

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
 Data File : BF081668.D
 Acq On : 17 Sep 2015 6:03
 Operator : UM/IZ
 Sample : G3624-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-SOURCE-5B

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	1.440	7	9	15	rBV	152386	419411	18.59%	2.179%
2	1.531	15	17	58	rVB	620046	2256616	100.00%	11.723%
3	4.480	271	275	293	rBV	318615	1005265	44.55%	5.222%
4	5.349	348	351	373	rBV	910554	1721922	76.31%	8.945%
5	7.612	544	549	553	rBV	914658	1742036	77.20%	9.050%
6	7.703	553	557	560	rVB	1019542	1754245	77.74%	9.113%
7	8.183	596	599	604	rBB	185486	288680	12.79%	1.500%
8	8.515	624	628	631	rBV	780766	1292034	57.26%	6.712%
9	9.486	708	713	716	rBV	606970	1143124	50.66%	5.938%
10	11.075	849	852	858	rBV	202783	360343	15.97%	1.872%
11	13.727	1079	1084	1087	rBV	1024271	1885893	83.57%	9.797%
12	14.778	1172	1176	1185	rBV	196079	328365	14.55%	1.706%
13	15.212	1210	1214	1219	rBB	224322	380313	16.85%	1.976%
14	16.607	1332	1336	1340	rBB	15192	28387	1.26%	0.147%
15	17.110	1376	1380	1387	rBV	587238	1193676	52.90%	6.201%
16	17.750	1433	1436	1444	rBV	23347	57194	2.53%	0.297%
17	18.710	1516	1520	1527	rVB	232178	396617	17.58%	2.060%
18	18.836	1527	1531	1534	rBV	20608	37514	1.66%	0.195%
19	20.470	1671	1674	1681	rBV	83465	186325	8.26%	0.968%
20	21.876	1795	1797	1804	rVV	17636	34277	1.52%	0.178%
21	22.082	1812	1815	1817	rBV	1331550	1646019	72.94%	8.551%
22	23.350	1921	1926	1929	rBV	338145	523439	23.20%	2.719%
23	23.693	1953	1956	1959	rBV2	14590	27734	1.23%	0.144%
24	24.013	1982	1984	1988	rVB2	27208	49088	2.18%	0.255%
25	24.368	2013	2015	2018	rVV	52392	74000	3.28%	0.384%
26	24.608	2034	2036	2038	rBV	30180	38994	1.73%	0.203%
27	24.790	2050	2052	2056	rVB	205879	221259	9.80%	1.149%
28	25.236	2089	2091	2100	rVB3	25043	74517	3.30%	0.387%
29	26.219	2174	2177	2182	rBV4	15849	42994	1.91%	0.223%
30	26.894	2232	2236	2244	rVB5	10413	39424	1.75%	0.205%

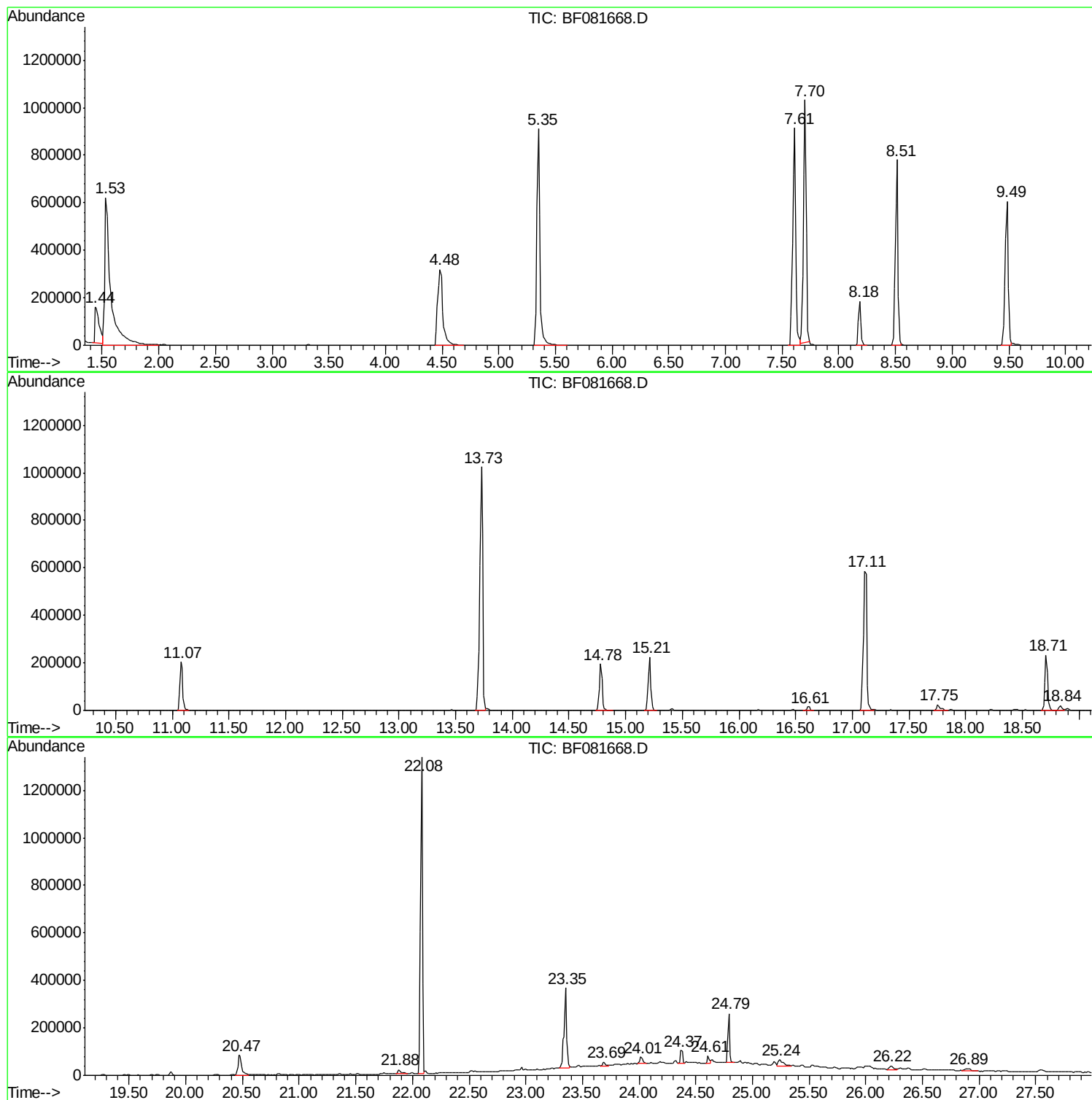
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ClientSampleId :
VITALE-FILL-SOURCE-5B

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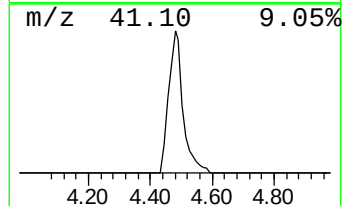
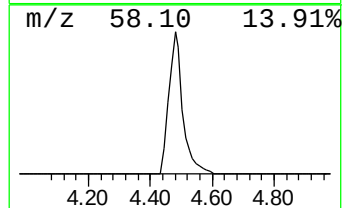
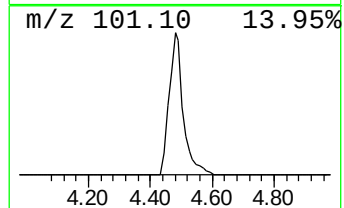
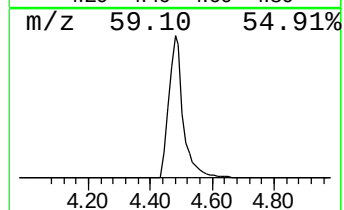
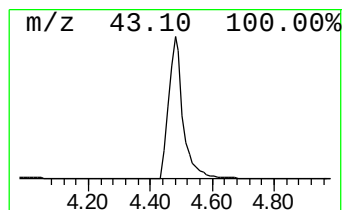
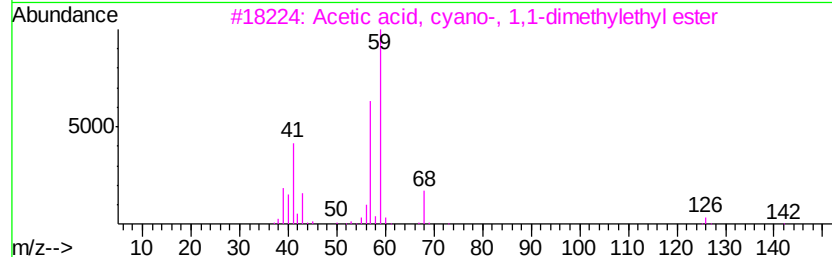
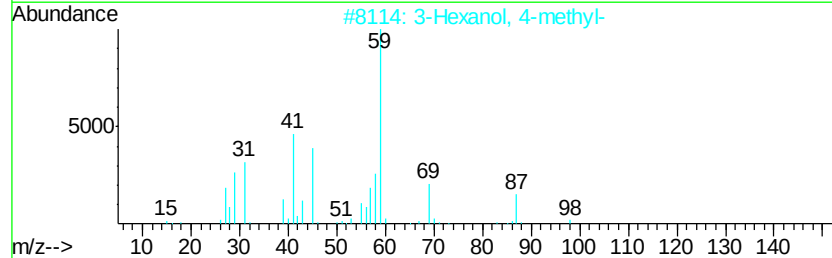
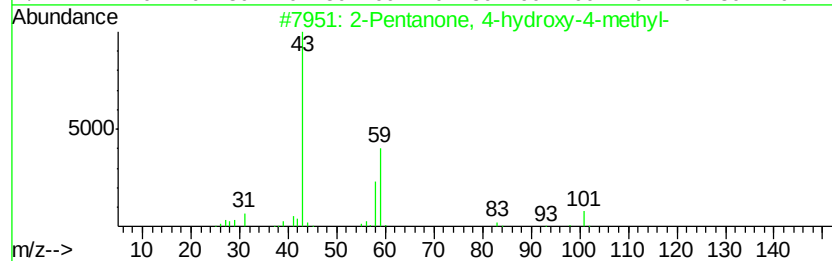
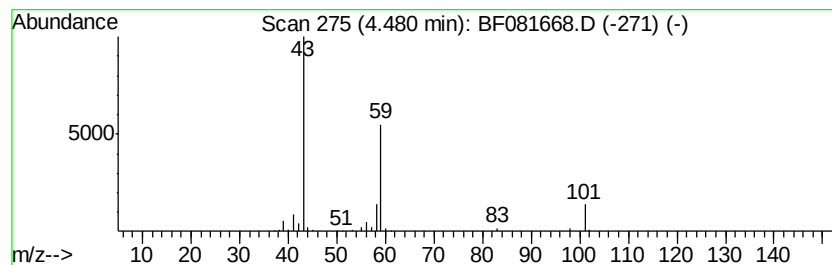
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	69.65 ng	1005270	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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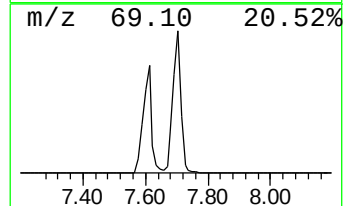
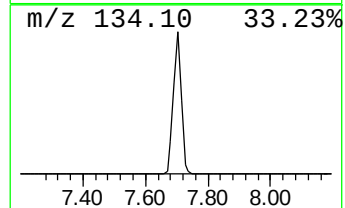
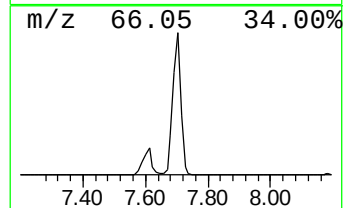
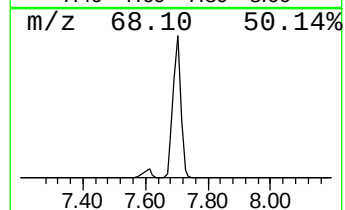
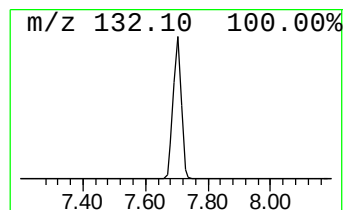
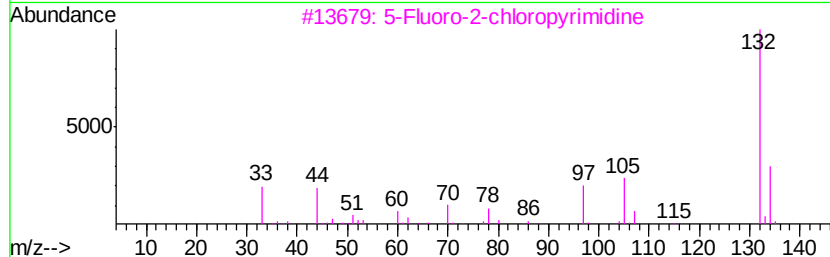
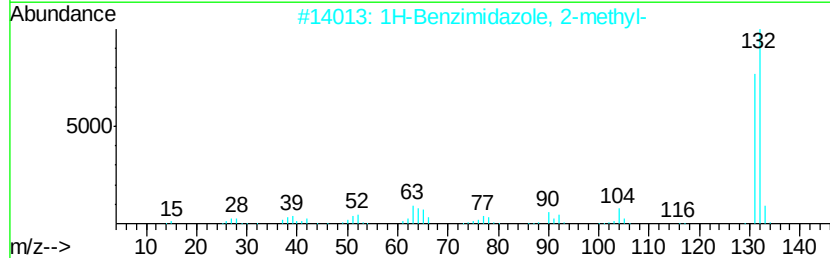
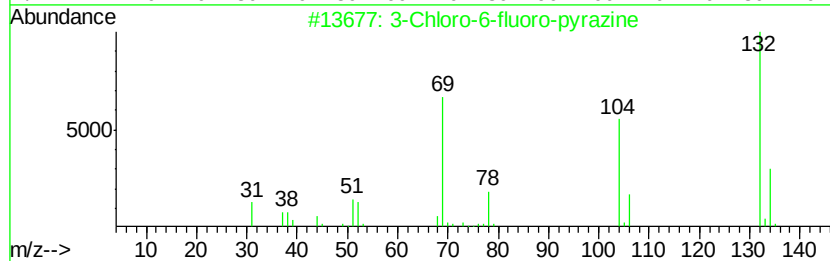
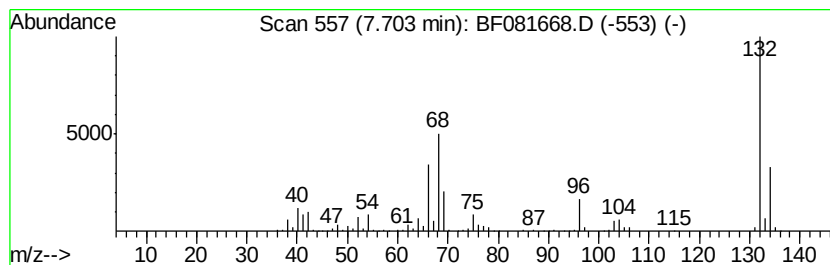
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Peak Number 4 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	121.54 ng	1754250	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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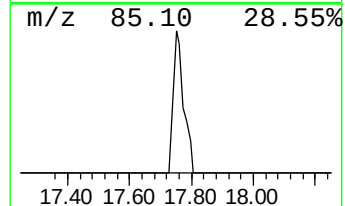
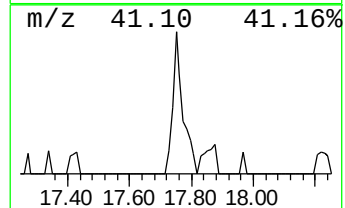
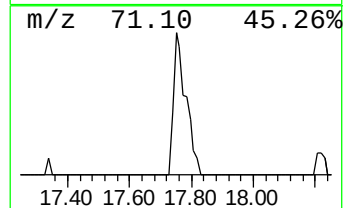
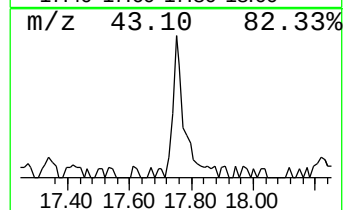
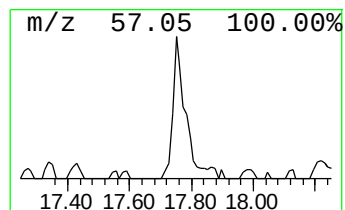
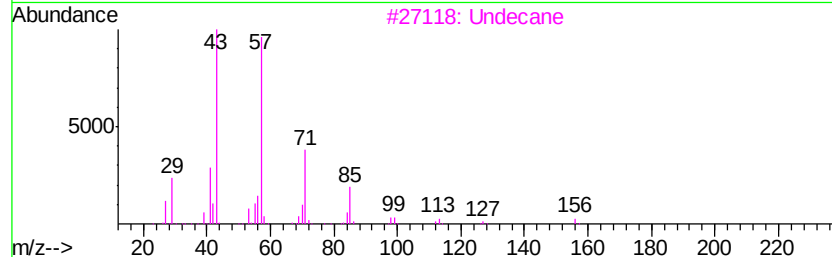
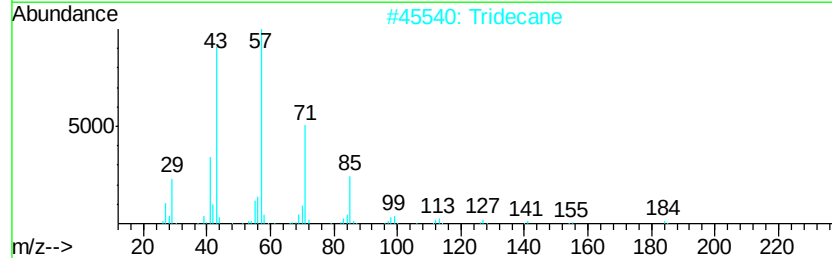
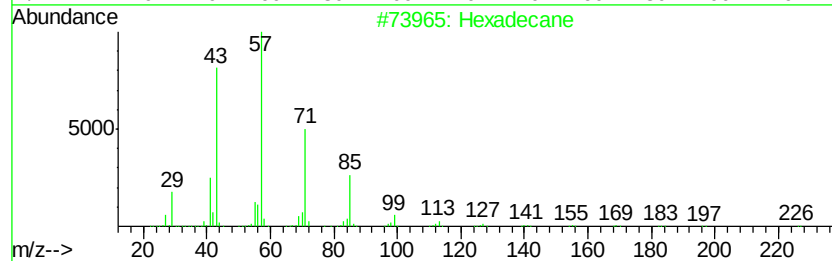
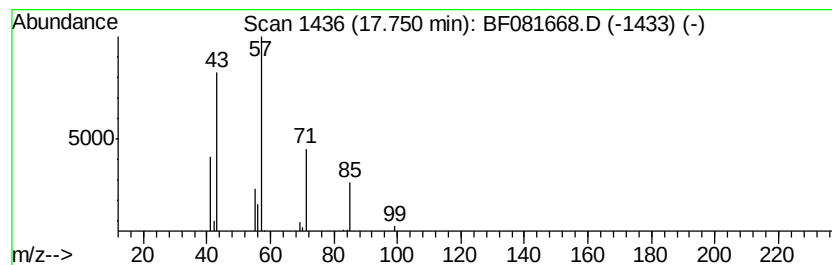
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Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.88 ng	57194	Phenanthrene-d10	18.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	83
2		Tridecane	184	C13H28	000629-50-5	78
3		Undecane	156	C11H24	001120-21-4	64
4		Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	59
5		Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	59



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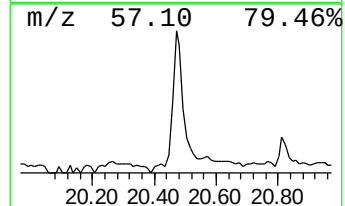
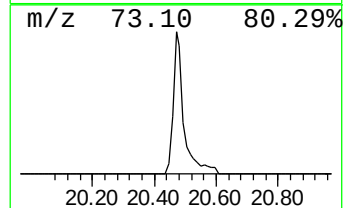
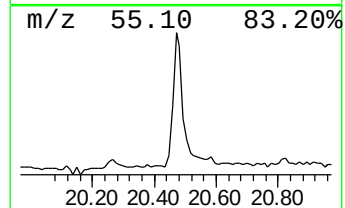
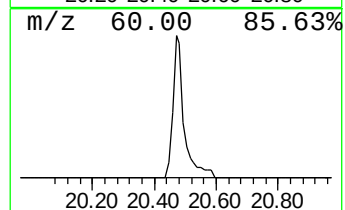
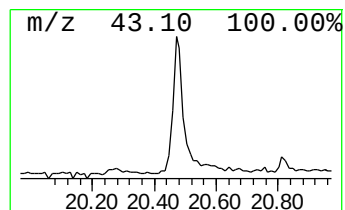
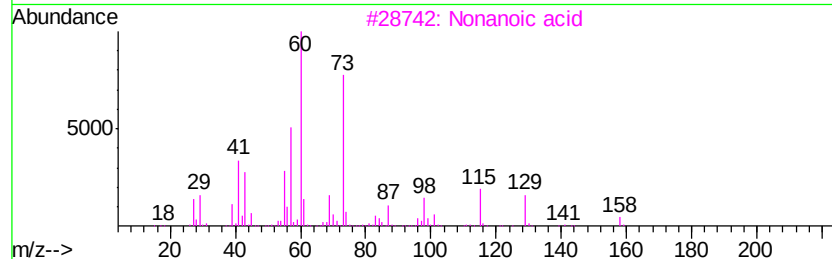
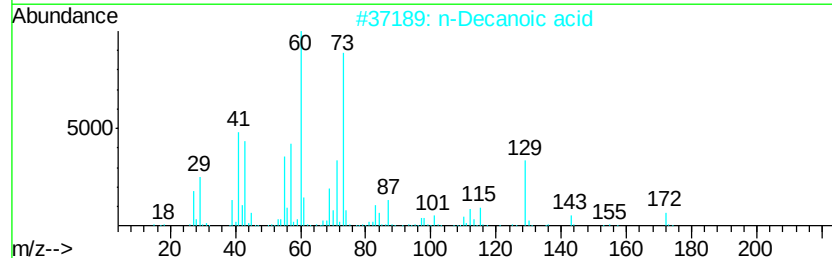
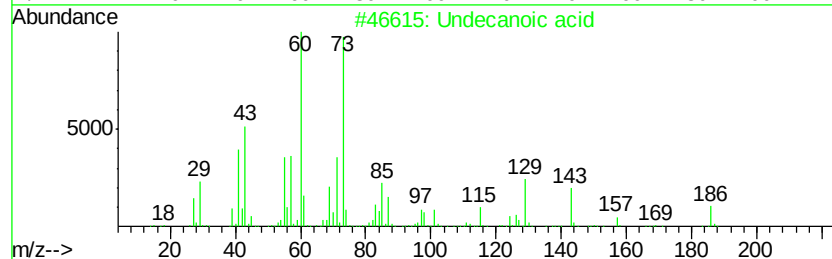
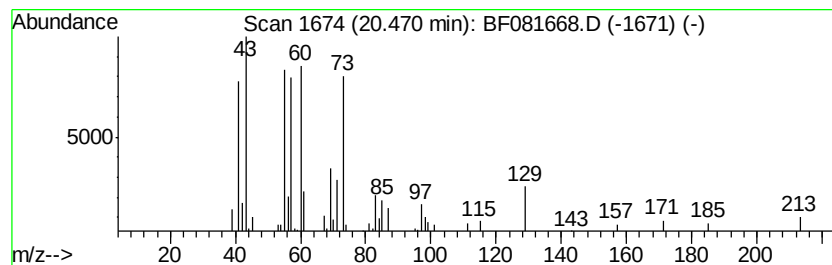
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	9.40 ng	186325	Phenanthrene-d10	18.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	80
2		n-Decanoic acid	172	C10H20O2	000334-48-5	53
3		Nonanoic acid	158	C9H18O2	000112-05-0	53
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50
5		Heptanoic acid	130	C7H14O2	000111-14-8	43



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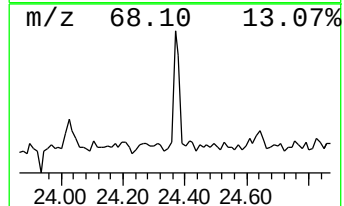
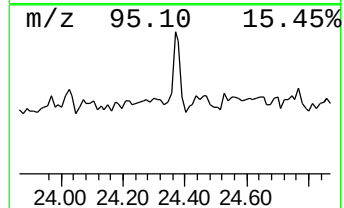
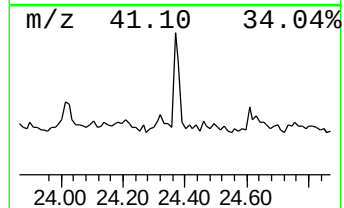
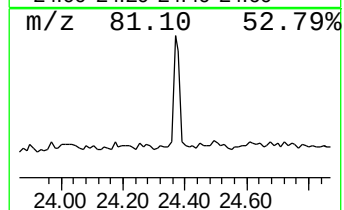
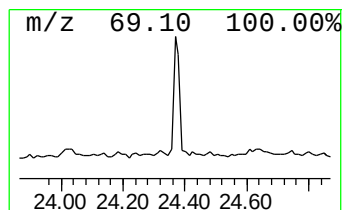
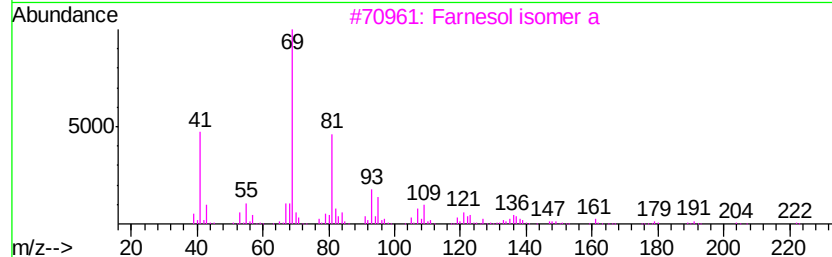
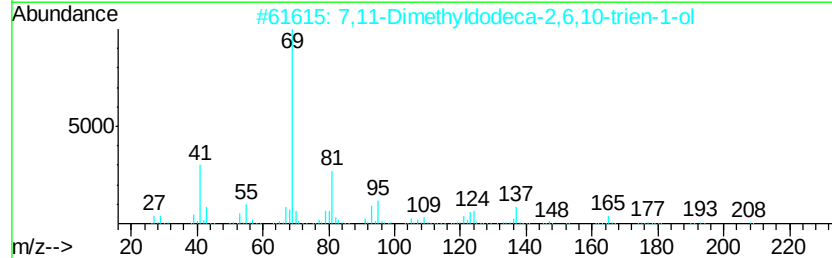
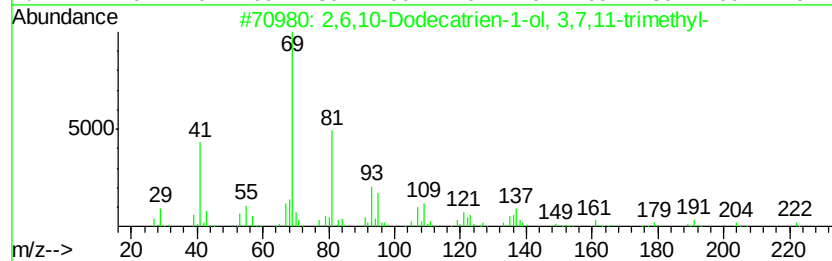
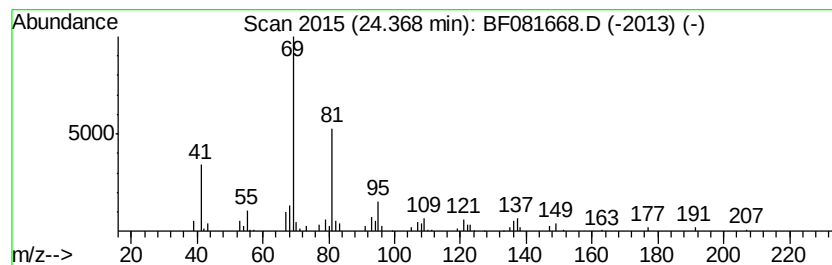
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Peak Number 8 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.37	6.69 ng	74000	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
2		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	56
3		Farnesol isomer a	222	C15H26O	1000108-92-4	56
4		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53
5		2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	53



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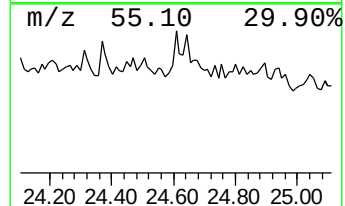
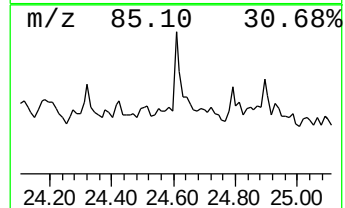
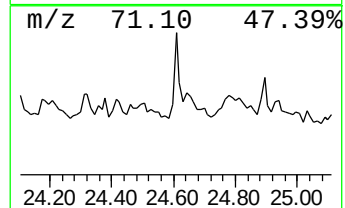
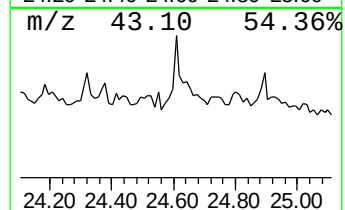
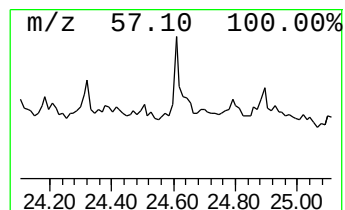
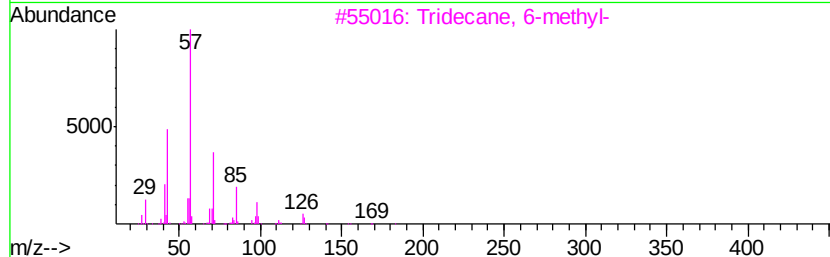
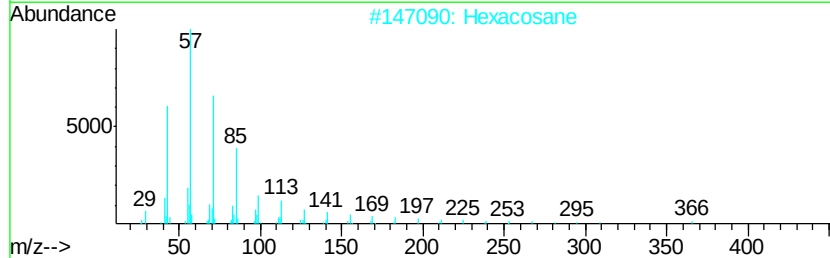
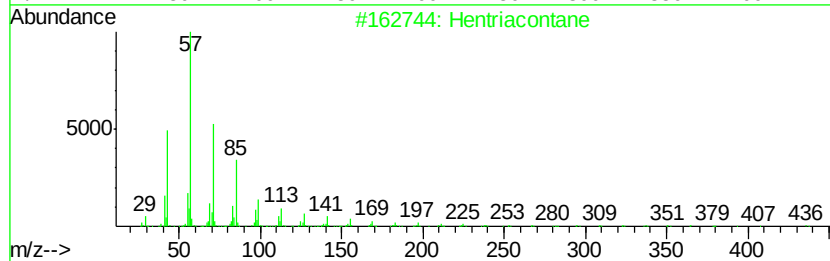
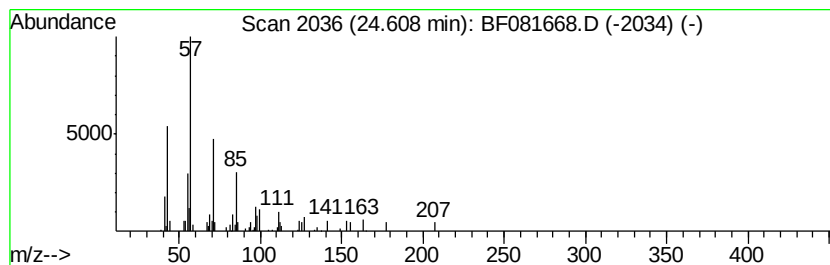
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.61	3.52 ng	38994	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	80
2		Hexacosane	366	C26H54	000630-01-3	64
3		Tridecane, 6-methyl-	198	C14H30	013287-21-3	53
4		Nonacosane	408	C29H60	000630-03-5	53
5		Undecane, 5-ethyl-	184	C13H28	017453-94-0	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081668.D
Acq On : 17 Sep 2015 6:03
Operator : UM/IZ
Sample : G3624-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-5B

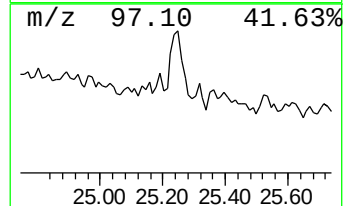
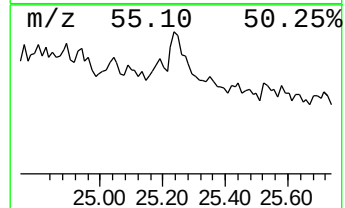
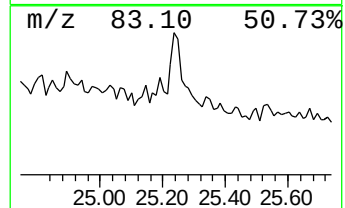
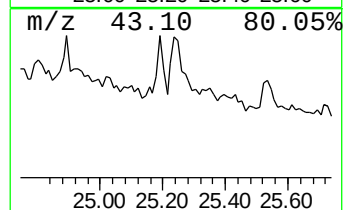
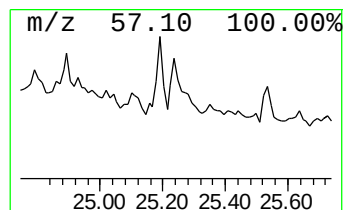
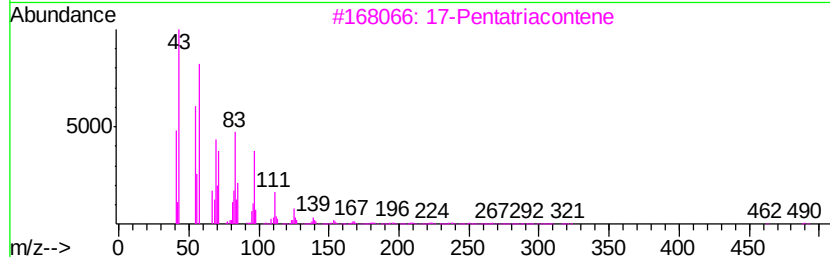
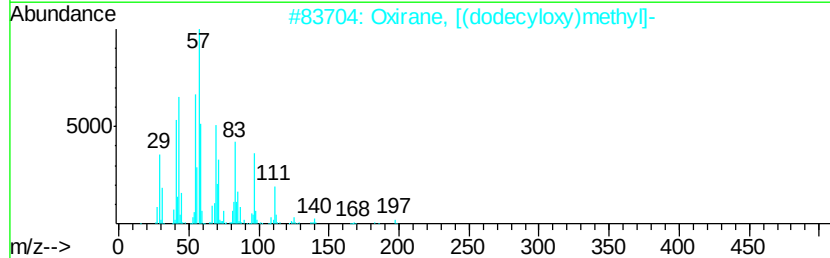
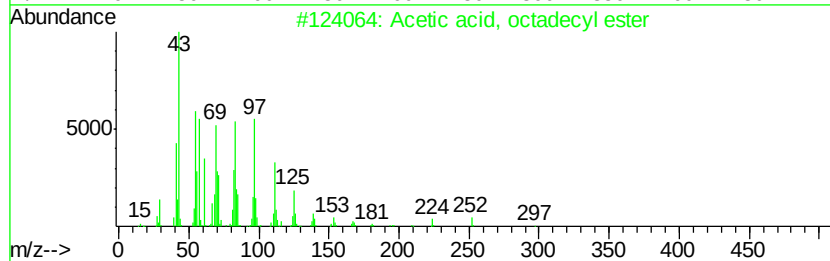
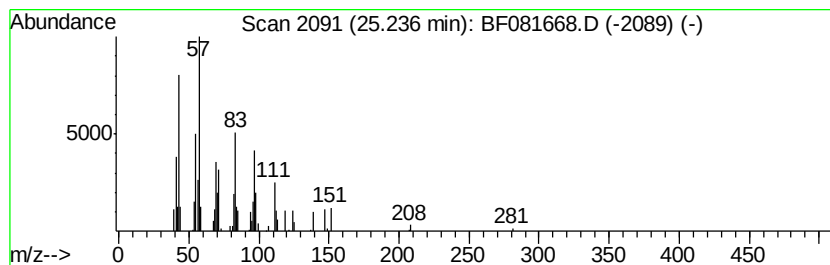
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Acetic acid, octadecyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.24	6.74 ng	74517	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	52
2		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	49
3		17-Pentatriacontene	491	C35H70	006971-40-0	46
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	27
5		Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081668.D
Acq On : 17 Sep 2015 6:03
Operator : UM/IZ
Sample : G3624-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-5B

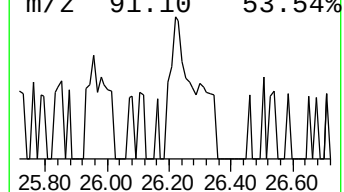
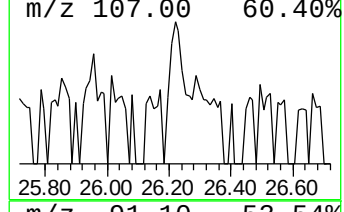
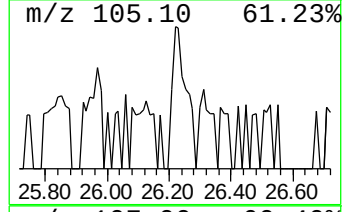
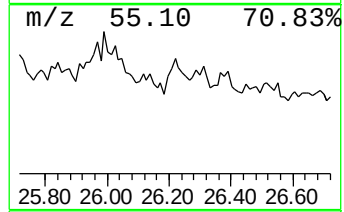
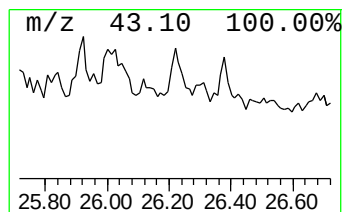
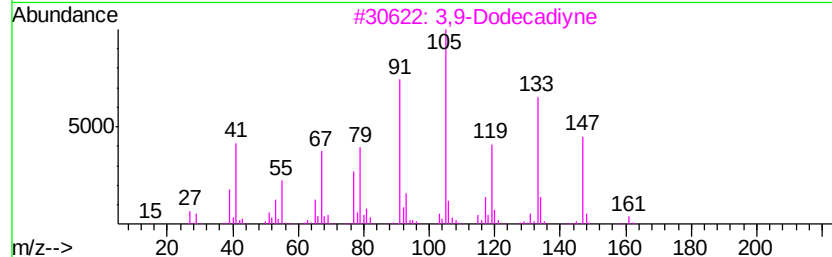
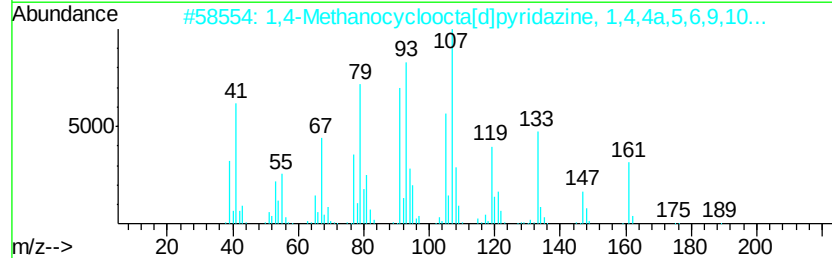
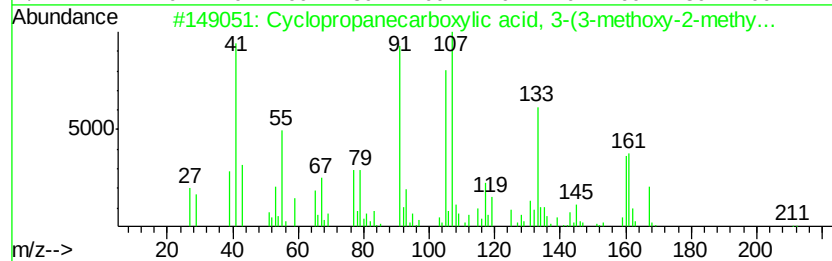
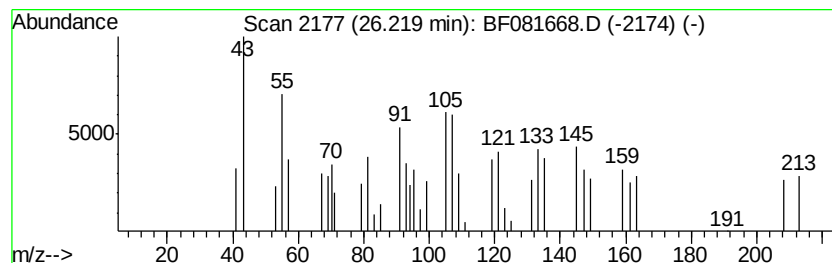
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown26.22 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.22	3.89 ng	42994	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanecarboxylic acid, 3-(...	372	C22H28O5	000121-29-9	27
2		1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	16
3		3,9-Dodecadiyne	162	C12H18	061827-89-2	10
4		Cyclopentanecarboxylic acid, 4-i...	208	C13H20O2	1000159-44-5	9
5		1,6-Bis[methyl(trimethylene)silyl...	286	C14H30O2Si2	1000217-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081668.D
Acq On : 17 Sep 2015 6:03
Operator : UM/IZ
Sample : G3624-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-5B

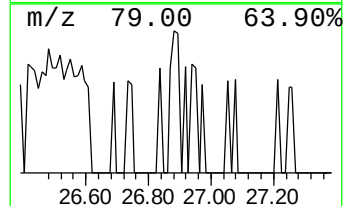
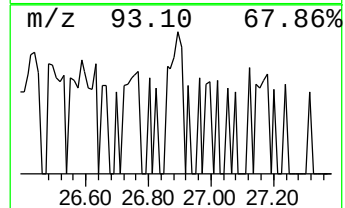
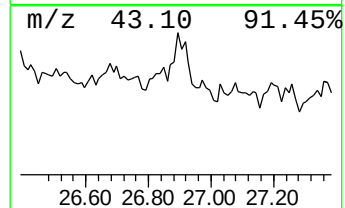
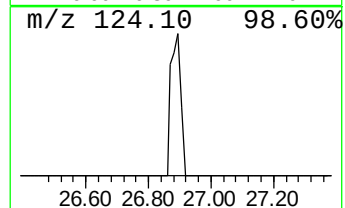
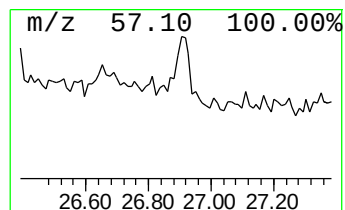
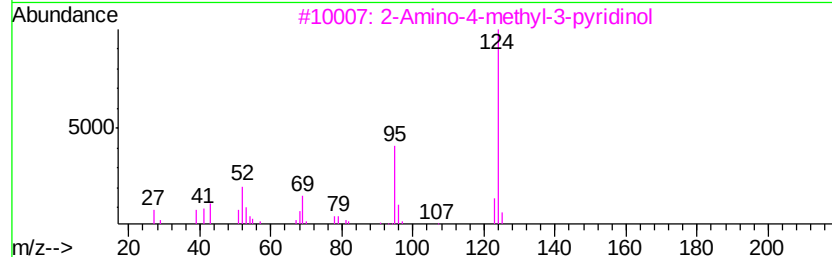
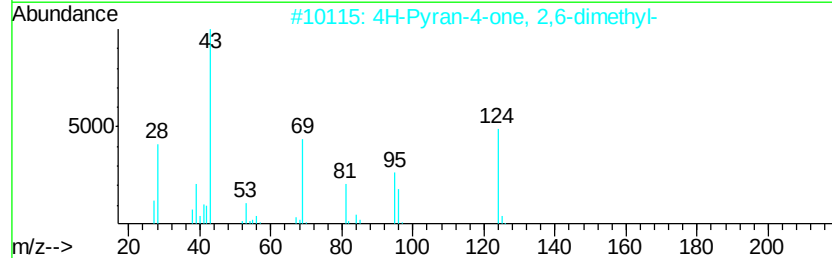
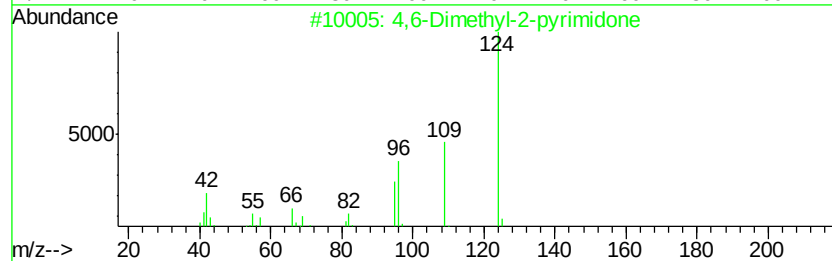
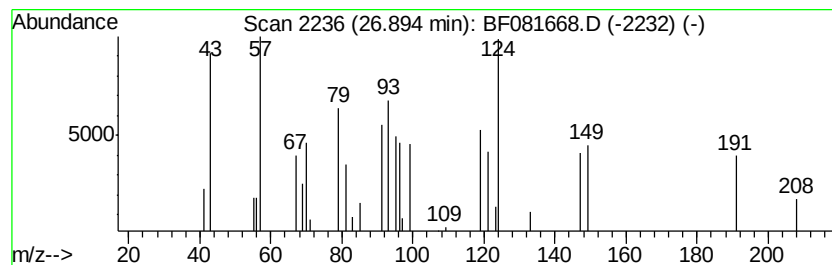
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown26.89 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.89	3.56 ng	39424	Perylene-d12	24.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Dimethyl-2-pyrimidone			124	C6H8N2O	000108-79-2	22
2	4H-Pyran-4-one, 2,6-dimethyl-			124	C7H8O2	001004-36-0	16
3	2-Amino-4-methyl-3-pyridinol			124	C6H8N2O	020348-18-9	10
4	Phenol, 3-methoxy-			124	C7H8O2	000150-19-6	9
5	1,4-Benzenediol, 2-methyl-			124	C7H8O2	000095-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081668.D
Acq On : 17 Sep 2015 6:03
Operator : UM/IZ
Sample : G3624-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-5B

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
2-Pentanone, 4-hy...	4.48	69.7	ng	1005270	1	8.18	288680	20.0
unknown7.70	7.70	121.5	ng	1754250	1	8.18	288680	20.0
Hexadecane	17.75	2.9	ng	57194	4	18.71	396617	20.0
Undecanoic acid	20.47	9.4	ng	186325	4	18.71	396617	20.0
2,6,10-Dodecatric...	24.37	6.7	ng	74000	6	24.79	221259	20.0
Hentriacontane	24.61	3.5	ng	38994	6	24.79	221259	20.0
Acetic acid, octa...	25.24	6.7	ng	74517	6	24.79	221259	20.0
unknown26.22	26.22	3.9	ng	42994	6	24.79	221259	20.0
unknown26.89	26.89	3.6	ng	39424	6	24.79	221259	20.0