

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
 Data File : BF083756.D
 Acq On : 14 Dec 2015 4:10
 Operator : UM/IZ
 Sample : G4731-01
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1-STOCKPILE-(0-2)

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-BF121315.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	2.224	9	12	18	rVB	40311	69532	1.88%	0.212%
2	5.116	262	265	270	rVB	743075	1047260	28.27%	3.197%
3	5.527	298	301	304	rBV	2660510	3249983	87.73%	9.921%
4	5.927	334	336	338	rVB	51232	43984	1.19%	0.134%
5	6.545	387	390	393	rBV	2406744	3324288	89.74%	10.148%
6	6.693	400	403	405	rBV	2786591	3704536	100.00%	11.308%
7	6.922	420	423	425	rBV	701672	726698	19.62%	2.218%
8	7.082	434	437	439	rVB	2469719	2928403	79.05%	8.939%
9	7.482	468	472	474	rBV	2189258	2427843	65.54%	7.411%
10	8.202	533	535	537	rBV	1114635	961906	25.97%	2.936%
11	9.276	626	629	632	rBV	3419242	3583892	96.74%	10.940%
12	9.665	661	663	666	rBV	508464	462368	12.48%	1.411%
13	9.893	681	683	686	rBV	74070	52249	1.41%	0.159%
14	9.951	686	688	691	rBV	950762	961275	25.95%	2.934%
15	10.396	723	727	728	rBV	75260	91577	2.47%	0.280%
16	10.613	742	746	747	rBV	28887	44908	1.21%	0.137%
17	10.739	754	757	759	rBV	2010712	1978194	53.40%	6.039%
18	10.865	765	768	772	rVB	85983	104232	2.81%	0.318%
19	11.311	803	807	809	rBV	64821	75282	2.03%	0.230%
20	11.436	816	818	820	rBV	767193	814268	21.98%	2.486%
21	11.494	820	823	825	rVB2	24136	41873	1.13%	0.128%
22	12.134	876	879	883	rBV2	28240	58352	1.58%	0.178%
23	12.637	921	923	926	rVB	42269	38645	1.04%	0.118%
24	12.842	939	941	945	rBV2	376780	380161	10.26%	1.160%
25	12.922	945	948	950	rVB2	93327	106390	2.87%	0.325%
26	13.014	954	956	959	rBV	2372712	2605704	70.34%	7.954%
27	13.551	1000	1003	1005	rBV	280727	275194	7.43%	0.840%
28	13.597	1005	1007	1010	rVV2	53122	78423	2.12%	0.239%
29	13.917	1032	1035	1039	rBV	164008	275510	7.44%	0.841%
30	14.054	1045	1047	1050	rBV2	603396	924527	24.96%	2.822%
31	14.237	1061	1063	1065	rBV	84139	111583	3.01%	0.341%
32	14.545	1088	1090	1091	rBV	94226	97398	2.63%	0.297%
33	14.694	1101	1103	1108	rVB	280145	292584	7.90%	0.893%
34	14.842	1115	1116	1118	rBV	56045	73876	1.99%	0.226%

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1-STOCKPILE-(0-2)

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 >
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35	15.505	1171	1174	1176	rBV	449345	554651	14.97%	1.693%
36	16.214	1234	1236	1242	rVB3	91319	191361	5.17%	0.584%

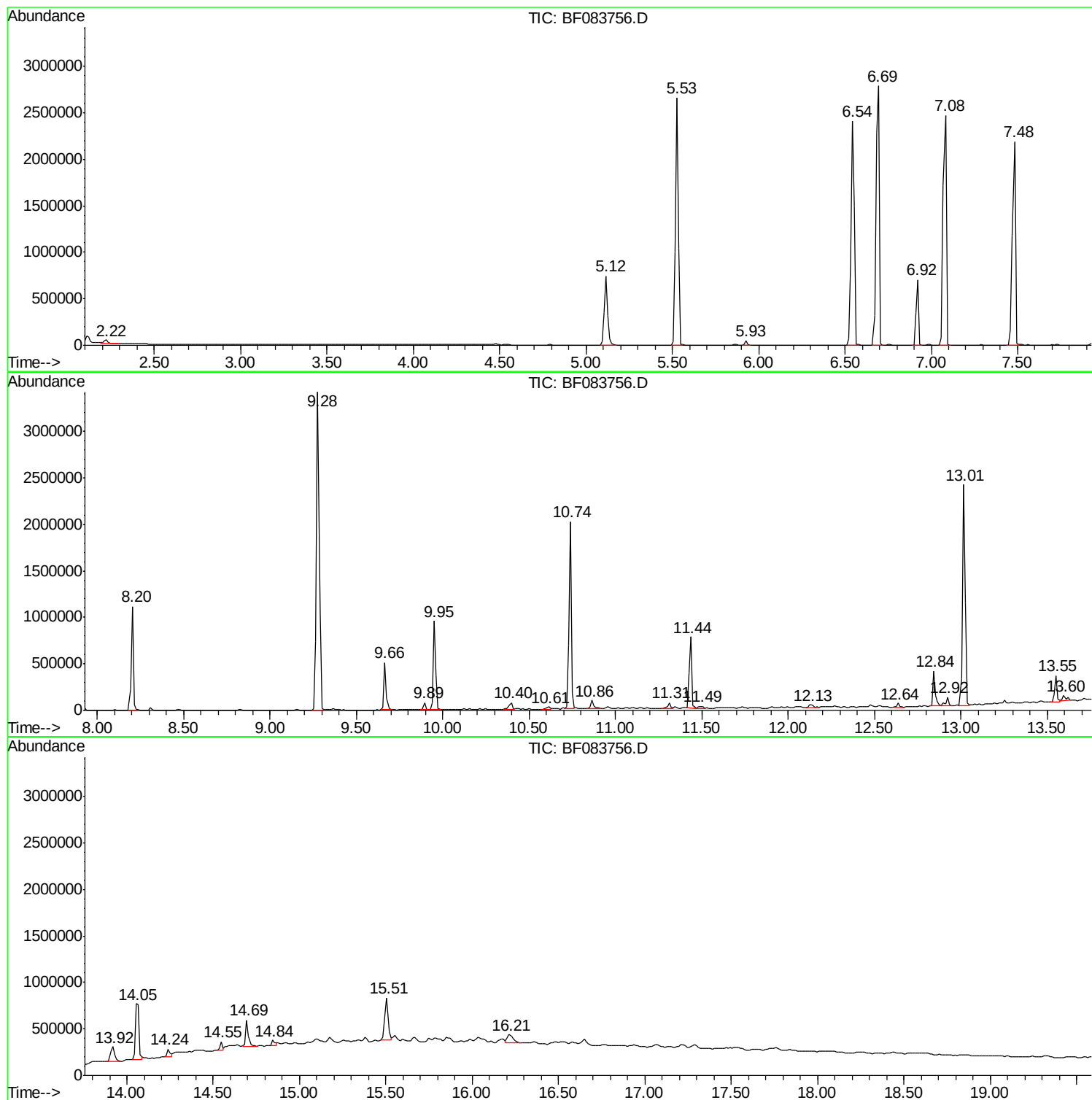
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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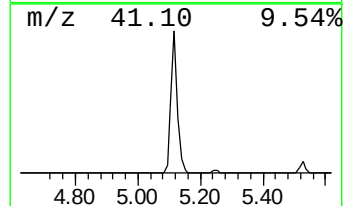
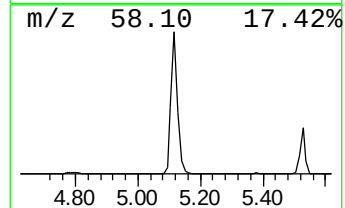
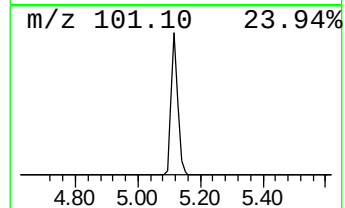
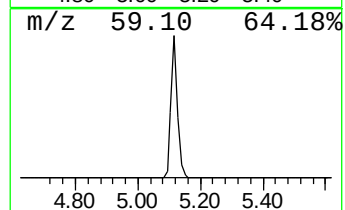
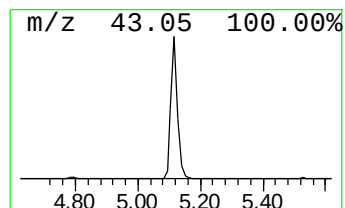
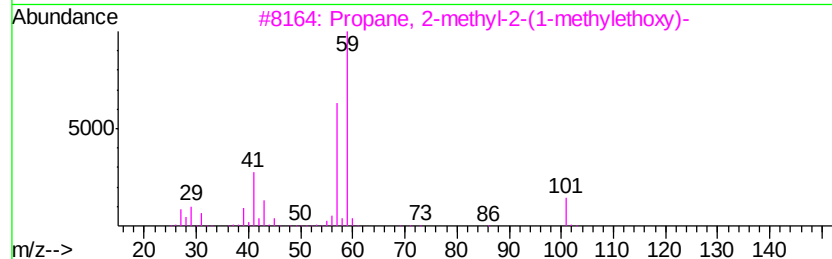
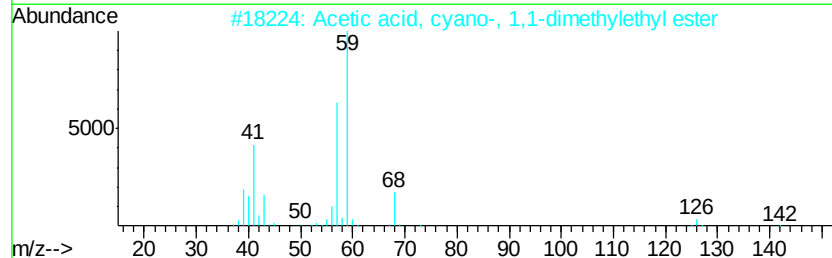
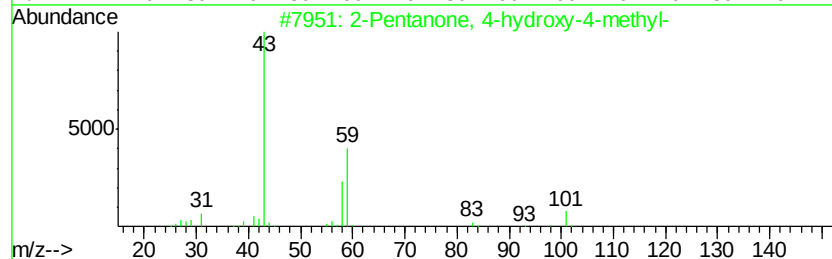
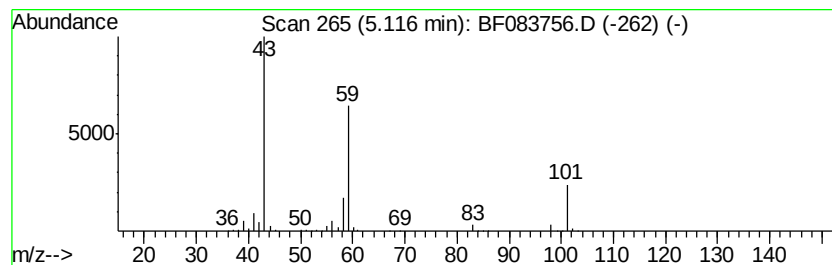
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	28.82 ng	1047260	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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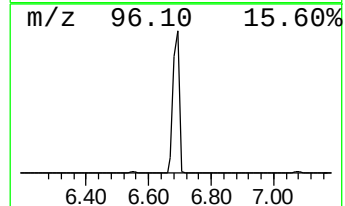
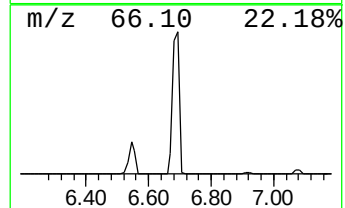
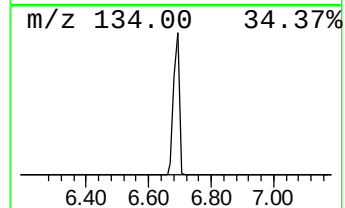
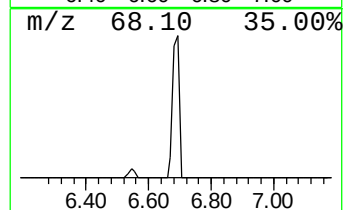
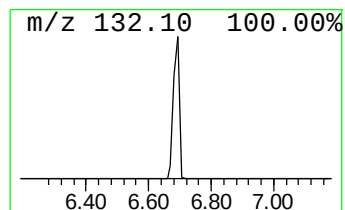
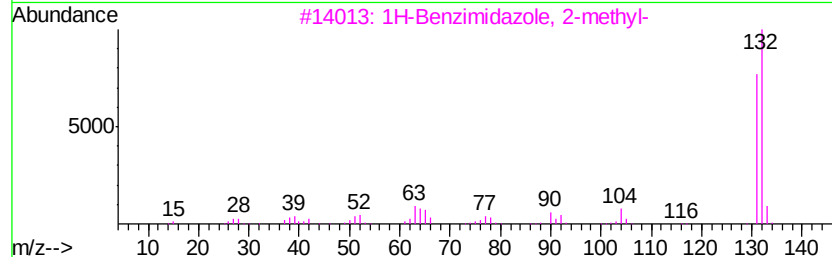
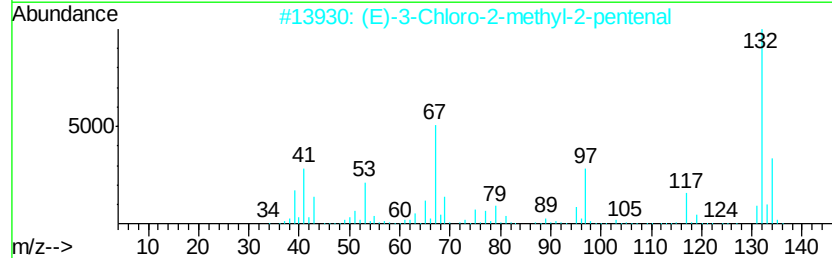
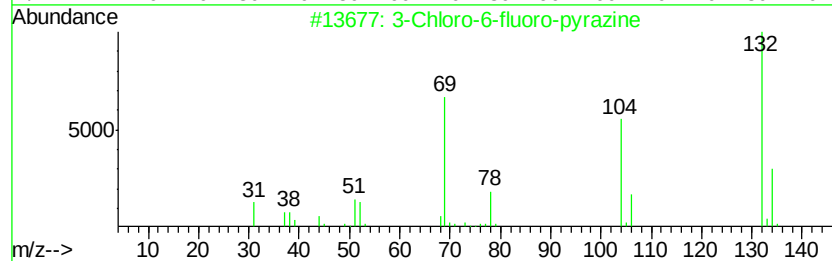
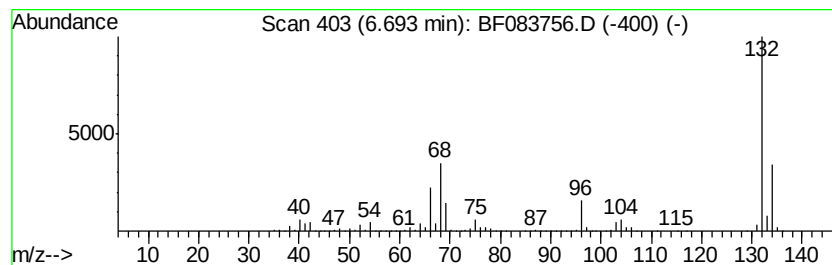
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	101.96 ng	3704540	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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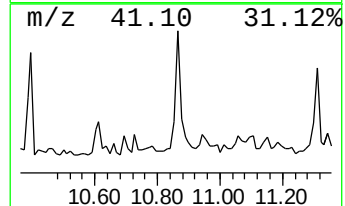
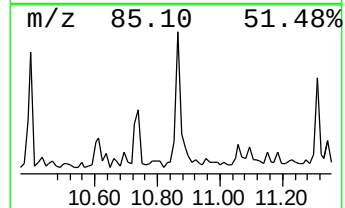
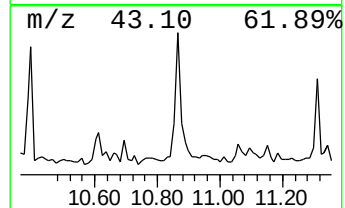
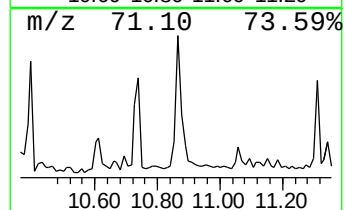
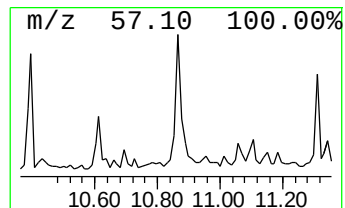
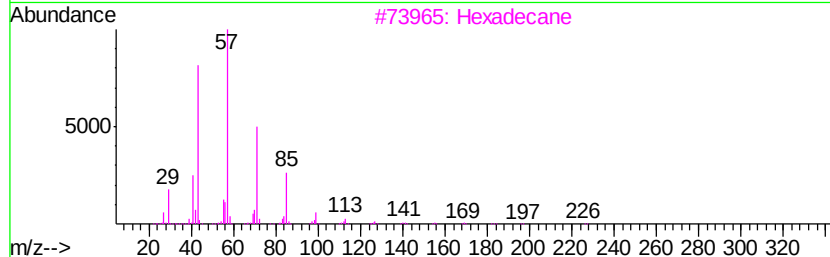
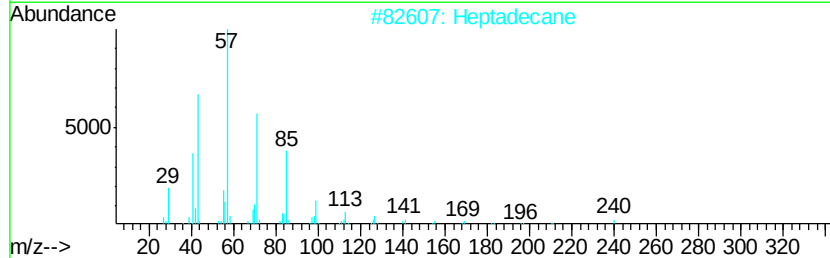
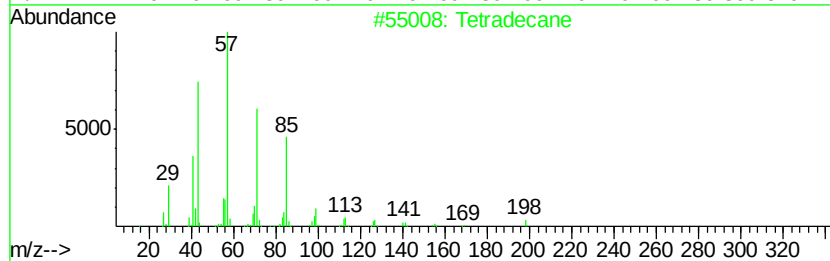
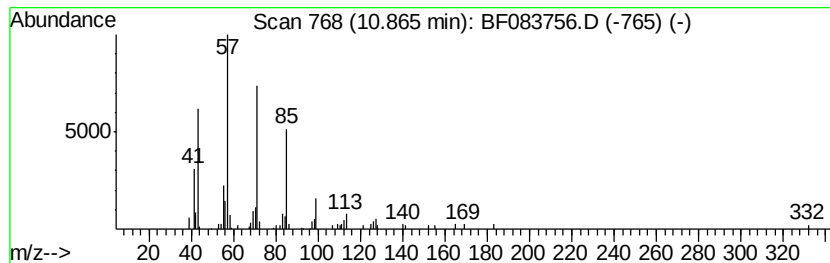
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.56 ng	104232	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Hexadecane	226	C16H34	000544-76-3	90
4		Nonadecane	268	C19H40	000629-92-5	90
5		Octadecane	254	C18H38	000593-45-3	90



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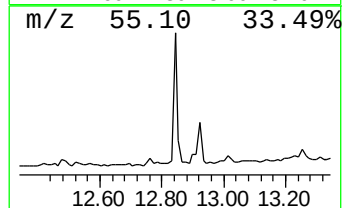
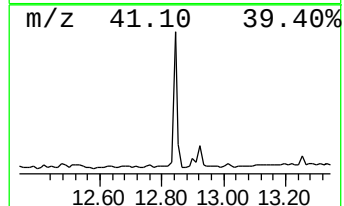
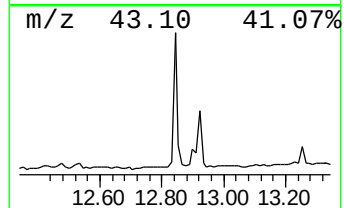
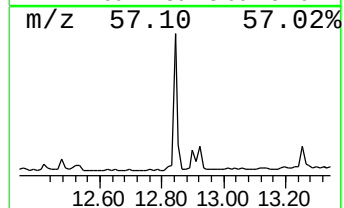
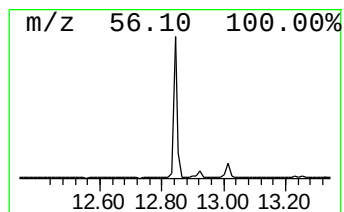
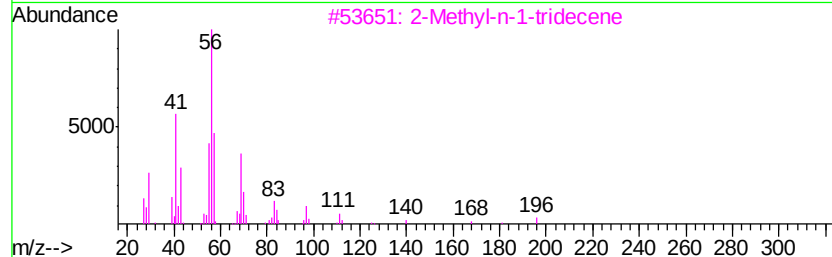
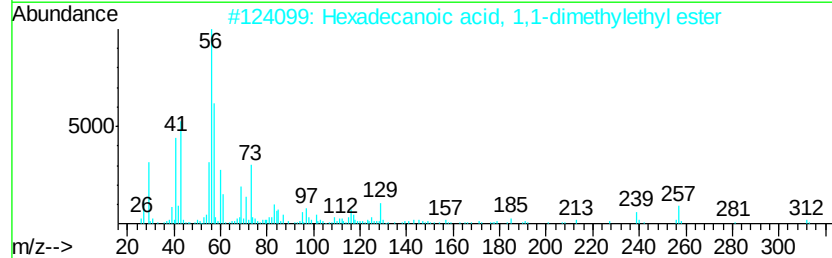
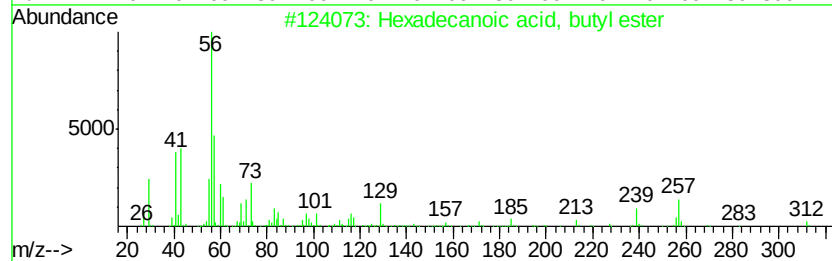
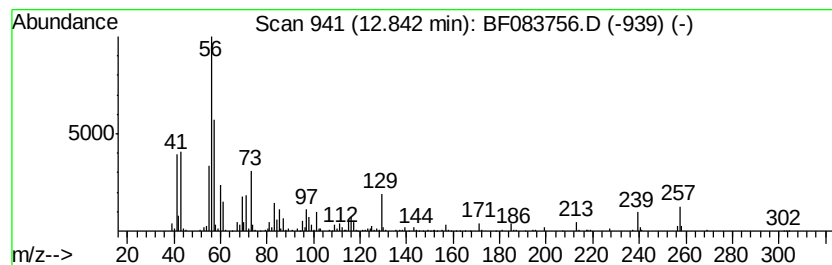
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	8.22 ng	380161	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4		Cyclohexanamine	99	C6H13N	000108-91-8	30
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



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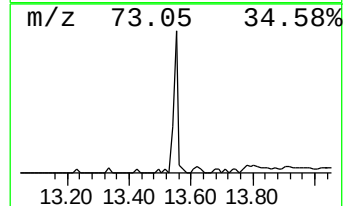
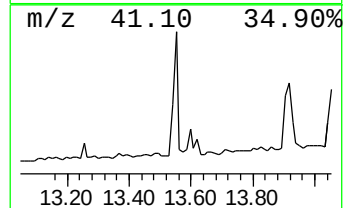
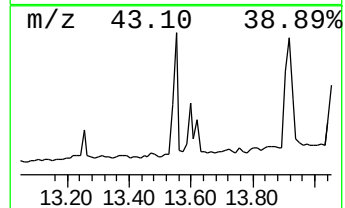
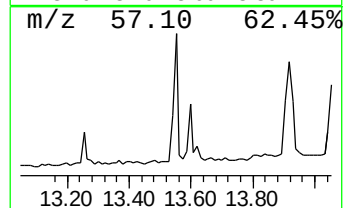
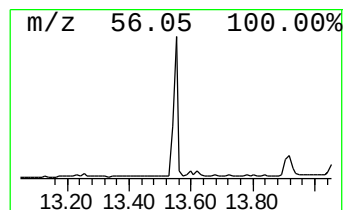
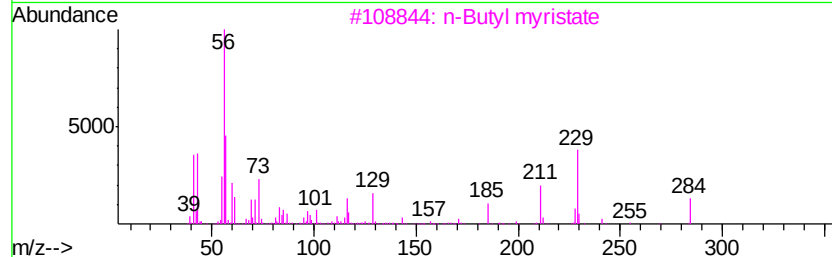
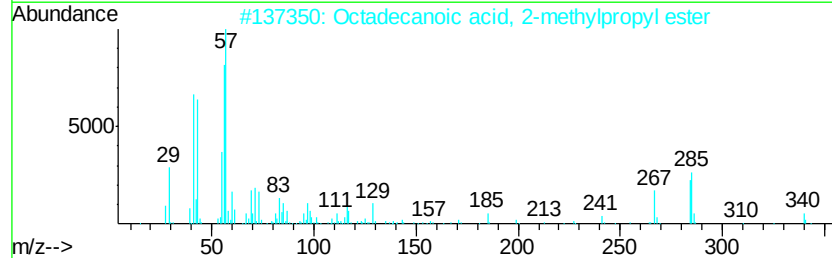
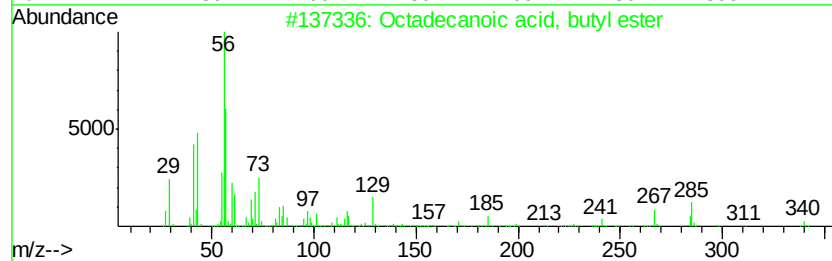
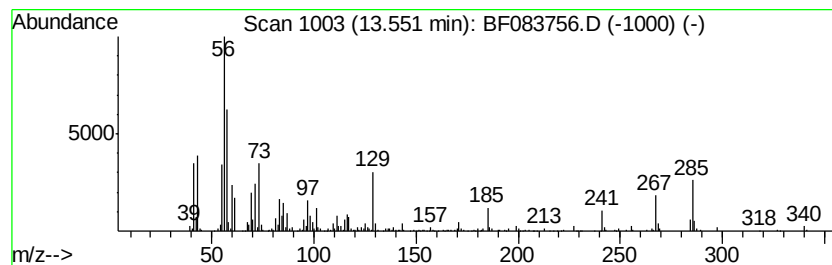
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	5.95 ng	275194	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	72
3		n-Butyl myristate	284	C18H36O2	000110-36-1	50
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30
5		2-Methylhexadec-1-ene	238	C17H34	061868-19-7	27



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Misc :
ALS Vial : 46 Sample Multiplier: 1

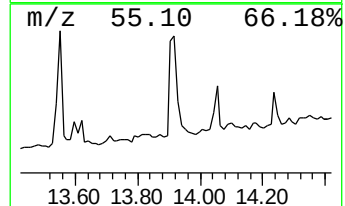
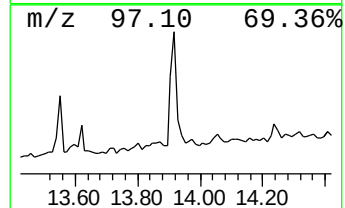
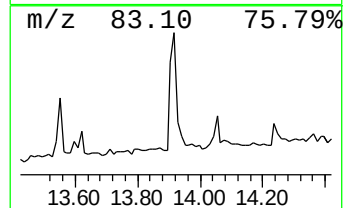
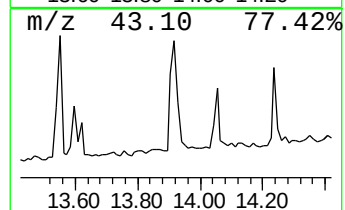
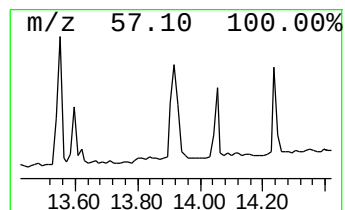
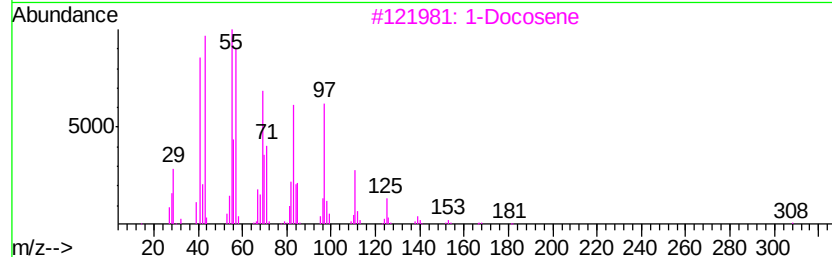
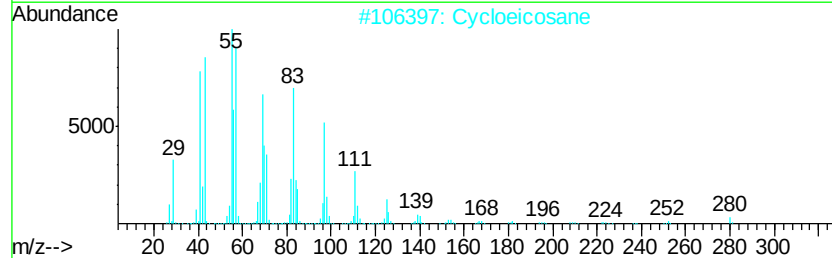
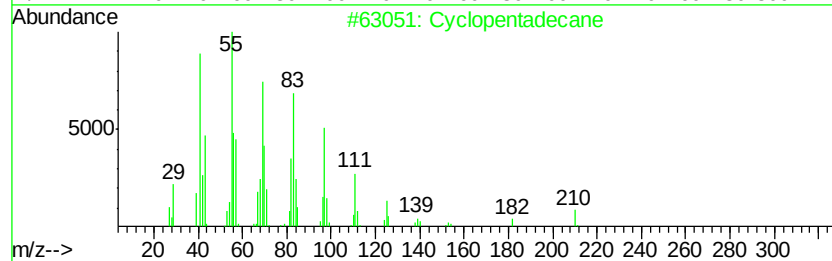
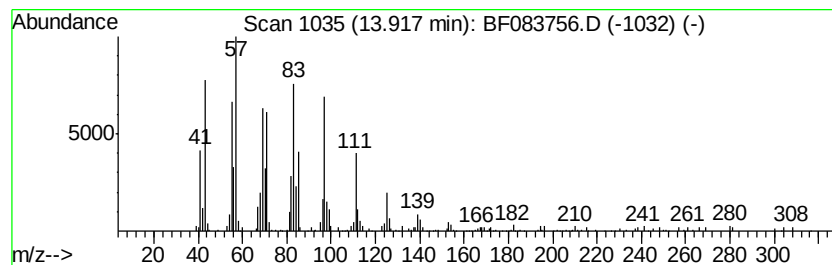
Instrument :
BNA_F
ClientSampleId :
1-STOCKPILE-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.92	5.96 ng	275510	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	98
2	Cycloeicosane	280	C20H40	000296-56-0	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083756.D
Acq On : 14 Dec 2015 4:10
Operator : UM/IZ
Sample : G4731-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

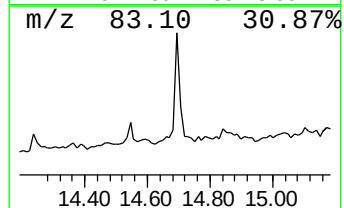
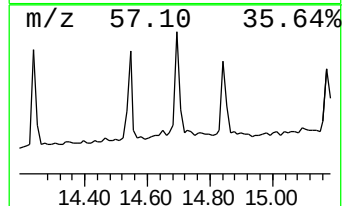
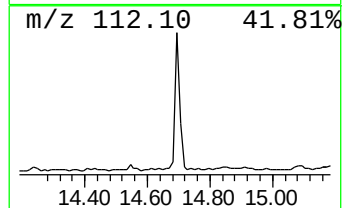
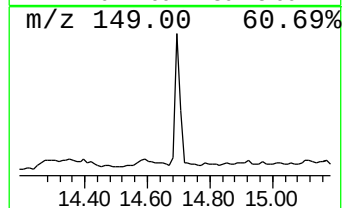
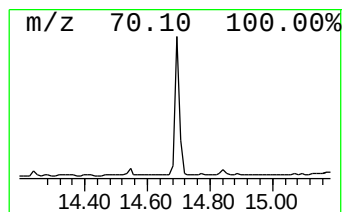
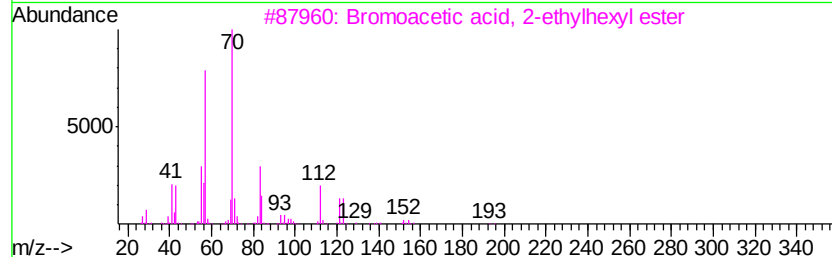
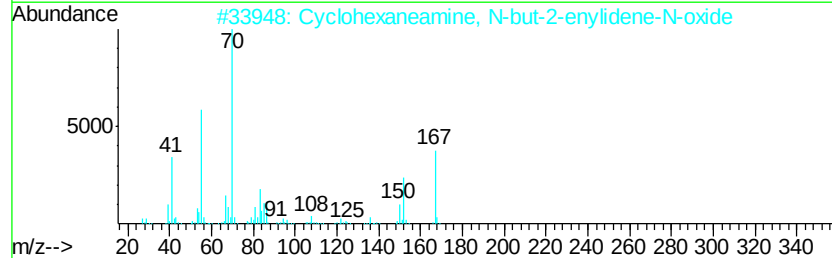
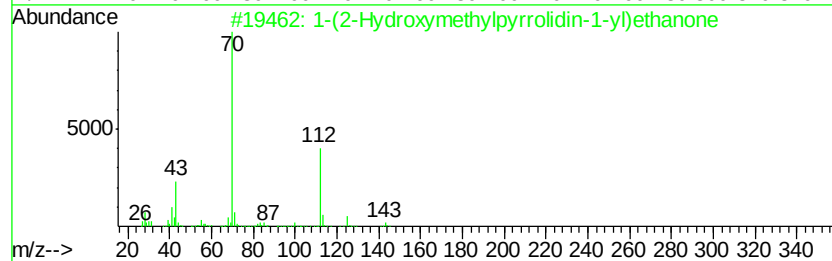
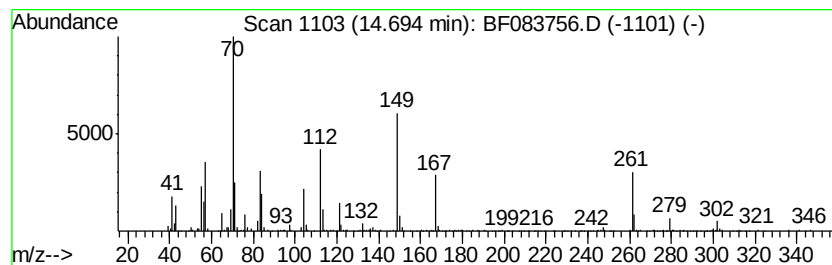
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ClientSampleId :
1-STOCKPILE-(0-2)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	6.33 ng	292584	Chrysene-d12	14.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-(2-Hydroxymethylpyrrolidin-1-yl)ethanone	143 C7H13NO2	1000192-83-2 35
2		Cyclohexaneamine, N-but-2-enylidene-N-oxide	167 C10H17NO	068048-01-1 27
3		Bromoacetic acid, 2-ethylhexyl ester	250 C10H19BrO2	068144-73-0 16
4		Cyclohexanamine, N-methyl-	113 C7H15N	000100-60-7 12
5		Aspidofractinine-3-methanol, (2S,3S,4S,5S,6S)-	310 C20H26N2O	002656-44-2 12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083756.D
Acq On : 14 Dec 2015 4:10
Operator : UM/IZ
Sample : G4731-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-STOCKPILE-(0-2)

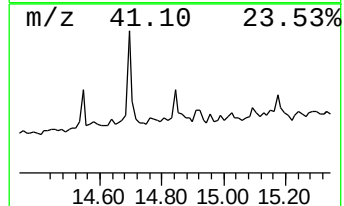
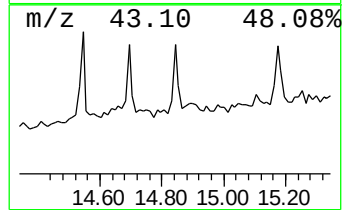
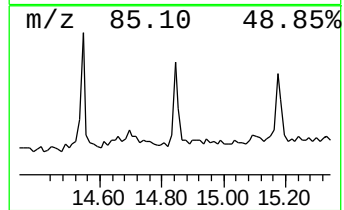
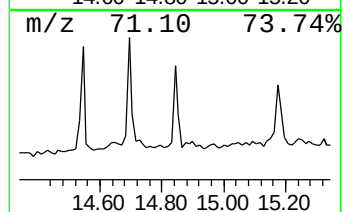
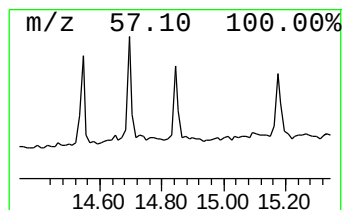
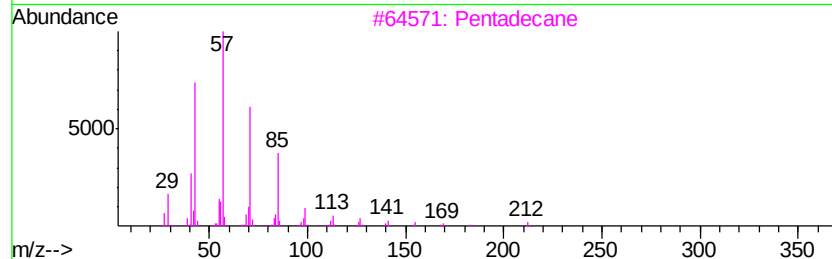
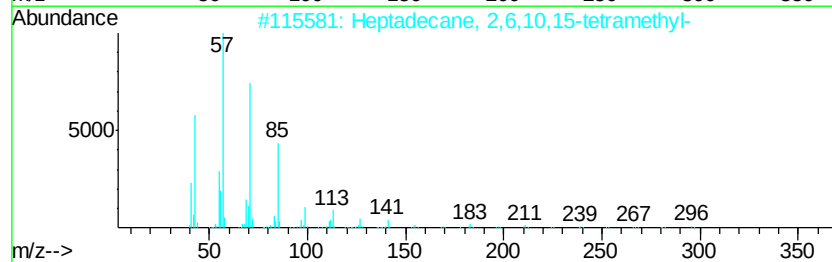
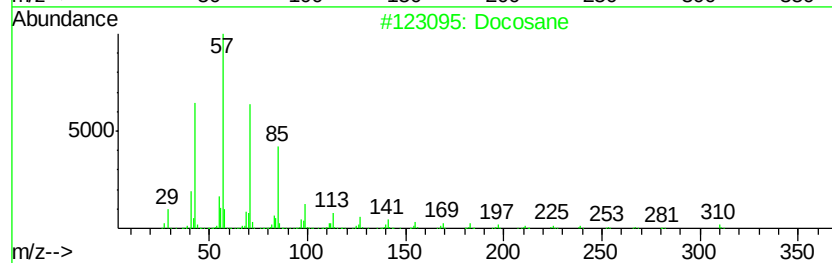
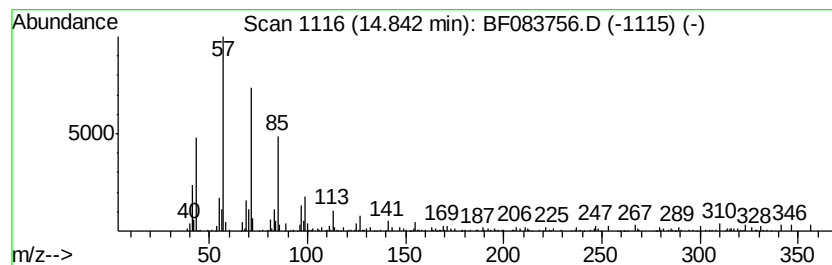
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.66 ng	73876	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	96
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3		Pentadecane	212	C15H32	000629-62-9	91
4		Tetradecane, 2-methyl-	212	C15H32	001560-95-8	90
5		Nonadecane	268	C19H40	000629-92-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083756.D
Acq On : 14 Dec 2015 4:10
Operator : UM/IZ
Sample : G4731-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-STOCKPILE-(0-2)

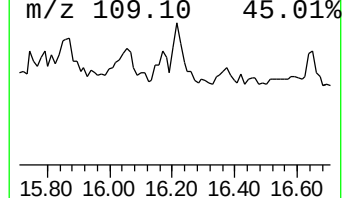
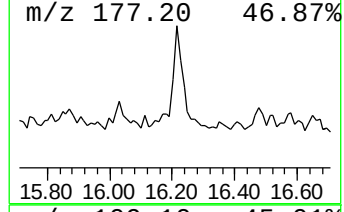
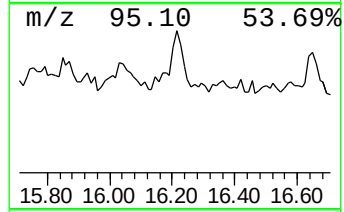
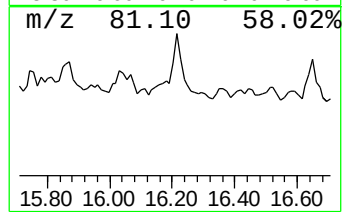
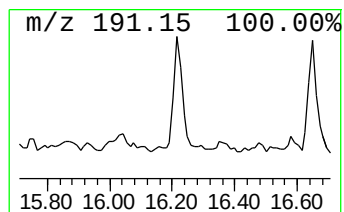
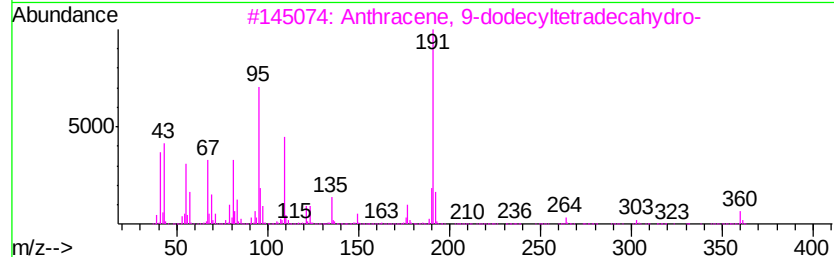
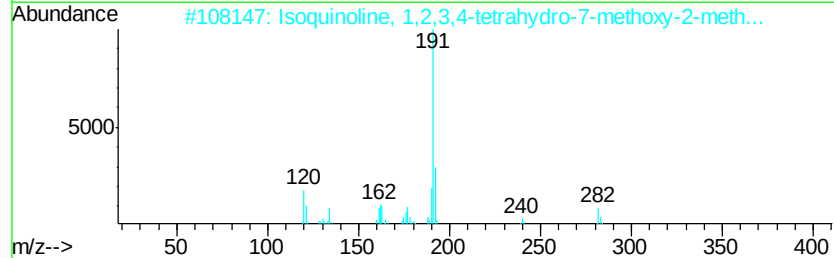
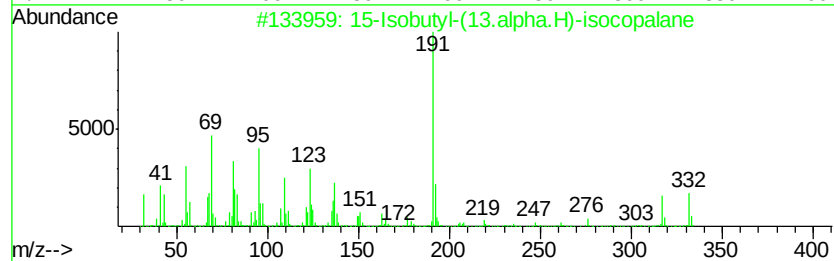
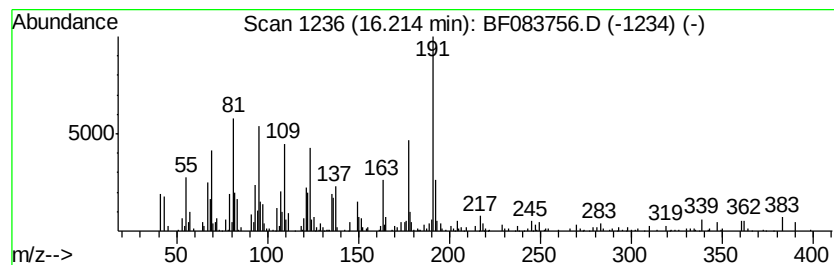
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 15-Isobutyl-(13.alpha.H)-is... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	6.90 ng	191361	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	52
2		Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21N02	036646-87-4	38
3		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37
4		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	37
5		28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083756.D
Acq On : 14 Dec 2015 4:10
Operator : UM/IZ
Sample : G4731-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-STOCKPILE-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.12	28.8	ng	1047260	1	6.92	726698	20.0
unknown6.69	6.69	102.0	ng	3704540	1	6.92	726698	20.0
Tetradecane	10.86	2.6	ng	104232	4	11.44	814268	20.0
Hexadecanoic acid...	12.84	8.2	ng	380161	5	14.07	924527	20.0
Octadecanoic acid...	13.55	6.0	ng	275194	5	14.07	924527	20.0
Cyclopentadecane	13.92	6.0	ng	275510	5	14.07	924527	20.0
unknown14.69	14.69	6.3	ng	292584	5	14.07	924527	20.0
Docosane	14.84	2.7	ng	73876	6	15.51	554651	20.0
15-Isobutyl-(13.a...	16.21	6.9	ng	191361	6	15.51	554651	20.0