 1,2,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
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9.36	17.63 ug/l	1067940	1,4-Difluorobenzene	8.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	90
2	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	87
3	Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	86
4	Heptane, 3-methylene-	112	C8H16	001632-16-2	72
5	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	72

 Peak Number 5 Cyclopentane, 1,1,2-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.84	15.00 ug/l	908418	1,4-Difluorobenzene	8.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	91
2	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	72
3	2-Chloro-2-methylnonane	176	C10H21Cl	004325-50-2	59
4	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	49
5	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	46

 Peak Number 6 Cyclohexane, 1,1-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.26	22.42 ug/l	1805710	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	94
2	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	80
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
4	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	50
5	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	50

 Peak Number 7 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.44	31.89 ug/l	2568600	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	94
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	90
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87
5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	87

Peak Number 8 1,3-Dimethyl-1-cyclohexene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	30.69 ug/l	2471570	Chlorobenzene-d5	11.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	64
2			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	64
3			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	58
4			Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	53
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	53

Peak Number 9 Bicyclo[3.3.1]nonane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	14.42 ug/l	1161060	Chlorobenzene-d5	11.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	68
2			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	52
3			Cyclohexene,3-propyl-	124	C9H16	003983-06-0	49
4			Cyclohexane, 1-propenyl-	124	C9H16	005364-83-0	49
5			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	46

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2,3-dimet...	4.53	29.0	ug/l	1081290	1	7.67	1862520	50.0
Pentane, 2,3-dime...	7.74	43.8	ug/l	1631750	1	7.67	1862520	50.0
Cyclopentane, 1,1...	9.05	17.3	ug/l	1048070	2	8.59	3028450	50.0
Cyclopentane, 1,2...	9.36	17.6	ug/l	1067940	2	8.59	3028450	50.0
Cyclopentane, 1,1...	9.84	15.0	ug/l	908418	2	8.59	3028450	50.0
Cyclohexane, 1,1-...	10.26	22.4	ug/l	1805710	3	11.41	4026740	50.0
Cyclohexane, 1,2-...	10.44	31.9	ug/l	2568600	3	11.41	4026740	50.0
1,3-Dimethyl-1-cy...	10.52	30.7	ug/l	2471570	3	11.41	4026740	50.0
Bicyclo[3.3.1]nonane	12.12	14.4	ug/l	1161060	3	11.41	4026740	50.0