

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071817\
 Data File : BM010884.D
 Acq On : 18 Jul 2017 23:18
 Operator : SJ/JU
 Sample : I4199-10
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3570-SPP4-DUP

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:\HPCHEM1\BNA_M\METHODS\8270-BM071217.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	4.634	292	297	306	rVB	181526	262910	1.34%	0.276%
2	5.081	366	373	383	rBV	2865782	4045828	20.62%	4.250%
3	6.634	629	637	646	rBV	1775238	2673219	13.62%	2.808%
4	6.981	686	696	705	rBV	5414154	8043553	41.00%	8.449%
5	7.440	767	774	782	rBV	1185257	1790315	9.12%	1.880%
6	7.757	820	828	835	rVB	4939691	7730321	39.40%	8.120%
7	8.587	961	969	976	rBV	4442804	6946050	35.40%	7.296%
8	10.198	1236	1243	1252	rBV	1485715	2410768	12.29%	2.532%
9	10.845	1344	1353	1360	rBV2	783515	1302571	6.64%	1.368%
10	12.704	1662	1669	1676	rBV	10641622	14842195	75.65%	15.590%
11	14.092	1899	1905	1913	rBV2	1959682	2933018	14.95%	3.081%
12	15.592	2153	2160	2175	rBV	7929548	10814850	55.12%	11.360%
13	16.845	2367	2373	2383	rVB2	2367695	3271482	16.67%	3.436%
14	19.503	2820	2825	2831	rBV	15255090	19620441	100.00%	20.609%
15	21.062	3085	3090	3096	rVB	3168056	4111015	20.95%	4.318%
16	21.909	3230	3234	3237	rBV2	356007	426556	2.17%	0.448%
17	23.192	3446	3452	3459	rVB	2290090	3979621	20.28%	4.180%

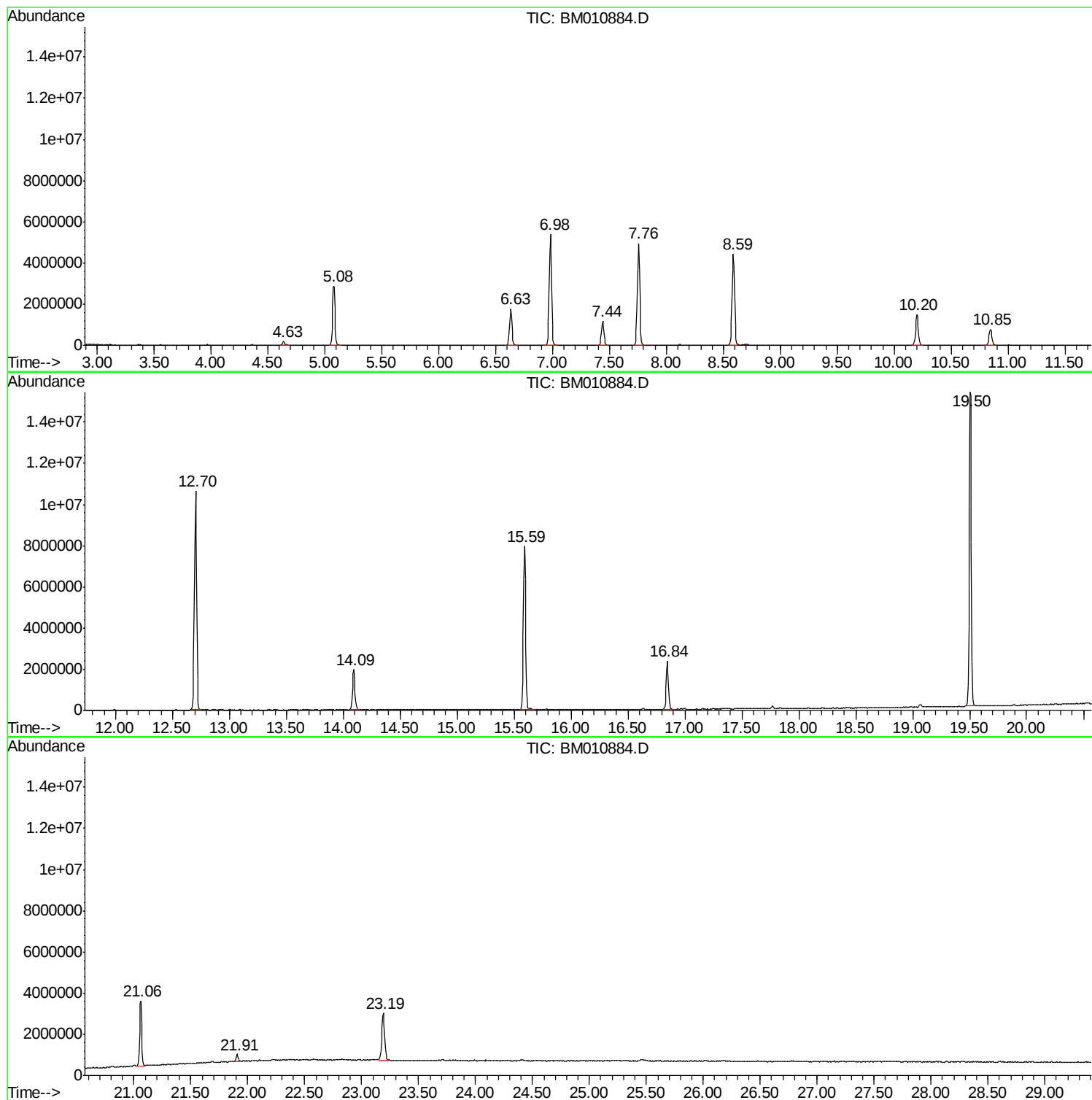
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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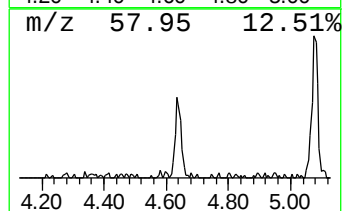
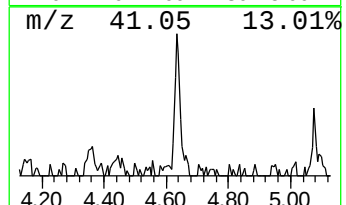
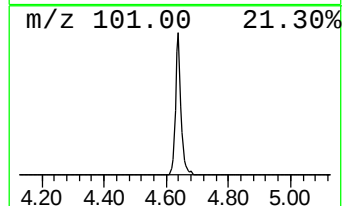
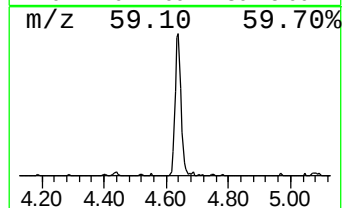
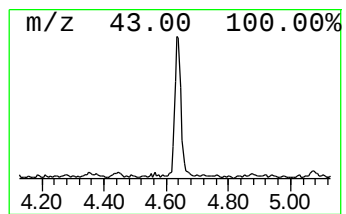
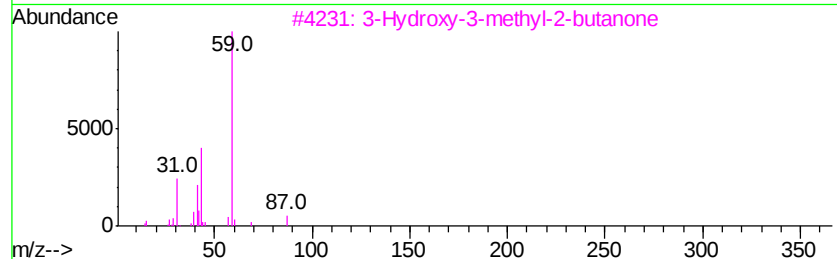
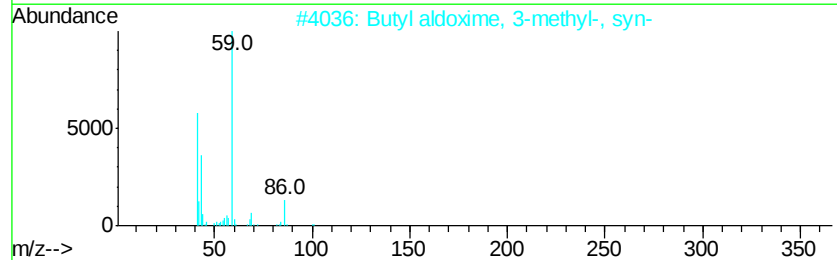
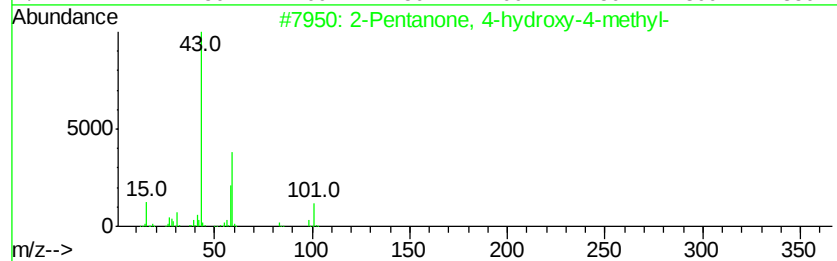
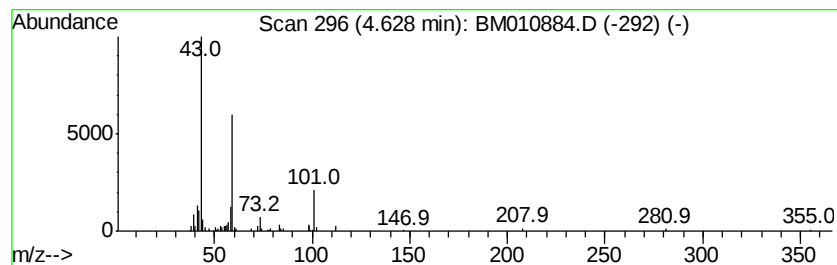
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	2.94 ng	262910	1,4-Dichlorobenzene-d4	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	32
5			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	32



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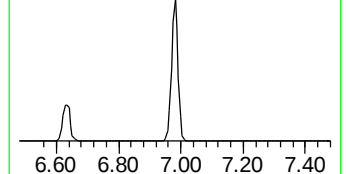
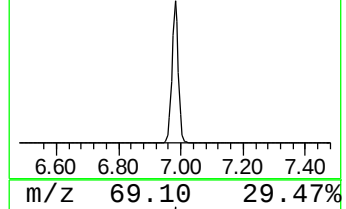
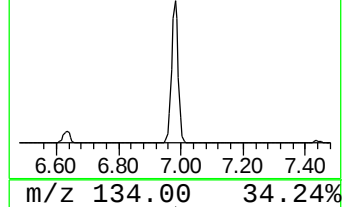
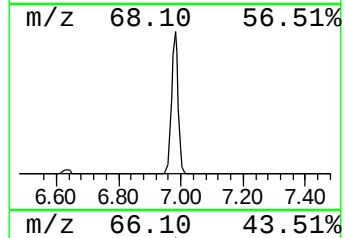
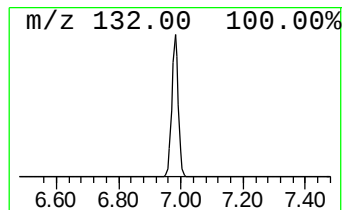
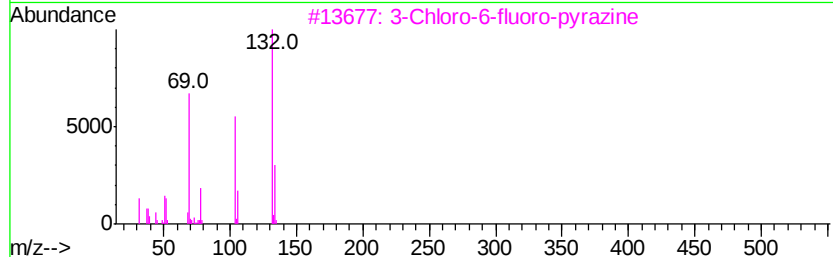
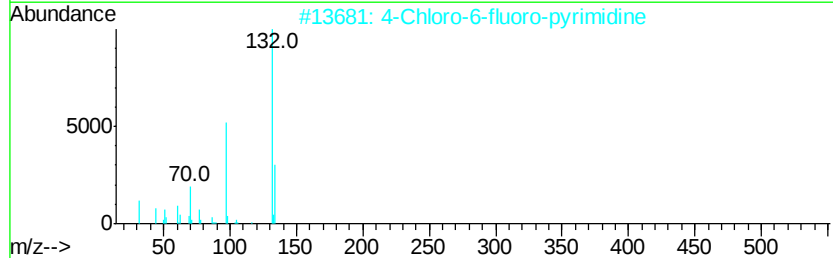
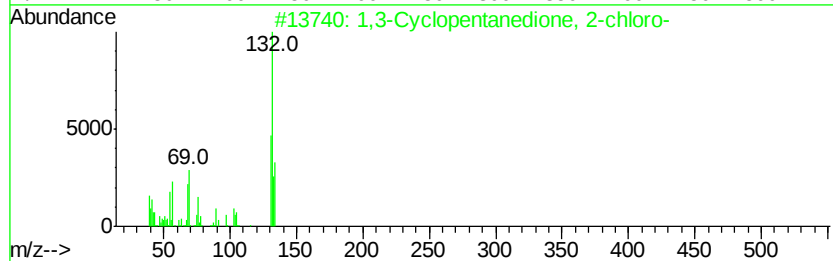
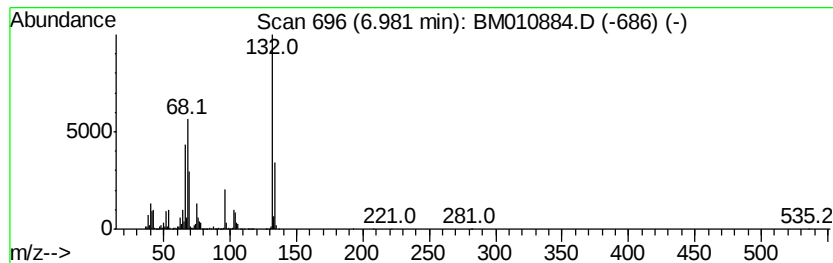
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	89.86 ng	8043550	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		Xenon	132	Xe	007440-63-3	9



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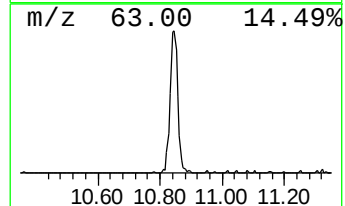
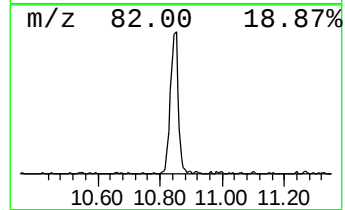
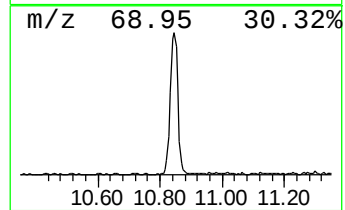
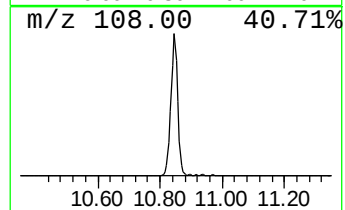
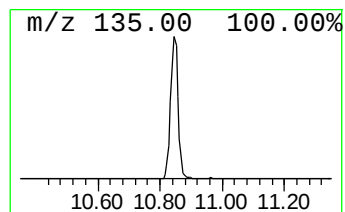
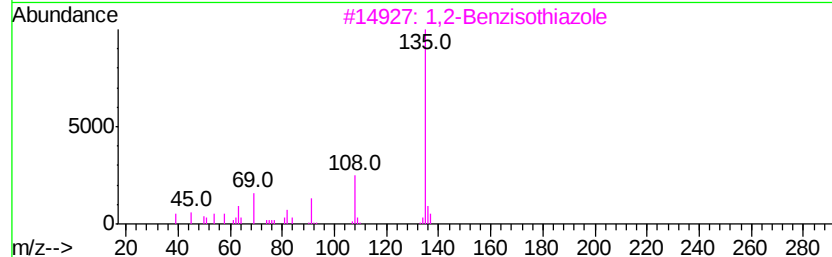
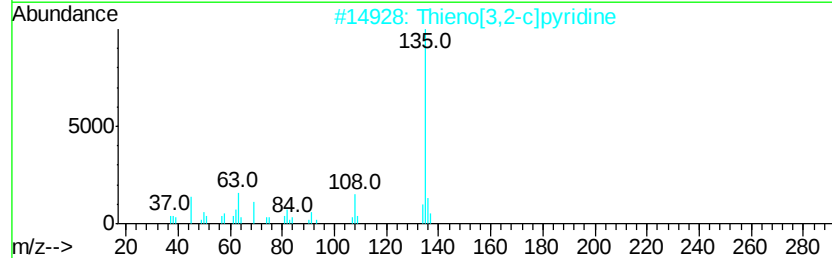
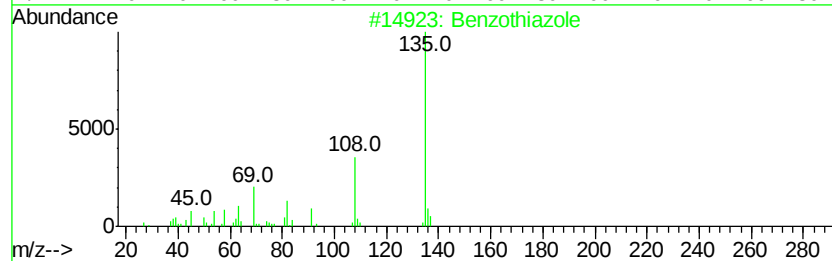
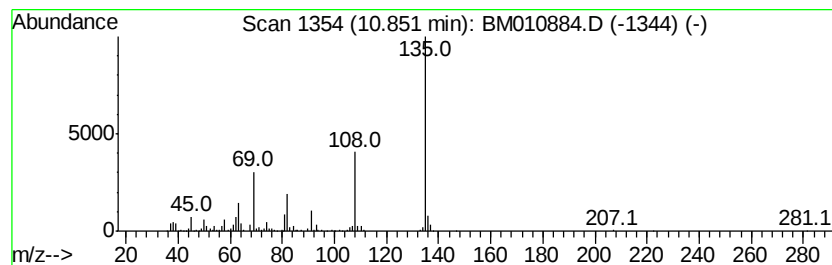
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Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	10.81 ng	1302570	Naphthalene-d8	10.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzothiazole	135 C7H5NS	000095-16-9 96
2		Thieno[3,2-c]pyridine	135 C7H5NS	000272-14-0 76
3		1,2-Benzisothiazole	135 C7H5NS	000272-16-2 72
4		3-Allylbenzothiazolium bromide	255 C10H10BrNS	016407-55-9 59
5		Adenine	135 C5H5N5	000073-24-5 47



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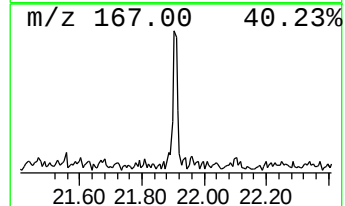
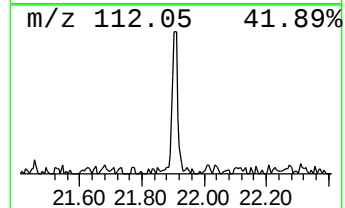
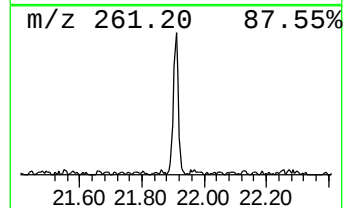
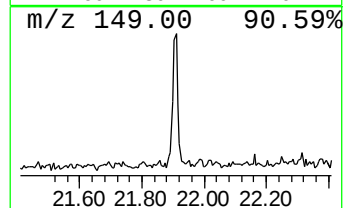
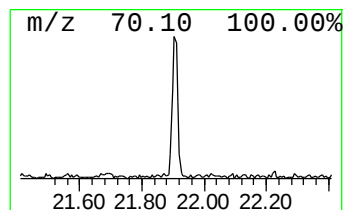
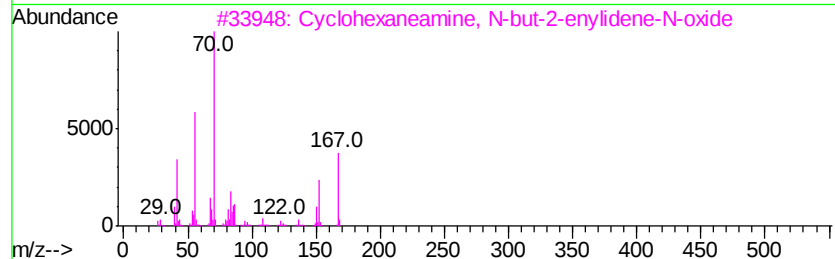
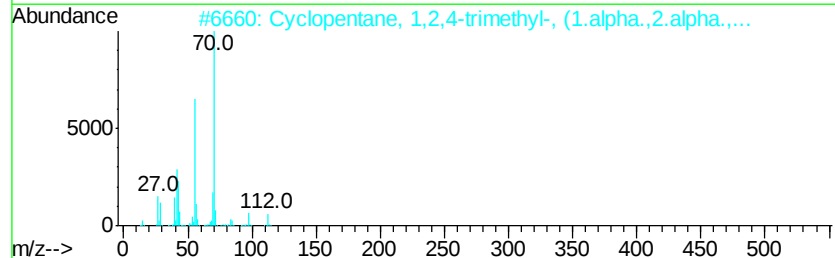
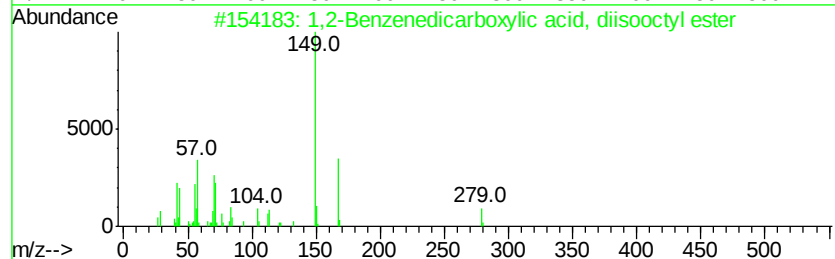
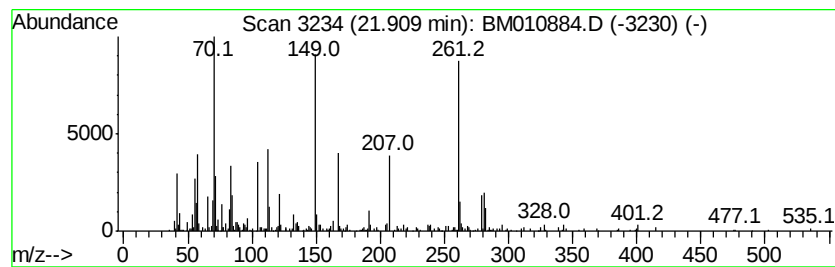
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Peak Number 5 unknown21.91 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.91	2.08 ng	426556	Chrysene-d12	21.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	22
2		Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	14
3		Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	14
4		t-Butyl hydrogen phthalate	222	C12H14O4	033693-84-4	14
5		Benzaldehyde, 3-(4-nitrophenoxy...	287	C15H13NO5	1000273-81-9	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	2.9	ng	262910	1	7.44	1790320	20.0
unknown6.98	6.98	89.9	ng	8043550	1	7.44	1790320	20.0
Benzothiazole	10.85	10.8	ng	1302570	2	10.20	2410770	20.0
unknown21.91	21.91	2.1	ng	426556	5	21.06	4111020	20.0