

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
 Data File : BF089263.D
 Acq On : 24 Jul 2016 6:35
 Operator : UM/SJ
 Sample : H4151-08
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-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-BF072016.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	1.712	9	11	47	rVB	425764	898669	65.18%	7.459%
2	4.707	270	273	281	rBV	40487	67476	4.89%	0.560%
3	5.164	311	313	331	rBV	855635	1227748	89.04%	10.190%
4	6.239	405	407	414	rBV	1010447	1306808	94.78%	10.846%
5	6.342	414	416	419	rBV	818139	1183348	85.82%	9.822%
6	6.582	434	437	448	rVB	207337	259279	18.80%	2.152%
7	6.730	448	450	453	rBV	900064	916005	66.43%	7.603%
8	7.153	485	487	502	rBV	616538	824628	59.81%	6.844%
9	7.862	547	549	560	rBV	384133	387451	28.10%	3.216%
10	8.947	641	644	646	rBV	1174077	1378828	100.00%	11.444%
11	9.336	676	678	681	rBV	139893	163057	11.83%	1.353%
12	9.610	699	702	704	rBV	365995	382729	27.76%	3.177%
13	10.388	768	770	773	rBV2	434542	642698	46.61%	5.334%
14	10.525	781	782	787	rVB	17421	24572	1.78%	0.204%
15	10.971	819	821	823	rBV	19479	19837	1.44%	0.165%
16	11.085	829	831	841	rVB	246842	326220	23.66%	2.708%
17	12.285	934	936	939	rBB	16497	15369	1.11%	0.128%
18	12.502	953	955	958	rBV2	157338	160734	11.66%	1.334%
19	12.582	961	962	964	rVB	24119	17927	1.30%	0.149%
20	12.662	967	969	972	rBV	847959	810213	58.76%	6.725%
21	13.211	1015	1017	1019	rBV	91899	86058	6.24%	0.714%
22	13.257	1019	1021	1025	rVB	12120	21113	1.53%	0.175%
23	13.371	1029	1031	1033	rBV	16219	14724	1.07%	0.122%
24	13.577	1047	1049	1057	rBV	46319	81038	5.88%	0.673%
25	13.702	1057	1060	1067	rVV	242810	273395	19.83%	2.269%
26	13.897	1075	1077	1079	rBV	17792	17365	1.26%	0.144%
27	14.011	1085	1087	1092	rVB	9655	14023	1.02%	0.116%
28	14.194	1101	1103	1110	rBV3	12407	38398	2.78%	0.319%
29	14.491	1124	1129	1132	rBV2	20298	31496	2.28%	0.261%
30	14.685	1144	1146	1151	rBV	10746	25839	1.87%	0.214%
31	14.777	1152	1154	1156	rBV	22031	21347	1.55%	0.177%
32	15.040	1175	1177	1180	rVV	159986	239093	17.34%	1.984%
33	15.097	1180	1182	1184	rVB	18781	24859	1.80%	0.206%
34	15.451	1210	1213	1216	rBV	16703	26446	1.92%	0.219%

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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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35	15.862	1246	1249	1256	rVB2	11737	24907	1.81%	0.207%
36	16.343	1287	1291	1295	rBV3	6056	15469	1.12%	0.128%
37	16.743	1322	1326	1327	rBV	9096	20165	1.46%	0.167%
38	16.777	1327	1329	1332	rVV2	10317	20690	1.50%	0.172%
39	16.891	1336	1339	1344	rVV3	8725	20135	1.46%	0.167%
40	16.994	1346	1348	1355	rVB7	5494	18238	1.32%	0.151%

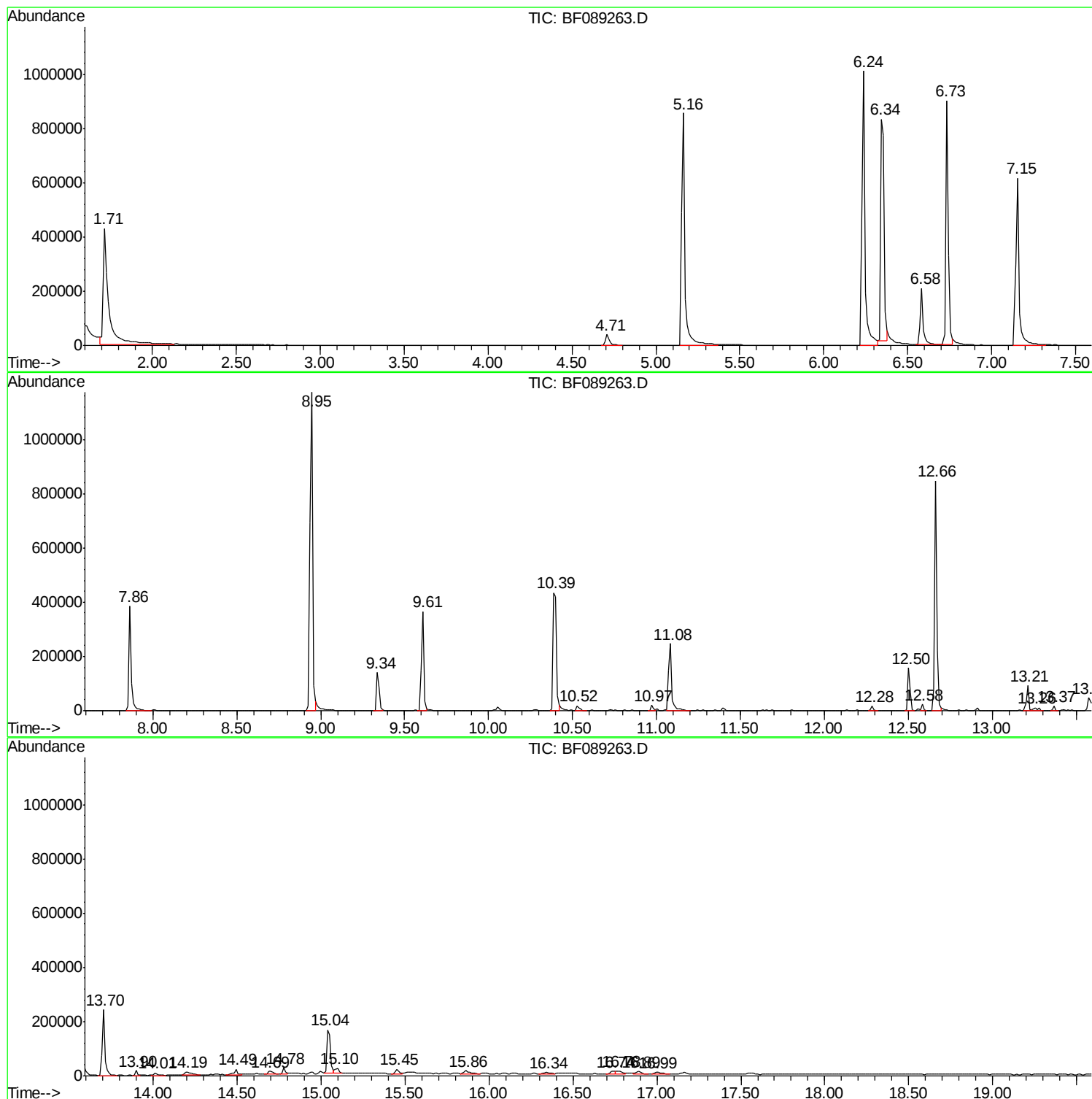
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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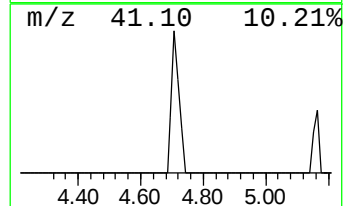
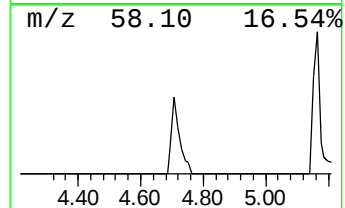
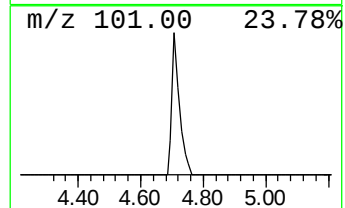
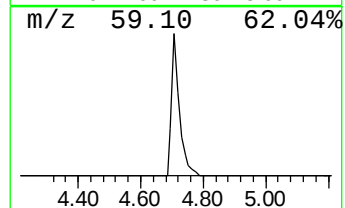
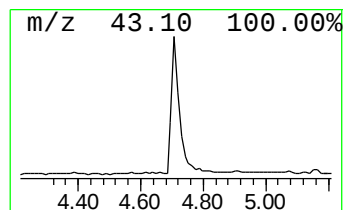
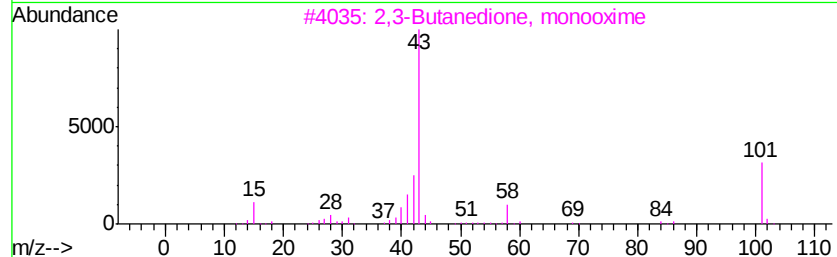
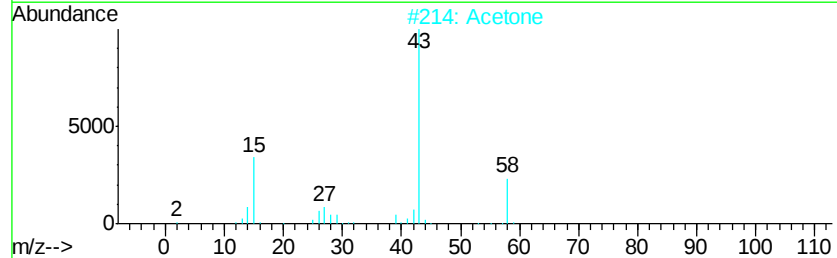
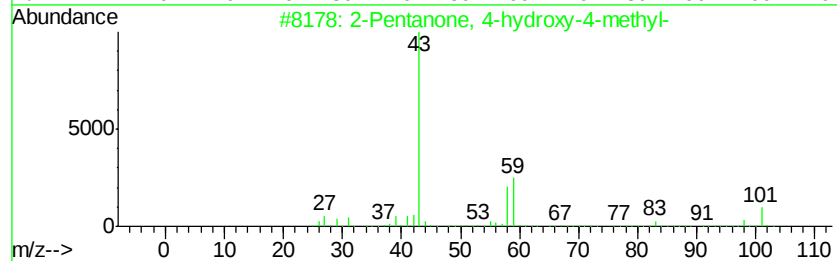
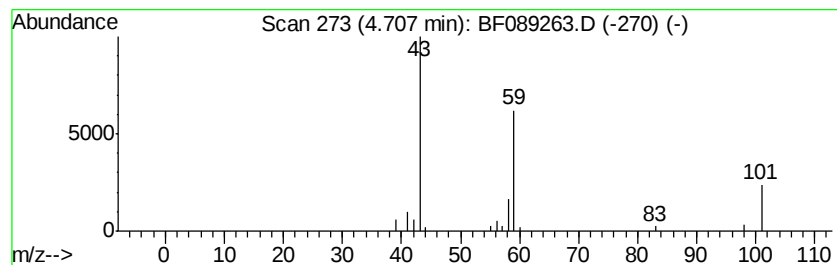
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	5.20 ng	67476	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetone	58	C3H6O	000067-64-1	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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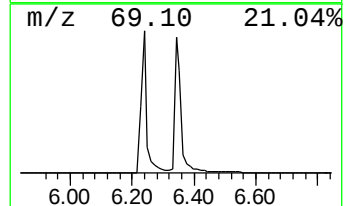
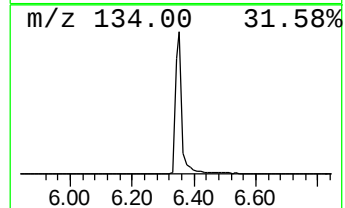
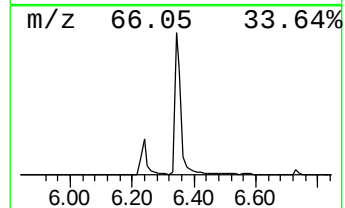
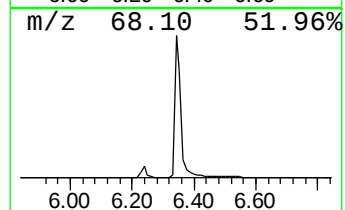
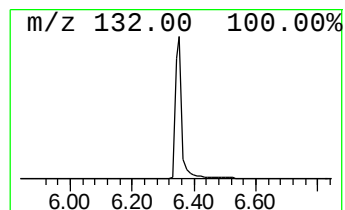
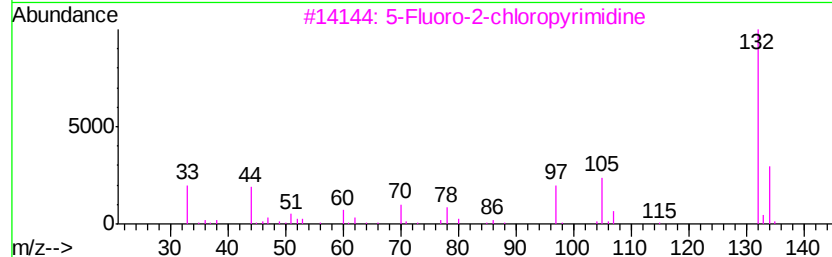
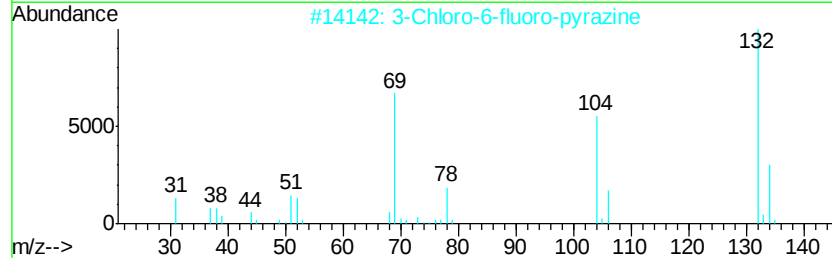
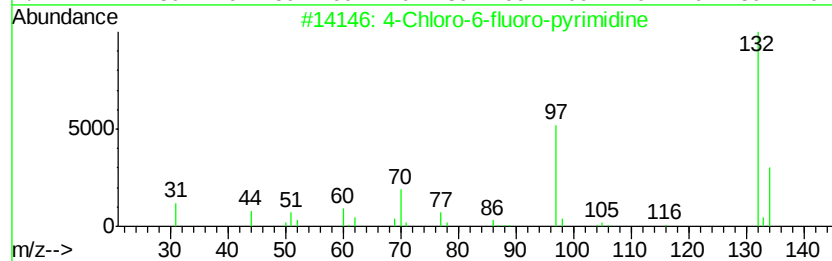
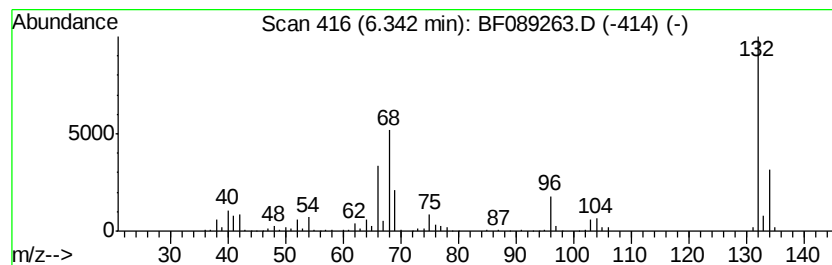
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Peak Number 3 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	91.28 ng	1183350	1,4-Dichlorobenzene-d4	6.58

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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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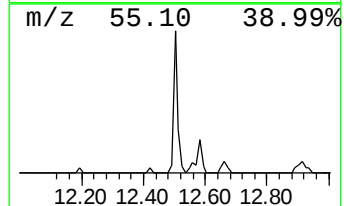
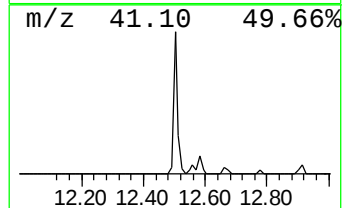
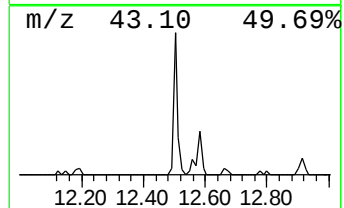
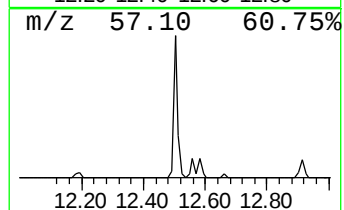
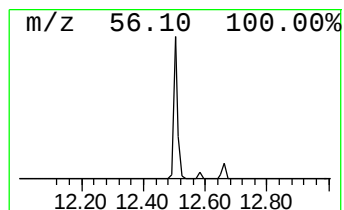
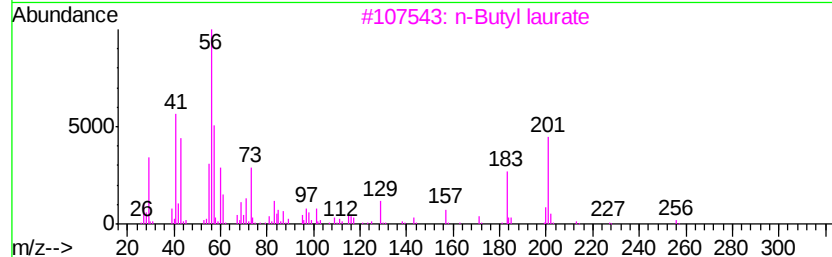
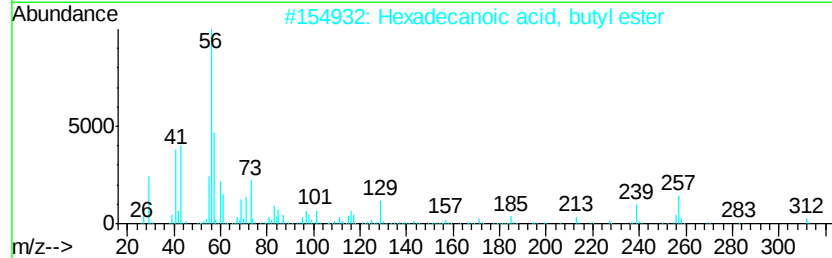
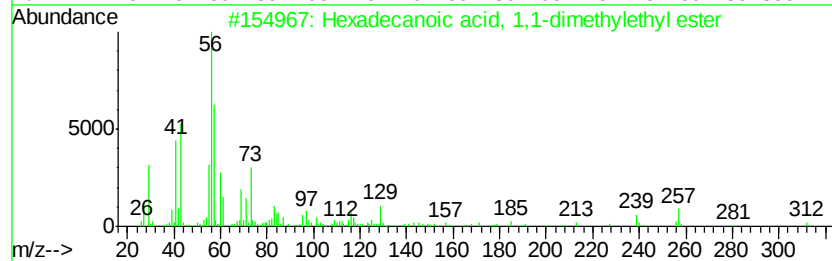
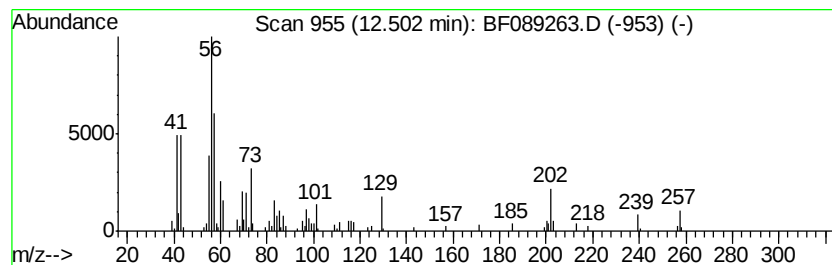
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	11.76 ng	160734	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	81
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
3		n-Butyl laurate	256	C16H32O2	000106-18-3	58
4		Dodecanoic acid tert-butyl ester	256	C16H32O2	007143-18-2	53
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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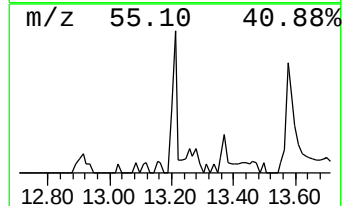
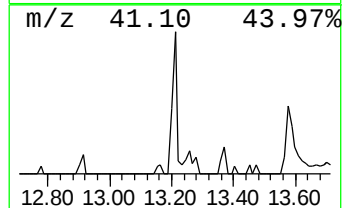
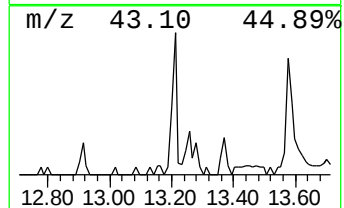
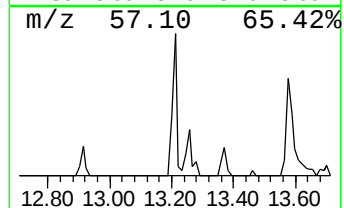
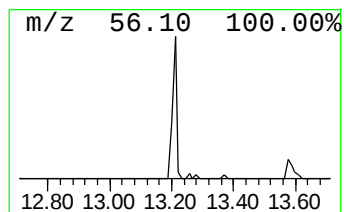
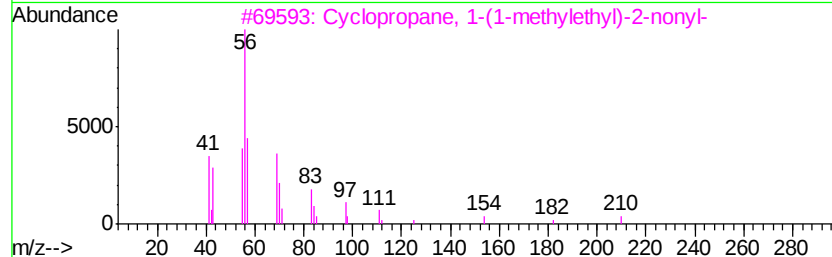
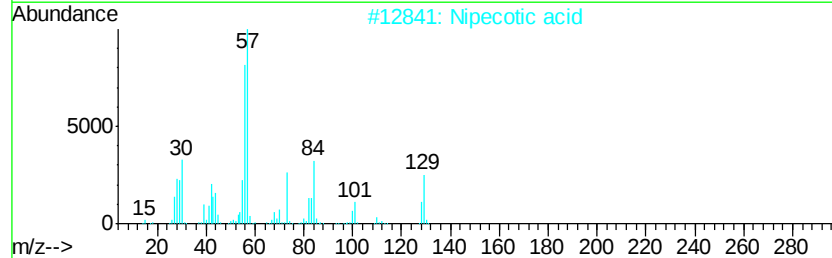
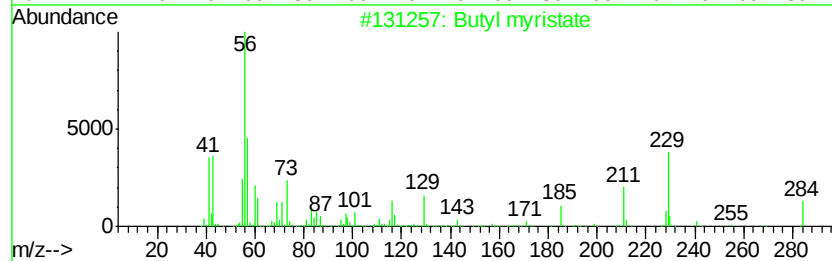
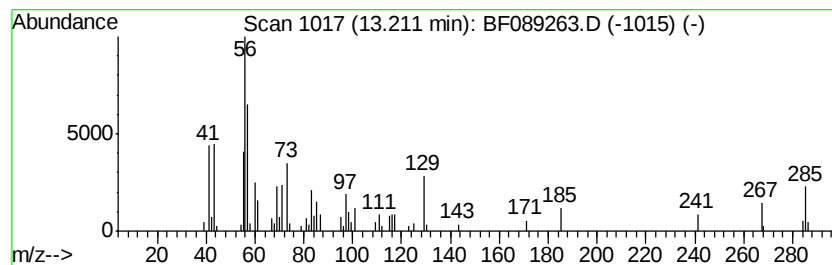
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Peak Number 6 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.21	6.30 ng	86058	Chrysene-d12	13.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	59
2	Nipecotic acid	129	C6H11NO2	000498-95-3	50
3	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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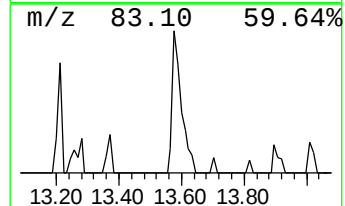
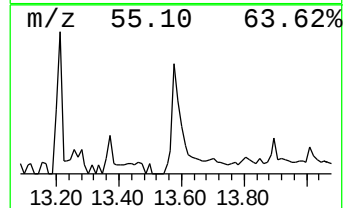
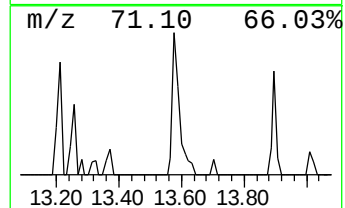
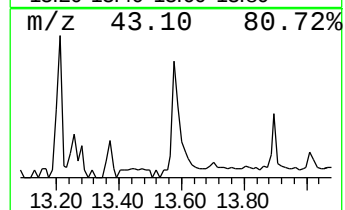
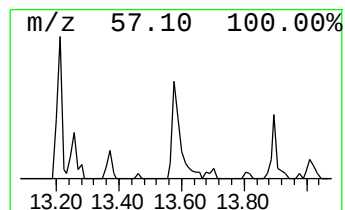
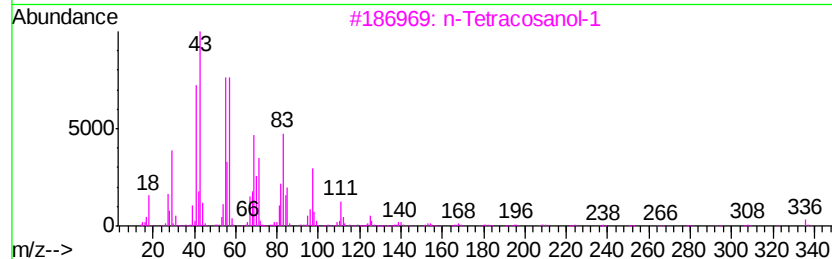
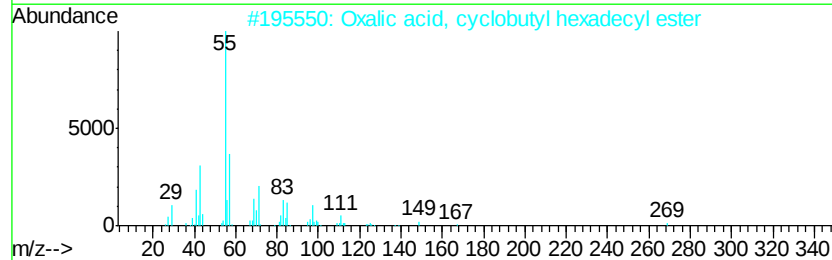
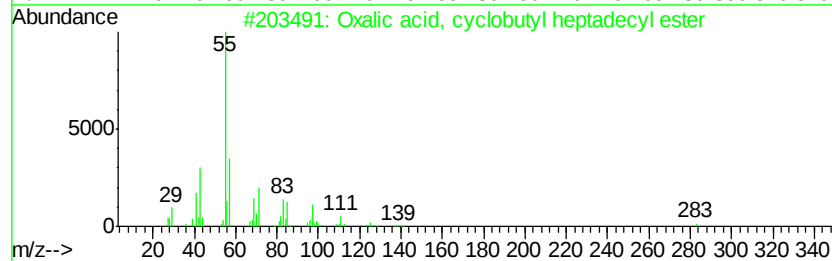
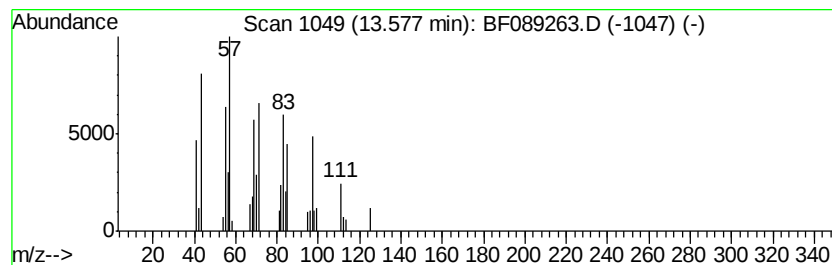
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Peak Number 7 Oxalic acid, cyclobutyl hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	5.93 ng	81038	Chrysene-d12	13.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	90
2			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	86
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	72
5			1-Hexacosanol	382	C26H54O	000506-52-5	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089263.D
Acq On : 24 Jul 2016 6:35
Operator : UM/SJ
Sample : H4151-08
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

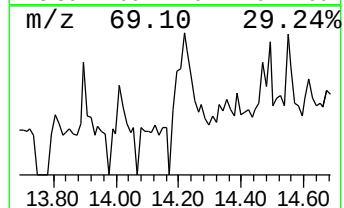
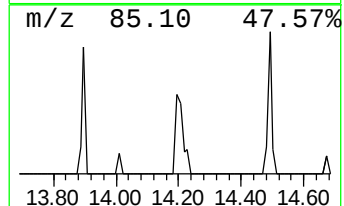
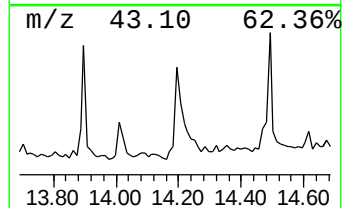
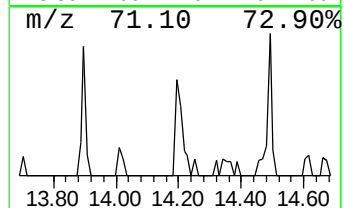
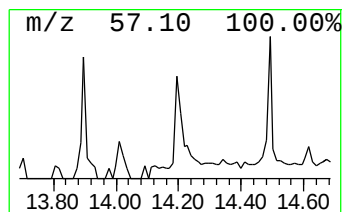
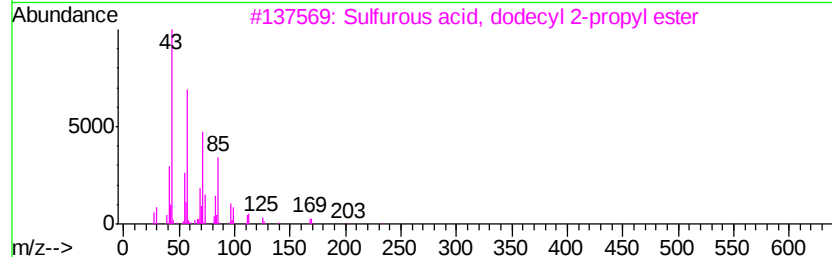
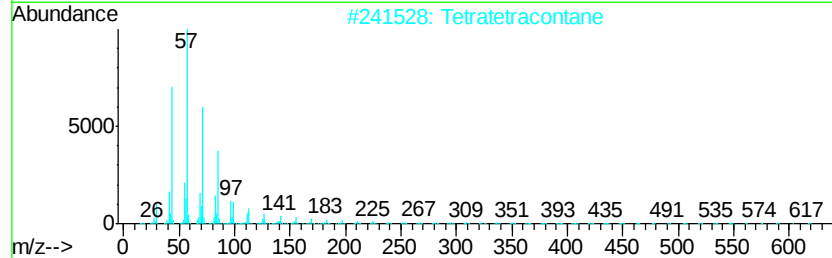
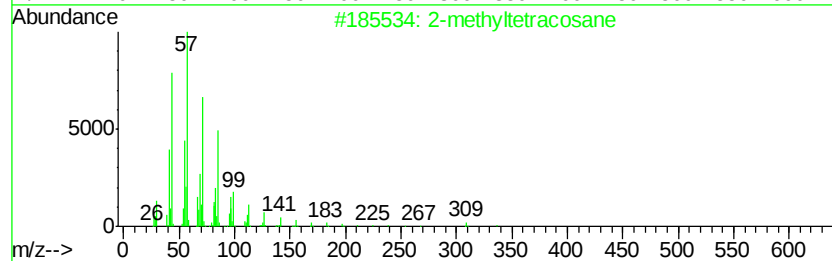
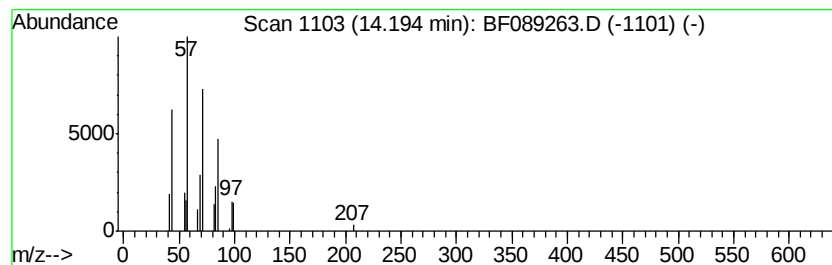
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyltetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.81 ng	38398	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyltetracosane	352	C25H52	1000376-72-6	78
2		Tetratetracontane	619	C44H90	007098-22-8	72
3		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	72
4		Tritetracontane	605	C43H88	007098-21-7	72
5		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
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Acq On : 24 Jul 2016 6:35
Operator : UM/SJ
Sample : H4151-08
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

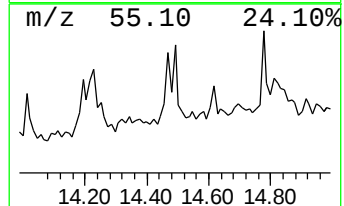
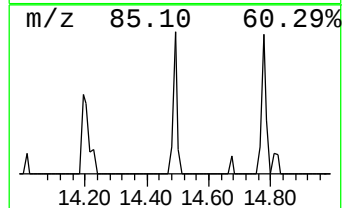
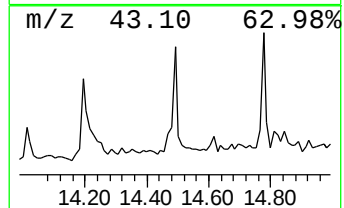
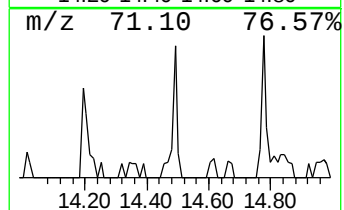
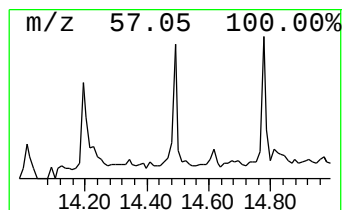
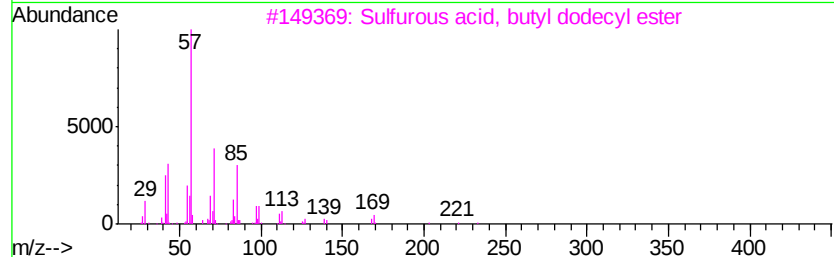
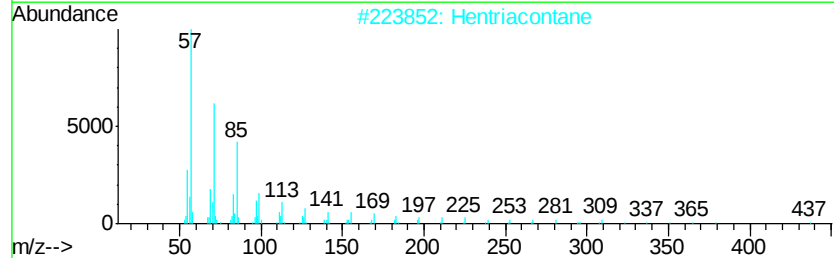
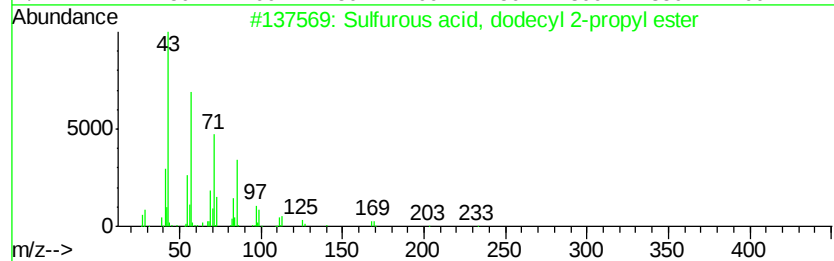
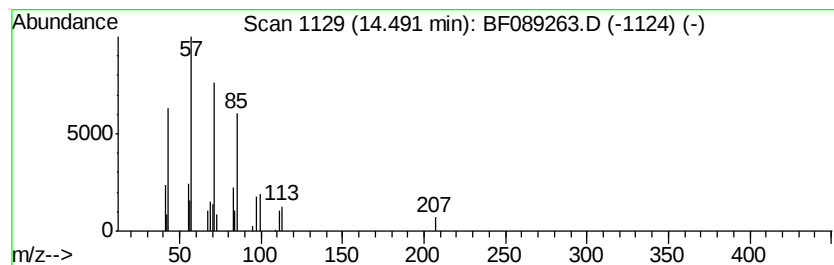
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, dodecyl 2-p... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.63 ng	31496	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	90
4		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86
5		Tritetracontane	605	C43H88	007098-21-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089263.D
Acq On : 24 Jul 2016 6:35
Operator : UM/SJ
Sample : H4151-08
Misc :
ALS Vial : 61 Sample Multiplier: 1

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ClientSampleId :
SB-06-COMP

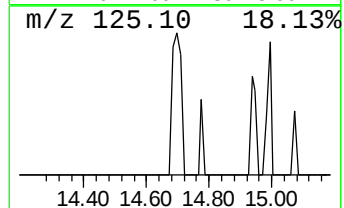
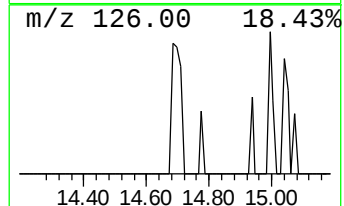
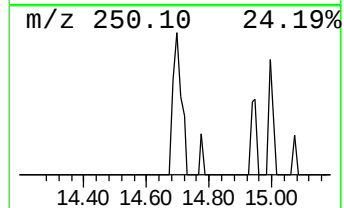
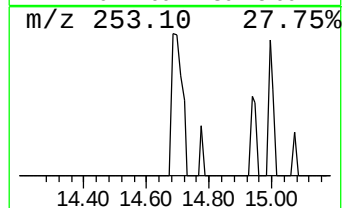
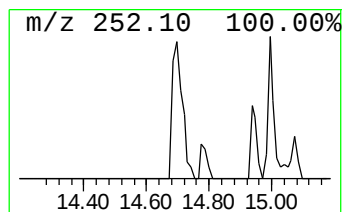
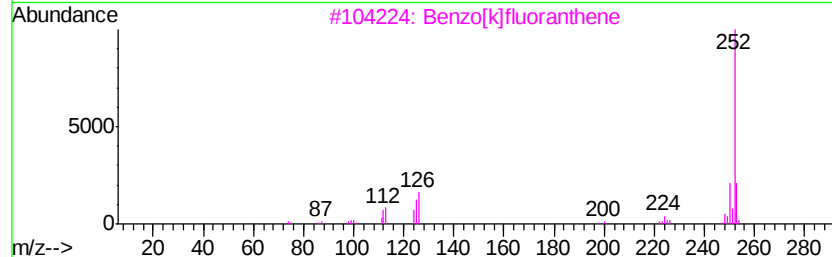
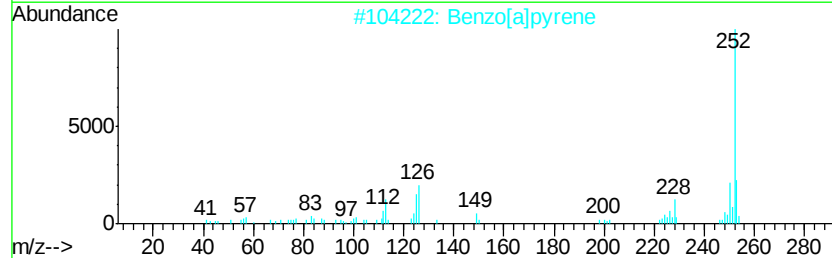
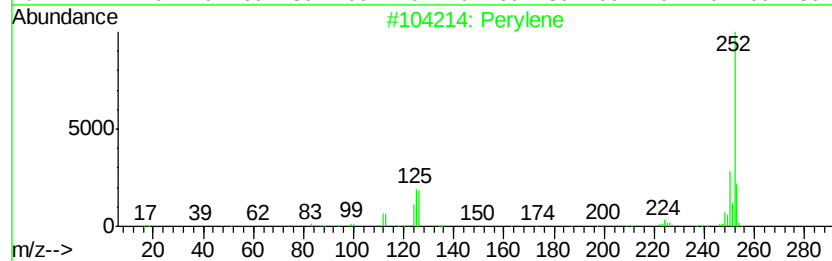
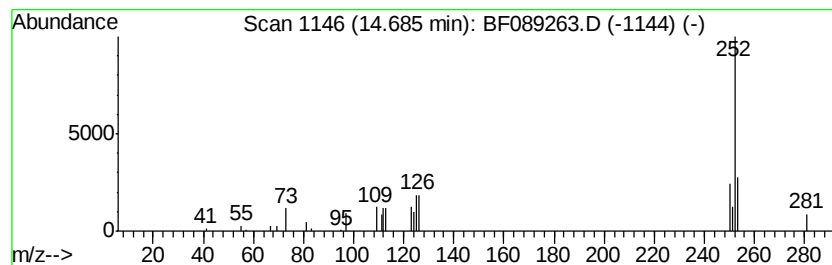
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.16 ng	25839	Perylene-d12	15.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	81
2	Benzo[a]pyrene		252	C20H12	000050-32-8	74
3	Benzo[k]fluoranthene		252	C20H12	000207-08-9	74
4	Benz[e]acephenanthrylene		252	C20H12	000205-99-2	74
5	Benzo[e]pyrene		252	C20H12	000192-97-2	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089263.D
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Operator : UM/SJ
Sample : H4151-08
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-06-COMP

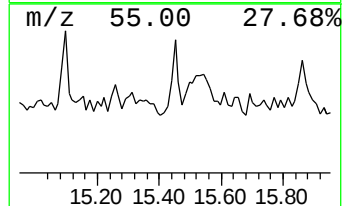
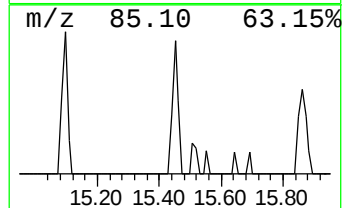
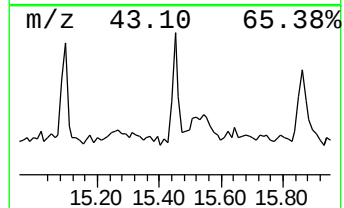
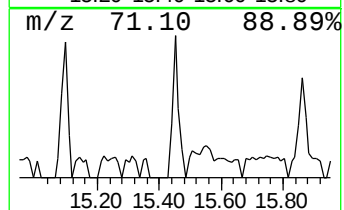
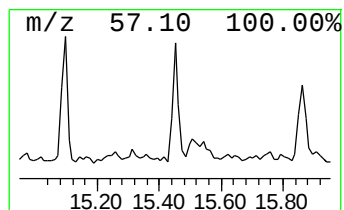
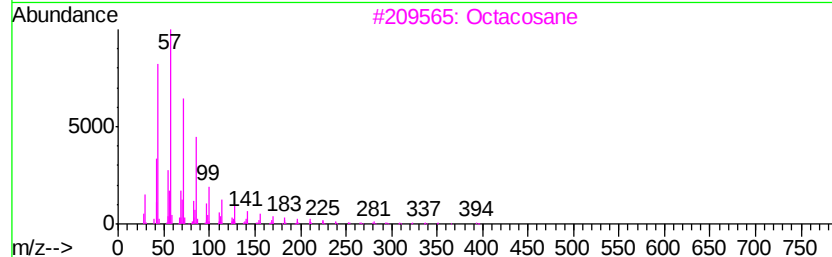
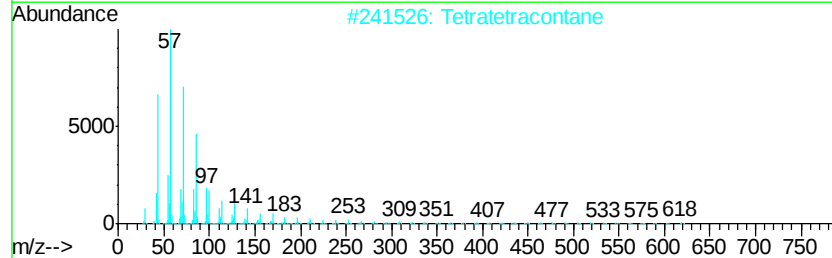
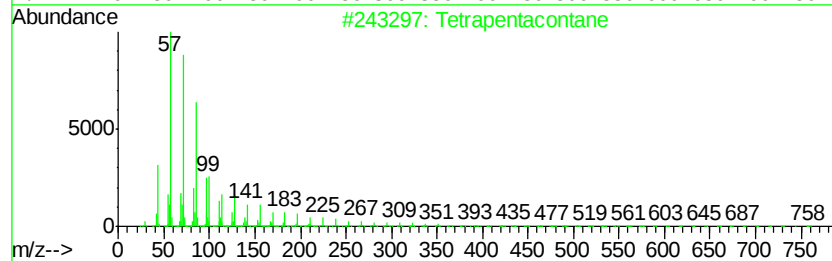
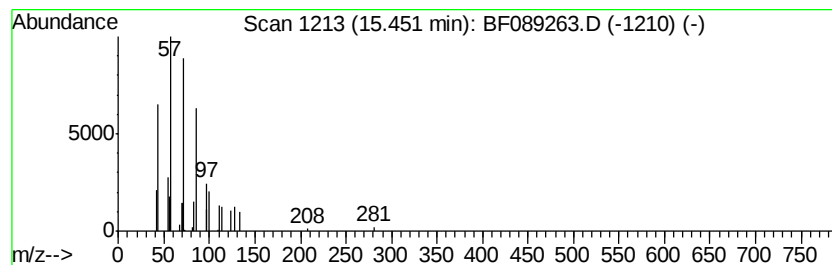
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetrapentacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.21 ng	26446	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane	759	C54H110	005856-66-6	80
2		Tetratetracontane	619	C44H90	007098-22-8	72
3		Octacosane	394	C28H58	000630-02-4	72
4		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64
5		Heptadecane	240	C17H36	000629-78-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
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Acq On : 24 Jul 2016 6:35
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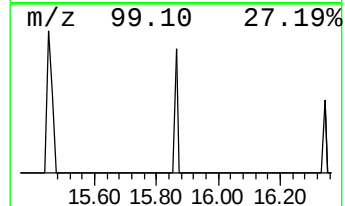
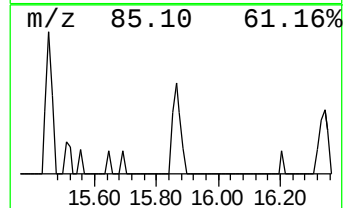
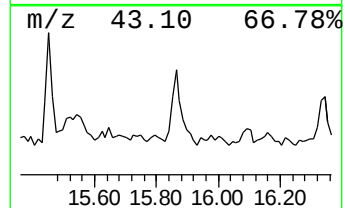
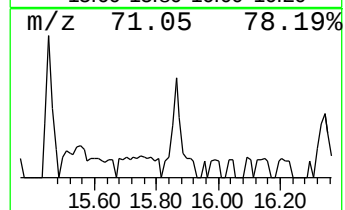
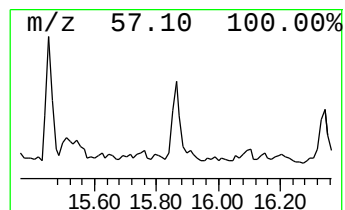
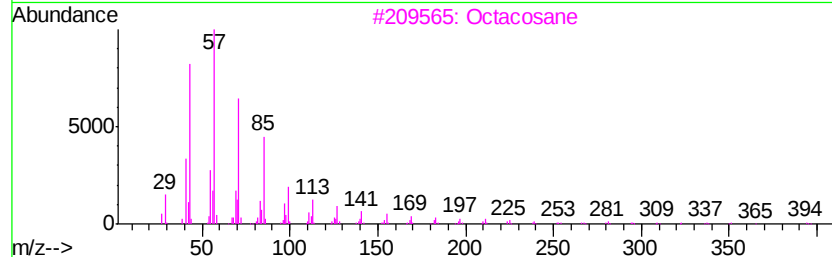
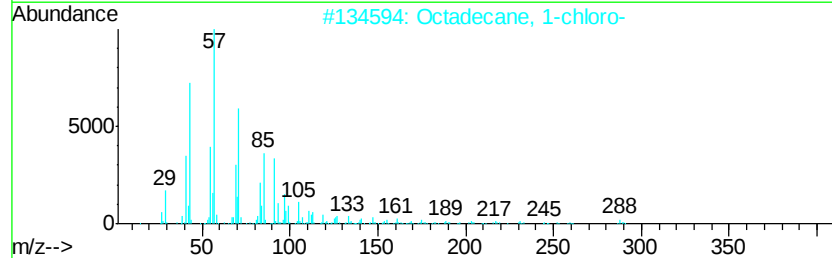
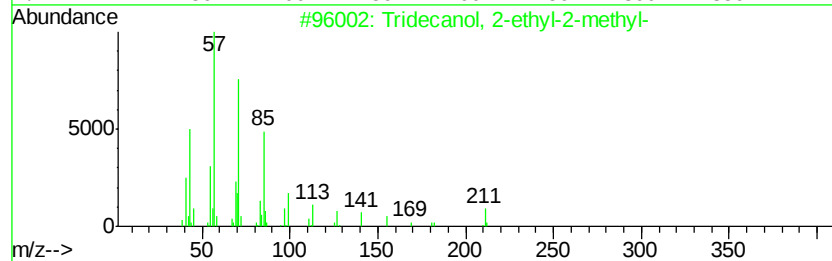
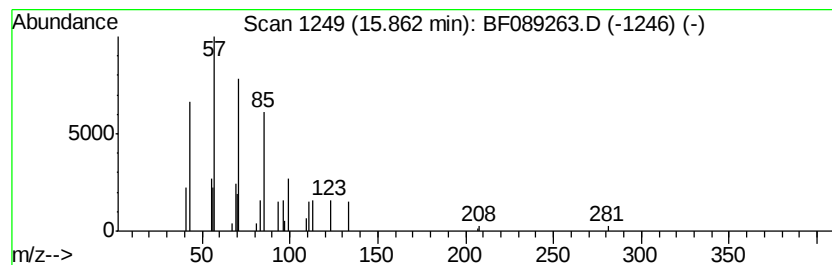
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.08 ng	24907	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	72
2		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	72
3		Octacosane	394	C28H58	000630-02-4	59
4		Tetrapentacontane	759	C54H110	005856-66-6	59
5		Dodecane	170	C12H26	000112-40-3	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
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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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unknown6.34	6.34	91.3	ng	1183350	1	6.58	259279	20.0
Hexadecanoic acid...	12.50	11.8	ng	160734	5	13.70	273395	20.0
Butyl myristate	13.21	6.3	ng	86058	5	13.70	273395	20.0
Oxalic acid, cycl...	13.58	5.9	ng	81038	5	13.70	273395	20.0
2-methyltetracosane	14.19	2.8	ng	38398	5	13.70	273395	20.0
Sulfurous acid, d...	14.49	2.6	ng	31496	6	15.05	239093	20.0
Perylene	14.69	2.2	ng	25839	6	15.05	239093	20.0
Tetrapentacontane	15.45	2.2	ng	26446	6	15.05	239093	20.0
Tridecanol, 2-eth...	15.86	2.1	ng	24907	6	15.05	239093	20.0