

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
 Data File : VY020821.D
 Acq On : 14 Jan 2025 14:23
 Operator : SY/MD
 Sample : Q1077-01
 Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 5 Sample Multiplier: 1

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\82Y010625S.M

Title : SW846 8260

Signal : TIC: VY020821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.757	4	6	9	rVB	408	383	13.13%	0.808%
2	1.812	13	15	16	rBV2	514	314	10.77%	0.662%
3	2.044	52	53	55	rBV2	414	293	10.05%	0.618%
4	2.092	58	61	62	rBV2	320	330	11.32%	0.696%
5	2.373	104	107	108	rBV2	259	326	11.18%	0.687%
6	2.885	189	191	194	rVB2	272	292	10.01%	0.616%
7	3.062	219	220	225	rVB2	268	346	11.87%	0.730%
8	3.111	225	228	230	rBV2	235	307	10.53%	0.647%
9	3.178	235	239	241	rBV2	267	376	12.89%	0.793%
10	3.482	286	289	294	rVB3	253	415	14.23%	0.875%
11	3.641	313	315	319	rVB2	357	417	14.30%	0.879%
12	3.690	319	323	324	rBV2	301	367	12.59%	0.774%
13	3.879	352	354	359	rVB	329	340	11.66%	0.717%
14	3.934	359	363	365	rBV2	224	321	11.01%	0.677%
15	4.555	462	465	468	rBV3	319	489	16.77%	1.031%
16	4.647	479	480	483	rVB	435	257	8.81%	0.542%
17	4.671	483	484	486	rBV2	432	352	12.07%	0.742%
18	4.714	489	491	494	rBV2	189	259	8.88%	0.546%
19	5.427	607	608	612	rVB3	301	304	10.43%	0.641%
20	5.555	624	629	631	rVB2	361	550	18.86%	1.160%
21	5.689	648	651	652	rVB3	341	255	8.74%	0.538%
22	5.872	678	681	683	rVB	353	278	9.53%	0.586%
23	6.110	718	720	723	rVB3	206	247	8.47%	0.521%
24	6.201	734	735	738	rVB2	263	265	9.09%	0.559%
25	6.232	738	740	741	rBV2	294	251	8.61%	0.529%
26	6.336	754	757	761	rVB2	194	280	9.60%	0.590%
27	6.689	809	815	816	rVB2	339	410	14.06%	0.865%
28	7.055	872	875	877	rVB3	295	310	10.63%	0.654%
29	7.085	877	880	882	rBV	256	339	11.63%	0.715%
30	7.134	885	888	891	rBV2	313	449	15.40%	0.947%
31	7.250	905	907	911	rBV2	294	283	9.71%	0.597%
32	7.390	926	930	933	rBV3	238	385	13.20%	0.812%
33	7.573	958	960	964	rVV2	292	298	10.22%	0.628%
34	7.610	964	966	969	rVB2	302	312	10.70%	0.658%
35	7.762	988	991	993	rVB2	327	379	13.00%	0.799%
36	8.256	1070	1072	1074	rVB2	310	263	9.02%	0.555%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
 Data File : VY020821.D
 Acq On : 14 Jan 2025 14:23
 Operator : SY/MD
 Sample : Q1077-01
 Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 5 Sample Multiplier: 1

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\82Y010625S.M
 Title : SW846 8260

37	8.329	1080	1084	1086	rBV2	232	304	10.43%	0.641%
38	8.561	1118	1122	1124	rVB2	323	320	10.97%	0.675%
39	8.634	1131	1134	1136	rVB2	261	302	10.36%	0.637%
40	8.695	1142	1144	1146	rVB	462	366	12.55%	0.772%
41	8.713	1146	1147	1149	rBV2	362	329	11.28%	0.694%
42	8.841	1166	1168	1171	rVB2	312	370	12.69%	0.780%
43	8.896	1171	1177	1178	rBV3	255	410	14.06%	0.865%
44	9.103	1209	1211	1214	rVB2	373	360	12.35%	0.759%
45	9.152	1214	1219	1220	rBV2	364	568	19.48%	1.198%
46	9.244	1232	1234	1236	rBV	260	253	8.68%	0.533%
47	9.548	1282	1284	1286	rVB2	324	248	8.50%	0.523%
48	9.603	1291	1293	1294	rBV	423	267	9.16%	0.563%
49	9.634	1297	1298	1301	rBV3	317	251	8.61%	0.529%
50	9.762	1317	1319	1321	rBV2	230	255	8.74%	0.538%
51	9.817	1325	1328	1331	rVV3	209	364	12.48%	0.768%
52	9.872	1335	1337	1340	rVB2	455	377	12.93%	0.795%
53	9.969	1351	1353	1355	rVB2	343	273	9.36%	0.576%
54	10.280	1402	1404	1406	rVB2	401	307	10.53%	0.647%
55	10.609	1455	1458	1460	rBV2	380	507	17.39%	1.069%
56	10.646	1463	1464	1467	rBV2	315	312	10.70%	0.658%
57	10.682	1467	1470	1471	rBV	274	319	10.94%	0.673%
58	10.701	1471	1473	1475	rVV2	532	356	12.21%	0.751%
59	10.743	1477	1480	1483	rVB3	697	799	27.40%	1.685%
60	10.774	1483	1485	1487	rBV	470	368	12.62%	0.776%
61	10.993	1518	1521	1523	rBV4	409	608	20.85%	1.282%
62	11.060	1530	1532	1533	rBV	354	294	10.08%	0.620%
63	11.115	1539	1541	1545	rBV2	611	853	29.25%	1.799%
64	11.213	1555	1557	1560	rVB2	594	444	15.23%	0.936%
65	11.249	1561	1563	1566	rBV2	302	360	12.35%	0.759%
66	11.286	1566	1569	1570	rBV3	378	260	8.92%	0.548%
67	11.304	1570	1572	1576	rBV4	301	406	13.92%	0.856%
68	11.347	1576	1579	1582	rBV6	1053	1494	51.23%	3.150%
69	11.377	1582	1584	1586	rBV3	829	1004	34.43%	2.117%
70	11.414	1586	1590	1591	rBV3	934	1315	45.10%	2.773%
71	11.536	1609	1610	1613	rBV3	480	500	17.15%	1.054%
72	11.597	1616	1620	1623	rBV5	567	829	28.43%	1.748%
73	11.633	1623	1626	1627	rBV2	572	633	21.71%	1.335%
74	11.658	1627	1630	1633	rBV4	1076	2066	70.85%	4.357%
75	11.920	1668	1673	1678	rVV9	1377	2916	100.00%	6.149%
76	11.963	1678	1680	1685	rVB6	1663	2013	69.03%	4.245%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

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_Y\methods\82Y010625S.M
Title : SW846 8260

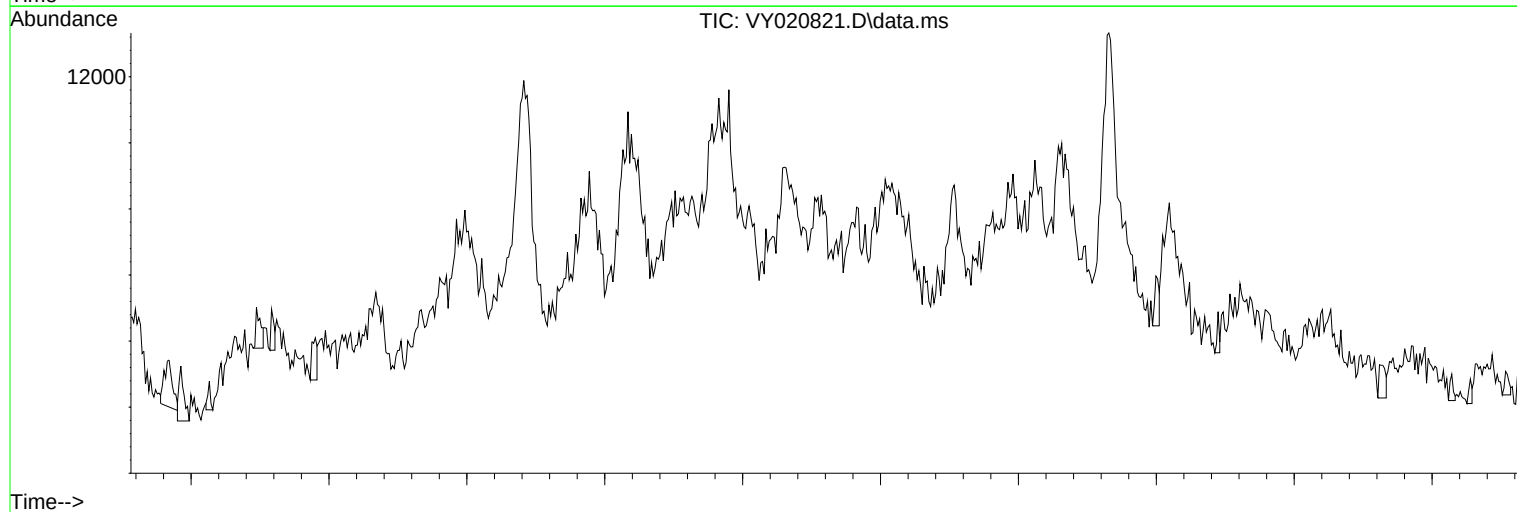
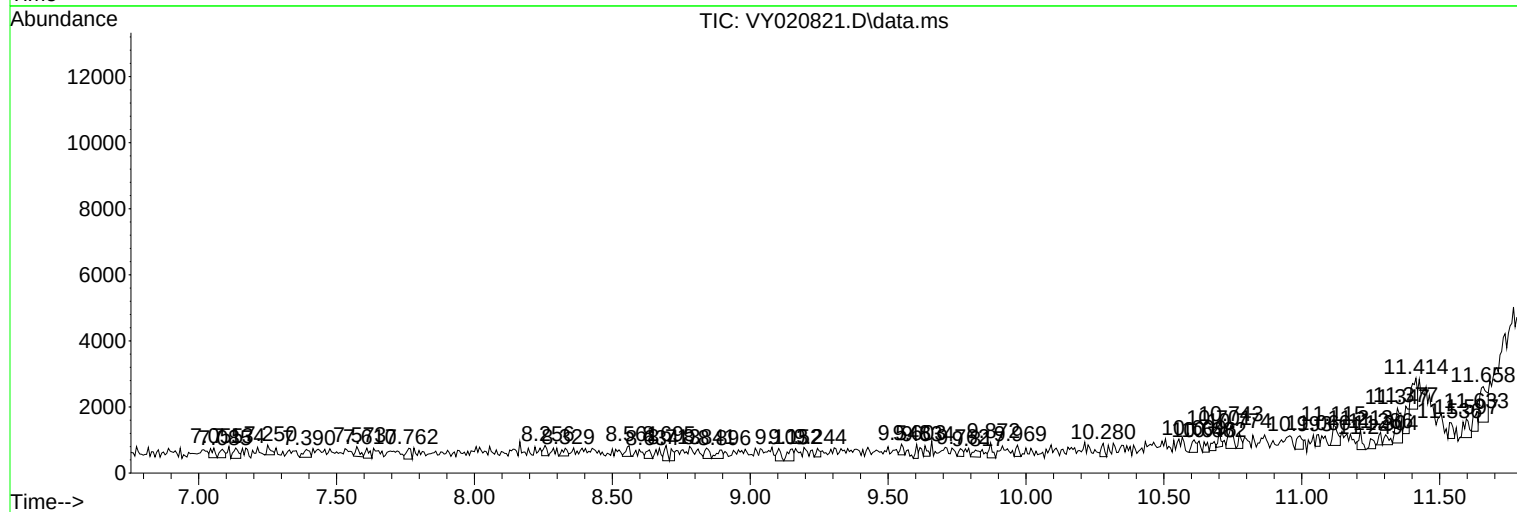
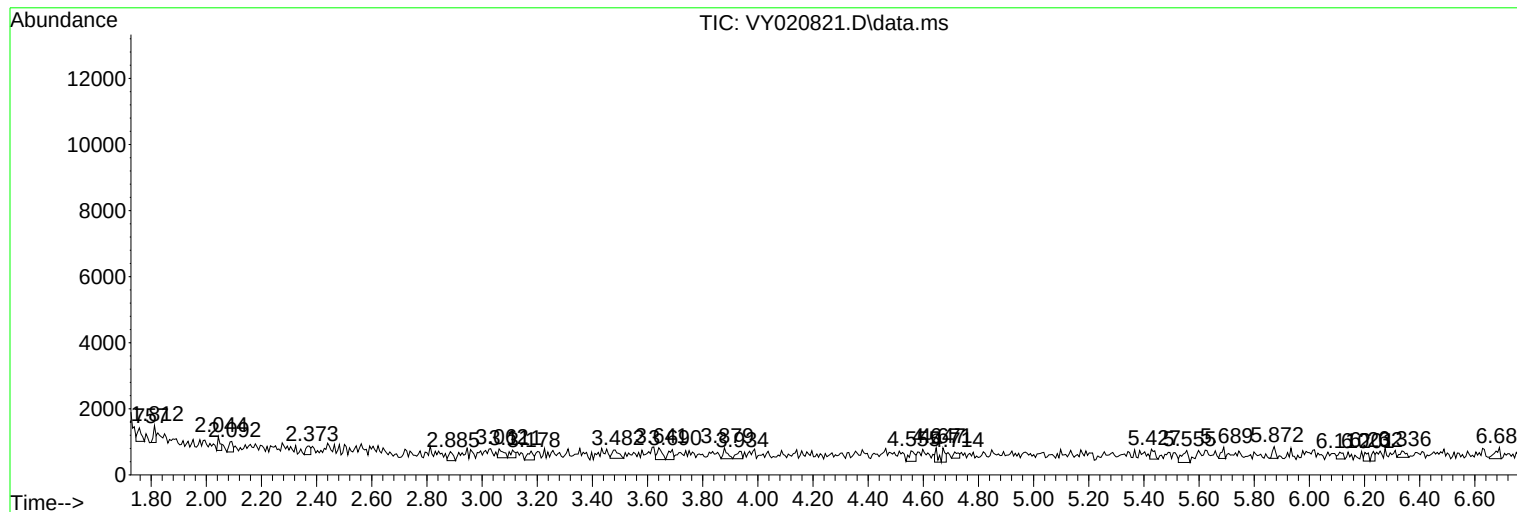
77	12.066	1695	1697	1699	rVB2	860	542	18.59%	1.143%
78	12.237	1723	1725	1729	rBV5	1234	1555	53.33%	3.279%
79	12.292	1733	1734	1736	rBV2	1242	1009	34.60%	2.128%
80	12.450	1757	1760	1761	rBV3	1275	1671	57.30%	3.524%
81	15.499	2258	2260	2262	rBV3	1505	1680	57.61%	3.543%
82	15.724	2295	2297	2298	rBV2	1244	669	22.94%	1.411%
83	16.309	2392	2393	2397	rBV4	1005	1653	56.69%	3.486%
84	16.572	2434	2436	2438	rBV3	799	652	22.36%	1.375%
85	16.639	2445	2447	2448	rBV2	743	584	20.03%	1.231%
86	16.767	2466	2468	2471	rBV4	712	786	26.95%	1.657%

Sum of corrected areas: 47423

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

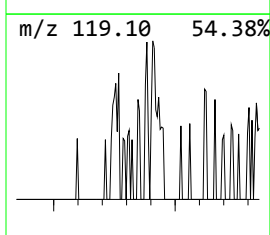
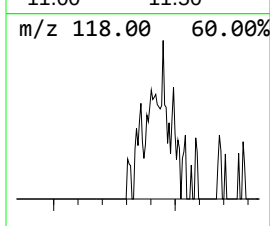
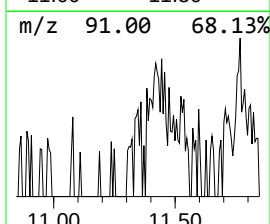
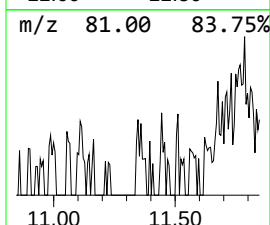
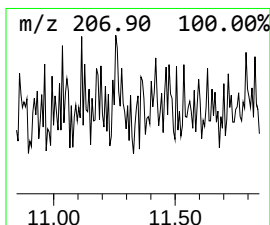
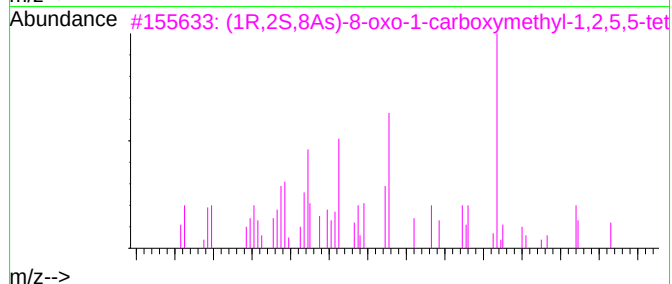
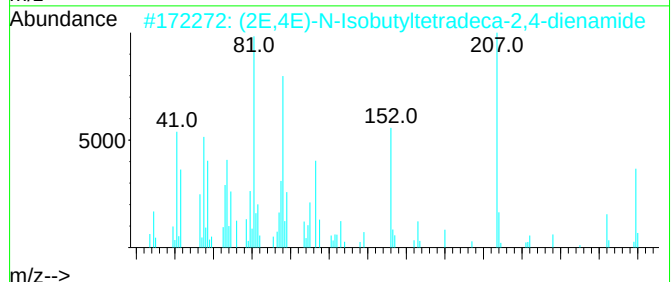
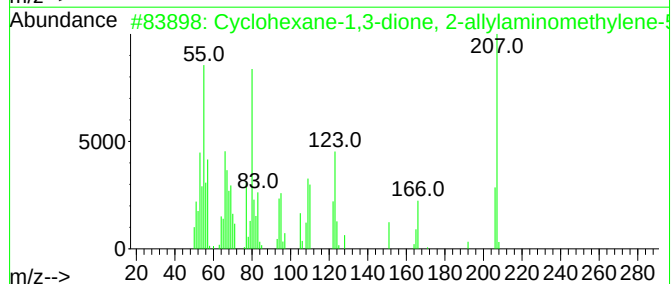
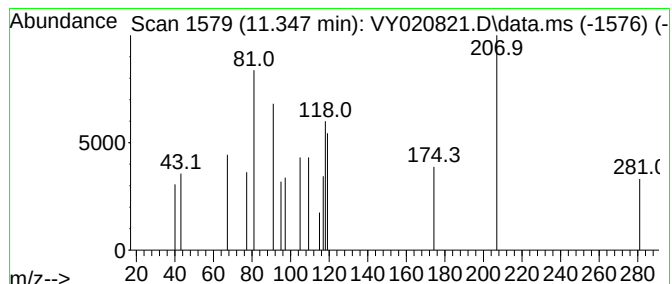
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown11.347 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.347	56.81 ug/l	1494	Chlorobenzene-d5	11.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	22
2	(2E,4E)-N-Isobutyltetradeca-2,4-...	279	C18H33NO	013891-73-1	17
3	(1R,2S,8As)-8-oxo-1-carboxymethy...	266	C16H26O3	1000298-98-2	12
4	Adamantane, cyclopropylidene-	174	C13H18	099298-53-0	10
5	Benzene, (1-azido-1-methylethyl)-	161	C9H11N3	032366-26-0	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

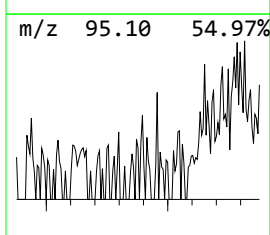
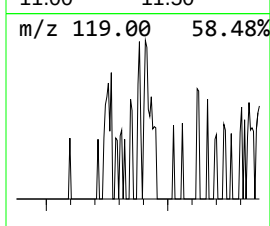
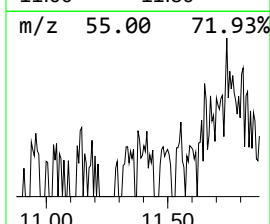
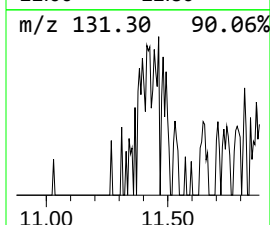
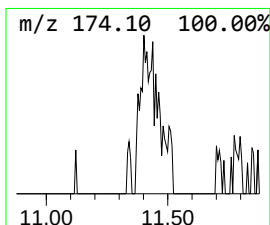
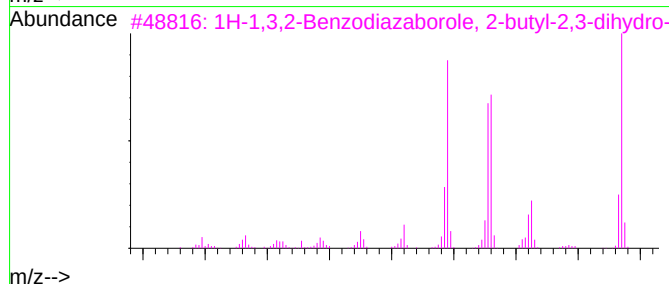
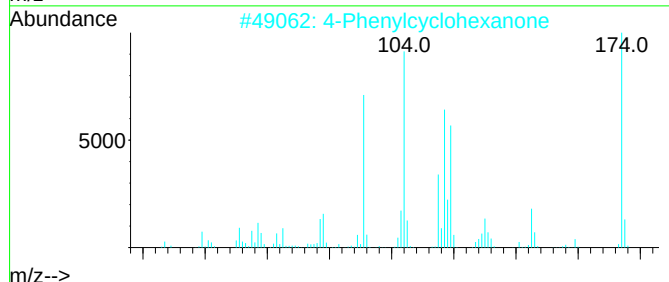
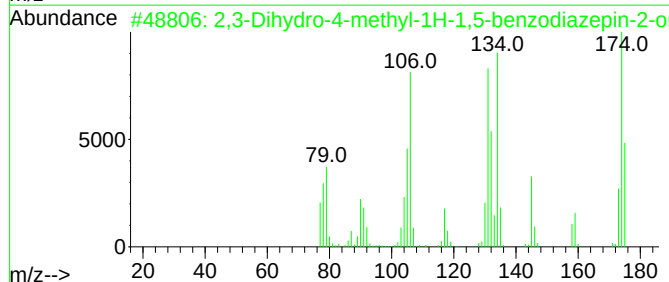
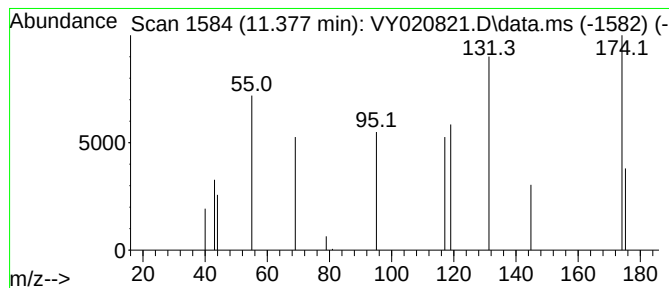
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown11.377 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.377	38.17 ug/l	1004	Chlorobenzene-d5	11.432

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-4-methyl-1H-1,5-benz...	174	C10H10N2O	006276-48-8	47		
2	4-Phenylcyclohexanone	174	C12H14O	004894-75-1	43		
3	1H-1,3,2-Benzodiazaborole, 2-but...	174	C10H15BN2	031748-14-8	9		
4	3-(Pent-1-en-1-yl)benzaldehyde	174	C12H14O	1000461-11-8	9		
5	trans-3'-Hydroxycotinine, penta...	338	C13H11F5N2O3	1000448-21-0	9		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

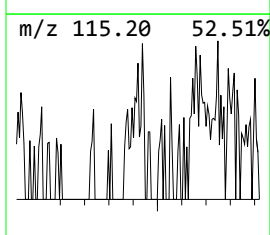
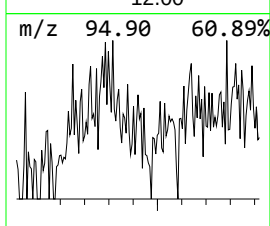
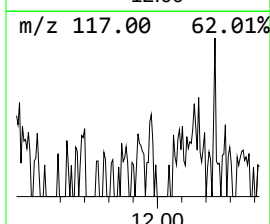
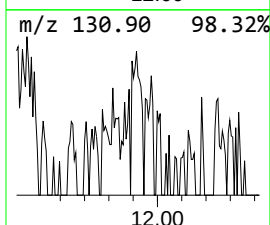
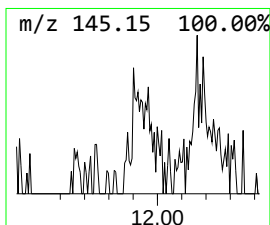
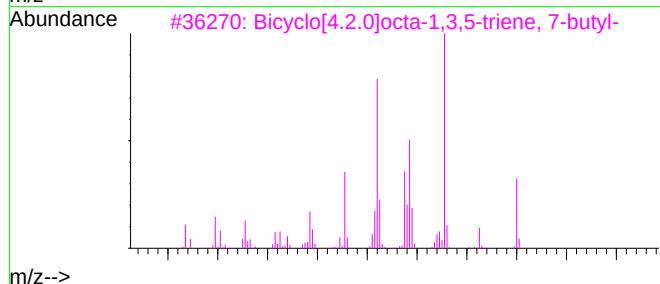
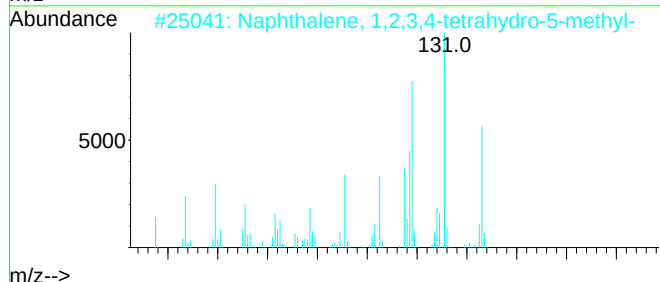
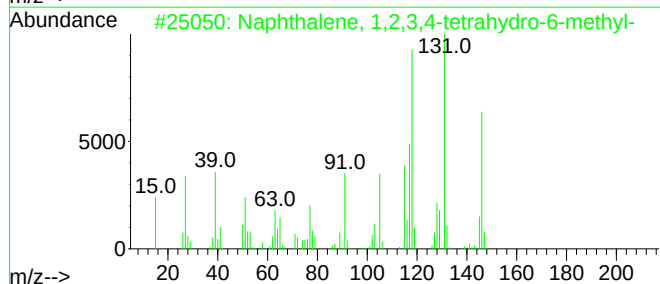
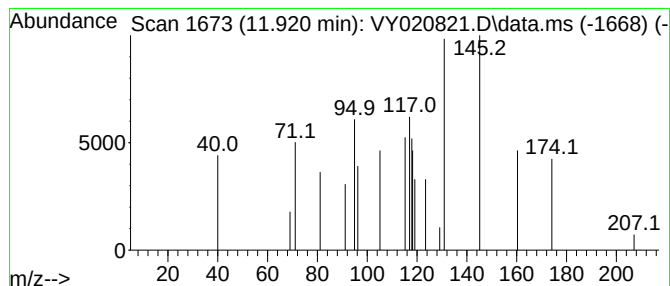
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown11.920 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.920	110.88 ug/l	2916	Chlorobenzene-d5	11.432

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	35
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	27
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	22
4			2-Chloro-6-fluorophenol, O-metho...	204	C8H6ClF03	1000487-73-2	12
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

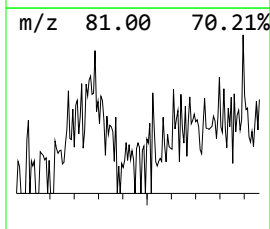
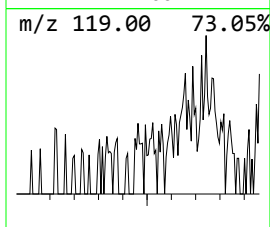
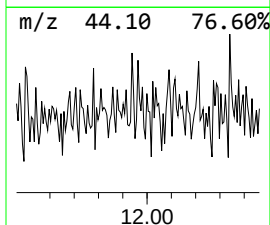
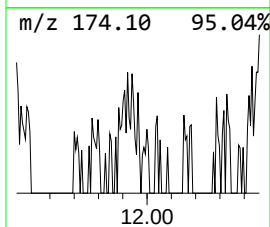
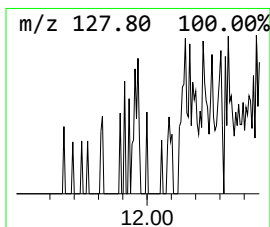
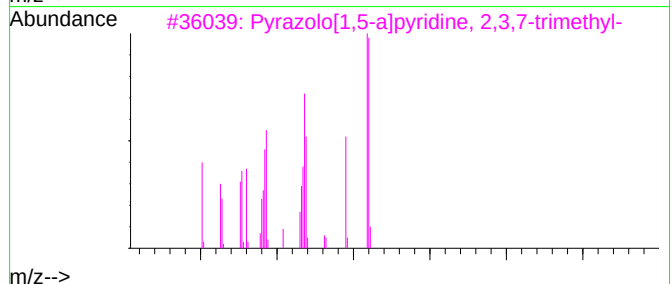
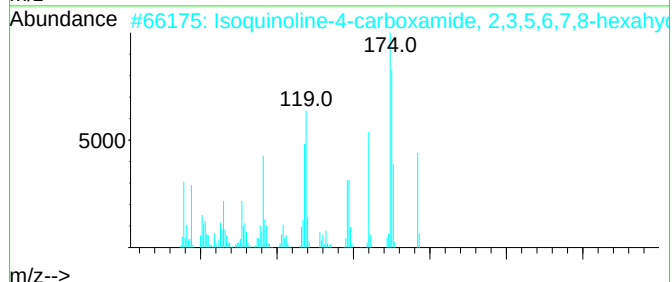
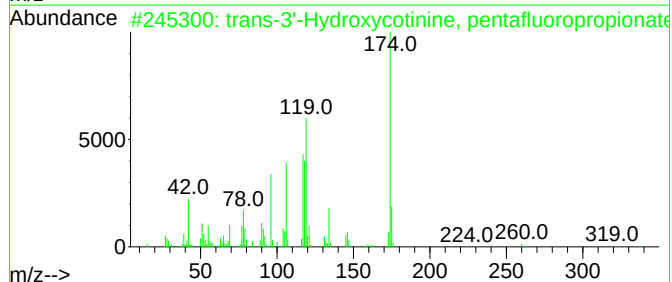
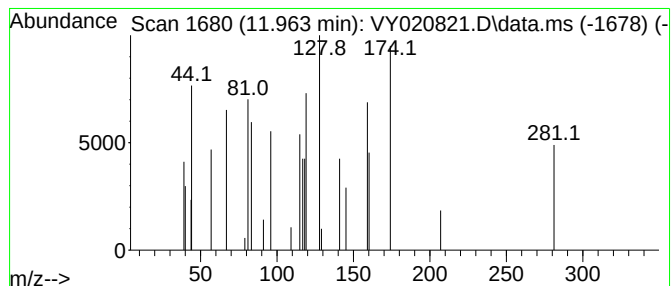
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown11.963 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	76.54 ug/l	2013	Chlorobenzene-d5	11.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-3'-Hydroxycotinine, penta...	338	C13H11F5N2O3	1000448-21-0	25
2	Isoquinoline-4-carboxamide, 2,3,...	192	C10H12N2O2	026862-51-1	16
3	Pyrazolo[1,5-a]pyridine, 2,3,7-t...	160	C10H12N2	017408-34-3	14
4	(1R,2R,4S,6S,7S,8S)-8-Isopropyl-...	220	C15H24O	124753-76-0	10
5	1-tert-Butyl-4-(prop-2-en-1-yl)b...	174	C13H18	1000486-84-1	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

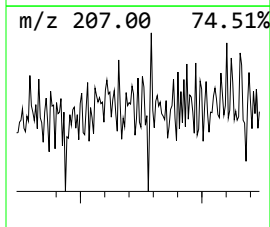
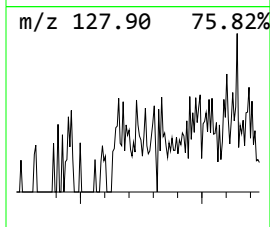
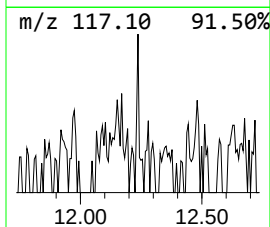
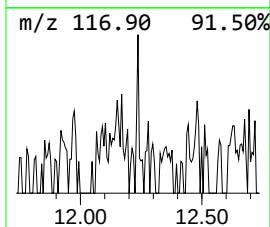
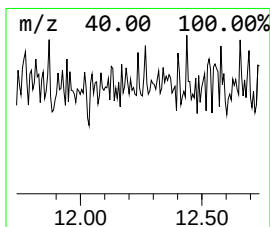
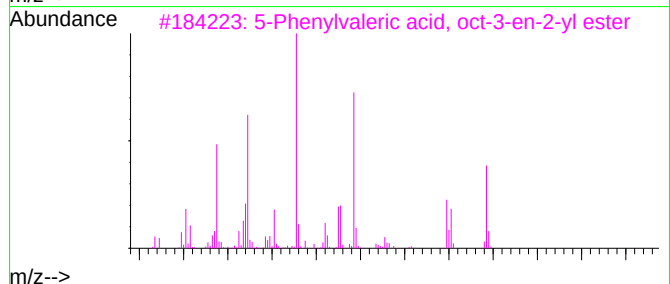
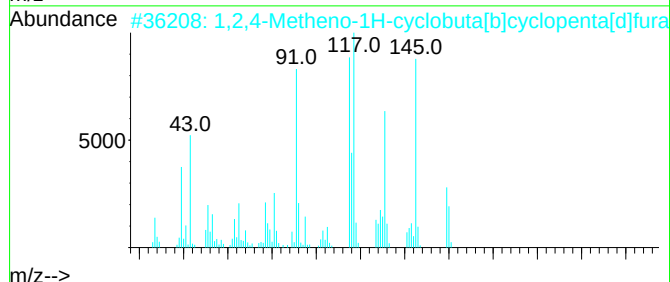
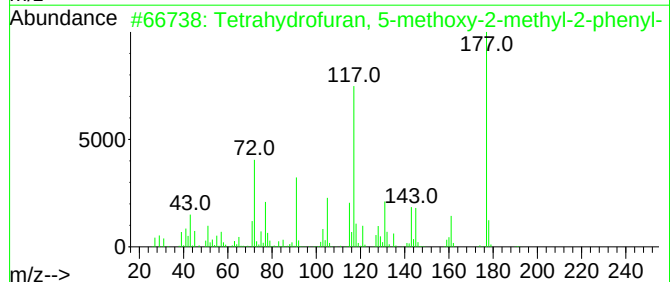
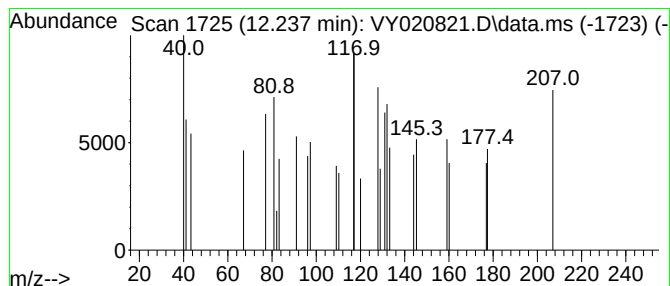
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown12.237 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.237	59.13 ug/l	1555	Chlorobenzene-d5	11.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrahydrofuran, 5-methoxy-2-met...	192	C12H16O2	082194-21-6	16
2	1,2,4-Metheno-1H-cyclobuta[b]cyc...	160	C11H12O	078323-74-7	12
3	5-Phenylvaleric acid, oct-3-en-2...	288	C19H28O2	1000406-93-6	10
4	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	10
5	3-Chloro-2-methylcyclopent-2-enol	132	C6H9ClO	1000192-84-7	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

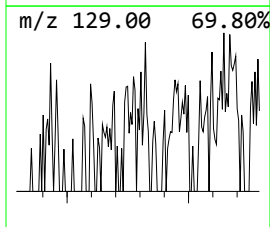
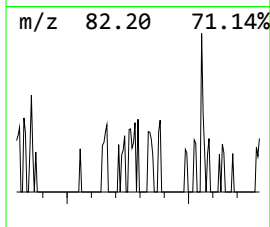
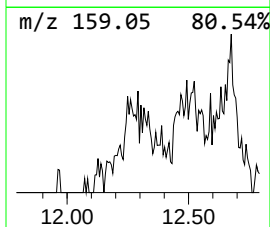
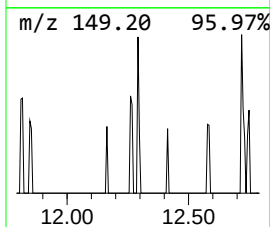
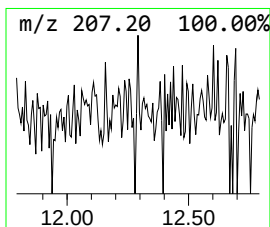
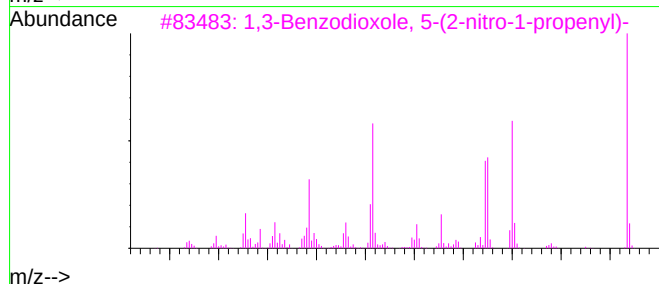
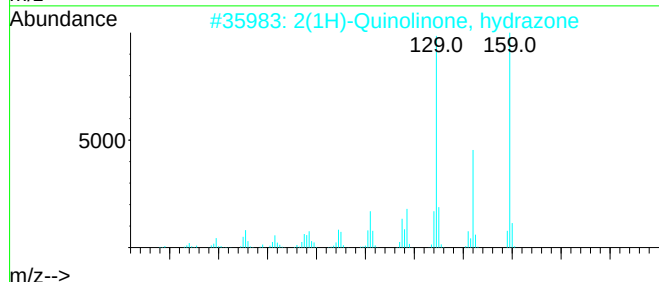
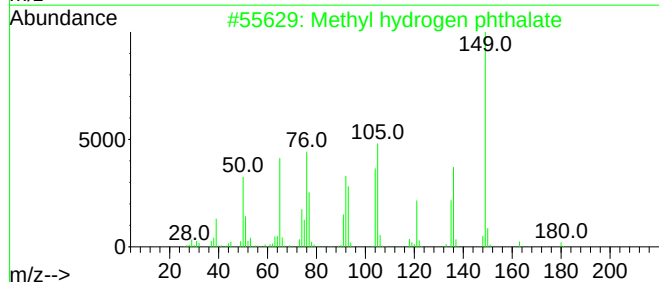
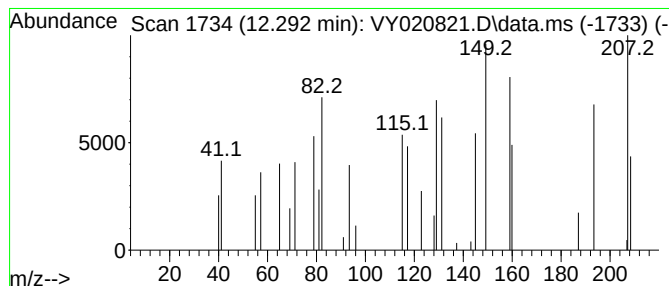
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown12.292 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.292	38.37 ug/l	1009	Chlorobenzene-d5	11.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl hydrogen phthalate	180	C9H8O4	004376-18-5	10
2	2(1H)-Quinolinone, hydrazone	159	C9H9N3	015793-77-8	10
3	1,3-Benzodioxole, 5-(2-nitro-1-p...	207	C10H9NO4	005438-41-5	9
4	Isoquinoline, 1-hydrazino-	159	C9H9N3	1000362-59-9	9
5	2,3,4-Trifluorobenzaldehyde	160	C7H3F3O	161793-17-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

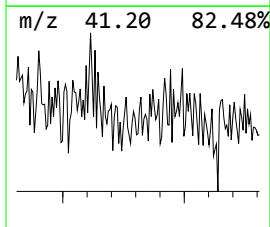
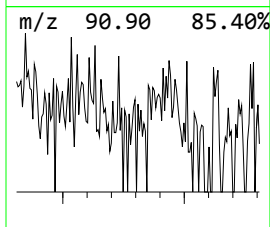
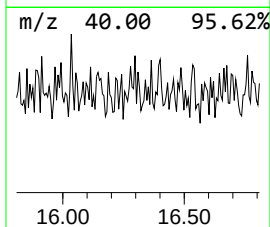
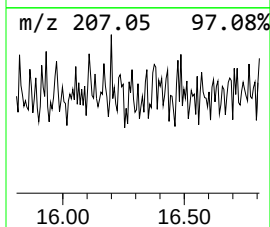
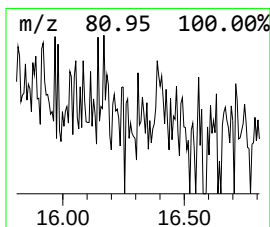
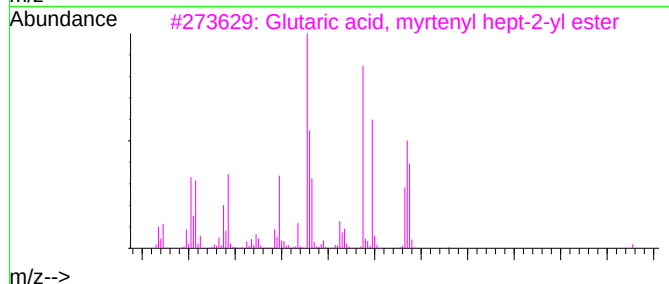
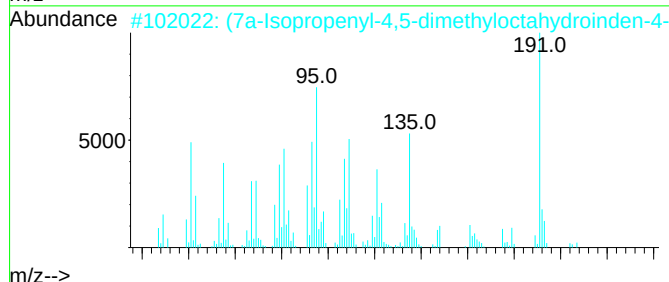
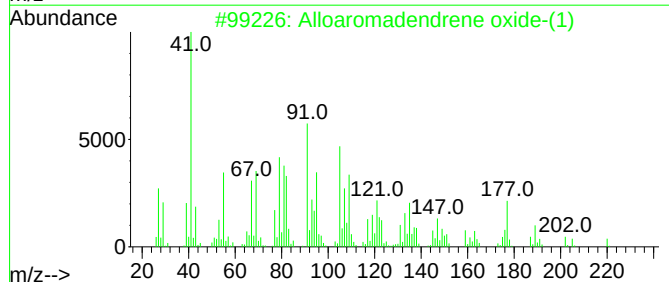
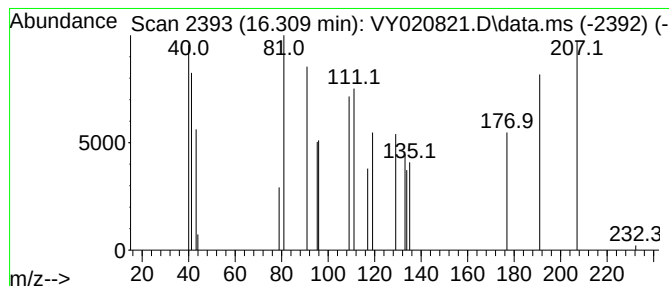
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.309 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	49.46 ug/l	1653	1,4-Dichlorobenzene-d4	13.365

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Alloaromadendrene oxide-(1)	220	C15H24O	1000156-12-8	10
2			(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1010187-02-9	10
3			Glutaric acid, myrtenyl hept-2-y...	364	C22H36O4	1000405-54-1	10
4			Isoxazole, trimethyl-	111	C6H9NO	010557-82-1	9
5			Anthranilic acid, N-methyl-, but...	207	C12H17NO2	015236-34-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011425\
Data File : VY020821.D
Acq On : 14 Jan 2025 14:23
Operator : SY/MD
Sample : Q1077-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010625S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown11.347	11.347	56.8	ug/l	1494	1	11.432	1315	50.0
unknown11.377	11.377	38.2	ug/l	1004	1	11.432	1315	50.0
unknown11.920	11.920	110.9	ug/l	2916	1	11.432	1315	50.0
unknown11.963	11.963	76.5	ug/l	2013	1	11.432	1315	50.0
unknown12.237	12.237	59.1	ug/l	1555	1	11.432	1315	50.0
unknown12.292	12.292	38.4	ug/l	1009	1	11.432	1315	50.0
unknown16.309	16.309	49.5	ug/l	1653	2	13.365	1671	50.0