

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
 Data File : BF082072.D
 Acq On : 6 Oct 2015 5:01
 Operator : UM/IZ
 Sample : G3891-19
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-4(0-24)

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-BF092815.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	2.331	15	17	24	rVB2	13346	30841	2.04%	0.206%
2	5.063	254	256	265	rBV	467835	640321	42.39%	4.284%
3	5.486	290	293	295	rBV	1460096	1430335	94.69%	9.570%
4	5.806	319	321	326	rVB4	11770	16932	1.12%	0.113%
5	6.320	363	366	368	rBV	12454	18774	1.24%	0.126%
6	6.514	381	383	386	rBV	1021692	1285263	85.09%	8.600%
7	6.652	393	395	398	rBV	1576794	1424476	94.30%	9.531%
8	6.709	398	400	402	rVV	18748	22886	1.52%	0.153%
9	6.754	402	404	407	rVB	14832	18003	1.19%	0.120%
10	6.892	413	416	418	rBV	335554	436608	28.90%	2.921%
11	6.937	418	420	425	rVB3	8267	16943	1.12%	0.113%
12	7.040	427	429	432	rBV	1310370	1182064	78.25%	7.909%
13	7.200	441	443	448	rBV4	11182	22459	1.49%	0.150%
14	7.280	448	450	457	rVB5	7299	17959	1.19%	0.120%
15	7.452	463	465	470	rBV	836862	792023	52.43%	5.299%
16	7.532	470	472	476	rVB	26258	31765	2.10%	0.213%
17	7.692	484	486	491	rVB	14094	23335	1.54%	0.156%
18	7.909	501	505	509	rBV2	15416	35797	2.37%	0.240%
19	8.103	519	522	525	rBV	129512	124073	8.21%	0.830%
20	8.172	526	528	530	rVB	624824	514031	34.03%	3.439%
21	8.469	550	554	556	rBV3	7213	17081	1.13%	0.114%
22	8.595	563	565	571	rVB2	15509	34192	2.26%	0.229%
23	8.709	573	575	578	rBV3	7135	17944	1.19%	0.120%
24	8.755	578	579	581	rVB	25927	29269	1.94%	0.196%
25	8.823	581	585	587	rBV	18959	23513	1.56%	0.157%
26	9.120	610	611	613	rBV	16157	15862	1.05%	0.106%
27	9.189	613	617	620	rVV	29934	36907	2.44%	0.247%
28	9.246	620	622	625	rVV	1274487	1510531	100.00%	10.107%
29	9.326	625	629	630	rVV	66181	78528	5.20%	0.525%
30	9.395	634	635	638	rVB	22811	23776	1.57%	0.159%
31	9.589	649	652	653	rBV2	20576	22986	1.52%	0.154%
32	9.646	655	657	659	rVV	283717	235903	15.62%	1.578%
33	9.795	668	670	671	rBV	19257	22644	1.50%	0.152%
34	9.852	671	675	677	rVB	49795	68129	4.51%	0.456%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.932	679	682	684	rVB	632867	562763	37.26%	3.765%
36	10.115	697	698	700	rBV	11996	15615	1.03%	0.104%
37	10.172	702	703	705	rBV2	11972	15267	1.01%	0.102%
38	10.332	715	717	718	rBV	18328	20728	1.37%	0.139%
39	10.355	718	719	721	rVB	86249	64057	4.24%	0.429%
40	10.572	735	738	742	rBV	33119	54488	3.61%	0.365%
41	10.721	748	751	754	rBV	819178	758328	50.20%	5.074%
42	10.801	756	758	759	rVV	14402	19203	1.27%	0.128%
43	10.835	759	761	763	rVV	71701	109160	7.23%	0.730%
44	10.915	766	768	770	rBV2	14636	21346	1.41%	0.143%
45	11.018	775	777	779	rBV2	8577	16672	1.10%	0.112%
46	11.281	797	800	801	rBV	61541	64642	4.28%	0.433%
47	11.303	801	802	805	rVB	34541	38172	2.53%	0.255%
48	11.372	806	808	810	rBV2	17031	19121	1.27%	0.128%
49	11.418	810	812	815	rBV	536275	502192	33.25%	3.360%
50	11.704	836	837	840	rVB2	51704	51815	3.43%	0.347%
51	11.944	856	858	862	rBV2	49550	69067	4.57%	0.462%
52	12.115	871	873	874	rBV	29001	25617	1.70%	0.171%
53	12.504	905	907	909	rVB	23737	23564	1.56%	0.158%
54	12.618	914	917	920	rBV2	27039	51483	3.41%	0.344%
55	13.007	948	951	954	rBV	1454888	1382579	91.53%	9.251%
56	13.898	1028	1029	1033	rBV	82477	133266	8.82%	0.892%
57	14.058	1041	1043	1046	rBV	325123	403176	26.69%	2.698%
58	15.521	1169	1171	1174	rVB	224476	301214	19.94%	2.015%

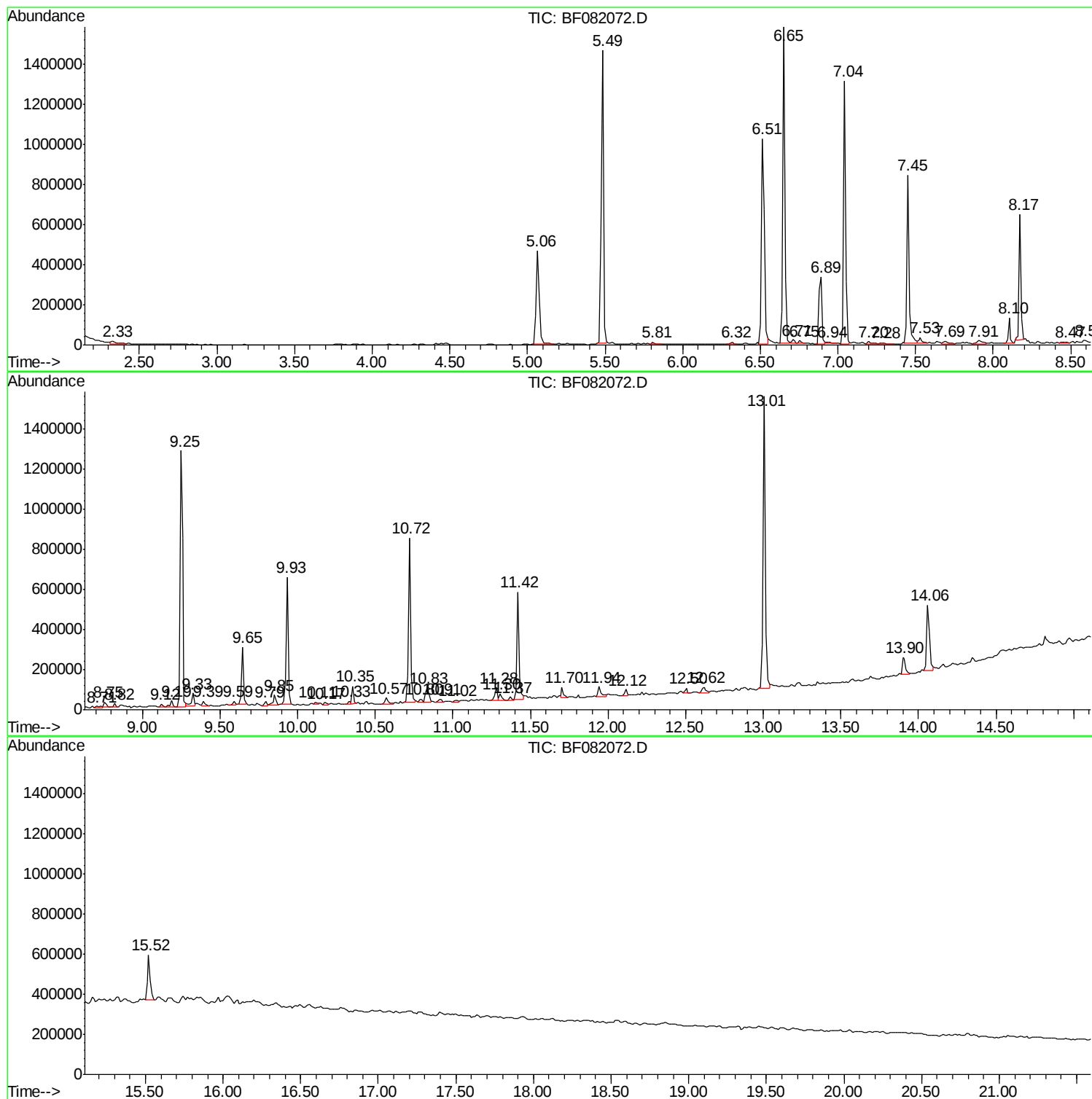
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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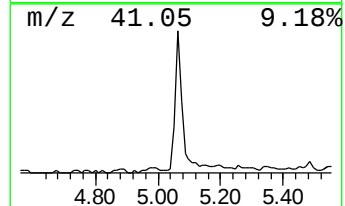
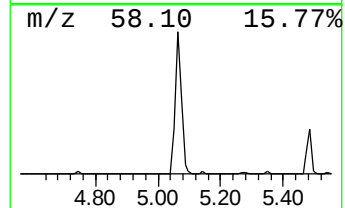
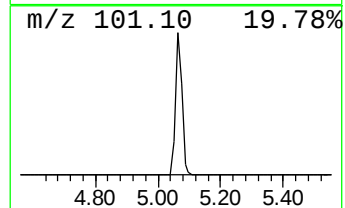
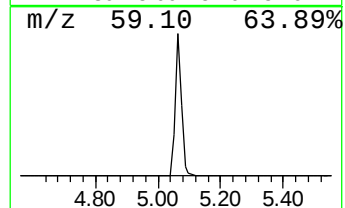
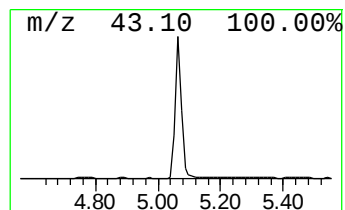
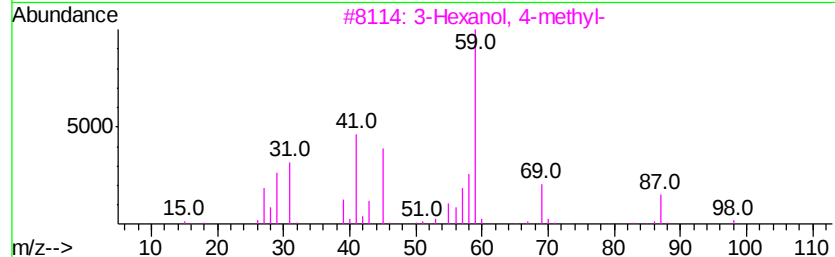
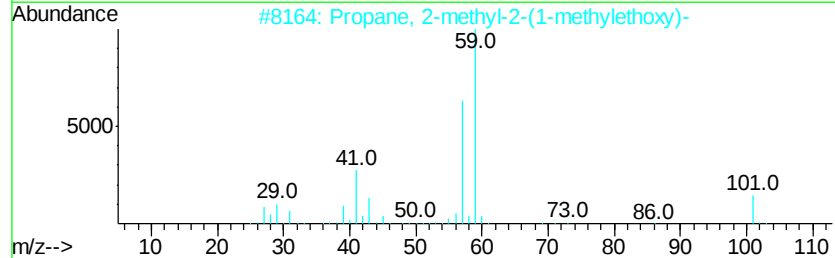
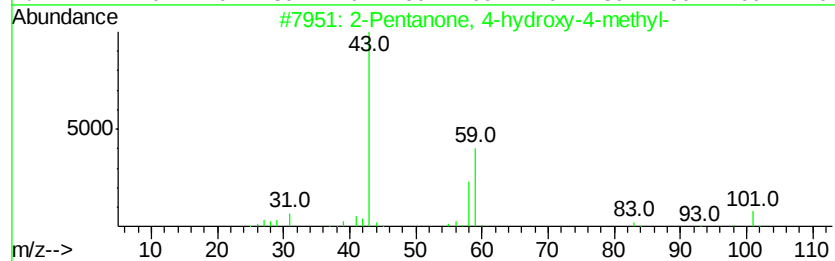
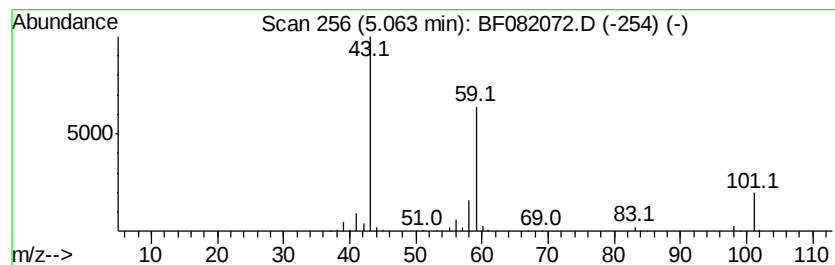
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	29.33 ng	640321	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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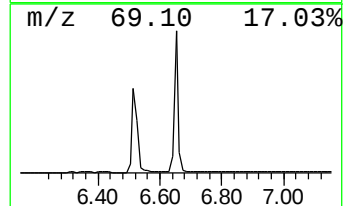
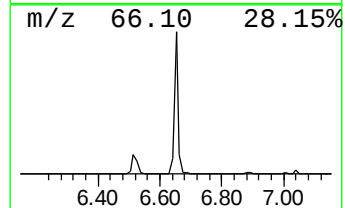
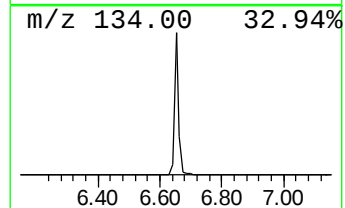
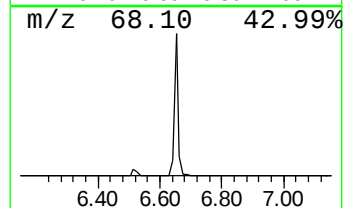
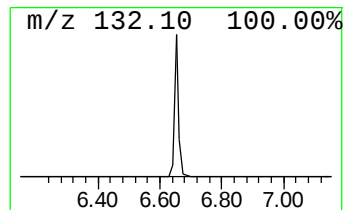
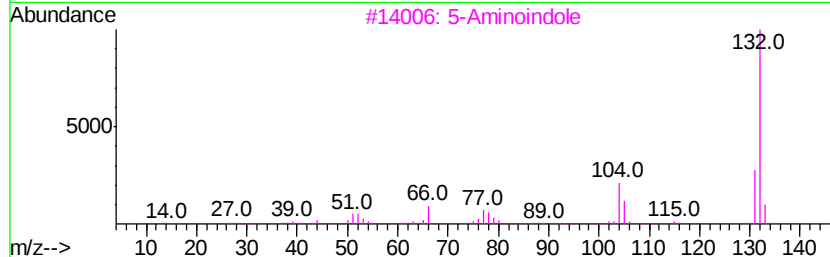
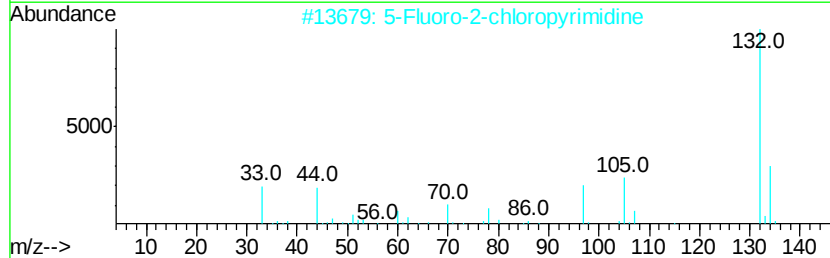
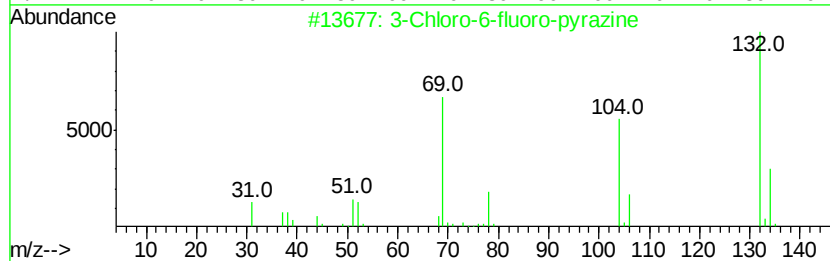
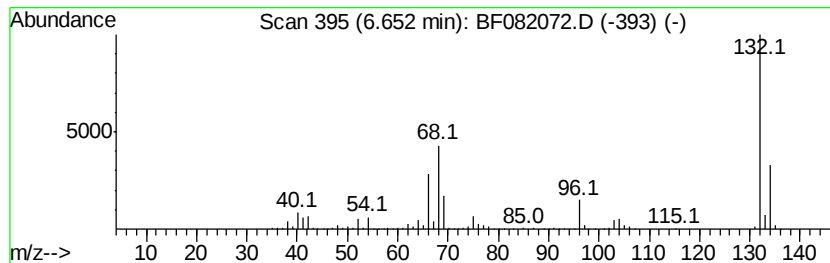
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	65.25 ng	1424480	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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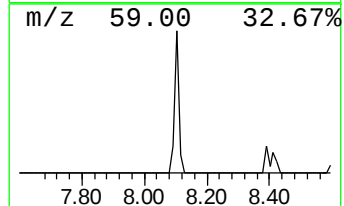
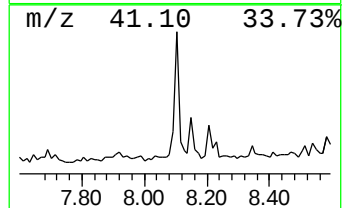
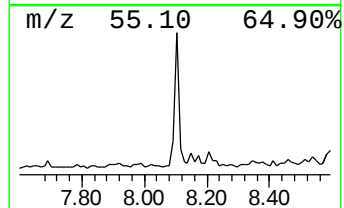
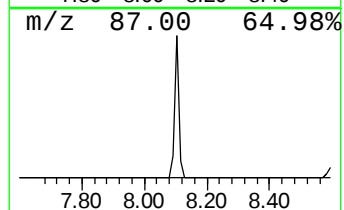
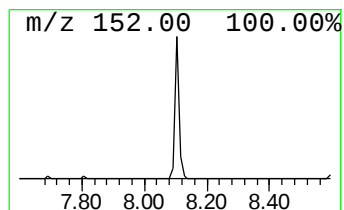
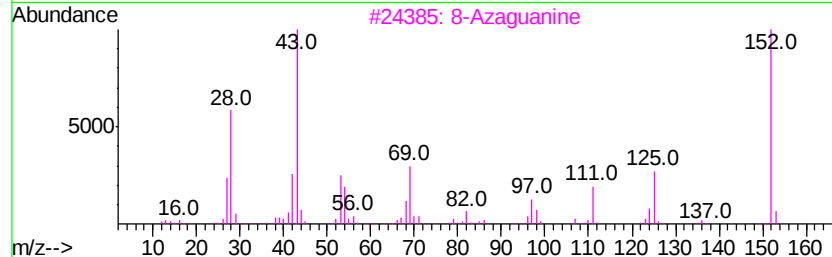
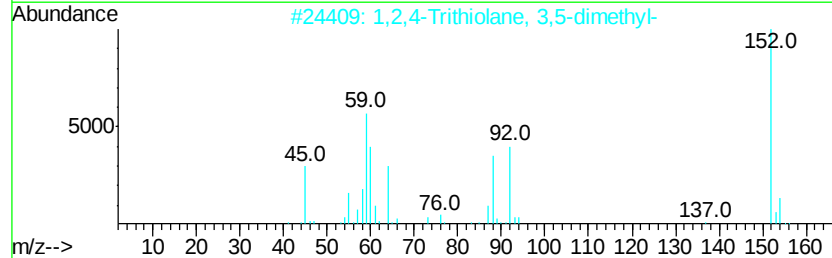
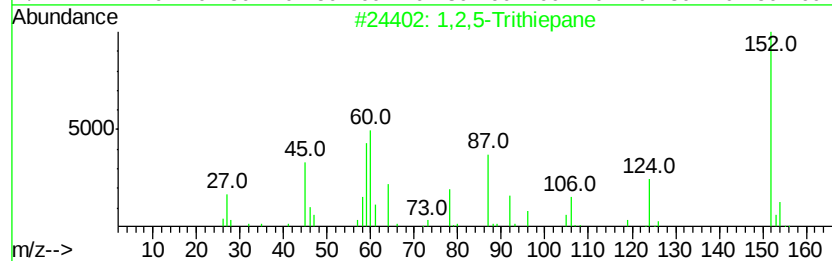
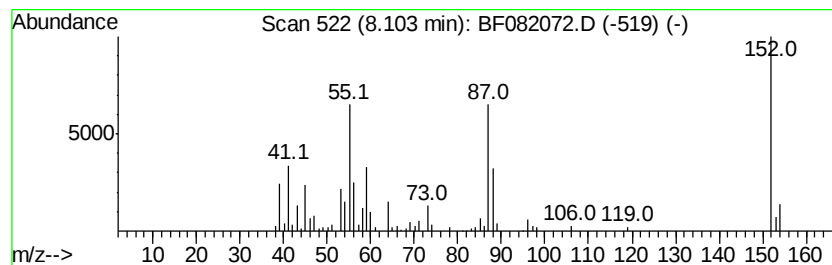
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.10	4.83 ng	124073	Naphthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	43
2		1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	37
3		8-Azaquanine	152	C4H4N6O	000134-58-7	22
4		2-Chlorobenzimidazole	152	C7H5ClN2	004857-06-1	22
5		Benzene, 1-(ethylthio)-4-methyl-	152	C9H12S	000622-63-9	22



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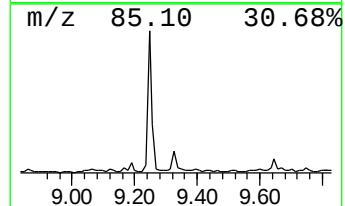
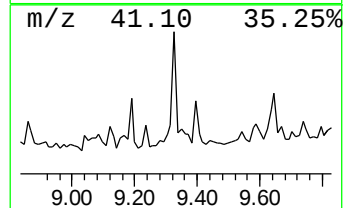
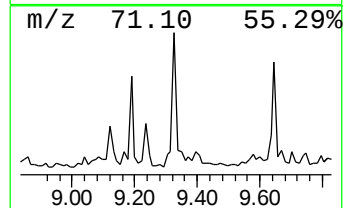
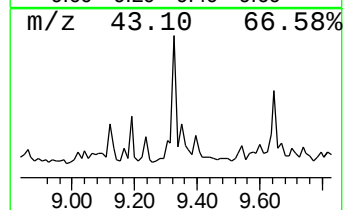
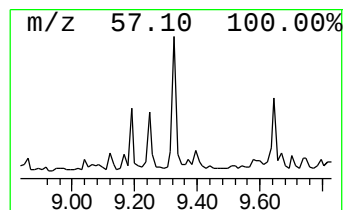
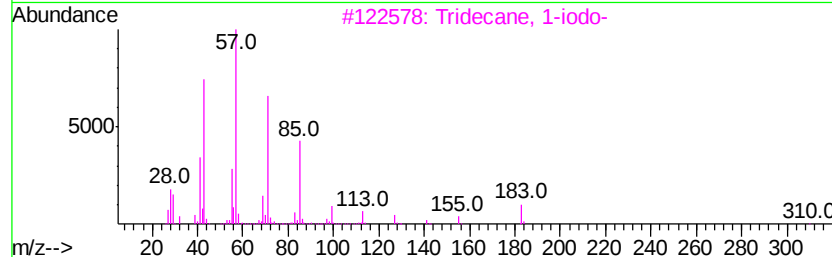
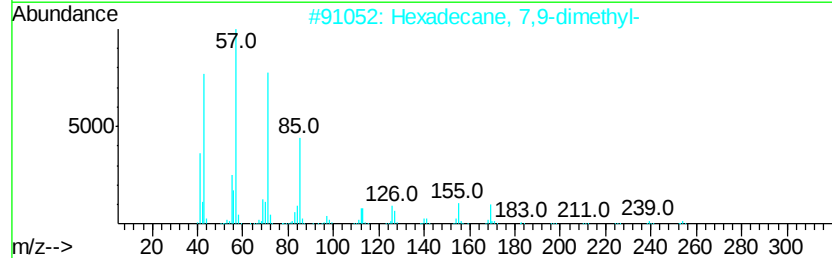
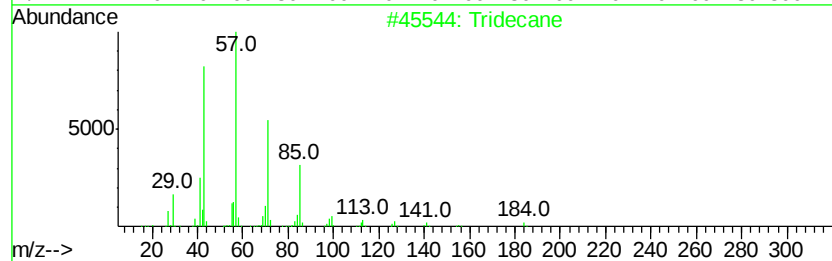
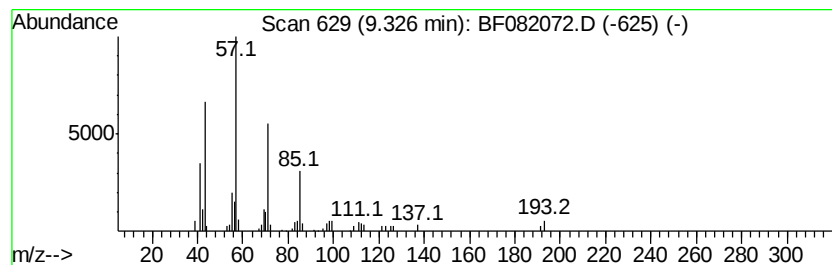
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.33	2.79 ng	78528	Acenaphthene-d10	9.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	72
2	Hexadecane, 7,9-dimethyl-		254	C18H38	021164-95-4	64
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	64
4	Tetradecane		198	C14H30	000629-59-4	64
5	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	64



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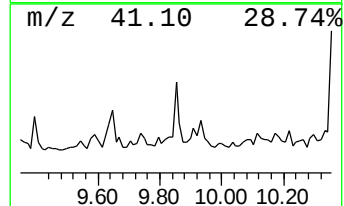
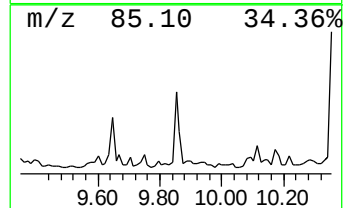
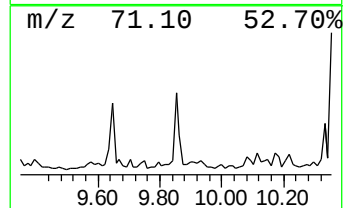
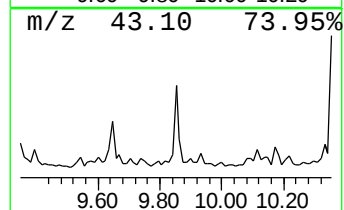
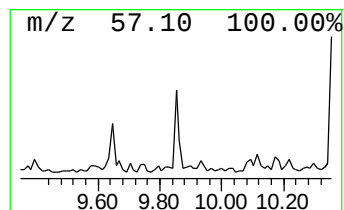
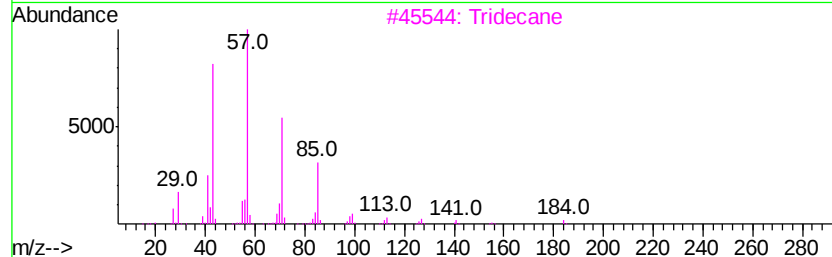
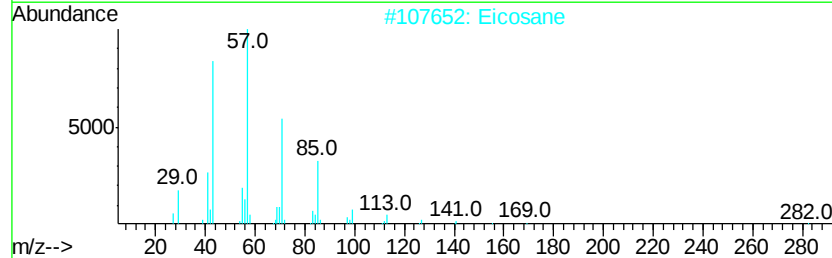
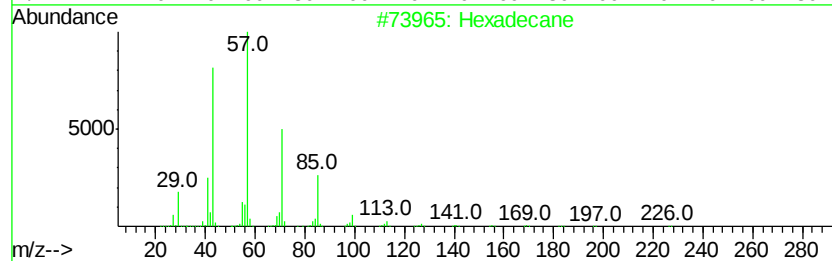
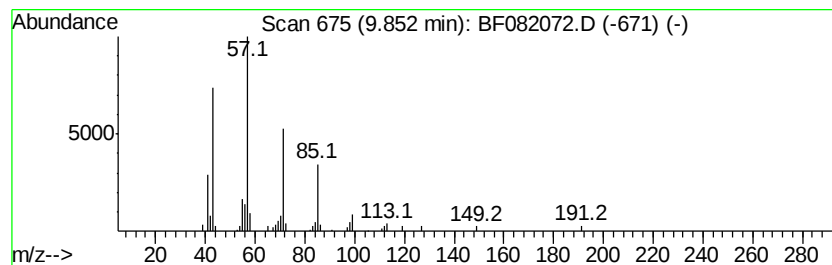
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.42 ng	68129	Acenaphthene-d10	9.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	86
2		Eicosane	282	C20H42	000112-95-8	78
3		Tridecane	184	C13H28	000629-50-5	72
4		Tetradecane	198	C14H30	000629-59-4	72
5		Pentadecane	212	C15H32	000629-62-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
Data File : BF082072.D
Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
ALS Vial : 29 Sample Multiplier: 1

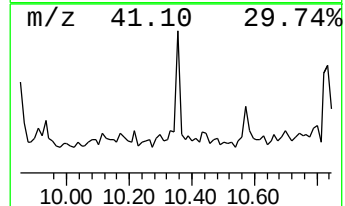
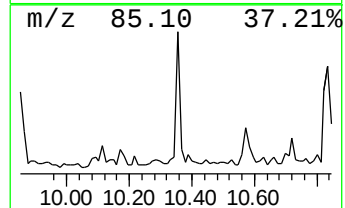
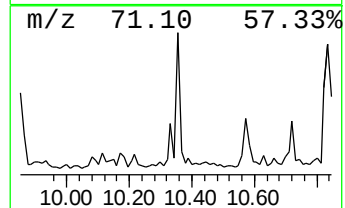
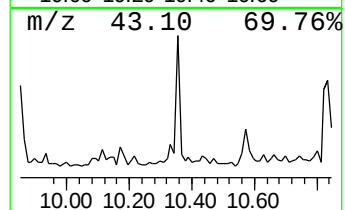
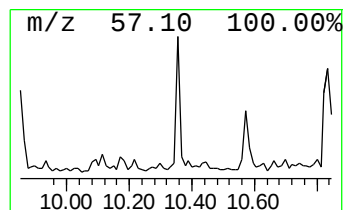
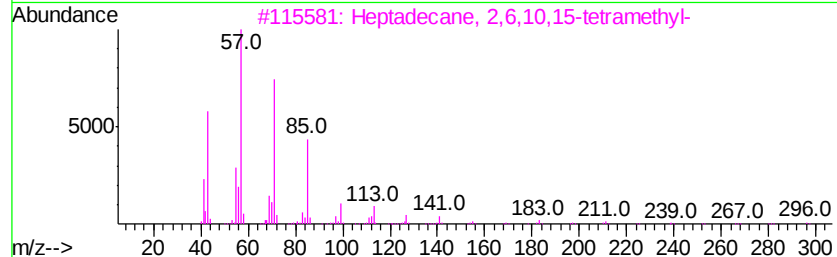
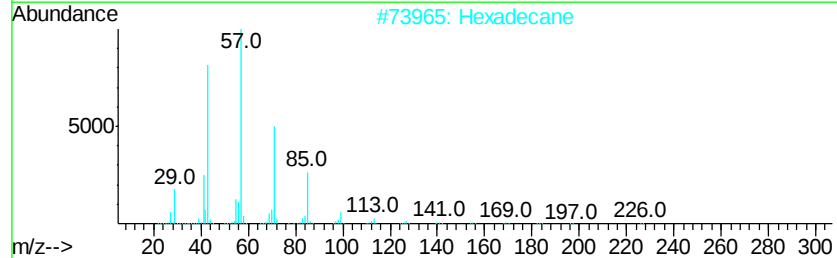
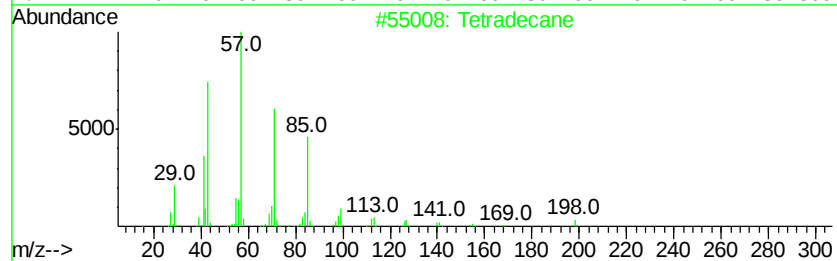
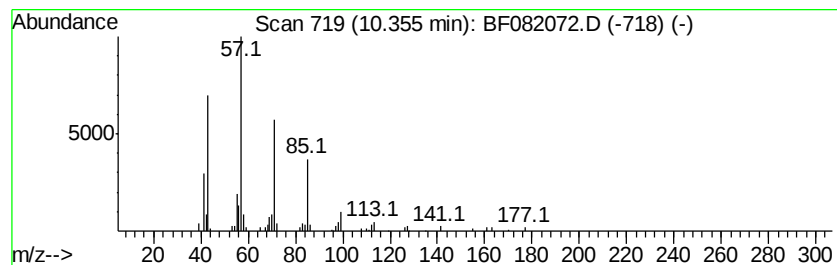
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ClientSampleId :
SS-4(0-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.28 ng	64057	Acenaphthene-d10	9.93
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 86
2		Hexadecane	226 C16H34	000544-76-3 83
3		Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6 80
4		Octadecane	254 C18H38	000593-45-3 78
5		Undecane, 3-methyl-	170 C12H26	001002-43-3 64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
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Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
ALS Vial : 29 Sample Multiplier: 1

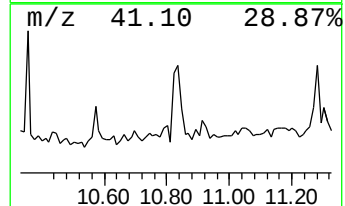
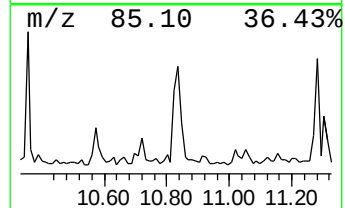
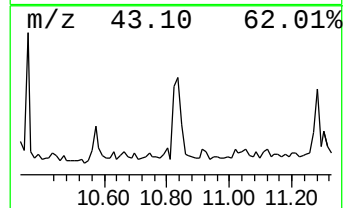
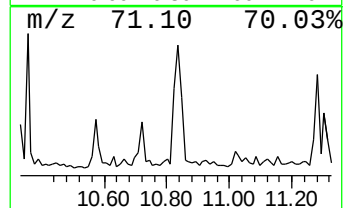
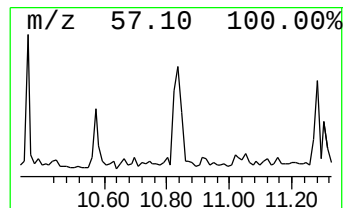
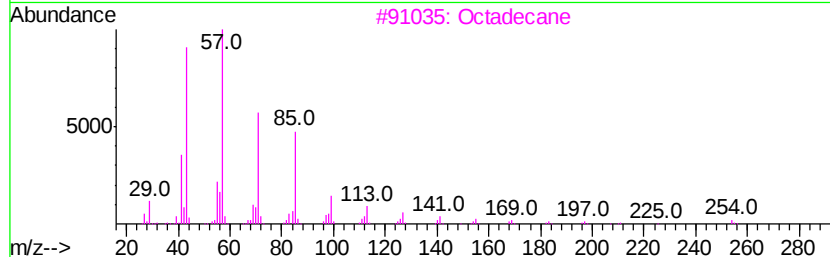
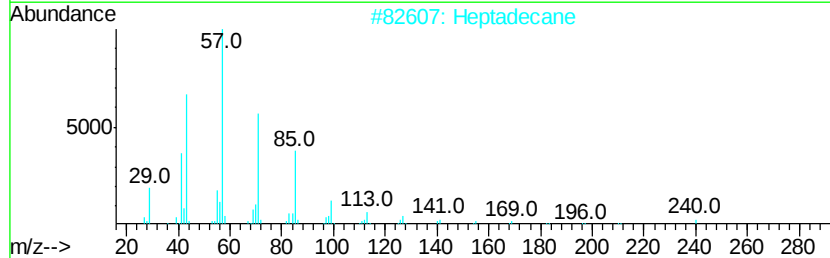
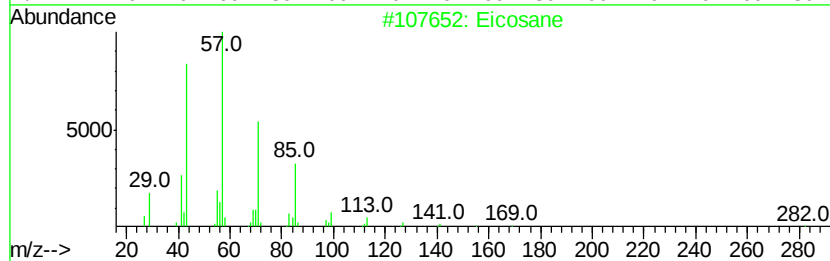
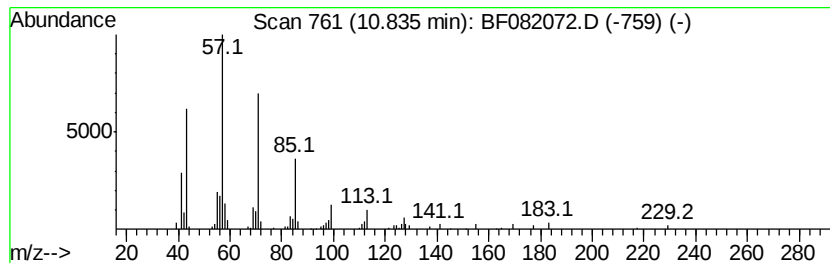
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.83	4.35 ng	109160	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
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Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
ALS Vial : 29 Sample Multiplier: 1

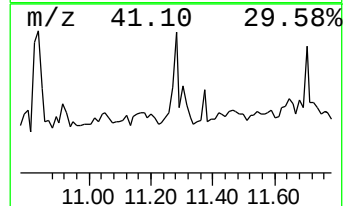
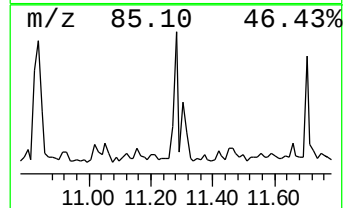
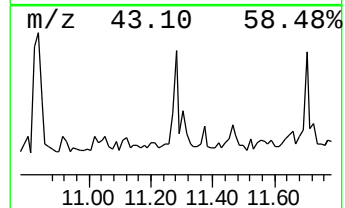
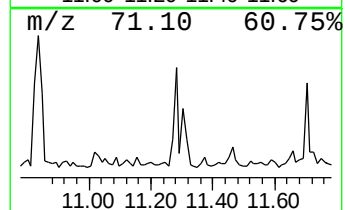
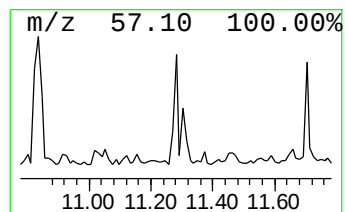
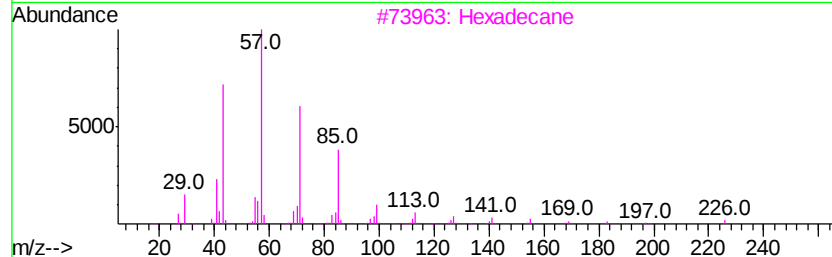
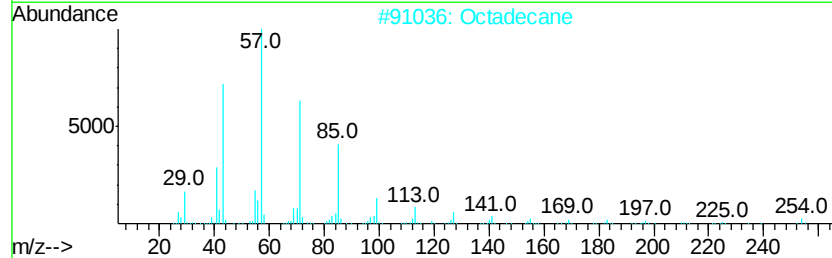
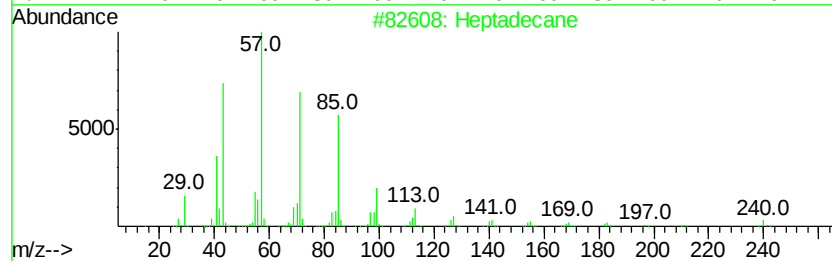
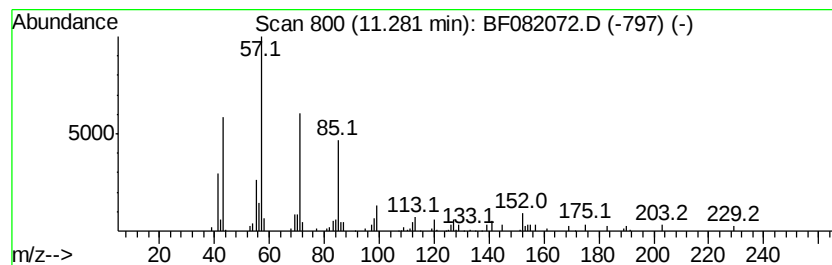
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.28	2.57 ng	64642	Phenanthrene-d10		11.42	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	87
2	Octadecane		254	C18H38	000593-45-3	87
3	Hexadecane		226	C16H34	000544-76-3	87
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	86
5	Tetracosane		338	C24H50	000646-31-1	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100515\
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Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
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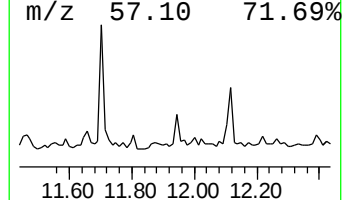
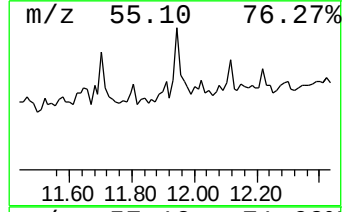
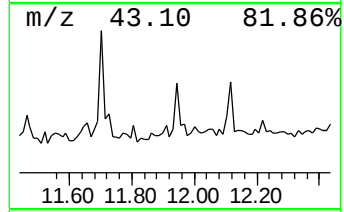
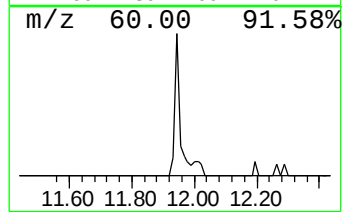
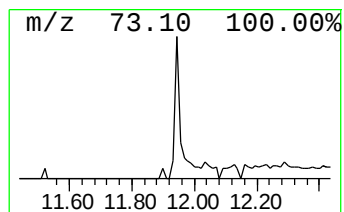
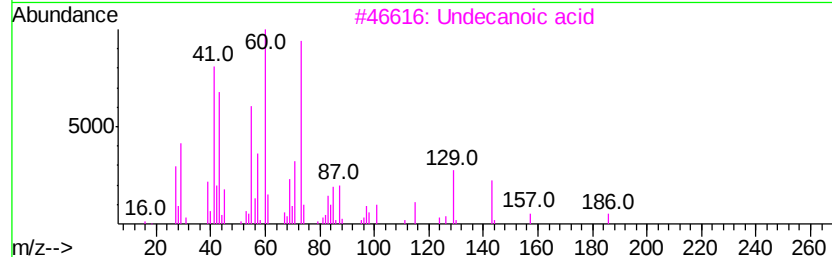
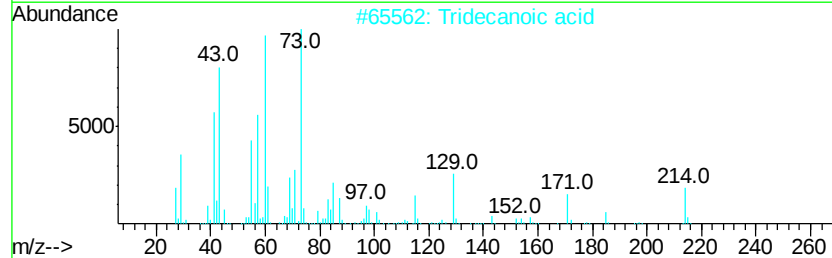
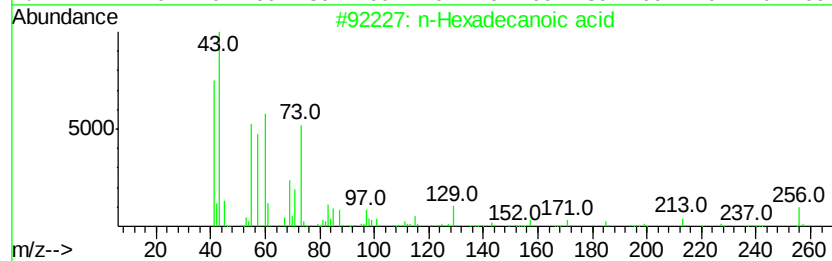
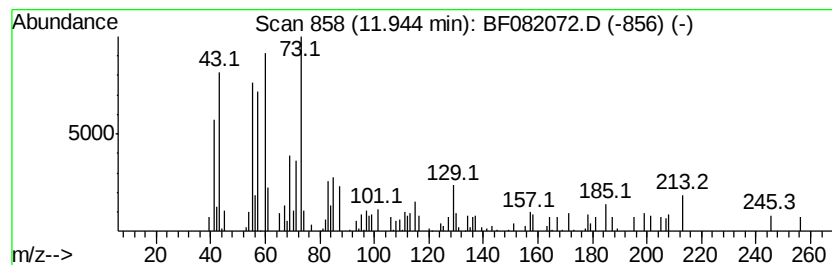
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.94	2.75 ng	69067	Phenanthrene-d10		11.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
Data File : BF082072.D
Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
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Instrument :
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ClientSampleId :
SS-4(0-24)

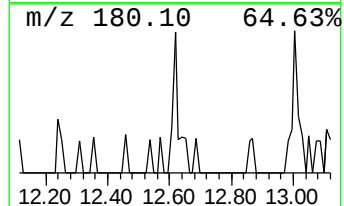
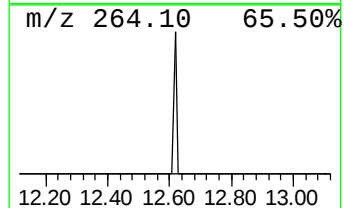
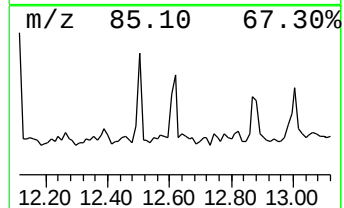
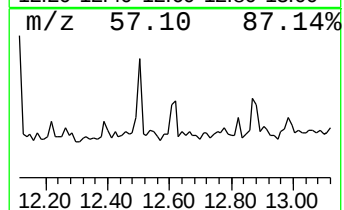
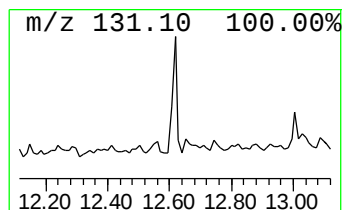
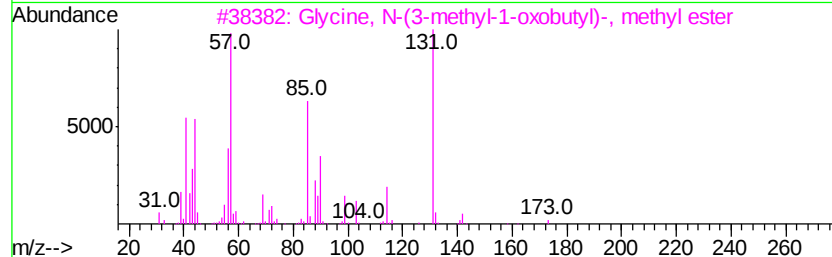
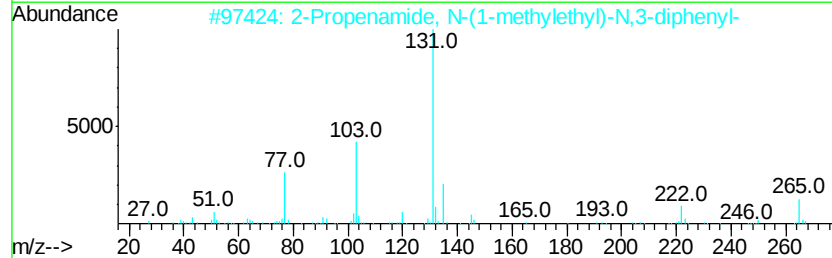
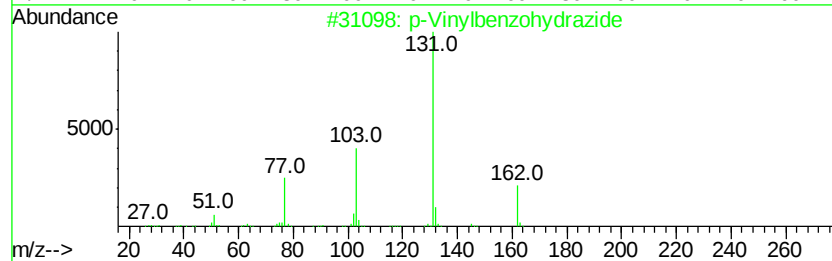
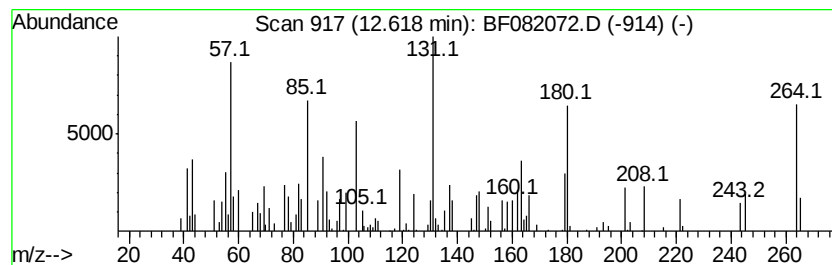
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown12.62 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	2.05 ng	51483	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	22
2		2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	16
3		Glycine, N-(3-methyl-1-oxobutyl)...	173	C8H15NO3	056009-37-1	16
4		2-Propenal, 3-(2-methoxyphenyl)-	162	C10H10O2	001504-74-1	14
5		2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	000103-26-4	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
Data File : BF082072.D
Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SS-4(0-24)

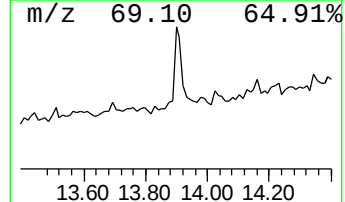
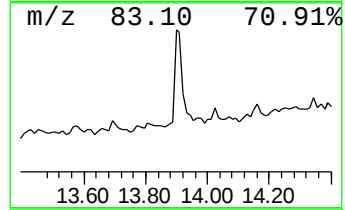
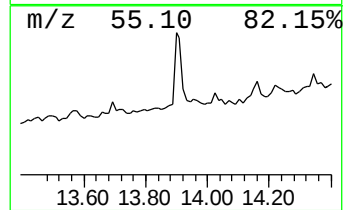
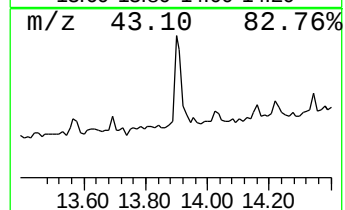
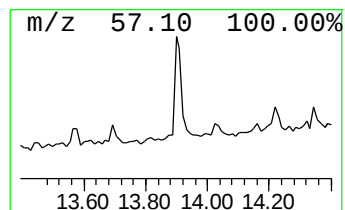
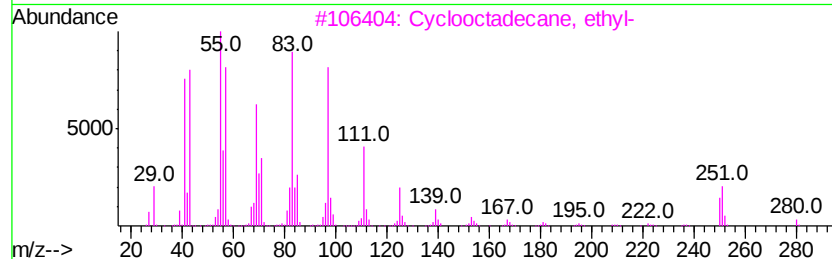
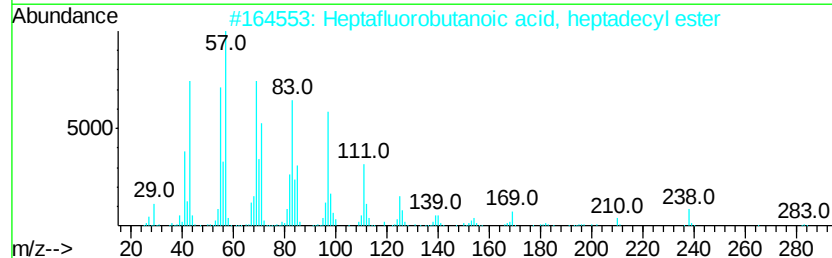
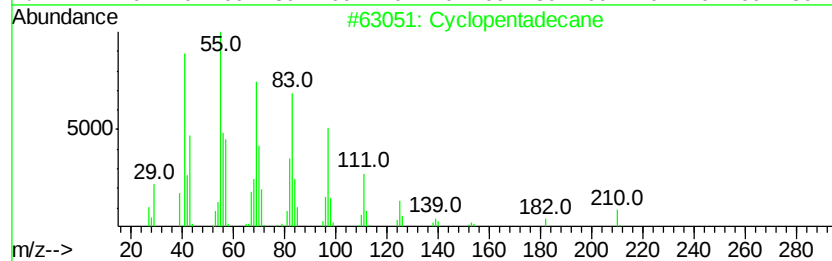
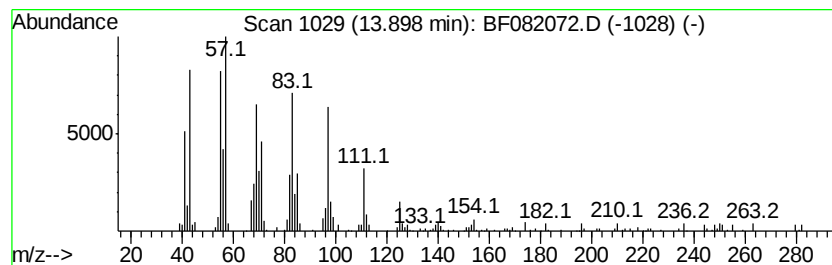
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.61 ng	133266	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	93
2			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3			Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	83
4			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	83
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100515\
Data File : BF082072.D
Acq On : 6 Oct 2015 5:01
Operator : UM/IZ
Sample : G3891-19
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-4(0-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.06	29.3	ng	640321	1	6.89	436608	20.0
unknown6.65	6.65	65.3	ng	1424480	1	6.89	436608	20.0
unknown8.10	8.10	4.8	ng	124073	2	8.17	514031	20.0
Tridecane	9.33	2.8	ng	78528	3	9.93	562763	20.0
Hexadecane	9.85	2.4	ng	68129	3	9.93	562763	20.0
Tetradecane	10.35	2.3	ng	64057	3	9.93	562763	20.0
Eicosane	10.83	4.3	ng	109160	4	11.42	502192	20.0
Heptadecane	11.28	2.6	ng	64642	4	11.42	502192	20.0
n-Hexadecanoic acid	11.94	2.8	ng	69067	4	11.42	502192	20.0
unknown12.62	12.62	2.0	ng	51483	4	11.42	502192	20.0
Cyclopentadecane	13.90	6.6	ng	133266	5	14.06	403176	20.0