

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
 Data File : BF084368.D
 Acq On : 10 Jan 2016 16:49
 Operator : SJ/UM
 Sample : H1043-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5COMP

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-BF123115.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	5.047	256	259	267	rVB	1304721	1911934	24.96%	2.897%
2	5.470	293	296	299	rBV	5615149	6345976	82.84%	9.617%
3	6.510	383	387	389	rBV	6230813	7660453	100.00%	11.609%
4	6.625	395	397	400	rBV	5151342	6658721	86.92%	10.091%
5	6.853	415	417	419	rBV	2056422	1657796	21.64%	2.512%
6	7.013	428	431	433	rBV	5860039	5282800	68.96%	8.006%
7	7.425	464	467	469	rBV	4739229	4979396	65.00%	7.546%
8	8.145	527	530	532	rBV	2033926	2146280	28.02%	3.252%
9	9.219	621	624	627	rBV	7274350	6684605	87.26%	10.130%
10	9.619	656	659	660	rBV	1304406	1472660	19.22%	2.232%
11	9.825	676	677	680	rBV	150727	195814	2.56%	0.297%
12	9.893	681	683	686	rVB	2654186	2318149	30.26%	3.513%
13	10.328	719	721	723	rVB	405252	354352	4.63%	0.537%
14	10.545	738	740	744	rBV	110472	214898	2.81%	0.326%
15	10.682	749	752	755	rBV2	3971018	4575273	59.73%	6.933%
16	10.808	760	763	767	rVB2	298979	554114	7.23%	0.840%
17	10.991	777	779	784	rVB2	45594	124338	1.62%	0.188%
18	11.254	800	802	803	rBV	227783	202755	2.65%	0.307%
19	11.276	803	804	808	rVB	65732	86311	1.13%	0.131%
20	11.379	811	813	815	rVV	2686972	2239247	29.23%	3.393%
21	11.436	815	818	822	rVB	42780	88701	1.16%	0.134%
22	12.797	935	937	939	rBV	239686	294466	3.84%	0.446%
23	12.854	939	942	946	rVV2	180098	336832	4.40%	0.510%
24	12.968	949	952	955	rBV	6012617	5725807	74.75%	8.677%
25	13.494	996	998	1000	rBV	225758	232604	3.04%	0.352%
26	13.871	1028	1031	1038	rBV	205695	314465	4.11%	0.477%
27	14.020	1041	1044	1046	rBV	1095744	1508218	19.69%	2.286%
28	14.385	1070	1076	1083	rBV4	26839	122210	1.60%	0.185%
29	14.488	1083	1085	1088	rBV	57170	80603	1.05%	0.122%
30	15.437	1165	1168	1171	rBV	848438	1276515	16.66%	1.934%
31	17.608	1355	1358	1366	rVB	45152	131192	1.71%	0.199%
32	18.397	1424	1427	1433	rVB	32573	106189	1.39%	0.161%
33	19.357	1506	1511	1515	rBV4	29150	105353	1.38%	0.160%

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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

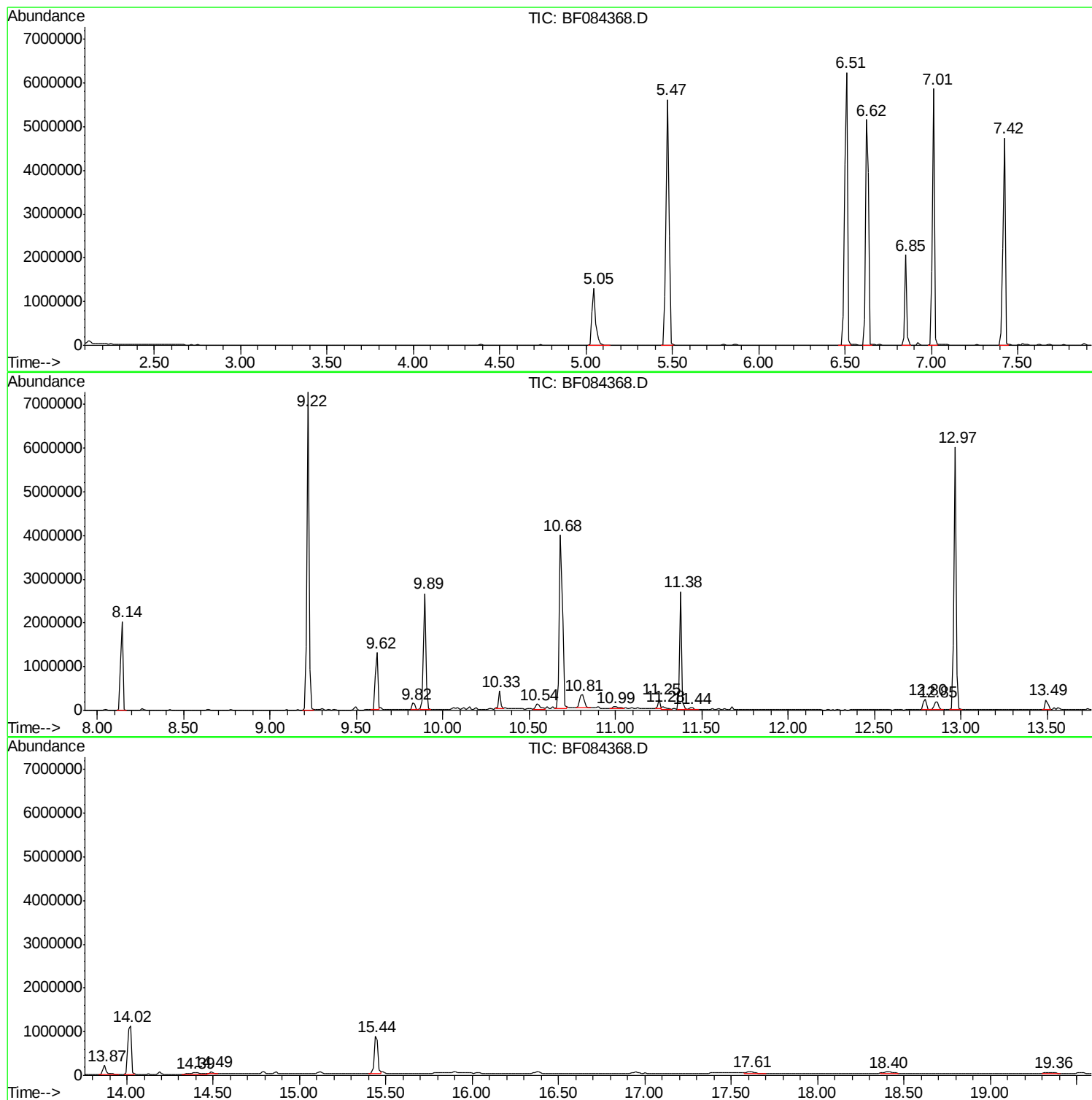
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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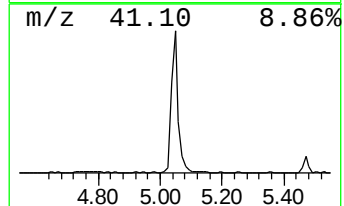
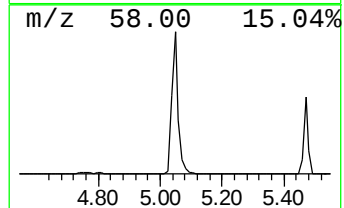
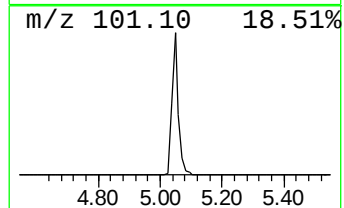
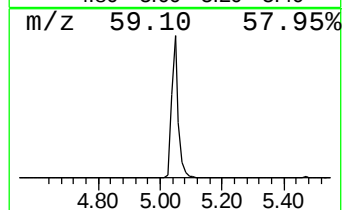
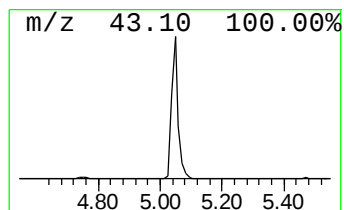
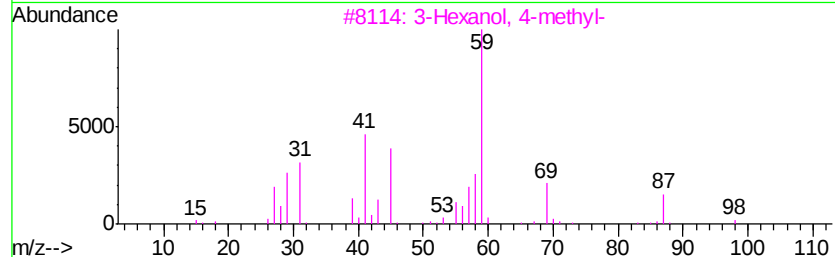
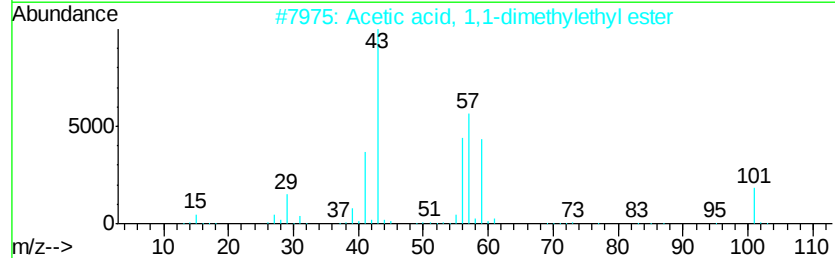
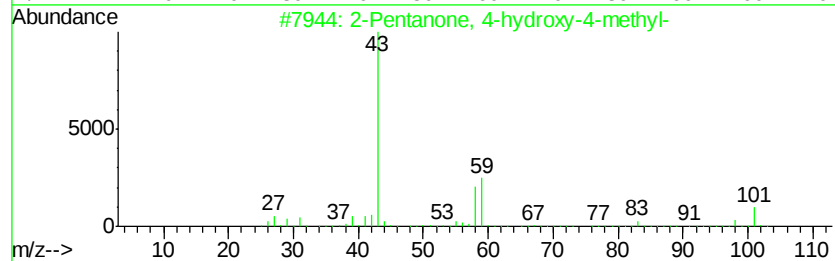
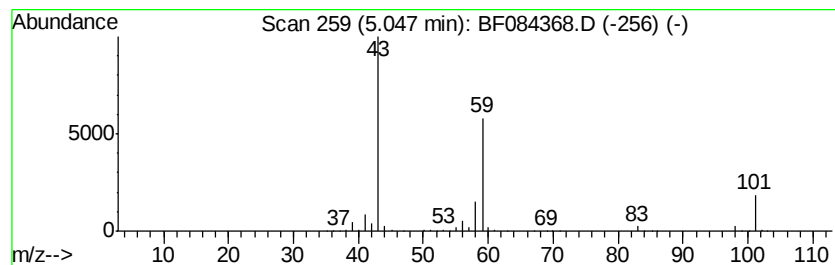
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	23.07 ng	1911930	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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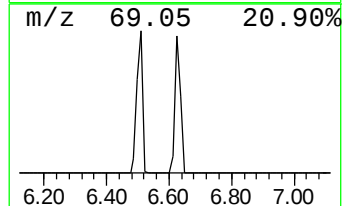
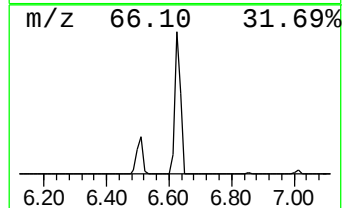
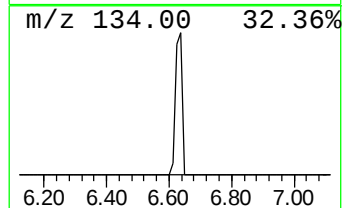
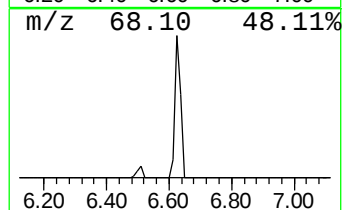
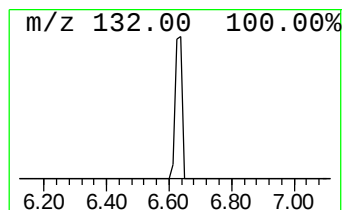
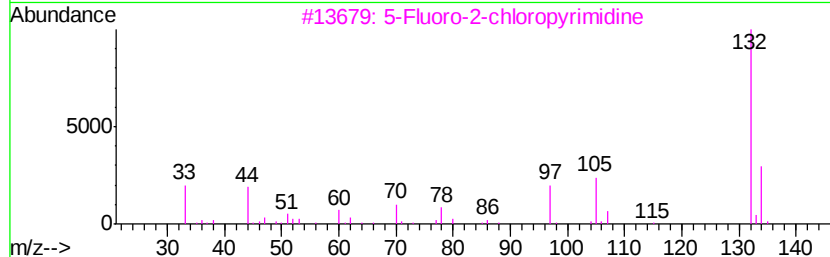
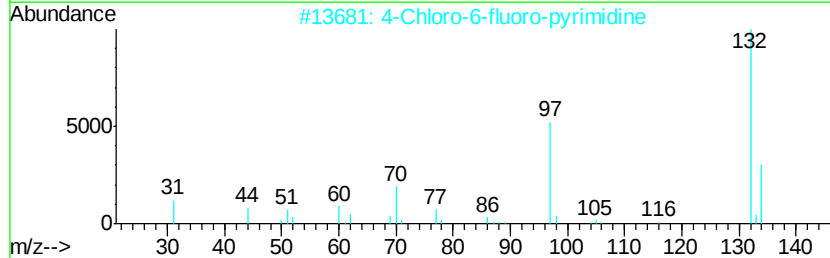
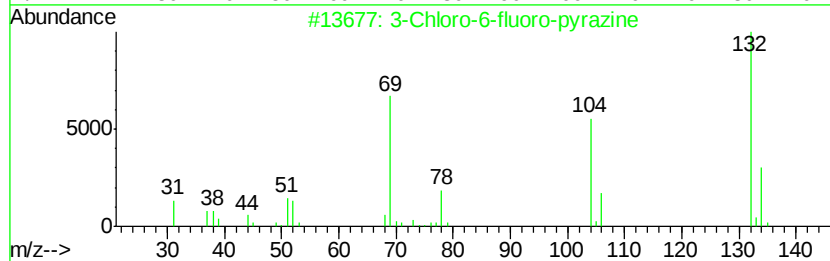
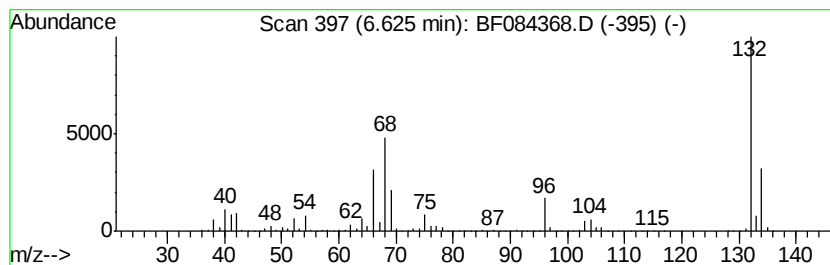
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.33 ng	6658720	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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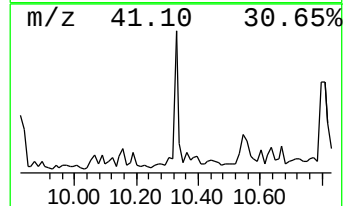
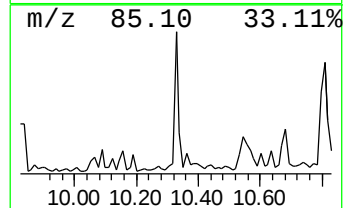
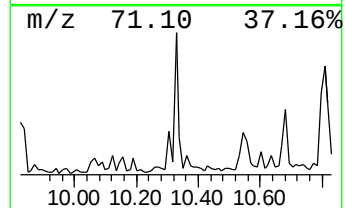
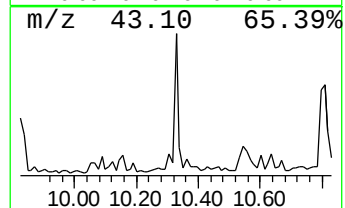
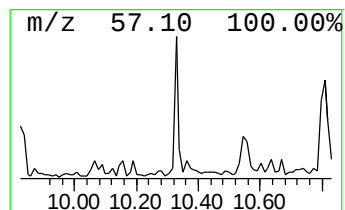
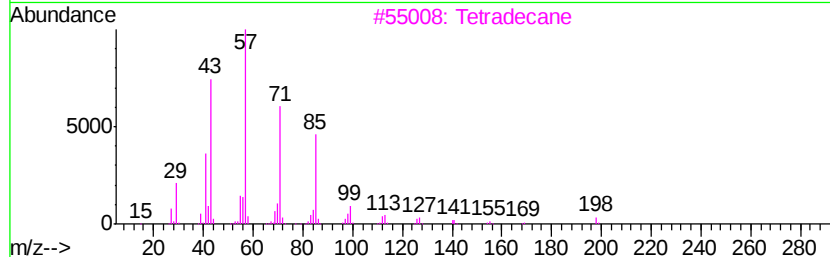
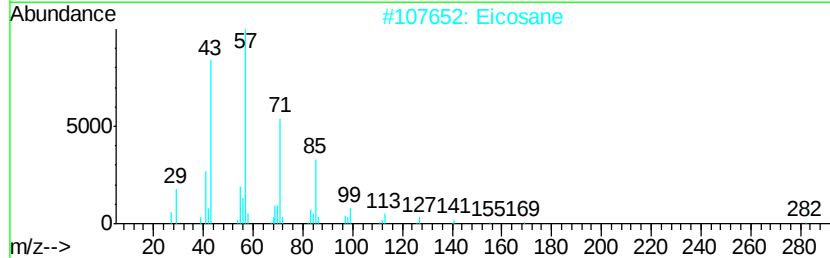
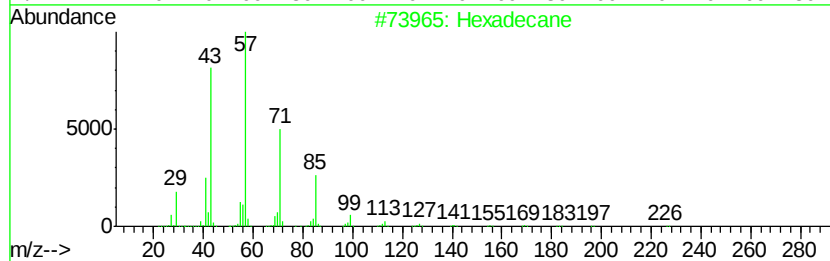
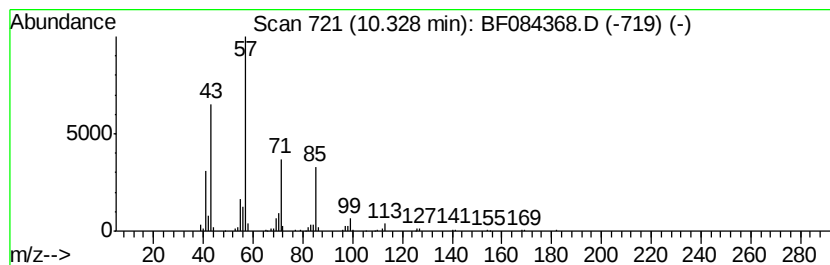
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.33	3.06 ng	354352	Acenaphthene-d10		9.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	80
3	Tetradecane	198	C14H30	000629-59-4	72
4	Undecane	156	C11H24	001120-21-4	59
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	59



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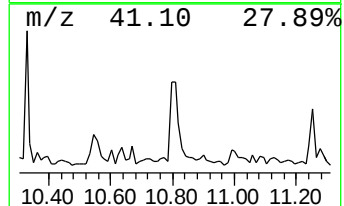
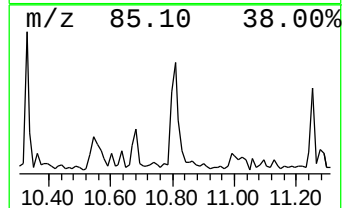
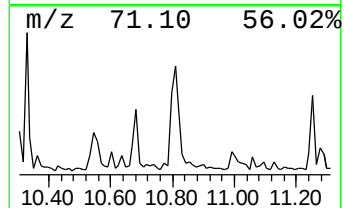
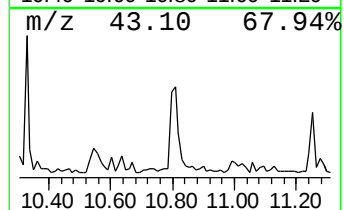
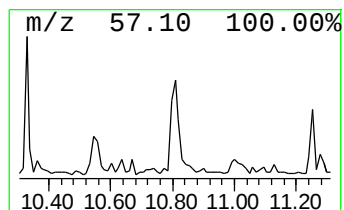
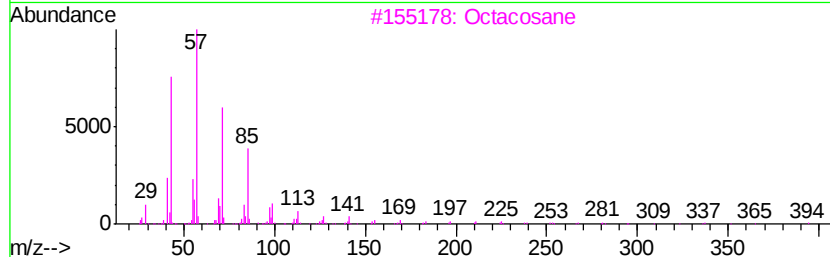
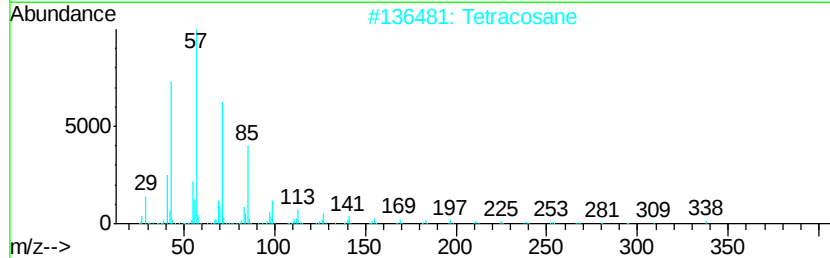
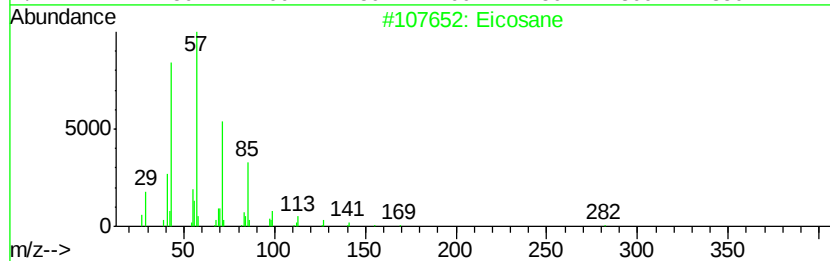
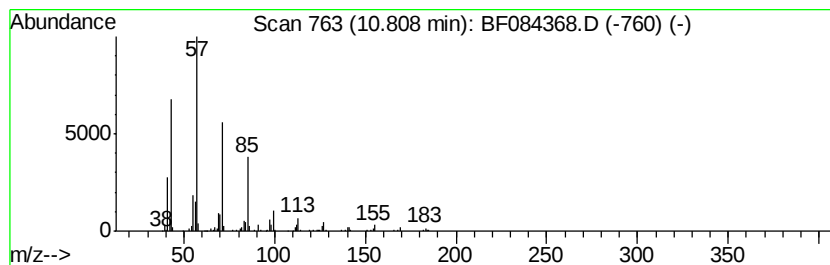
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	4.95 ng	554114	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86



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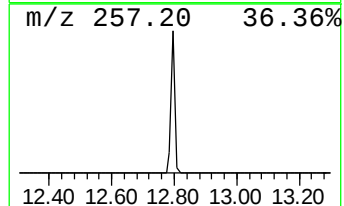
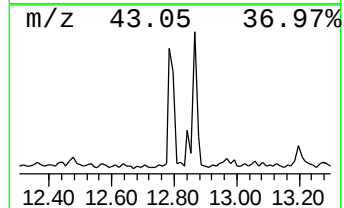
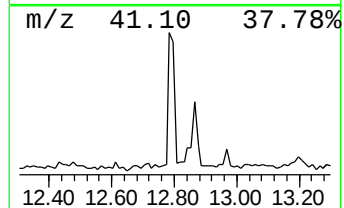
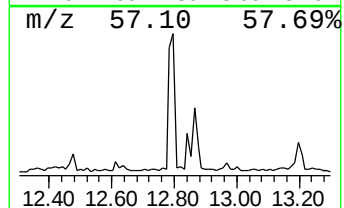
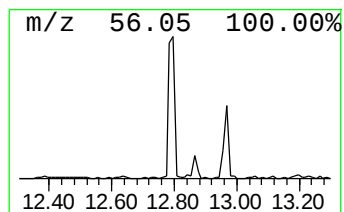
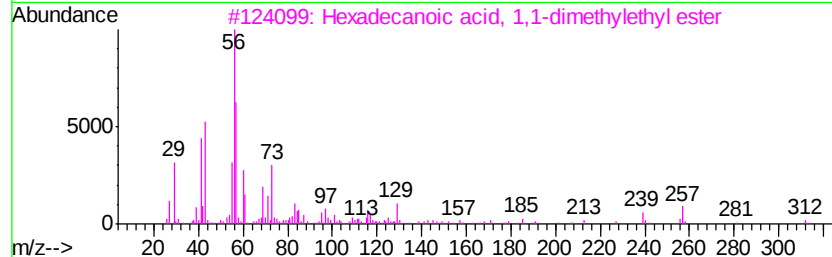
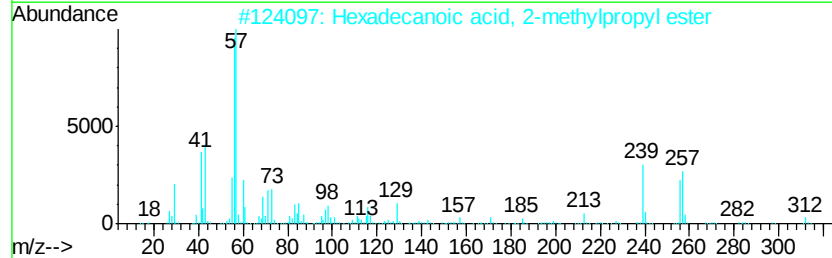
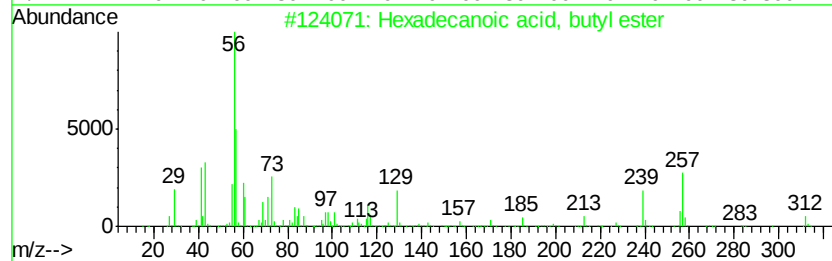
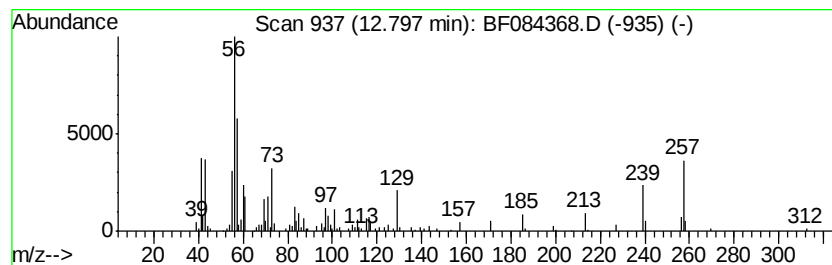
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	3.90 ng	294466	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	53
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	30
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22



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SB-5COMP

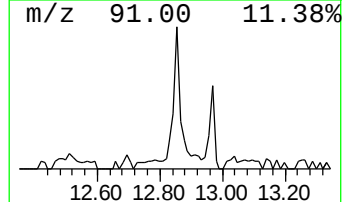
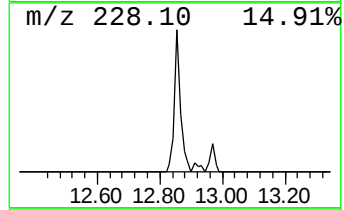
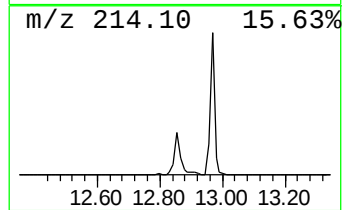
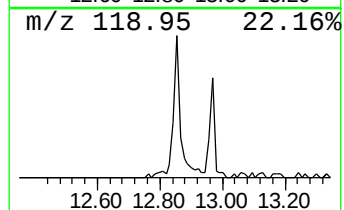
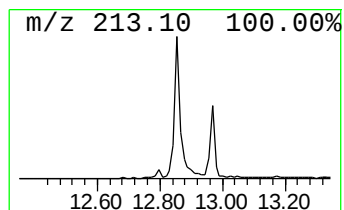
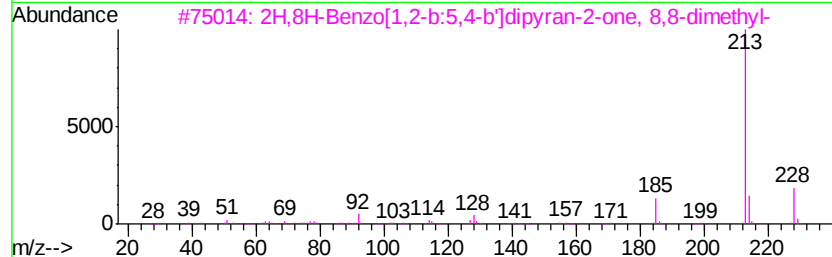
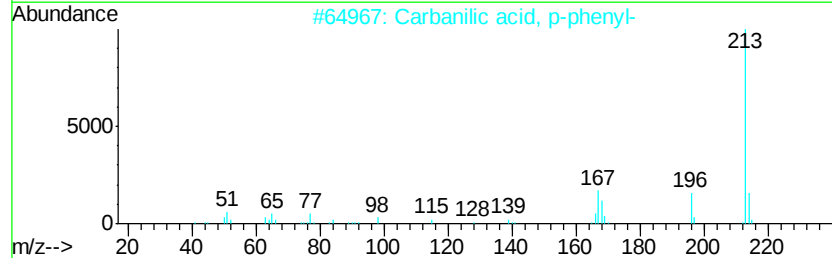
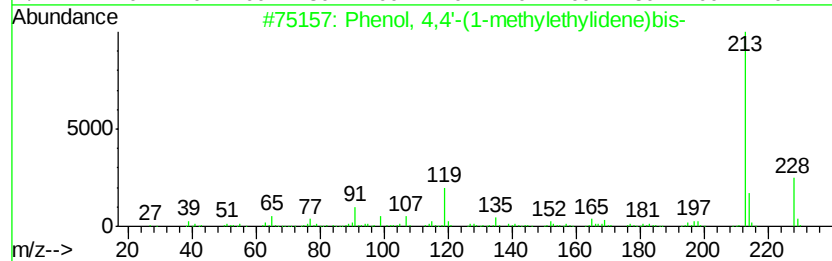
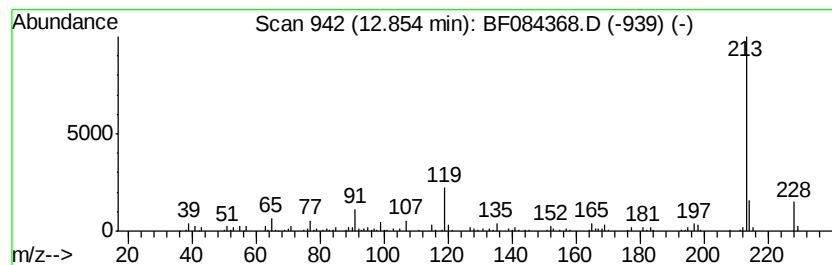
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	4.47 ng	336832	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	96
2		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
3		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50
4		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	50
5		2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
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 Acq On : 10 Jan 2016 16:49
 Operator : SJ/UM
 Sample : H1043-20
 Misc :
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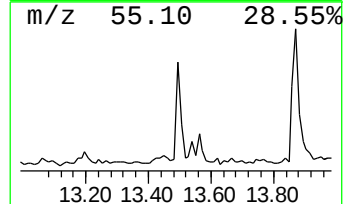
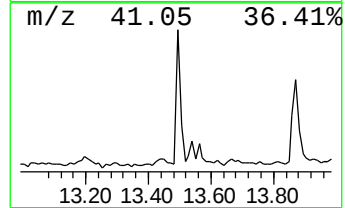
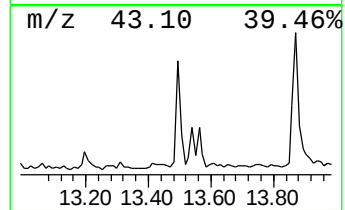
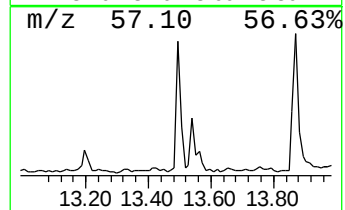
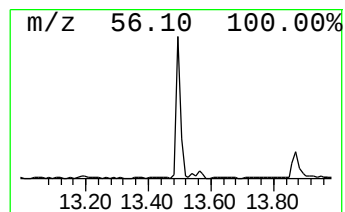
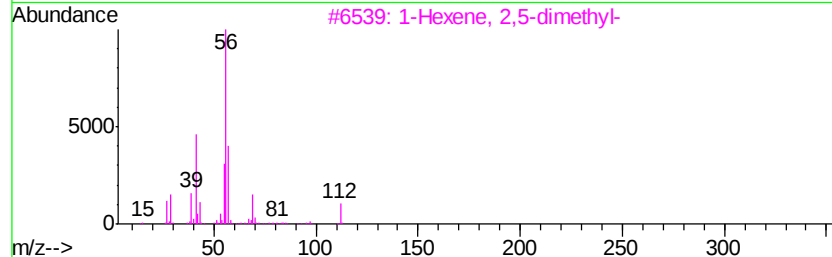
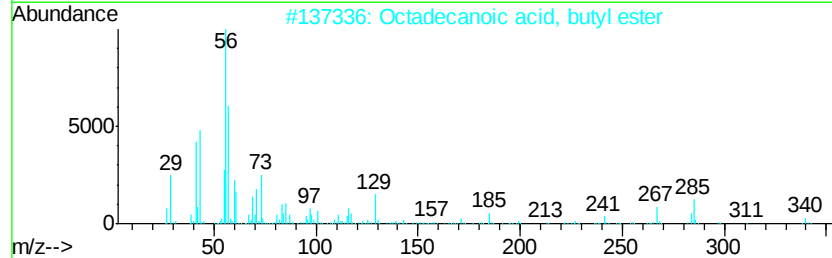
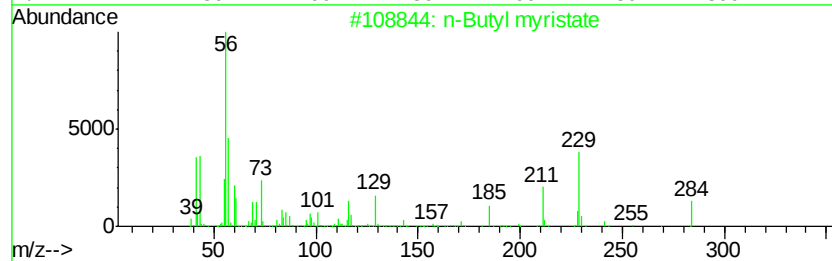
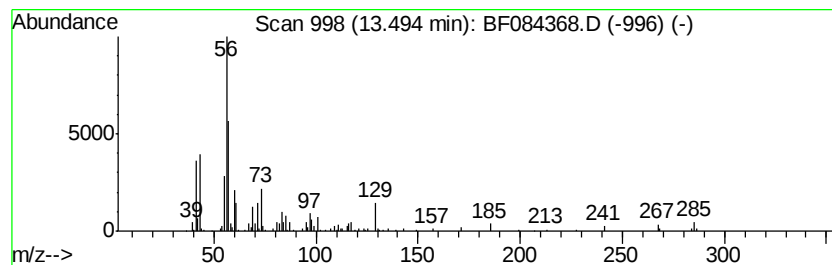
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 SB-5COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 n-Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	3.08 ng	232604	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	86
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	47
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084368.D
Acq On : 10 Jan 2016 16:49
Operator : SJ/UM
Sample : H1043-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5COMP

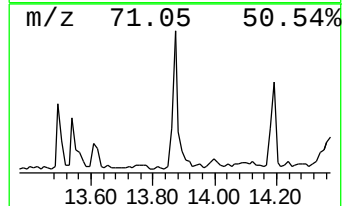
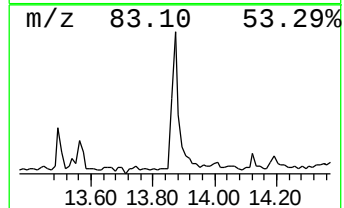
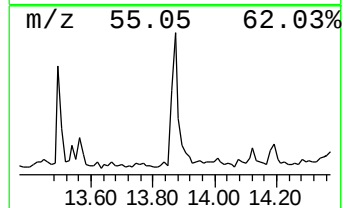
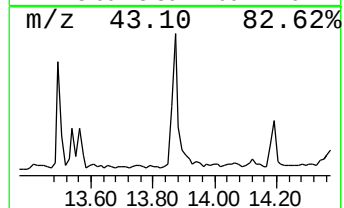
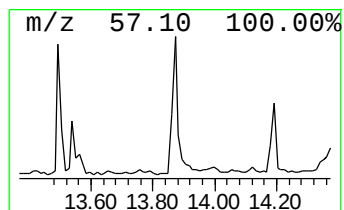
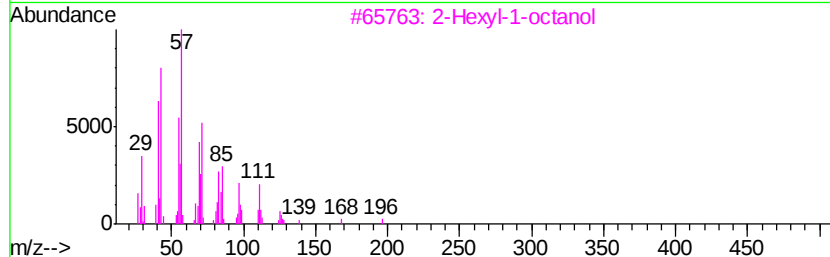
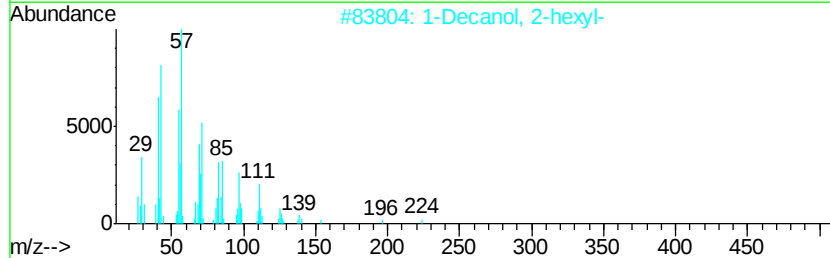
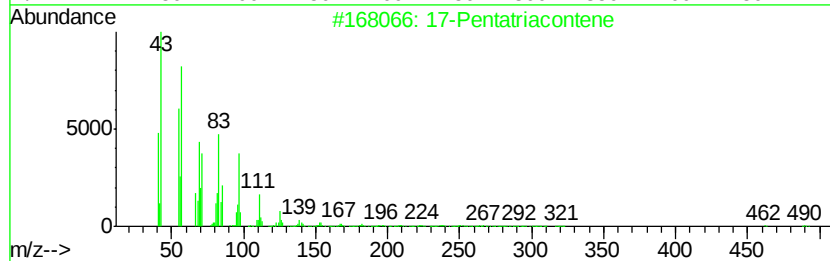
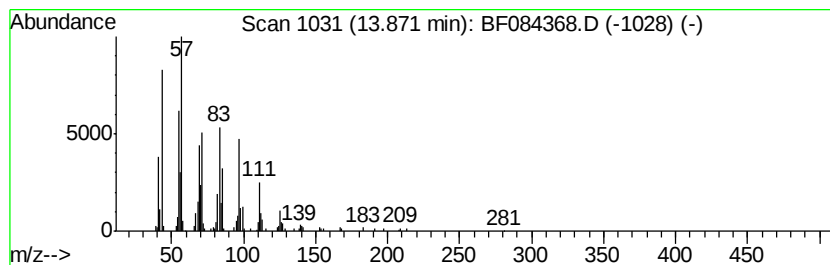
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.17 ng	314465	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	90
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
3		2-Hexyl-1-octanol	214	C14H30O	019780-79-1	68
4		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	64
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084368.D
Acq On : 10 Jan 2016 16:49
Operator : SJ/UM
Sample : H1043-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5COMP

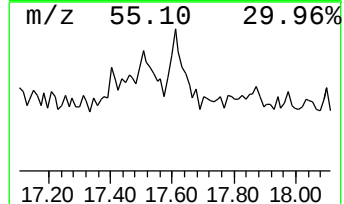
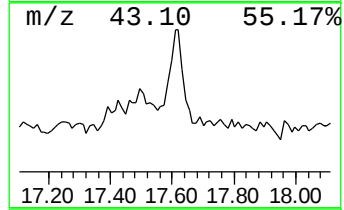
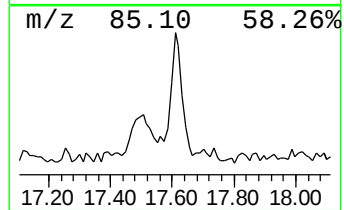
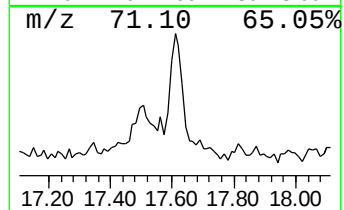
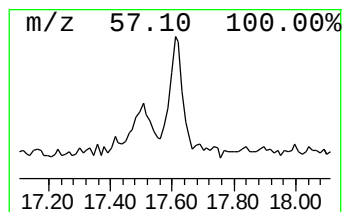
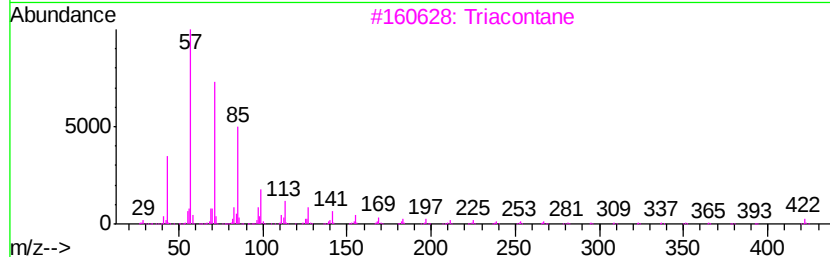
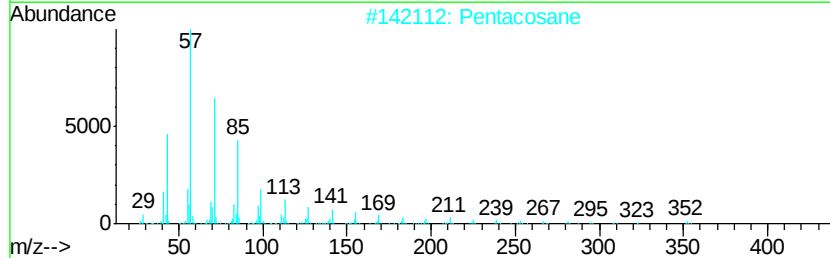
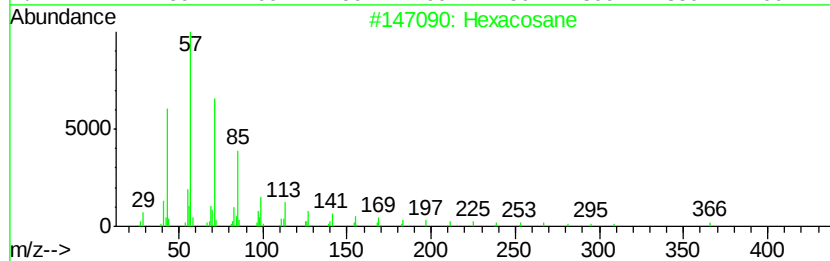
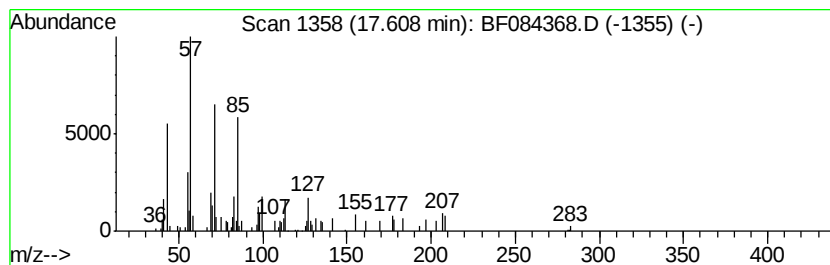
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	2.06 ng	131192	Perylene-d12	15.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Pentacosane	352	C25H52	000629-99-2	86
3			Triacontane	422	C30H62	000638-68-6	80
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5			Nonacosane	408	C29H60	000630-03-5	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084368.D
Acq On : 10 Jan 2016 16:49
Operator : SJ/UM
Sample : H1043-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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...	5.05	23.1	ng	1911930	1	6.85	1657800	20.0
unknown6.62	6.62	80.3	ng	6658720	1	6.85	1657800	20.0
Hexadecane	10.33	3.1	ng	354352	3	9.89	2318150	20.0
Eicosane	10.81	5.0	ng	554114	4	11.38	2239250	20.0
Hexadecanoic acid...	12.80	3.9	ng	294466	5	14.02	1508220	20.0
Phenol, 4,4'-(1-m...	12.85	4.5	ng	336832	5	14.02	1508220	20.0
n-Butyl myristate	13.49	3.1	ng	232604	5	14.02	1508220	20.0
17-Pentatriacontene	13.87	4.2	ng	314465	5	14.02	1508220	20.0
Hexacosane	17.61	2.1	ng	131192	6	15.45	1276520	20.0