

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
 Data File : BF087341.D
 Acq On : 24 May 2016 14:35
 Operator : UM/SJ
 Sample : H3169-10
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-COMP

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-BF052316.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	1.678	7	8	56	rVB	2553156	7080813	100.00%	12.914%
2	4.902	288	290	308	rBV	227960	707523	9.99%	1.290%
3	5.530	342	345	375	rBV	2689717	4965756	70.13%	9.057%
4	7.153	484	487	490	rBV	2757505	4866403	68.73%	8.875%
5	7.267	494	497	506	rVB	3555195	4896370	69.15%	8.930%
6	7.610	525	527	540	rVB	722586	948020	13.39%	1.729%
7	7.850	545	548	559	rBV	2721857	3796563	53.62%	6.924%
8	8.525	604	607	622	rBV	2240318	3282506	46.36%	5.987%
9	9.645	702	705	718	rBV	754174	1244498	17.58%	2.270%
10	11.428	857	861	863	rBV	3489102	5458539	77.09%	9.955%
11	12.114	918	921	925	rBV	324953	493351	6.97%	0.900%
12	12.468	949	952	958	rBV	1029615	1388444	19.61%	2.532%
13	13.302	1021	1025	1028	rVB	110929	134783	1.90%	0.246%
14	13.771	1062	1066	1068	rBV	2092255	3101147	43.80%	5.656%
15	14.080	1090	1093	1098	rBV	103974	179118	2.53%	0.327%
16	14.811	1154	1157	1159	rBV	66172	80785	1.14%	0.147%
17	14.868	1160	1162	1172	rVB	789368	1213370	17.14%	2.213%
18	15.634	1226	1229	1232	rVB	215367	257339	3.63%	0.469%
19	16.594	1310	1313	1314	rBV	686702	687588	9.71%	1.254%
20	16.628	1314	1316	1321	rVV	842210	957959	13.53%	1.747%
21	16.754	1325	1327	1330	rBV	135083	136363	1.93%	0.249%
22	17.051	1351	1353	1356	rBV	83561	86964	1.23%	0.159%
23	17.211	1364	1367	1370	rBV	3074433	4307118	60.83%	7.855%
24	18.549	1482	1484	1487	rBV	547425	882972	12.47%	1.610%
25	18.606	1487	1489	1492	rVB	141285	223068	3.15%	0.407%
26	19.006	1518	1524	1529	rBV	60162	85018	1.20%	0.155%
27	19.246	1542	1545	1547	rBV	56138	74239	1.05%	0.135%
28	19.360	1549	1555	1557	rBV3	21810	76537	1.08%	0.140%
29	19.577	1571	1574	1575	rBV	95163	108598	1.53%	0.198%
30	19.612	1575	1577	1580	rVB	58981	78358	1.11%	0.143%
31	19.966	1605	1608	1611	rBV	1758858	2023038	28.57%	3.690%
32	20.217	1628	1630	1636	rBV	479621	697739	9.85%	1.273%
33	20.674	1667	1670	1675	rVB	137683	194302	2.74%	0.354%
34	21.315	1723	1726	1731	rBV	61009	114884	1.62%	0.210%

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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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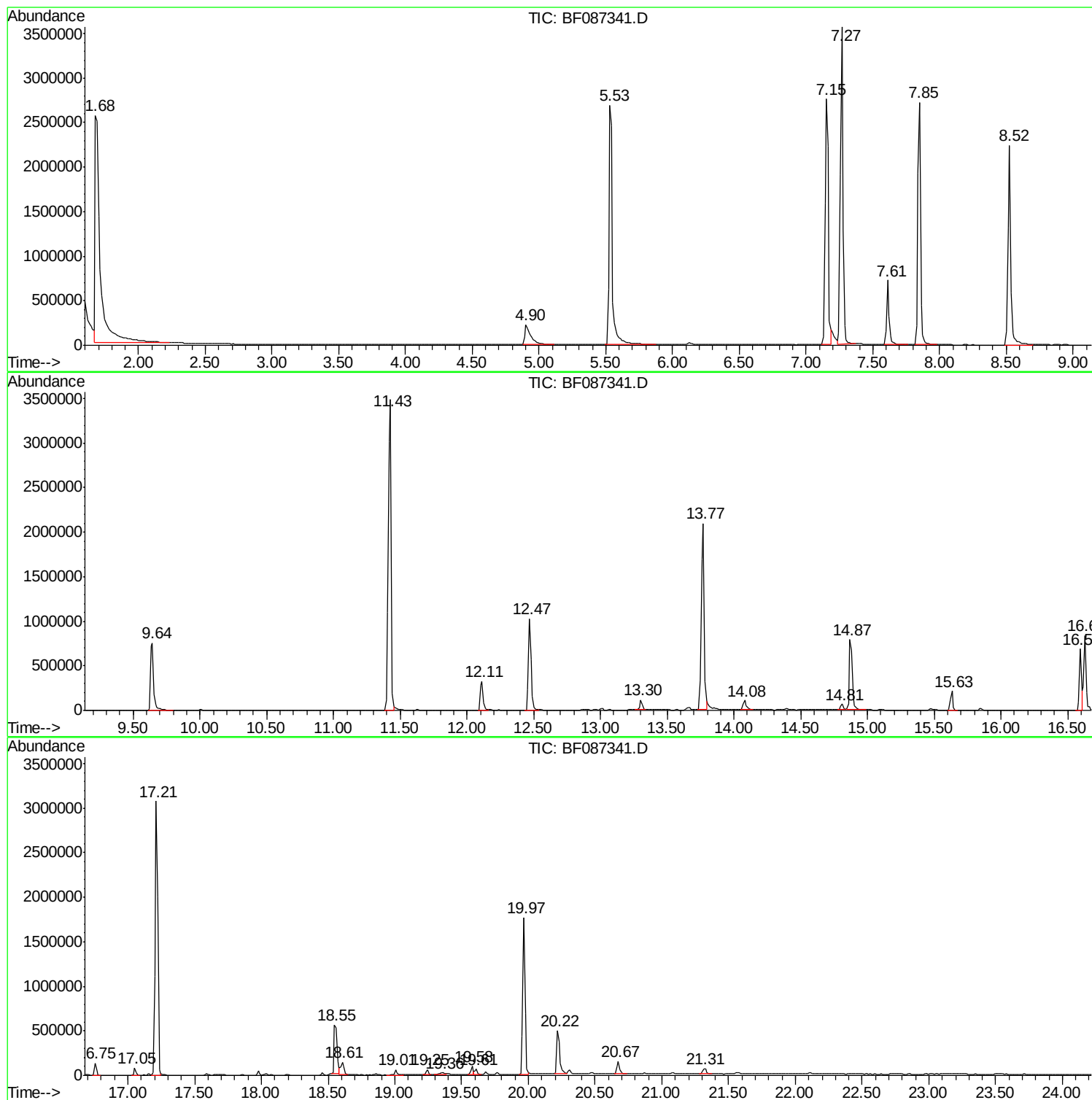
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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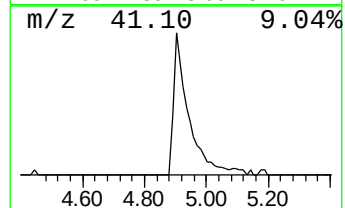
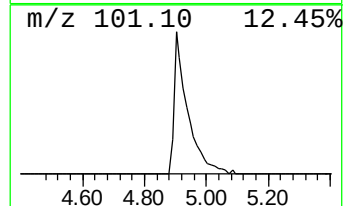
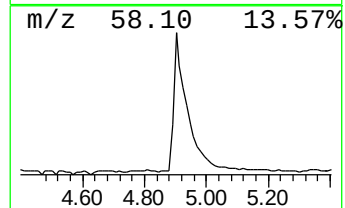
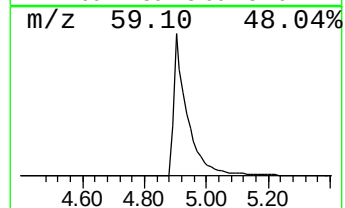
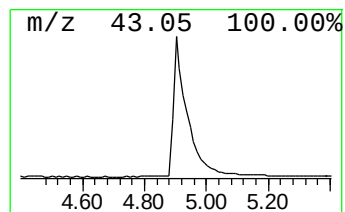
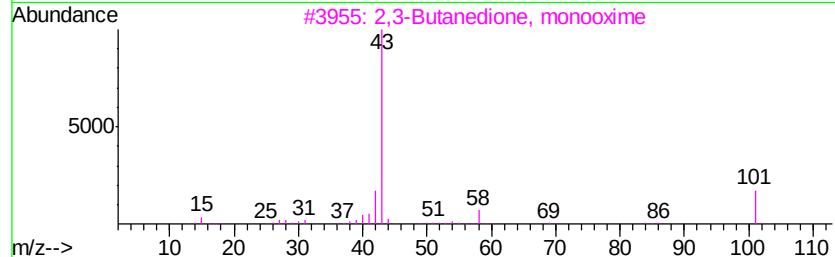
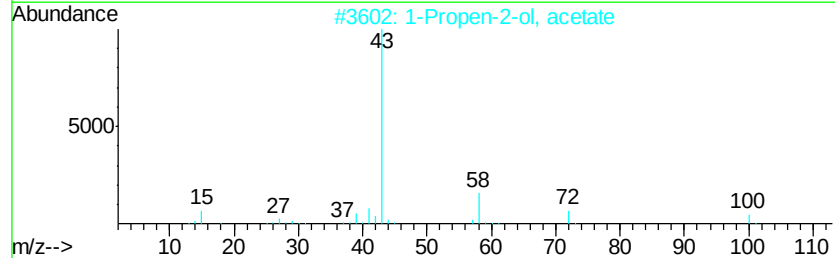
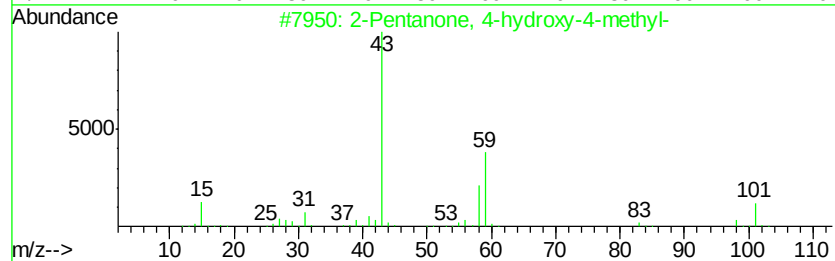
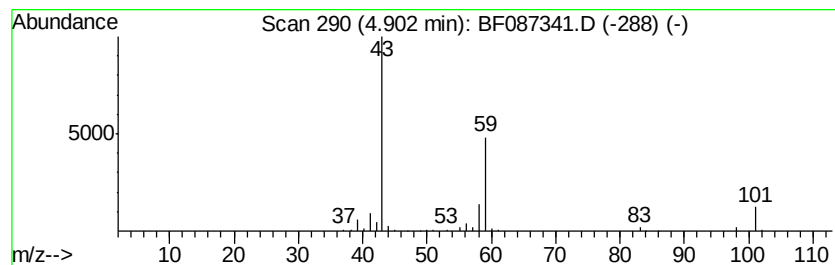
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	14.93 ng	707523	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane	58	C4H10	000106-97-8	9
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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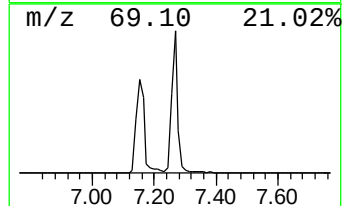
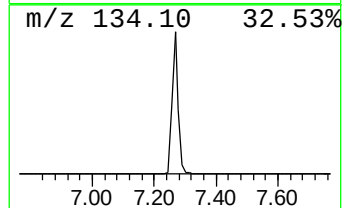
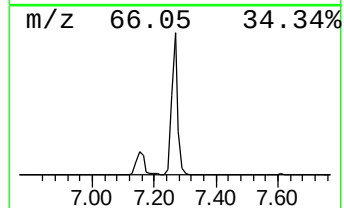
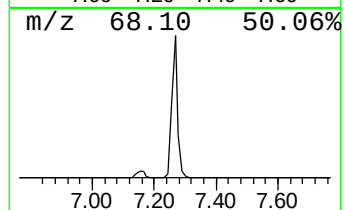
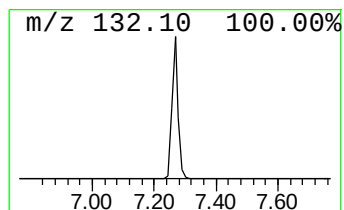
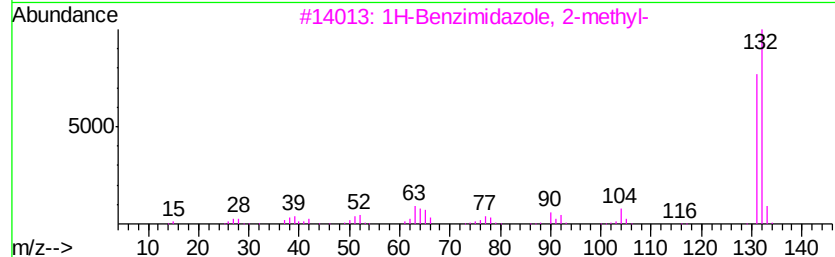
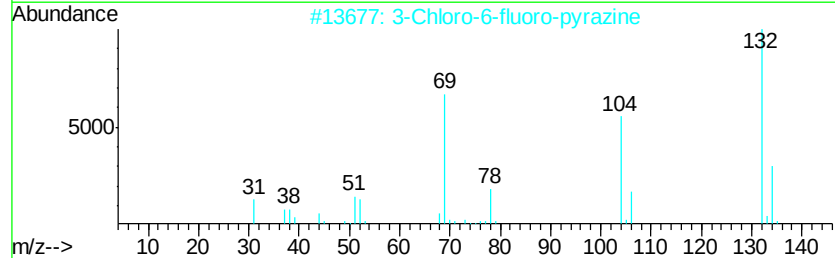
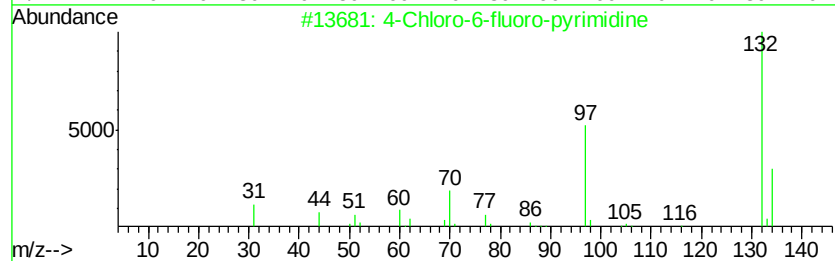
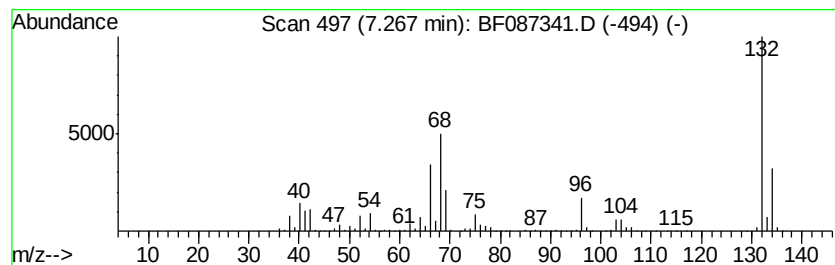
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	103.30 ng	4896370	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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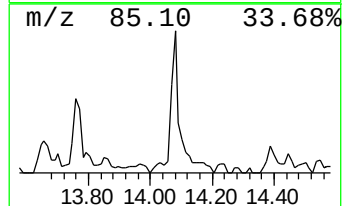
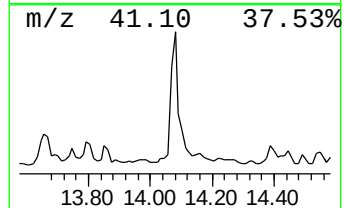
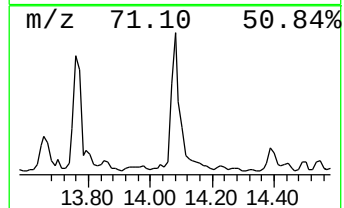
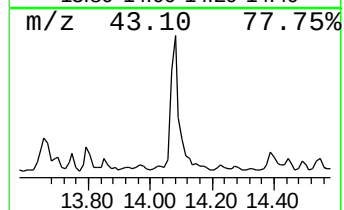
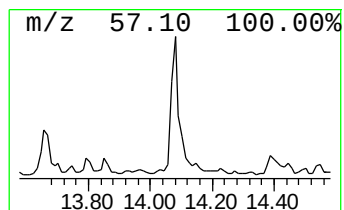
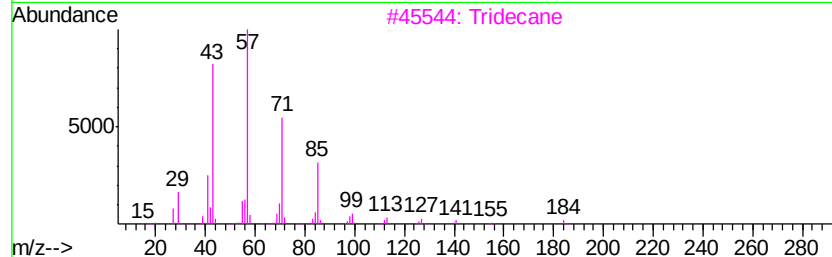
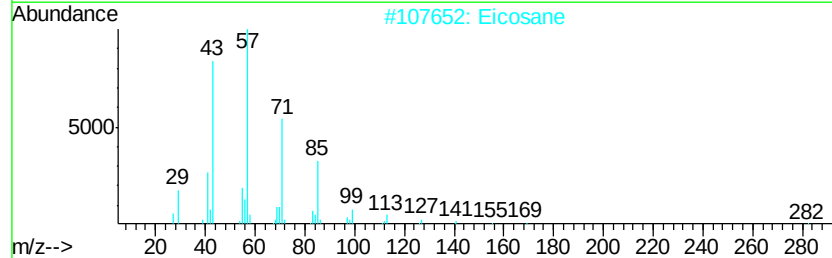
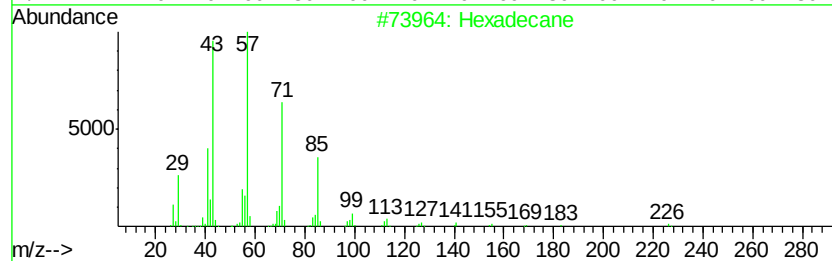
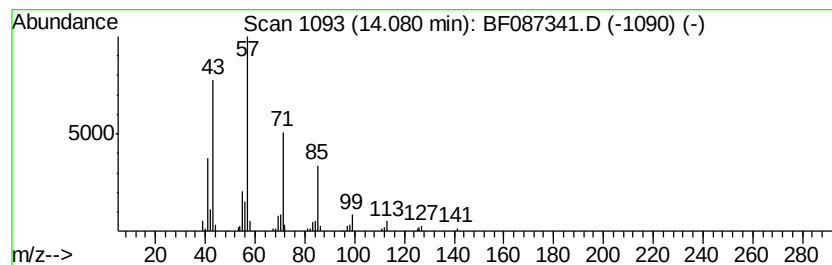
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.95 ng	179118	Phenanthrene-d10	14.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Tridecane		184	C13H28	000629-50-5	86
4	Tetradecane		198	C14H30	000629-59-4	80
5	Tetracosane		338	C24H50	000646-31-1	78



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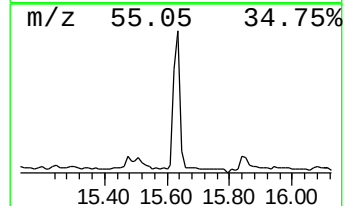
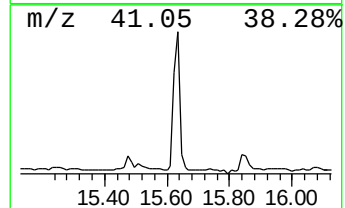
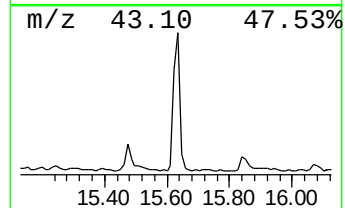
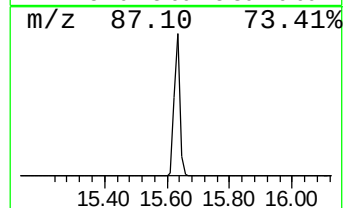
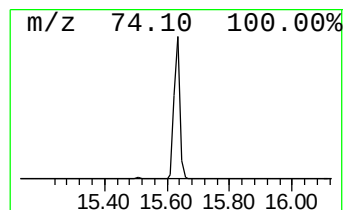
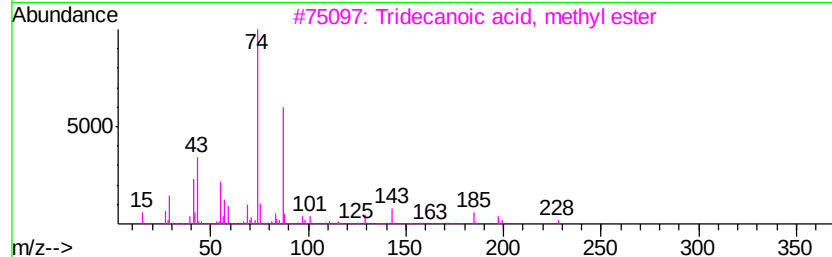
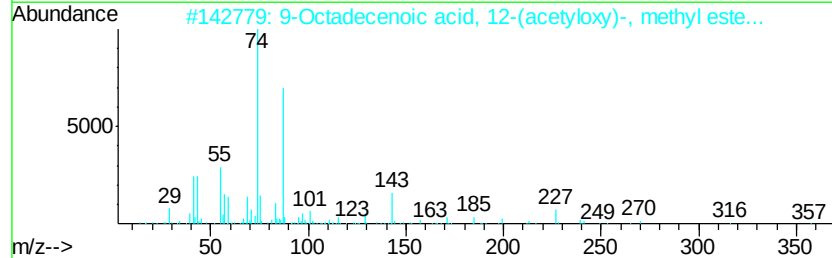
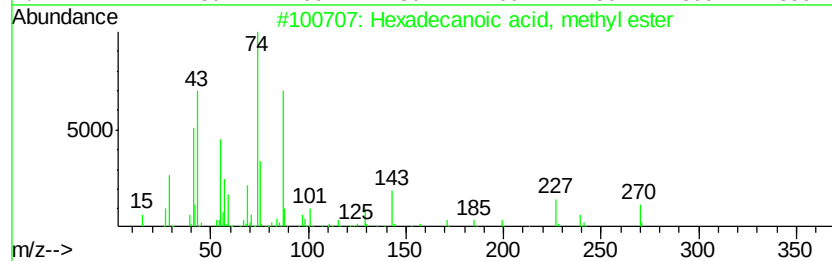
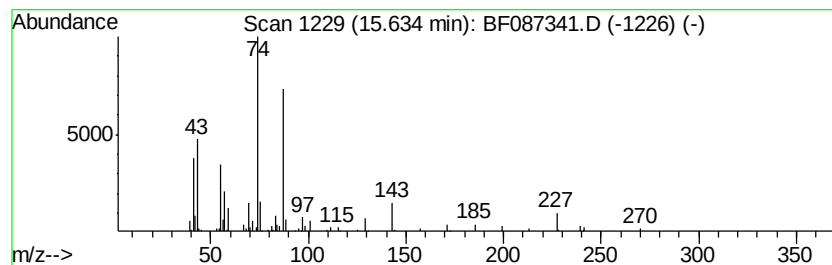
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	4.24 ng	257339	Phenanthrene-d10	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	91
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90



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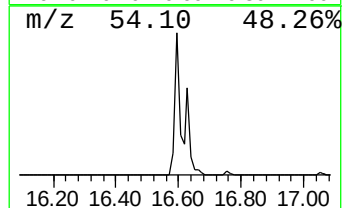
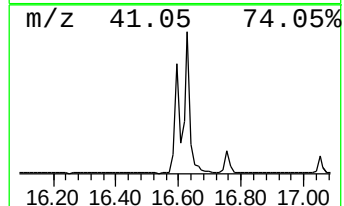
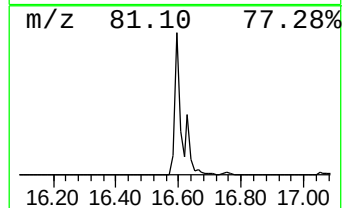
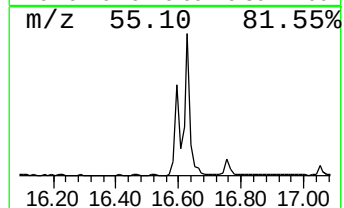
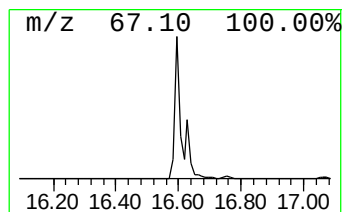
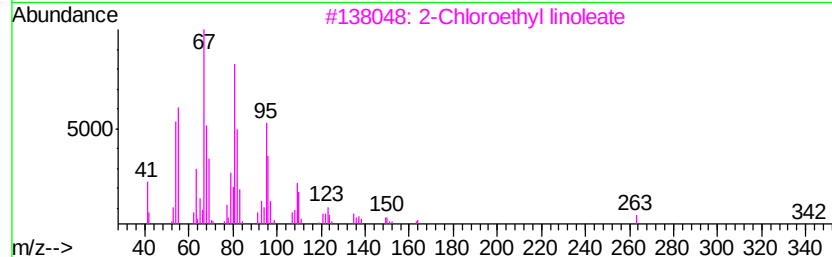
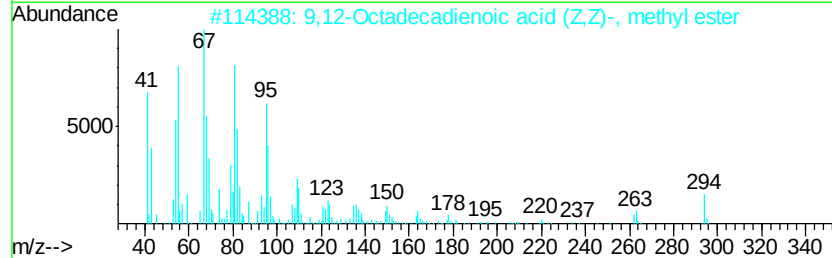
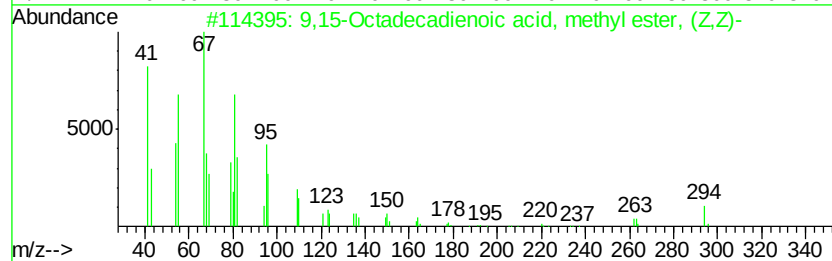
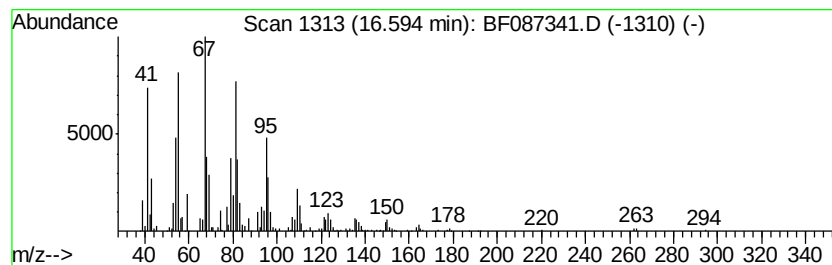
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 9,15-Octadecadienoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	11.33 ng	687588	Phenanthrene-d10	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	91
5		11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	91



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SB-05-COMP

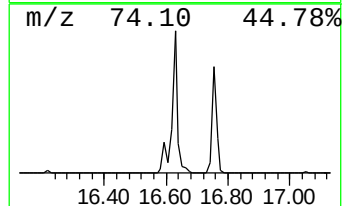
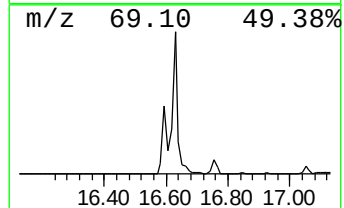
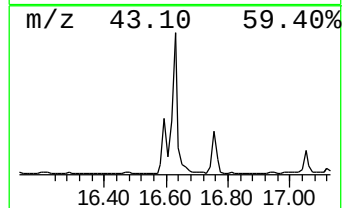
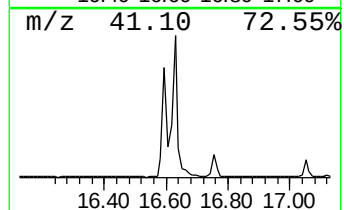
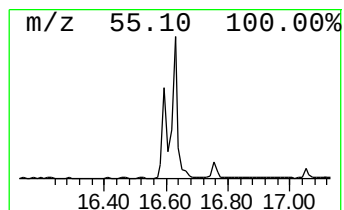
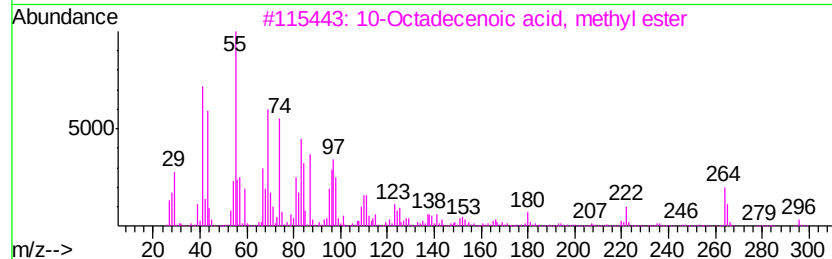
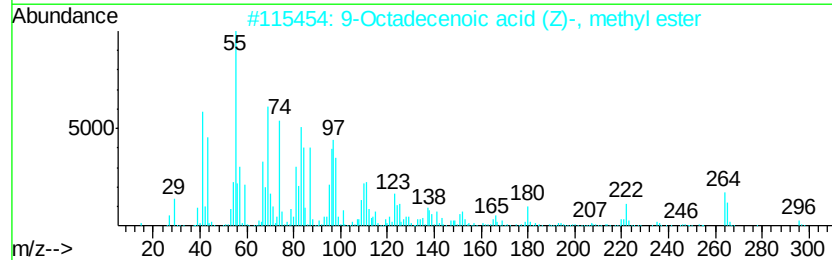
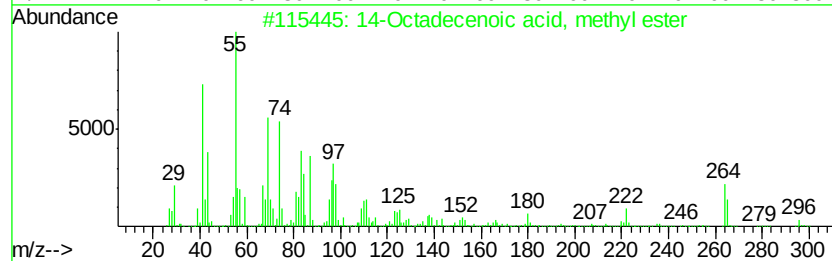
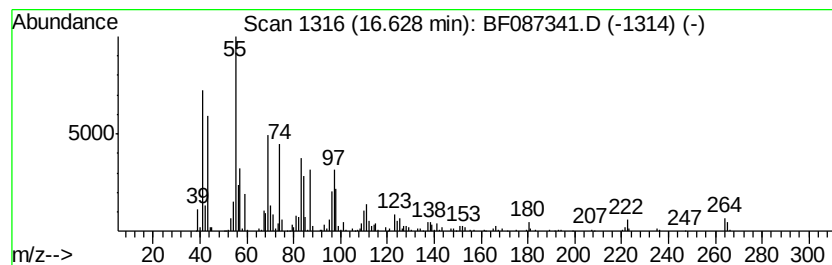
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 14-Octadecenoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	15.79 ng	957959	Phenanthrene-d10	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
2		9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	91
3		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
5		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087341.D
Acq On : 24 May 2016 14:35
Operator : UM/SJ
Sample : H3169-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

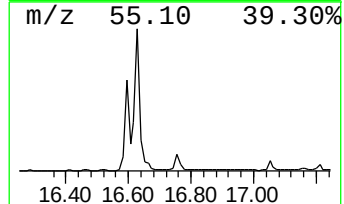
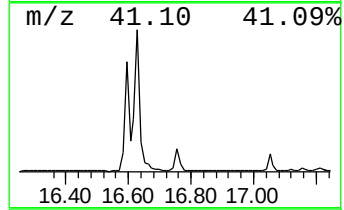
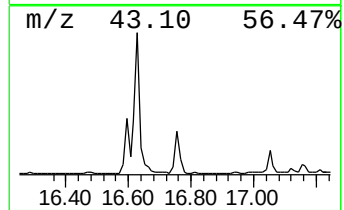
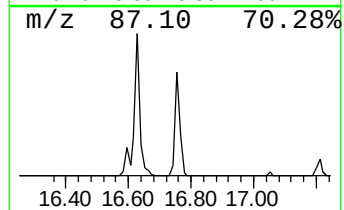
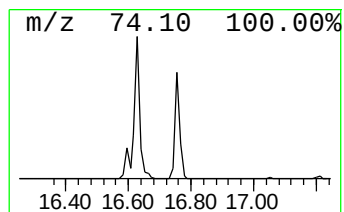
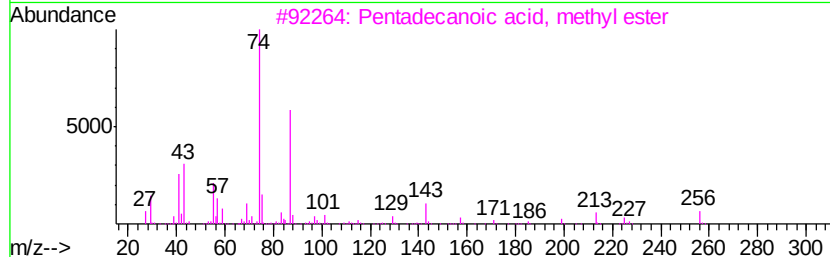
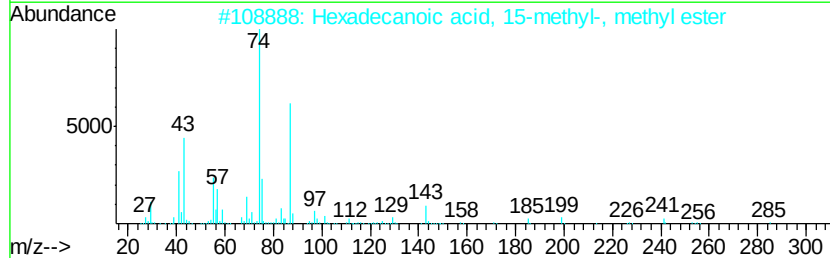
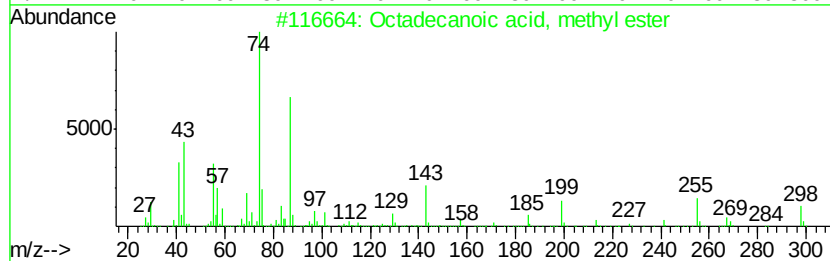
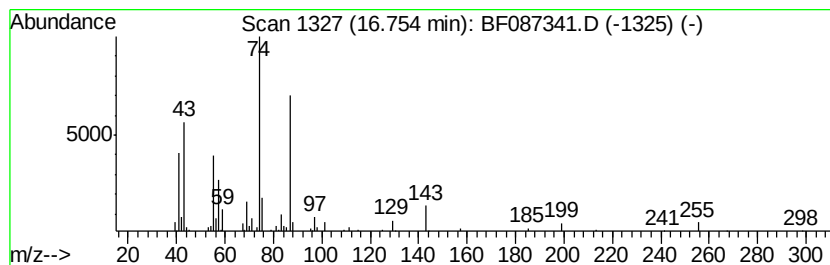
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, methyl e... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.75	3.09 ng	136363	Chrysene-d12	18.56		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	97
2		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	90
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087341.D
Acq On : 24 May 2016 14:35
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ClientSampleId :
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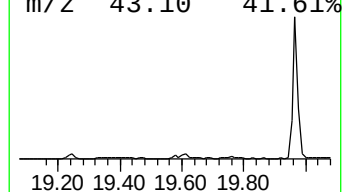
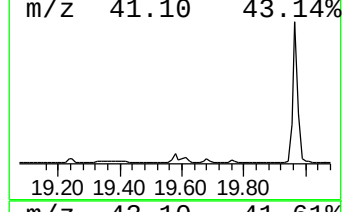
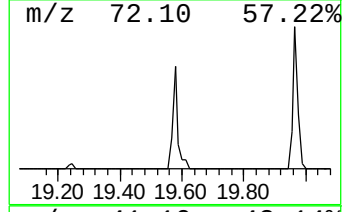
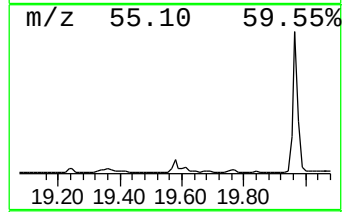
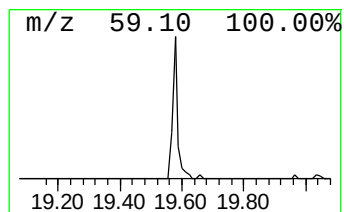
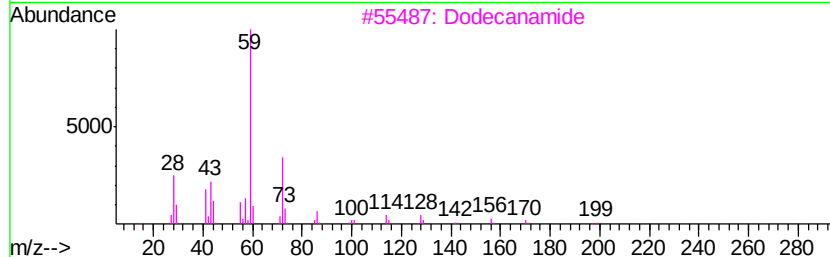
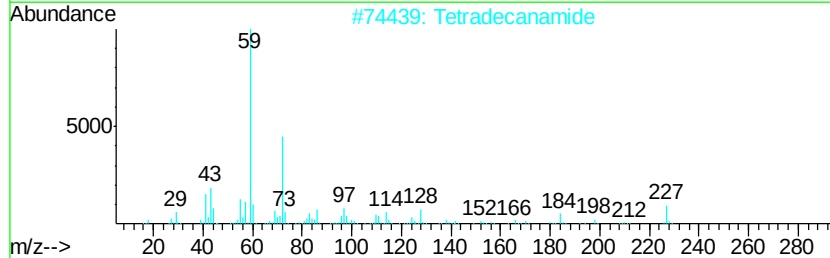
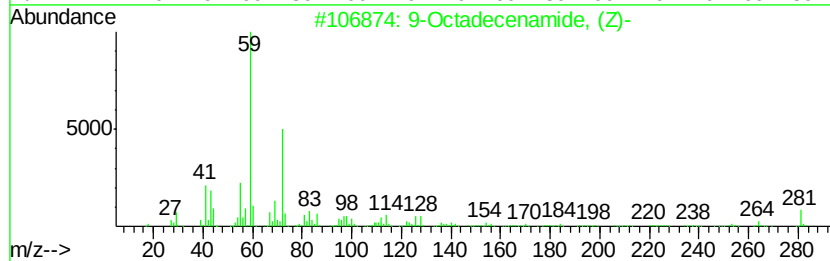
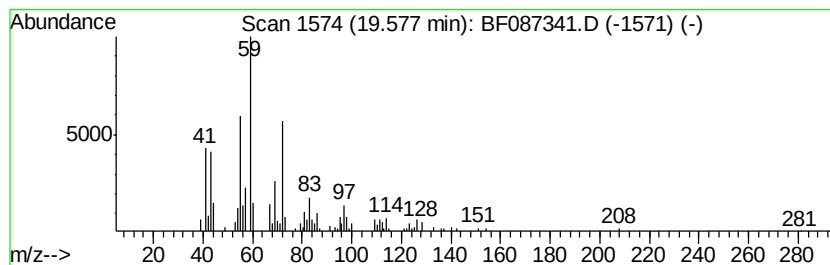
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.58	3.11 ng	108598	Perylene-d12	20.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2			Tetradecanamide	227	C14H29NO	000638-58-4	64
3			Dodecanamide	199	C12H25NO	001120-16-7	53
4			Decanamide-	171	C10H21NO	002319-29-1	50
5			Hexanamide	115	C6H13NO	000628-02-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
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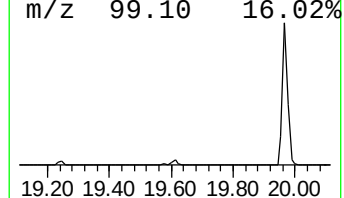
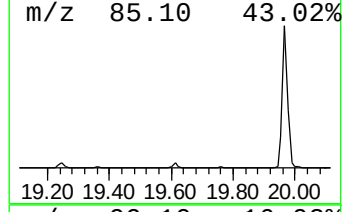
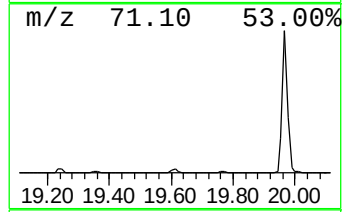
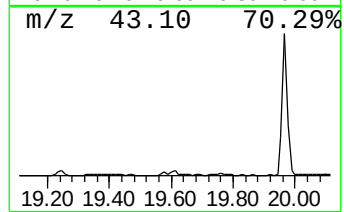
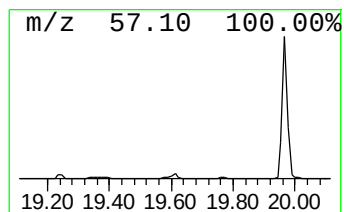
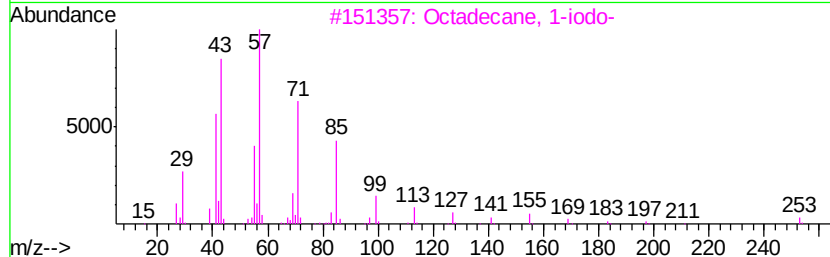
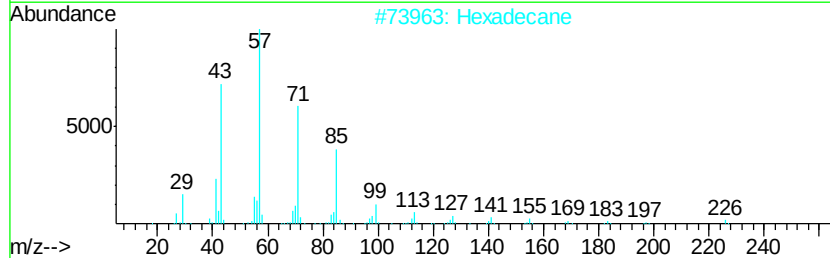
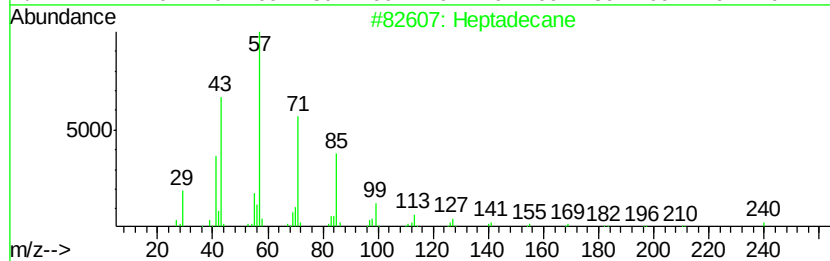
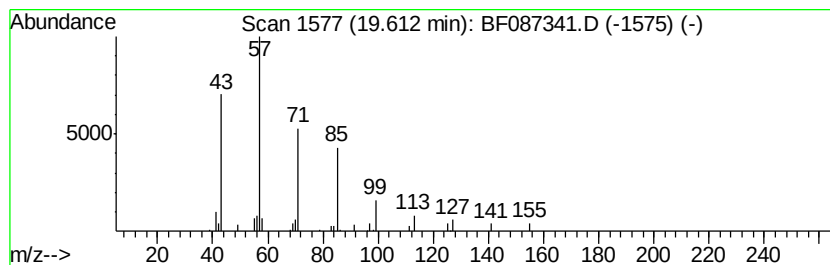
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.25 ng	78358	Perylene-d12	20.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	78
2	Hexadecane	226 C16H34	000544-76-3	78
3	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	78
4	Tetradecane, 6,9-dimethyl-	226 C16H34	055045-13-1	72
5	Undecane, 2,10-dimethyl-	184 C13H28	017301-27-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087341.D
Acq On : 24 May 2016 14:35
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Misc :
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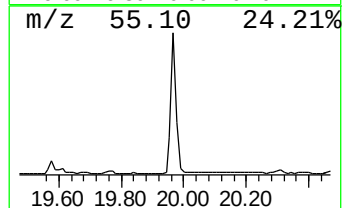
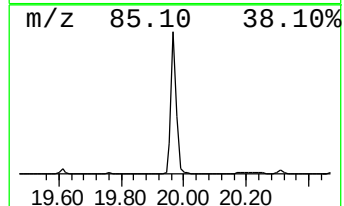
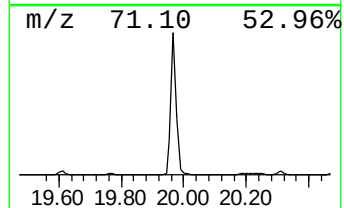
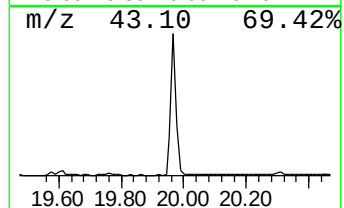
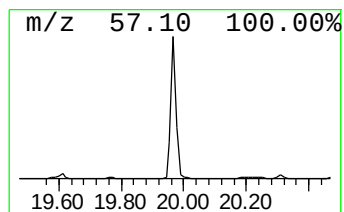
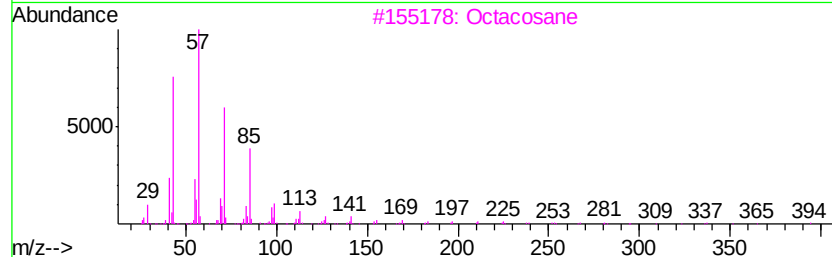
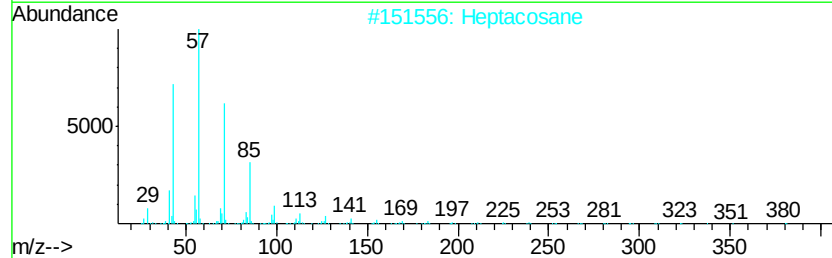
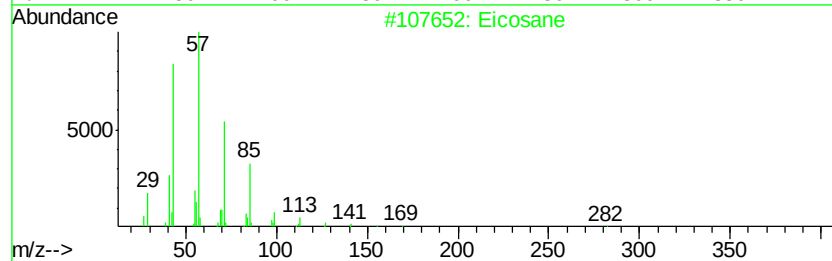
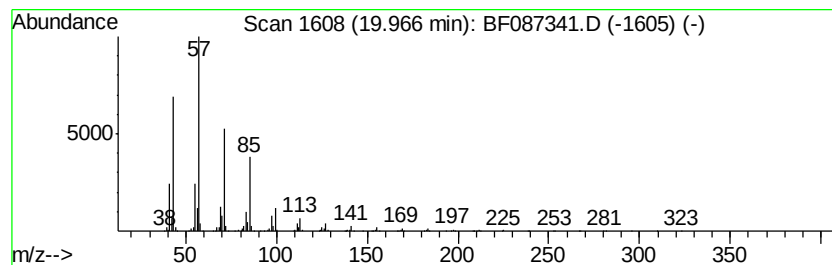
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.97	57.99 ng	2023040	Perylene-d12	20.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetratriacontane	479	C34H70	014167-59-0	90
5		Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087341.D
Acq On : 24 May 2016 14:35
Operator : UM/SJ
Sample : H3169-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

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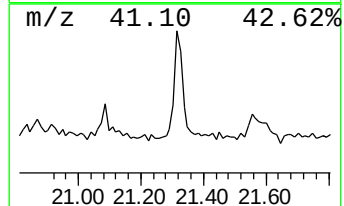
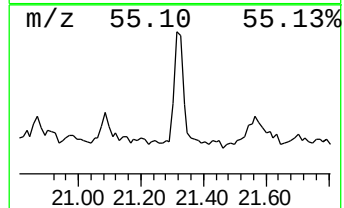
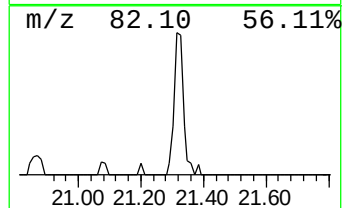
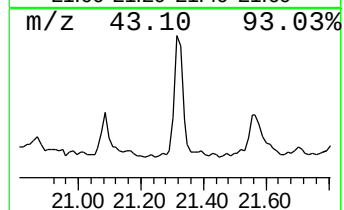
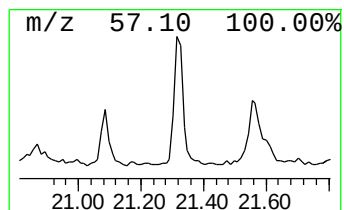
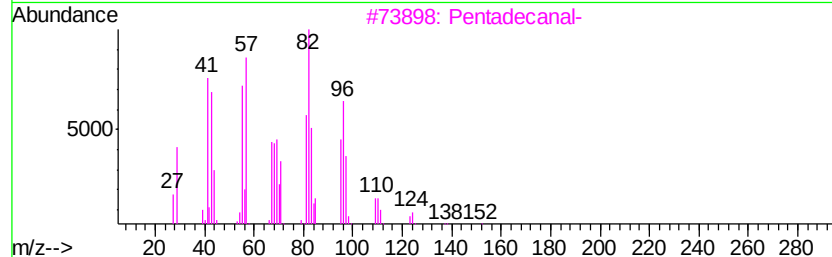
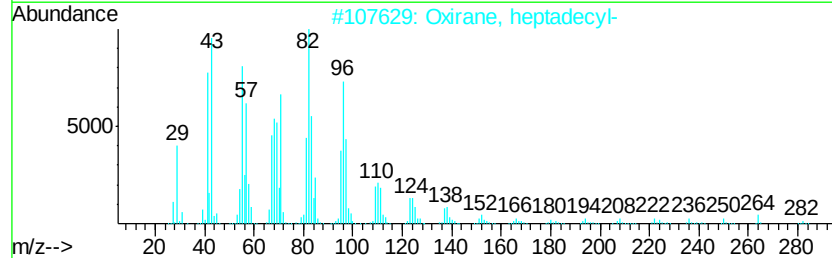
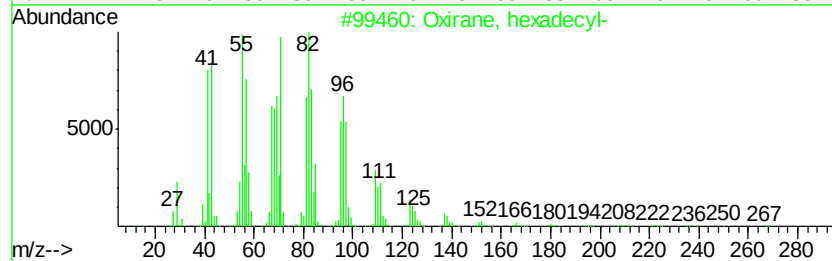
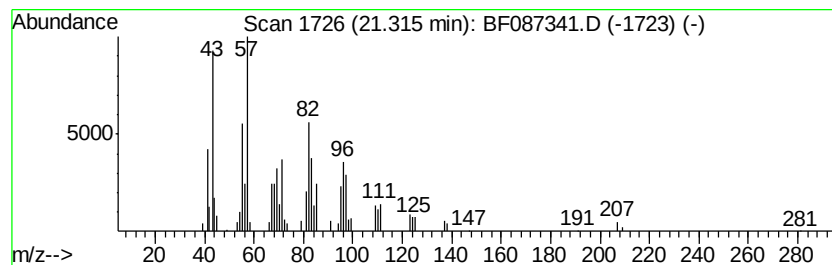
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.29 ng	114884	Perylene-d12	20.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
3		Pentadecanal-	226	C15H30O	002765-11-9	83
4		Hexadecanal	240	C16H32O	000629-80-1	80
5		Octadecanal	268	C18H36O	000638-66-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
 Data File : BF087341.D
 Acq On : 24 May 2016 14:35
 Operator : UM/SJ
 Sample : H3169-10
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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 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...	4.90	14.9	ng	707523	1	7.61	948020	20.0
unknown7.27	7.27	103.3	ng	4896370	1	7.61	948020	20.0
Hexadecane	14.08	3.0	ng	179118	4	14.87	1213370	20.0
Hexadecanoic acid...	15.63	4.2	ng	257339	4	14.87	1213370	20.0
9,15-Octadecadien...	16.59	11.3	ng	687588	4	14.87	1213370	20.0
14-Octadecenoic a...	16.63	15.8	ng	957959	4	14.87	1213370	20.0
Octadecanoic acid...	16.75	3.1	ng	136363	5	18.56	882972	20.0
9-Octadecenamide,...	19.58	3.1	ng	108598	6	20.22	697739	20.0
Heptadecane	19.61	2.3	ng	78358	6	20.22	697739	20.0
Eicosane	19.97	58.0	ng	2023040	6	20.22	697739	20.0
Oxirane, hexadecyl-	21.31	3.3	ng	114884	6	20.22	697739	20.0