

Data Path : Z:\HPCHEM1\BNA F\DATA\BF090315\
 Data File : BF081407.D
 Acq On : 4 Sep 2015 7:22
 Operator : UM/IZ
 Sample : G3505-06
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P005-BF003-01

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	3.541	169	171	178	rBB	10844	23159	1.42%	0.156%
2	4.410	244	247	257	rVB	553446	958345	58.66%	6.473%
3	4.913	289	291	294	rBV	1099499	1436873	87.96%	9.705%
4	6.033	387	389	392	rBV	1235308	1353168	82.83%	9.139%
5	6.136	396	398	400	rBV	1725677	1527060	93.48%	10.314%
6	6.364	416	418	421	rVB	430656	373322	22.85%	2.521%
7	6.524	430	432	434	rBV	1247828	1145196	70.10%	7.735%
8	6.947	466	469	471	rBV	983731	1051324	64.36%	7.101%
9	7.656	529	531	533	rBV	592073	483192	29.58%	3.263%
10	8.742	623	626	628	rBV	1853204	1633623	100.00%	11.033%
11	9.142	659	661	664	rBV	360708	324163	19.84%	2.189%
12	9.393	681	683	686	rVB	460359	477041	29.20%	3.222%
13	10.182	749	752	754	rBV	951019	937508	57.39%	6.332%
14	10.330	763	765	768	rBV	35458	38750	2.37%	0.262%
15	10.776	802	804	805	rBV	31286	25481	1.56%	0.172%
16	10.856	809	811	814	rBV	422149	474056	29.02%	3.202%
17	11.439	860	862	868	rBV	101546	113398	6.94%	0.766%
18	12.445	947	950	953	rBV	1482917	1350948	82.70%	9.124%
19	13.371	1028	1031	1037	rBV	78590	127485	7.80%	0.861%
20	13.462	1037	1039	1042	rBV	304444	371131	22.72%	2.507%
21	13.988	1083	1085	1089	rBV	20154	35442	2.17%	0.239%
22	14.411	1119	1122	1124	rBV	30108	37097	2.27%	0.251%
23	14.559	1133	1135	1143	rBV2	24252	71288	4.36%	0.481%
24	14.777	1152	1154	1156	rBV	246060	255787	15.66%	1.728%
25	14.994	1171	1173	1176	rVB	22240	25528	1.56%	0.172%
26	15.165	1185	1188	1190	rBV	29296	40691	2.49%	0.275%
27	15.737	1235	1238	1241	rBV	17214	27894	1.71%	0.188%
28	15.965	1254	1258	1261	rBV3	14419	35306	2.16%	0.238%
29	16.080	1266	1268	1274	rVB5	14909	31483	1.93%	0.213%
30	16.754	1323	1327	1331	rVB2	8168	20387	1.25%	0.138%

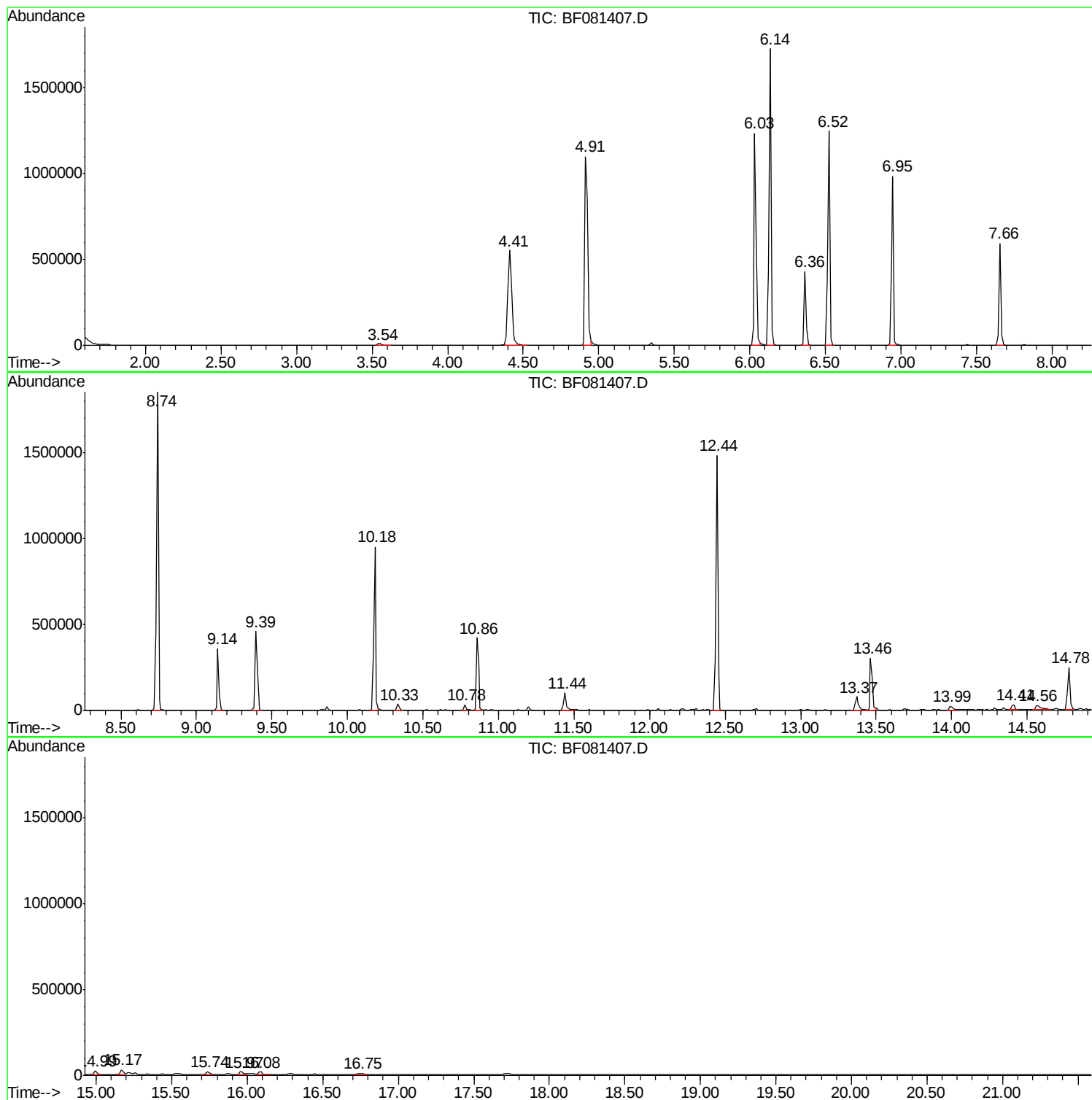
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ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-BF003-01

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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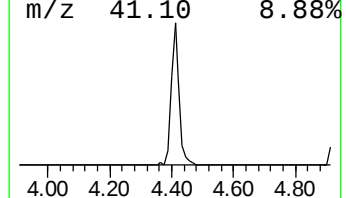
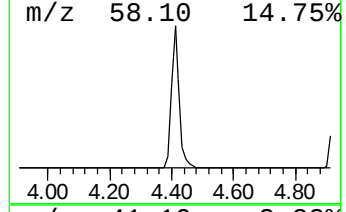
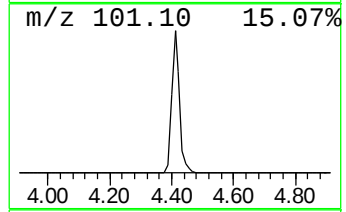
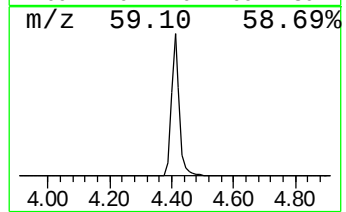
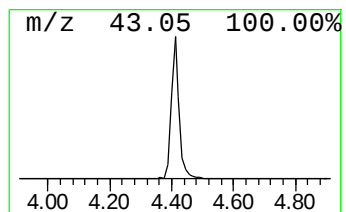
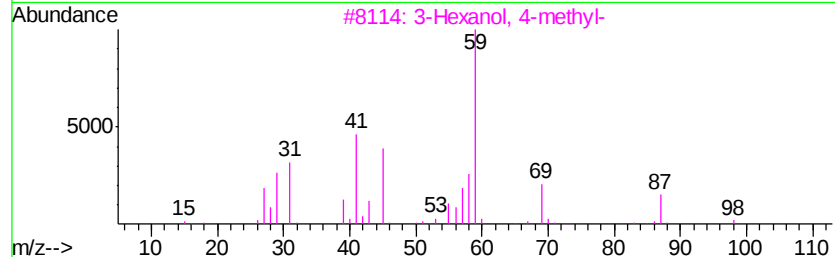
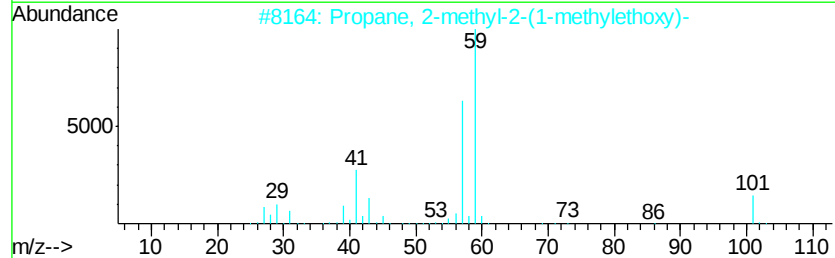
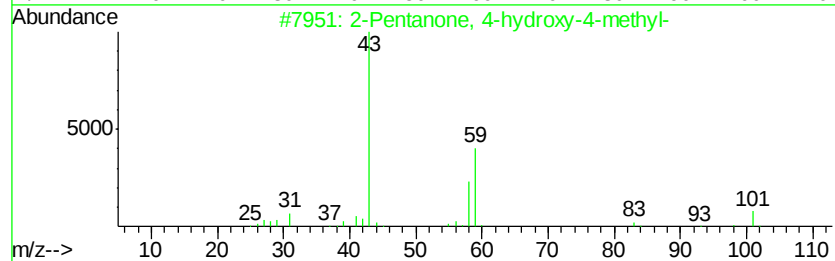
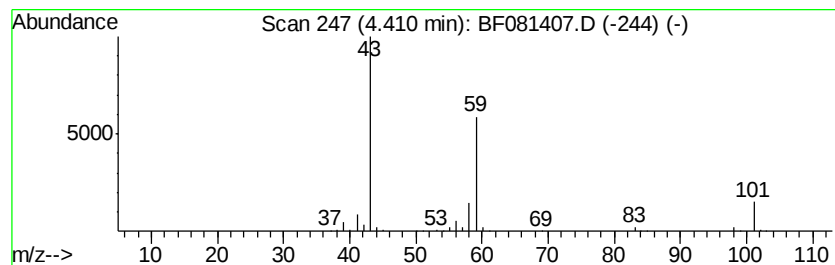
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.41	51.34 ng	958345	1,4-Dichlorobenzene-d4	6.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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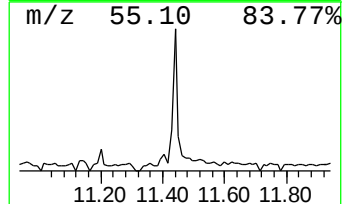
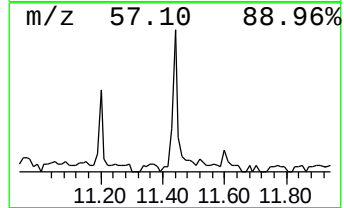
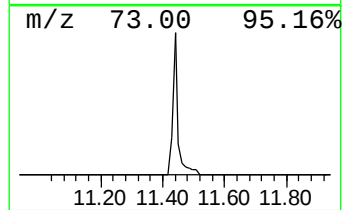
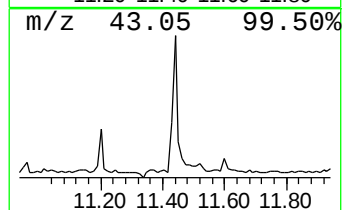
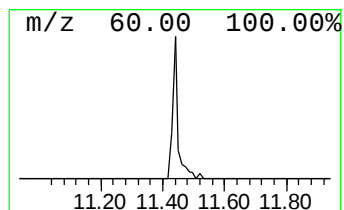
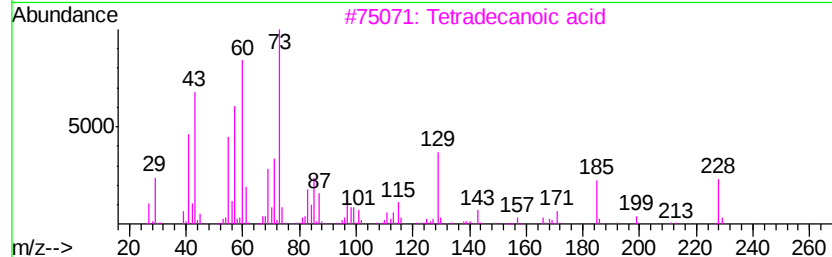
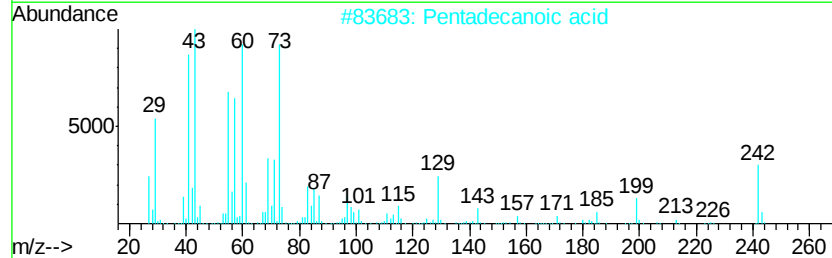
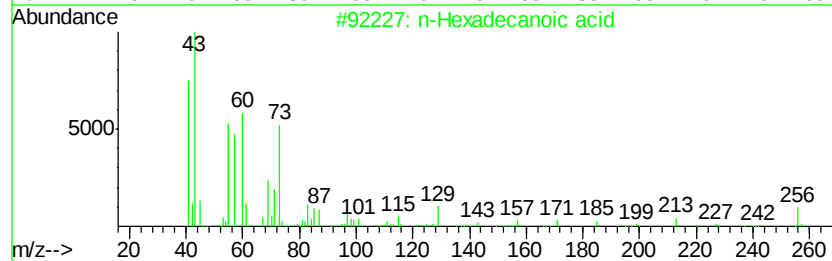
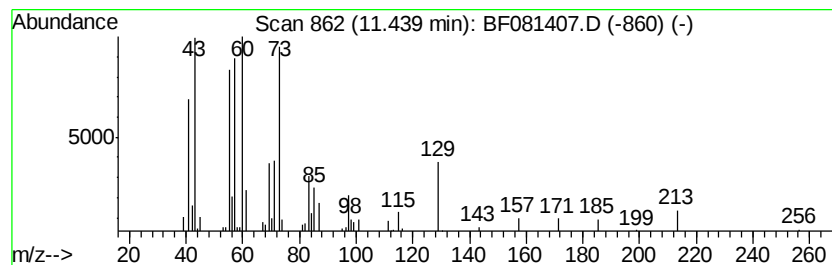
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.44	4.78 ng	113398	Phenanthrene-d10		10.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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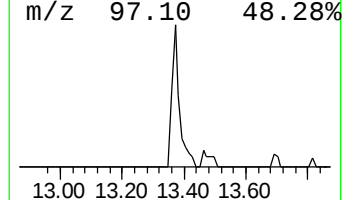
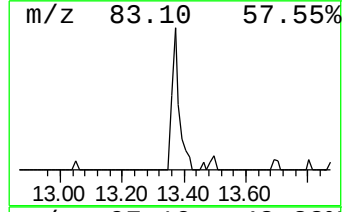
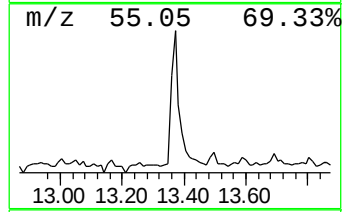
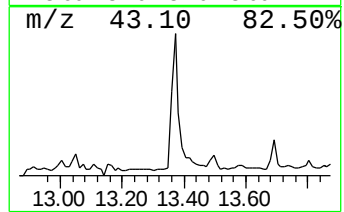
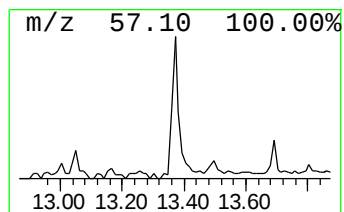
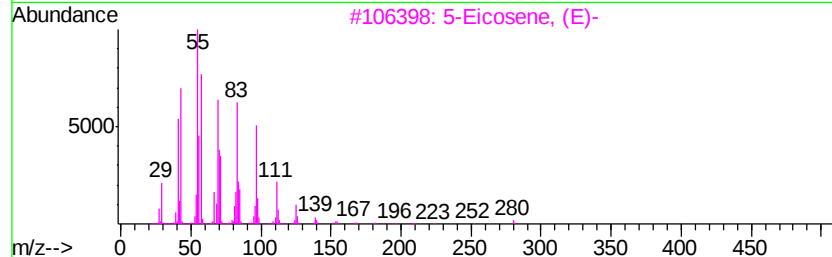
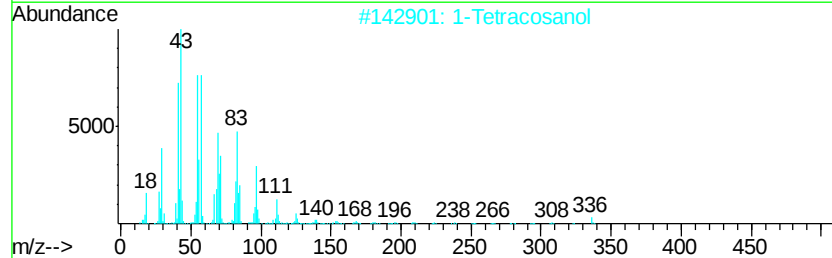
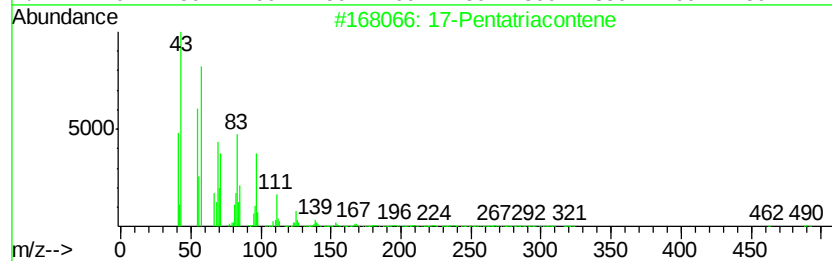
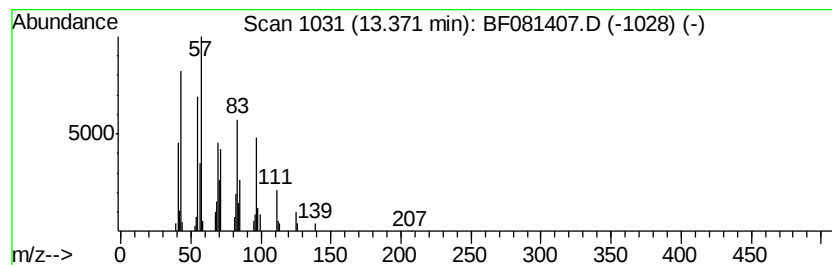
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Peak Number 5 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	6.87 ng	127485	Chrysene-d12	13.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	90
2		1-Tetracosanol	354	C24H50O	000506-51-4	72
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	68
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	62
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	58



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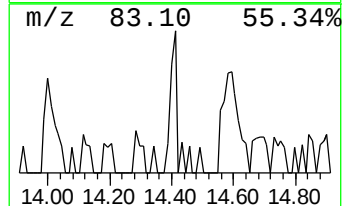
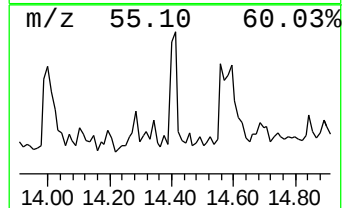
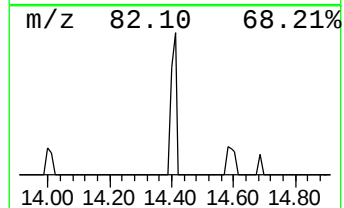
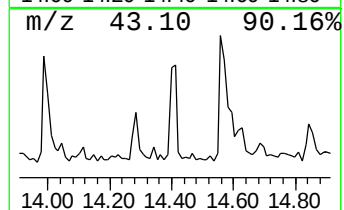
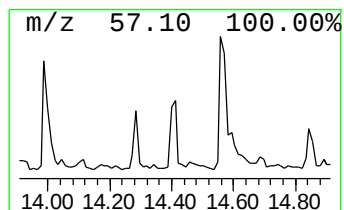
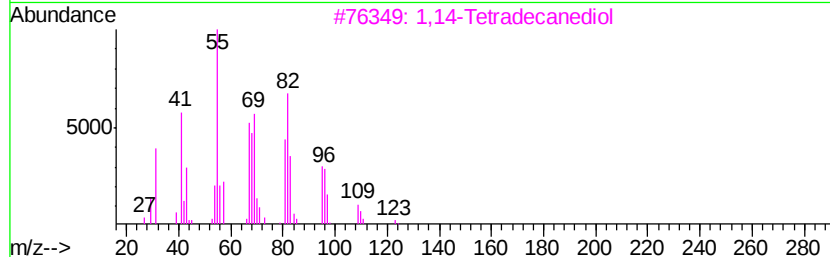
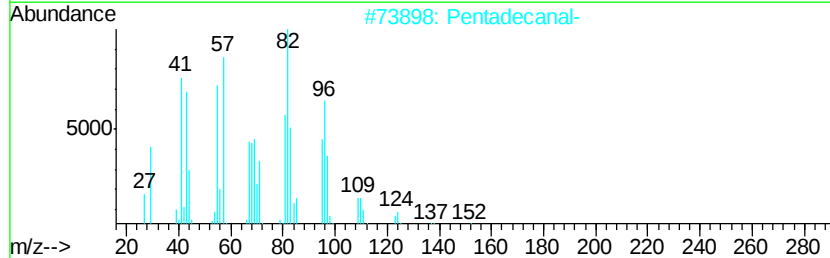
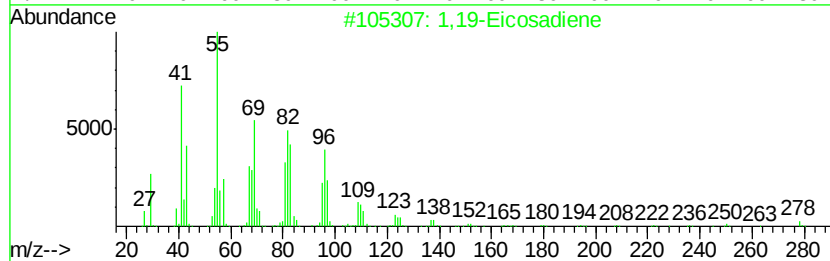
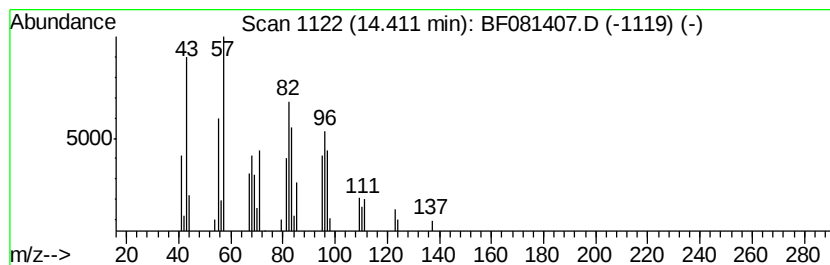
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Peak Number 6 1,19-Eicosadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.41	2.90 ng	37097	Perylene-d12	14.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	72
2	Pentadecanal-	226	C15H30O	002765-11-9	58
3	1,14-Tetradecanediol	230	C14H30O2	019812-64-7	53
4	Oxirane, dodecyl-	212	C14H28O	003234-28-4	53
5	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	35



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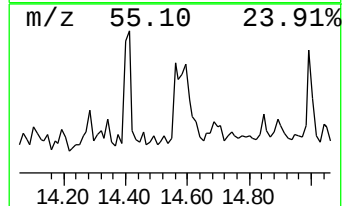
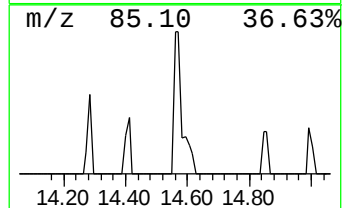
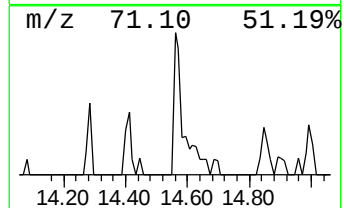
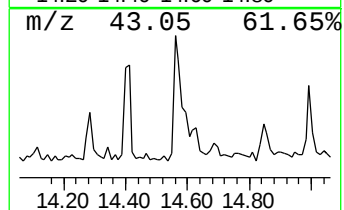
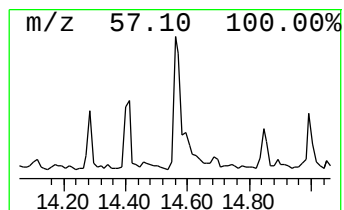
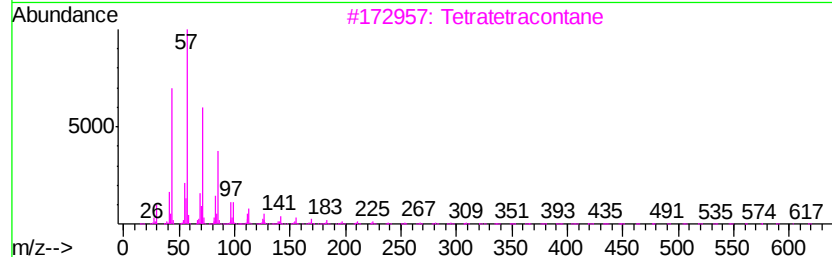
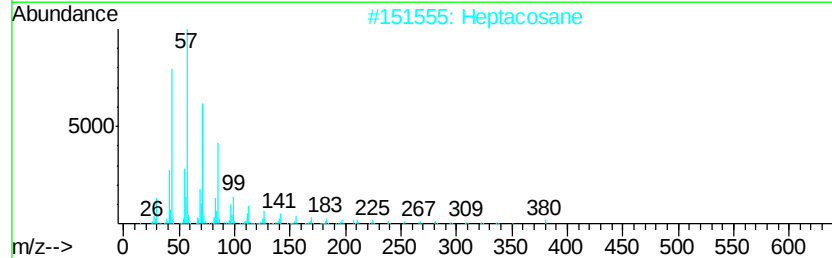
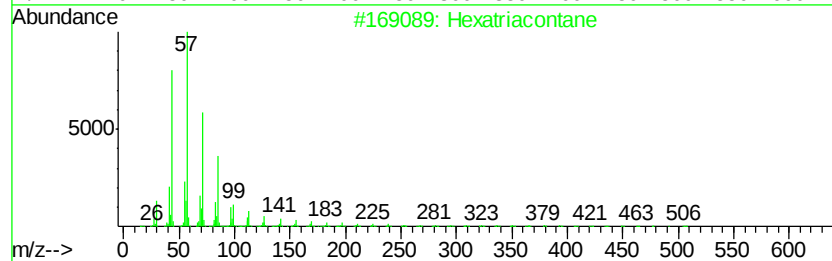
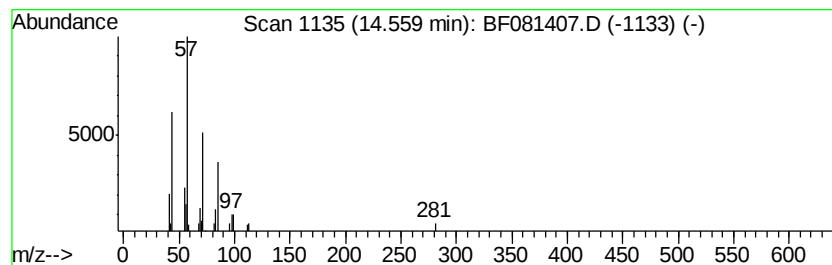
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Hexatriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	5.57 ng	71288	Perylene-d12	14.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane		507	C36H74	000630-06-8	86
2	Heptacosane		380	C27H56	000593-49-7	80
3	Tetratetracontane		619	C44H90	007098-22-8	78
4	Hentriacontane		437	C31H64	000630-04-6	78
5	Pentacosane		352	C25H52	000629-99-2	78



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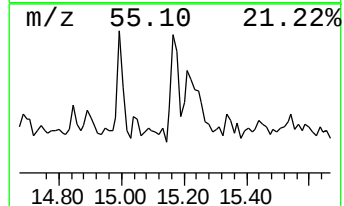
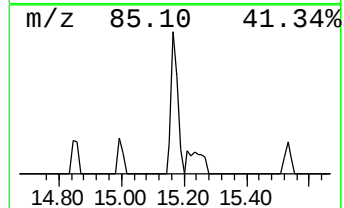
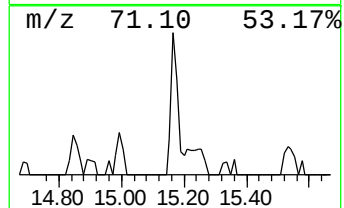
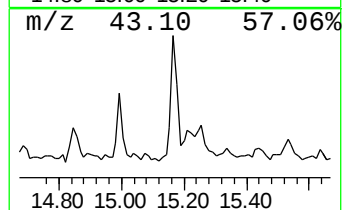
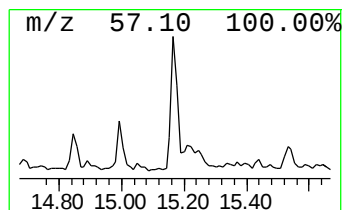
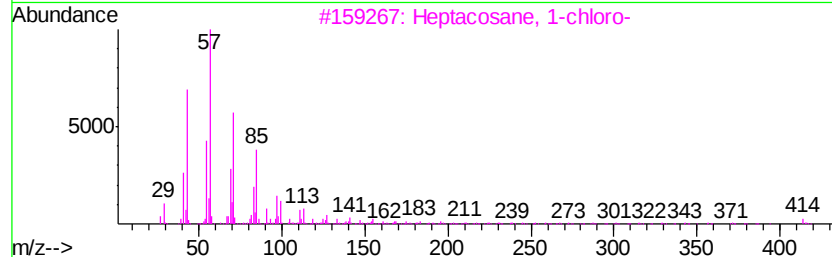
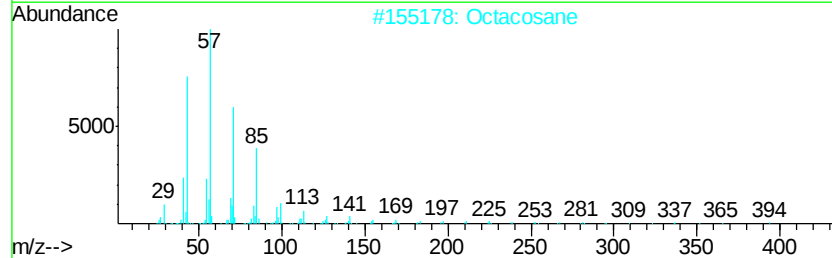
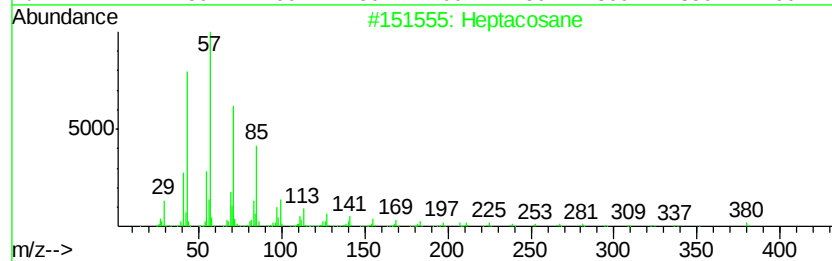
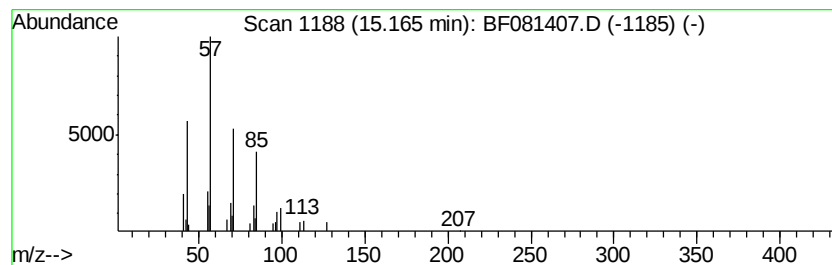
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.18 ng	40691	Perylene-d12	14.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	86
2	Octacosane		394	C28H58	000630-02-4	86
3	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	86
4	Tetratetracontane		619	C44H90	007098-22-8	86
5	10-Methylnonadecane		282	C20H42	056862-62-5	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081407.D
Acq On : 4 Sep 2015 7:22
Operator : UM/IZ
Sample : G3505-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-BF003-01

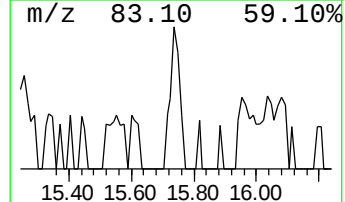
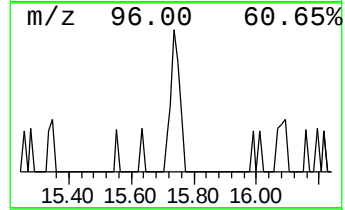
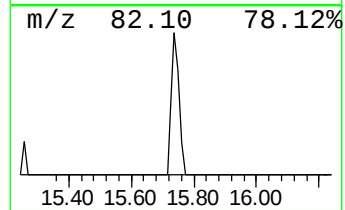
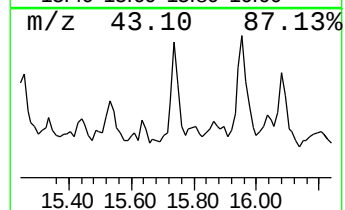
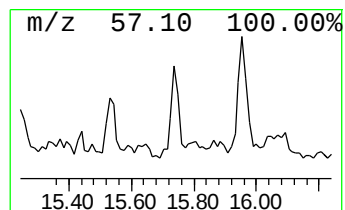
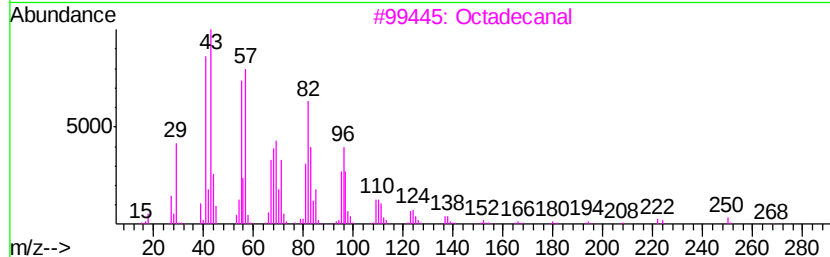
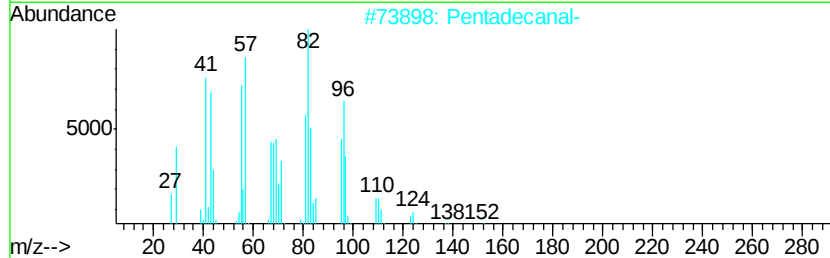
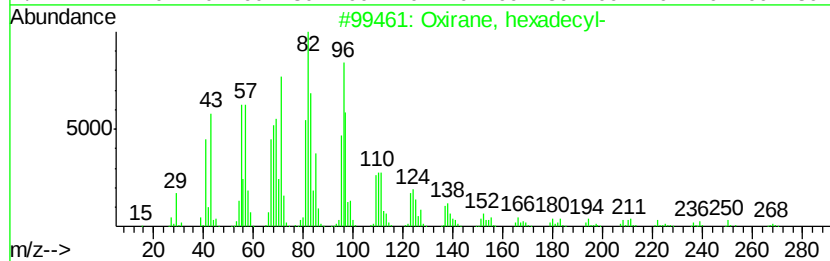
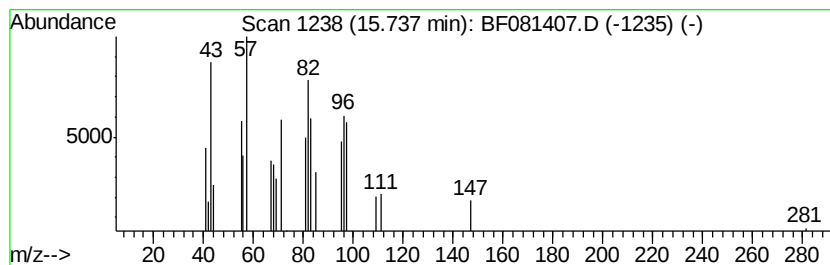
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.18 ng	27894	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Pentadecanal-	226	C15H30O	002765-11-9	64
3		Octadecanal	268	C18H36O	000638-66-4	64
4		E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	59
5		1,19-Eicosadiene	278	C20H38	014811-95-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081407.D
Acq On : 4 Sep 2015 7:22
Operator : UM/IZ
Sample : G3505-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-BF003-01

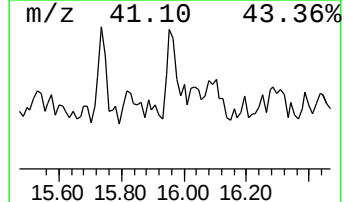
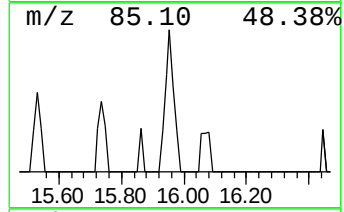
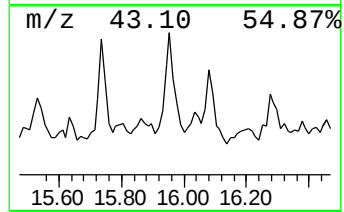
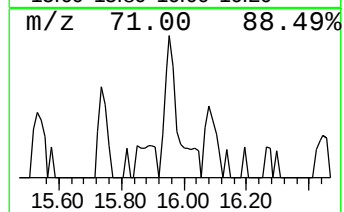
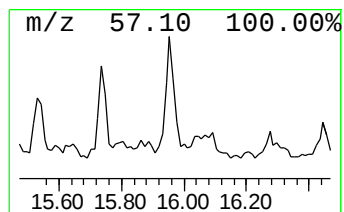
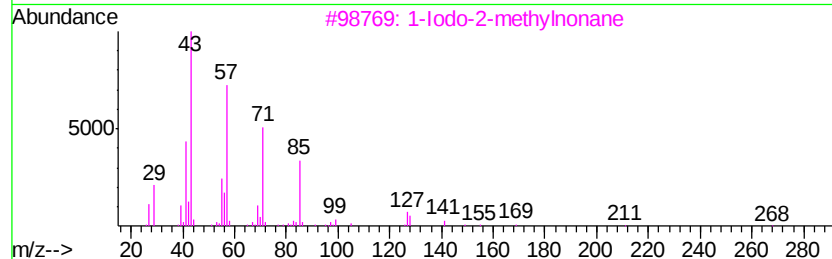
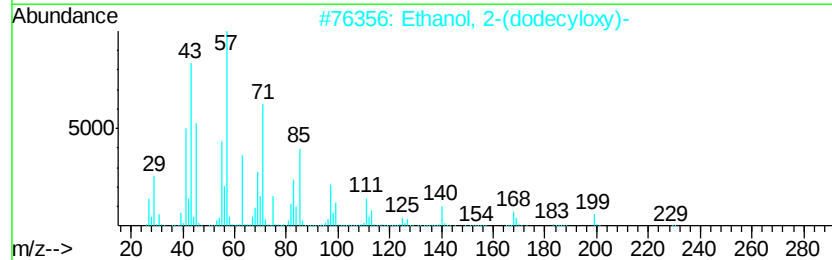
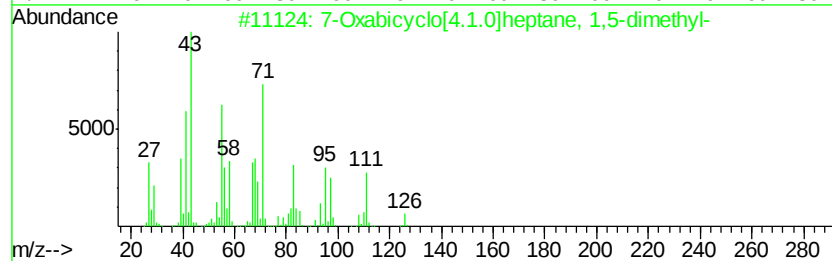
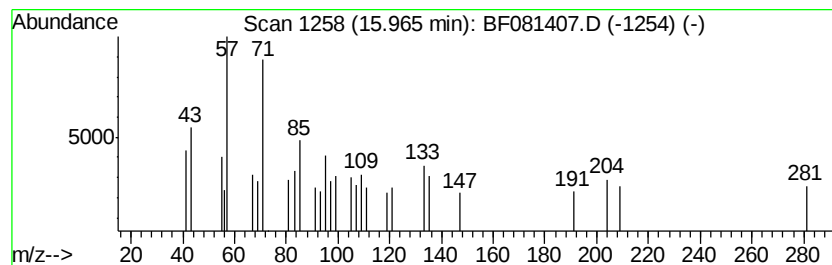
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.76 ng	35306	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	27
2		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	27
3		1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	27
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	27
5		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF090315\
Data File : BF081407.D
Acq On : 4 Sep 2015 7:22
Operator : UM/IZ
Sample : G3505-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-BF003-01

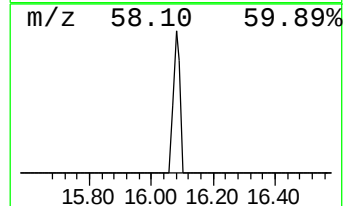
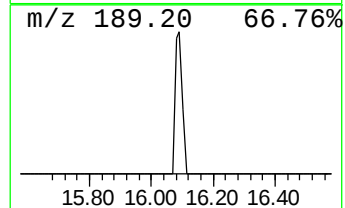
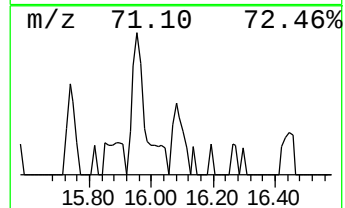
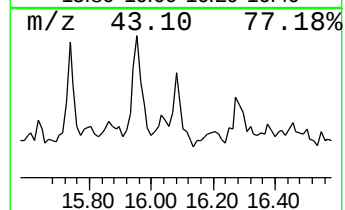
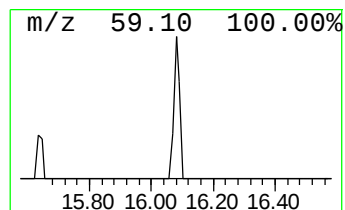
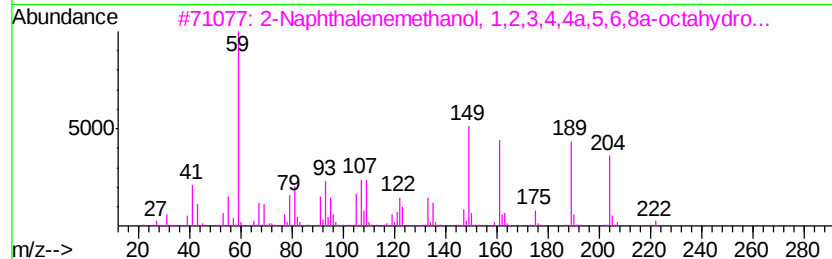
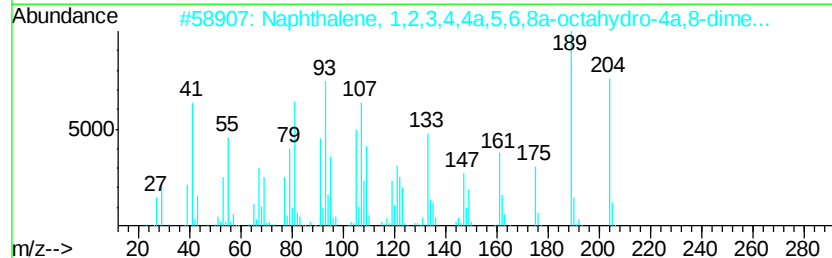
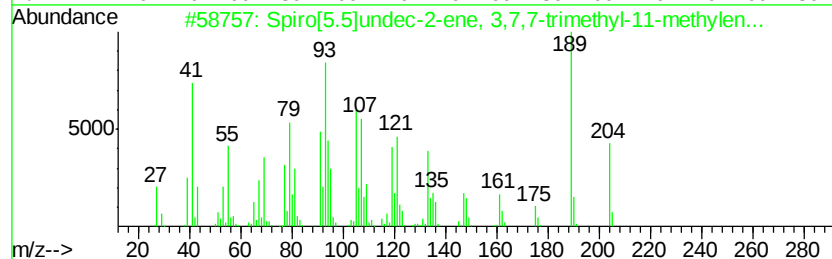
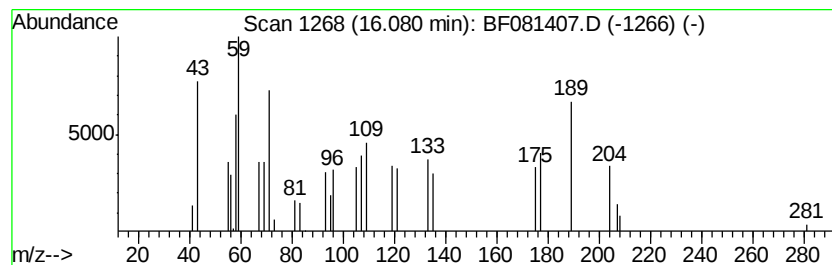
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	2.46 ng	31483	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	35
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	35
3		2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	000473-16-5	28
4		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	27
5		2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	079254-46-9	23



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081407.D
Acq On : 4 Sep 2015 7:22
Operator : UM/IZ
Sample : G3505-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-BF003-01

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...	4.41	51.3	ng	958345	1	6.36	373322	20.0
n-Hexadecanoic acid	11.44	4.8	ng	113398	4	10.86	474056	20.0
17-Pentatriacontene	13.37	6.9	ng	127485	5	13.46	371131	20.0
1,19-Eicosadiene	14.41	2.9	ng	37097	6	14.78	255787	20.0
Hexatriacontane	14.56	5.6	ng	71288	6	14.78	255787	20.0
Heptacosane	15.17	3.2	ng	40691	6	14.78	255787	20.0
Oxirane, hexadecyl-	15.74	2.2	ng	27894	6	14.78	255787	20.0
unknown15.97	15.97	2.8	ng	35306	6	14.78	255787	20.0
unknown16.08	16.08	2.5	ng	31483	6	14.78	255787	20.0