

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
 Data File : BF092964.D
 Acq On : 15 Feb 2017 21:20
 Operator : SJ/MA
 Sample : I1837-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-1

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-BF013017.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	3.127	89	91	106	rBV	145696	303768	1.19%	0.498%
2	3.401	112	115	125	rVB	466705	964204	3.79%	1.580%
3	4.453	198	207	209	rBV	6631411	25452980	100.00%	41.721%
4	5.093	256	263	265	rBV	4595207	12060923	47.39%	19.769%
5	6.864	416	418	421	rBV	801078	894353	3.51%	1.466%
6	7.024	430	432	435	rBV	2744528	2464883	9.68%	4.040%
7	7.196	444	447	449	rBV	635977	545173	2.14%	0.894%
8	7.436	465	468	470	rBV	2260779	2122519	8.34%	3.479%
9	8.156	528	531	533	rBV	1443687	1342795	5.28%	2.201%
10	9.230	622	625	627	rBV	4019170	3778896	14.85%	6.194%
11	9.619	657	659	661	rBV	307991	362386	1.42%	0.594%
12	9.905	682	684	686	rBV	1723634	1445665	5.68%	2.370%
13	11.391	811	814	815	rBV	1599604	1495223	5.87%	2.451%
14	12.602	917	920	922	rBV	455382	524597	2.06%	0.860%
15	12.831	936	940	942	rBV2	311751	485038	1.91%	0.795%
16	12.979	950	953	955	rVB	2680326	3650596	14.34%	5.984%
17	14.019	1041	1044	1050	rVB2	1176615	1565372	6.15%	2.566%
18	14.774	1107	1110	1115	rBV2	304654	491523	1.93%	0.806%
19	15.460	1167	1170	1176	rVB	657194	1056930	4.15%	1.732%

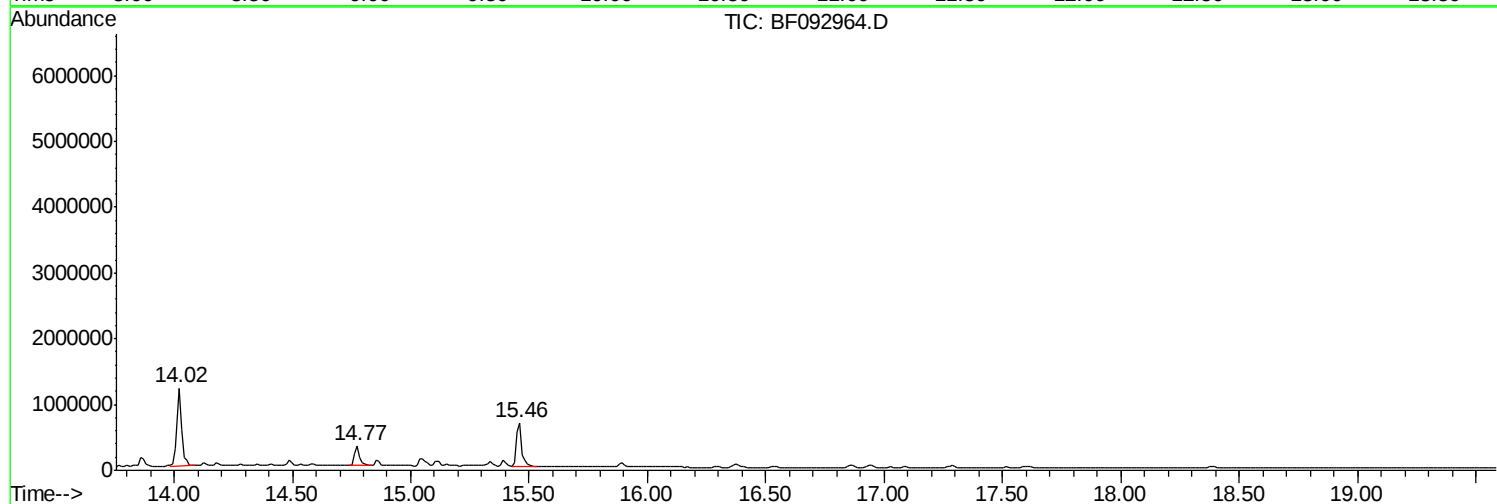
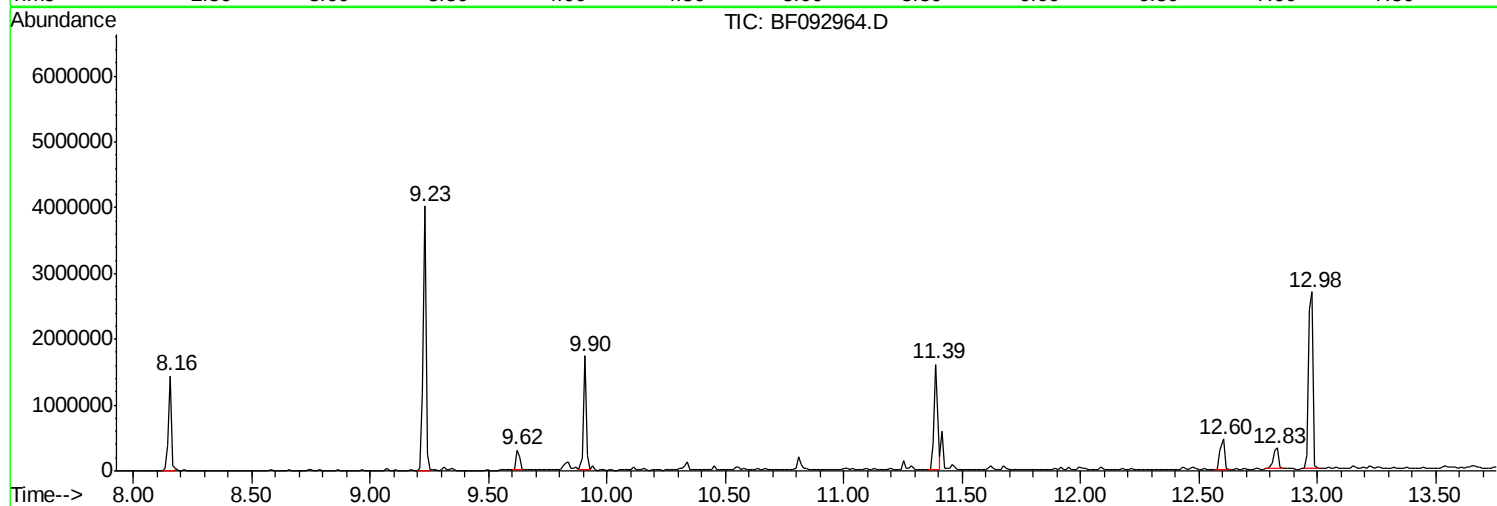
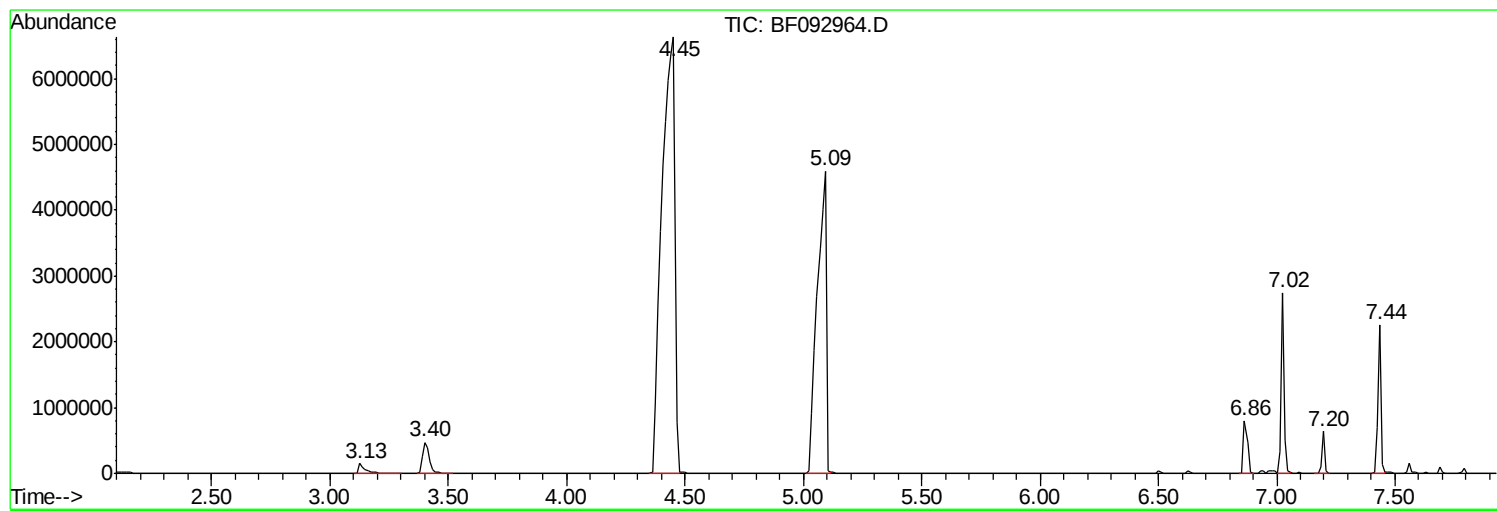
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : SJ/MA
Sample : I1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
P-1

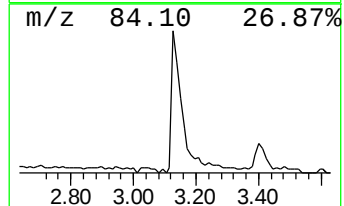
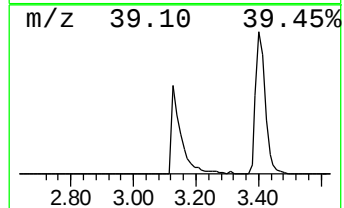
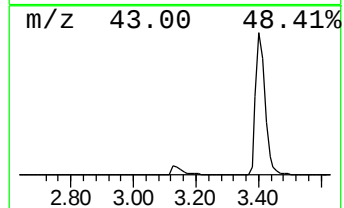
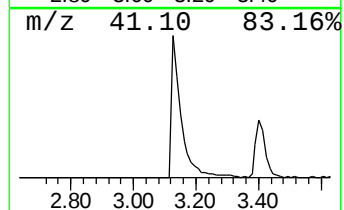
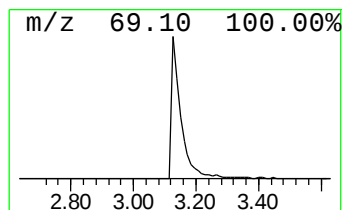
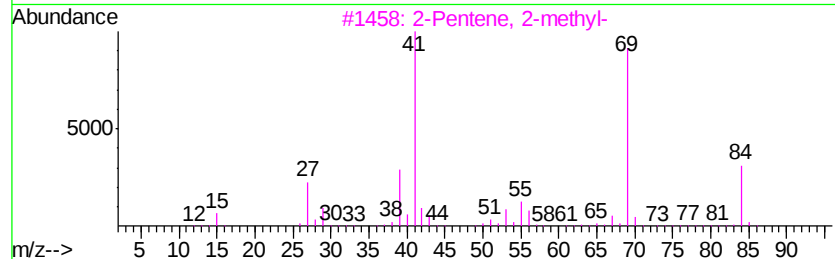
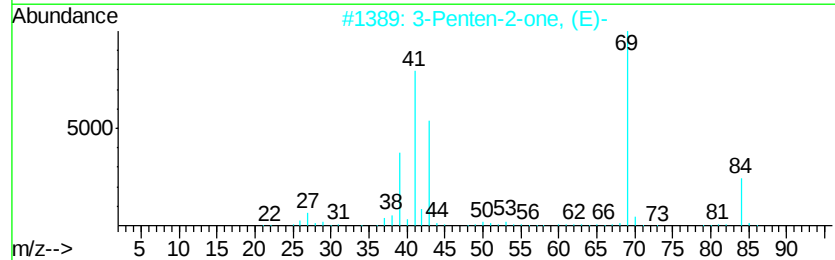
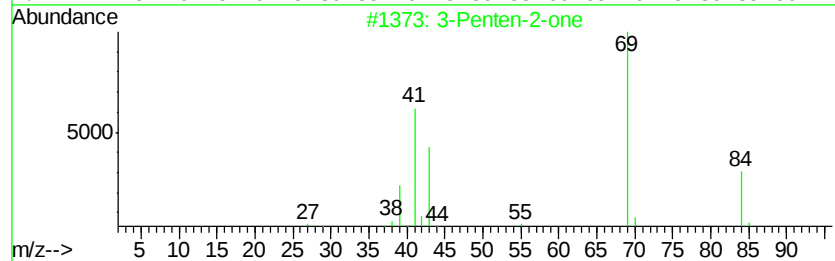
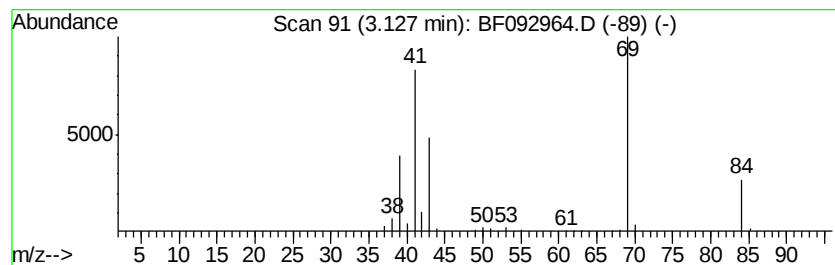
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	6.79 ng	303768	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one	84	C5H8O	000625-33-2	78
2		3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	76
3		2-Pentene, 2-methyl-	84	C6H12	000625-27-4	58
4		2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	58
5		1-Butene, 2,3-dimethyl-	84	C6H12	000563-78-0	58



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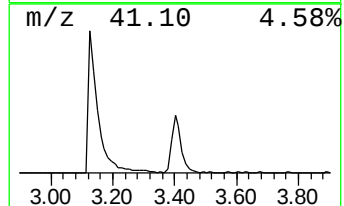
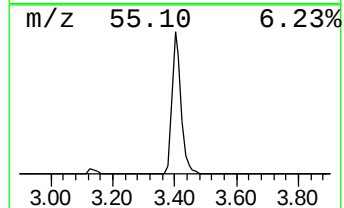
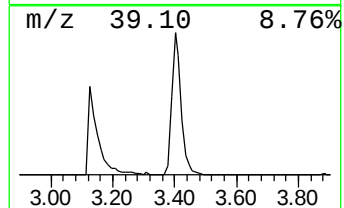
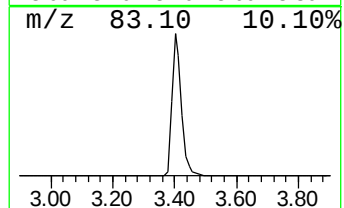
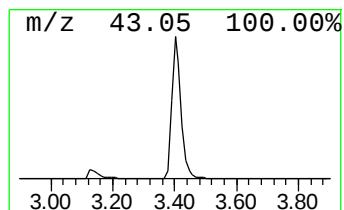
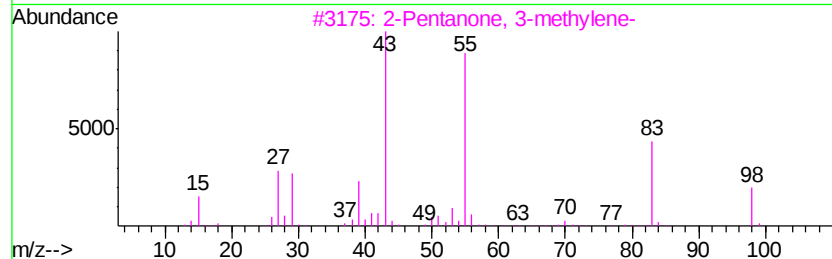
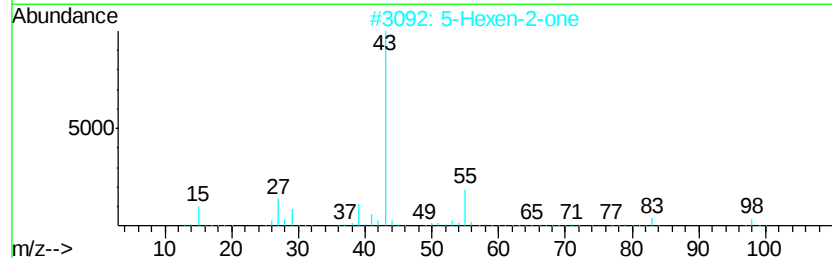
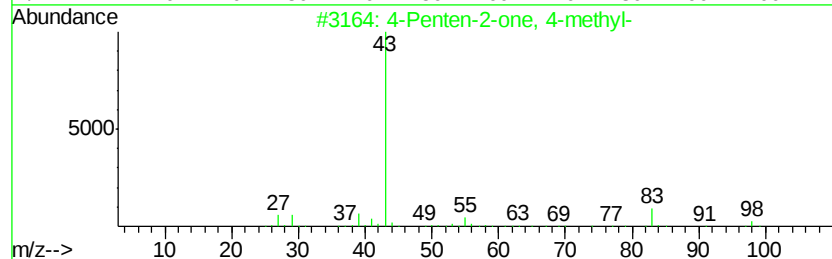
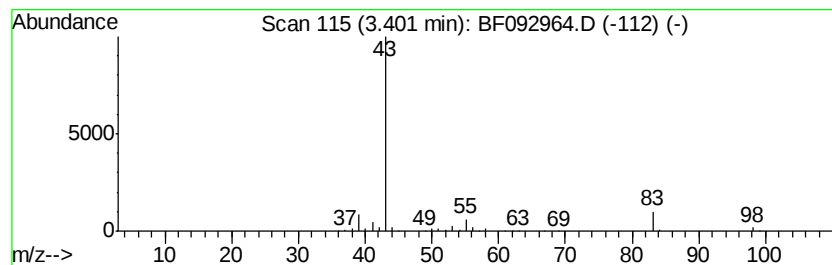
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.40	21.56 ng	964204	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			5-Hexen-2-one	98	C6H10O	000109-49-9	35
3			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9
4			4-Hexen-2-one	98	C6H10O	025659-22-7	9
5			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9



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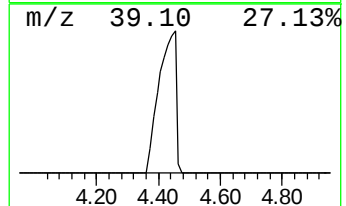
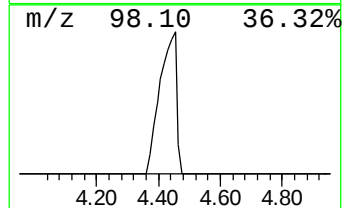
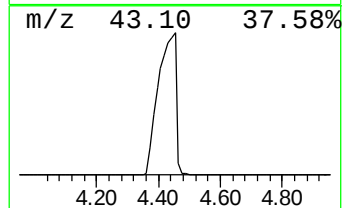
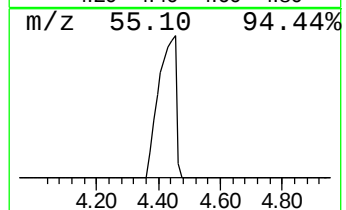
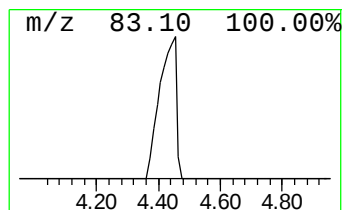
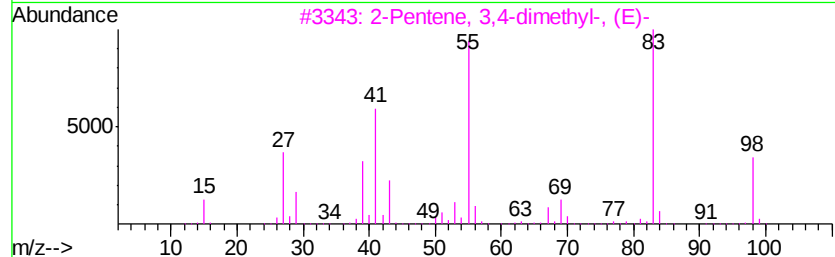
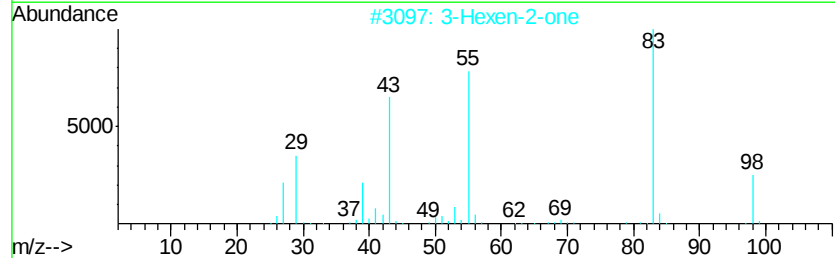
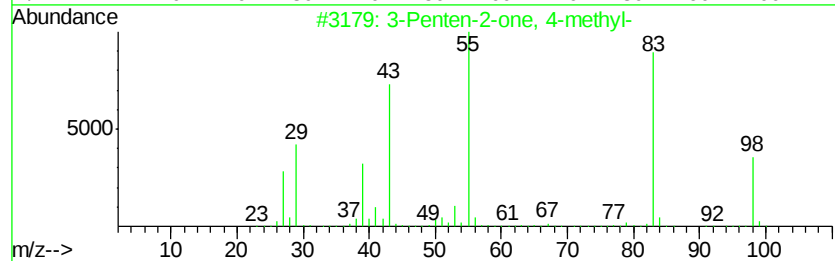
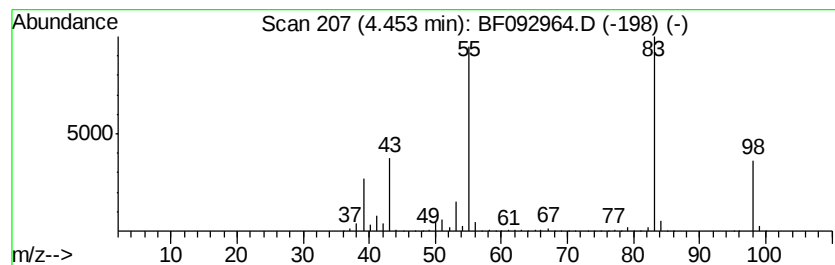
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	569.19 ng	25453000	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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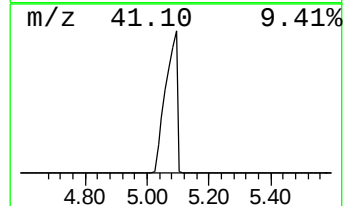
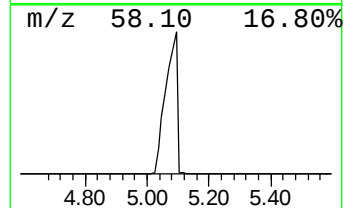
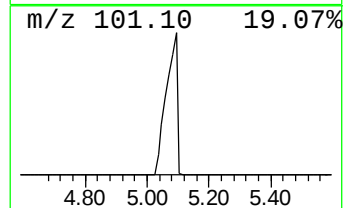
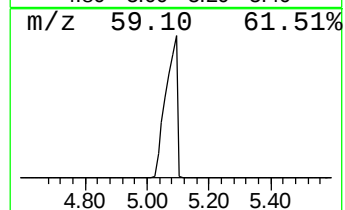
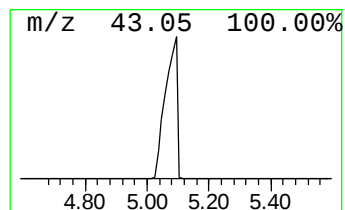
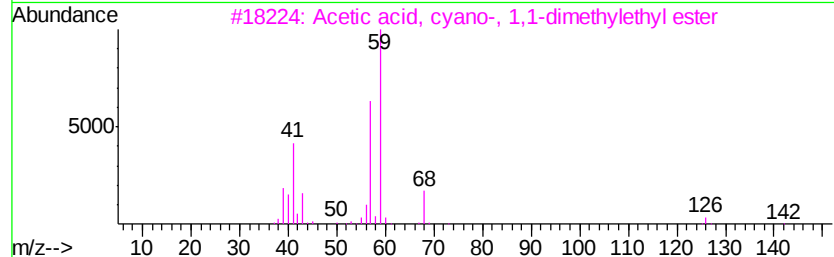
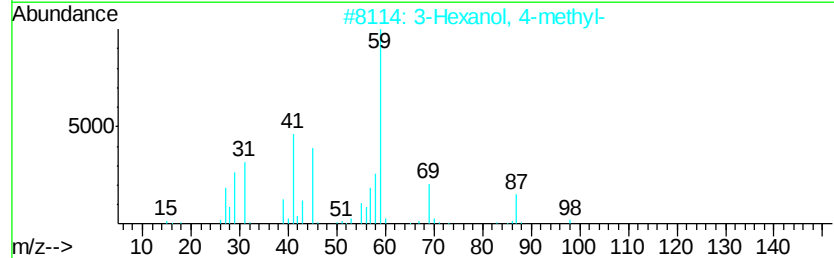
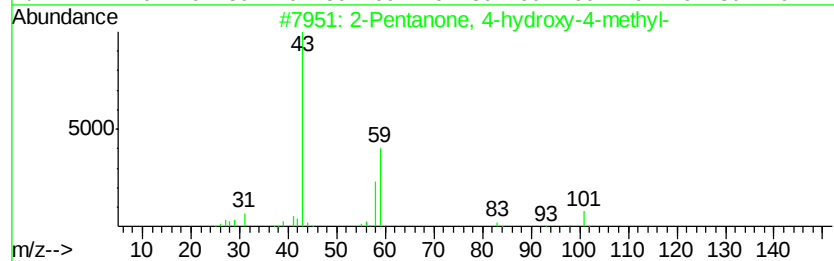
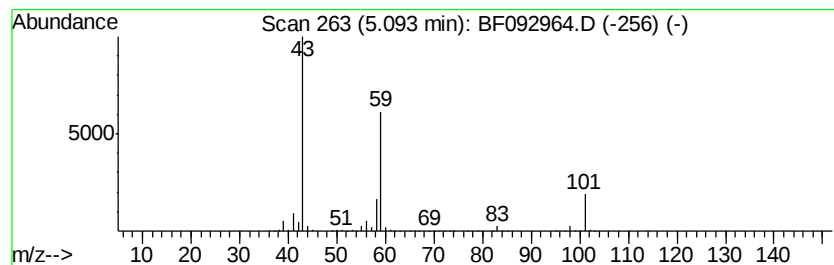
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	269.71 ng	12060900	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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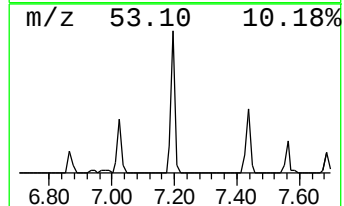
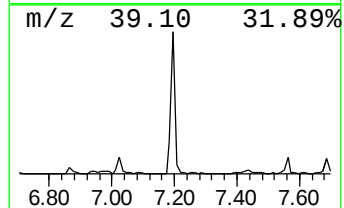
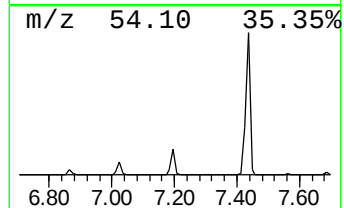
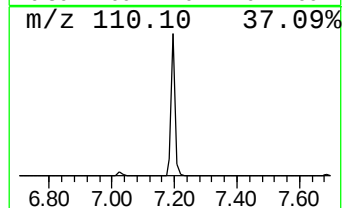
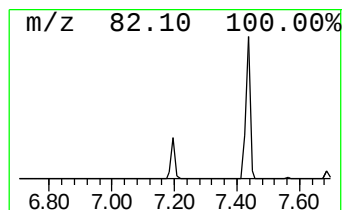
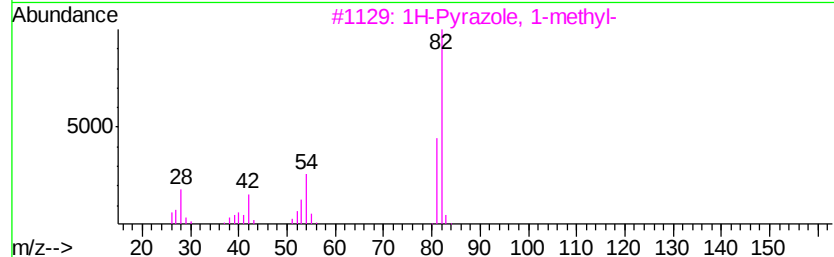
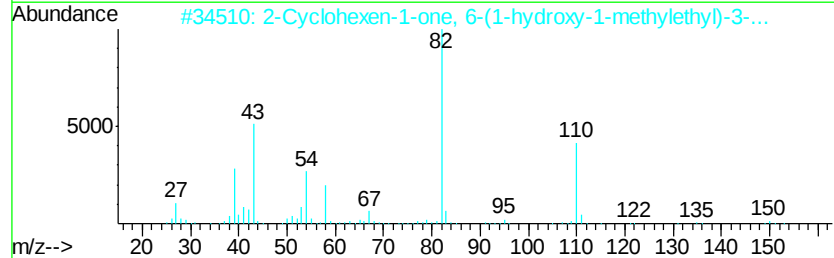
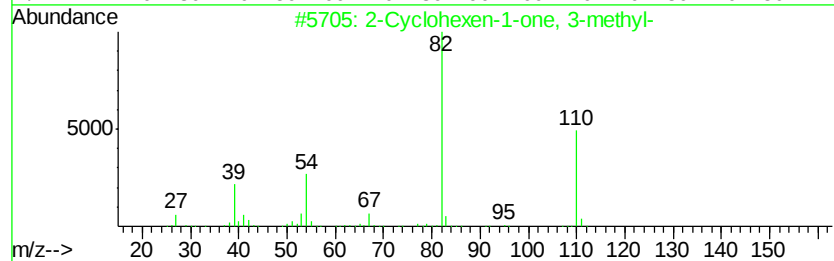
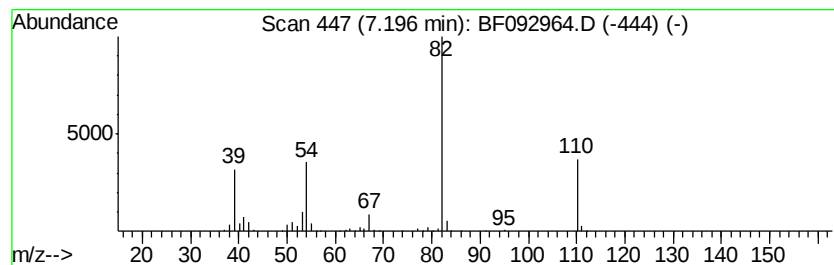
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	12.19 ng	545173	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2		2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
3		1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	53
4		Azeleoneitrile	150	C9H14N2	001675-69-0	50
5		Betazole	111	C5H9N3	000105-20-4	47



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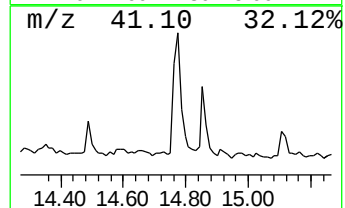
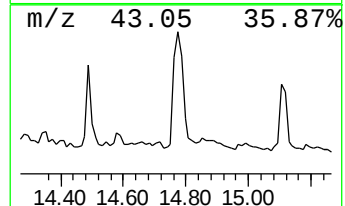
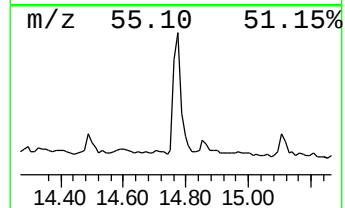
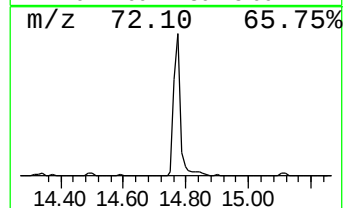
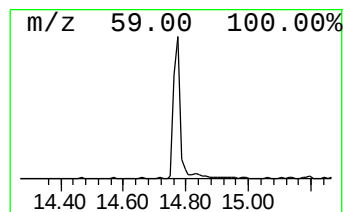
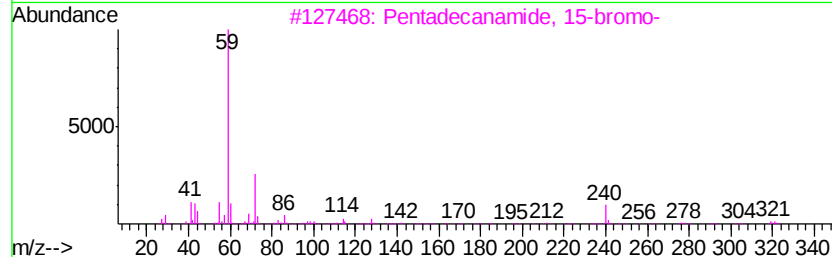
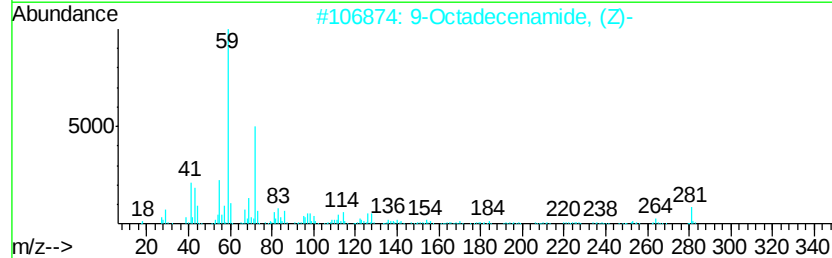
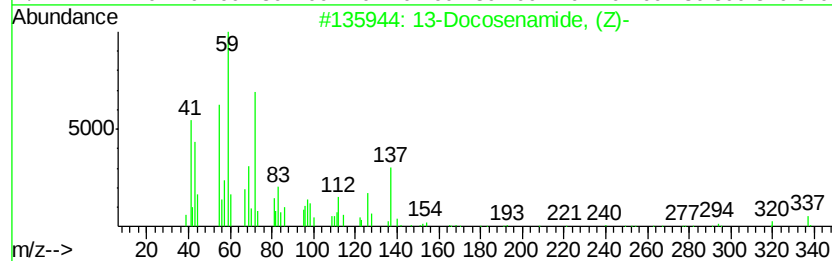
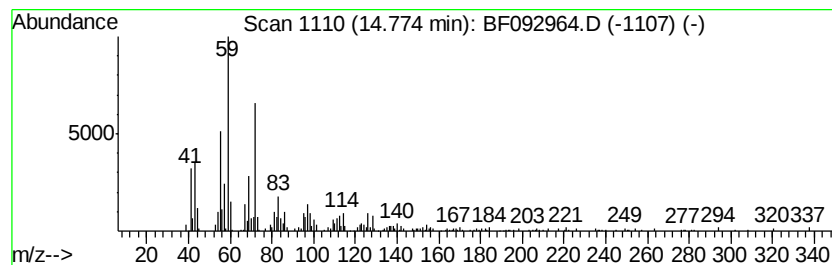
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	9.30 ng	491523	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
4		Dodecanamide	199	C12H25NO	001120-16-7	50
5		Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
Data File : BF092964.D
Acq On : 15 Feb 2017 21:20
Operator : SJ/MA
Sample : I1837-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one	3.13	6.8	ng	303768	1	6.86	894353	20.0
4-Penten-2-one, 4...	3.40	21.6	ng	964204	1	6.86	894353	20.0
3-Penten-2-one, 4...	4.45	569.2	ng	25453000	1	6.86	894353	20.0
2-Pentanone, 4-hy...	5.09	269.7	ng	12060900	1	6.86	894353	20.0
2-Cyclohexen-1-on...	7.20	12.2	ng	545173	1	6.86	894353	20.0
13-Docosenamide, ...	14.77	9.3	ng	491523	6	15.46	1056930	20.0