

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
 Data File : VN054628.D
 Acq On : 24 Mar 2019 2:58
 Operator : JC/SP
 Sample : K2043-07
 Misc : 6.42g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WP022SB441-190319-(23-25)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	2.516	203	231	233	rBV3	46199	140419	4.94%	0.862%
2	2.558	234	244	259	rVB	262476	422603	14.85%	2.594%
3	6.822	1546	1570	1594	rBV2	73792	227038	7.98%	1.394%
4	7.590	1789	1809	1819	rBV	351376	859937	30.22%	5.278%
5	7.661	1819	1831	1849	rVB	615085	1440721	50.64%	8.843%
6	8.024	1925	1944	1966	rBV	397266	940364	33.05%	5.772%
7	8.584	2103	2118	2173	rVB	939937	2142141	75.29%	13.148%
8	10.088	2565	2586	2634	rBV	1407585	2845229	100.00%	17.464%
9	11.407	2982	2996	3025	rBV	1240806	2313834	81.32%	14.202%
10	12.043	3185	3194	3205	rVB3	25340	45454	1.60%	0.279%
11	12.152	3205	3228	3239	rBV6	24682	73032	2.57%	0.448%
12	12.400	3293	3305	3328	rVB	990003	1702457	59.84%	10.450%
13	12.963	3472	3480	3494	rVB4	41089	74514	2.62%	0.457%
14	13.091	3511	3520	3529	rBV9	18139	39665	1.39%	0.243%
15	13.143	3531	3536	3549	rVB9	18679	33510	1.18%	0.206%
16	13.284	3572	3580	3585	rBV5	31894	50843	1.79%	0.312%
17	13.342	3585	3598	3616	rVB	1136969	1952531	68.62%	11.984%
18	13.657	3690	3696	3705	rVB	34092	67993	2.39%	0.417%
19	14.040	3808	3815	3819	rBV7	32288	50306	1.77%	0.309%
20	14.191	3856	3862	3881	rVB2	164099	314195	11.04%	1.929%
21	14.300	3888	3896	3910	rBV	129301	224537	7.89%	1.378%
22	14.847	4060	4066	4074	rVB2	71526	102647	3.61%	0.630%
23	14.902	4076	4083	4103	rVV5	78750	228194	8.02%	1.401%

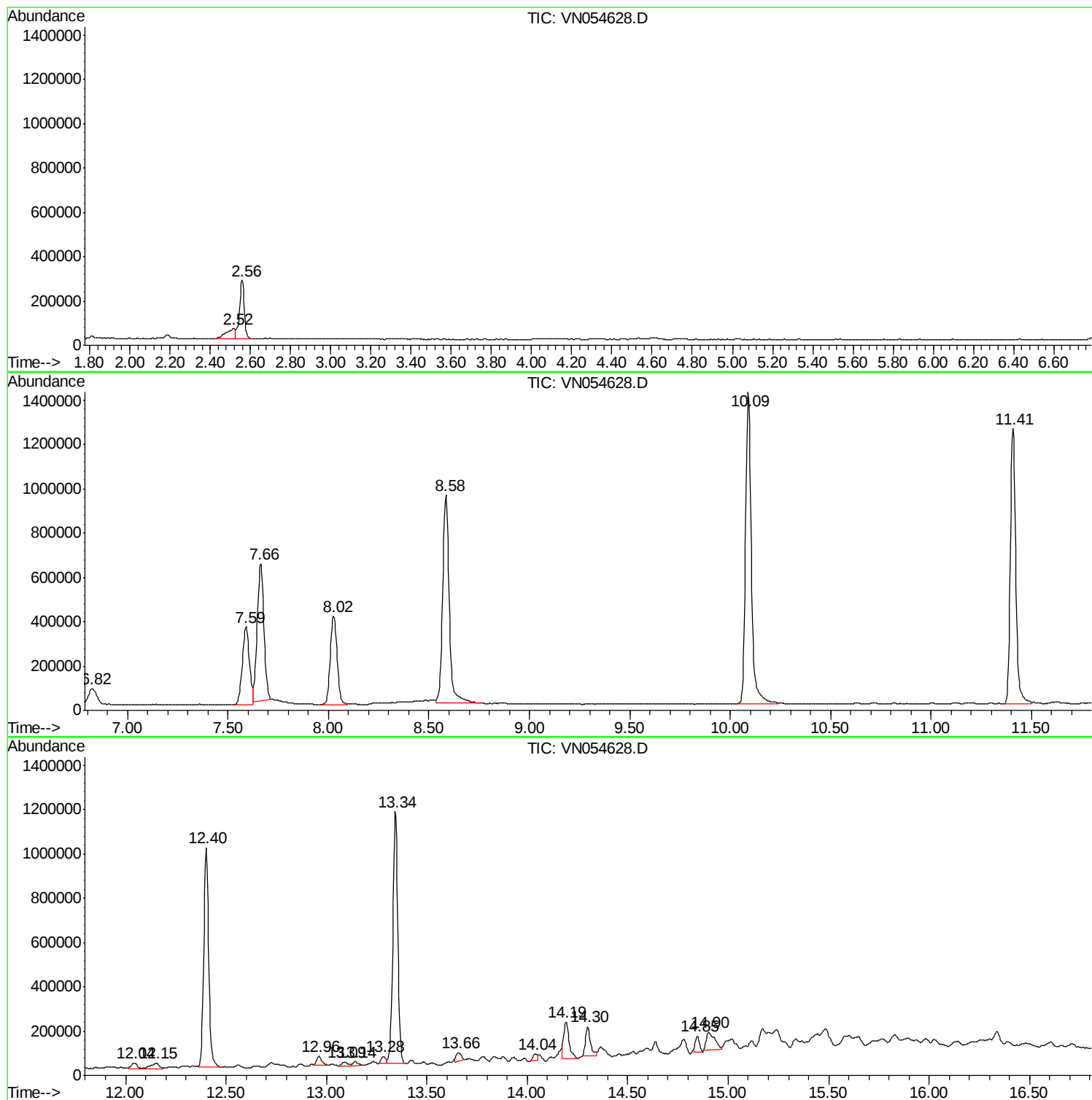
Sum of corrected areas: 16292164

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



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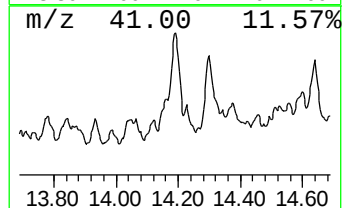
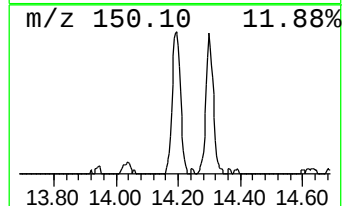
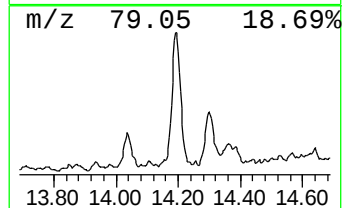
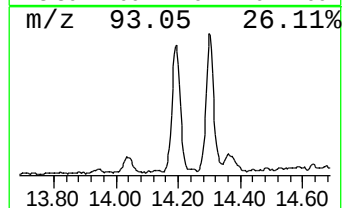
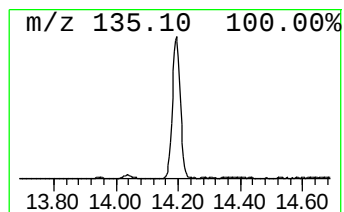
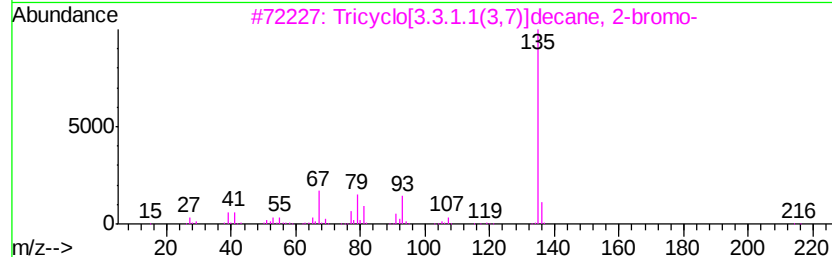
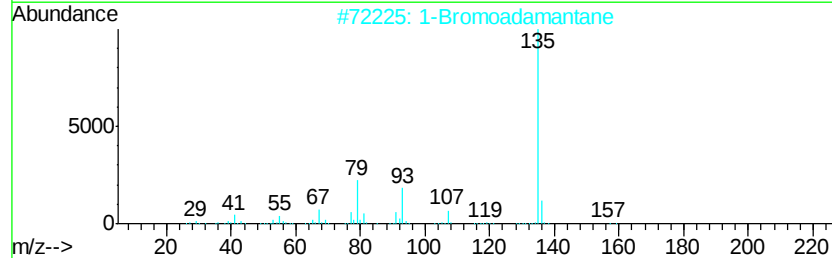
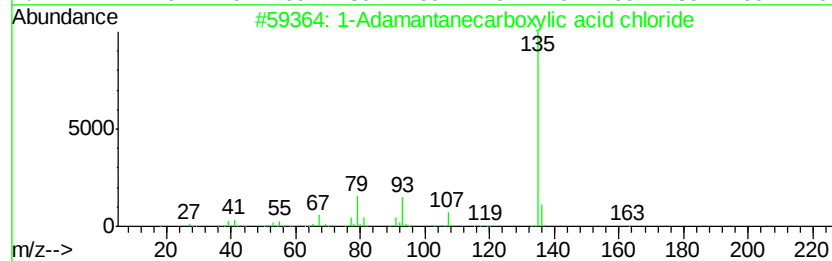
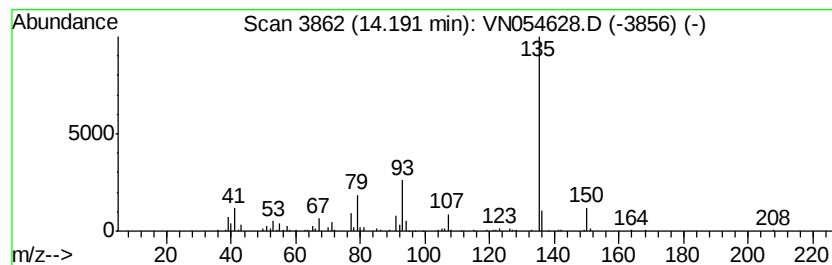
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Adamantanecarboxylic acid... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	8.05 ug/l	314195	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	72
2		1-Bromoadamantane	214	C10H15Br	000768-90-1	72
3		Tricyclo[3.3.1.1(3,7)]decane, 2-...	214	C10H15Br	007314-85-4	72
4		Ethyladamantane-1-carboxylate	208	C13H20O2	002094-73-7	72
5		Adamantane-1-carboxylic acid, (2...	332	C23H24O2	294876-57-6	64



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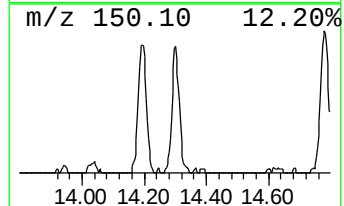
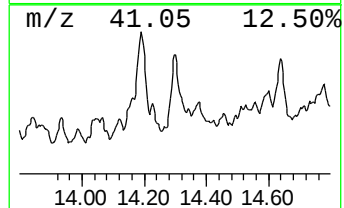
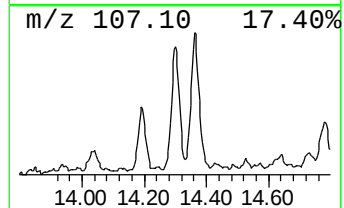
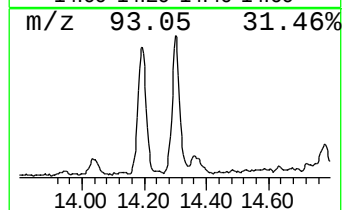
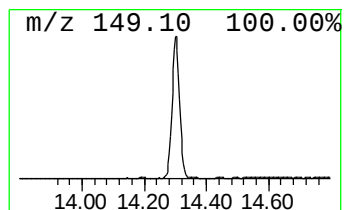
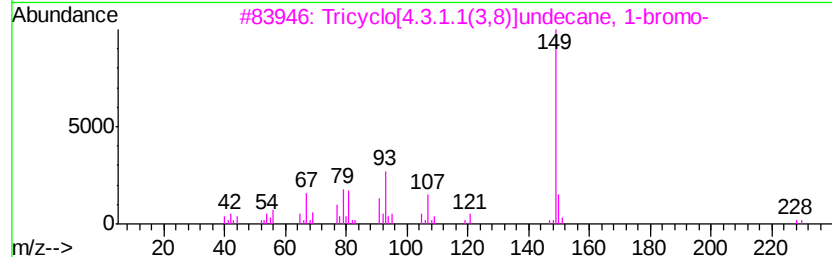
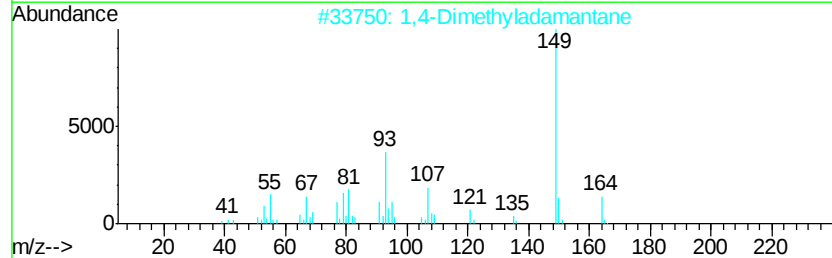
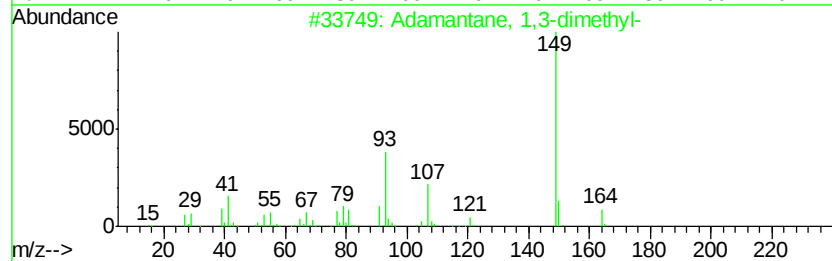
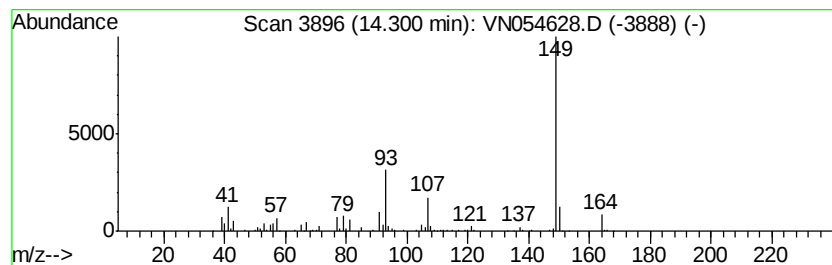
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Peak Number 3 Adamantane, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	5.75 ug/l	224537	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Adamantane, 1,3-dimethyl-	164 C12H20	000702-79-4	91
2	1,4-Dimethyladamantane	164 C12H20	024145-89-9	64
3	Tricyclo[4.3.1.1(3,8)]undecane, ...	228 C11H17Br	021898-96-4	56
4	Pyridinium, 1-(acetyl-amino)-2,6-...	164 C9H12N2O	031020-35-6	45
5	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149 C6H7N5	1000244-21-4	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Adamantanecarbo...	14.19	8.1	ug/l	314195	4	13.34	1952530	50.0
Adamantane, 1,3-d...	14.30	5.8	ug/l	224537	4	13.34	1952530	50.0