

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
 Data File : BF083562.D
 Acq On : 7 Dec 2015 17:59
 Operator : UM/IZ
 Sample : G4634-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K203-20-21

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-BF120415.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	3.573	162	165	186	rVB	621123	1502100	24.85%	2.791%
2	4.007	201	203	223	rBV	4386952	5875602	97.18%	10.916%
3	5.287	312	315	323	rBV	4113977	5856378	96.87%	10.880%
4	5.413	323	326	329	rBV	3679857	5634971	93.20%	10.469%
5	5.721	351	353	363	rVB	746210	946034	15.65%	1.758%
6	5.939	369	372	385	rVB	3415846	4269878	70.63%	7.933%
7	6.556	423	426	428	rBV	2368298	3711827	61.40%	6.896%
8	6.842	448	451	460	rBV	49656	105190	1.74%	0.195%
9	7.619	517	519	531	rVB	853086	1289394	21.33%	2.395%
10	8.362	580	584	593	rBV4	16661	75559	1.25%	0.140%
11	9.185	652	656	659	rVB	36277	61173	1.01%	0.114%
12	9.368	668	672	675	rBV	4060189	6045792	100.00%	11.232%
13	10.053	729	732	735	rBV	1070961	1322014	21.87%	2.456%
14	10.408	760	763	769	rBV	1021682	1582066	26.17%	2.939%
15	11.253	834	837	840	rVB	152810	197473	3.27%	0.367%
16	11.619	864	869	871	rBV	58209	133725	2.21%	0.248%
17	11.699	873	876	879	rBV2	2311218	3672272	60.74%	6.822%
18	12.031	902	905	909	rBV	142932	316097	5.23%	0.587%
19	12.099	909	911	914	rVB2	39853	67651	1.12%	0.126%
20	12.339	930	932	936	rBV2	27830	76699	1.27%	0.142%
21	12.442	939	941	944	rBV	43828	63749	1.05%	0.118%
22	12.762	966	969	971	rBV	84319	114399	1.89%	0.213%
23	12.808	971	973	980	rVB	1091210	1498498	24.79%	2.784%
24	13.859	1061	1065	1070	rBV3	80344	160526	2.66%	0.298%
25	14.579	1126	1128	1132	rVV2	75651	176373	2.92%	0.328%
26	14.648	1132	1134	1139	rVB	29513	62541	1.03%	0.116%
27	15.140	1175	1177	1181	rBV	88660	140433	2.32%	0.261%
28	15.448	1200	1204	1207	rBV	3449305	5379925	88.99%	9.995%
29	15.722	1225	1228	1232	rBV	67760	154050	2.55%	0.286%
30	15.951	1245	1248	1253	rVB	37158	71158	1.18%	0.132%
31	16.248	1270	1274	1277	rVV	77773	148075	2.45%	0.275%
32	16.328	1278	1281	1288	rVV3	40131	97685	1.62%	0.181%
33	16.454	1289	1292	1296	rVV	76551	162812	2.69%	0.302%
34	16.523	1296	1298	1301	rVV	129137	186282	3.08%	0.346%

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Instrument :
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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-BF120415.M
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35	16.580	1301	1303	1306	rVB	56546	76072	1.26%	0.141%
36	16.934	1332	1334	1339	rBV2	137697	318192	5.26%	0.591%
37	17.014	1339	1341	1349	rVB	924733	1297651	21.46%	2.411%
38	18.168	1439	1442	1444	rVB	63311	74004	1.22%	0.137%
39	18.648	1482	1484	1491	rBV	597910	901996	14.92%	1.676%

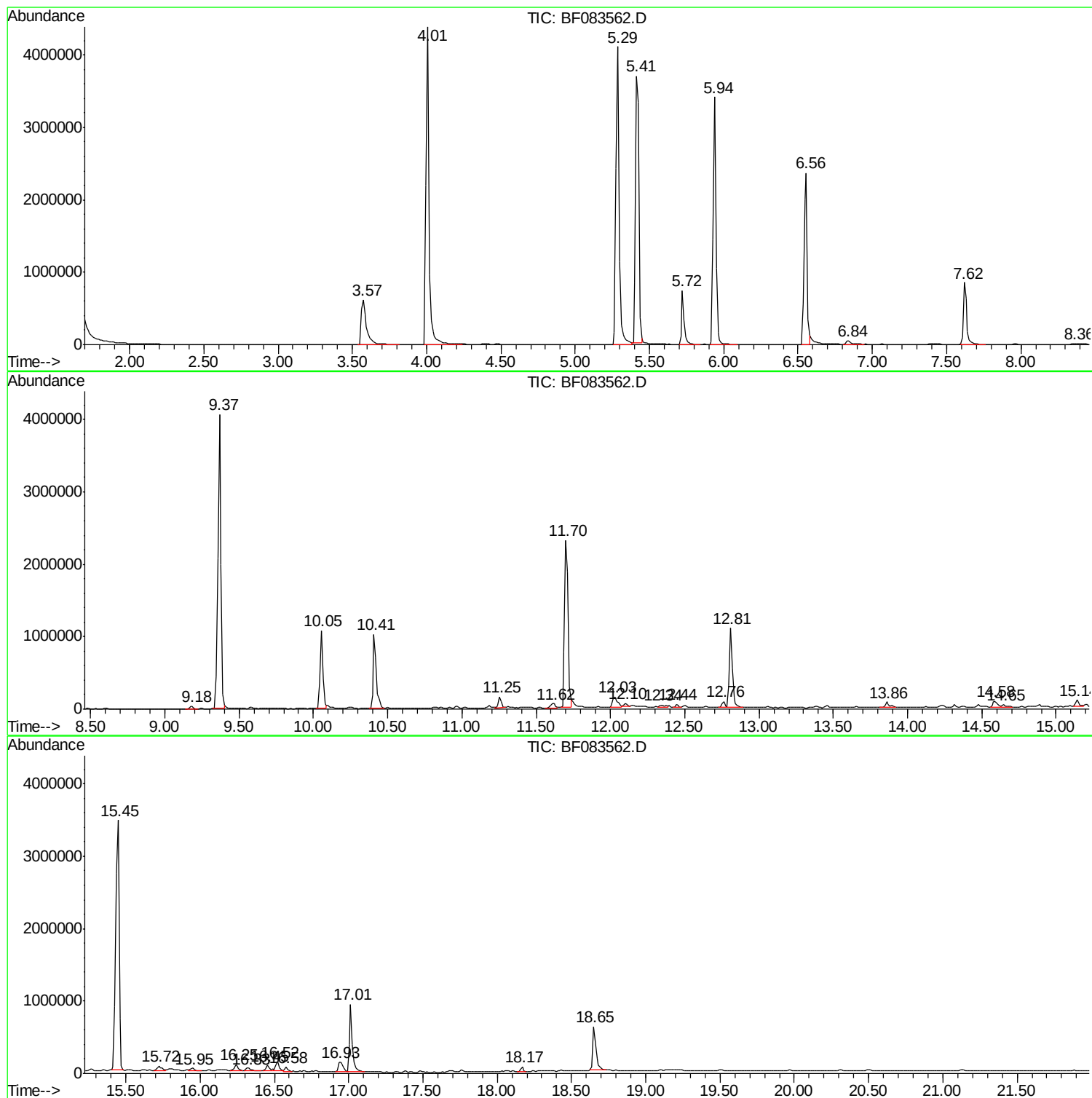
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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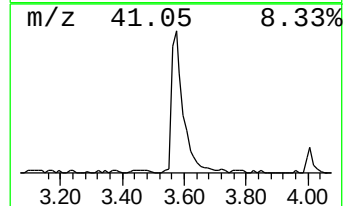
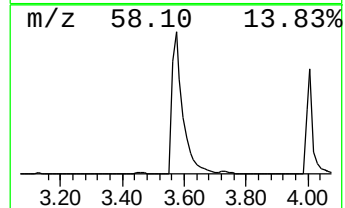
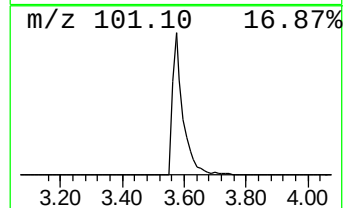
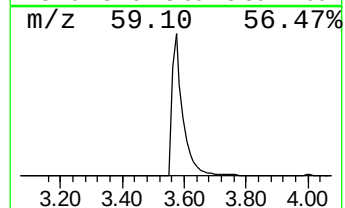
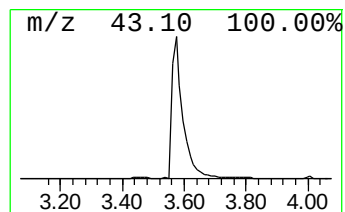
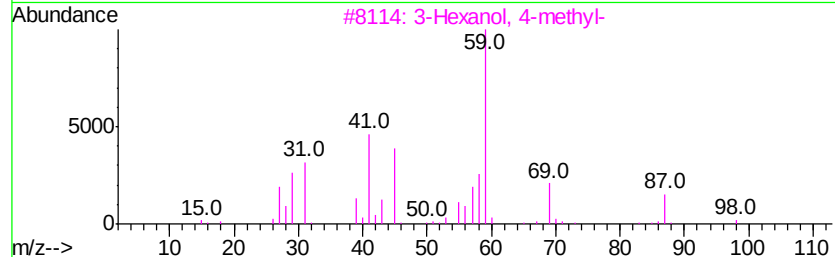
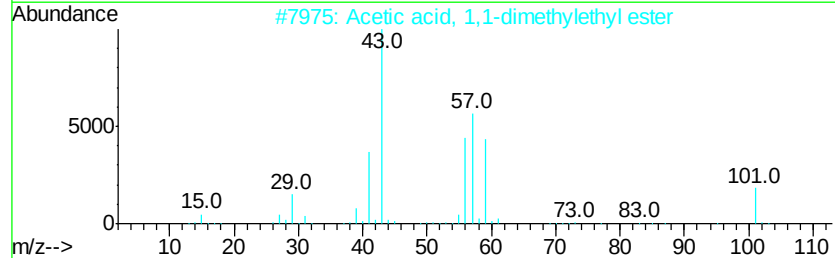
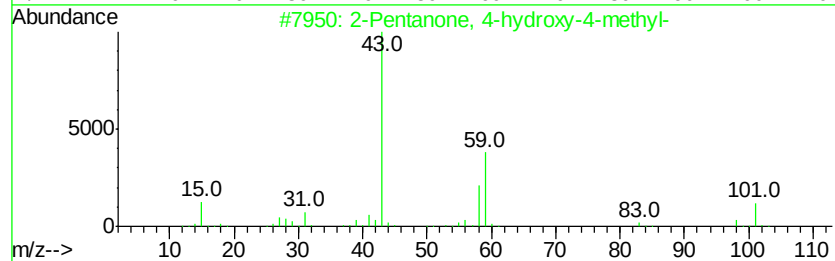
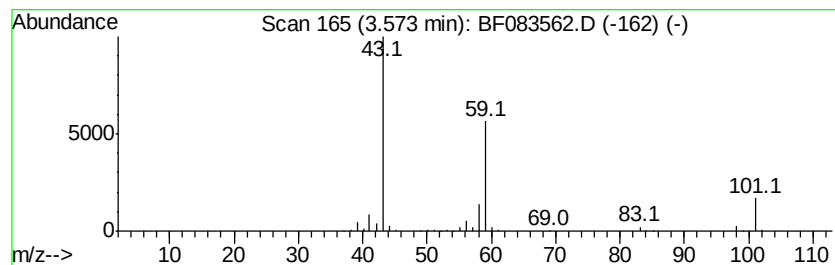
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	31.76 ng	1502100	1,4-Dichlorobenzene-d4	5.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		3-Hexanol	102	C6H14O	000623-37-0	33



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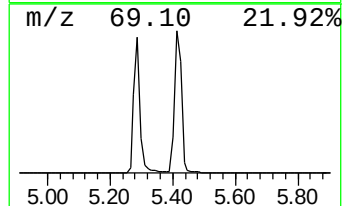
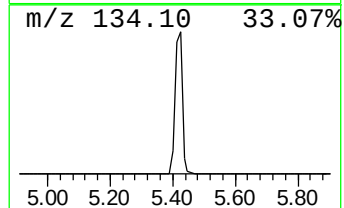
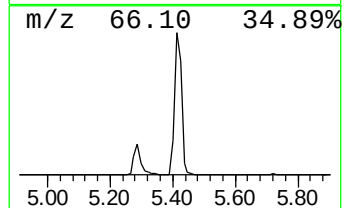
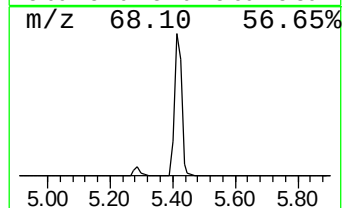
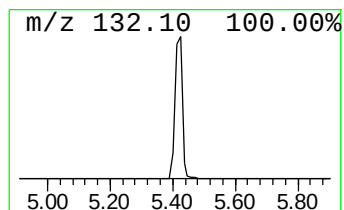
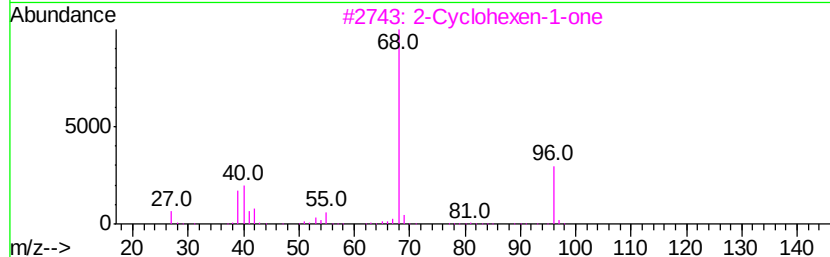
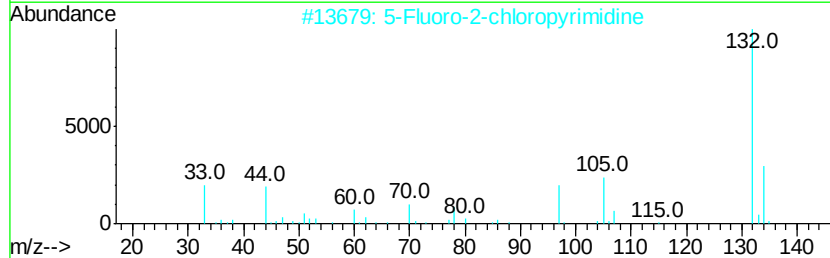
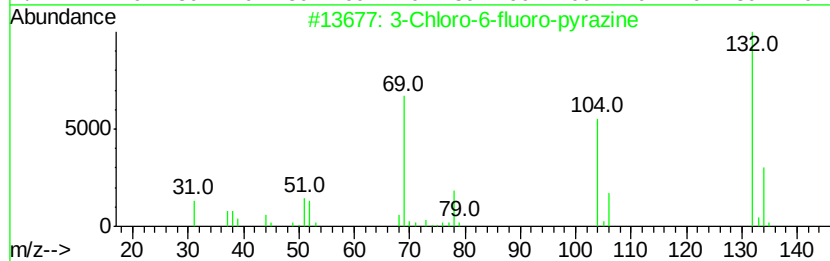
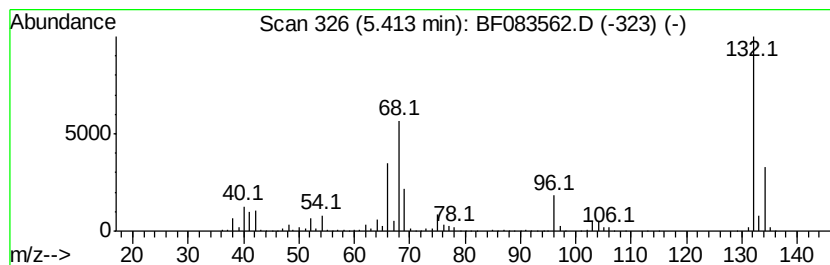
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.41	119.13 ng	5634970	1,4-Dichlorobenzene-d4	5.72

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	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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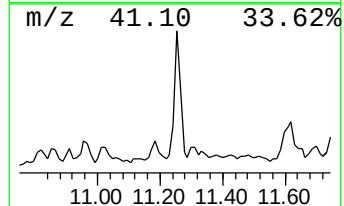
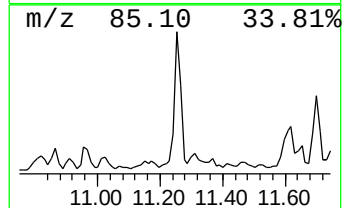
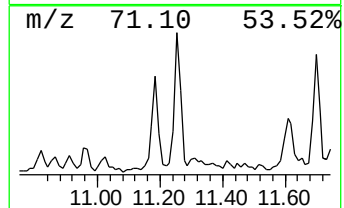
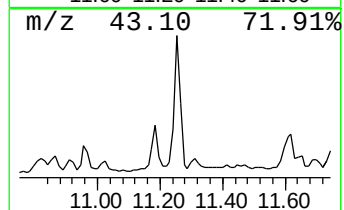
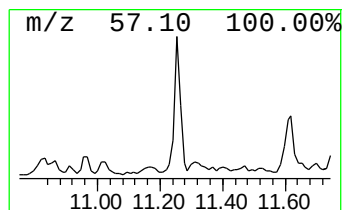
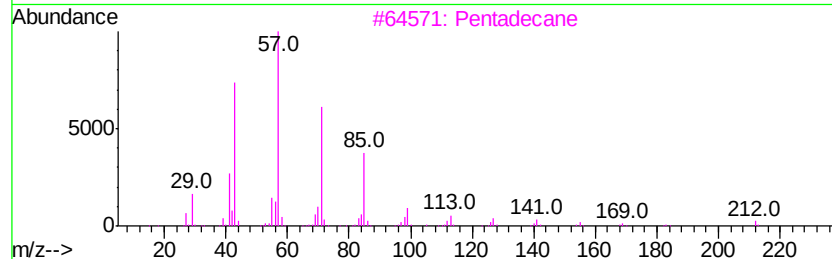
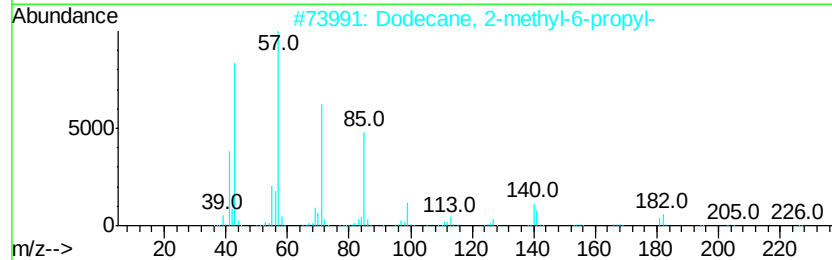
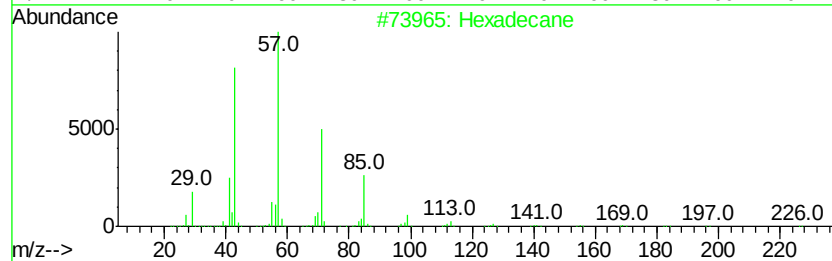
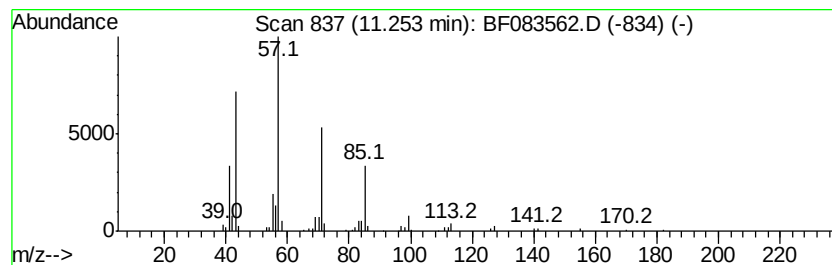
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.50 ng	197473	Acenaphthene-d10	10.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3		Pentadecane	212	C15H32	000629-62-9	83
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	80



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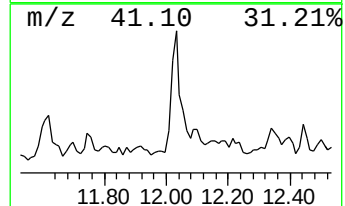
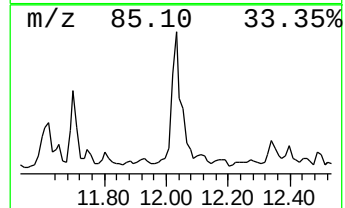
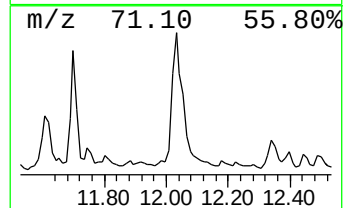
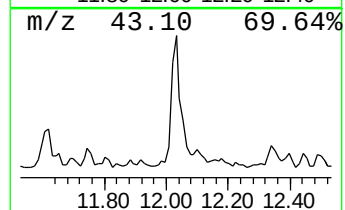
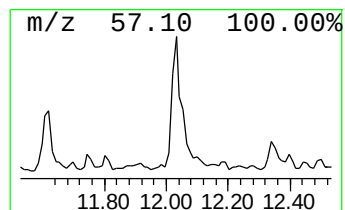
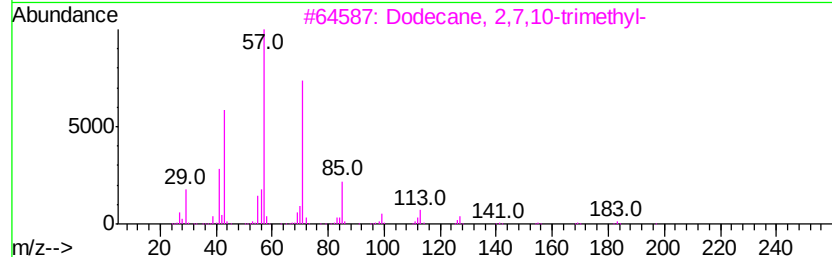
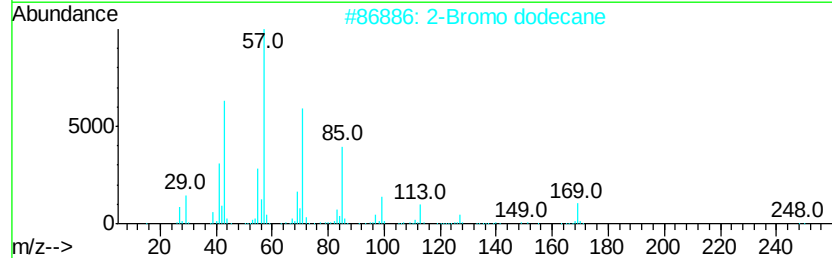
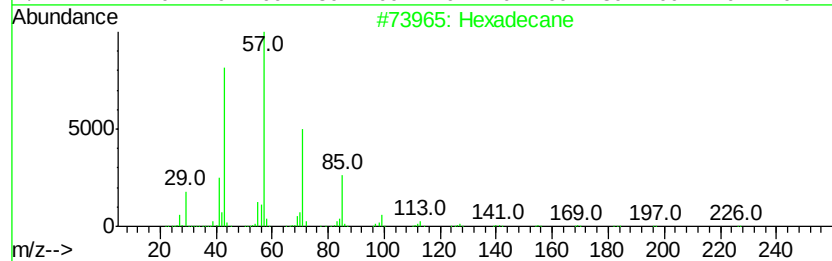
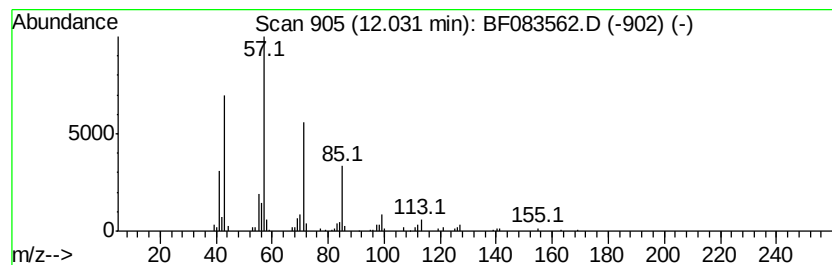
Instrument :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	4.22 ng	316097	Phenanthrene-d10	12.81
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	86
2	2-Bromo dodecane	248 C12H25Br	013187-99-0	83
3	Dodecane, 2,7,10-trimethyl-	212 C15H32	074645-98-0	80
4	Pentadecane	212 C15H32	000629-62-9	80
5	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	72



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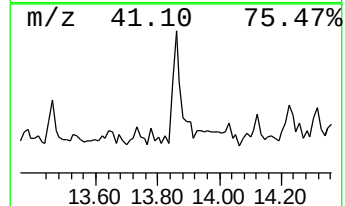
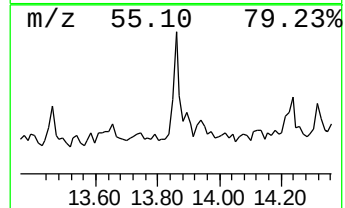
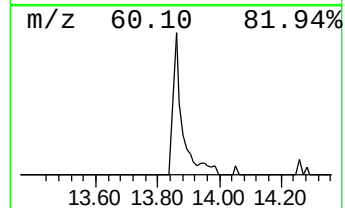
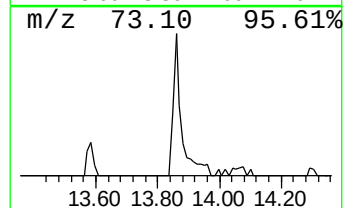
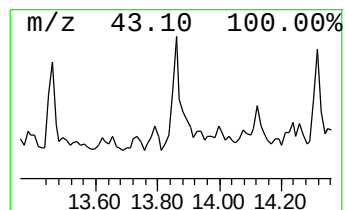
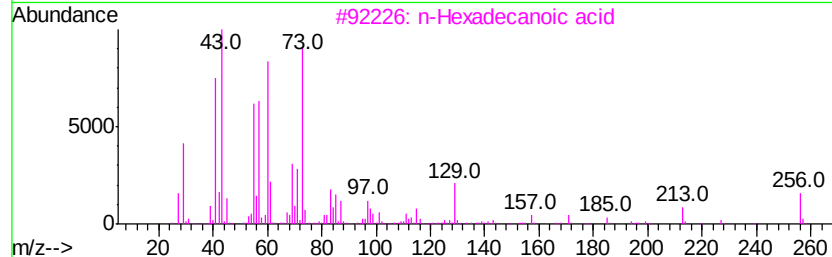
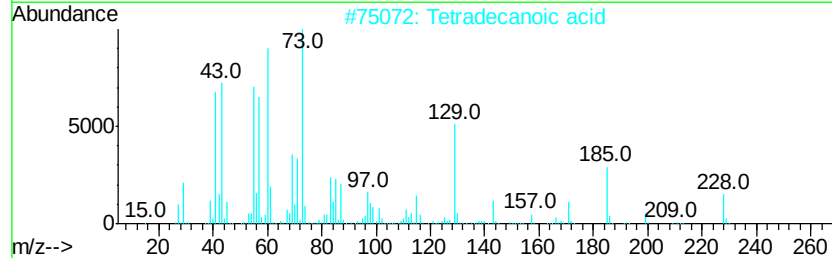
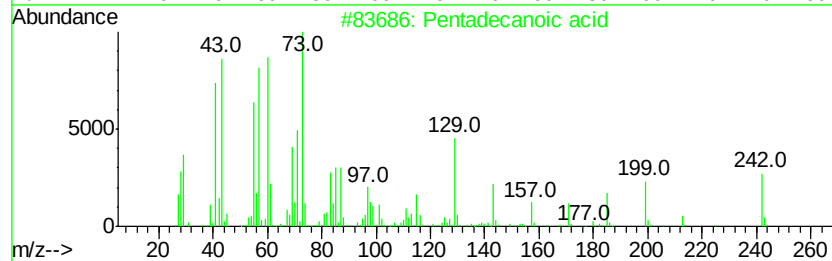
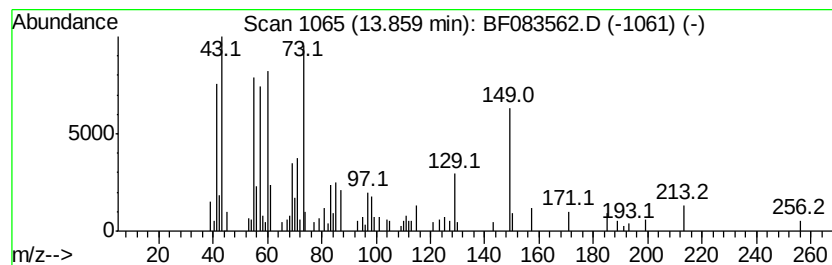
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	2.14 ng	160526	Phenanthrene-d10	12.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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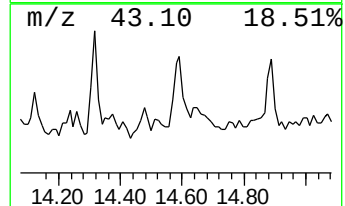
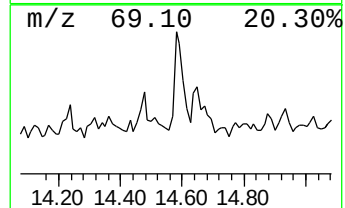
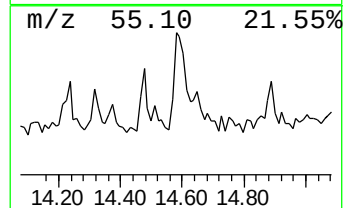
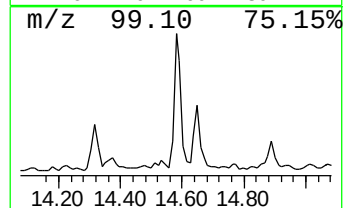
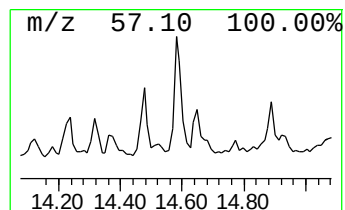
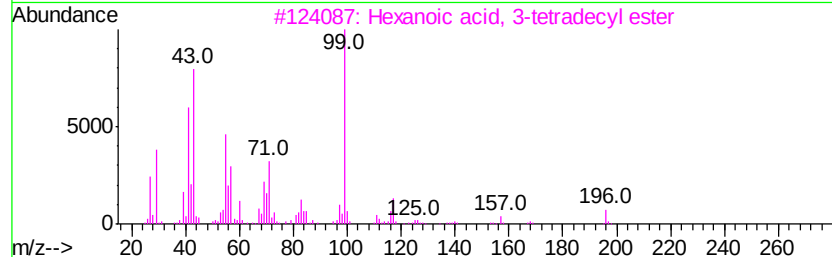
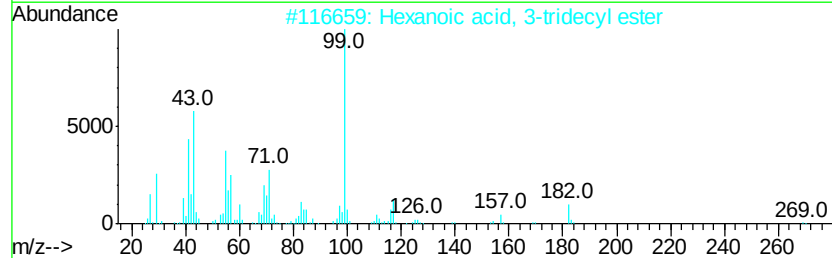
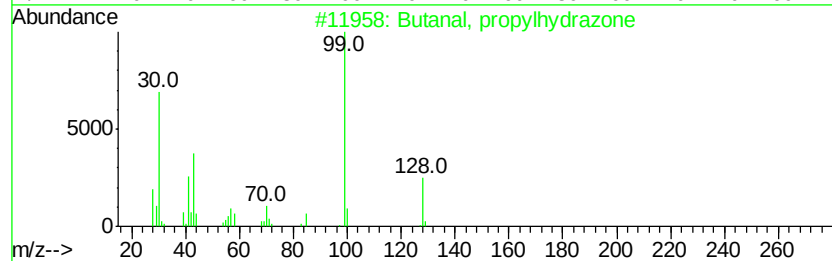
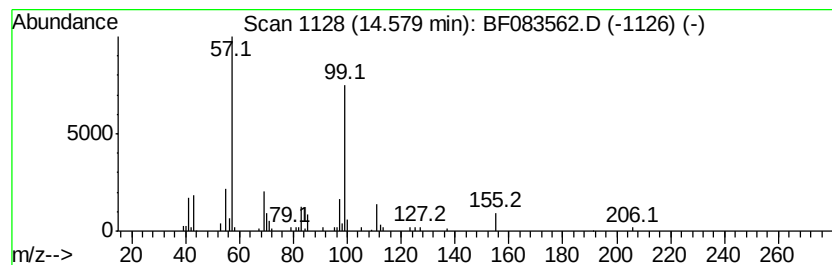
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ClientSampled :
K203-20-21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.58 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.58	2.35 ng	176373	Phenanthrene-d10	12.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, propylhydrazone	128	C7H16N2	020607-76-5	47
2	Hexanoic acid, 3-tridecyl ester	298	C19H38O2	1000279-29-2	42
3	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1000279-29-7	42
4	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	42
5	Diaziridine, 1,2-dipropyl-	128	C7H16N2	006794-92-9	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
Data File : BF083562.D
Acq On : 7 Dec 2015 17:59
Operator : UM/IZ
Sample : G4634-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K203-20-21

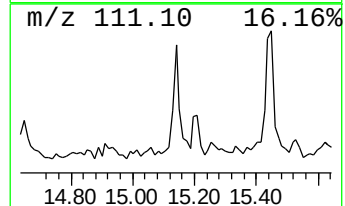
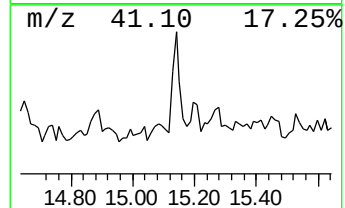
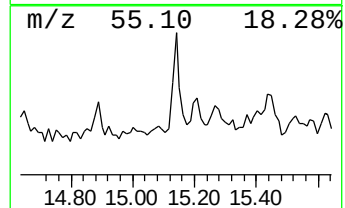
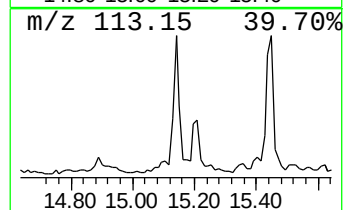
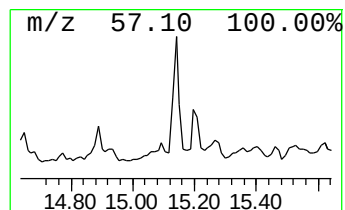
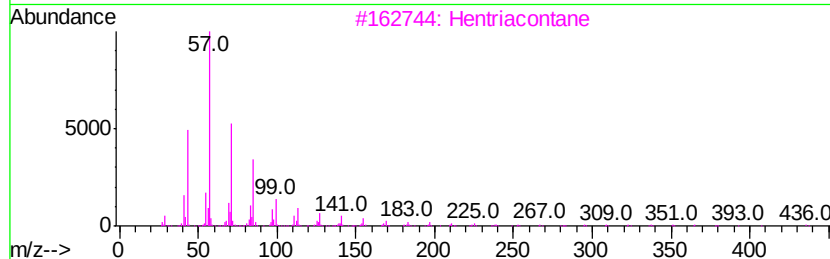
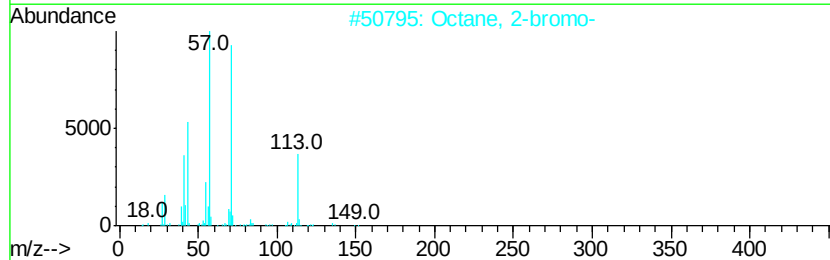
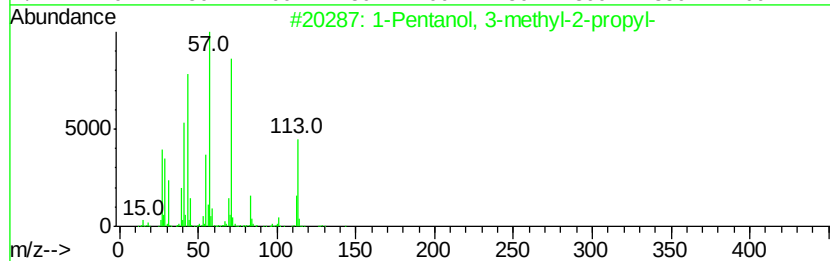
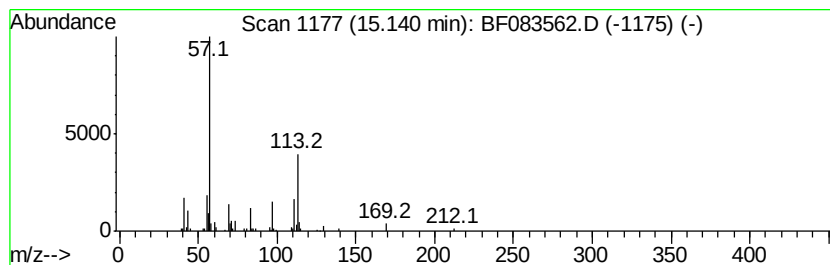
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.14 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.16 ng	140433	Chrysene-d12	17.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	42
2		Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
3		Hentriacontane	437	C31H64	000630-04-6	28
4		6-Undecen-3-one, 5-butyl-2,2-dim...	252	C17H32O	055976-05-1	25
5		2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
Data File : BF083562.D
Acq On : 7 Dec 2015 17:59
Operator : UM/IZ
Sample : G4634-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

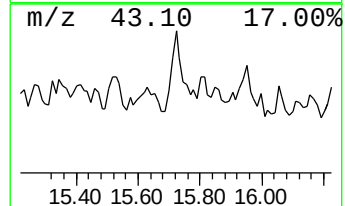
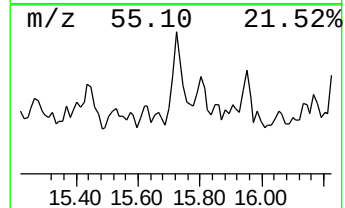
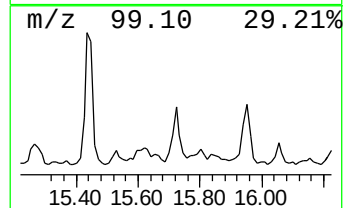
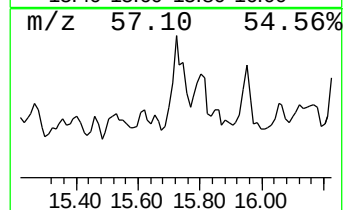
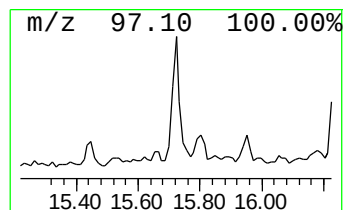
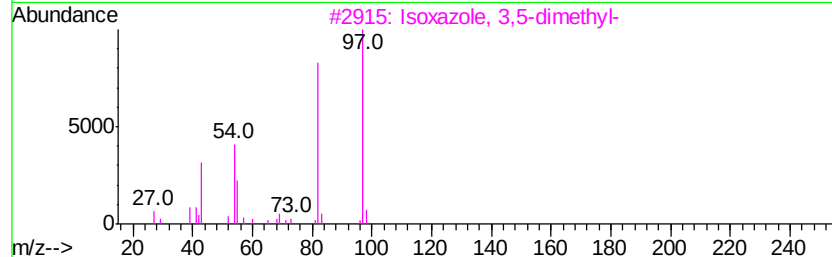
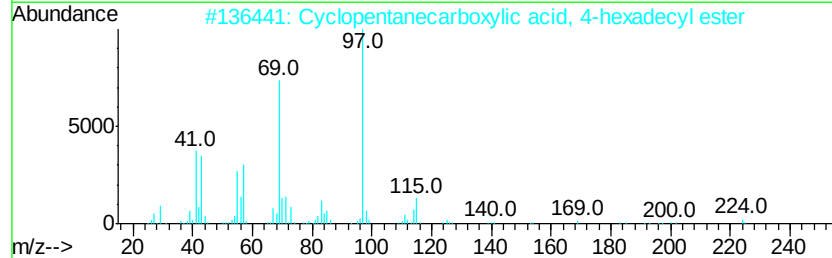
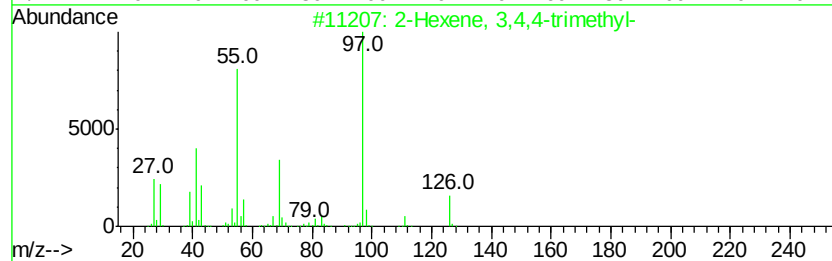
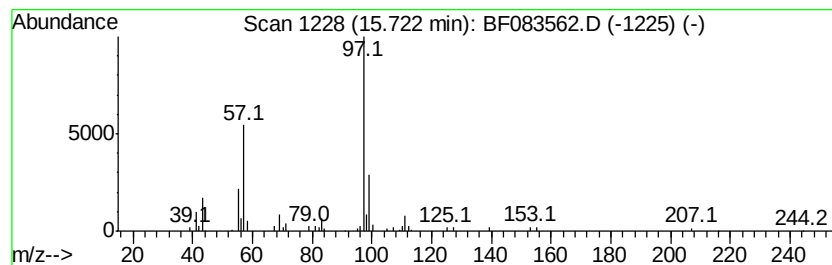
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Hexene, 3,4,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.37 ng	154050	Chrysene-d12	17.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Hexene, 3,4,4-trimethyl-	126 C9H18	053941-19-8	59
2	Cyclopentanecarboxylic acid, 4-h...	338 C22H42O2	1000282-77-5	53
3	Isoxazole, 3,5-dimethyl-	97 C5H7NO	000300-87-8	50
4	Oxazole, 2,4-dimethyl-	97 C5H7NO	007208-05-1	50
5	Cyclohexanone, 3-(3,3-dimethylbu...	182 C12H22O	040564-94-1	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120715\
Data File : BF083562.D
Acq On : 7 Dec 2015 17:59
Operator : UM/IZ
Sample : G4634-04
Misc :
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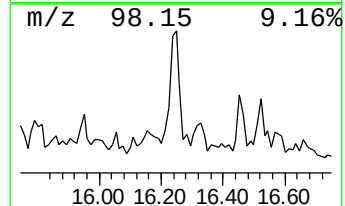
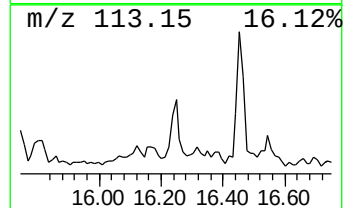
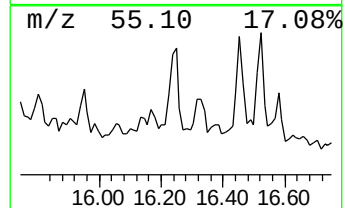
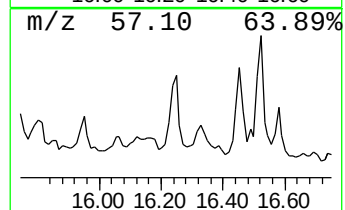
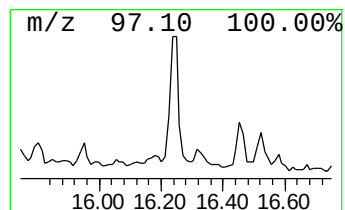
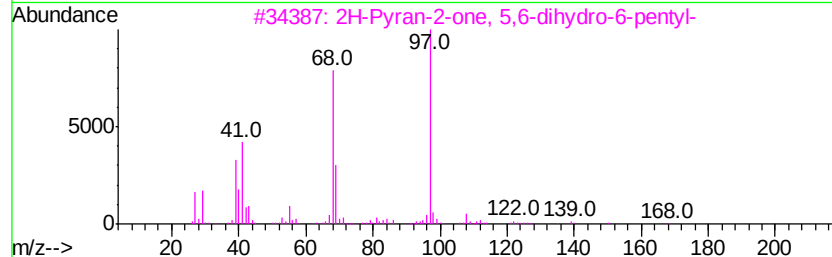
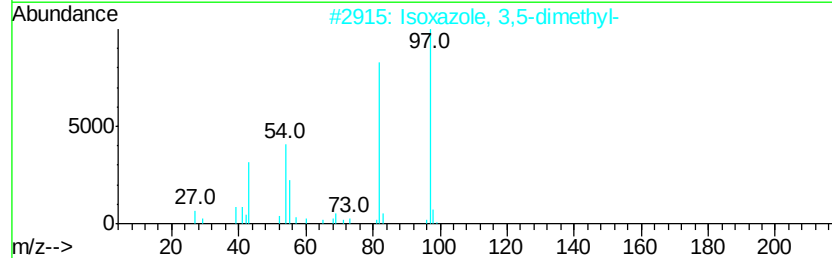
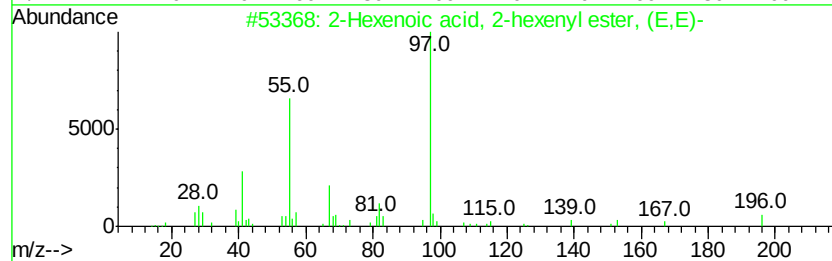
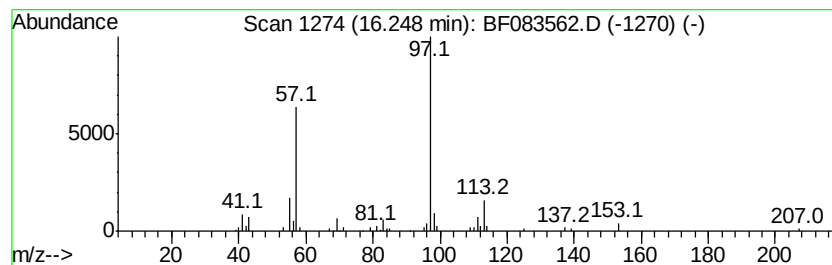
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Hexenoic acid, 2-hexenyl ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.25	2.28 ng	148075	Chrysene-d12	17.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenoic acid, 2-hexenyl ester...	196	C12H20O2	054845-28-2	59
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	59
3	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	53
4	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	50
5	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
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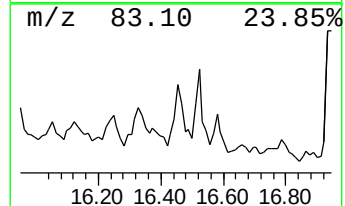
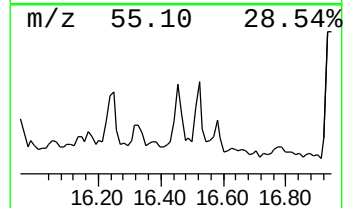
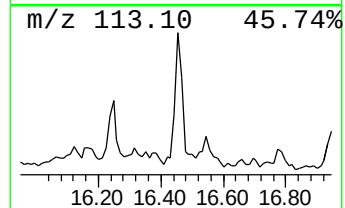
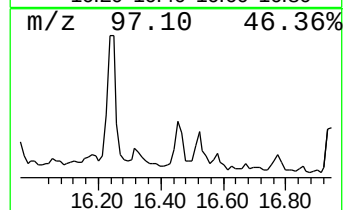
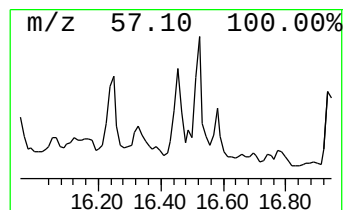
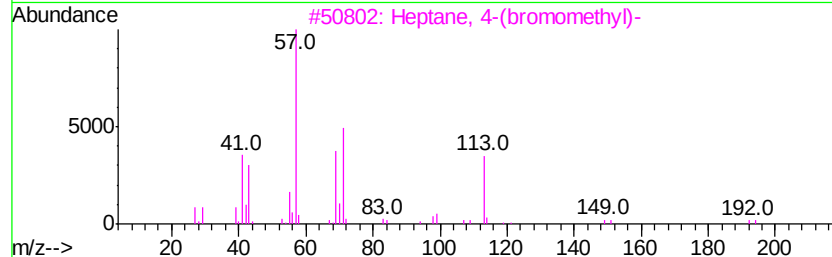
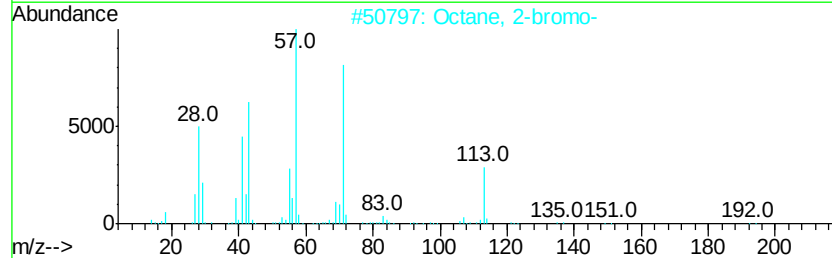
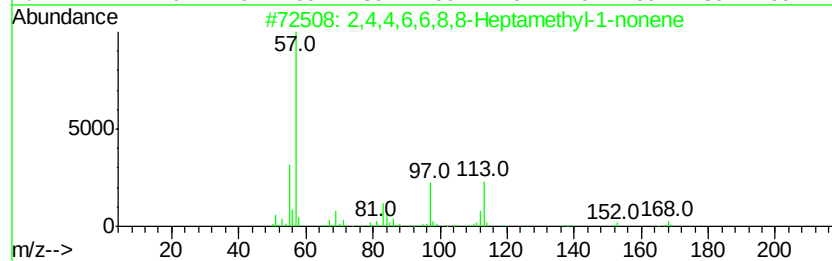
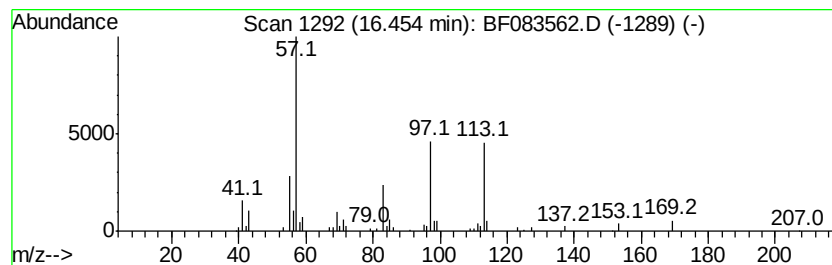
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.45	2.51 ng	162812	Chrysene-d12	17.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	83
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	23
4	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	14
5	6-Tridecene, 2,2,4,10,12,12-hexa...	392	C28H56	055255-73-7	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
Data File : BF083562.D
Acq On : 7 Dec 2015 17:59
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K203-20-21

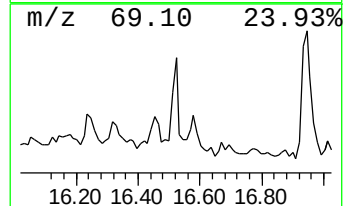
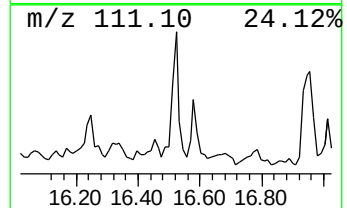
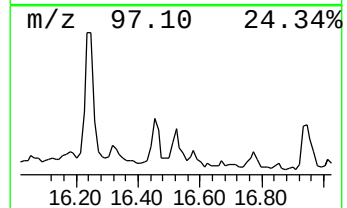
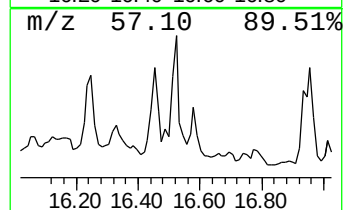
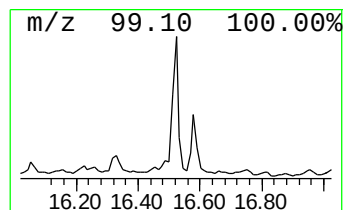
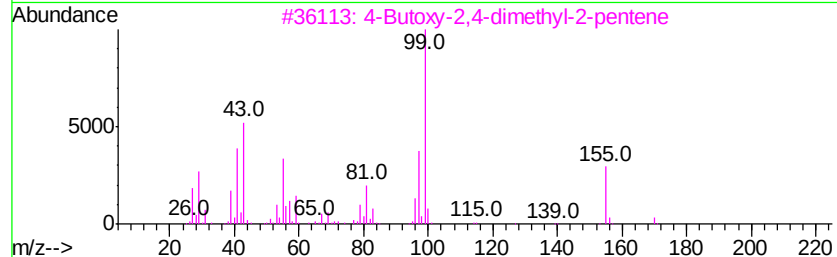
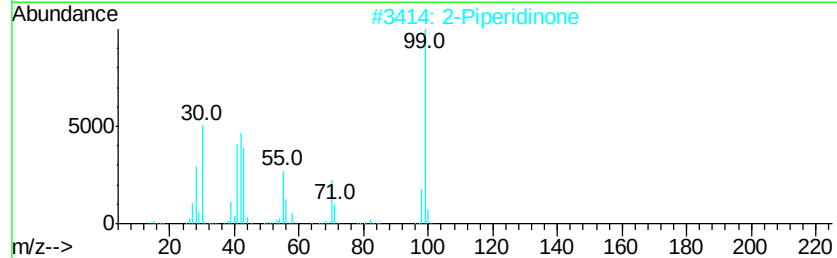
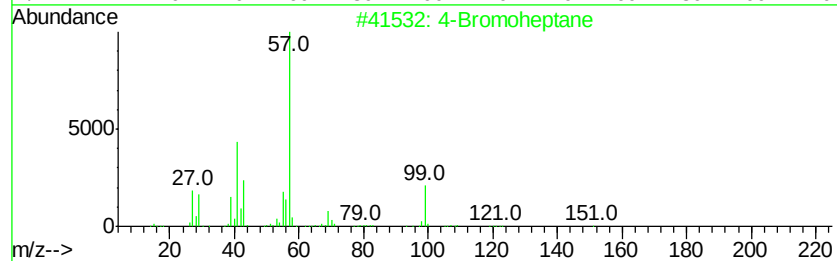
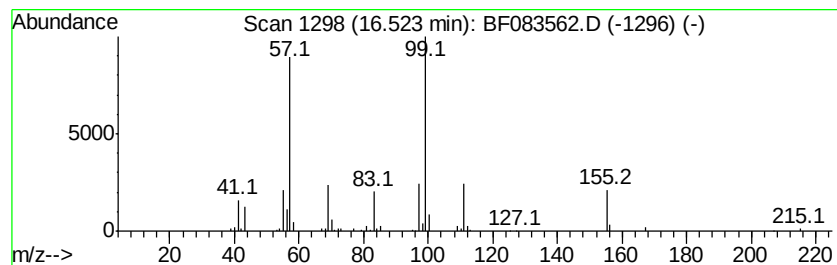
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.52 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	2.87 ng	186282	Chrysene-d12	17.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Bromoheptane	178	C7H15Br	000998-93-6	37
2		2-Piperidinone	99	C5H9NO	000675-20-7	35
3		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	32
4		1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	28
5		2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
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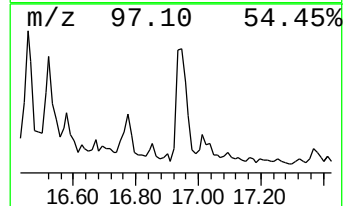
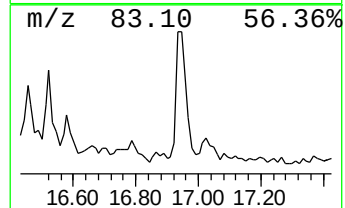
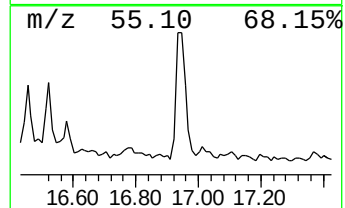
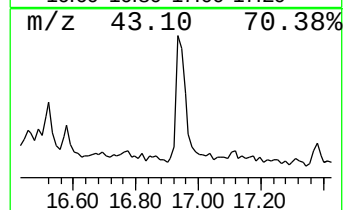
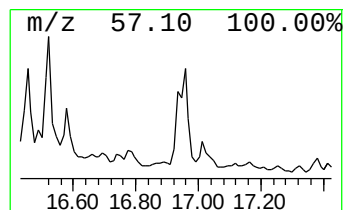
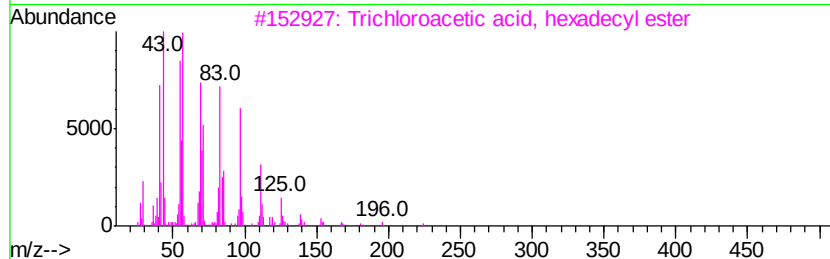
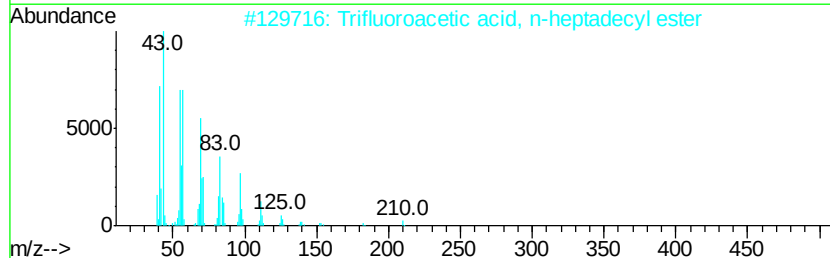
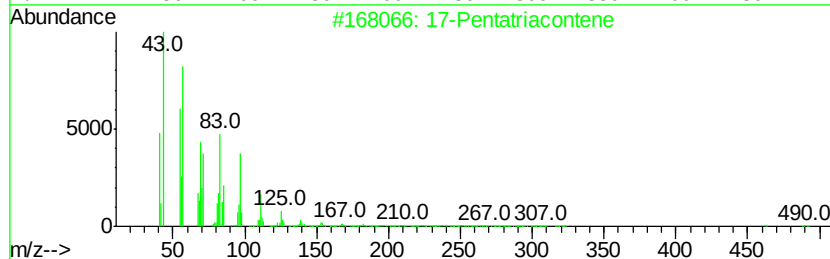
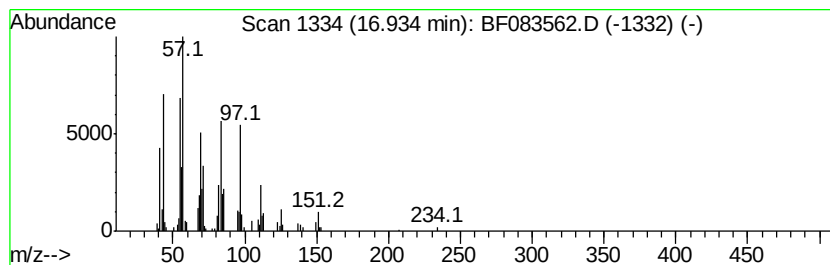
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.93	4.90 ng	318192	Chrysene-d12	17.01		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	58
2		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	58
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
4		1-Hexacosanol	382	C26H54O	000506-52-5	52
5		1-Docosene	308	C22H44	001599-67-3	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120715\
Data File : BF083562.D
Acq On : 7 Dec 2015 17:59
Operator : UM/IZ
Sample : G4634-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K203-20-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.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
unknown3.57	3.57	31.8	ng	1502100	1	5.72	946034	20.0
unknown5.41	5.41	119.1	ng	5634970	1	5.72	946034	20.0
Hexadecane	11.25	2.5	ng	197473	3	10.41	1582070	20.0
2-Bromo dodecane	12.03	4.2	ng	316097	4	12.81	1498500	20.0
Pentadecanoic acid	13.86	2.1	ng	160526	4	12.81	1498500	20.0
unknown14.58	14.58	2.4	ng	176373	4	12.81	1498500	20.0
unknown15.14	15.14	2.2	ng	140433	5	17.01	1297650	20.0
2-Hexene, 3,4,4-t...	15.72	2.4	ng	154050	5	17.01	1297650	20.0
2-Hexenoic acid, ...	16.25	2.3	ng	148075	5	17.01	1297650	20.0
2,4,4,6,6,8,8-Hep...	16.45	2.5	ng	162812	5	17.01	1297650	20.0
unknown16.52	16.52	2.9	ng	186282	5	17.01	1297650	20.0
17-Pentatriacontene	16.93	4.9	ng	318192	5	17.01	1297650	20.0