

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102324\
 Data File : VY019994.D
 Acq On : 23 Oct 2024 15:09
 Operator : SY/MD
 Sample : P4486-01
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EO-03-102224

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\82Y1009245.M
 Title : SW846 8260

Signal : TIC: VY019994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.080	51	59	60	rBV2	4884	9399	17.56%	2.995%
2	2.604	144	145	149	rBV3	1589	1528	2.86%	0.487%
3	3.464	281	286	289	rBV3	606	992	1.85%	0.316%
4	3.848	345	349	354	rVB4	1235	2078	3.88%	0.662%
5	4.000	370	374	376	rVB	714	1005	1.88%	0.320%
6	4.311	422	425	429	rBV2	895	1238	2.31%	0.394%
7	4.354	429	432	435	rVB2	1093	1567	2.93%	0.499%
8	4.500	454	456	459	rVB2	1186	1183	2.21%	0.377%
9	4.531	459	461	464	rBV2	1270	1294	2.42%	0.412%
10	5.110	553	556	559	rBV3	1040	1142	2.13%	0.364%
11	5.360	594	597	599	rBV2	896	1125	2.10%	0.358%
12	5.585	629	634	635	rBV3	792	1179	2.20%	0.376%
13	5.756	661	662	666	rBV2	985	988	1.85%	0.315%
14	5.908	685	687	691	rVB	874	1062	1.98%	0.338%
15	6.030	705	707	710	rVB3	871	1062	1.98%	0.338%
16	6.073	713	714	719	rBV2	1063	1345	2.51%	0.429%
17	6.512	784	786	792	rVB3	961	990	1.85%	0.315%
18	6.866	840	844	846	rBV4	1591	2826	5.28%	0.900%
19	6.884	846	847	853	rVV5	2340	3844	7.18%	1.225%
20	6.951	855	858	859	rVB2	1413	1313	2.45%	0.418%
21	7.219	898	902	905	rVB2	786	1402	2.62%	0.447%
22	7.256	905	908	910	rBV2	1017	1213	2.27%	0.386%
23	7.530	949	953	955	rVB2	991	1148	2.15%	0.366%
24	7.634	963	970	975	rBV2	7659	15890	29.69%	5.063%
25	7.707	976	982	991	rVB3	14740	32947	61.57%	10.497%
26	7.774	991	993	995	rBV2	991	994	1.86%	0.317%
27	7.908	1013	1015	1017	rVB2	1107	979	1.83%	0.312%
28	7.932	1017	1019	1022	rBV	801	1089	2.04%	0.347%
29	8.060	1033	1040	1047	rBV6	7682	19103	35.70%	6.086%
30	8.615	1124	1131	1138	rBV	21675	40406	75.51%	12.874%
31	9.115	1210	1213	1217	rVB2	923	1092	2.04%	0.348%
32	9.621	1294	1296	1298	rBV3	782	971	1.81%	0.309%
33	9.908	1342	1343	1347	rVB3	965	1273	2.38%	0.406%
34	10.103	1369	1375	1384	rBV	28370	53513	100.00%	17.050%
35	10.883	1499	1503	1506	rBV5	1929	2853	5.33%	0.909%
36	11.249	1561	1563	1566	rVB2	1026	1015	1.90%	0.323%

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Integrator: RTE

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Peak Location: TOP

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

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37	11.359	1578	1581	1583	rBV2	855	1025	1.92%	0.327%
38	11.420	1583	1591	1600	rBV3	21234	39664	74.12%	12.638%
39	11.517	1602	1607	1609	rBV4	1040	1958	3.66%	0.624%
40	12.224	1718	1723	1724	rBV4	1953	2894	5.41%	0.922%
41	12.407	1748	1753	1758	rBV6	9715	15985	29.87%	5.093%
42	12.517	1765	1771	1774	rVB5	2487	4476	8.36%	1.426%
43	12.822	1819	1821	1823	rBV2	1514	988	1.85%	0.315%
44	13.139	1868	1873	1874	rBV4	2522	4228	7.90%	1.347%
45	13.242	1888	1890	1891	rBV2	1234	1027	1.92%	0.327%
46	13.279	1894	1896	1901	rVB5	1195	1505	2.81%	0.480%
47	13.346	1902	1907	1914	rBV7	6145	11991	22.41%	3.821%
48	13.462	1923	1926	1928	rBV3	981	981	1.83%	0.313%
49	13.657	1955	1958	1962	rVV6	1304	1905	3.56%	0.607%
50	13.694	1962	1964	1968	rVB4	1512	1945	3.63%	0.620%
51	13.944	2003	2005	2007	rBV3	1090	1008	1.88%	0.321%
52	14.011	2010	2016	2018	rBV4	1205	1813	3.39%	0.578%
53	14.450	2086	2088	2091	rBV4	1042	1064	1.99%	0.339%
54	15.376	2238	2240	2242	rBV3	1345	991	1.85%	0.316%
55	15.584	2273	2274	2278	rVB3	1668	1296	2.42%	0.413%
56	15.760	2300	2303	2304	rBV3	1391	1268	2.37%	0.404%
57	15.870	2318	2321	2326	rBV5	1047	1835	3.43%	0.585%
58	16.266	2384	2386	2389	rVB3	1163	964	1.80%	0.307%

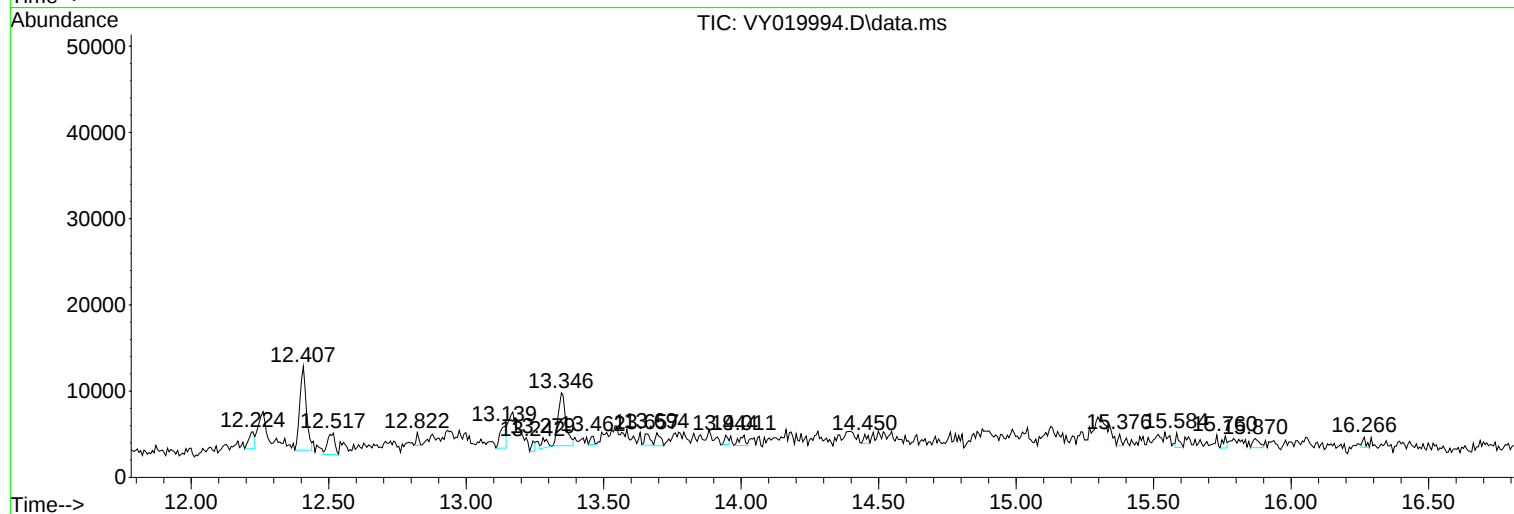
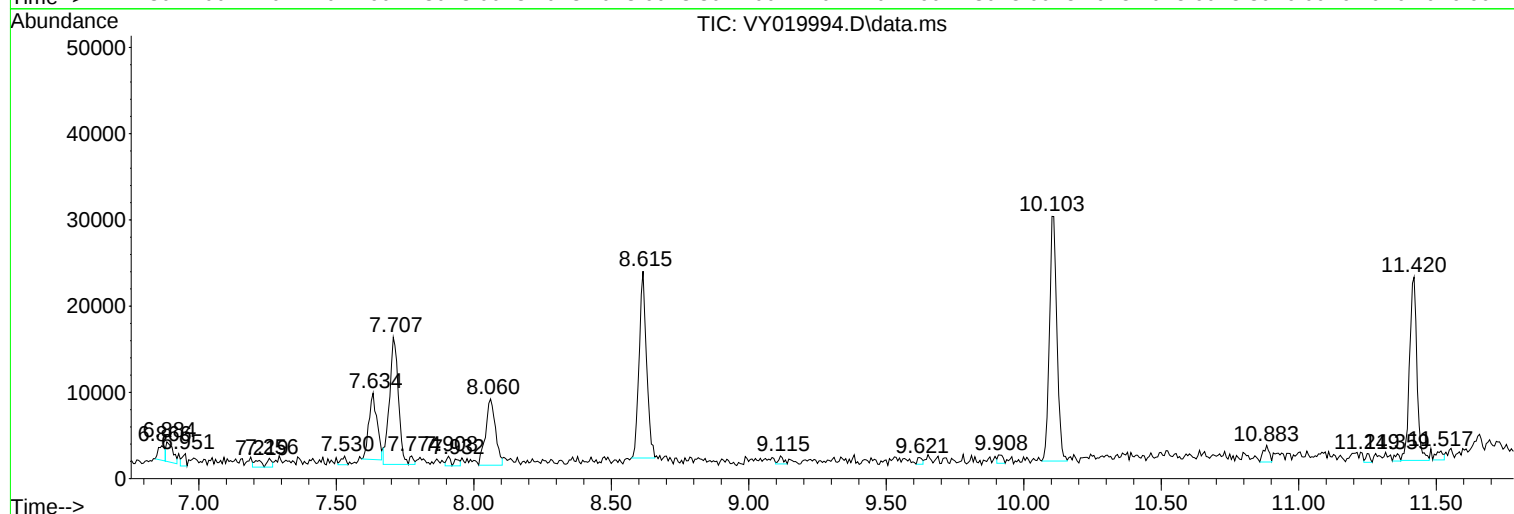
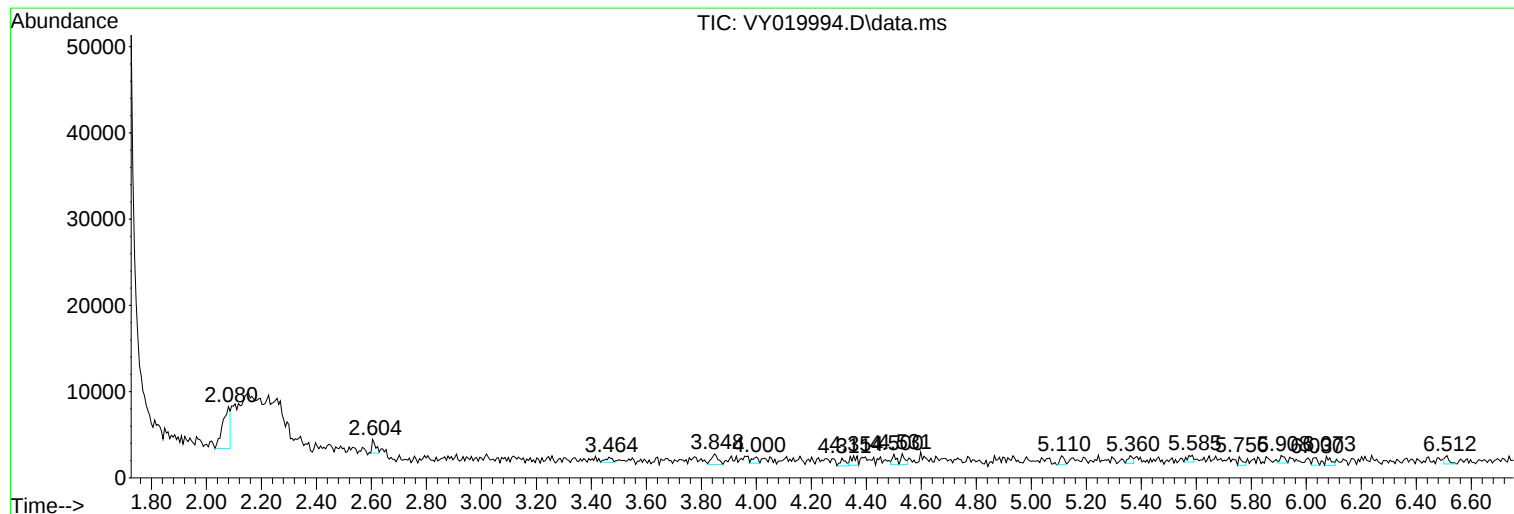
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Quant Title : SW846 8260

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



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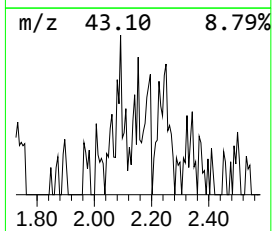
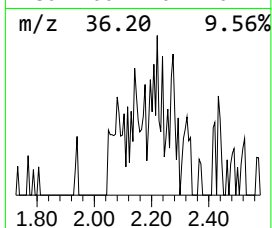
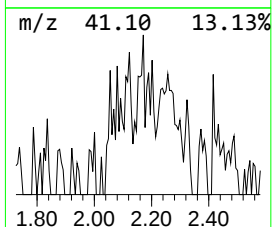
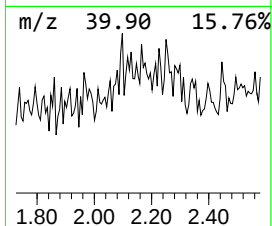
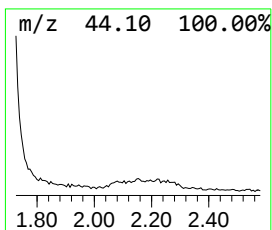
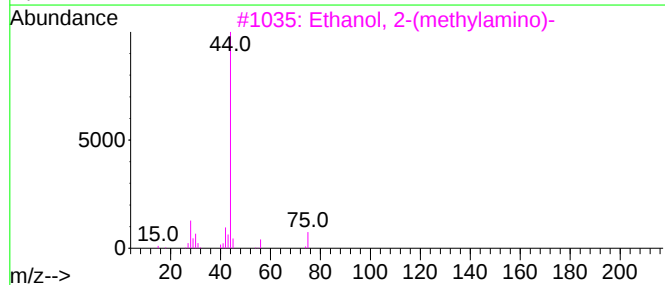
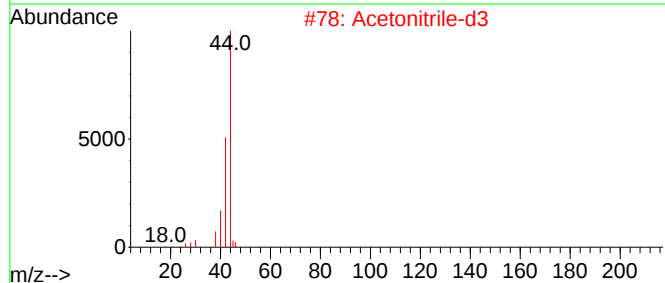
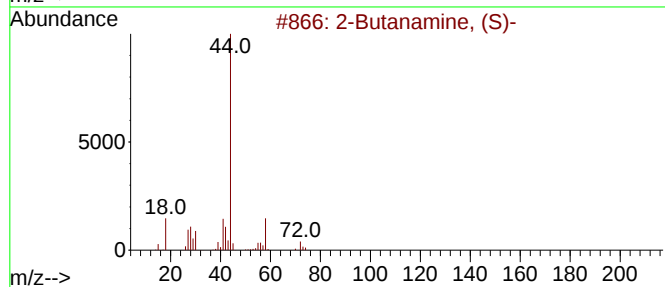
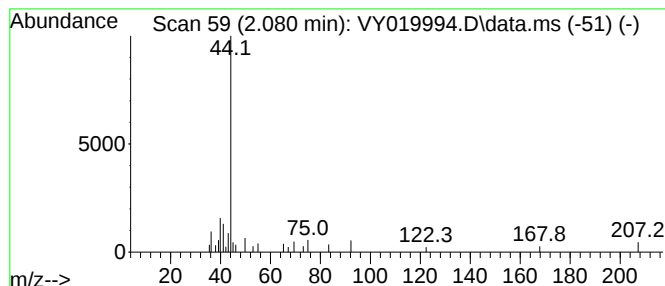
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Quant Title : SW846 8260

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

Peak Number 1 unknown2.080 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.080	14.26 ug/l	9399	Pentafluorobenzene	7.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanamine, (S)-			73	C4H11N	000513-49-5	28
2	Acetonitrile-d3			44	C2D3N	002206-26-0	7
3	Ethanol, 2-(methylamino)-			75	C3H9NO	000109-83-1	7
4	Hydrazinecarboxamide			75	CH5N3O	000057-56-7	5
5	N-Desmethyltapentadol			207	C13H21NO	1246819-18-0	5



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ALS Vial : 11 Sample Multiplier: 1

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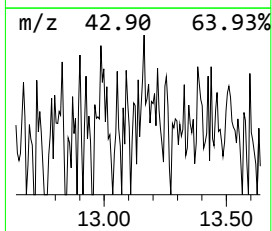
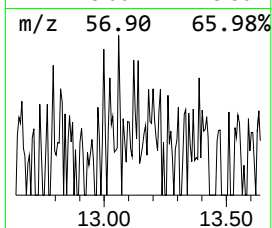
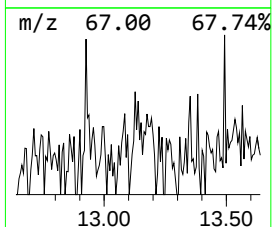
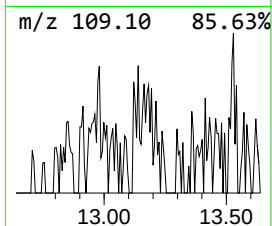
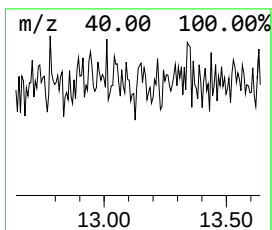
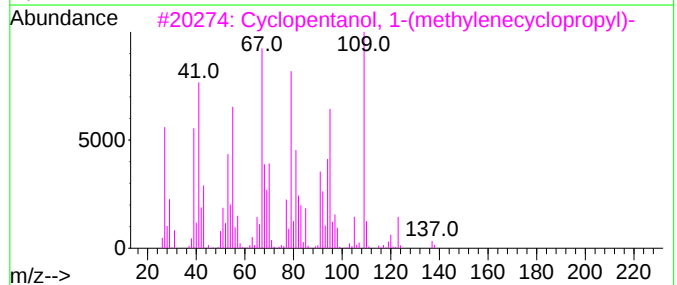
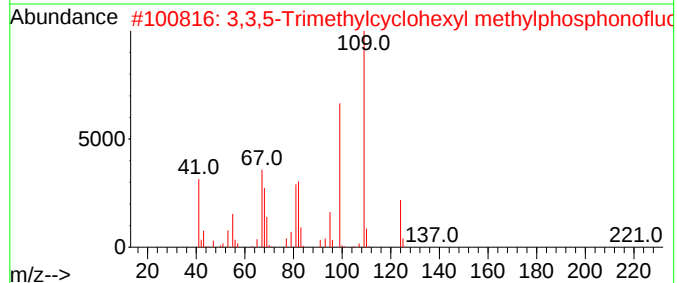
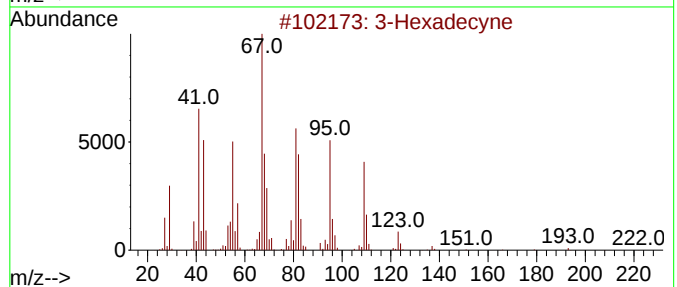
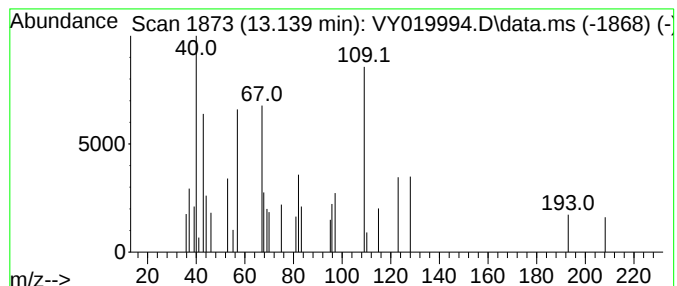
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.139 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	17.63 ug/l	4228	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexadecyne			222	C16H30	061886-62-2	32
2	3,3,5-Trimethylcyclohexyl methyl...			222	C10H20F02P	1000298-38-1	25
3	Cyclopentanol, 1-(methylenecyclo...			138	C9H14O	086951-58-8	25
4	N-[4-(5-Methyl-4H-1,2,4-triazol-...			208	C7H8N6O2	1000459-92-2	14
5	Hexane, 1-(isopropylidenecyclopr...			166	C12H22	024524-53-6	14



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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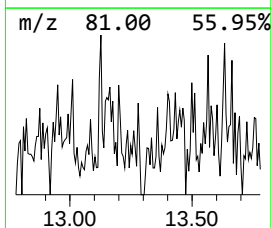
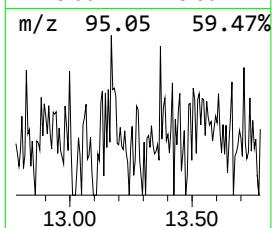
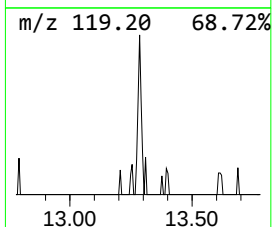
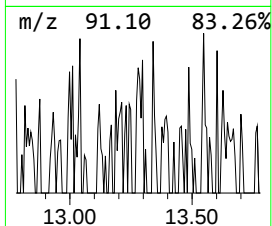
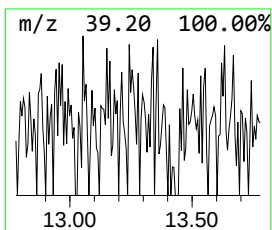
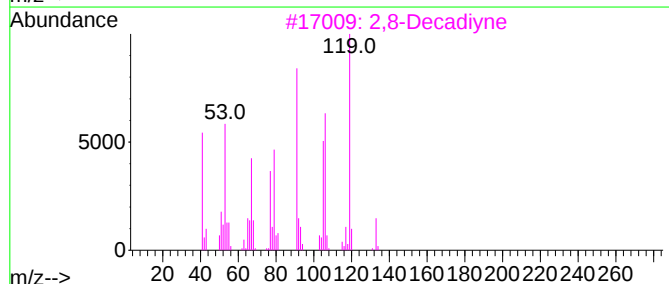
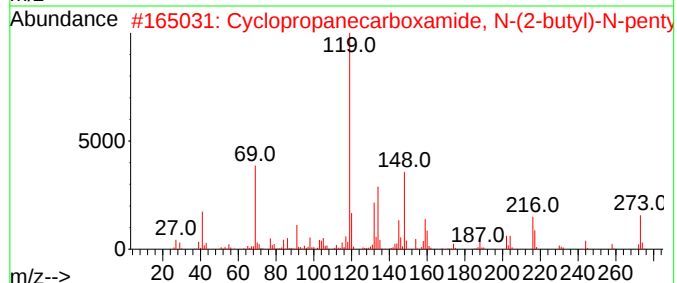
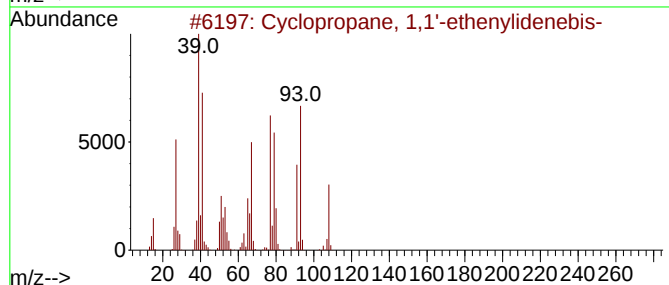
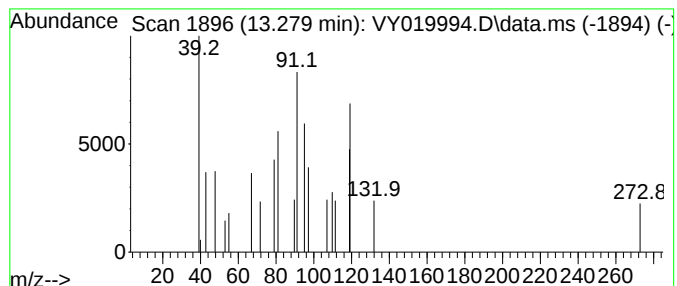
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.279 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.279	6.28 ug/l	1505	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1'-ethenylidenebis-	108	C8H12	000822-93-5	25
2			Cyclopropanecarboxamide, N-(2-bu...	273	C18H27NO	1000491-75-2	9
3			2,8-Decadiyne	134	C10H14	004116-93-2	8
4			Benzene, (2-propynyloxy)-	132	C9H8O	013610-02-1	5
5			2-Furancarboxylic acid, 2-ethylc...	222	C13H18O3	1000278-83-7	4



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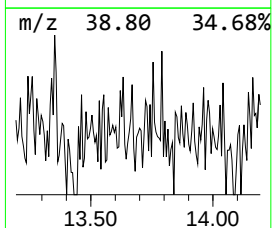
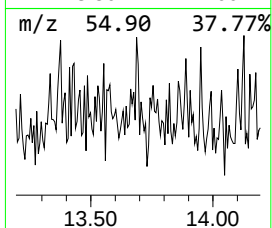
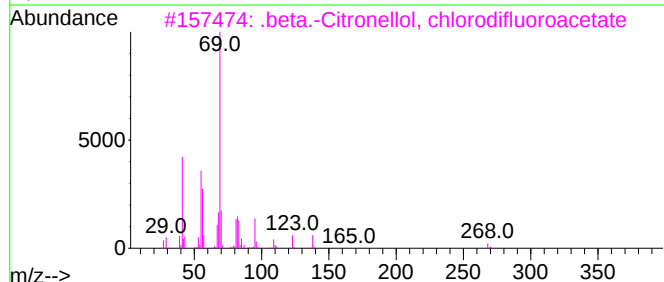
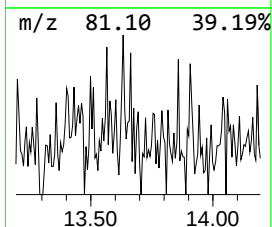
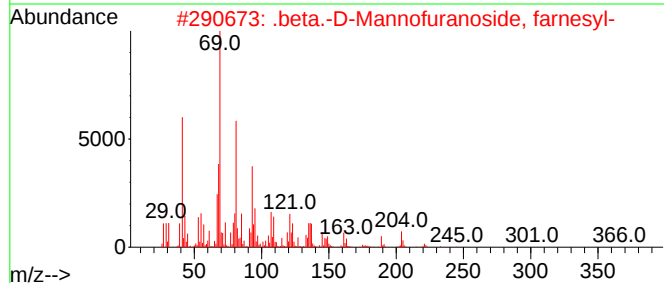
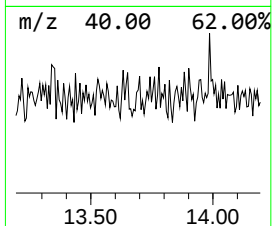
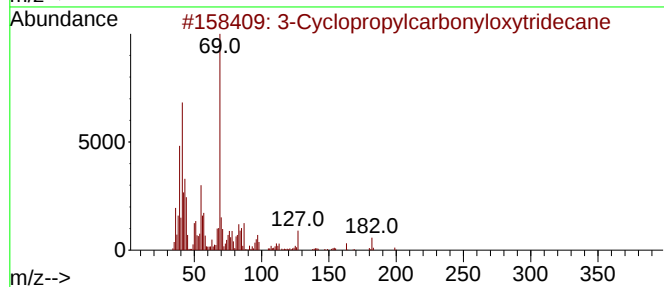
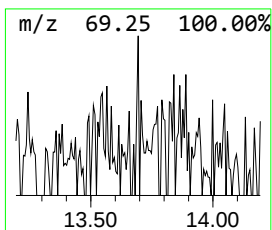
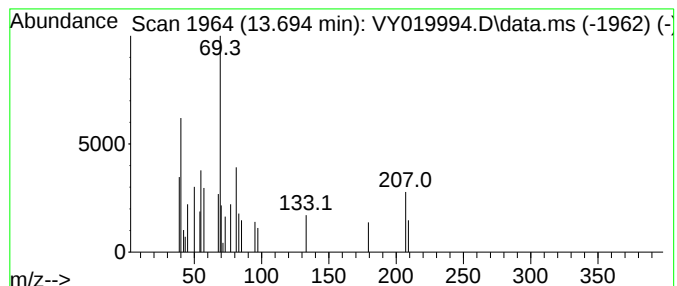
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 7 unknown13.694 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.694	8.11 ug/l	1945	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Cyclopropylcarbonyloxytridecane	268	C17H32O2	1000245-58-4	37
2			.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	37
3			.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	23
4			2-Undecene, 4,5-dimethyl-, [R*,R...	182	C13H26	055170-92-8	17
5			Isoxazole	69	C3H3NO	000288-14-2	9



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ClientSampleId :
EO-03-102224

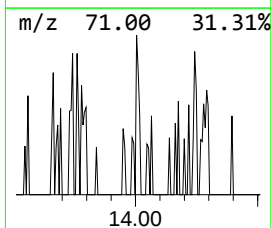
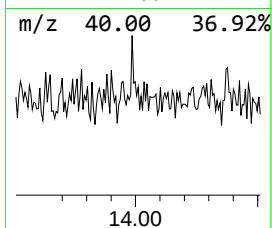
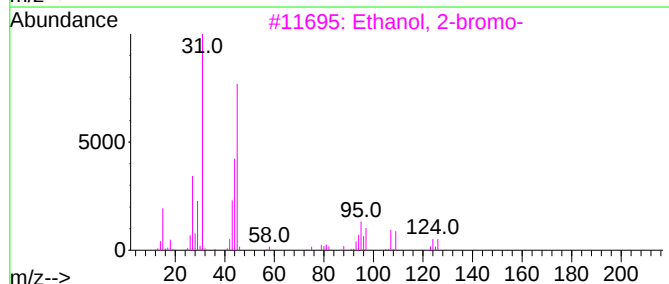
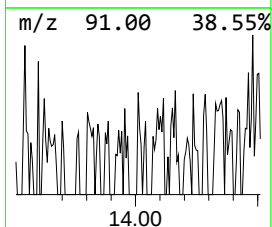
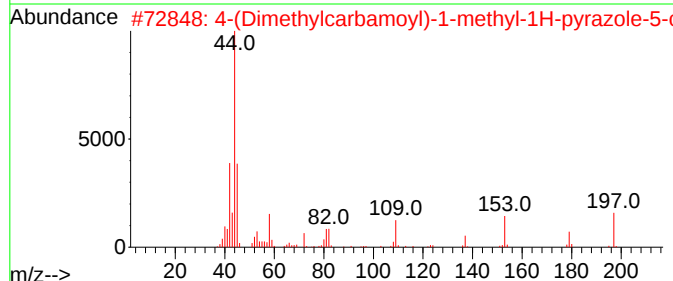
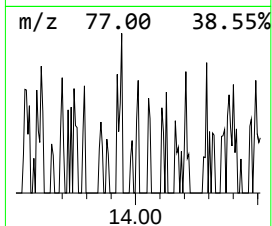
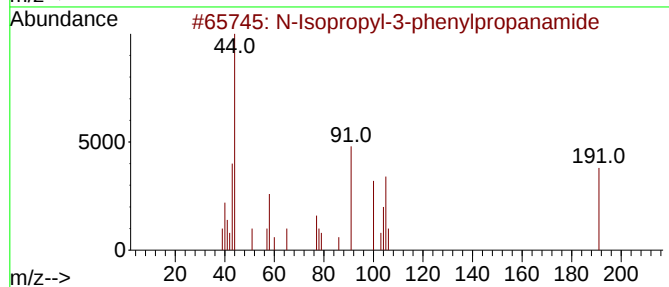
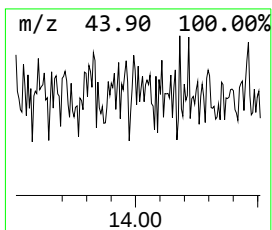
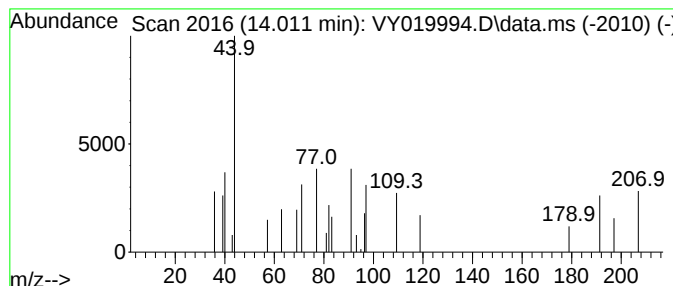
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.011 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.011	7.56 ug/l	1813	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Isopropyl-3-phenylpropanamide	191	C12H17NO	056146-87-3	25
2			4-(Dimethylcarbamoyl)-1-methyl-1...	197	C8H11N3O3	1000386-95-3	9
3			Ethanol, 2-bromo-	124	C2H5BrO	000540-51-2	9
4			(2-Chloroethyl)(methyl)amine	93	C3H8ClN	032315-92-7	5
5			Acetamide, 2-fluoro-	77	C2H4FNO	000640-19-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102324\
Data File : VY019994.D
Acq On : 23 Oct 2024 15:09
Operator : SY/MD
Sample : P4486-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EO-03-102224

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.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
unknown2.080	2.080	14.3	ug/l	9399	1	7.713	32947	50.0
unknown13.139	13.139	17.6	ug/l	4228	4	13.346	11991	50.0
unknown13.279	13.279	6.3	ug/l	1505	4	13.346	11991	50.0
unknown13.694	13.694	8.1	ug/l	1945	4	13.346	11991	50.0
unknown14.011	14.011	7.6	ug/l	1813	4	13.346	11991	50.0