

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092215\
 Data File : BF081745.D
 Acq On : 22 Sep 2015 18:12
 Operator : UM/IZ
 Sample : G3753-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-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-BF090115.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	1.213	8	11	14	rVB	919224	959479	16.33%	4.800%
2	1.430	28	30	36	rBV	251194	659109	11.22%	3.297%
3	1.521	36	38	86	rVB	1600251	5875916	100.00%	29.397%
4	4.413	287	291	312	rBV	213011	646764	11.01%	3.236%
5	5.293	366	368	388	rBV	491869	1119430	19.05%	5.600%
6	7.579	564	568	572	rBV	601453	1051599	17.90%	5.261%
7	7.659	572	575	594	rVB	695006	1307846	22.26%	6.543%
8	8.139	614	617	623	rBB	133519	236890	4.03%	1.185%
9	8.459	642	645	655	rBB	541408	884214	15.05%	4.424%
10	9.442	727	731	750	rBB	435438	759277	12.92%	3.799%
11	11.031	867	870	883	rBB	167985	288566	4.91%	1.444%
12	13.682	1097	1102	1105	rBV	692097	1269939	21.61%	6.353%
13	14.734	1191	1194	1200	rBV	136551	219410	3.73%	1.098%
14	15.157	1228	1231	1236	rBV2	168774	279763	4.76%	1.400%
15	17.066	1394	1398	1407	rBB	346166	623059	10.60%	3.117%
16	18.666	1535	1538	1541	rBV	143919	252642	4.30%	1.264%
17	18.723	1541	1543	1546	rVV	44783	78514	1.34%	0.393%
18	20.426	1689	1692	1699	rBV	41132	84176	1.43%	0.421%
19	21.363	1771	1774	1779	rVB	127275	197094	3.35%	0.986%
20	21.706	1802	1804	1810	rBV	130546	212962	3.62%	1.065%
21	22.049	1831	1834	1836	rBV	670481	835344	14.22%	4.179%
22	23.329	1940	1946	1947	rBV3	241975	489640	8.33%	2.450%
23	23.363	1947	1949	1951	rVV2	69848	116065	1.98%	0.581%
24	23.992	2002	2004	2007	rVB	61745	83784	1.43%	0.419%
25	24.426	2040	2042	2047	rBV	115076	250349	4.26%	1.252%
26	24.586	2054	2056	2062	rBV2	78900	179830	3.06%	0.900%
27	24.678	2062	2064	2066	rBV	82440	90365	1.54%	0.452%
28	24.724	2066	2068	2070	rVV	132392	141941	2.42%	0.710%
29	24.769	2070	2072	2076	rVV	198280	239118	4.07%	1.196%
30	25.169	2104	2107	2108	rBV	67828	114478	1.95%	0.573%
31	25.249	2111	2114	2117	rVB	80718	148342	2.52%	0.742%
32	25.535	2137	2139	2143	rVB3	68667	99909	1.70%	0.500%
33	25.798	2160	2162	2166	rVB	55865	109879	1.87%	0.550%
34	26.107	2187	2189	2192	rBV2	40407	82741	1.41%	0.414%

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

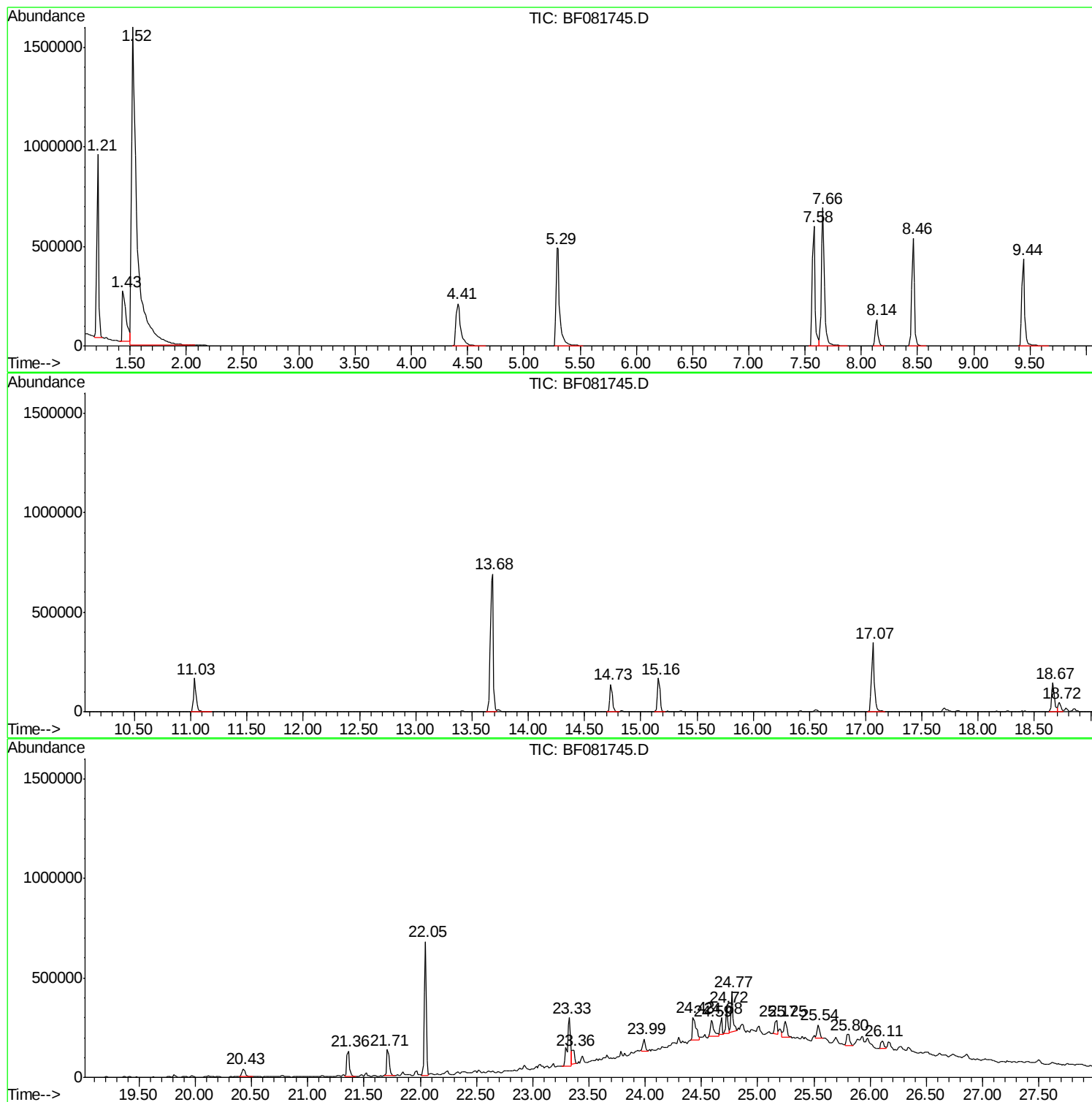
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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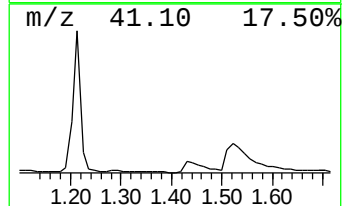
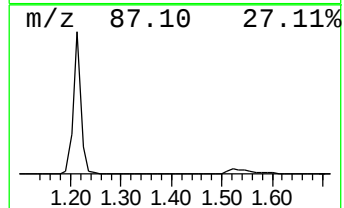
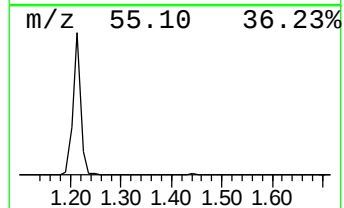
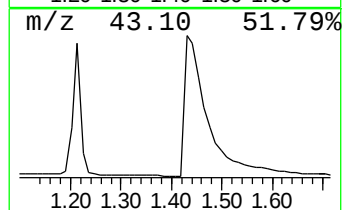
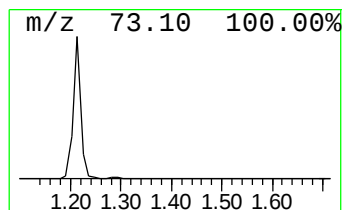
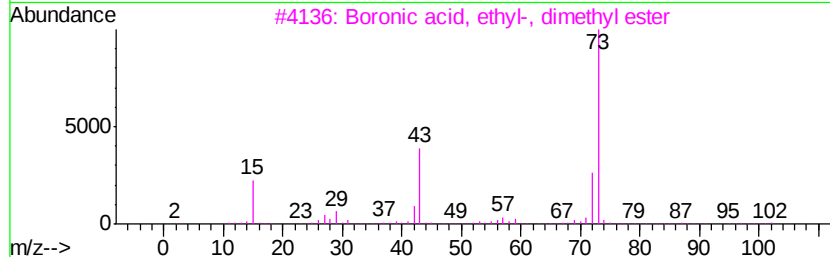
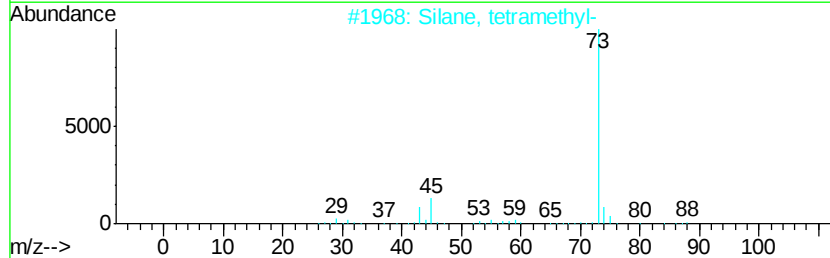
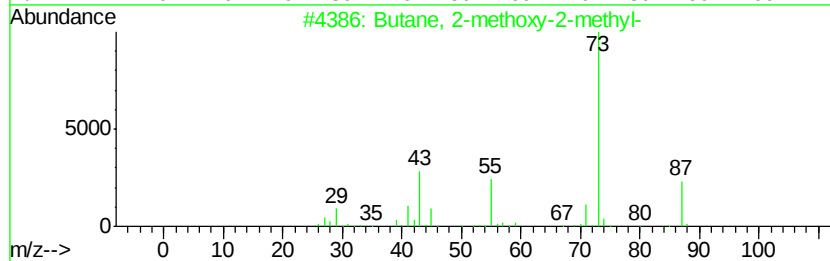
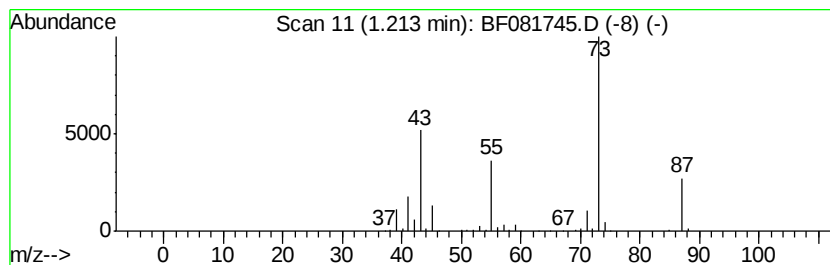
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.21	81.01 ng	959479	1,4-Dichlorobenzene-d4	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
3		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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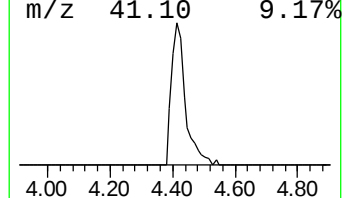
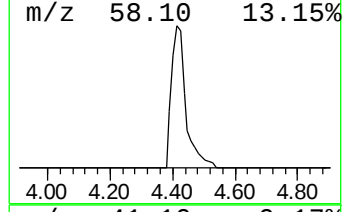
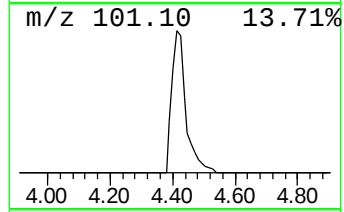
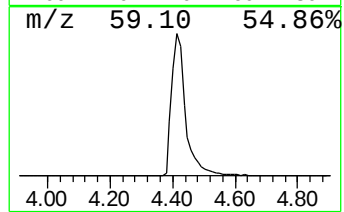
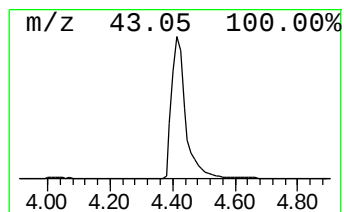
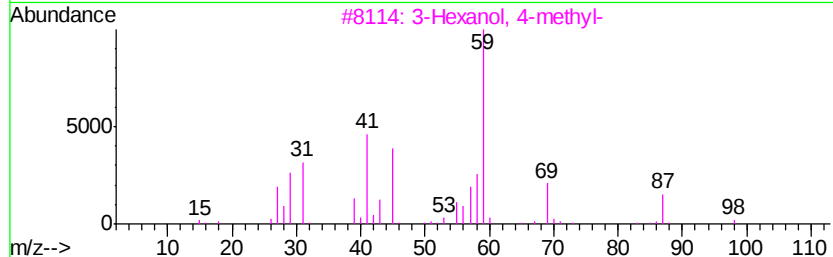
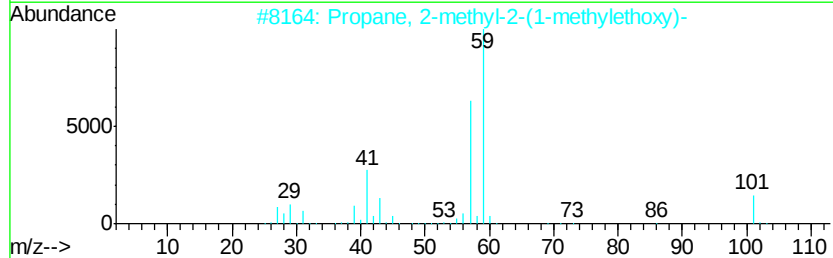
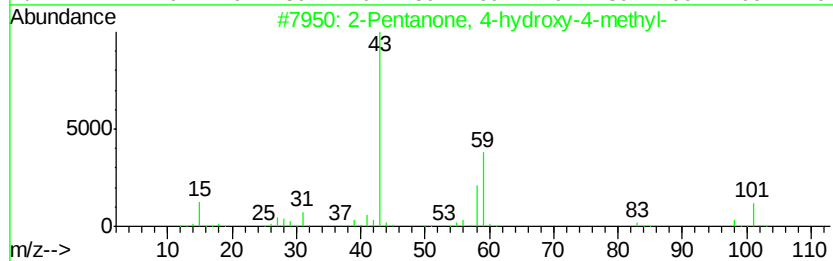
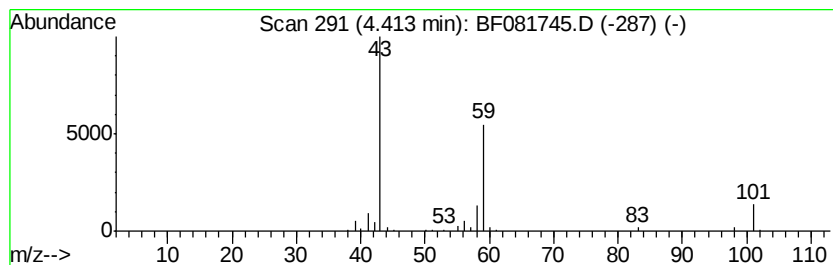
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	54.60 ng	646764	1,4-Dichlorobenzene-d4	8.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	32		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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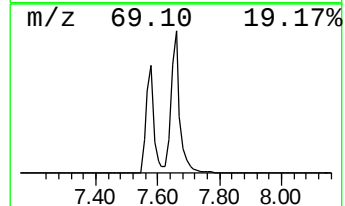
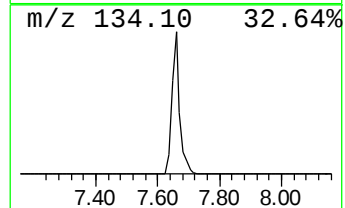
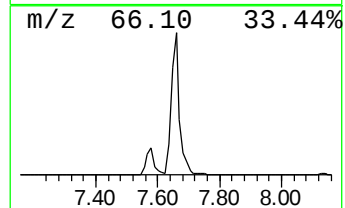
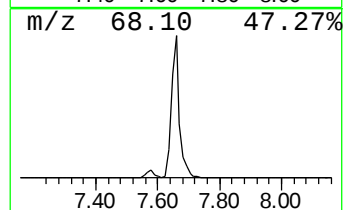
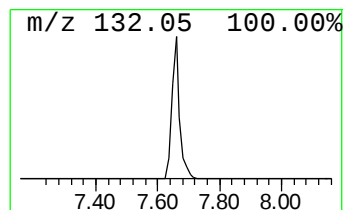
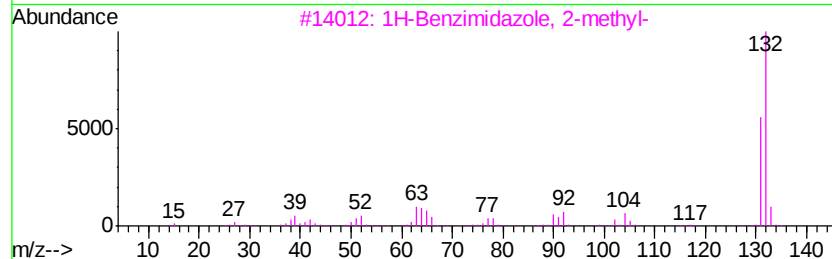
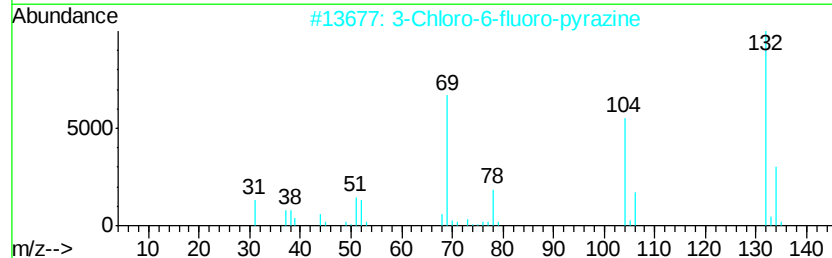
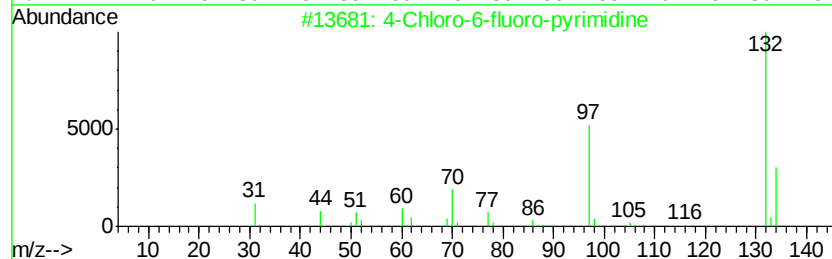
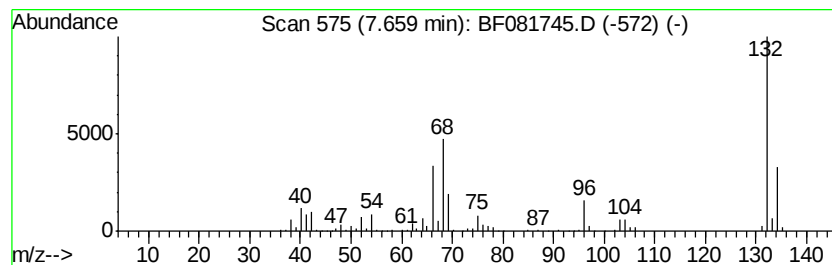
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	110.42 ng	1307850	1,4-Dichlorobenzene-d4	8.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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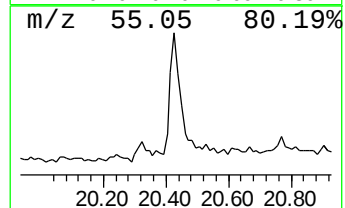
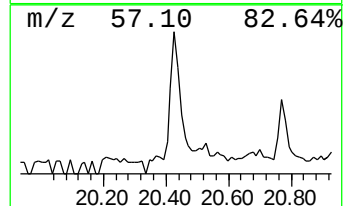
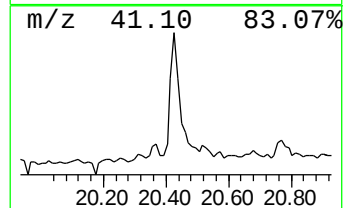
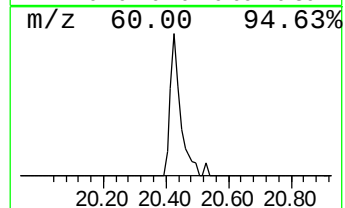
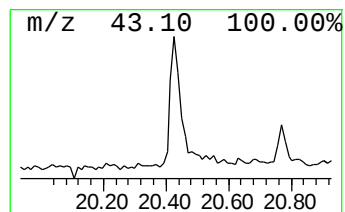
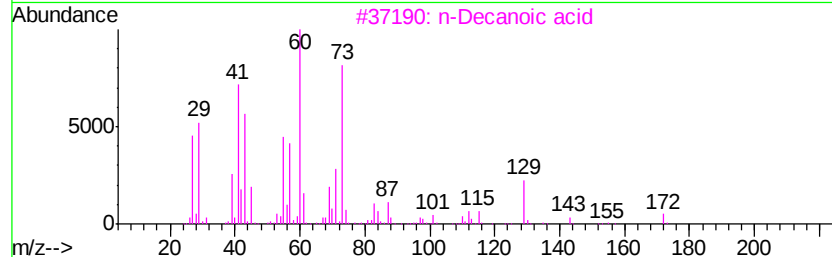
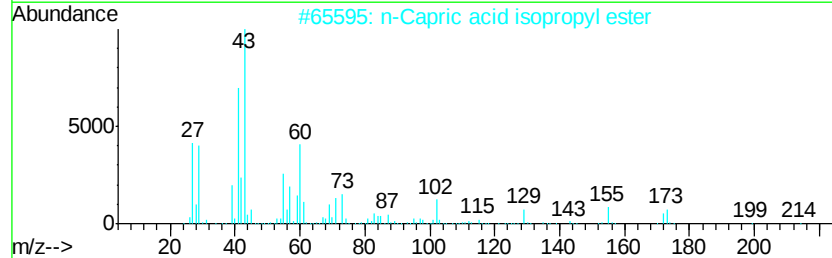
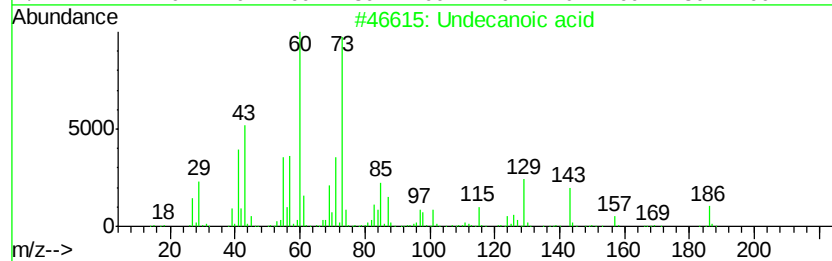
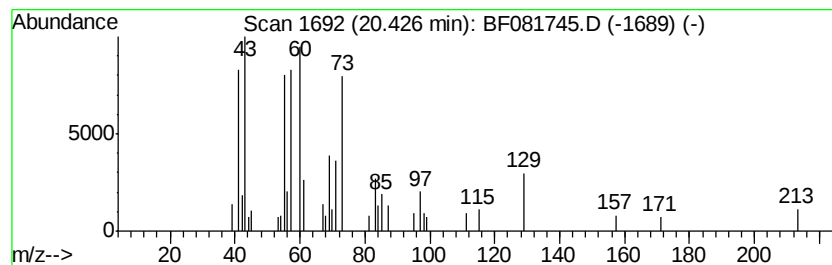
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Undecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	6.66 ng	84176	Phenanthrene-d10	18.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	64
2		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		Amvl Nitrite	117	C5H11NO2	000110-46-3	27
5		4-Propionyloxypentadecane	284	C18H36O2	1000245-63-2	14



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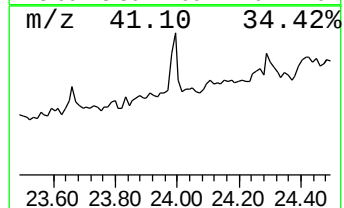
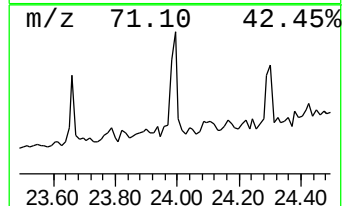
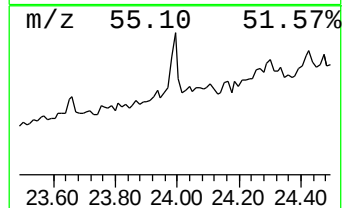
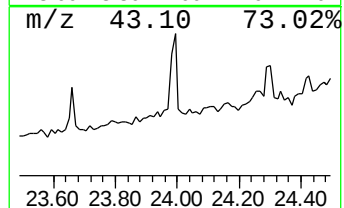
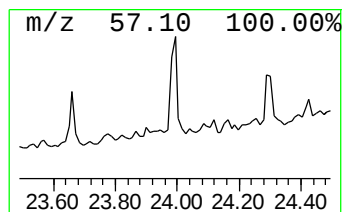
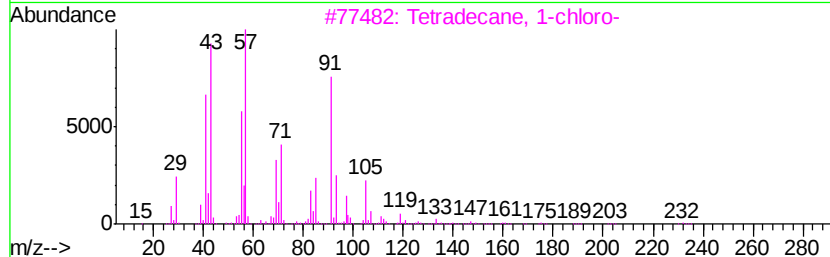
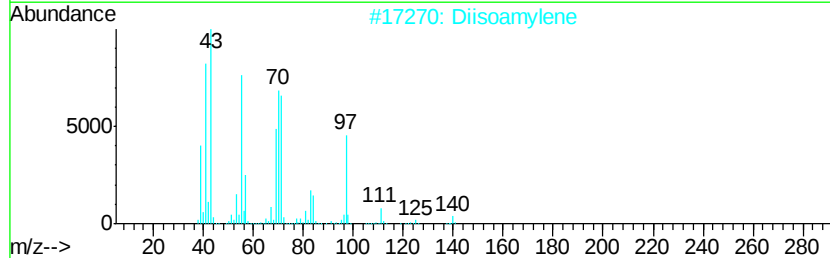
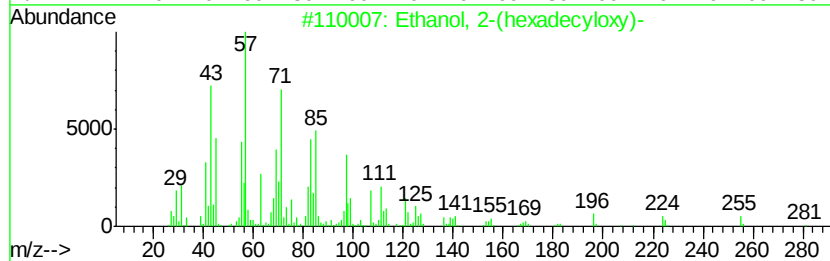
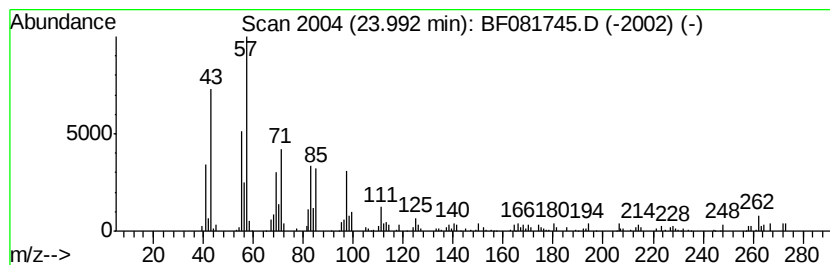
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanol, 2-(hexadecyloxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.42 ng	83784	Chrysene-d12	23.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	58
2		Diisiamylene	140	C10H20	054063-09-1	50
3		Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	49
4		Undecane	156	C11H24	001120-21-4	45
5		Tetradecane	198	C14H30	000629-59-4	43



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ClientSampleId :
SP-2

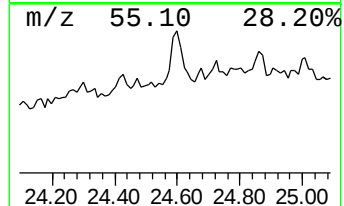
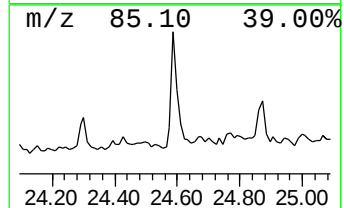
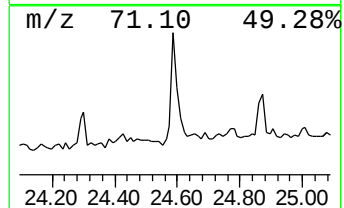
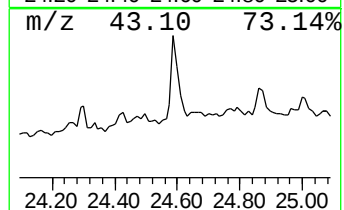
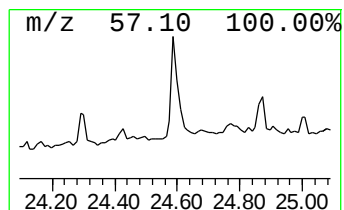
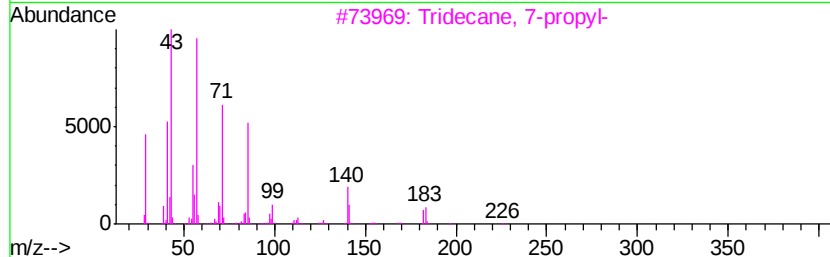
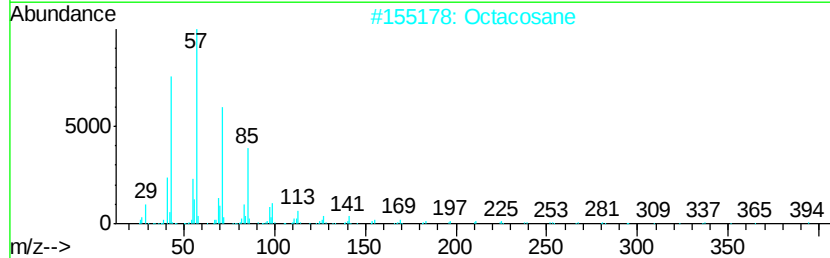
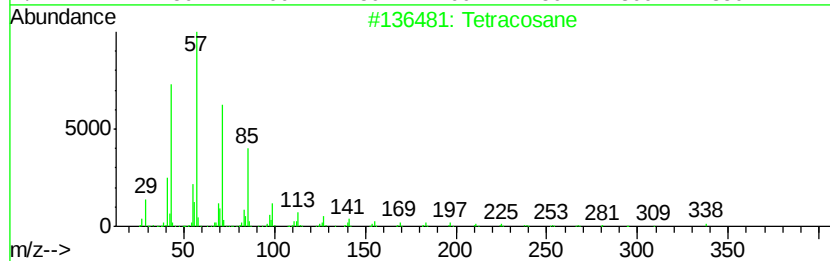
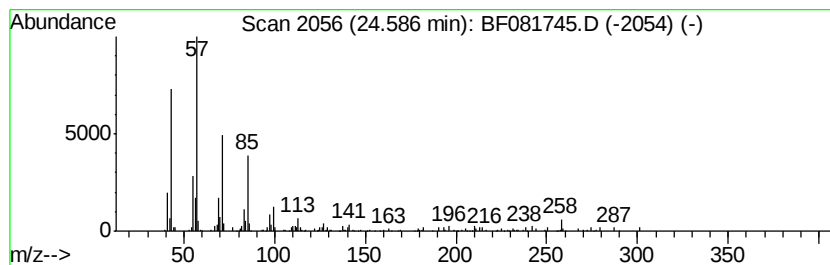
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.59	15.04 ng	179830	Perylene-d12	24.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane		338	C24H50	000646-31-1	87
2	Octacosane		394	C28H58	000630-02-4	83
3	Tridecane, 7-propyl-		226	C16H34	055045-09-5	83
4	Eicosane		282	C20H42	000112-95-8	80
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081745.D
Acq On : 22 Sep 2015 18:12
Operator : UM/IZ
Sample : G3753-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

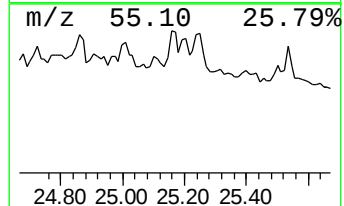
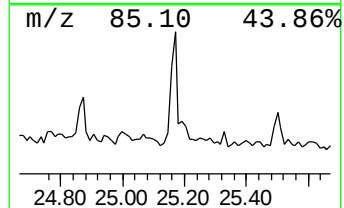
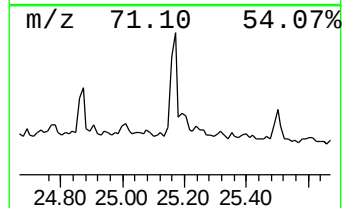
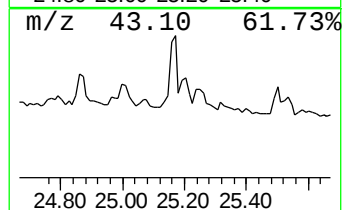
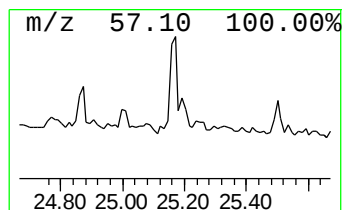
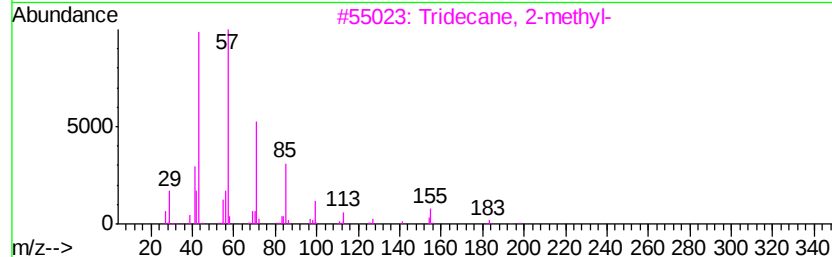
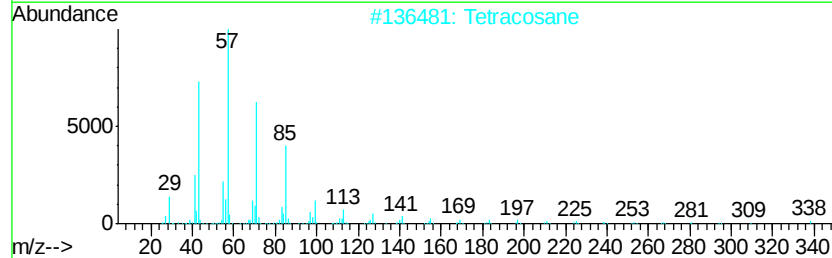
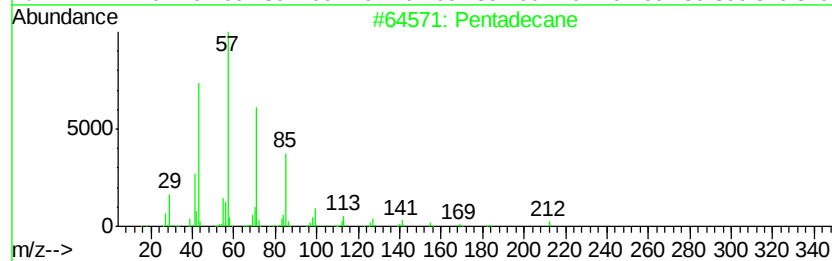
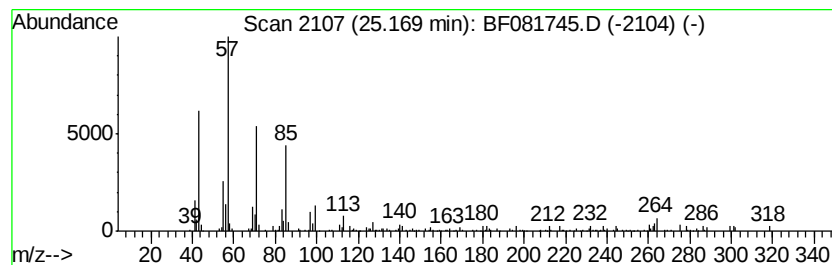
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.17	9.58 ng	114478	Perylene-d12	24.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	96
2	Tetracosane		338	C24H50	000646-31-1	83
3	Tridecane, 2-methyl-		198	C14H30	001560-96-9	74
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72
5	Octadecane		254	C18H38	000593-45-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081745.D
Acq On : 22 Sep 2015 18:12
Operator : UM/IZ
Sample : G3753-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

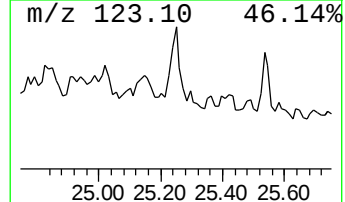
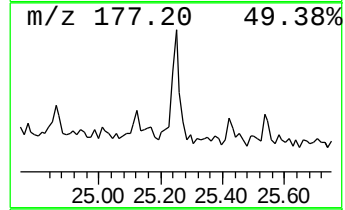
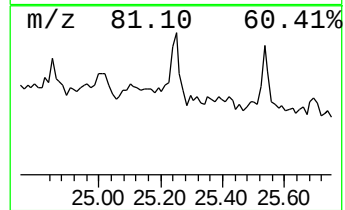
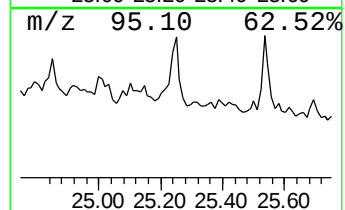
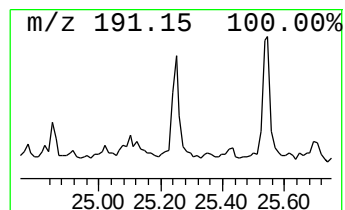
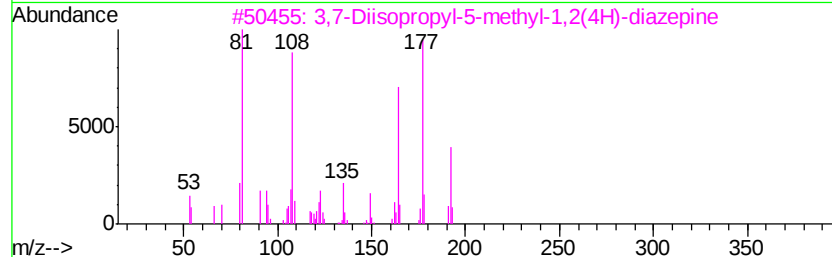
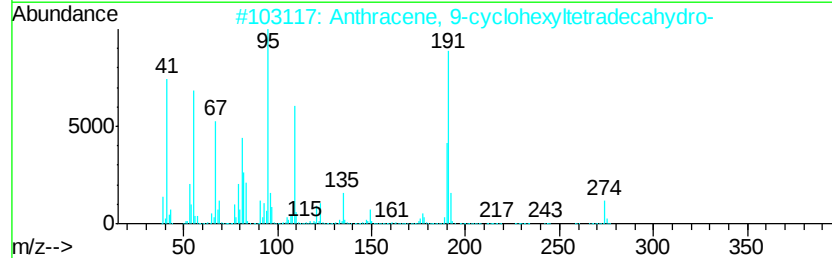
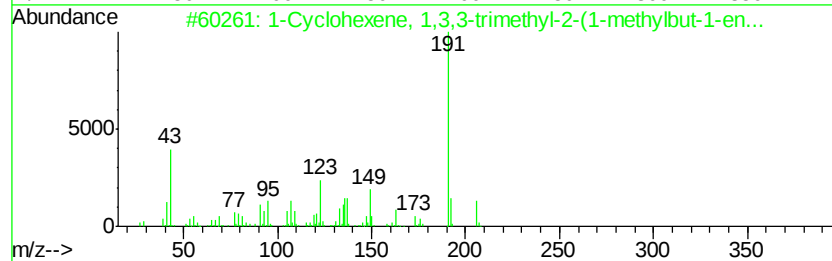
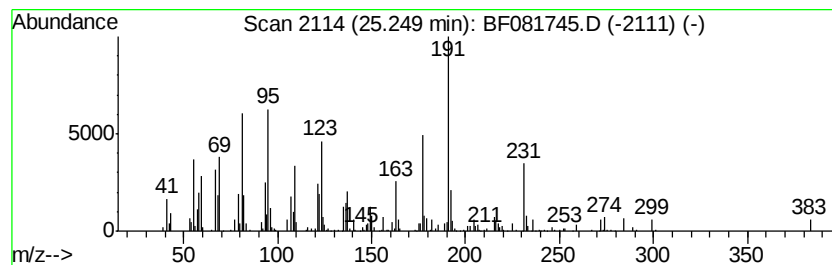
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown25.25 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.25	12.41 ng	148342	Perylene-d12	24.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
2		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
3		3,7-Diisopropyl-5-methyl-1,2(4H)...	192	C12H20N2	088829-71-4	25
4		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	22
5		Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092215\
Data File : BF081745.D
Acq On : 22 Sep 2015 18:12
Operator : UM/IZ
Sample : G3753-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

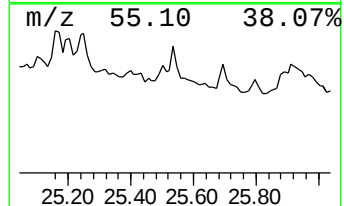
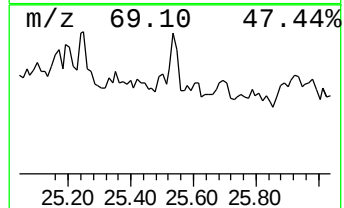
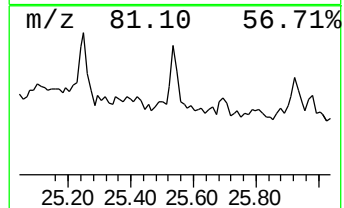
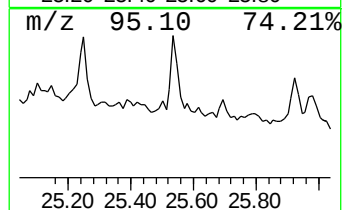
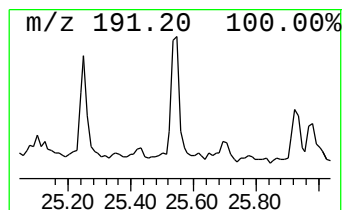
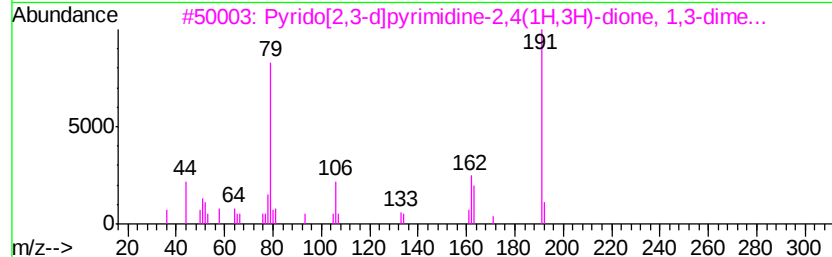
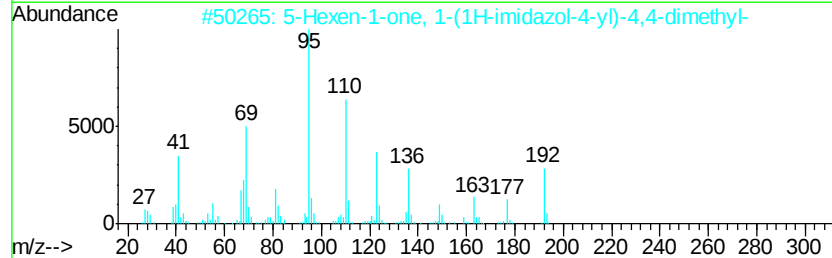
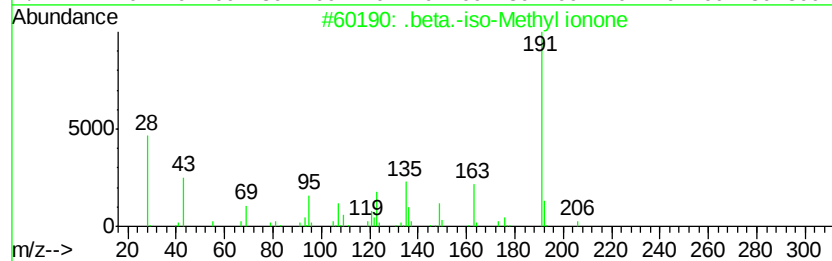
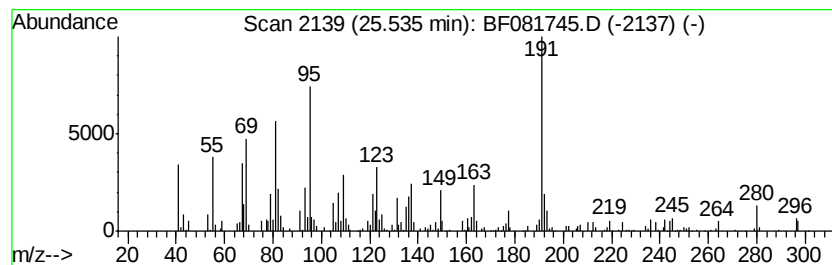
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown25.54 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.54	8.36 ng	99909	Perylene-d12	24.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	35
2		5-Hexen-1-one, 1-(1H-imidazol-4-yl)-4,4-dimethyl-	192	C11H16N2O	069393-41-5	30
3		Pyrrolo[2,3-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-	191	C9H9N3O2	024410-21-7	27
4		Indolizine, 6-carbethoxy-7,8-dihydro-	191	C11H13NO2	1000131-05-8	27
5		1-Penten-3-one, 1-(2,6,6-trimethyl-4-oxocyclohex-1-en-1-yl)-	206	C14H22O	000127-43-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092215\
Data File : BF081745.D
Acq On : 22 Sep 2015 18:12
Operator : UM/IZ
Sample : G3753-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.21	81.0	ng	959479	1	8.14	236890	20.0
2-Pentanone, 4-hy...	4.41	54.6	ng	646764	1	8.14	236890	20.0
unknown7.66	7.66	110.4	ng	1307850	1	8.14	236890	20.0
Undecanoic acid	20.43	6.7	ng	84176	4	18.67	252642	20.0
Ethanol, 2-(hexad...	23.99	3.4	ng	83784	5	23.33	489640	20.0
Tetracosane	24.59	15.0	ng	179830	6	24.77	239118	20.0
Pentadecane	25.17	9.6	ng	114478	6	24.77	239118	20.0
unknown25.25	25.25	12.4	ng	148342	6	24.77	239118	20.0
unknown25.54	25.54	8.4	ng	99909	6	24.77	239118	20.0