

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052216\
 Data File : BF087286.D
 Acq On : 22 May 2016 12:56
 Operator : UM/SJ
 Sample : H3172-02
 Misc :
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-05

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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	1.701	9	10	65	rVB	3160529	6542213	100.00%	15.880%
2	4.684	268	271	283	rBV	92402	231107	3.53%	0.561%
3	5.141	309	311	332	rBV	1549518	2246947	34.35%	5.454%
4	6.227	404	406	413	rBV	1297995	1506396	23.03%	3.656%
5	6.330	413	415	420	rVV	3973226	4030296	61.60%	9.783%
6	6.559	432	435	441	rVB	704091	869708	13.29%	2.111%
7	6.707	446	448	451	rBV	3202681	3199743	48.91%	7.767%
8	7.142	483	486	488	rBV	2155588	3163104	48.35%	7.678%
9	7.542	519	521	529	rBV3	122771	263215	4.02%	0.639%
10	7.793	537	543	546	rBV4	24712	71372	1.09%	0.173%
11	7.839	546	547	550	rBV2	870689	1131655	17.30%	2.747%
12	8.296	584	587	592	rBV2	72144	181439	2.77%	0.440%
13	8.868	630	637	639	rBV3	63558	230362	3.52%	0.559%
14	8.925	639	642	644	rBV	5158924	4876979	74.55%	11.838%
15	9.096	654	657	660	rVB3	61272	108480	1.66%	0.263%
16	9.153	660	662	666	rBV3	45818	71592	1.09%	0.174%
17	9.245	667	670	672	rBV2	64189	117988	1.80%	0.286%
18	9.416	681	685	687	rBV3	36939	88824	1.36%	0.216%
19	9.588	698	700	704	rBV	1365135	1269169	19.40%	3.081%
20	9.896	722	727	730	rBV5	140246	387271	5.92%	0.940%
21	9.976	731	734	737	rVV4	84739	195185	2.98%	0.474%
22	10.033	737	739	742	rVB3	46923	80058	1.22%	0.194%
23	10.388	767	770	772	rBV2	2187447	2969279	45.39%	7.207%
24	10.936	814	818	820	rBV3	131400	198571	3.04%	0.482%
25	11.062	828	829	832	rVV	794239	1046447	16.00%	2.540%
26	11.622	876	878	885	rVB4	68621	143861	2.20%	0.349%
27	12.479	951	953	956	rVB	371521	345880	5.29%	0.840%
28	12.559	958	960	962	rVB	88071	78867	1.21%	0.191%
29	12.651	965	968	970	rBV	3916821	3771719	57.65%	9.155%
30	13.177	1012	1014	1017	rBV2	166473	208625	3.19%	0.506%
31	13.554	1045	1047	1054	rVB	44747	79716	1.22%	0.193%
32	13.691	1057	1059	1066	rVB	636866	791059	12.09%	1.920%
33	15.051	1175	1178	1187	rVB	499266	701343	10.72%	1.702%

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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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

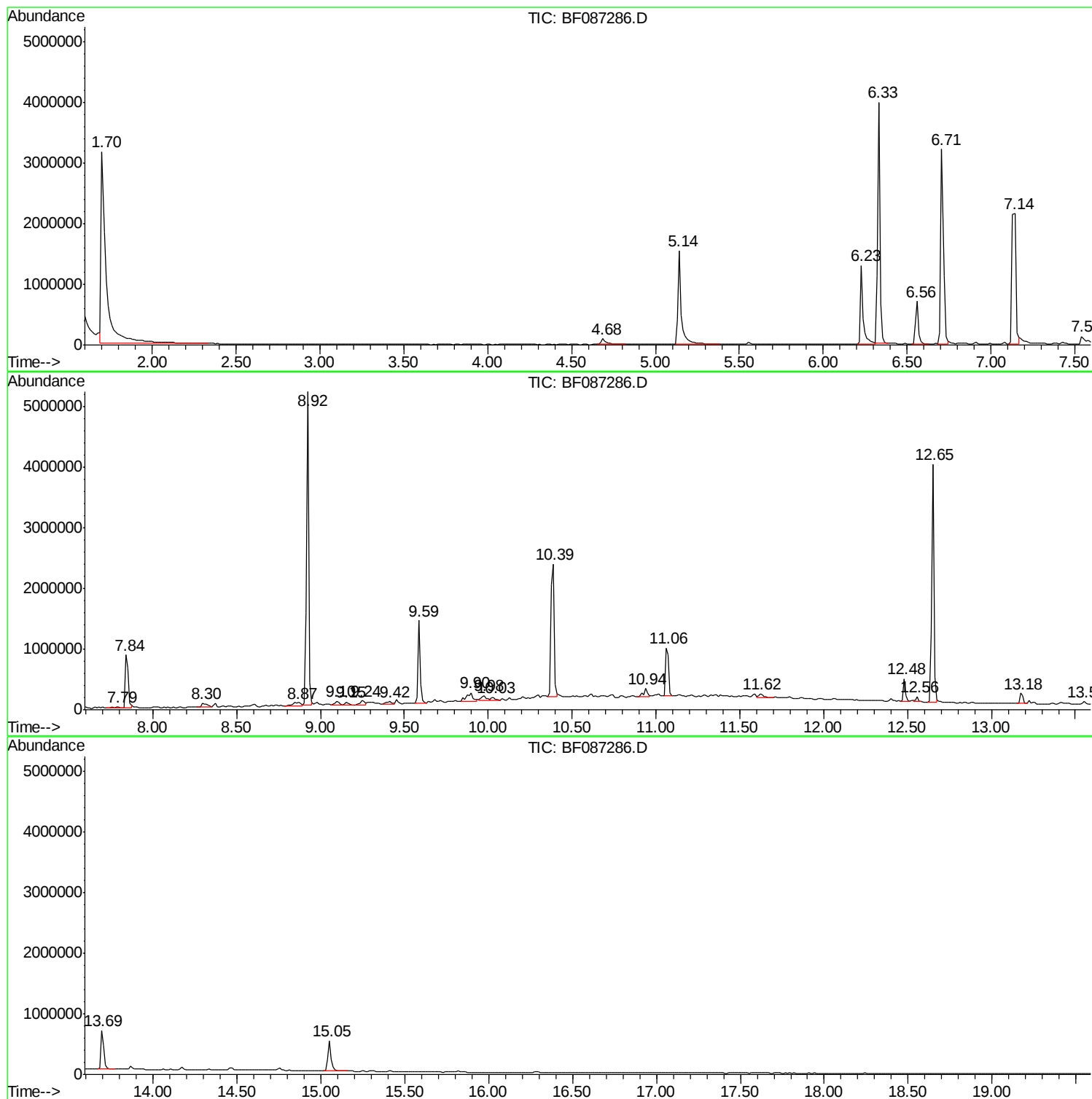
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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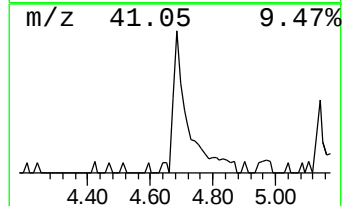
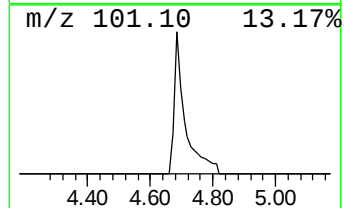
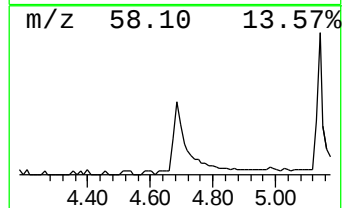
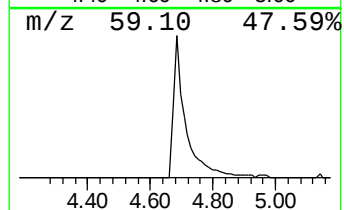
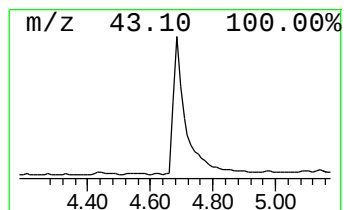
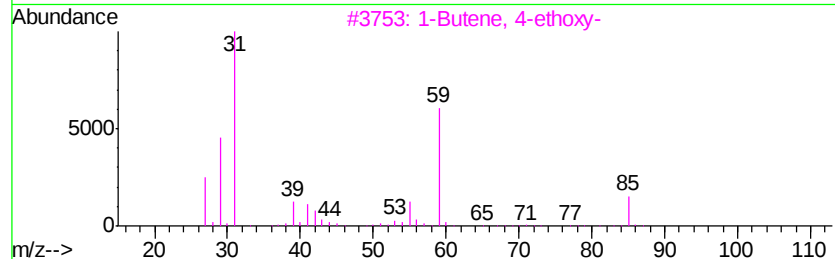
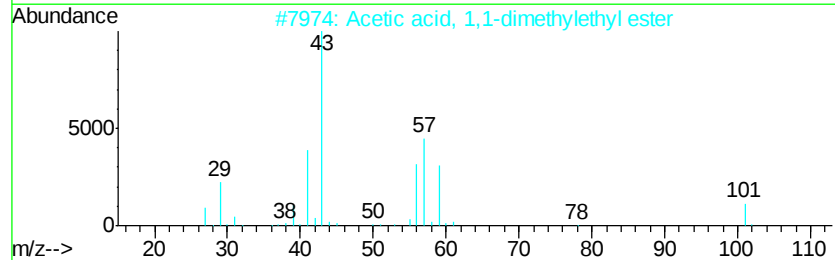
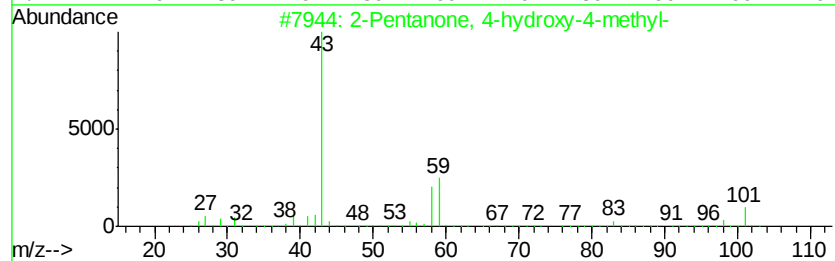
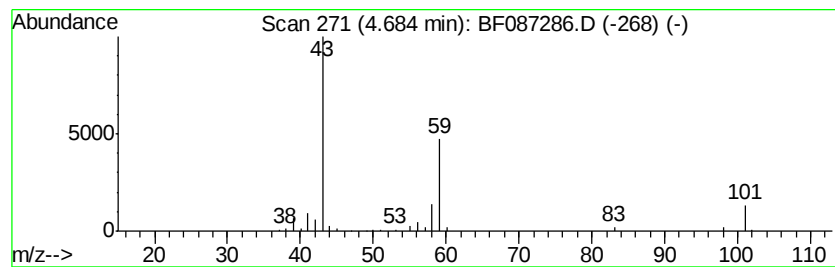
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	5.31 ng	231107	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Diacetamide	101	C4H7NO2	000625-77-4	9	



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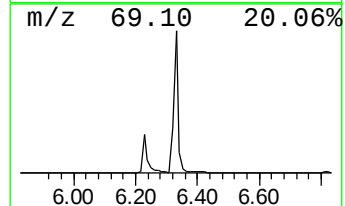
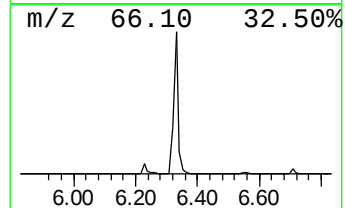
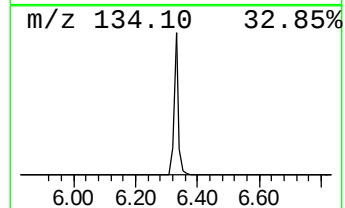
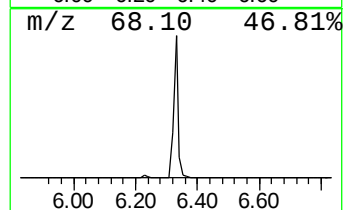
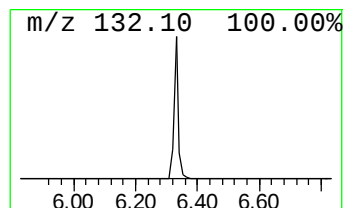
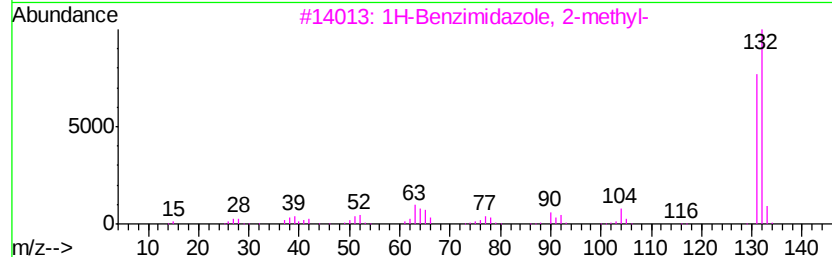
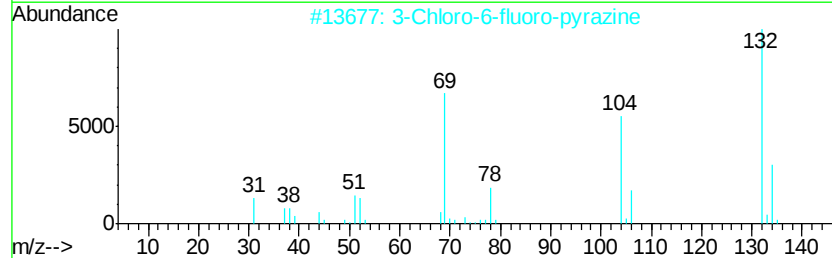
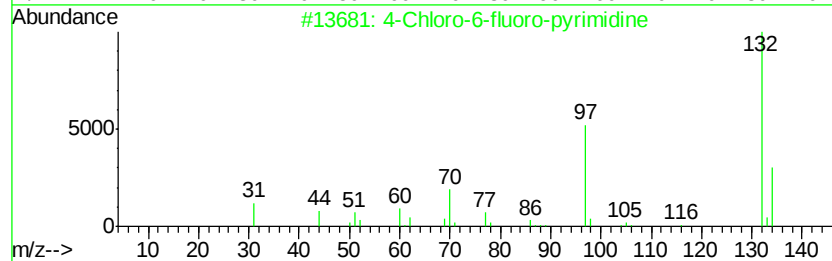
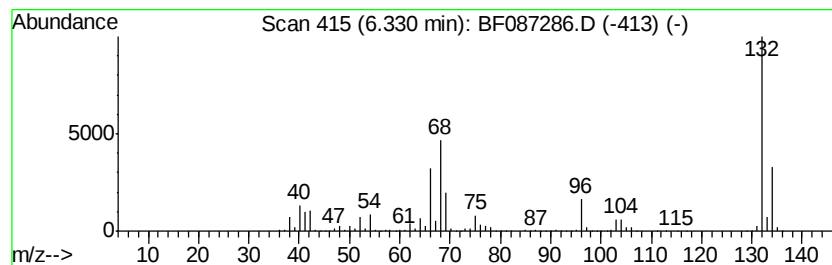
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	92.68 ng	4030300	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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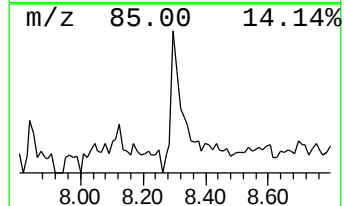
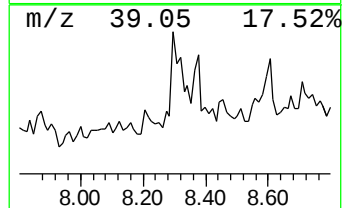
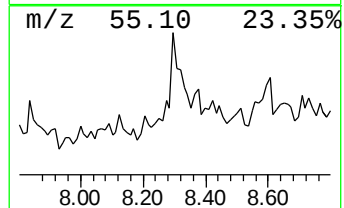
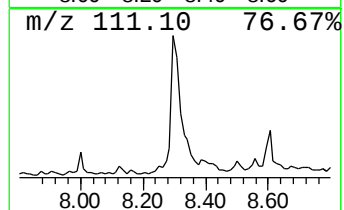
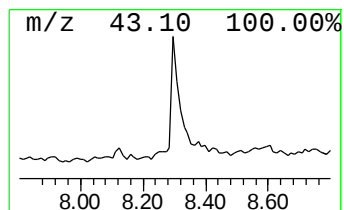
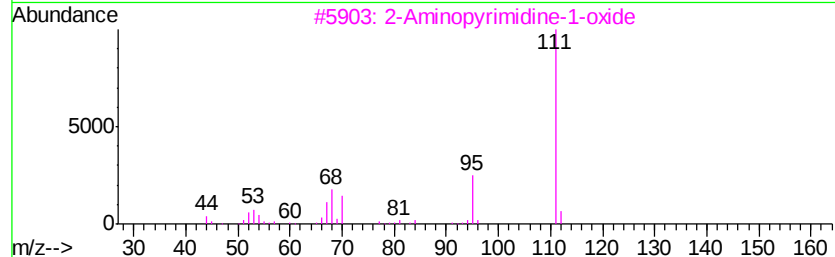
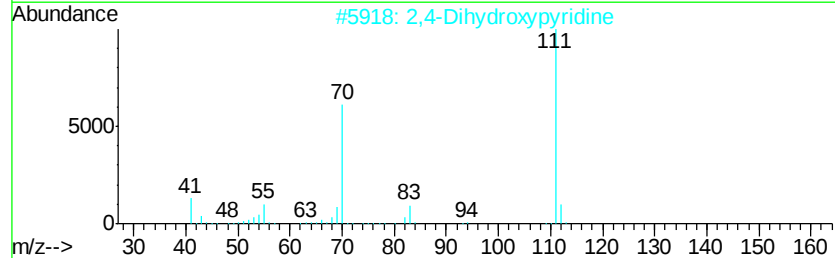
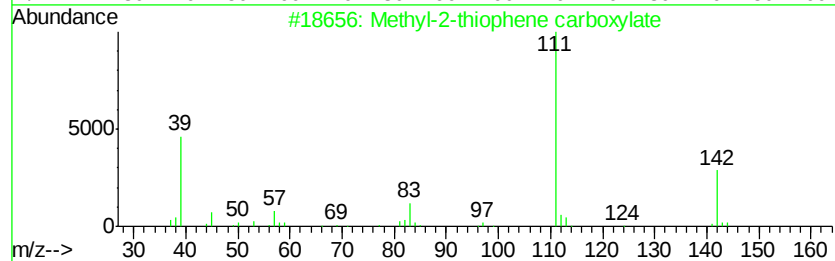
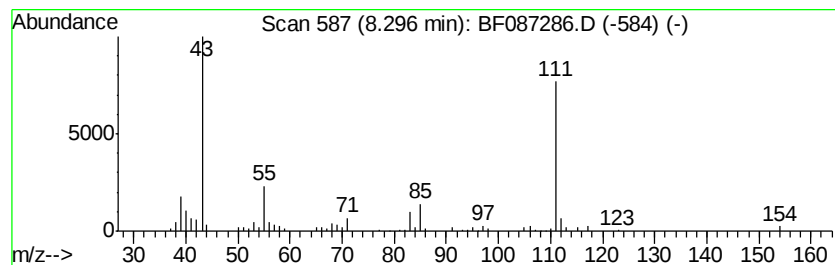
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Methyl-2-thiophene carboxylate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.30	3.21 ng	181439	Napthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl-2-thiophene carboxylate	142	C6H6O2S	005380-42-7	53
2		2,4-Dihydroxypyridine	111	C5H5NO2	000626-03-9	53
3		2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	53
4		4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	47
5		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	40



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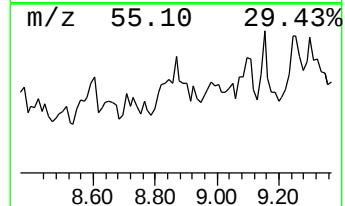
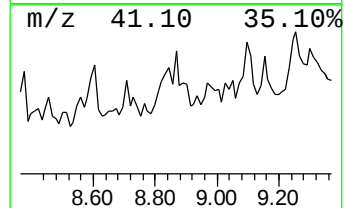
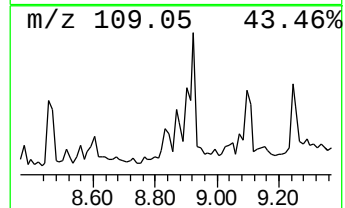
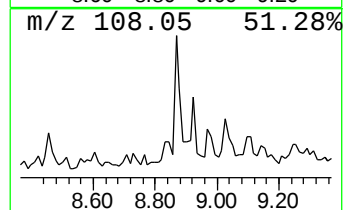
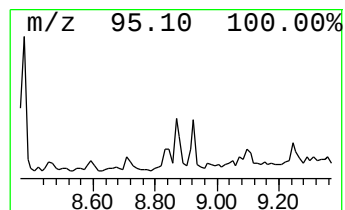
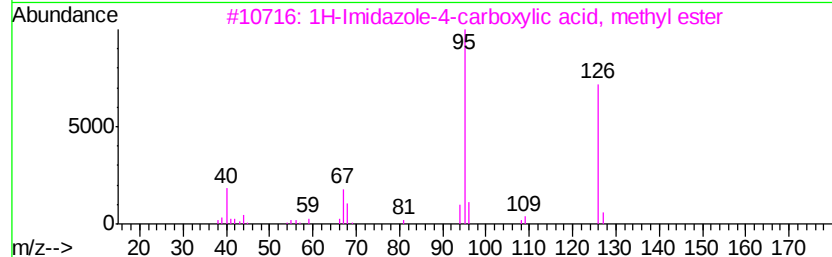
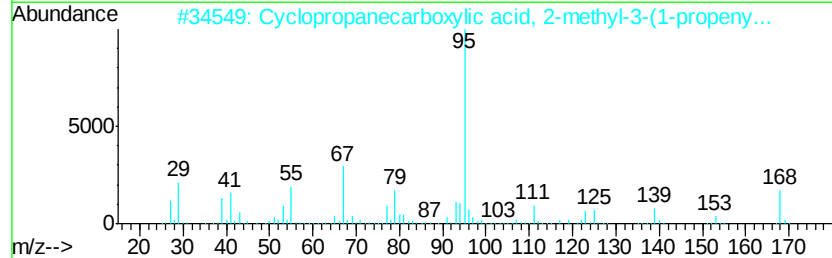
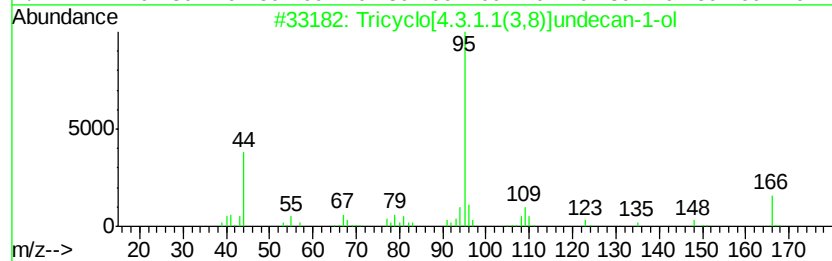
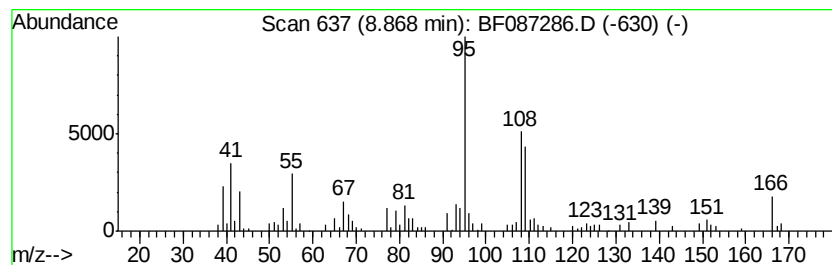
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown8.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.87	3.63 ng	230362	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricyclo[4.3.1.1(3,8)]undecan-1-ol	166	C11H18O	031061-64-0	46
2		Cyclopropanecarboxylic acid, 2-methyl-3-(1-propeny...	168	C10H16O2	030626-51-8	43
3		1H-Imidazole-4-carboxylic acid, ...	126	C5H6N2O2	017325-26-7	43
4		1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	35
5		2-Pyrimidinamine	95	C4H5N3	000109-12-6	35



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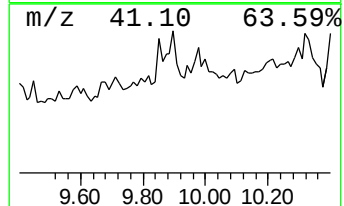
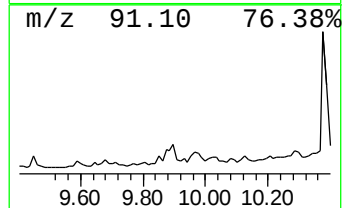
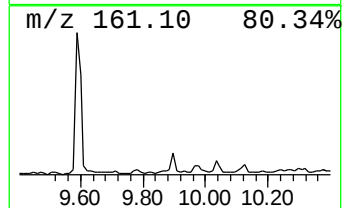
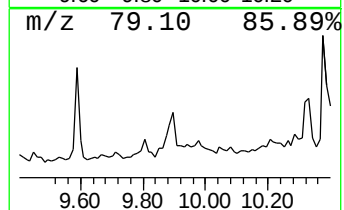
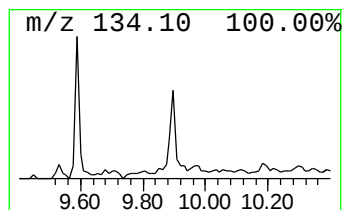
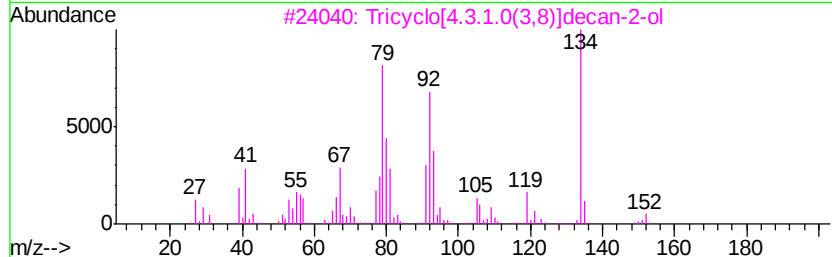
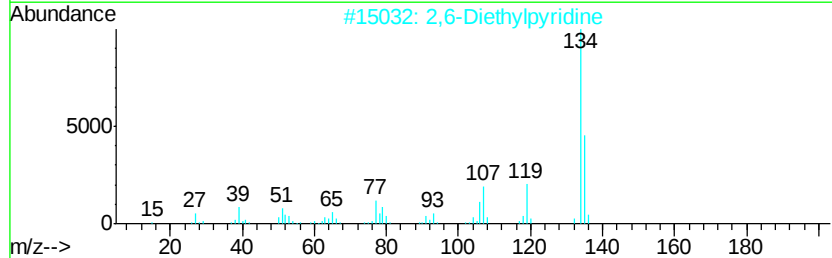
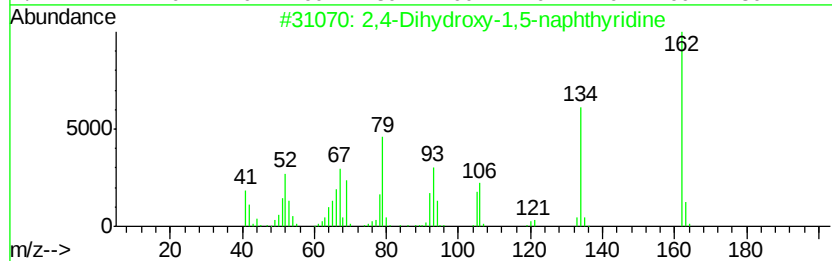
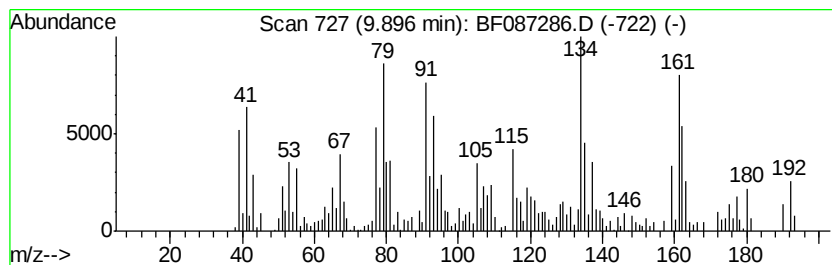
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Peak Number 7 unknown9.90 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	6.10 ng	387271	Acenaphthene-d10	9.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dihydroxy	162	C8H6N2O2	060058-16-4	43		
2	2,6-Diethylpyridine	135	C9H13N	000935-28-4	35		
3	Tricyclo[4.3.1.0(3,8)]decan-2-ol	152	C10H16O	1000197-64-5	30		
4	Pyridine, 2-ethyl-4,6-dimethyl-	135	C9H13N	001124-35-2	18		
5	4(3H)-Pteridinone, 3-methoxy-6-m...	192	C8H8N4O2	024898-65-5	15		



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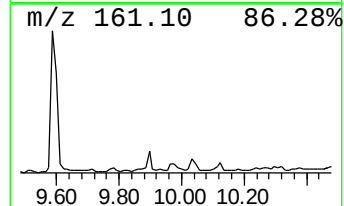
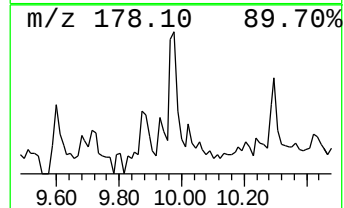
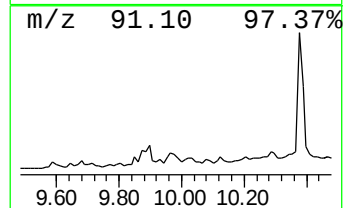
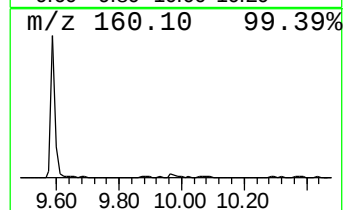
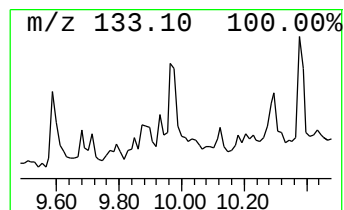
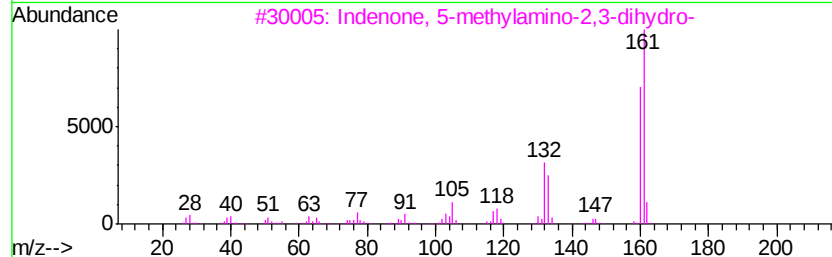
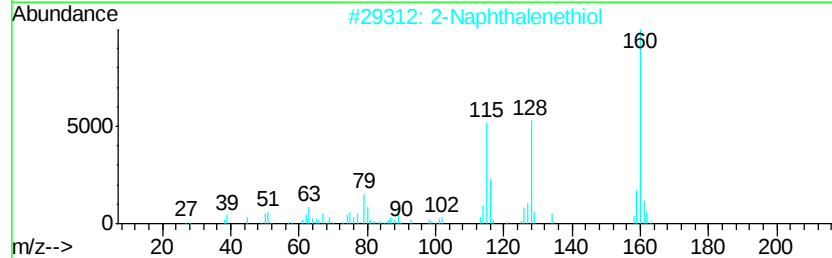
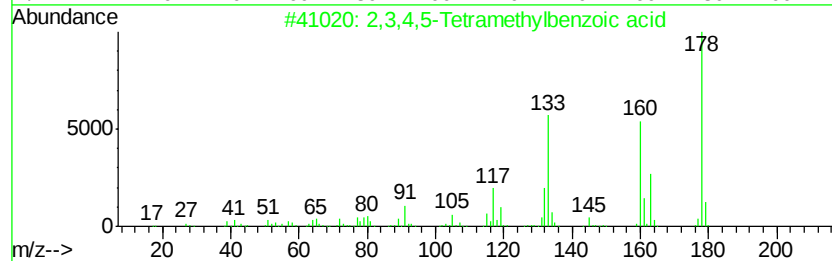
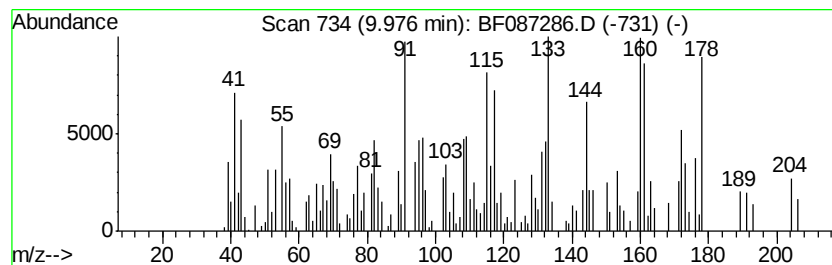
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.98 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	3.08 ng	195185	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3,4,5-Tetramethylbenzoic acid	178	C11H14O2	002529-39-7	43
2		2-Naphthalenethiol	160	C10H8S	000091-60-1	25
3		Indenone, 5-methylamino-2,3-dihydro...	161	C10H11NO	1000153-18-7	18
4		2-Benzyl-1,3-oxazol-2-ine	161	C10H11NO	010431-95-5	18
5		2H-1-Benzopyran-2-one, 6-methyl-	160	C10H8O2	000092-48-8	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052216\
Data File : BF087286.D
Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

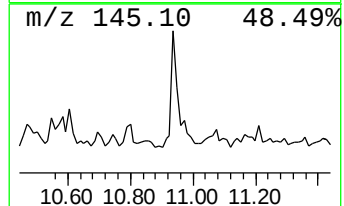
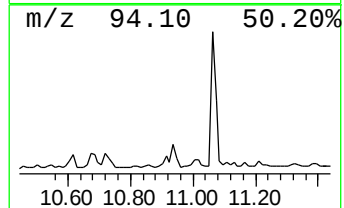
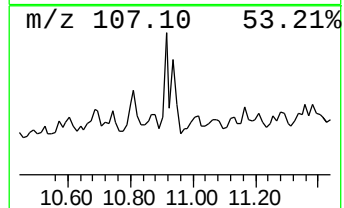
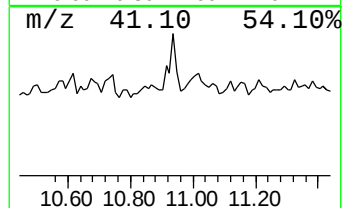
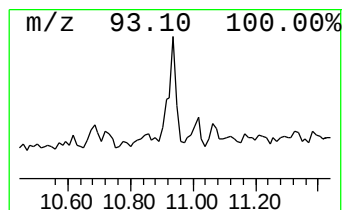
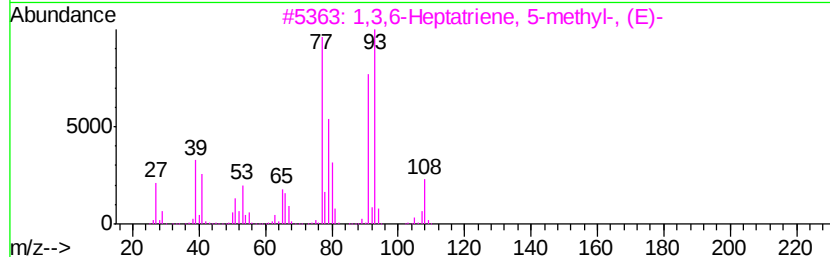
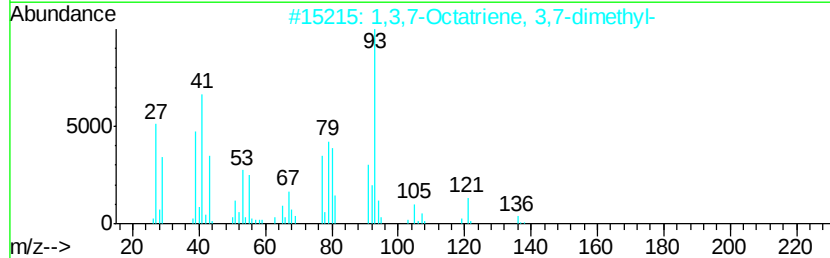
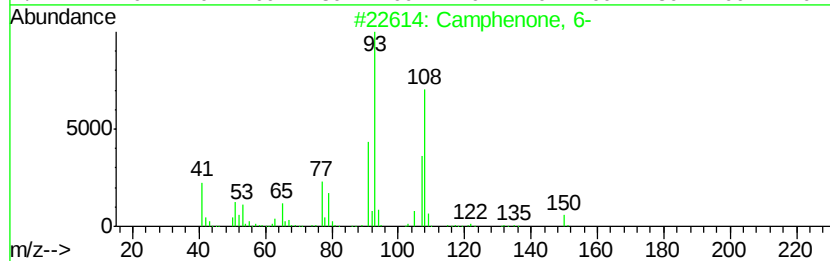
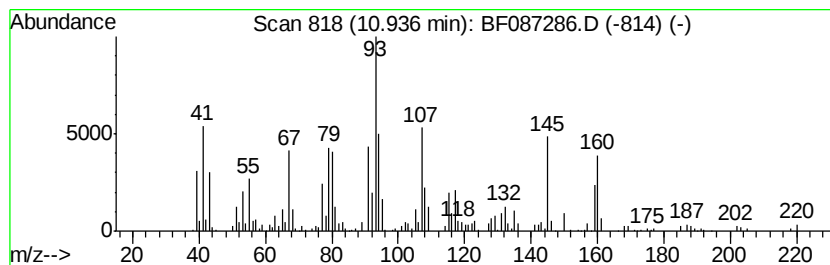
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	3.80 ng	198571	Phenanthrene-d10	11.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphenone, 6-	150	C10H14O	055659-42-2	30
2		1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	30
3		1,3,6-Heptatriene, 5-methyl-, (E)-	108	C8H12	000818-48-4	27
4		Cyclohexanol, 2-methyl-5-(1-meth...	154	C10H18O	018675-33-7	22
5		Cyclobutane, 2-ethylidene-1-vinyl-	108	C8H12	1000150-32-4	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052216\
Data File : BF087286.D
Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
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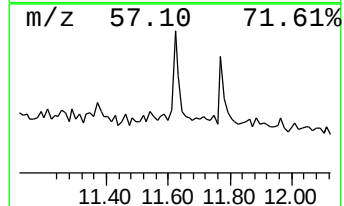
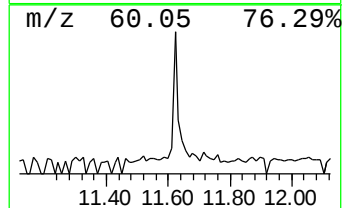
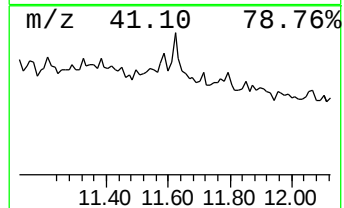
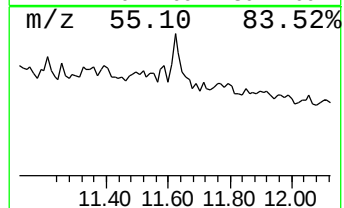
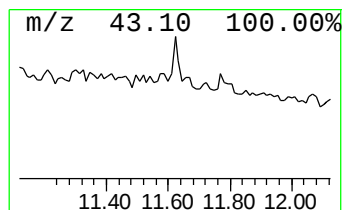
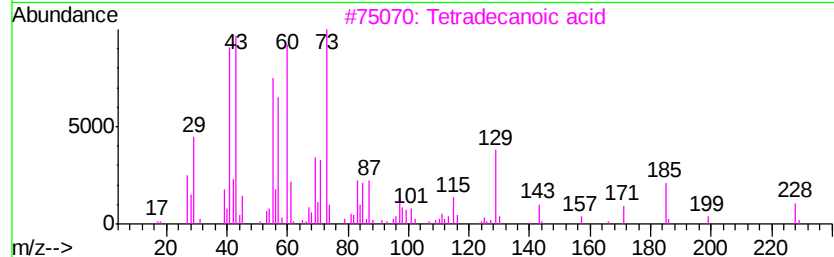
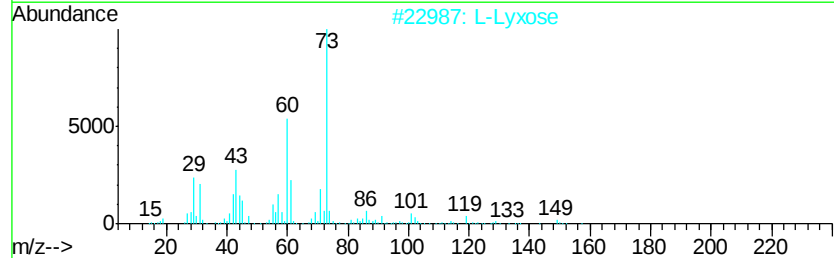
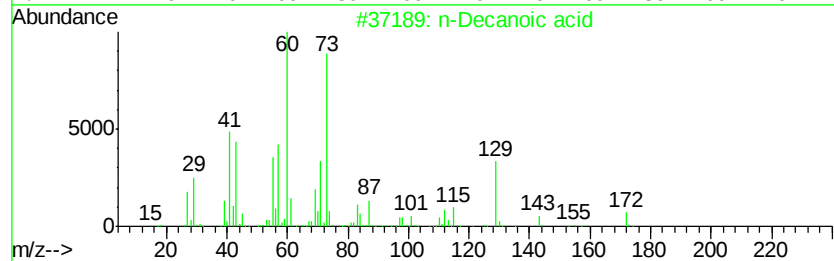
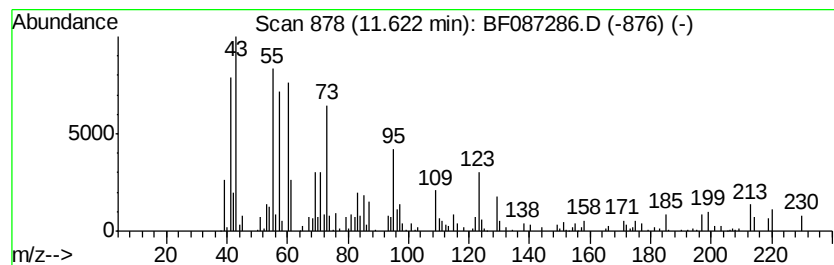
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown11.62 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.62	2.75 ng	143861	Phenanthrene-d10		11.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	38
2	L-Lyxose	150	C5H10O5	001949-78-6	35
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	30
4	Tridecanoic acid	214	C13H26O2	000638-53-9	30
5	Nonanoic acid	158	C9H18O2	000112-05-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052216\
Data File : BF087286.D
Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

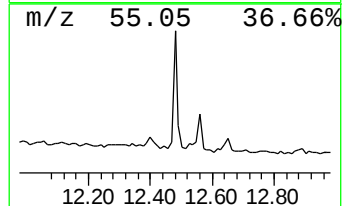
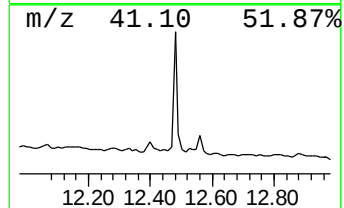
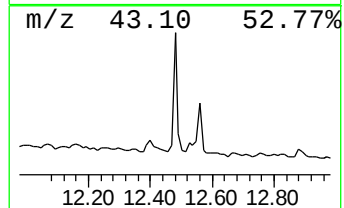
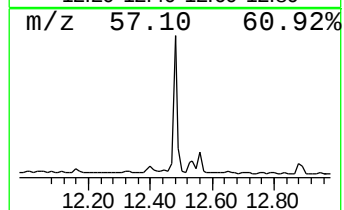
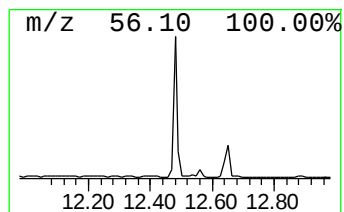
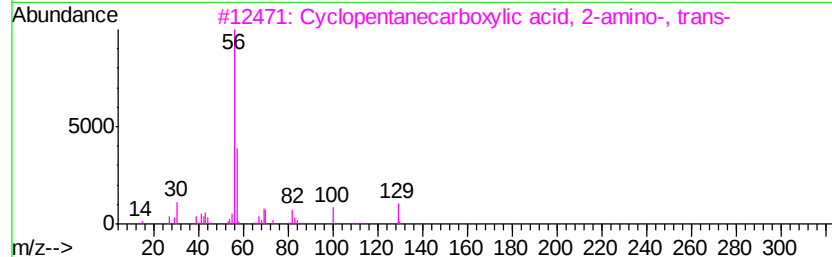
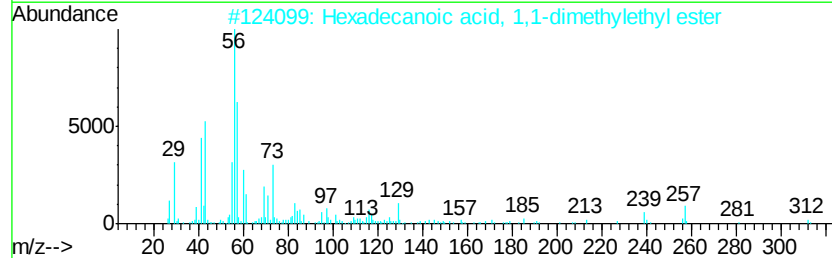
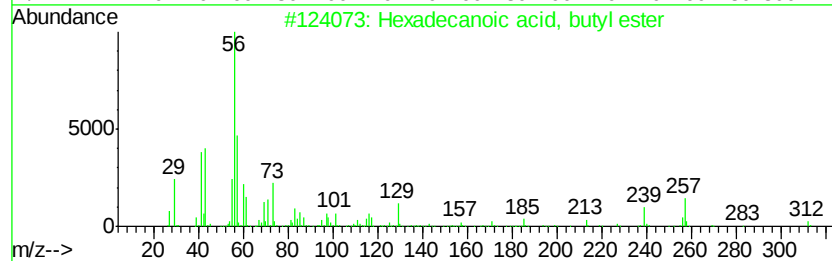
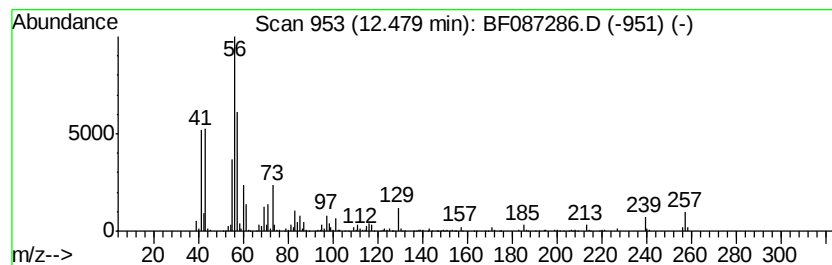
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	8.74 ng	345880	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052216\
Data File : BF087286.D
Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-05

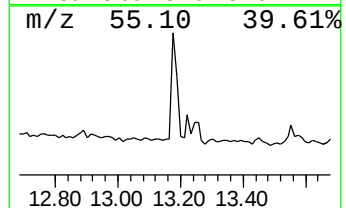
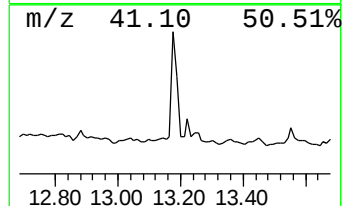
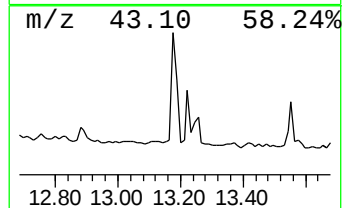
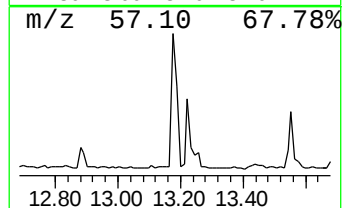
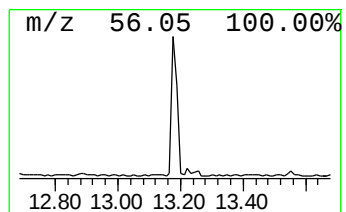
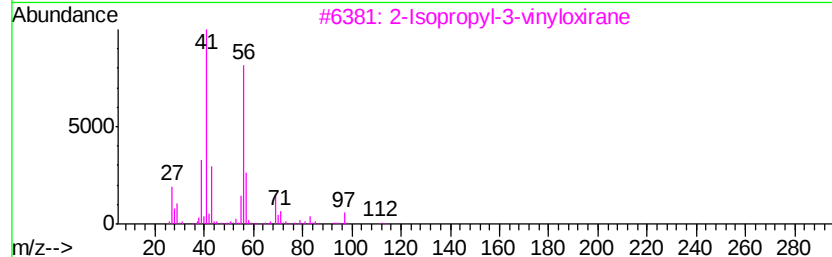
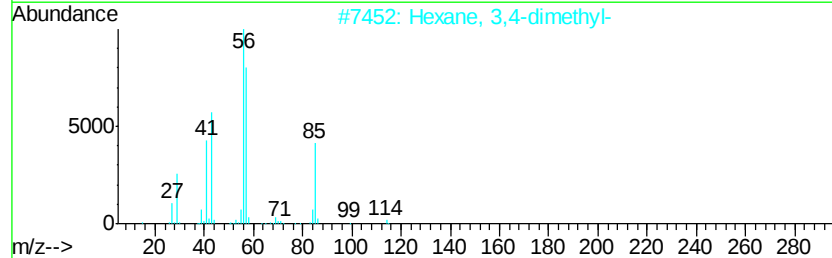
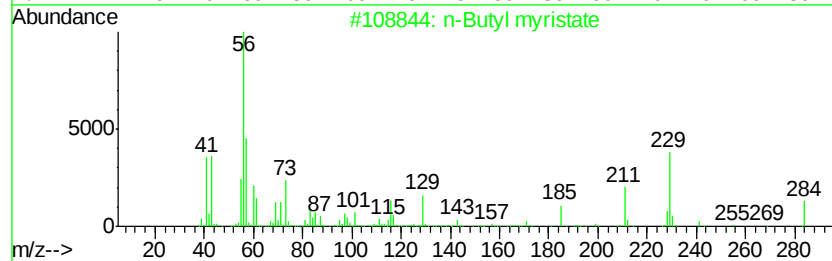
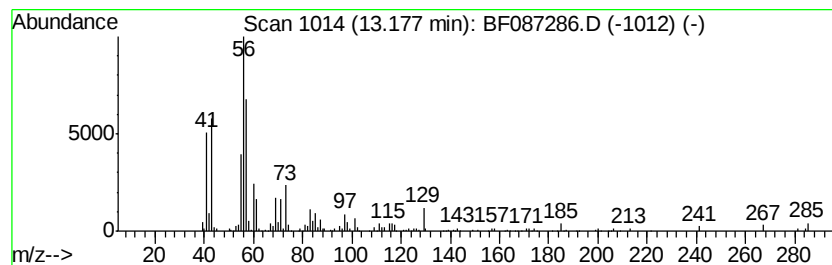
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	5.27 ng	208625	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Butyl myristate	284	C18H36O2	000110-36-1	72
2		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	43
3		2-Isopropyl-3-vinylloxirane	112	C7H12O	070777-23-0	38
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5		Cyclopropane, propyl-	84	C6H12	002415-72-7	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052216\
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Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

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ClientSampleId :
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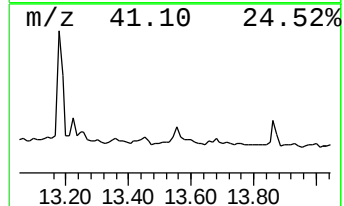
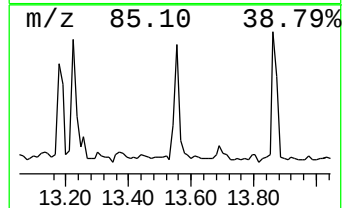
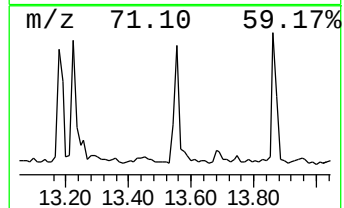
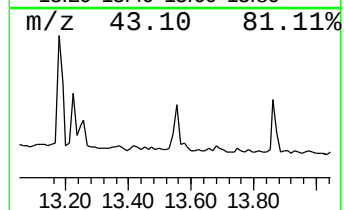
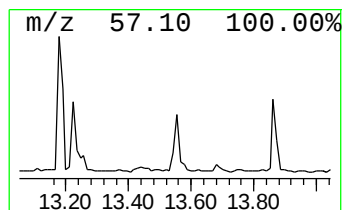
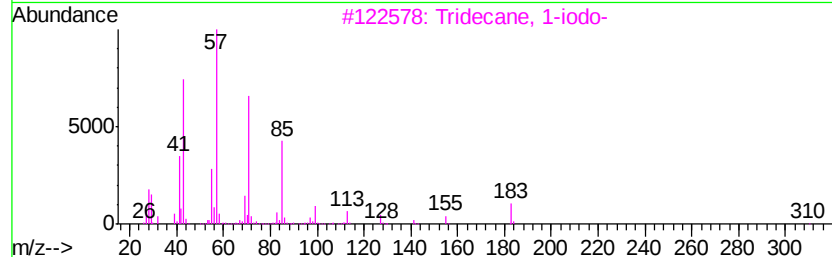
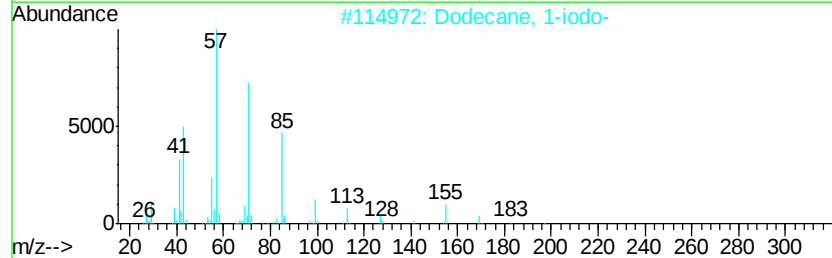
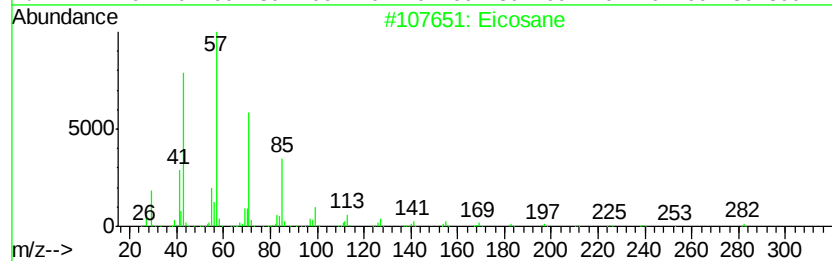
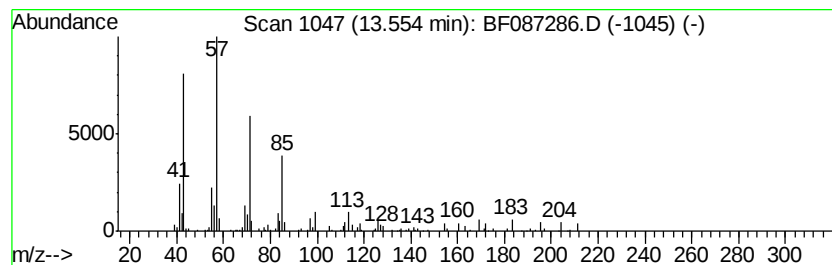
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.02 ng	79716	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	80
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
4		Nonacosane	408	C29H60	000630-03-5	64
5		triacontane	422	C30H62	000638-68-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052216\
Data File : BF087286.D
Acq On : 22 May 2016 12:56
Operator : UM/SJ
Sample : H3172-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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
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unknown6.33	6.33	92.7	ng	4030300	1	6.56	869708	20.0
Methyl-2-thiophen...	8.30	3.2	ng	181439	2	7.84	1131660	20.0
unknown8.87	8.87	3.6	ng	230362	3	9.59	1269170	20.0
unknown9.90	9.90	6.1	ng	387271	3	9.59	1269170	20.0
unknown9.98	9.98	3.1	ng	195185	3	9.59	1269170	20.0
unknown10.94	10.94	3.8	ng	198571	4	11.07	1046450	20.0
unknown11.62	11.62	2.8	ng	143861	4	11.07	1046450	20.0
Hexadecanoic acid...	12.48	8.7	ng	345880	5	13.69	791059	20.0
n-Butyl myristate	13.18	5.3	ng	208625	5	13.69	791059	20.0
Eicosane	13.55	2.0	ng	79716	5	13.69	791059	20.0