

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
 Data File : BF083757.D
 Acq On : 14 Dec 2015 4:37
 Operator : UM/IZ
 Sample : G4731-03
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-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	2.235	11	13	28	rVB4	56092	128107	3.38%	0.399%
2	5.116	262	265	273	rVB	683511	999967	26.37%	3.111%
3	5.527	298	301	304	rBV	2323078	3385391	89.27%	10.531%
4	5.927	334	336	338	rVB	46705	39689	1.05%	0.123%
5	6.544	387	390	393	rBV	2267407	3362845	88.67%	10.461%
6	6.693	400	403	405	rBV	2900712	3582625	94.47%	11.144%
7	6.922	421	423	425	rBV	754251	728082	19.20%	2.265%
8	7.082	434	437	439	rVB	2565921	2870715	75.70%	8.930%
9	7.482	469	472	474	rBV	2086058	2302016	60.70%	7.161%
10	8.202	532	535	537	rBV	1118459	960242	25.32%	2.987%
11	9.276	626	629	632	rBV	3095325	3792385	100.00%	11.797%
12	9.665	661	663	666	rBV	499255	506434	13.35%	1.575%
13	9.893	681	683	686	rBV	85770	72860	1.92%	0.227%
14	9.950	686	688	691	rVV	838487	954588	25.17%	2.969%
15	10.396	723	727	728	rBV	96449	98187	2.59%	0.305%
16	10.613	743	746	749	rBV	31438	55675	1.47%	0.173%
17	10.739	754	757	760	rBV	1999305	1926686	50.80%	5.993%
18	10.865	766	768	773	rVB	106387	120948	3.19%	0.376%
19	11.310	803	807	809	rBV	68356	72720	1.92%	0.226%
20	11.436	816	818	820	rBV	906537	845747	22.30%	2.631%
21	12.133	877	879	883	rBV2	24286	46398	1.22%	0.144%
22	12.842	939	941	945	rBV2	266262	298538	7.87%	0.929%
23	12.922	945	948	950	rVB2	79474	88919	2.34%	0.277%
24	13.014	954	956	959	rBV	2314146	2679532	70.66%	8.335%
25	13.551	1001	1003	1005	rVV	213682	203262	5.36%	0.632%
26	13.596	1005	1007	1010	rVB2	45177	68051	1.79%	0.212%
27	13.814	1021	1026	1027	rBV5	19683	53020	1.40%	0.165%
28	13.916	1032	1035	1038	rBV2	94293	163667	4.32%	0.509%
29	14.065	1045	1048	1050	rBV	623911	730981	19.27%	2.274%
30	14.236	1061	1063	1065	rBV	66354	65829	1.74%	0.205%
31	14.545	1088	1090	1091	rBV	83624	91449	2.41%	0.284%
32	14.842	1114	1116	1121	rVB	63703	96298	2.54%	0.300%
33	15.174	1143	1145	1148	rBV	42757	58534	1.54%	0.182%
34	15.505	1171	1174	1177	rBV	410089	607846	16.03%	1.891%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
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35	15.985	1213	1216	1218	rBV	33658	47479	1.25%	0.148%
36	16.477	1257	1259	1263	rBV3	21629	41386	1.09%	0.129%

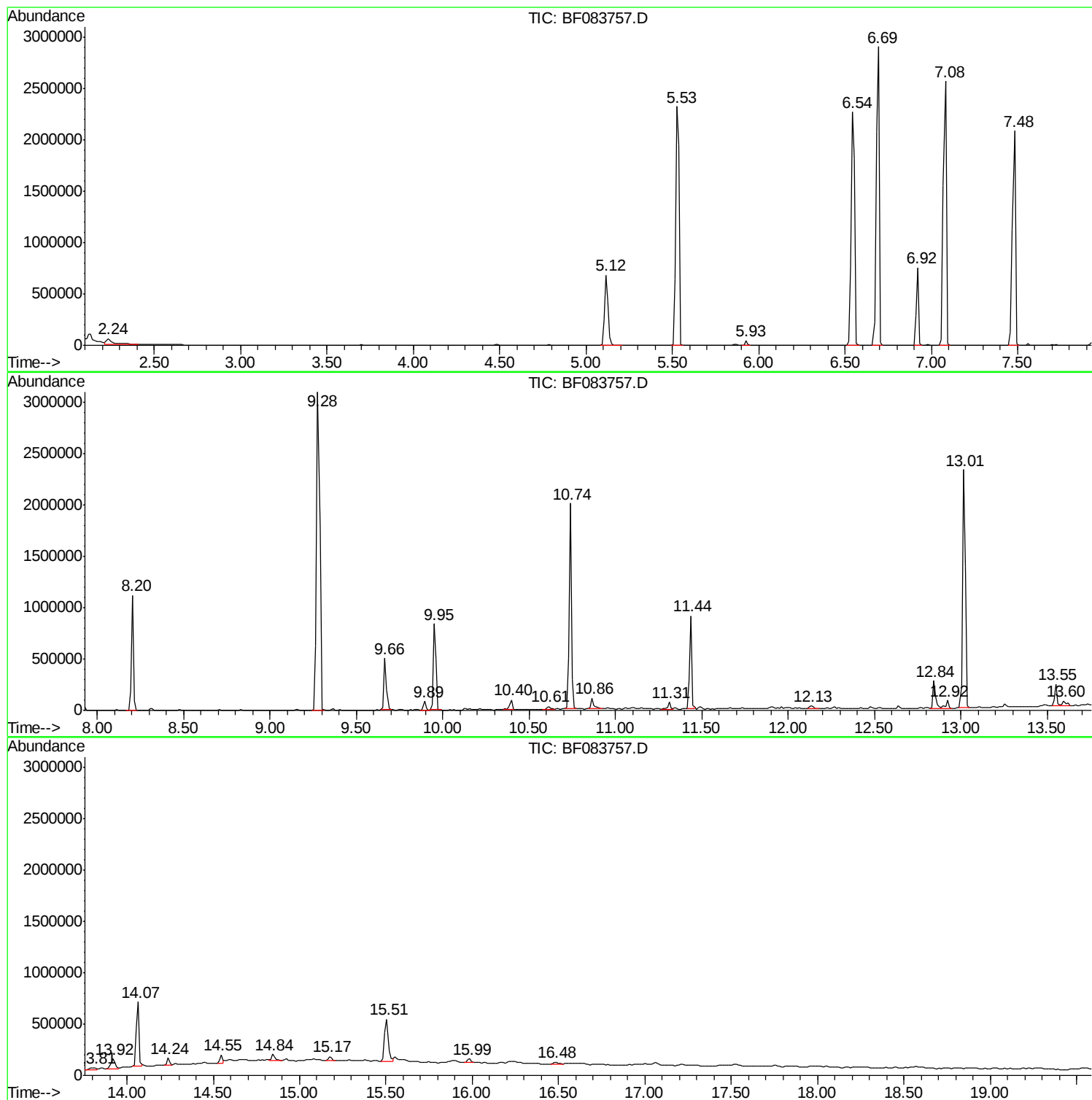
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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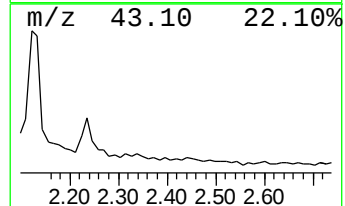
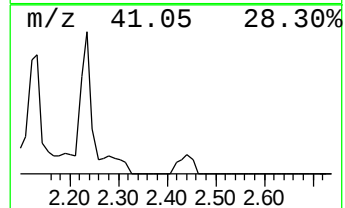
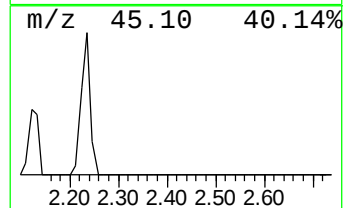
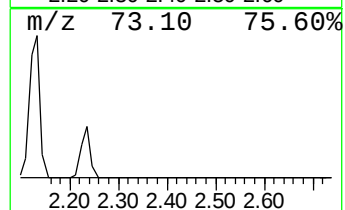
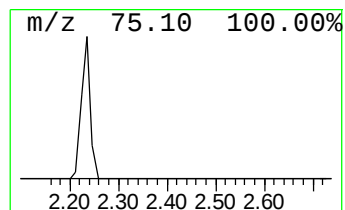
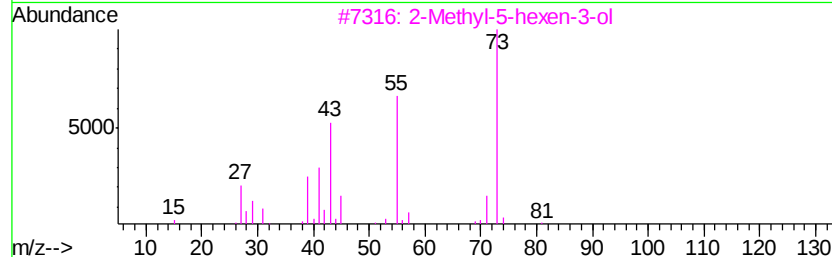
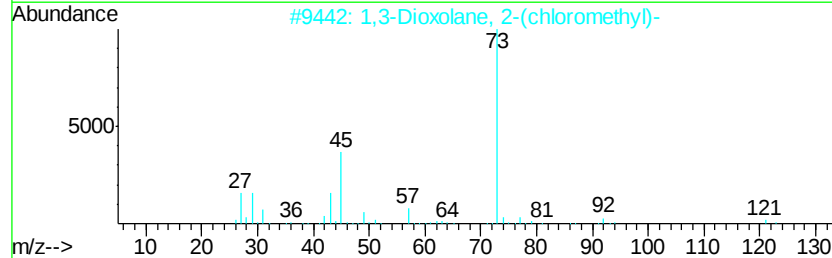
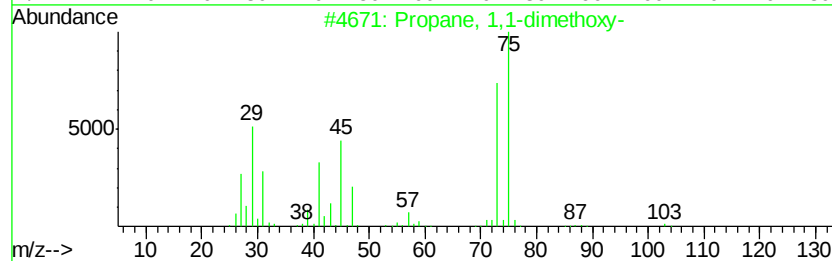
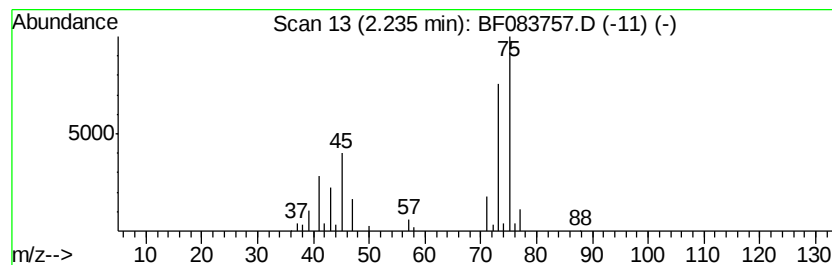
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	3.52 ng	128107	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	59
2			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
4			Silane, methylenebis-	76	CH8Si2	001759-88-2	7
5			Glycine	75	C2H5NO2	000056-40-6	5



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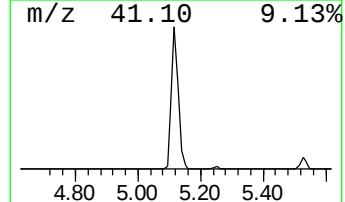
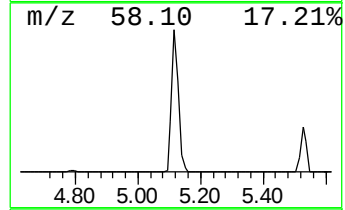
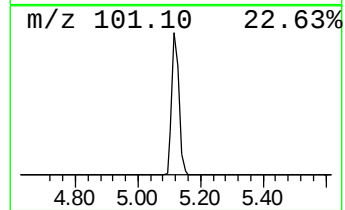
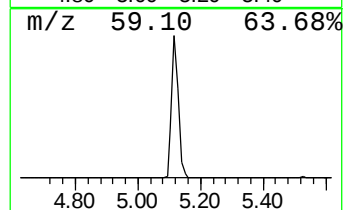
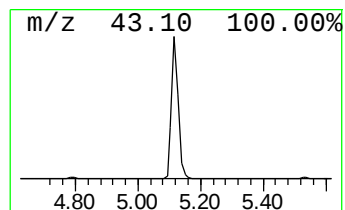
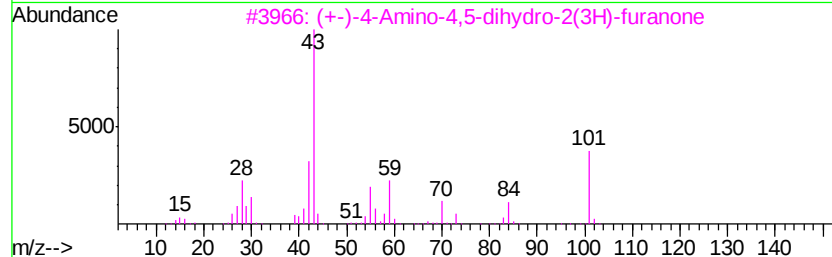
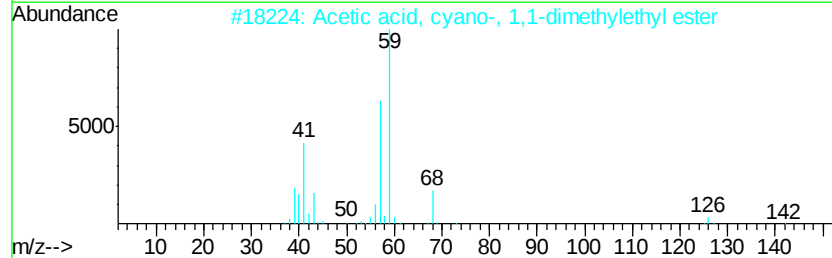
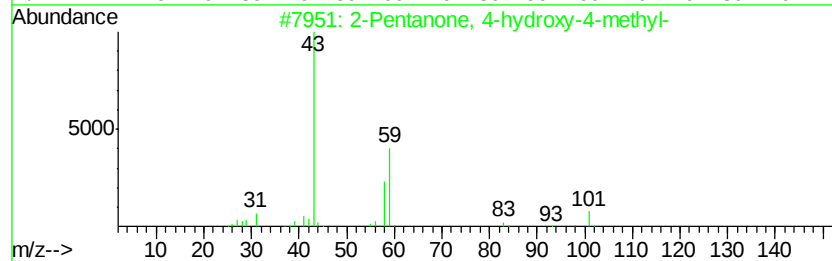
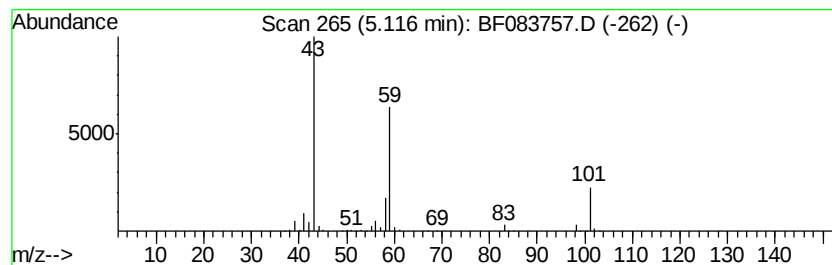
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	27.47 ng	999967	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	23
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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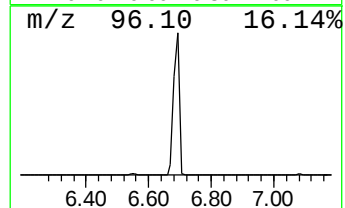
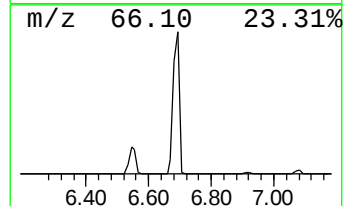
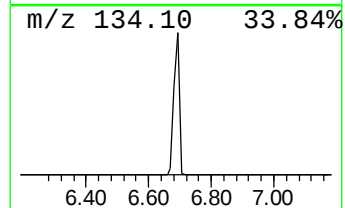
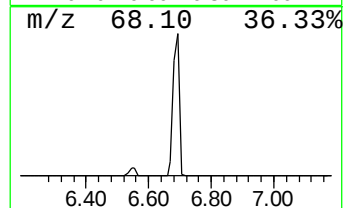
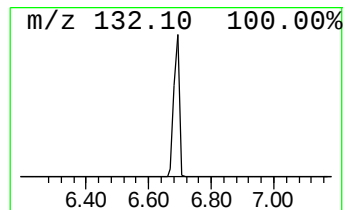
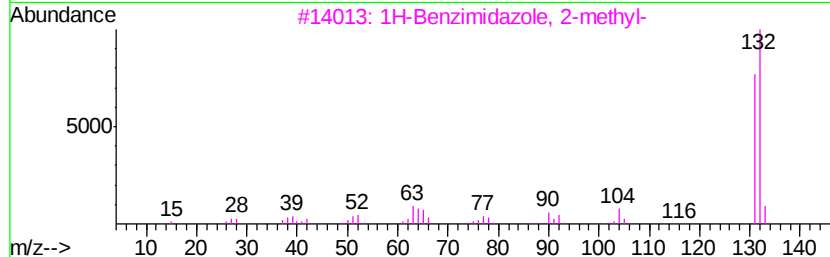
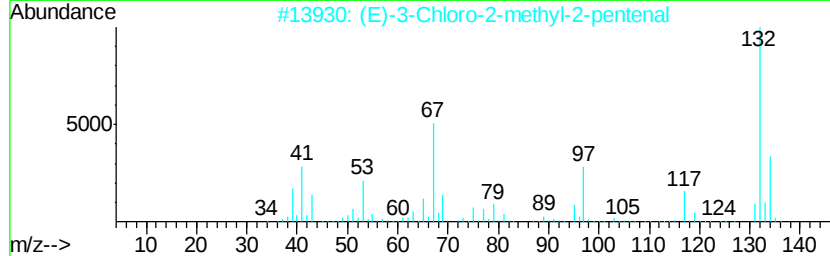
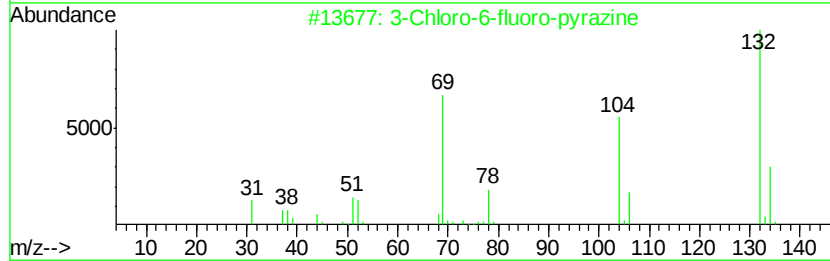
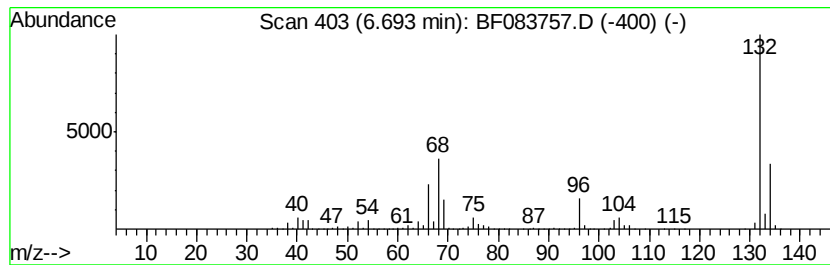
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	98.41 ng	3582630	1,4-Dichlorobenzene-d4	6.92

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	Benzene, 1,3,5-trifluoro-			132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9



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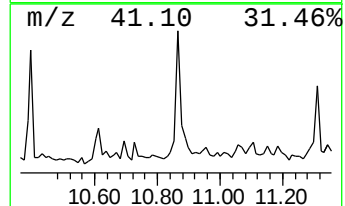
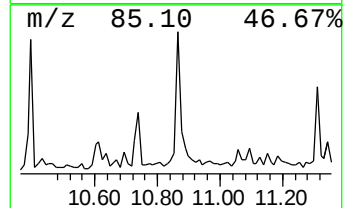
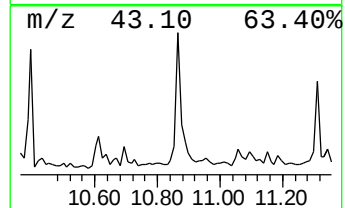
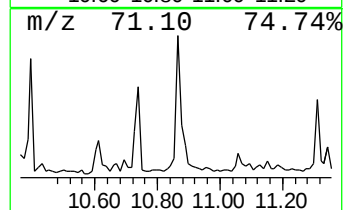
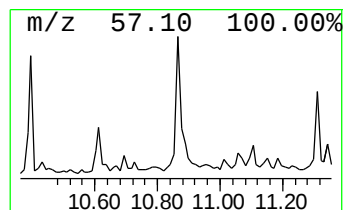
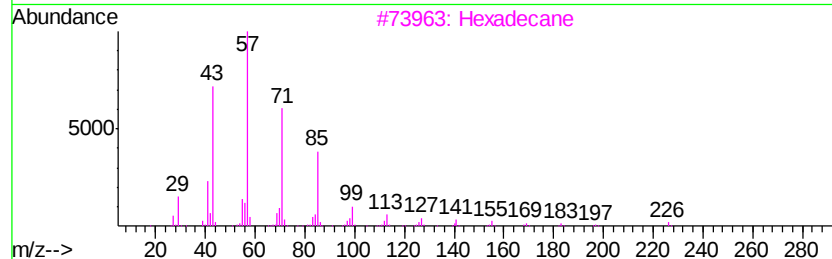
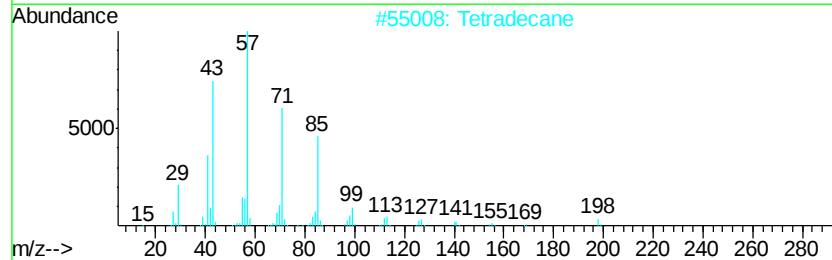
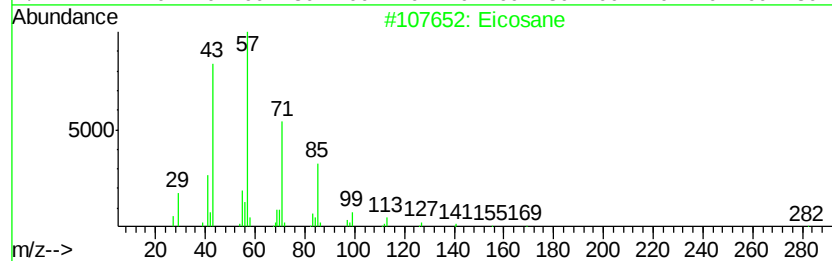
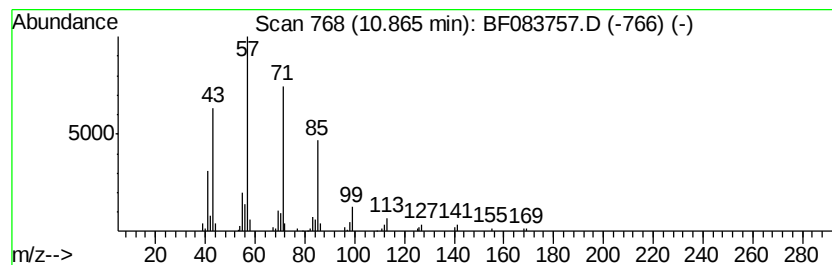
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.86 ng	120948	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tetradecane		198	C14H30	000629-59-4	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetracosane		338	C24H50	000646-31-1	86
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86



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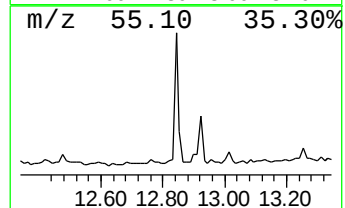
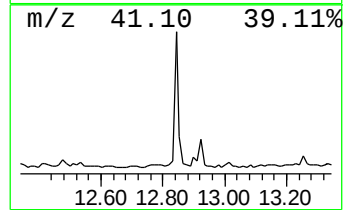
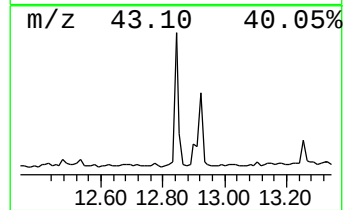
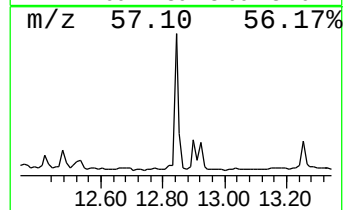
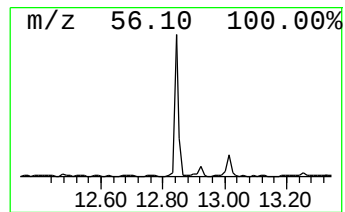
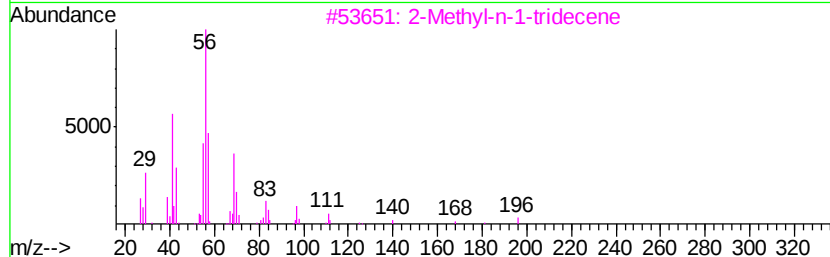
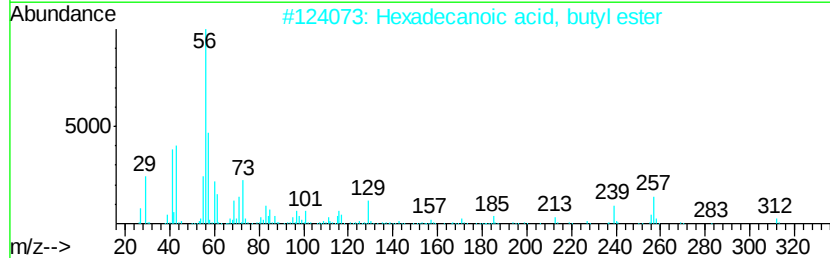
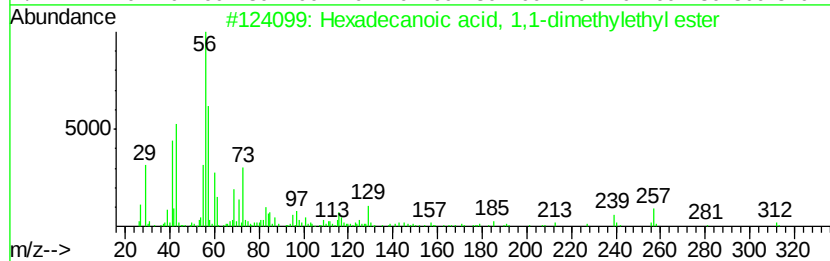
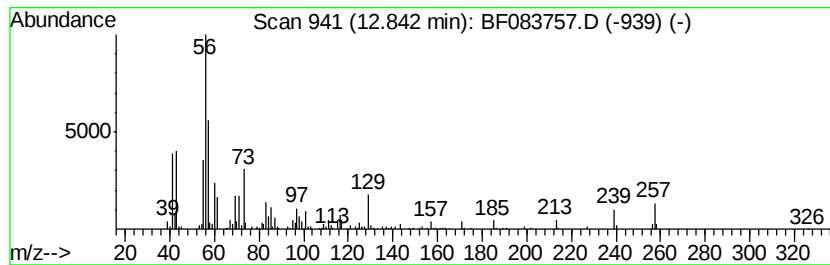
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	8.17 ng	298538	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083757.D
Acq On : 14 Dec 2015 4:37
Operator : UM/IZ
Sample : G4731-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

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

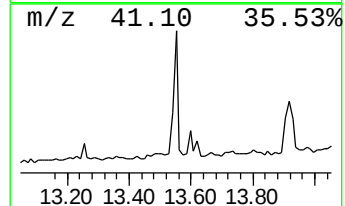
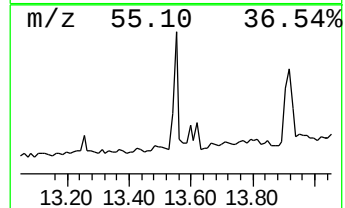
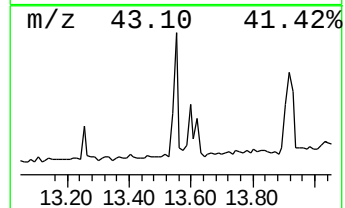
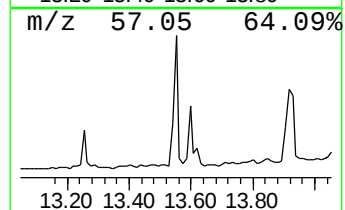
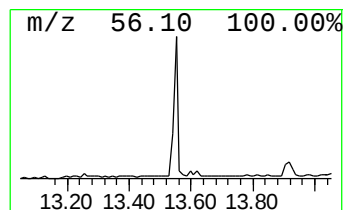
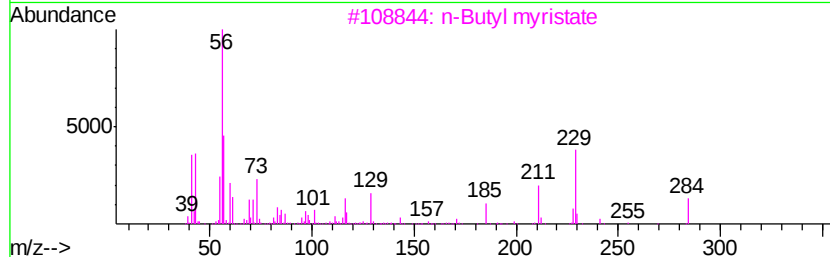
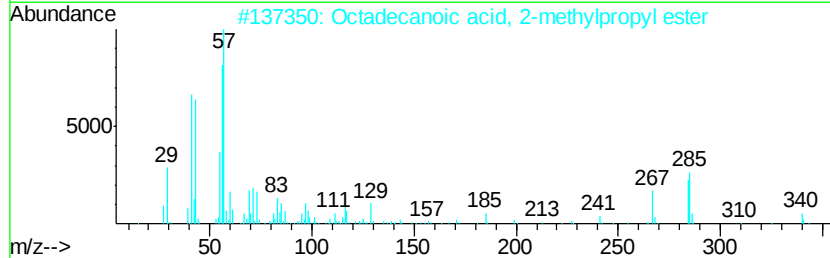
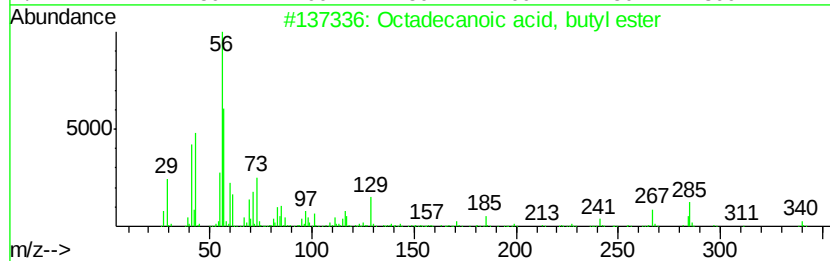
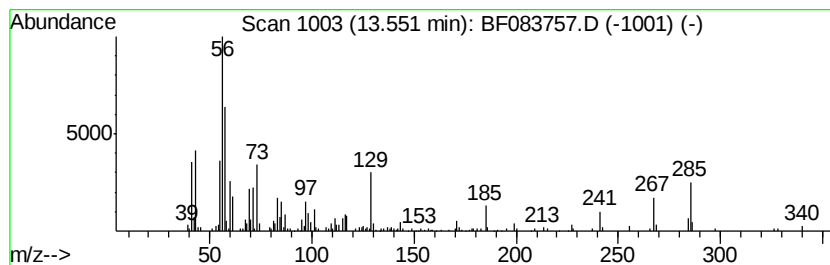
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	5.56 ng	203262	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	98
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	64
3		n-Butyl myristate	284	C18H36O2	000110-36-1	50
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32
5		Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083757.D
Acq On : 14 Dec 2015 4:37
Operator : UM/IZ
Sample : G4731-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

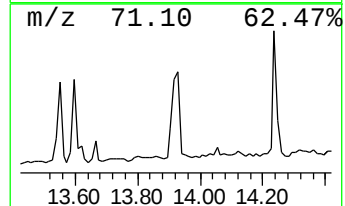
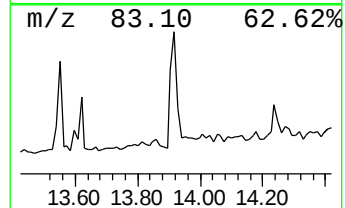
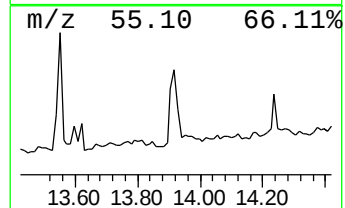
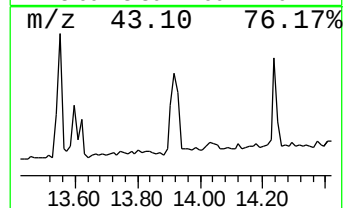
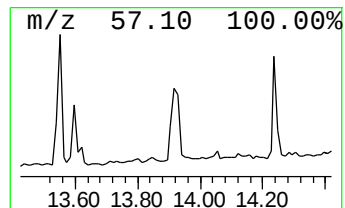
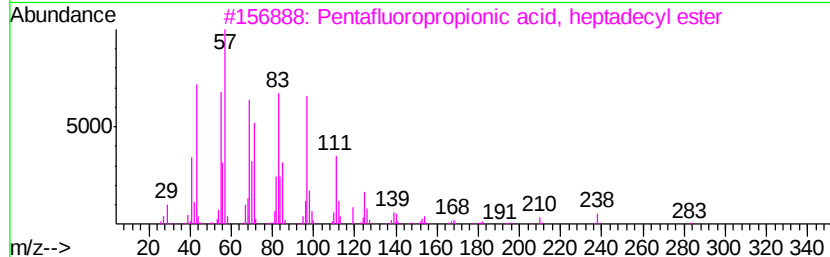
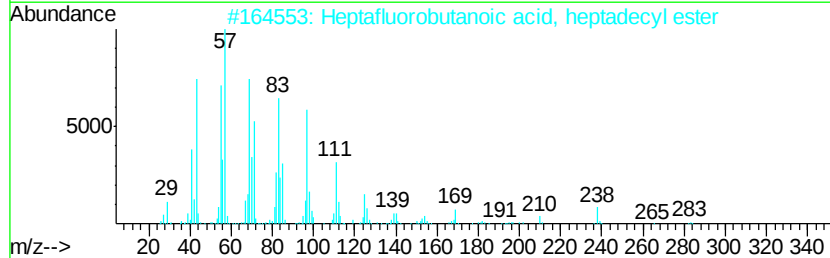
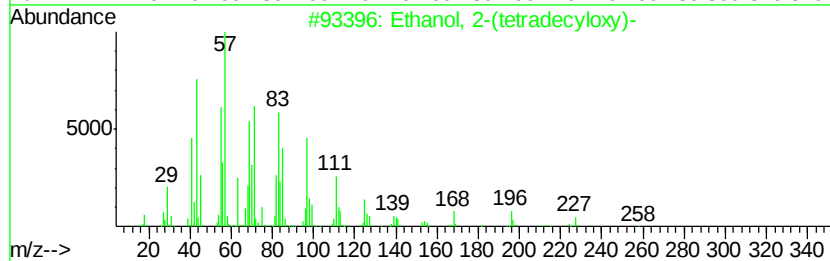
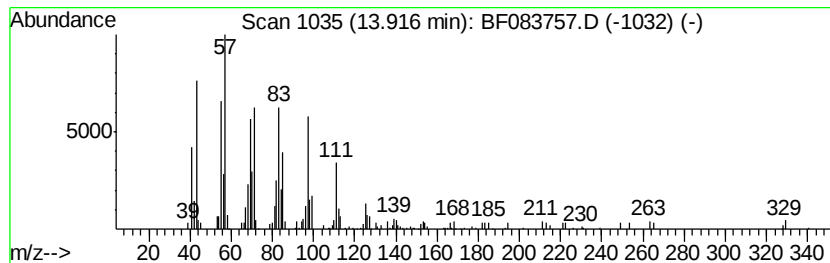
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ClientSampleId :
2-STOCKPILE-(0-2)

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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 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.92	4.48 ng	163667	Chrysene-d12	14.07		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083757.D
Acq On : 14 Dec 2015 4:37
Operator : UM/IZ
Sample : G4731-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

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

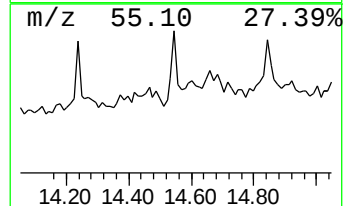
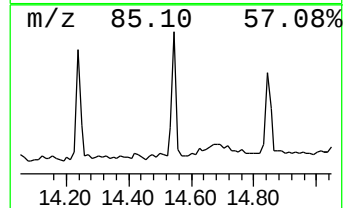
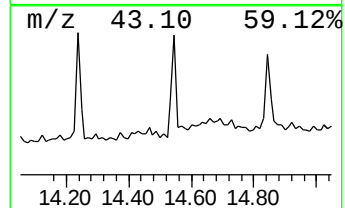
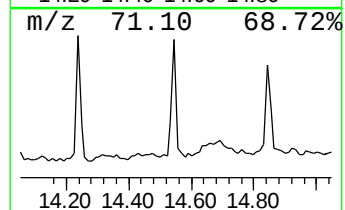
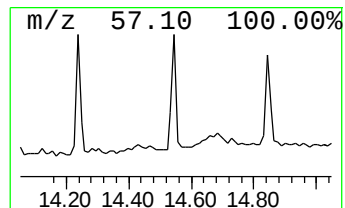
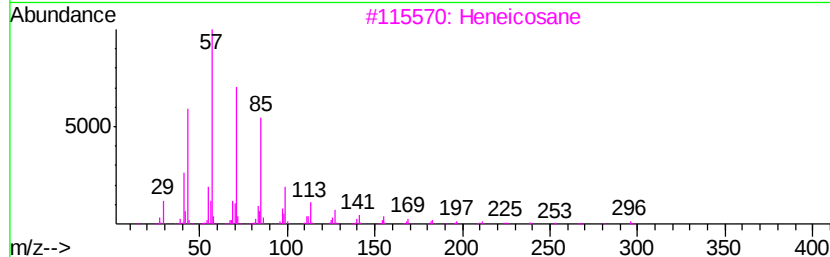
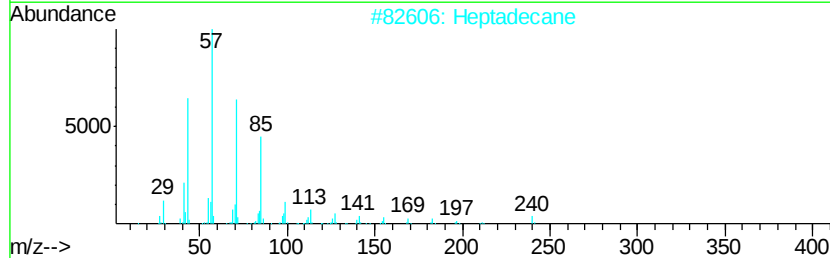
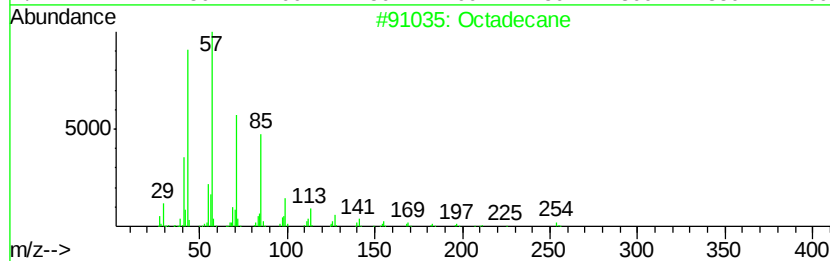
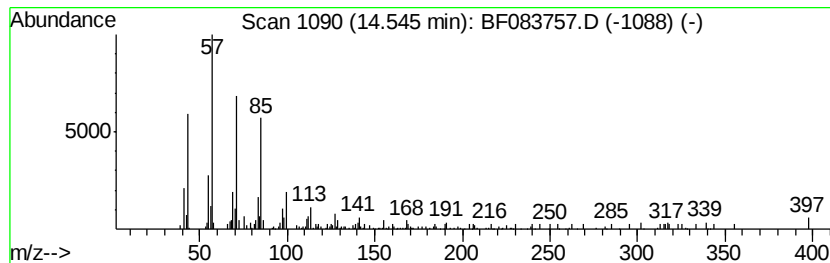
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.50 ng	91449	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	93
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Eicosane	282	C20H42	000112-95-8	90
5		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083757.D
Acq On : 14 Dec 2015 4:37
Operator : UM/IZ
Sample : G4731-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

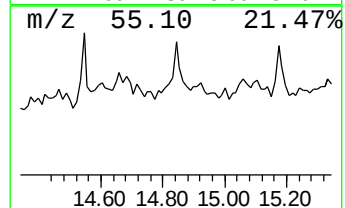
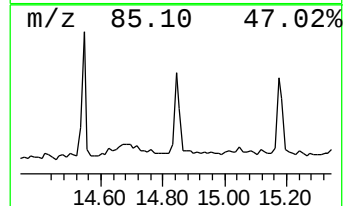
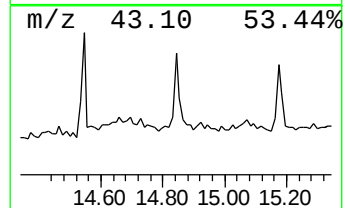
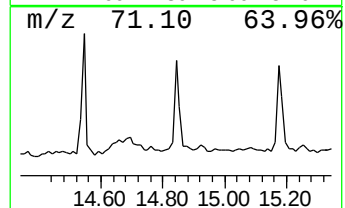
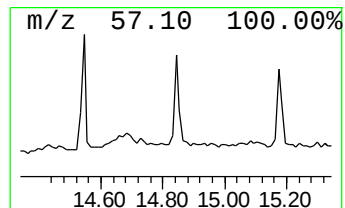
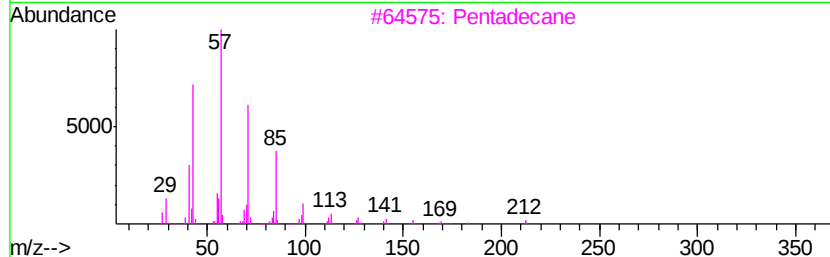
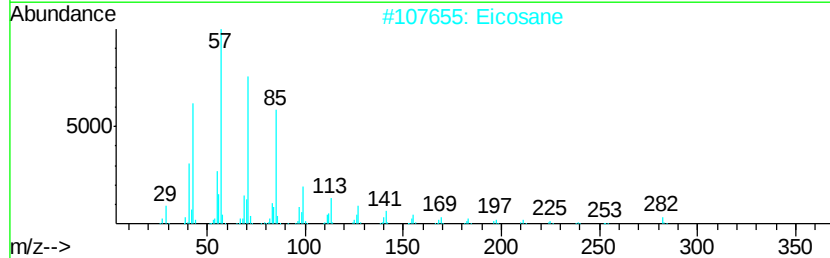
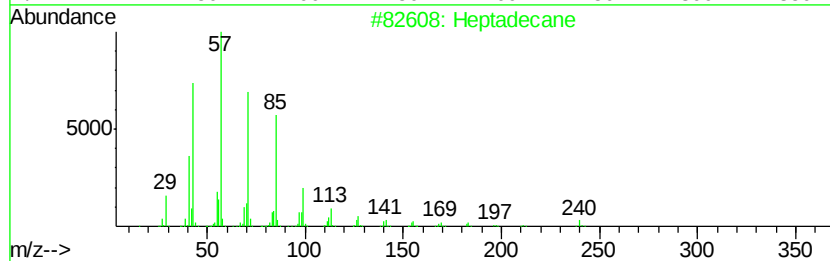
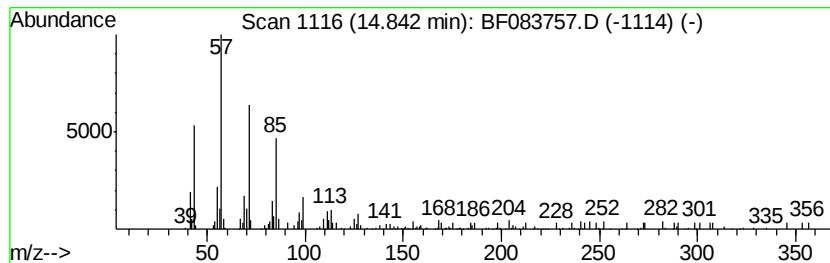
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.17 ng	96298	Perylene-d12	15.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	96
2	Eicosane	282 C20H42	000112-95-8	93
3	Pentadecane	212 C15H32	000629-62-9	70
4	Tetradecane	198 C14H30	000629-59-4	64
5	Tridecane	184 C13H28	000629-50-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083757.D
Acq On : 14 Dec 2015 4:37
Operator : UM/IZ
Sample : G4731-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
2-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
Propane, 1,1-dime...	2.24	3.5	ng	128107	1	6.92	728082	20.0
2-Pentanone, 4-hy...	5.12	27.5	ng	999967	1	6.92	728082	20.0
unknown6.69	6.69	98.4	ng	3582630	1	6.92	728082	20.0
Eicosane	10.86	2.9	ng	120948	4	11.44	845747	20.0
Hexadecanoic acid...	12.84	8.2	ng	298538	5	14.07	730981	20.0
Octadecanoic acid...	13.55	5.6	ng	203262	5	14.07	730981	20.0
Ethanol, 2-(tetra...	13.92	4.5	ng	163667	5	14.07	730981	20.0
Octadecane	14.55	2.5	ng	91449	5	14.07	730981	20.0
Heptadecane	14.84	3.2	ng	96298	6	15.51	607846	20.0