

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
 Data File : BF089051.D
 Acq On : 16 Jul 2016 13:07
 Operator : UM/SJ
 Sample : H3951-04 5X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LSS-SB-SB02(0-2in)

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-BF063016.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	1.770	14	16	59	rVB	1200092	2256127	100.00%	26.327%
2	4.776	278	279	283	rVB	29349	40963	1.82%	0.478%
3	5.244	318	320	323	rBV	295025	300497	13.32%	3.507%
4	6.307	411	413	416	rBV	392646	339357	15.04%	3.960%
5	6.433	422	424	426	rBB	287472	319868	14.18%	3.733%
6	6.662	442	444	446	rBB	459465	377716	16.74%	4.408%
7	6.810	455	457	460	rBB	209470	233250	10.34%	2.722%
8	7.222	491	493	495	rBV	214613	172689	7.65%	2.015%
9	7.942	554	556	559	rBV	331395	460281	20.40%	5.371%
10	9.028	648	651	653	rBV	388876	342518	15.18%	3.997%
11	9.428	683	686	688	rVB	158907	139153	6.17%	1.624%
12	9.702	707	710	712	rBV	543595	516325	22.89%	6.025%
13	10.479	776	778	781	rBV2	143893	133328	5.91%	1.556%
14	11.176	836	839	840	rBV	557709	464969	20.61%	5.426%
15	11.199	840	841	842	rVV	76757	54203	2.40%	0.633%
16	11.245	842	845	847	rVB3	14769	22777	1.01%	0.266%
17	11.782	890	892	896	rVB2	24285	33522	1.49%	0.391%
18	12.377	942	944	947	rVB	90427	93405	4.14%	1.090%
19	12.605	961	964	966	rBV	105973	100743	4.47%	1.176%
20	12.754	976	977	980	rVB	178839	195678	8.67%	2.283%
21	12.937	989	993	995	rVB	18236	26992	1.20%	0.315%
22	13.005	995	999	1001	rBV3	15253	28607	1.27%	0.334%
23	13.131	1006	1010	1011	rBV	15242	22652	1.00%	0.264%
24	13.680	1054	1058	1061	rBV2	23662	38160	1.69%	0.445%
25	13.805	1066	1069	1070	rBV2	323972	402869	17.86%	4.701%
26	13.908	1075	1078	1080	rBV3	11343	24439	1.08%	0.285%
27	14.182	1100	1102	1104	rVV	16678	27347	1.21%	0.319%
28	14.297	1110	1112	1117	rBV3	27146	55010	2.44%	0.642%
29	14.594	1134	1138	1140	rBV4	21582	52061	2.31%	0.608%
30	14.651	1141	1143	1145	rVV	23833	37360	1.66%	0.436%
31	14.800	1153	1156	1160	rBV	47340	96077	4.26%	1.121%
32	14.891	1162	1164	1166	rBV	116337	123283	5.46%	1.439%
33	15.063	1176	1179	1181	rVB	28186	43667	1.94%	0.510%
34	15.108	1181	1183	1185	rBV	79097	103482	4.59%	1.208%

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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

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35	15.165	1185	1188	1191	rBV	206176	293971	13.03%	3.430%
36	15.360	1203	1205	1206	rBV	18216	24947	1.11%	0.291%
37	15.394	1206	1208	1212	rVB3	34394	55122	2.44%	0.643%
38	15.611	1224	1227	1230	rBV	152258	261563	11.59%	3.052%
39	16.297	1284	1287	1290	rVB4	21391	45083	2.00%	0.526%
40	16.446	1297	1300	1306	rVB2	15147	35553	1.58%	0.415%
41	16.548	1307	1309	1312	rBV	15727	33524	1.49%	0.391%
42	16.823	1331	1333	1338	rVB	17540	36573	1.62%	0.427%
43	17.337	1376	1378	1381	rBV2	15992	37842	1.68%	0.442%
44	17.840	1418	1422	1428	rVB7	19366	65923	2.92%	0.769%

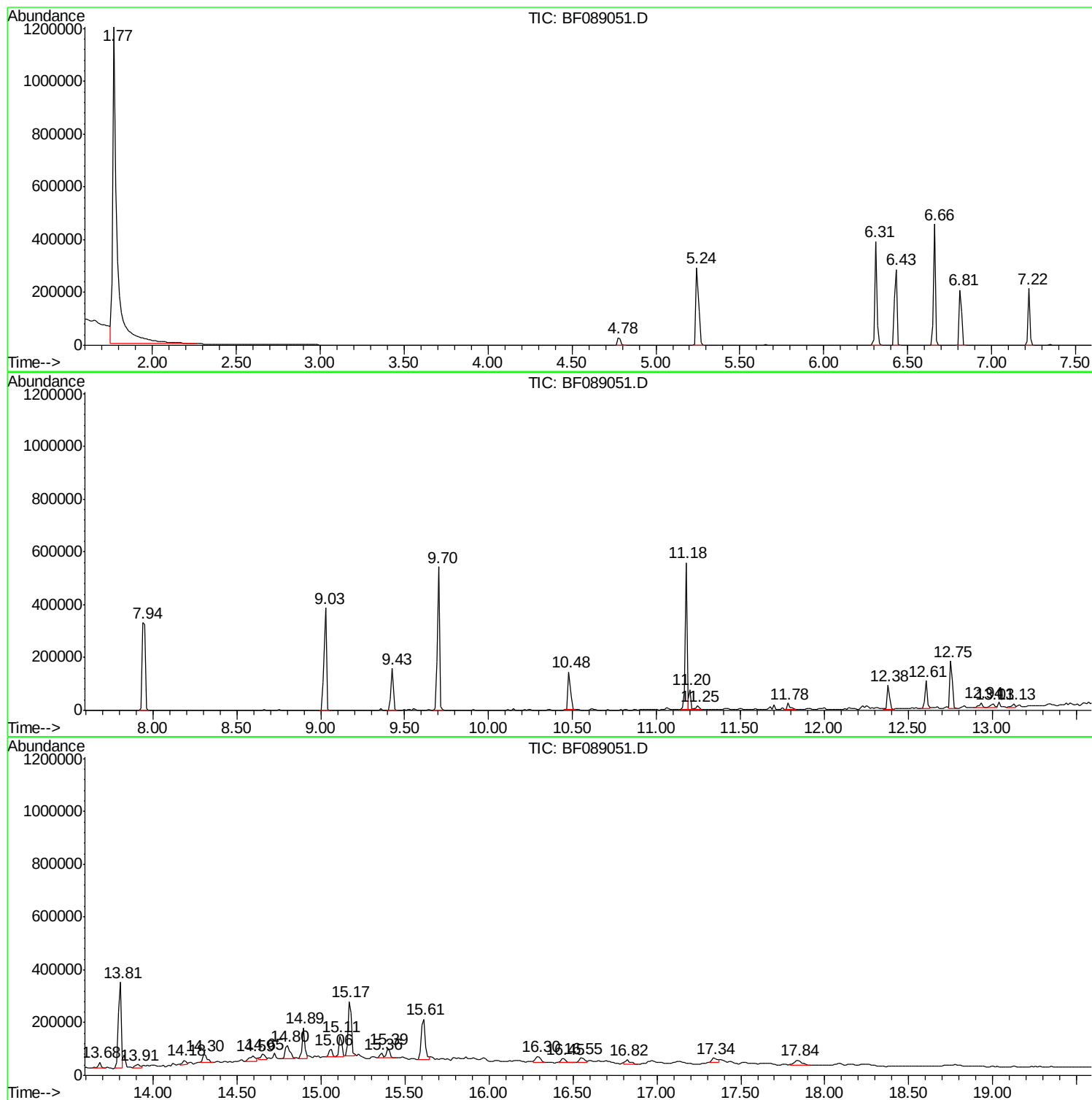
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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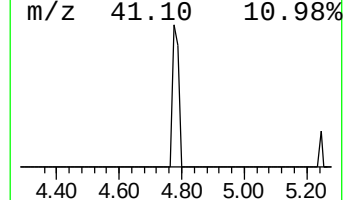
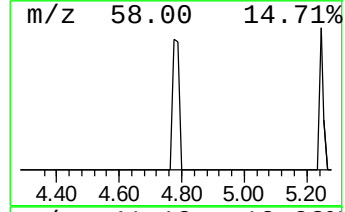
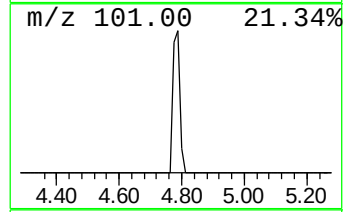
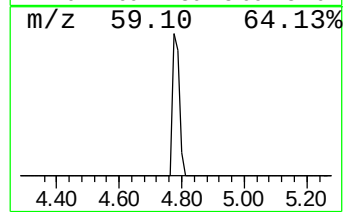
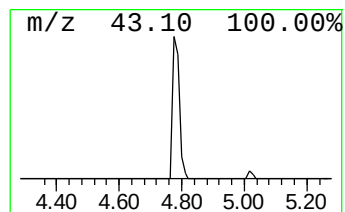
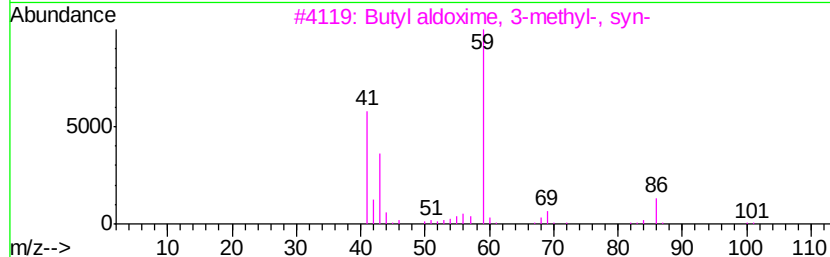
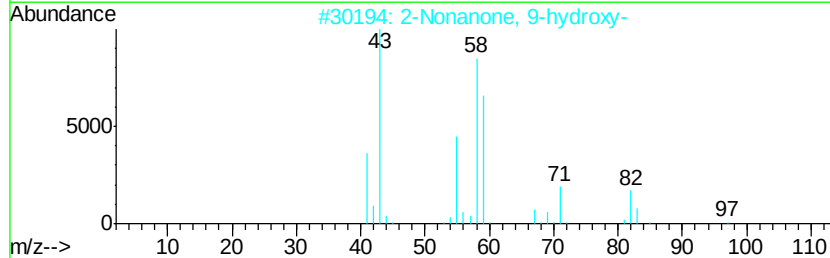
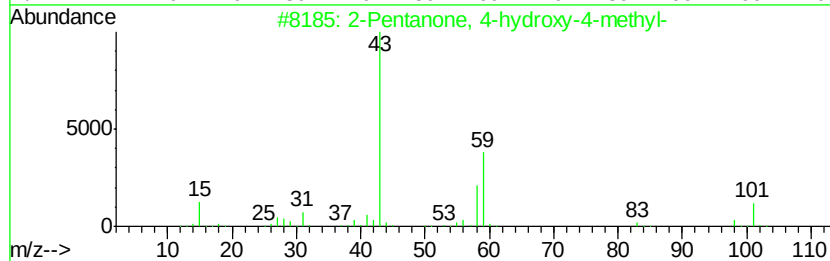
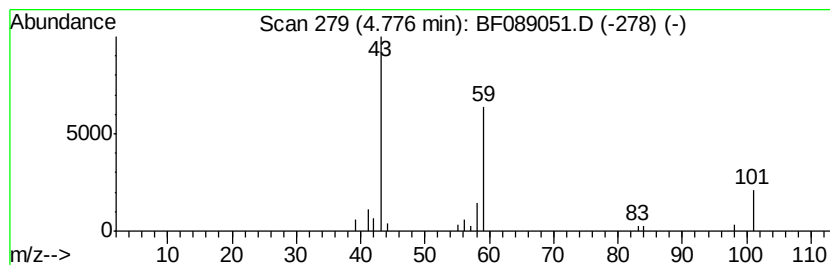
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	2.17 ng	40963	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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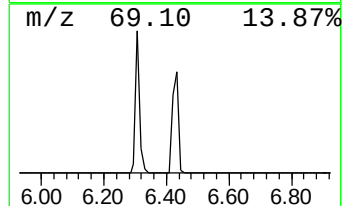
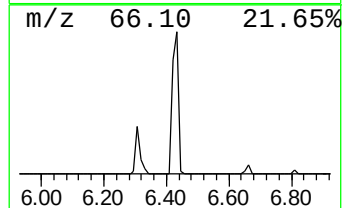
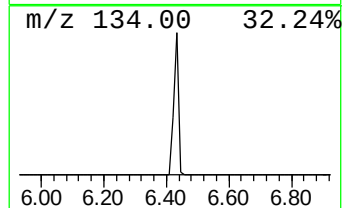
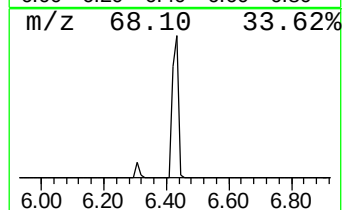
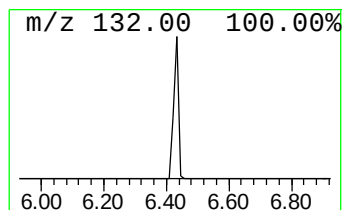
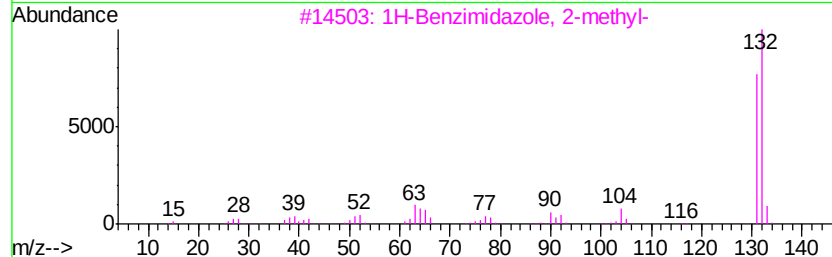
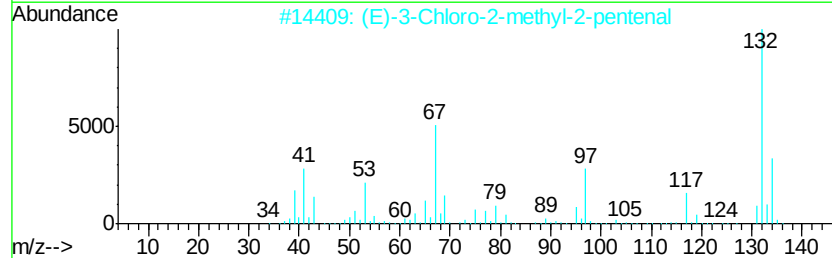
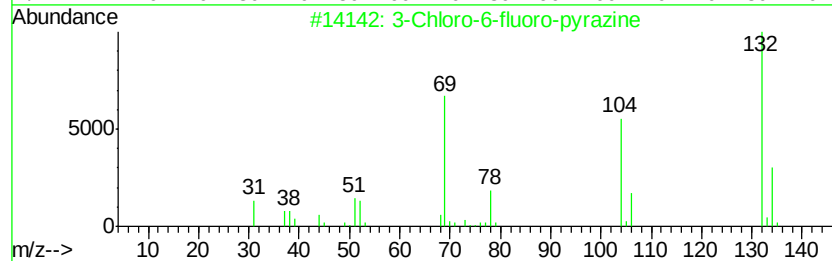
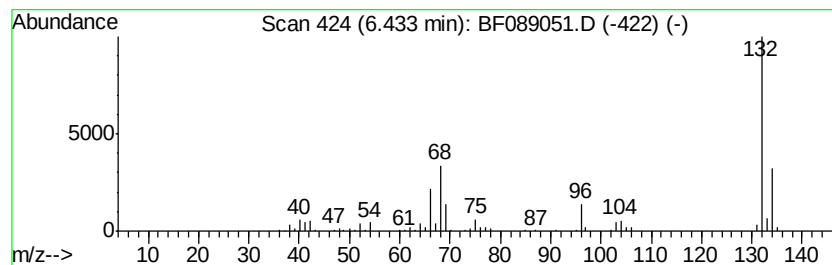
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Peak Number 3 unknown6.43 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	16.94 ng	319868	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	10
4	(5-Methyl-2-pyridyl)acetonitrile			132	C8H8N2	1000241-93-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9



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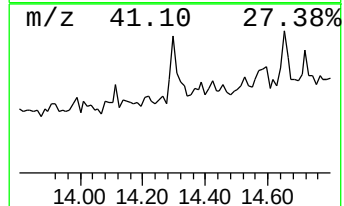
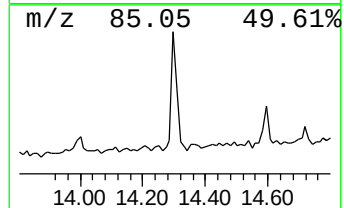
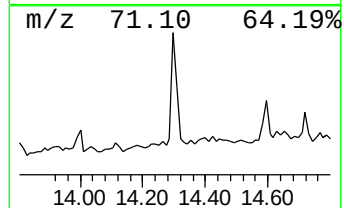
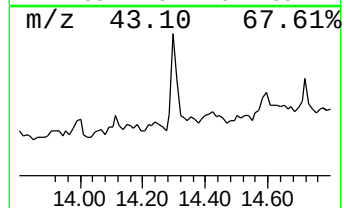
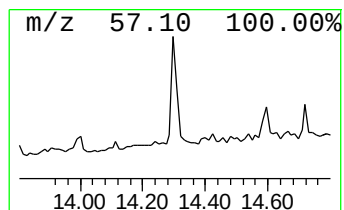
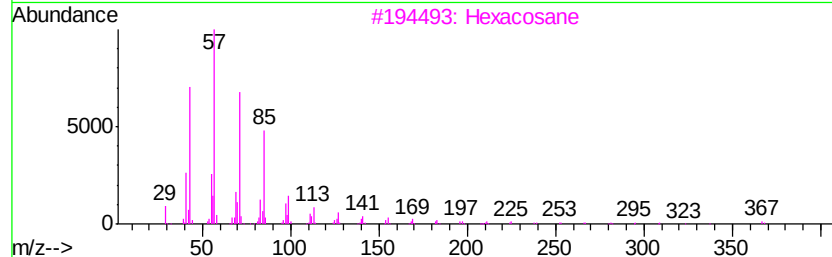
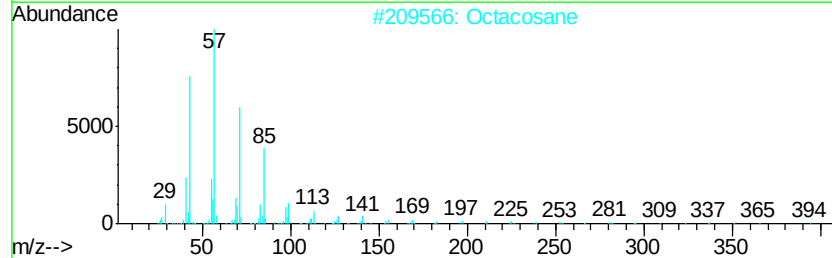
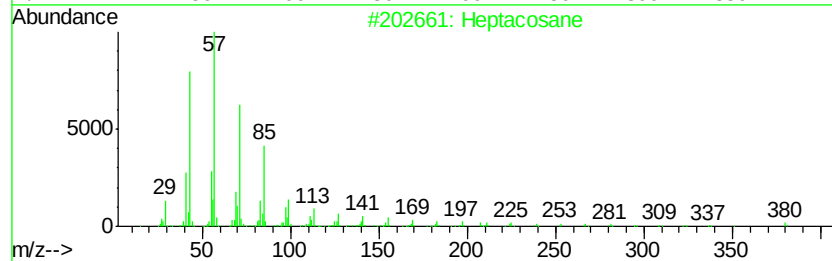
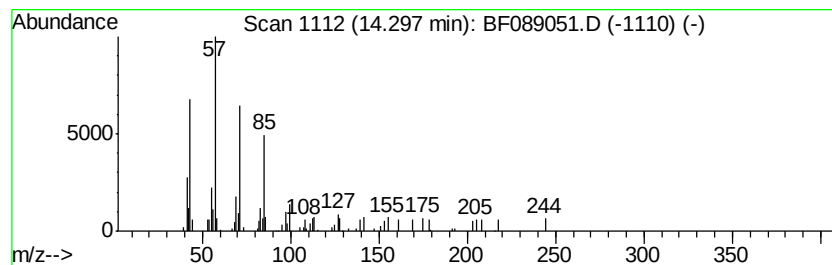
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.73 ng	55010	Chrysene-d12	13.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	81
2	Octacosane		394	C28H58	000630-02-4	74
3	Hexacosane		366	C26H54	000630-01-3	74
4	Heneicosane		296	C21H44	000629-94-7	74
5	Hentriacontane		437	C31H64	000630-04-6	72



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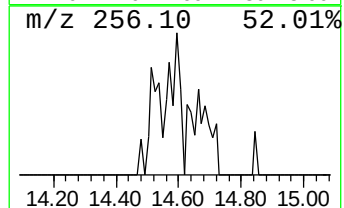
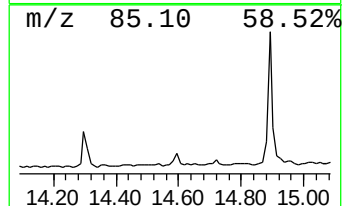
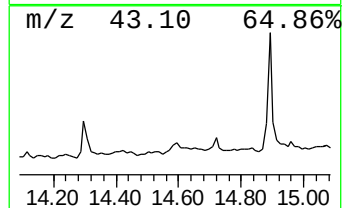
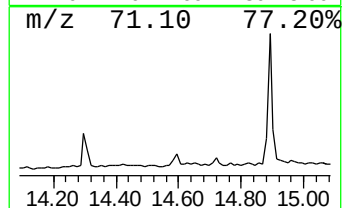
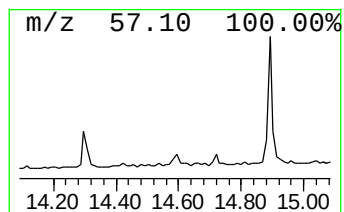
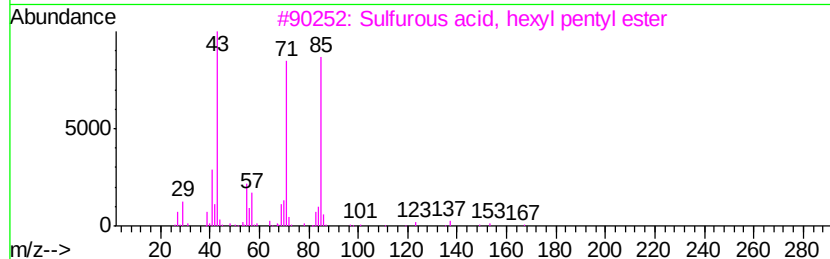
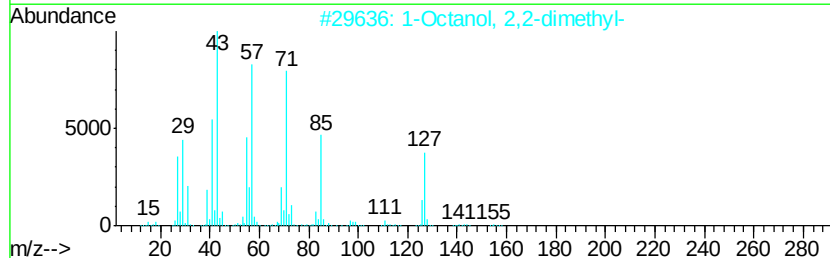
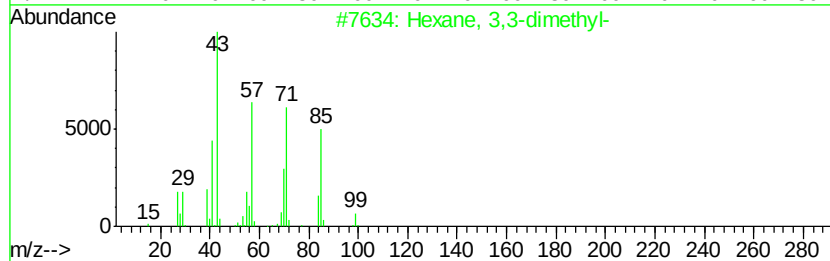
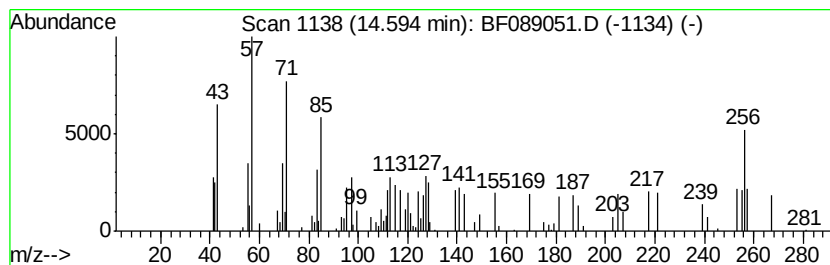
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown14.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.54 ng	52061	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	27
2		1-Octanol, 2,2-dimethyl-	158	C10H22O	002370-14-1	27
3		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	27
4		5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	27
5		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	27



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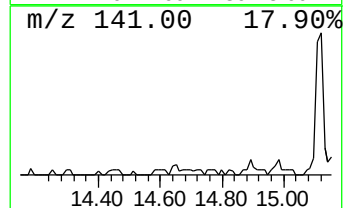
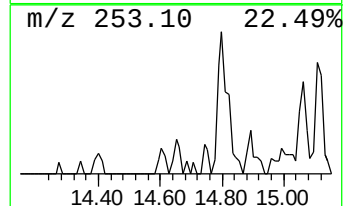
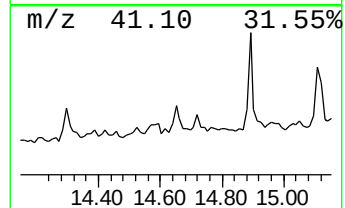
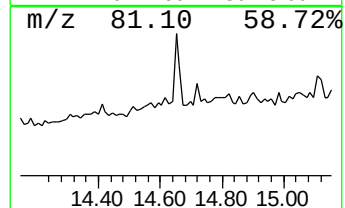
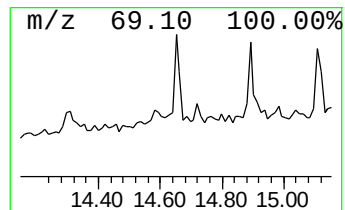
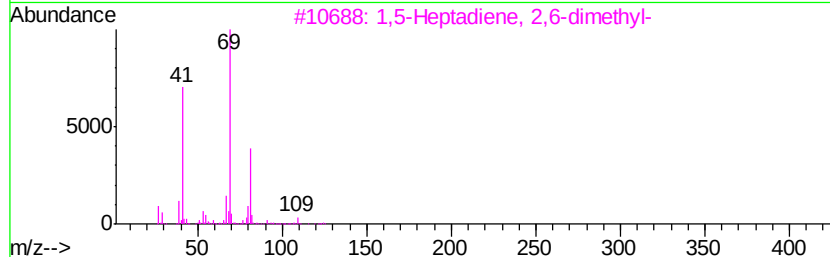
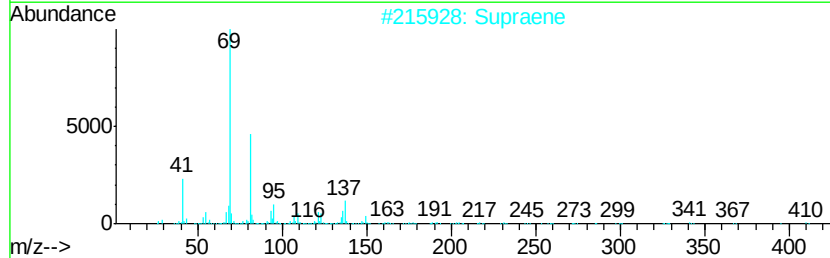
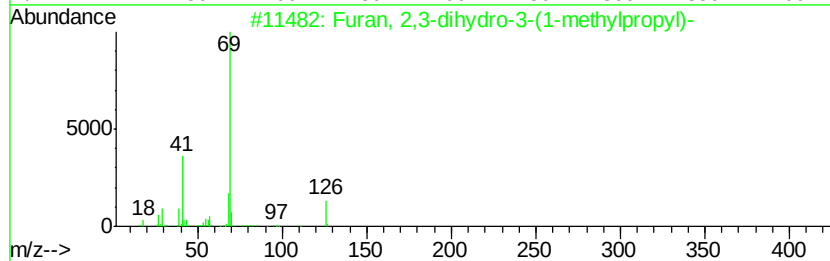
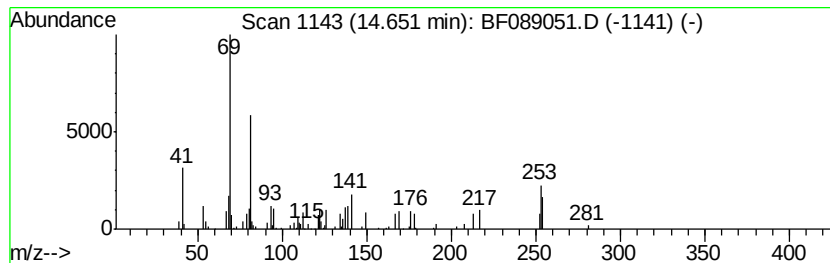
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Peak Number 7 unknown14.65 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.54 ng	37360	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, 2,3-dihydro-3-(1-methylpr...	126	C8H14O	056805-32-4	38
2		Supraene	410	C30H50	007683-64-9	38
3		1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	35
4		1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	35
5		3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089051.D
Acq On : 16 Jul 2016 13:07
Operator : UM/SJ
Sample : H3951-04 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSS-SB-SB02(0-2in)

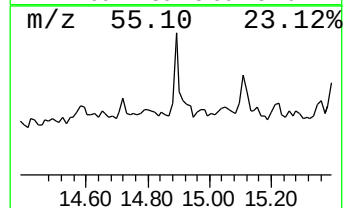
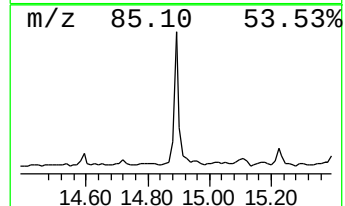
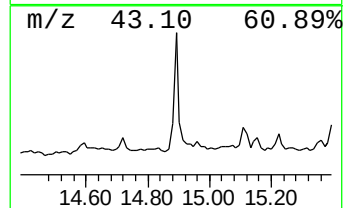
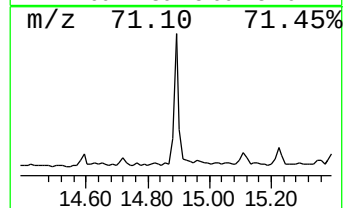
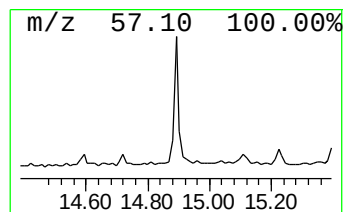
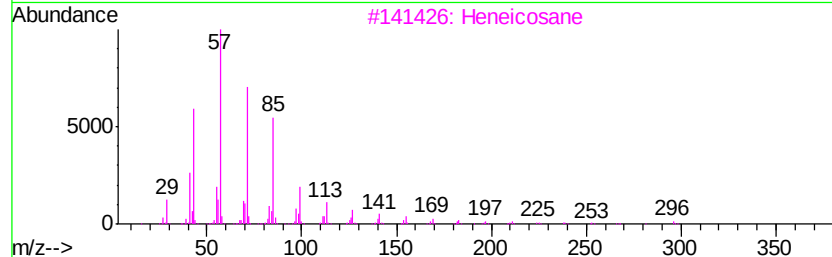
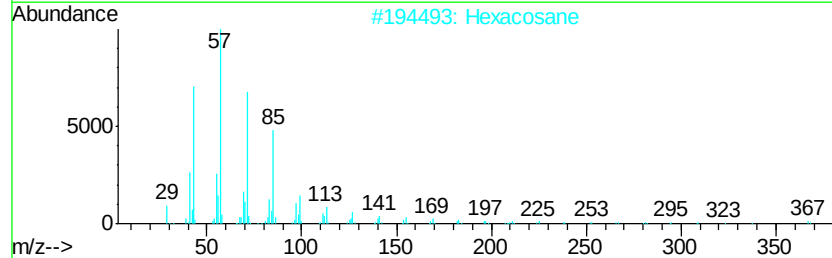
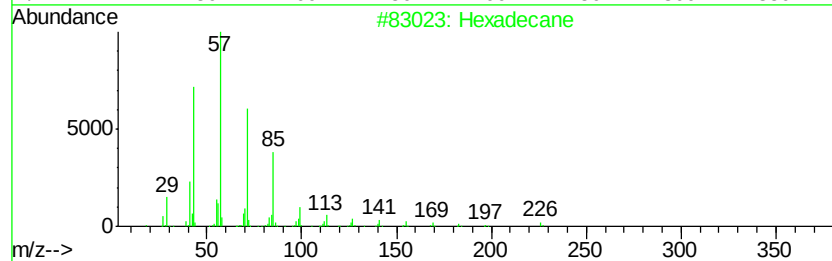
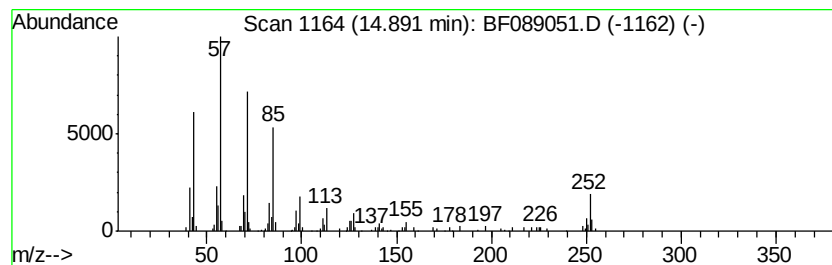
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	8.39 ng	123283	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	94
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		triacontane	422	C30H62	000638-68-6	86
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
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Sample : H3951-04 5X
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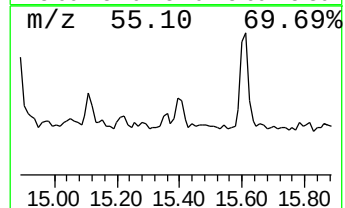
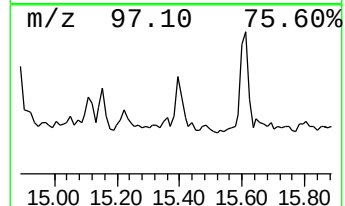
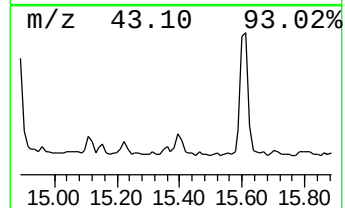
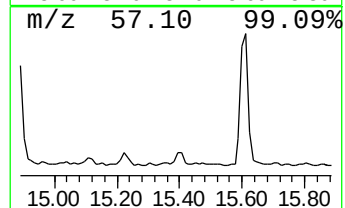
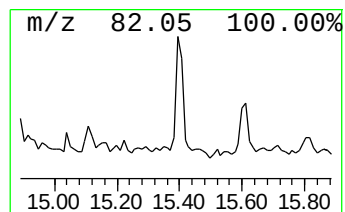
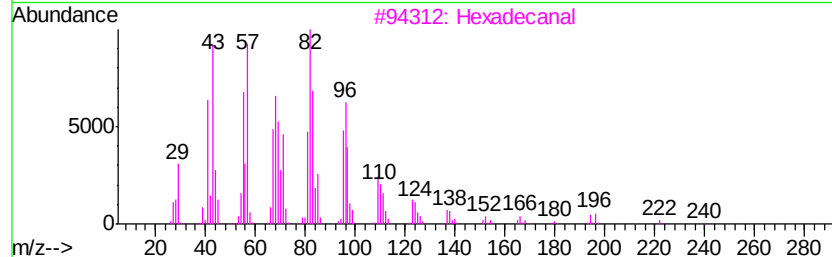
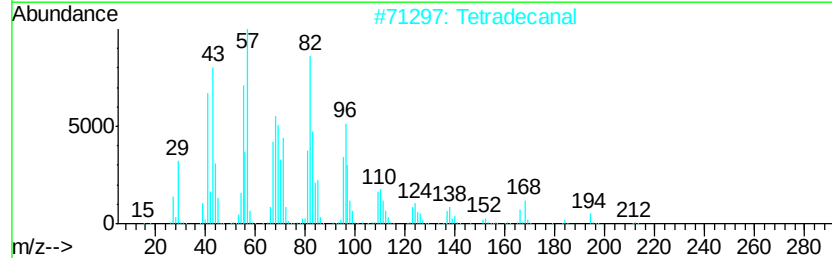
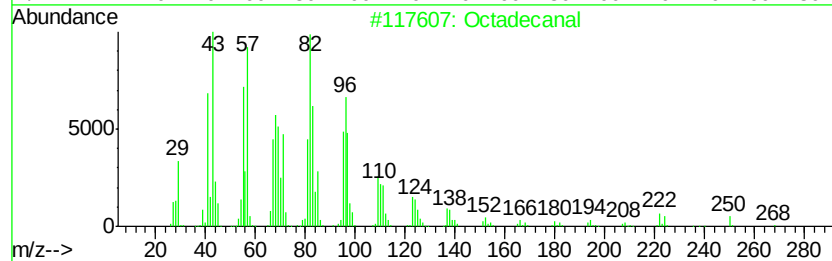
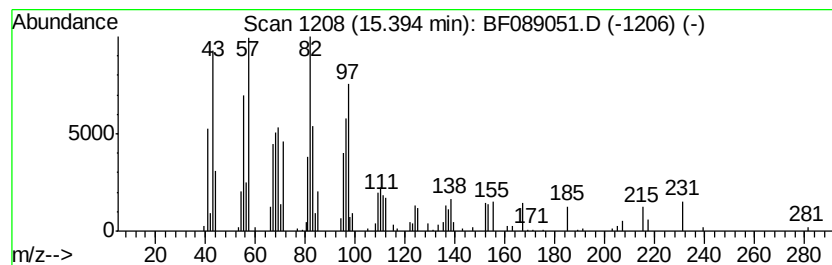
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.39	3.75 ng	55122	Perylene-d12		15.17
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	87
2	Tetradecanal	212	C14H28O	000124-25-4	83
3	Hexadecanal	240	C16H32O	000629-80-1	80
4	Heptadecanal	254	C17H34O	1000376-70-0	74
5	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089051.D
Acq On : 16 Jul 2016 13:07
Operator : UM/SJ
Sample : H3951-04 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

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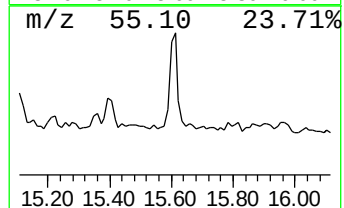
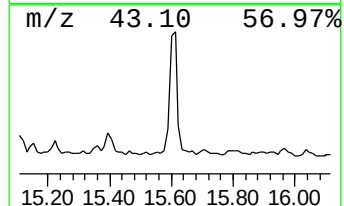
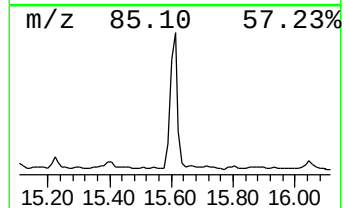
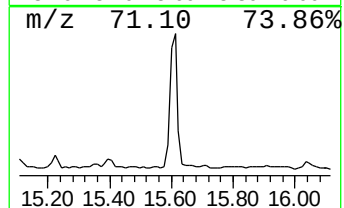
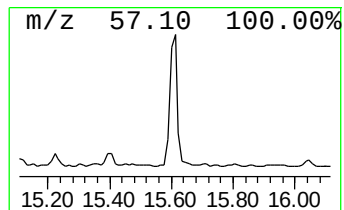
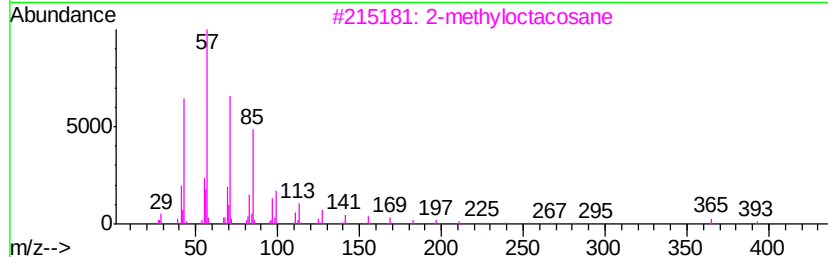
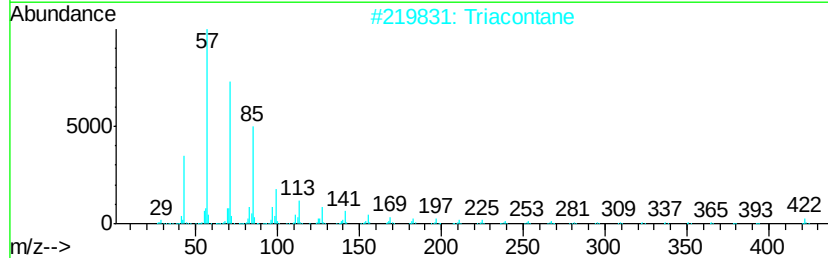
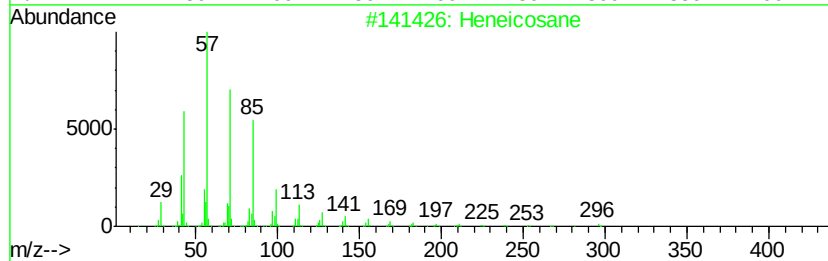
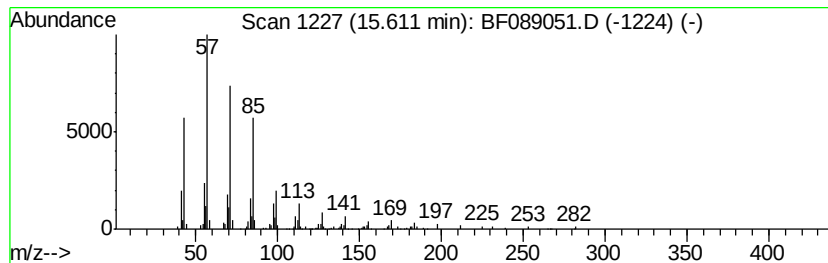
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	17.80 ng	261563	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089051.D
Acq On : 16 Jul 2016 13:07
Operator : UM/SJ
Sample : H3951-04 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-SB-SB02(0-2in)

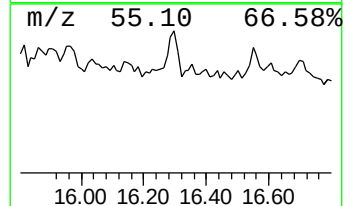
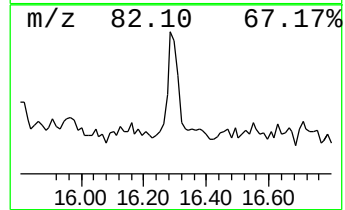
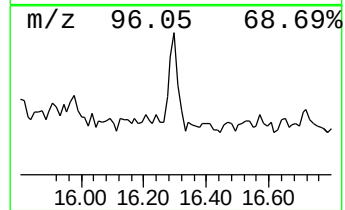
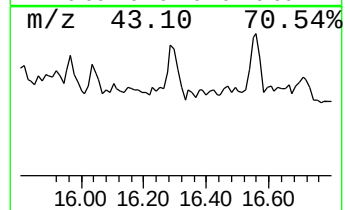
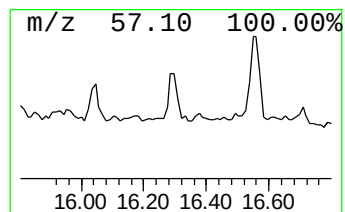
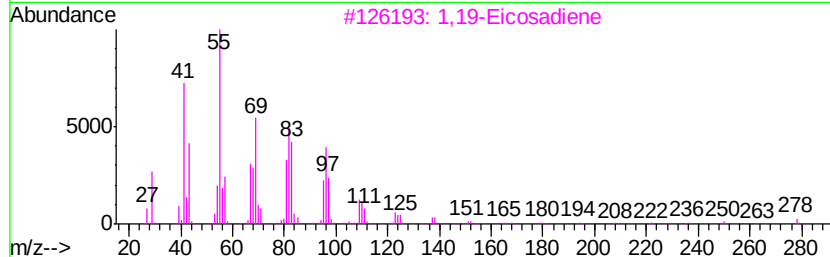
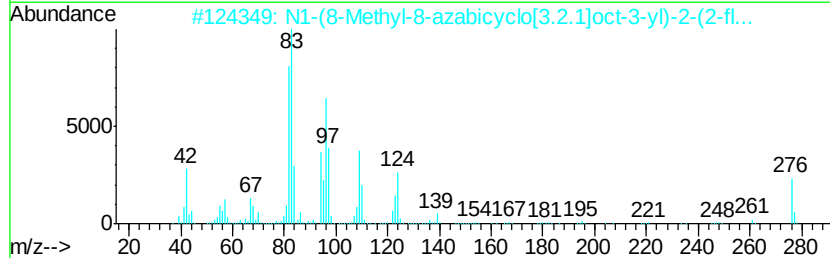
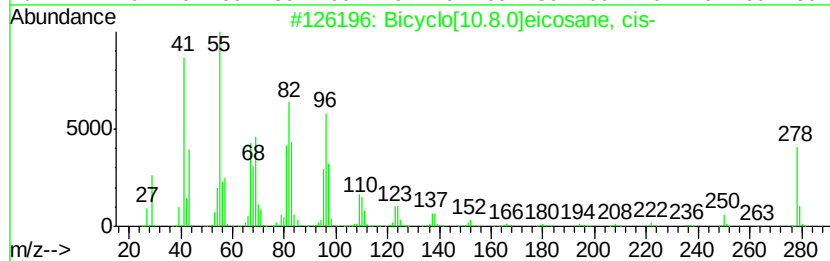
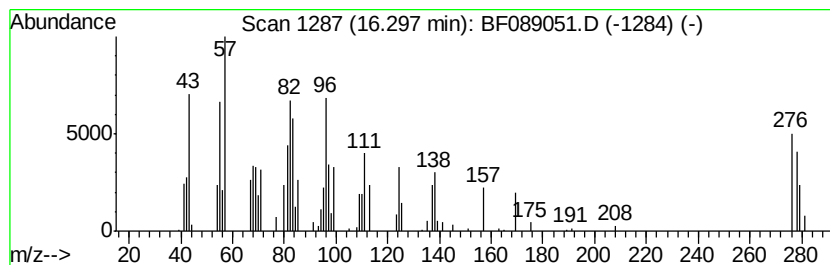
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	3.07 ng	45083	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	30
2		N1-(8-Methyl-8-azabicyclo[3.2.1]...	276	C16H21FN2O	247565-70-4	22
3		1,19-Eicosadiene	278	C20H38	014811-95-1	22
4		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	18
5		Z-2-Octadecen-1-ol acetate	310	C20H38O2	1000131-08-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089051.D
Acq On : 16 Jul 2016 13:07
Operator : UM/SJ
Sample : H3951-04 5X
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Instrument :
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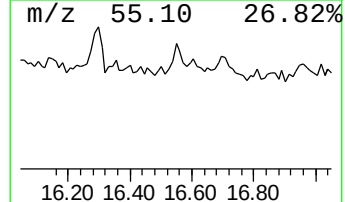
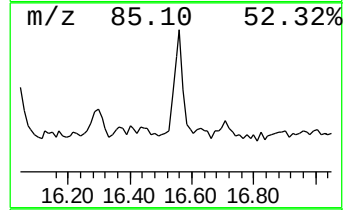
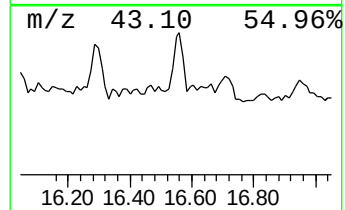
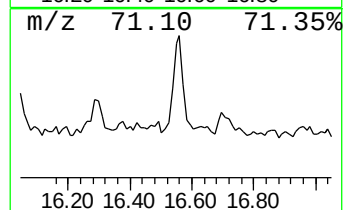
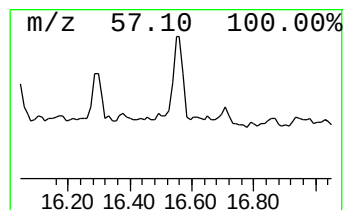
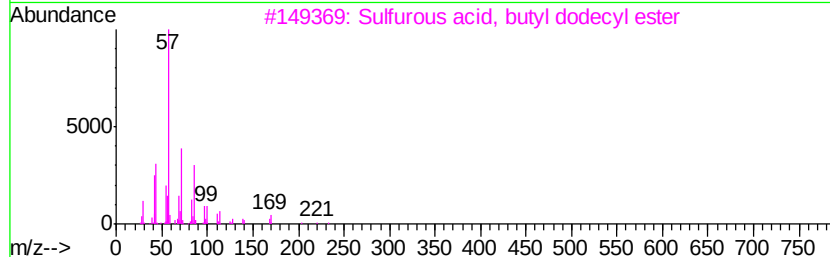
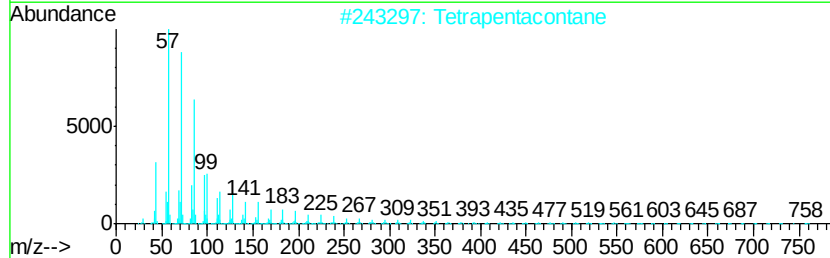
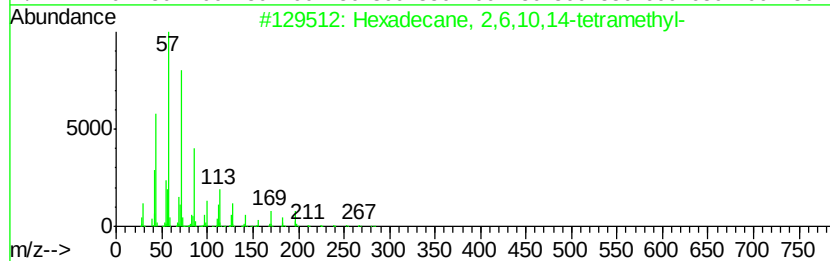
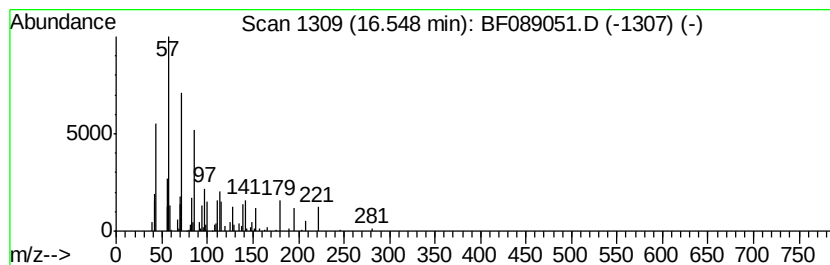
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.55 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.28 ng	33524	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	47
2		Tetrapentacontane	759	C54H110	005856-66-6	47
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	43
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	38
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089051.D
Acq On : 16 Jul 2016 13:07
Operator : UM/SJ
Sample : H3951-04 5X
Misc :
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ClientSampleId :
LSS-SB-SB02(0-2in)

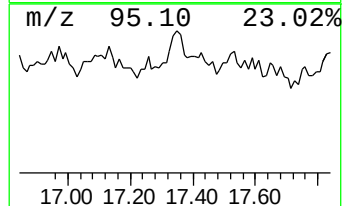
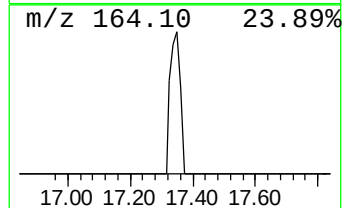
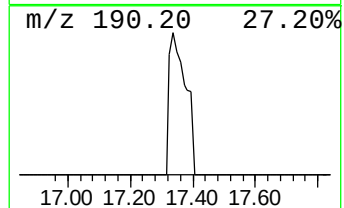
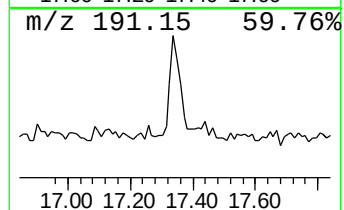
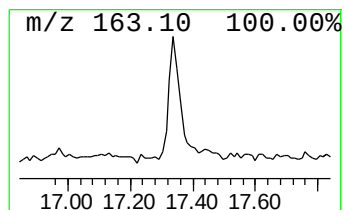
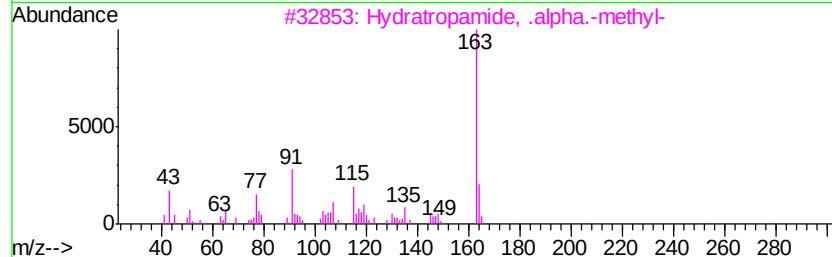
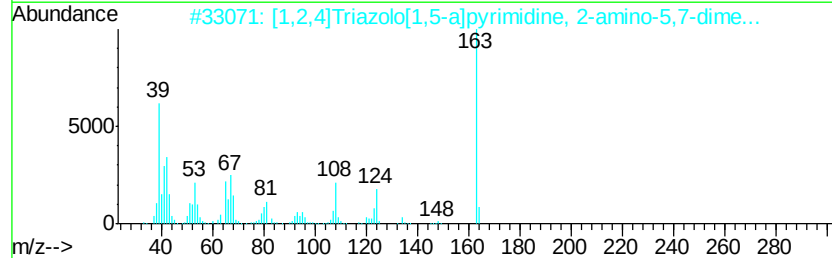
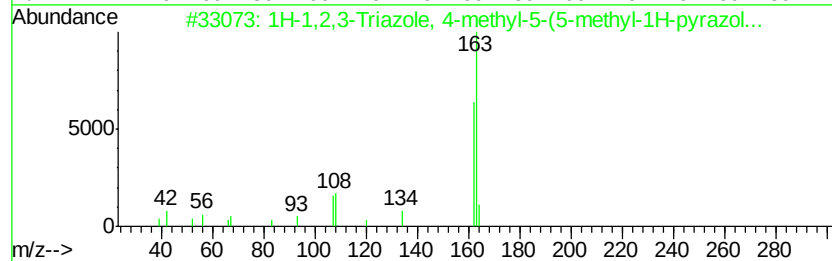
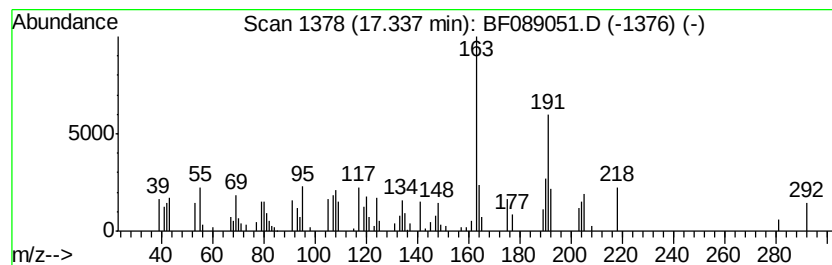
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.34 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.57 ng	37842	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-1,2,3-Triazole, 4-methyl-5-(5...	163	C7H9N5	051719-86-9	27
2		[1,2,4]Triazolo[1,5-a]pyrimidine...	163	C7H9N5	007135-02-6	27
3		Hydratropamide, .alpha.-methyl-	163	C10H13NO	000826-54-0	25
4		4-Aminocinnamic acid	163	C9H9NO2	002393-18-2	22
5		Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089051.D
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LSS-SB-SB02(0-2in)

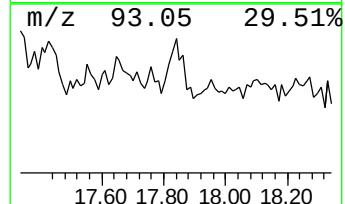
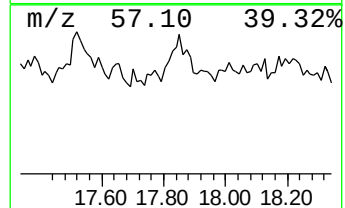
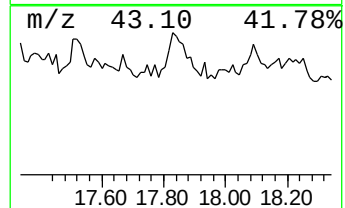
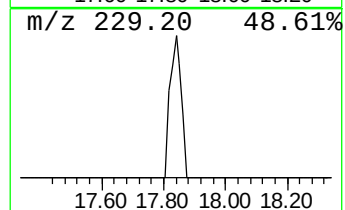
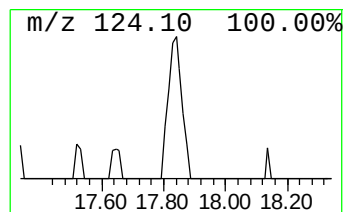
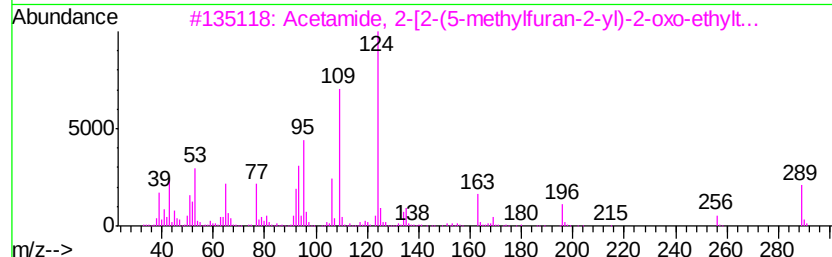
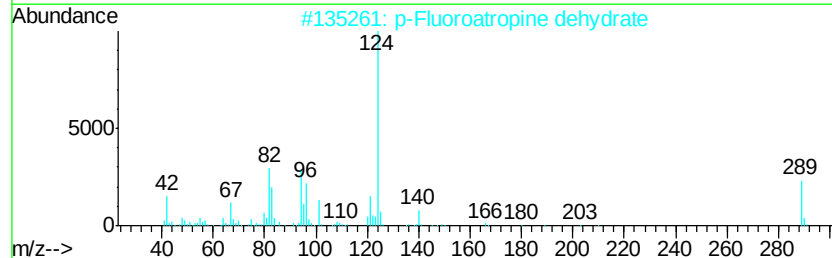
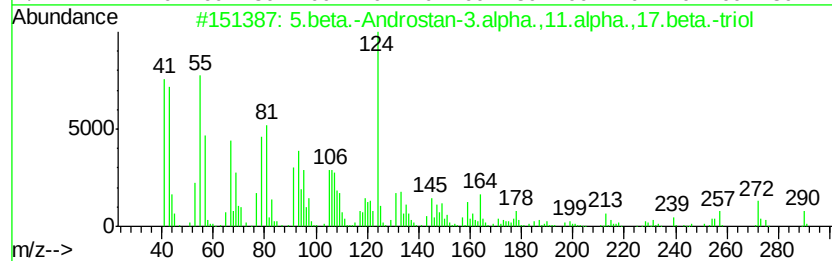
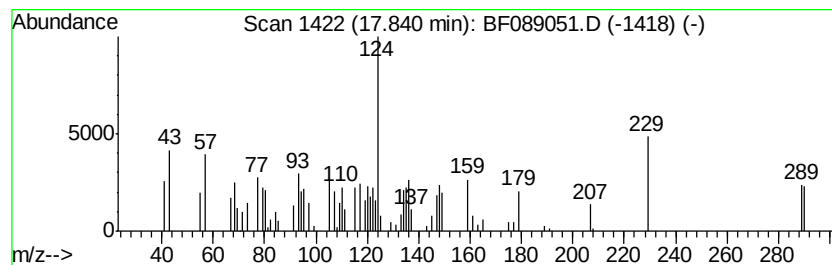
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.84 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	4.49 ng	65923	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5.beta.-Androstan-3.alpha.,11.alpha.,17.beta.-triol	308	C19H32O3	032212-61-6	16
2		p-Fluoroatropine dehydrate	289	C17H20FN02	1000212-74-8	12
3		Acetamide, 2-[2-(5-methylfuran-2-yl)-2-oxo-ethyl]-	289	C15H15N03S	1000259-79-3	12
4		4H-Pyran-4-one, 3,5-dimethyl-	124	C7H8O2	019083-61-5	11
5		Isonicotinic acid, octyl ester	235	C14H21N02	1000299-88-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
 Data File : BF089051.D
 Acq On : 16 Jul 2016 13:07
 Operator : UM/SJ
 Sample : H3951-04 5X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LSS-SB-SB02(0-2in)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
 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
2-Pentanone, 4-hy...	4.78	2.2	ng	40963	1	6.66	377716	20.0
unknown6.43	6.43	16.9	ng	319868	1	6.66	377716	20.0
Heptacosane	14.30	2.7	ng	55010	5	13.81	402869	20.0
unknown14.59	14.59	3.5	ng	52061	6	15.17	293971	20.0
unknown14.65	14.65	2.5	ng	37360	6	15.17	293971	20.0
Hexadecane	14.89	8.4	ng	123283	6	15.17	293971	20.0
Octadecanal	15.39	3.8	ng	55122	6	15.17	293971	20.0
Heneicosane	15.61	17.8	ng	261563	6	15.17	293971	20.0
unknown16.30	16.30	3.1	ng	45083	6	15.17	293971	20.0
unknown16.55	16.55	2.3	ng	33524	6	15.17	293971	20.0
unknown17.34	17.34	2.6	ng	37842	6	15.17	293971	20.0
unknown17.84	17.84	4.5	ng	65923	6	15.17	293971	20.0