

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
 Data File : BF081273.D
 Acq On : 29 Aug 2015 16:19
 Operator : UM/IZ
 Sample : G3489-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SES-EFFLUENT-CS-3

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-BF081715.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.548	244	246	258	rVB	158733	205040	12.07%	1.756%
2	5.029	286	288	291	rBV	413318	398171	23.44%	3.410%
3	6.126	382	384	386	rBV	286511	244608	14.40%	2.095%
4	6.240	392	394	397	rBV	888168	754597	44.43%	6.462%
5	6.480	413	415	417	rBV	349813	296015	17.43%	2.535%
6	6.640	426	429	431	rBV	1083113	1233367	72.62%	10.561%
7	7.052	462	465	468	rBV	916103	933802	54.98%	7.996%
8	7.772	525	528	530	rBV	300060	366951	21.60%	3.142%
9	8.846	620	622	625	rBV	1273448	1698455	100.00%	14.544%
10	9.246	656	657	659	rBB	29790	23882	1.41%	0.205%
11	9.509	678	680	683	rBB	493730	407465	23.99%	3.489%
12	10.286	746	748	751	rBV2	498993	613209	36.10%	5.251%
13	10.435	760	761	768	rVB	25140	33540	1.97%	0.287%
14	10.686	782	783	785	rBV	20748	17112	1.01%	0.147%
15	10.881	798	800	802	rBV	23138	21408	1.26%	0.183%
16	10.972	806	808	811	rBV2	358788	401183	23.62%	3.435%
17	11.246	830	832	836	rBV	17234	30250	1.78%	0.259%
18	11.463	849	851	856	rBV	84366	91130	5.37%	0.780%
19	11.543	856	858	868	rVV	165419	171556	10.10%	1.469%
20	11.795	878	880	882	rVB	33378	37012	2.18%	0.317%
21	12.069	901	904	909	rVB2	16106	28612	1.68%	0.245%
22	12.241	916	919	924	rBV	19701	27841	1.64%	0.238%
23	12.561	944	947	950	rBV	1246656	1459123	85.91%	12.494%
24	13.487	1025	1028	1033	rBV	71278	115325	6.79%	0.988%
25	13.589	1035	1037	1039	rBV	435914	392651	23.12%	3.362%
26	14.458	1110	1113	1115	rBV	1073004	1040063	61.24%	8.906%
27	14.835	1139	1146	1148	rVB3	11425	21321	1.26%	0.183%
28	14.915	1150	1153	1155	rVB	253300	306896	18.07%	2.628%
29	15.384	1190	1194	1201	rBV3	9022	29018	1.71%	0.248%
30	15.498	1201	1204	1208	rVV	21049	41771	2.46%	0.358%
31	15.624	1212	1215	1219	rVB2	16097	30576	1.80%	0.262%
32	15.910	1236	1240	1245	rVB2	7685	18960	1.12%	0.162%
33	16.401	1279	1283	1289	rVB	18520	49388	2.91%	0.423%
34	17.647	1386	1392	1400	rVB2	17599	54499	3.21%	0.467%

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Instrument :
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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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35	19.224	1523	1530	1535	rBV5	8673	41757	2.46%	0.358%
36	19.407	1541	1546	1555	rVB4	9873	41590	2.45%	0.356%

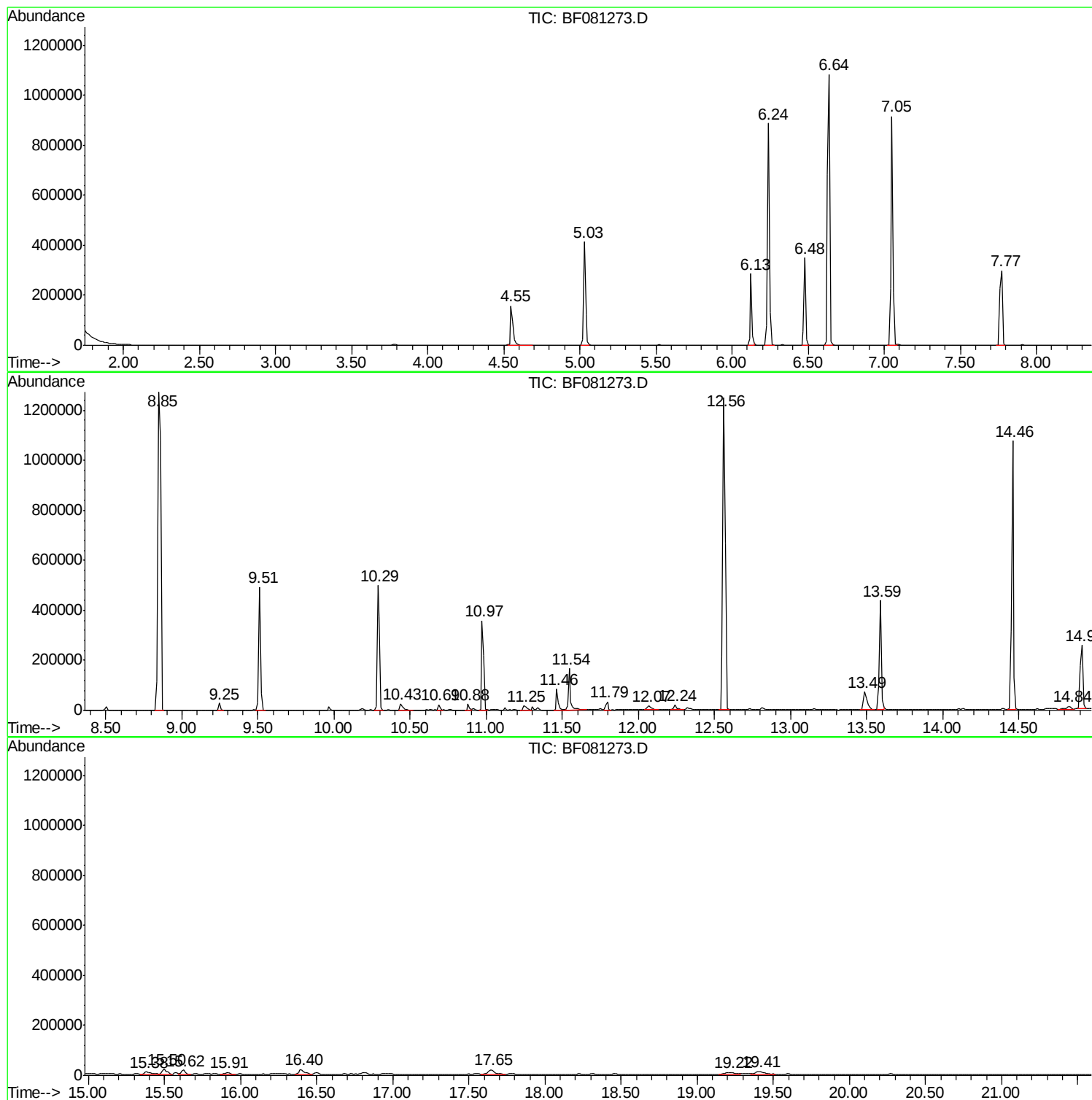
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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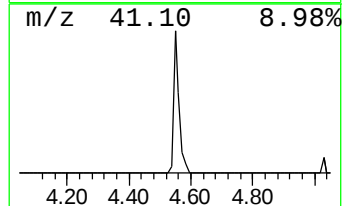
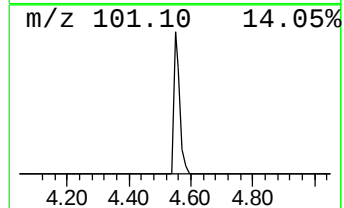
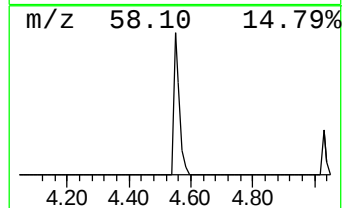
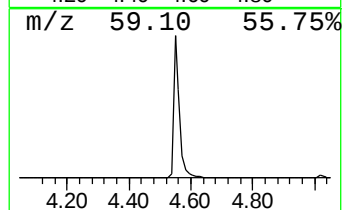
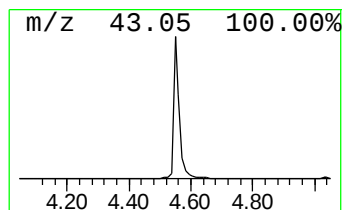
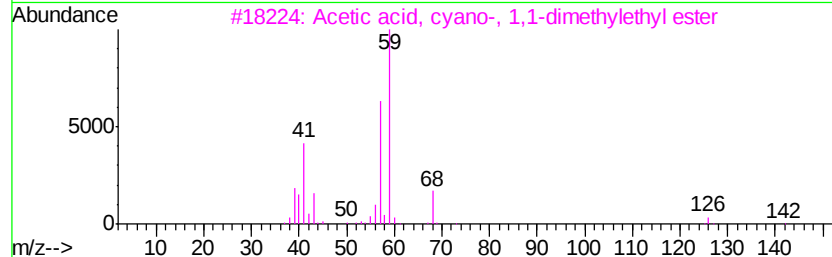
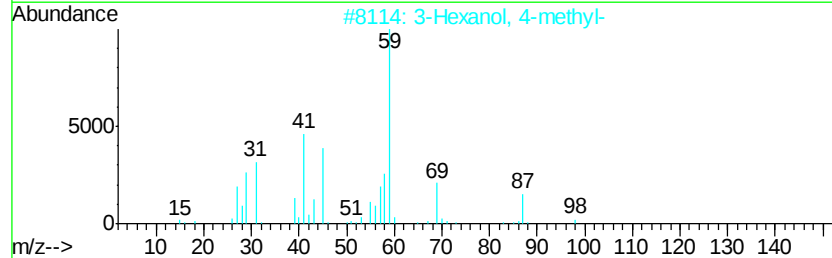
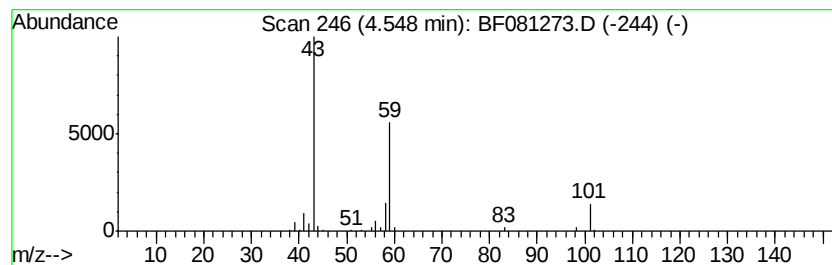
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	13.85 ng	205040	1,4-Dichlorobenzene-d4	6.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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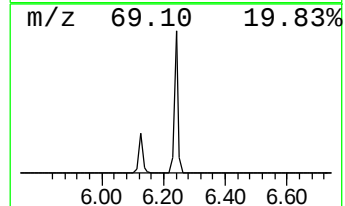
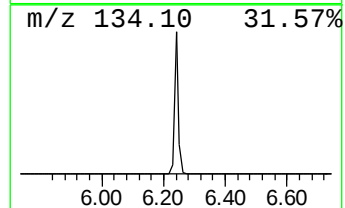
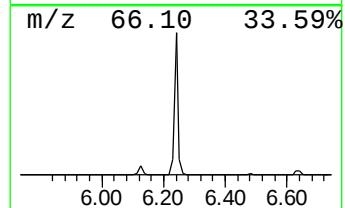
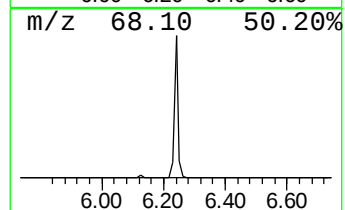
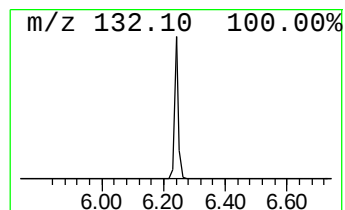
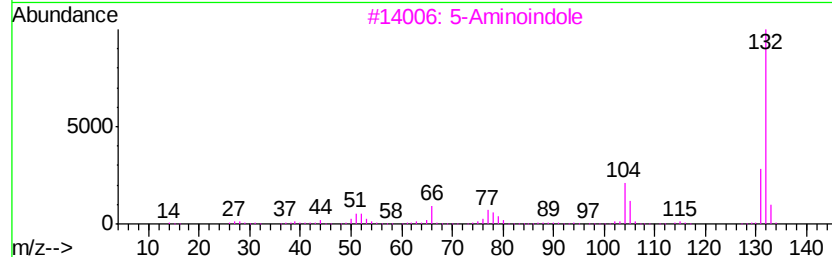
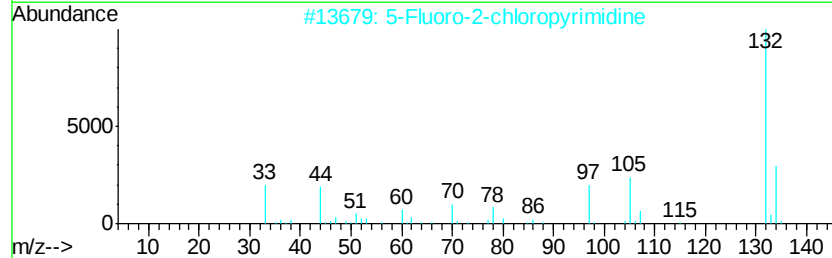
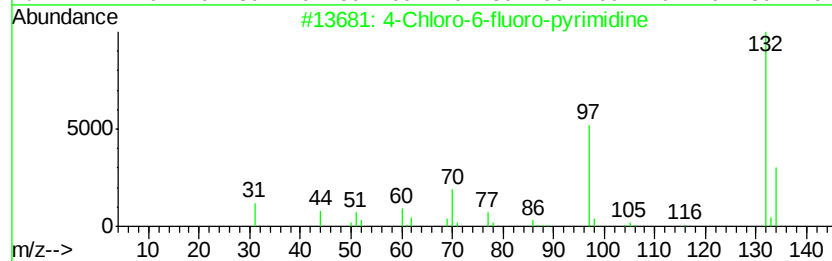
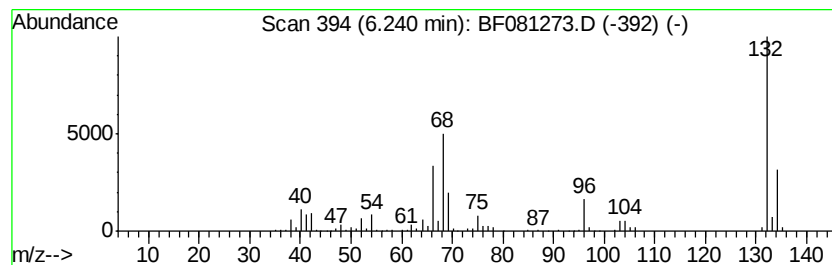
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	50.98 ng	754597	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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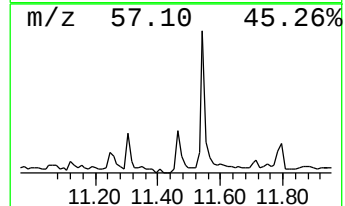
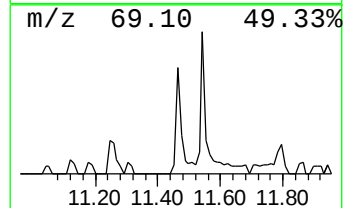
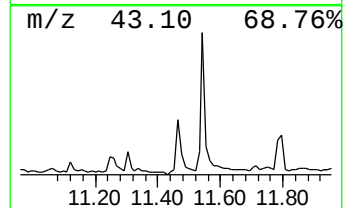
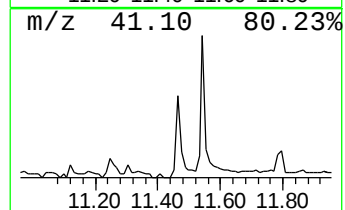
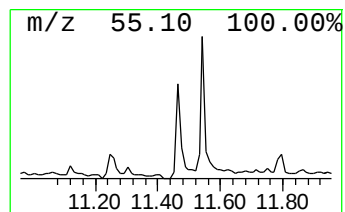
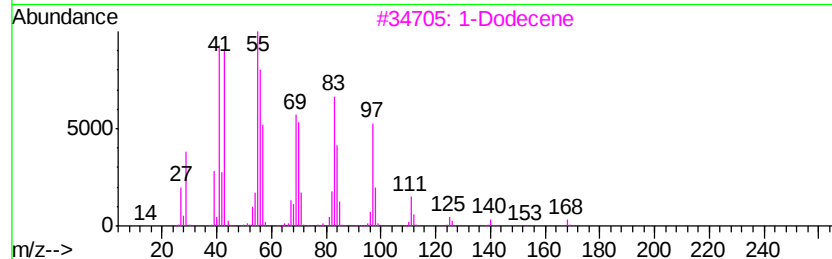
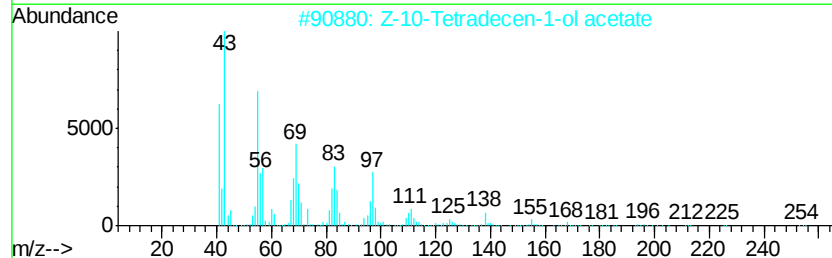
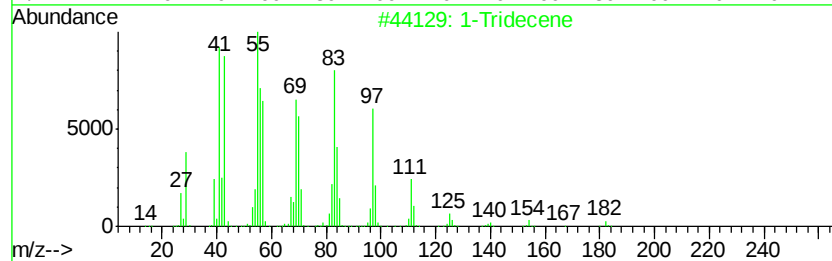
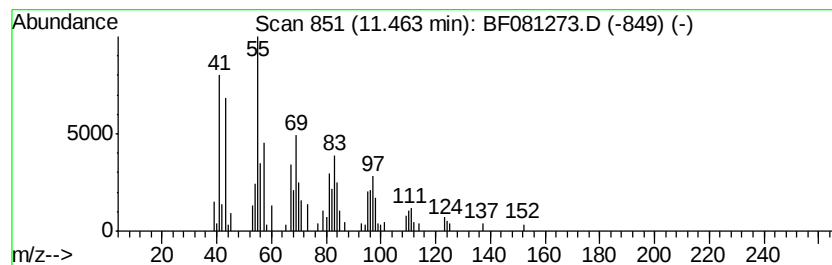
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Tridecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.46	4.54 ng	91130	Phenanthrene-d10		10.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	58
2	Z-10-Tetradecen-1-ol acetate	254	C16H30O2	1000130-99-3	53
3	1-Dodecene	168	C12H24	000112-41-4	52
4	1-Hexadecanol	242	C16H34O	036653-82-4	49
5	1-Hexadecene	224	C16H32	000629-73-2	49



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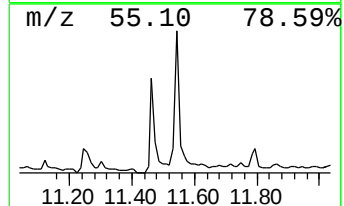
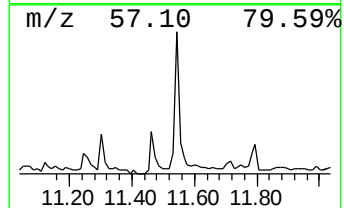
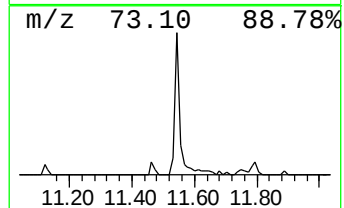
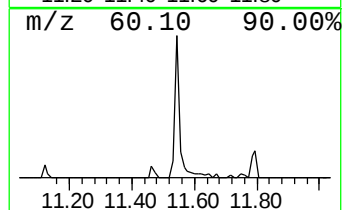
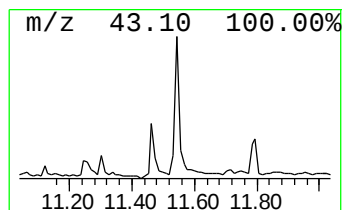
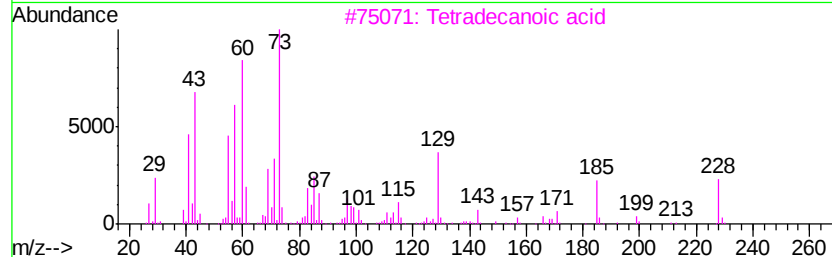
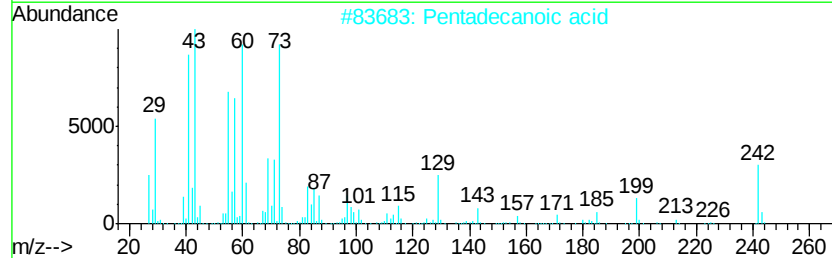
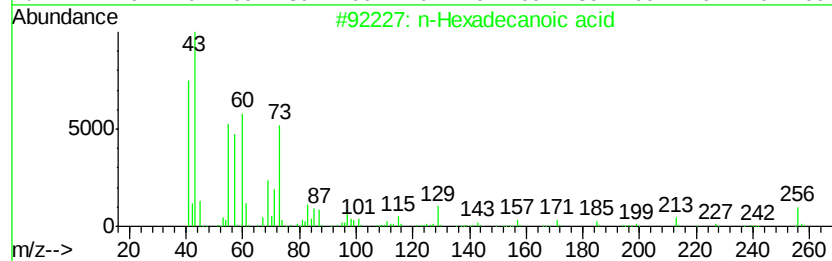
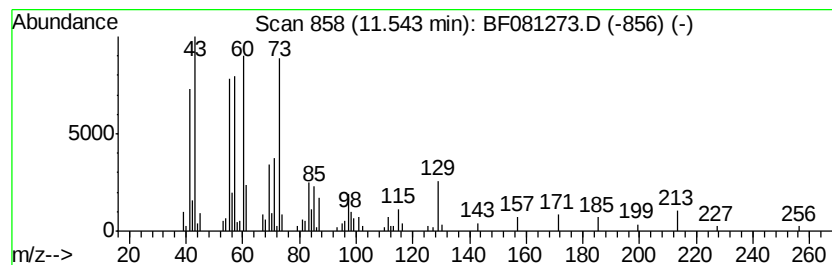
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	8.55 ng	171556	Phenanthrene-d10	10.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Undecanoic acid	186	C11H22O2	000112-37-8	80
5		Tridecanoic acid	214	C13H26O2	000638-53-9	78



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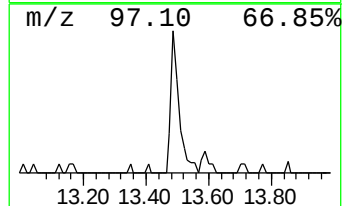
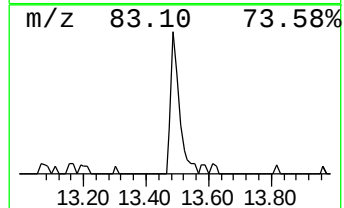
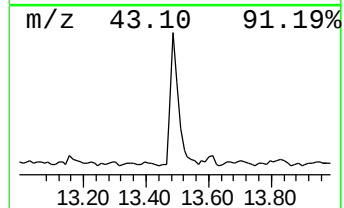
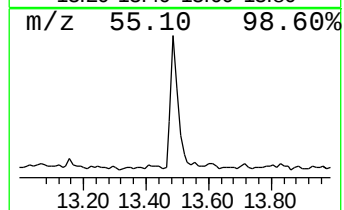
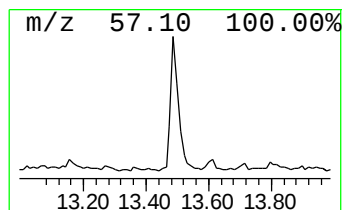
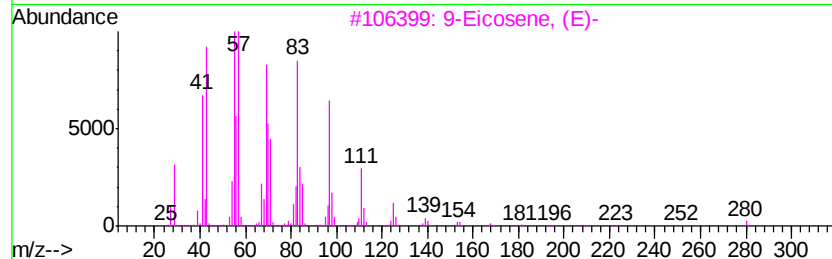
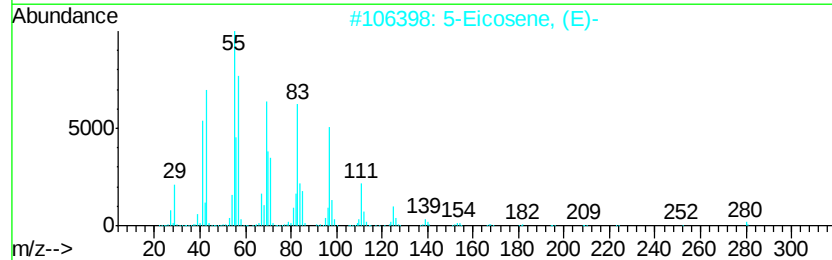
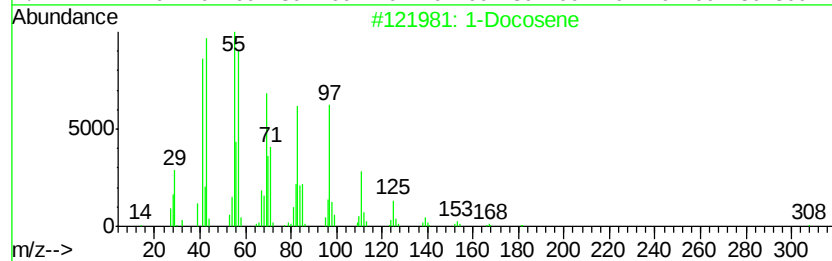
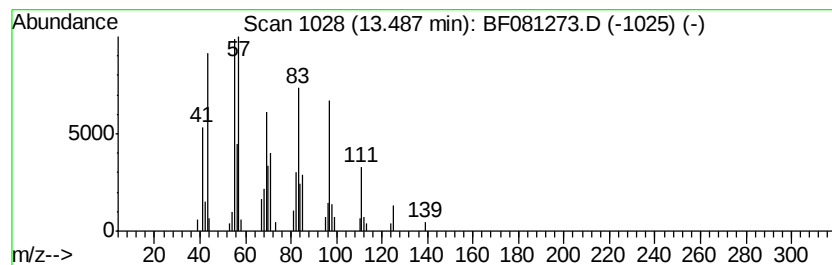
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	5.87 ng	115325	Chrysene-d12	13.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		11-Tricosene	322	C23H46	052078-56-5	86



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ALS Vial : 6 Sample Multiplier: 1

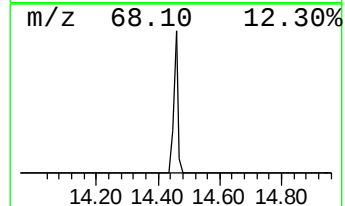
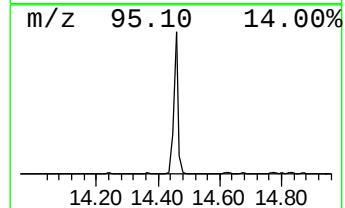
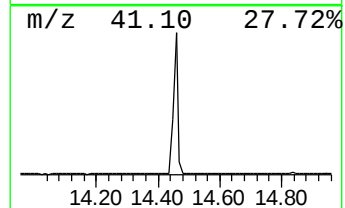
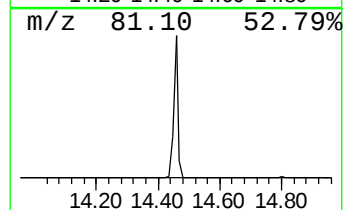
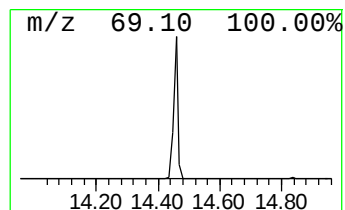
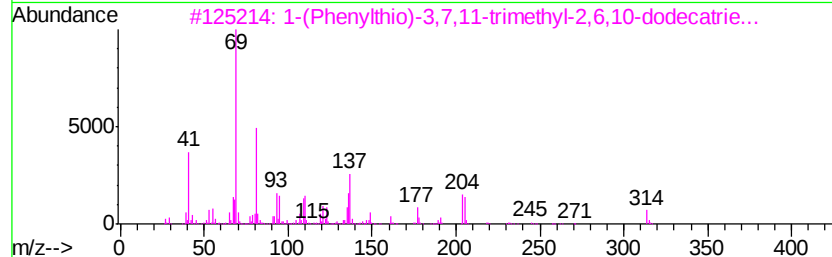
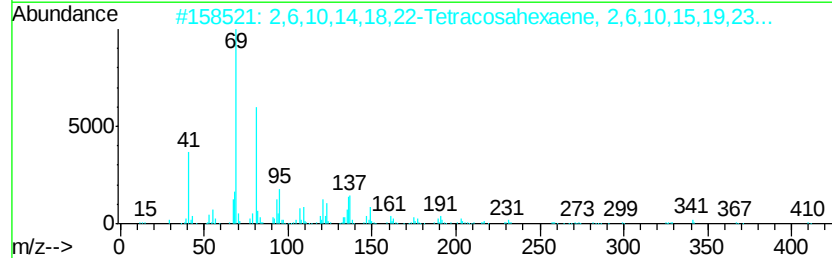
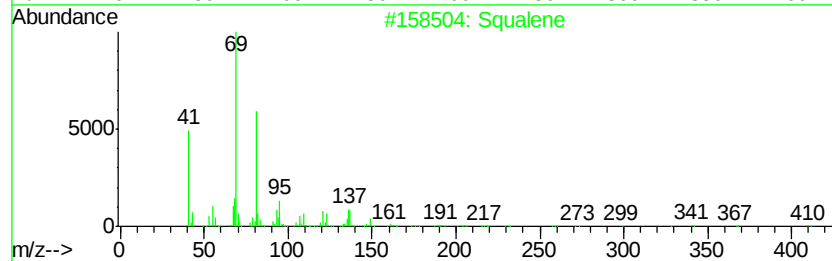
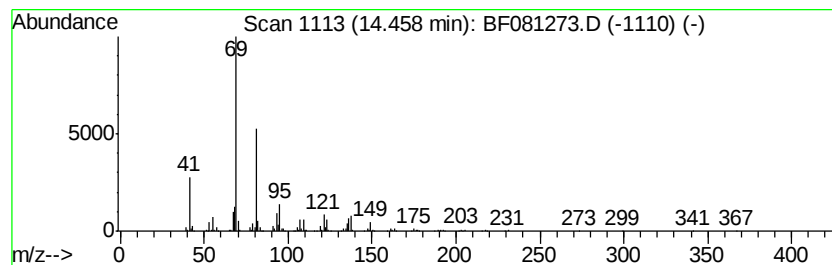
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ClientSampleId :
SES-EFFLUENT-CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	67.78 ng	1040060	Perylene-d12	14.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
3	1-(Phenylthio)-3,7,11-trimethyl-...	314 C21H30S	028413-57-2	83
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	83
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264 C17H28O2	004128-17-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081273.D
Acq On : 29 Aug 2015 16:19
Operator : UM/IZ
Sample : G3489-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SES-EFFLUENT-CS-3

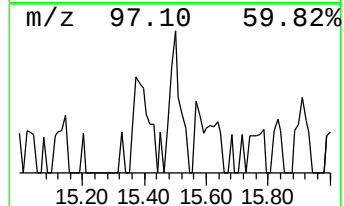
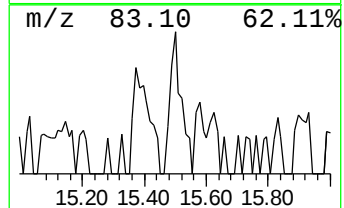
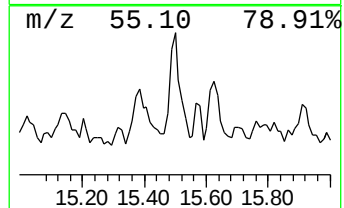
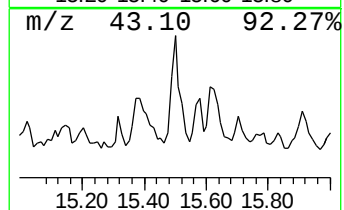
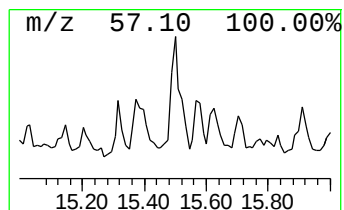
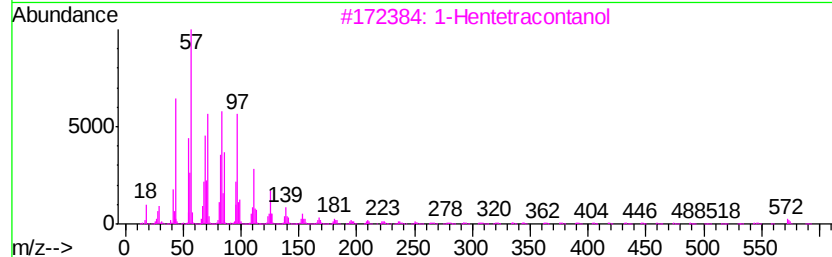
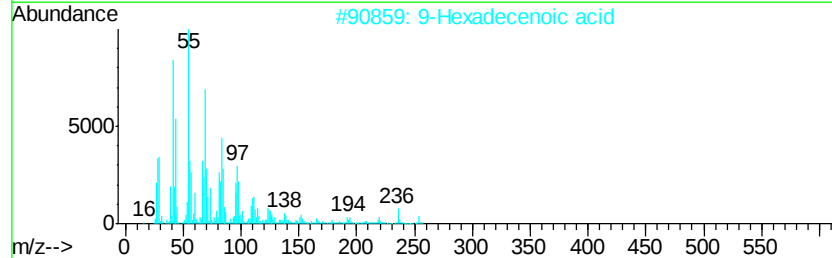
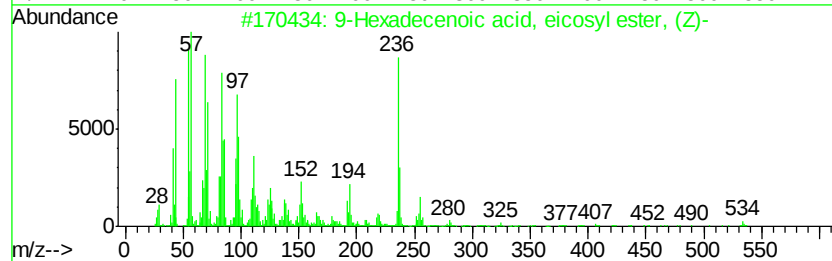
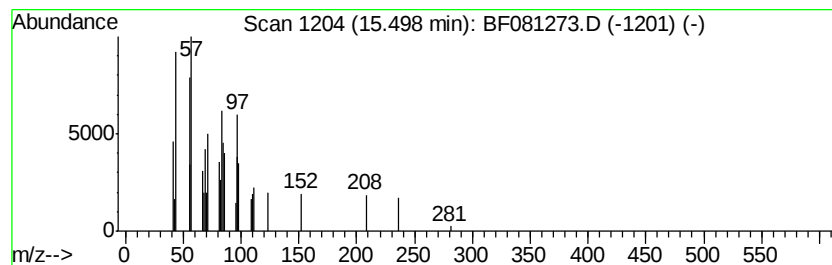
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Hexadecenoic acid, eicosy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	2.72 ng	41771	Perylene-d12	14.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Hexadecenoic acid, eicosyl est...	535	C36H70O2	022522-34-5	64
2		9-Hexadecenoic acid	254	C16H30O2	002091-29-4	47
3		1-Hentetracontanol	593	C41H84O	040710-42-7	38
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	35
5		17-Pentatriacontene	491	C35H70	006971-40-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081273.D
Acq On : 29 Aug 2015 16:19
Operator : UM/IZ
Sample : G3489-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

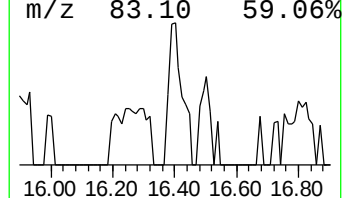
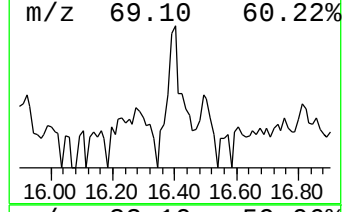
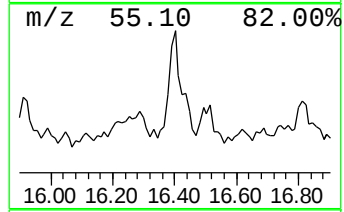
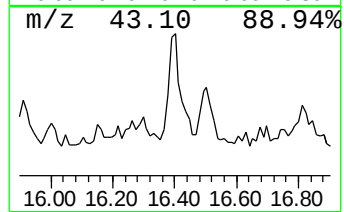
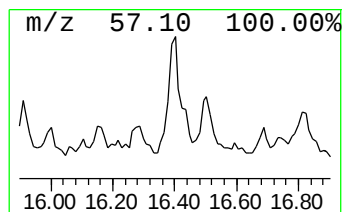
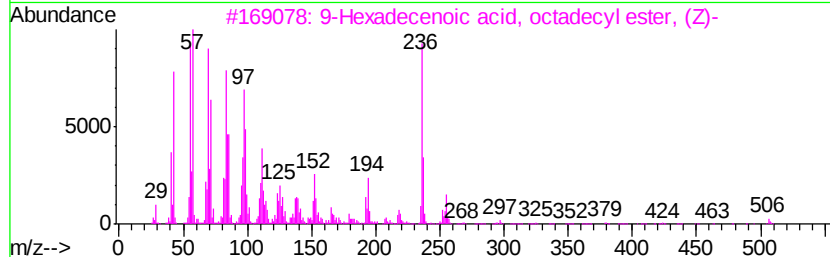
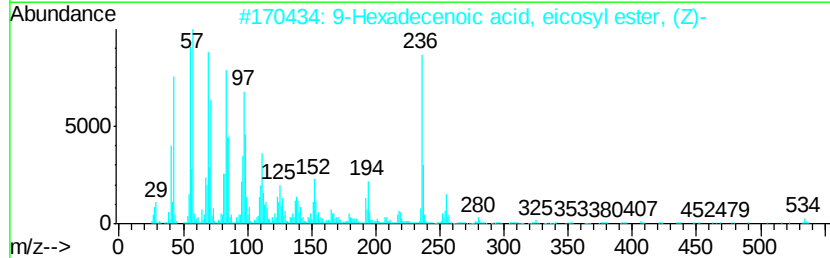
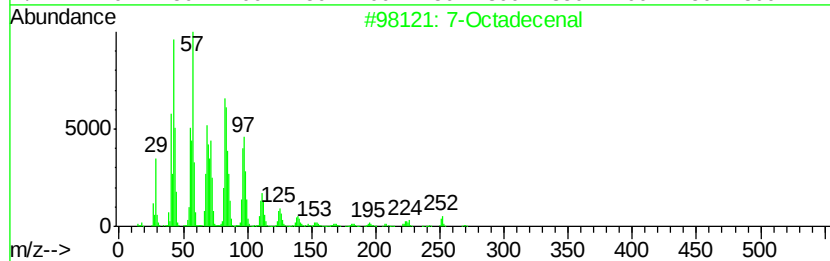
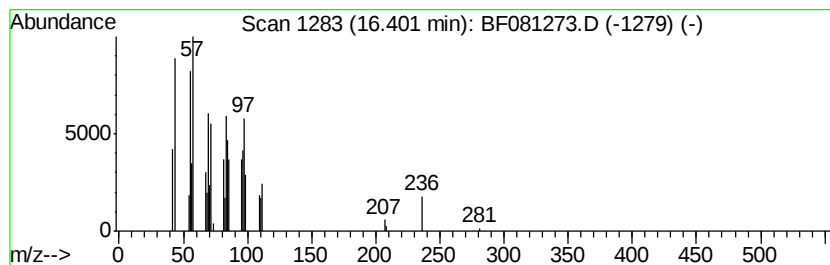
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ClientSampleId :
SES-EFFLUENT-CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 7-Octadecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	3.22 ng	49388	Perylene-d12	14.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	7-Octadecenal	266 C18H34O	056555-00-1	86
2	9-Hexadecenoic acid, eicosyl est...	535 C36H70O2	022522-34-5	64
3	9-Hexadecenoic acid, octadecyl e...	507 C34H66O2	022393-84-6	64
4	17-Pentatriacontene	491 C35H70	006971-40-0	53
5	2-Piperidinone, N-[4-bromo-n-but...	233 C9H16BrNO	195194-80-0	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081273.D
Acq On : 29 Aug 2015 16:19
Operator : UM/IZ
Sample : G3489-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SES-EFFLUENT-CS-3

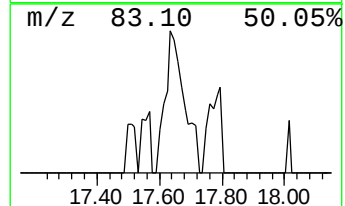
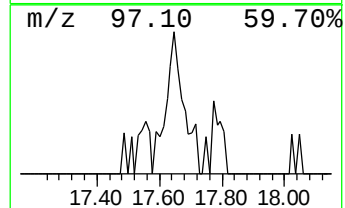
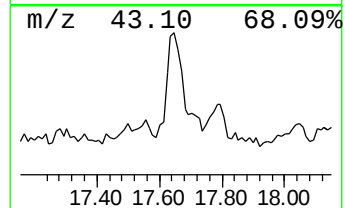
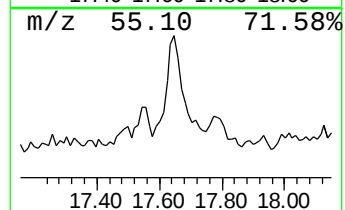
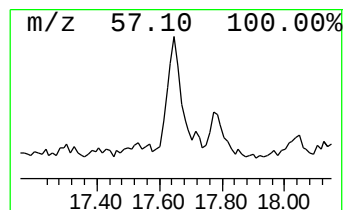
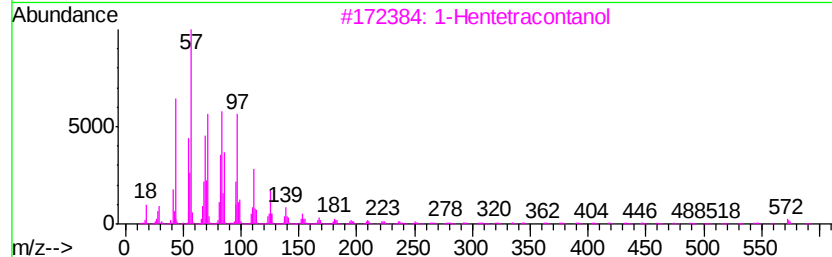
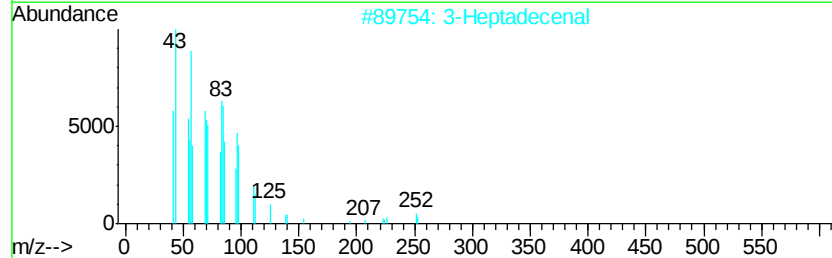
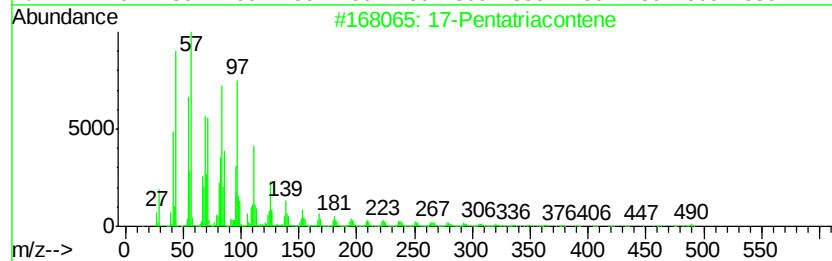
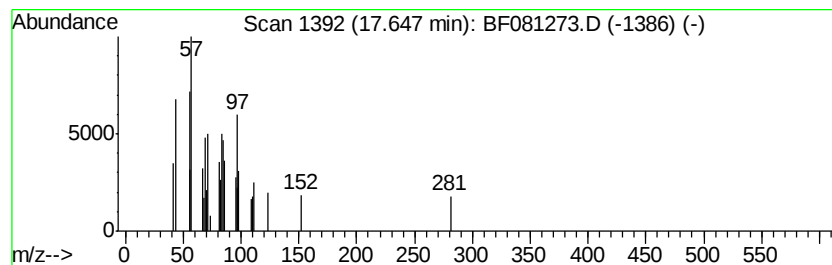
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	3.55 ng	54499	Perylene-d12	14.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	52
2			3-Heptadecenal	252	C17H32O	1000143-48-7	52
3			1-Hentetracontanol	593	C41H84O	040710-42-7	49
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	49
5			Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
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Acq On : 29 Aug 2015 16:19
Operator : UM/IZ
Sample : G3489-01
Misc :
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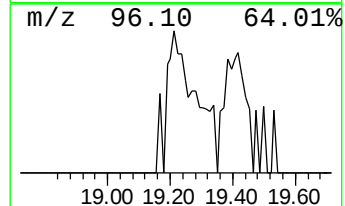
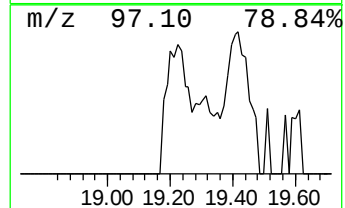
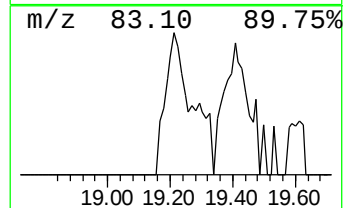
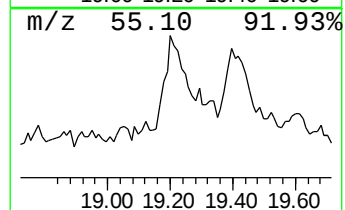
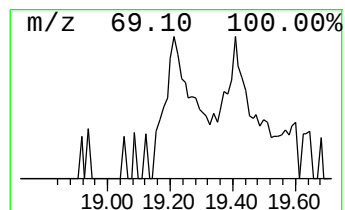
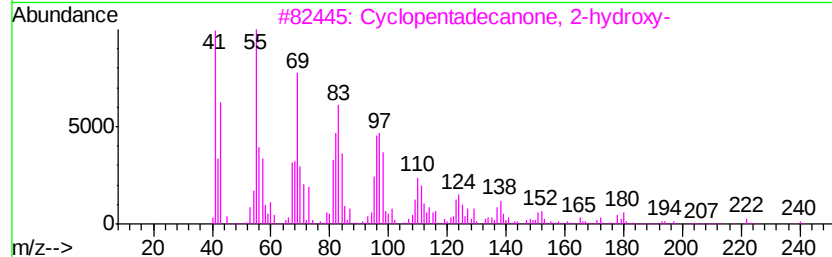
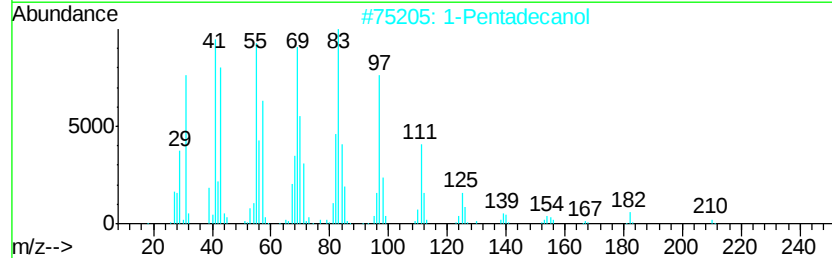
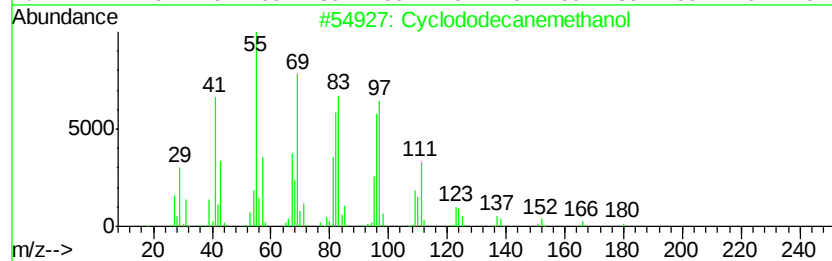
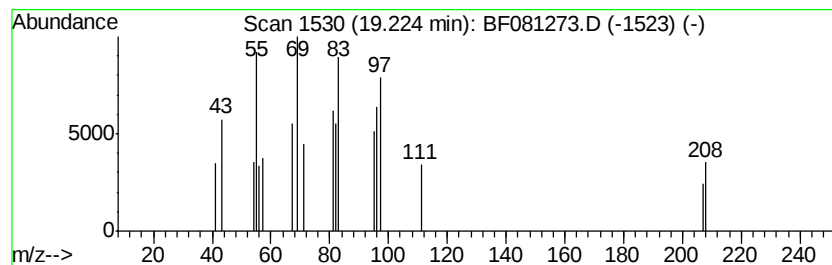
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclododecanemethanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.22	2.72 ng	41757	Perylene-d12	14.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanemethanol	198	C13H26O	001892-12-2	59
2	1-Pentadecanol	228	C15H32O	000629-76-5	53
3	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	50
4	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	50
5	Oxirane, 2-decyl-3-(5-methylhexy...	282	C19H38O	057457-72-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081273.D
Acq On : 29 Aug 2015 16:19
Operator : UM/IZ
Sample : G3489-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

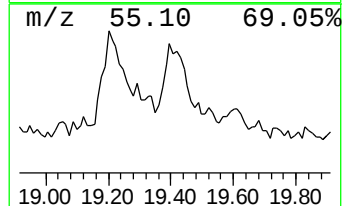
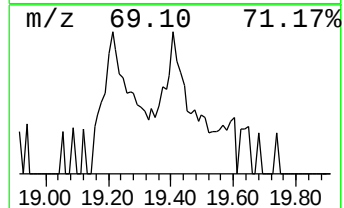
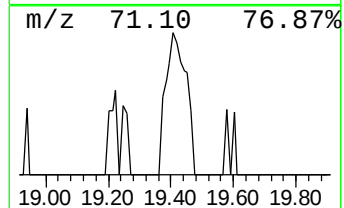
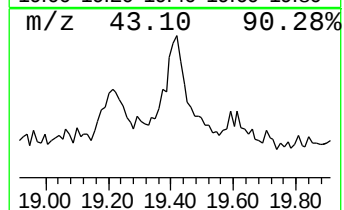
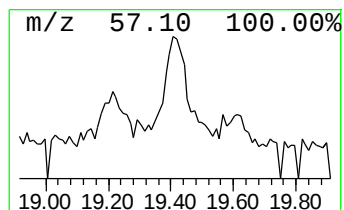
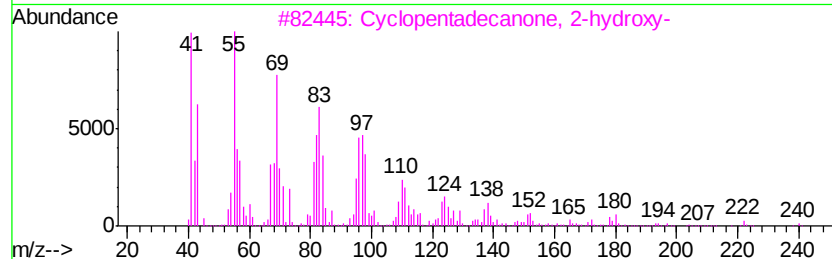
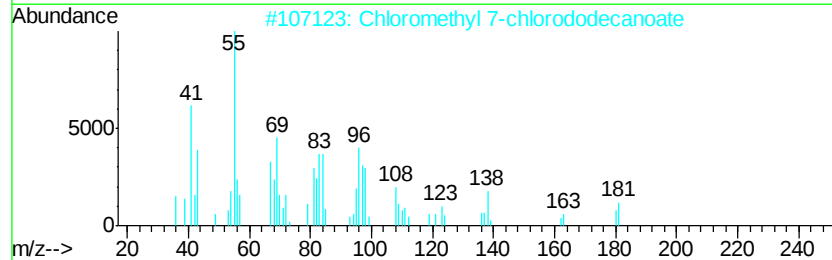
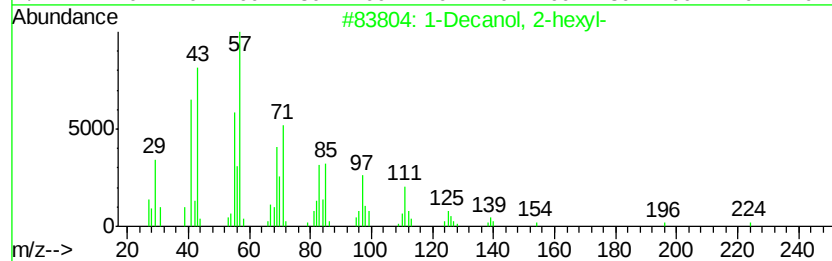
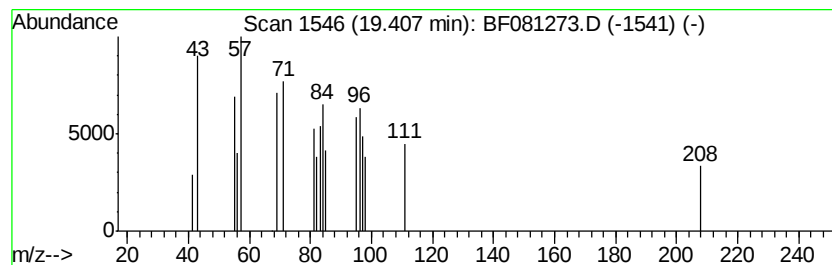
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown19.41 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.41	2.71 ng	41590	Perylene-d12	14.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47
2	Chloromethyl 7-chlorododecanoate	282	C13H24Cl2O2	080419-03-0	38
3	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	35
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	35
5	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
 Data File : BF081273.D
 Acq On : 29 Aug 2015 16:19
 Operator : UM/IZ
 Sample : G3489-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 SES-EFFLUENT-CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.55	13.9	ng	205040	1	6.48	296015	20.0
unknown6.24	6.24	51.0	ng	754597	1	6.48	296015	20.0
1-Tridecene	11.46	4.5	ng	91130	4	10.97	401183	20.0
n-Hexadecanoic acid	11.54	8.6	ng	171556	4	10.97	401183	20.0
1-Docosene	13.49	5.9	ng	115325	5	13.59	392651	20.0
Squalene	14.46	67.8	ng	1040060	6	14.92	306896	20.0
9-Hexadecenoic ac...	15.50	2.7	ng	41771	6	14.92	306896	20.0
7-Octadecenal	16.40	3.2	ng	49388	6	14.92	306896	20.0
17-Pentatriacontene	17.65	3.5	ng	54499	6	14.92	306896	20.0
Cyclododecanemeth...	19.22	2.7	ng	41757	6	14.92	306896	20.0
unknown19.41	19.41	2.7	ng	41590	6	14.92	306896	20.0