

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
 Data File : BF082628.D
 Acq On : 31 Oct 2015 18:29
 Operator : UM/IZ
 Sample : G4180-03
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3

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-BF103015.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	5.104	260	264	271	rBV	2374308	3309176	43.00%	4.822%
2	5.516	297	300	302	rBV	5762965	6015539	78.16%	8.766%
3	6.533	386	389	392	rBV	5385707	6189230	80.42%	9.019%
4	6.670	398	401	404	rBV	6153580	6108878	79.38%	8.902%
5	6.899	419	421	424	rVB	1501940	1475157	19.17%	2.150%
6	7.059	432	435	438	rBV	4819039	4649075	60.41%	6.774%
7	7.470	467	471	473	rBV	3447378	4727714	61.43%	6.889%
8	7.562	475	479	481	rVV	135905	194112	2.52%	0.283%
9	8.190	531	534	536	rBV	2302517	1970159	25.60%	2.871%
10	9.276	625	629	631	rBV	7098165	7696157	100.00%	11.214%
11	9.665	660	663	665	rBV	2078290	1781341	23.15%	2.596%
12	9.893	680	683	685	rVB	206191	186612	2.42%	0.272%
13	9.951	685	688	690	rBV	2125837	2191124	28.47%	3.193%
14	10.145	701	705	707	rBV3	48926	132439	1.72%	0.193%
15	10.396	723	727	728	rBV	233372	355437	4.62%	0.518%
16	10.613	743	746	749	rBV	107218	164835	2.14%	0.240%
17	10.739	754	757	759	rVV	4317291	4998973	64.95%	7.284%
18	10.865	766	768	775	rBV	396430	443739	5.77%	0.647%
19	11.059	783	785	787	rBV	61853	80578	1.05%	0.117%
20	11.311	805	807	809	rBV	265109	227766	2.96%	0.332%
21	11.425	815	817	820	rBV	1406351	1971877	25.62%	2.873%
22	11.494	820	823	825	rVB2	55254	80064	1.04%	0.117%
23	11.745	842	845	847	rVB	78822	100924	1.31%	0.147%
24	11.894	855	858	860	rBV2	42649	84515	1.10%	0.123%
25	11.974	863	865	867	rBV	778970	870294	11.31%	1.268%
26	12.145	876	880	886	rVB	56308	92265	1.20%	0.134%
27	12.637	922	923	924	rBV	106020	113785	1.48%	0.166%
28	12.682	924	927	931	rVV3	100688	272844	3.55%	0.398%
29	12.751	931	933	939	rVV2	389743	593577	7.71%	0.865%
30	12.854	940	942	946	rVB2	342580	382834	4.97%	0.558%
31	13.025	954	957	959	rBV	6618765	6237574	81.05%	9.089%
32	13.562	1002	1004	1006	rBV	204702	191231	2.48%	0.279%
33	13.928	1034	1036	1046	rBV	355813	536828	6.98%	0.782%
34	14.065	1046	1048	1051	rBV	1277772	1557324	20.24%	2.269%

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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-BF103015.M
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35	14.568	1089	1092	1094	rBV2	62836	92901	1.21%	0.135%
36	14.945	1123	1125	1128	rBV	96718	124624	1.62%	0.182%
37	15.105	1136	1139	1144	rVB	39703	86606	1.13%	0.126%
38	15.208	1146	1148	1150	rVV	54506	83386	1.08%	0.122%
39	15.243	1150	1151	1160	rVB2	56518	108388	1.41%	0.158%
40	15.528	1173	1176	1179	rBV	1003791	1247020	16.20%	1.817%
41	16.020	1216	1219	1222	rBV	59893	89809	1.17%	0.131%
42	16.088	1222	1225	1231	rBV3	36707	102634	1.33%	0.150%
43	17.117	1311	1315	1318	rBV	40065	93911	1.22%	0.137%
44	17.288	1327	1330	1332	rBV2	55317	112148	1.46%	0.163%
45	17.334	1332	1334	1340	rVB3	120878	275424	3.58%	0.401%
46	17.574	1351	1355	1362	rBV3	79246	226100	2.94%	0.329%

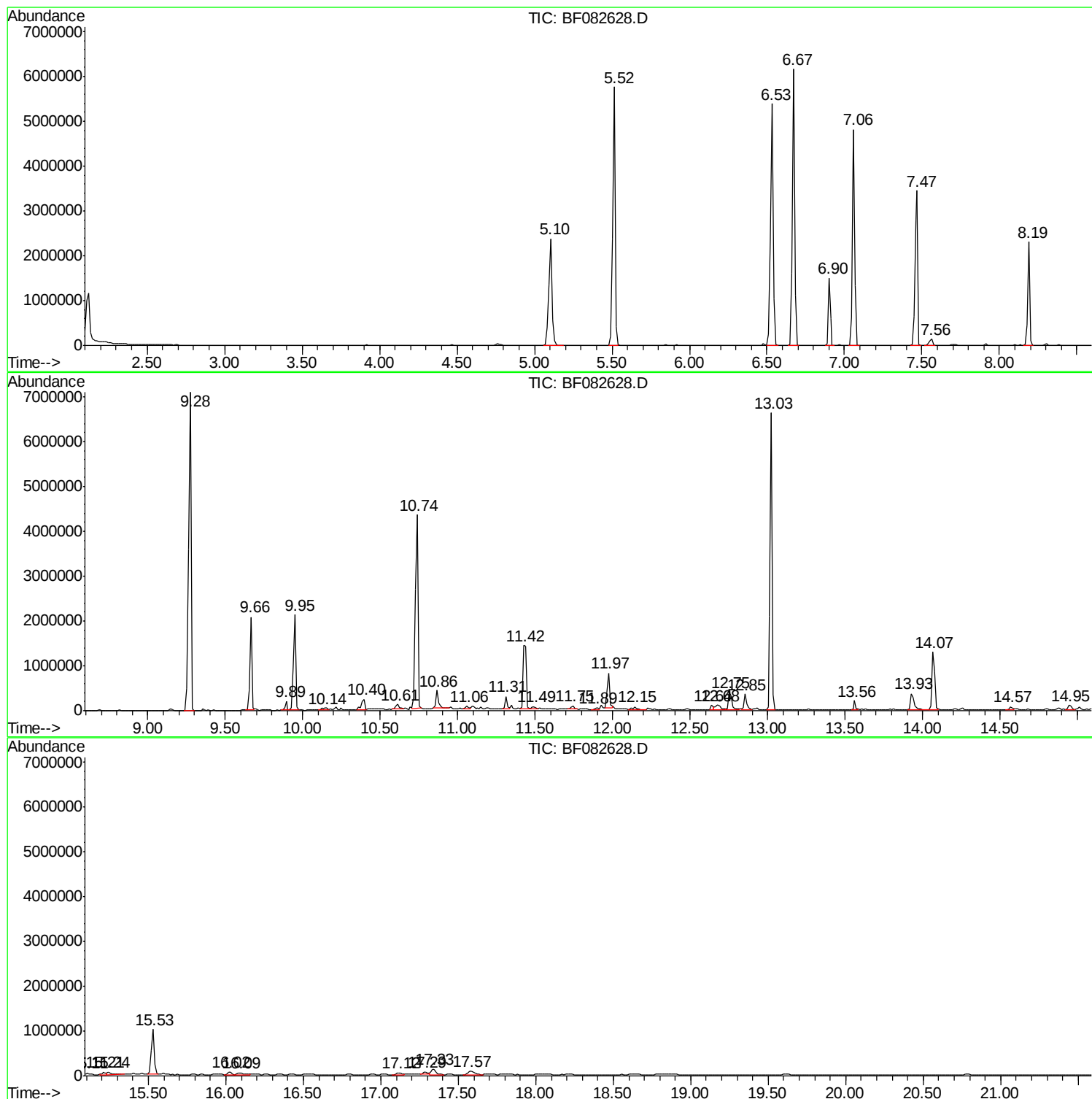
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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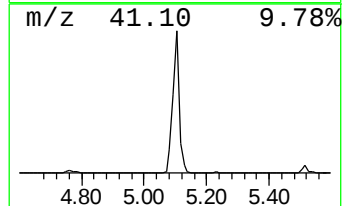
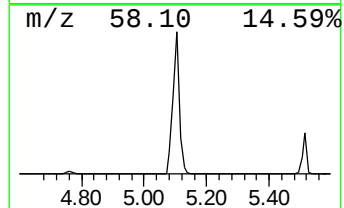
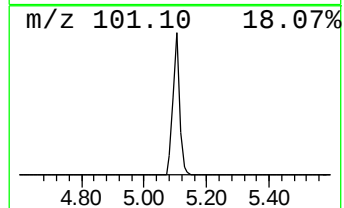
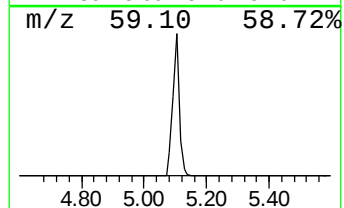
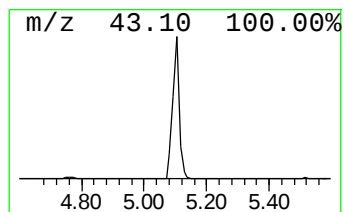
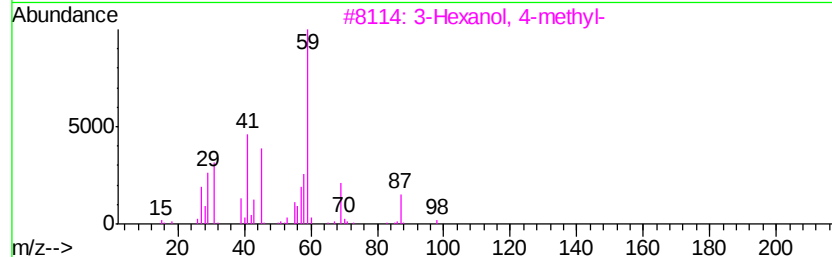
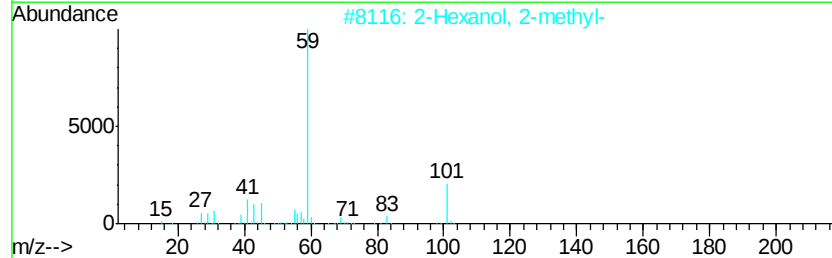
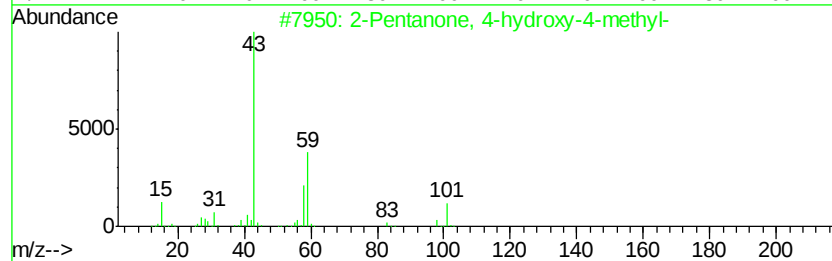
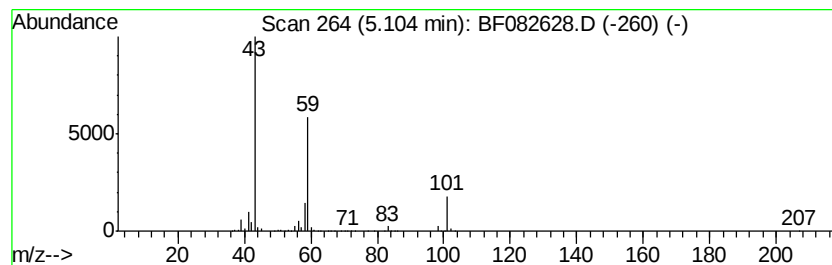
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	44.87 ng	3309180	1,4-Dichlorobenzene-d4	6.90

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		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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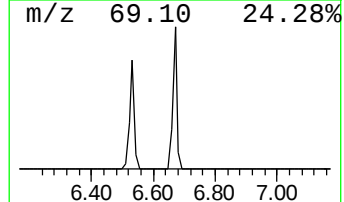
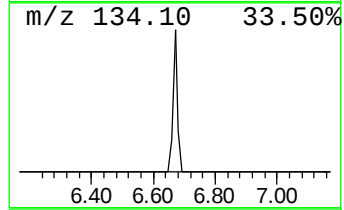
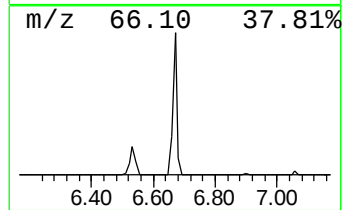
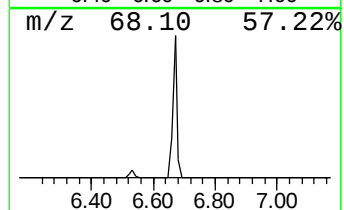
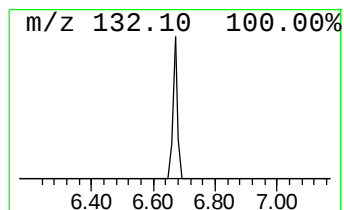
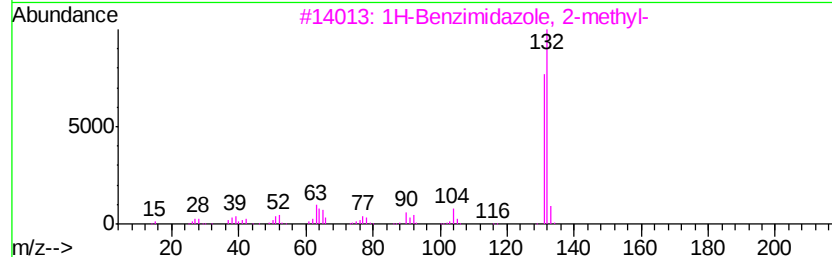
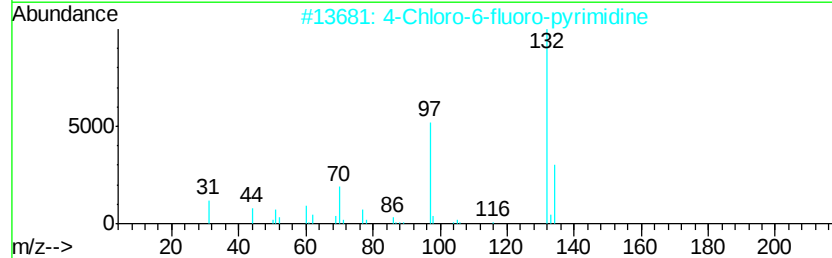
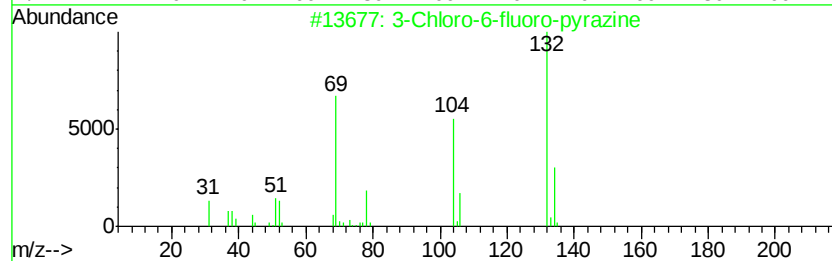
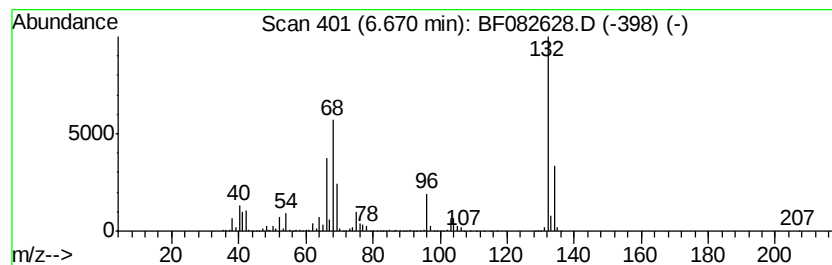
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	82.82 ng	6108880	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11



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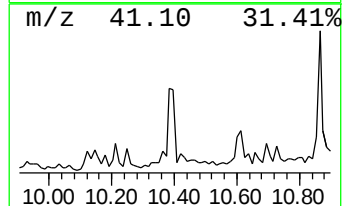
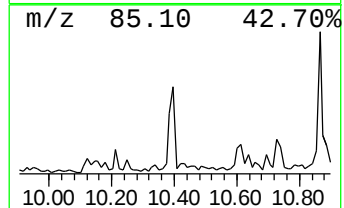
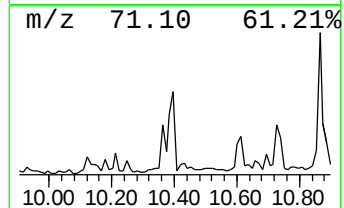
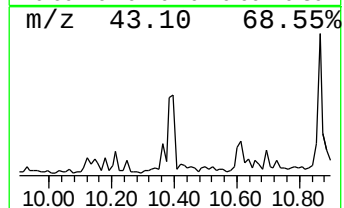
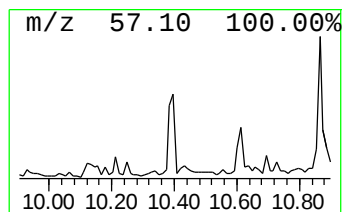
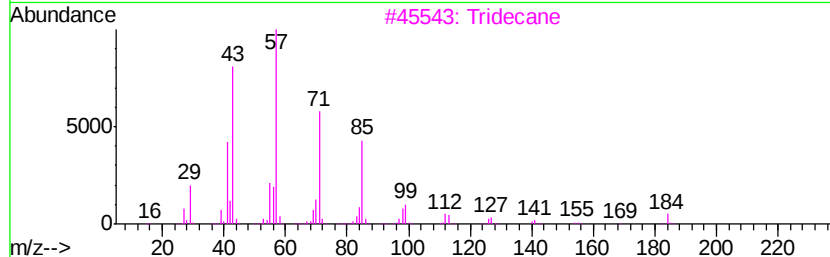
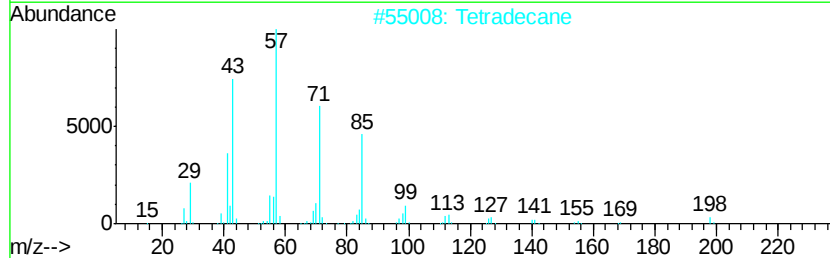
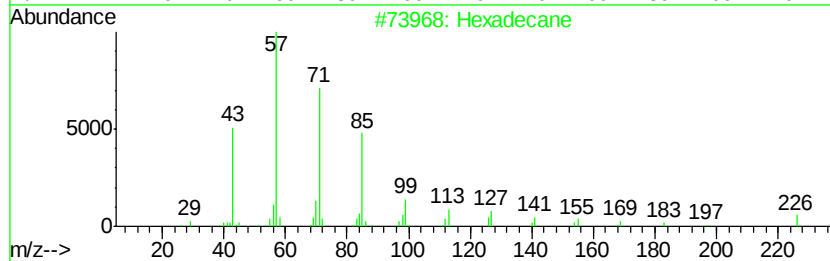
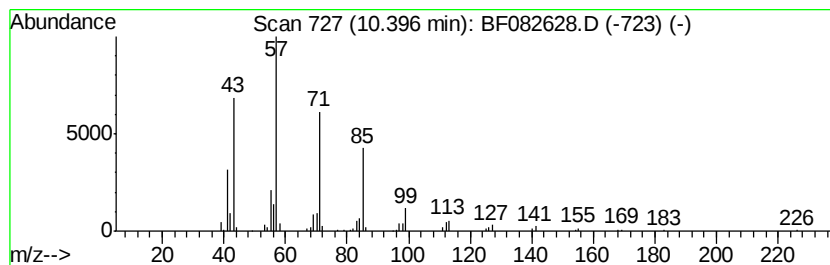
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.40	3.24 ng	355437	Acenaphthene-d10		9.95
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Tetradecane	198	C14H30	000629-59-4	91
3	Tridecane	184	C13H28	000629-50-5	87
4	Heneicosane	296	C21H44	000629-94-7	83
5	Heptadecane	240	C17H36	000629-78-7	74



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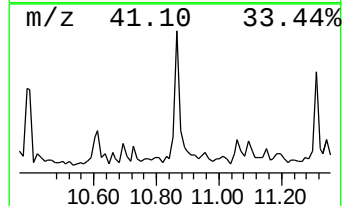
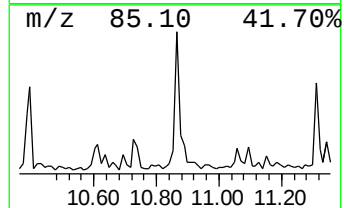
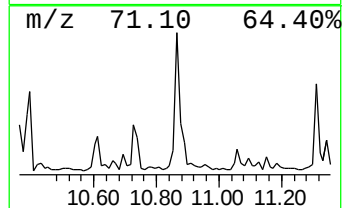
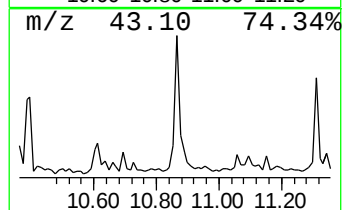
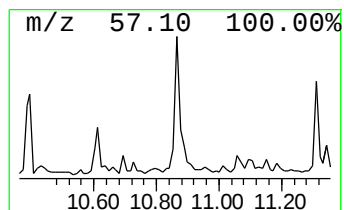
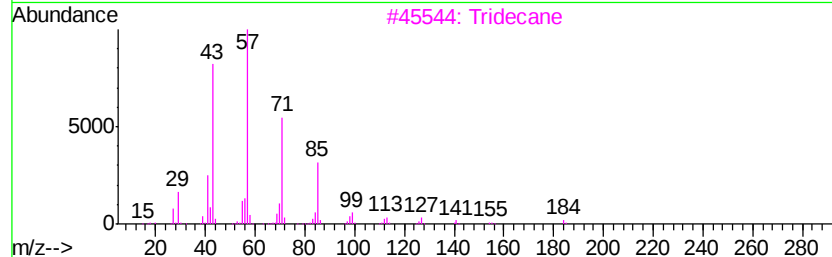
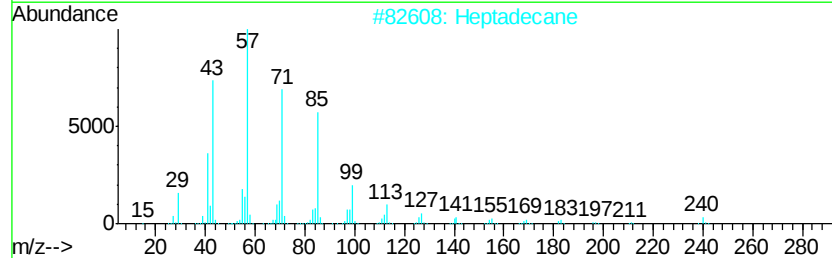
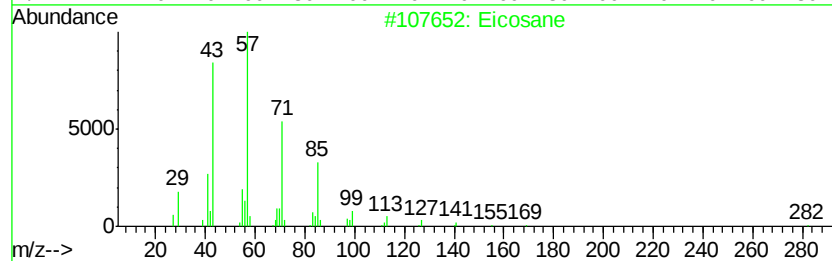
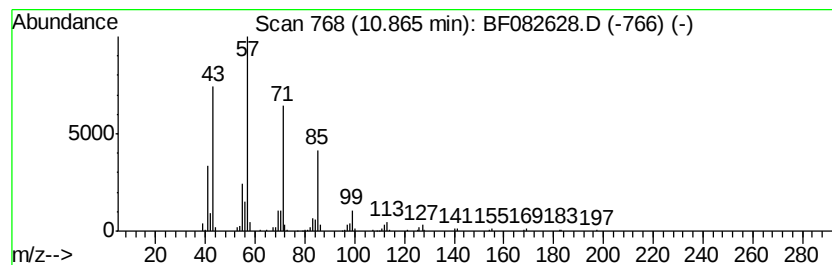
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	4.50 ng	443739	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	90
3	Tridecane		184	C13H28	000629-50-5	86
4	10-Methylnonadecane		282	C20H42	056862-62-5	86
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	80



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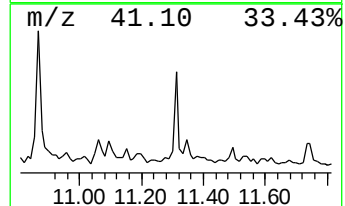
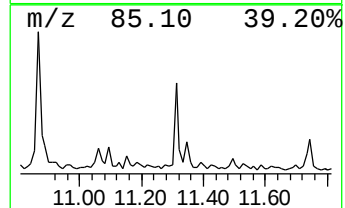
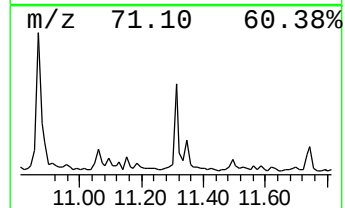
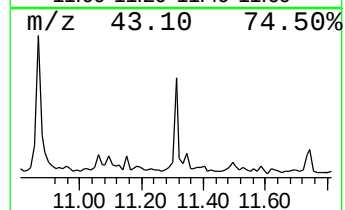
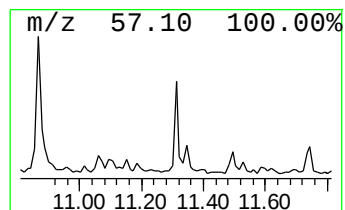
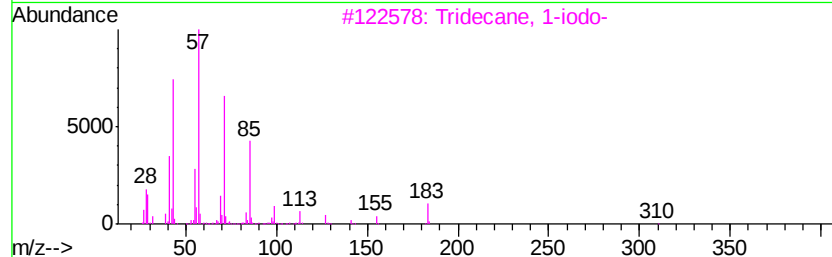
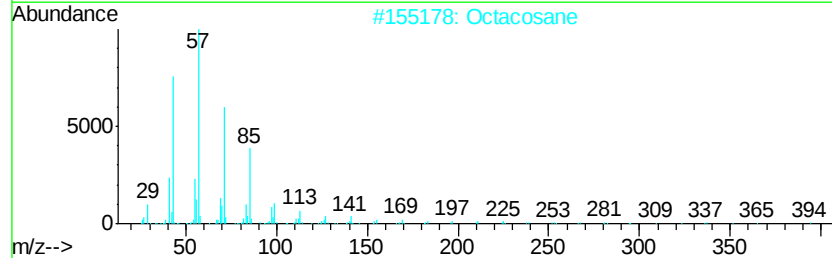
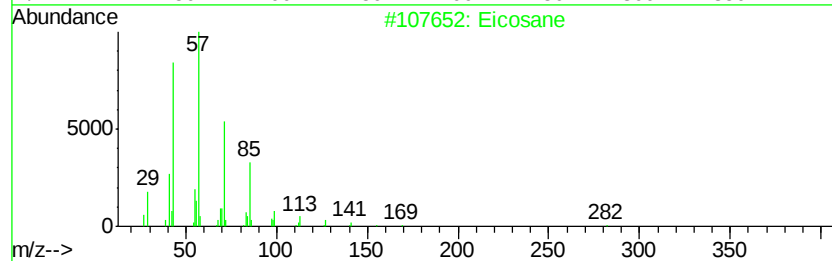
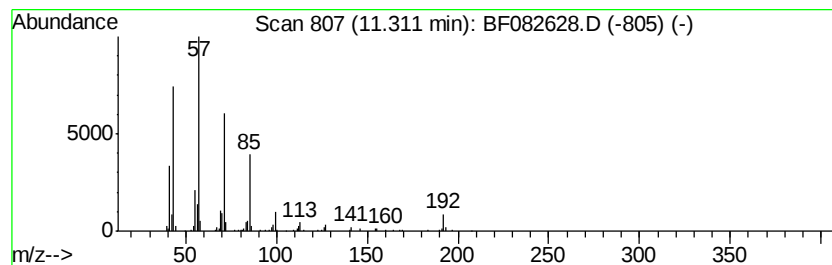
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.31	2.31 ng	227766	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5		Tetradecane	198	C14H30	000629-59-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
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Operator : UM/IZ
Sample : G4180-03
Misc :
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ClientSampleId :
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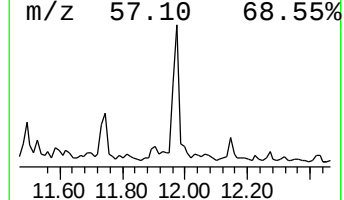
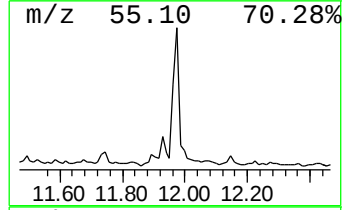
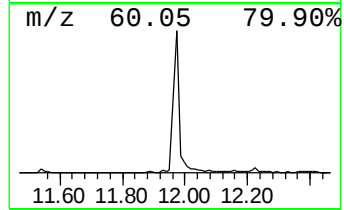
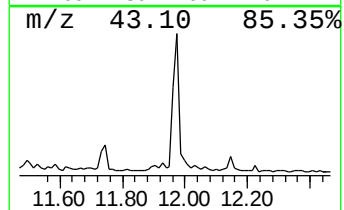
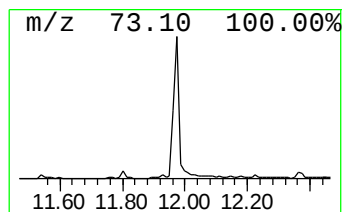
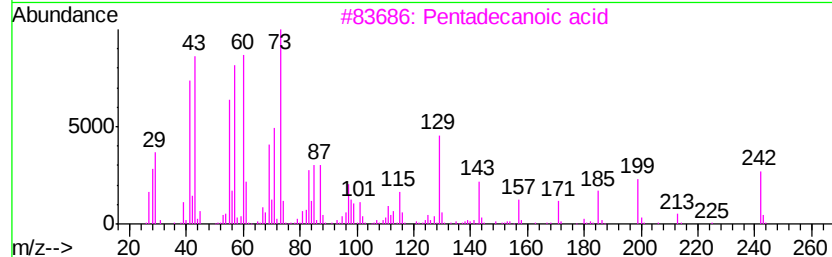
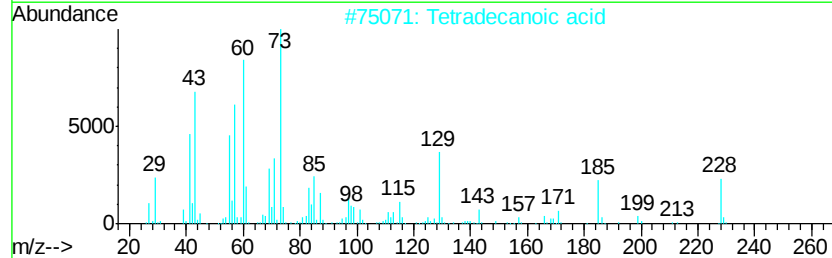
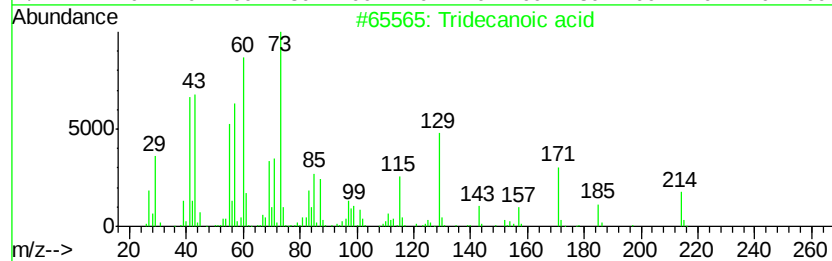
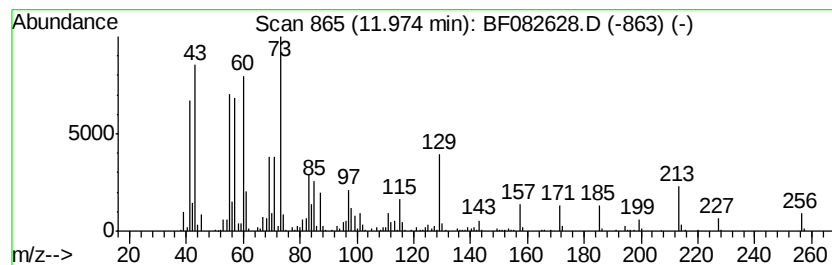
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	8.83 ng	870294	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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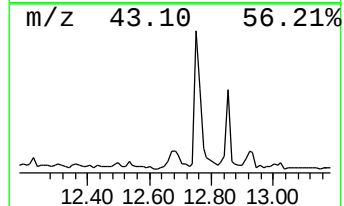
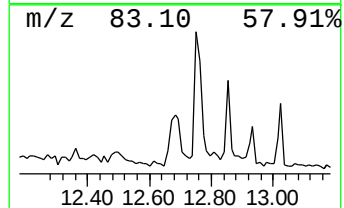
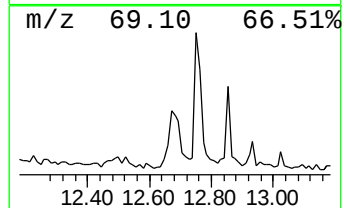
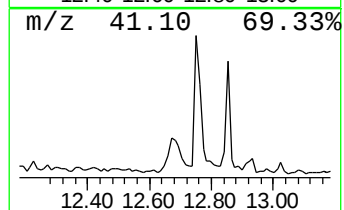
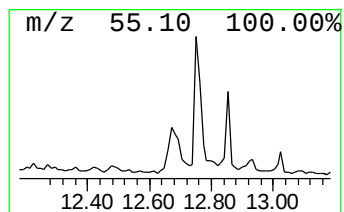
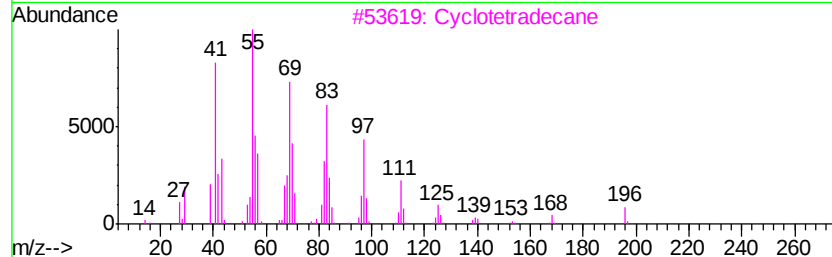
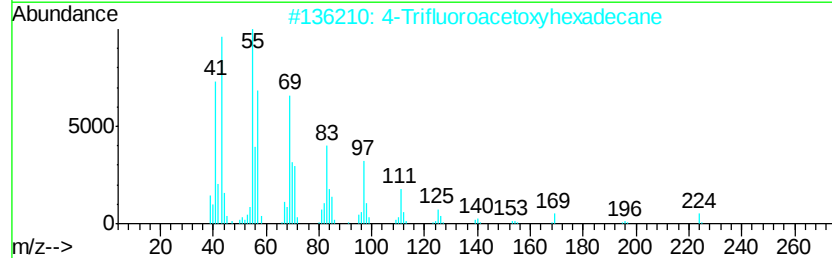
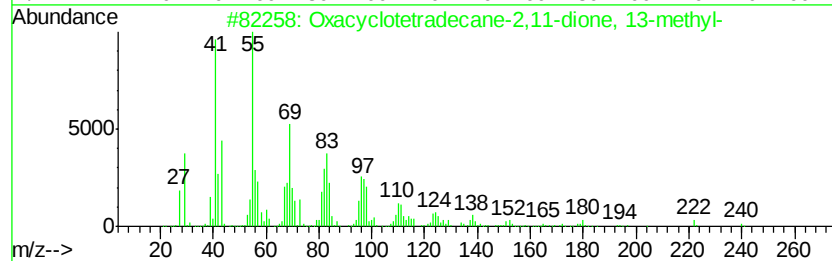
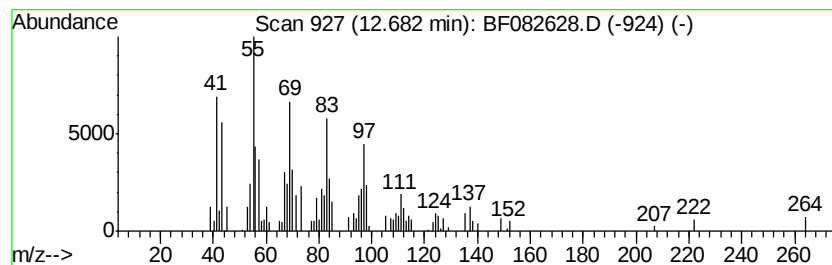
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxacyclotetradecane-2,11-di... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.77 ng	272844	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	64
2		4-Trifluoroacetoxyhexadecane	338	C18H33F3O2	1000215-97-5	58
3		Cyclotetradecane	196	C14H28	000295-17-0	58
4		Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	53
5		1-Hexadecene	224	C16H32	000629-73-2	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
Acq On : 31 Oct 2015 18:29
Operator : UM/IZ
Sample : G4180-03
Misc :
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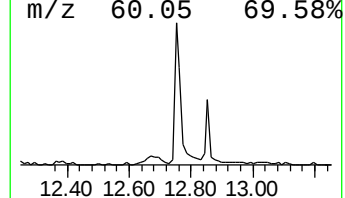
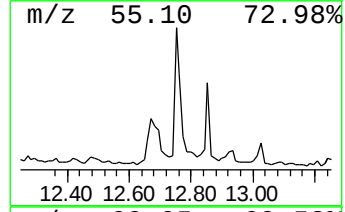
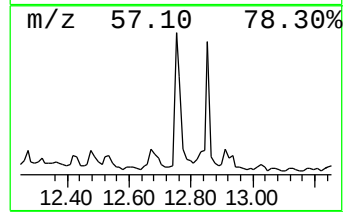
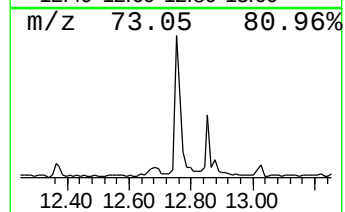
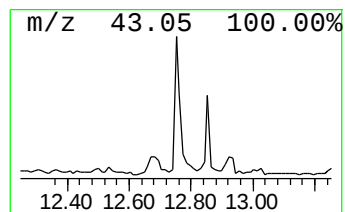
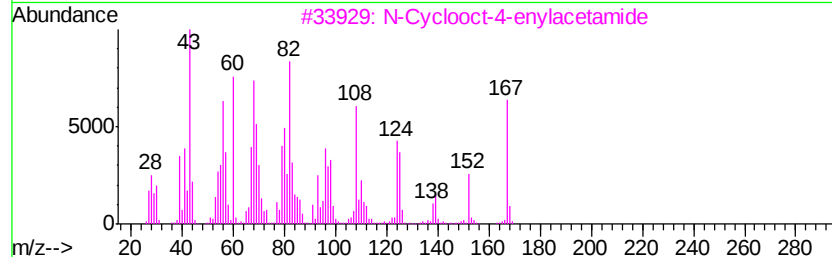
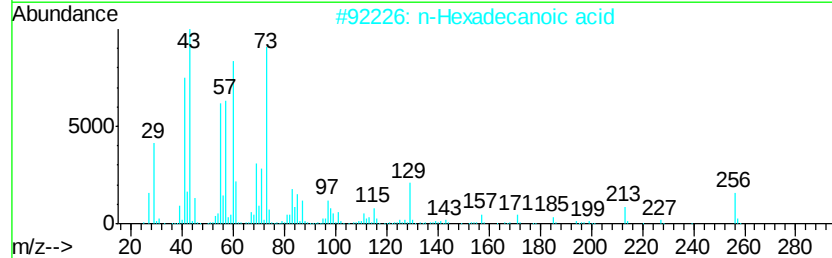
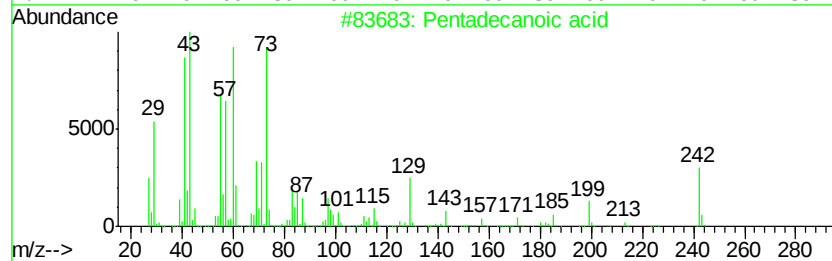
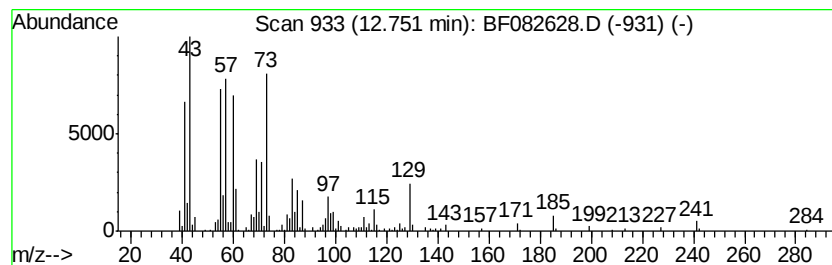
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	7.62 ng	593577	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	22
4		Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	18
5		2H-Pyran, 2-(2-heptadecynyloxy)t...	336	C22H40O2	069502-96-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
Acq On : 31 Oct 2015 18:29
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Misc :
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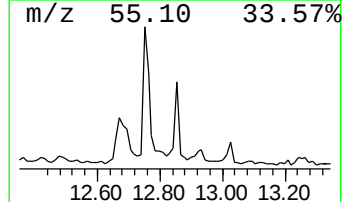
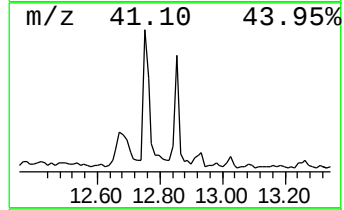
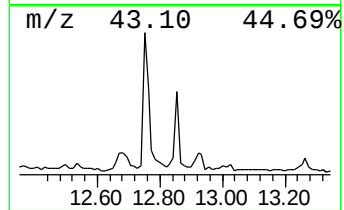
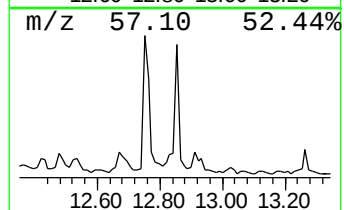
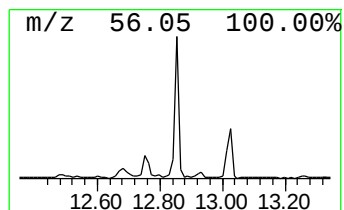
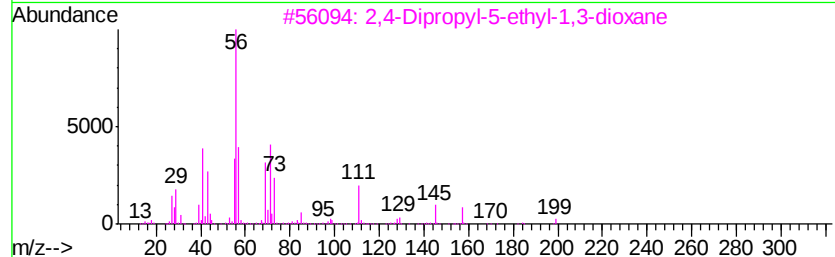
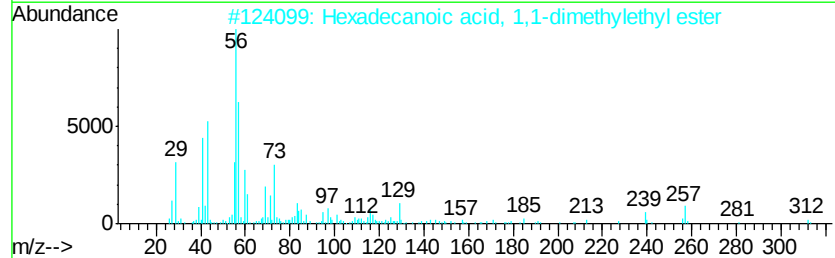
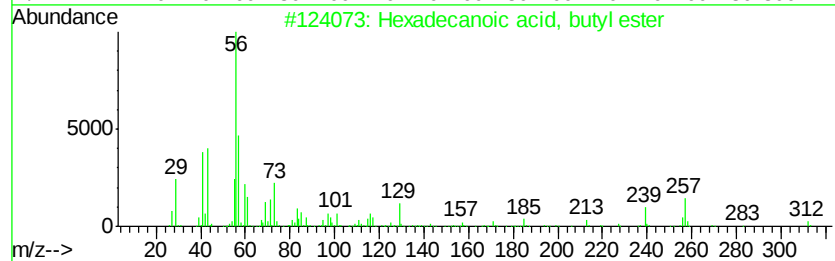
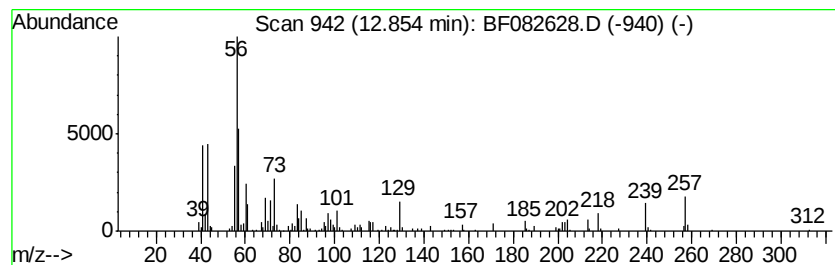
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	4.92 ng	382834	Chrysene-d12	14.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	47
3			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			Cyclohexanol,2-amino-,trans-	115	C6H13NO	006982-39-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
Acq On : 31 Oct 2015 18:29
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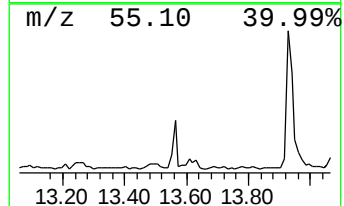
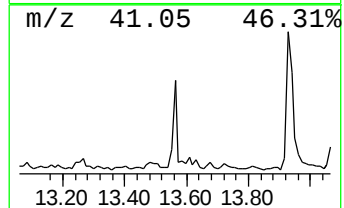
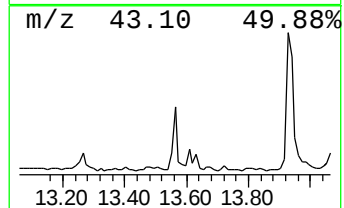
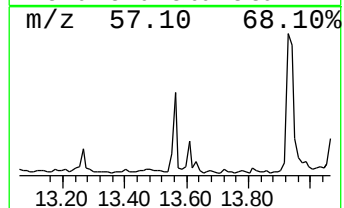
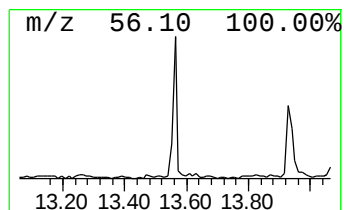
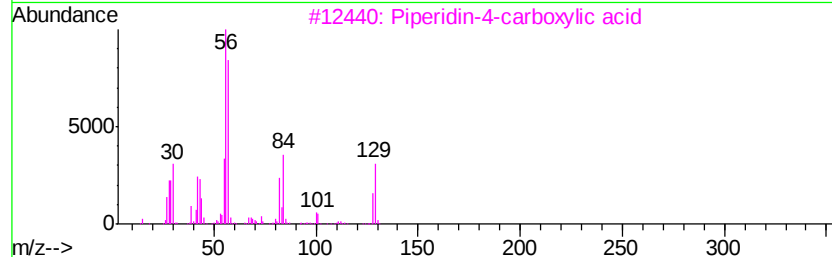
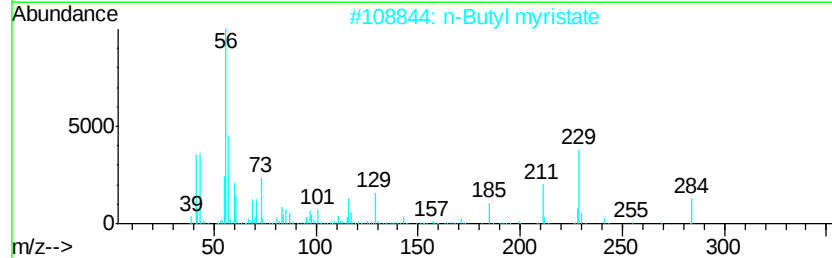
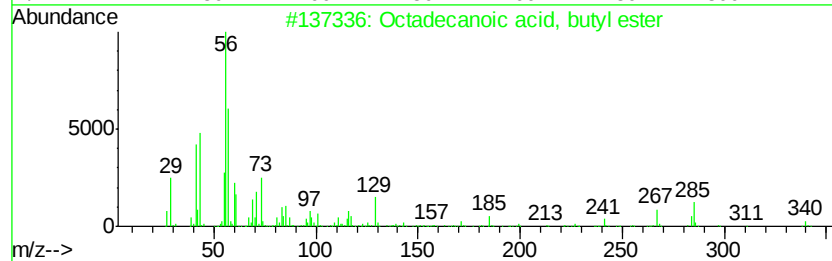
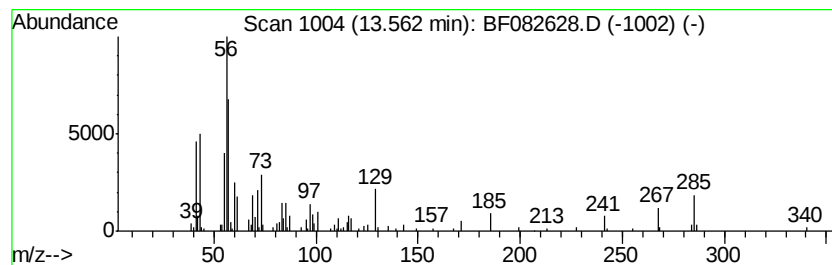
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid, butyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	2.46 ng	191231	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		n-Butyl myristate	284	C18H36O2	000110-36-1	72
3		Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
Acq On : 31 Oct 2015 18:29
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Sample : G4180-03
Misc :
ALS Vial : 43 Sample Multiplier: 1

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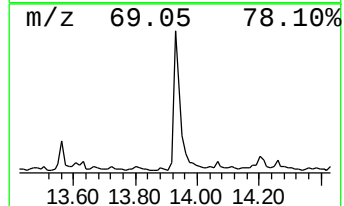
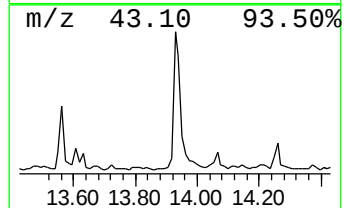
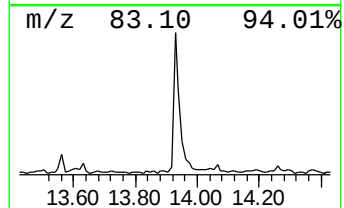
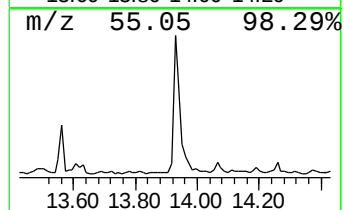
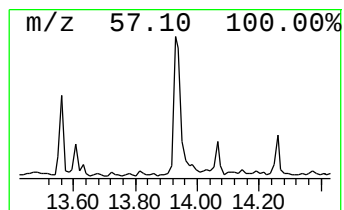
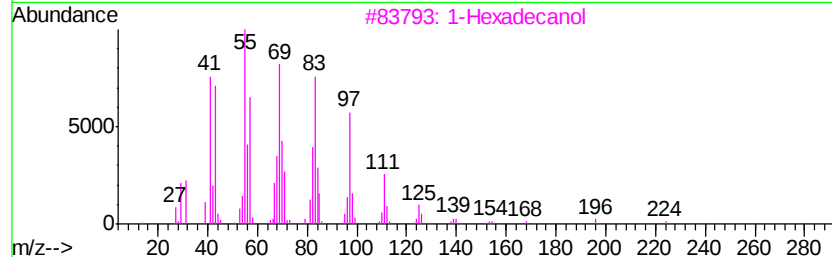
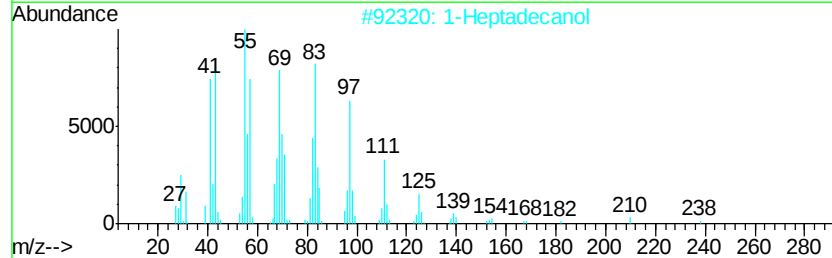
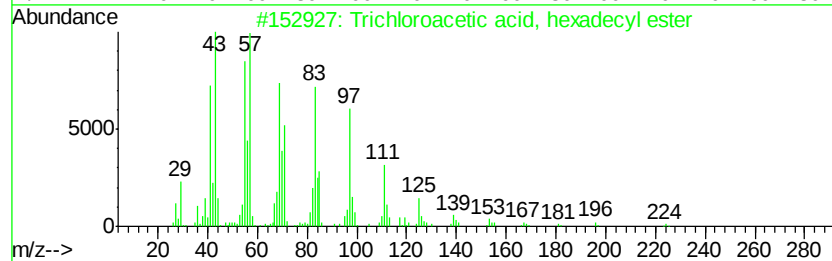
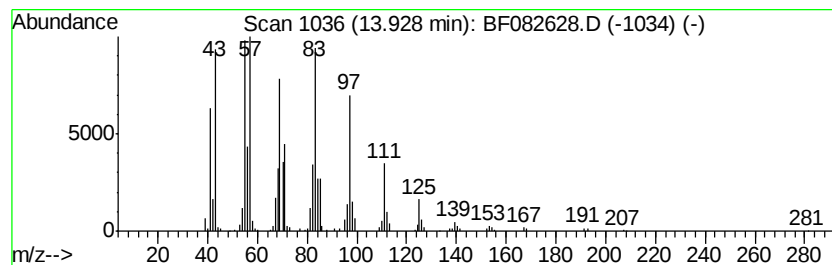
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	6.89 ng	536828	Chrysene-d12	14.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			1-Heptadecanol	256	C17H36O	001454-85-9	90
3			1-Hexadecanol	242	C16H34O	036653-82-4	87
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	83
5			1-Nonadecene	266	C19H38	018435-45-5	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
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Acq On : 31 Oct 2015 18:29
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Sample : G4180-03
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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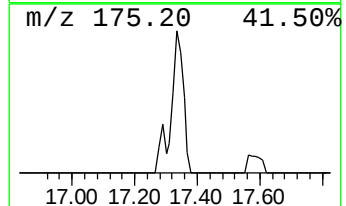
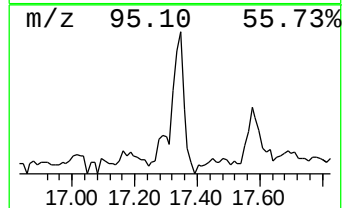
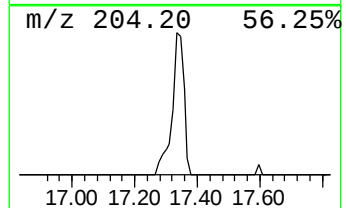
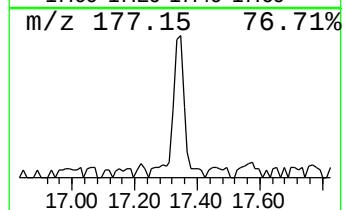
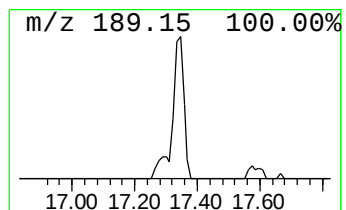
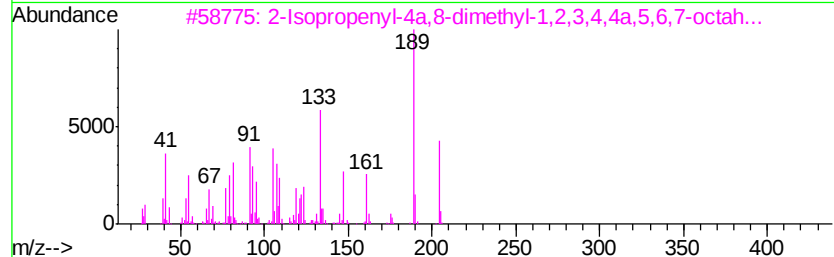
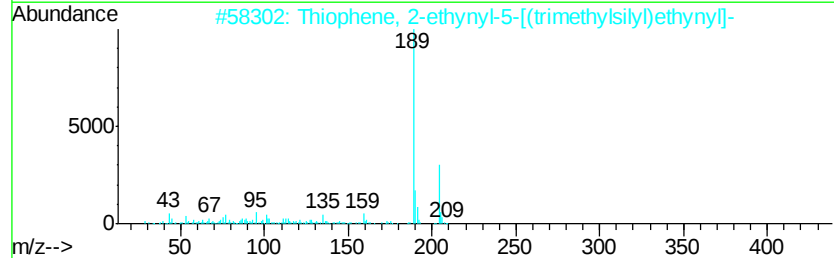
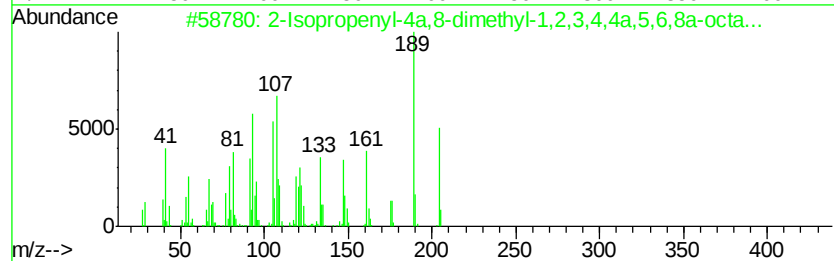
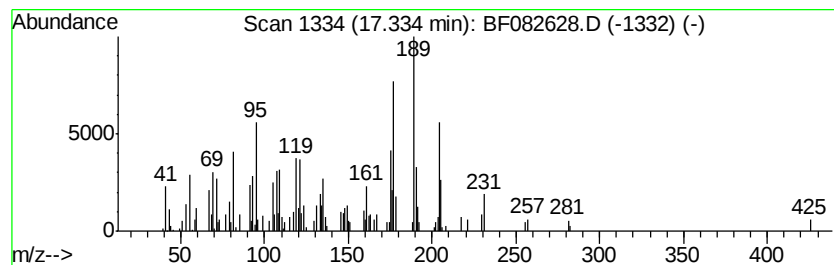
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	4.42 ng	275424	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	52
2		Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	43
3		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	35
4		Aciphyllene	204	C15H24	087745-31-1	30
5		Benzenepropanal, 3-(1,1-dimethyl...	204	C14H20O	062518-65-4	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103015\
Data File : BF082628.D
Acq On : 31 Oct 2015 18:29
Operator : UM/IZ
Sample : G4180-03
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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...	5.10	44.9	ng	3309180	1	6.90	1475160	20.0
unknown6.67	6.67	82.8	ng	6108880	1	6.90	1475160	20.0
Hexadecane	10.40	3.2	ng	355437	3	9.95	2191120	20.0
Eicosane	10.86	4.5	ng	443739	4	11.44	1971880	20.0
Octacosane	11.31	2.3	ng	227766	4	11.44	1971880	20.0
Tridecanoic acid	11.97	8.8	ng	870294	4	11.44	1971880	20.0
Oxacyclotetradeca...	12.68	2.8	ng	272844	4	11.44	1971880	20.0
Pentadecanoic acid	12.75	7.6	ng	593577	5	14.07	1557320	20.0
Hexadecanoic acid...	12.85	4.9	ng	382834	5	14.07	1557320	20.0
Octadecanoic acid...	13.56	2.5	ng	191231	5	14.07	1557320	20.0
Trichloroacetic a...	13.93	6.9	ng	536828	5	14.07	1557320	20.0
2-Isopropenyl-4a,...	17.33	4.4	ng	275424	6	15.53	1247020	20.0