

Data Path : Z:\VOASRV\HPCHEM1\MSVOA W\DATA\VW091119\
 Data File : VW012913.D
 Acq On : 11 Sep 2019 13:24
 Operator : SY/VA
 Sample : K4692-15
 Misc : 5.04G/5ML/MSVOA W/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 SB-27-8.5-9.0

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_W\METHOD\82W090719S.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	2.154	35	41	50	rBV	31226	56405	6.09%	0.917%
2	2.660	113	124	125	rBV9	12830	29823	3.22%	0.485%
3	4.123	354	364	372	rBV2	4617	14485	1.56%	0.236%
4	4.903	479	492	507	rBV2	17913	62654	6.77%	1.019%
5	5.933	648	661	675	rBV3	33173	104546	11.29%	1.700%
6	7.878	970	980	985	rBV2	123027	284539	30.74%	4.627%
7	7.945	985	991	1003	rVB	244360	549270	59.34%	8.932%
8	8.299	1039	1049	1061	rBV	125763	284368	30.72%	4.624%
9	8.841	1129	1138	1150	rBV	344764	691194	74.67%	11.240%
10	10.323	1372	1381	1389	rBV	531205	925695	100.00%	15.053%
11	10.707	1438	1444	1449	rVB2	25039	41363	4.47%	0.673%
12	11.231	1525	1530	1535	rVB3	5504	9363	1.01%	0.152%
13	11.627	1587	1595	1604	rBV	437595	743049	80.27%	12.083%
14	11.835	1620	1629	1631	rBV6	6940	13444	1.45%	0.219%
15	11.871	1633	1635	1639	rVV4	8672	12845	1.39%	0.209%
16	12.133	1671	1678	1682	rBV5	11510	25347	2.74%	0.412%
17	12.249	1693	1697	1701	rVB2	8309	13287	1.44%	0.216%
18	12.335	1701	1711	1713	rBV8	9423	21170	2.29%	0.344%
19	12.615	1750	1757	1766	rBV2	353833	588377	63.56%	9.568%
20	12.780	1780	1784	1790	rVB6	7558	15703	1.70%	0.255%
21	12.865	1792	1798	1802	rBV5	7586	18704	2.02%	0.304%
22	12.938	1805	1810	1815	rVB5	14233	26071	2.82%	0.424%
23	13.164	1843	1847	1851	rVV5	9555	13229	1.43%	0.215%
24	13.493	1896	1901	1905	rVB6	5947	10613	1.15%	0.173%
25	13.554	1905	1911	1921	rVB	368920	636979	68.81%	10.358%
26	13.877	1958	1964	1969	rBV3	21282	40462	4.37%	0.658%
27	14.072	1992	1996	1997	rBV4	9345	12379	1.34%	0.201%
28	14.200	2012	2017	2022	rBV7	15449	30142	3.26%	0.490%
29	14.261	2022	2027	2034	rVV3	35066	68164	7.36%	1.108%
30	14.340	2034	2040	2043	rVV7	9184	21334	2.30%	0.347%
31	14.414	2043	2052	2058	rVV	88520	183973	19.87%	2.992%
32	14.523	2063	2070	2076	rVV	68401	141975	15.34%	2.309%
33	14.584	2076	2080	2089	rVB4	26726	58116	6.28%	0.945%
34	14.724	2099	2103	2108	rBV4	18303	32110	3.47%	0.522%

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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 >
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35	14.804	2110	2116	2119	rBV6	23711	53911	5.82%	0.877%
36	14.840	2119	2122	2129	rVB3	28577	55861	6.03%	0.908%
37	15.005	2146	2149	2153	rVB2	15792	20408	2.20%	0.332%
38	15.066	2154	2159	2164	rBV4	22589	42189	4.56%	0.686%
39	15.127	2164	2169	2171	rBV4	21924	35819	3.87%	0.582%
40	15.328	2197	2202	2208	rBV2	38838	71471	7.72%	1.162%
41	15.413	2211	2216	2217	rBV4	20518	31845	3.44%	0.518%
42	15.627	2248	2251	2253	rBV4	10503	16189	1.75%	0.263%
43	16.291	2355	2360	2366	rVB3	21494	40561	4.38%	0.660%

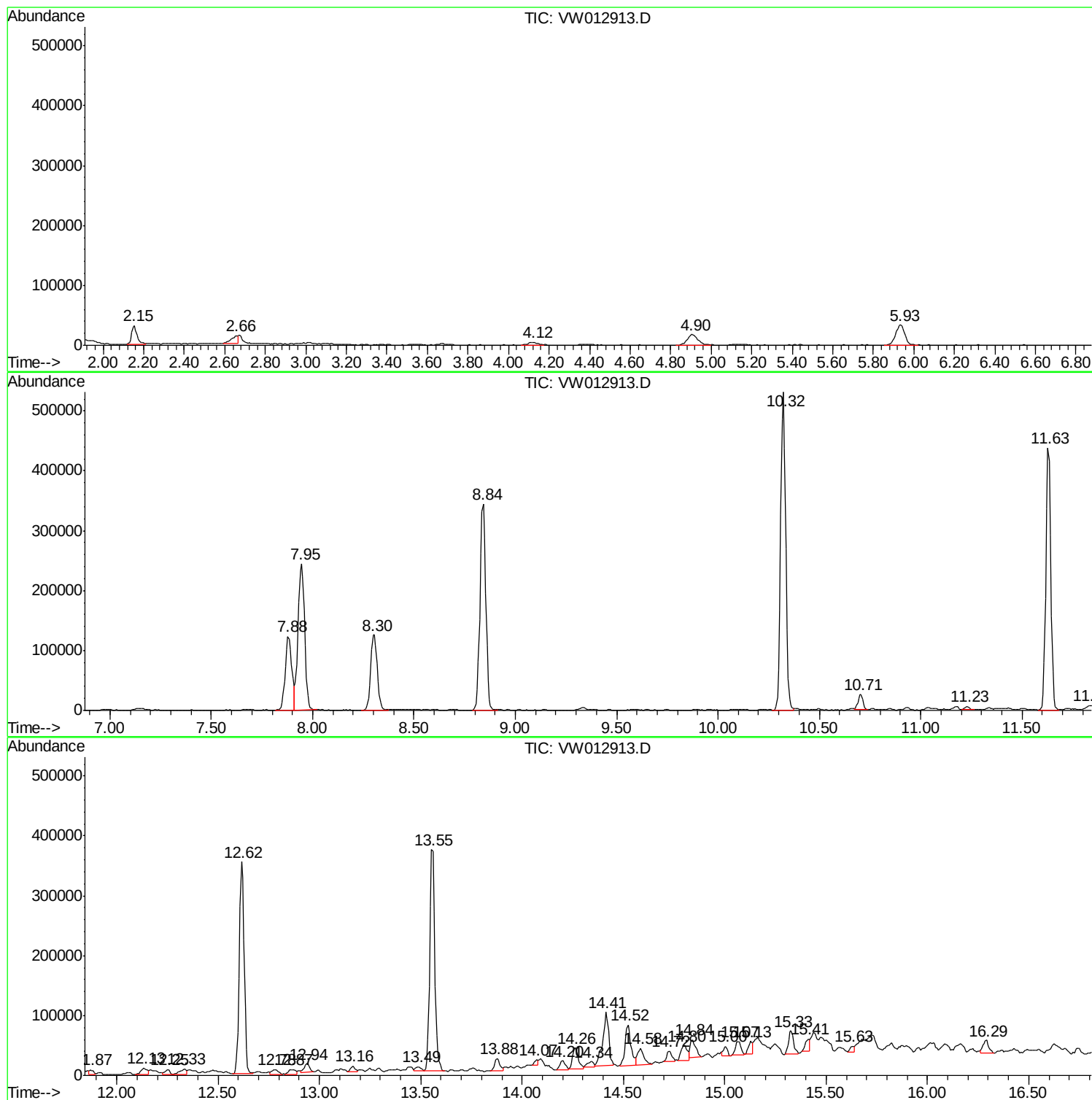
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Quant Title : SW846 8260

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



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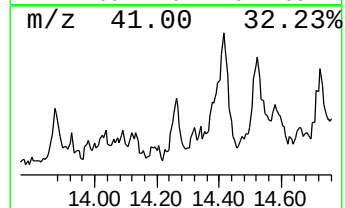
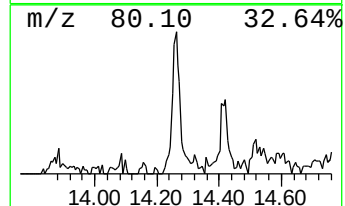
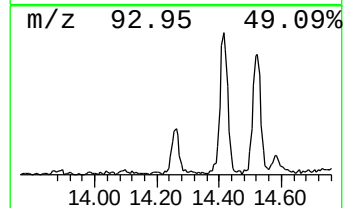
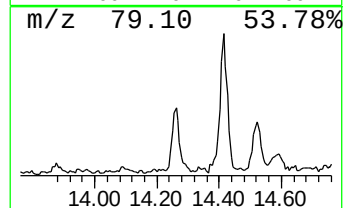
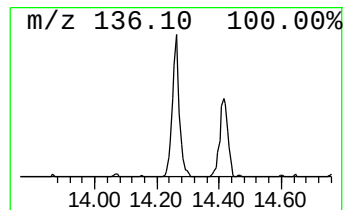
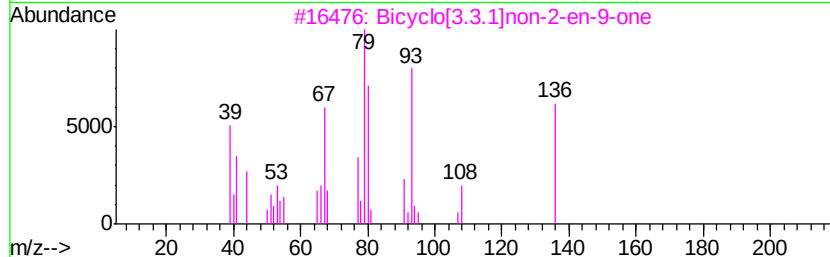
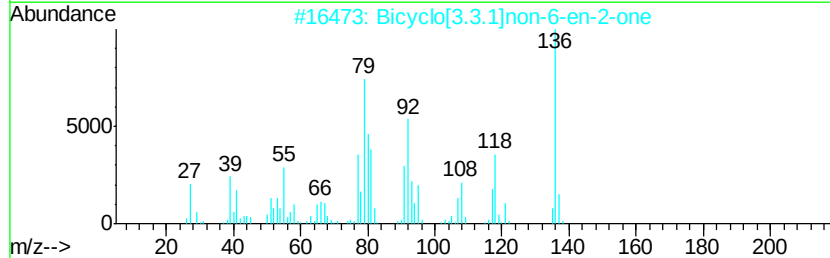
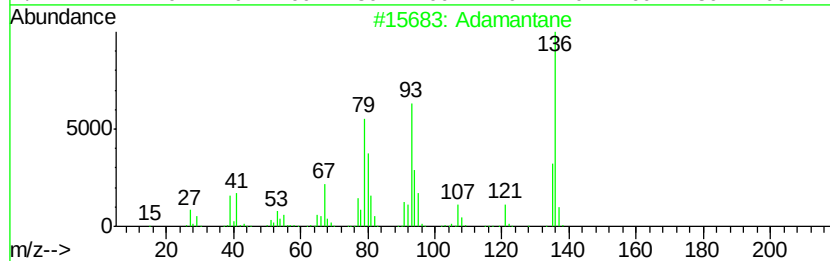
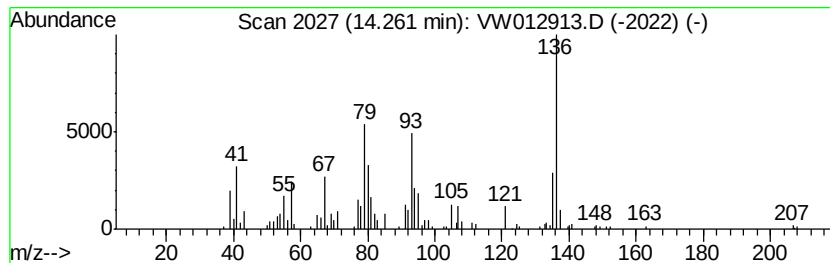
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_W\METHOD\82W090719S.M
Quant Title : SW846 8260

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

Peak Number 3 Adamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	5.35 ug/l	68164	1,4-Dichlorobenzene-d4	13.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane		136	C10H16	000281-23-2	98
2	Bicyclo[3.3.1]non-6-en-2-one		136	C9H12O	022482-58-2	68
3	Bicyclo[3.3.1]non-2-en-9-one		136	C9H12O	004844-11-5	64
4	3-Methylene-bicyclo[3.2.1]oct-6-...		136	C9H12O	1000193-00-0	62
5	1,3-Cyclohexadiene, 5-butyl-		136	C10H16	030168-57-1	47



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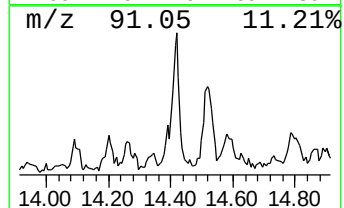
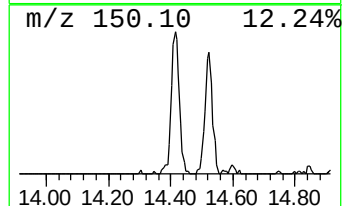
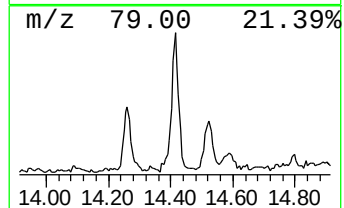
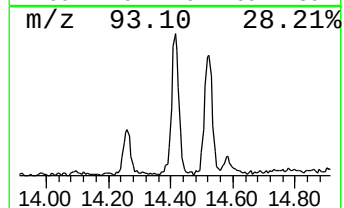
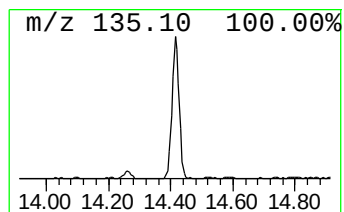
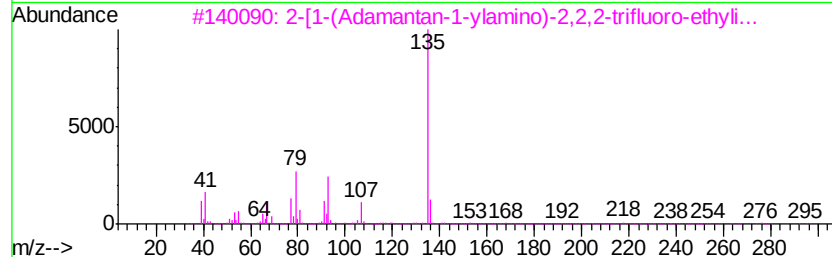
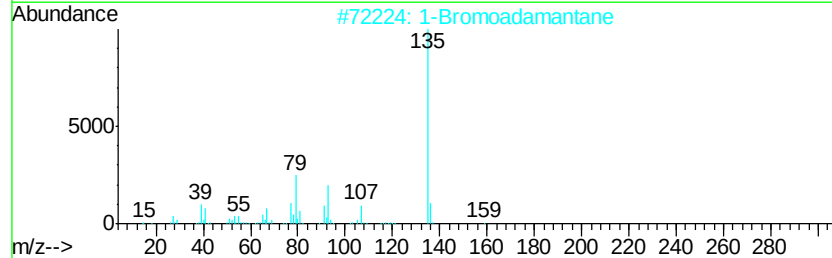
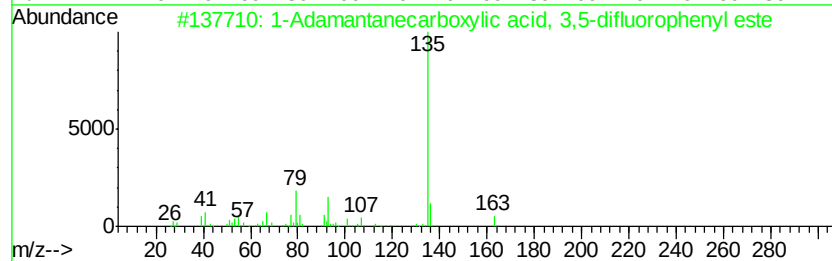
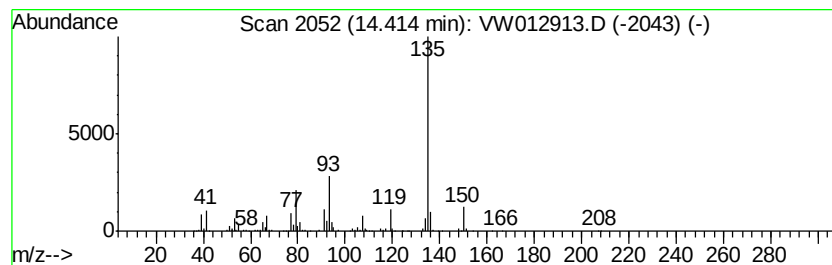
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Peak Number 4 1-Adamantanecarboxylic acid... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	14.44 ug/l	183973	1,4-Dichlorobenzene-d4	13.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanecarboxylic acid, 3,5...	292	C17H18F2O2	1000293-75-1	64	
2	1-Bromoadamantane	214	C10H15Br	000768-90-1	64	
3	2-[1-(Adamantan-1-ylamino)-2,2,2...	295	C15H16F3N3	1000275-90-9	64	
4	Adamantane-1-carboxylic acid, 4-...	284	C18H20O3	1000276-61-1	59	
5	Adamantane-1-carbohydrazide, N2-...	316	C18H21FN2O2	332037-11-3	59	



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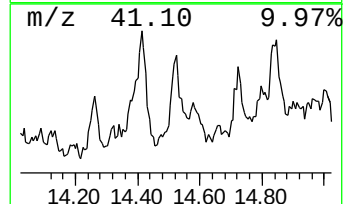
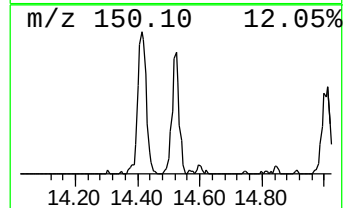
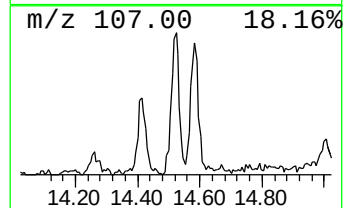
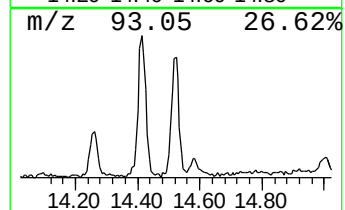
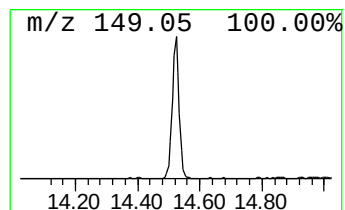
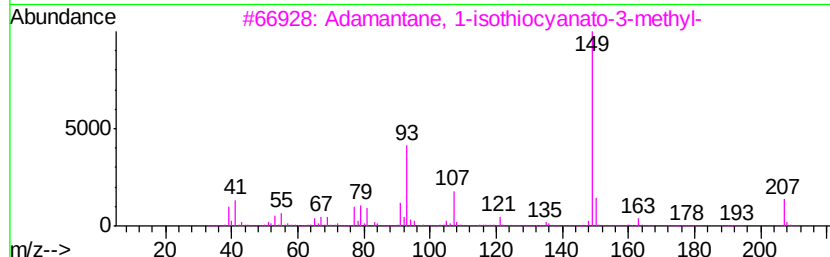
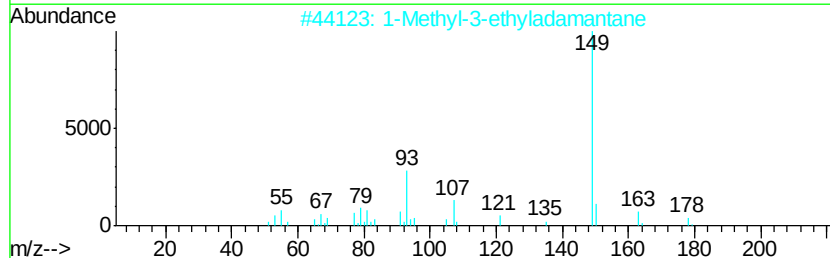
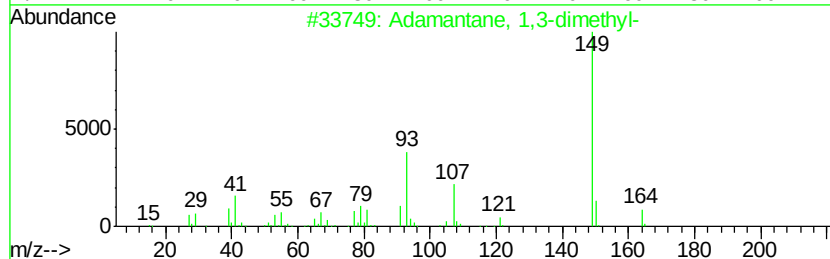
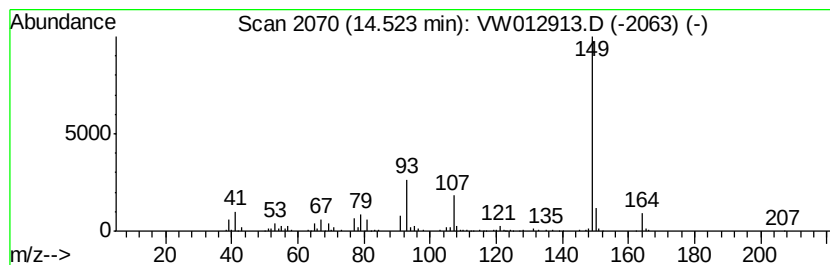
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	11.14 ug/l	141975	1,4-Dichlorobenzene-d4	13.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	91
2		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	72
3		Adamantane, 1-isothiocyanato-3-methyl-	207	C12H17NS	136860-48-5	56
4		Phthalic acid, butyl tridec-2-ynyl-	400	C25H36O4	1000315-43-7	50
5		2-((Octan-2-yloxy)carbonyl)benzoic acid	278	C16H22O4	1000373-83-2	50



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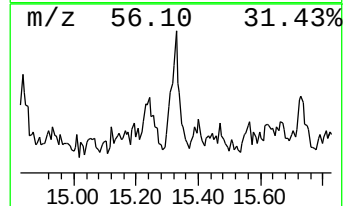
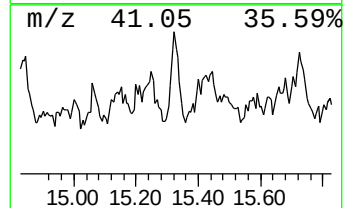
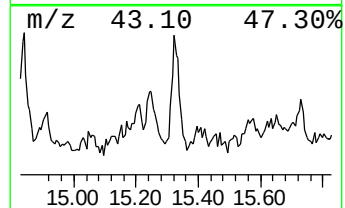
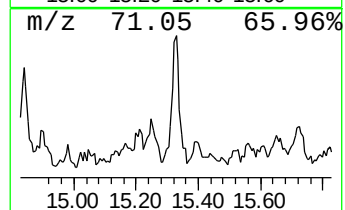
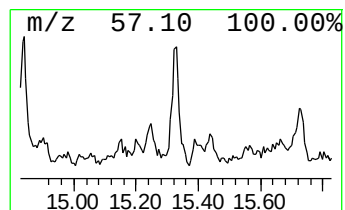
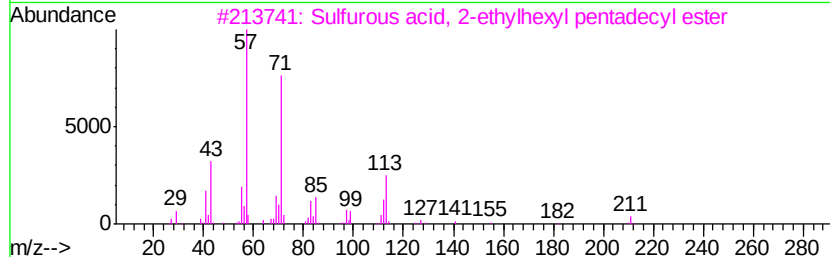
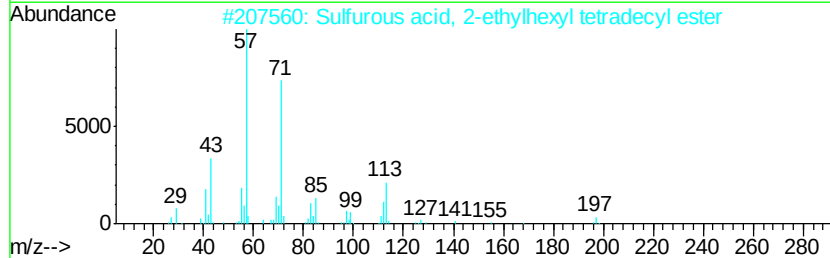
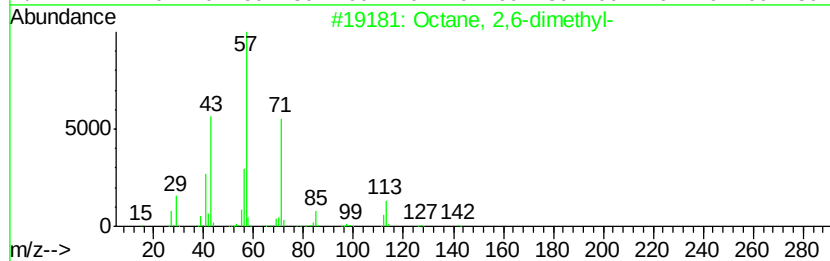
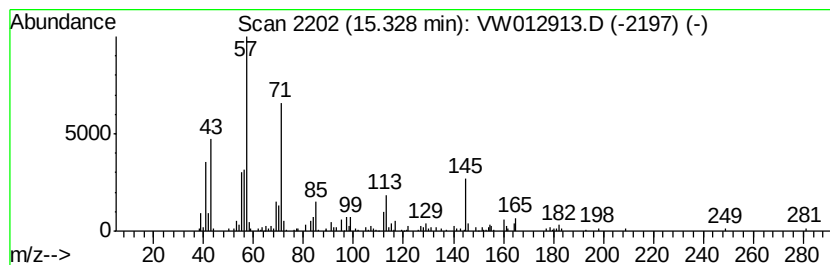
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	5.61 ug/l	71471	1,4-Dichlorobenzene-d4	13.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
2		Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	62
3		Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	62
4		Nonane, 3-methyl-	142	C10H22	005911-04-6	59
5		Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	58



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Adamantane	14.26	5.4	ug/l	68164	4	13.56	636979	50.0
1-Adamantanecarbo...	14.41	14.4	ug/l	183973	4	13.56	636979	50.0
Adamantane, 1,3-d...	14.52	11.1	ug/l	141975	4	13.56	636979	50.0
Octane, 2,6-dimet...	15.33	5.6	ug/l	71471	4	13.56	636979	50.0