

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD062819\
 Data File : VD062961.D
 Acq On : 28 Jun 2019 12:56
 Operator : VA/AP
 Sample : K3552-14
 Misc : 5.02g/5ml/MSVOA D/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 M-7A

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_D\METHOD\82D061919S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.736	26	31	32	rBV2	8046	15709	4.93%	0.779%
2	1.765	32	34	36	rVV	4269	7130	2.24%	0.354%
3	1.932	49	51	52	rVB	3567	3926	1.23%	0.195%
4	1.962	52	54	55	rBV	3797	3977	1.25%	0.197%
5	1.982	55	56	58	rBV2	3005	3892	1.22%	0.193%
6	2.090	64	67	72	rVB3	10289	27555	8.65%	1.366%
7	2.169	74	75	77	rBV2	5240	5305	1.67%	0.263%
8	2.287	84	87	89	rVB2	3597	7459	2.34%	0.370%
9	2.316	89	90	96	rVB2	4969	12559	3.94%	0.623%
10	2.385	96	97	99	rBV2	4063	5007	1.57%	0.248%
11	2.474	103	106	107	rBV3	3521	5392	1.69%	0.267%
12	2.582	115	117	119	rVB2	4658	6680	2.10%	0.331%
13	2.631	119	122	123	rBV2	5107	6756	2.12%	0.335%
14	2.671	123	126	127	rVV2	2943	6407	2.01%	0.318%
15	2.691	127	128	131	rVV2	5660	6348	1.99%	0.315%
16	2.730	131	132	133	rVB	5707	3370	1.06%	0.167%
17	2.858	142	145	147	rVV3	4587	9024	2.83%	0.448%
18	2.907	147	150	151	rVV2	3453	6174	1.94%	0.306%
19	2.966	155	156	157	rVV	7584	6098	1.91%	0.302%
20	3.006	159	160	163	rVV3	6876	11010	3.46%	0.546%
21	3.055	163	165	166	rVV	7886	9194	2.89%	0.456%
22	3.084	166	168	169	rVV2	6070	8697	2.73%	0.431%
23	3.143	172	174	176	rVV	9205	14076	4.42%	0.698%
24	3.193	176	179	186	rVB	9400	28036	8.80%	1.390%
25	3.439	201	204	206	rBV2	2784	5255	1.65%	0.261%
26	3.606	219	221	225	rVB	1931	3995	1.25%	0.198%
27	3.783	237	239	246	rVB	3877	9052	2.84%	0.449%
28	3.960	253	257	262	rVB2	3618	10816	3.40%	0.536%
29	5.093	369	372	375	rVB	1804	3901	1.22%	0.193%
30	5.900	451	454	458	rBV2	1328	3778	1.19%	0.187%
31	6.136	471	478	487	rBV	58545	203526	63.89%	10.093%
32	6.727	534	538	543	rBB	1184	3583	1.12%	0.178%
33	6.894	549	555	562	rBV	48258	133711	41.98%	6.631%
34	7.012	562	567	574	rVB3	36996	97356	30.56%	4.828%

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35	7.426	604	609	617	rBV	57747	156876	49.25%	7.779%
36	7.514	617	618	622	rVB	2477	3191	1.00%	0.158%
37	8.193	681	687	692	rBV	66859	168462	52.88%	8.354%
38	8.253	692	693	695	rVB	4321	3835	1.20%	0.190%
39	10.389	905	910	915	rBV	63252	142319	44.68%	7.058%
40	11.216	990	994	999	rBV2	9199	19762	6.20%	0.980%
41	11.856	1056	1059	1063	rBV	7874	13742	4.31%	0.681%
42	12.348	1105	1109	1117	rVB	136660	213505	67.02%	10.588%
43	12.495	1122	1124	1130	rVB	1409	4154	1.30%	0.206%
44	12.653	1138	1140	1141	rBV	5217	4262	1.34%	0.211%
45	12.673	1141	1142	1146	rVB2	4405	5527	1.74%	0.274%
46	12.820	1154	1157	1161	rBV2	2065	4966	1.56%	0.246%
47	13.037	1178	1179	1183	rBV	1962	3678	1.15%	0.182%
48	13.539	1227	1230	1236	rVB	165028	228910	71.86%	11.352%
49	13.854	1258	1262	1263	rVB	2112	3730	1.17%	0.185%
50	14.218	1296	1299	1305	rBB	3040	6651	2.09%	0.330%
51	14.504	1325	1328	1333	rVB	259006	318548	100.00%	15.797%
52	15.567	1433	1436	1438	rBV	1614	3613	1.13%	0.179%
53	16.108	1489	1491	1496	rBV	2110	3459	1.09%	0.172%
54	17.260	1607	1608	1613	rBV	1285	3646	1.14%	0.181%
55	17.447	1621	1627	1629	rVB	2209	5613	1.76%	0.278%
56	17.487	1629	1631	1636	rBV	1693	3330	1.05%	0.165%

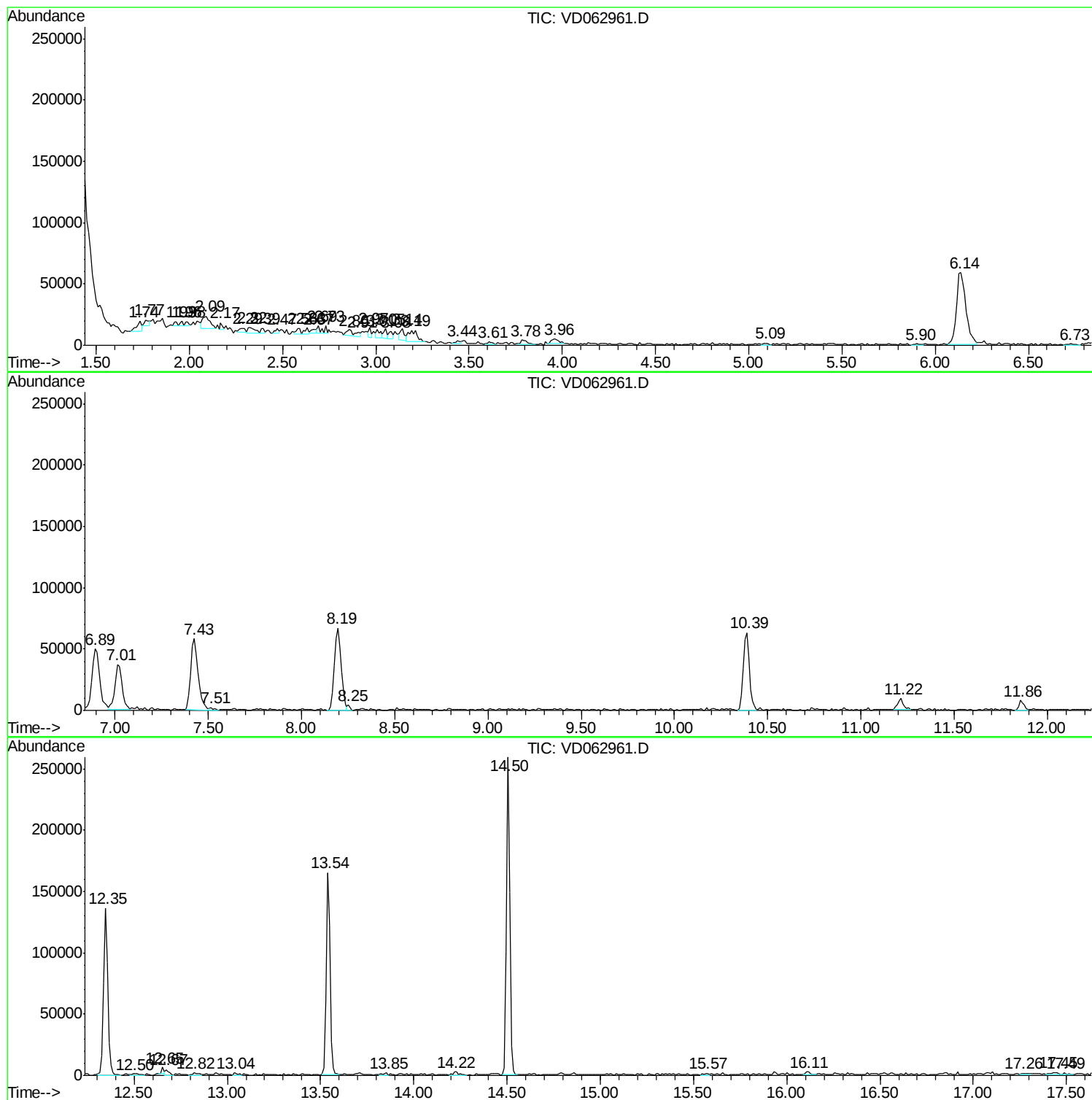
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D061919S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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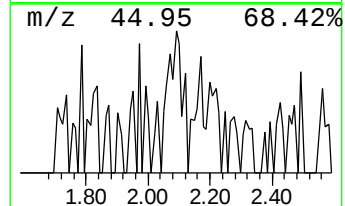
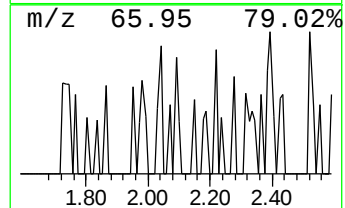
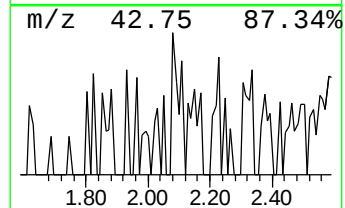
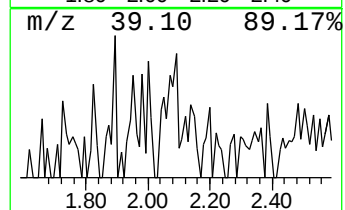
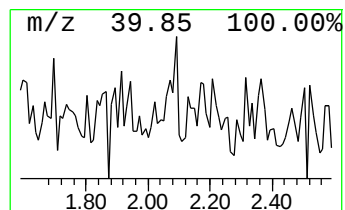
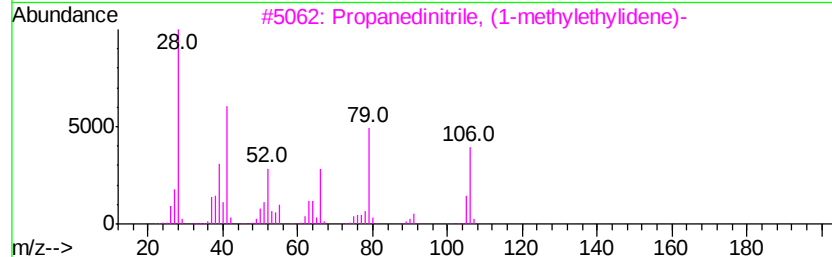
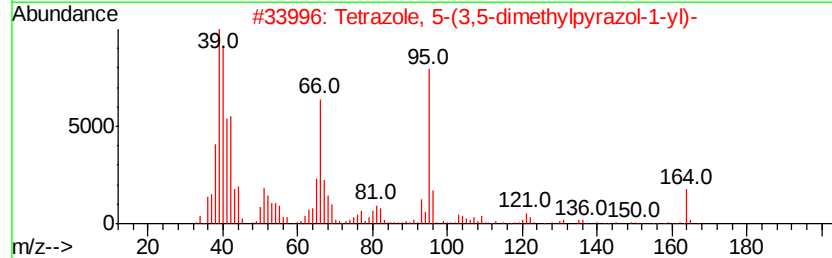
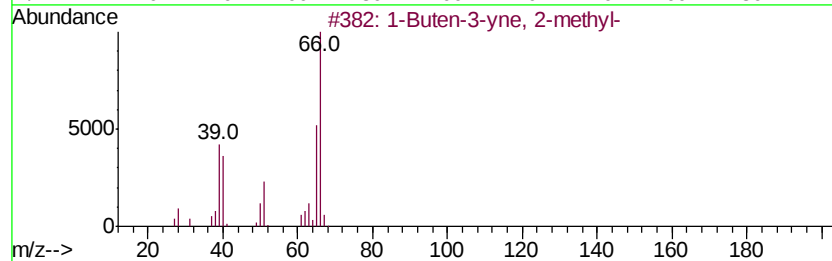
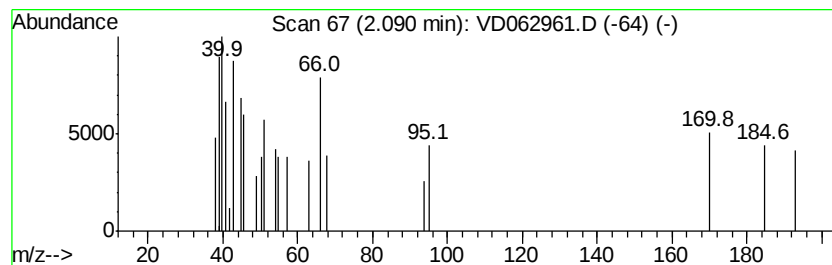
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D061919S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.09 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	14.15 ug/l	27555	Pentafluorobenzene	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Buten-3-yne, 2-methyl-	66	C5H6	000078-80-8	43
2		Tetrazole, 5-(3,5-dimethylpyrazol...	164	C6H8N6	297763-48-5	38
3		Propanedinitrile, (1-methylethylidene)-	106	C6H6N2	013166-10-4	36
4		Allene	40	C3H4	000463-49-0	16
5		Benzisoxazole-2-acetic acid, hyd...	191	C9H9N3O2	055244-10-5	12



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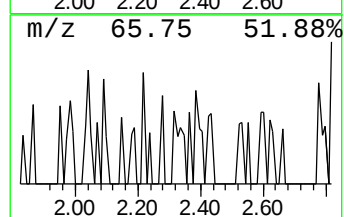
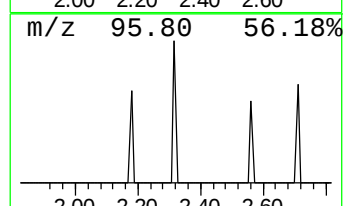
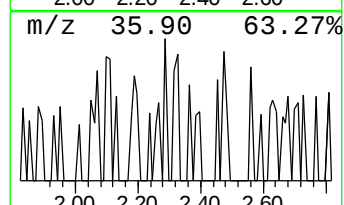
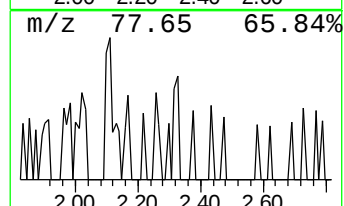
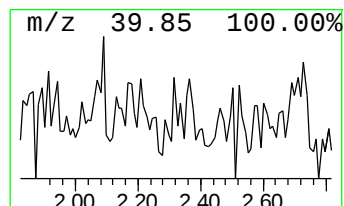
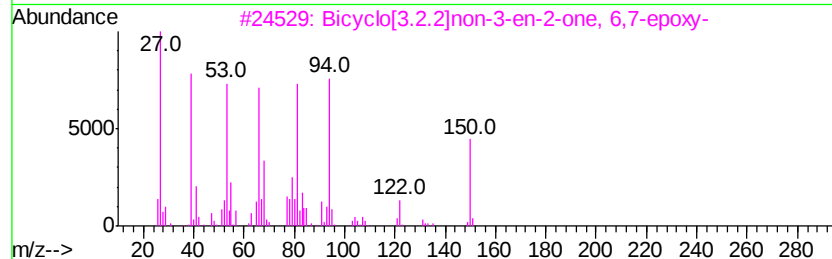
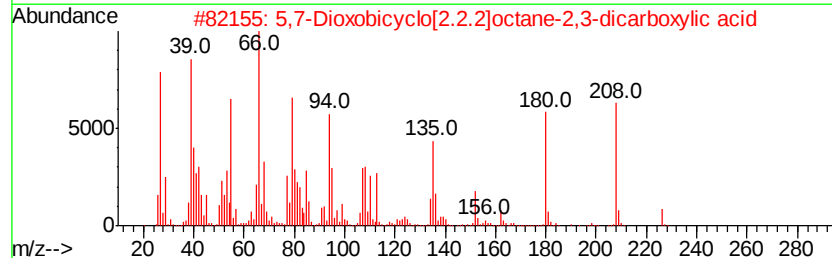
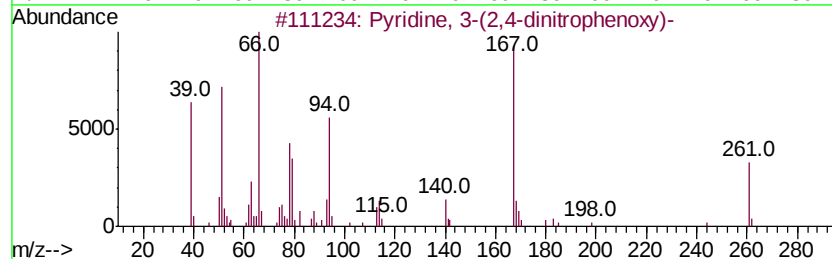
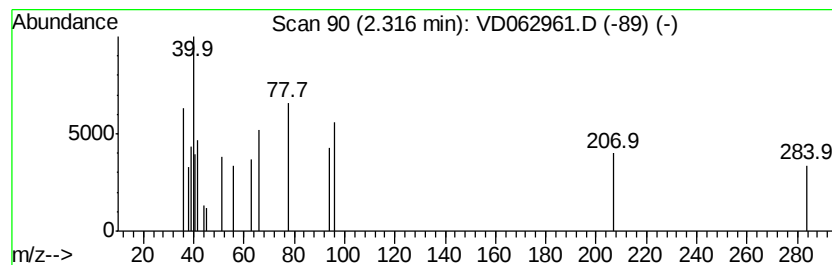
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown2.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	6.45 ug/l	12559	Pentafluorobenzene	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridine, 3-(2,4-dinitrophenoxv)-	261	C11H7N3O5	040604-27-1	28
2		5,7-Dioxobicyclo[2.2.2]octane-2,...	226	C10H10O6	099745-78-5	9
3		Bicyclo[3.2.2]non-3-en-2-one, 6,...	150	C9H10O2	1000155-95-4	9
4		cis-1,2-Dihydrocatechol	112	C6H8O2	017793-95-2	9
5		Pyridine, 3-(4-trifluoromethyl-2...	284	C12H7F3N2O3	1000276-57-5	9



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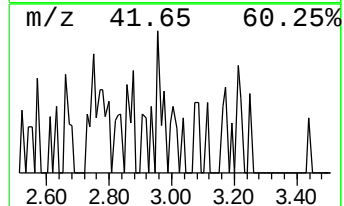
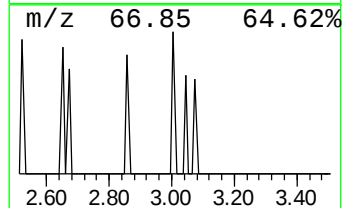
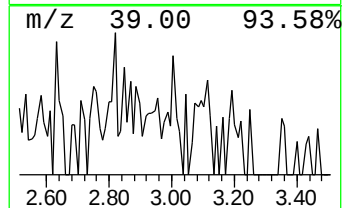
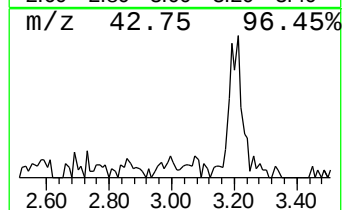
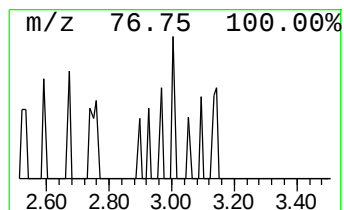
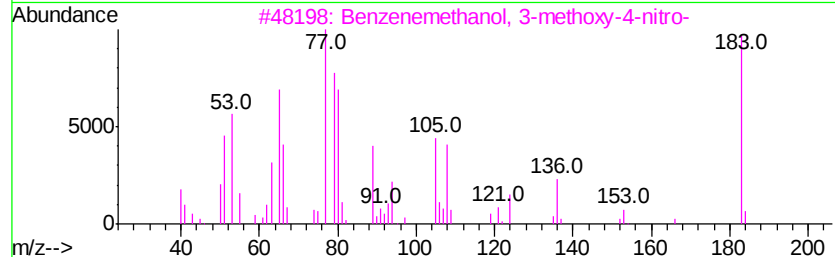
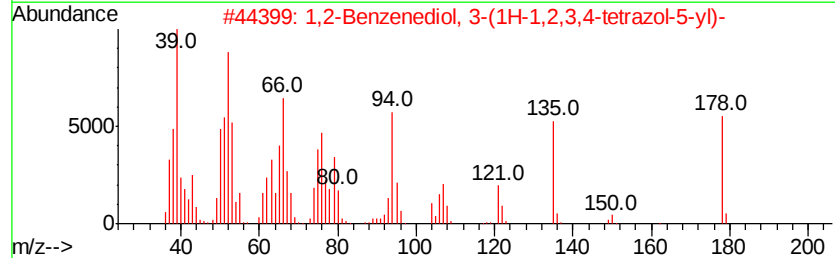
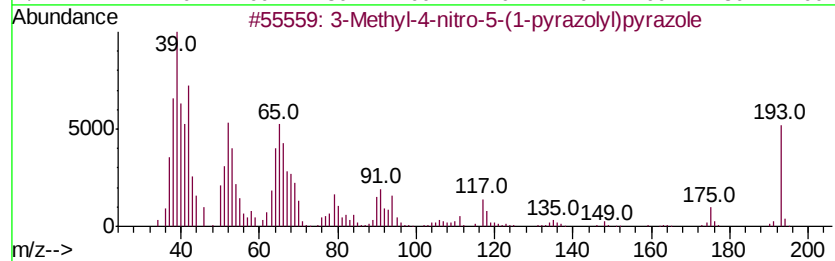
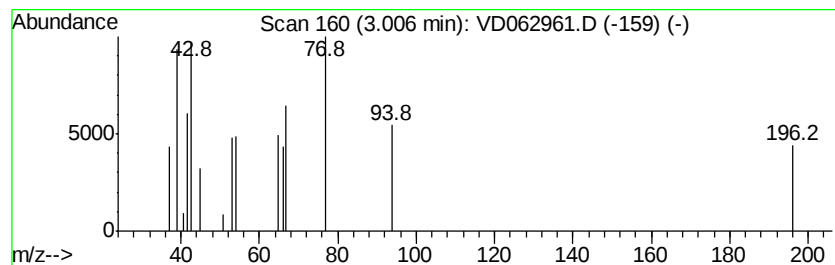
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Peak Number 4 3-Methyl-4-nitro-5-(1-pyrazolyl)pyrazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	5.65 ug/l	11010	Pentafluorobenzene	7.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methyl-4-nitro-5-(1-pyrazolyl)pyrazole	193	C7H7N5O2	292855-42-6	64
2		1,2-Benzenediol, 3-(1H-1,2,3,4-tetrazol-5-yl)-	178	C7H6N4O2	1000362-63-3	40
3		Benzenemethanol, 3-methoxy-4-nitro-	183	C8H9NO4	080866-88-2	39
4		7-Norcarancarboxylic acid, methyl ester	154	C9H14O2	1000222-16-2	32
5		Cyclohexane, cyclopropylidene-	122	C9H14	014114-06-8	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.09	2.09	14.2	ug/l	27555	1	7.01	97356	50.0
unknown2.32	2.32	6.5	ug/l	12559	1	7.01	97356	50.0
3-Methyl-4-nitro-...	3.01	5.7	ug/l	11010	1	7.01	97356	50.0