

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
 Data File : BF089525.D
 Acq On : 1 Aug 2016 22:26
 Operator : UM/SJ
 Sample : H4269-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-DUP-02-072716

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-BF072716.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.655	4	6	46	rVB	518888	1238138	100.00%	12.620%
2	4.558	257	260	269	rBV	203814	328787	26.55%	3.351%
3	5.038	301	302	322	rBV	489938	862512	69.66%	8.792%
4	5.461	337	339	347	rVB	14213	15684	1.27%	0.160%
5	6.136	396	398	406	rBV	600019	855088	69.06%	8.716%
6	6.239	406	407	410	rBV	580047	870116	70.28%	8.869%
7	6.479	426	428	439	rVB	216649	238646	19.27%	2.433%
8	6.627	439	441	444	rBV	554154	628370	50.75%	6.405%
9	7.050	476	478	496	rBV	472137	573890	46.35%	5.850%
10	7.770	539	541	547	rBV	194015	307915	24.87%	3.139%
11	8.845	633	635	637	rBV	1080101	976072	78.83%	9.949%
12	9.245	668	670	675	rBV	160559	140008	11.31%	1.427%
13	9.462	687	689	691	rBV	11714	13703	1.11%	0.140%
14	9.507	691	693	695	rBV	336394	324070	26.17%	3.303%
15	9.965	726	733	734	rBV	26518	29140	2.35%	0.297%
16	10.182	748	752	753	rBV	13597	17174	1.39%	0.175%
17	10.285	760	761	764	rBV2	331926	431835	34.88%	4.402%
18	10.433	772	774	778	rBV	31323	44479	3.59%	0.453%
19	10.879	811	813	814	rBV	16085	17455	1.41%	0.178%
20	10.982	819	822	827	rBV	164837	245642	19.84%	2.504%
21	11.531	869	870	874	rBV	11910	18628	1.50%	0.190%
22	12.079	916	918	923	rBV2	11518	23000	1.86%	0.234%
23	12.559	958	960	962	rBV	670526	639284	51.63%	6.516%
24	13.474	1037	1040	1043	rBV	44890	66744	5.39%	0.680%
25	13.599	1048	1051	1059	rVV	172056	260847	21.07%	2.659%
26	13.794	1066	1068	1073	rVB4	8773	16453	1.33%	0.168%
27	13.896	1073	1077	1079	rBV5	6873	19156	1.55%	0.195%
28	14.102	1092	1095	1099	rBV3	12204	25832	2.09%	0.263%
29	14.697	1143	1147	1151	rBV3	15903	44503	3.59%	0.454%
30	14.868	1160	1162	1165	rBV3	12052	21107	1.70%	0.215%
31	14.925	1165	1167	1170	rBV	231299	263043	21.25%	2.681%
32	15.314	1199	1201	1204	rBV2	14941	31674	2.56%	0.323%
33	15.702	1233	1235	1237	rBV	17507	23069	1.86%	0.235%
34	15.794	1241	1243	1249	rVB3	24194	48782	3.94%	0.497%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.160	1272	1275	1276	rBV	16470	30711	2.48%	0.313%
36	16.240	1280	1282	1285	rVV3	18833	38268	3.09%	0.390%
37	16.297	1285	1287	1293	rVB4	18814	40351	3.26%	0.411%
38	17.314	1373	1376	1380	rVB4	16753	40418	3.26%	0.412%

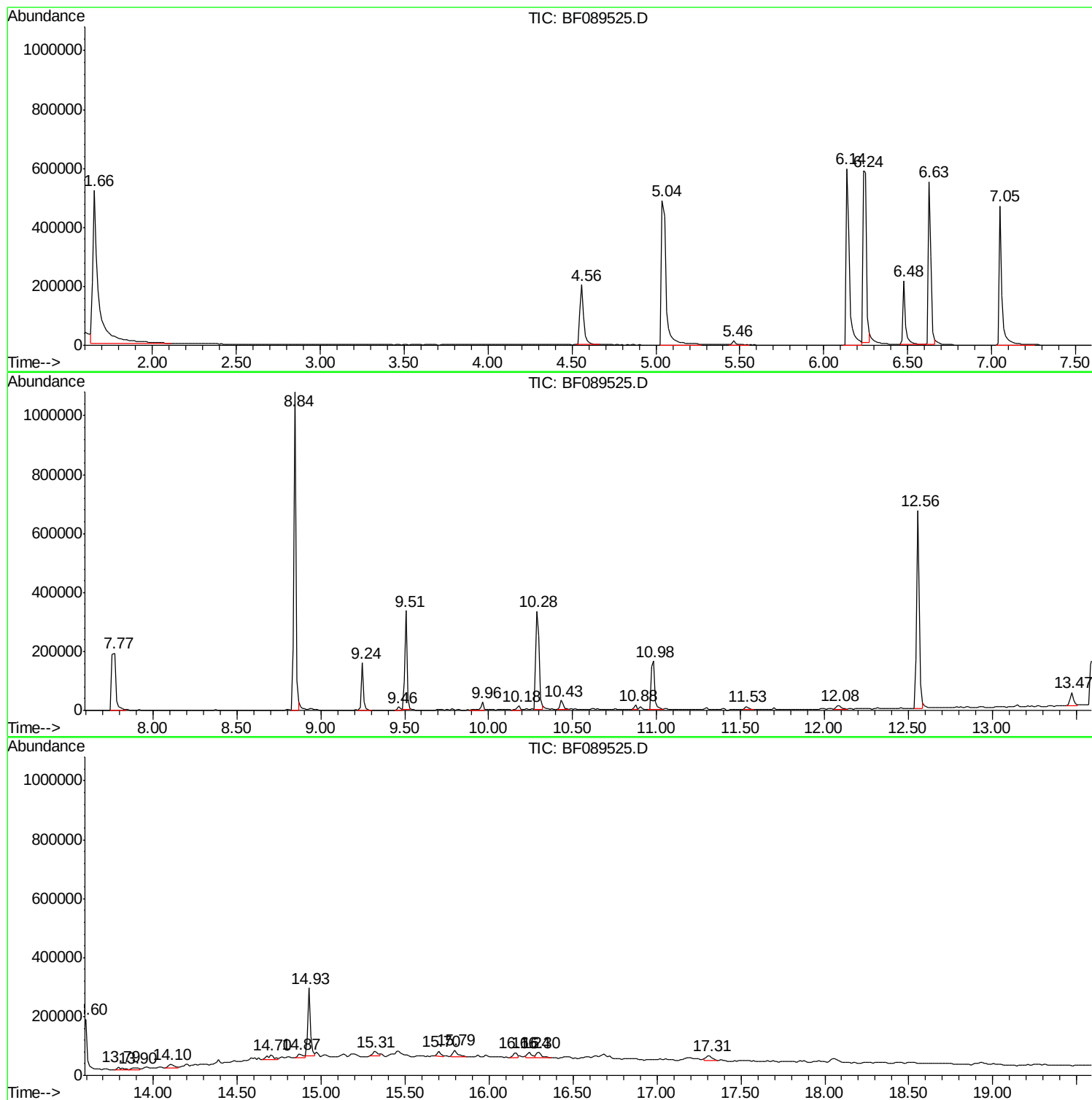
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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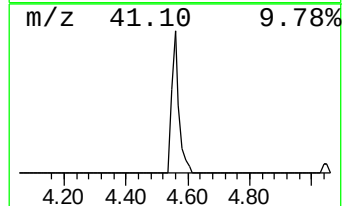
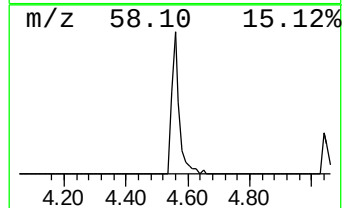
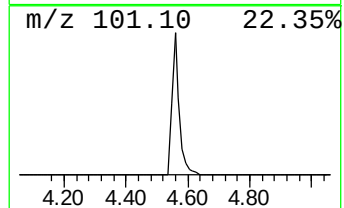
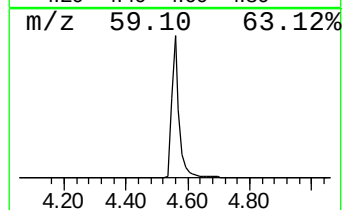
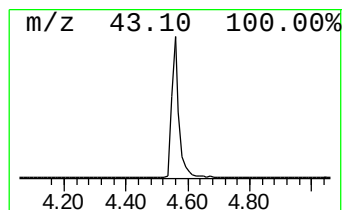
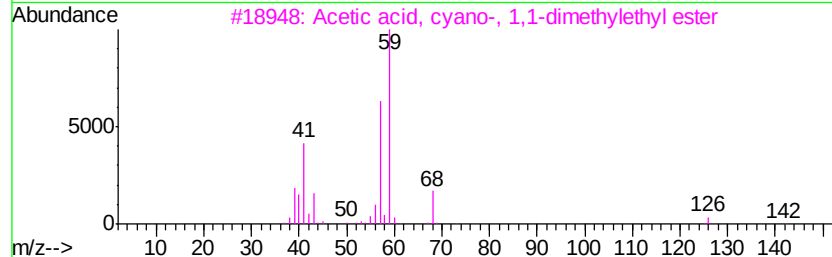
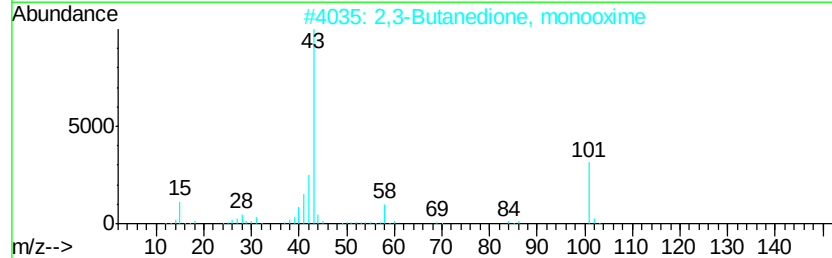
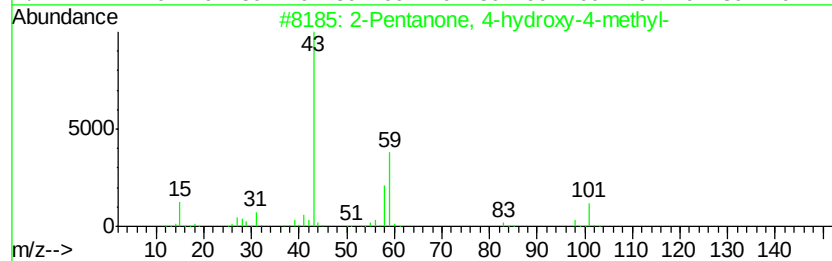
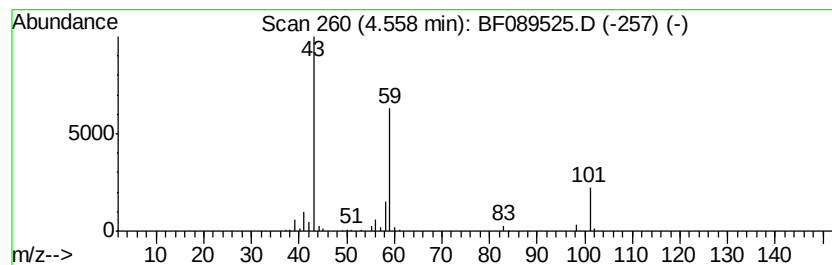
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	27.55 ng	328787	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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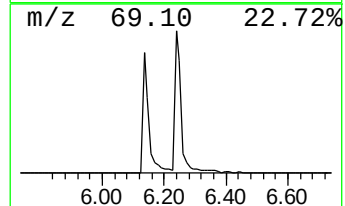
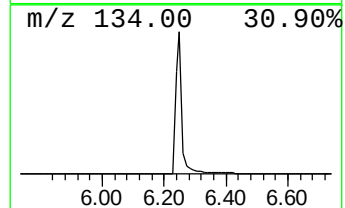
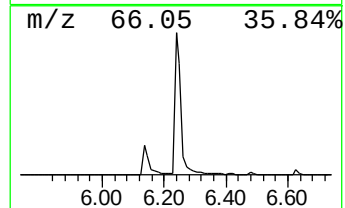
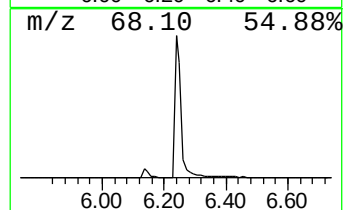
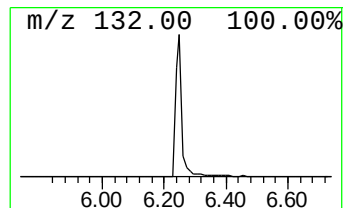
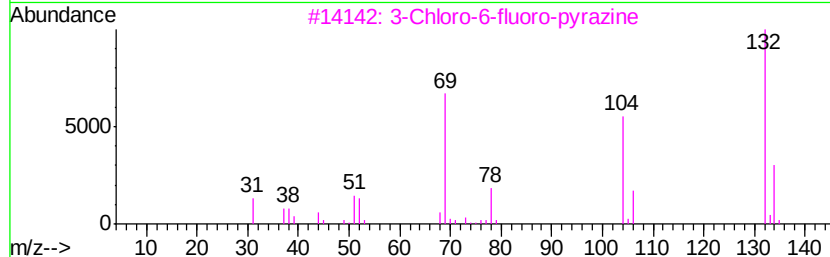
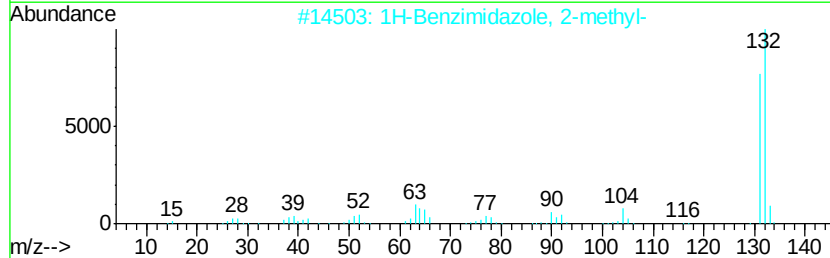
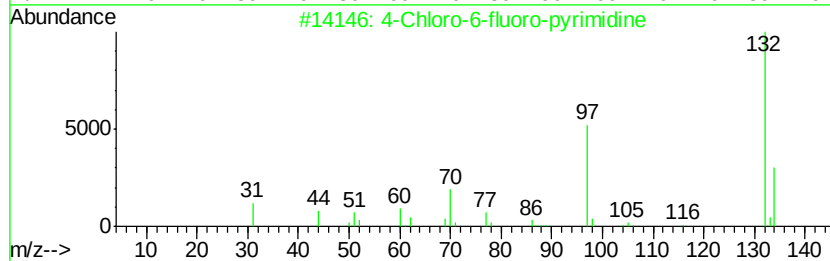
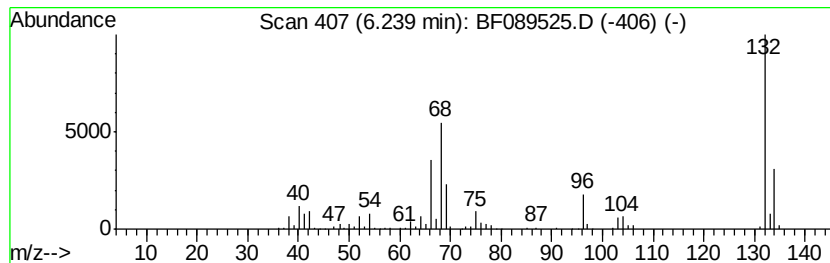
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	72.92 ng	870116	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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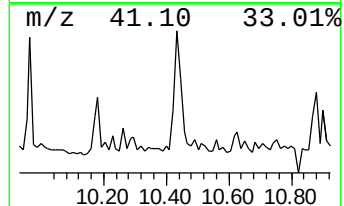
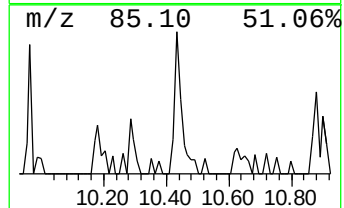
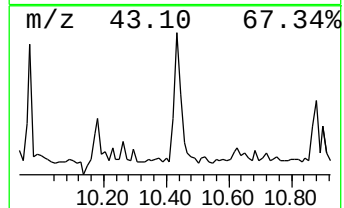
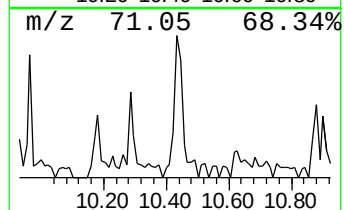
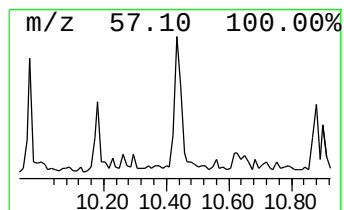
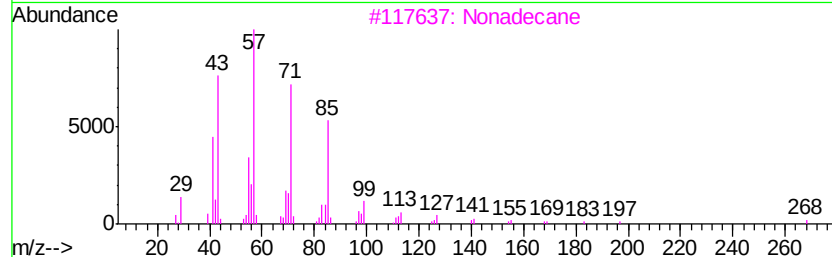
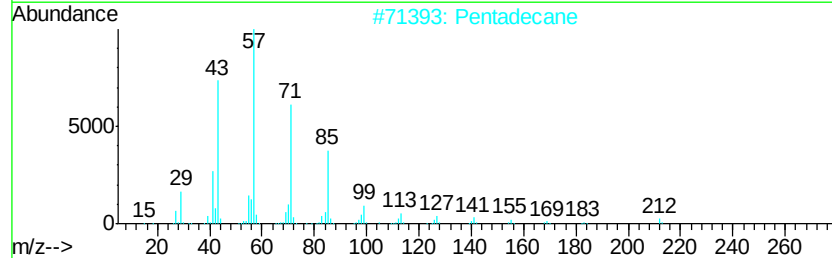
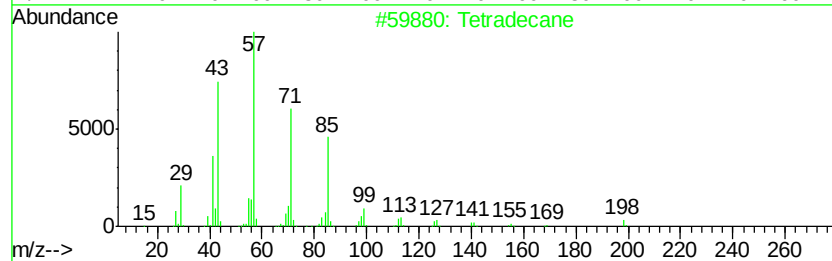
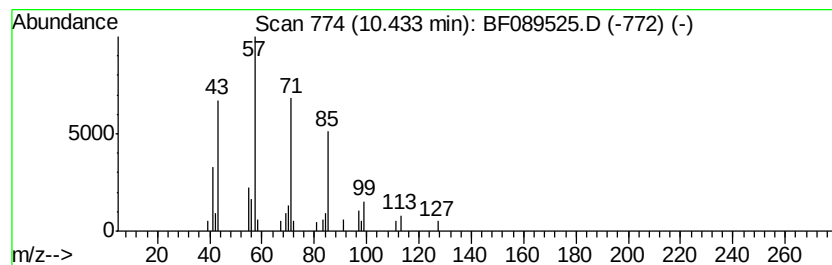
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	3.62 ng	44479	Phenanthrene-d10		10.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Pentadecane	212	C15H32	000629-62-9	86
3	Nonadecane	268	C19H40	000629-92-5	83
4	Heptadecane	240	C17H36	000629-78-7	78
5	Tridecane	184	C13H28	000629-50-5	78



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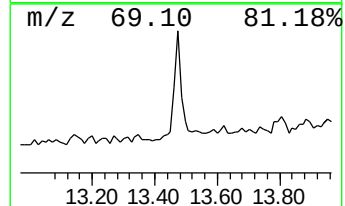
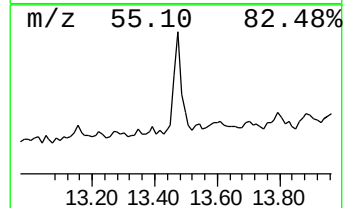
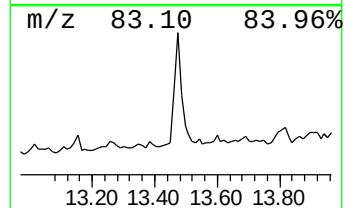
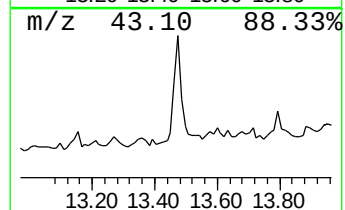
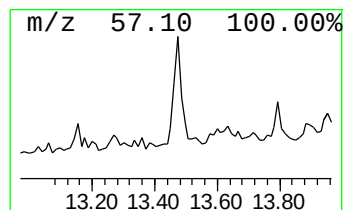
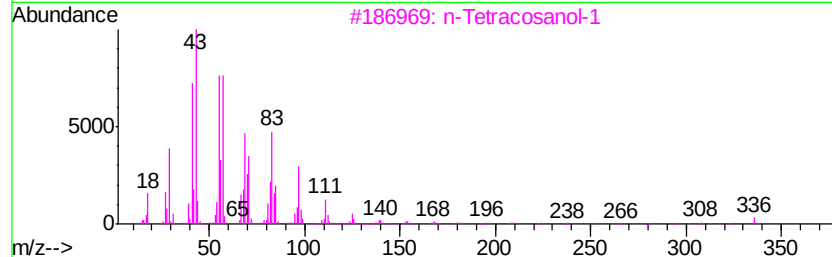
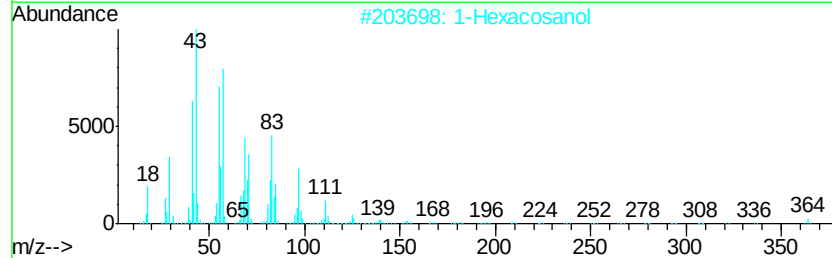
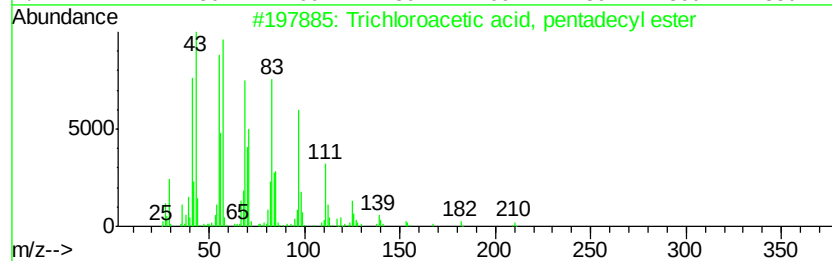
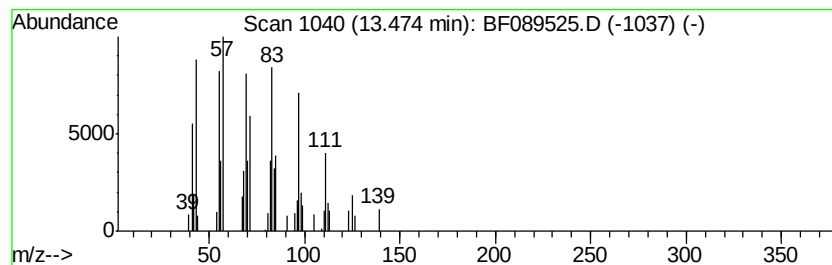
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.12 ng	66744	Chrysene-d12	13.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		1-Hexacosanol	382	C26H54O	000506-52-5	90
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4		11-Tricosene	322	C23H46	052078-56-5	83
5		1-Hexadecanol	242	C16H34O	036653-82-4	76



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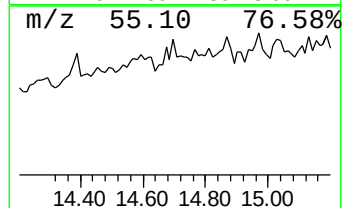
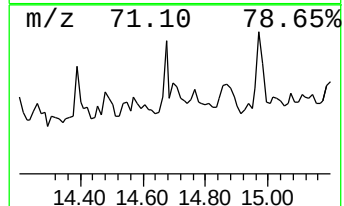
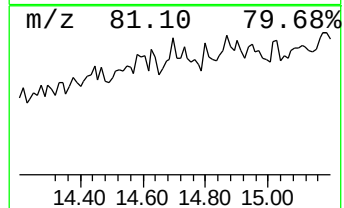
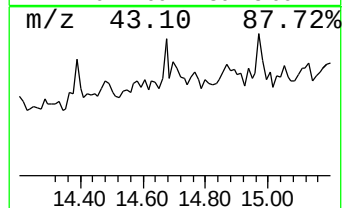
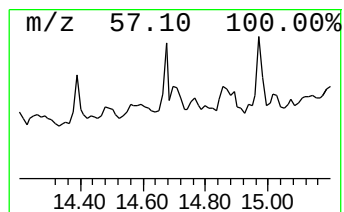
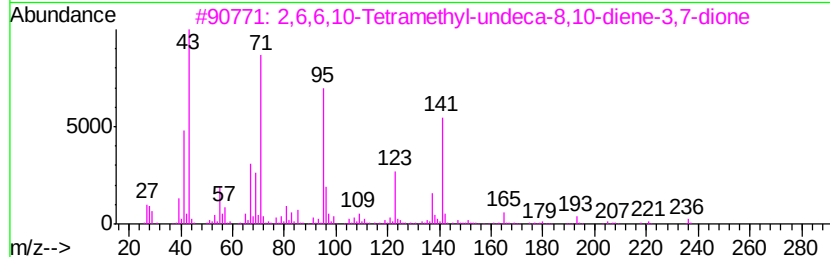
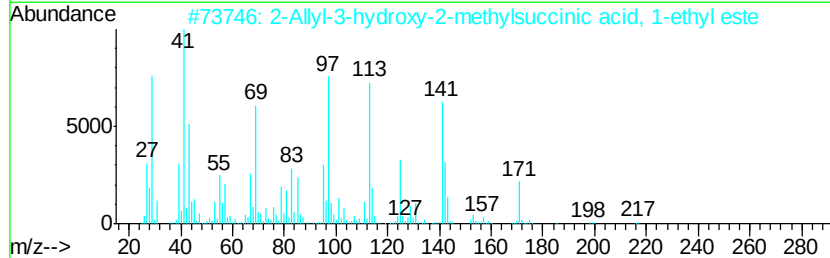
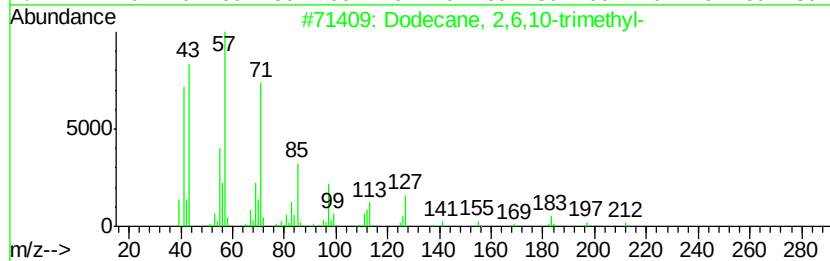
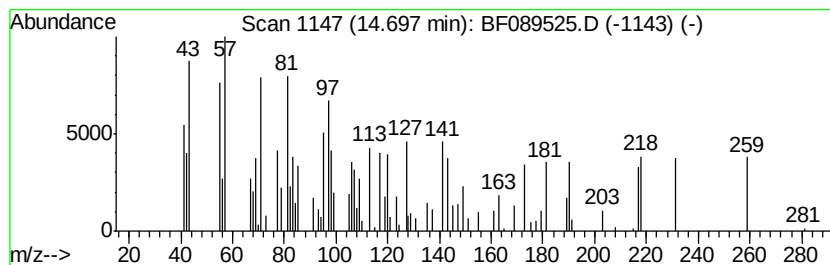
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Peak Number 7 unknown14.70 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	3.38 ng	44503	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	14
2		2-Allyl-3-hydroxy-2-methylsuccin...	216	C10H16O5	111832-94-1	10
3		2,6,6,10-Tetramethyl-undeca-8,10...	236	C15H24O2	098419-16-0	10
4		Silacyclopent-3-ene, 3-methyl-	98	C5H10Si	054077-65-5	10
5		5-Ethoxy-4-ethoxycarbonylmethylo...	199	C9H13NO4	010500-74-0	10



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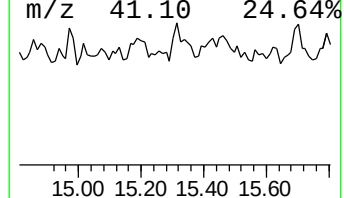
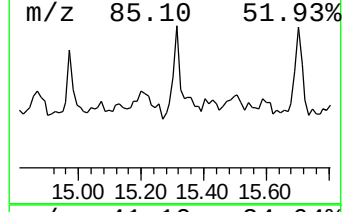
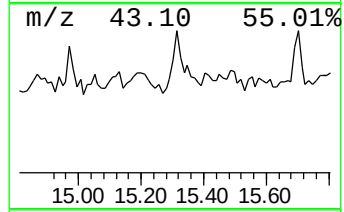
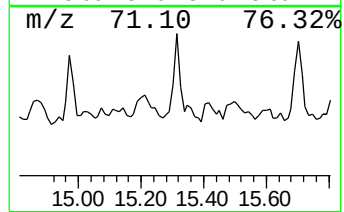
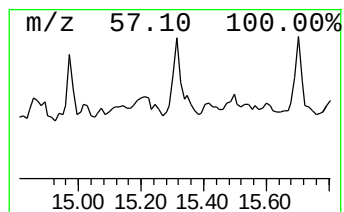
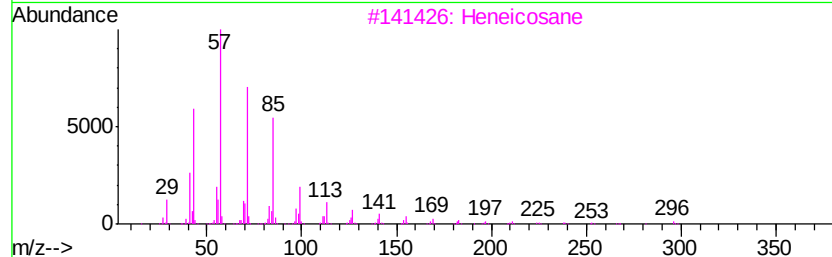
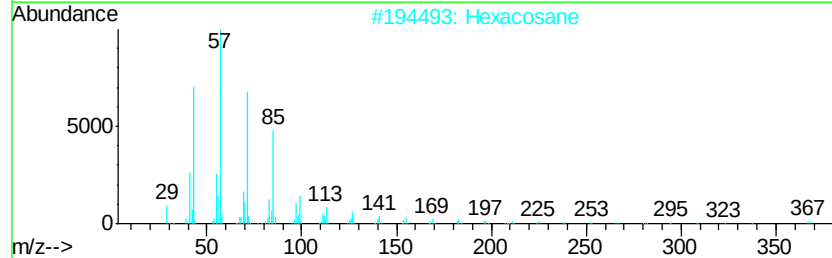
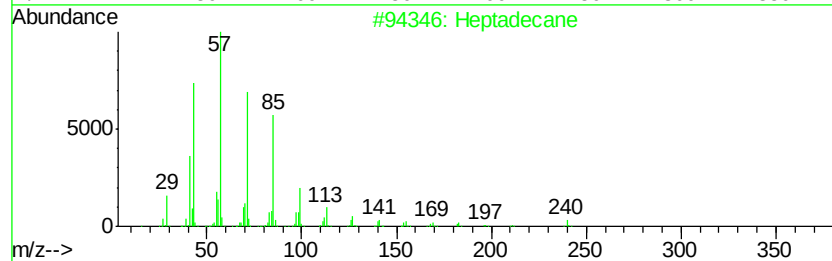
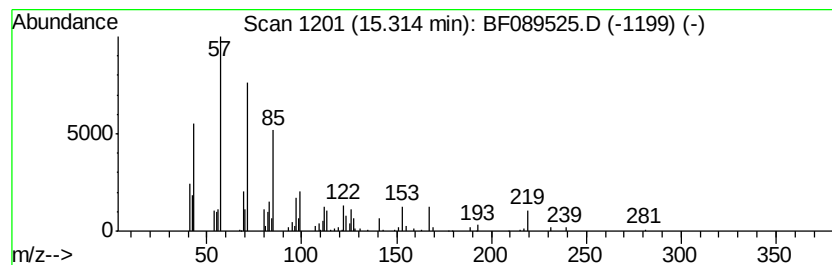
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.41 ng	31674	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	59
2		Hexacosane	366	C26H54	000630-01-3	58
3		Heneicosane	296	C21H44	000629-94-7	58
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	53
5		Hentriacontane	437	C31H64	000630-04-6	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089525.D
Acq On : 1 Aug 2016 22:26
Operator : UM/SJ
Sample : H4269-08
Misc :
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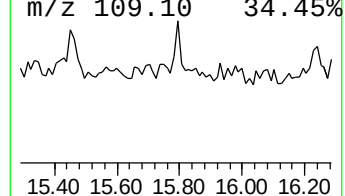
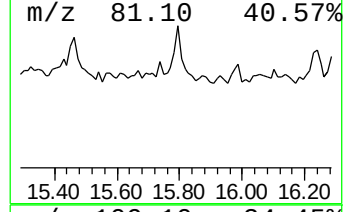
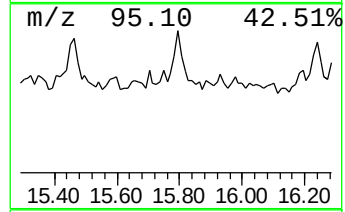
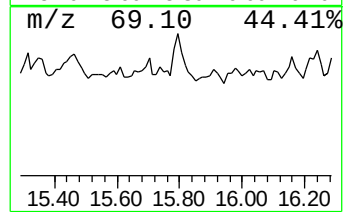
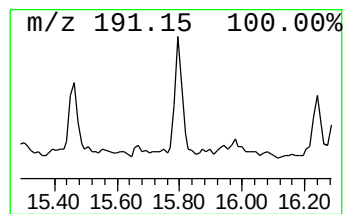
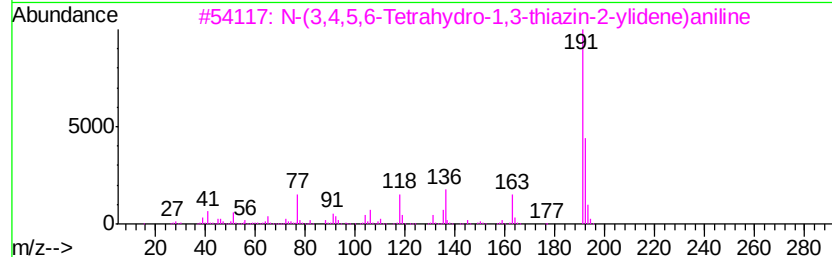
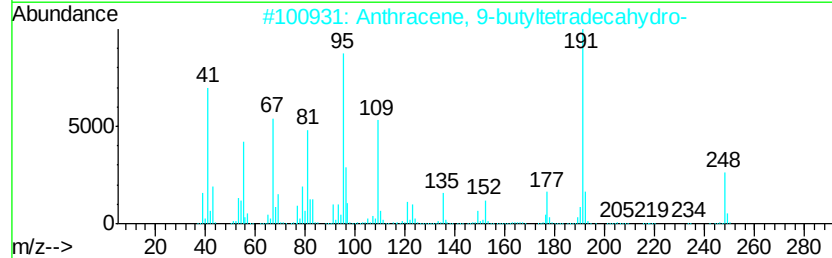
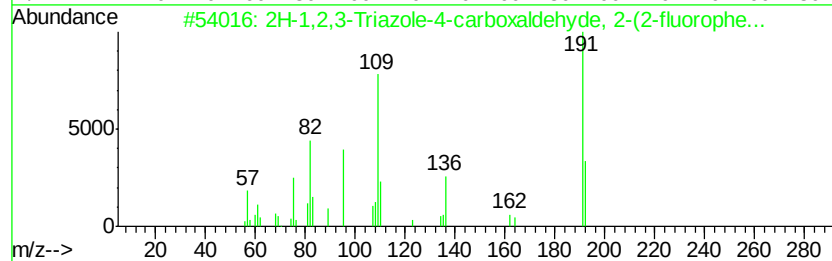
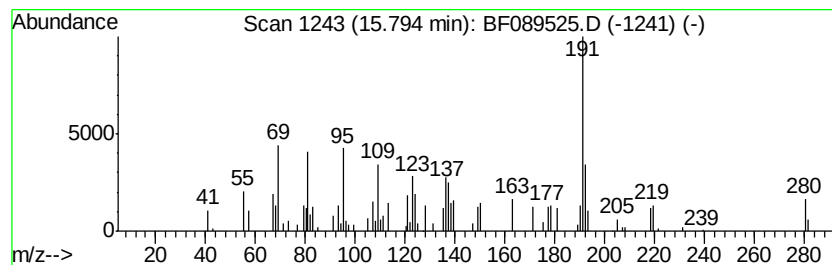
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2H-1,2,3-Triazole-4-carboxa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.79	3.71 ng	48782	Perylene-d12	14.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	50	
2	Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	47	
3	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	35	
4	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	35	
5	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	27	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
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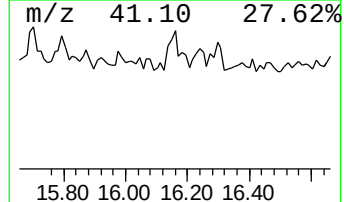
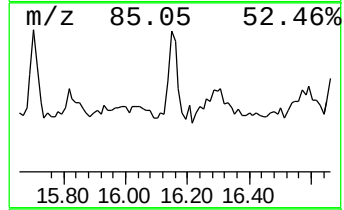
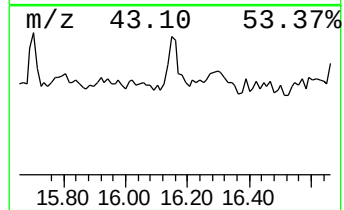
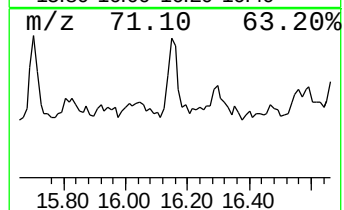
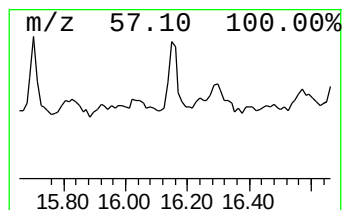
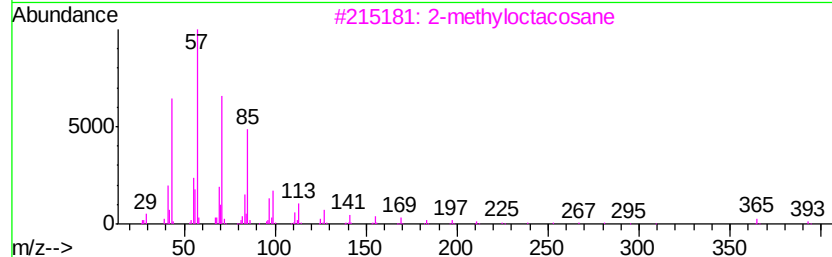
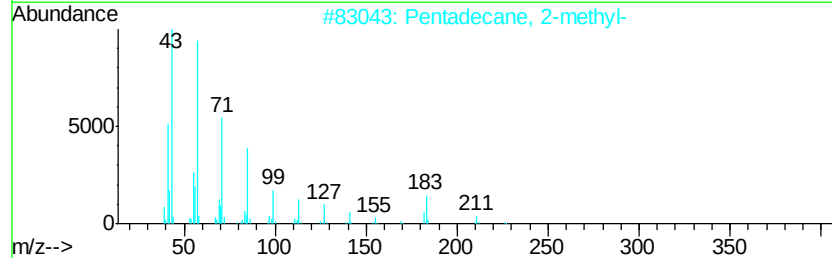
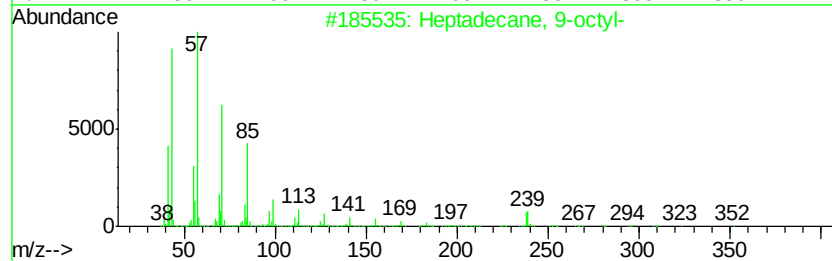
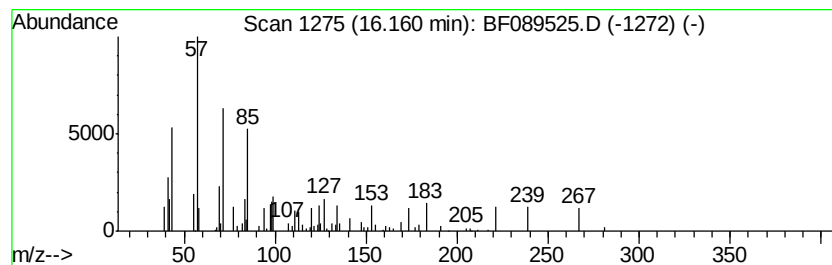
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.16 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	2.34 ng	30711	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	49
2		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	47
3		2-methyloctacosane	408	C29H60	1000376-72-8	46
4		Tetratetracontane	619	C44H90	007098-22-8	46
5		Hentriacontane	437	C31H64	000630-04-6	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
Data File : BF089525.D
Acq On : 1 Aug 2016 22:26
Operator : UM/SJ
Sample : H4269-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-DUP-02-072716

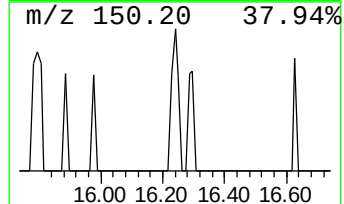
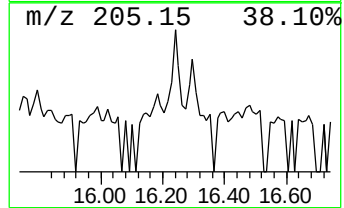
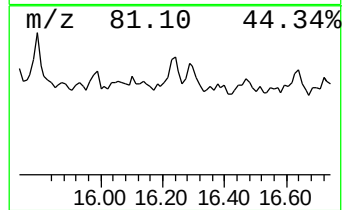
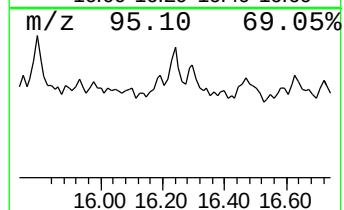
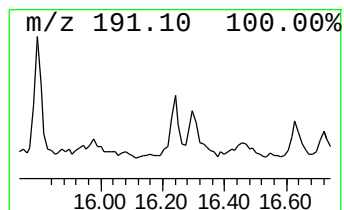
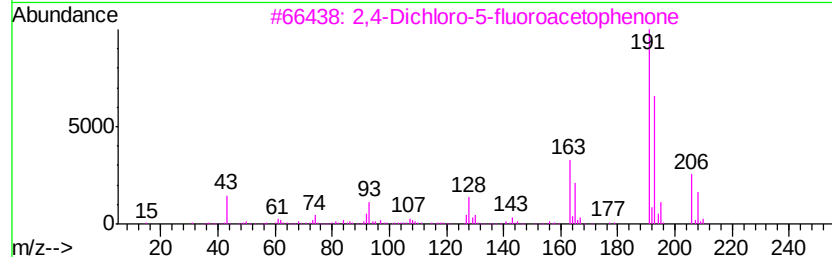
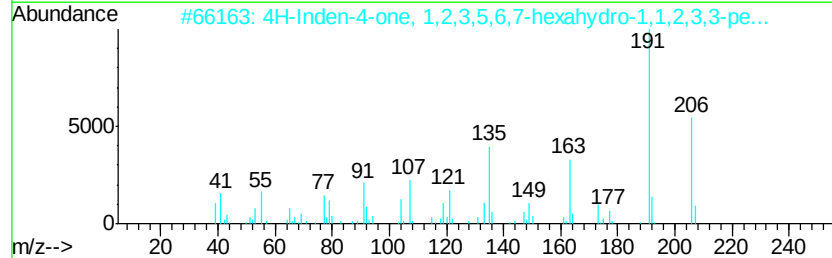
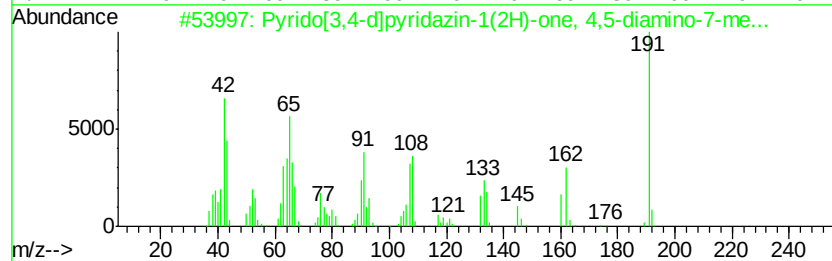
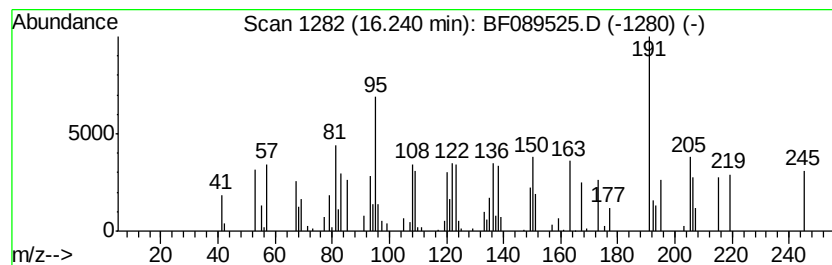
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown16.24 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	2.91 ng	38268	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	35
2		4H-Inden-4-one, 1,2,3,5,6,7-hexa...	206	C14H22O	033704-61-9	27
3		2,4-Dichloro-5-fluoroacetophenone	206	C8H5Cl2FO	000704-10-9	27
4		1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	27
5		9H-Purine, 6-methyl-9-(trimethyl...	206	C9H14N4Si	032865-79-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
Data File : BF089525.D
Acq On : 1 Aug 2016 22:26
Operator : UM/SJ
Sample : H4269-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

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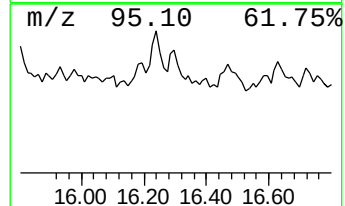
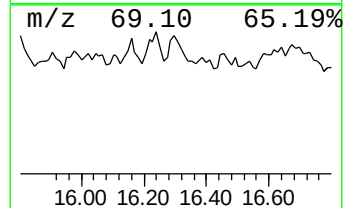
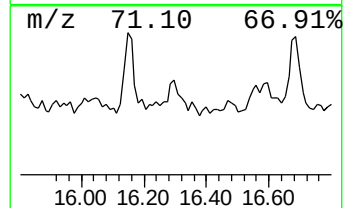
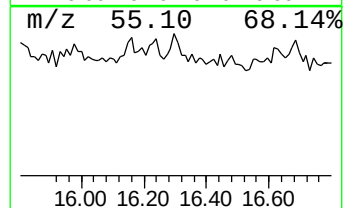
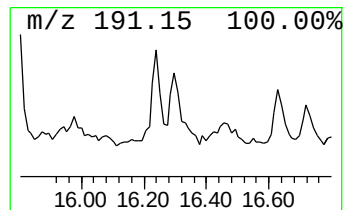
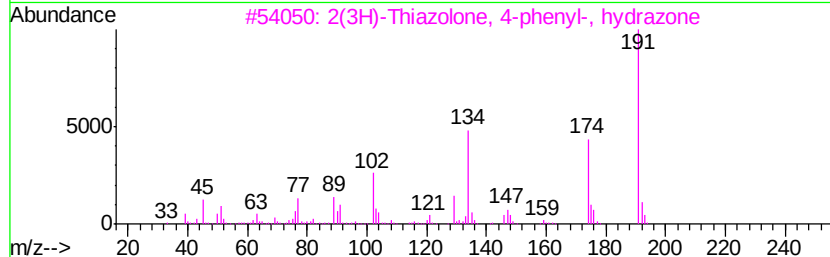
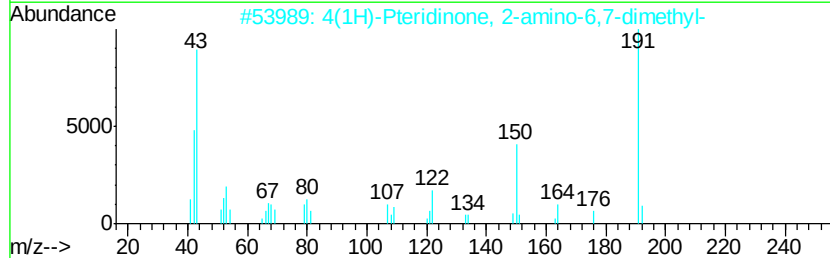
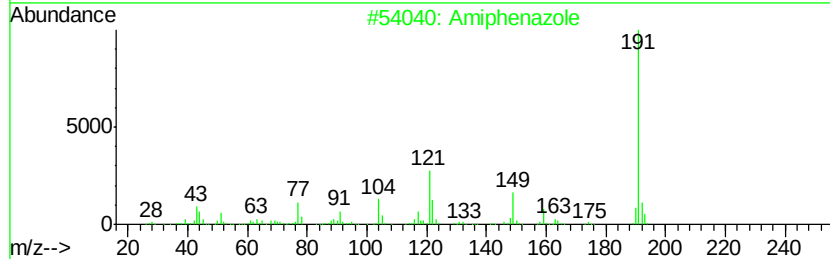
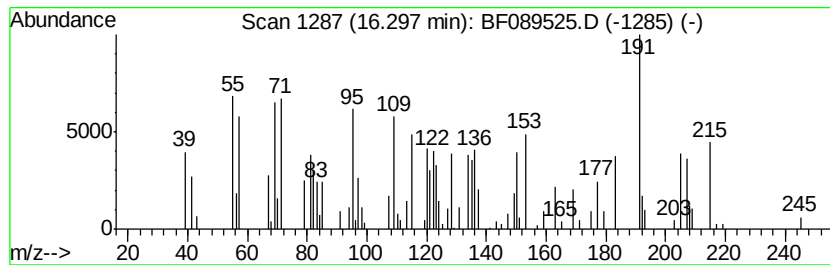
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown16.30 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	3.07 ng	40351	Perylene-d12	14.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Amiphenazole	191	C9H9N3S	000490-55-1	11
2		4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	10
3		2(3H)-Thiazolone, 4-phenyl-, hyd...	191	C9H9N3S	034176-52-8	10
4		Carbamic acid, 3-methylphenyl-, ...	191	C11H13N02	1000314-77-3	10
5		3-Methyl-2-thioxo-1,2-dihydro-3H...	191	C9H9N3S	121361-81-7	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089525.D
Acq On : 1 Aug 2016 22:26
Operator : UM/SJ
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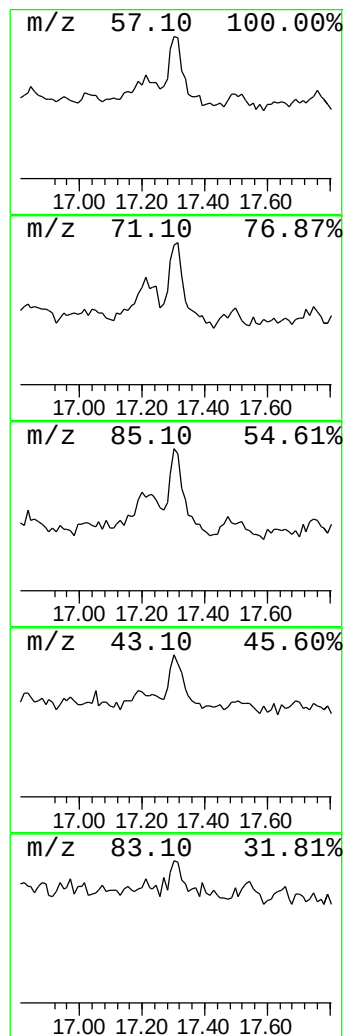
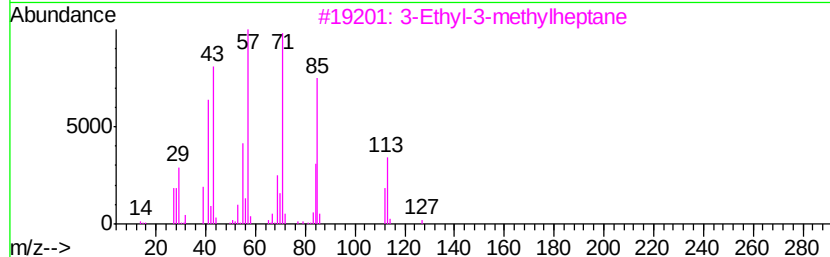
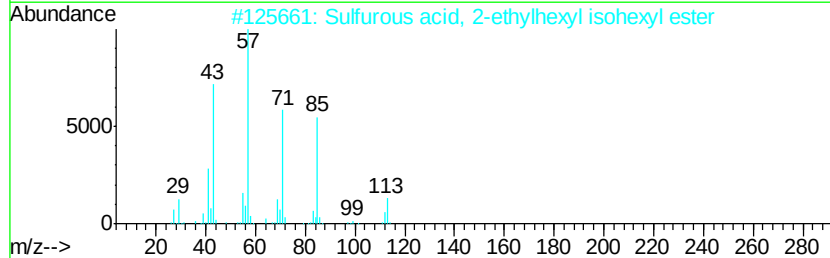
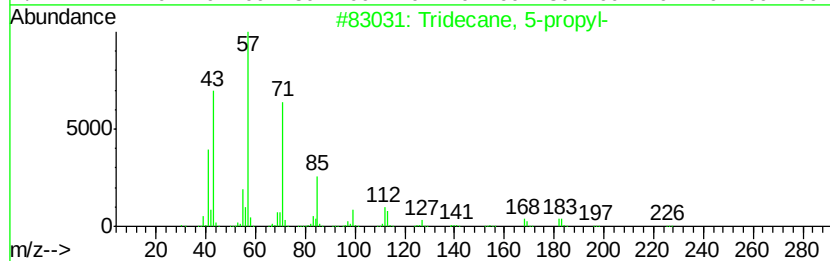
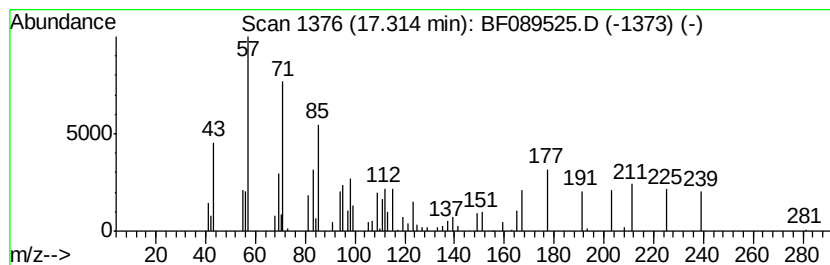
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown17.31 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	3.07 ng	40418	Perylene-d12	14.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	38
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	35
3			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	35
4			5,5-Diethyltridecane	240	C17H36	1000360-41-3	35
5			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
Data File : BF089525.D
Acq On : 1 Aug 2016 22:26
Operator : UM/SJ
Sample : H4269-08
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.24	6.24	72.9	ng	870116	1	6.48	238646	20.0
Tetradecane	10.43	3.6	ng	44479	4	10.98	245642	20.0
Trichloroacetic a...	13.47	5.1	ng	66744	5	13.60	260847	20.0
unknown14.70	14.70	3.4	ng	44503	6	14.93	263043	20.0
Heptadecane	15.31	2.4	ng	31674	6	14.93	263043	20.0
2H-1,2,3-Triazole...	15.79	3.7	ng	48782	6	14.93	263043	20.0
unknown16.16	16.16	2.3	ng	30711	6	14.93	263043	20.0
unknown16.24	16.24	2.9	ng	38268	6	14.93	263043	20.0
unknown16.30	16.30	3.1	ng	40351	6	14.93	263043	20.0
unknown17.31	17.31	3.1	ng	40418	6	14.93	263043	20.0