

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030217\
 Data File : BF093358.D
 Acq On : 3 Mar 2017 12:55
 Operator : SJ/MA
 Sample : I2057-15
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 34B-4

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-BF013017.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	4.259	187	190	205	rBV	423283	664986	19.70%	1.899%
2	4.944	247	250	261	rBV	1282956	1708198	50.59%	4.879%
3	5.390	287	289	300	rBV	2778889	2988193	88.50%	8.535%
4	6.385	374	376	379	rVB	51431	49614	1.47%	0.142%
5	6.442	379	381	389	rBV	2418161	3376389	100.00%	9.644%
6	6.567	389	392	394	rVV	3348895	3169661	93.88%	9.054%
7	6.613	394	396	399	rVB	102887	107398	3.18%	0.307%
8	6.796	410	412	415	rBV	1019125	909115	26.93%	2.597%
9	6.853	415	417	421	rVB2	51506	60987	1.81%	0.174%
10	6.956	423	426	428	rBV	2359845	2601501	77.05%	7.431%
11	7.116	438	440	445	rVB2	31531	47432	1.40%	0.135%
12	7.367	460	462	465	rBV	2071180	2045382	60.58%	5.842%
13	8.088	523	525	528	rBV	1261061	1241264	36.76%	3.546%
14	9.173	617	620	623	rBV	3621485	3333521	98.73%	9.522%
15	9.573	653	655	657	rBV	485043	413048	12.23%	1.180%
16	9.859	677	680	682	rBV	961408	1254687	37.16%	3.584%
17	10.282	712	717	721	rBV3	72753	109998	3.26%	0.314%
18	10.408	724	728	731	rVB2	32458	52600	1.56%	0.150%
19	10.499	734	736	740	rVB	25367	43417	1.29%	0.124%
20	10.648	747	749	752	rBV	969928	974877	28.87%	2.785%
21	10.762	757	759	763	rBV2	125102	194929	5.77%	0.557%
22	10.956	773	776	778	rBV3	20083	39997	1.18%	0.114%
23	11.082	785	787	790	rBV3	21887	50225	1.49%	0.143%
24	11.208	795	798	799	rVV	136023	136952	4.06%	0.391%
25	11.242	799	801	804	rVB2	50366	75610	2.24%	0.216%
26	11.345	808	810	811	rBV	1403084	1256263	37.21%	3.588%
27	11.425	814	817	819	rVB	70020	86111	2.55%	0.246%
28	11.585	829	831	834	rBV2	56941	65053	1.93%	0.186%
29	11.631	834	835	838	rVV	110919	103980	3.08%	0.297%
30	11.848	852	854	855	rBV	62484	64516	1.91%	0.184%
31	11.882	855	857	860	rVV3	58135	117037	3.47%	0.334%
32	11.962	862	864	869	rVB2	95030	193692	5.74%	0.553%
33	12.042	869	871	873	rBV	70444	83867	2.48%	0.240%
34	12.397	899	902	903	rBV2	65856	101805	3.02%	0.291%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.431	903	905	908	rVV3	65673	132454	3.92%	0.378%
36	12.488	908	910	911	rVV2	46112	58275	1.73%	0.166%
37	12.557	914	916	919	rVV	690193	626367	18.55%	1.789%
38	12.785	933	936	938	rBV	572330	605181	17.92%	1.729%
39	12.922	946	948	951	rBV	2139540	2399886	71.08%	6.855%
40	13.002	951	955	959	rVV5	31846	98375	2.91%	0.281%
41	13.814	1024	1026	1029	rBV3	194846	372425	11.03%	1.064%
42	13.974	1038	1040	1044	rVB2	708391	1248372	36.97%	3.566%
43	15.403	1163	1165	1176	rVB	695832	1745506	51.70%	4.986%

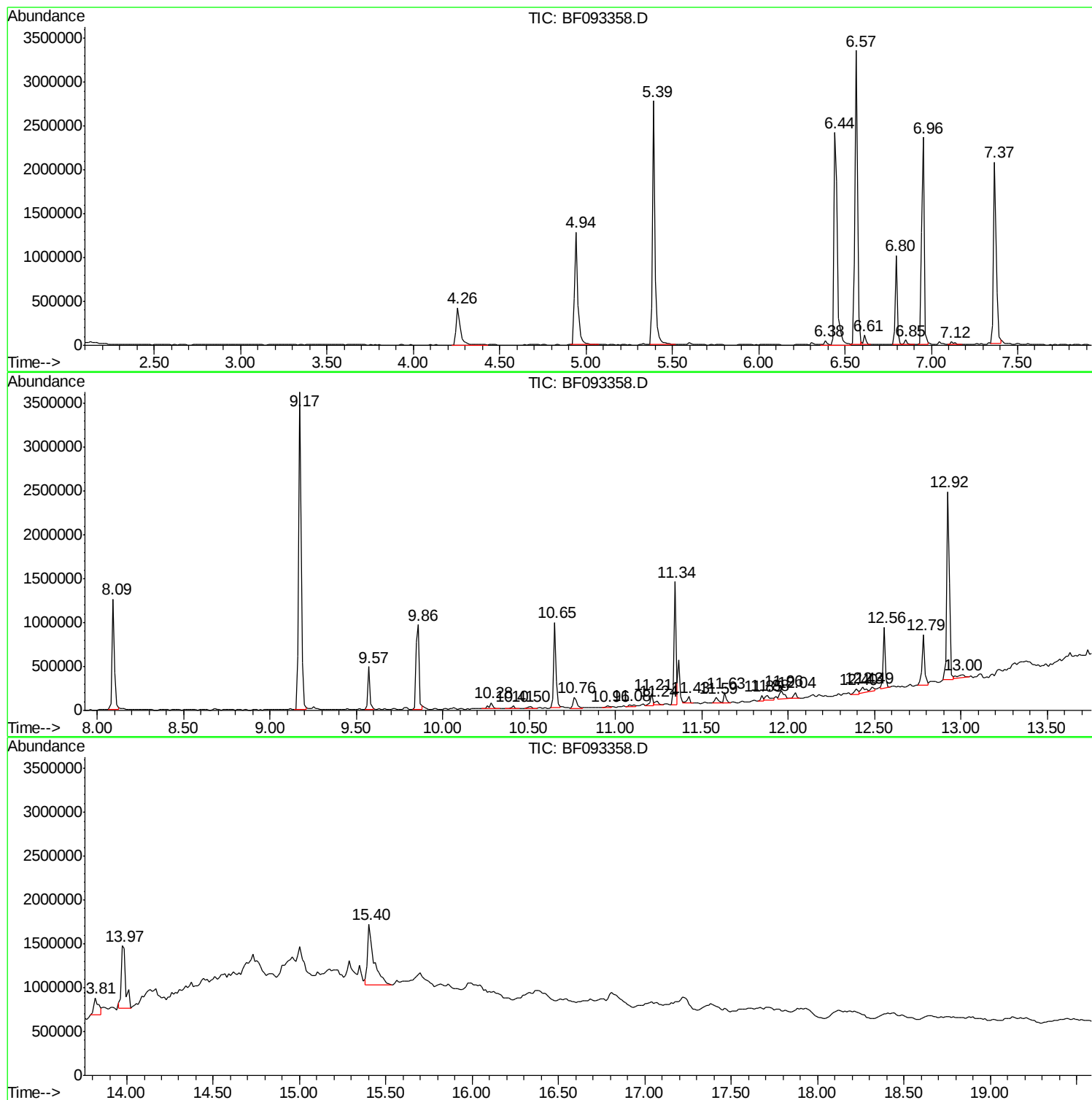
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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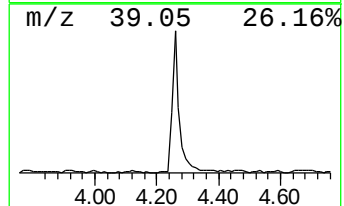
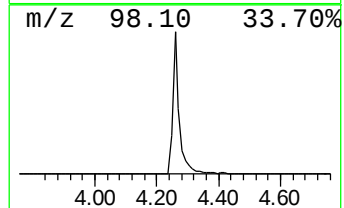
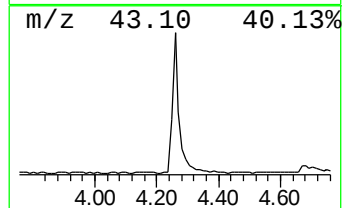
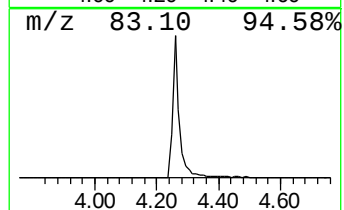
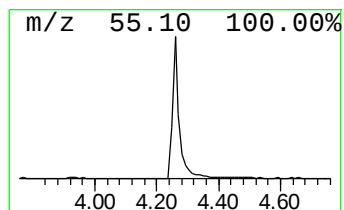
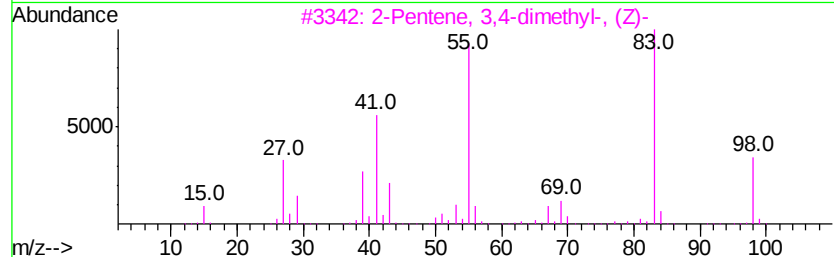
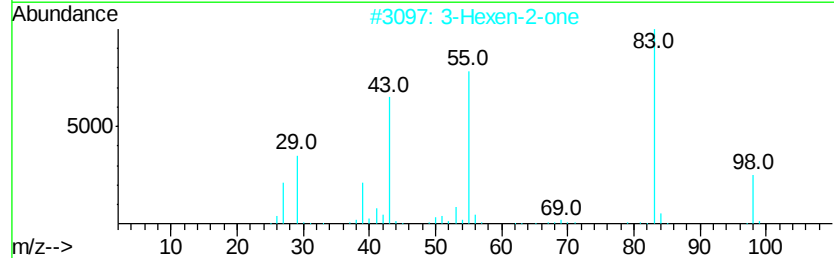
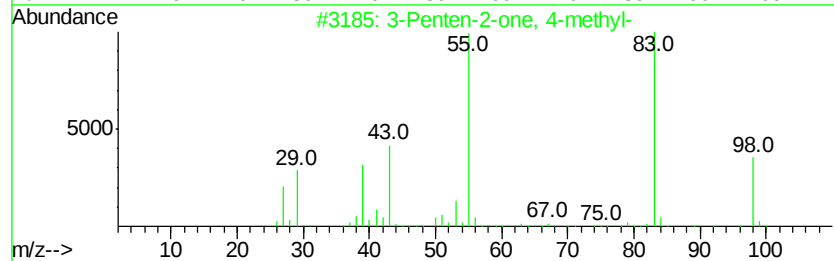
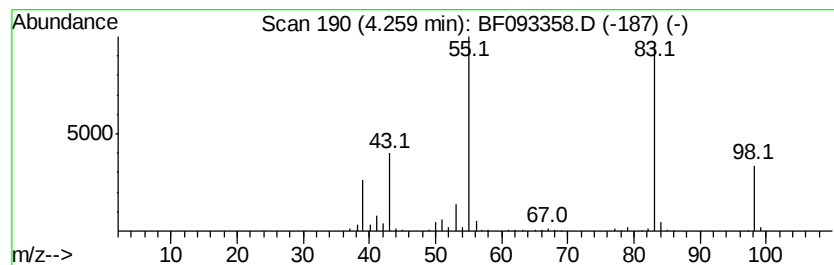
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	14.63 ng	664986	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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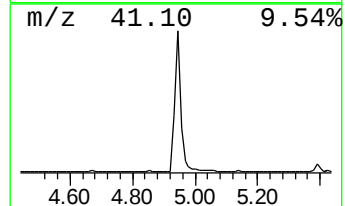
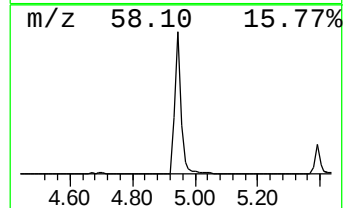
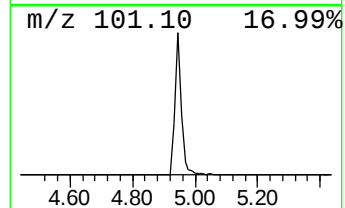
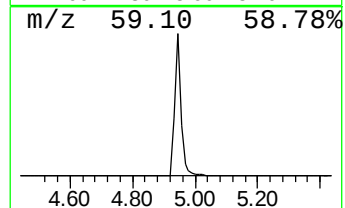
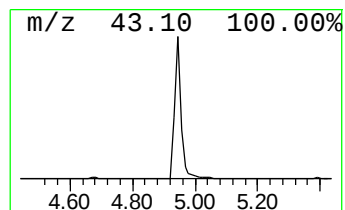
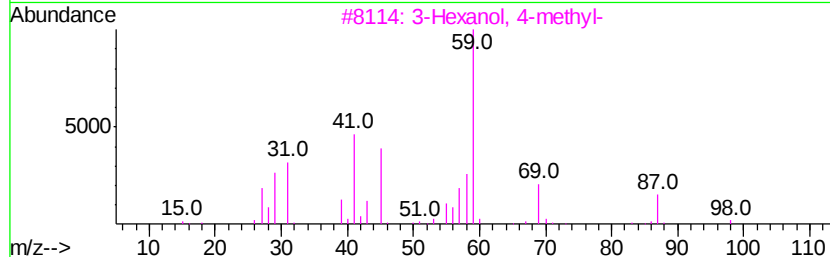
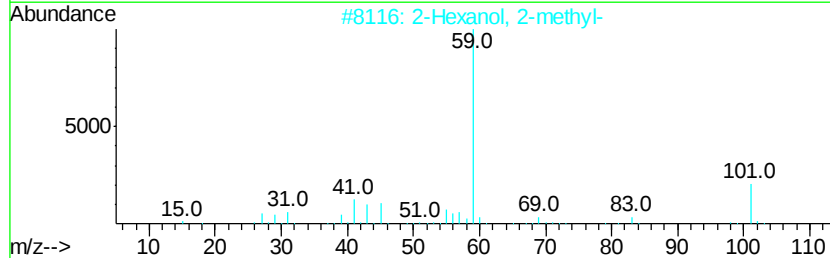
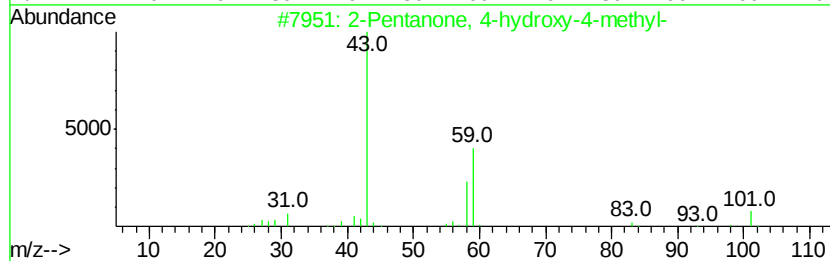
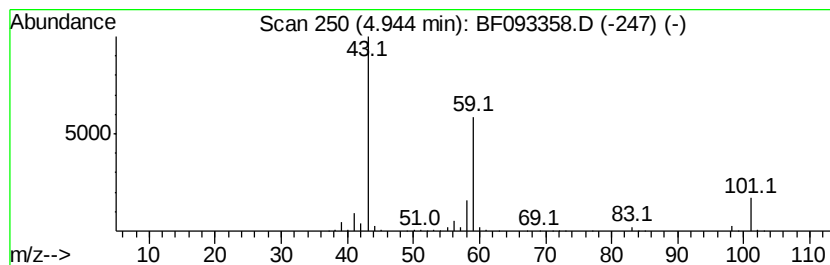
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	37.58 ng	1708200	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32



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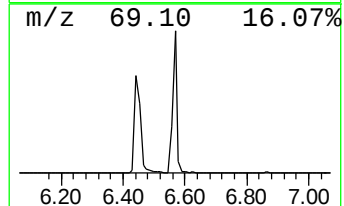
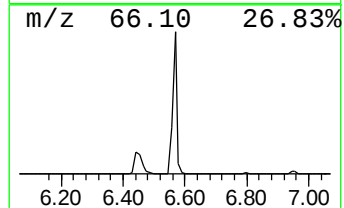
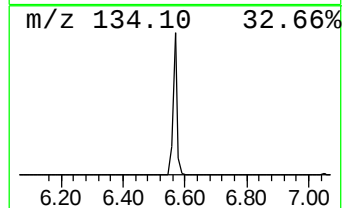
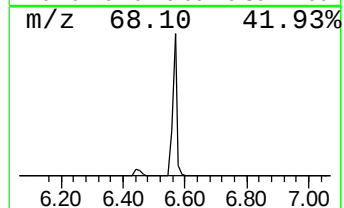
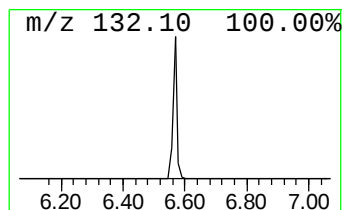
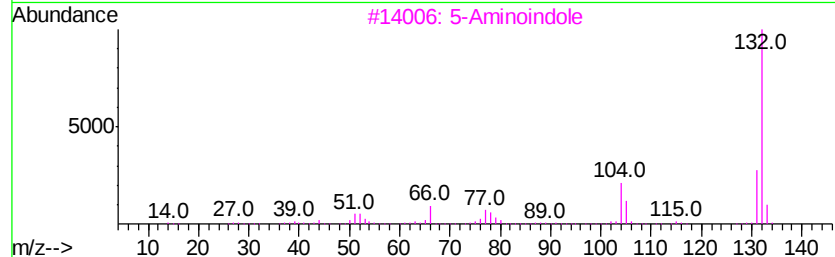
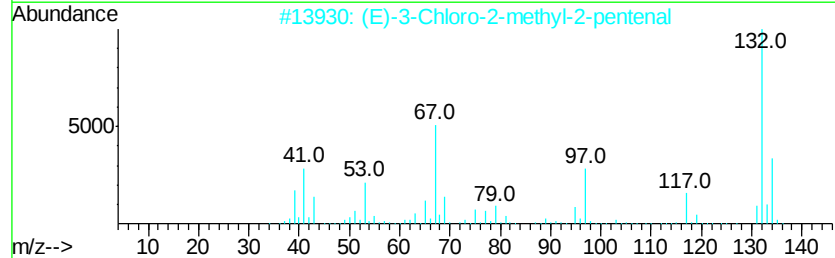
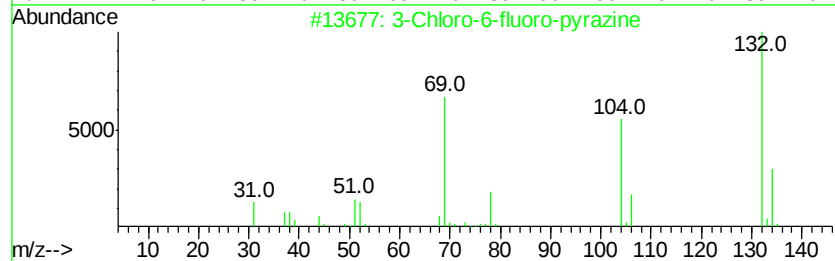
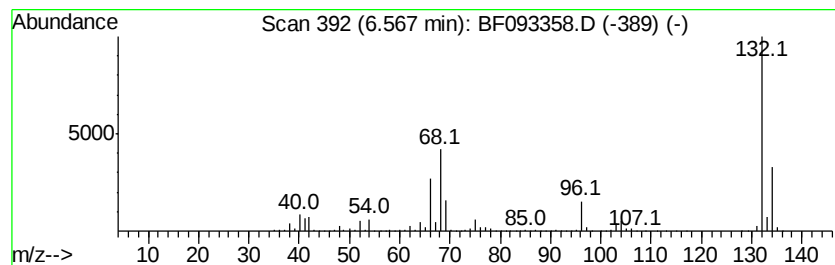
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	69.73 ng	3169660	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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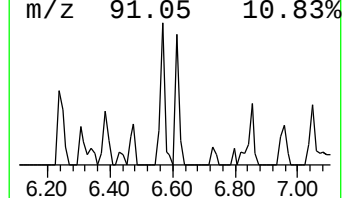
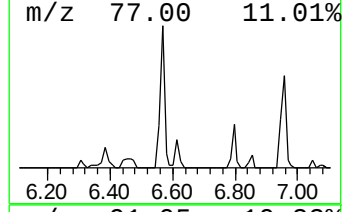
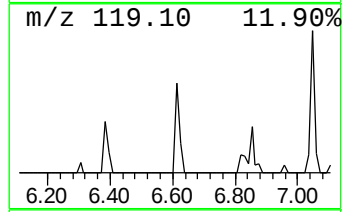
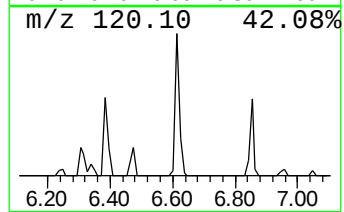
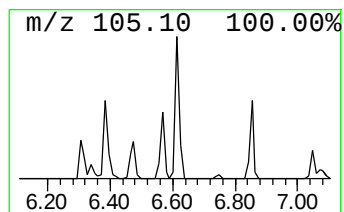
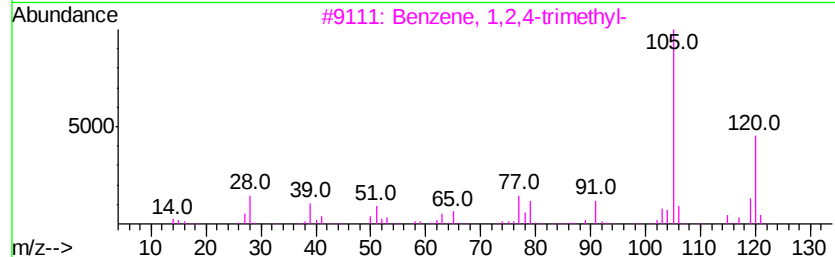
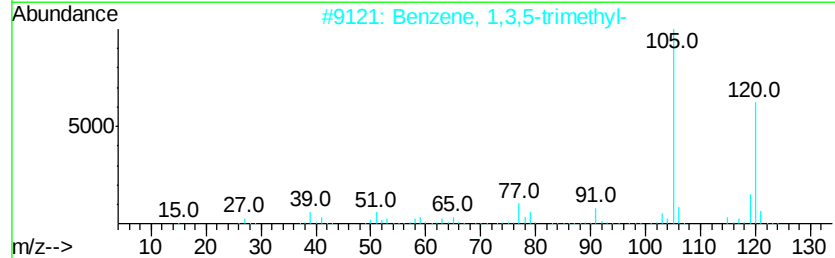
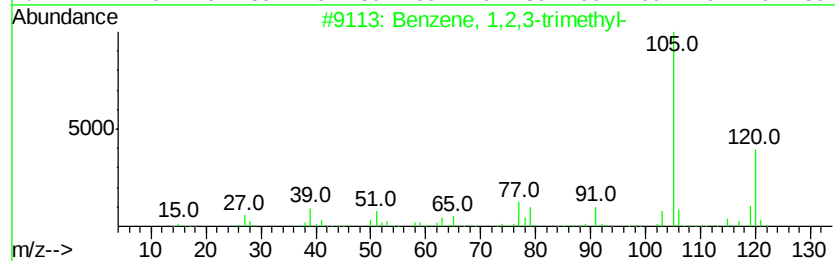
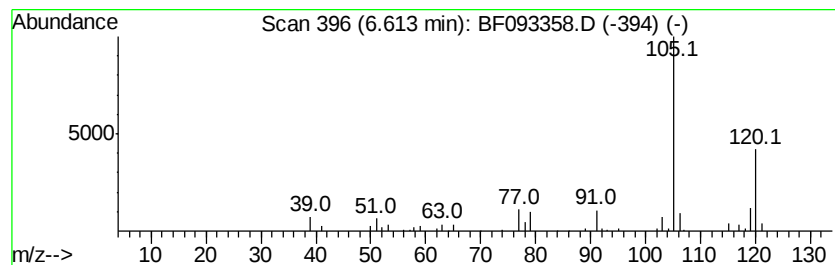
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	2.36 ng	107398	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



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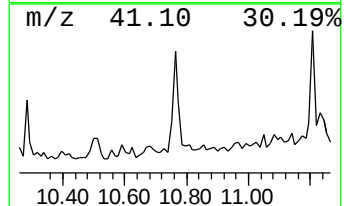
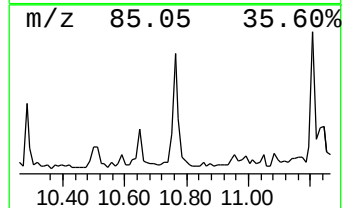
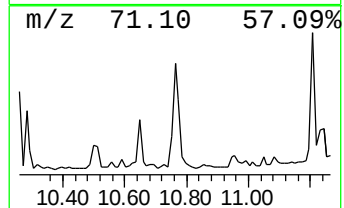
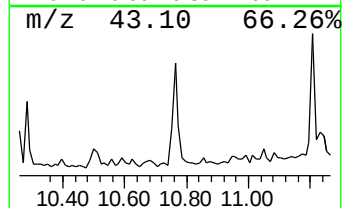
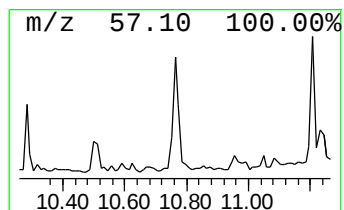
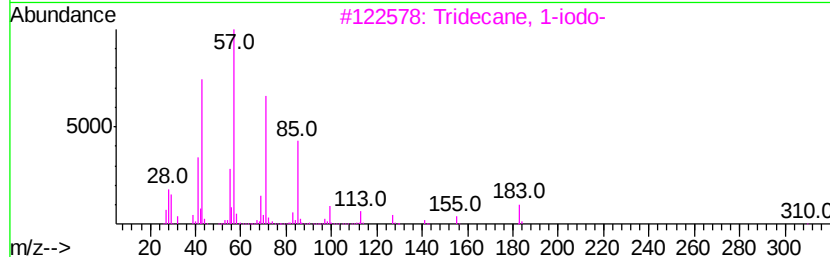
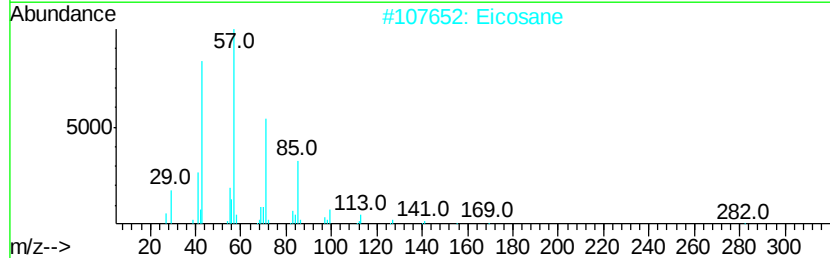
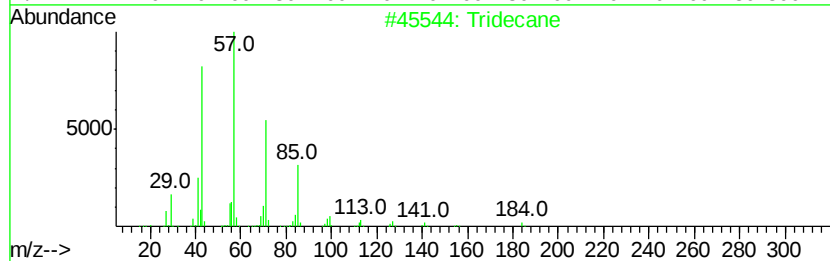
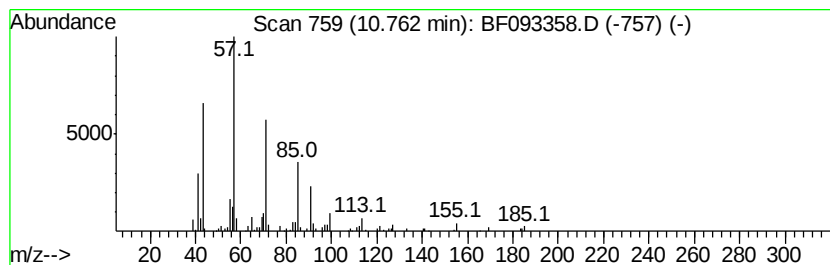
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.76	3.10 ng	194929	Phenanthrene-d10		11.35
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane	282	C20H42	000112-95-8	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030217\
Data File : BF093358.D
Acq On : 3 Mar 2017 12:55
Operator : SJ/MA
Sample : I2057-15
Misc :
ALS Vial : 40 Sample Multiplier: 1

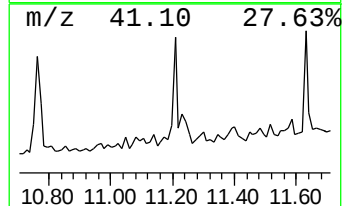
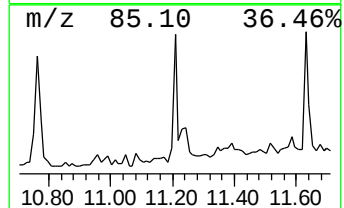
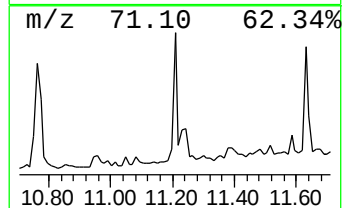
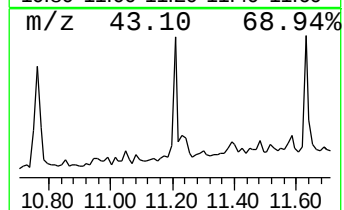
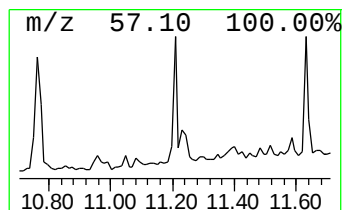
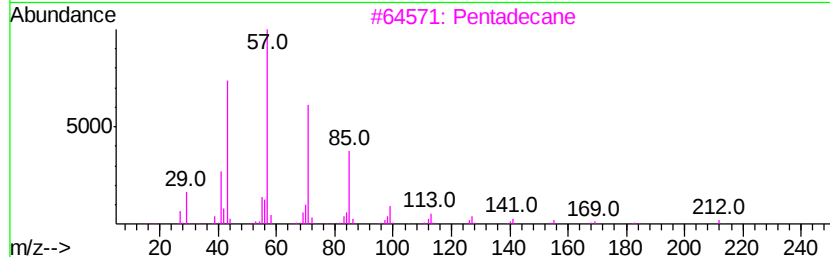
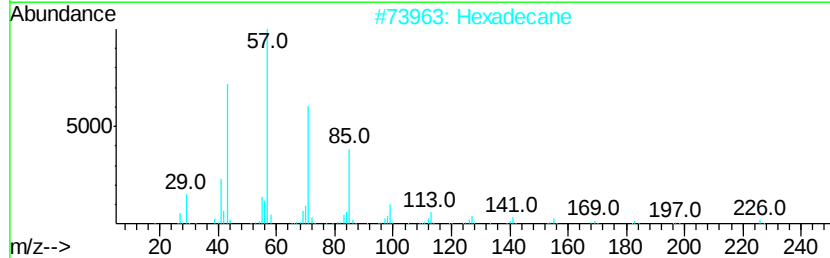
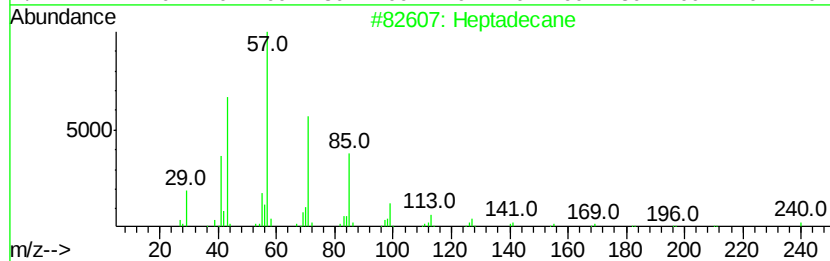
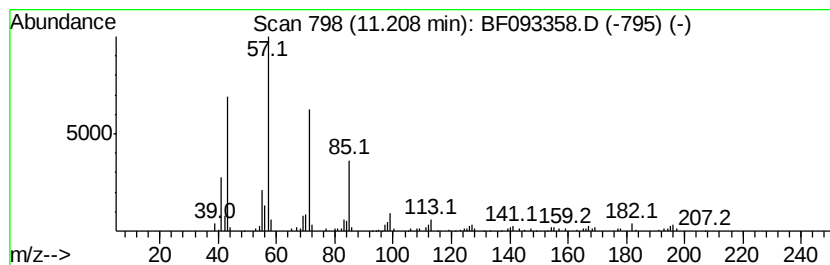
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BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.21	2.18 ng	136952	Phenanthrene-d10		11.35		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	87
2			Hexadecane	226	C16H34	000544-76-3	87
3			Pentadecane	212	C15H32	000629-62-9	87
4			Tetradecane	198	C14H30	000629-59-4	86
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030217\
Data File : BF093358.D
Acq On : 3 Mar 2017 12:55
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Sample : I2057-15
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Instrument :
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ClientSampleId :
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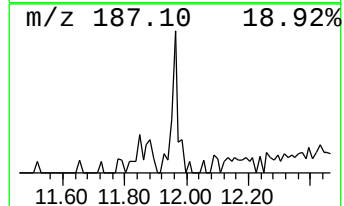
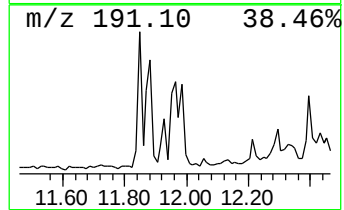
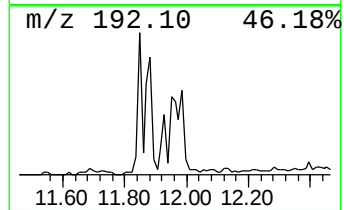
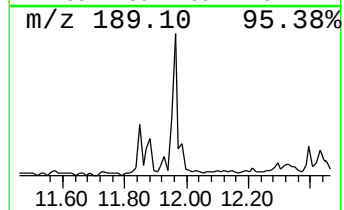
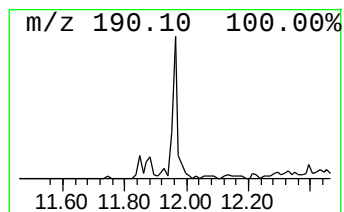
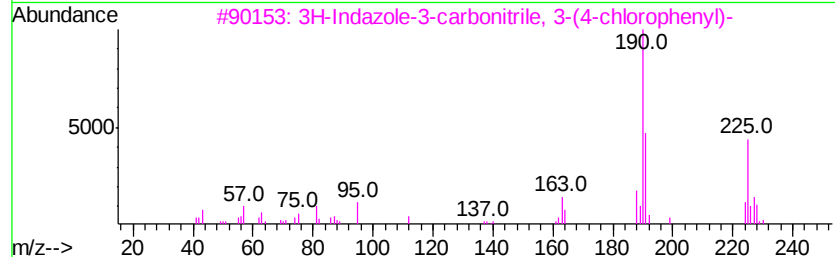
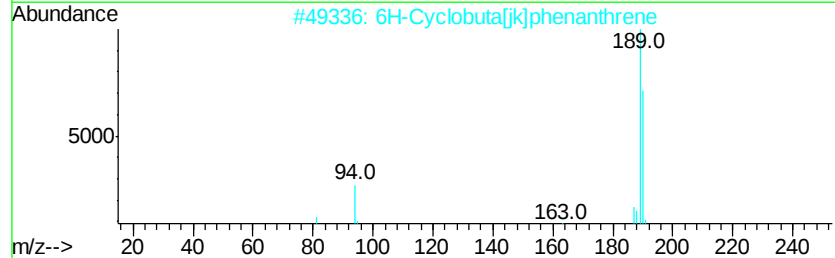
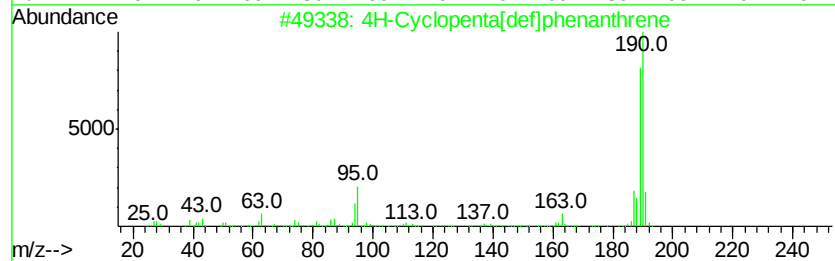
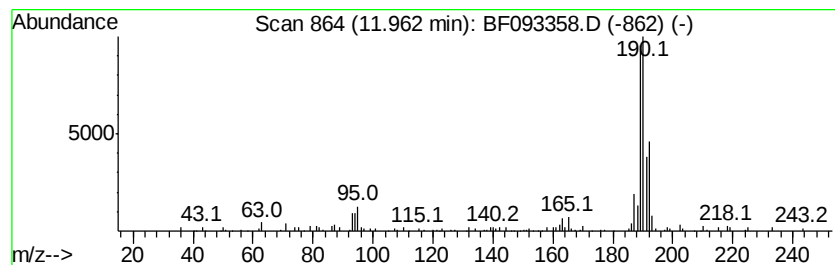
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	3.08 ng	193692	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3		3H-Indazole-3-carbonitrile, 3-(4...	253	C14H8ClN3	056630-97-8	23
4		4-(4-Chlorophenyl)pyridine	189	C11H8ClN	005957-96-0	17
5		1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030217\
Data File : BF093358.D
Acq On : 3 Mar 2017 12:55
Operator : SJ/MA
Sample : I2057-15
Misc :
ALS Vial : 40 Sample Multiplier: 1

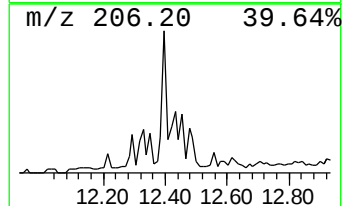
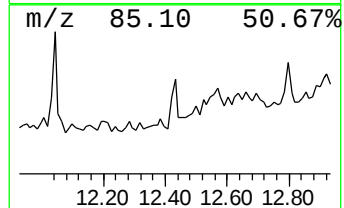
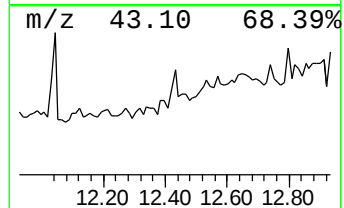
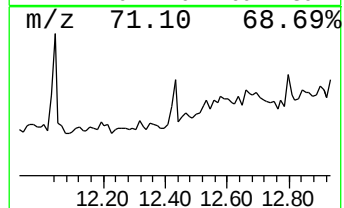
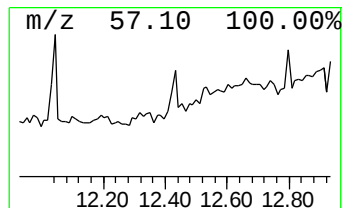
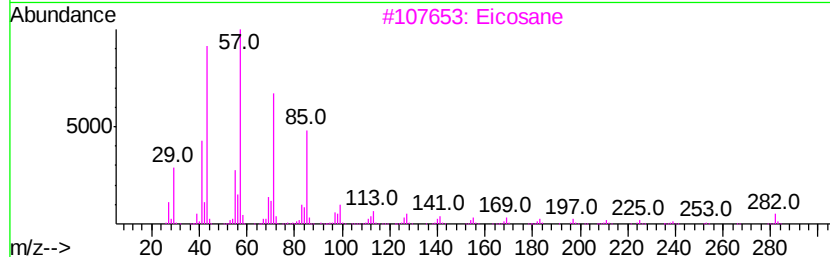
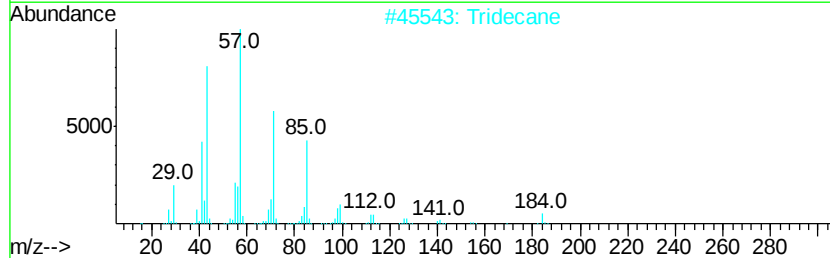
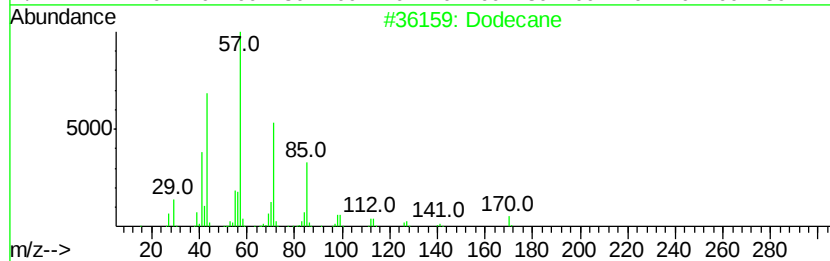
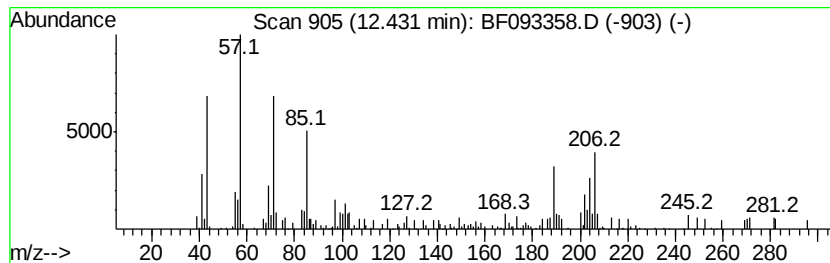
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.43 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	2.11 ng	132454	Phenanthrene-d10	11.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane	170 C12H26	000112-40-3	42
2	Tridecane	184 C13H28	000629-50-5	42
3	Eicosane	282 C20H42	000112-95-8	38
4	Decane, 2,3,8-trimethyl-	184 C13H28	062238-14-6	27
5	2-Bromo dodecane	248 C12H25Br	013187-99-0	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030217\
Data File : BF093358.D
Acq On : 3 Mar 2017 12:55
Operator : SJ/MA
Sample : I2057-15
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
34B-4

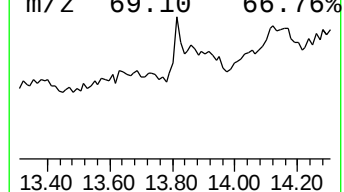
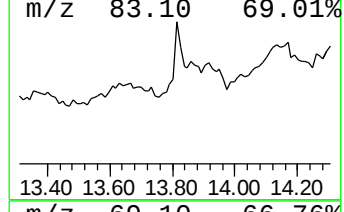
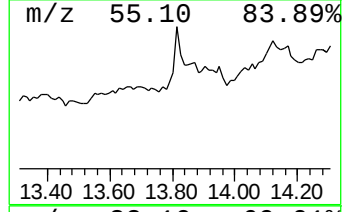
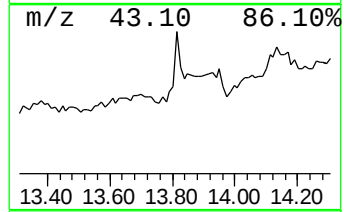
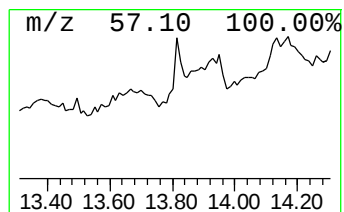
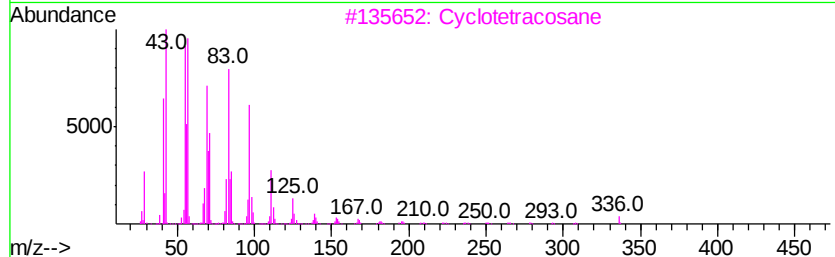
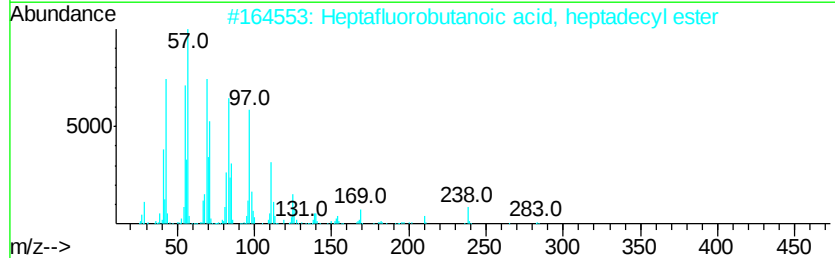
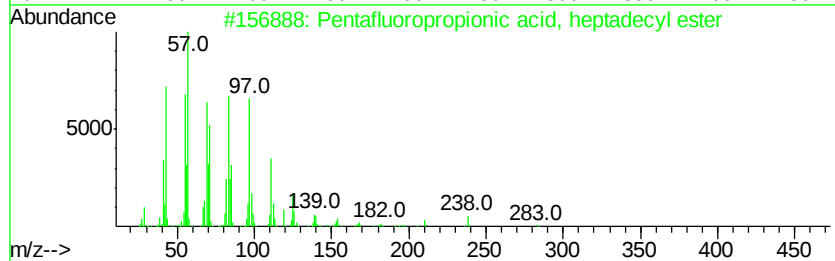
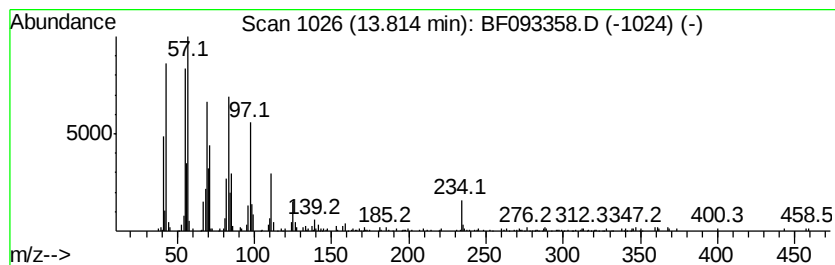
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.97 ng	372425	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
3		Cyclotetracosane	336	C24H48	000297-03-0	90
4		1-Tricosene	322	C23H46	018835-32-0	90
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90



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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
3-Penten-2-one, 4...	4.26	14.6	ng	664986	1	6.80	909115	20.0
2-Pentanone, 4-hy...	4.94	37.6	ng	1708200	1	6.80	909115	20.0
unknown6.57	6.57	69.7	ng	3169660	1	6.80	909115	20.0
Benzene, 1,2,3-tr...	6.61	2.4	ng	107398	1	6.80	909115	20.0
Tridecane	10.76	3.1	ng	194929	4	11.35	1256260	20.0
Heptadecane	11.21	2.2	ng	136952	4	11.35	1256260	20.0
4H-Cyclopenta[def...	11.96	3.1	ng	193692	4	11.35	1256260	20.0
unknown12.43	12.43	2.1	ng	132454	4	11.35	1256260	20.0
Pentafluoropropio...	13.81	6.0	ng	372425	5	13.99	1248370	20.0