

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100224\
 Data File : VY019759.D
 Acq On : 02 Oct 2024 13:03
 Operator : SY/MD
 Sample : P4225-01
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TR-04-092724

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\82Y090924S.M

Title : SW846 8260

Signal : TIC: VY019759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.995	43	45	48	rBV2	1120	1295	5.16%	0.631%
2	2.105	52	63	65	rBV4	4669	13342	53.21%	6.504%
3	2.123	65	66	68	rVV	1969	1107	4.41%	0.540%
4	2.288	92	93	98	rVB4	996	1163	4.64%	0.567%
5	2.330	98	100	101	rBV2	1113	770	3.07%	0.375%
6	2.428	114	116	119	rBV3	654	944	3.76%	0.460%
7	2.550	134	136	139	rVB	827	921	3.67%	0.449%
8	2.623	144	148	151	rVB5	1287	2037	8.12%	0.993%
9	2.794	174	176	179	rBV3	747	900	3.59%	0.439%
10	2.824	179	181	185	rBV	590	870	3.47%	0.424%
11	2.885	189	191	194	rBV2	752	766	3.05%	0.373%
12	3.196	238	242	245	rVB4	754	794	3.17%	0.387%
13	3.574	301	304	307	rBV2	687	771	3.07%	0.376%
14	3.952	363	366	368	rBV2	924	841	3.35%	0.410%
15	4.184	400	404	407	rBV3	786	1287	5.13%	0.627%
16	4.373	431	435	438	rVB3	568	756	3.01%	0.369%
17	4.665	480	483	489	rVB4	537	1124	4.48%	0.548%
18	5.037	541	544	546	rVB2	782	1034	4.12%	0.504%
19	5.378	597	600	601	rBV2	724	755	3.01%	0.368%
20	5.628	640	641	646	rBV3	1068	1410	5.62%	0.687%
21	6.220	734	738	741	rBV2	622	979	3.90%	0.477%
22	6.311	750	753	756	rVB2	585	850	3.39%	0.414%
23	6.567	793	795	800	rBV2	629	887	3.54%	0.432%
24	6.866	840	844	845	rBV	1690	1801	7.18%	0.878%
25	7.634	961	970	976	rBV5	3548	8502	33.90%	4.144%
26	7.713	976	983	992	rVB4	5883	14424	57.52%	7.031%
27	7.854	1003	1006	1007	rBV	909	903	3.60%	0.440%
28	7.866	1007	1008	1013	rVB2	1001	1067	4.26%	0.520%
29	8.061	1035	1040	1047	rVB3	4705	9929	39.60%	4.840%
30	8.616	1124	1131	1139	rBV	10705	21983	87.67%	10.716%
31	8.884	1173	1175	1179	rVB2	635	991	3.95%	0.483%
32	9.055	1196	1203	1205	rVB3	557	1166	4.65%	0.568%
33	9.085	1205	1208	1210	rBV	896	909	3.62%	0.443%
34	9.737	1311	1315	1317	rBV2	658	898	3.58%	0.438%
35	10.109	1370	1376	1383	rVB	14622	25076	100.00%	12.223%
36	10.170	1383	1386	1390	rBV3	830	1105	4.41%	0.539%

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Integrator: RTE

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37	10.353	1411	1416	1417	rVB3	589	776	3.09%	0.378%
38	10.548	1444	1448	1450	rBV2	758	790	3.15%	0.385%
39	11.414	1585	1590	1599	rVB2	12386	21785	86.88%	10.619%
40	11.487	1599	1602	1604	rBV3	735	912	3.64%	0.445%
41	11.585	1615	1618	1621	rBV2	452	758	3.02%	0.369%
42	11.621	1621	1624	1632	rVB4	814	1909	7.61%	0.931%
43	11.944	1676	1677	1680	rBV3	768	805	3.21%	0.392%
44	12.066	1694	1697	1702	rBV4	760	1187	4.73%	0.579%
45	12.249	1722	1727	1728	rBV3	737	970	3.87%	0.473%
46	12.408	1748	1753	1762	rBV5	4865	8202	32.71%	3.998%
47	12.591	1779	1783	1785	rBV2	628	815	3.25%	0.397%
48	12.676	1794	1797	1800	rBV2	1137	1055	4.21%	0.514%
49	12.895	1831	1833	1836	rVB2	938	811	3.23%	0.395%
50	12.938	1836	1840	1841	rBV	641	821	3.27%	0.400%
51	13.090	1862	1865	1866	rVB3	853	834	3.33%	0.407%
52	13.115	1866	1869	1872	rBV3	828	1177	4.69%	0.574%
53	13.151	1872	1875	1878	rVB2	889	1011	4.03%	0.493%
54	13.347	1901	1907	1911	rVB4	2697	4757	18.97%	2.319%
55	13.554	1934	1941	1942	rBV2	640	960	3.83%	0.468%
56	13.572	1942	1944	1947	rVB2	913	870	3.47%	0.424%
57	13.877	1992	1994	1995	rBV2	985	892	3.56%	0.435%
58	14.121	2029	2034	2038	rVB3	790	1627	6.49%	0.793%
59	14.188	2042	2045	2046	rBV3	850	795	3.17%	0.388%
60	14.383	2075	2077	2080	rBV4	639	793	3.16%	0.387%
61	14.560	2102	2106	2108	rVB3	790	990	3.95%	0.483%
62	14.590	2108	2111	2115	rBV4	877	1405	5.60%	0.685%
63	14.682	2124	2126	2128	rVB3	789	777	3.10%	0.379%
64	14.712	2128	2131	2132	rBV2	1009	836	3.33%	0.408%
65	14.840	2150	2152	2157	rVB5	675	1119	4.46%	0.545%
66	15.084	2191	2192	2194	rVB	1222	860	3.43%	0.419%
67	15.108	2194	2196	2198	rBV3	900	931	3.71%	0.454%
68	15.139	2198	2201	2204	rBV4	1335	2349	9.37%	1.145%
69	15.316	2229	2230	2233	rBV2	1115	1165	4.65%	0.568%
70	15.450	2248	2252	2254	rBV4	635	1155	4.61%	0.563%
71	15.517	2260	2263	2264	rBV	905	1002	4.00%	0.488%
72	15.767	2300	2304	2305	rVB4	793	818	3.26%	0.399%
73	15.992	2338	2341	2345	rBV3	851	1113	4.44%	0.543%
74	16.066	2351	2353	2356	rVB3	785	833	3.32%	0.406%
75	16.133	2363	2364	2367	rBV3	784	915	3.65%	0.446%
76	16.224	2377	2379	2381	rBV2	840	794	3.17%	0.387%

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77	16.285	2384	2389	2391	rBV5	903	1536	6.13%	0.749%
78	16.358	2399	2401	2403	rBV3	1090	1232	4.91%	0.601%
79	16.383	2403	2405	2409	rVB3	913	1333	5.32%	0.650%
80	16.456	2414	2417	2420	rVB5	1213	1406	5.61%	0.685%
81	16.492	2420	2423	2424	rBV3	1247	1032	4.12%	0.503%
82	16.596	2437	2440	2441	rVB3	933	780	3.11%	0.380%
83	16.700	2455	2457	2460	rVB4	1147	1099	4.38%	0.536%

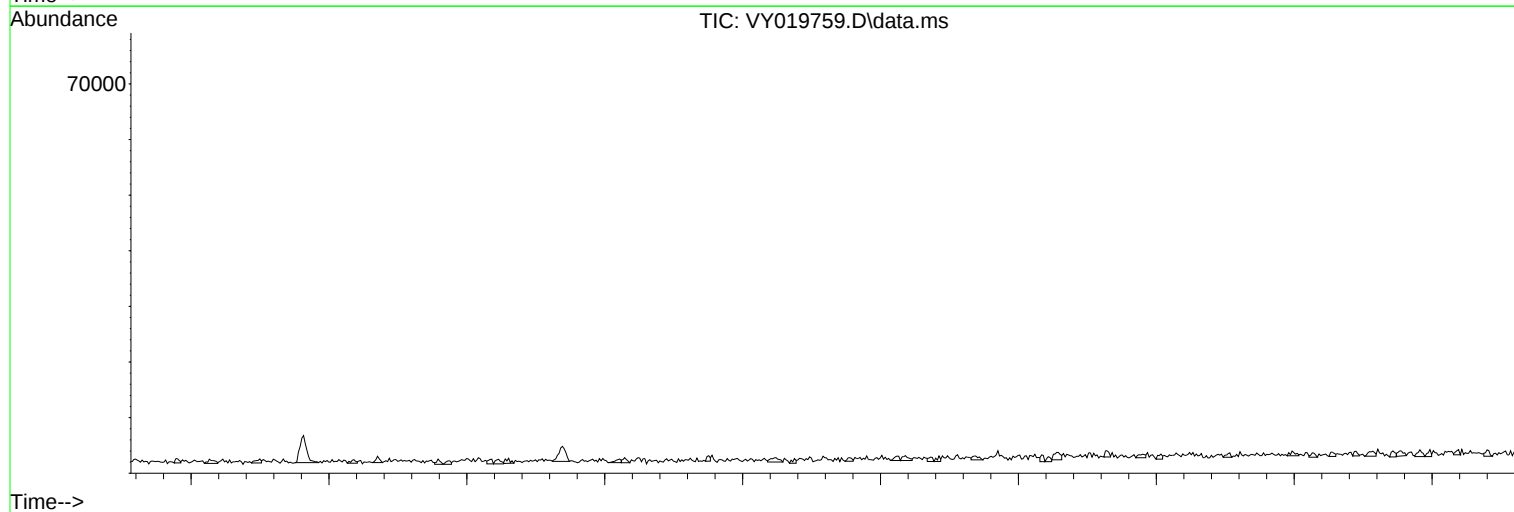
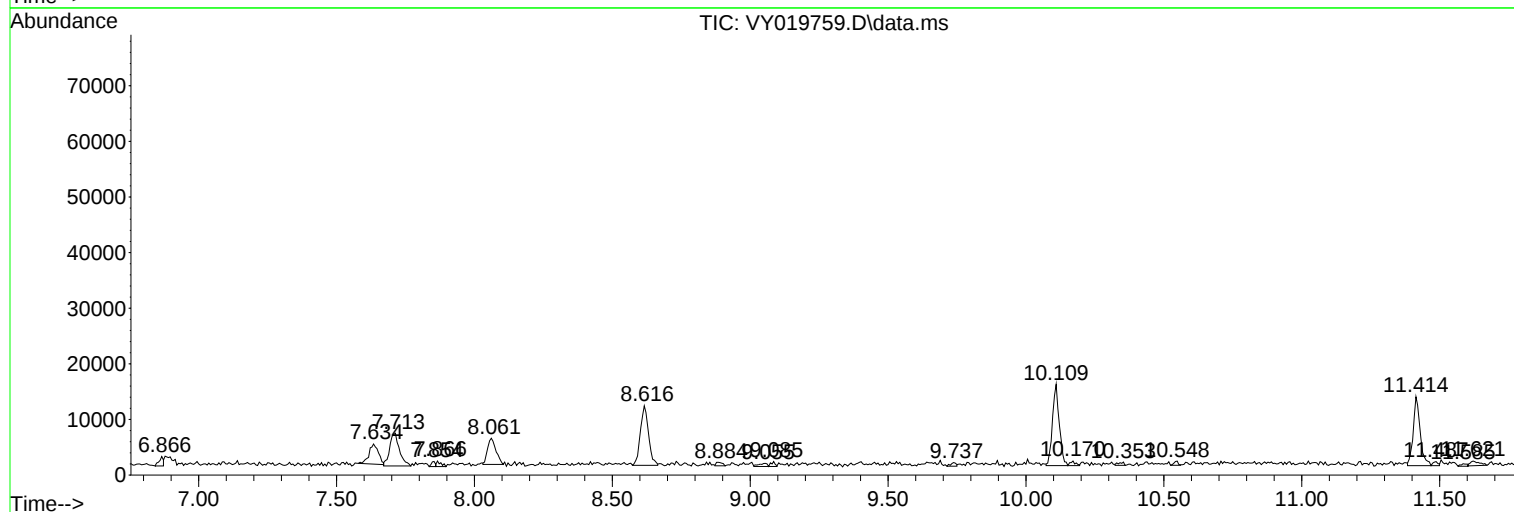
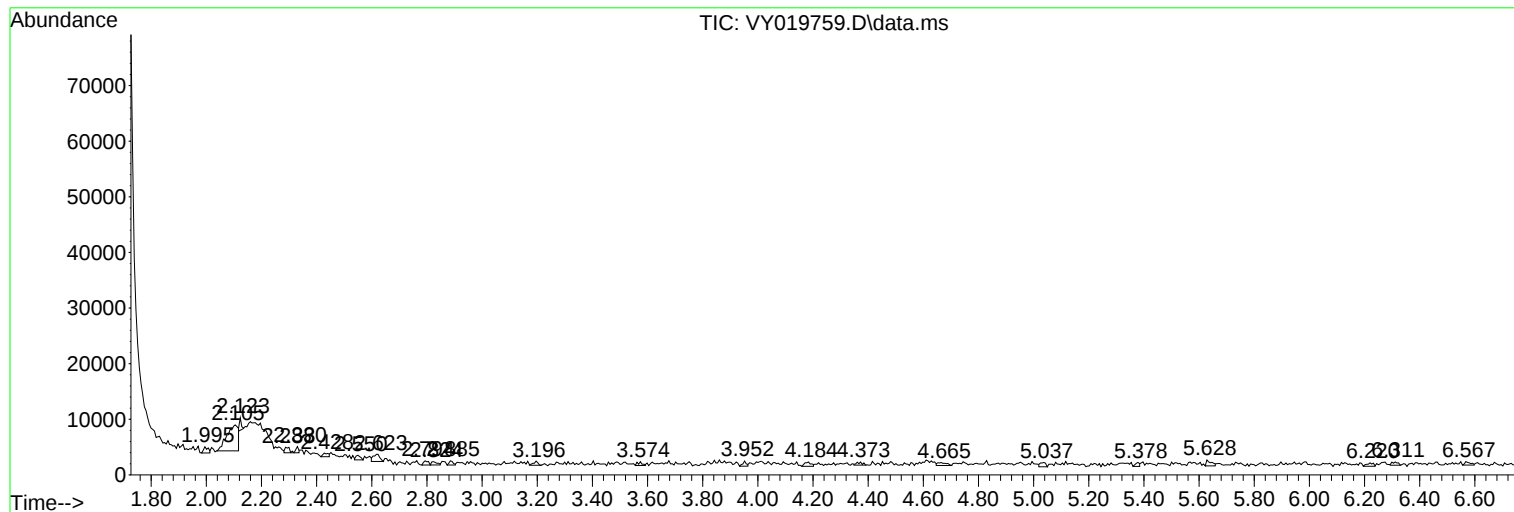
Sum of corrected areas: 205149

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
TR-04-092724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

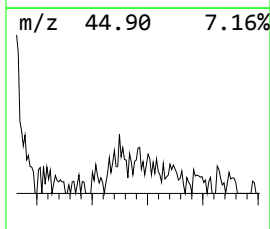
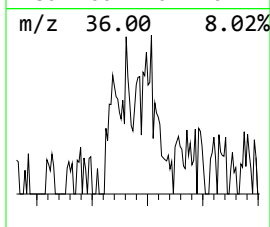
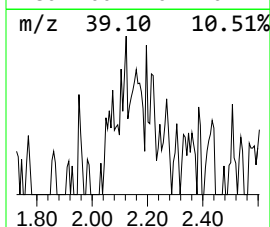
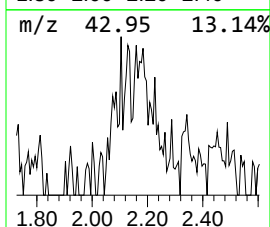
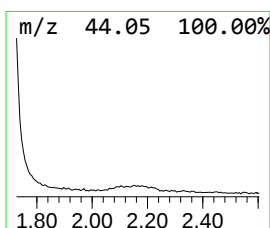
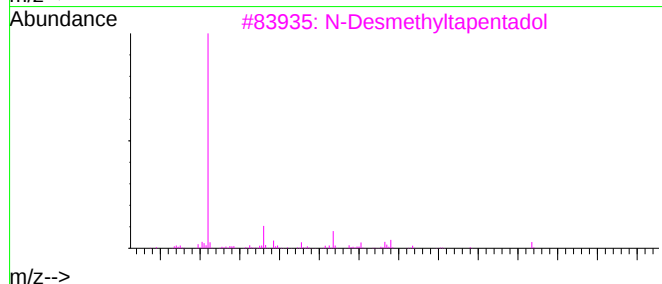
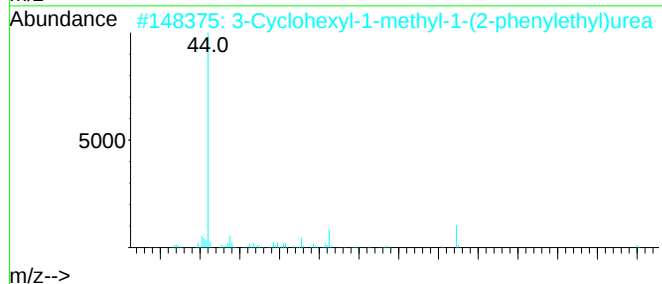
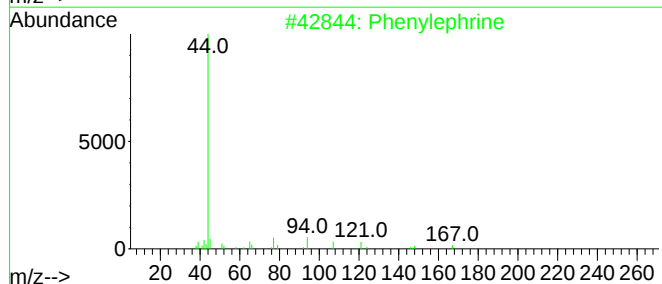
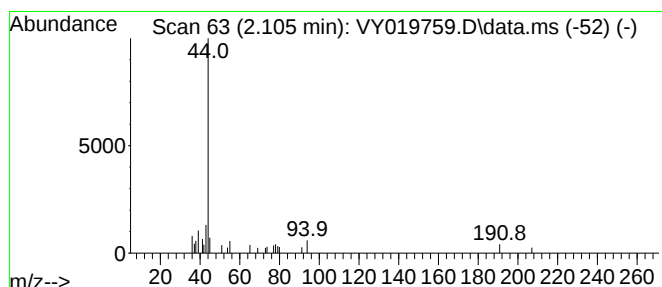
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Phenylephrine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	46.25 ug/l	13342	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylephrine	167	C9H13NO2	000059-42-7	56
2	3-Cyclohexyl-1-methyl-1-(2-pheny...	260	C16H24N2O	1024470-80-1	38
3	N-Desmethyltapentadol	207	C13H21NO	1246819-18-0	9
4	Amphetamine-3-methyl	149	C10H15N	000588-06-7	9
5	Paradrine	151	C9H13NO	000103-86-6	9



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Instrument :
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TR-04-092724

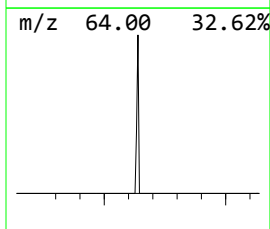
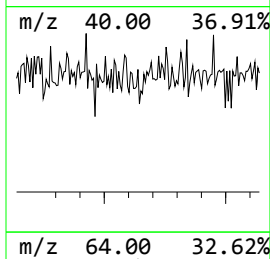
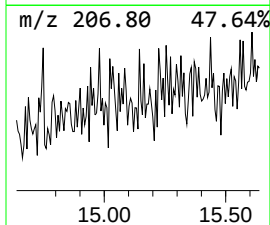
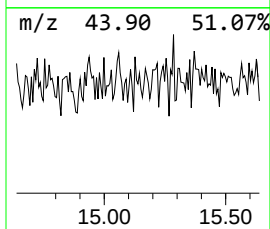
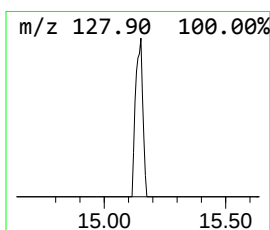
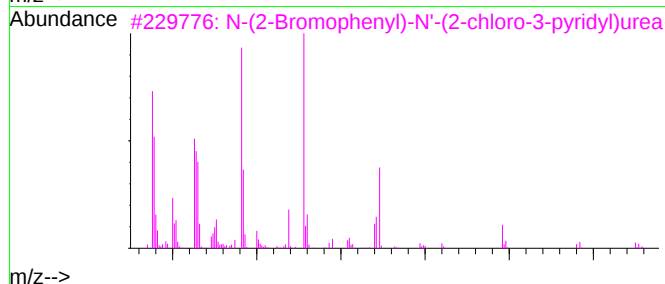
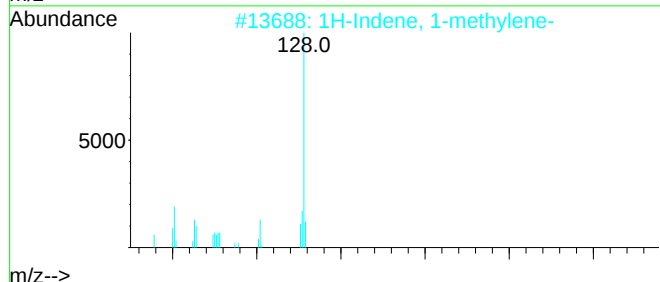
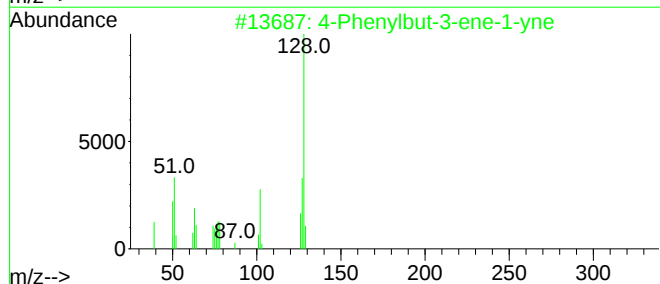
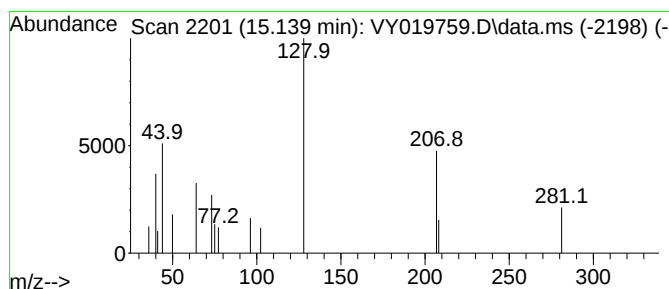
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.139 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	24.69 ug/l	2349	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	10
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	9
3			N-(2-Bromophenyl)-N'-(2-chloro-3...	325	C12H9BrClN3O	1000223-08-1	9
4			Quinoline-2-carboxylic acid carb...	229	C12H11N3O2	1000274-24-1	9
5			2-Propenenitrile, 3-(2-bromophen...	207	C9H6BrN	178809-30-8	9



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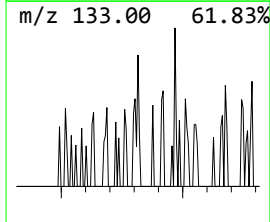
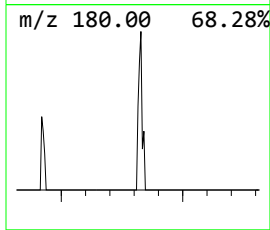
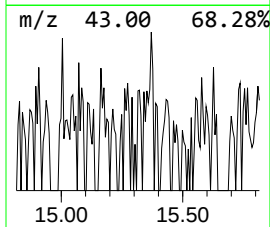
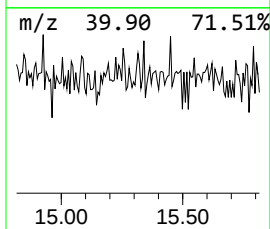
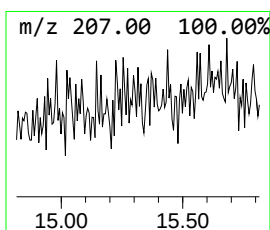
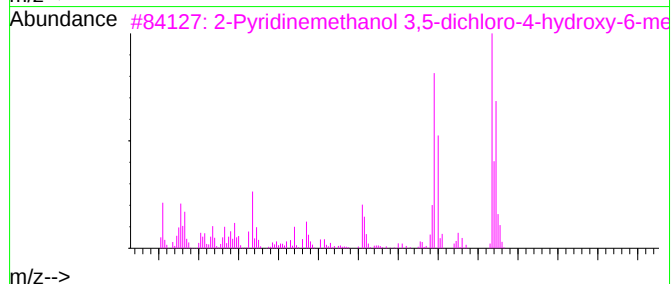
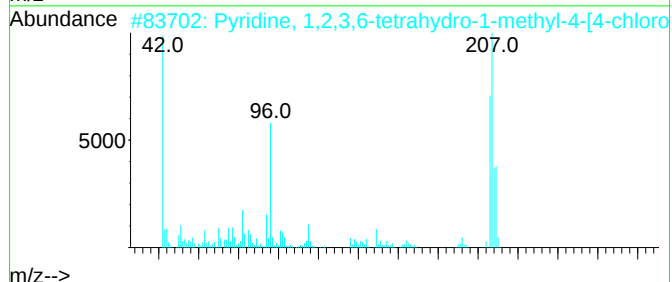
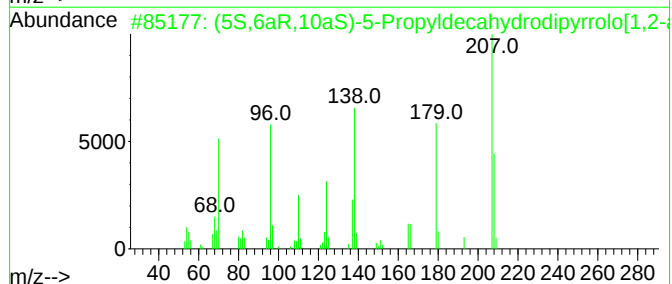
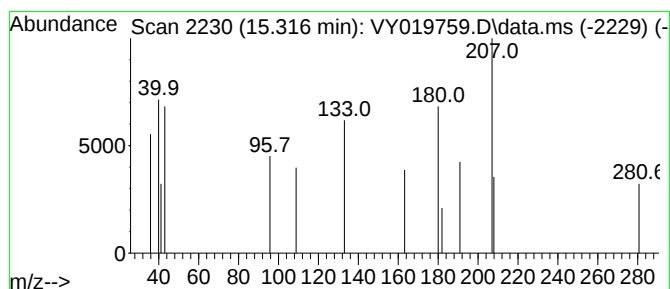
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown15.316 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.316	12.25 ug/l	1165	1,4-Dichlorobenzene-d4	13.347

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(5S,6aR,10aS)-5-Propyldecahydrod...	208	C13H24N2	172139-30-9	16	
2	Pyridine, 1,2,3,6-tetrahydro-1-m...	207	C12H14ClN	005048-08-8	12	
3	2-Pyridinemethanol 3,5-dichloro-...	207	C7H7Cl2NO2	055042-78-9	12	
4	2,5,5,6,8a-Pentamethyl-trans-4a,...	208	C14H24O	1000215-77-8	9	
5	1,11-Tridecadiene	180	C13H24	1000130-76-4	9	



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Quant Title : SW846 8260

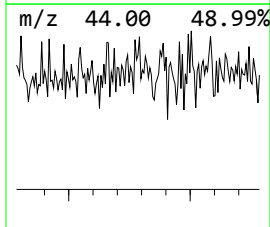
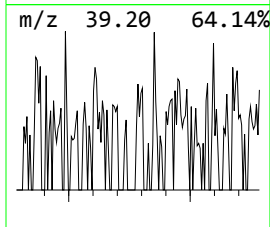
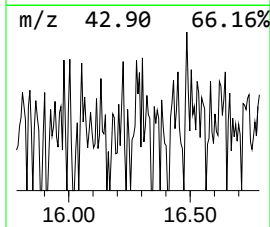
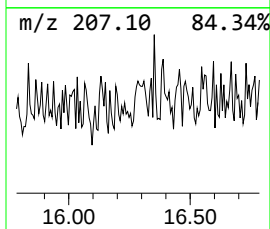
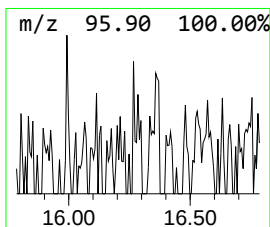
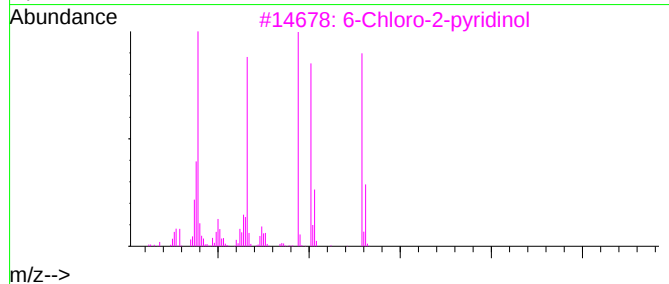
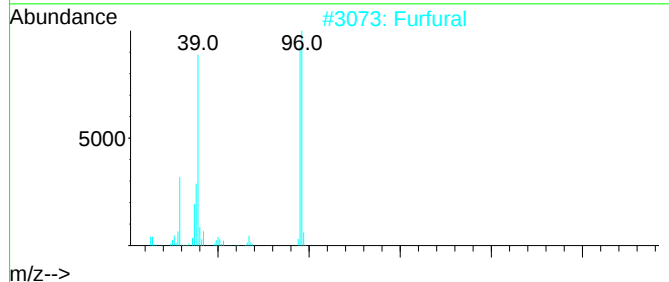
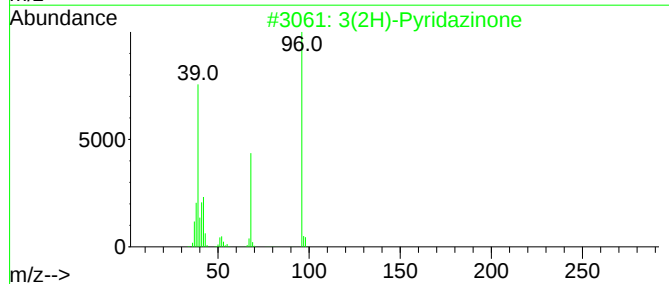
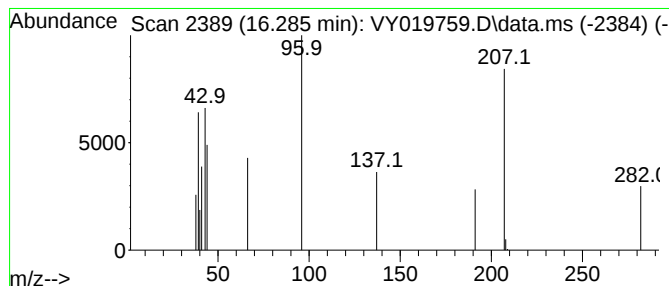
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown16.285 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.285	16.14 ug/l	1536	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3(2H)-Pyridazinone	96	C4H4N2O	000504-30-3	10
2			Furfural	96	C5H4O2	000098-01-1	10
3			6-Chloro-2-pyridinol	129	C5H4ClNO	073018-09-4	9
4			2-(Prop-2-yn-1-yl)-2,3-dihydrois...	157	C6H7NO2S	1000481-51-0	9
5			Pyridin-2-amine, N,N-bis(trifluo...	358	C7H4F6N2O4S2	145100-50-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100224\
Data File : VY019759.D
Acq On : 02 Oct 2024 13:03
Operator : SY/MD
Sample : P4225-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-04-092724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

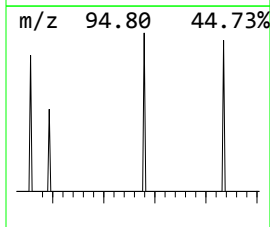
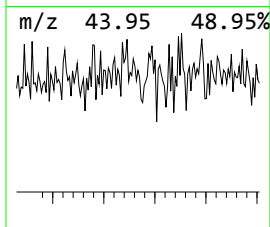
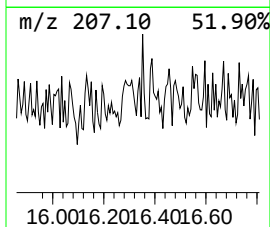
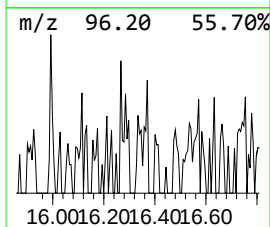
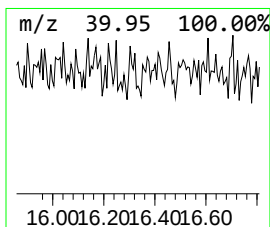
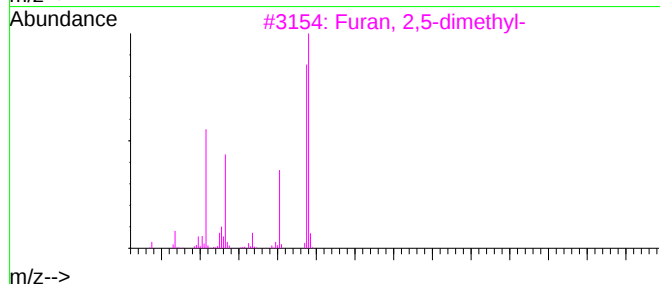
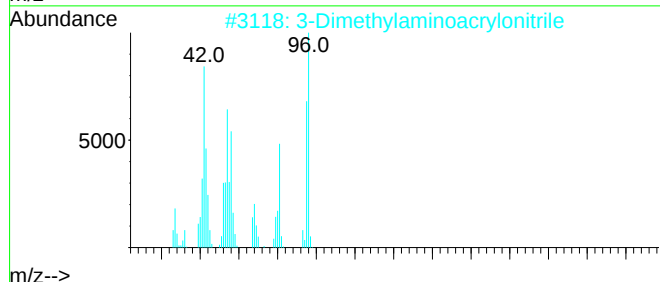
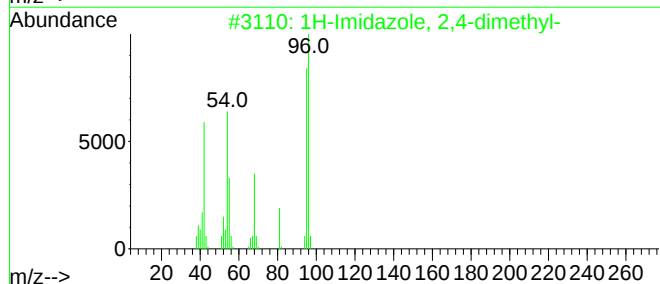
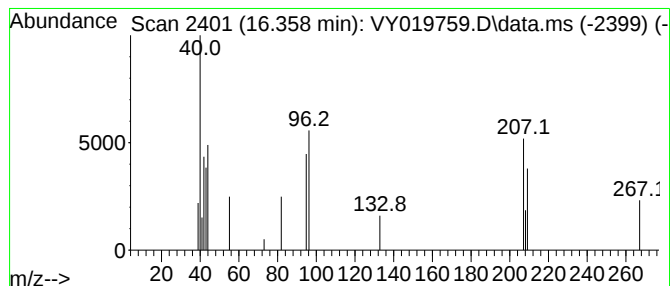
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown16.358 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.358	12.95 ug/l	1232	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 2,4-dimethyl-	96	C5H8N2	000930-62-1	27
2	3-Dimethylaminoacrylonitrile	96	C5H8N2	002407-68-3	25
3	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	9
4	5-Methyl-1H-pyrrol-2-amine	96	C5H8N2	1000436-81-3	9
5	3,5-Dimethylpyrazole	96	C5H8N2	000067-51-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100224\
Data File : VY019759.D
Acq On : 02 Oct 2024 13:03
Operator : SY/MD
Sample : P4225-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TR-04-092724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.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
Phenylephrine	2.105	46.3	ug/l	13342	1	7.707	14424	50.0
unknown15.139	15.139	24.7	ug/l	2349	4	13.347	4757	50.0
unknown15.316	15.316	12.3	ug/l	1165	4	13.347	4757	50.0
unknown16.285	16.285	16.1	ug/l	1536	4	13.347	4757	50.0
unknown16.358	16.358	12.9	ug/l	1232	4	13.347	4757	50.0