

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092022\
 Data File : VY010581.D
 Acq On : 20 Sep 2022 17:34
 Operator : KP/MD
 Sample : N4697-07
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-31-6.5-7.0

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\82Y091922S.M

Title : SW846 8260

Signal : TIC: VY010581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	4	7	10	rVB3	753	971	1.06%	0.148%
2	2.125	42	50	51	rBV3	3017	5704	6.23%	0.867%
3	2.284	73	76	79	rBV2	760	1076	1.18%	0.164%
4	2.497	107	111	112	rBV3	1228	1219	1.33%	0.185%
5	3.052	200	202	212	rVB4	3755	7958	8.69%	1.209%
6	3.241	228	233	240	rVB5	1249	3062	3.35%	0.465%
7	4.192	383	389	397	rBV5	1039	2652	2.90%	0.403%
8	4.704	463	473	485	rBV4	5357	15650	17.10%	2.378%
9	5.734	636	642	652	rVB7	2070	5631	6.15%	0.856%
10	6.972	835	845	856	rBV	15782	48077	52.53%	7.305%
11	7.716	957	967	972	rBV2	12745	30245	33.05%	4.596%
12	7.783	972	978	989	rVB	23536	53183	58.11%	8.081%
13	8.130	1023	1035	1046	rBV3	18795	60680	66.30%	9.221%
14	8.685	1117	1126	1134	rBV2	34483	69377	75.80%	10.542%
15	10.179	1364	1371	1380	rBV	52039	91524	100.00%	13.907%
16	10.575	1430	1436	1443	rBV	5122	9420	10.29%	1.431%
17	10.941	1492	1496	1505	rBV3	3389	5430	5.93%	0.825%
18	11.032	1507	1511	1516	rVB3	968	1502	1.64%	0.228%
19	11.319	1553	1558	1564	rBV2	5011	8743	9.55%	1.329%
20	11.489	1576	1586	1595	rBV	49476	80601	88.07%	12.248%
21	12.483	1741	1749	1757	rBV2	38690	67583	73.84%	10.269%
22	12.733	1787	1790	1794	rBV3	750	998	1.09%	0.152%
23	13.178	1860	1863	1870	rVB2	602	973	1.06%	0.148%
24	13.422	1897	1903	1910	rVB	40158	61749	67.47%	9.383%
25	13.635	1931	1938	1940	rBV5	1107	1919	2.10%	0.292%
26	13.959	1987	1991	1998	rBV3	1003	2088	2.28%	0.317%
27	14.227	2029	2035	2042	rVB5	515	1015	1.11%	0.154%
28	15.233	2194	2200	2206	rBV	5507	9822	10.73%	1.492%
29	15.312	2209	2213	2220	rVB3	2648	4489	4.90%	0.682%
30	15.501	2240	2244	2247	rBV4	587	1275	1.39%	0.194%
31	16.287	2370	2373	2379	rVB5	849	1348	1.47%	0.205%
32	16.489	2401	2406	2412	rBV8	1197	2131	2.33%	0.324%

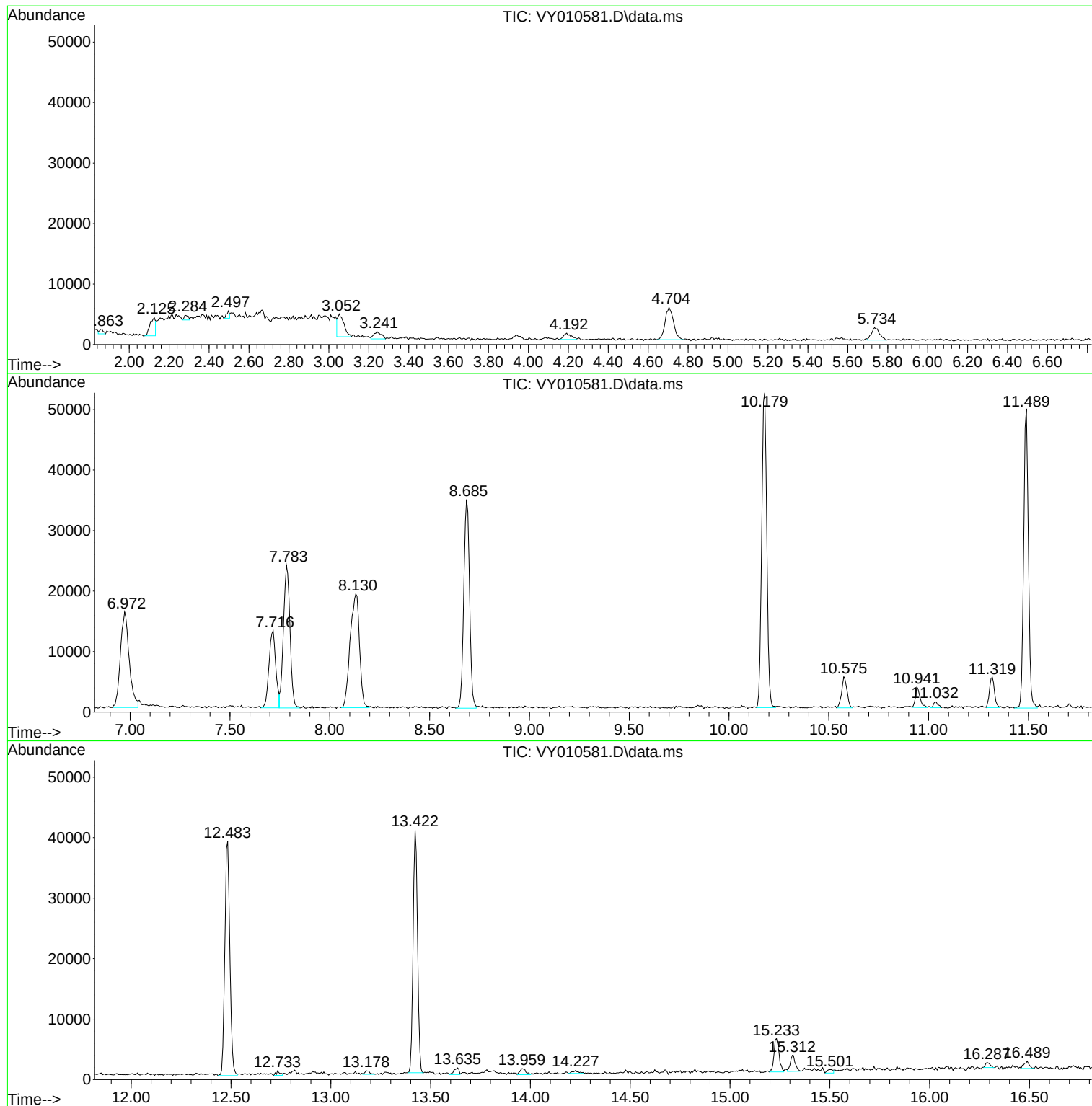
Sum of corrected areas: 658095

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SB-31-6.5-7.0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
Quant Title : SW846 8260

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



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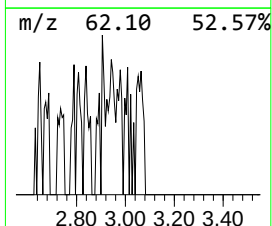
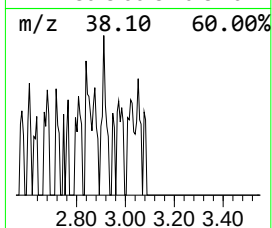
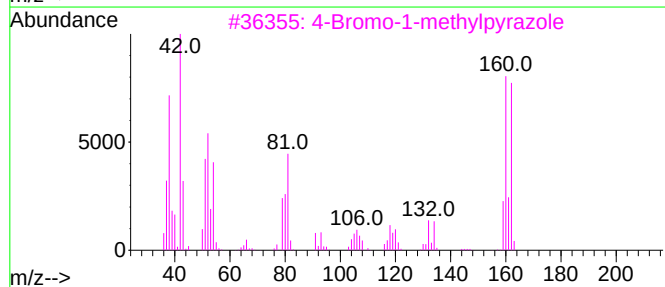
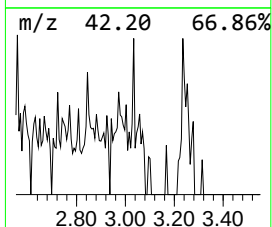
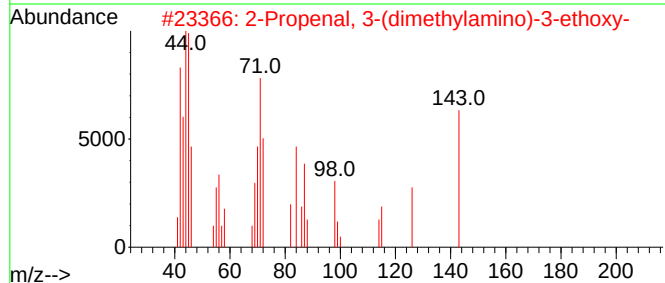
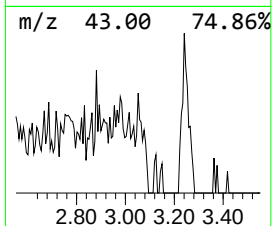
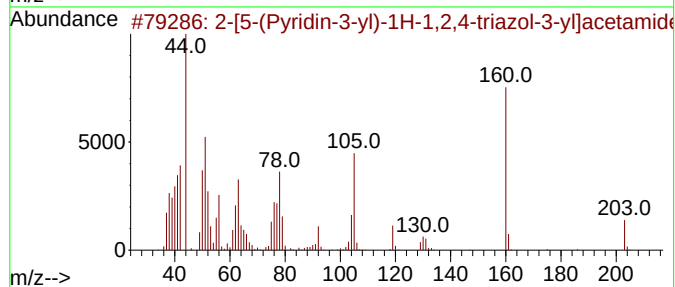
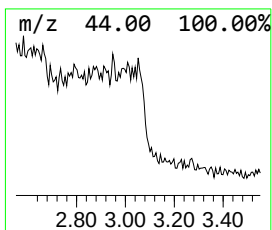
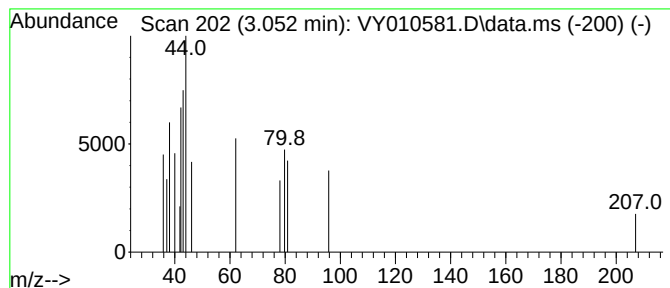
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091922S.M
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.052 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	7.48 ug/l	7958	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		[5-(Pyridin-3-yl)-1H-1,2,4-tri...	203	C9H9N5O	1000410-33-9	33
2	2		Propenal, 3-(dimethylamino)-3-...	143	C7H13NO2	026387-77-9	9
3	4		Bromo-1-methylpyrazole	160	C4H5BrN2	015803-02-8	9
4	3,4		Furandicarboxylic acid	156	C6H4O5	003387-26-6	9
5	3		Cyano-2,5-dimethylpyrazine	133	C7H7N3	002435-47-4	9



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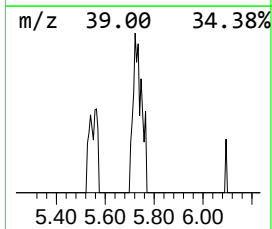
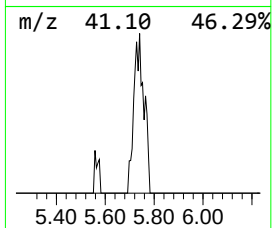
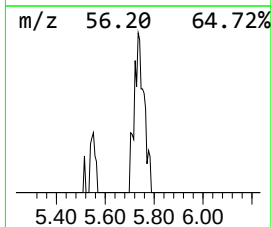
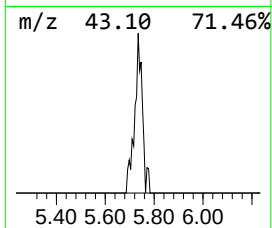
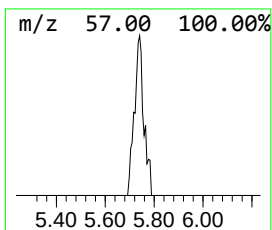
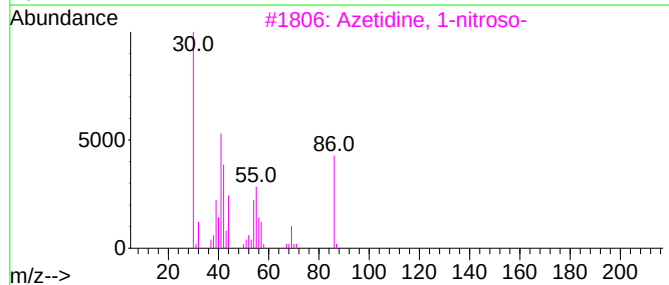
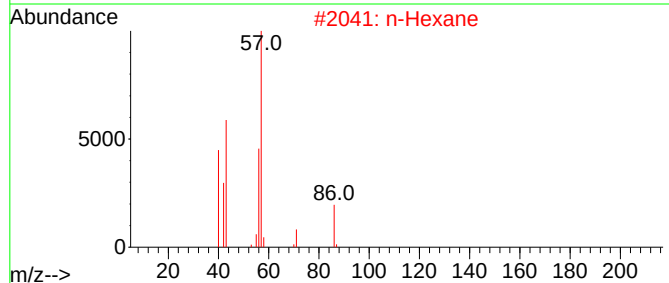
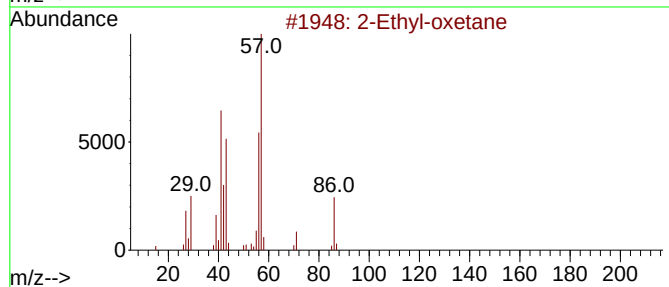
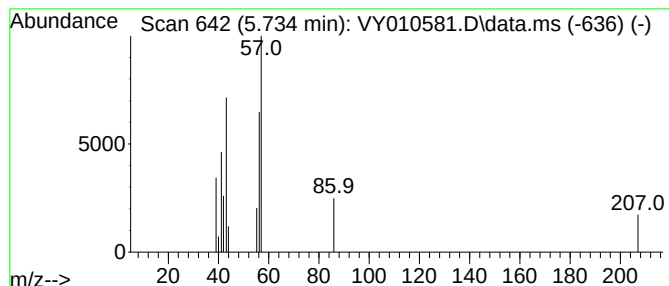
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Ethyl-oxetane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.734	5.29 ug/l	5631	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	50
2			n-Hexane	86	C6H14	000110-54-3	40
3			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
4			Trichloroacetic acid, decyl ester	302	C12H21Cl3O2	065611-33-8	9
5			Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.052	3.052	7.5	ug/l	7958	1	7.789	53183	50.0
2-Ethyl-oxetane	5.734	5.3	ug/l	5631	1	7.789	53183	50.0