

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081423\
 Data File : VD077005.D
 Acq On : 14 Aug 2023 17:07
 Operator : JC/SY
 Sample : 03961-03
 Misc : 5.05G/5.0ml/MSVOA_D/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 20071

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_D\Method\82D080823S.M
 Title : SW846 8260

Signal : TIC: VD077005.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	18	26	36	rVB	400173	742930	100.00%	9.231%
2	2.246	107	112	116	rBV2	12682	17471	2.35%	0.217%
3	4.028	408	415	424	rVB3	6034	16553	2.23%	0.206%
4	5.052	576	589	590	rBV3	12646	26467	3.56%	0.329%
5	7.075	921	933	945	rBV	98206	286527	38.57%	3.560%
6	7.363	971	982	991	rBV2	34350	91794	12.36%	1.141%
7	7.804	1048	1057	1063	rBV	113305	279507	37.62%	3.473%
8	7.875	1063	1069	1080	rVB	155732	354493	47.72%	4.405%
9	8.228	1120	1129	1141	rVB2	90037	205105	27.61%	2.549%
10	8.416	1153	1161	1165	rBV3	5168	13260	1.78%	0.165%
11	8.646	1193	1200	1209	rVB5	3811	9669	1.30%	0.120%
12	8.775	1213	1222	1233	rVV	275231	561813	75.62%	6.981%
13	9.163	1281	1288	1293	rBV5	3844	8352	1.12%	0.104%
14	9.228	1293	1299	1303	rBV2	11863	20181	2.72%	0.251%
15	9.534	1346	1351	1357	rVB3	8749	15041	2.02%	0.187%
16	9.610	1357	1364	1372	rVB2	15404	30592	4.12%	0.380%
17	10.063	1429	1441	1451	rVB7	4914	16110	2.17%	0.200%
18	10.163	1451	1458	1460	rBV4	5622	8965	1.21%	0.111%
19	10.269	1468	1476	1483	rBV	390592	699338	94.13%	8.690%
20	10.334	1483	1487	1493	rVB2	20169	34878	4.69%	0.433%
21	10.457	1501	1508	1512	rBV6	4803	7868	1.06%	0.098%
22	10.575	1523	1528	1537	rVB3	3626	7679	1.03%	0.095%
23	10.804	1557	1567	1573	rVB8	16976	40951	5.51%	0.509%
24	10.922	1579	1587	1592	rBV4	12542	25349	3.41%	0.315%
25	11.028	1599	1605	1610	rBV4	9217	16118	2.17%	0.200%
26	11.581	1691	1699	1708	rBV	386036	651240	87.66%	8.092%
27	11.687	1710	1717	1723	rVB	19544	35606	4.79%	0.442%
28	11.792	1728	1735	1747	rVB	43116	98641	13.28%	1.226%
29	12.122	1784	1791	1799	rVB3	28853	51880	6.98%	0.645%
30	12.198	1799	1804	1811	rBV2	11450	17993	2.42%	0.224%
31	12.298	1811	1821	1824	rBV8	7959	18238	2.45%	0.227%
32	12.575	1861	1868	1875	rVB	231518	375133	50.49%	4.661%
33	12.828	1905	1911	1918	rBV4	22571	59261	7.98%	0.736%
34	12.898	1918	1923	1930	rVB4	36170	65183	8.77%	0.810%
35	13.057	1945	1950	1955	rVB3	7749	15160	2.04%	0.188%
36	13.210	1971	1976	1981	rBV	33173	56751	7.64%	0.705%

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37	13.404	1995	2009	2014	rBV	17993	56088	7.55%	0.697%
38	13.516	2021	2028	2038	rVB	233784	415030	55.86%	5.157%
39	13.616	2042	2045	2051	rVB4	15067	22449	3.02%	0.279%
40	13.710	2056	2061	2066	rBV8	15938	34378	4.63%	0.427%
41	13.839	2077	2083	2088	rBV4	65151	113046	15.22%	1.405%
42	13.939	2095	2100	2102	rBV4	18533	28540	3.84%	0.355%
43	14.057	2115	2120	2133	rVB4	32675	74202	9.99%	0.922%
44	14.169	2134	2139	2143	rBV6	26972	47949	6.45%	0.596%
45	14.222	2143	2148	2156	rBV8	41156	92181	12.41%	1.145%
46	14.298	2156	2161	2165	rBV8	24504	48144	6.48%	0.598%
47	14.351	2165	2170	2171	rBV5	54895	69637	9.37%	0.865%
48	14.380	2171	2175	2181	rVB	84481	157413	21.19%	1.956%
49	14.486	2186	2193	2197	rBV	91000	204209	27.49%	2.537%
50	14.563	2200	2206	2212	rVB6	59383	146975	19.78%	1.826%
51	14.704	2226	2230	2234	rVB5	38555	52300	7.04%	0.650%
52	14.763	2235	2240	2241	rBV3	61176	84967	11.44%	1.056%
53	14.822	2247	2250	2256	rVB6	69622	113067	15.22%	1.405%
54	14.933	2265	2269	2270	rBV4	41201	56033	7.54%	0.696%
55	14.969	2272	2275	2282	rVB3	93260	141164	19.00%	1.754%
56	15.039	2282	2287	2291	rBV3	106522	159879	21.52%	1.987%
57	15.098	2292	2297	2300	rBV	90883	174887	23.54%	2.173%
58	15.380	2340	2345	2351	rBV6	116558	296142	39.86%	3.680%
59	15.827	2419	2421	2428	rVB5	82971	126856	17.08%	1.576%
60	16.592	2547	2551	2559	rVB9	166371	350173	47.13%	4.351%

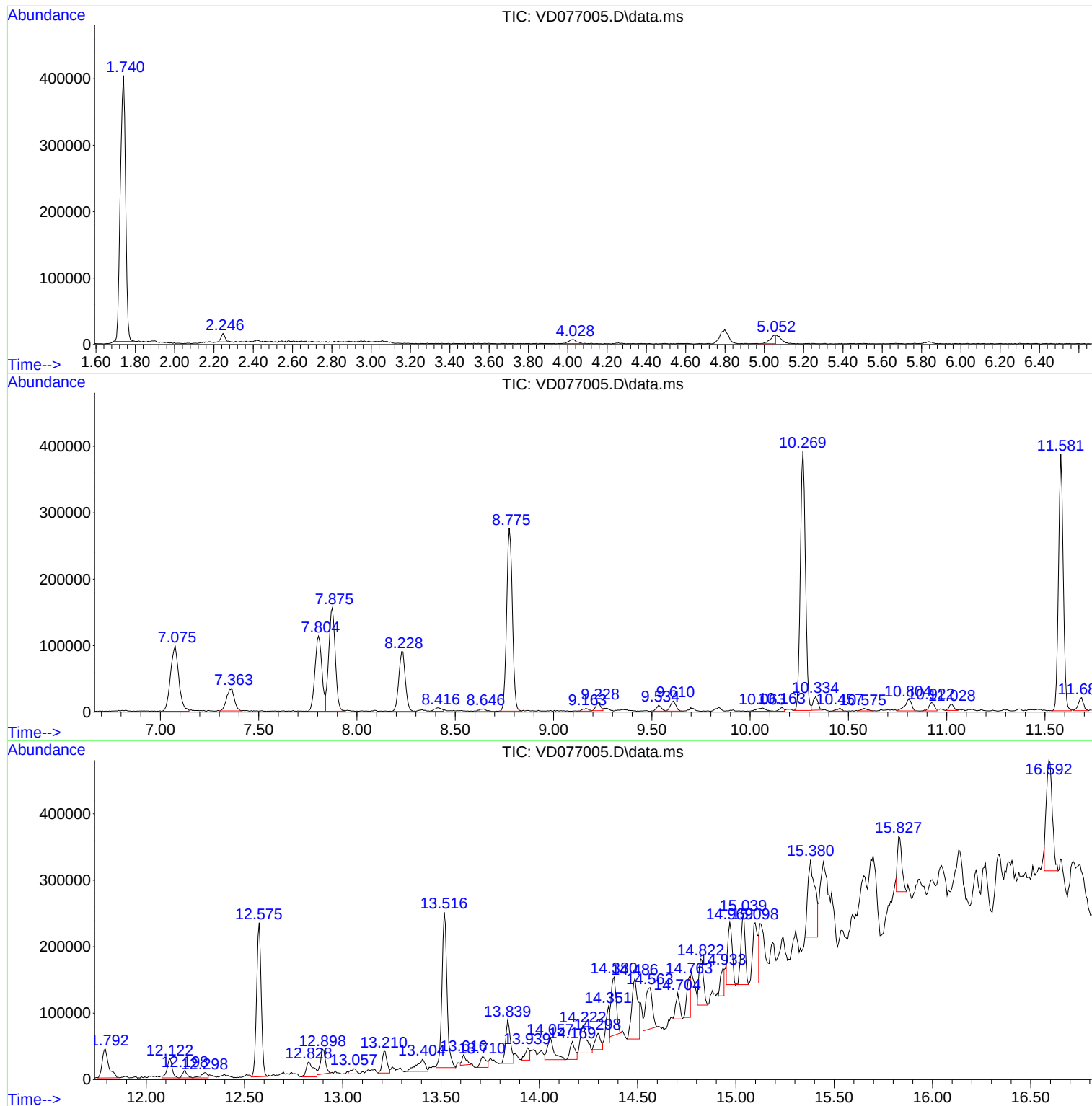
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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MSVOA_D
ClientSampleId :
20071

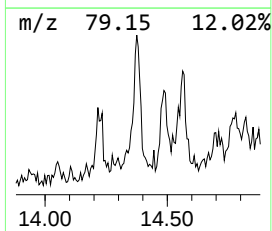
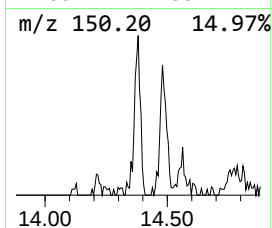
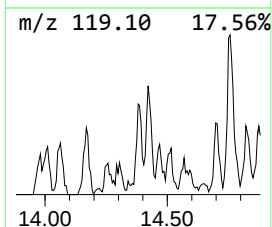
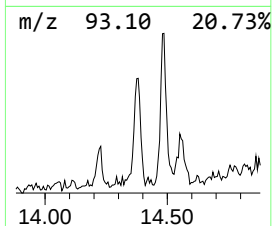
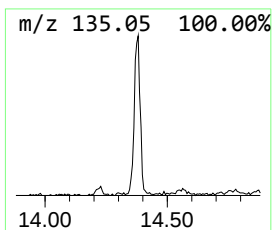
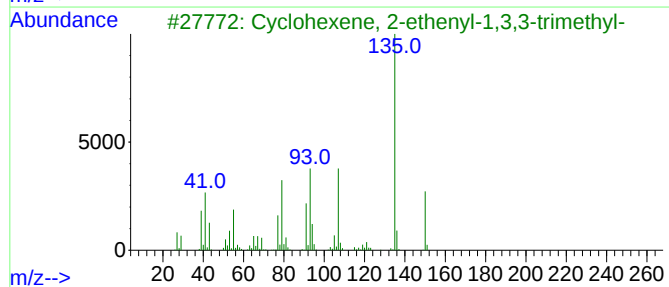
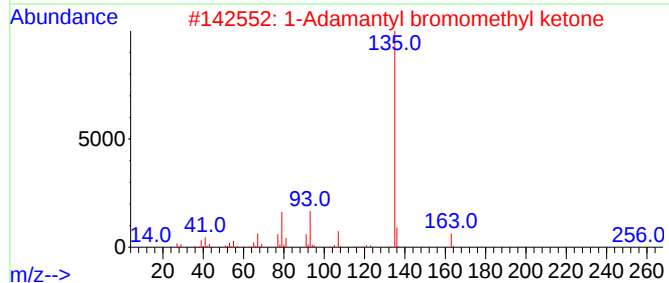
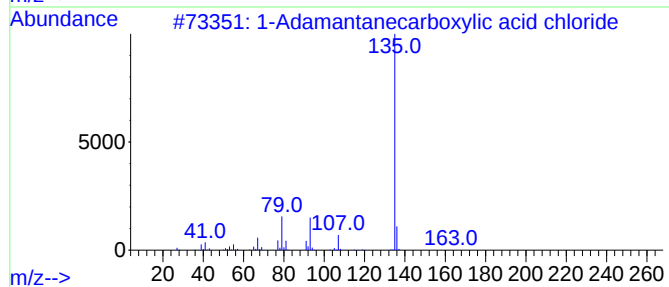
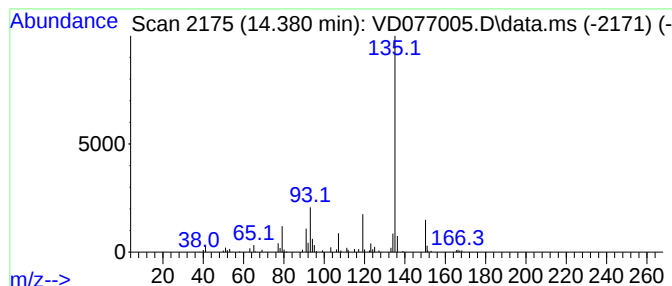
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D080823S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Adamantanecarboxylic acid... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.381	18.96 ug/l	157413	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	59
2			1-Adamantyl bromomethyl ketone	256	C12H17BrO	005122-82-7	59
3			Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	59
4			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	53
5			1-isocyanatocyclopropyl tricyclo...	233	C14H19NO2	1000396-40-9	53



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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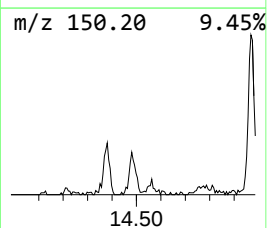
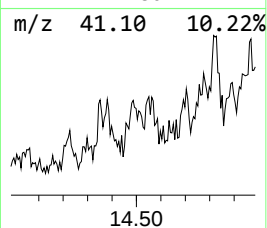
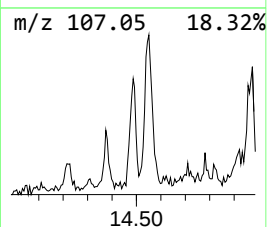
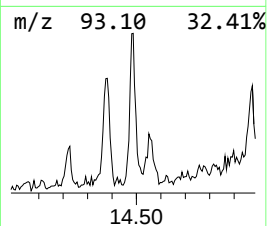
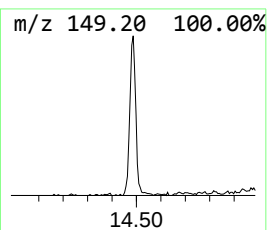
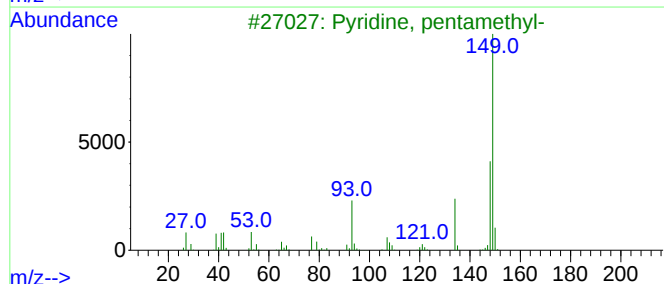
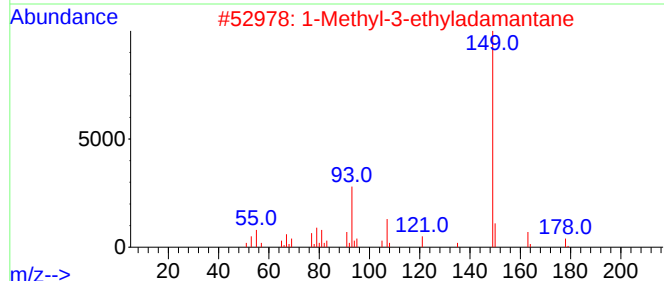
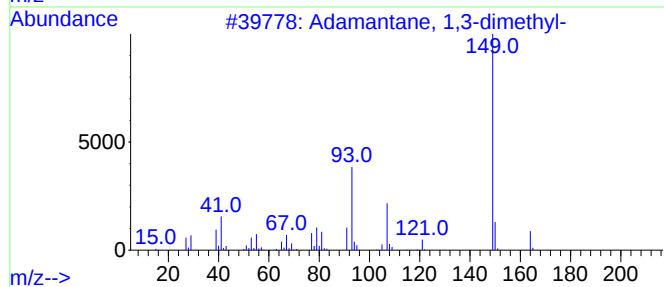
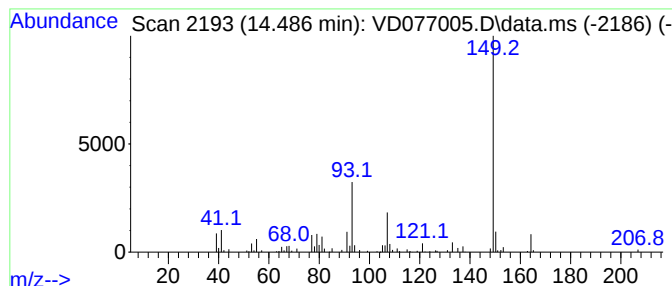
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D080823S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Adamantane, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	24.60 ug/l	204209	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	95
2			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	78
3			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	64
4			Adamantane, 1-isothiocyanato-3-m...	207	C12H17NS	136860-48-5	58
5			Phthalic acid, 2,7-dimethyloct-7...	356	C22H28O4	1000315-49-7	53



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Misc : 5.05G/5.0ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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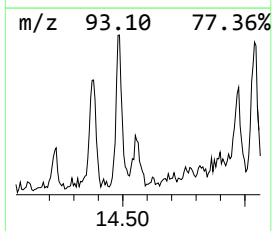
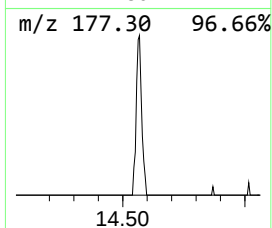
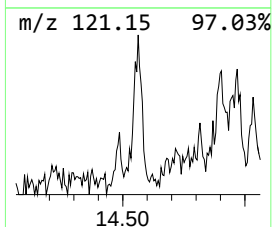
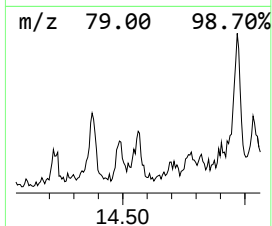
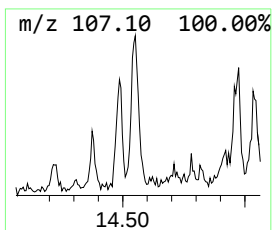
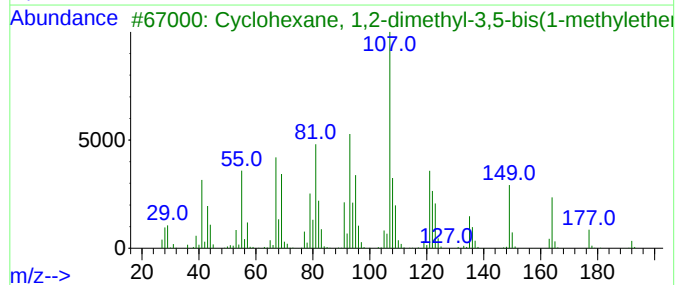
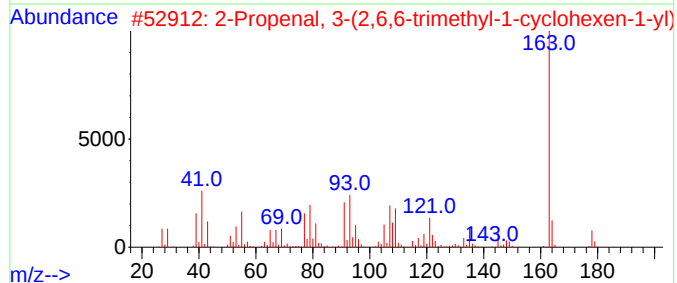
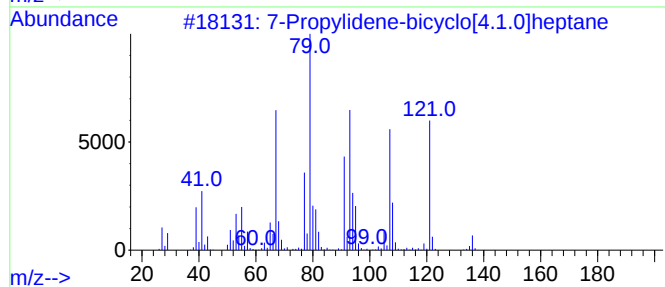
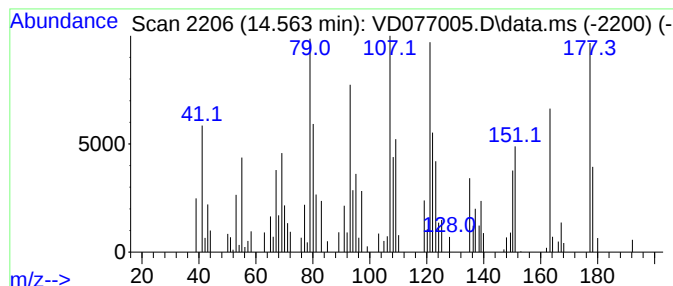
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.563 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	17.71 ug/l	146975	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Propylidene-bicyclo[4.1.0]heptane	136	C10H16	082253-09-6	38
2			2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	25
3			Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	062337-99-9	25
4			2H-1-Benzopyran-2-one, 3-amino-4...	177	C9H7NO3	1000351-60-2	18
5			1,5-Heptadiene, 2,5-dimethyl-3-m...	136	C10H16	074663-83-5	18



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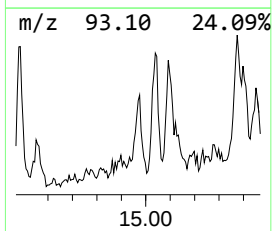
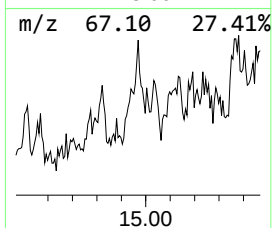
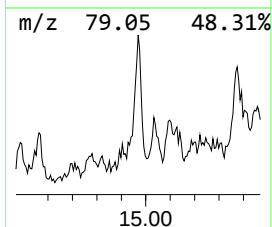
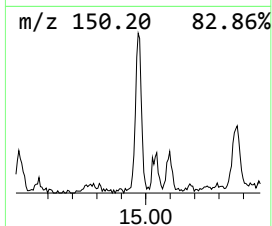
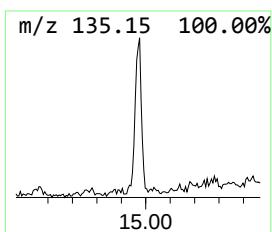
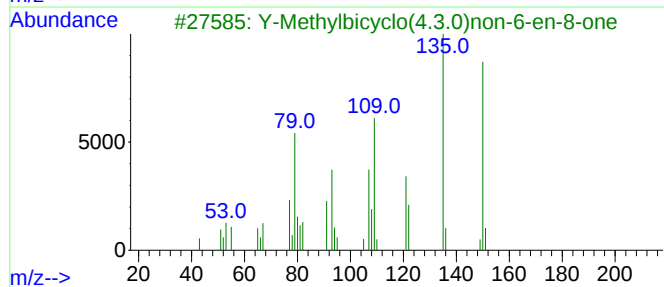
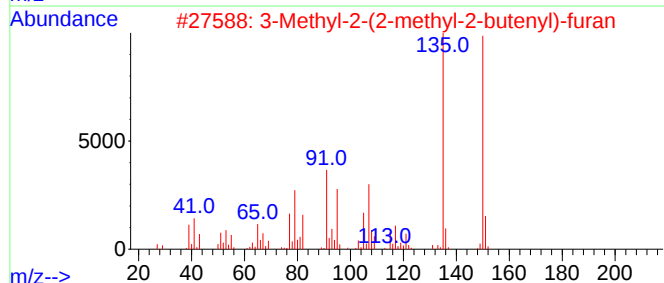
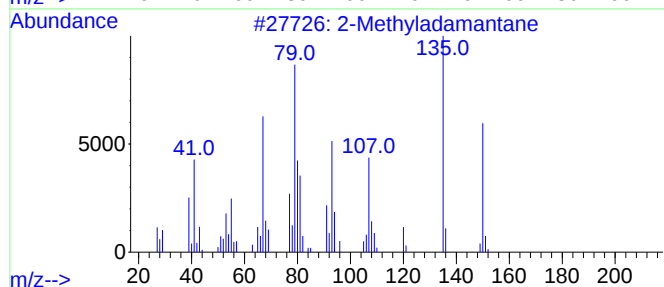
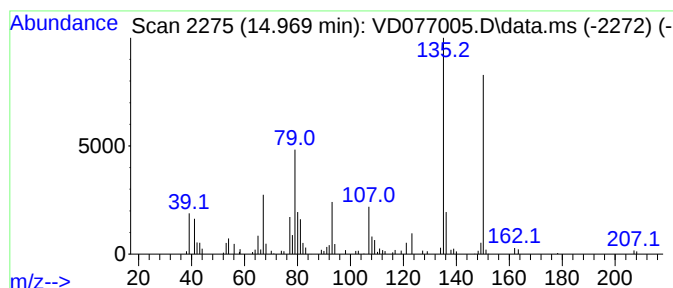
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 2-Methyladamantane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.969	17.01 ug/l	141164	1,4-Dichlorobenzene-d4		13.516	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Methyladamantane		150	C11H18	000700-56-1	90
2	3-Methyl-2-(2-methyl-2-butenyl)-...		150	C10H14O	015186-51-3	52
3	Y-Methylbicyclo(4.3.0)non-6-en-8...		150	C10H14O	1000424-65-9	50
4	Ethyltetramethylcyclopentadiene		150	C11H18	057693-77-3	47
5	Phenol, 5-ethenyl-2-methoxy-		150	C9H10O2	000621-58-9	47



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ClientSampleId :
20071

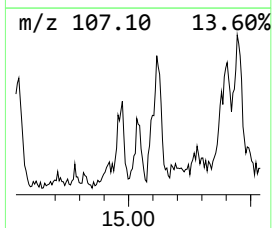
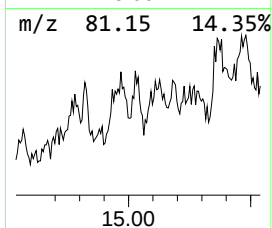
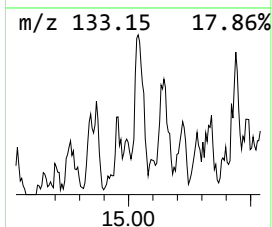
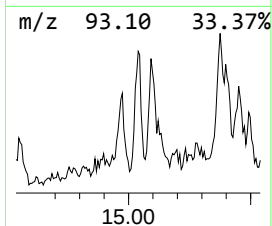
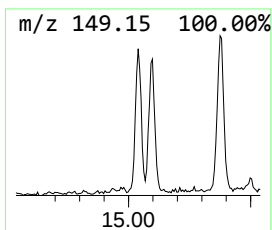
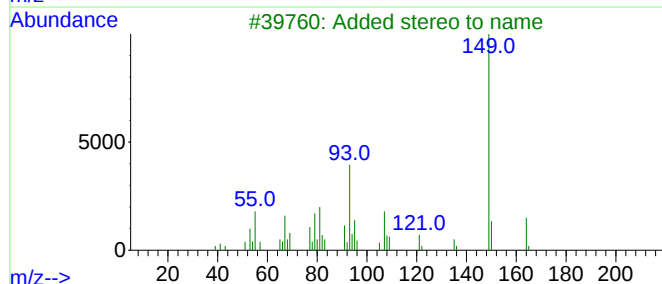
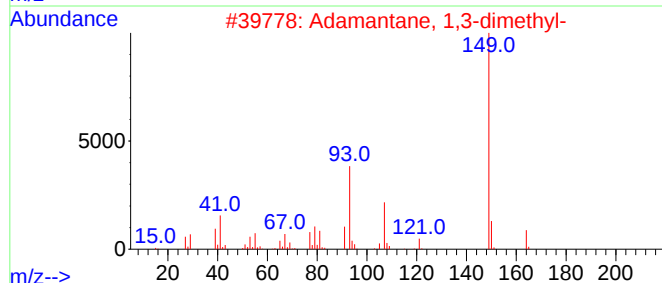
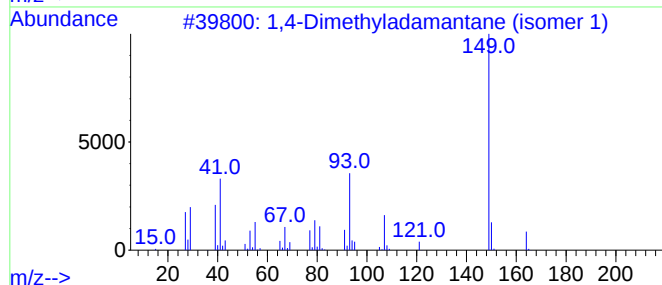
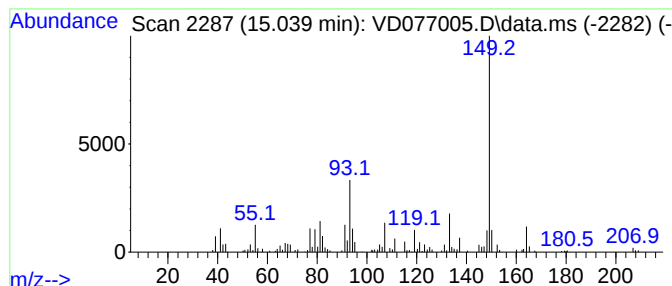
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	19.26 ug/l	159879	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	76
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	76
3			Added stereo to name	164	C12H20	024145-88-8	74
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	68
5			Tricyclo[4.3.1.1(3,8)]undecane-3...	208	C13H20O2	031061-61-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081423\
Data File : VD077005.D
Acq On : 14 Aug 2023 17:07
Operator : JC/SY
Sample : 03961-03
Misc : 5.05G/5.0ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
20071

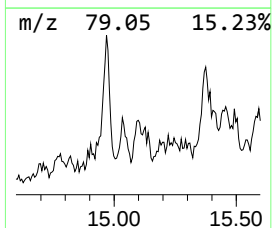
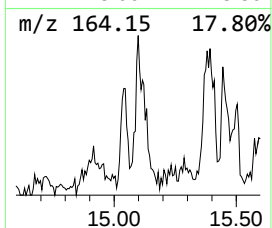
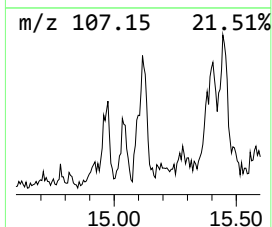
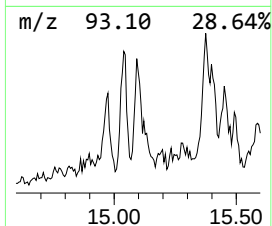
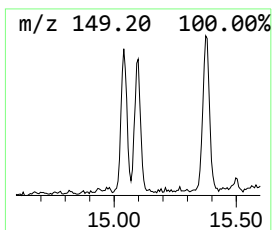
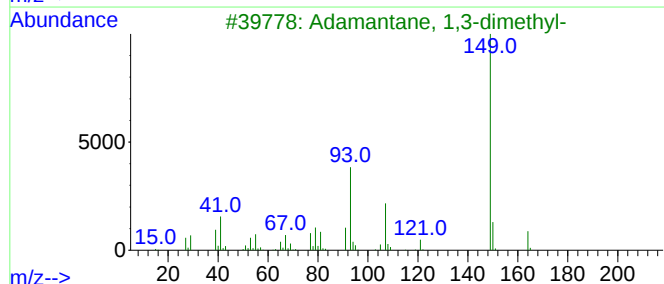
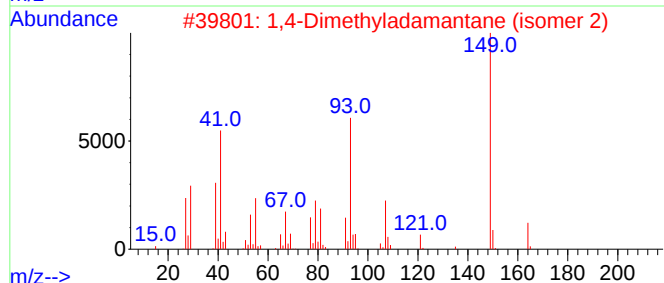
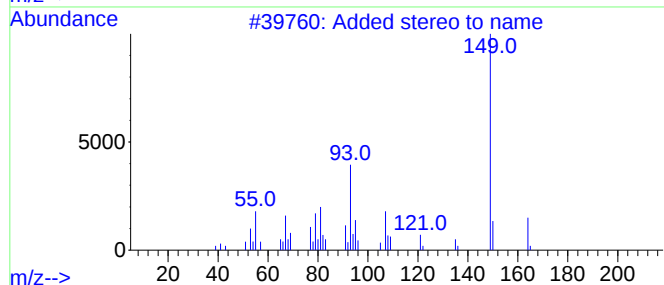
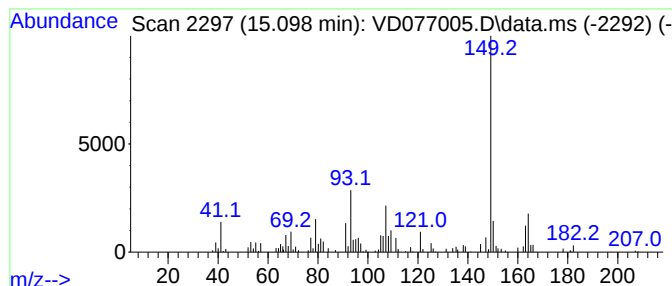
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1,4-Dimethyladamantane (iso... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	21.07 ug/l	174887	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	87
2	1,4-Dimethyladamantane (isomer 2)			164	C12H20	1000460-67-1	70
3	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	62
4	Benzene, 1-butyl-4-methoxy-			164	C11H16O	018272-84-9	60
5	1-Methyl-3-ethyladamantane			178	C13H22	001687-34-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081423\
Data File : VD077005.D
Acq On : 14 Aug 2023 17:07
Operator : JC/SY
Sample : 03961-03
Misc : 5.05G/5.0ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
20071

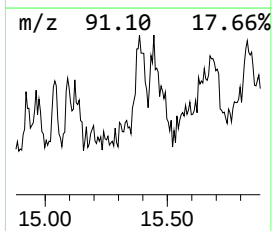
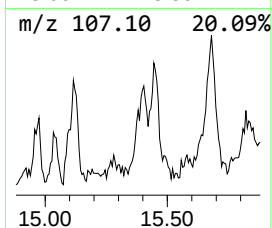
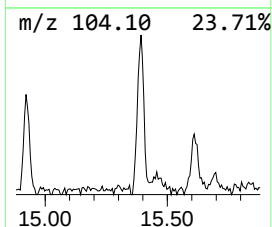
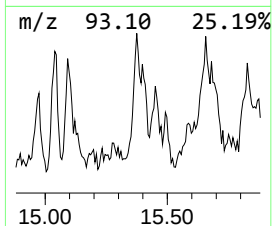
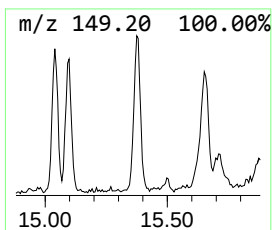
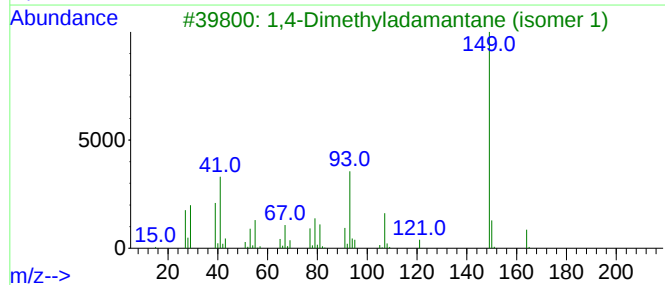
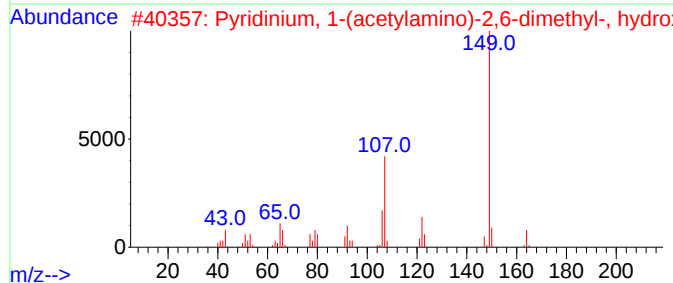
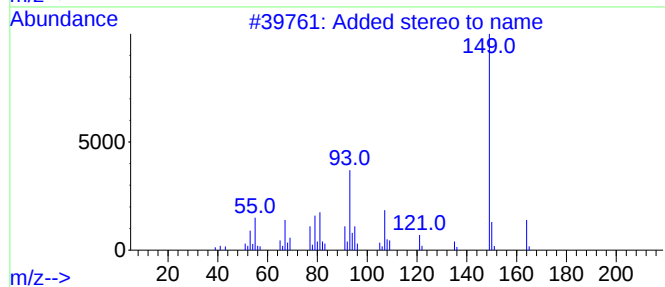
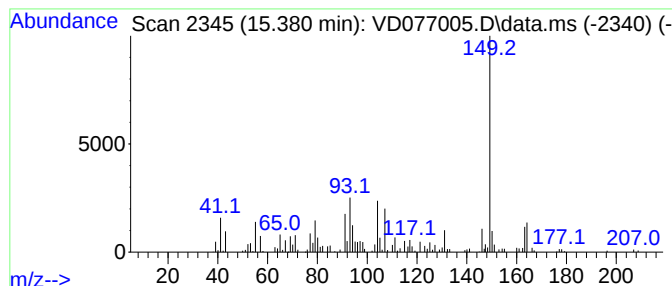
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown15.380 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	35.68 ug/l	296142	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	50
2	Pyridinium, 1-(acetylamino)-2,6-...			164	C9H12N2O	031020-35-6	47
3	1,4-Dimethyladamantane (isomer 1)			164	C12H20	1000460-67-0	46
4	2'-Hydroxy-4',5'-dimethylacetoph...			164	C10H12O2	036436-65-4	43
5	Methyl (1s,3s,5R,7S)-3-methylada...			208	C13H20O2	1010504-39-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081423\
Data File : VD077005.D
Acq On : 14 Aug 2023 17:07
Operator : JC/SY
Sample : 03961-03
Misc : 5.05G/5.0ml/MSVOA_D/SOIL
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D080823S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Adamantane, 1,3...	14.486	24.6	ug/l	204209	4	13.516	415030	50.0
unknown14.563	14.563	17.7	ug/l	146975	4	13.516	415030	50.0
2-Methyladamantane	14.969	17.0	ug/l	141164	4	13.516	415030	50.0
1,4-Dimethylada...	15.039	19.3	ug/l	159879	4	13.516	415030	50.0
1,4-Dimethylada...	15.098	21.1	ug/l	174887	4	13.516	415030	50.0
unknown15.380	15.380	35.7	ug/l	296142	4	13.516	415030	50.0