

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072423\
 Data File : BF134439.D
 Acq On : 24 Jul 2023 20:38
 Operator : CG\JU
 Sample : PB154372BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154372BL

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.481	401	407	410	rBV	1397834	1678064	63.50%	9.146%
2	5.093	504	511	529	rBV	1106984	1752607	66.32%	9.553%
3	5.487	573	578	594	rBV	1803704	1940836	73.45%	10.579%
4	5.857	638	641	647	rBV	65207	57789	2.19%	0.315%
5	6.481	742	747	750	rBV	1812842	1831242	69.30%	9.981%
6	6.834	803	807	815	rBV	464029	372489	14.10%	2.030%
7	7.398	899	903	906	rBV	1215244	1208200	45.72%	6.585%
8	8.110	1021	1024	1037	rBV	574494	489710	18.53%	2.669%
9	9.192	1203	1208	1211	rBV	2819658	2313439	87.55%	12.610%
10	9.869	1319	1323	1332	rBV	679792	541312	20.48%	2.950%
11	10.669	1454	1459	1462	rBV	1779068	1612390	61.02%	8.788%
12	11.363	1574	1577	1585	rBV	636580	583532	22.08%	3.181%
13	12.969	1845	1850	1853	rBV	2771372	2642494	100.00%	14.403%
14	14.027	2026	2030	2039	rBV	611654	557494	21.10%	3.039%
15	15.533	2280	2286	2299	rBV	383181	546744	20.69%	2.980%
16	16.004	2360	2366	2371	rBV2	22915	36559	1.38%	0.199%
17	16.533	2449	2456	2462	rBV4	22766	44283	1.68%	0.241%
18	17.162	2557	2563	2571	rVB3	15004	33850	1.28%	0.185%
19	17.480	2605	2617	2622	rBV2	21754	76815	2.91%	0.419%
20	17.904	2682	2689	2699	rVB7	12070	26877	1.02%	0.146%

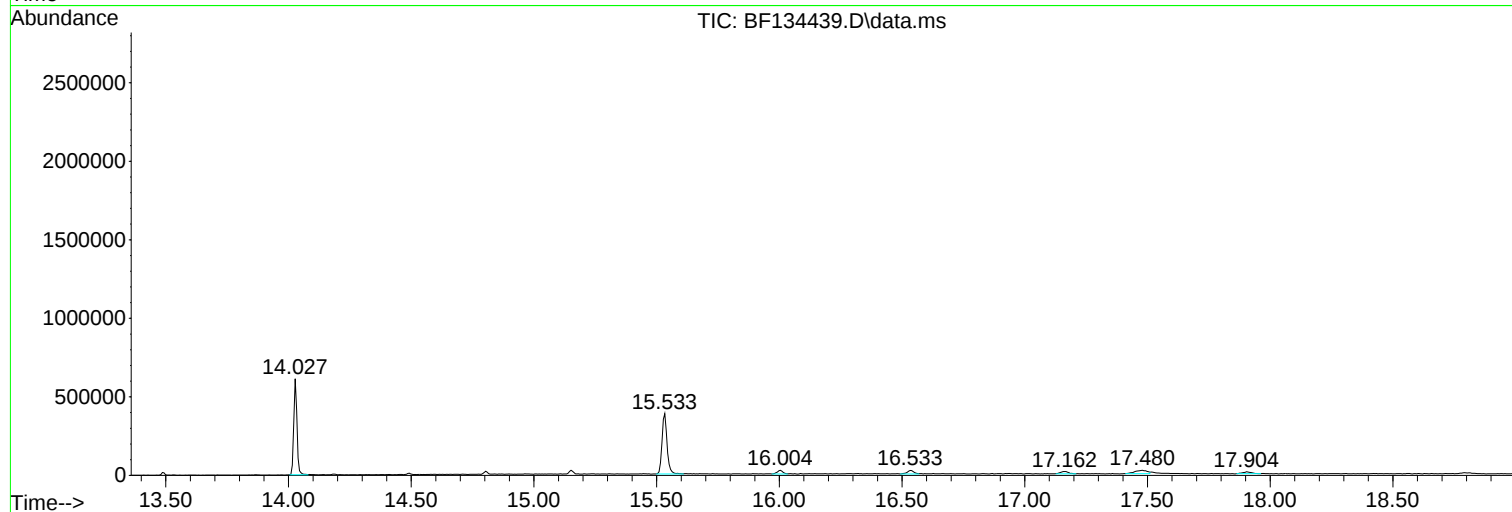
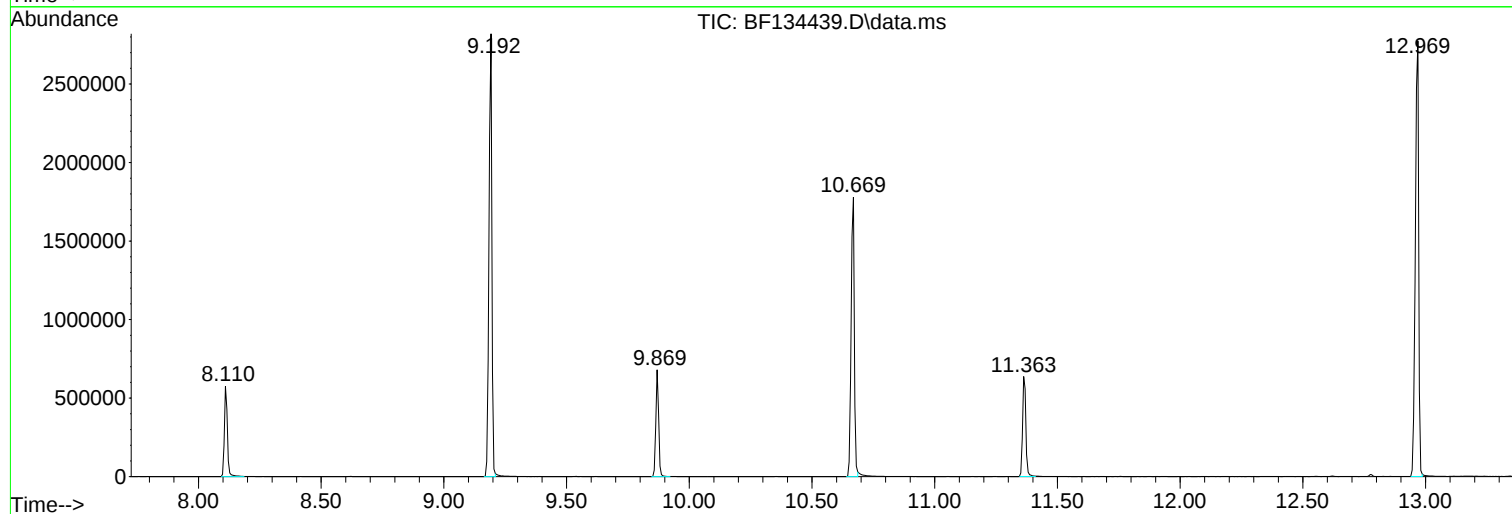
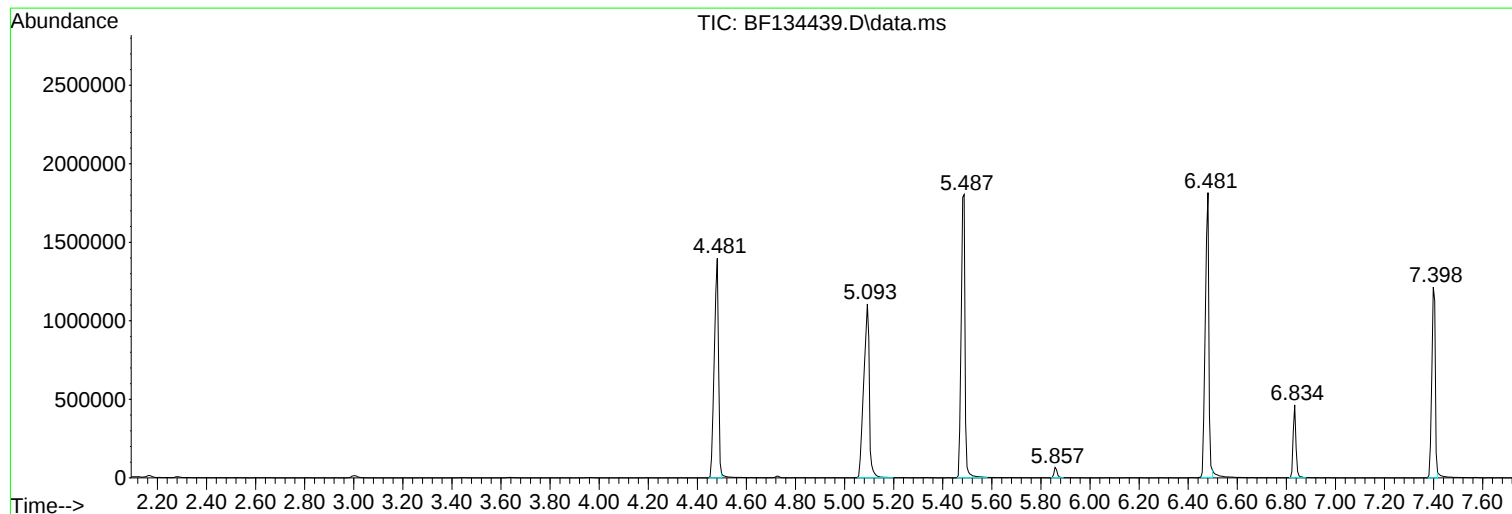
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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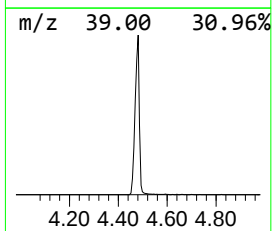
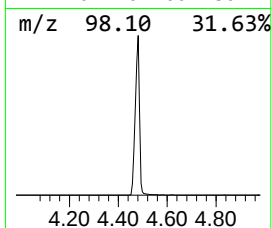
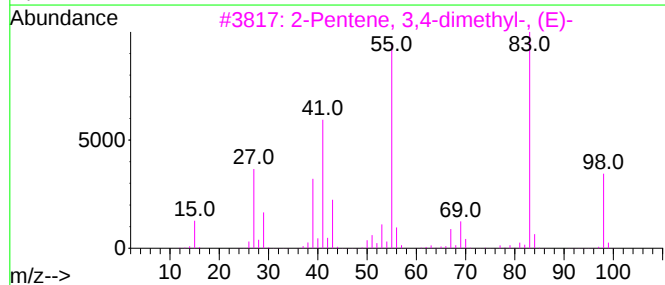
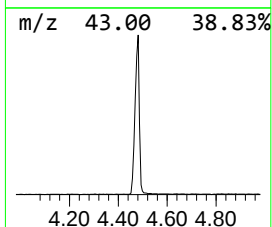
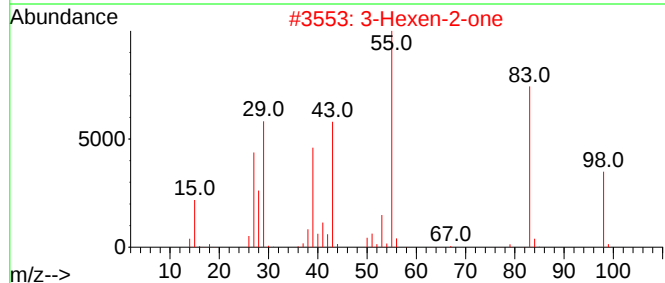
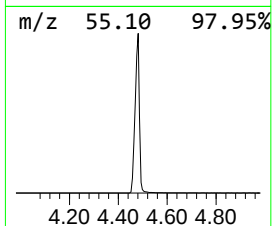
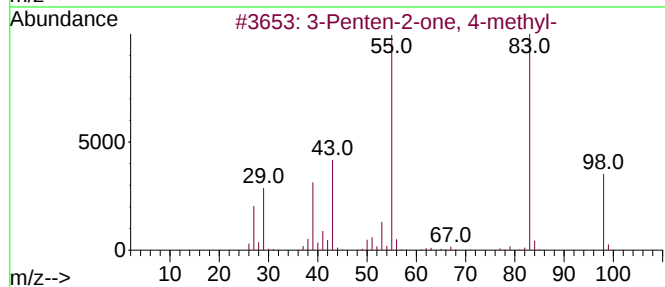
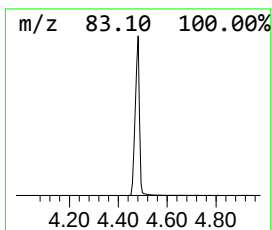
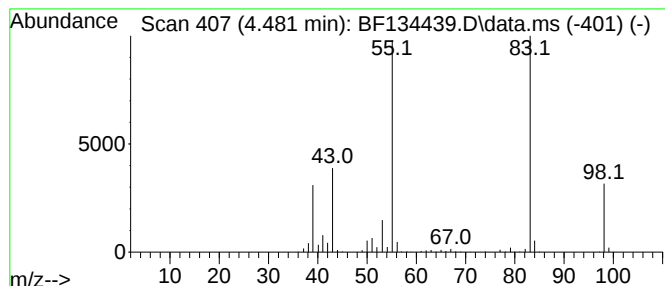
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	90.10 ng	1678060	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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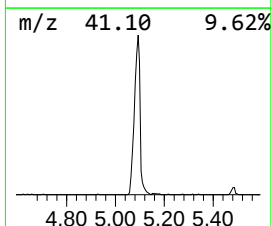
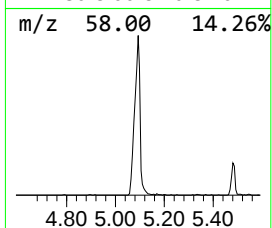
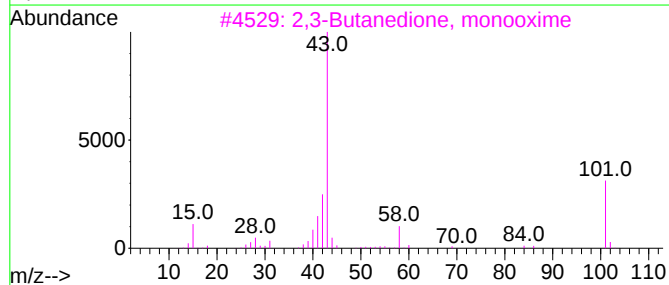
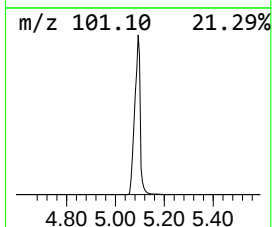
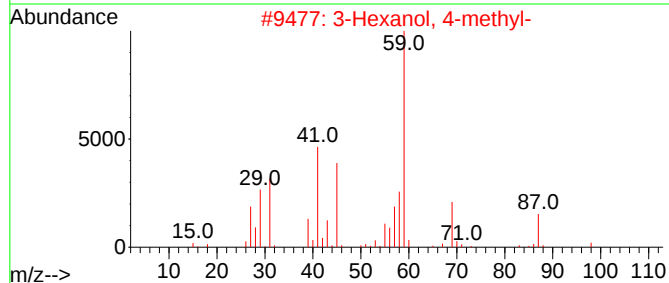
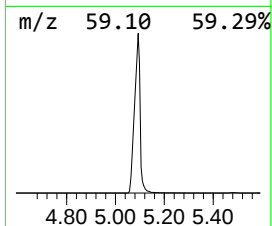
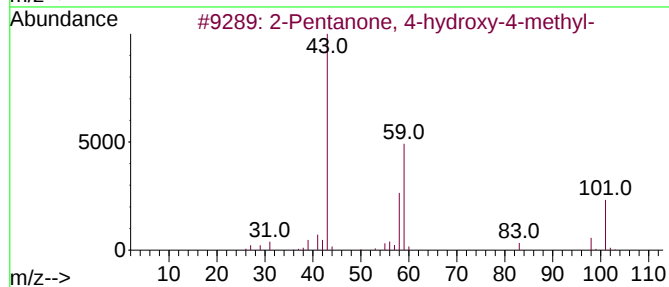
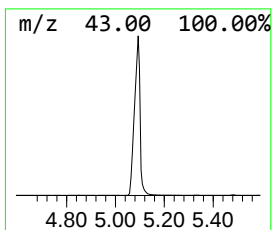
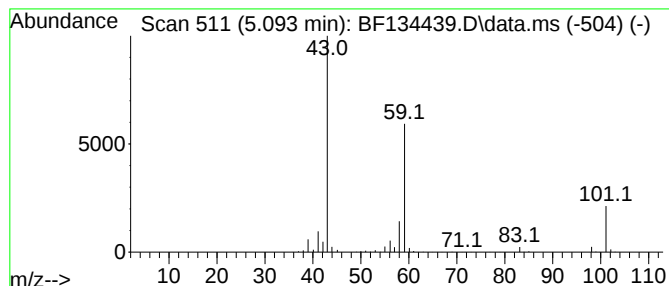
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	94.10 ng	1752610	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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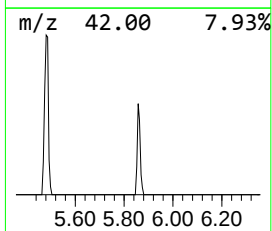
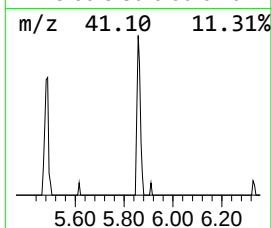
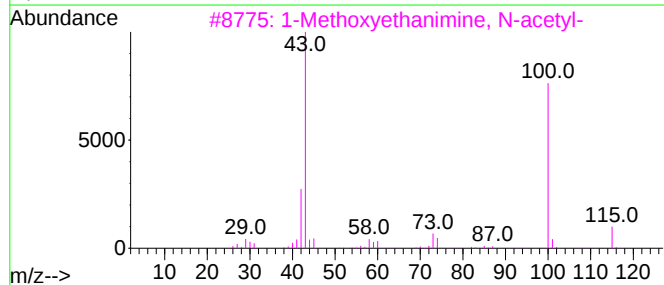
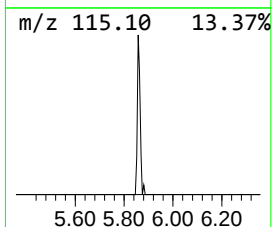
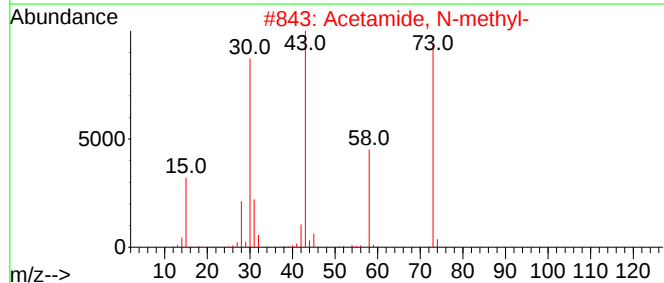
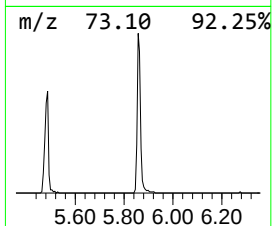
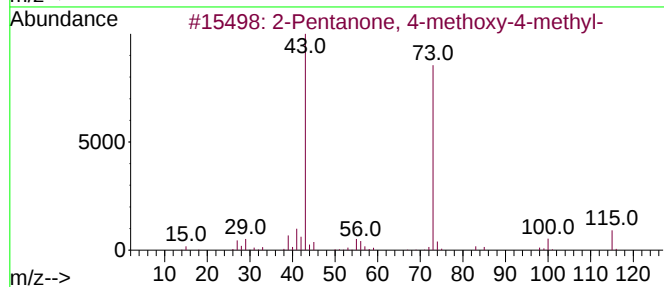
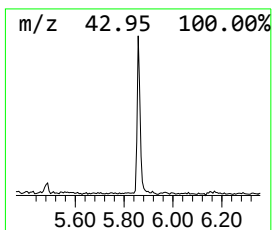
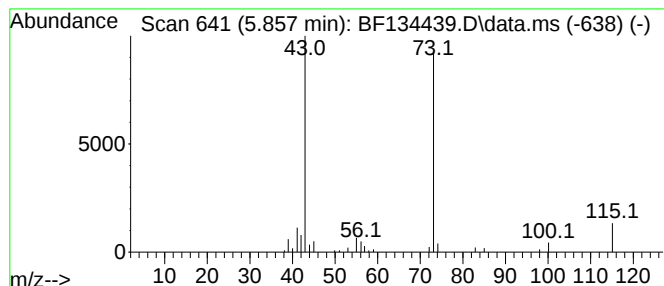
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.857	3.10 ng	57789	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	49		
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25		
4	N-Ethylformamide	73	C3H7NO	000627-45-2	12		
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9		



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ALS Vial : 3 Sample Multiplier: 1

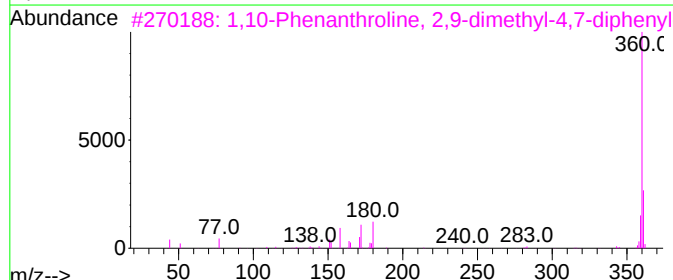
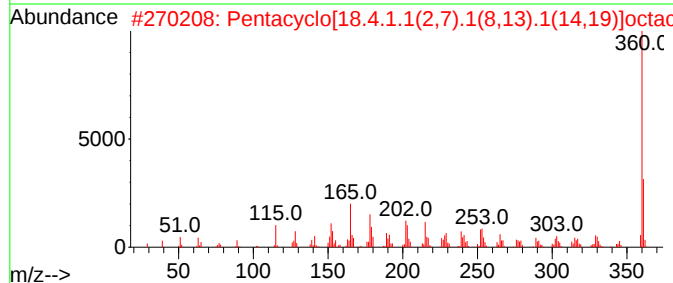
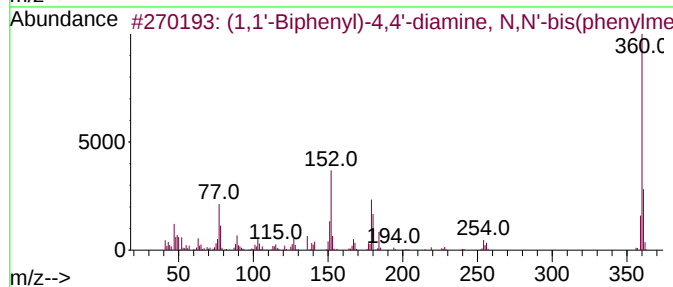
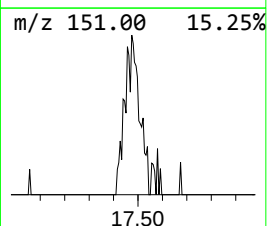
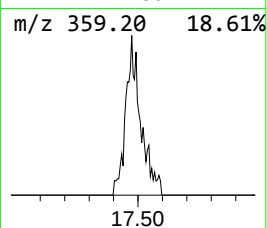
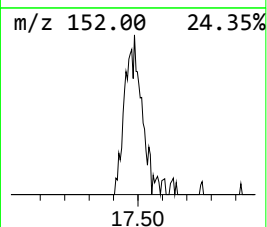
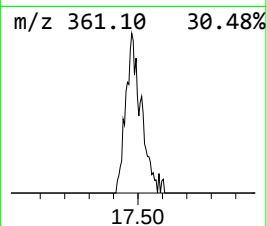
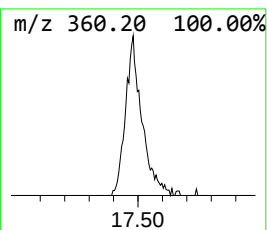
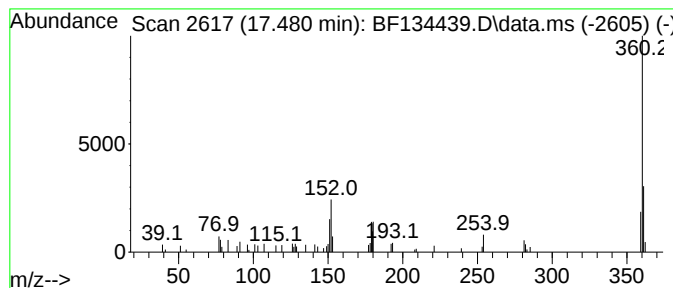
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.480	2.81 ng	76815	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N...	360	C26H20N2	006311-48-4	93
2	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	53
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	52
4	1H-isoindole-1,3(2H)-dione, 2-[5...	360	C21H16N2O4	1000398-48-8	52
5	4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	50



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.481	90.1	ng	1678060	1	6.834	372489	20.0
2-Pentanone, 4-...	5.093	94.1	ng	1752610	1	6.834	372489	20.0
2-Pentanone, 4-...	5.857	3.1	ng	57789	1	6.834	372489	20.0
(1,1'-Biphenyl)...	17.480	2.8	ng	76815	6	15.533	546744	20.0