

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
 Data File : BF084510.D
 Acq On : 16 Jan 2016 00:41
 Operator : SJ/UM
 Sample : H1148-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13

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_F\METHODS\8270-BF123115.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	4.327	194	196	200	rBV	244468	334215	3.45%	0.523%
2	5.001	252	255	257	rBV	1662362	2267858	23.43%	3.551%
3	5.424	290	292	295	rBV	3982072	3975207	41.07%	6.225%
4	5.824	325	327	330	rBV	467866	396567	4.10%	0.621%
5	6.464	380	383	385	rBV	2513837	2727430	28.18%	4.271%
6	6.590	391	394	397	rBV	6867519	6460549	66.75%	10.117%
7	6.819	412	414	416	rBV	2065633	1702937	17.60%	2.667%
8	6.979	425	428	430	rBV	7296764	6599945	68.19%	10.335%
9	7.390	461	464	466	rBV	5440494	5647112	58.35%	8.843%
10	8.110	524	527	529	rBV	2198698	2218385	22.92%	3.474%
11	9.196	618	622	624	rBV	6664083	9678410	100.00%	15.156%
12	9.585	654	656	657	rBV	171363	151331	1.56%	0.237%
13	9.859	678	680	683	rVB2	2053220	2274401	23.50%	3.562%
14	10.293	715	718	720	rBV2	93827	187999	1.94%	0.294%
15	10.659	747	750	752	rBV	4272683	5611411	57.98%	8.787%
16	10.773	757	760	764	rVB	111964	130861	1.35%	0.205%
17	11.345	808	810	813	rBV	2546494	2181264	22.54%	3.416%
18	12.934	946	949	952	rBV	6001991	7409487	76.56%	11.603%
19	13.860	1026	1030	1036	rBV2	65767	157405	1.63%	0.246%
20	13.985	1038	1041	1043	rBV	1639392	1752912	18.11%	2.745%
21	15.403	1162	1165	1168	rBV	1264095	1540540	15.92%	2.412%
22	15.963	1206	1214	1224	rVB2	86550	453286	4.68%	0.710%

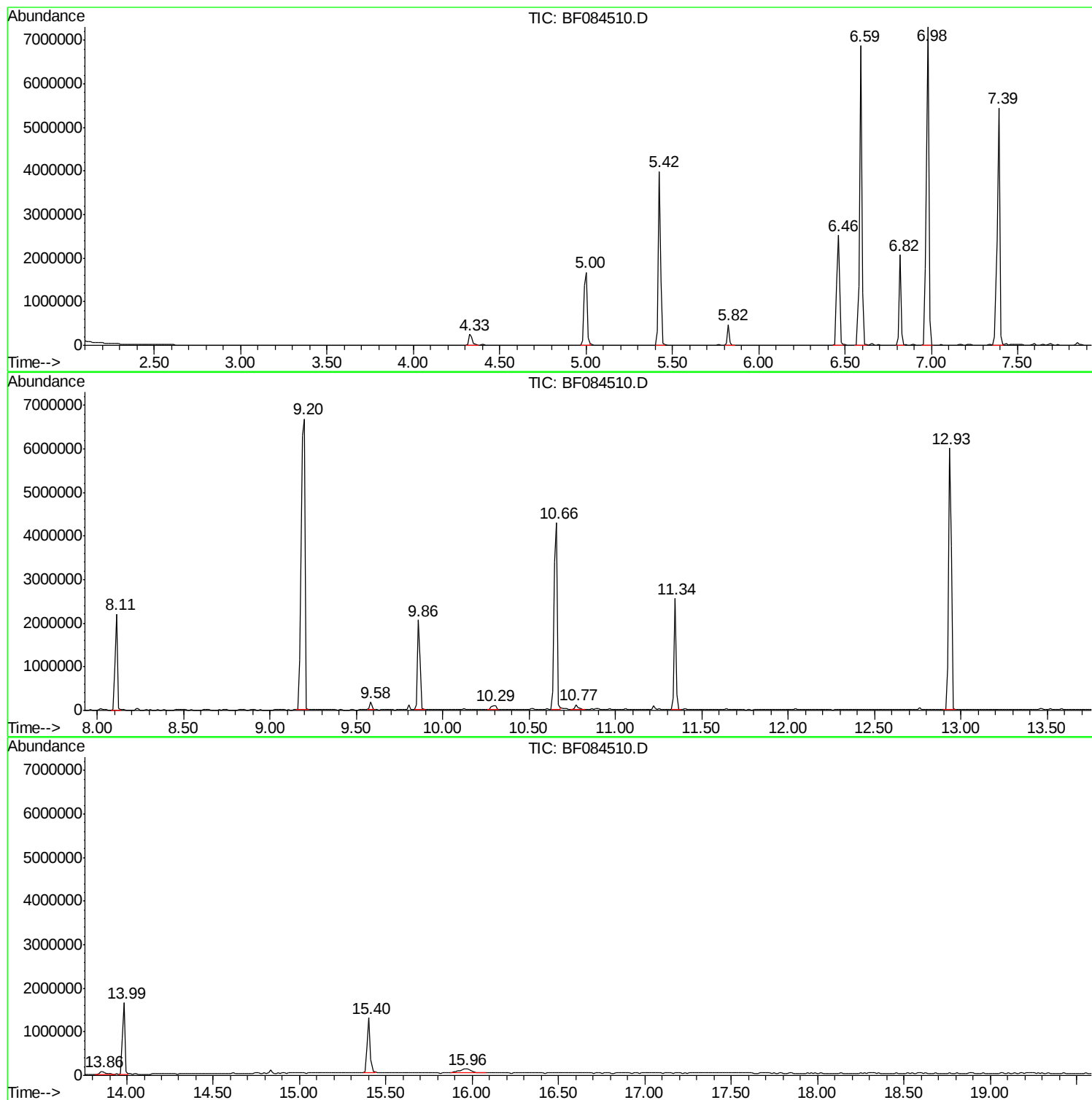
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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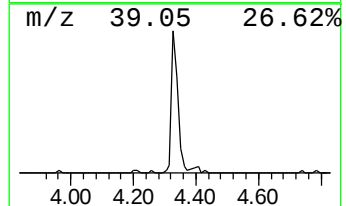
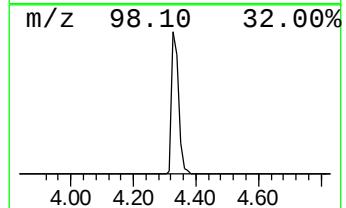
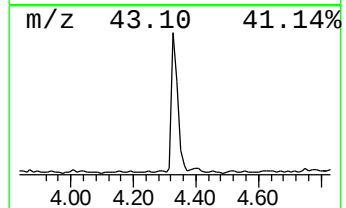
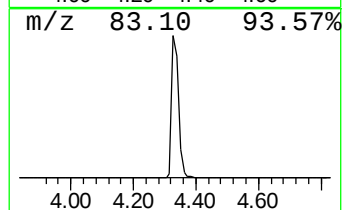
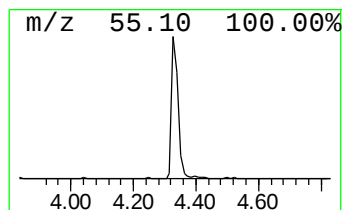
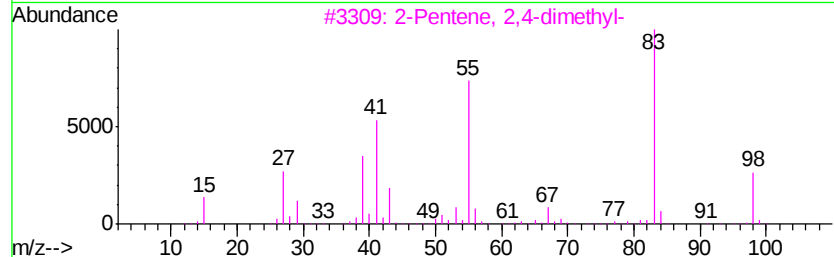
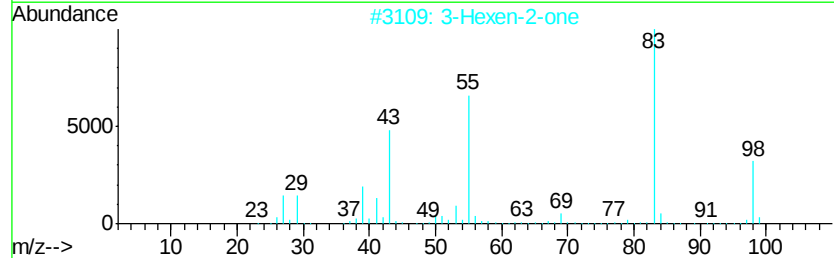
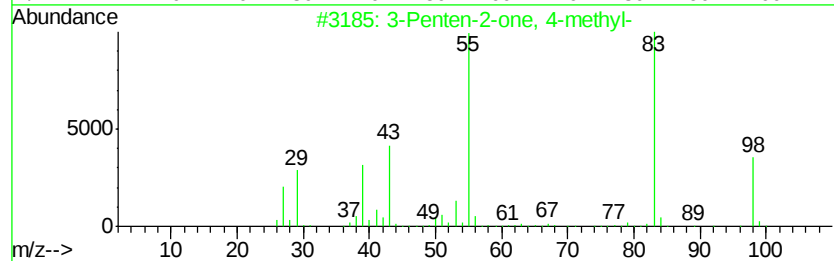
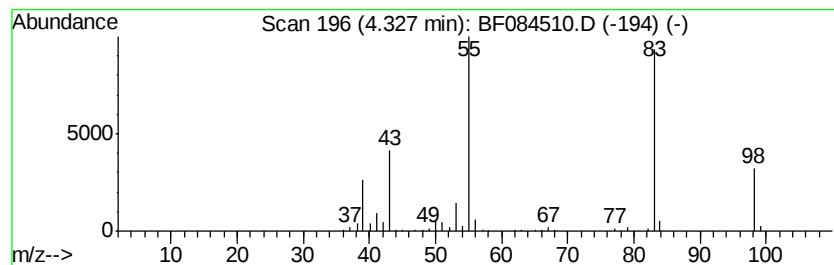
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	3.93 ng	334215	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4			Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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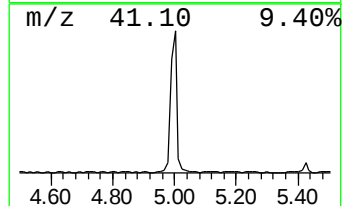
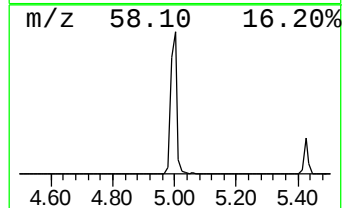
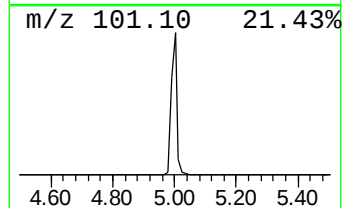
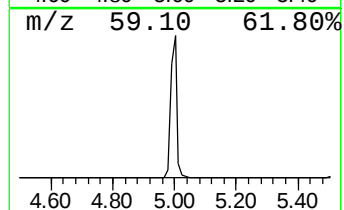
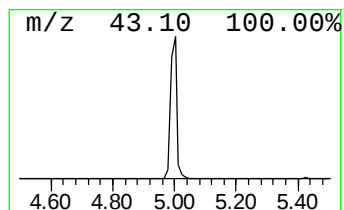
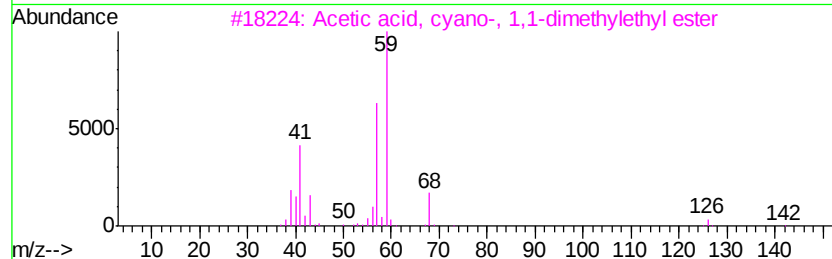
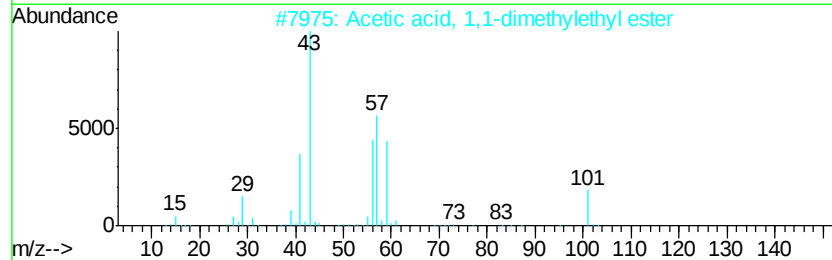
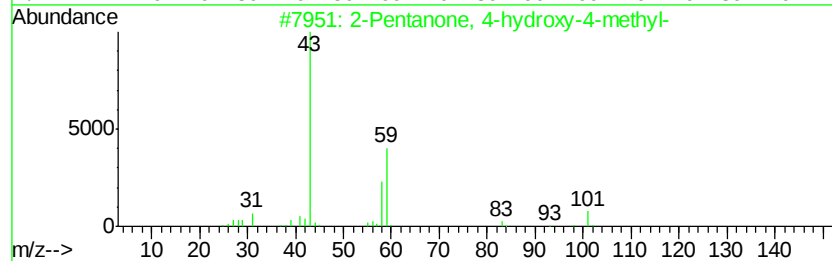
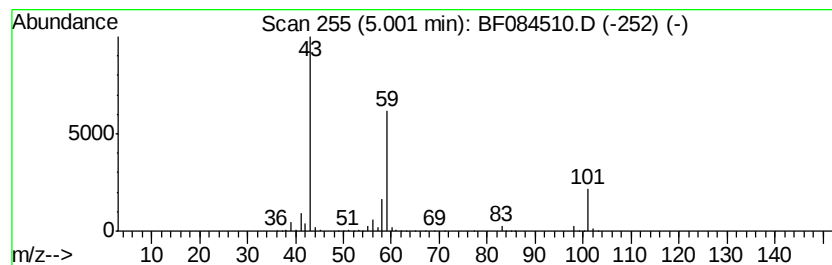
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	26.63 ng	2267860	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	9



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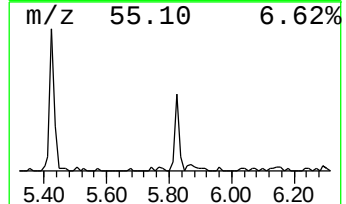
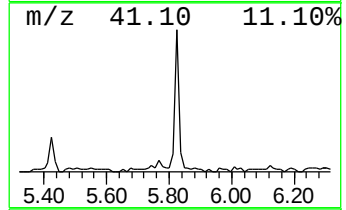
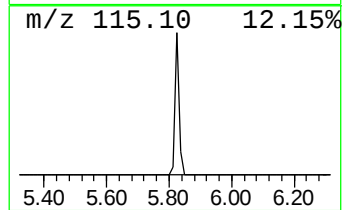
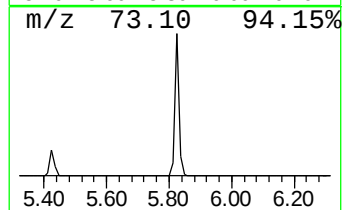
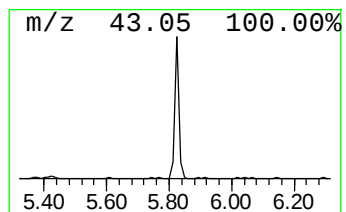
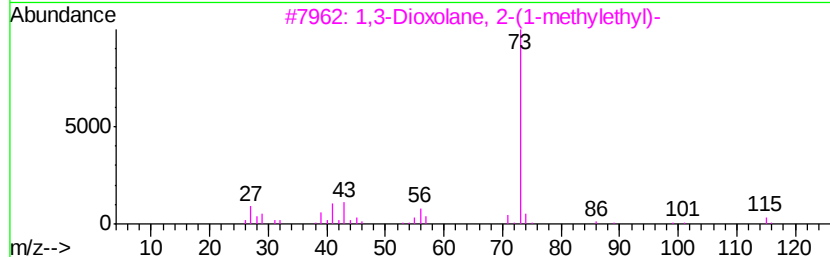
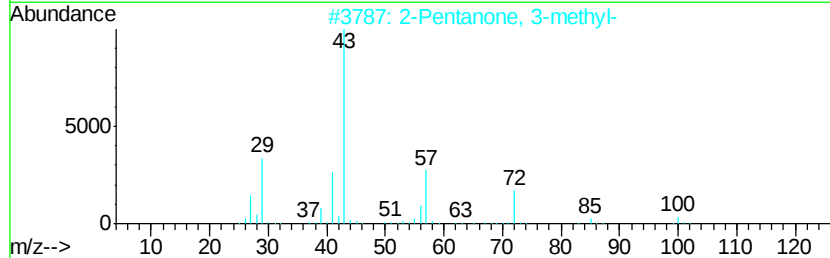
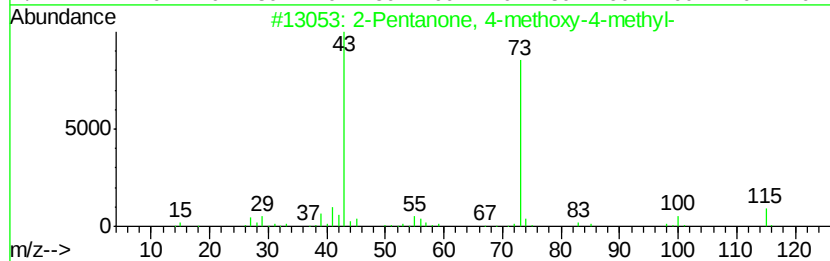
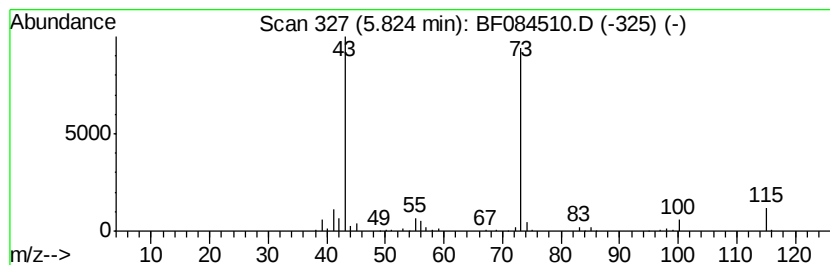
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	4.66 ng	396567	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10		
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10		
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10		
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9		



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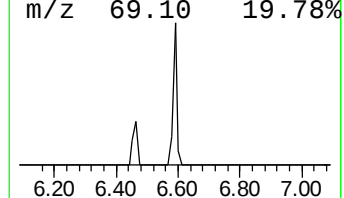
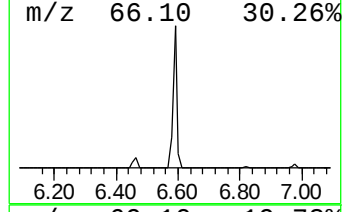
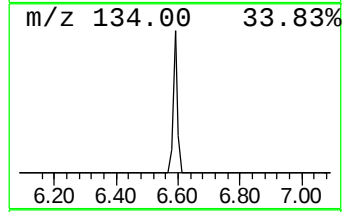
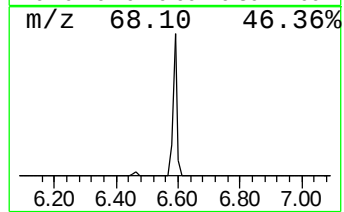
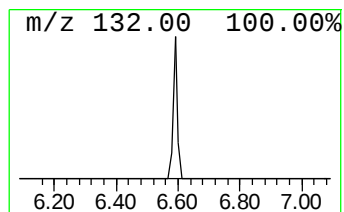
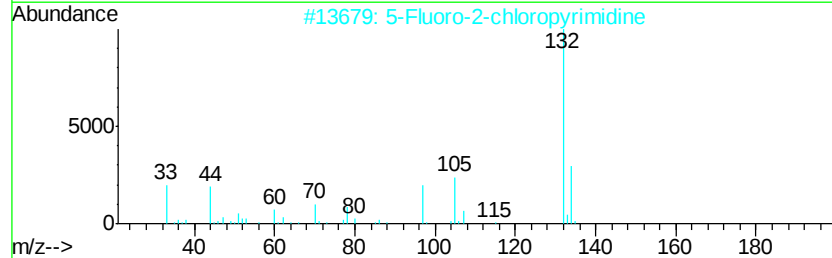
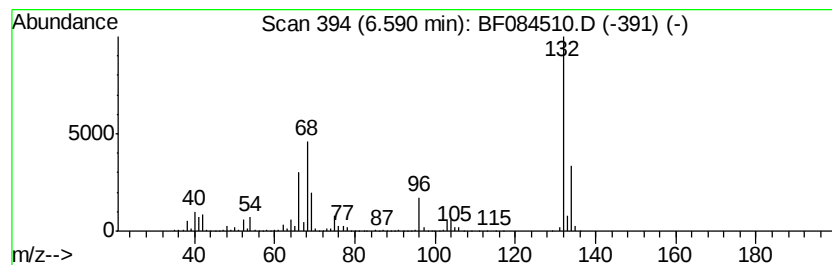
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	75.88 ng	6460550	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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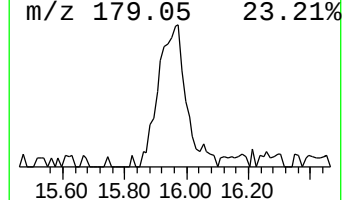
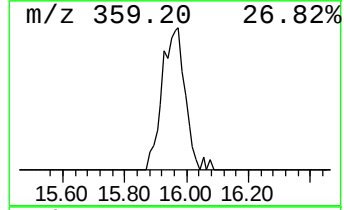
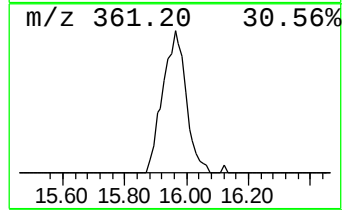
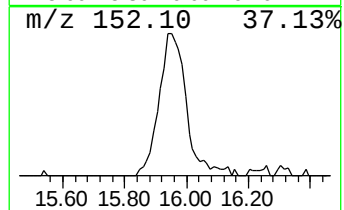
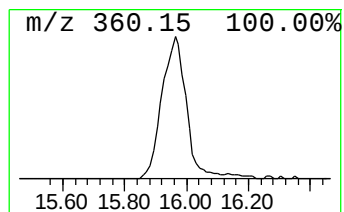
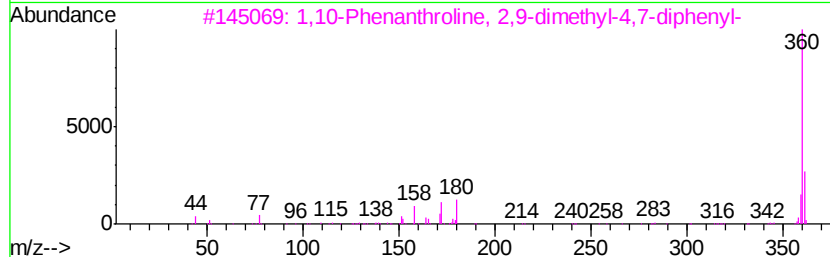
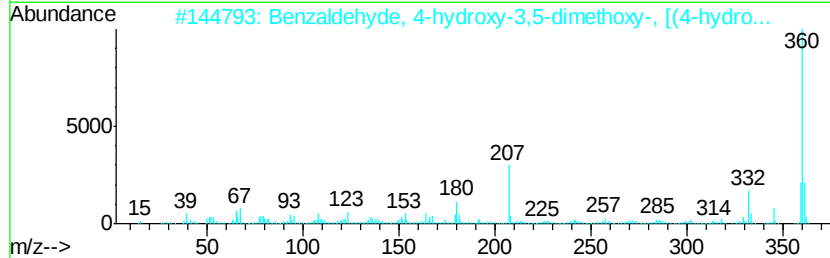
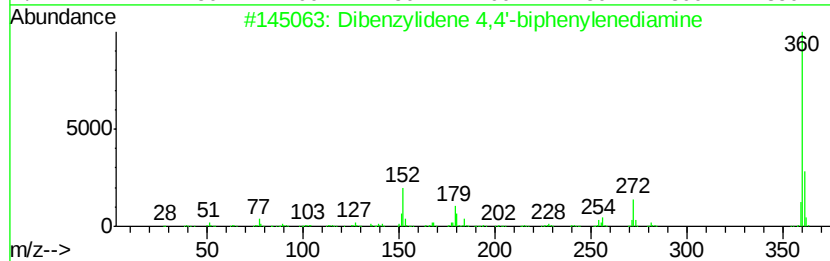
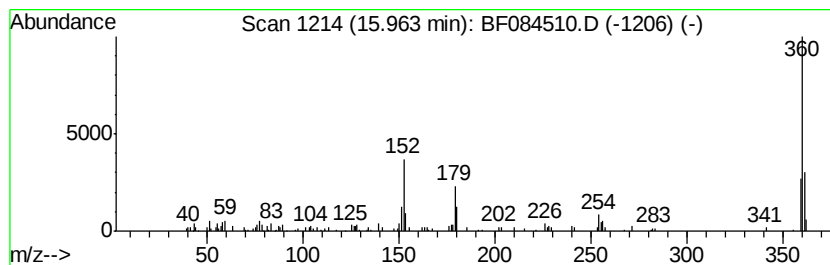
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	5.88 ng	453286	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	52
3		1,10-Phenanthroline, 2,9-dimethv...	360	C26H20N2	004733-39-5	52
4		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	49
5		Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47



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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
3-Penten-2-one, 4...	4.33	3.9	ng	334215	1	6.82	1702940	20.0
2-Pentanone, 4-hy...	5.00	26.6	ng	2267860	1	6.82	1702940	20.0
2-Pentanone, 4-me...	5.82	4.7	ng	396567	1	6.82	1702940	20.0
unknown6.59	6.59	75.9	ng	6460550	1	6.82	1702940	20.0
Dibenzylidene 4,4...	15.96	5.9	ng	453286	6	15.40	1540540	20.0