

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052616\
 Data File : BF087421.D
 Acq On : 26 May 2016 22:26
 Operator : UM/SJ
 Sample : H3240-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HSR-WC-46-052316

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-BF052316.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	2.055	39	41	56	rVB	113037	215401	5.02%	0.617%
2	2.650	90	93	99	rBV	180831	389635	9.08%	1.117%
3	3.781	189	192	211	rBV	638634	1523341	35.49%	4.366%
4	4.204	226	229	236	rVB	44299	87484	2.04%	0.251%
5	4.799	279	281	300	rBV	108384	329815	7.68%	0.945%
6	5.439	334	337	358	rBV	1881143	3684065	85.82%	10.559%
7	7.062	476	479	485	rBV	2196310	3202182	74.60%	9.178%
8	7.165	485	488	501	rVB	2941545	4003301	93.26%	11.474%
9	7.507	515	518	523	rBV	563759	760997	17.73%	2.181%
10	7.736	535	538	541	rBV	2040081	2880184	67.09%	8.255%
11	8.056	564	566	573	rBV2	40213	100007	2.33%	0.287%
12	8.422	595	598	600	rBV	1825809	2511053	58.50%	7.197%
13	9.531	692	695	716	rBV	653953	972902	22.66%	2.788%
14	11.314	847	851	854	rBV	2981676	4185278	97.50%	11.996%
15	12.365	940	943	955	rBV	544157	904464	21.07%	2.592%
16	13.657	1053	1056	1079	rBV	1922669	2841169	66.19%	8.143%
17	14.765	1150	1153	1162	rBV	647439	1033004	24.06%	2.961%
18	17.120	1356	1359	1362	rBV	3537672	4292726	100.00%	12.304%
19	18.457	1474	1476	1487	rBV	631681	820061	19.10%	2.350%
20	20.149	1621	1624	1629	rBV2	69588	153050	3.57%	0.439%

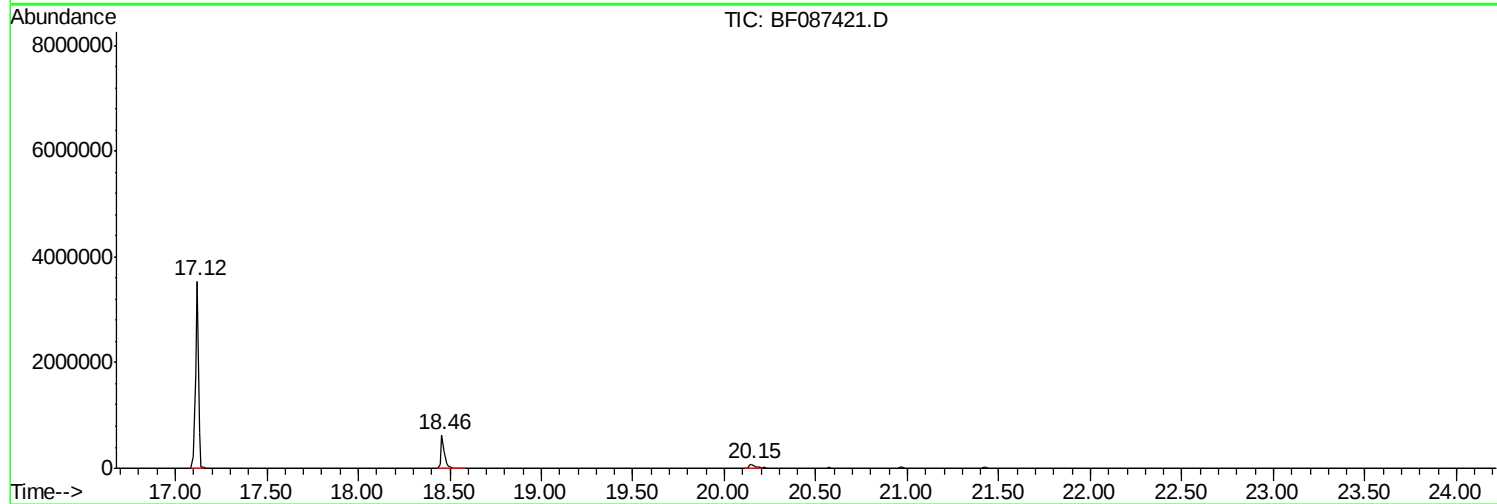
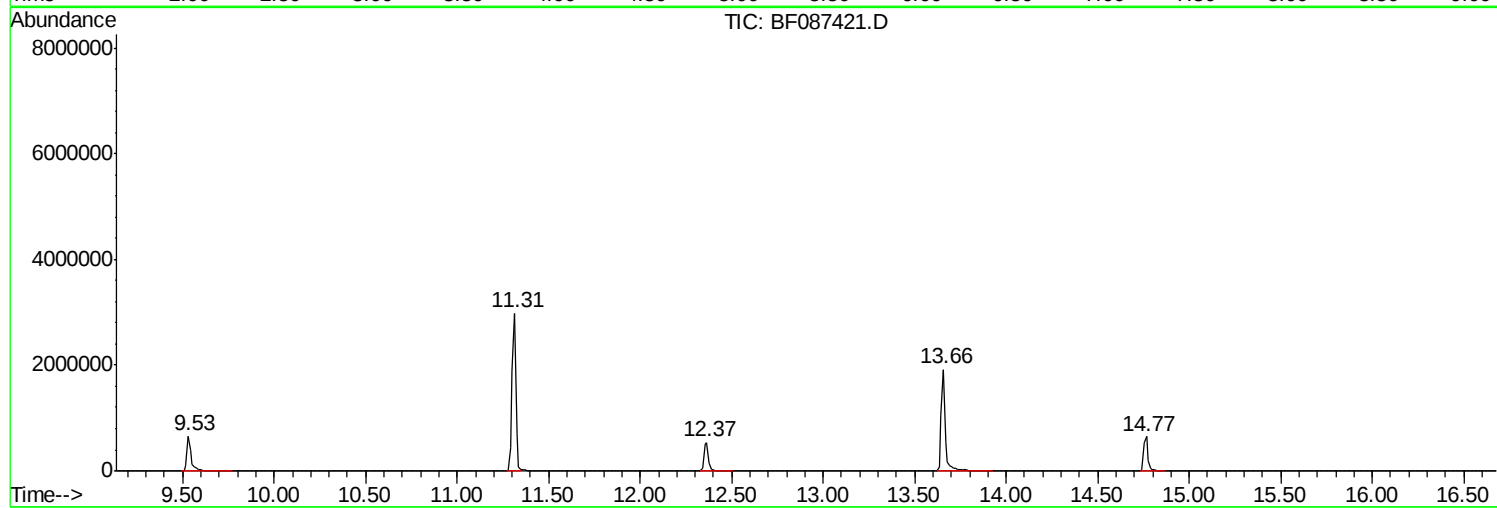
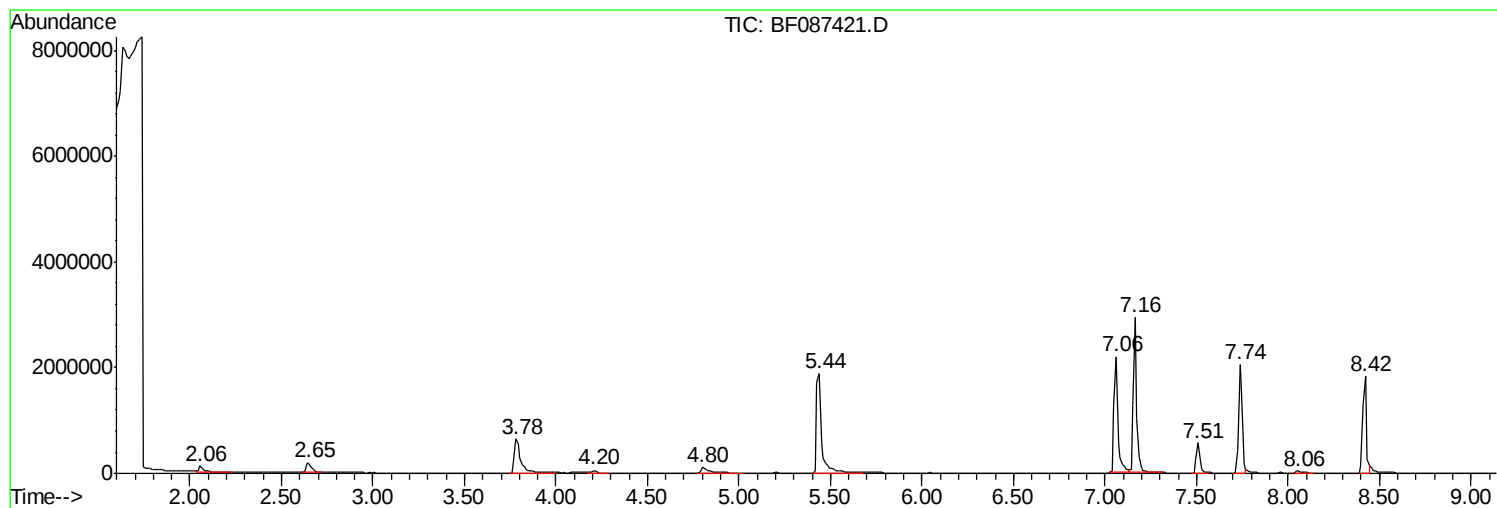
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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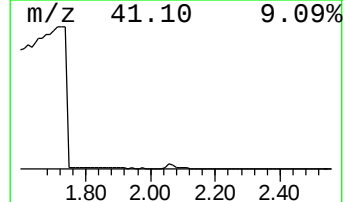
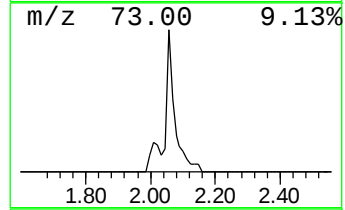
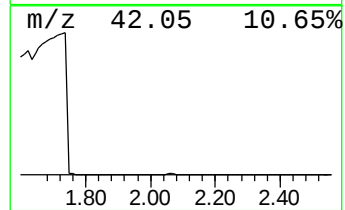
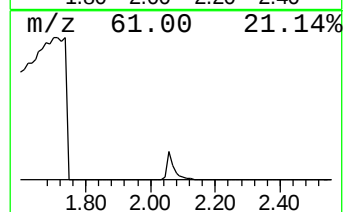
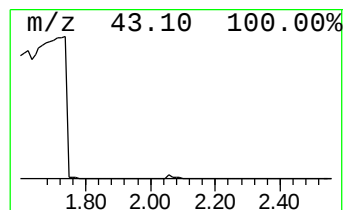
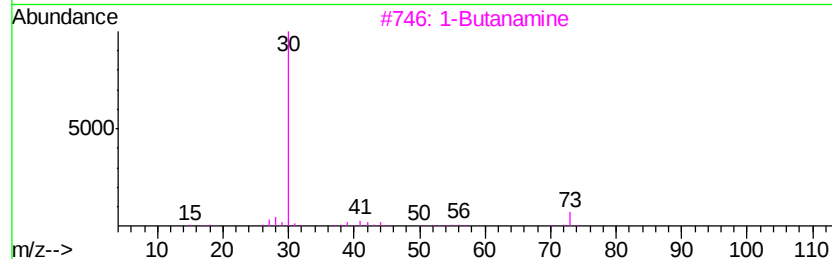
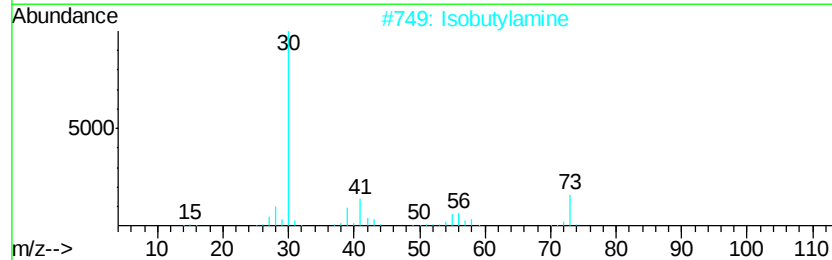
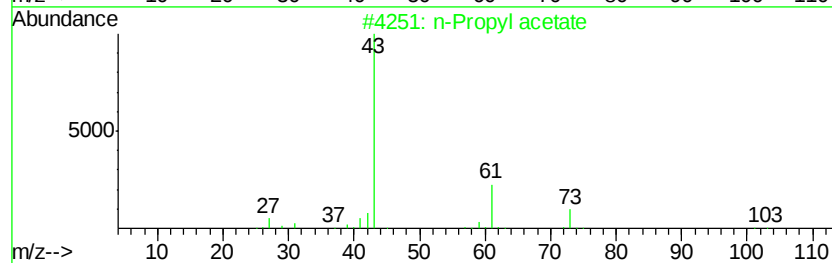
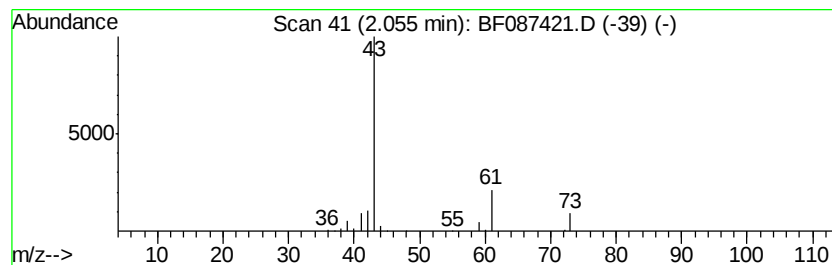
Instrument :
BNA_F
ClientSampleId :
HSR-WC-46-052316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.06	5.66 ng	215401	1,4-Dichlorobenzene-d4	7.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isobutylamine	73	C4H11N	000078-81-9	5
3	1-Butanamine	73	C4H11N	000109-73-9	4
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5	Hydrogen azide	43	HN3	007782-79-8	4



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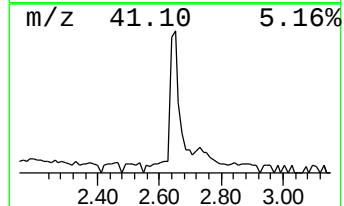
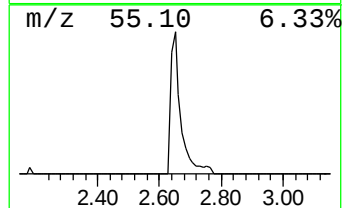
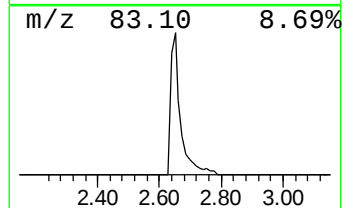
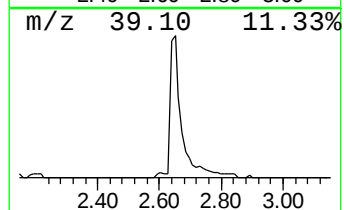
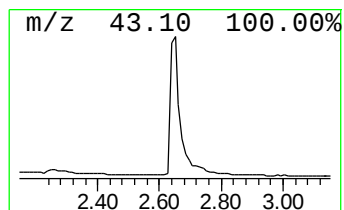
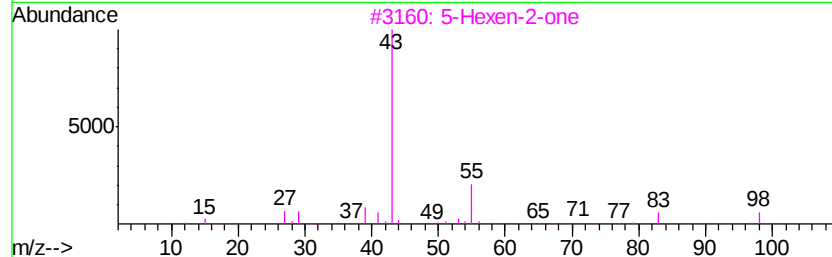
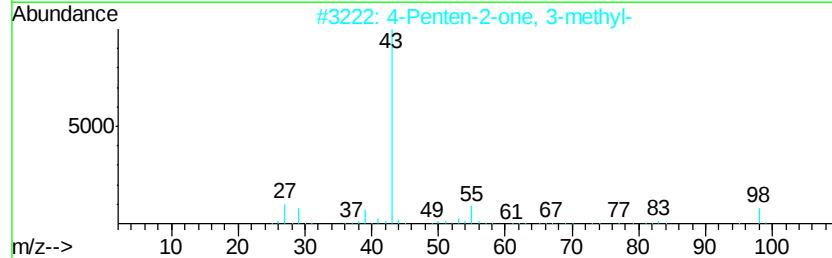
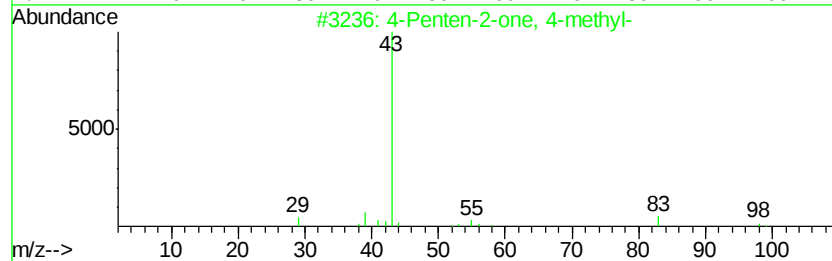
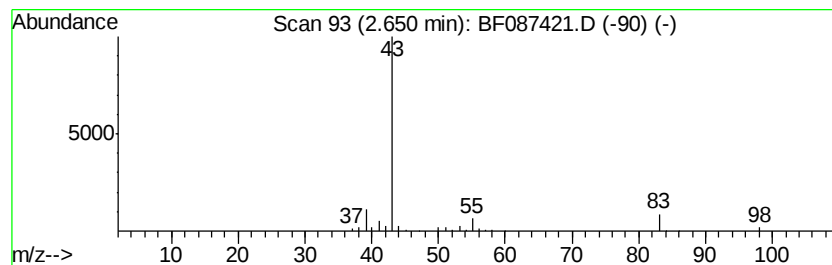
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
2.65	10.24 ng	389635	1,4-Dichlorobenzene-d4	7.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	59
3			5-Hexen-2-one	98	C6H10O	000109-49-9	42
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
5			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9



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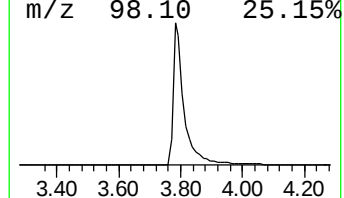
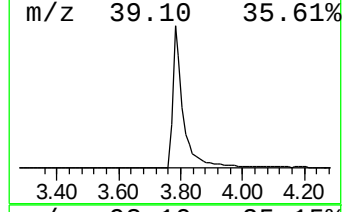
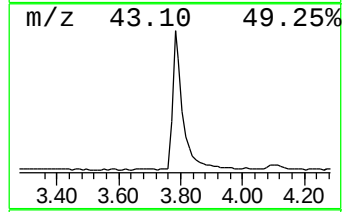
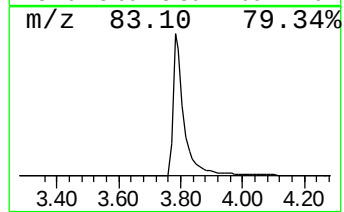
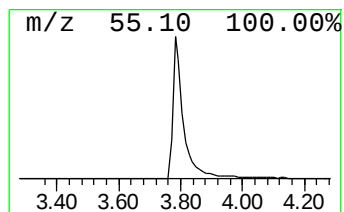
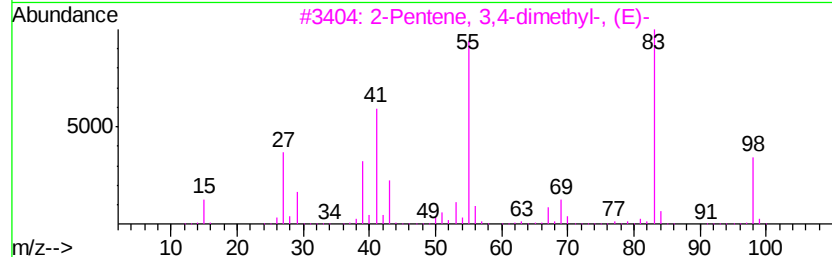
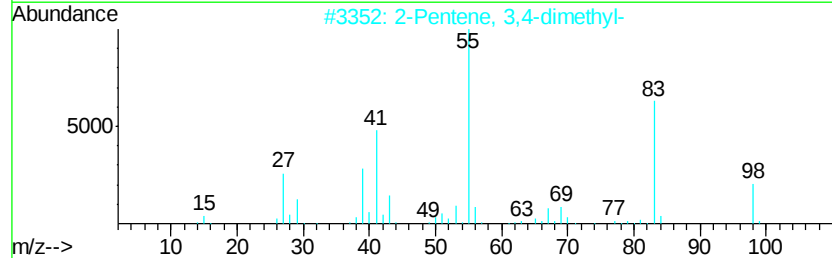
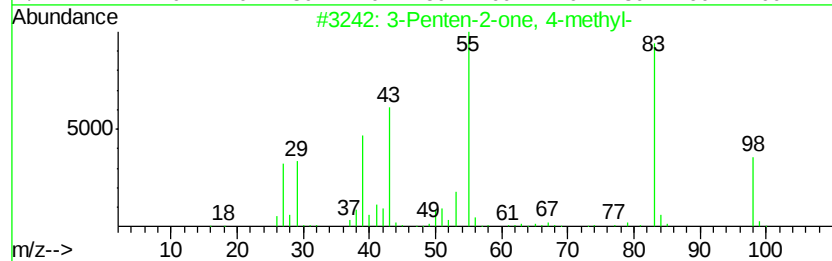
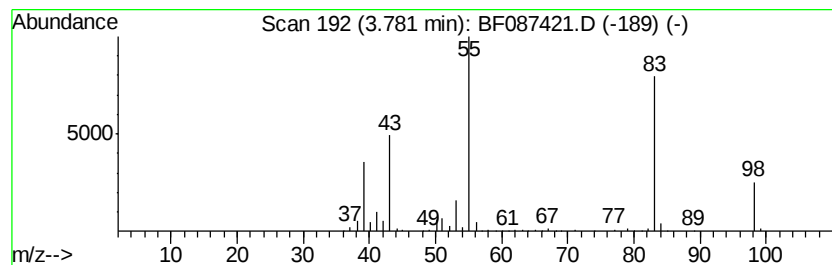
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.78	40.04 ng	1523340	1,4-Dichlorobenzene-d4	7.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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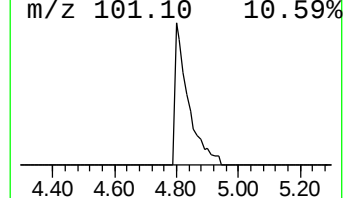
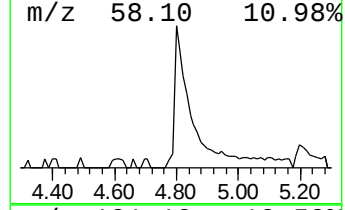
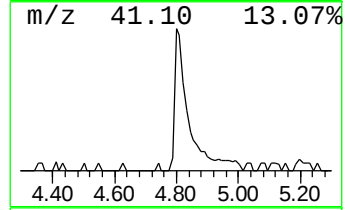
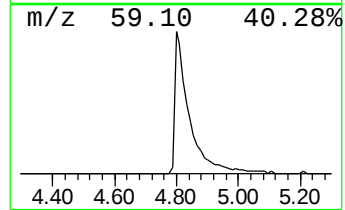
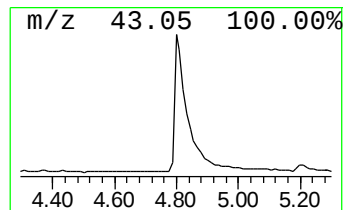
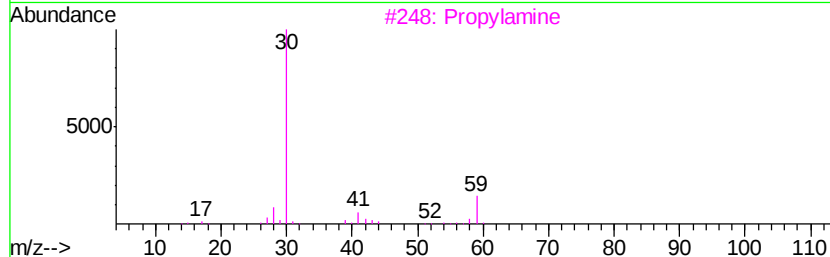
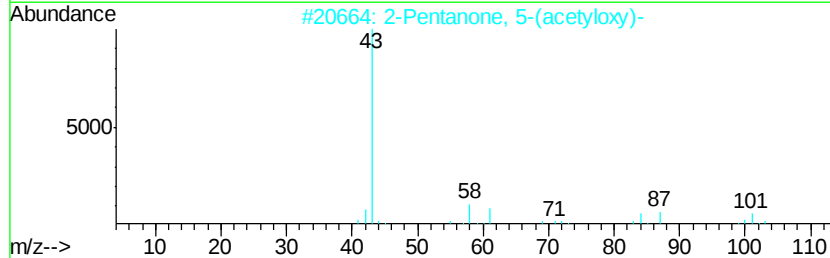
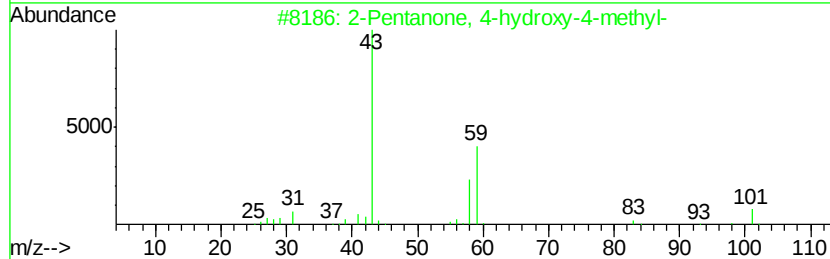
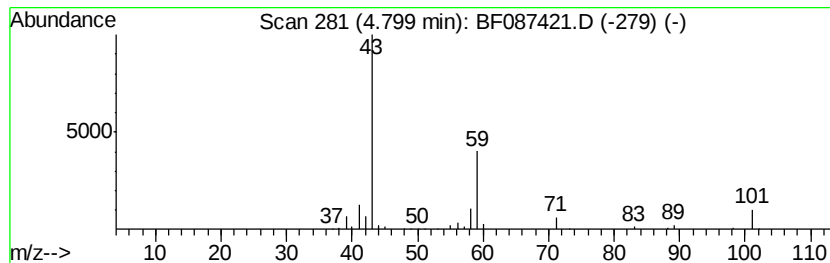
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	8.67 ng	329815	1,4-Dichlorobenzene-d4	7.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	12
3		Propylamine	59	C3H9N	000107-10-8	9
4		Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
5		Butane	58	C4H10	000106-97-8	9



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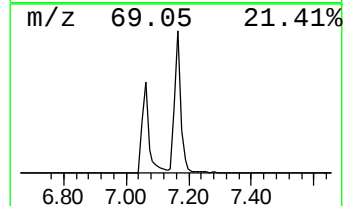
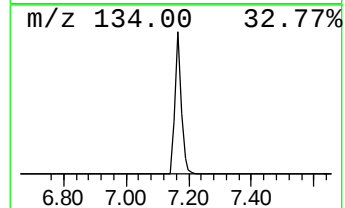
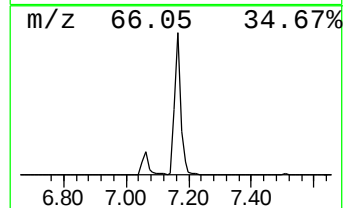
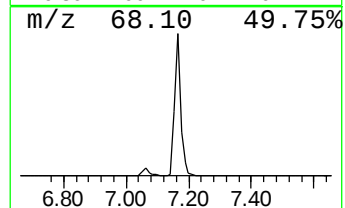
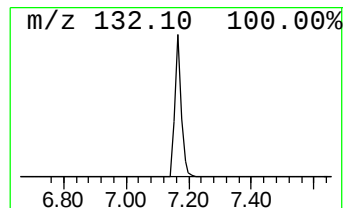
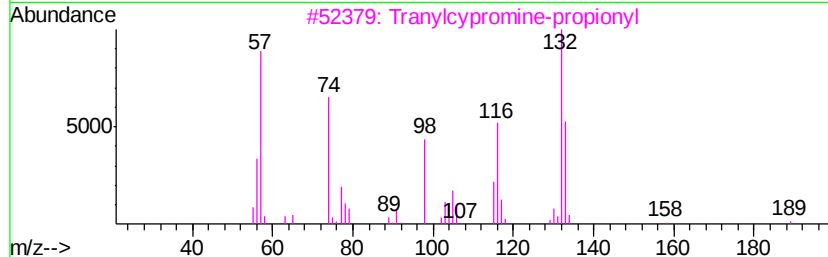
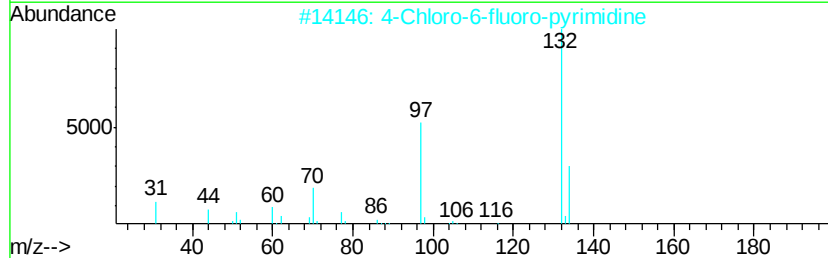
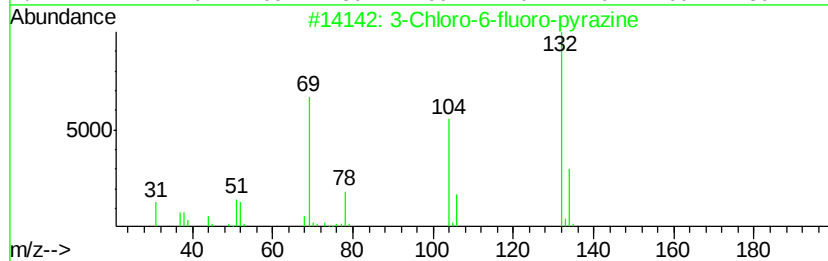
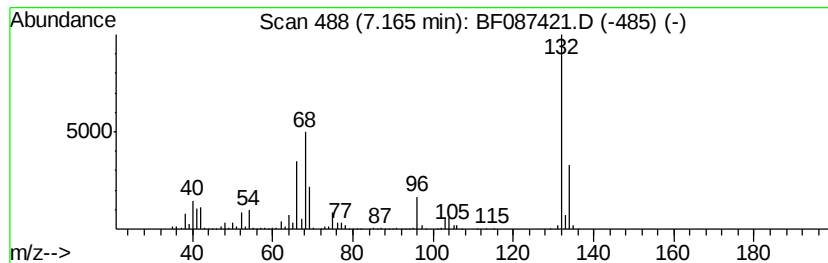
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Peak Number 6 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	105.21 ng	4003300	1,4-Dichlorobenzene-d4	7.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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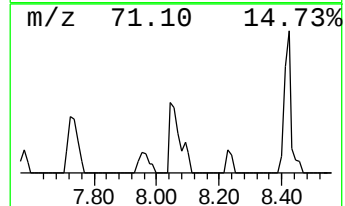
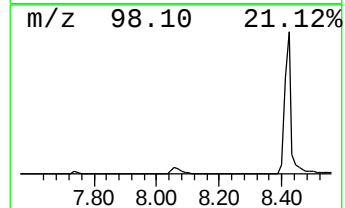
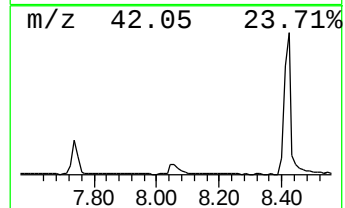
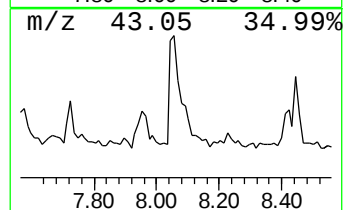
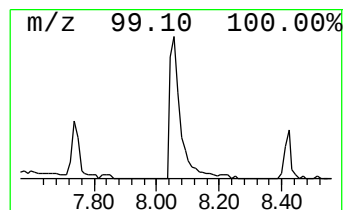
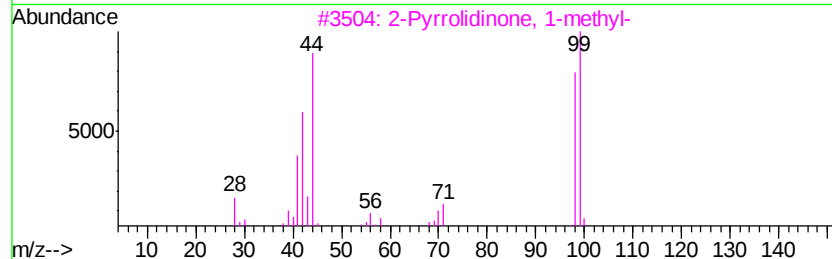
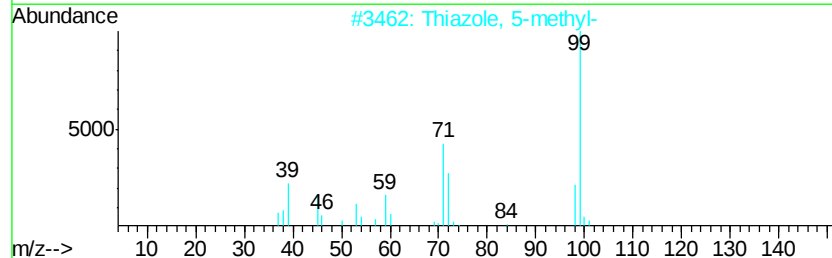
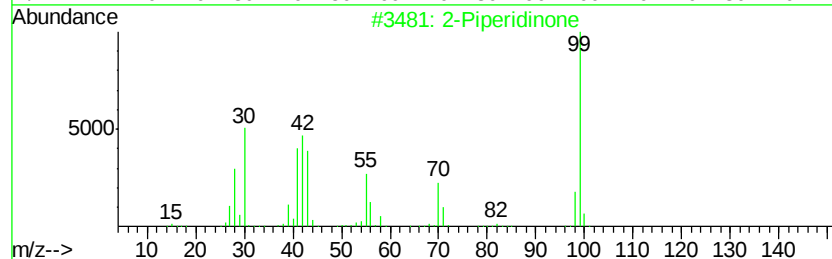
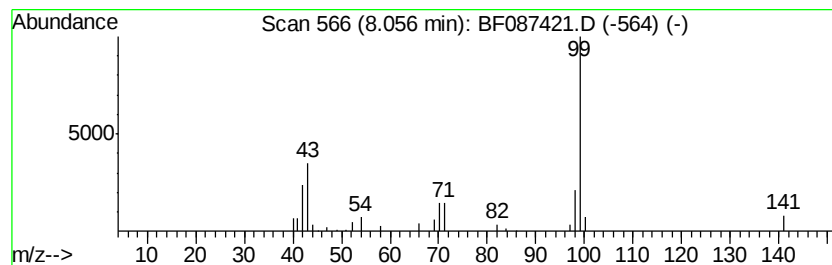
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2-Piperidinone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	2.63 ng	100007	1,4-Dichlorobenzene-d4	7.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Piperidinone	99	C5H9NO	000675-20-7	72
2			Thiazole, 5-methyl-	99	C4H5NS	003581-89-3	58
3			2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	50
4			Benzo[1,2,5]thiadiazole, 4-bromo...	376	C11H13BrN4O2S2	1000296-37-8	42
5			4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052616\
Data File : BF087421.D
Acq On : 26 May 2016 22:26
Operator : UM/SJ
Sample : H3240-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HSR-WC-46-052316

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.06	5.7	ng	215401	1	7.51	760997	20.0
4-Penten-2-one, 4...	2.65	10.2	ng	389635	1	7.51	760997	20.0
3-Penten-2-one, 4...	3.78	40.0	ng	1523340	1	7.51	760997	20.0
2-Pentanone, 4-hy...	4.80	8.7	ng	329815	1	7.51	760997	20.0
unknown7.16	7.16	105.2	ng	4003300	1	7.51	760997	20.0
2-Piperidinone	8.06	2.6	ng	100007	1	7.51	760997	20.0