

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020722\
 Data File : VY007411.D
 Acq On : 07 Feb 2022 14:31
 Operator : SY/MD
 Sample : N1387-05
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 26601

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_Y\methods\82Y020222S.M
 Title : SW846 8260

Signal : TIC: VY007411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.016	30	32	37	rVB	383	559	1.13%	0.171%
2	2.387	90	93	97	rBV3	584	772	1.56%	0.236%
3	2.637	131	134	135	rVV2	506	519	1.05%	0.159%
4	2.668	137	139	146	rVB4	801	1236	2.50%	0.379%
5	3.058	200	203	206	rVB2	525	627	1.27%	0.192%
6	4.722	470	476	482	rVB5	1155	2459	4.97%	0.753%
7	5.765	641	647	650	rBV2	380	547	1.11%	0.168%
8	7.722	960	968	974	rBV	6497	15190	30.73%	4.652%
9	7.795	974	980	990	rVB	13269	30222	61.14%	9.256%
10	7.966	1002	1008	1011	rBV	285	541	1.09%	0.166%
11	8.149	1031	1038	1047	rVB3	6672	15084	30.52%	4.620%
12	8.691	1116	1127	1134	rBV	20216	40125	81.18%	12.289%
13	10.185	1364	1372	1378	rBV	27906	49430	100.00%	15.138%
14	10.252	1378	1383	1387	rVB2	1310	2014	4.07%	0.617%
15	10.612	1439	1442	1448	rVB2	328	544	1.10%	0.167%
16	11.489	1580	1586	1594	rBV	22723	38031	76.94%	11.647%
17	11.587	1599	1602	1606	rVB3	525	559	1.13%	0.171%
18	12.038	1672	1676	1678	rBV3	494	562	1.14%	0.172%
19	12.483	1742	1749	1758	rBV2	15486	23382	47.30%	7.161%
20	13.428	1898	1904	1909	rBV	12963	20911	42.30%	6.404%
21	14.263	2037	2041	2042	rVV3	682	832	1.68%	0.255%
22	14.294	2042	2046	2052	rVB7	1459	2977	6.02%	0.912%
23	14.391	2058	2062	2066	rBV4	1843	3257	6.59%	0.997%
24	14.458	2069	2073	2074	rBV2	1210	1274	2.58%	0.390%
25	14.477	2074	2076	2083	rVB5	1342	2152	4.35%	0.659%
26	14.599	2091	2096	2098	rBV3	585	1056	2.14%	0.323%
27	14.647	2101	2104	2105	rBV3	736	689	1.39%	0.211%
28	14.666	2105	2107	2111	rBV4	579	1102	2.23%	0.337%
29	14.727	2115	2117	2120	rVB3	910	1054	2.13%	0.323%
30	14.782	2124	2126	2130	rBV4	724	1249	2.53%	0.383%
31	14.879	2131	2142	2147	rVB6	3529	8581	17.36%	2.628%
32	14.940	2147	2152	2156	rBV6	3288	5981	12.10%	1.832%
33	15.007	2158	2163	2164	rBV4	2324	3585	7.25%	1.098%
34	15.031	2164	2167	2173	rVB8	2559	4268	8.63%	1.307%
35	15.092	2173	2177	2178	rBV3	1304	1742	3.52%	0.534%
36	15.153	2185	2187	2188	rVB2	1134	679	1.37%	0.208%

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Integrator: RTE

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	15.178	2188	2191	2194	rBV3	829	1301	2.63%	0.398%
38	15.239	2199	2201	2202	rBV2	706	495	1.00%	0.152%
39	15.281	2202	2208	2209	rBV5	3428	5923	11.98%	1.814%
40	15.355	2215	2220	2225	rVB7	3122	6047	12.23%	1.852%
41	15.391	2225	2226	2230	rVB4	1750	1659	3.36%	0.508%
42	15.440	2230	2234	2236	rBV5	1201	1521	3.08%	0.466%
43	15.489	2238	2242	2245	rBV6	1499	2673	5.41%	0.819%
44	15.525	2247	2248	2250	rBV2	902	923	1.87%	0.283%
45	15.690	2273	2275	2276	rBV2	906	632	1.28%	0.194%
46	15.714	2276	2279	2284	rVV6	2651	5863	11.86%	1.796%
47	15.848	2299	2301	2303	rVB3	1063	698	1.41%	0.214%
48	15.915	2310	2312	2313	rBV2	928	771	1.56%	0.236%
49	16.013	2326	2328	2335	rVB6	1427	2479	5.02%	0.759%
50	16.111	2341	2344	2351	rVB8	701	1258	2.55%	0.385%
51	16.269	2365	2370	2374	rBV7	1555	2947	5.96%	0.903%
52	16.336	2379	2381	2383	rVV3	821	958	1.94%	0.293%
53	16.373	2385	2387	2390	rVV4	1126	1509	3.05%	0.462%
54	16.403	2390	2392	2394	rVV3	1118	1206	2.44%	0.369%
55	16.446	2397	2399	2402	rVV4	887	1291	2.61%	0.395%
56	16.470	2402	2403	2407	rVV3	1021	1140	2.31%	0.349%
57	16.763	2448	2451	2455	rVB4	1082	1434	2.90%	0.439%

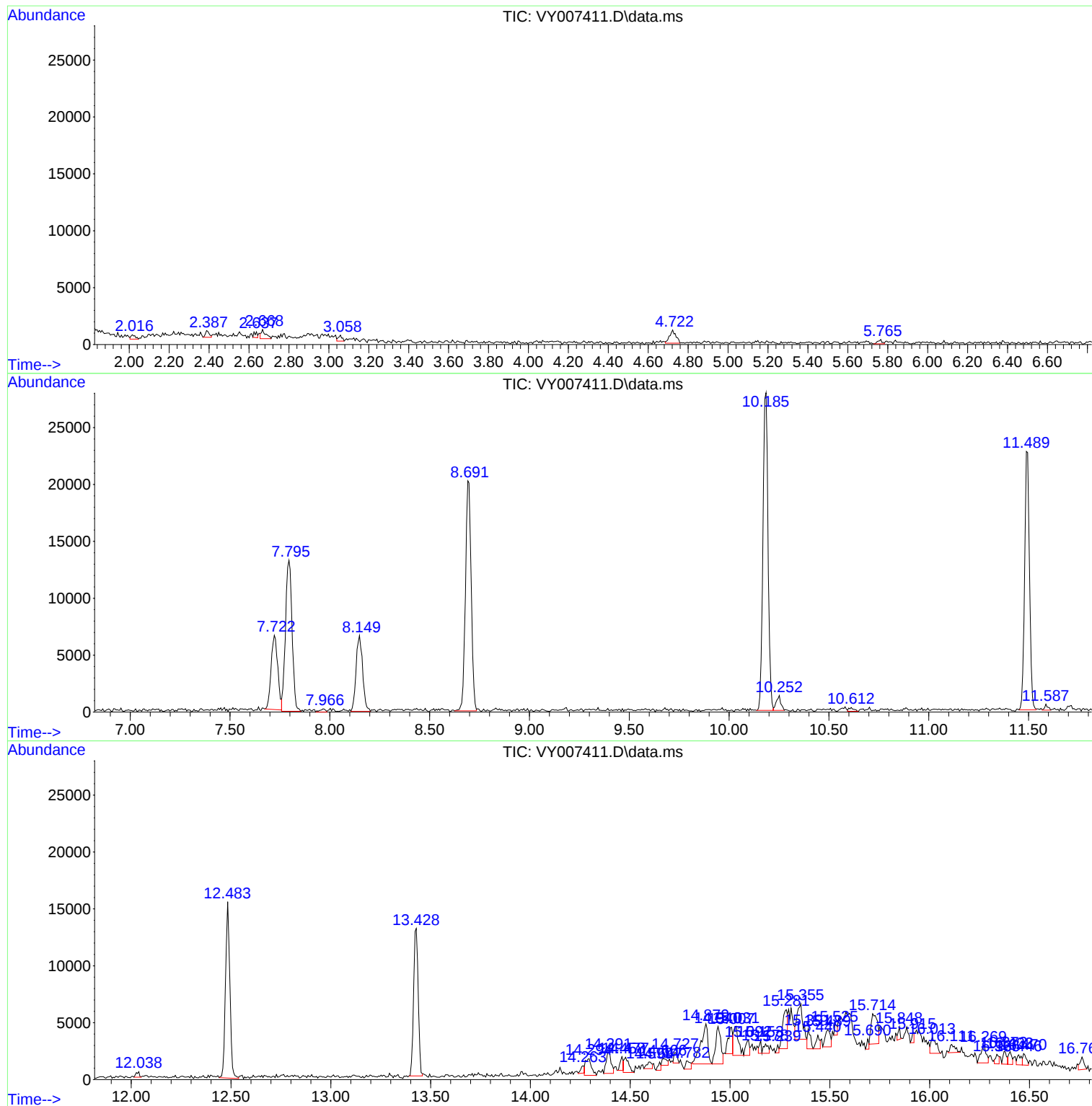
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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



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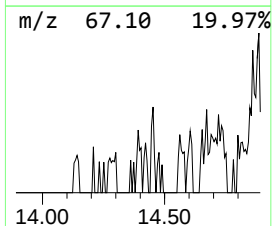
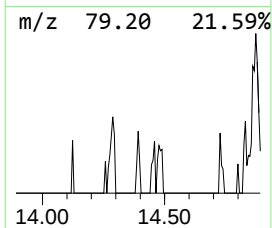
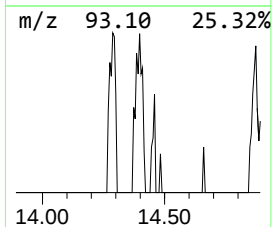
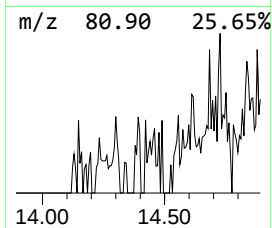
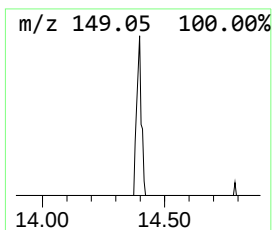
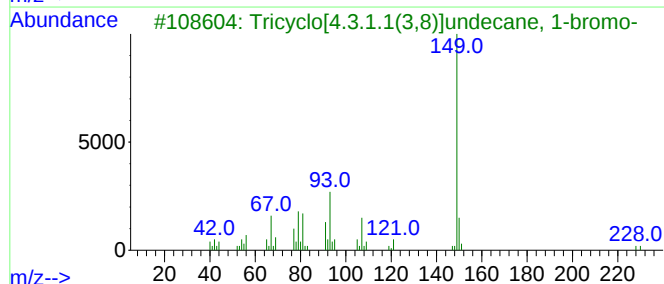
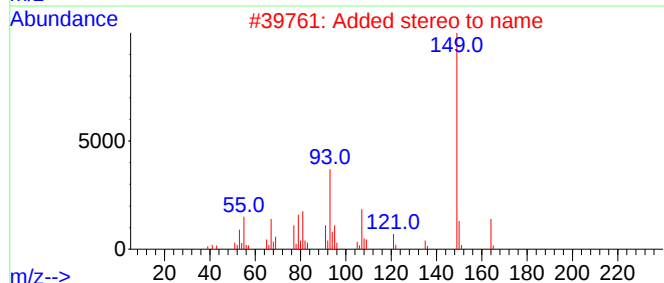
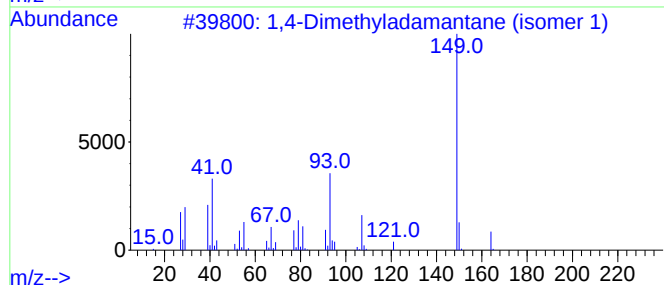
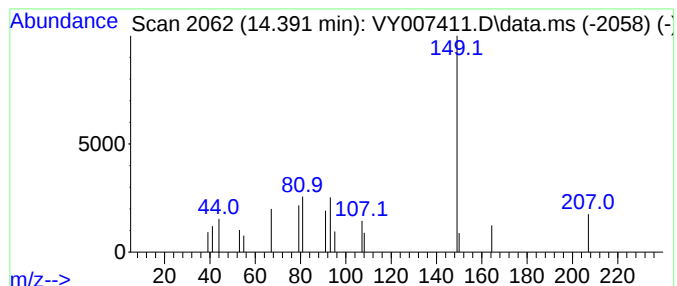
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 2 1,4-Dimethyladamantane (iso... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.391	7.79 ug/l	3257	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	59
2			Added stereo to name	164	C12H20	024145-89-9	58
3			Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	56
4			4-(2-Methyl-cyclohex-1-enyl)-but...	164	C11H16O	041437-92-7	50
5			1H-Indene, 1-ethylideneoctahydro...	164	C12H20	056362-87-9	49



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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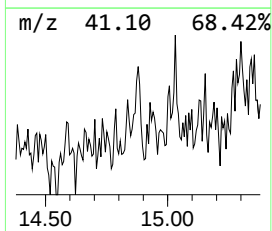
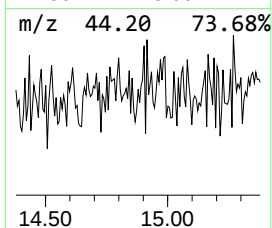
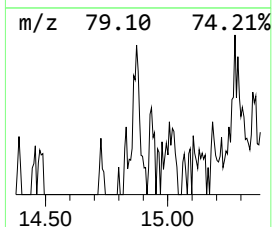
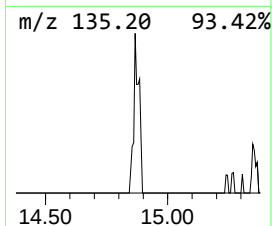
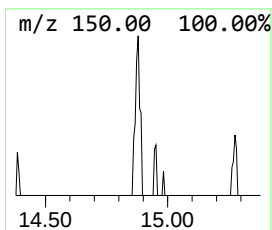
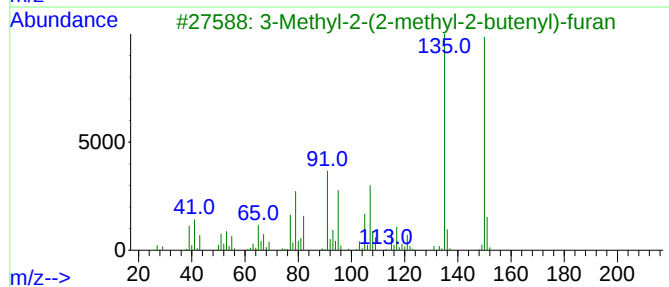
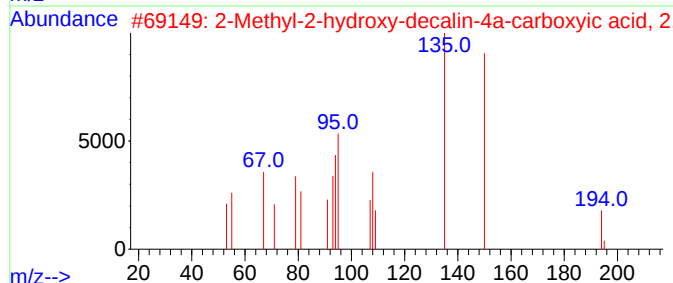
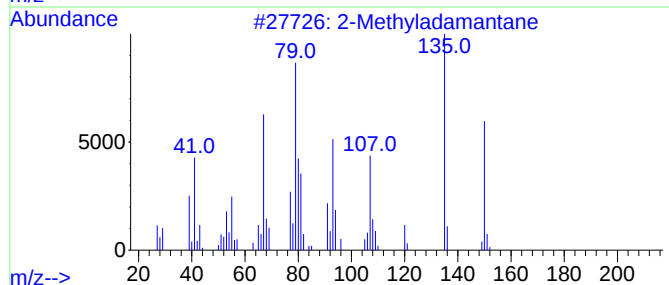
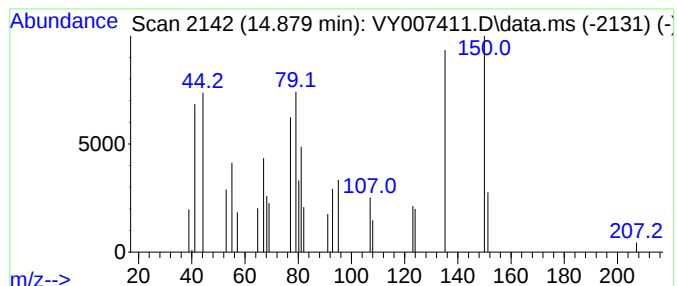
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 3 2-Methyladamantane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.879	20.52 ug/l	8581	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyladamantane	150	C11H18	000700-56-1	52
2			2-Methyl-2-hydroxy-decalin-4a-ca...	194	C12H18O2	1000146-22-6	43
3			3-Methyl-2-(2-methyl-2-butenyl)-...	150	C10H14O	015186-51-3	43
4			Tricyclo[5.2.1.0(2,6)]decan-10-one	150	C10H14O	103385-97-3	38
5			Bicyclo[5.1.0]octane, 8-(1-methy...	150	C11H18	054166-47-1	38



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Misc : 5.07g/5.0mL/MSVOA_Y/soil
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
26601

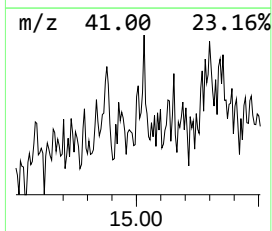
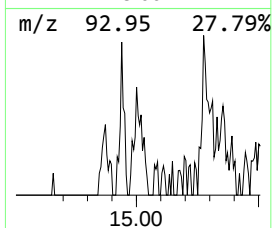
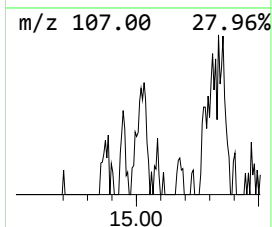
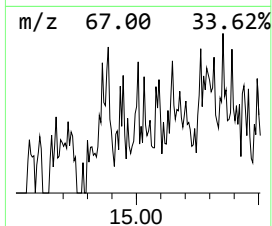
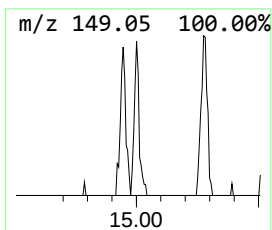
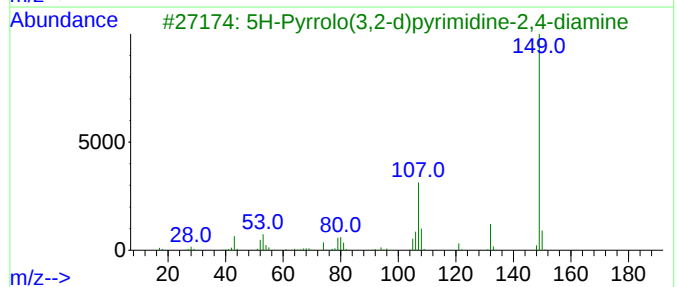
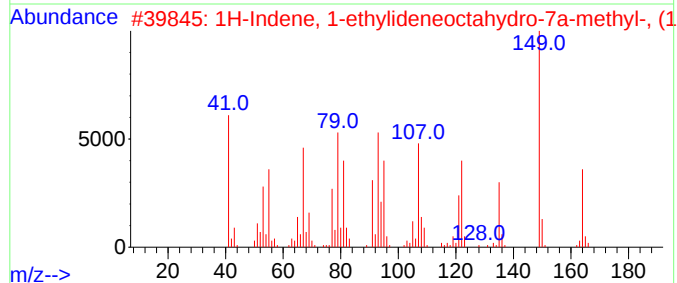
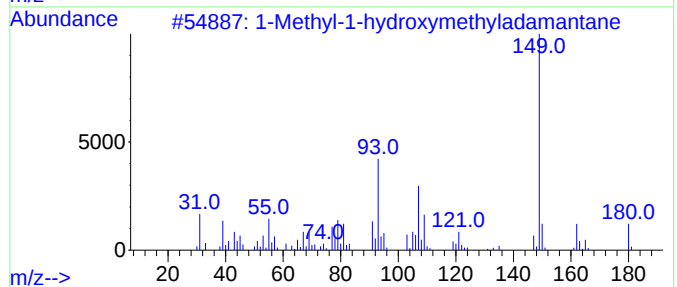
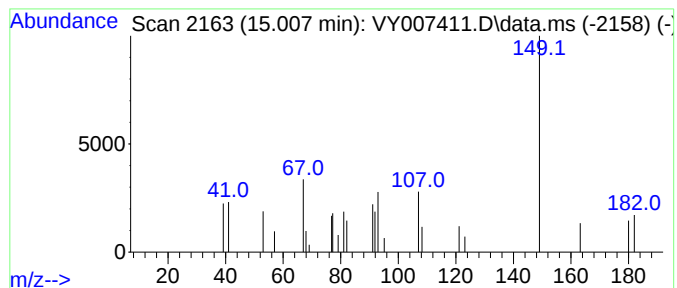
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 5 1-Methyl-1-hydroxymethyladamantane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.007	8.57 ug/l	3585	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1-hydroxymethyladamantane	180	C12H20O	001200-78-8	59
2			1H-Indene, 1-ethylideneoctahydro...	164	C12H20	056324-69-7	42
3			5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	37
4			Myrtene acid bromide	228	C10H13BrO	1000159-35-0	36
5			1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	33



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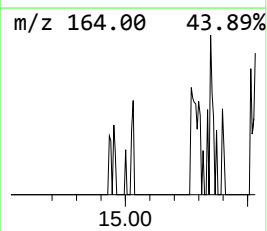
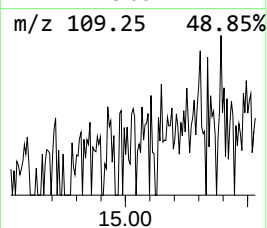
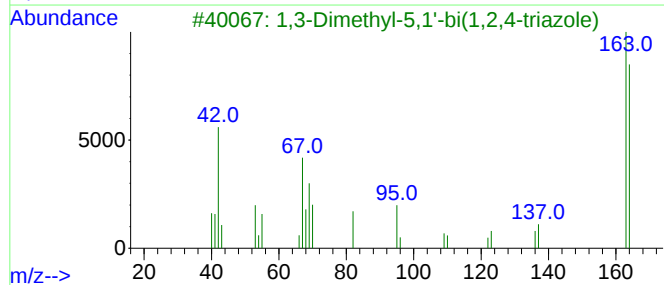
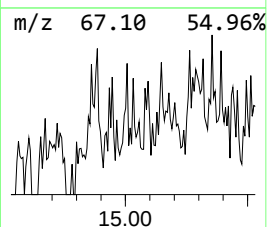
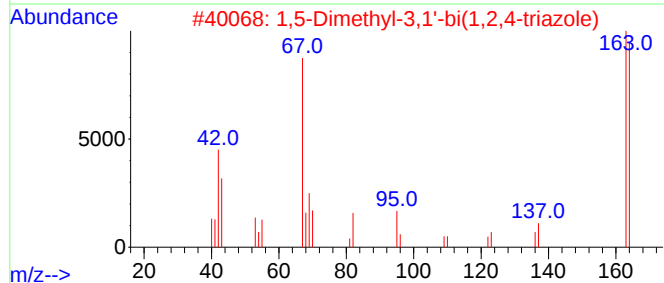
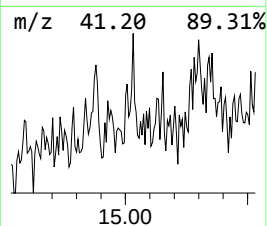
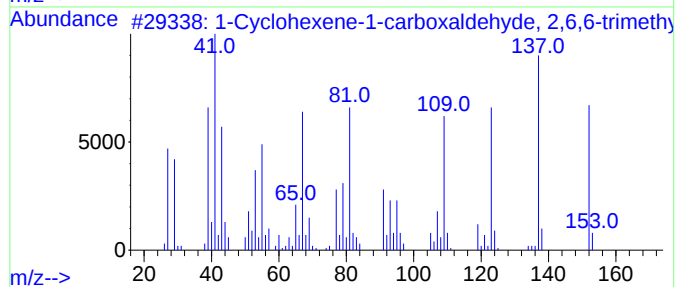
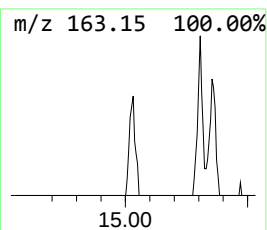
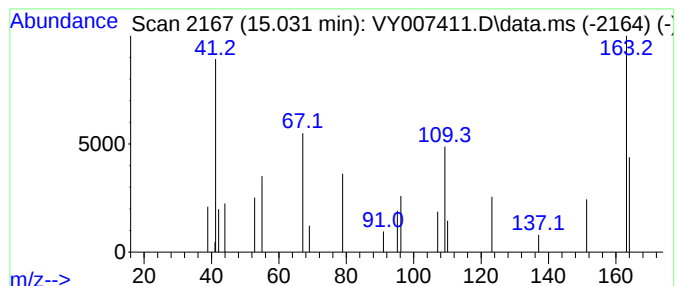
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown15.031 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.031	10.21 ug/l	4268	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-25-7	27
2			1,5-Dimethyl-3,1'-bi(1,2,4-triaz...	164	C6H8N6	063523-88-6	25
3			1,3-Dimethyl-5,1'-bi(1,2,4-triaz...	164	C6H8N6	063523-86-4	23
4			Isoneral	152	C10H16O	1000414-18-0	22
5			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	12



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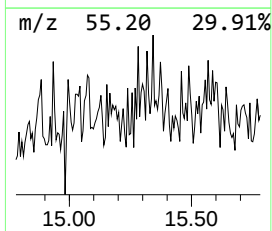
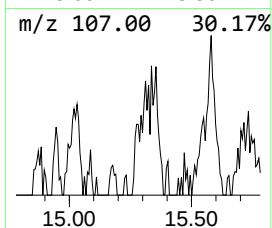
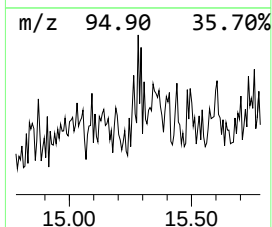
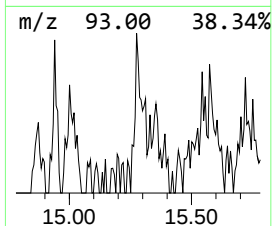
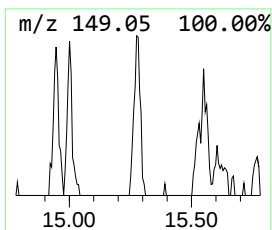
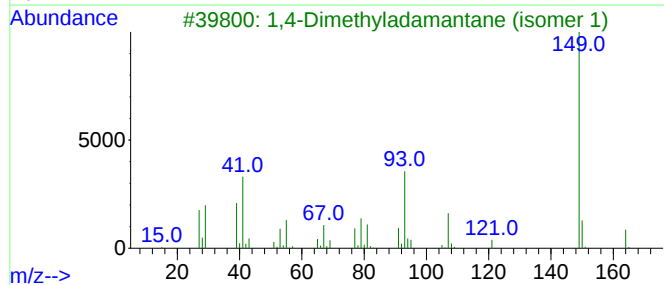
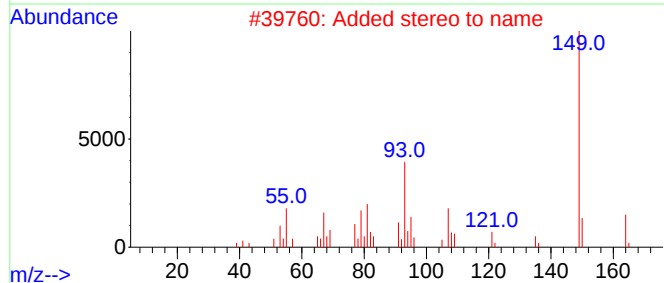
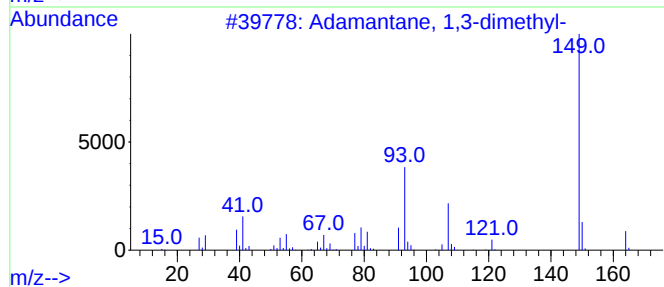
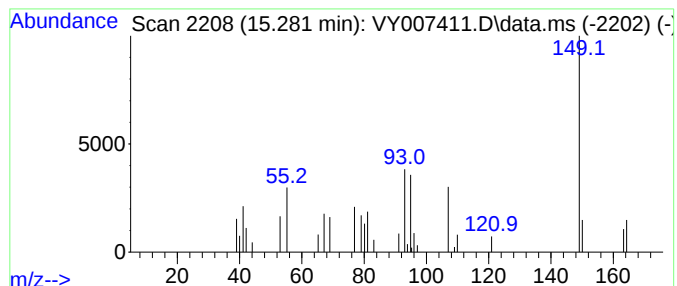
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Quant Title : SW846 8260

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

Peak Number 7 Adamantane, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.281	14.16 ug/l	5923	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	62
2			Added stereo to name	164	C12H20	024145-88-8	59
3			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	58
4			Added stereo to name	164	C12H20	024145-89-9	58
5			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY0720222\
Data File : VY07411.D
Acq On : 07 Feb 2022 14:31
Operator : SY/MD
Sample : N1387-05
Misc : 5.07g/5.0mL/MSVOA_Y/soil
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
26601

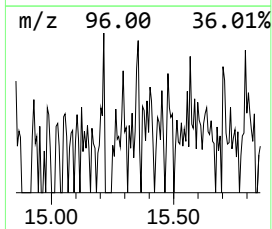
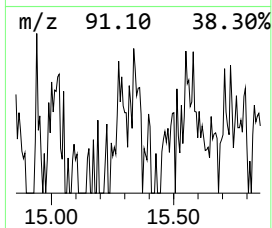
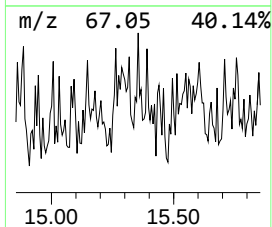
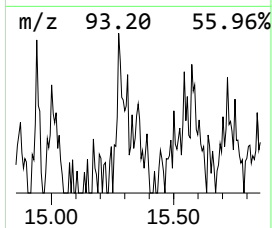
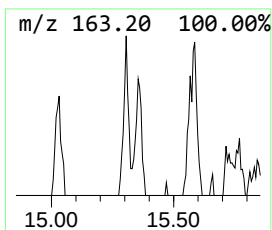
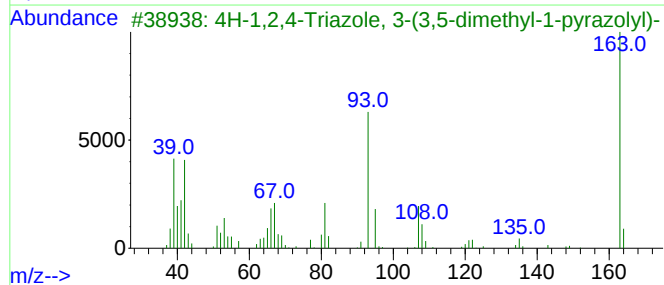
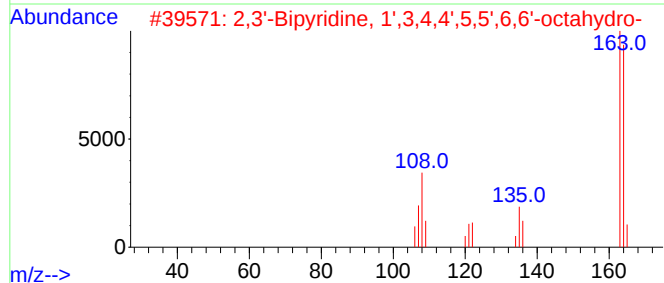
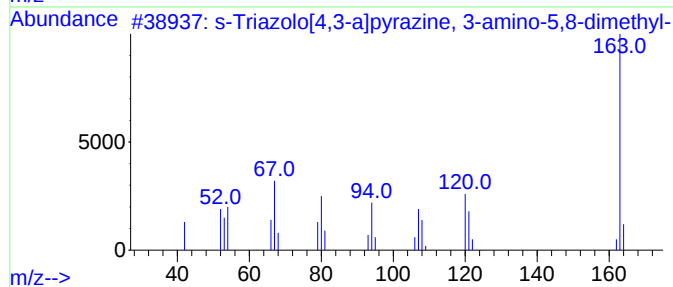
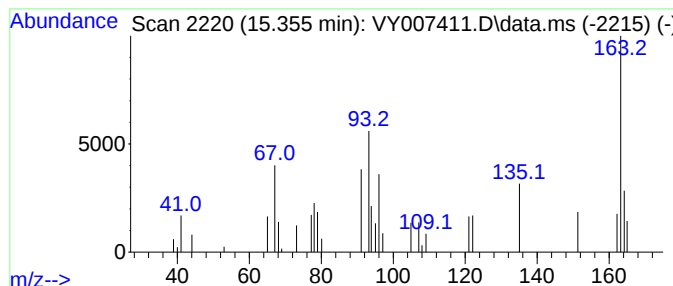
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.355 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.355	14.46 ug/l	6047	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			s-Triazolo[4,3-a]pyrazine, 3-ami...	163	C7H9N5	019855-02-8	43
2			2,3'-Bipyridine, 1',3,4,4',5,5',...	164	C10H16N2	018017-50-0	42
3			4H-1,2,4-Triazole, 3-(3,5-dimeth...	163	C7H9N5	003310-78-9	32
4			Diethylphosphinothioic azide	163	C4H10N3PS	058347-14-1	32
5			2-(1-Oxobut-2-ynyl)cyclohexanone	164	C10H12O2	1000191-07-1	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020722\
Data File : VY007411.D
Acq On : 07 Feb 2022 14:31
Operator : SY/MD
Sample : N1387-05
Misc : 5.07g/5.0mL/MSVOA_Y/soil
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
26601

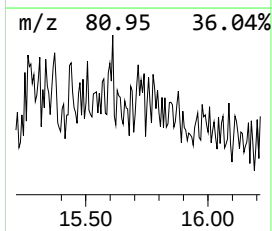
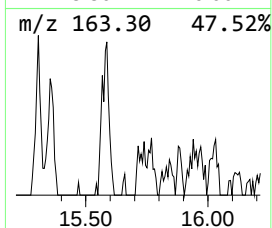
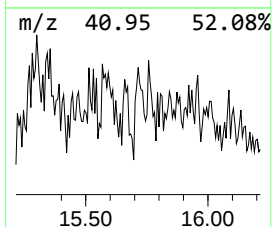
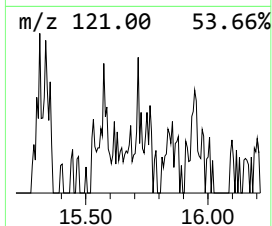
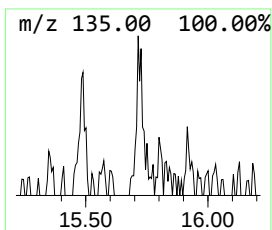
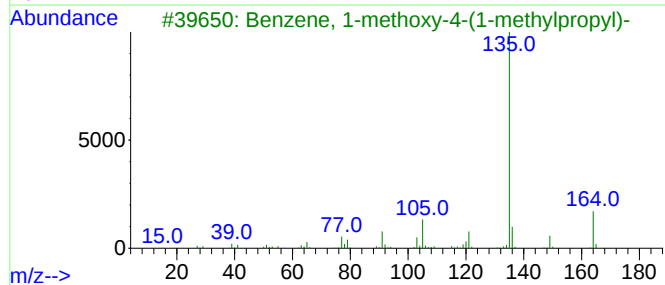
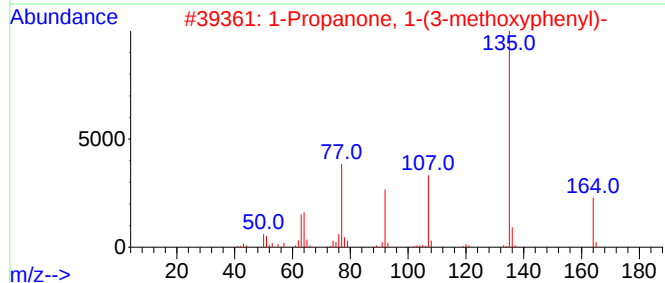
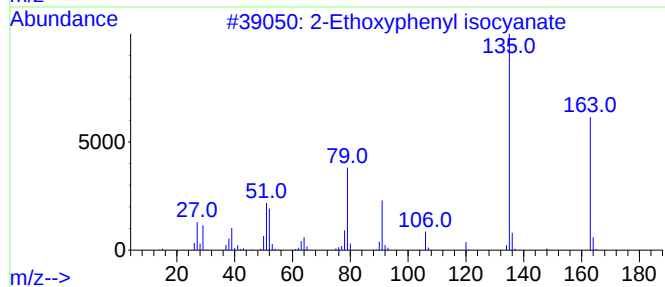
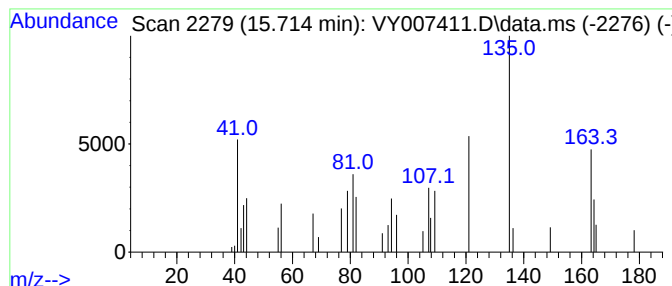
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.714 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.714	14.02 ug/l	5863	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethoxyphenyl isocyanate	163	C9H9NO2	005395-71-1	43
2			1-Propanone, 1-(3-methoxyphenyl)-	164	C10H12O2	037951-49-8	43
3			Benzene, 1-methoxy-4-(1-methylpr...	164	C11H16O	004917-90-2	38
4			1,3-Benzodioxole, 5-propyl-	164	C10H12O2	000094-58-6	38
5			2-(Adamantan-1-ylamino)-ethanol	195	C12H21NO	1000300-19-1	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020722\
Data File : VY007411.D
Acq On : 07 Feb 2022 14:31
Operator : SY/MD
Sample : N1387-05
Misc : 5.07g/5.0mL/MSVOA_Y/soil
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
26601

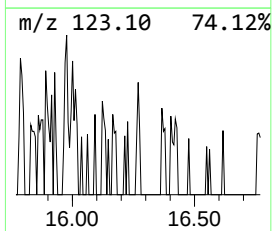
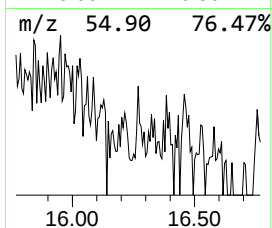
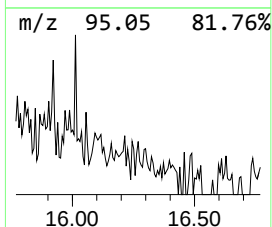
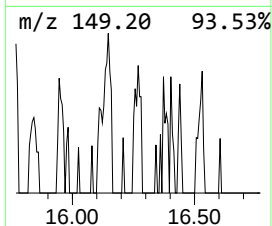
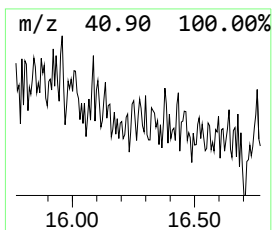
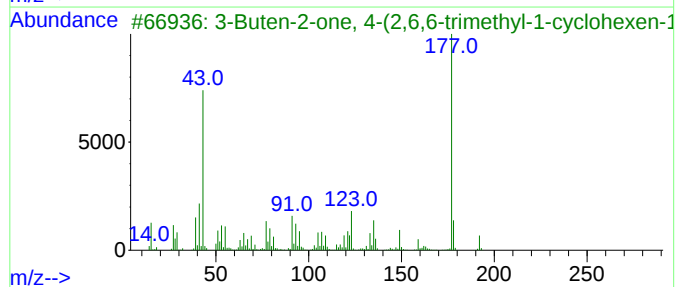
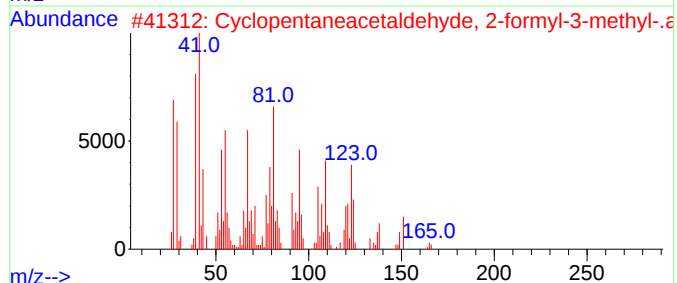
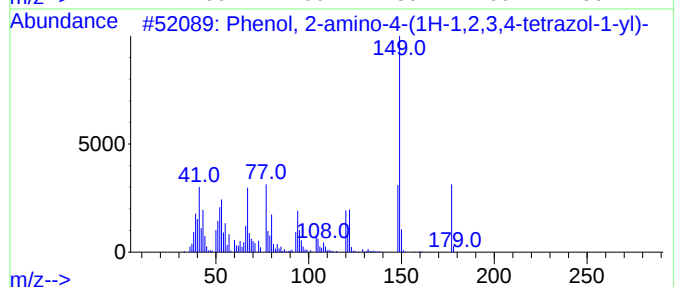
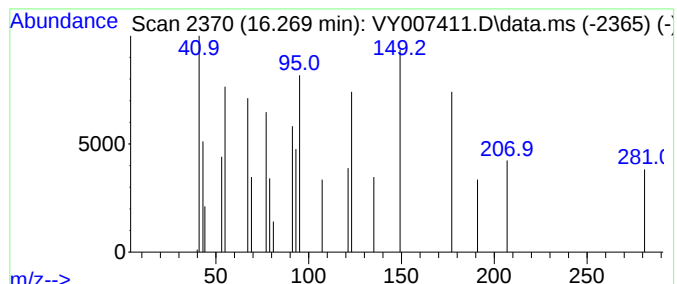
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.269 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	7.05 ug/l	2947	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-amino-4-(1H-1,2,3,4-te...	177	C7H7N5O	1000362-63-1	32
2			Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	25
3			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	22
4			Cyclopropanecarboxylic acid, 2,2...	328	C21H28O3	000121-21-1	12
5			2-Heptenoic acid, 7-(methylenecy...	194	C12H18O2	1000158-04-1	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY020722\
Data File : VY007411.D
Acq On : 07 Feb 2022 14:31
Operator : SY/MD
Sample : N1387-05
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
26601

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y020222S.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
1,4-Dimethylada...	14.391	7.8	ug/l	3257	4	13.422	20911	50.0
2-Methyladamantane	14.879	20.5	ug/l	8581	4	13.422	20911	50.0
1-Methyl-1-hydr...	15.007	8.6	ug/l	3585	4	13.422	20911	50.0
unknown15.031	15.031	10.2	ug/l	4268	4	13.422	20911	50.0
Adamantane, 1,3...	15.281	14.2	ug/l	5923	4	13.422	20911	50.0
unknown15.355	15.355	14.5	ug/l	6047	4	13.422	20911	50.0
unknown15.714	15.714	14.0	ug/l	5863	4	13.422	20911	50.0
unknown16.269	16.269	7.0	ug/l	2947	4	13.422	20911	50.0