

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
 Data File : BF087812.D
 Acq On : 8 Jun 2016 16:22
 Operator : UM/SJ
 Sample : H3378-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-20

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-BF060716.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	1.644	3	5	7	rVB	2909021	3654216	100.00%	16.657%
2	1.758	13	15	24	rVB	126973	266524	7.29%	1.215%
3	1.884	24	26	38	rVB	2092826	3290612	90.05%	15.000%
4	2.044	38	40	81	rVB2	87937	589430	16.13%	2.687%
5	4.981	296	297	303	rVB	81953	117269	3.21%	0.535%
6	5.416	332	335	337	rBV	1107483	1140131	31.20%	5.197%
7	6.456	423	426	428	rBV	1262557	1247673	34.14%	5.687%
8	6.593	435	438	440	rBV	1116900	1212392	33.18%	5.526%
9	6.822	456	458	461	rBV	668481	583216	15.96%	2.658%
10	6.982	469	472	474	rBB	1009714	870810	23.83%	3.969%
11	7.382	505	507	510	rBV	604753	657764	18.00%	2.998%
12	8.113	568	571	573	rBV	914762	840350	23.00%	3.831%
13	9.188	663	665	668	rVB	1162335	1146540	31.38%	5.226%
14	9.588	698	700	702	rBV	335105	268562	7.35%	1.224%
15	9.873	722	725	727	rBV	767404	851334	23.30%	3.881%
16	10.651	791	793	796	rBV	666172	693181	18.97%	3.160%
17	11.348	852	854	858	rBV2	647290	816463	22.34%	3.722%
18	12.559	958	960	963	rVB	175501	157616	4.31%	0.718%
19	12.788	977	980	983	rBV	145299	157031	4.30%	0.716%
20	12.948	991	994	996	rVB	665424	910805	24.92%	4.152%
21	13.851	1070	1073	1077	rBV	30891	58502	1.60%	0.267%
22	13.988	1082	1085	1091	rVB	648684	750681	20.54%	3.422%
23	14.857	1158	1161	1165	rVB	24407	41326	1.13%	0.188%
24	15.005	1171	1174	1178	rBV	80062	161085	4.41%	0.734%
25	15.108	1181	1183	1185	rVB	38012	43087	1.18%	0.196%
26	15.291	1197	1199	1202	rVB	45624	63128	1.73%	0.288%
27	15.348	1202	1204	1207	rBV	44563	69431	1.90%	0.316%
28	15.417	1207	1210	1213	rBV	454959	579677	15.86%	2.642%
29	15.897	1249	1252	1255	rBV	25961	53109	1.45%	0.242%
30	16.800	1328	1331	1336	rBV2	22264	47924	1.31%	0.218%
31	17.211	1365	1367	1373	rVB	17901	39251	1.07%	0.179%
32	17.394	1379	1383	1394	rBV6	47772	210039	5.75%	0.957%
33	17.828	1417	1421	1426	rBV5	20632	82322	2.25%	0.375%
34	17.920	1426	1429	1436	rVB5	36602	110479	3.02%	0.504%

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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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.160	1445	1450	1451	rBV4	24778	65502	1.79%	0.299%
36	19.360	1549	1555	1565	rVB3	23894	90605	2.48%	0.413%

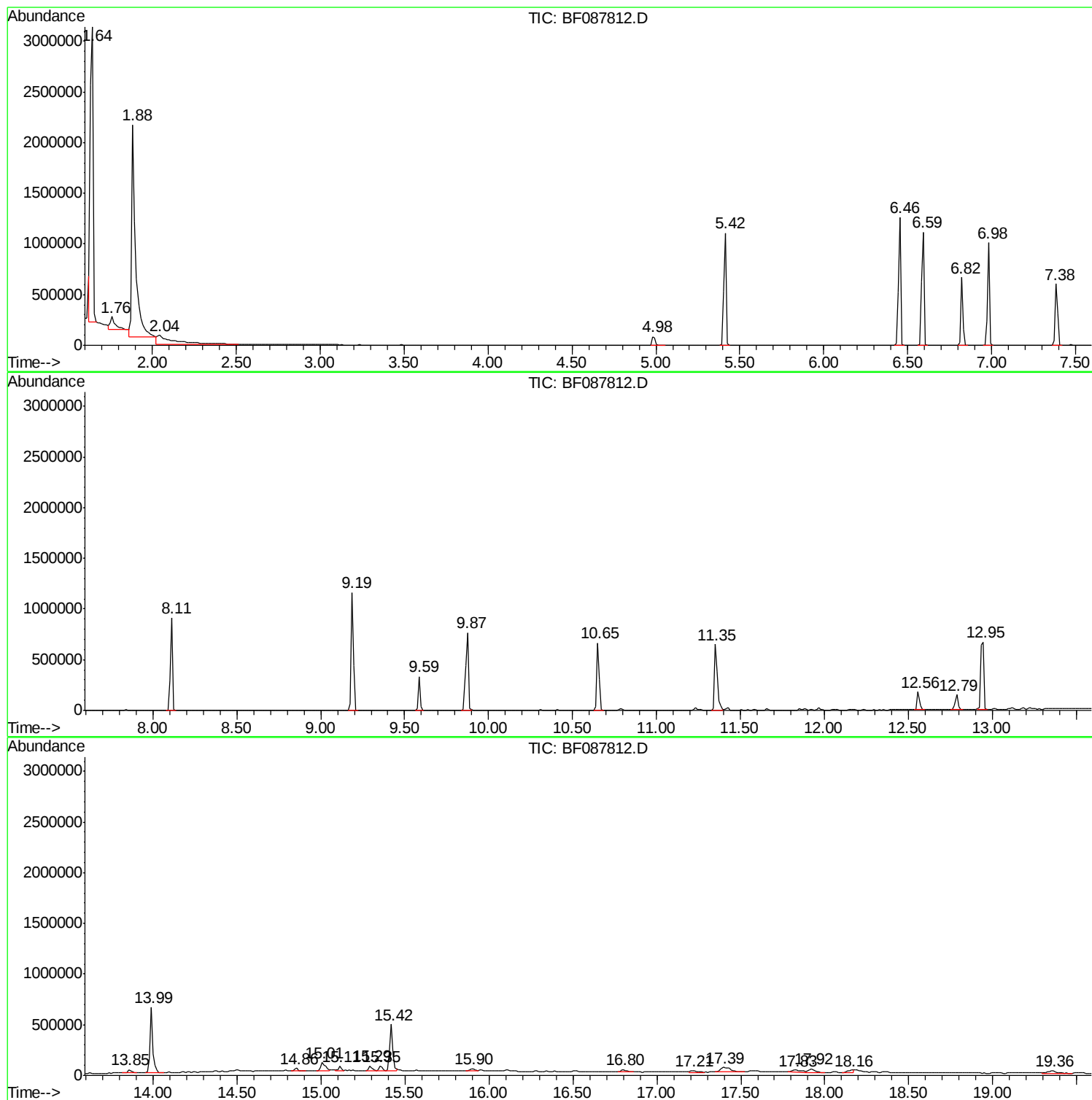
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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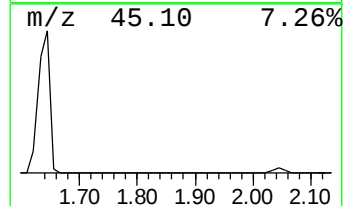
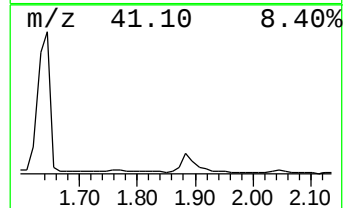
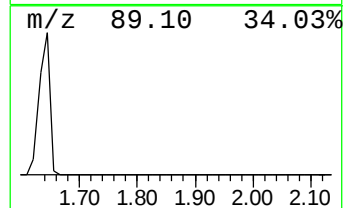
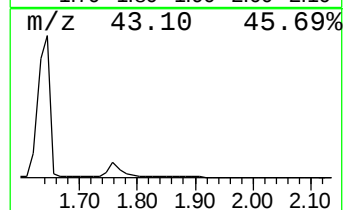
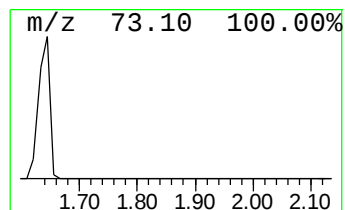
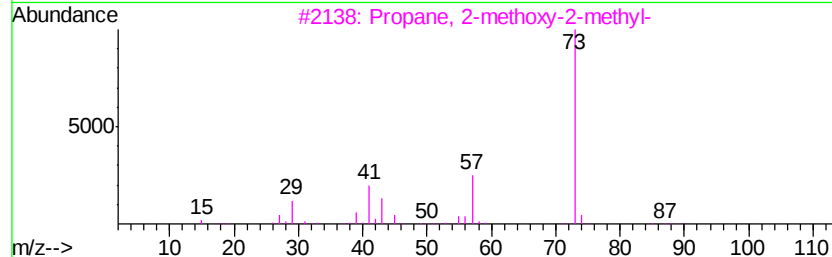
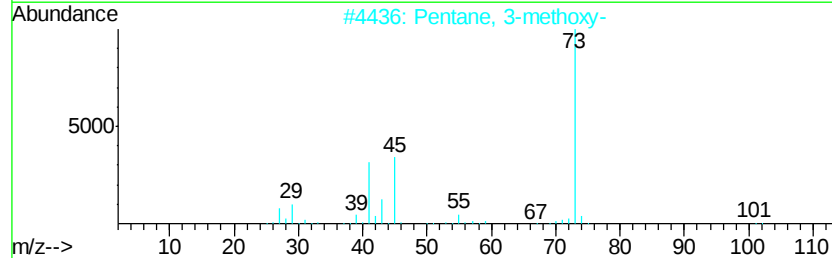
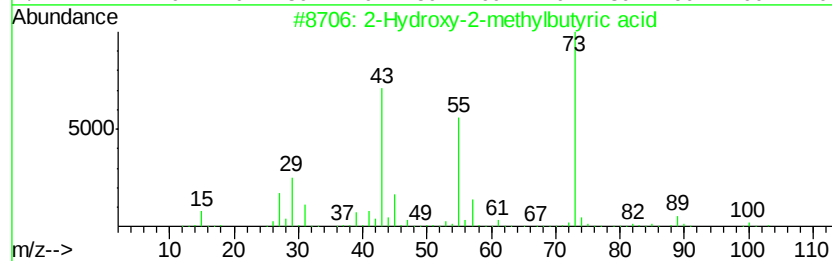
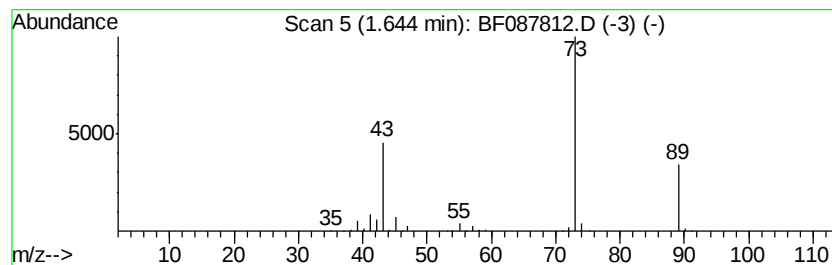
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	125.31 ng	3654220	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	9
5			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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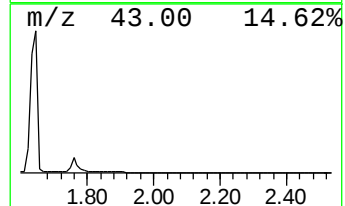
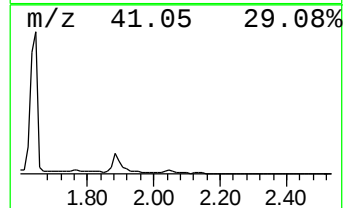
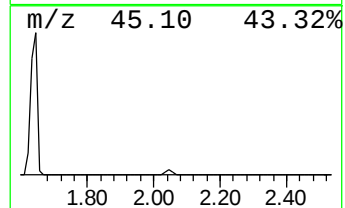
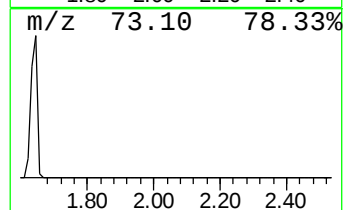
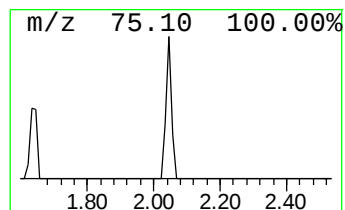
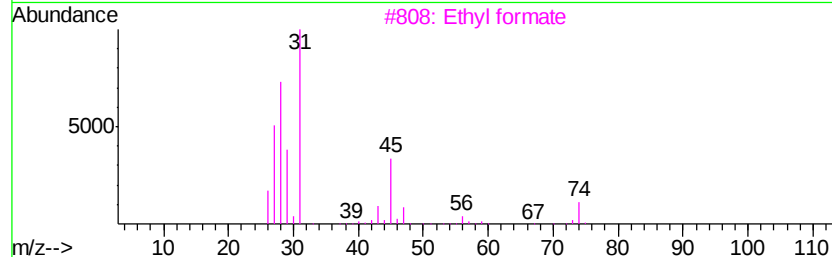
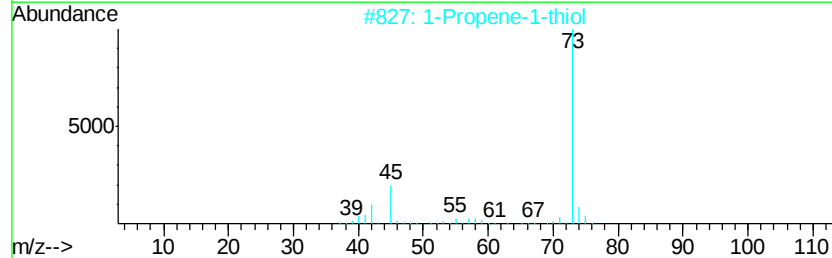
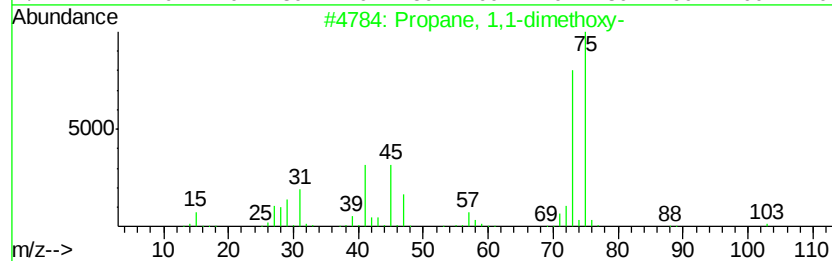
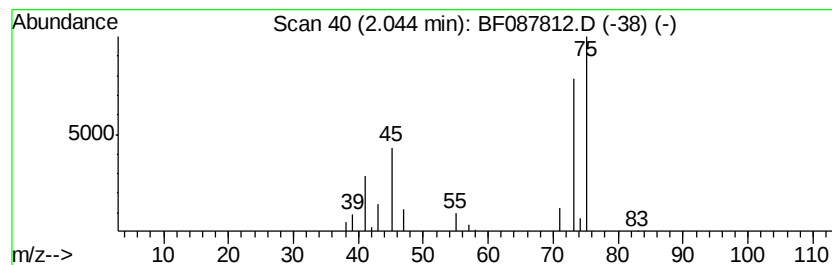
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown2.04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	20.21 ng	589430	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
2		1-Propene-1-thiol	74	C3H6S	000925-89-3	4
3		Ethyl formate	74	C3H6O2	000109-94-4	4
4		Formamide, N-methylthio	75	C2H5NS	018952-41-5	4
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	4



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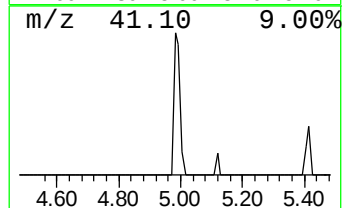
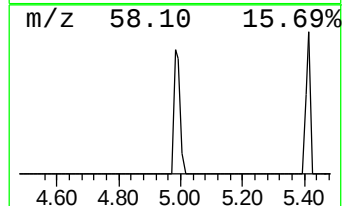
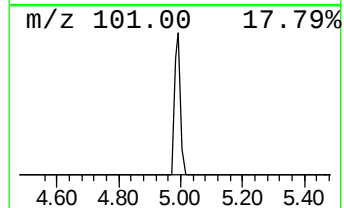
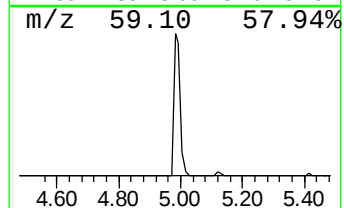
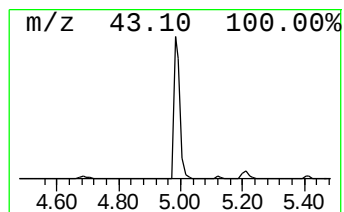
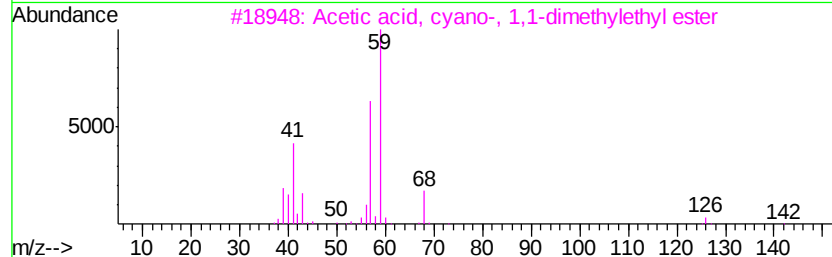
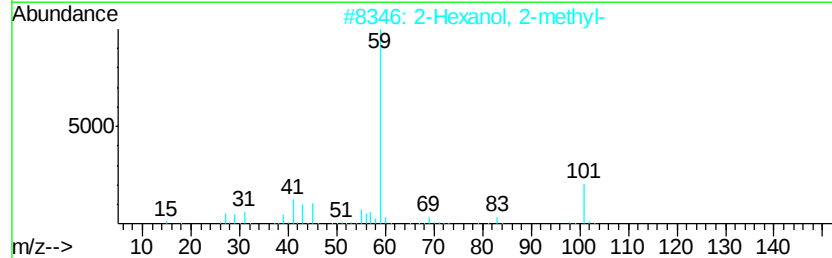
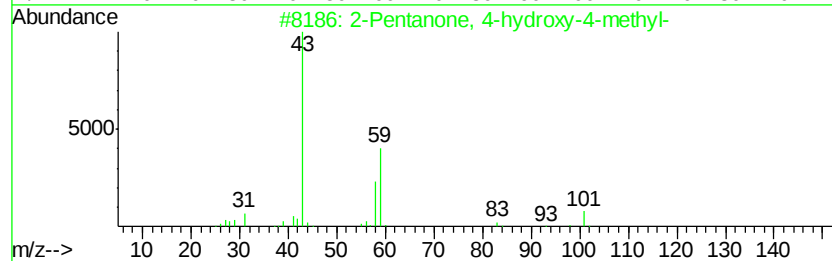
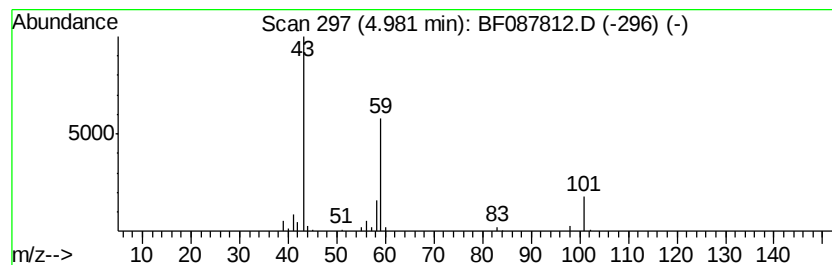
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown4.98 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	4.02 ng	117269	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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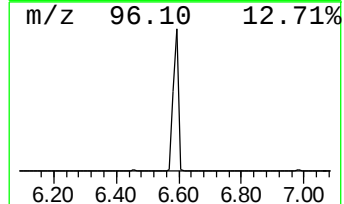
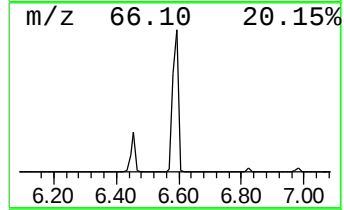
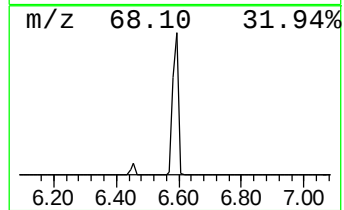
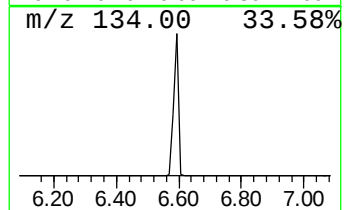
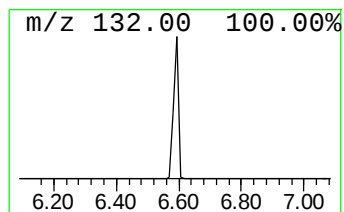
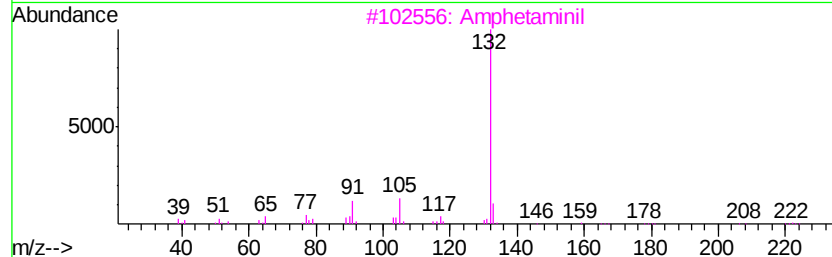
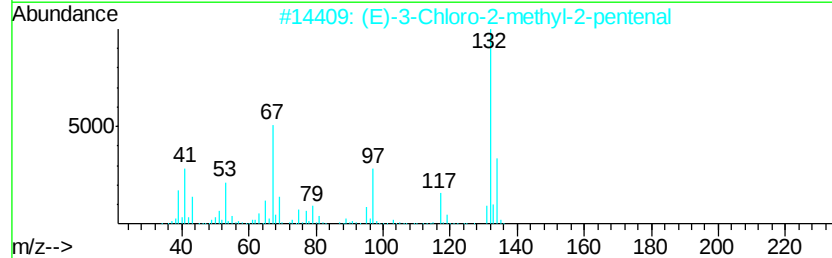
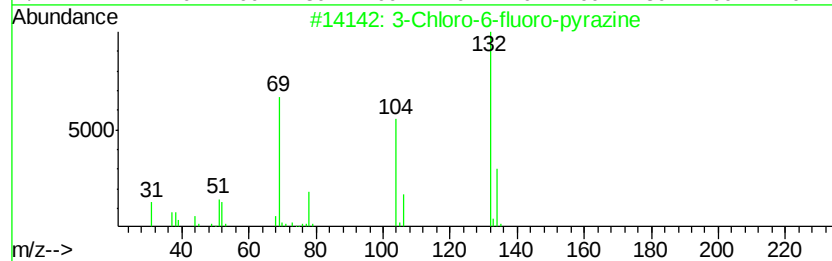
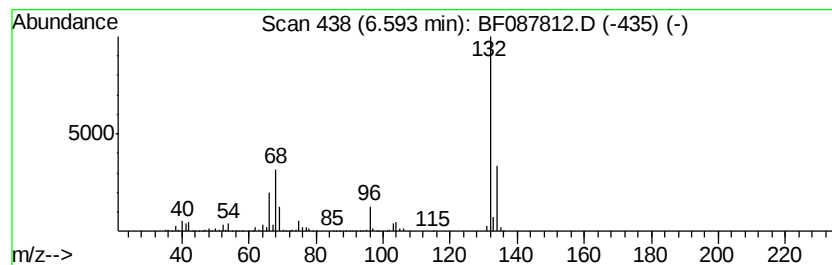
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	41.58 ng	1212390	1,4-Dichlorobenzene-d4	6.82

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	17
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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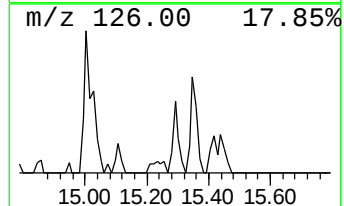
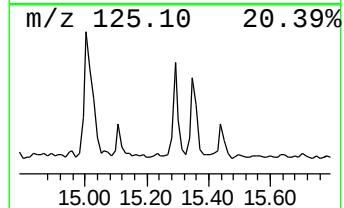
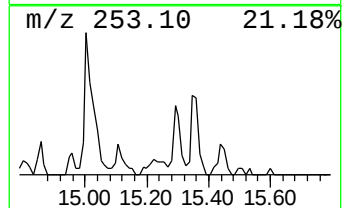
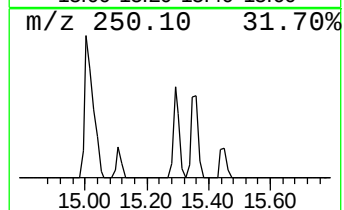
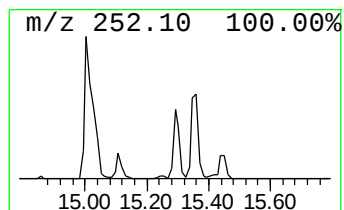
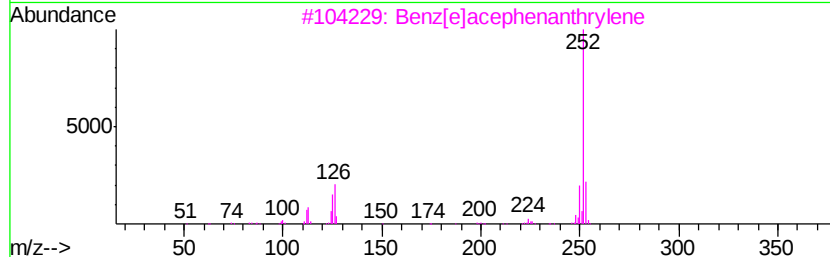
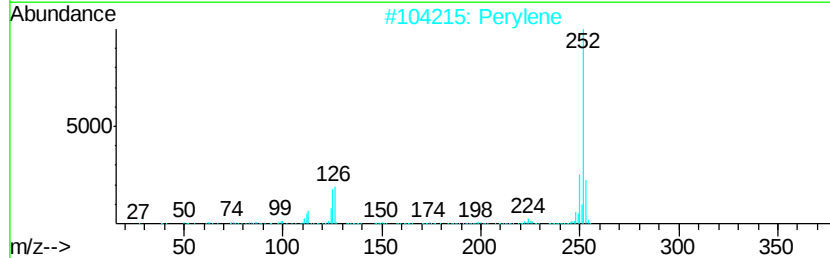
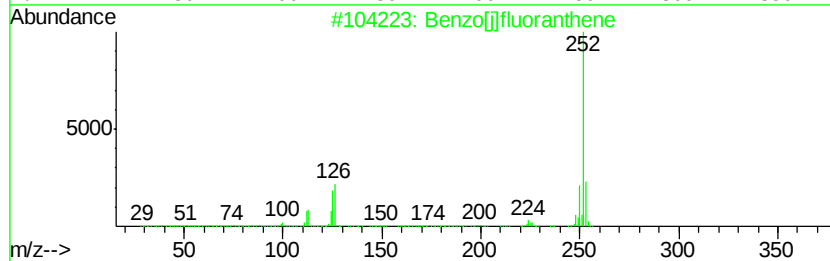
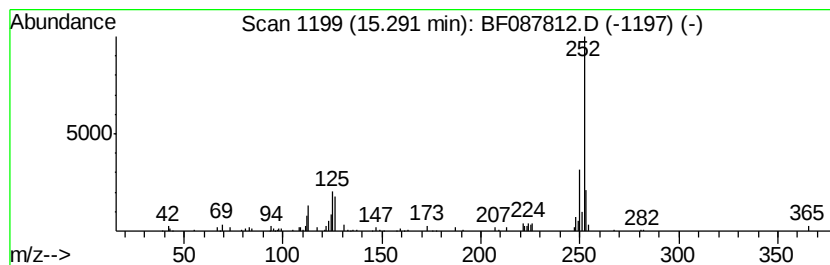
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 Benzo[j]fluoranthene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.18 ng	63128	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[i]fluoranthene	252	C20H12	000205-82-3	96
2		Perylene	252	C20H12	000198-55-0	96
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5		Benzo[e]pyrene	252	C20H12	000192-97-2	95



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Misc :
ALS Vial : 7 Sample Multiplier: 1

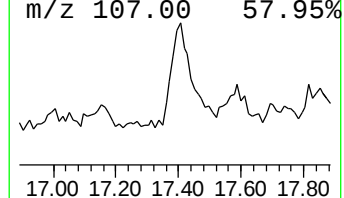
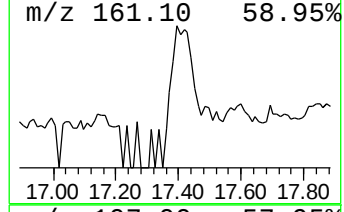
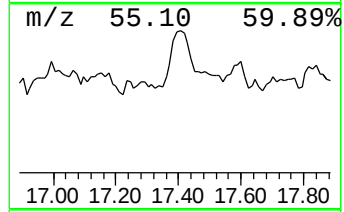
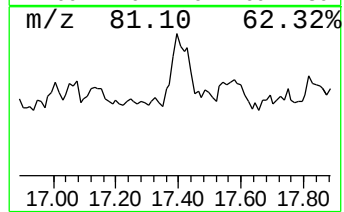
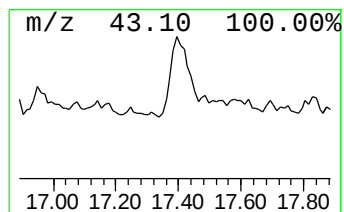
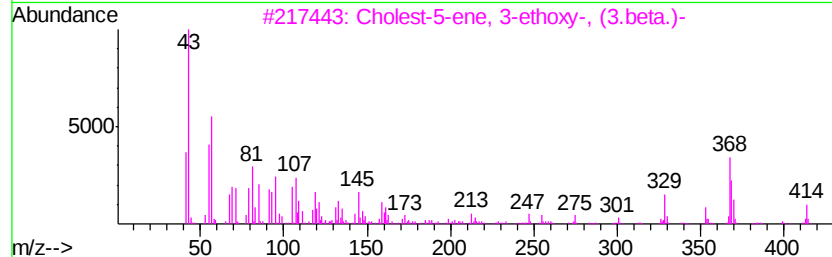
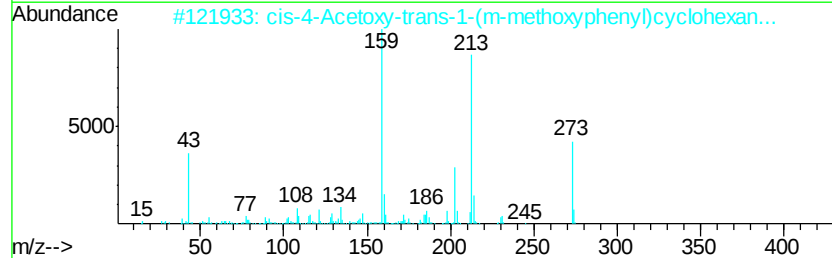
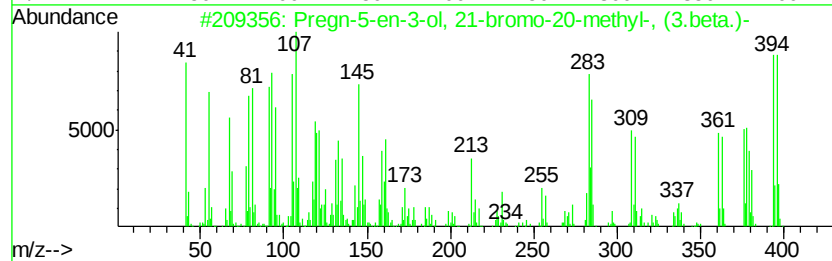
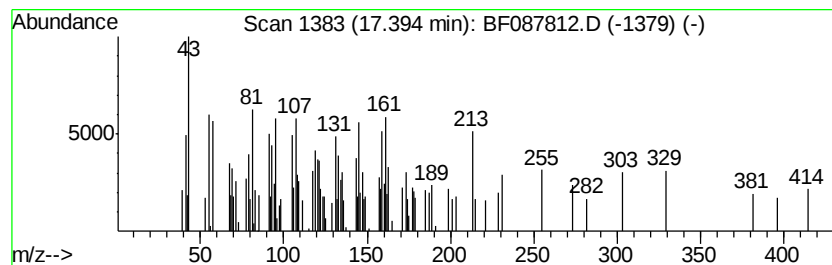
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.39 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	7.25 ng	210039	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pregn-5-en-3-ol, 21-bromo-20-met...	394 C22H35BrO	055103-80-5	27
2	cis-4-Acetoxy-trans-1-(m-methoxy...	273 C16H19NO3	1000241-10-4	22
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H50O	000986-19-6	18
4	Spirost-5-en-3-ol, acetate, (3.b...	456 C29H44O4	001061-54-7	14
5	1H-Pyrrole-1-carboxylic acid, 2-...	329 C15H24BrN02	168106-33-0	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087812.D
Acq On : 8 Jun 2016 16:22
Operator : UM/SJ
Sample : H3378-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-20

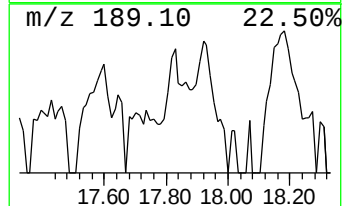
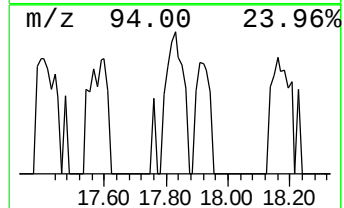
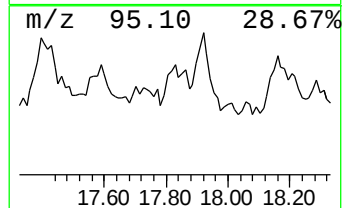
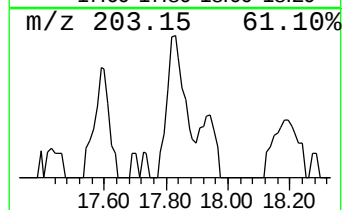
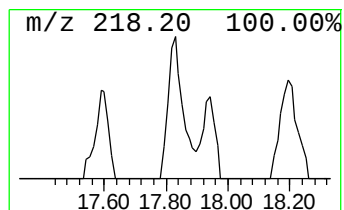
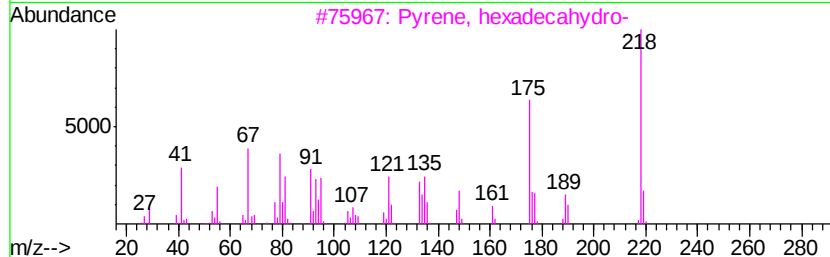
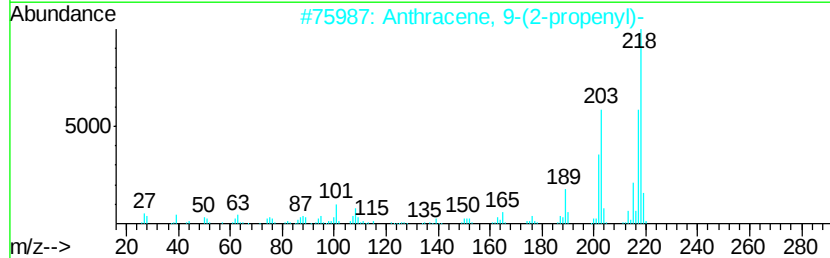
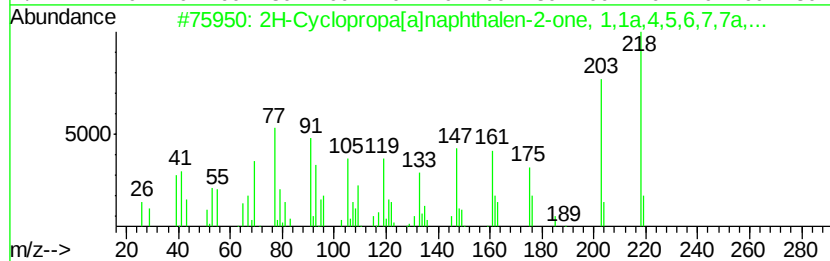
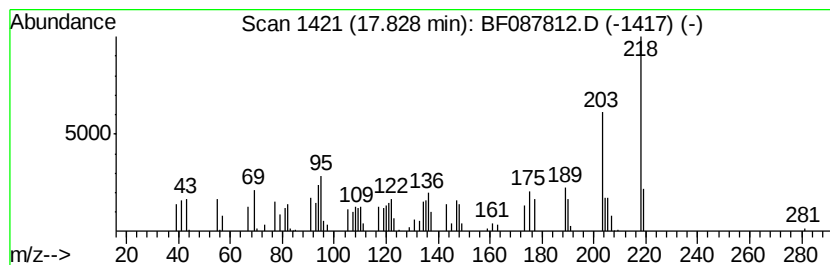
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2H-Cyclopropa[a]naphthalen-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	2.84 ng	82322	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	64
2		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	52
3		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	49
4		2-Chloro-5,6-dimethyl-1-(2-propyl...	218	C12H11ClN2	080276-20-6	49
5		6H-[1,2]Dioxeto[3',4':4,5]furo[3...	260	C14H12O5	129812-24-4	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087812.D
Acq On : 8 Jun 2016 16:22
Operator : UM/SJ
Sample : H3378-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SS-20

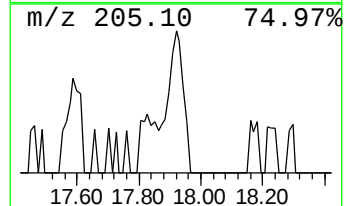
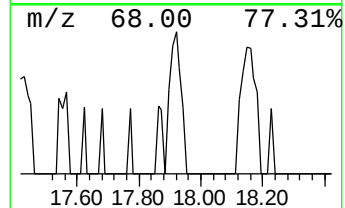
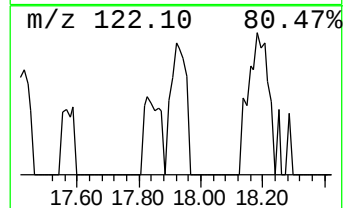
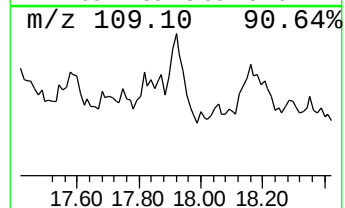
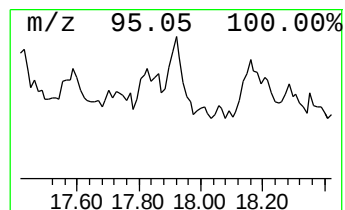
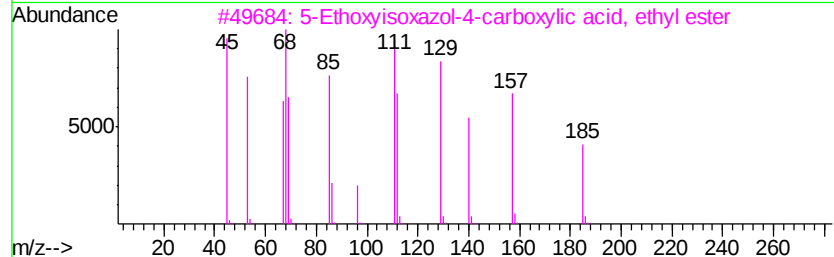
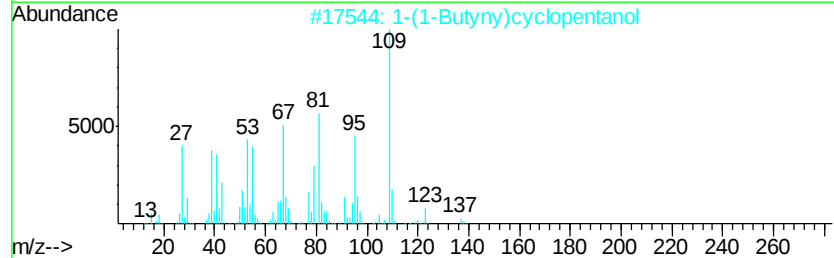
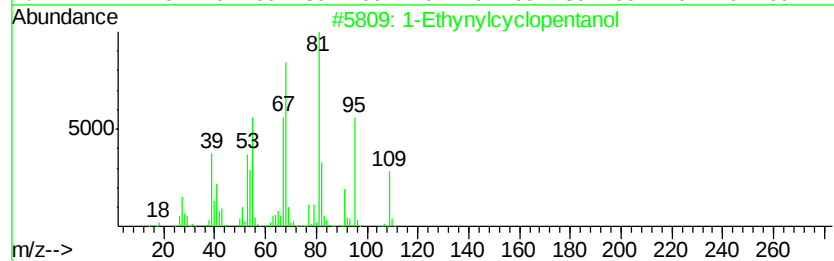
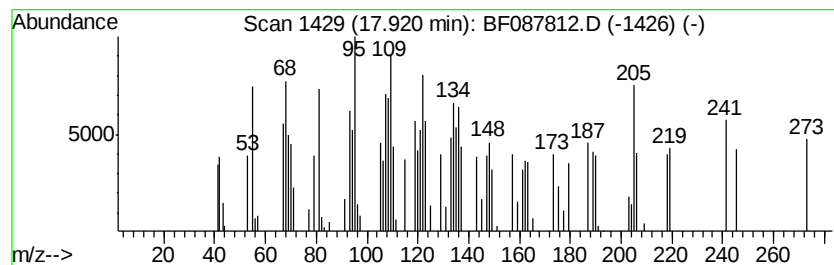
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.92 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	3.81 ng	110479	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethynylcyclopentanol	110	C7H10O	017356-19-3	35
2			1-(1-Butynyl)cyclopentanol	138	C9H14O	1000342-86-5	27
3			5-Ethoxyisoxazol-4-carboxylic ac...	185	C8H11NO4	1000306-38-6	25
4			1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	22
5			Cyclohexane, 1-methyl-4-methylene-	110	C8H14	002808-80-2	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087812.D
Acq On : 8 Jun 2016 16:22
Operator : UM/SJ
Sample : H3378-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-20

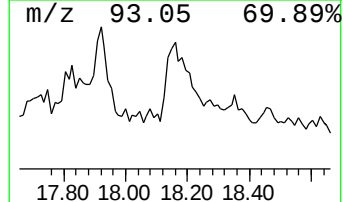
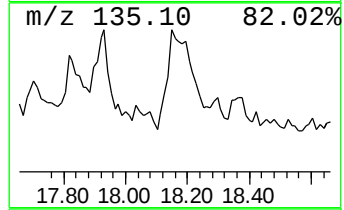
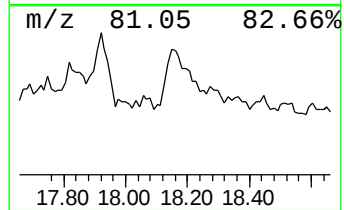
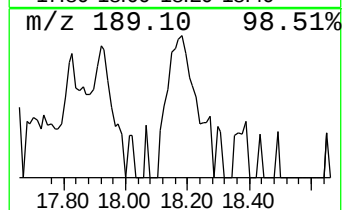
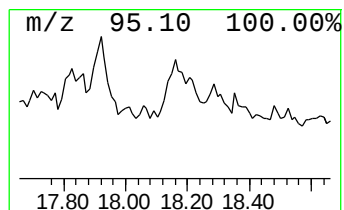
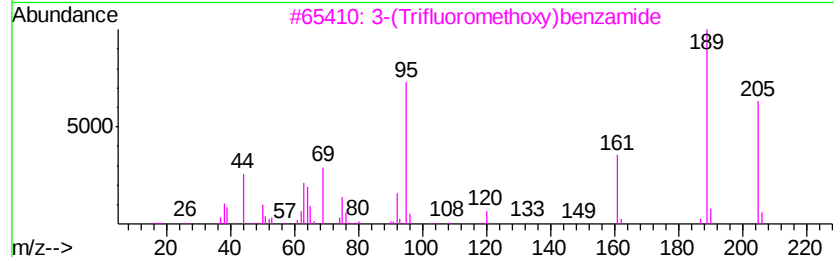
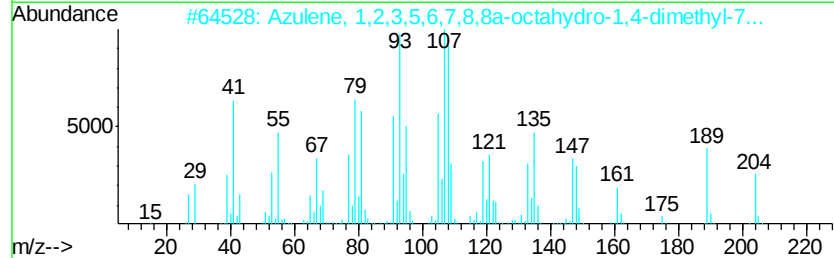
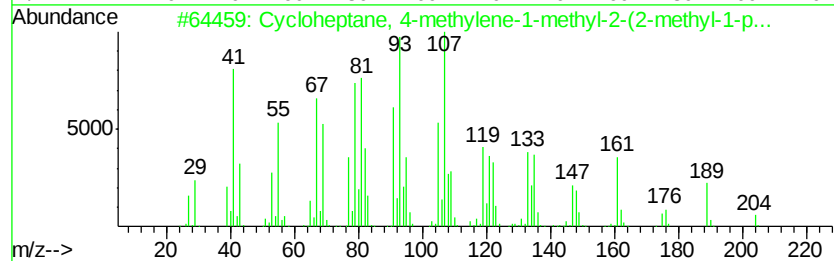
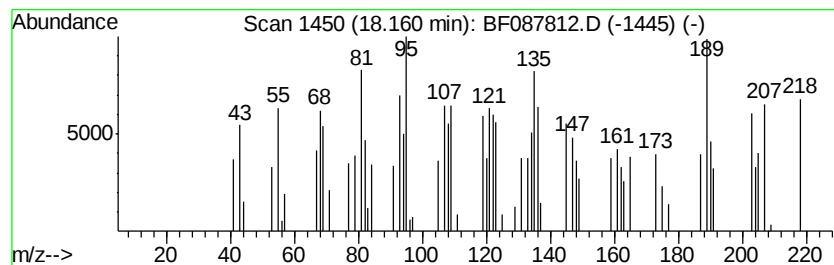
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.16 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	2.26 ng	65502	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	38
2		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	35
3		3-(Trifluoromethoxy)benzamide	205	C8H6F3NO2	000658-91-3	27
4		2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	18
5		1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087812.D
Acq On : 8 Jun 2016 16:22
Operator : UM/SJ
Sample : H3378-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

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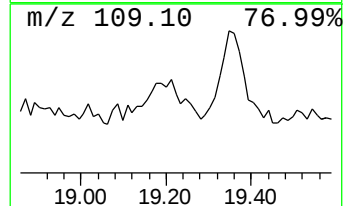
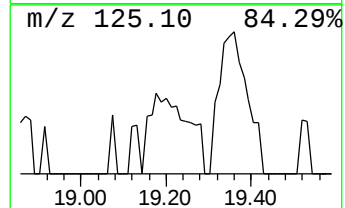
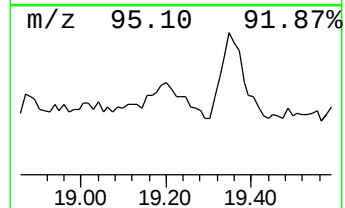
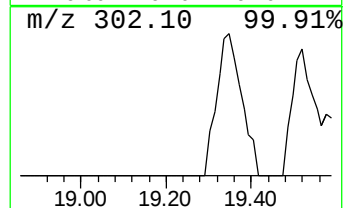
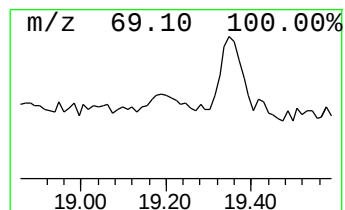
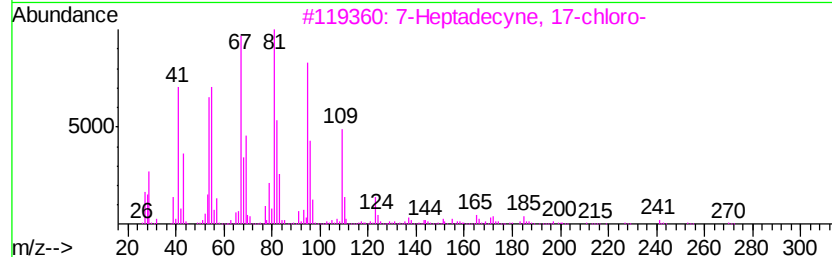
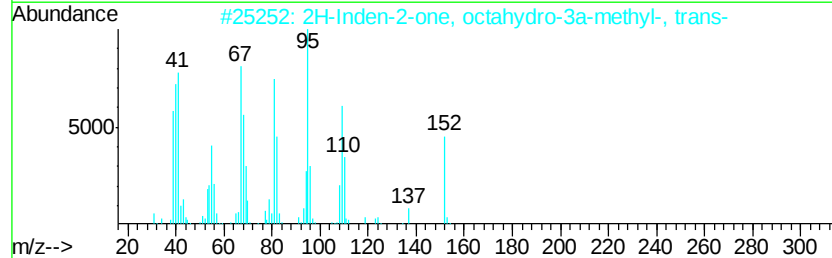
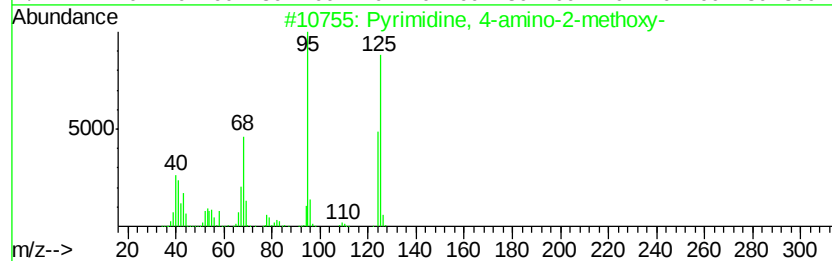
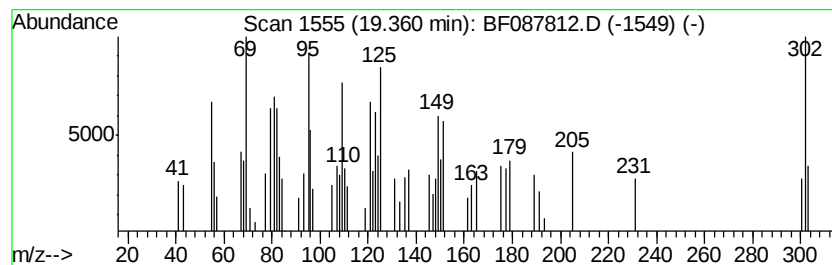
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.36 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.36	3.13 ng	90605	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrimidine, 4-amino-2-methoxy-	125	C5H7N3O	003289-47-2	18
2		2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	020379-99-1	14
3		7-Heptadecyne, 17-chloro-	270	C17H31Cl	056554-75-7	14
4		2-Hydroxyphenol bis(trifluoroact...	302	C10H4F6O4	023529-06-8	14
5		1-Cyclopentyl-4-(1-methylethyl)c...	194	C14H26	1000215-44-4	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
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Acq On : 8 Jun 2016 16:22
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Sample : H3378-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-20

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
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unknown2.04	2.04	20.2	ng	589430	1	6.82	583216	20.0
unknown4.98	4.98	4.0	ng	117269	1	6.82	583216	20.0
unknown6.59	6.59	41.6	ng	1212390	1	6.82	583216	20.0
Benzo[j]fluoranthene	15.29	2.2	ng	63128	6	15.42	579677	20.0
unknown17.39	17.39	7.3	ng	210039	6	15.42	579677	20.0
2H-Cyclopropa[a]n...	17.83	2.8	ng	82322	6	15.42	579677	20.0
unknown17.92	17.92	3.8	ng	110479	6	15.42	579677	20.0
unknown18.16	18.16	2.3	ng	65502	6	15.42	579677	20.0
unknown19.36	19.36	3.1	ng	90605	6	15.42	579677	20.0