

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
 Data File : BF090864.D
 Acq On : 27 Oct 2016 2:14
 Operator : UM/SJ
 Sample : H5396-08 5X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P5-S1

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-BF102616.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	4.933	246	249	261	rBV	126959	164060	12.33%	1.177%
2	5.367	285	287	299	rBV	602719	730478	54.89%	5.238%
3	6.419	377	379	388	rBV	640644	711919	53.50%	5.105%
4	6.544	388	390	401	rVB	543699	726565	54.60%	5.210%
5	6.784	409	411	417	rBV	902207	872830	65.59%	6.259%
6	6.944	423	425	427	rBV	439417	564476	42.42%	4.048%
7	7.344	458	460	467	rBV	279698	427422	32.12%	3.065%
8	7.447	467	469	476	rVB4	10751	34048	2.56%	0.244%
9	8.076	521	524	526	rBV	1277464	1213735	91.21%	8.704%
10	9.150	616	618	620	rBV	1073304	902497	67.82%	6.472%
11	9.550	650	653	655	rBV	176523	171383	12.88%	1.229%
12	9.825	675	677	680	rBV	1534740	1330754	100.00%	9.543%
13	10.613	743	746	752	rBV	443028	429631	32.28%	3.081%
14	10.739	755	757	761	rVB	29755	34309	2.58%	0.246%
15	11.311	805	807	809	rBV	1231013	1108728	83.32%	7.951%
16	12.522	910	913	915	rBV	54824	62330	4.68%	0.447%
17	12.751	930	933	935	rBV	43626	61809	4.64%	0.443%
18	12.899	943	946	948	rBV	617818	688316	51.72%	4.936%
19	13.139	963	967	969	rBV3	10531	16308	1.23%	0.117%
20	13.596	1005	1007	1010	rBV3	23274	31786	2.39%	0.228%
21	13.825	1022	1027	1030	rBV3	64476	145849	10.96%	1.046%
22	13.951	1035	1038	1040	rBV	778395	1011589	76.02%	7.254%
23	14.122	1052	1053	1055	rBV	18223	18300	1.38%	0.131%
24	14.431	1078	1080	1083	rBV2	59537	113457	8.53%	0.814%
25	14.728	1104	1106	1109	rBV	26167	38085	2.86%	0.273%
26	14.831	1110	1115	1116	rBV2	48515	137030	10.30%	0.983%
27	14.865	1116	1118	1122	rVB2	63027	101781	7.65%	0.730%
28	14.957	1124	1126	1130	rVB	42517	83224	6.25%	0.597%
29	15.048	1131	1134	1136	rBV	115261	141295	10.62%	1.013%
30	15.242	1149	1151	1154	rVB	32021	48333	3.63%	0.347%
31	15.299	1154	1156	1159	rBV	24720	49257	3.70%	0.353%
32	15.357	1159	1161	1164	rVV	624661	918395	69.01%	6.586%
33	15.402	1164	1165	1170	rVB	51389	68826	5.17%	0.494%
34	15.585	1179	1181	1185	rVB3	40476	57241	4.30%	0.410%

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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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.814	1198	1201	1203	rBV	90070	160192	12.04%	1.149%
36	15.951	1211	1213	1217	rVB3	27166	39056	2.93%	0.280%
37	16.271	1239	1241	1244	rBV	20084	37604	2.83%	0.270%
38	16.545	1262	1265	1271	rVB4	34314	77526	5.83%	0.556%
39	16.820	1287	1289	1292	rBV	22159	46897	3.52%	0.336%
40	16.877	1292	1294	1299	rVB5	25476	57803	4.34%	0.415%
41	17.277	1326	1329	1332	rBV4	24040	75962	5.71%	0.545%
42	18.214	1408	1411	1417	rVB4	25431	77035	5.79%	0.552%
43	19.174	1490	1495	1502	rVB6	45829	156372	11.75%	1.121%

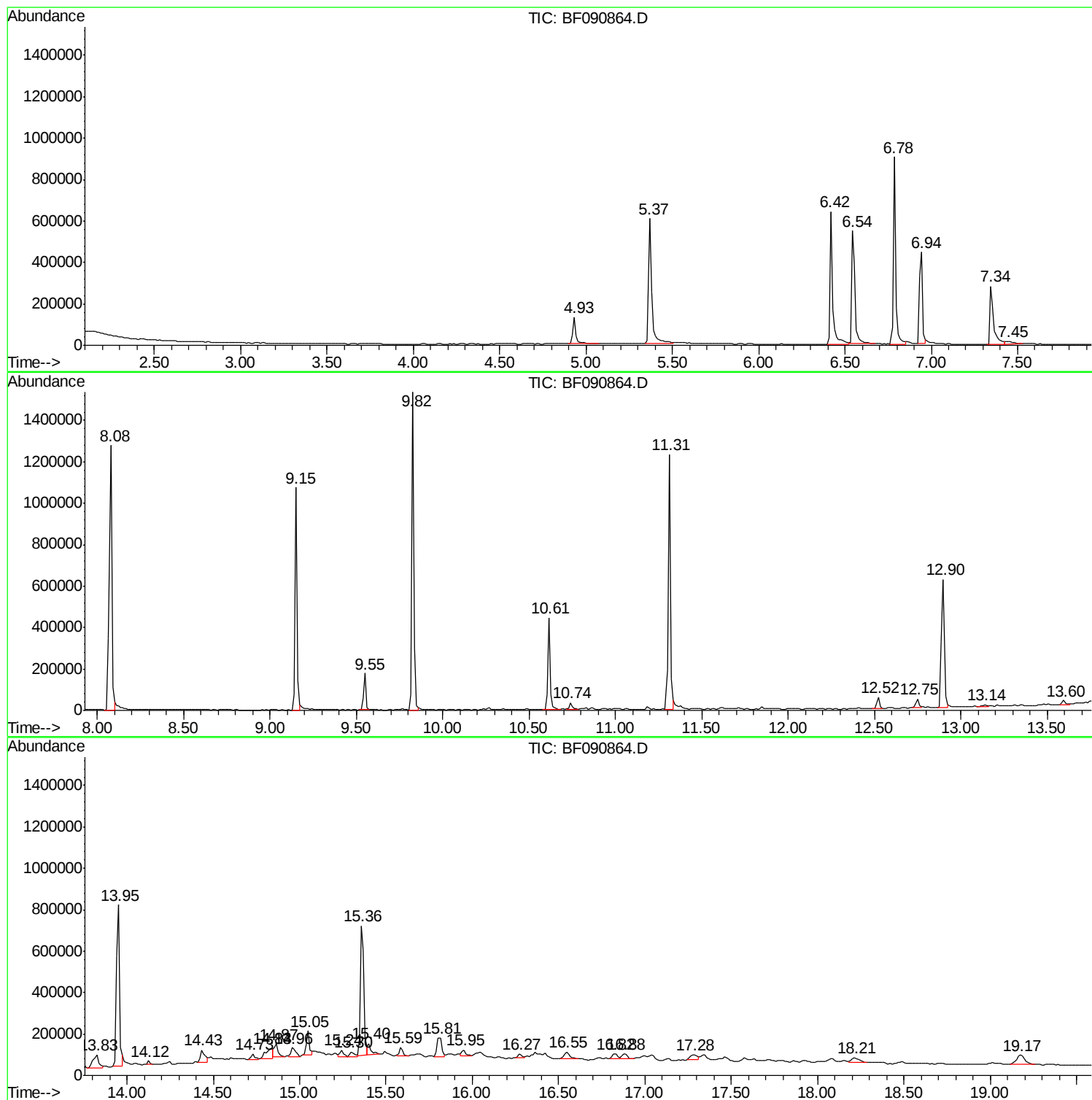
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Instrument :
BNA_F
ClientSampled :
P5-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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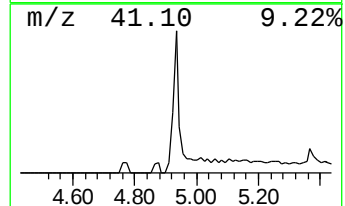
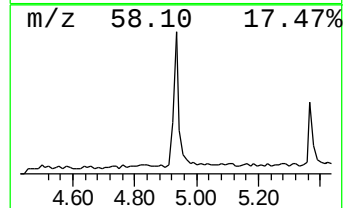
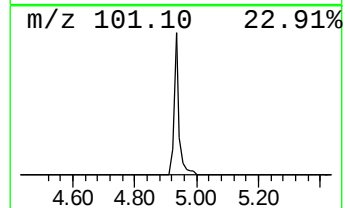
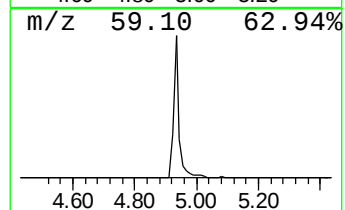
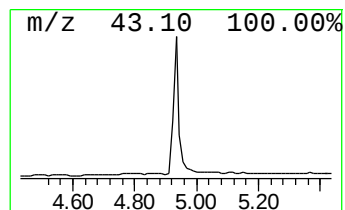
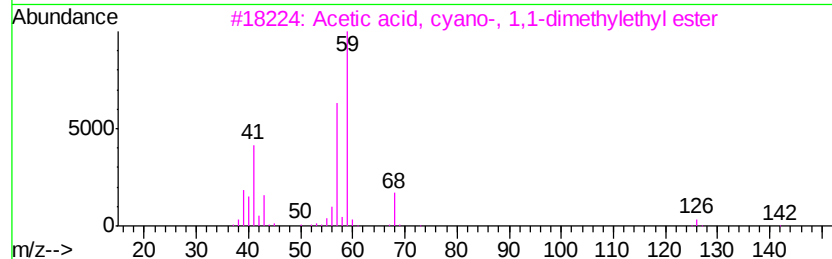
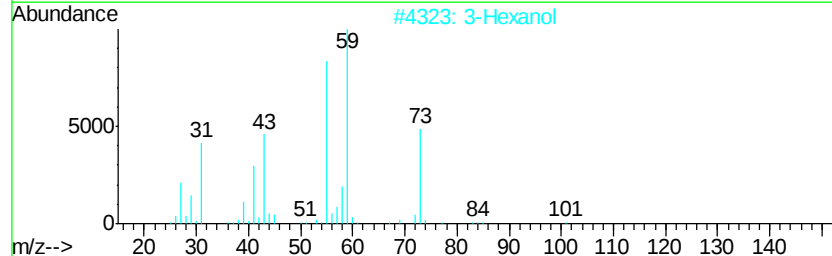
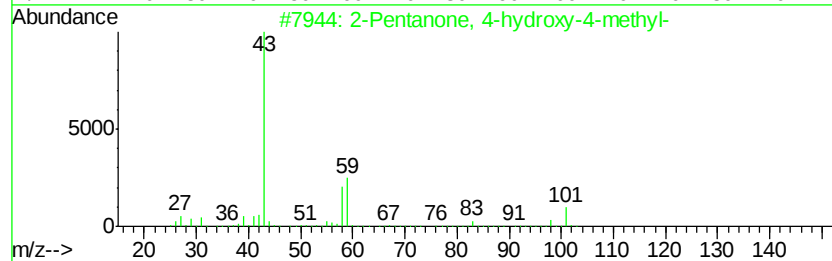
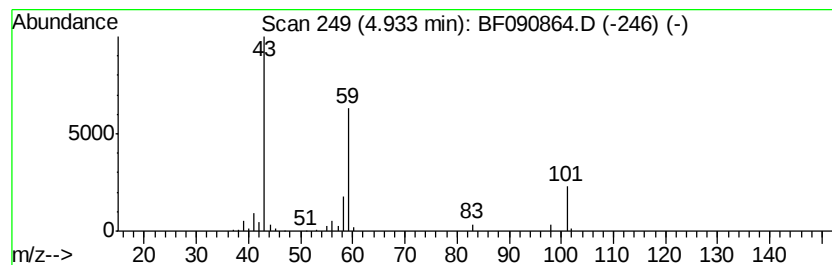
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.93	3.76 ng	164060	1,4-Dichlorobenzene-d4	6.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	3-Hexanol	102	C6H14O	000623-37-0	28	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
4	Acetone	58	C3H6O	000067-64-1	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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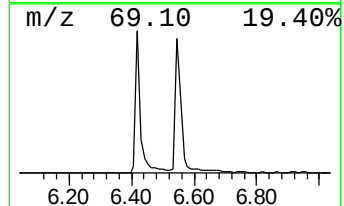
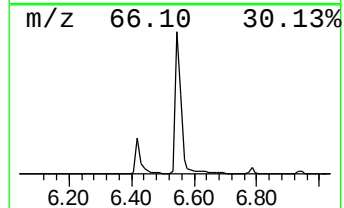
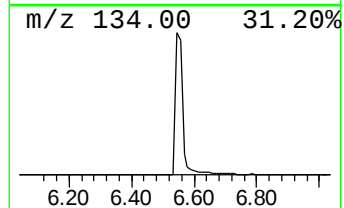
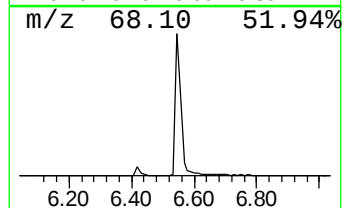
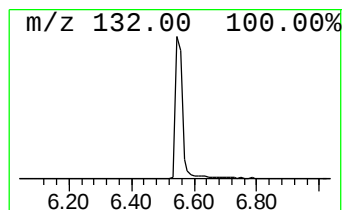
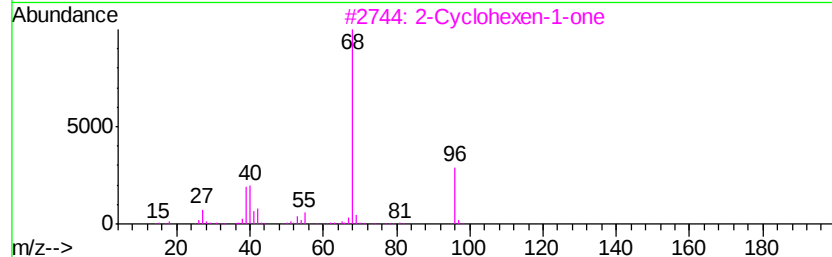
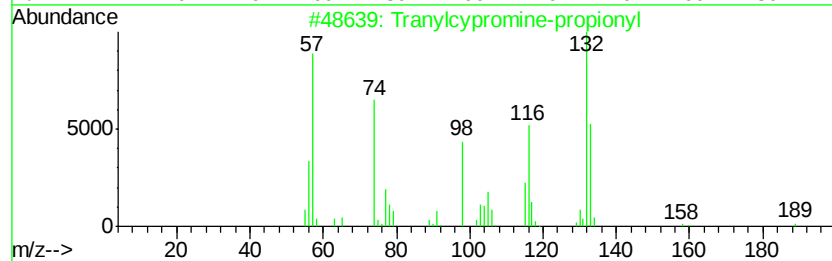
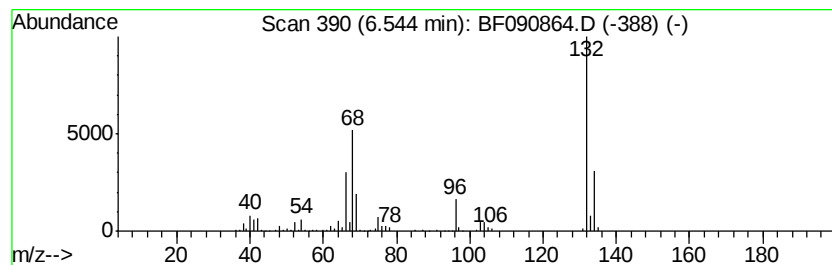
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	16.65 ng	726565	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		5-Aminoindole	132	C8H8N2	005192-03-0	10
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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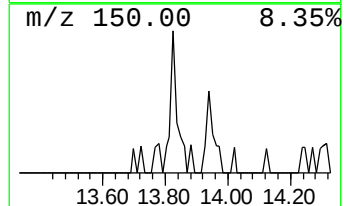
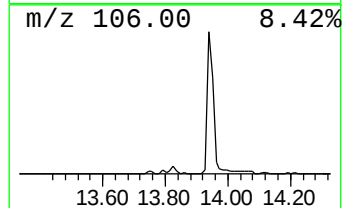
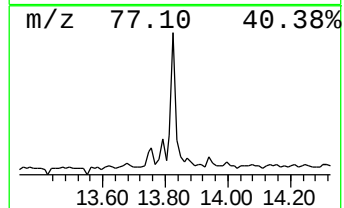
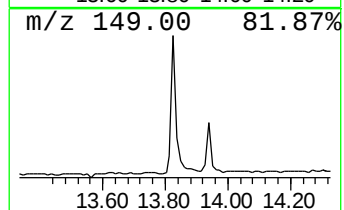
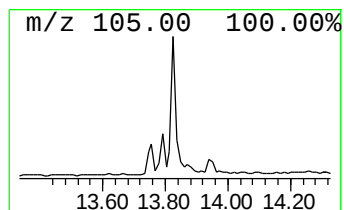
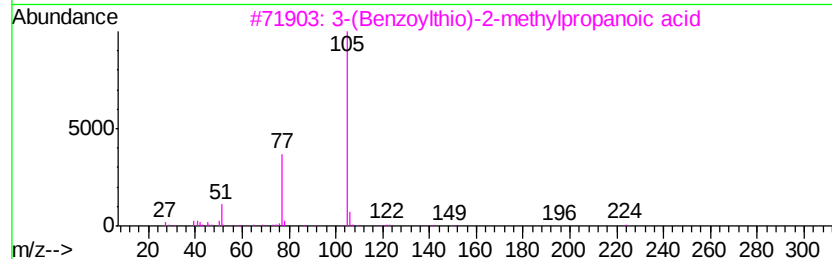
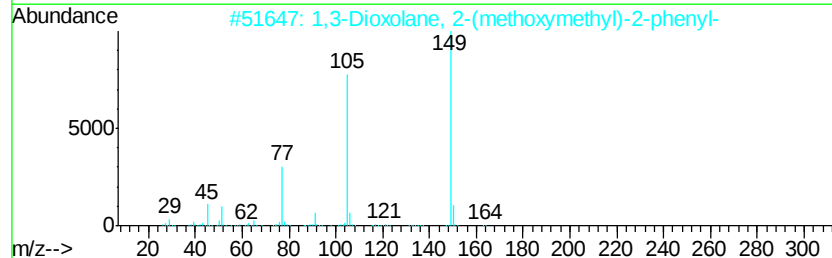
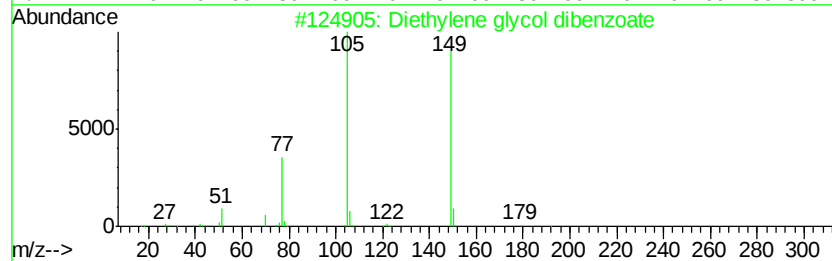
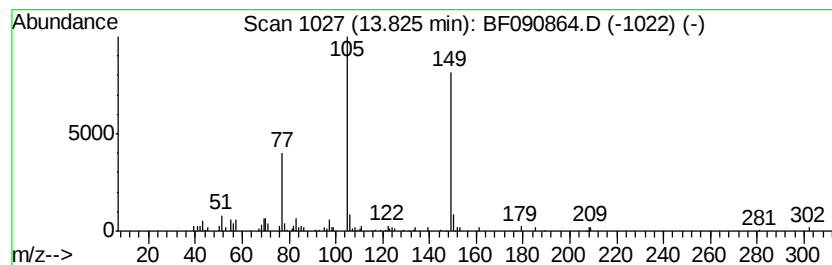
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.88 ng	145849	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2		1,3-Dioxolane, 2-(methoxymethyl)-2-phenyl-	194	C11H14O3	1000156-71-2	78
3		3-(Benzoylthio)-2-methylpropanoic acid	224	C11H12O3S	067714-34-5	27
4		Benzo[b]thiophene-3-carboxylic acid	343	C18H17NO4S	096334-43-9	27
5		Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	27



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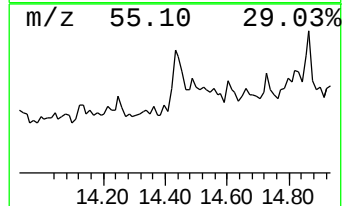
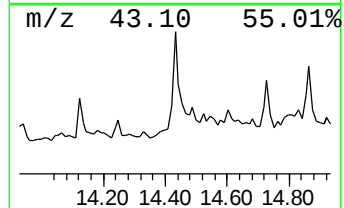
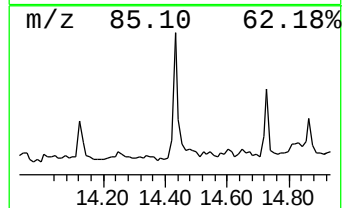
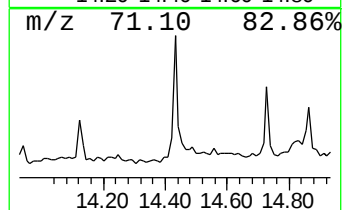
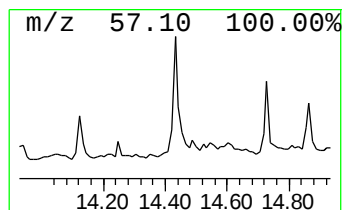
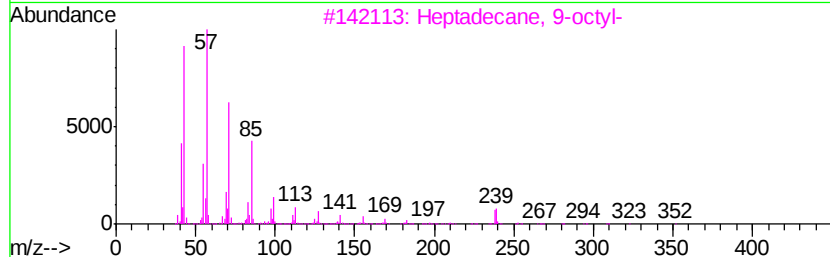
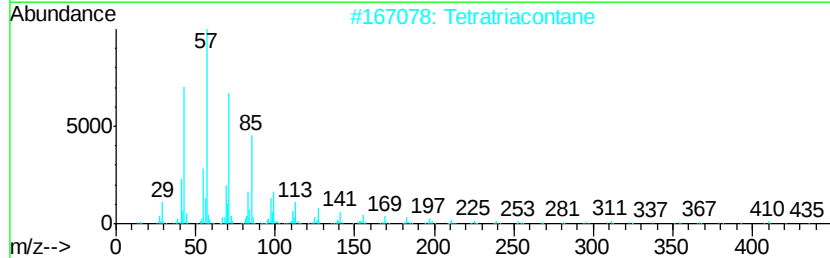
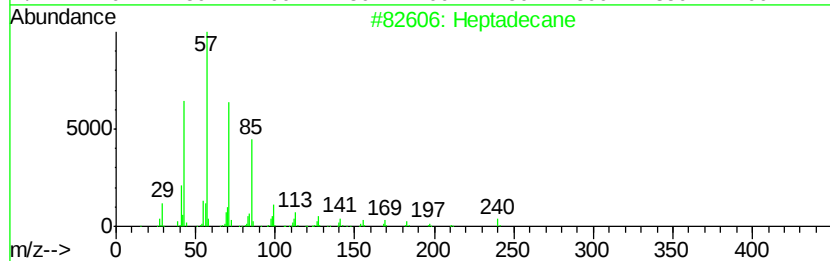
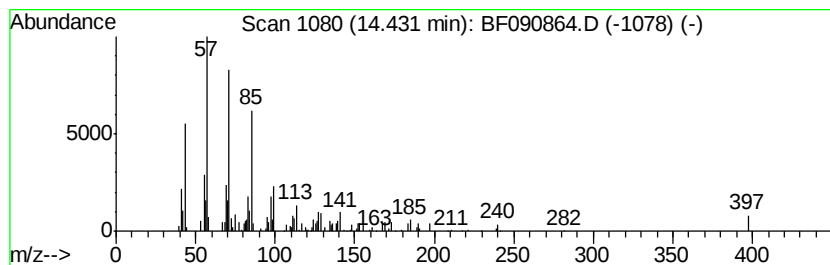
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.24 ng	113457	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	93
2	Tetratriacontane		479	C34H70	014167-59-0	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Eicosane		282	C20H42	000112-95-8	91
5	Hentriacontane		437	C31H64	000630-04-6	91



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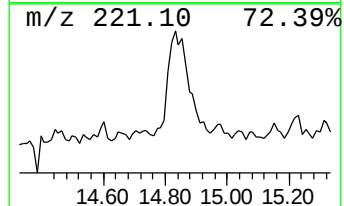
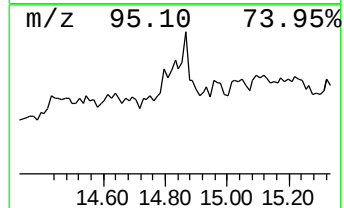
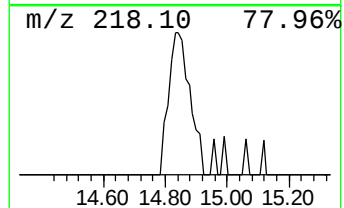
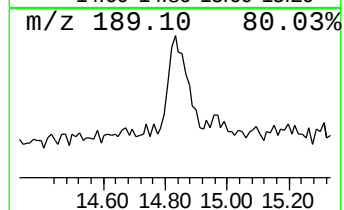
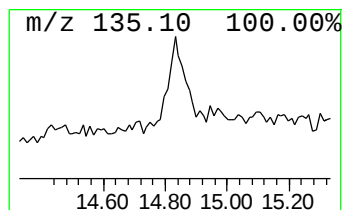
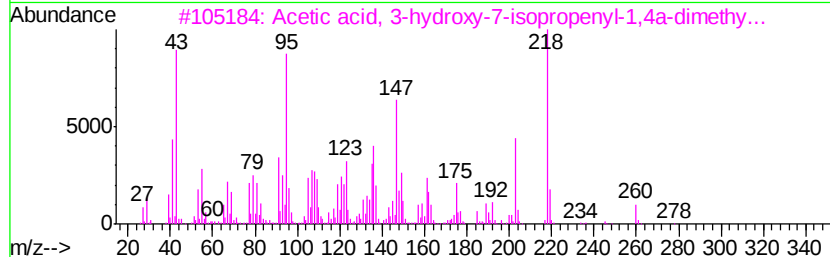
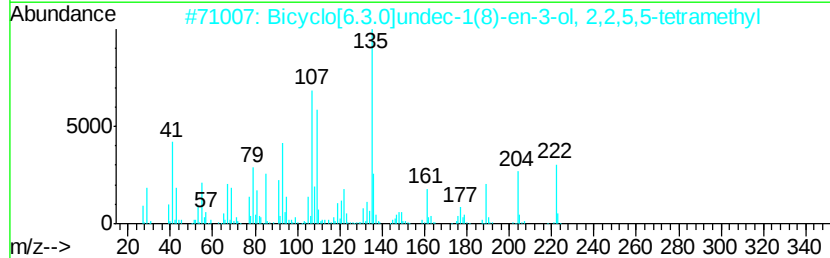
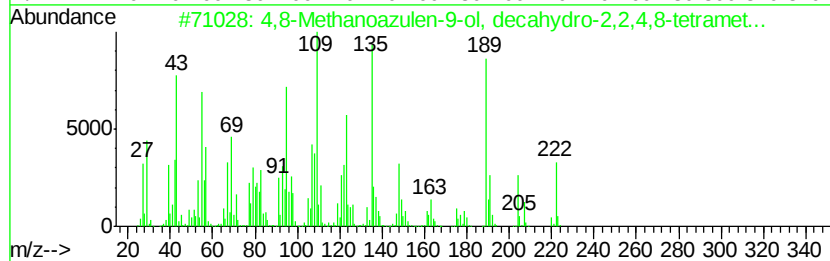
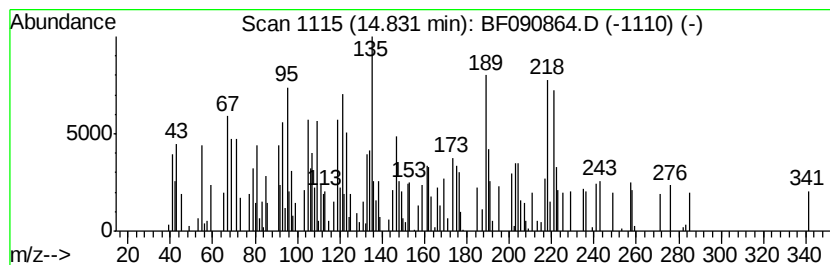
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Peak Number 6 4,8-Methanoazulen-9-ol, dec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.98 ng	137030	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,8-Methanoazulen-9-ol, decahydr...	222	C15H26O	004586-22-5	70
2		Bicyclo[6.3.0]undec-1(8)-en-3-ol...	222	C15H26O	1000164-02-6	46
3		Acetic acid, 3-hydroxy-7-isoprop...	278	C17H26O3	1000187-37-6	27
4		2-Amino-4-cyanomethyl-6-piperidi...	218	C10H14N6	1000241-05-9	18
5		1-Hydroxypyrene	218	C16H10O	005315-79-7	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
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Operator : UM/SJ
Sample : H5396-08 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

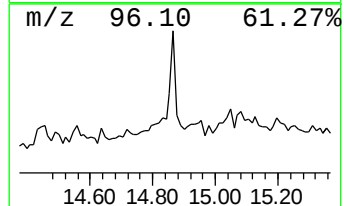
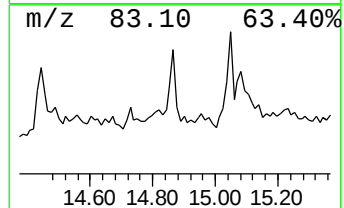
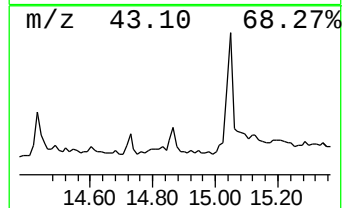
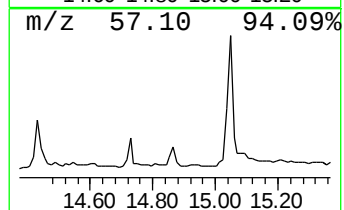
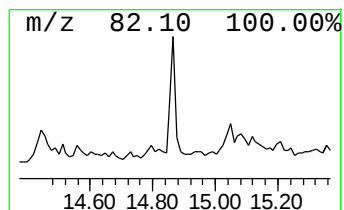
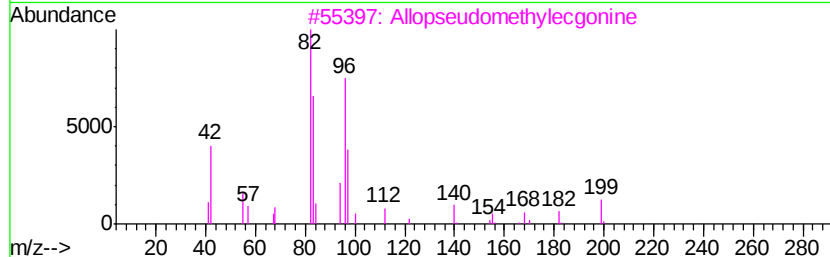
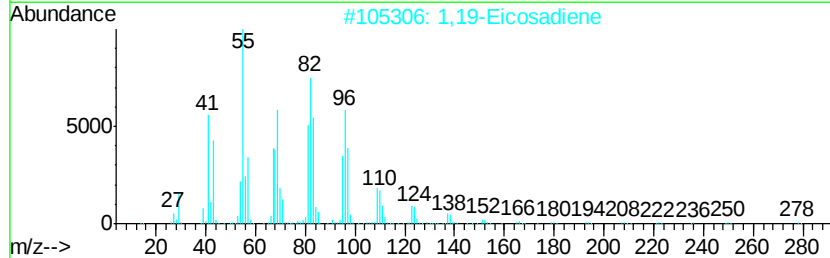
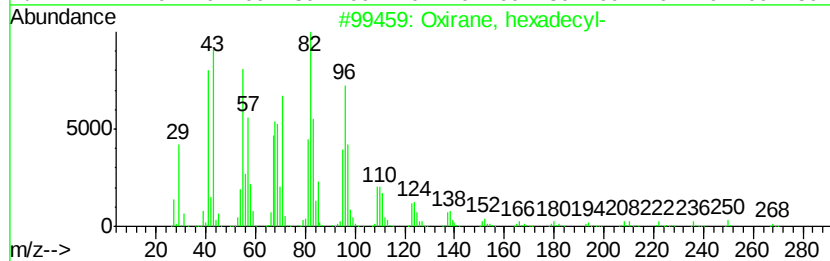
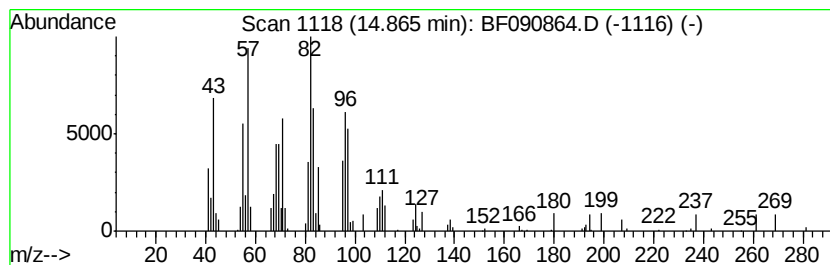
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.22 ng	101781	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 78
2		1,19-Eicosadiene	278 C20H38	014811-95-1 72
3		Allopseudomethylecgonine	199 C10H17NO3	1000120-22-1 43
4		Cyclopentane, (4-octyldodecyl)-	350 C25H50	005638-09-5 43
5		2,6,10-Trimethylundeca-1,3-diene	194 C14H26	1000222-09-1 38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
Data File : BF090864.D
Acq On : 27 Oct 2016 2:14
Operator : UM/SJ
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Misc :
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Instrument :
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ClientSampleId :
P5-S1

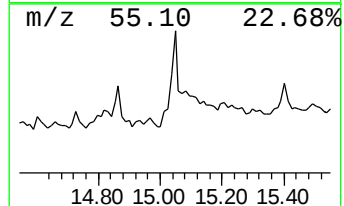
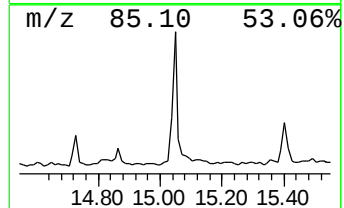
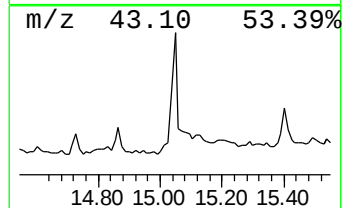
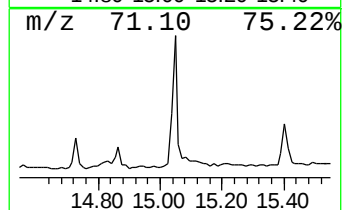
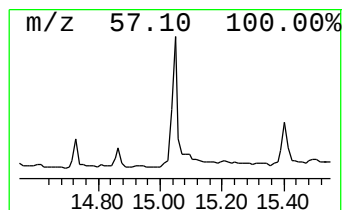
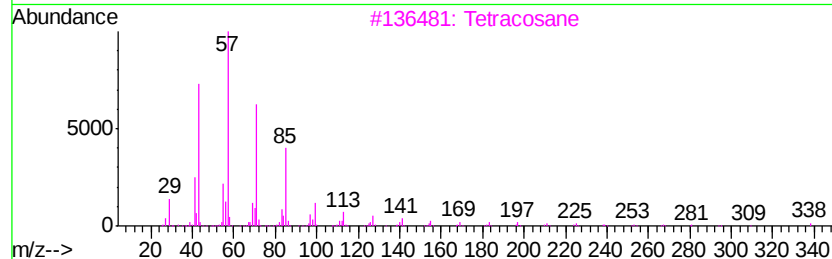
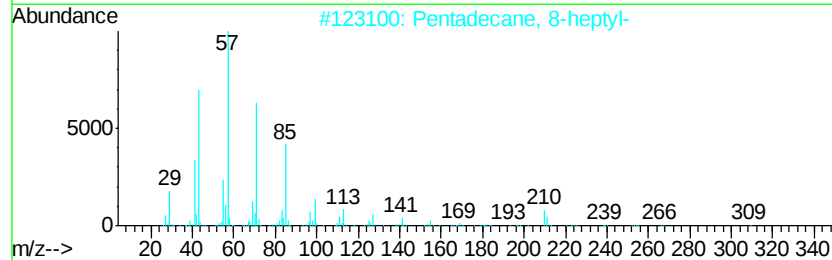
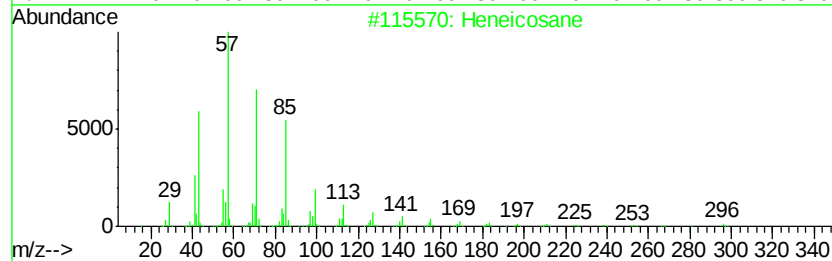
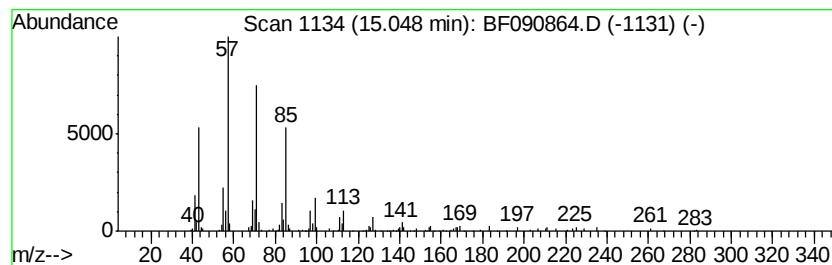
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	3.08 ng	141295	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Nonacosane		408	C29H60	000630-03-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
Data File : BF090864.D
Acq On : 27 Oct 2016 2:14
Operator : UM/SJ
Sample : H5396-08 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P5-S1

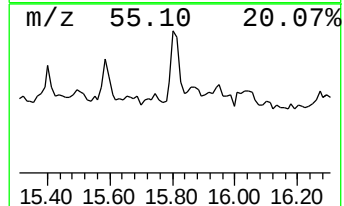
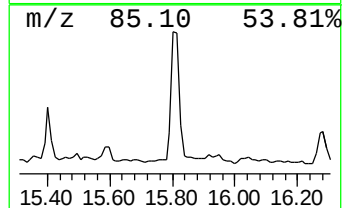
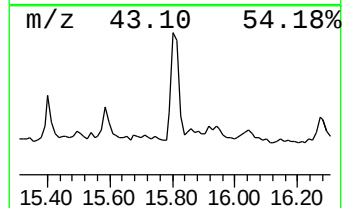
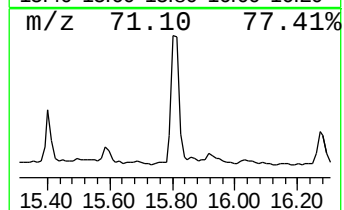
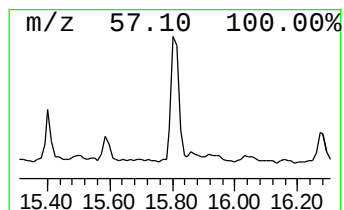
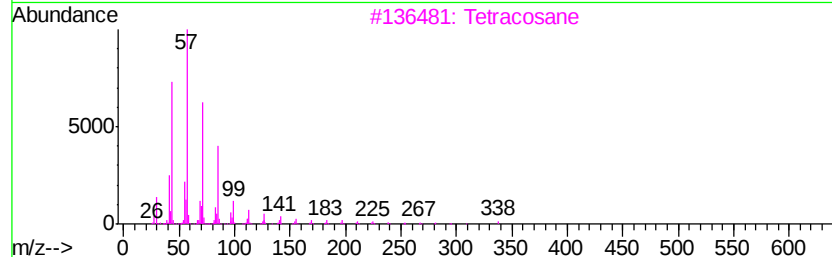
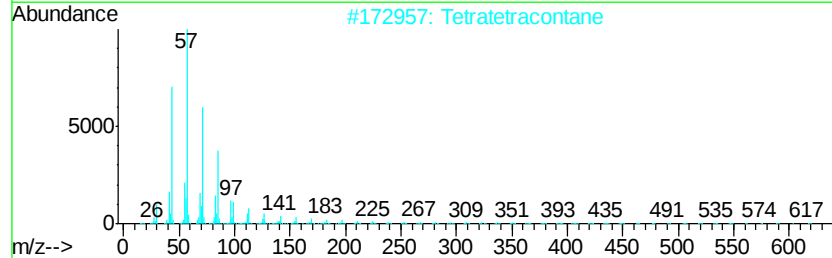
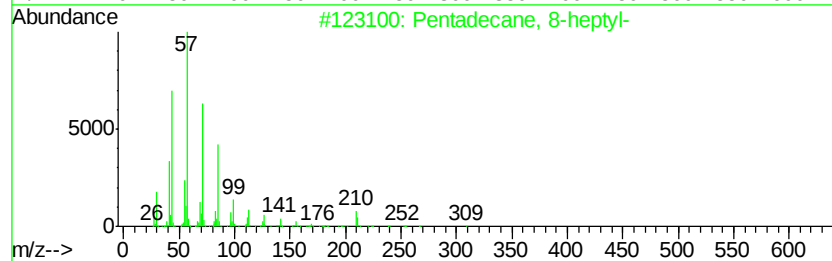
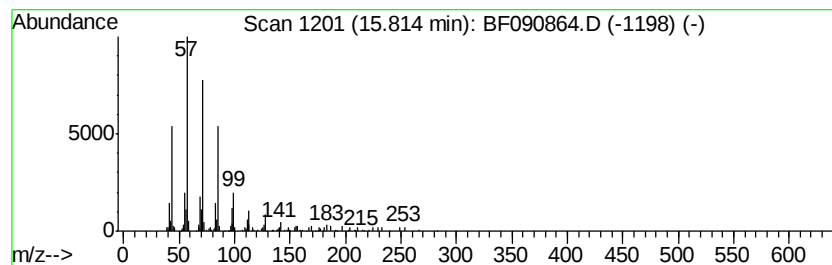
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	3.49 ng	160192	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Docosane	310	C22H46	000629-97-0	86
5		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
Data File : BF090864.D
Acq On : 27 Oct 2016 2:14
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Misc :
ALS Vial : 23 Sample Multiplier: 1

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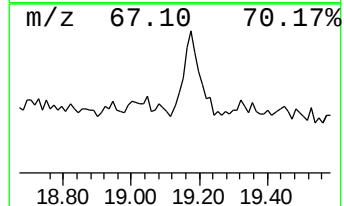
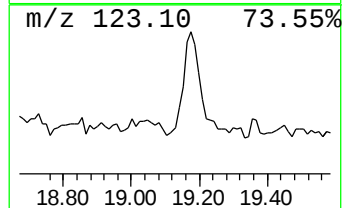
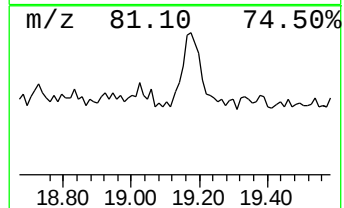
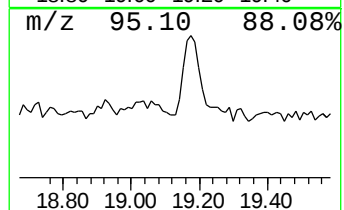
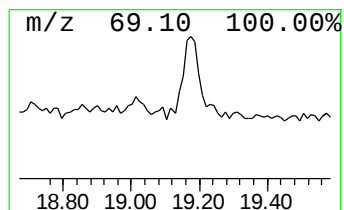
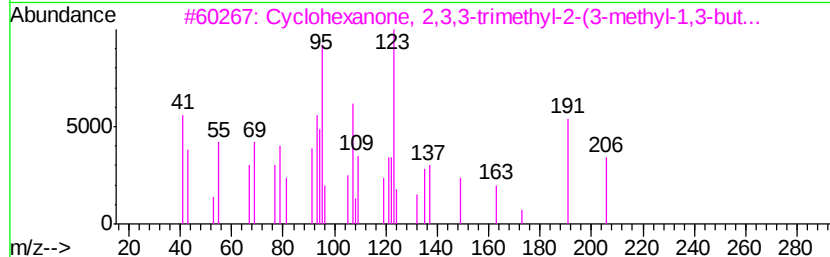
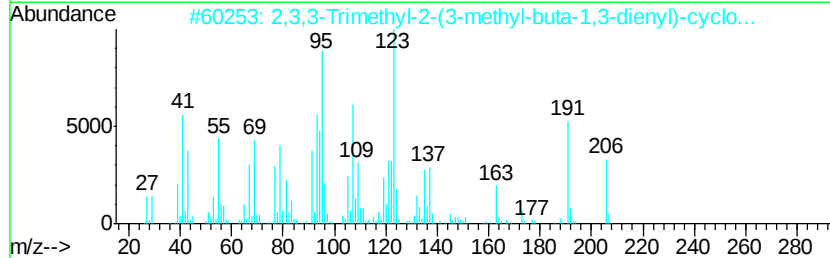
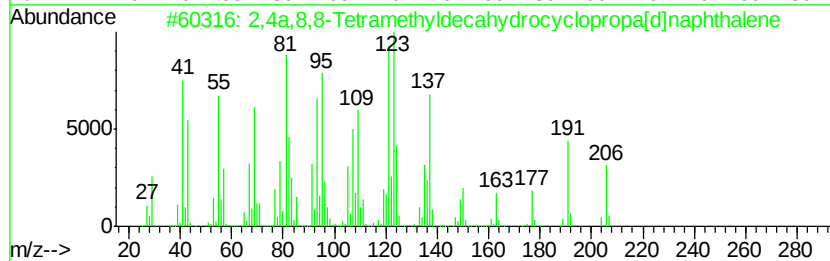
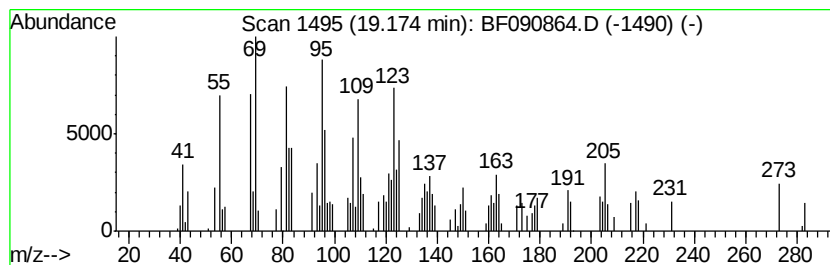
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown19.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	3.41 ng	156372	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	49
2		2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	38
3		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	38
4		Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	30
5		Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
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Acq On : 27 Oct 2016 2:14
Operator : UM/SJ
Sample : H5396-08 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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
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unknown6.54	6.54	16.6	ng	726565	1	6.78	872830	20.0
Diethylene glycol...	13.83	2.9	ng	145849	5	13.95	1011590	20.0
Heptadecane	14.43	2.2	ng	113457	5	13.95	1011590	20.0
4,8-Methanoazulen...	14.83	3.0	ng	137030	6	15.36	918395	20.0
Oxirane, hexadecyl-	14.87	2.2	ng	101781	6	15.36	918395	20.0
Heneicosane	15.05	3.1	ng	141295	6	15.36	918395	20.0
Pentadecane, 8-he...	15.81	3.5	ng	160192	6	15.36	918395	20.0
unknown19.17	19.17	3.4	ng	156372	6	15.36	918395	20.0