

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
 Data File : BF097612.D
 Acq On : 12 Aug 2017 00:35
 Operator : SJ/JU
 Sample : I4631-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VE-1-2

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-BF081117.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	4.751	518	521	532	rBV3	22922	62286	2.10%	0.223%
2	5.428	632	636	658	rBV	474233	1150902	38.87%	4.119%
3	7.075	913	916	928	rBV	292208	680187	22.97%	2.434%
4	7.169	928	932	947	rVB	1221108	2050778	69.25%	7.340%
5	7.510	986	990	1012	rVB	362427	530542	17.92%	1.899%
6	7.745	1025	1030	1043	rBV	1250918	1659926	56.05%	5.941%
7	8.339	1128	1131	1140	rBV3	43927	115296	3.89%	0.413%
8	8.422	1140	1145	1159	rVV	957930	1523089	51.43%	5.451%
9	8.528	1160	1163	1170	rVV2	30779	53167	1.80%	0.190%
10	8.598	1170	1175	1181	rVV4	21420	35640	1.20%	0.128%
11	9.386	1302	1309	1314	rBV6	17679	38467	1.30%	0.138%
12	9.475	1320	1324	1328	rBV5	26371	45846	1.55%	0.164%
13	9.539	1330	1335	1340	rVV	500273	666839	22.52%	2.387%
14	9.604	1342	1346	1350	rVB5	40883	75022	2.53%	0.268%
15	9.804	1375	1380	1387	rBV10	14043	31113	1.05%	0.111%
16	9.875	1387	1392	1397	rBV8	21445	45731	1.54%	0.164%
17	10.028	1414	1418	1424	rBV6	49743	96658	3.26%	0.346%
18	10.086	1425	1428	1433	rVB4	63724	84977	2.87%	0.304%
19	10.157	1437	1440	1447	rVB5	37069	59794	2.02%	0.214%
20	10.239	1449	1454	1459	rBV	89693	193250	6.53%	0.692%
21	10.310	1461	1466	1473	rVV7	73956	198981	6.72%	0.712%
22	10.380	1474	1478	1482	rVB6	61182	96195	3.25%	0.344%
23	10.480	1487	1495	1498	rBV6	68767	183614	6.20%	0.657%
24	10.622	1512	1519	1524	rBV7	92916	227697	7.69%	0.815%
25	10.675	1524	1528	1537	rVB5	97106	181644	6.13%	0.650%
26	10.775	1539	1545	1550	rBV6	91769	195154	6.59%	0.698%
27	10.833	1552	1555	1558	rVV2	37211	49364	1.67%	0.177%
28	10.998	1580	1583	1587	rBV5	72344	142215	4.80%	0.509%
29	11.316	1632	1637	1644	rVB	1596211	2196665	74.18%	7.862%
30	11.380	1645	1648	1651	rBV4	107721	174440	5.89%	0.624%
31	12.369	1812	1816	1819	rBV	351193	443314	14.97%	1.587%
32	12.657	1862	1865	1868	rBV4	163902	315992	10.67%	1.131%
33	13.674	2034	2038	2042	rVB	423972	549137	18.54%	1.965%
34	14.774	2222	2225	2229	rVB	247441	301579	10.18%	1.079%

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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-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.163	2286	2291	2296	rBV6	296975	755432	25.51%	2.704%
36	17.133	2622	2626	2630	rVB2	992399	1207095	40.76%	4.320%
37	18.104	2788	2791	2794	rBV4	136026	233673	7.89%	0.836%
38	18.474	2851	2854	2860	rVB	382909	459872	15.53%	1.646%
39	19.015	2943	2946	2949	rBV5	123607	220405	7.44%	0.789%
40	19.439	3013	3018	3026	rVB5	740813	1344933	45.42%	4.813%
41	19.792	3073	3078	3087	rBV4	816598	1464636	49.46%	5.242%
42	20.009	3112	3115	3120	rBV6	109894	238470	8.05%	0.853%
43	20.139	3132	3137	3147	rVB3	1891106	2961247	100.00%	10.598%
44	20.280	3159	3161	3163	rBV2	63309	49137	1.66%	0.176%
45	20.474	3190	3194	3202	rVB	1067769	1567020	52.92%	5.608%
46	20.856	3253	3259	3270	rVB	1360360	2399285	81.02%	8.587%
47	21.292	3328	3333	3339	rVB	197747	355533	12.01%	1.272%
48	21.791	3414	3418	3426	rVB3	110898	228958	7.73%	0.819%

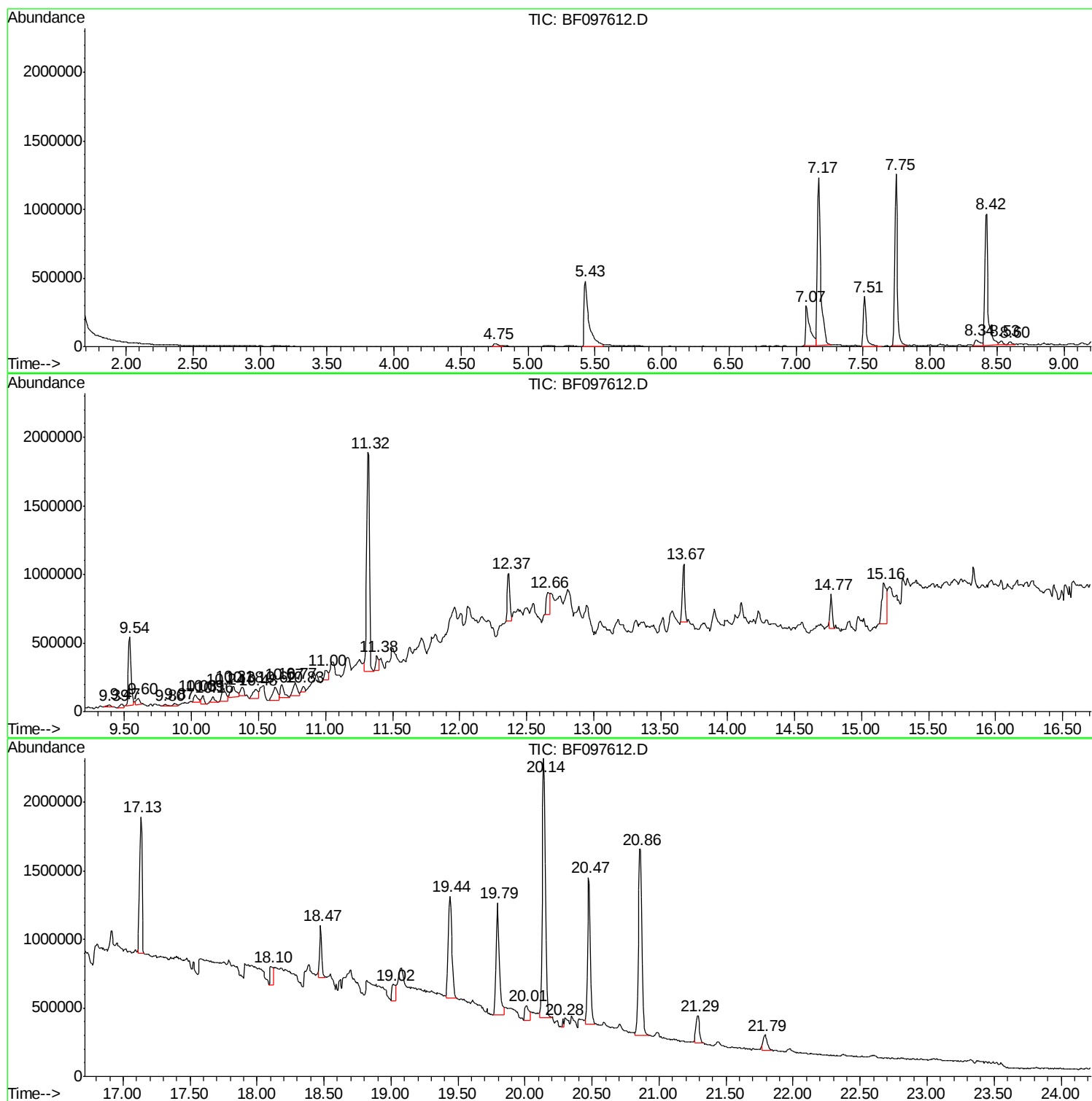
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ClientSampled :
VE-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE-1-2

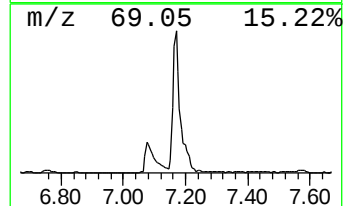
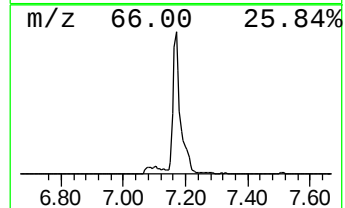
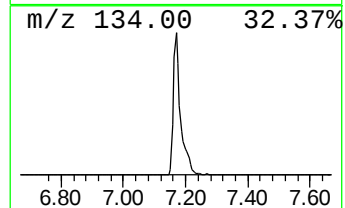
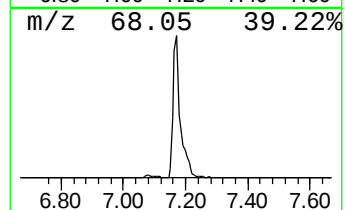
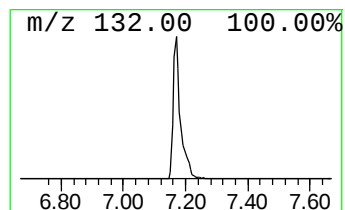
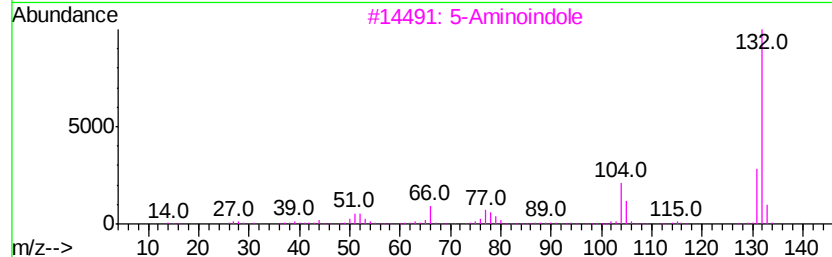
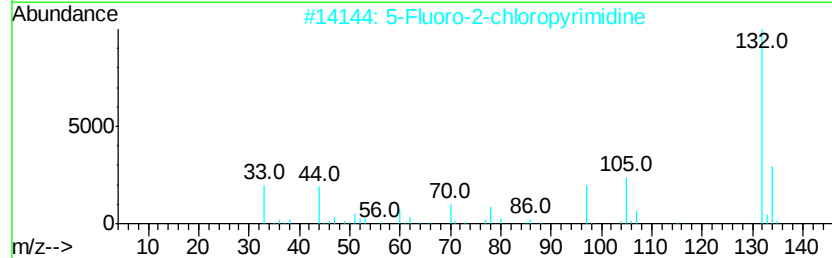
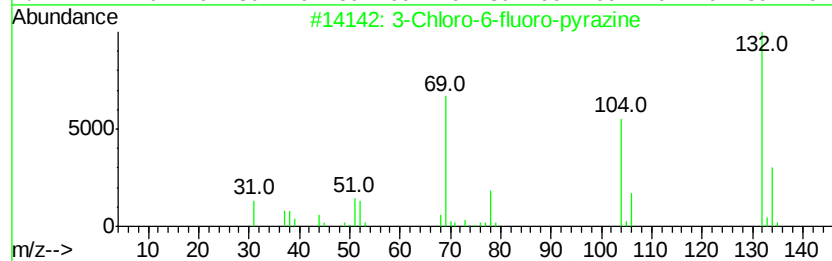
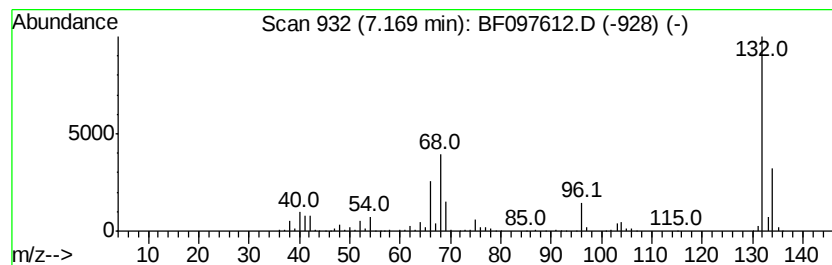
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	77.31 ng	2050780	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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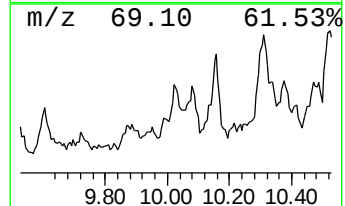
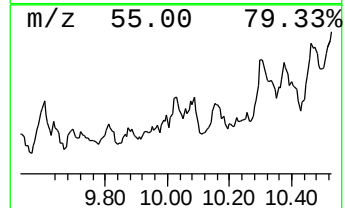
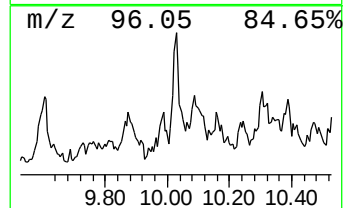
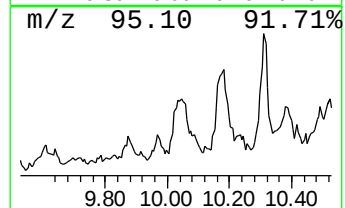
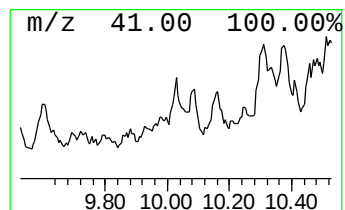
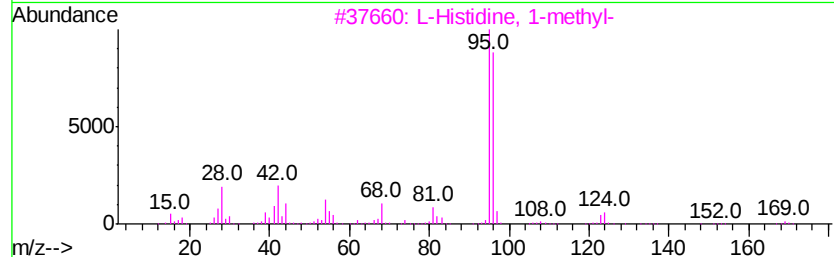
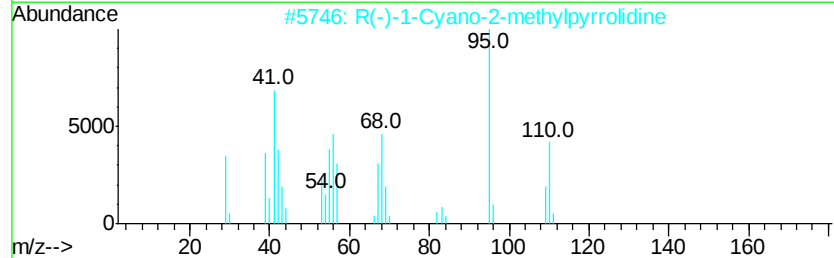
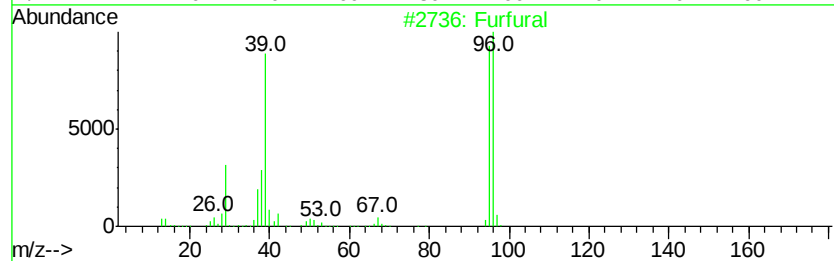
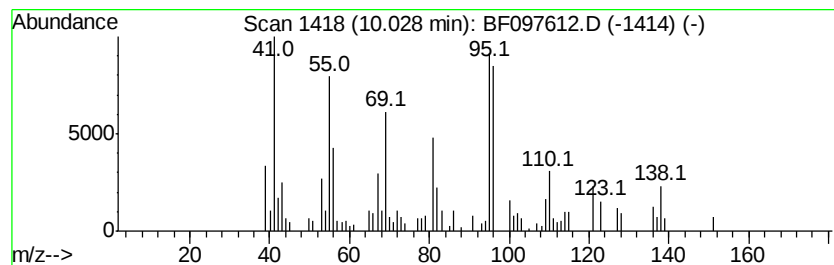
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.03 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.90 ng	96658	Napthalene-d8	9.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Furfural		96 C5H4O2	000098-01-1 46
2	R(-)-1-Cyano-2-methylpyrrolidine		110 C6H10N2	1000145-01-8 43
3	L-Histidine, 1-methyl-		169 C7H11N3O2	000332-80-9 43
4	1H-Pyrazole, 3,4-dimethyl-		96 C5H8N2	002820-37-3 43
5	o-Menth-8-ene		138 C10H18	015193-25-6 41



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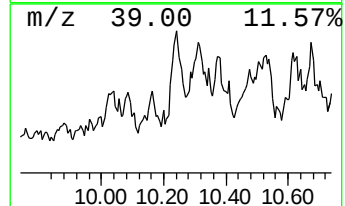
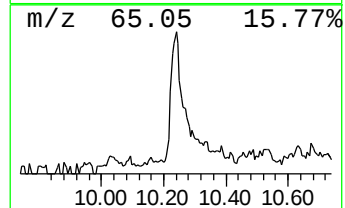
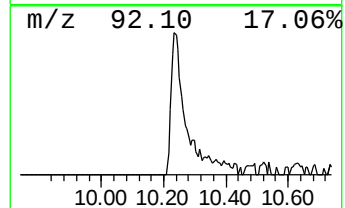
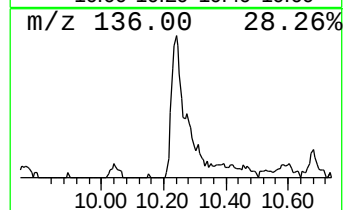
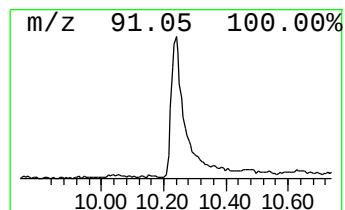
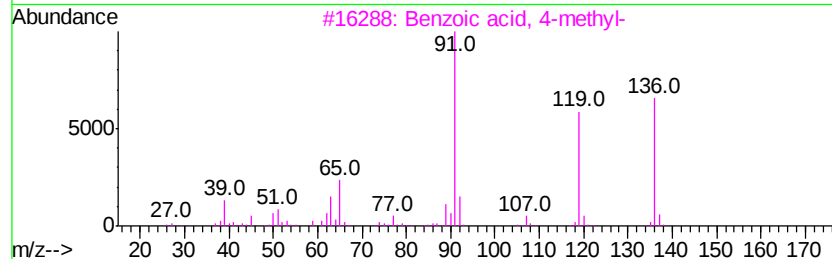
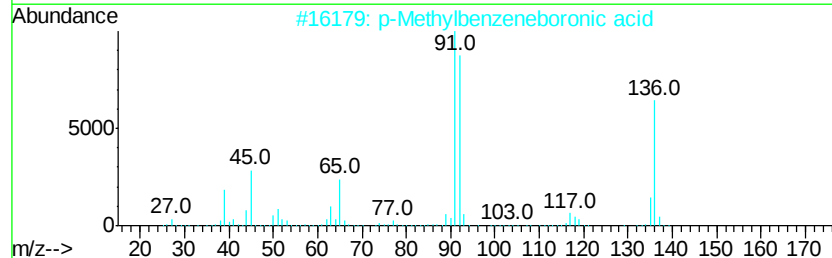
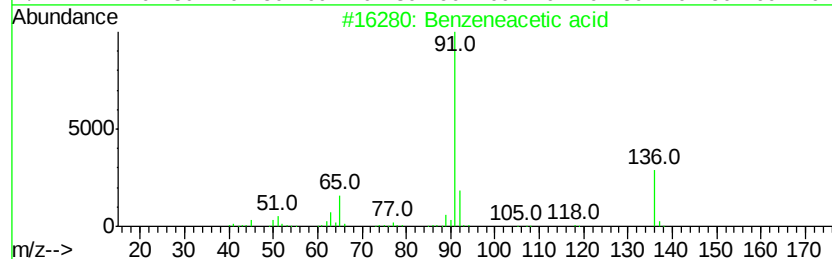
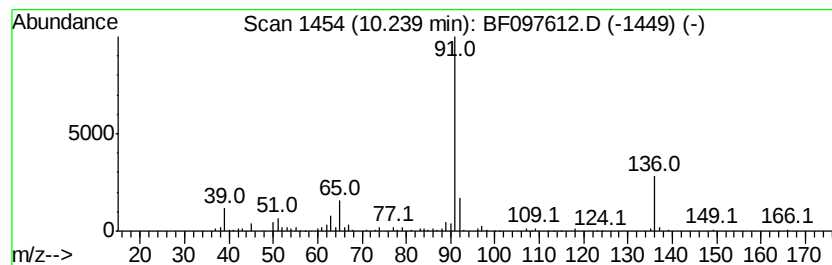
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzeneacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	5.80 ng	193250	Napthalene-d8	9.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzeneacetic acid	136 C8H8O2	000103-82-2 90
2		p-Methylbenzeneboronic acid	136 C7H9BO2	005720-05-8 59
3		Benzoic acid, 4-methyl-	136 C8H8O2	000099-94-5 53
4		Phenylacetic acid, pent-2-en-4-v...	200 C13H12O2	1000292-61-1 50
5		Benzyl 2-chloroethyl sulfone	218 C9H11ClO2S	066998-67-2 47



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
VE-1-2

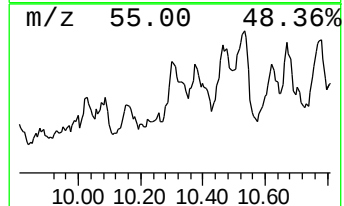
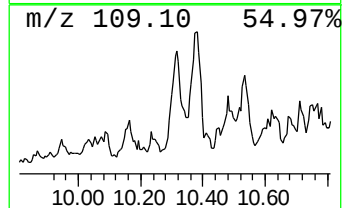
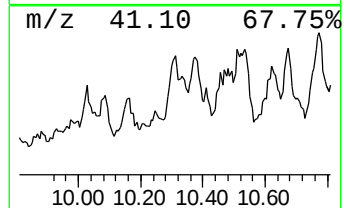
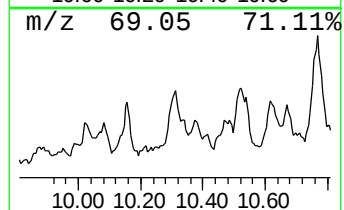
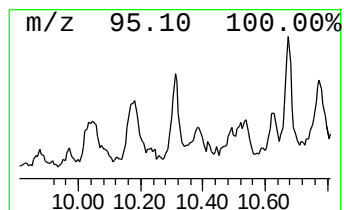
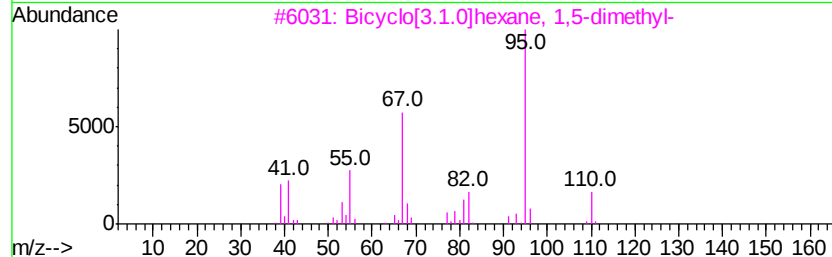
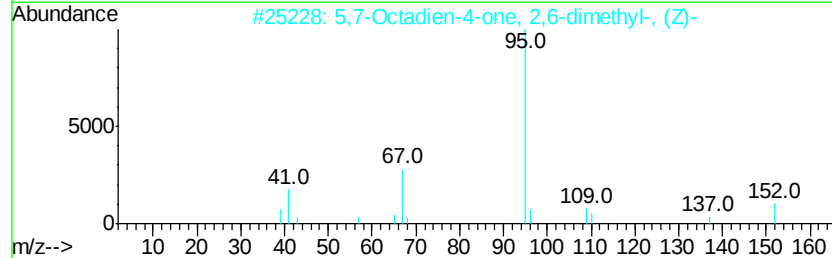
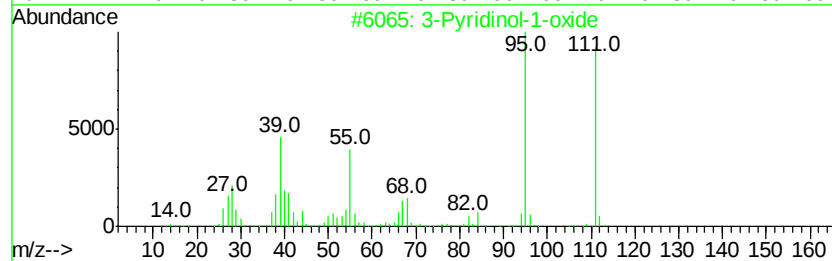
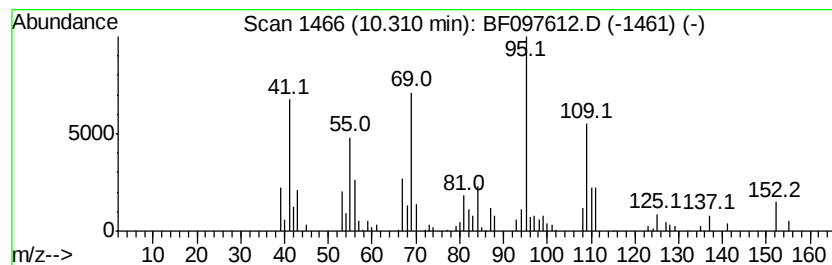
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.31 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.31	5.97 ng	198981	Naphthalene-d8	9.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Pyridinol-1-oxide	111	C5H5NO2	006602-28-4	43
2	5,7		Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	38
3	Bicvclo[3.1.0]		hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	38
4	2-Isopropv		limidazole	110	C6H10N2	036947-68-9	38
5	4-Pyridinol			95	C5H5NO	000626-64-2	35



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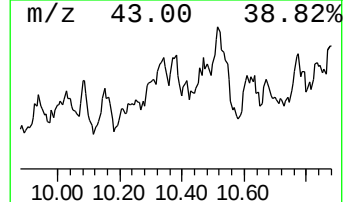
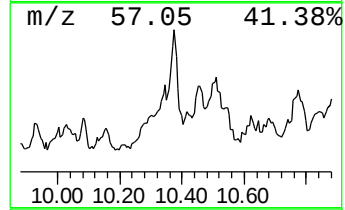
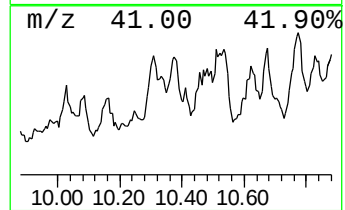
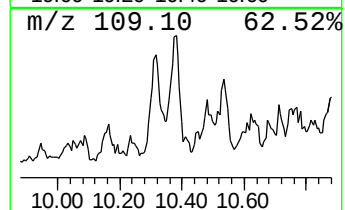
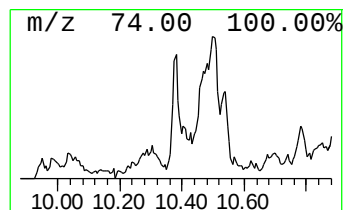
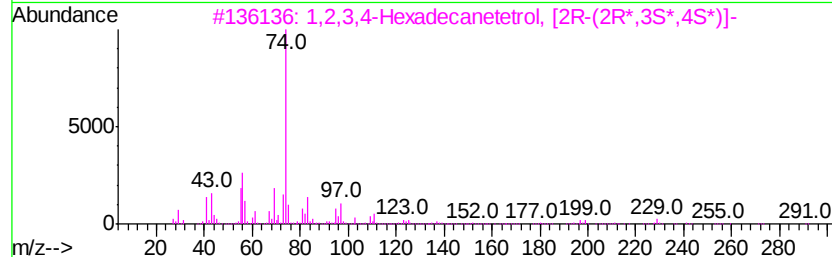
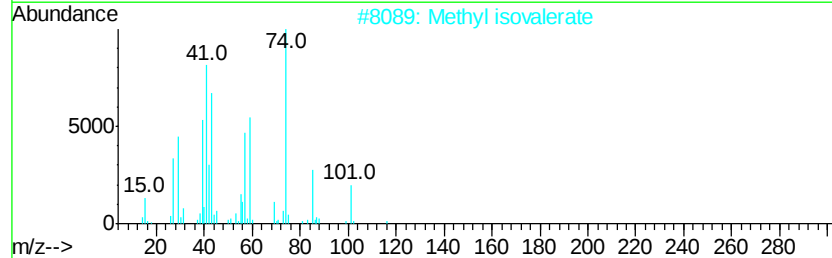
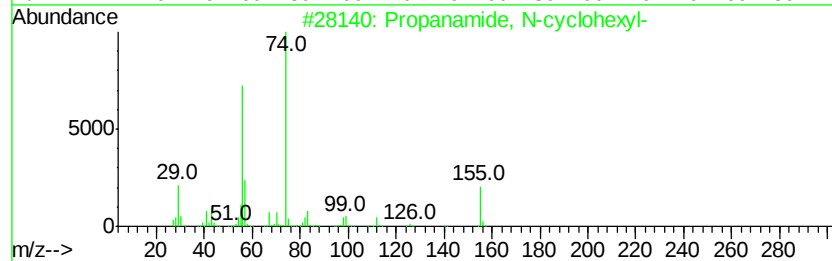
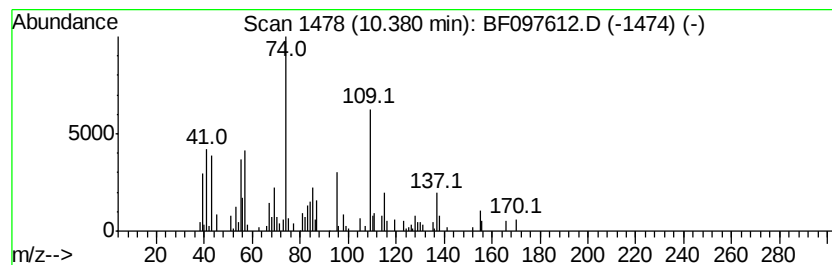
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.38 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.89 ng	96195	Naphthalene-d8	9.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanamide, N-cyclohexyl-	155	C9H17NO	001126-56-3	27
2		Methyl isovalerate	116	C6H12O2	000556-24-1	25
3		1,2,3,4-Hexadecanetetrol, [2R-(2...	290	C16H34O4	136953-06-5	12
4		6-Heptenoic acid, methyl ester	142	C8H14O2	001745-17-1	12
5		2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
Operator : SJ/JU
Sample : I4631-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

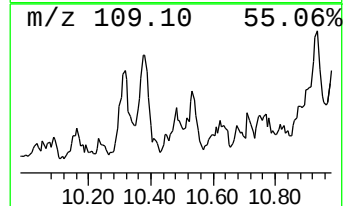
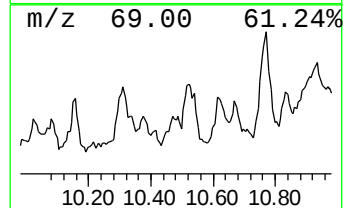
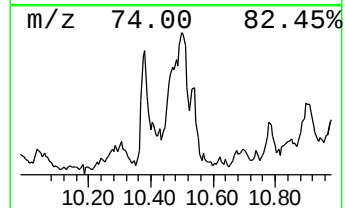
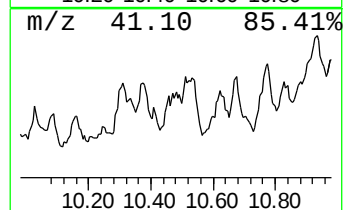
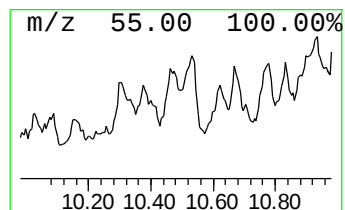
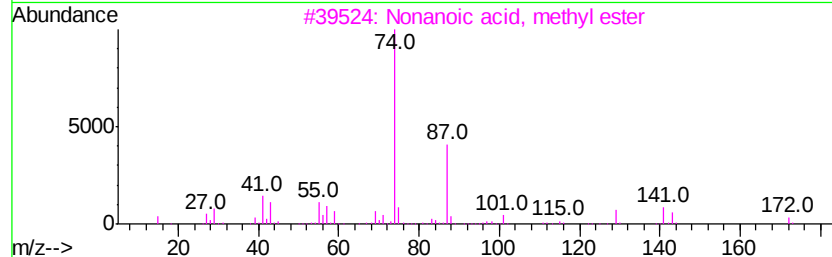
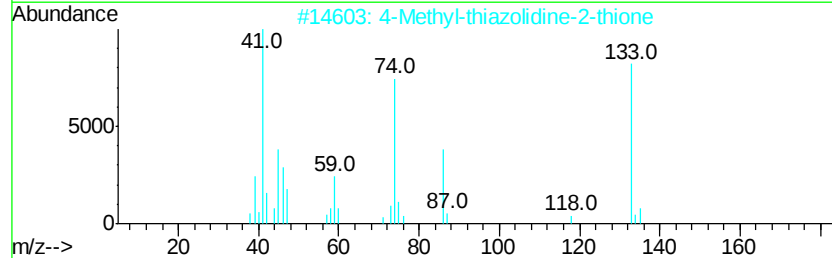
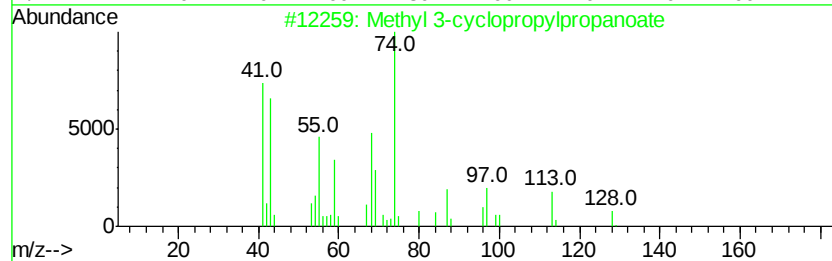
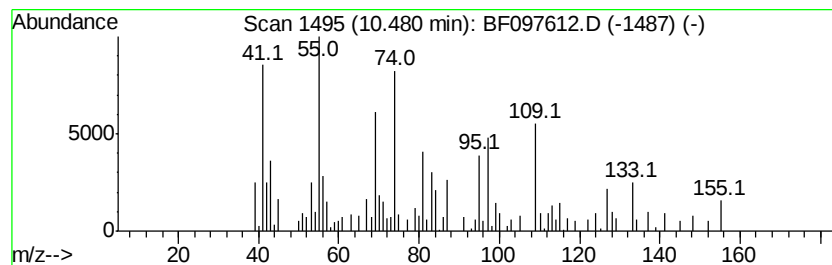
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.48 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.48	5.51 ng	183614	Napthalene-d8	9.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 3-cyclopropylpropanoate	128	C7H12O2	062021-34-5	27
2	4-Methyl-thiazolidine-2-thione	133	C4H7NS2	1000143-27-4	22
3	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	12
4	3-Hexene, 2,4-dimethyl-	112	C8H16	082085-14-1	10
5	Succinamic acid	117	C4H7NO3	000638-32-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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Acq On : 12 Aug 2017 00:35
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Misc :
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Instrument :
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ClientSampleId :
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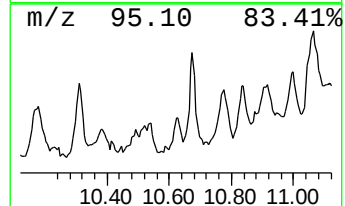
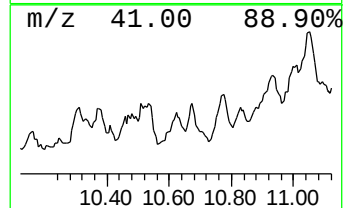
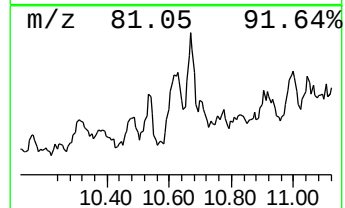
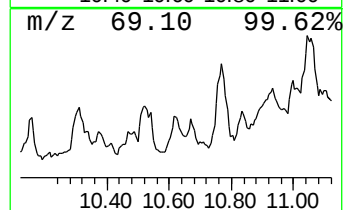
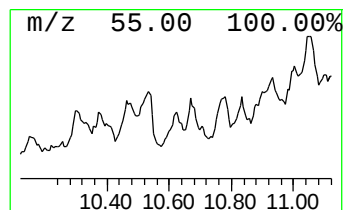
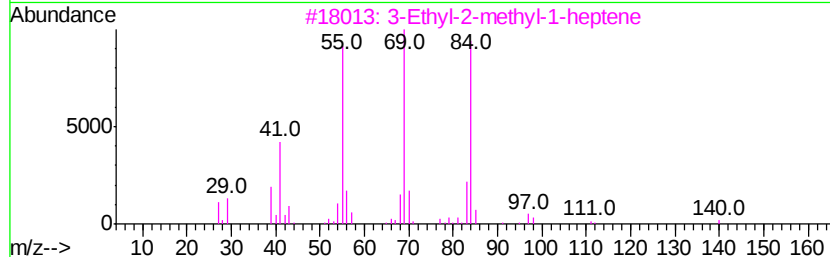
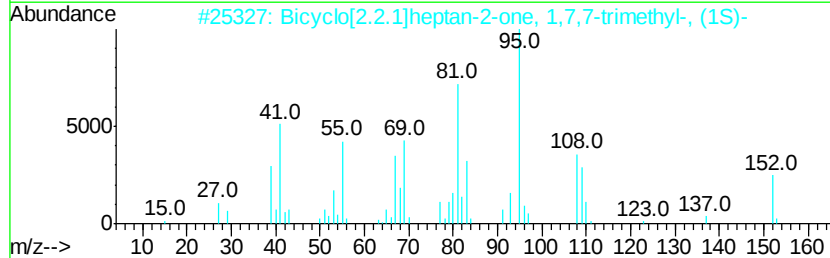
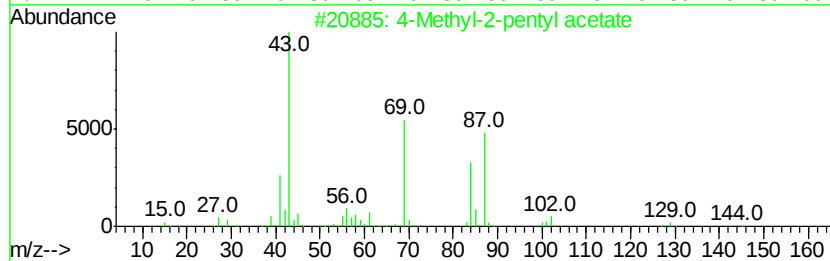
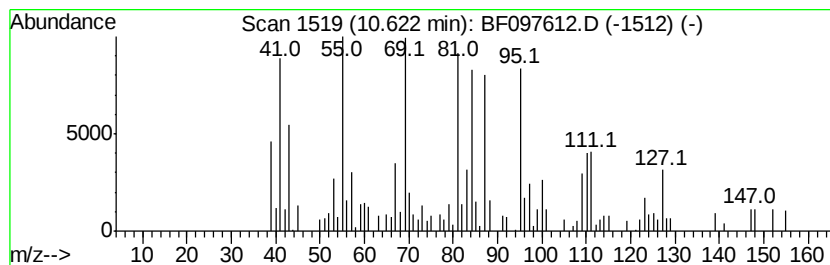
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.62 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	6.83 ng	227697	Naphthalene-d8	9.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-2-pentyl acetate	144	C8H16O2	000108-84-9	35
2		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	25
3		3-Ethyl-2-methyl-1-heptene	140	C10H20	019780-60-0	14
4		1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	14
5		Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
Operator : SJ/JU
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Misc :
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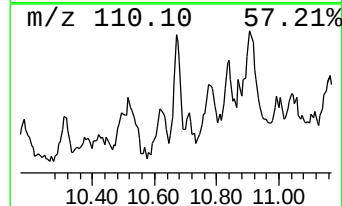
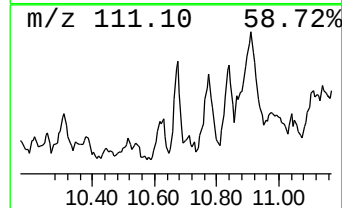
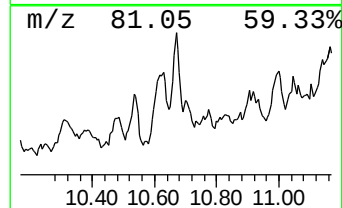
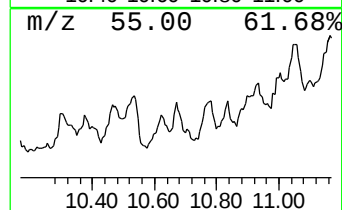
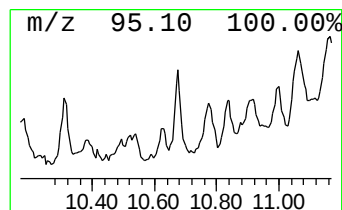
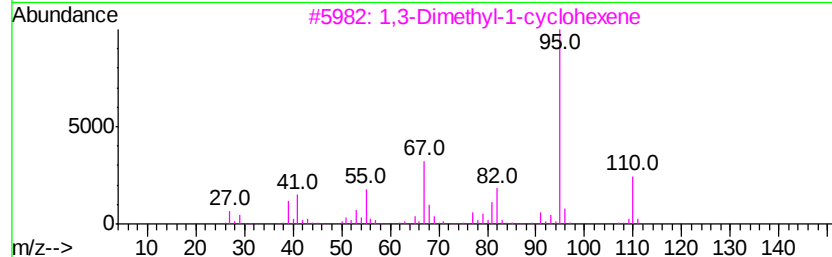
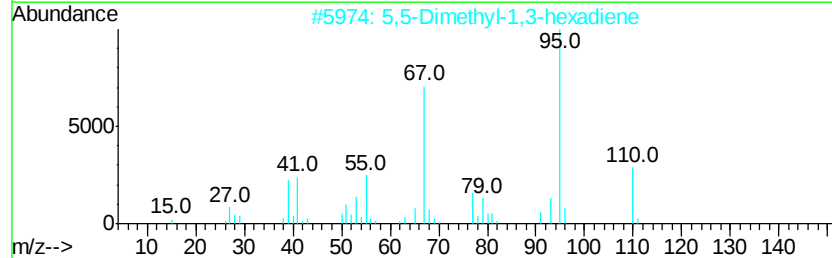
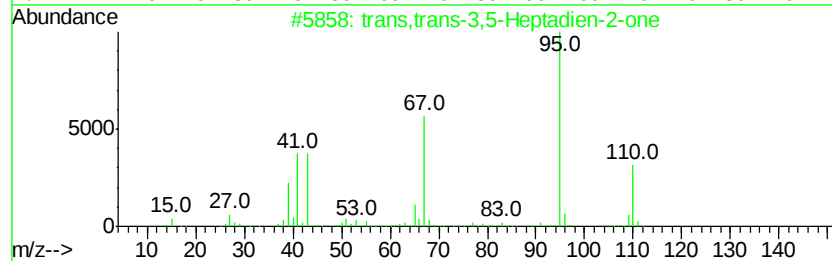
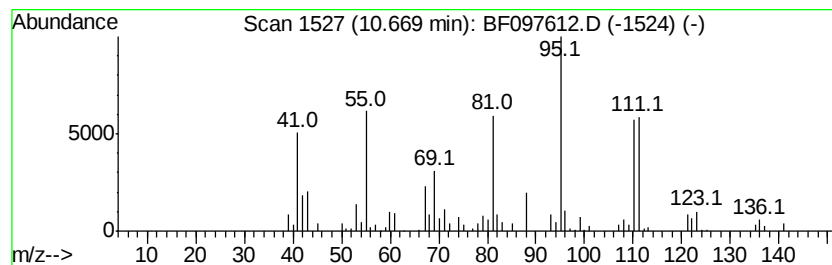
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 trans,trans-3,5-Heptadien-2... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	5.45 ng	181644	Napthalene-d8	9.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	50		
2	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	50		
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	50		
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	50		
5	2-Nonyne	124	C9H16	019447-29-1	50		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
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Sample : I4631-04
Misc :
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Instrument :
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ClientSampleId :
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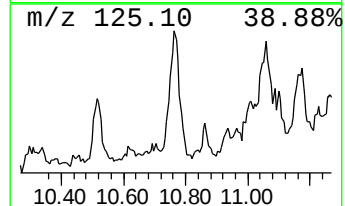
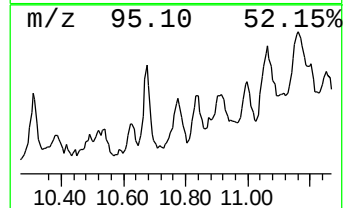
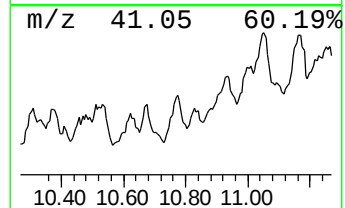
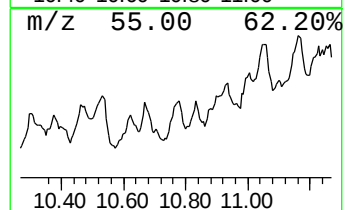
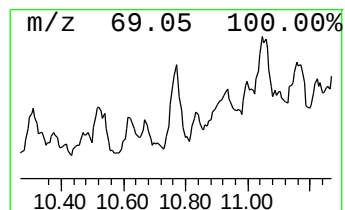
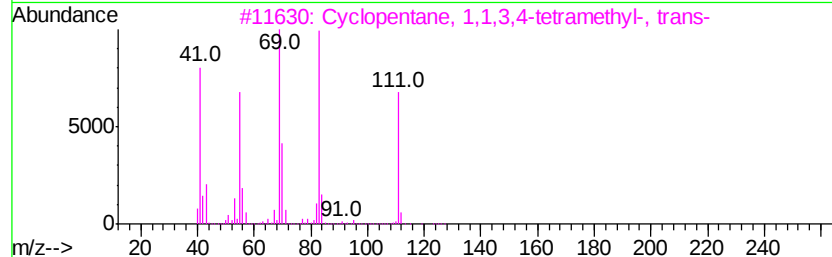
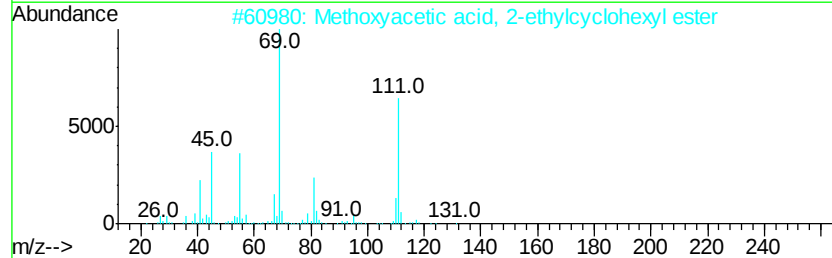
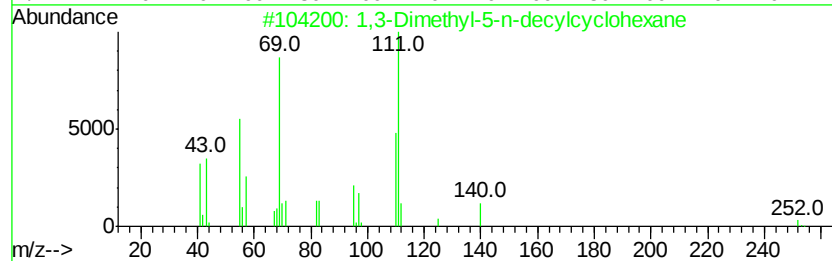
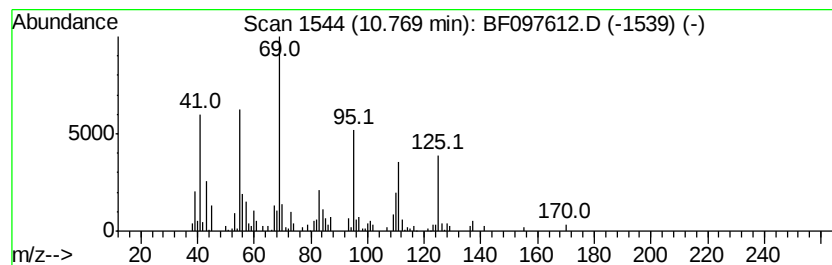
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.77 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	5.85 ng	195154	Napthalene-d8	9.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-5-n-decylcyclohexane	252	C18H36	086710-36-3	43
2			Methoxyacetic acid, 2-ethylcyclo...	200	C11H20O3	1000282-69-7	35
3			Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	35
4			Cyclohexane, 2-ethyl-1,3-dimethyl-	140	C10H20	007045-67-2	35
5			Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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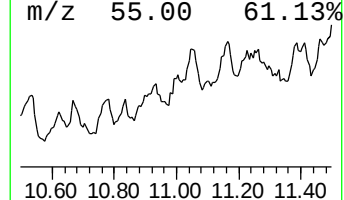
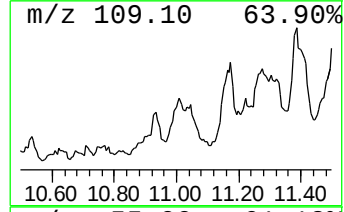
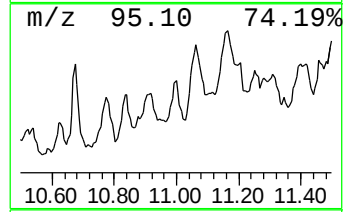
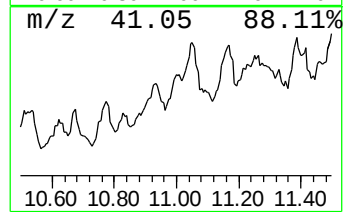
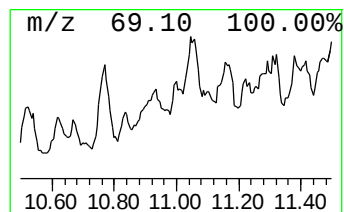
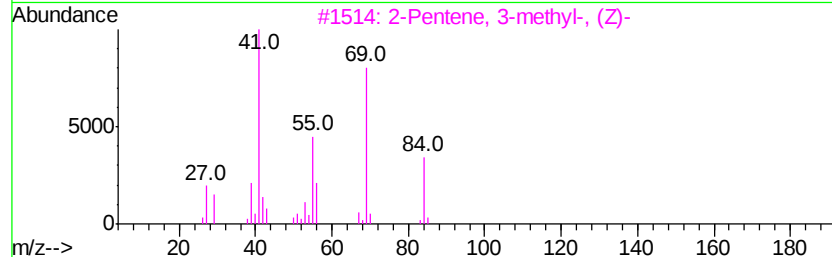
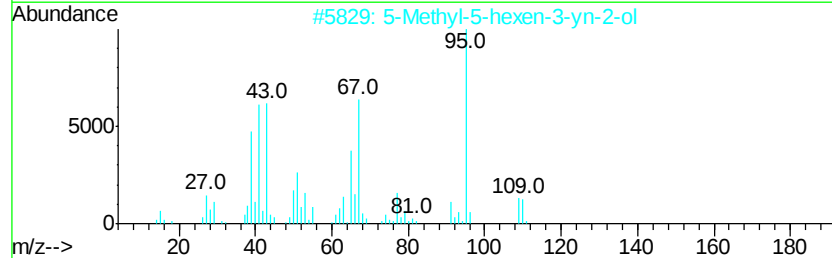
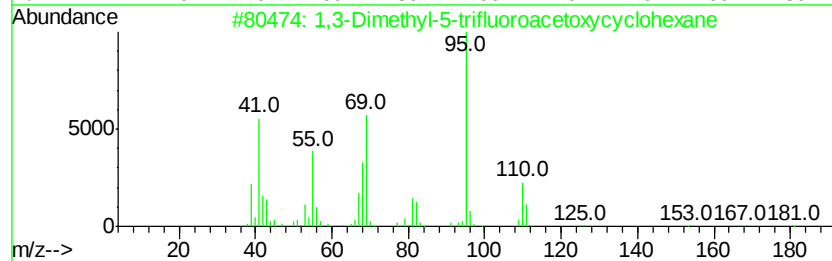
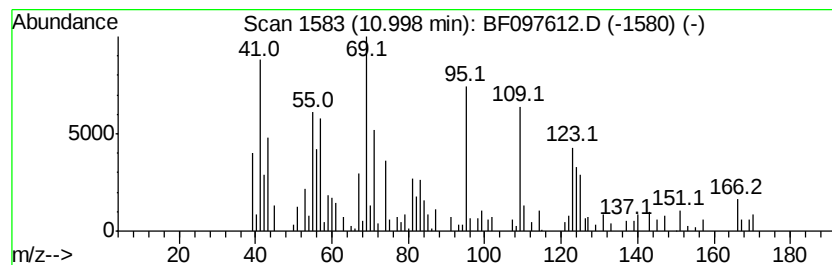
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown11.00 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	6.42 ng	142215	Acenaphthene-d10	12.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-5-trifluoroacetoxyc...	224	C10H15F3O2	1000216-63-7	35
2			5-Methyl-5-hexen-3-yn-2-ol	110	C7H10O	068017-33-4	15
3			2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	14
4			2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	14
5			Cyclopentene, 1-isopropyl-4,5-di...	138	C10H18	007712-74-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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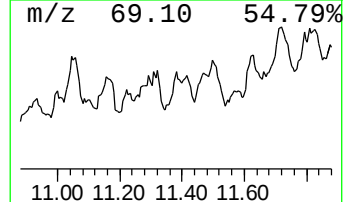
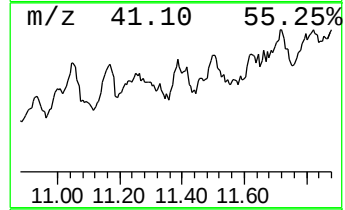
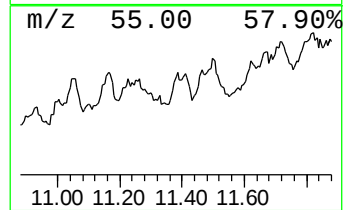
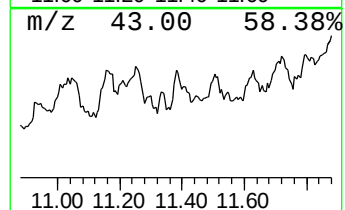
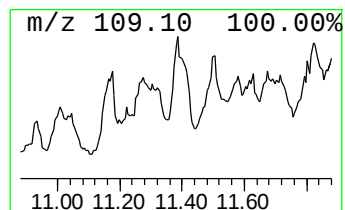
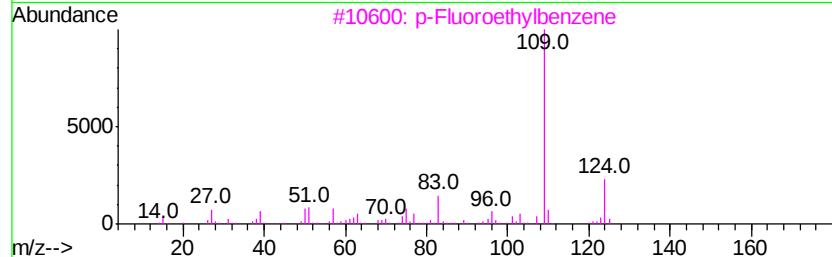
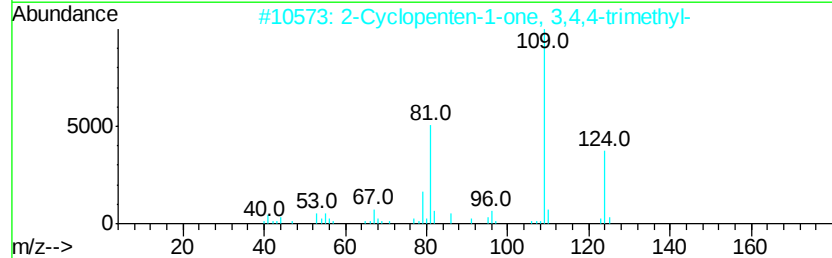
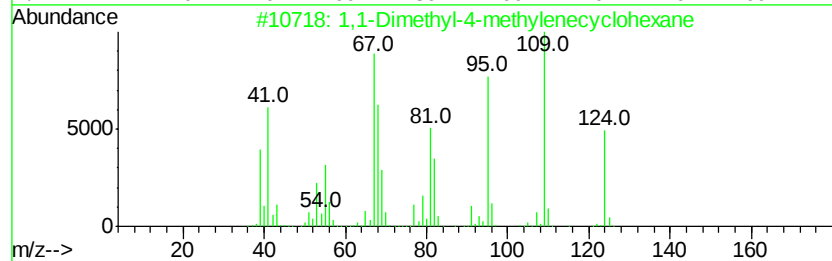
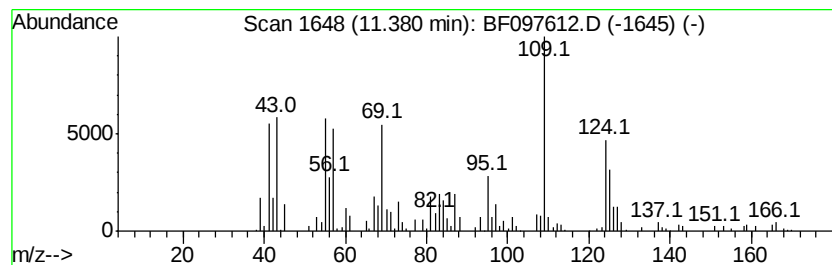
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown11.38 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.38	7.87 ng	174440	Acenaphthene-d10	12.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	46
2	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	46
3	p-Fluoroethylbenzene	124	C8H9F	000459-47-2	46
4	2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	46
5	6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
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ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
VE-1-2

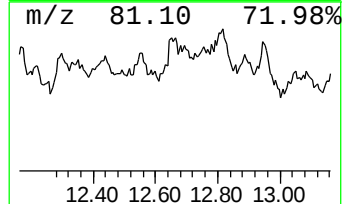
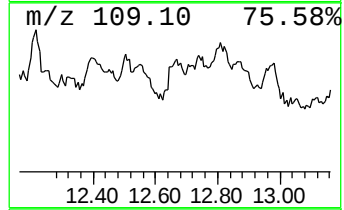
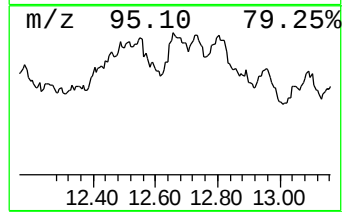
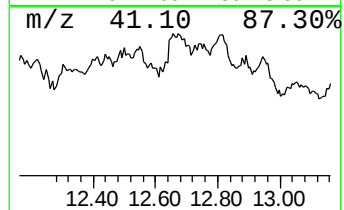
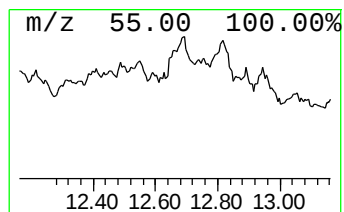
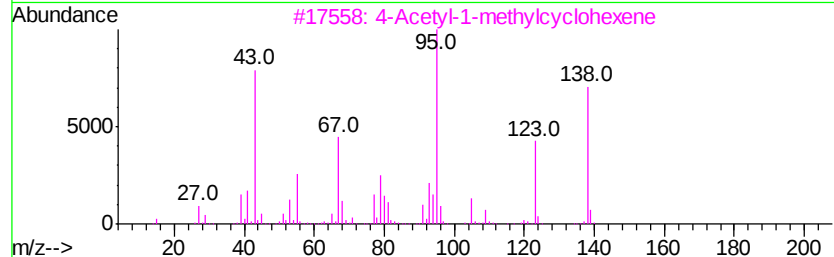
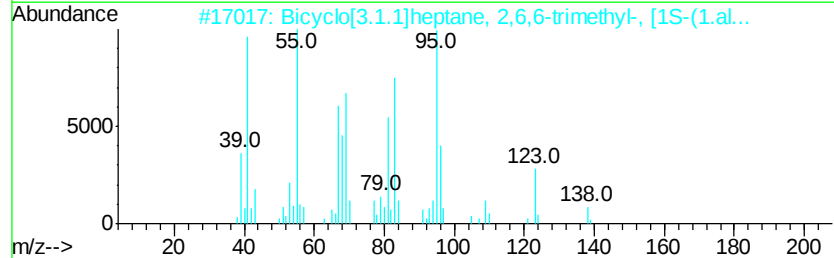
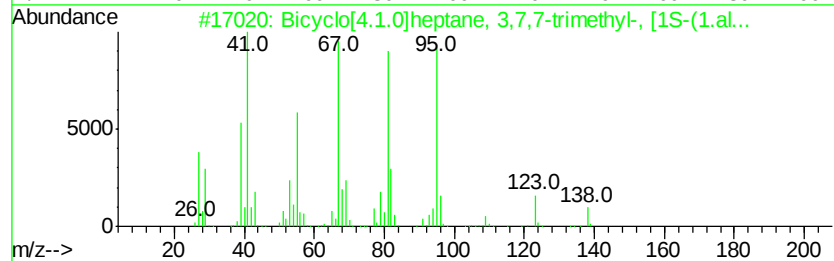
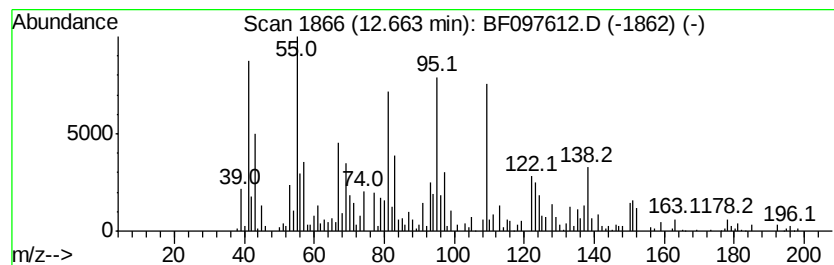
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Bicyclo[4.1.0]heptane, 3,7,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	14.26 ng	315992	Acenaphthene-d10	12.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	60
2		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	49
3		4-Acetyl-1-methylcyclohexene	138	C9H14O	006090-09-1	49
4		Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	46
5		Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
Operator : SJ/JU
Sample : I4631-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE-1-2

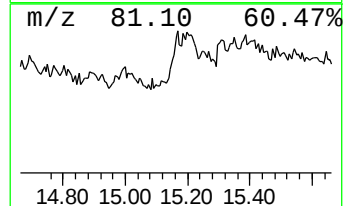
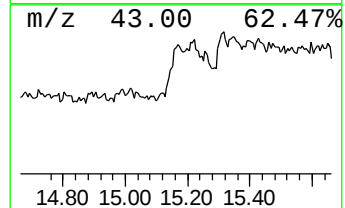
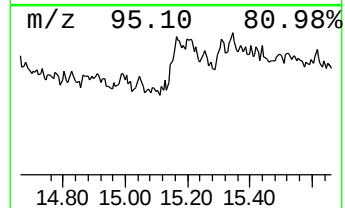
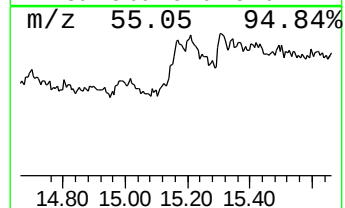
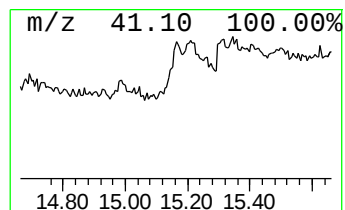
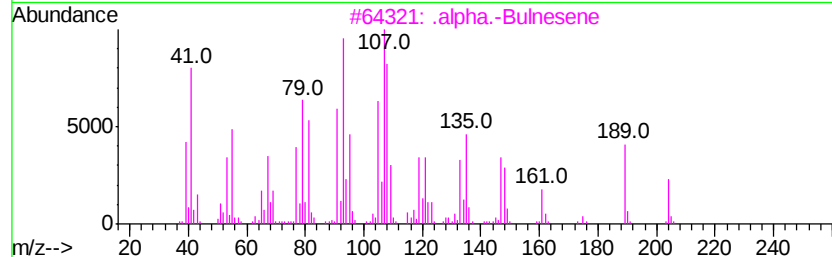
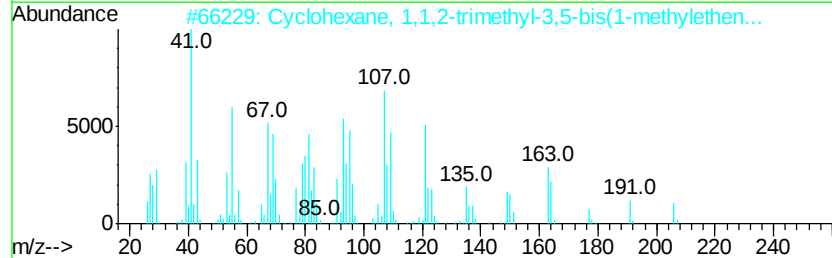
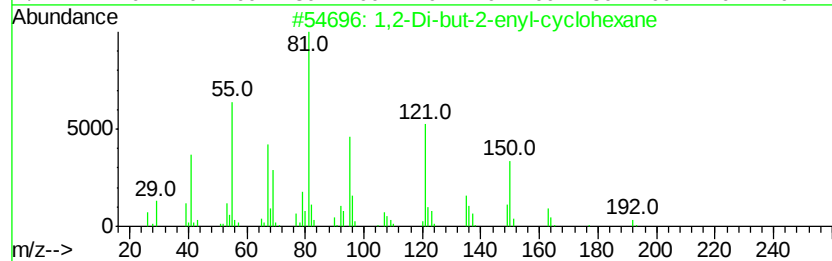
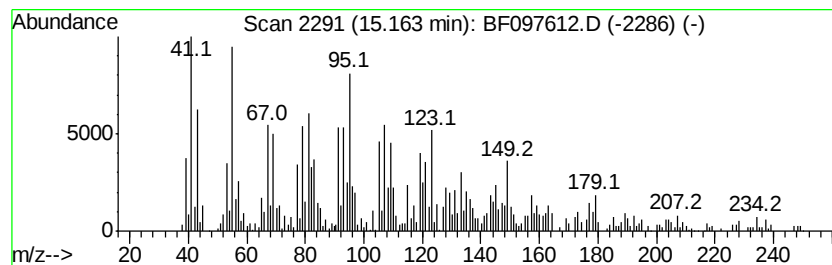
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1,2-Di-but-2-enyl-cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	50.10 ng	755432	Phenanthrene-d10	14.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Di-but-2-enyl-cvclohexane	192	C14H24	1000188-05-3	50
2			Cyclohexane, 1,1,2-trimethyl-3,5...	206	C15H26	062337-96-6	48
3			.alpha.-Bulnesene	204	C15H24	1000374-19-9	47
4			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	46
5			4-Ethenylhexahydro-4,7a-dimethyl...	194	C12H18O2	086003-24-9	44



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
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Acq On : 12 Aug 2017 00:35
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Sample : I4631-04
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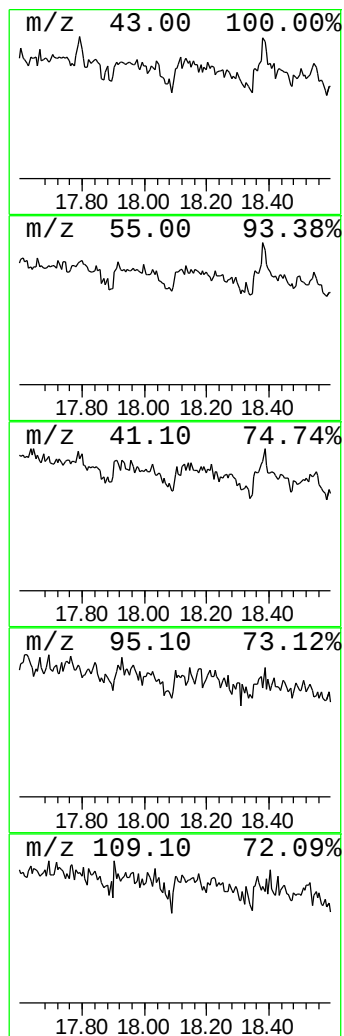
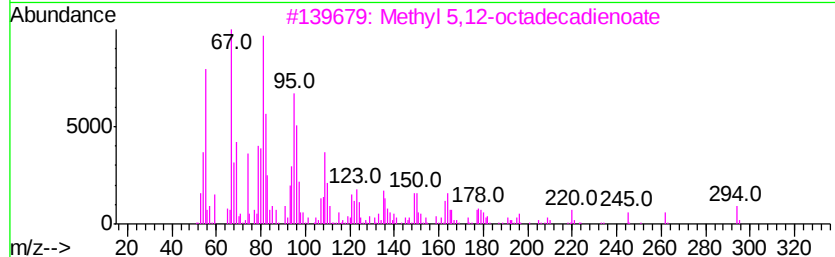
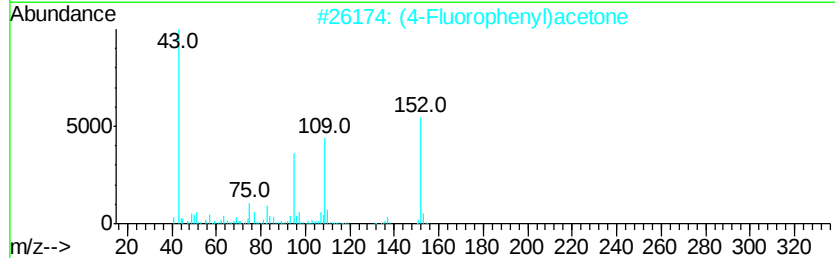
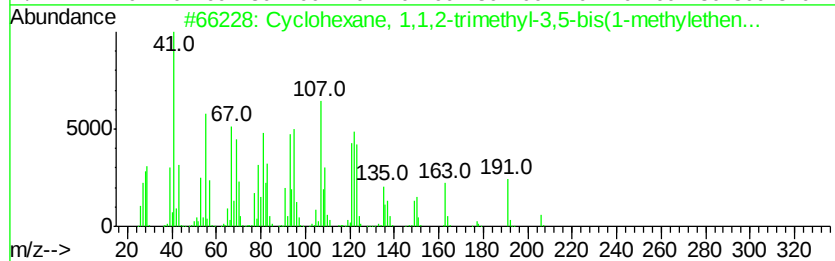
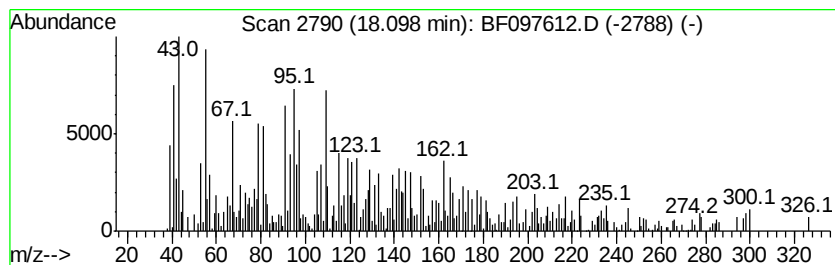
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ClientSampleId :
VE-1-2

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown18.10 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	10.16 ng	233673	Chrysene-d12	18.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1,1,2-trimethyl-3,5...	206 C15H26	062337-97-7 25
2		(4-Fluorophenyl)acetone	152 C9H9FO	000459-03-0 25
3		Methyl 5,12-octadecadienoate	294 C19H34O2	1000336-43-1 25
4		Silane, chlorodiethyl(dodec-9-yn...	302 C16H31ClOSi	1000363-59-2 25
5		Cyclopropa[c,d]pentalene-1,3-dio...	232 C15H20O2	094609-18-4 25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
Operator : SJ/JU
Sample : I4631-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VE-1-2

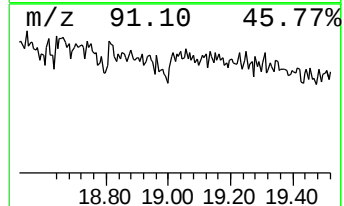
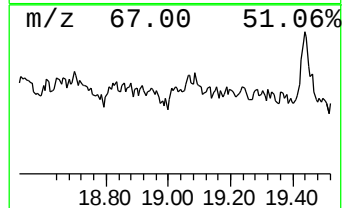
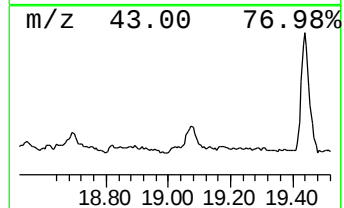
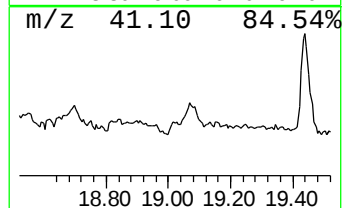
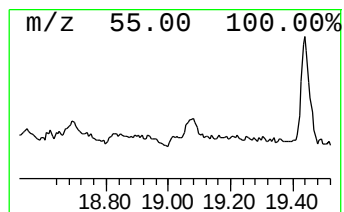
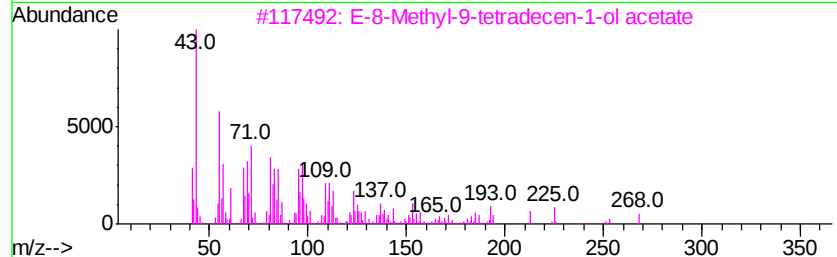
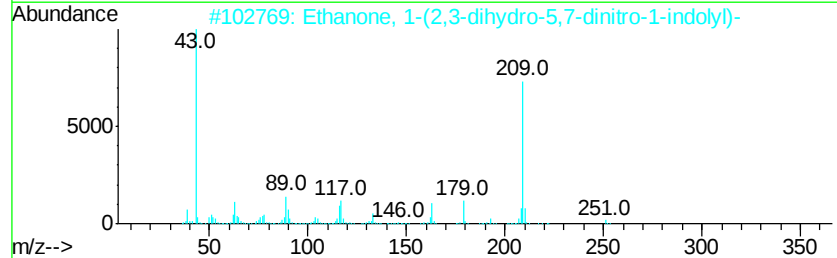
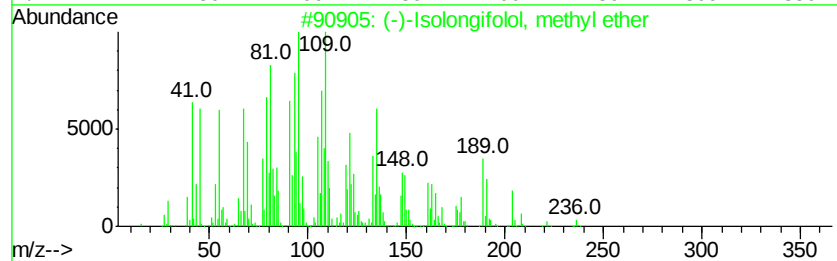
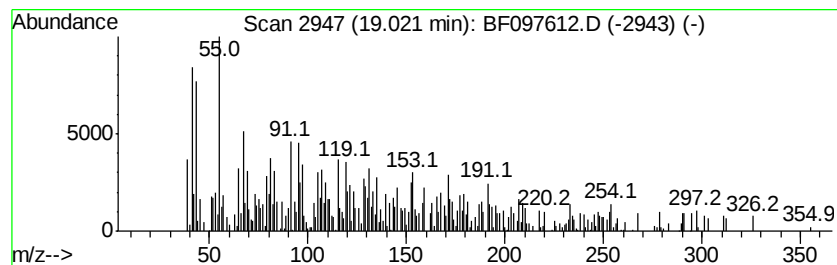
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 (-)-Isolongifolol, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	9.59 ng	220405	Chrysene-d12	18.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	52
2			Ethanone, 1-(2,3-dihydro-5,7-din...	251	C10H9N3O5	062796-78-5	25
3			E-8-Methyl-9-tetradecen-1-ol ace...	268	C17H32O2	1000130-81-4	25
4			Cyclopentaneacetic acid, 3-oxo-2...	224	C13H20O3	042536-97-0	22
5			5,6,6-Trimethyl-5-(3-oxobut-1-en...	236	C14H20O3	1000192-73-9	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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Operator : SJ/JU
Sample : I4631-04
Misc :
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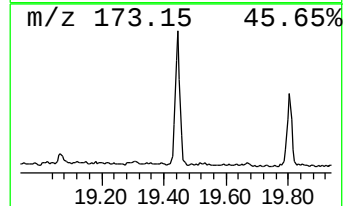
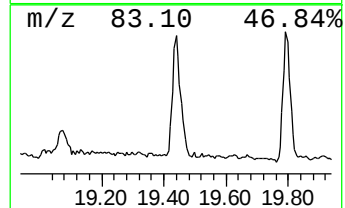
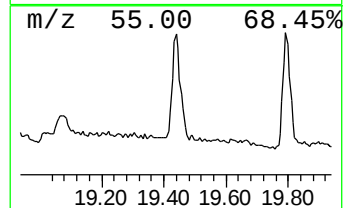
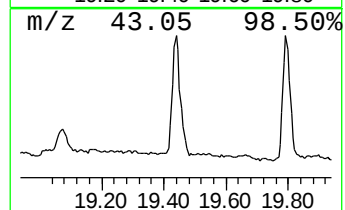
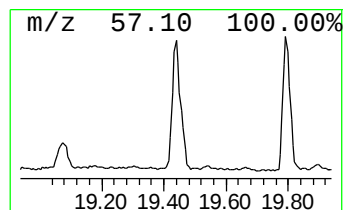
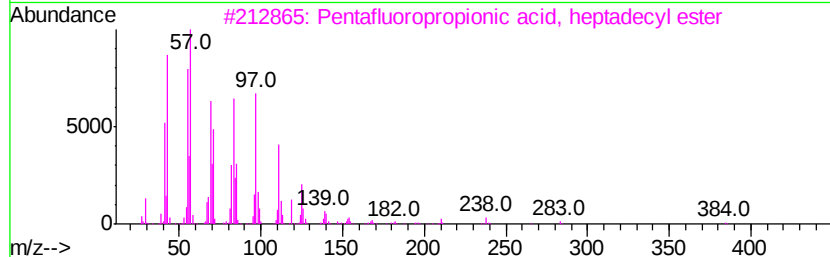
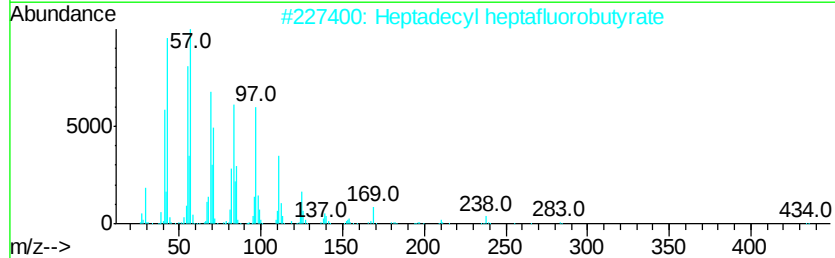
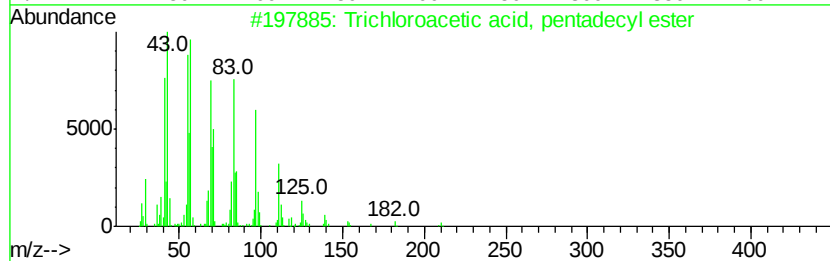
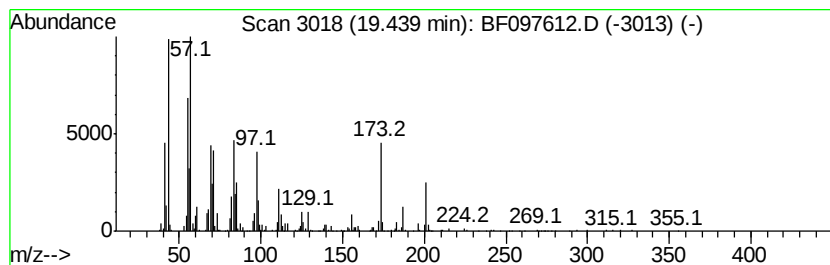
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Trichloroacetic acid, penta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.44	9.08 ng	1344930	Perylene-d12	20.14		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	70
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	70
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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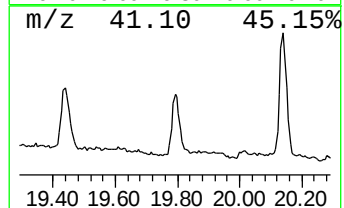
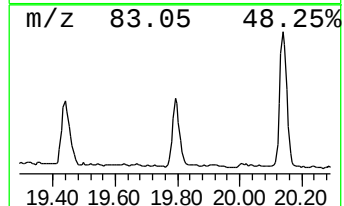
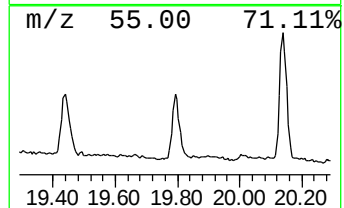
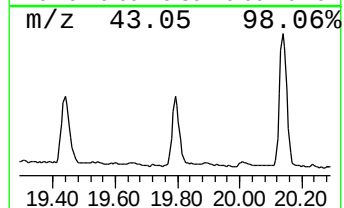
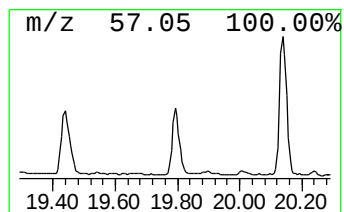
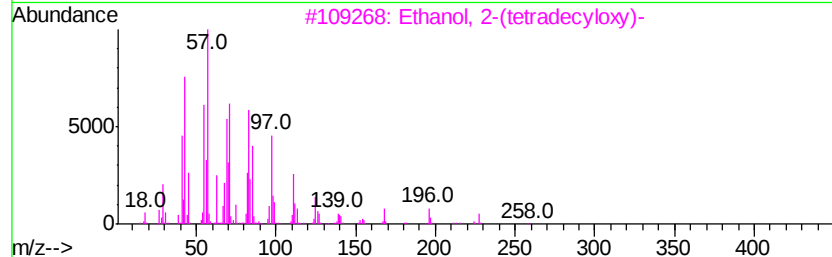
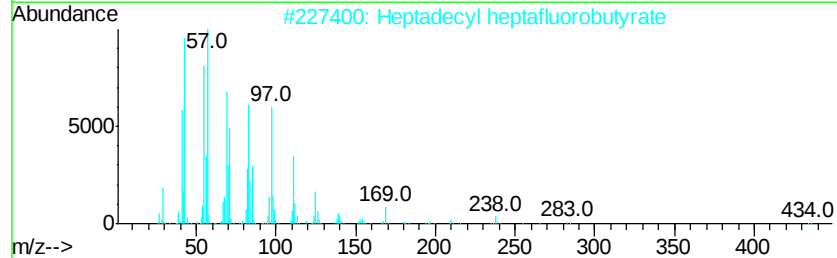
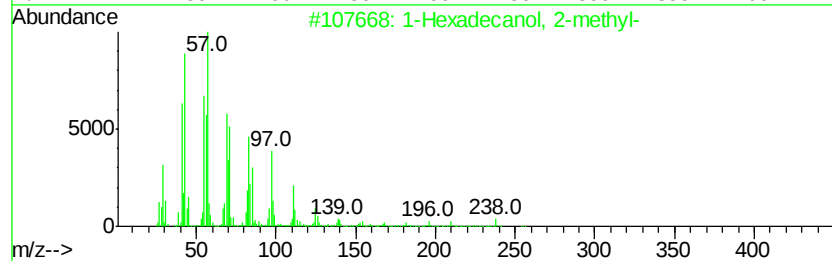
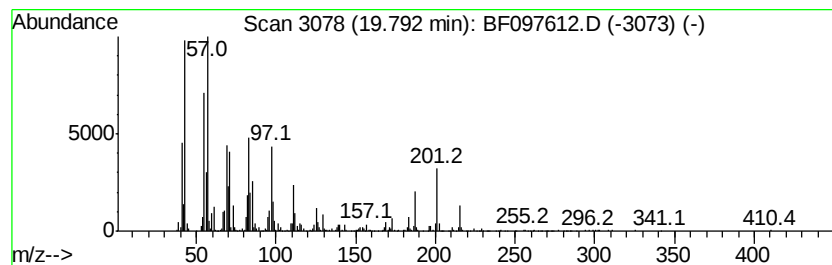
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 1-Hexadecanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.79	9.89 ng	1464640	Perylene-d12	20.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	86
4	1-Tricosene	322	C23H46	018835-32-0	81
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097612.D
Acq On : 12 Aug 2017 00:35
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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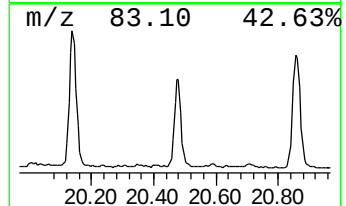
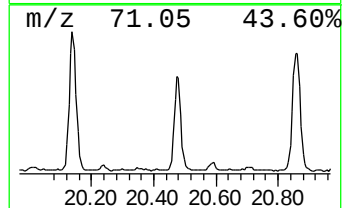
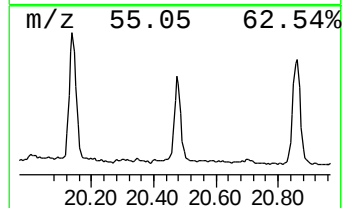
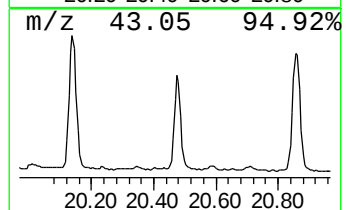
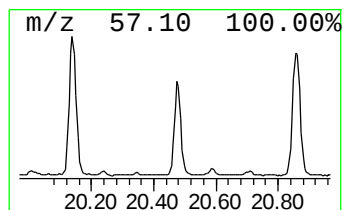
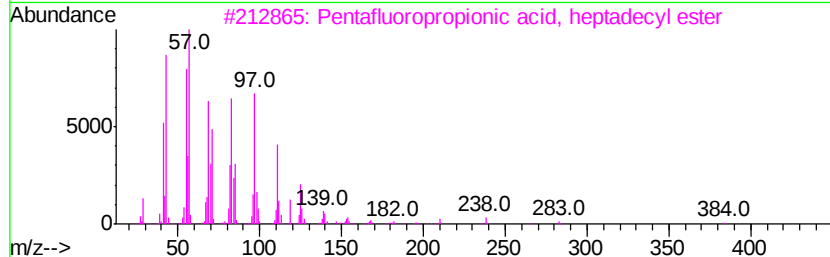
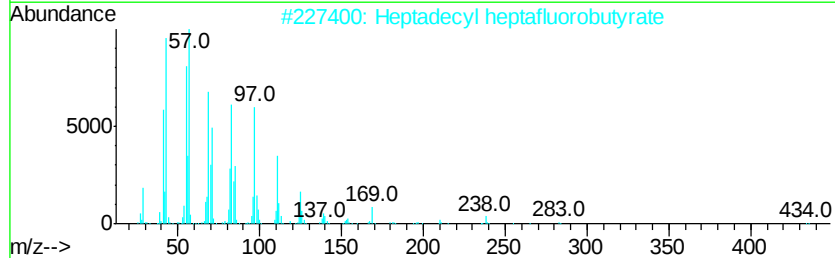
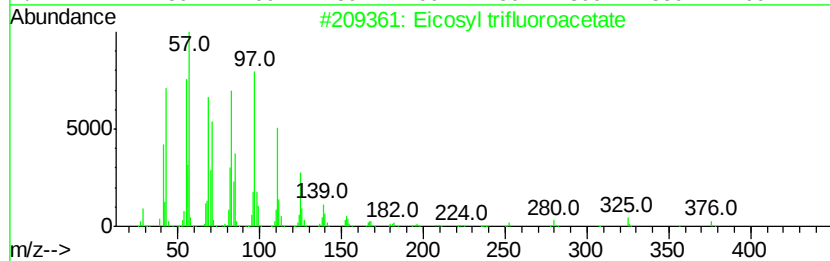
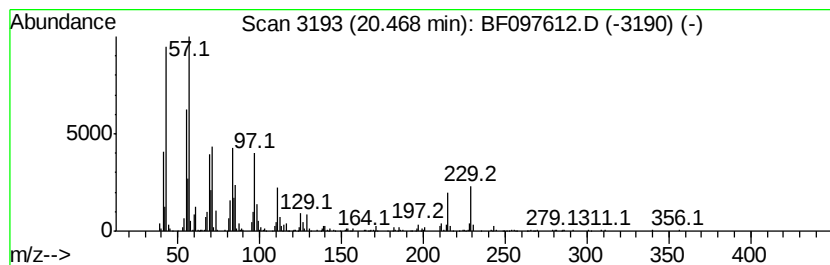
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Eicosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	10.58 ng	1567020	Perylene-d12	20.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	76
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	76
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	76
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
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Acq On : 12 Aug 2017 00:35
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Sample : I4631-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE-1-2

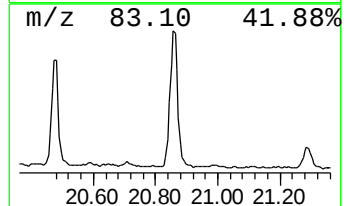
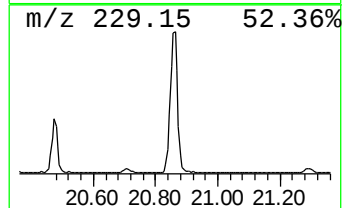
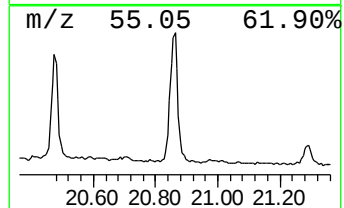
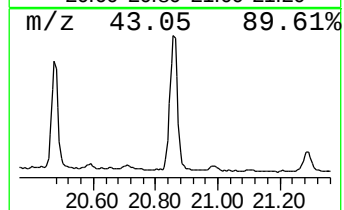
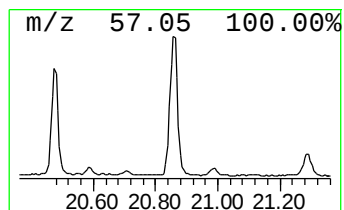
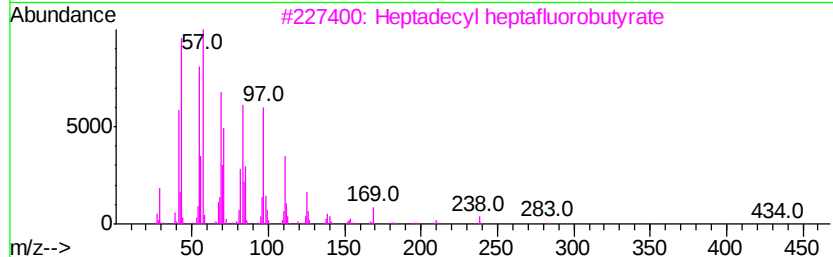
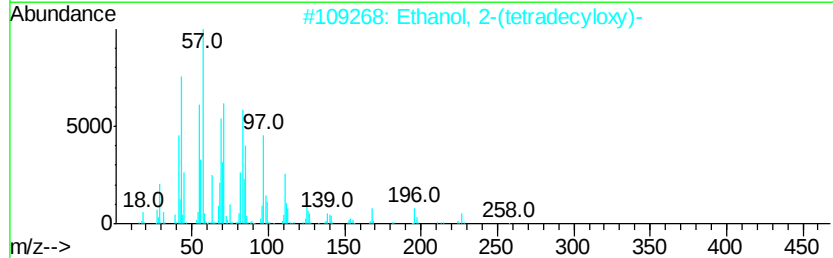
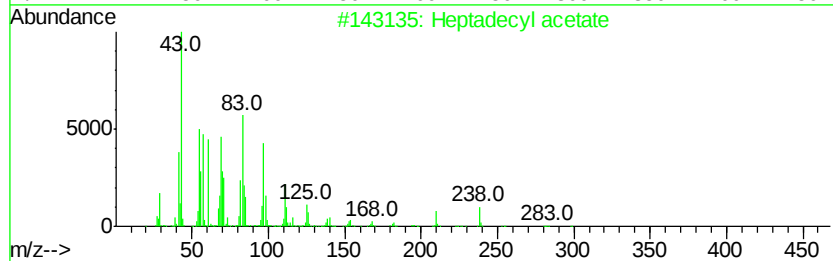
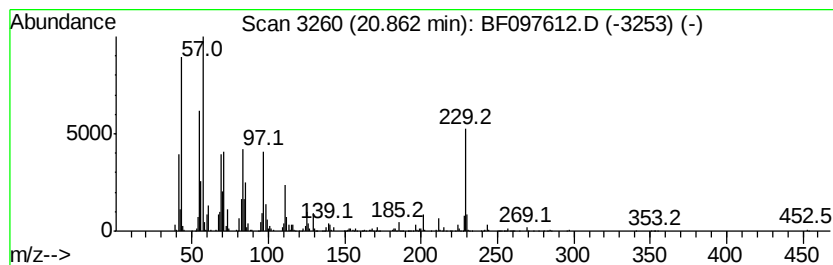
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Heptadecyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	16.20 ng	2399290	Perylene-d12	20.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl acetate	298	C19H38O2	000822-20-8	89
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	89
3		Heptadecyl heptafluorobutylate	452	C21H35F7O2	959085-66-6	89
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	76
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
 Data File : BF097612.D
 Acq On : 12 Aug 2017 00:35
 Operator : SJ/JU
 Sample : I4631-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VE-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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
unknown7.17	7.17	77.3	ng	2050780	1	7.51	530542	20.0
unknown10.03	10.03	2.9	ng	96658	2	9.54	666839	20.0
Benzeneacetic acid	10.24	5.8	ng	193250	2	9.54	666839	20.0
unknown10.31	10.31	6.0	ng	198981	2	9.54	666839	20.0
unknown10.38	10.38	2.9	ng	96195	2	9.54	666839	20.0
unknown10.48	10.48	5.5	ng	183614	2	9.54	666839	20.0
unknown10.62	10.62	6.8	ng	227697	2	9.54	666839	20.0
trans,trans-3,5-H...	10.67	5.5	ng	181644	2	9.54	666839	20.0
unknown10.77	10.77	5.8	ng	195154	2	9.54	666839	20.0
unknown11.00	11.00	6.4	ng	142215	3	12.37	443314	20.0
unknown11.38	11.38	7.9	ng	174440	3	12.37	443314	20.0
Bicyclo[4.1.0]hep...	12.66	14.3	ng	315992	3	12.37	443314	20.0
1,2-Di-but-2-enyl...	15.16	50.1	ng	755432	4	14.77	301579	20.0
unknown18.10	18.10	10.2	ng	233673	5	18.47	459872	20.0
(-)-Isolongifolol...	19.02	9.6	ng	220405	5	18.47	459872	20.0
Trichloroacetic a...	19.44	9.1	ng	1344930	6	20.14	2961250	20.0
1-Hexadecanol, 2-...	19.79	9.9	ng	1464640	6	20.14	2961250	20.0
Eicosyl trifluoro...	20.47	10.6	ng	1567020	6	20.14	2961250	20.0
Heptadecyl acetate	20.86	16.2	ng	2399290	6	20.14	2961250	20.0