

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071717\
 Data File : BM010859.D
 Acq On : 18 Jul 2017 05:56
 Operator : SJ/JU
 Sample : I4199-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 3567-SPP2

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	293	297	304	rVB	181271	262028	1.22%	0.255%
2	5.081	366	373	382	rVB	2722206	3733196	17.41%	3.639%
3	6.634	630	637	646	rBV	1683048	2515172	11.73%	2.452%
4	6.981	689	696	704	rBV	5082895	7706672	35.94%	7.512%
5	7.440	768	774	782	rBV	1297576	2003528	9.34%	1.953%
6	7.757	820	828	836	rBV	4767140	7412557	34.57%	7.226%
7	8.587	960	969	978	rBV	4126214	6730755	31.39%	6.561%
8	10.204	1237	1244	1251	rVB	1681305	2725372	12.71%	2.657%
9	10.845	1343	1353	1363	rBV	1907030	3305596	15.42%	3.222%
10	12.704	1663	1669	1677	rVB	10324654	15175272	70.77%	14.793%
11	14.092	1899	1905	1913	rVB3	2397337	3596992	16.77%	3.506%
12	15.592	2152	2160	2169	rBV	8481286	11972739	55.83%	11.671%
13	15.786	2187	2193	2201	rBV	271920	440238	2.05%	0.429%
14	16.851	2368	2374	2380	rVB2	2881046	4108261	19.16%	4.005%
15	17.768	2525	2530	2537	rBV2	271638	421380	1.97%	0.411%
16	18.080	2579	2583	2590	rVB2	191917	268238	1.25%	0.261%
17	19.068	2747	2751	2756	rBV2	273367	335415	1.56%	0.327%
18	19.509	2820	2826	2832	rBV	17918584	21443291	100.00%	20.903%
19	21.062	3085	3090	3095	rBV	3718080	4471930	20.85%	4.359%
20	23.192	3446	3452	3460	rVB	2317756	3957883	18.46%	3.858%

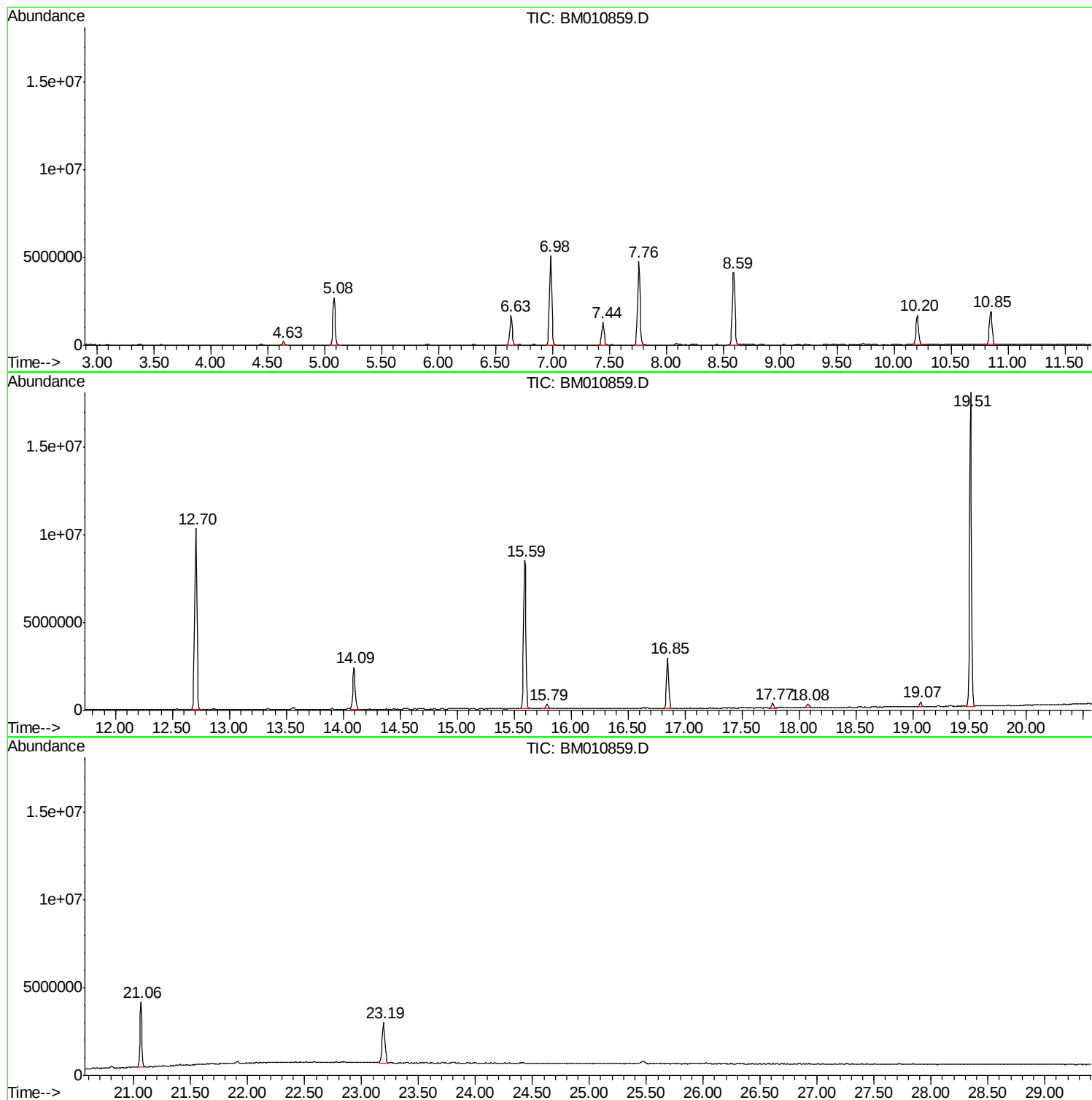
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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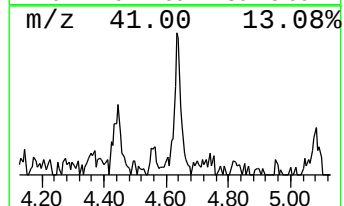
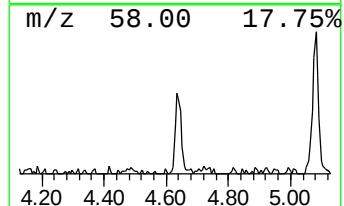
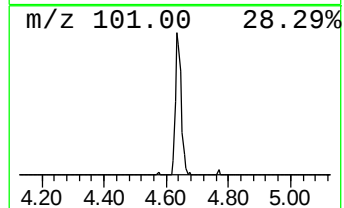
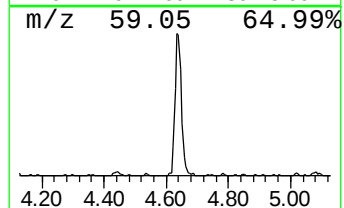
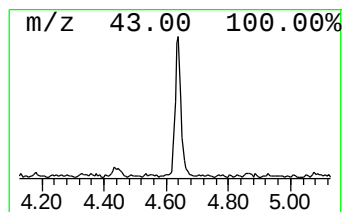
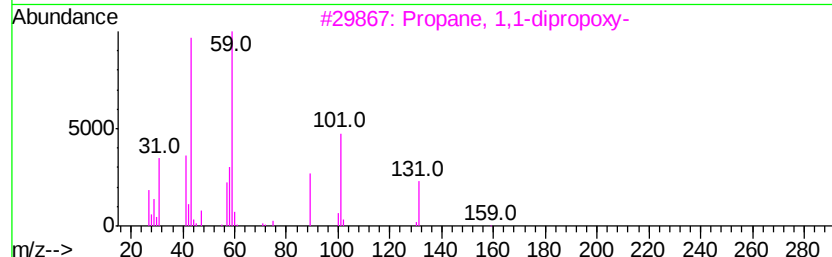
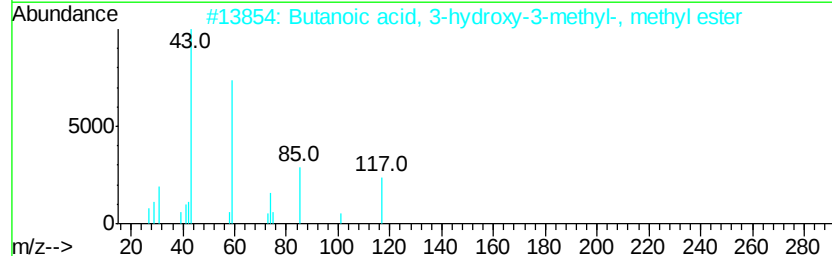
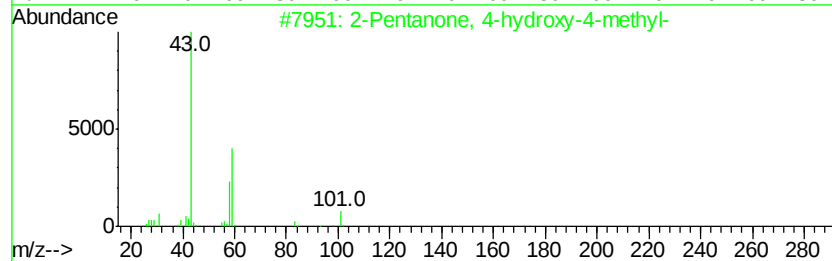
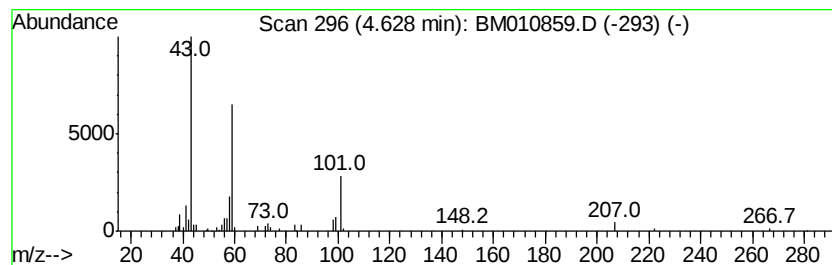
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	2.62 ng	262028	1,4-Dichlorobenzene-d4	7.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Butanoic acid, 3-hydroxy-3-methyl-	132	C6H12O3	006149-45-7	40
3			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	35
5			5-Hydroxypentanehydroxylamine, N...	245	C11H19NO5	104556-13-0	27



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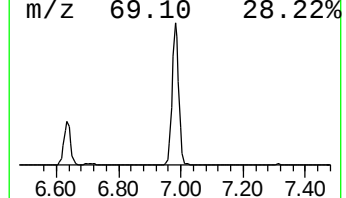
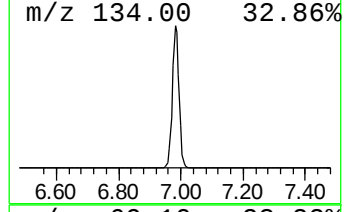
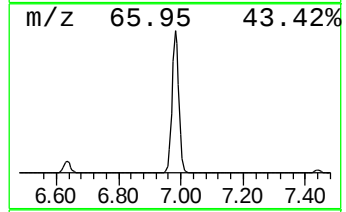
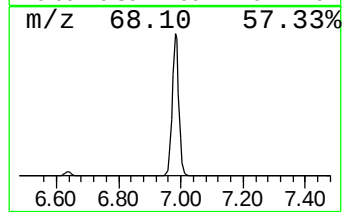
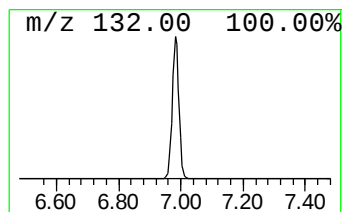
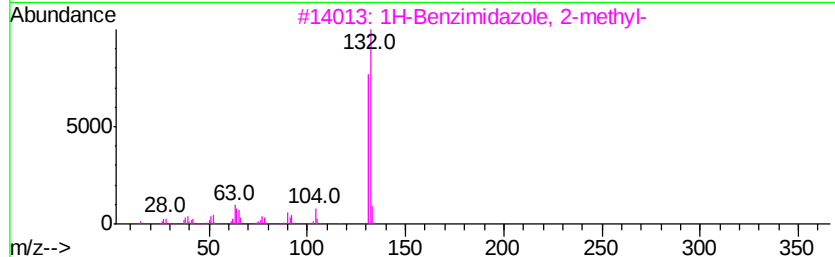
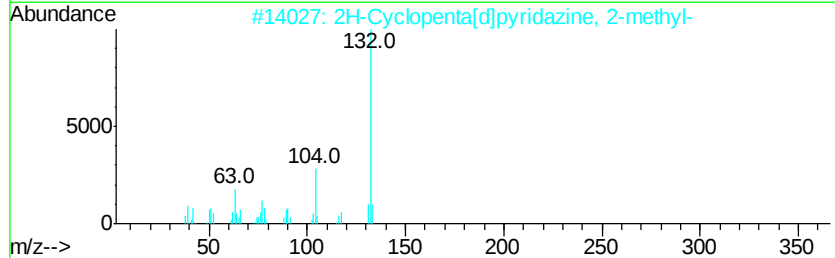
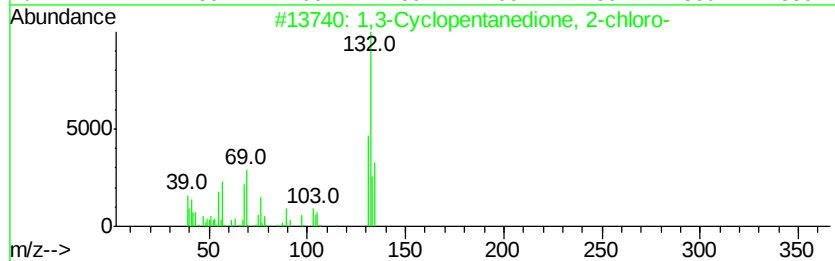
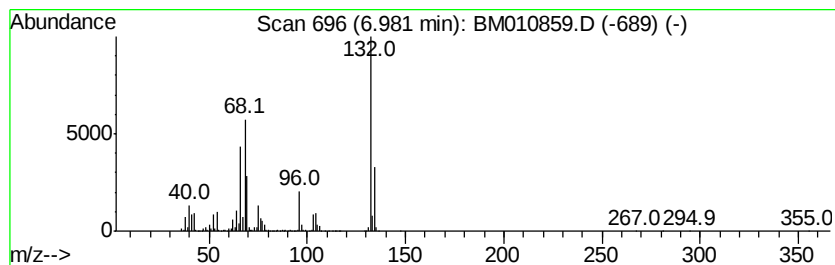
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	76.93 ng	7706670	1,4-Dichlorobenzene-d4	7.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10



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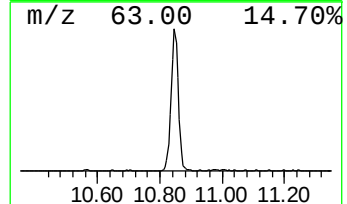
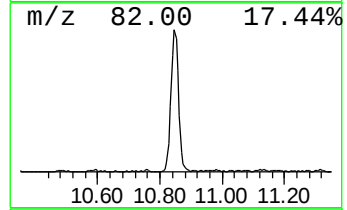
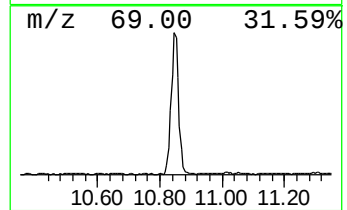
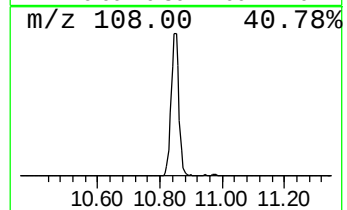
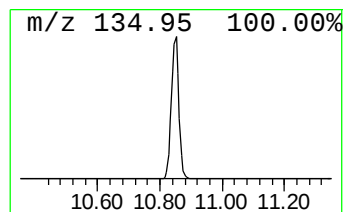
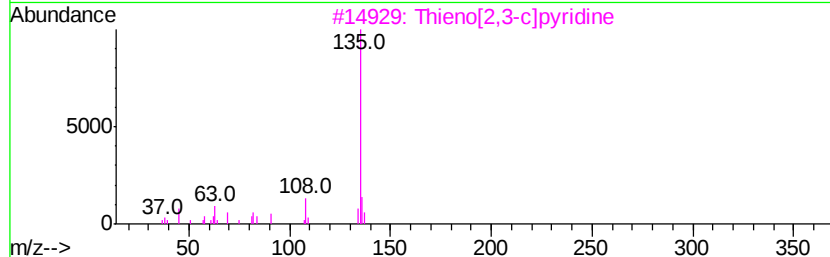
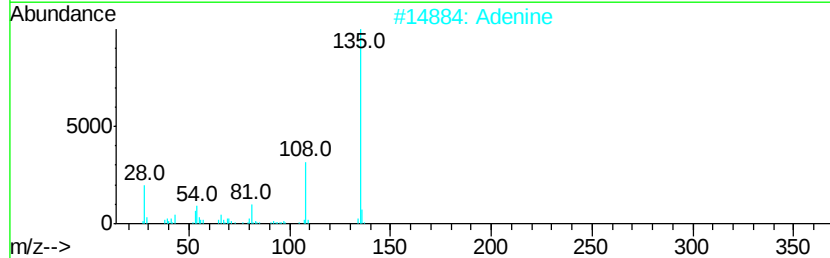
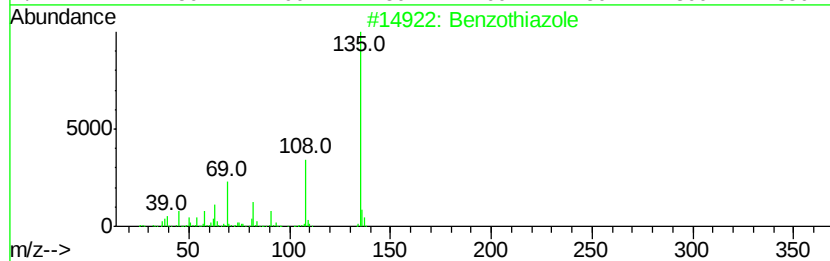
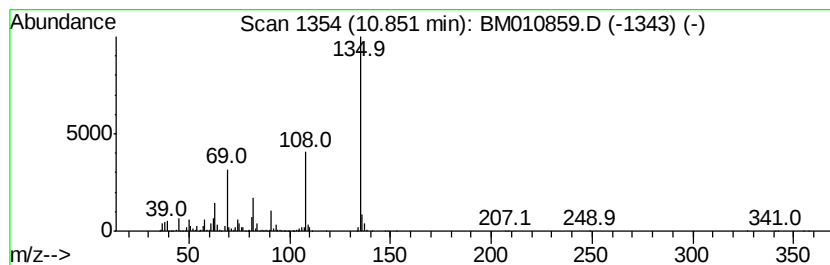
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Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	24.26 ng	3305600	Naphthalene-d8	10.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	96
2		Adenine	135	C5H5N5	000073-24-5	59
3		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	59
4		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	58
5		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	53



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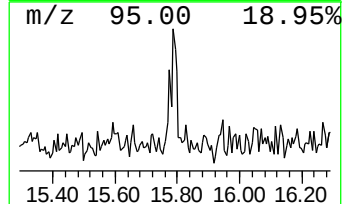
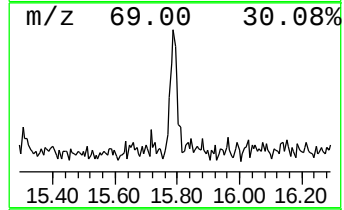
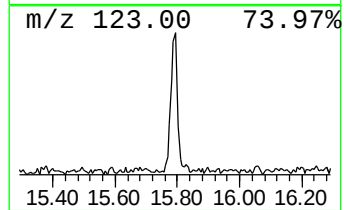
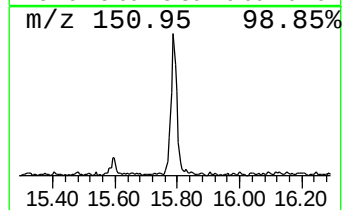
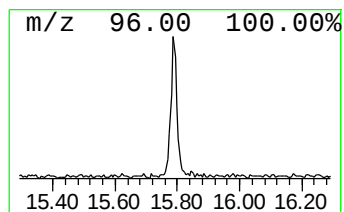
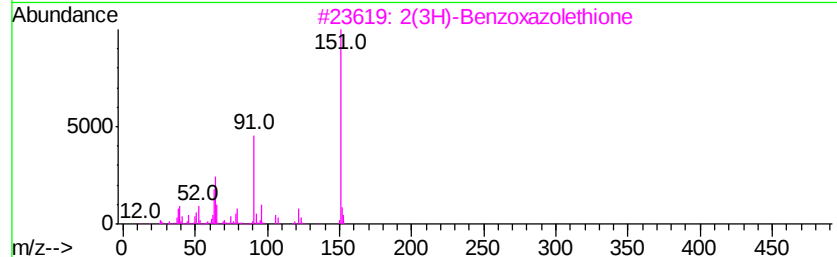
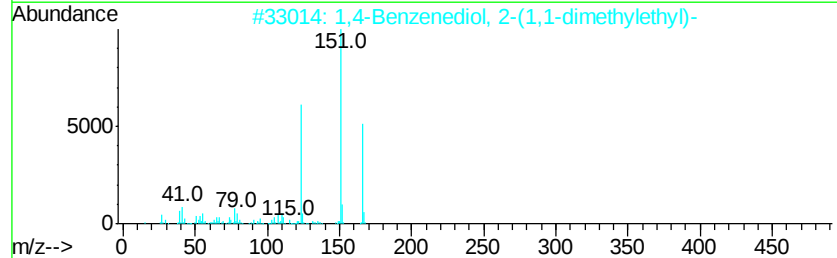
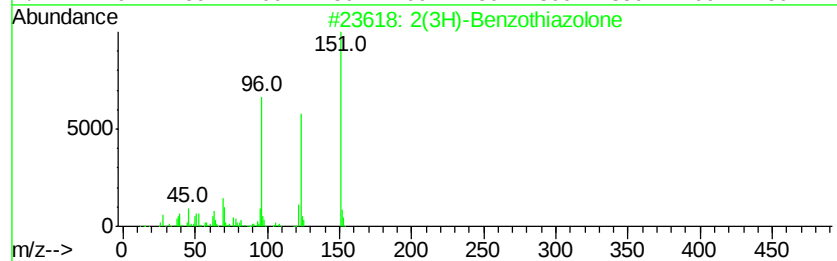
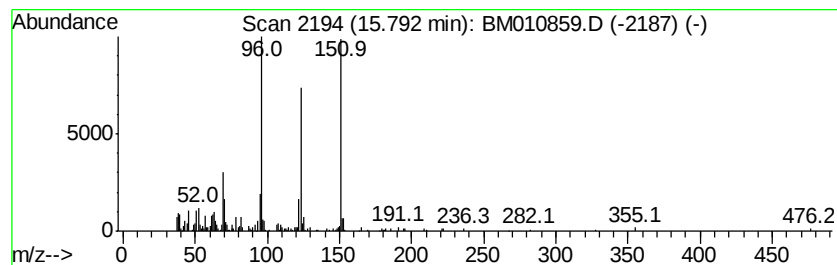
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.14 ng	440238	Phenanthrene-d10	16.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2		1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	43
3		2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	27
4		4-Methoxyvformanilide	151	C8H9NO2	023896-88-0	27
5		5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	25



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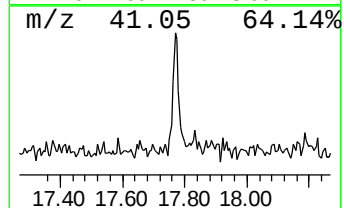
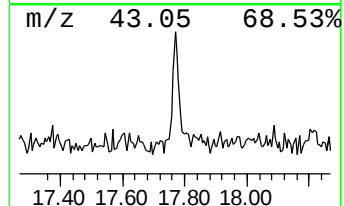
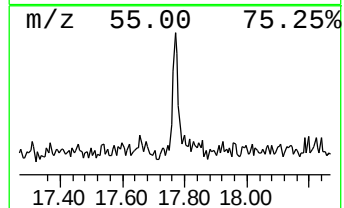
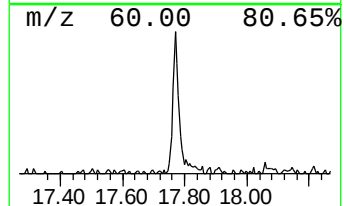
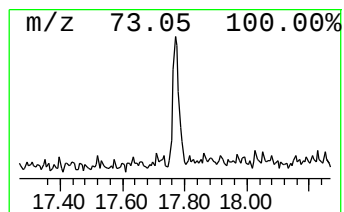
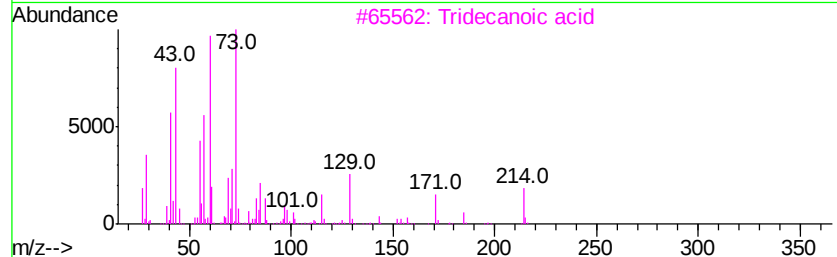
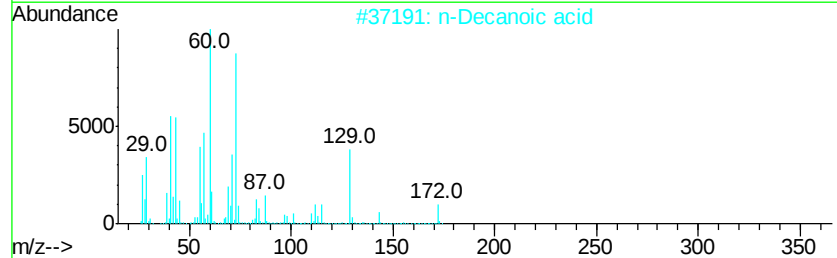
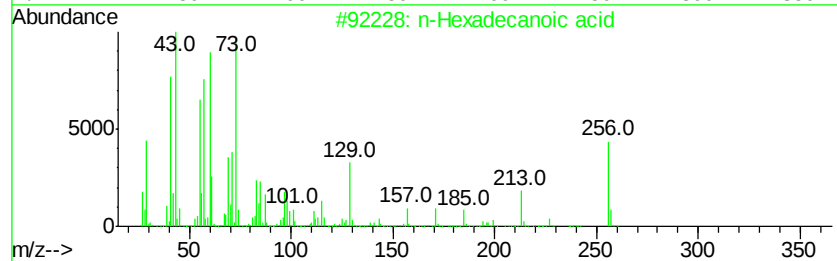
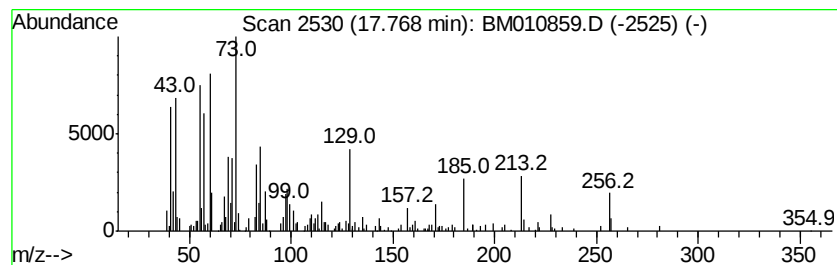
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	2.05 ng	421380	Phenanthrene-d10	16.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		n-Decanoic acid	172	C10H20O2	000334-48-5	70
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	50



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	2.6	ng	262028	1	7.45	2003530	20.0
unknown6.98	6.98	76.9	ng	7706670	1	7.45	2003530	20.0
Benzothiazole	10.85	24.3	ng	3305600	2	10.20	2725370	20.0
2(3H)-Benzothiazo...	15.79	2.1	ng	440238	4	16.85	4108260	20.0
n-Hexadecanoic acid	17.77	2.0	ng	421380	4	16.85	4108260	20.0