

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040617\
 Data File : BG026577.D
 Acq On : 6 Apr 2017 22:21
 Operator : SJ/MA
 Sample : I2532-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 54C

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:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.147	344	350	361	rBV	149882	237046	2.53%	0.536%
2	5.617	424	430	443	rBV	974291	1567988	16.75%	3.548%
3	7.203	693	700	711	rBV	631633	1085097	11.59%	2.455%
4	7.573	756	763	774	rBV	1862166	3306967	35.34%	7.482%
5	8.043	834	843	849	rBV	538145	929309	9.93%	2.103%
6	8.366	888	898	907	rBV	1997667	3467308	37.05%	7.845%
7	9.201	1032	1040	1051	rBV	1314200	2415518	25.81%	5.465%
8	10.840	1308	1319	1330	rBV	712448	1298018	13.87%	2.937%
9	11.257	1384	1390	1397	rVB2	85246	142260	1.52%	0.322%
10	11.398	1405	1414	1424	rBV	86499	165427	1.77%	0.374%
11	13.272	1726	1733	1744	rBV	4310581	6767176	72.31%	15.311%
12	14.559	1946	1952	1957	rVV	137116	217099	2.32%	0.491%
13	14.647	1961	1967	1978	rVB2	1111591	1746405	18.66%	3.951%
14	15.029	2027	2032	2038	rVB2	76908	115970	1.24%	0.262%
15	16.128	2211	2219	2238	rBV	2299602	3580434	38.26%	8.101%
16	17.379	2426	2432	2445	rBV2	1401325	2159841	23.08%	4.887%
17	19.659	2814	2820	2826	rBV	96920	131257	1.40%	0.297%
18	19.976	2868	2874	2885	rBV	6561398	9358716	100.00%	21.175%
19	21.627	3148	3155	3166	rBV	1648628	2759642	29.49%	6.244%
20	24.806	3686	3696	3714	rVB2	949705	2746037	29.34%	6.213%

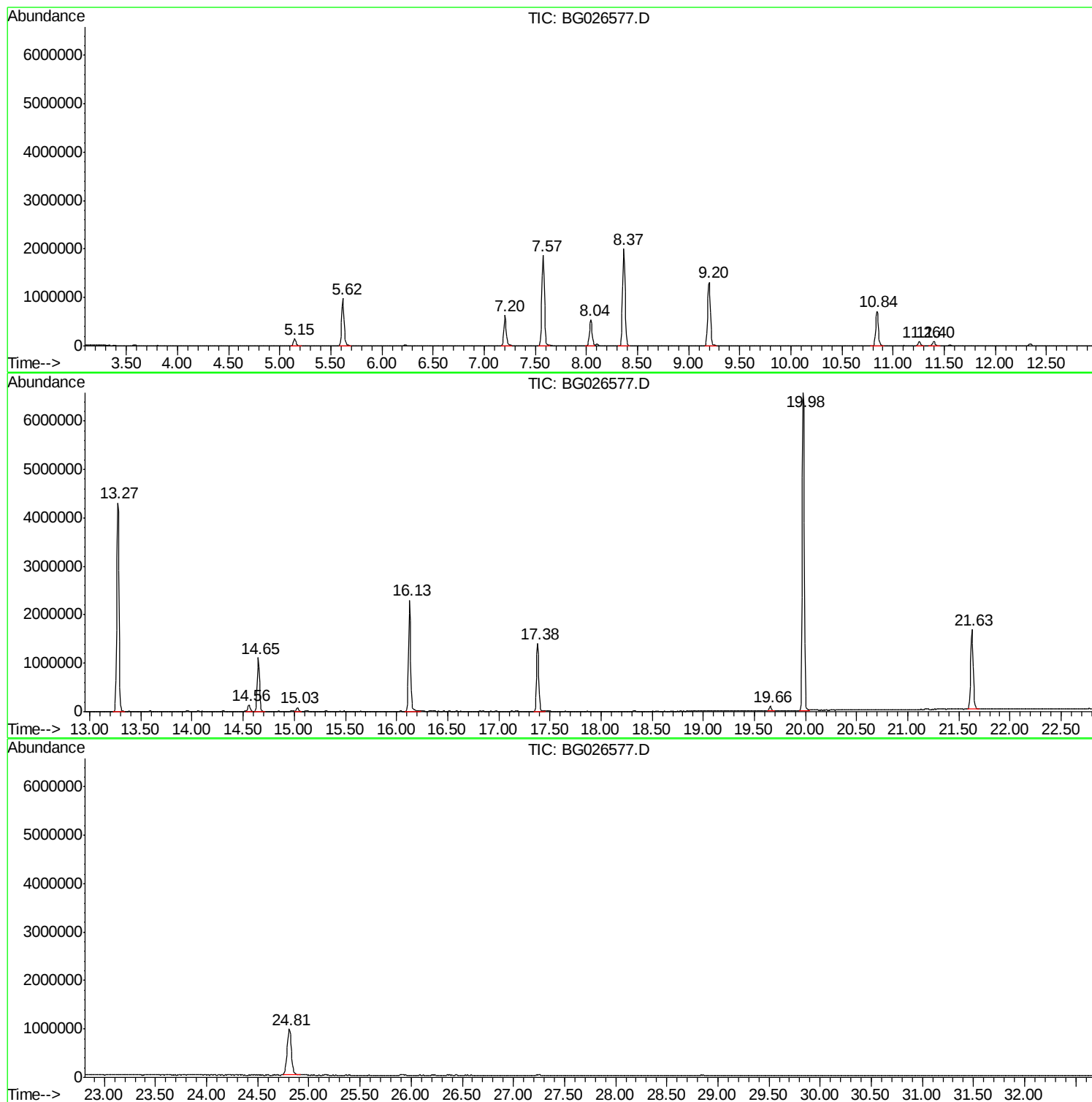
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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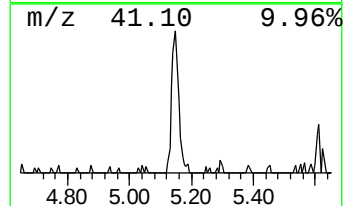
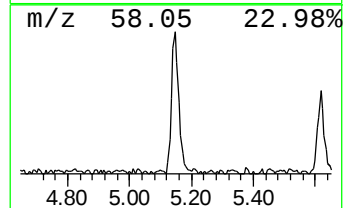
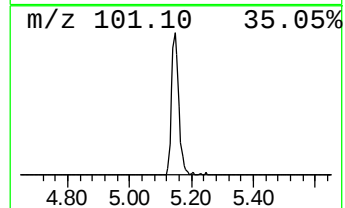
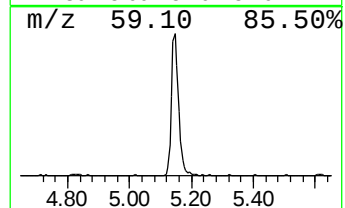
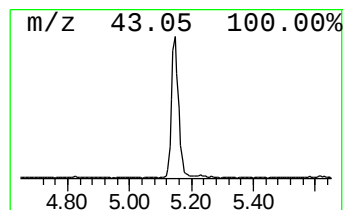
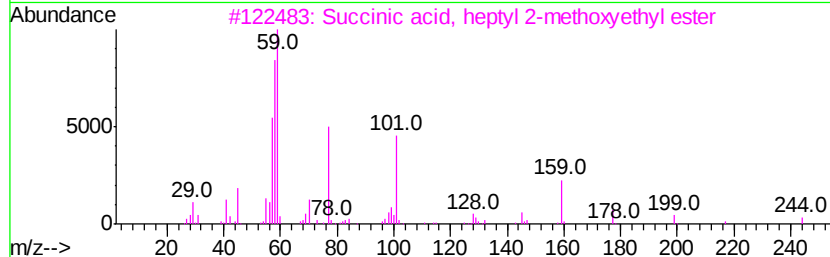
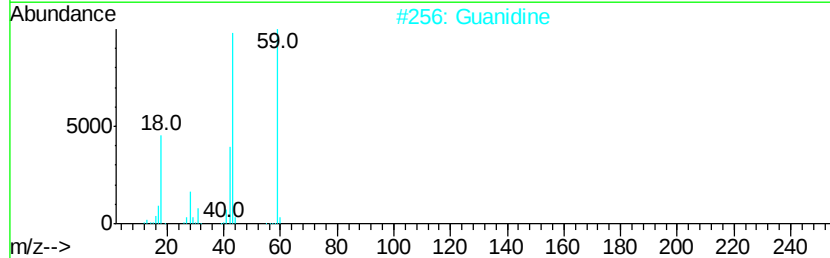
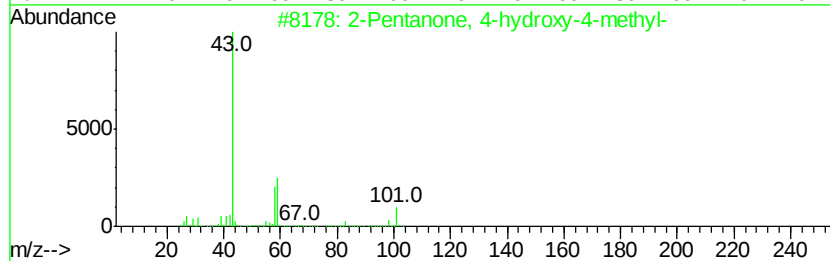
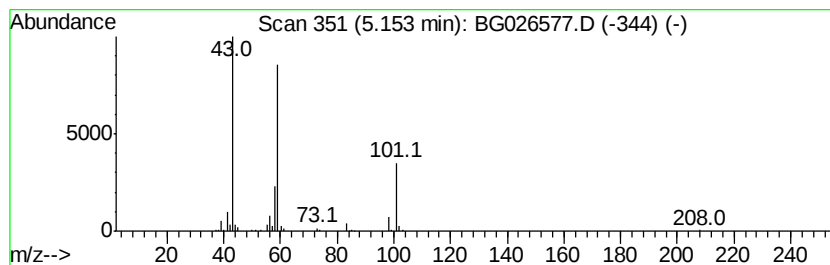
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.10 ng	237046	1,4-Dichlorobenzene-d4	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Guanidine	59	CH5N3	000113-00-8	50
3			Succinic acid, heptyl 2-methoxyve...	274	C14H26O5	1000325-80-7	33
4			2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	33
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33



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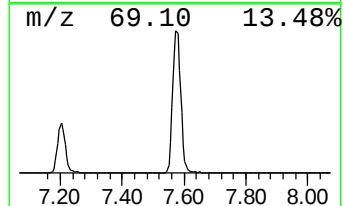
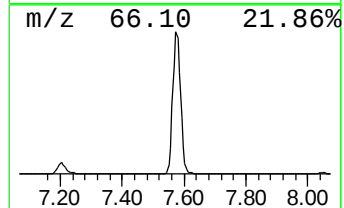
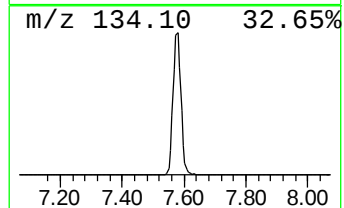
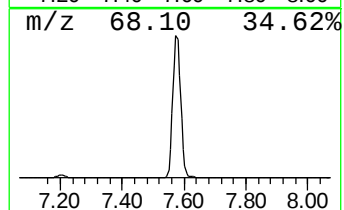
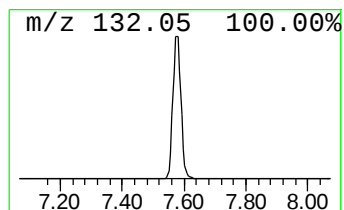
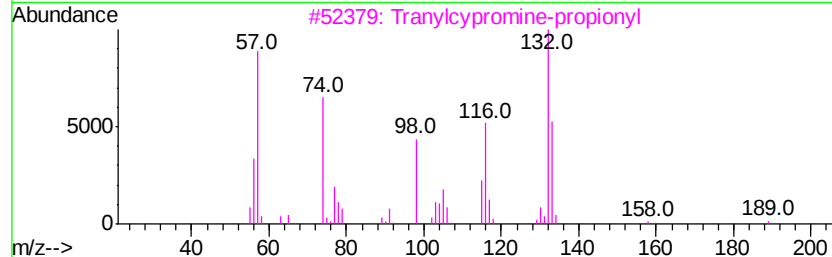
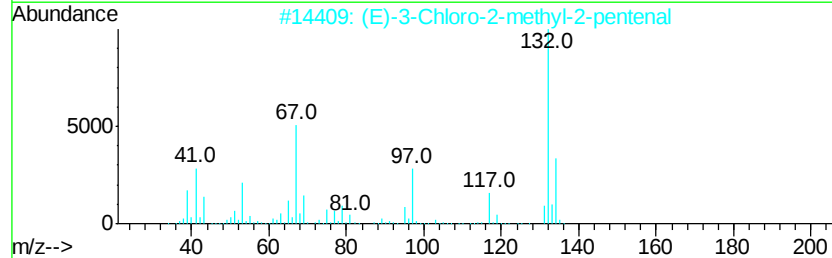
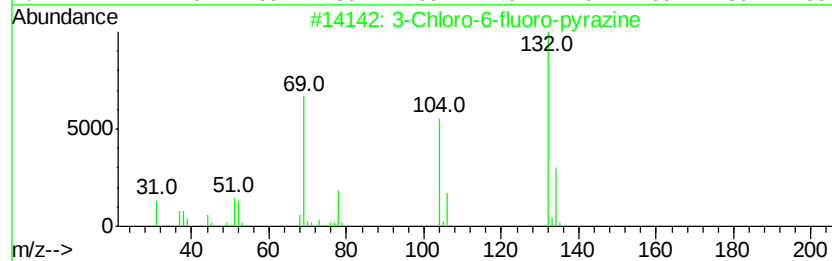
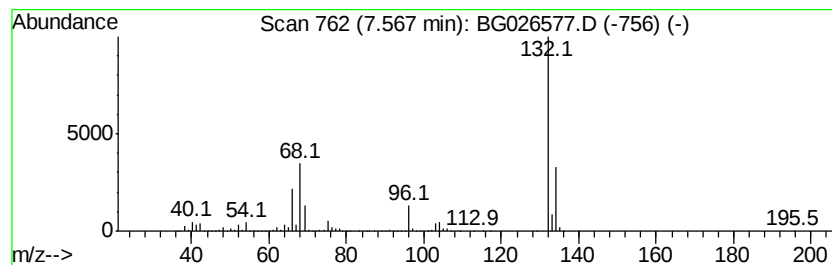
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	71.17 ng	3306970	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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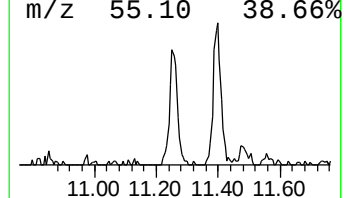
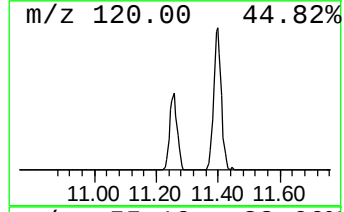
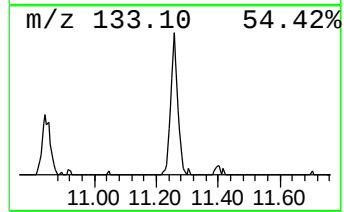
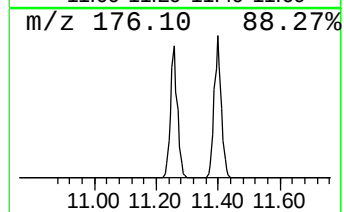
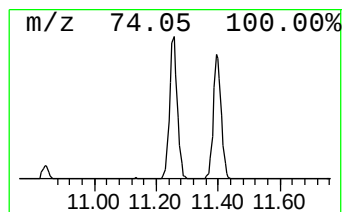
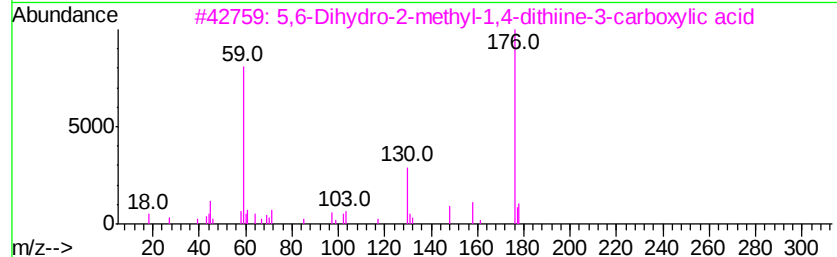
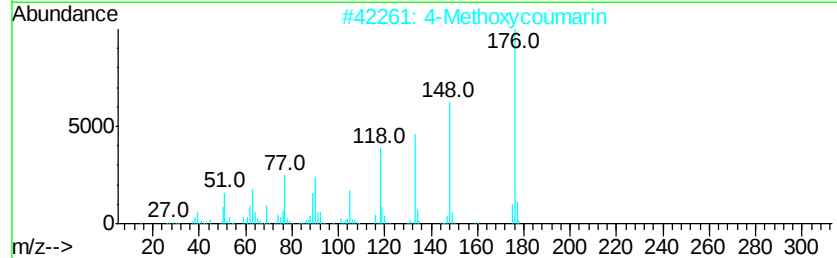
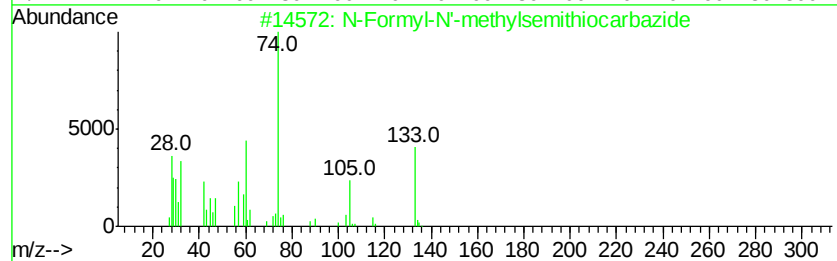
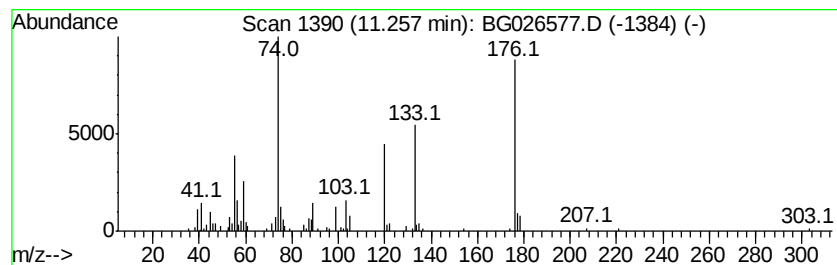
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Peak Number 4 unknown11.26 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.19 ng	142260	Naphthalene-d8	10.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Formyl-N'-methylsemithiocarbazide	133	C3H7N3OS	058064-52-1	35
2		4-Methoxycoumarin	176	C10H8O3	020280-81-3	35
3		5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	22
4		2-Thiazolamine, 4-phenyl-	176	C9H8N2S	002010-06-2	22
5		8H-[1,2,5]-Thiadiazolo[3,4-E]ben...	176	C7H4N4S	019546-85-1	14



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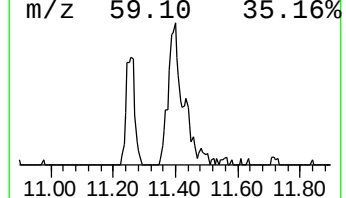
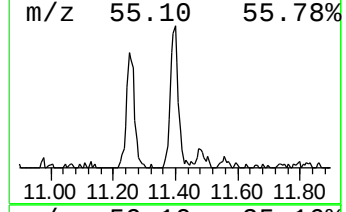
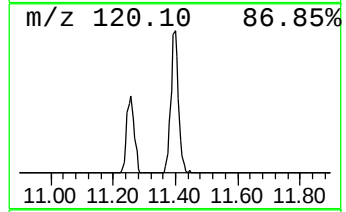
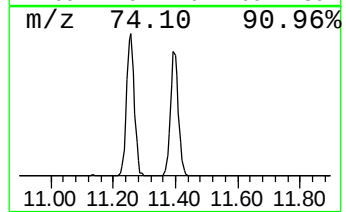
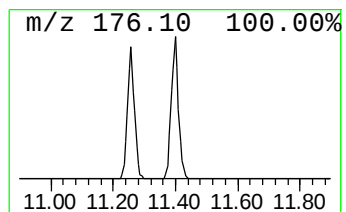
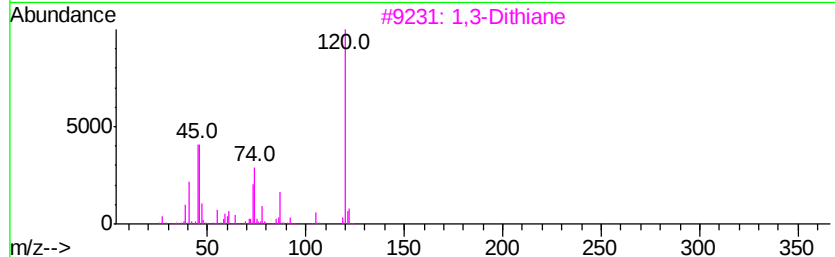
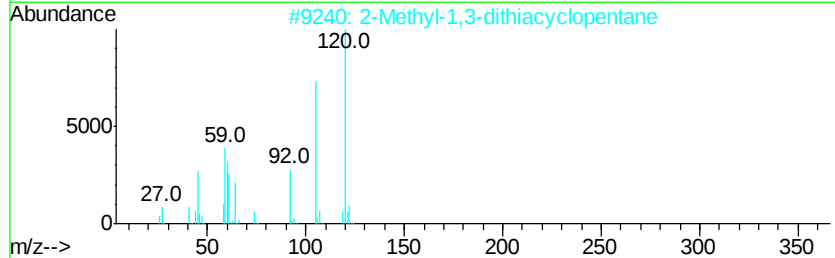
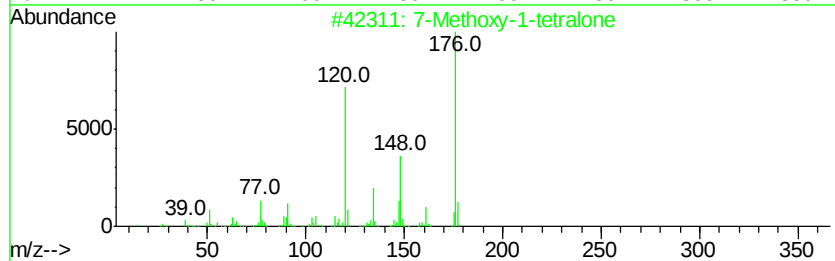
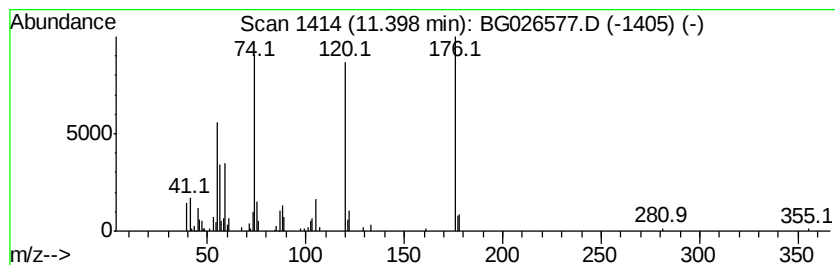
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Peak Number 5 unknown11.40 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	2.55 ng	165427	Naphthalene-d8	10.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	32
2		2-Methyl-1,3-dithiacyclopentane	120	C4H8S2	005616-51-3	25
3		1,3-Dithiane	120	C4H8S2	000505-23-7	22
4		1,2-Dithiane	120	C4H8S2	000505-20-4	22
5		5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	14



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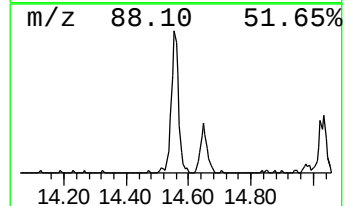
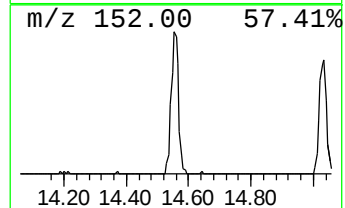
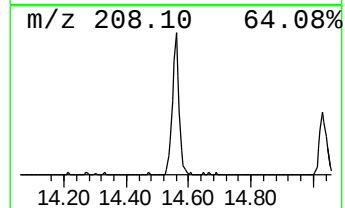
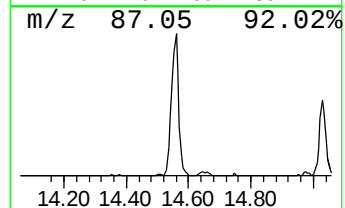
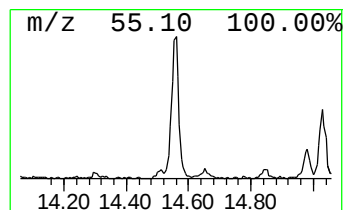
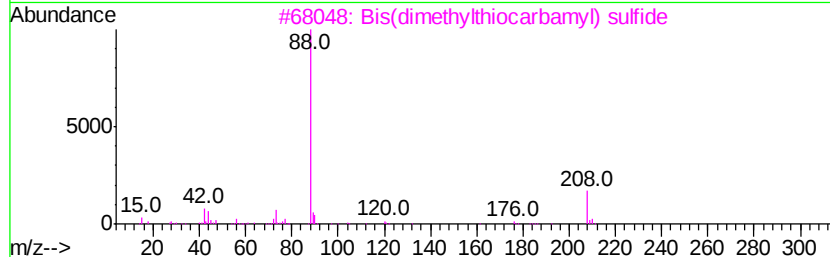
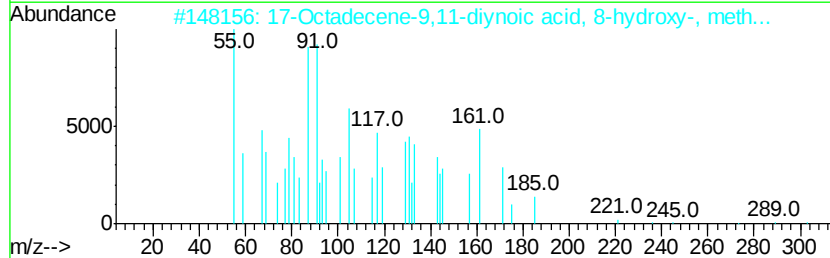
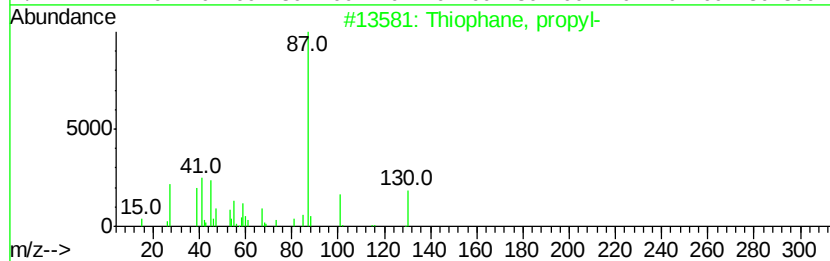
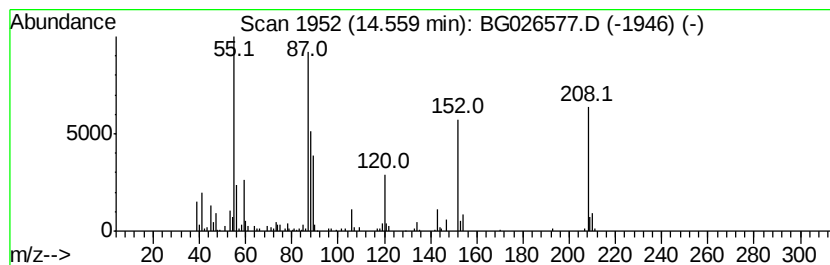
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Peak Number 6 unknown14.56 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.49 ng	217099	Acenaphthene-d10	14.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Thiophane, propyl-	130 C7H14S	001551-34-4 14
2		17-Octadecene-9,11-diyonic acid,...	304 C19H28O3	006084-79-3 14
3		Bis(dimethylthiocarbamyl) sulfide	208 C6H12N2S3	000097-74-5 14
4		Butane(dithioic) acid, methyl ester	134 C5H10S2	013831-08-8 12
5		4-O-Methyl-d-arabinose	164 C6H12O5	1000129-77-8 12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	5.1	ng	237046	1	8.04	929309	20.0
unknown7.57	7.57	71.2	ng	3306970	1	8.04	929309	20.0
unknown11.26	11.26	2.2	ng	142260	2	10.84	1298020	20.0
unknown11.40	11.40	2.5	ng	165427	2	10.84	1298020	20.0
unknown14.56	14.56	2.5	ng	217099	3	14.65	1746410	20.0