

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032715\
 Data File : BF078043.D
 Acq On : 27 Mar 2015 18:19
 Operator : TP/IZ
 Sample : G1654-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-8-3-24-15

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-BF031115.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	1.344	37	40	43	rVB	196195	276526	16.79%	2.700%
2	1.504	51	54	57	rVB	242973	296736	18.01%	2.898%
3	1.630	64	65	71	rVB	11715	17916	1.09%	0.175%
4	1.744	73	75	84	rVB	95455	204406	12.41%	1.996%
5	4.819	342	344	348	rBV	32740	49235	2.99%	0.481%
6	5.367	390	392	395	rBV	328232	372412	22.61%	3.637%
7	6.670	503	506	509	rBV	246991	223099	13.54%	2.179%
8	6.796	514	517	519	rBV	672611	782870	47.52%	7.645%
9	7.070	539	541	544	rBB	206578	196006	11.90%	1.914%
10	7.265	555	558	560	rVB	610623	810151	49.18%	7.911%
11	7.768	600	602	605	rBV	605480	590972	35.87%	5.771%
12	8.579	667	673	677	rBV3	19480	44940	2.73%	0.439%
13	8.648	677	679	682	rBV	304957	286350	17.38%	2.796%
14	9.253	730	732	735	rVB2	18106	23056	1.40%	0.225%
15	9.311	735	737	739	rBV	29356	27350	1.66%	0.267%
16	9.539	754	757	758	rBV2	9303	17306	1.05%	0.169%
17	9.574	758	760	763	rVB2	14489	22447	1.36%	0.219%
18	9.734	770	774	778	rVB6	10981	28136	1.71%	0.275%
19	9.928	789	791	795	rBV2	28677	52311	3.18%	0.511%
20	9.996	795	797	800	rVB	1530285	1339034	81.29%	13.076%
21	10.134	806	809	812	rBV5	11195	30646	1.86%	0.299%
22	10.214	815	816	819	rVB	34811	35566	2.16%	0.347%
23	10.271	819	821	825	rBV5	6750	20709	1.26%	0.202%
24	10.396	828	832	833	rBV3	17384	34973	2.12%	0.342%
25	10.579	847	848	851	rBV3	11407	16846	1.02%	0.165%
26	10.659	853	855	858	rVB3	13866	21715	1.32%	0.212%
27	10.785	858	866	867	rBV4	14584	58829	3.57%	0.574%
28	10.819	867	869	871	rBV	332468	341497	20.73%	3.335%
29	10.922	876	878	880	rBV2	14387	18844	1.14%	0.184%
30	11.151	895	898	899	rBV2	13606	21703	1.32%	0.212%
31	11.277	907	909	913	rVB5	17353	29492	1.79%	0.288%
32	11.802	952	955	957	rBV	571624	804089	48.81%	7.852%
33	12.500	1014	1016	1019	rVB2	21826	26627	1.62%	0.260%
34	12.648	1027	1029	1032	rBV	338401	366657	22.26%	3.580%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
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35	13.128	1068	1071	1074	rVB	11787	20864	1.27%	0.204%
36	14.648	1201	1204	1207	rBV	1585741	1647314	100.00%	16.086%
37	15.391	1267	1269	1272	rBV	38502	47084	2.86%	0.460%
38	15.826	1304	1307	1309	rBV	34184	53957	3.28%	0.527%
39	15.928	1313	1316	1318	rVV	355089	418431	25.40%	4.086%
40	17.083	1414	1417	1423	rBV2	51053	96632	5.87%	0.944%
41	17.574	1457	1460	1462	rBV	19606	28744	1.74%	0.281%
42	17.620	1462	1464	1467	rBV	313028	409185	24.84%	3.996%
43	18.032	1498	1500	1503	rVB2	18957	29009	1.76%	0.283%

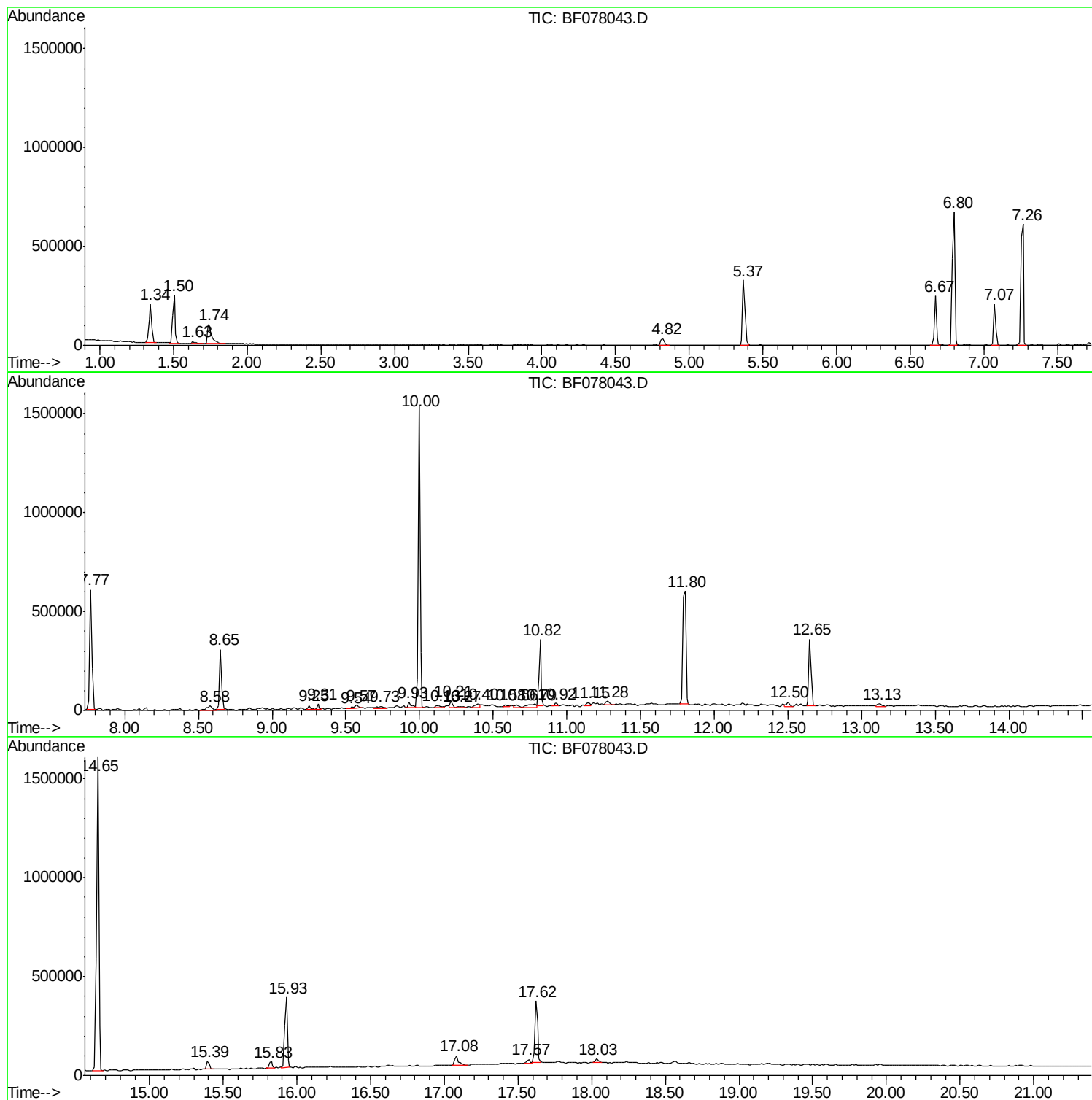
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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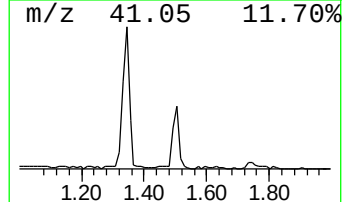
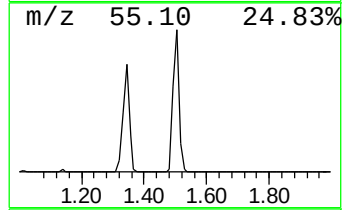
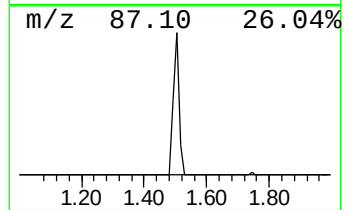
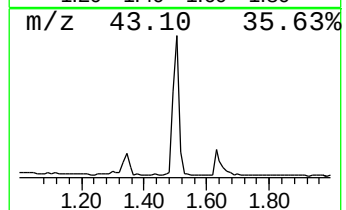
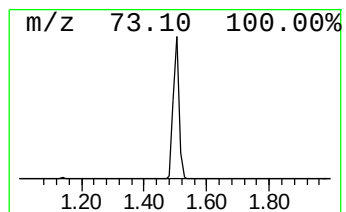
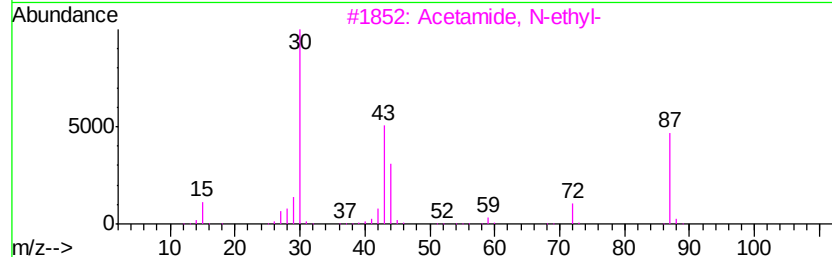
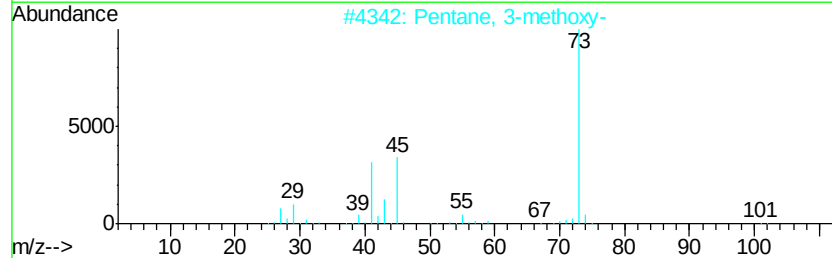
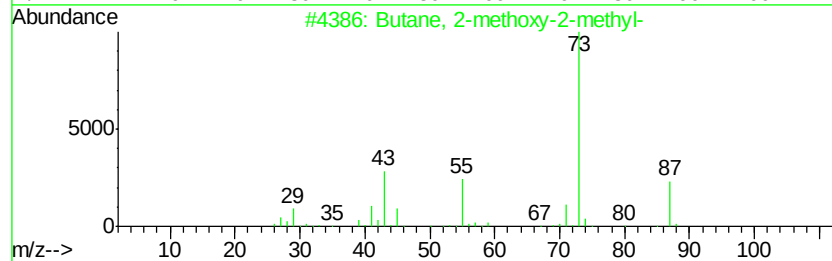
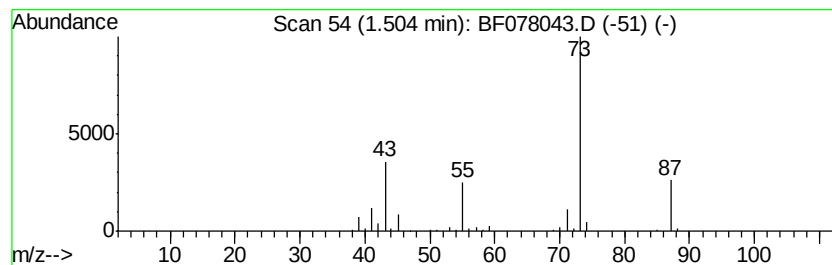
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	30.28 ng	296736	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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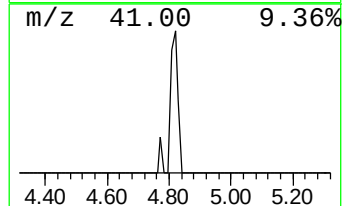
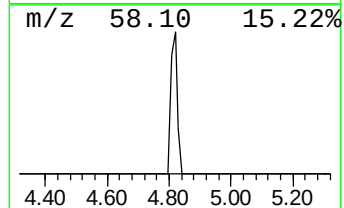
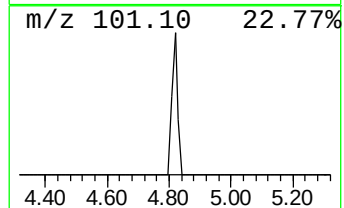
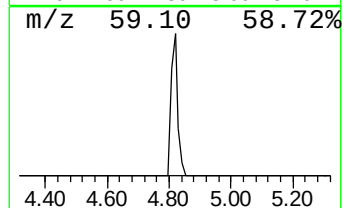
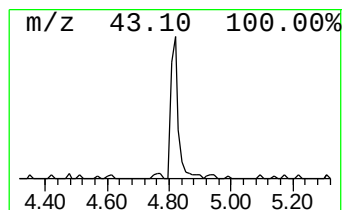
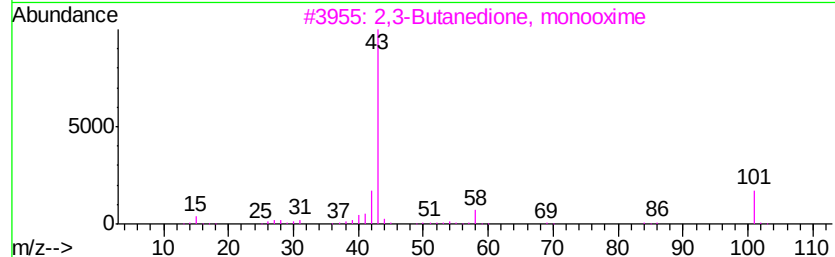
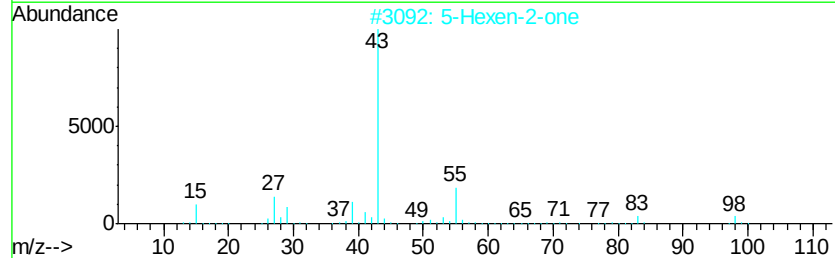
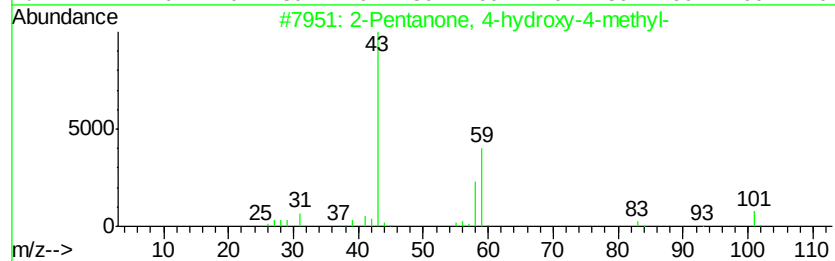
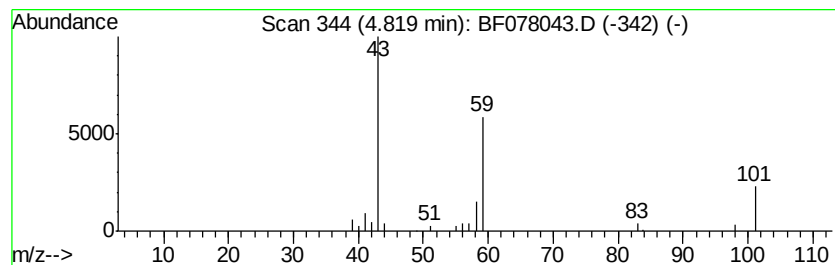
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	5.02 ng	49235	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		5-Hexen-2-one	98	C6H10O	000109-49-9	12
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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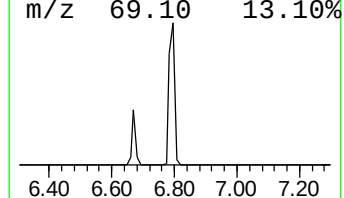
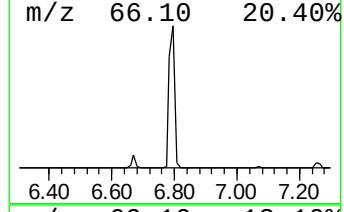
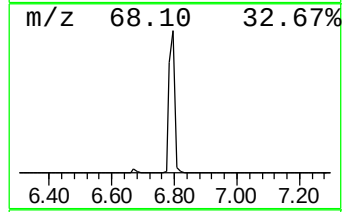
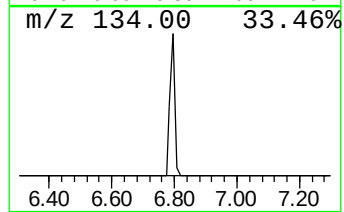
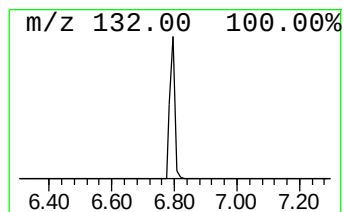
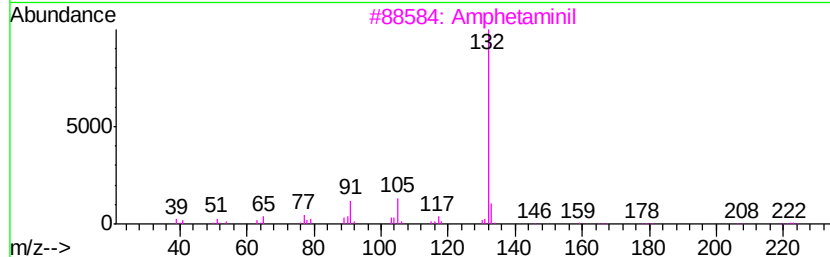
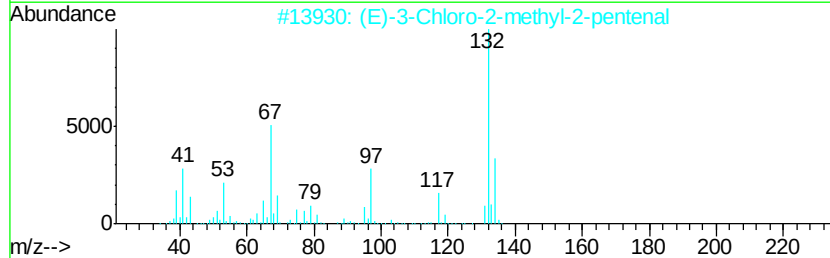
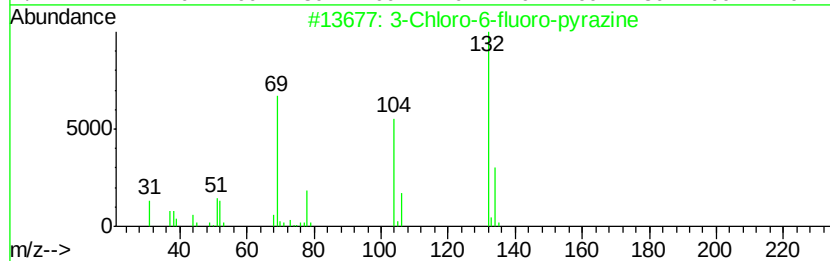
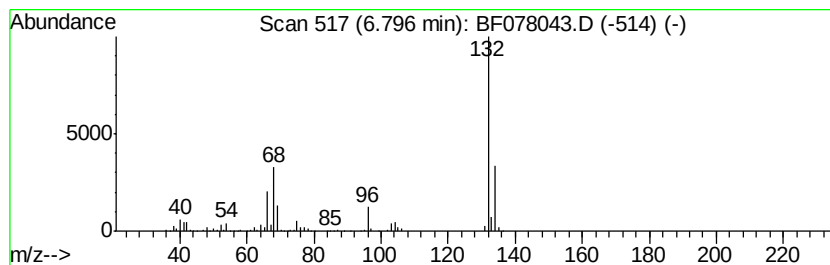
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	79.88 ng	782870	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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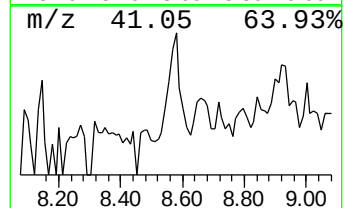
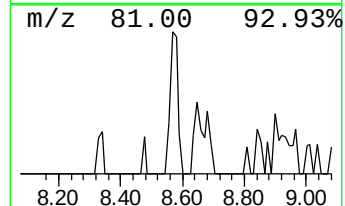
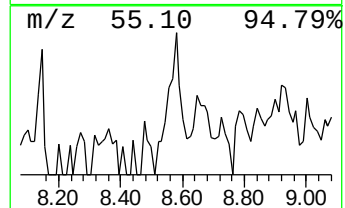
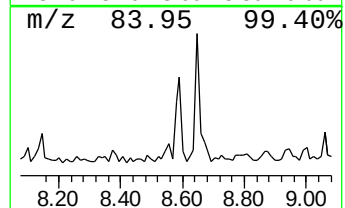
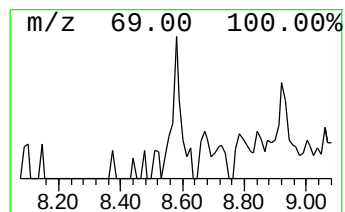
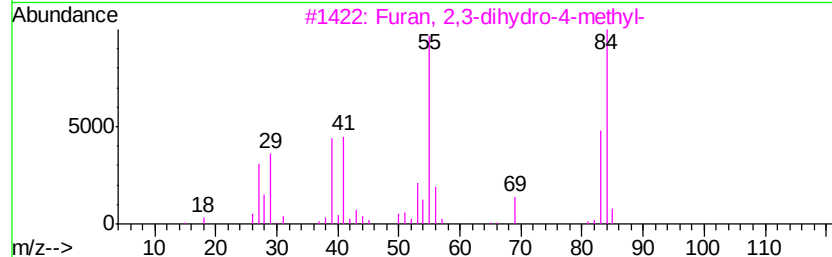
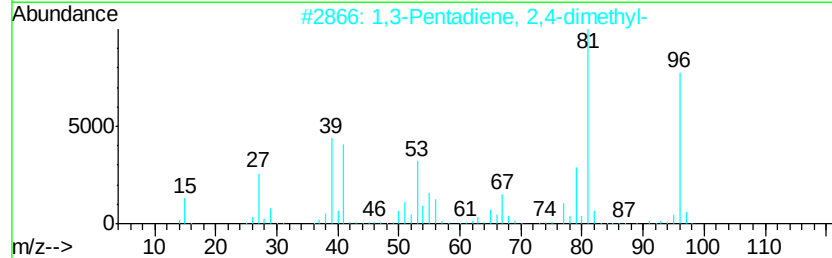
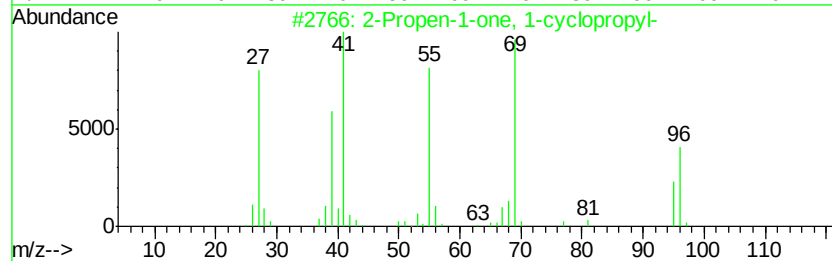
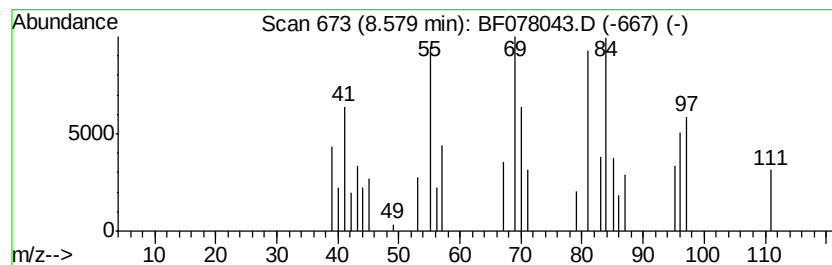
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown8.58 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	3.14 ng	44940	Napthalene-d8	8.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propen-1-one, 1-cyclopropyl-	96	C6H8O	059819-62-4	14
2		1,3-Pentadiene, 2,4-dimethyl-	96	C7H12	001000-86-8	11
3		Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	10
4		1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	10
5		1-Methyl-2-trifluoroacetoxycyclo...	210	C9H13F3O2	1000216-63-9	10



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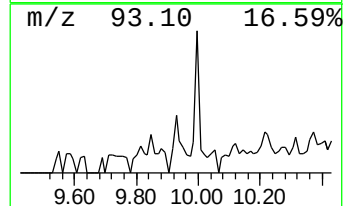
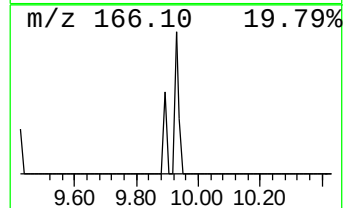
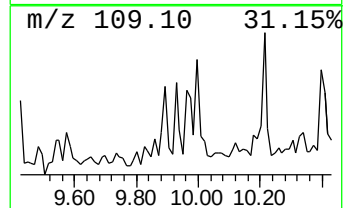
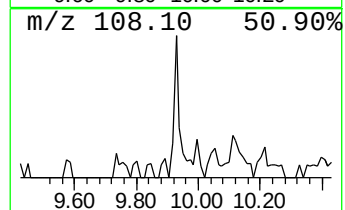
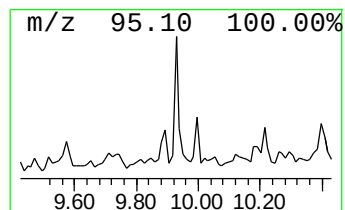
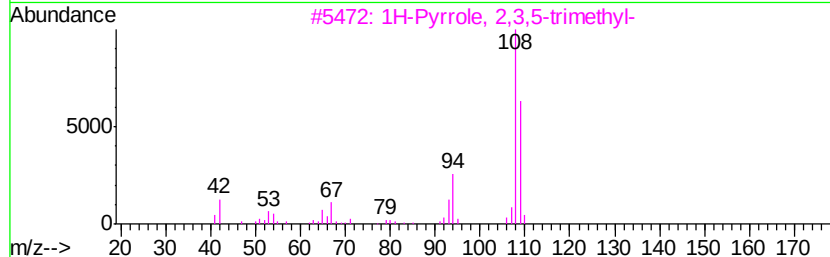
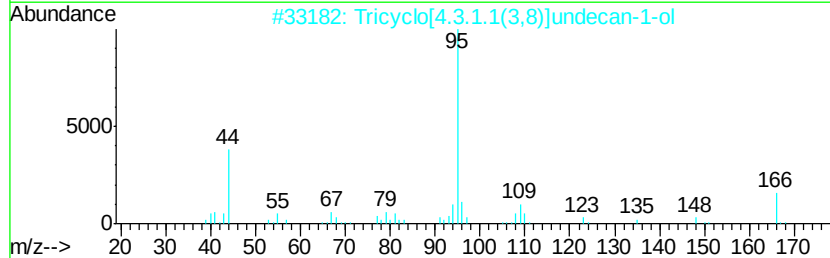
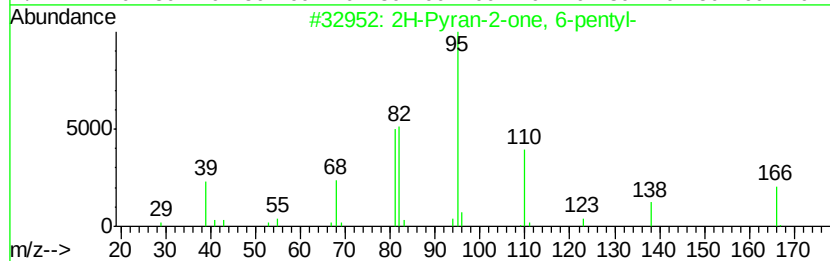
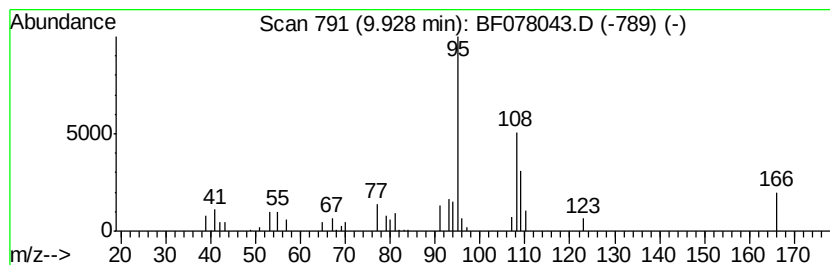
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Peak Number 8 unknown9.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	3.06 ng	52311	Acenaphthene-d10	10.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran-2-one, 6-pentyl-	166	C10H14O2	027593-23-3	43
2		Tricyclo[4.3.1.1(3,8)]undecan-1-ol	166	C11H18O	031061-64-0	36
3		1H-Pyrrole, 2,3,5-trimethyl-	109	C7H11N	002199-41-9	27
4		Cyclopropane, tetramethylmethylen-	110	C8H14	054376-39-5	25
5		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032715\
Data File : BF078043.D
Acq On : 27 Mar 2015 18:19
Operator : TP/IZ
Sample : G1654-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

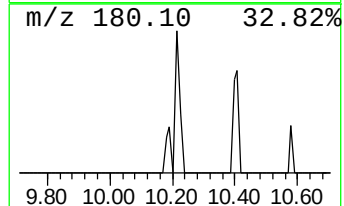
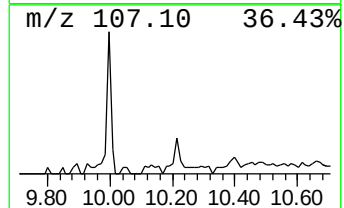
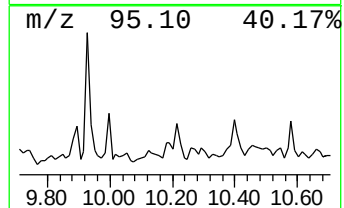
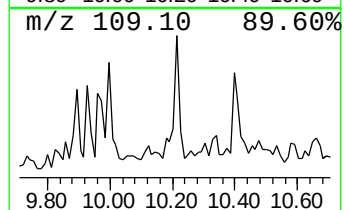
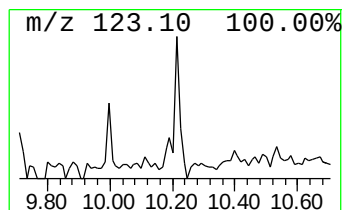
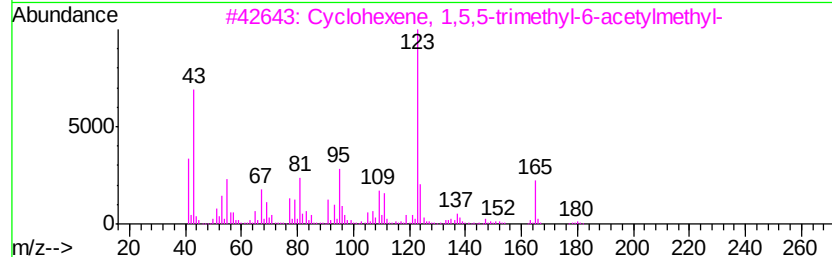
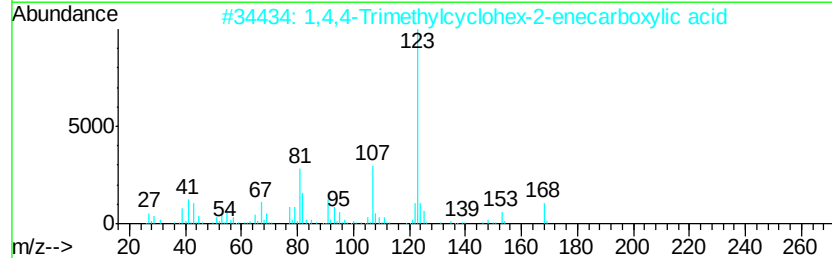
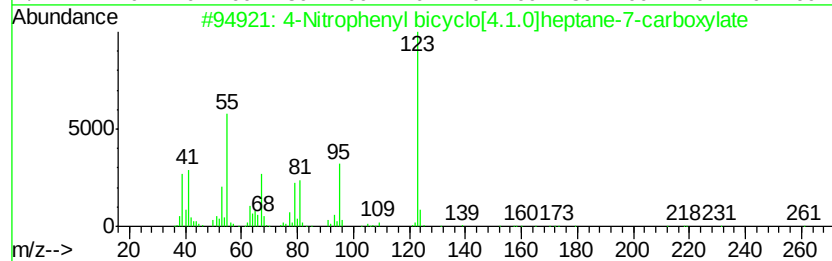
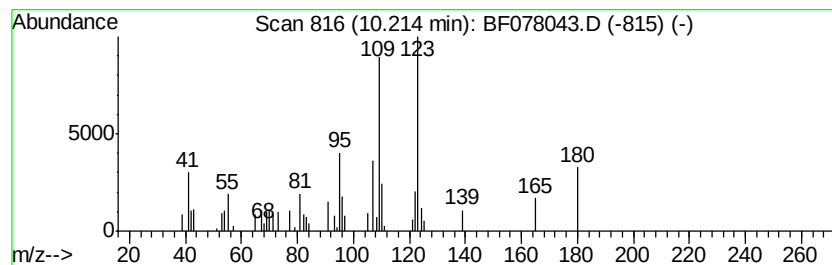
Instrument :
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ClientSampleId :
PZ-8-3-24-15

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.21 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	2.08 ng	35566	Acenaphthene-d10	10.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		4-Nitrophenyl bicyclo[4.1.0]hept...	261 C14H15N04	328938-65-4 27
2		1,4,4-Trimethylcyclohex-2-enecar...	168 C10H16O2	103262-04-0 27
3		Cyclohexene, 1,5,5-trimethyl-6-a...	180 C12H20O	211563-96-1 25
4		4-Fluorobenzoic acid, undec-10-e...	292 C18H25FO2	1000279-02-8 25
5		Cyclopropanecarboxylic acid, 2,2...	328 C21H28O3	000121-21-1 22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032715\
Data File : BF078043.D
Acq On : 27 Mar 2015 18:19
Operator : TP/IZ
Sample : G1654-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-8-3-24-15

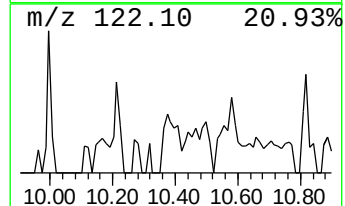
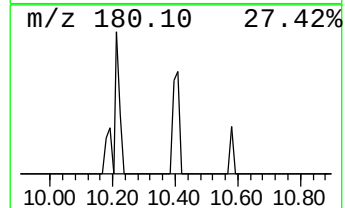
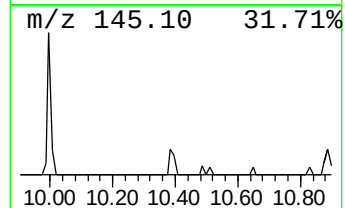
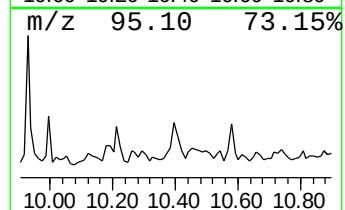
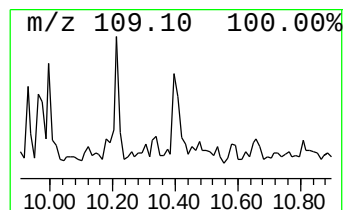
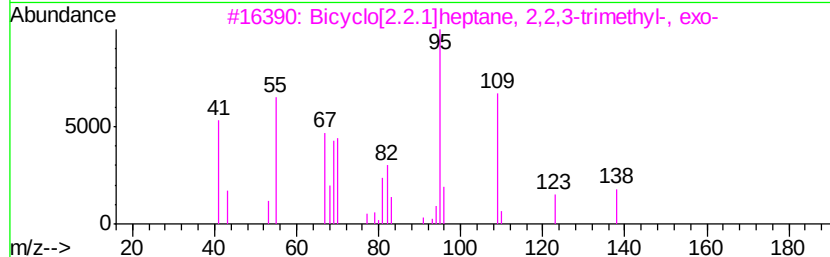
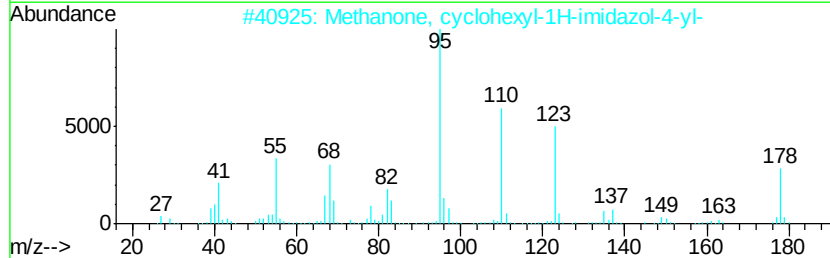
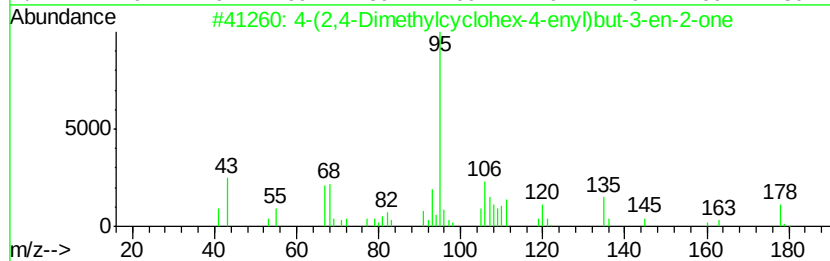
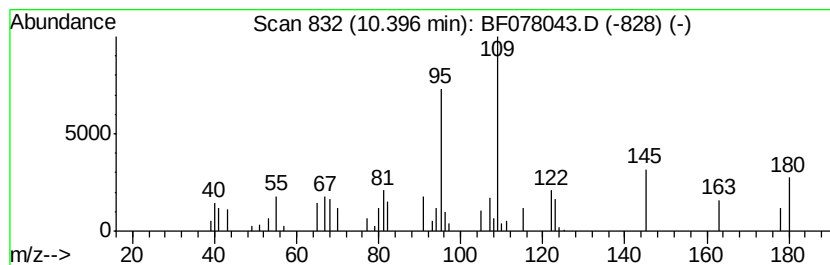
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.40 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.05 ng	34973	Acenaphthene-d10	10.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-(2,4-Dimethylcyclohex-4-enyl)b...	178	C12H18O	1000215-26-2	27
2		Methanone, cyclohexyl-1H-imidazo...	178	C10H14N2O	061985-29-3	27
3		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	25
4		4,7-Methanobenzofuran, 2,2'-oxyb...	374	C24H38O3	087248-50-8	25
5		Tricyclo[4.3.1.1(3,8)]undecan-1-ol	166	C11H18O	031061-64-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032715\
Data File : BF078043.D
Acq On : 27 Mar 2015 18:19
Operator : TP/IZ
Sample : G1654-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

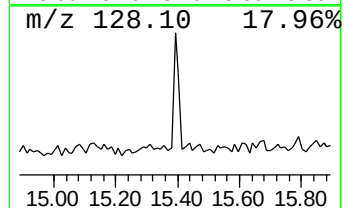
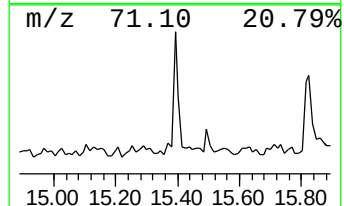
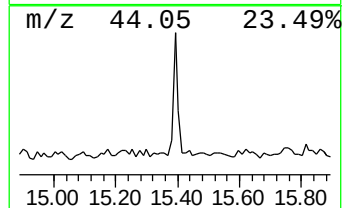
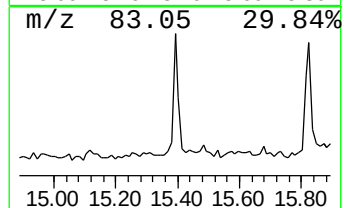
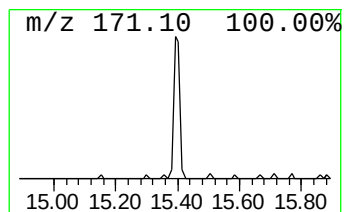
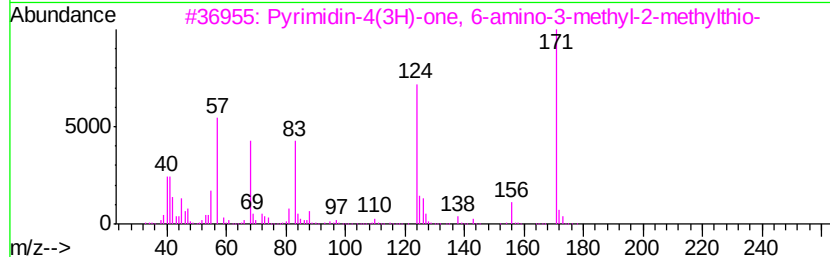
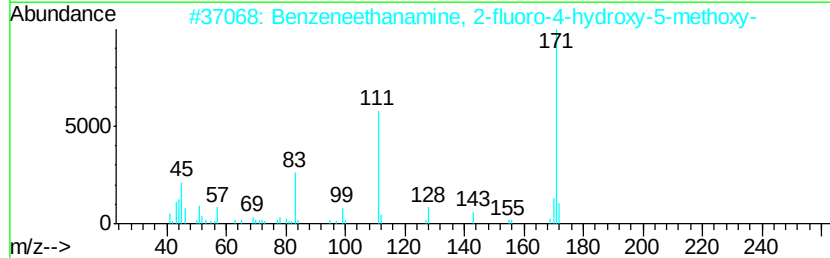
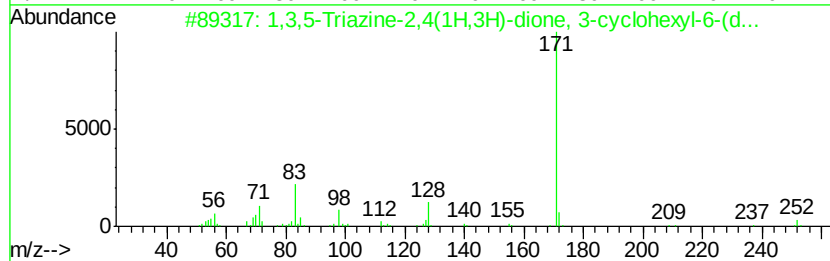
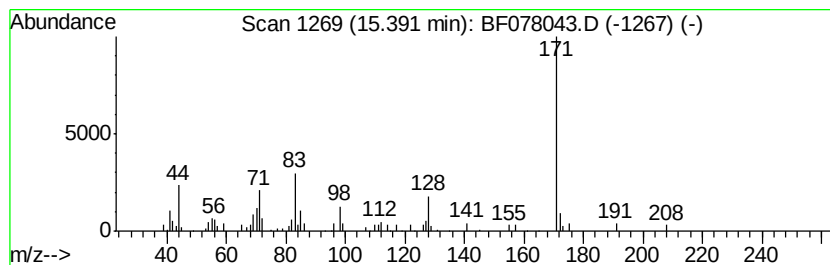
Instrument :
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ClientSampleId :
PZ-8-3-24-15

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.39	2.25 ng	47084	Chrysene-d12	15.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	91
2		Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	50
3		Pvrimidin-4(3H)-one, 6-amino-3-m...	171	C6H9N3OS	102363-06-4	43
4		N-Methoxy-2-carbethoxy-2-carbamo...	188	C7H12N2O4	063859-03-0	42
5		3H,6H-Thieno[3,4-c]isoxazole, 3a...	171	C8H13NOS	127865-49-0	39



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032715\
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Sample : G1654-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-8-3-24-15

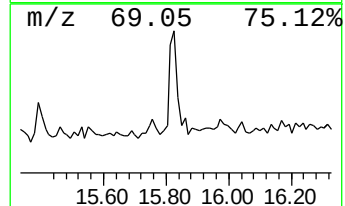
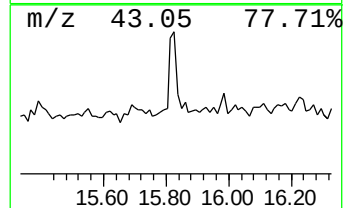
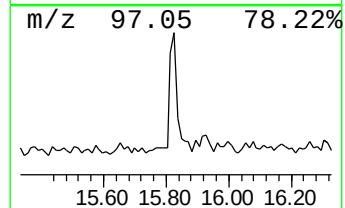
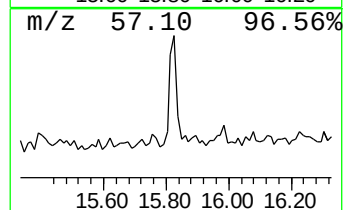
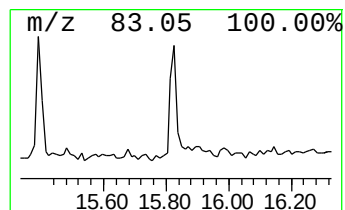
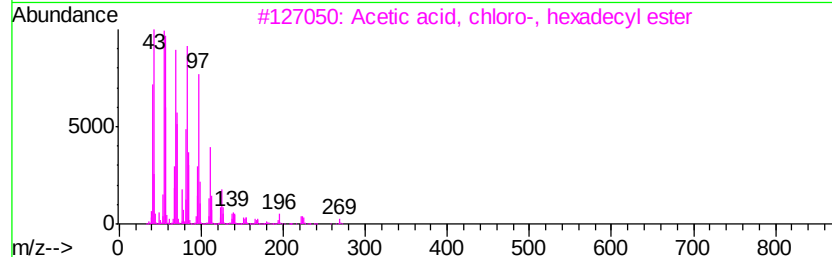
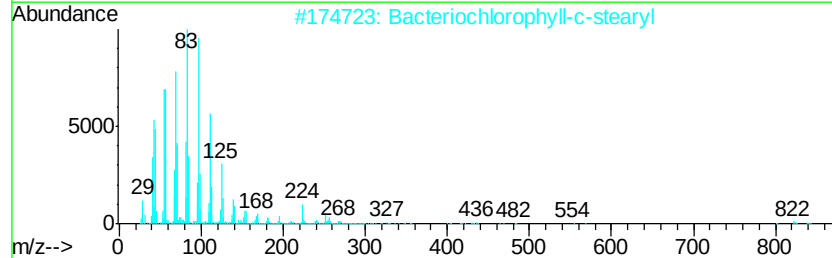
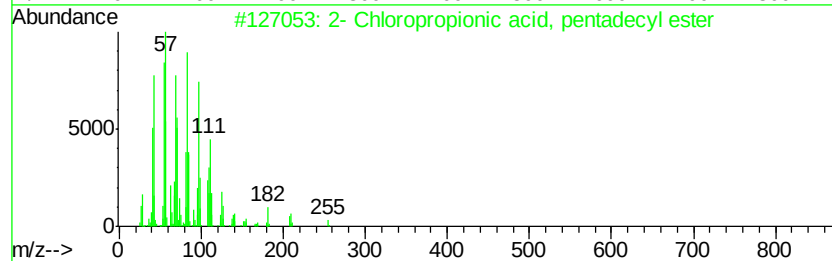
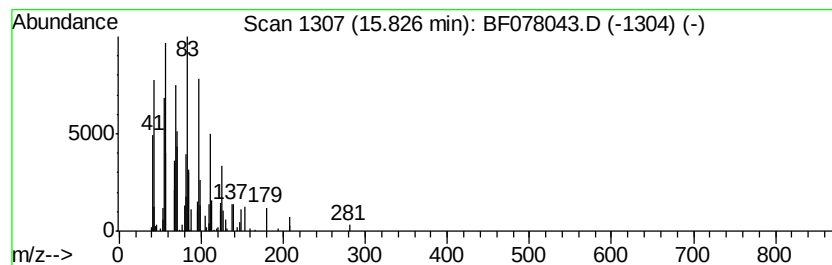
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2- Chloropropionic acid, pe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.58 ng	53957	Chrysene-d12	15.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
2			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	91
3			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
4			1-Octadecanol	270	C18H38O	000112-92-5	91
5			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032715\
Data File : BF078043.D
Acq On : 27 Mar 2015 18:19
Operator : TP/IZ
Sample : G1654-07
Misc :
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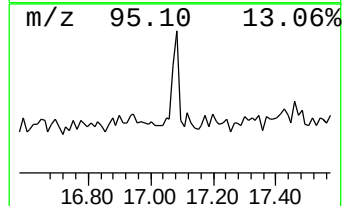
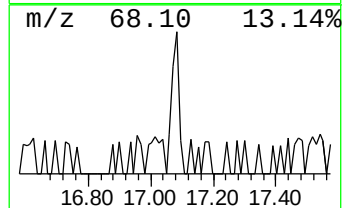
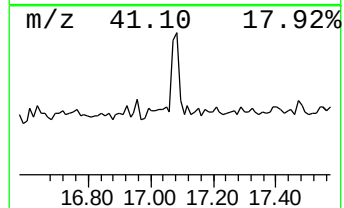
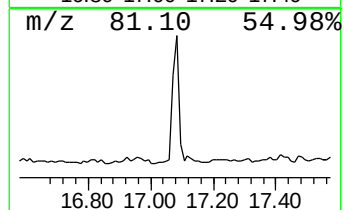
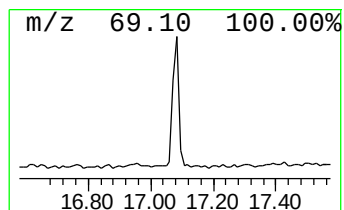
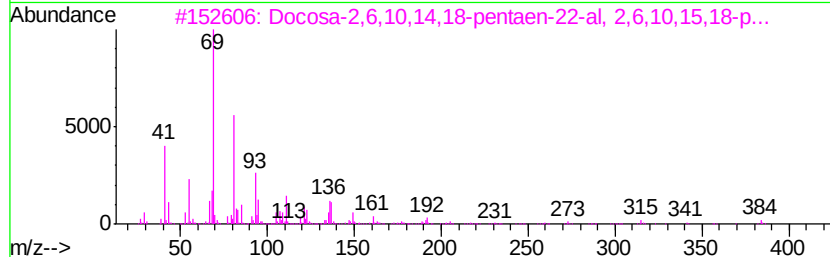
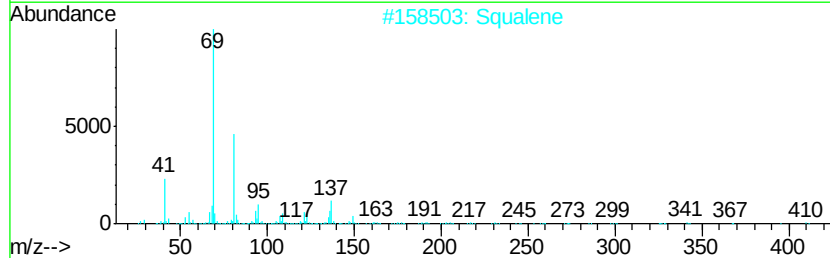
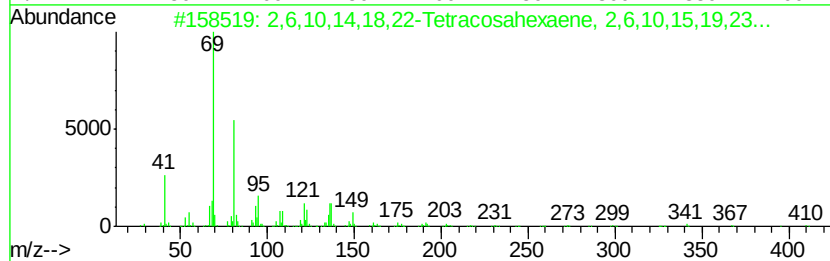
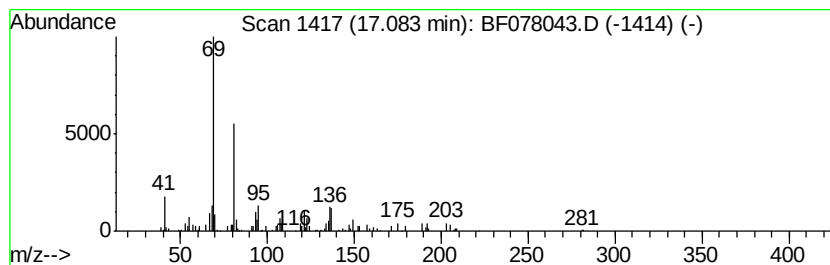
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.08	4.72 ng	96632	Perylene-d12	17.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	87
2	Squalene	410 C30H50	007683-64-9	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384 C27H44O	1000163-04-7	83
4	3,7,11-Trimethyl-dodeca-2,6,10-t...	236 C15H24O2	007548-13-2	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032715\
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Acq On : 27 Mar 2015 18:19
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Sample : G1654-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
Butane, 2-methoxy...	1.50	30.3	ng	296736	1	7.07	196006	20.0
2-Pentanone, 4-hy...	4.82	5.0	ng	49235	1	7.07	196006	20.0
unknown6.80	6.80	79.9	ng	782870	1	7.07	196006	20.0
unknown8.58	8.58	3.1	ng	44940	2	8.65	286350	20.0
unknown9.93	9.93	3.1	ng	52311	3	10.82	341497	20.0
unknown10.21	10.21	2.1	ng	35566	3	10.82	341497	20.0
unknown10.40	10.40	2.0	ng	34973	3	10.82	341497	20.0
1,3,5-Triazine-2,...	15.39	2.3	ng	47084	5	15.93	418431	20.0
2-Chloropropioni...	15.83	2.6	ng	53957	5	15.93	418431	20.0
2,6,10,14,18,22-T...	17.08	4.7	ng	96632	6	17.62	409185	20.0