LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

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\82Y060225S.M
Title : SW846 8260

Signal : TIC: VY022593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.105	50	63	64	rBV3	14268	43897	37.35%	6.058%
2	3.812	339	343	346	rBV3	733	1192	1.01%	0.165%
3	6.238	739	741	746	rBV2	813	1216	1.03%	0.168%
4	7.238	900	905	908	rBV3	836	1574	1.34%	0.217%
5	7.628	962	969	975	rBV3	11573	27704	23.57%	3.823%
6	7.707	975	982	993	rVB	40375	90824	77.27%	12.534%
7	8.061	1032	1040	1048	rBV3	10639	24461	20.81%	3.376%
8	8.610	1123	1130	1139	rBV	47536	95256	81.04%	13.146%
9	9.103	1208	1211	1216	rVB3	1216	1821	1.55%	0.251%
10	9.878	1335	1338	1341	rVB3	1157	1350	1.15%	0.186%
11	10.060	1365	1368	1369	rBV2	1198	1294	1.10%	0.179%
12	10.103	1369	1375	1383	rVV	64496	117542	100.00%	16.221%
13	10.164	1383	1385	1388	rVV4	1275	1437	1.22%	0.198%
14	10.658	1463	1466	1468	rBV4	969	1206	1.03%	0.166%
15	11.127	1542	1543	1546	rVV3	1038	1187	1.01%	0.164%
16	11.164	1546	1549	1551	rVV3	1633	2097	1.78%	0.289%
17	11.188	1551	1553	1556	rVV4	2491	3070	2.61%	0.424%
18	11.231	1558	1560	1565	rVV6	2035	3321	2.83%	0.458%
19	11.280	1565	1568	1571	rVV5	1202	1728	1.47%	0.238%
20	11.335	1574	1577	1578	rBV3	1176	1366	1.16%	0.189%
21	11.414	1584	1590	1596	rBV	43602	73531	62.56%	10.148%
22	11.481	1599	1601	1603	rBV3	1194	1415	1.20%	0.195%
23	11.579	1609	1617	1619	rBV8	3626	7418	6.31%	1.024%
24	11.828	1656	1658	1661	rBV4	901	1177	1.00%	0.162%
25	11.975	1681	1682	1684	rBV2	1675	1390	1.18%	0.192%
26	12.042	1689	1693	1695	rBV5	2074	2461	2.09%	0.340%
27	12.072	1695	1698	1701	rVV5	1671	2752	2.34%	0.380%
28	12.188	1715	1717	1718	rBV2	2421	1692	1.44%	0.234%
29	12.255	1725	1728	1739	rVB3	23265	47963	40.80%	6.619%
30	12.402	1748	1752	1759	rVB	23711	38961	33.15%	5.377%
31	12.651	1791	1793	1798	rVB5	1783	1857	1.58%	0.256%
32	12.725	1798	1805	1808	rBV8	2913	6805	5.79%	0.939%
33	12.840	1821	1824	1825	rBV3	2198	2332	1.98%	0.322%
34	13.084	1862	1864	1866	rBV3	2298	3161	2.69%	0.436%
35	13.255	1890	1892	1894	rVV3	2249	1483	1.26%	0.205%
36	13.286	1896	1897	1899	rVV2	2403	1571	1.34%	0.217%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

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\82Y060225S.M
Title : SW846 8260

37	13.346	1901	1907	1912	rBV	21015	34357	29.23%	4.741%
38	13.481	1925	1929	1931	rBV5	3210	4490	3.82%	0.620%
39	13.505	1931	1933	1935	rVV3	1876	2305	1.96%	0.318%
40	13.609	1948	1950	1952	rBV2	1367	1255	1.07%	0.173%
41	13.834	1983	1987	1988	rBV4	2297	2413	2.05%	0.333%
42	14.023	2017	2018	2020	rBV2	1880	1273	1.08%	0.176%
43	14.084	2026	2028	2033	rVV6	1013	1728	1.47%	0.238%
44	14.206	2044	2048	2051	rVV6	2116	2724	2.32%	0.376%
45	14.237	2051	2053	2055	rVB3	2259	1277	1.09%	0.176%
46	14.285	2060	2061	2065	rBV4	2057	2544	2.16%	0.351%
47	14.389	2076	2078	2083	rBV6	1355	1889	1.61%	0.261%
48	14.438	2083	2086	2087	rBV3	1180	1351	1.15%	0.186%
49	14.584	2108	2110	2114	rBV5	1801	2390	2.03%	0.330%
50	14.749	2131	2137	2139	rVV6	2342	3678	3.13%	0.508%
51	14.901	2161	2162	2164	rBV2	1271	1228	1.04%	0.169%
52	15.005	2176	2179	2188	rVB10	3799	9179	7.81%	1.267%
53	15.108	2191	2196	2197	rBV5	1473	2408	2.05%	0.332%
54	15.127	2197	2199	2201	rBV3	1403	1551	1.32%	0.214%
55	15.273	2216	2223	2228	rBV8	4752	11332	9.64%	1.564%
56	15.468	2250	2255	2256	rBV4	1216	1519	1.29%	0.210%
57	15.761	2300	2303	2305	rVB3	1172	1190	1.01%	0.164%
58	15.785	2305	2307	2309	rBV2	1407	1188	1.01%	0.164%
59	15.846	2314	2317	2320	rVV3	1105	1460	1.24%	0.201%
60	15.883	2320	2323	2326	rVV4	999	1225	1.04%	0.169%
61	15.919	2326	2329	2334	rVB6	1368	2308	1.96%	0.319%
62	16.005	2340	2343	2346	rVB4	1300	1996	1.70%	0.275%
63	16.120	2360	2362	2365	rBV4	992	1272	1.08%	0.176%
64	16.425	2406	2412	2415	rBV3	983	1992	1.69%	0.275%
65	16.706	2456	2458	2463	rVB3	995	1576	1.34%	0.217%

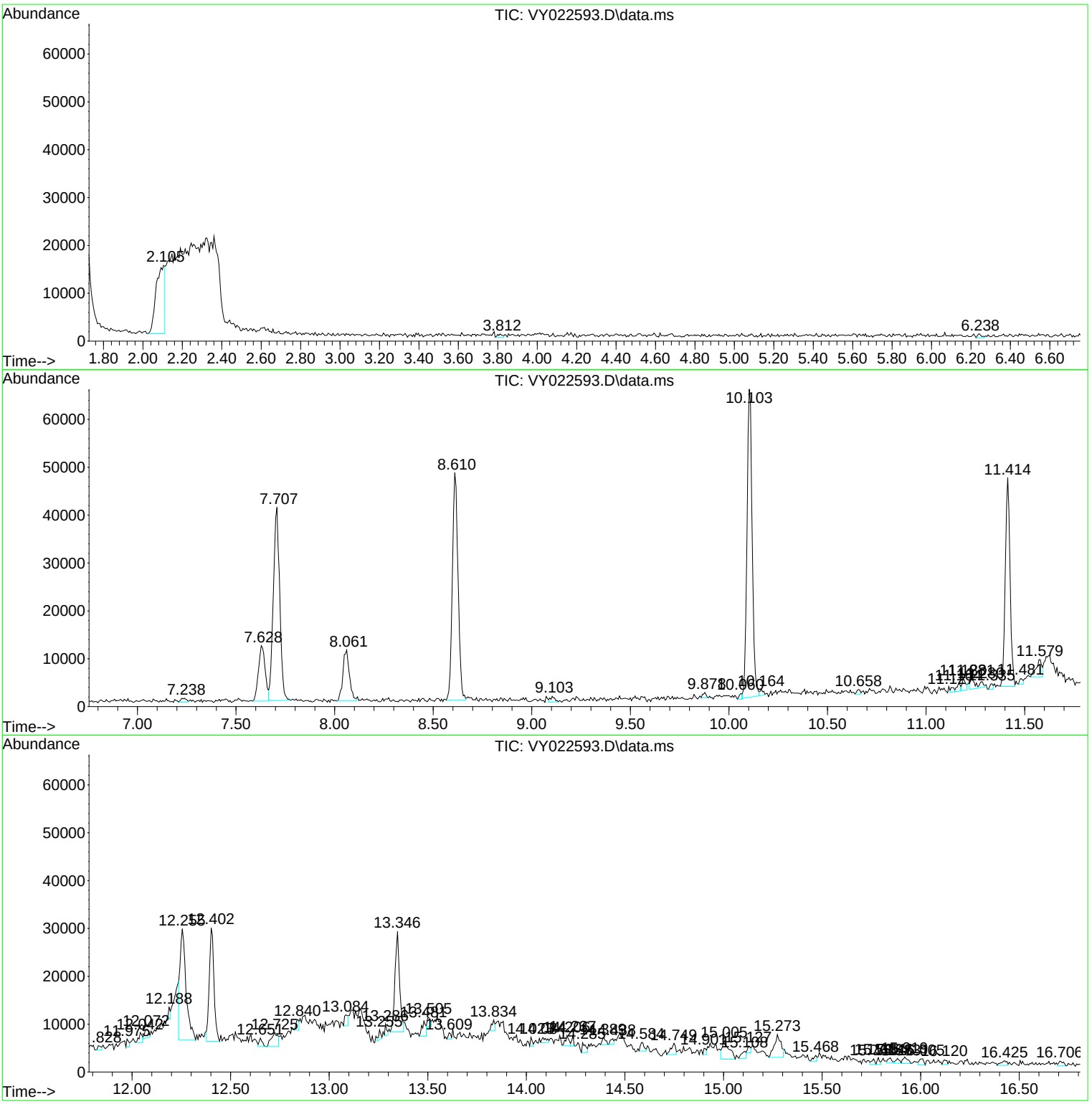
Sum of corrected areas: 724610

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

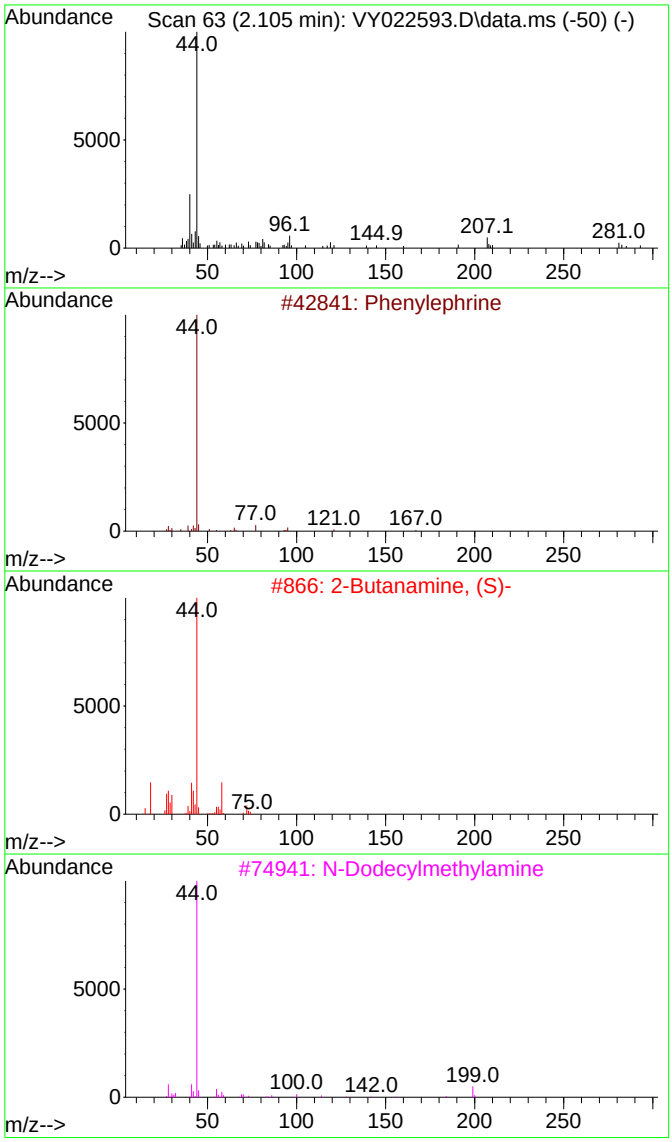
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

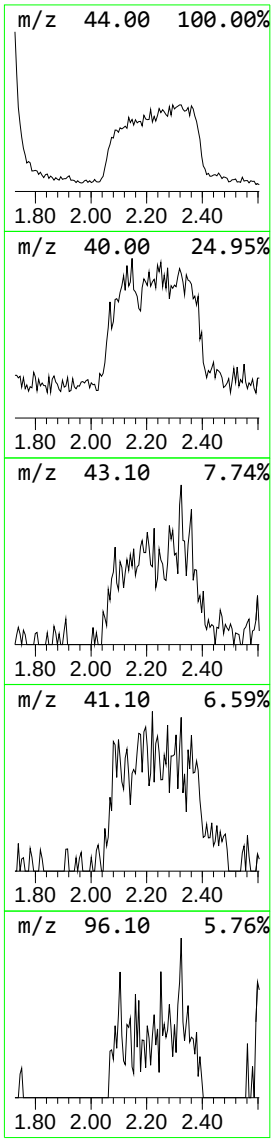
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Phenylephrine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	24.17 ug/l	43897	Pentafluorobenzene	7.701

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylephrine	167	C9H13NO2	000059-42-7	59
2	2-Butanamine, (S)-	73	C4H11N	000513-49-5	59
3	N-Dodecylmethylamine	199	C13H29N	1000342-26-1	45
4	1-Hexadecanamine, N-methyl-	255	C17H37N	013417-08-8	45
5	(S)-(+)-1-Cyclohexylethylamine	127	C8H17N	017430-98-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

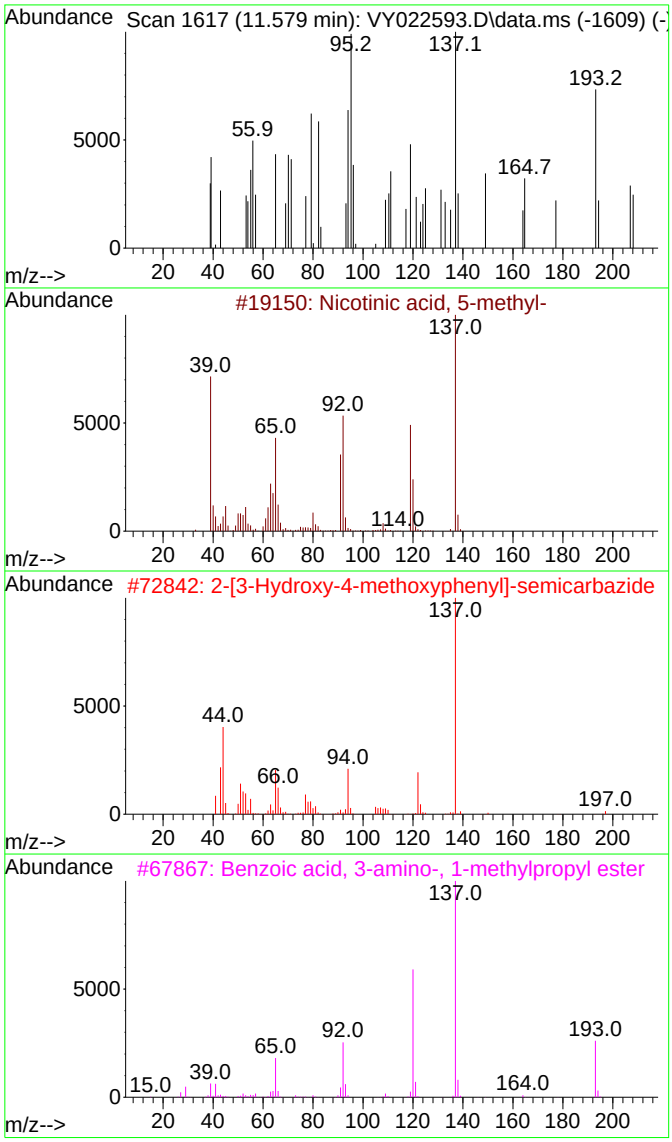
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

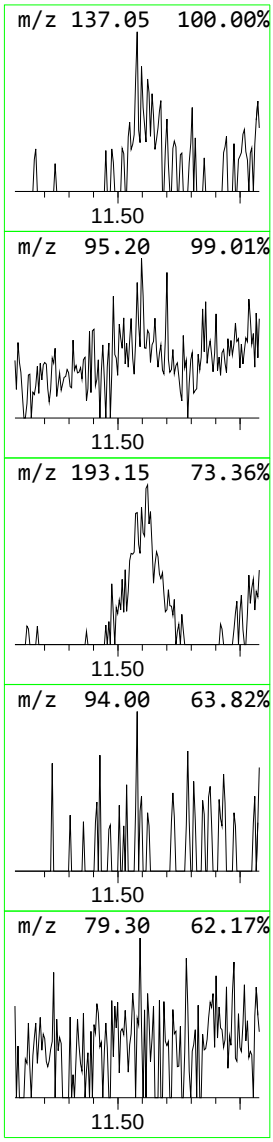
****

Peak Number 2 unknown11.579 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.579	5.04 ug/l	7418	Chlorobenzene-d5	11.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nicotinic acid, 5-methyl-	137	C7H7NO2	003222-49-9	35
2	2-[3-Hydroxy-4-methoxyphenyl]-se...	197	C8H11N3O3	1000116-96-7	25
3	Benzoic acid, 3-amino-, 1-methyl...	193	C11H15NO2	1000375-45-4	16
4	Methyl (1-nitrocyclohexane)propi...	215	C10H17NO4	1010370-34-2	14
5	cis-4a-Methyl-decahydronaphthalene	152	C11H20	002547-26-4	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

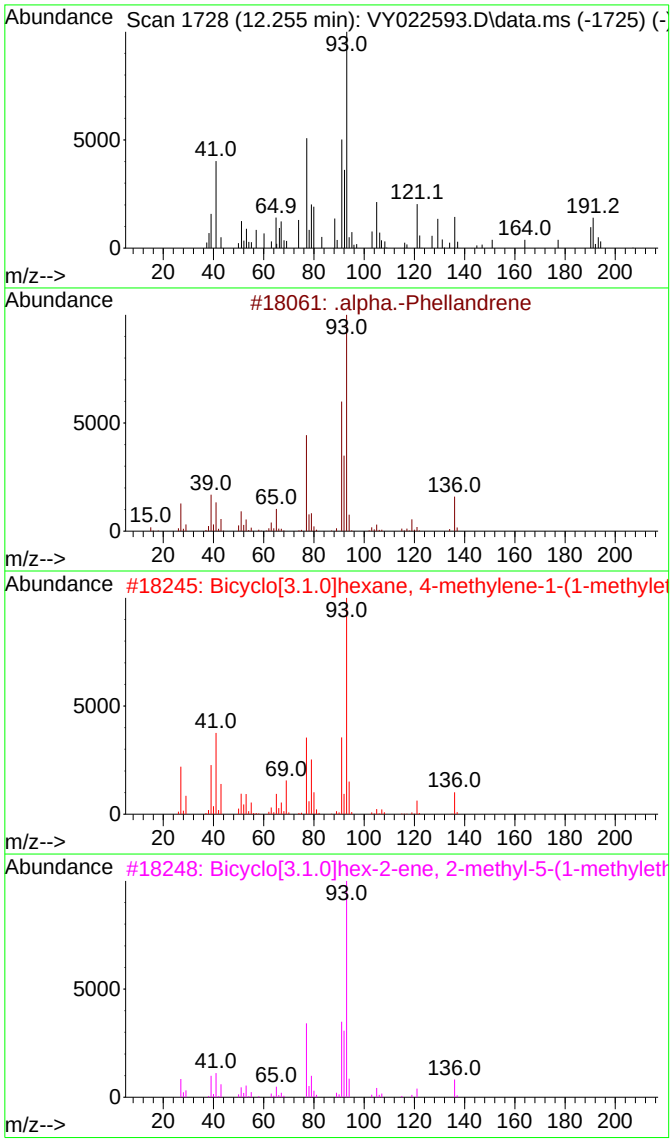
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

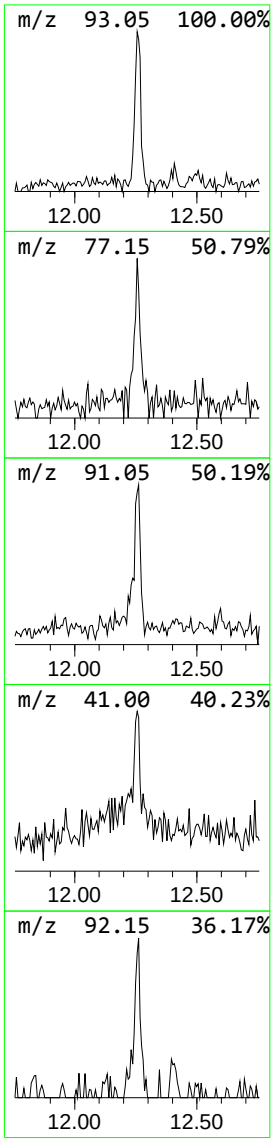
****

Peak Number 3 .alpha.-Phellandrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.255	32.61 ug/l	47963	Chlorobenzene-d5	11.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Phellandrene	136	C10H16	000099-83-2	58
2	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	50
3	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	50
4	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	50
5	3-Carene	136	C10H16	013466-78-9	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

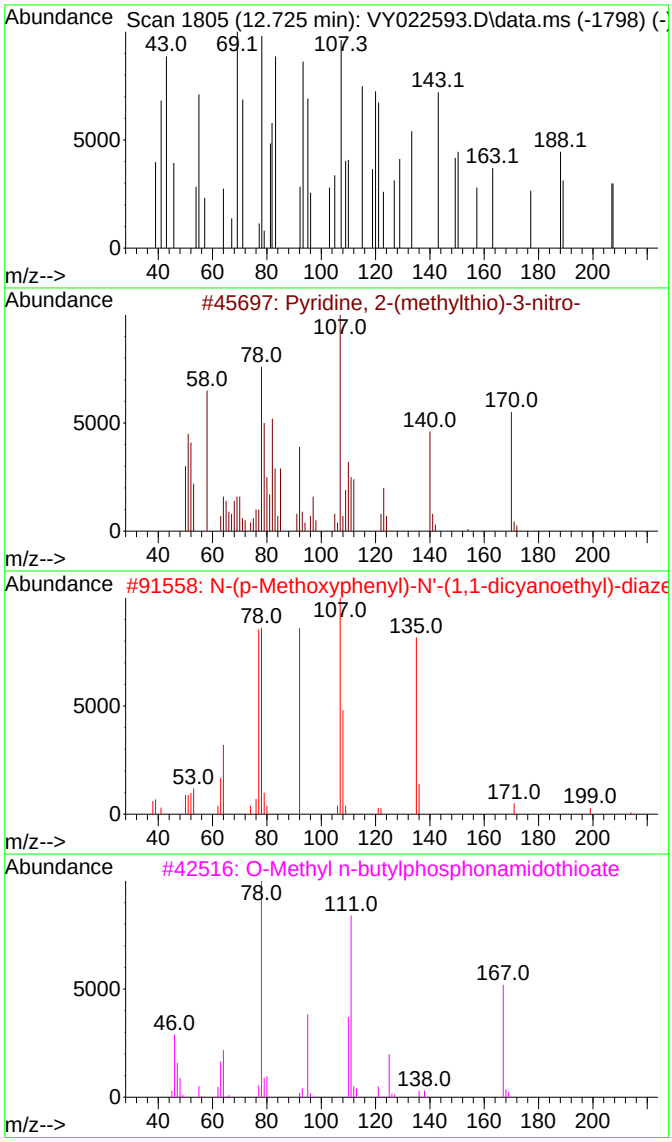
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

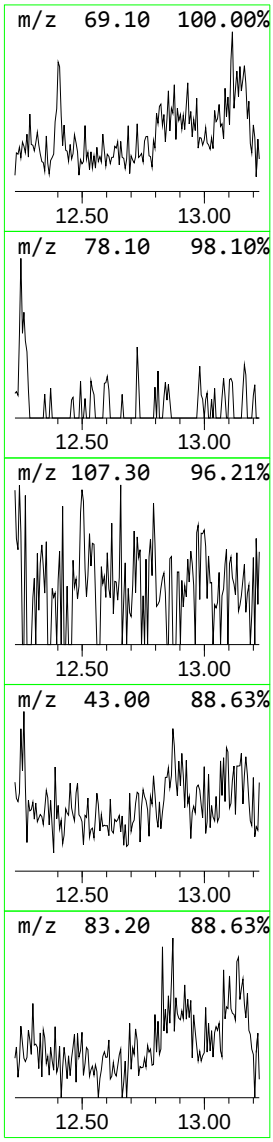
****

Peak Number 4 unknown12.725 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.725	9.90 ug/l	6805	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-(methylthio)-3-nitro-	170	C6H6N2O2S	022746-79-8	37
2	N-(p-Methoxyphenyl)-N'-(1,1-dicy...	214	C11H10N4O	040620-38-0	25
3	O-Methyl n-butylphosphonamidothi...	167	C5H14NOPS	1000306-05-2	23
4	Lenthionine	188	C2H4S5	000292-46-6	23
5	O-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-3	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

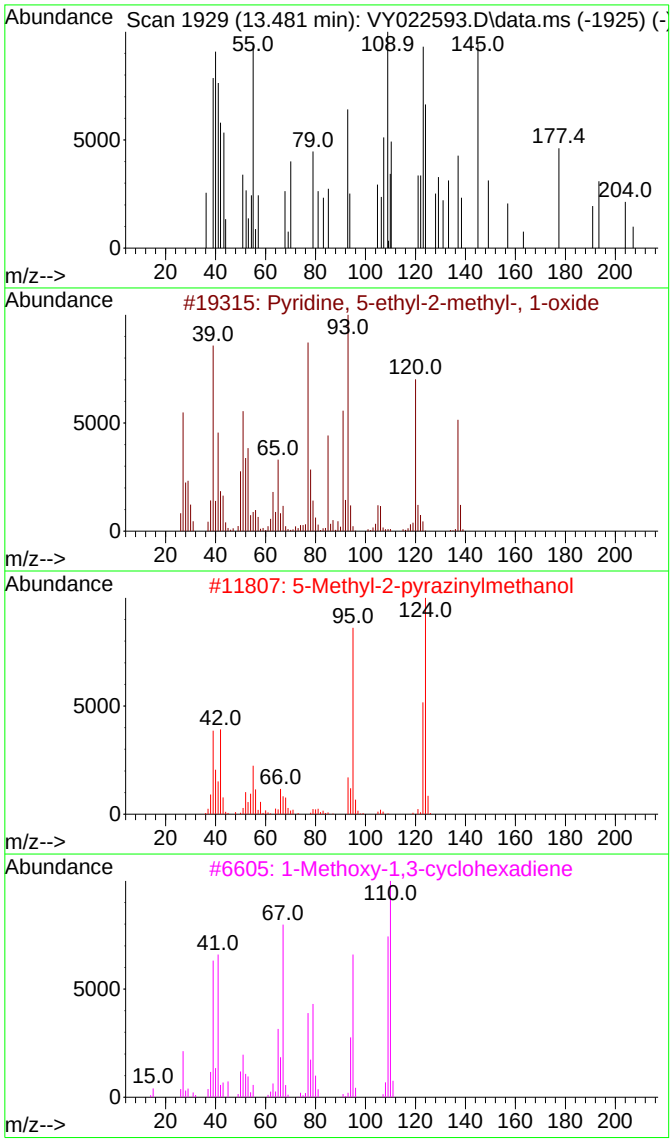
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

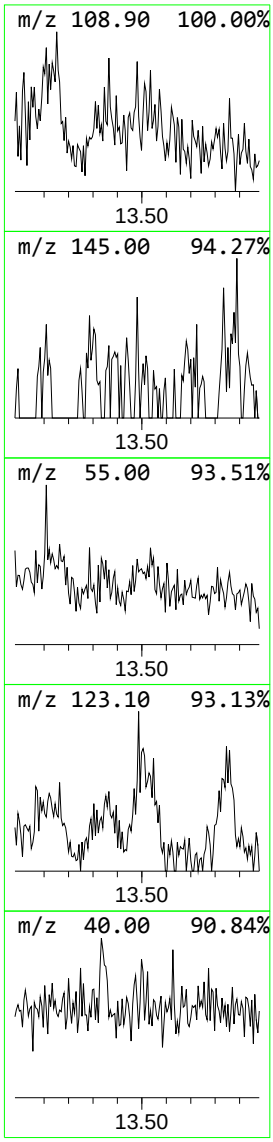
****

Peak Number 5 unknown13.481 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.481	6.53 ug/l	4490	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 5-ethyl-2-methyl-, 1-o...	137	C8H11NO	000768-44-5	43
2	5-Methyl-2-pyrazinylmethanol	124	C6H8N2O	061892-95-3	38
3	1-Methoxy-1,3-cyclohexadiene	110	C7H10O	002161-90-2	38
4	2-Hexyn-1-ol	98	C6H10O	000764-60-3	35
5	1H-Pyrazole-1-propanenitrile, 3,...	149	C8H11N3	005589-97-9	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

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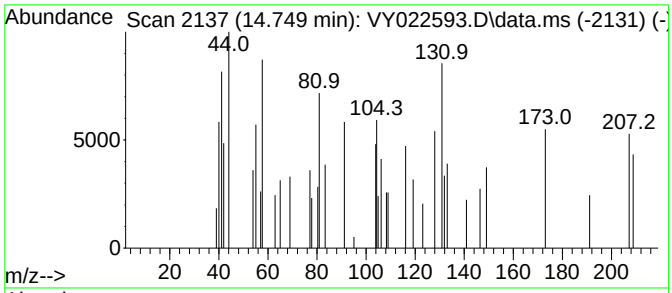
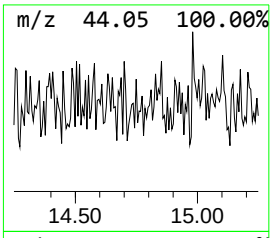
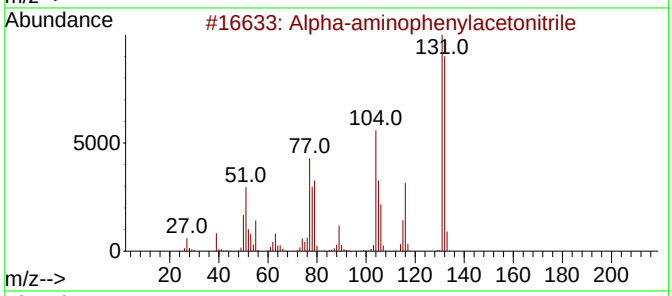
Peak Number 6 unknown14.749 Concentration Rank 7

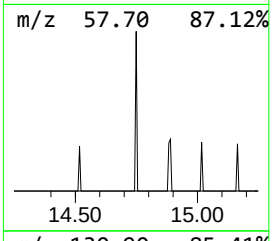
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.749	5.35 ug/l	3678	1,4-Dichlorobenzene-d4	13.347

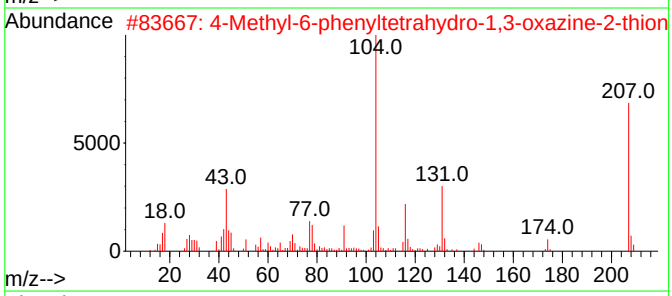
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Alpha-aminophenylacetonitrile	132	C8H8N2	016750-42-8	25
2	4-Methyl-6-phenyltetrahydro-1,3-...	207	C11H13NOS	086071-94-5	11
3	Azetidine, 2-phenyl-	133	C9H11N	022610-18-0	10
4	Thiourea, dimethylaminomethyl	133	C4H11N3S	109858-55-1	9
5	Benzeneacetonitrile, 4-methyl-	131	C9H9N	002947-61-7	9

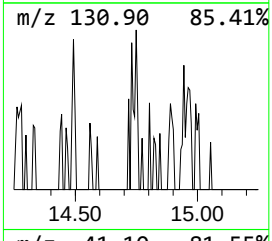


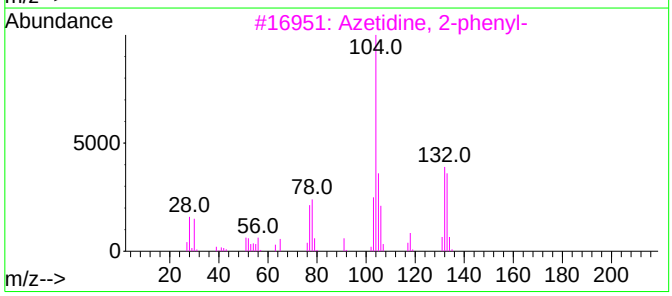


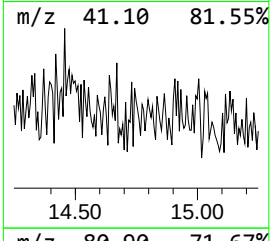


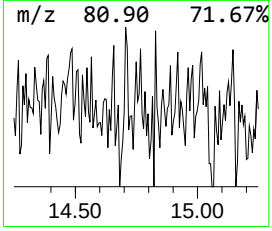












Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

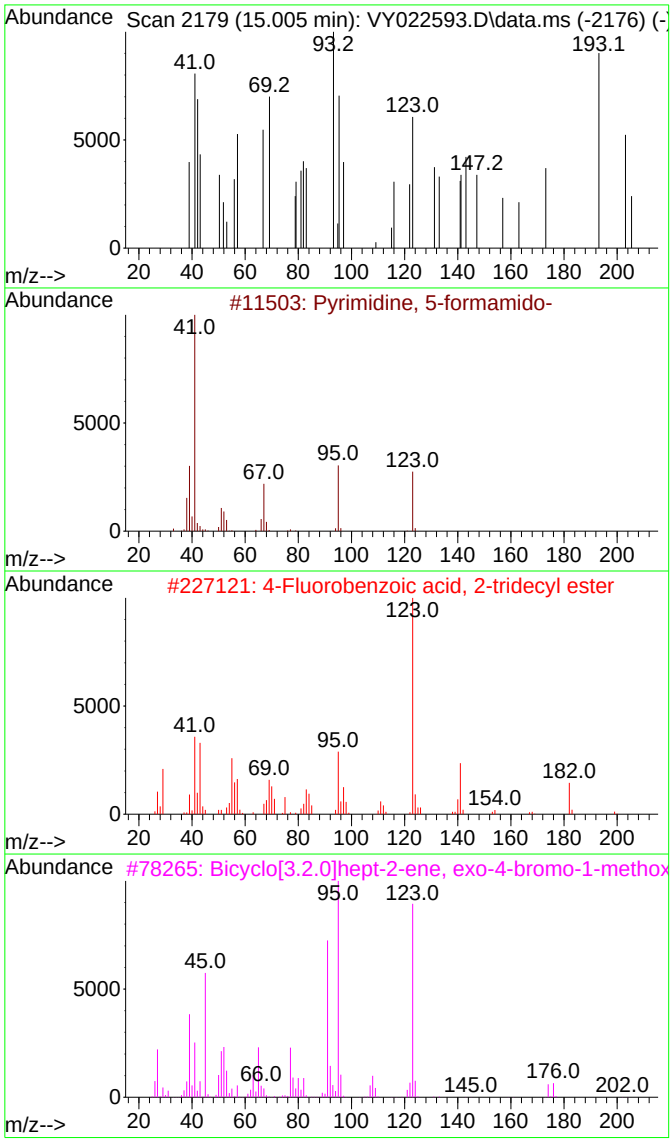
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

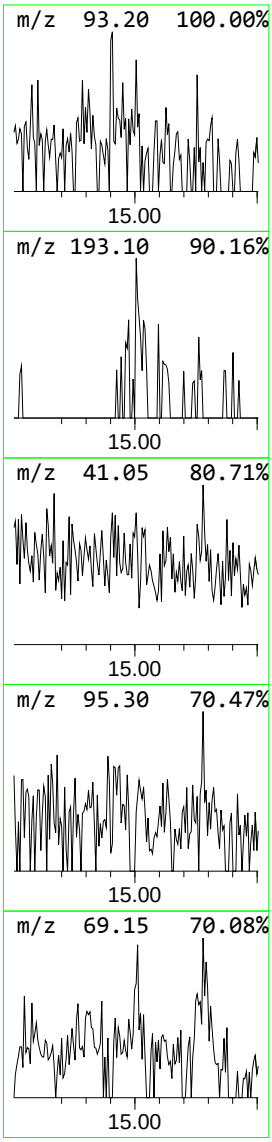
****

Peak Number 7 unknown15.005 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.005	13.36 ug/l	9179	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine, 5-formamido-	123	C5H5N3O	056621-84-2	22
2	4-Fluorobenzoic acid, 2-tridecyl...	322	C20H31FO2	1000280-67-8	10
3	Bicyclo[3.2.0]hept-2-ene, exo-4-...	202	C8H11BrO	1000155-39-6	10
4	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	9
5	N,N-Dimethyl-2-pyridinamine	122	C7H10N2	005683-33-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

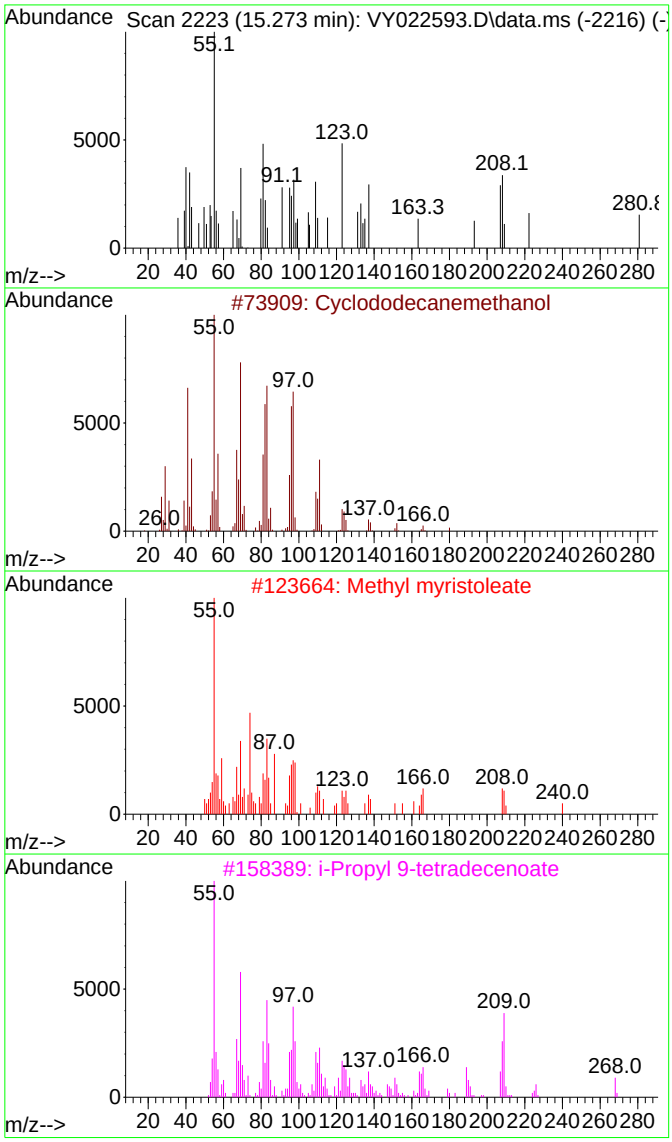
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

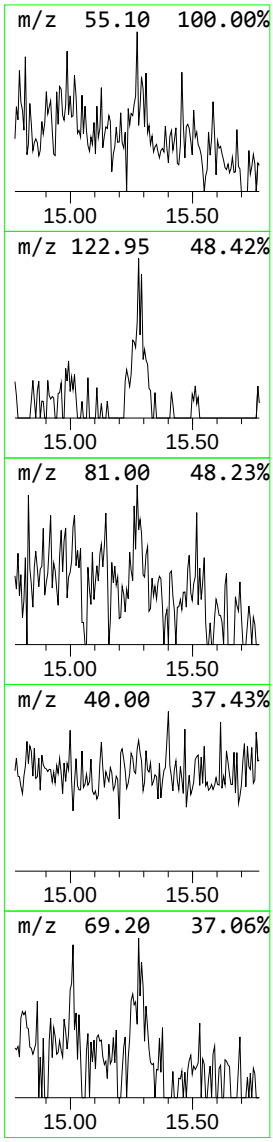
****

Peak Number 8 unknown15.273 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.273	16.49 ug/l	11332	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanemethanol	198	C13H26O	001892-12-2	22
2	Methyl myristoleate	240	C15H28O2	056219-06-8	16
3	i-Propyl 9-tetradecenoate	268	C17H32O2	1000336-60-7	12
4	Cyclohexaneacetonitrile, 2-oxo-	137	C8H11NO	042185-27-3	10
5	1,1'-Bicyclohexyl, 4-methyl-4'-p...	222	C16H30	092343-70-9	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060625\
Data File : VY022593.D
Acq On : 06 Jun 2025 12:26
Operator : SY/MD
Sample : Q2199-04
Misc : 5.30g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-231

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060225S.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Phenylephrine	2.105	24.2	ug/l	43897	1	7.701	90824	50.0
unknown11.579	11.579	5.0	ug/l	7418	3	11.414	73531	50.0
.alpha.-Phellan...	12.255	32.6	ug/l	47963	3	11.414	73531	50.0
unknown12.725	12.725	9.9	ug/l	6805	4	13.347	34357	50.0
unknown13.481	13.481	6.5	ug/l	4490	4	13.347	34357	50.0
unknown14.749	14.749	5.3	ug/l	3678	4	13.347	34357	50.0
unknown15.005	15.005	13.4	ug/l	9179	4	13.347	34357	50.0
unknown15.273	15.273	16.5	ug/l	11332	4	13.347	34357	50.0