

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN032319\
 Data File : VN054630.D
 Acq On : 24 Mar 2019 3:53
 Operator : JC/SP
 Sample : K2043-11ME
 Misc : 5.68g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WP022SB430-190319-(23-26)ME

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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	2.188	119	129	137	rVB2	19735	29531	1.03%	0.171%
2	2.510	203	229	231	rBV5	43427	127048	4.43%	0.734%
3	2.558	236	244	258	rVB	306370	473233	16.49%	2.735%
4	6.822	1550	1570	1591	rBV2	141621	408059	14.22%	2.358%
5	7.587	1790	1808	1819	rBV2	355916	870109	30.32%	5.028%
6	7.661	1819	1831	1852	rVB	619641	1490534	51.94%	8.614%
7	8.024	1928	1944	1964	rBV	410666	951845	33.17%	5.501%
8	8.584	2103	2118	2155	rVB	950470	2096220	73.05%	12.114%
9	10.088	2565	2586	2620	rBV	1420408	2869726	100.00%	16.584%
10	11.407	2981	2996	3027	rBV	1244800	2329385	81.17%	13.461%
11	12.043	3182	3194	3204	rVB3	33852	57274	2.00%	0.331%
12	12.153	3222	3228	3238	rVB2	24395	39348	1.37%	0.227%
13	12.336	3279	3285	3289	rBV4	23306	30381	1.06%	0.176%
14	12.400	3295	3305	3326	rVB	984611	1733723	60.41%	10.019%
15	12.654	3368	3384	3395	rBV9	18545	50058	1.74%	0.289%
16	12.725	3396	3406	3412	rBV3	53522	96702	3.37%	0.559%
17	12.876	3446	3453	3460	rVB2	25335	35916	1.25%	0.208%
18	12.927	3462	3469	3472	rBV2	30478	39686	1.38%	0.229%
19	12.963	3472	3480	3493	rVB2	136078	219931	7.66%	1.271%
20	13.088	3512	3519	3528	rBV4	28952	50543	1.76%	0.292%
21	13.140	3529	3535	3549	rVB3	38962	72225	2.52%	0.417%
22	13.284	3572	3580	3585	rBV2	73045	110193	3.84%	0.637%
23	13.345	3586	3599	3612	rVV	1165085	2105092	73.36%	12.165%
24	13.423	3616	3623	3635	rVB2	77625	120513	4.20%	0.696%
25	13.831	3743	3750	3759	rBV7	43764	78395	2.73%	0.453%
26	13.931	3775	3781	3790	rVB2	49209	66582	2.32%	0.385%
27	14.191	3843	3862	3870	rBV6	162036	439437	15.31%	2.539%
28	14.297	3889	3895	3903	rBV3	77251	107823	3.76%	0.623%
29	14.638	3995	4001	4017	rVB5	122669	204889	7.14%	1.184%

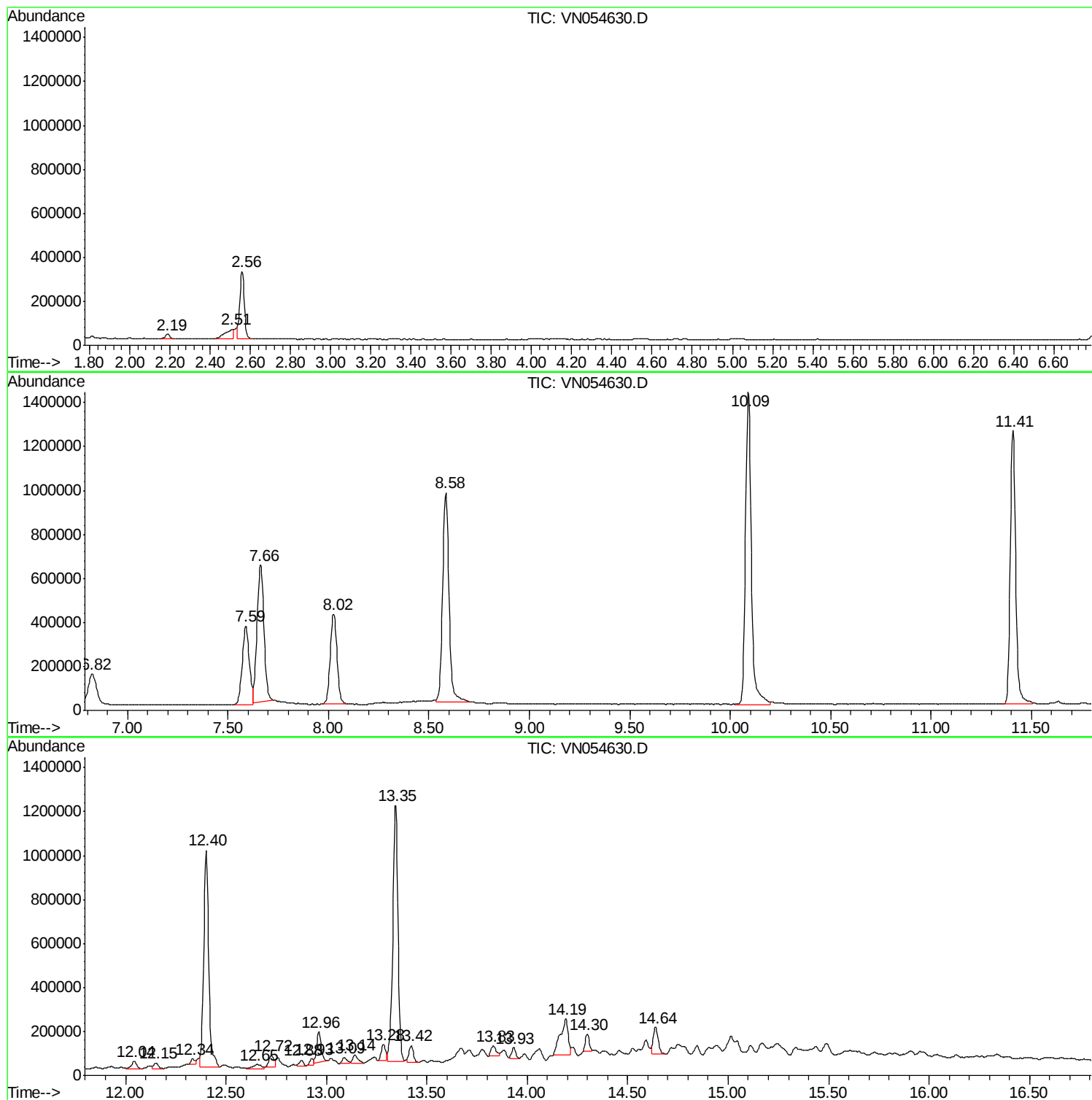
Sum of corrected areas: 17304401

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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



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 Quant Title : SW846 8260

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 TIC Integration Parameters: LSCINT.P

 Peak Number 1 Octane, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	5.22 ug/l	219931	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octane, 3,3-dimethyl-	142 C10H22	004110-44-5 83
2		Heptane, 3,3,5-trimethyl-	142 C10H22	007154-80-5 78
3		Decane, 4-methyl-	156 C11H24	002847-72-5 70
4		Undecane, 4-methyl-	170 C12H26	002980-69-0 59
5		Heptane, 5-ethyl-2-methyl-	142 C10H22	013475-78-0 50

 Peak Number 2 unknown14.19 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	10.44 ug/l	439437	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tricyclo[3.3.1.1(3,7)]decane, 1-...	181 C10H15N02	007575-82-8 49
2		1-Adamantanecarboxylic acid chlo...	198 C11H15ClO	002094-72-6 46
3		2-Adamantan-1-yl-5-(4-nitro-1H-p...	315 C14H17N7O2	1000301-14-4 46
4		2-[1-(Adamantan-1-ylamino)-2,2,2...	295 C15H16F3N3	1000275-90-9 46
5		Phosphonic dichloride, 1-adamantyl-	252 C10H15Cl2OP	1000294-15-7 46

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane, 3,3-dimet...	12.96	5.2	ug/l	219931	4	13.34	2105090	50.0
unknown14.19	14.19	10.4	ug/l	439437	4	13.34	2105090	50.0