

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
 Data File : BF088767.D
 Acq On : 7 Jul 2016 7:13
 Operator : UM/SJ
 Sample : H3870-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-COMP

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-BF063016.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	1.701	9	10	16	rVB	134526	182673	6.79%	0.764%
2	1.827	19	21	32	rVB	1126138	1690772	62.80%	7.070%
3	2.935	115	118	125	rBV	41835	85550	3.18%	0.358%
4	4.913	289	291	297	rBB	79784	133799	4.97%	0.560%
5	5.347	326	329	331	rBV	2024340	2427806	90.18%	10.152%
6	6.387	417	420	423	rBV	1725442	2170396	80.62%	9.076%
7	6.513	428	431	434	rBV	1745575	2353853	87.43%	9.843%
8	6.753	449	452	453	rBV	478215	553326	20.55%	2.314%
9	6.902	463	465	468	rVB	1502088	1760115	65.38%	7.360%
10	7.313	498	501	504	rBV	1322930	1364184	50.67%	5.705%
11	8.033	561	564	566	rBV	952153	784539	29.14%	3.281%
12	9.119	656	659	661	rBV	2097713	2692256	100.00%	11.258%
13	9.508	691	693	695	rBV	613614	501345	18.62%	2.096%
14	9.782	715	717	720	rVB	892182	774566	28.77%	3.239%
15	10.228	755	756	758	rVB	47364	33703	1.25%	0.141%
16	10.570	783	786	788	rBV	1439065	1419804	52.74%	5.937%
17	10.696	796	797	802	rVV	52275	63243	2.35%	0.264%
18	11.142	834	836	838	rBV	97219	99558	3.70%	0.416%
19	11.256	844	846	849	rVB	754193	657443	24.42%	2.749%
20	11.325	849	852	856	rVV2	26227	59863	2.22%	0.250%
21	11.485	865	866	871	rVV3	14706	37759	1.40%	0.158%
22	11.565	871	873	876	rVV	67087	94073	3.49%	0.393%
23	11.976	906	909	911	rBV2	22050	36335	1.35%	0.152%
24	12.365	940	943	946	rVB2	30055	53582	1.99%	0.224%
25	12.674	968	970	973	rBV2	238266	304433	11.31%	1.273%
26	12.754	976	977	979	rVB	73463	55393	2.06%	0.232%
27	12.845	982	985	987	rBV	2024676	1841618	68.40%	7.701%
28	13.382	1030	1032	1034	rBV	231963	189755	7.05%	0.794%
29	13.748	1062	1064	1073	rVB	91251	125728	4.67%	0.526%
30	13.885	1073	1076	1078	rBV	481113	535794	19.90%	2.241%
31	14.068	1090	1092	1095	rBV	39085	40297	1.50%	0.169%
32	14.377	1116	1119	1123	rBV	38057	46939	1.74%	0.196%
33	14.662	1142	1144	1147	rVB	27405	37158	1.38%	0.155%
34	14.971	1169	1171	1174	rBV	31737	38986	1.45%	0.163%

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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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.268	1194	1197	1199	rBV	401878	487228	18.10%	2.037%
36	15.325	1199	1202	1205	rVB	26367	41936	1.56%	0.175%
37	15.714	1233	1236	1238	rBV	23775	33627	1.25%	0.141%
38	16.171	1271	1276	1285	rVB4	19323	49224	1.83%	0.206%
39	17.120	1356	1359	1364	rBV4	12323	27495	1.02%	0.115%
40	18.057	1435	1441	1449	rVB6	5423	27478	1.02%	0.115%

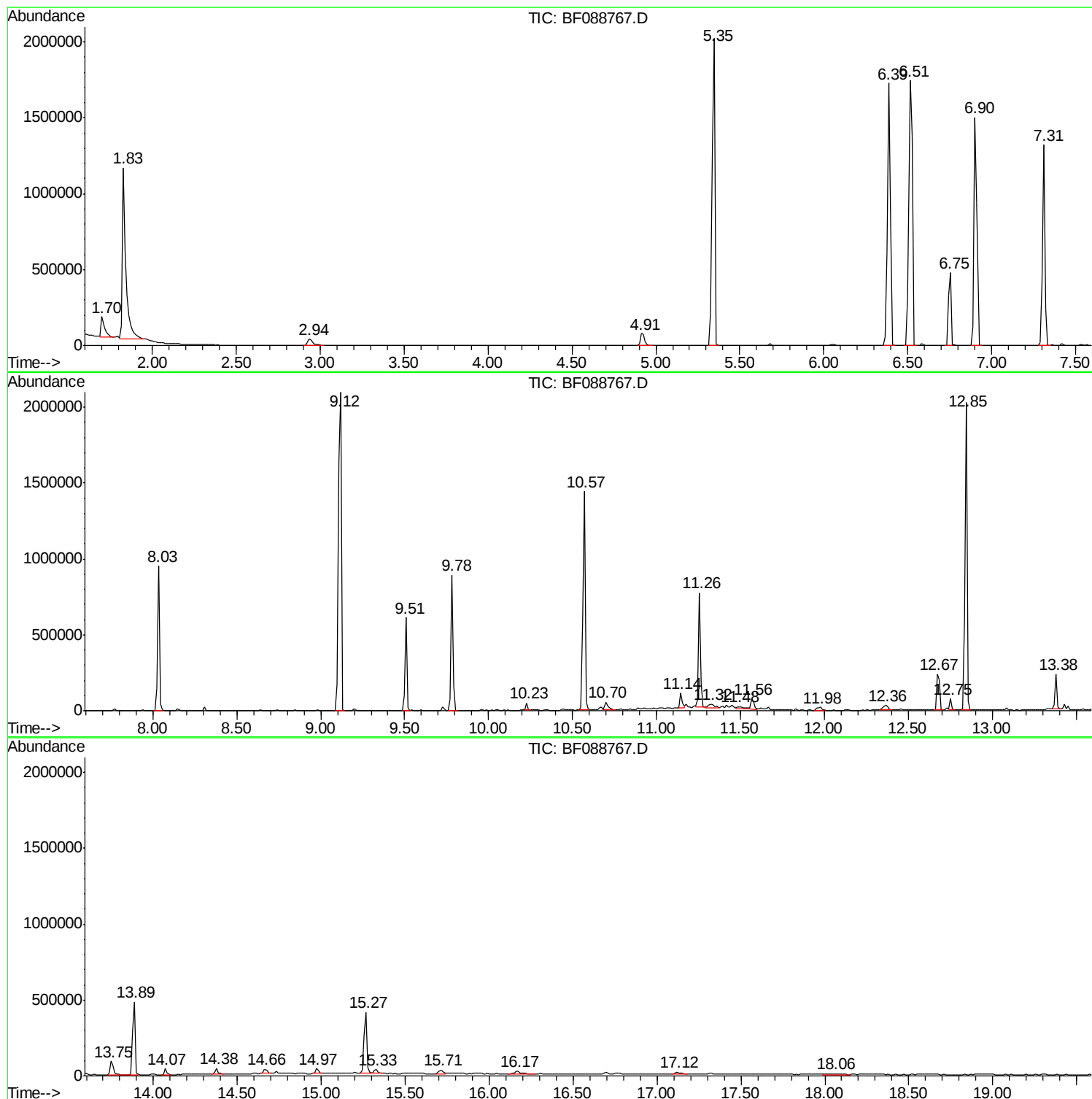
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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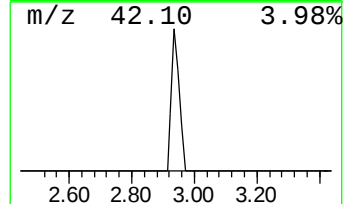
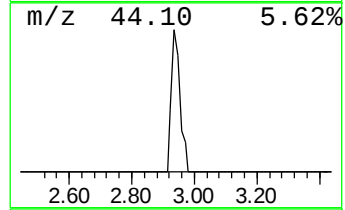
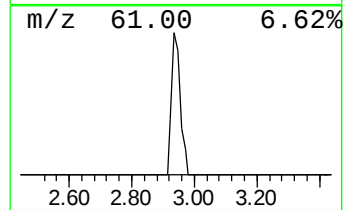
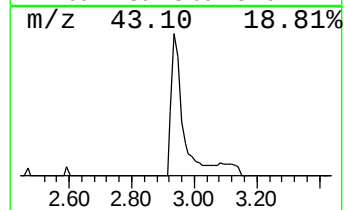
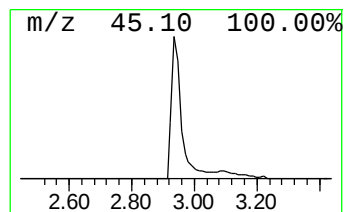
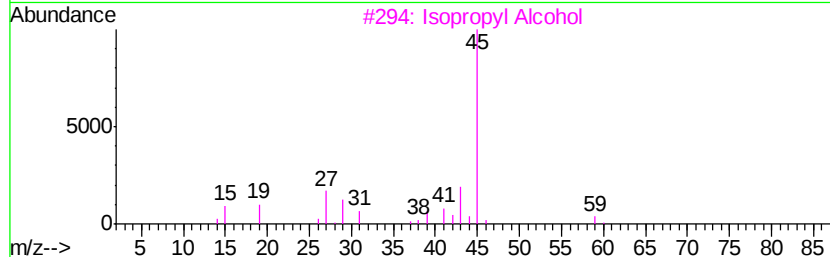
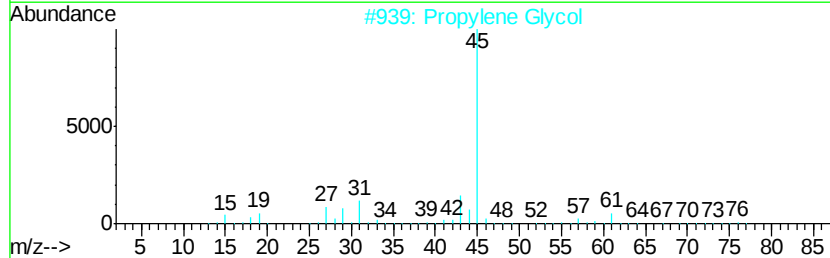
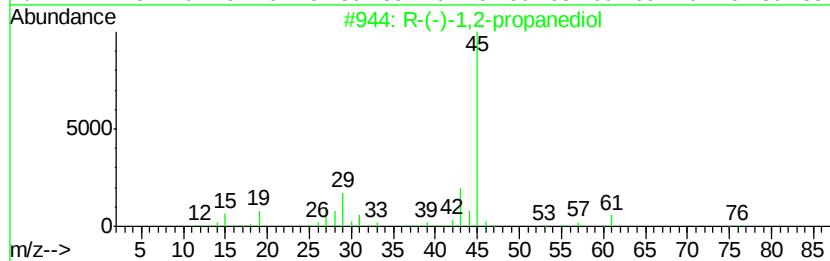
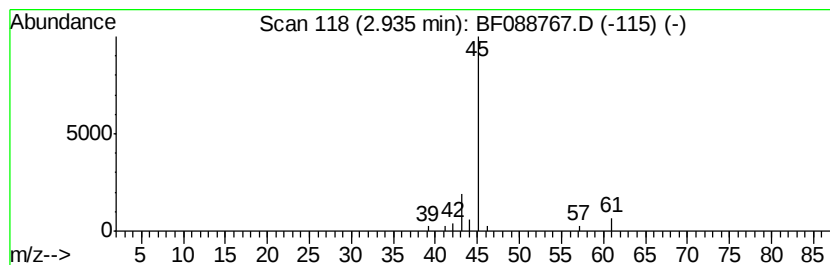
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	3.09 ng	85550	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		Propylene Glycol	76	C3H8O2	000057-55-6	9
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Formamide	45	CH3NO	000075-12-7	7
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	4



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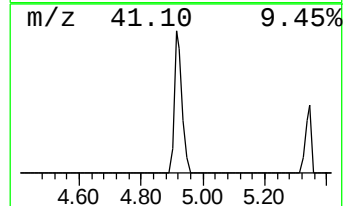
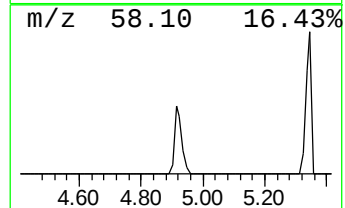
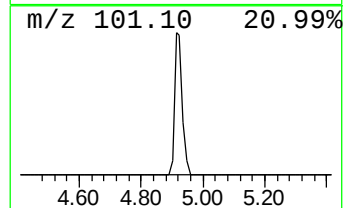
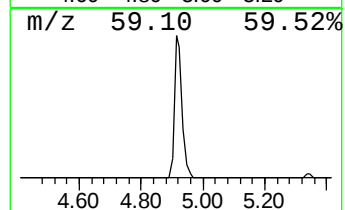
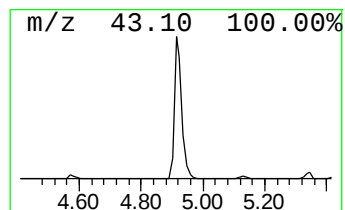
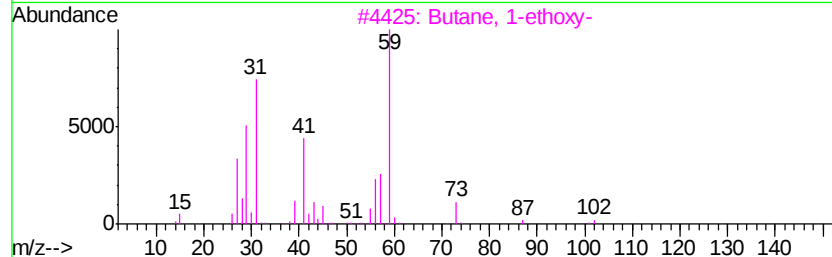
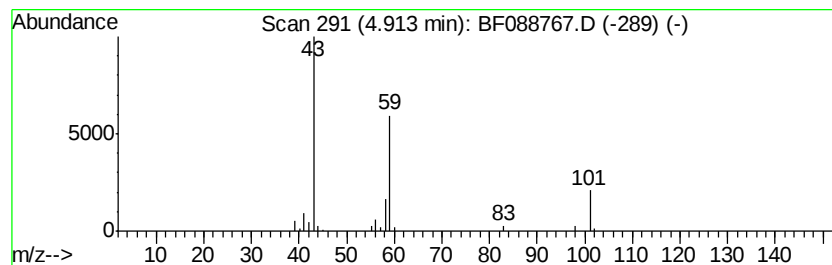
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.84 ng	133799	1,4-Dichlorobenzene-d4	6.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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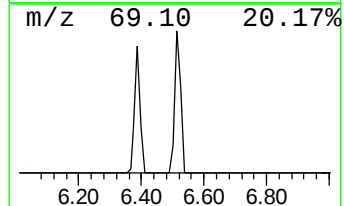
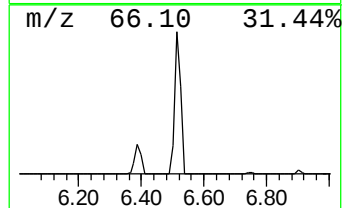
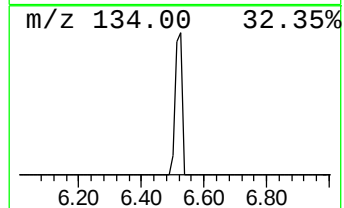
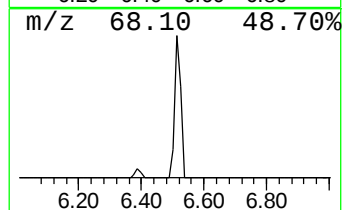
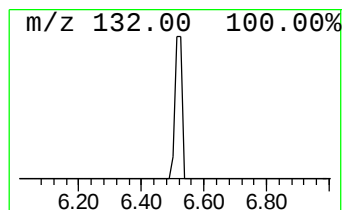
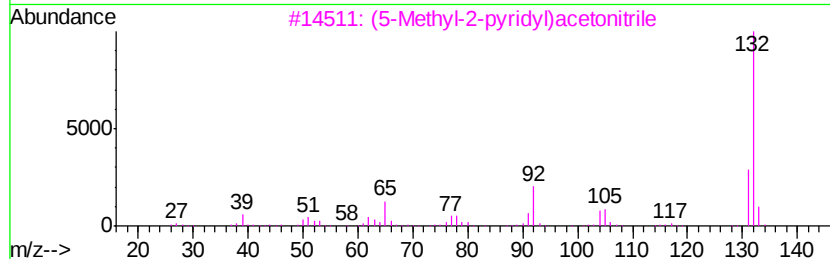
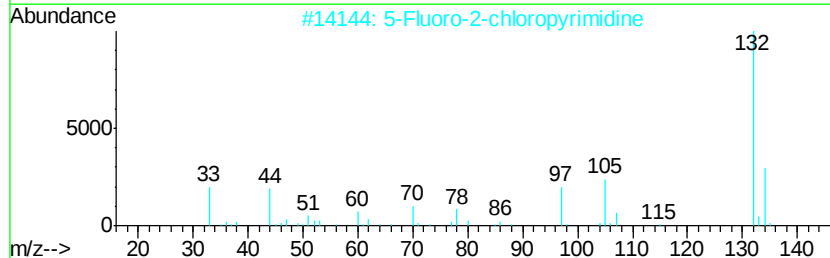
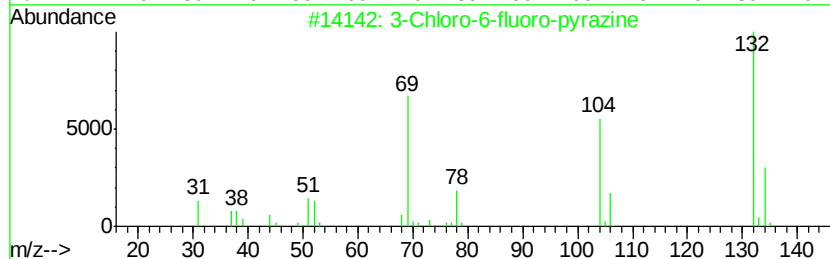
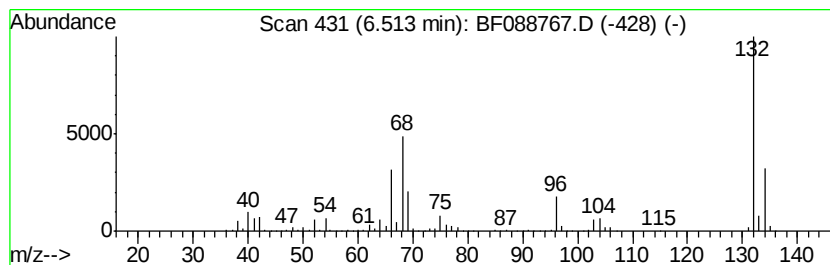
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	85.08 ng	2353850	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10	
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10	
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	



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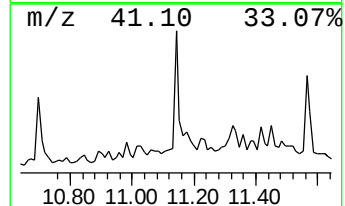
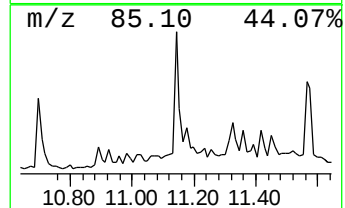
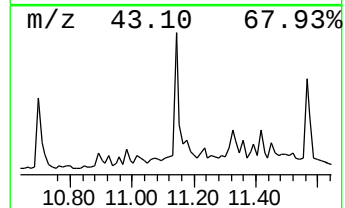
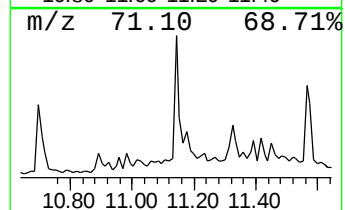
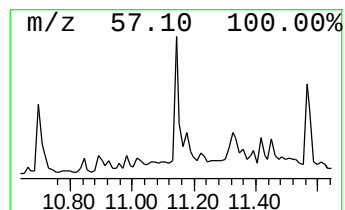
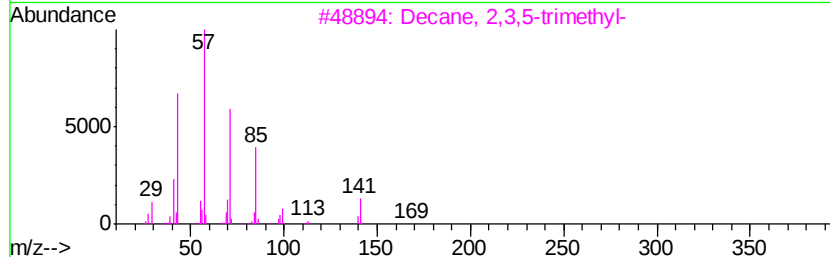
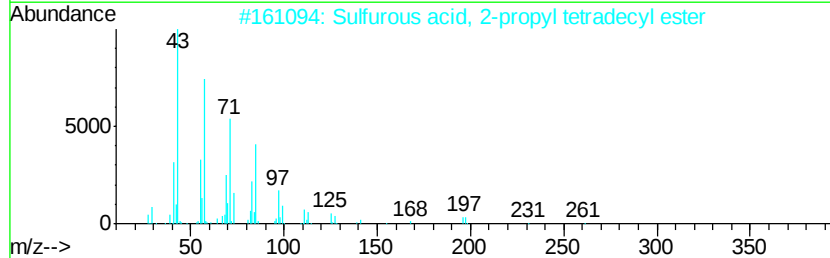
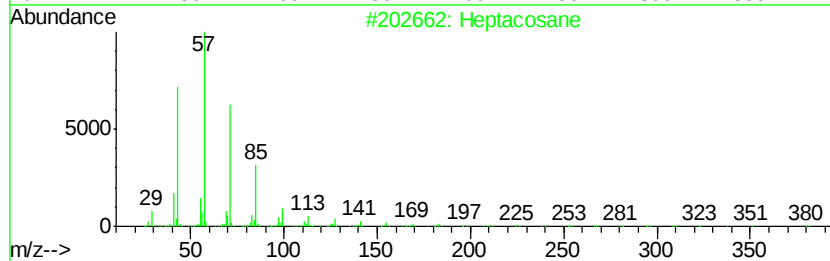
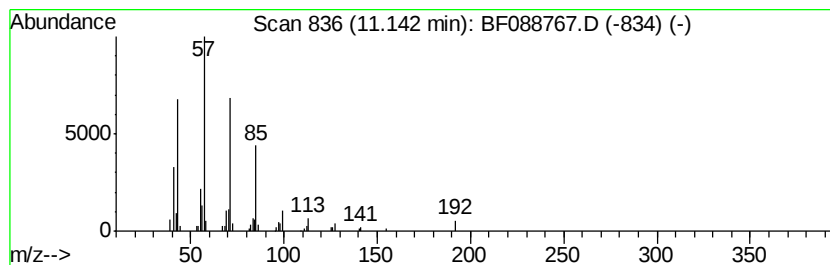
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	3.03 ng	99558	Phenanthrene-d10	11.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Sulfurous acid, 2-propyl tetradec...		320	C17H36O3S	1000309-12-5	86
3	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	86
4	Pentadecane		212	C15H32	000629-62-9	86
5	Tridecane		184	C13H28	000629-50-5	86



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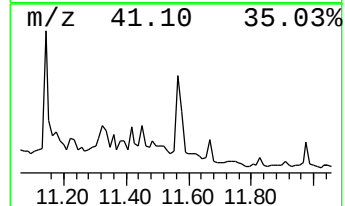
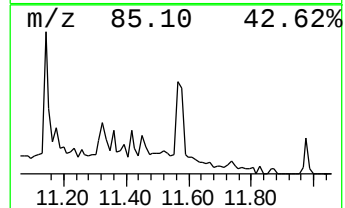
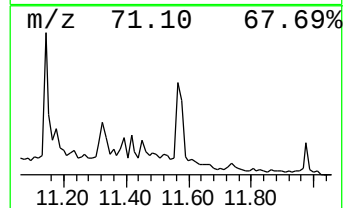
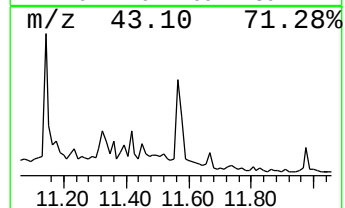
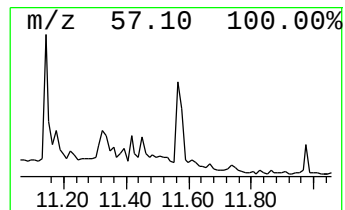
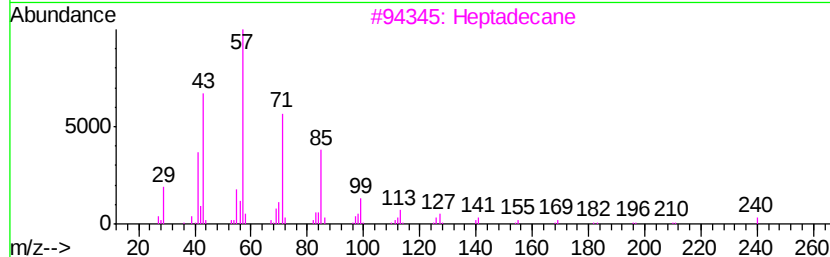
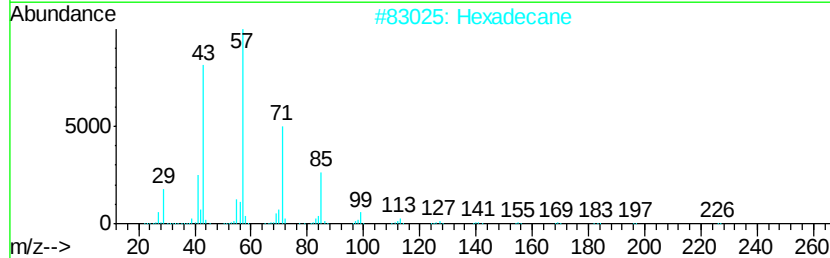
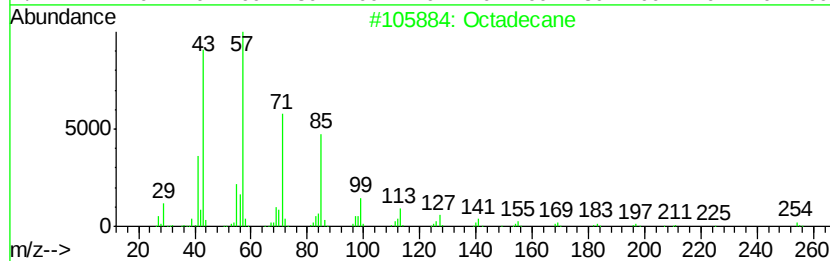
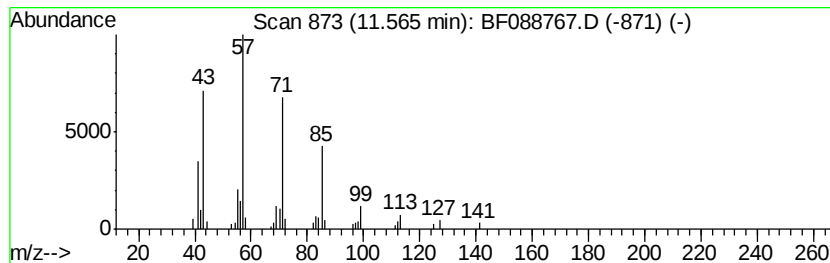
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Peak Number 8 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.56	2.86 ng	94073	Phenanthrene-d10		11.26	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heptadecane		240	C17H36	000629-78-7	90
4	Sulfurous acid, 2-propyl tetradec...		320	C17H36O3S	1000309-12-5	86
5	Pentadecane		212	C15H32	000629-62-9	86



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SB-02-COMP

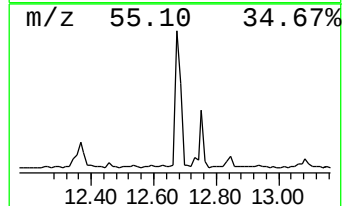
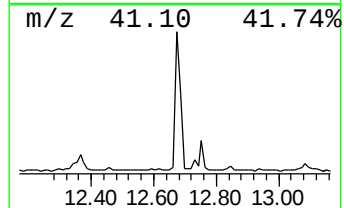
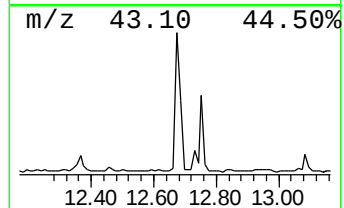
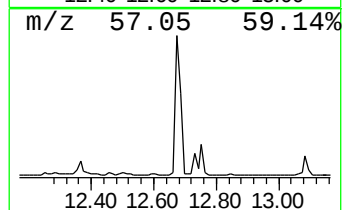
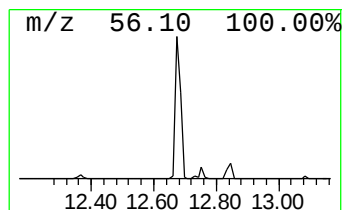
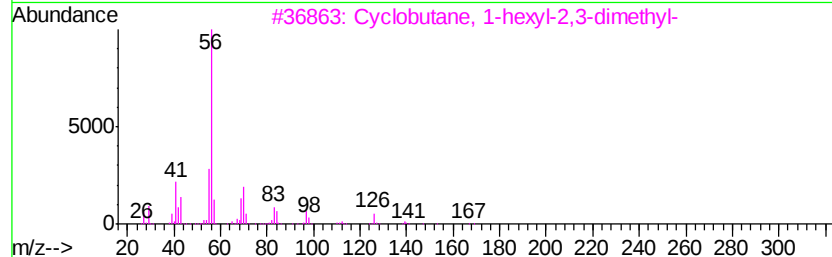
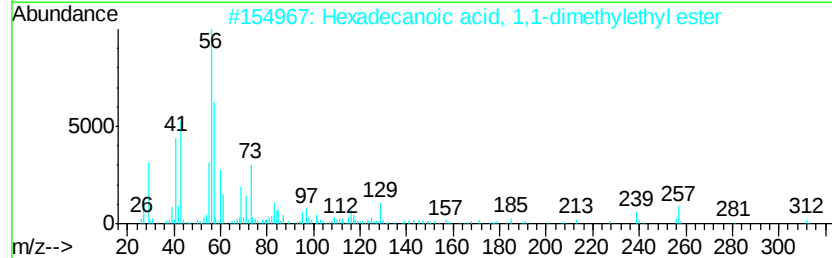
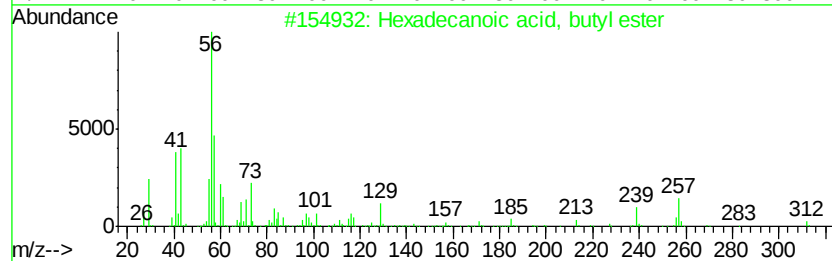
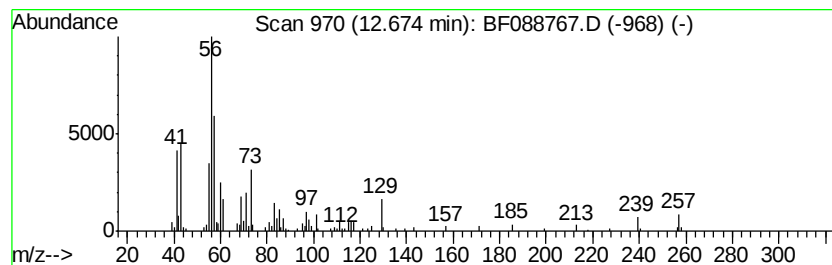
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown12.67 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	11.36 ng	304433	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088767.D
Acq On : 7 Jul 2016 7:13
Operator : UM/SJ
Sample : H3870-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

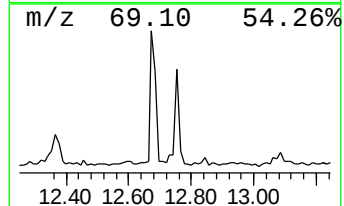
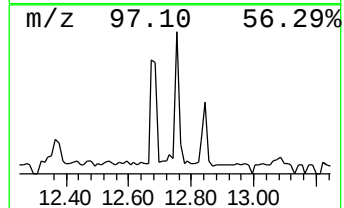
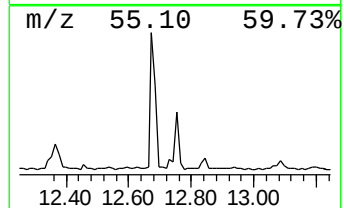
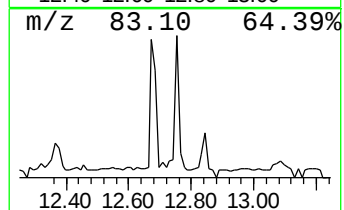
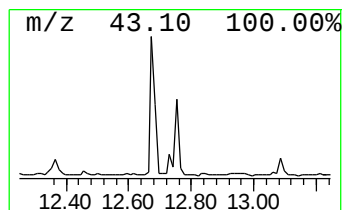
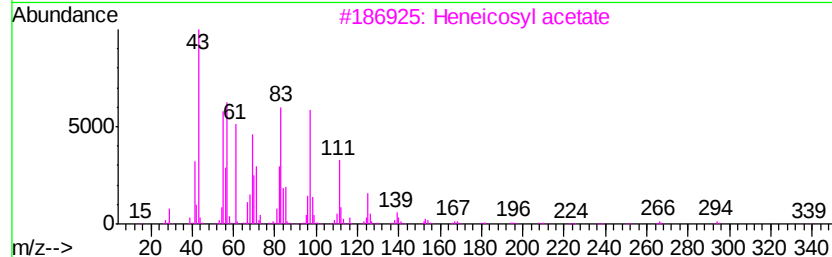
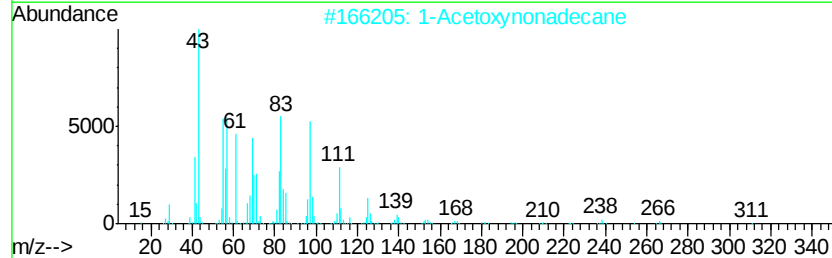
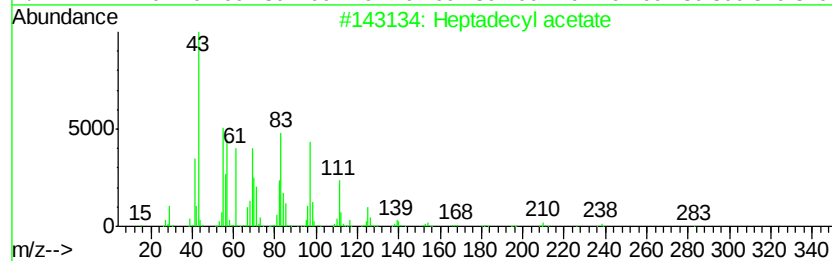
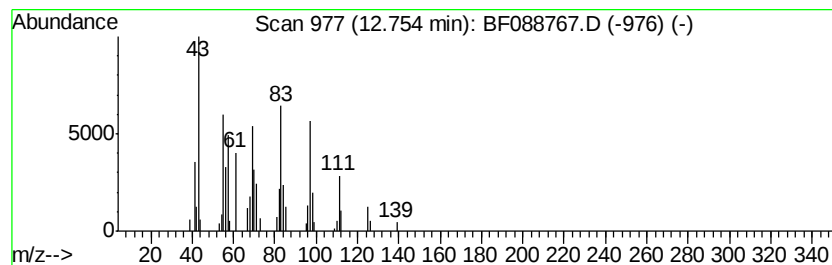
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heptadecyl acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.07 ng	55393	Chrysene-d12	13.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl acetate	298	C19H38O2	000822-20-8	91
2			1-Acetoxynonadecane	326	C21H42O2	001577-43-1	90
3			Heneicosyl acetate	354	C23H46O2	1000351-77-3	87
4			5-Octadecene, (E)-	252	C18H36	007206-21-5	64
5			17-Pentatriacontene	491	C35H70	006971-40-0	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088767.D
Acq On : 7 Jul 2016 7:13
Operator : UM/SJ
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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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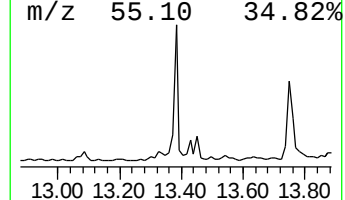
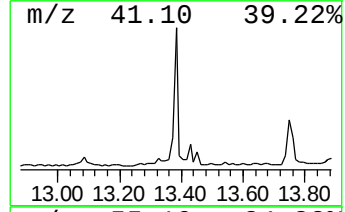
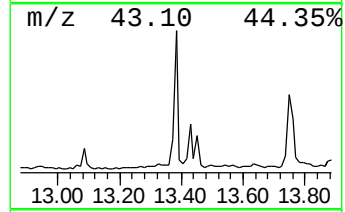
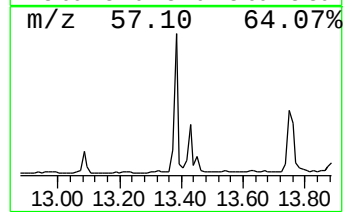
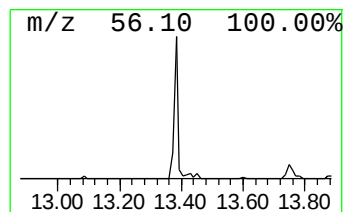
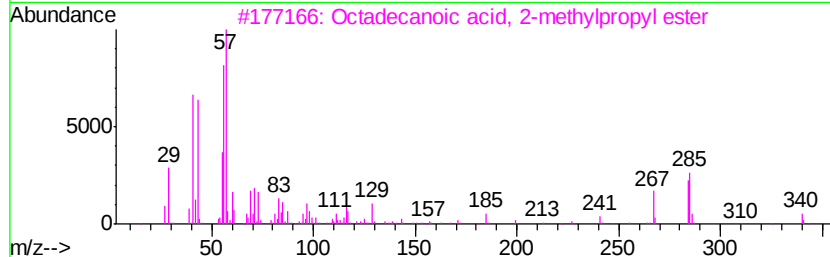
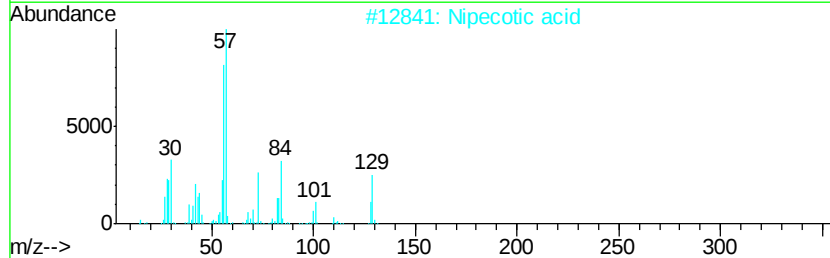
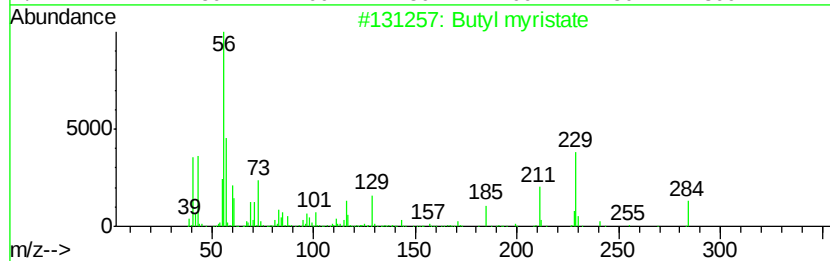
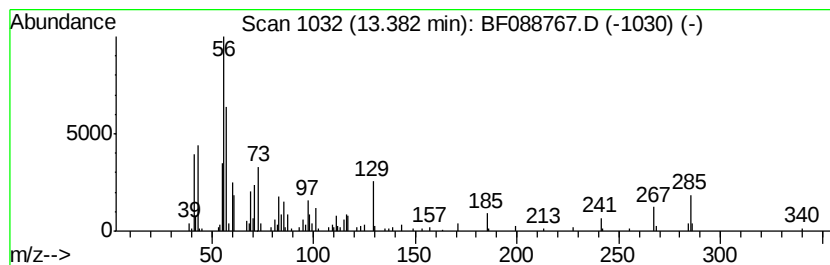
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	7.08 ng	189755	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl myristate	284	C18H36O2	000110-36-1	53
2		Nipecotic acid	129	C6H11NO2	000498-95-3	50
3		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	38
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088767.D
Acq On : 7 Jul 2016 7:13
Operator : UM/SJ
Sample : H3870-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

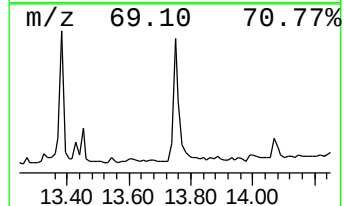
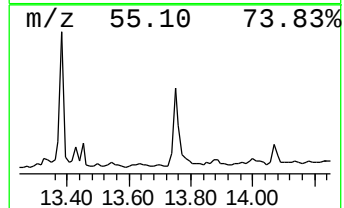
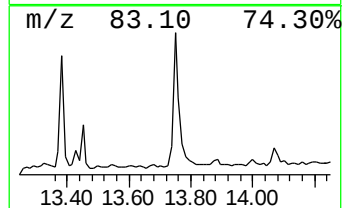
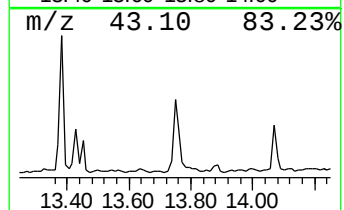
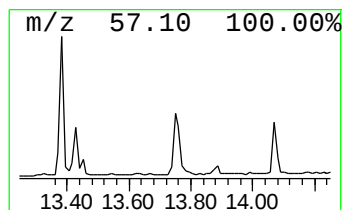
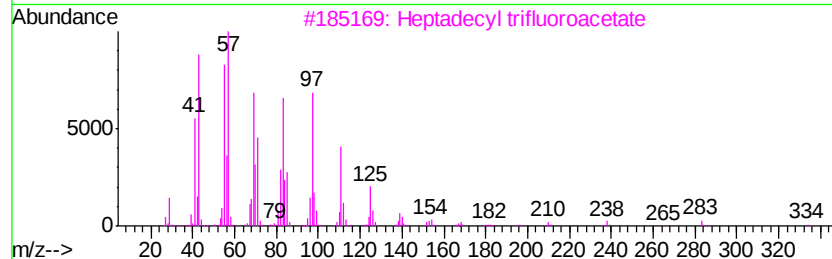
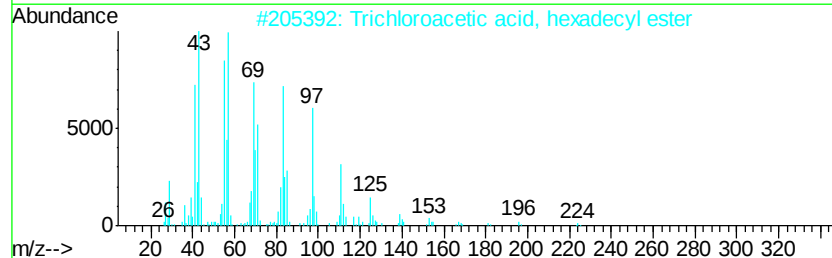
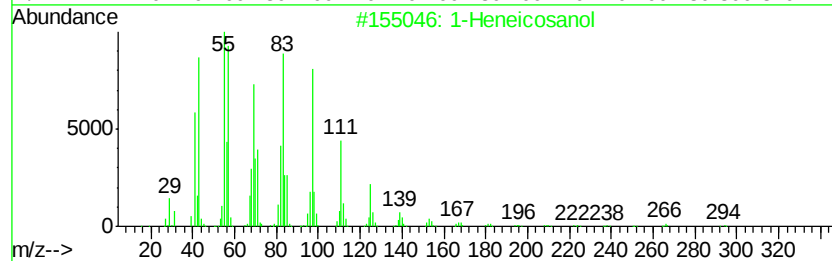
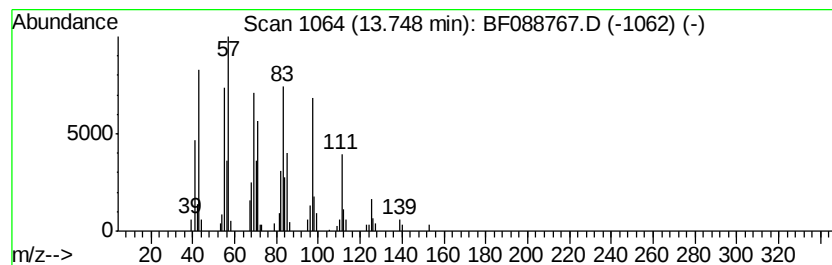
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.69 ng	125728	Chrysene-d12	13.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol		312 C21H44O	015594-90-8 93
2	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 90
3	Heptadecyl trifluoroacetate		352 C19H35F3O2	1000351-87-0 90
4	Isobutyl tetradecyl carbonate		314 C19H38O3	959275-58-2 86
5	5-Eicosene, (E)-		280 C20H40	074685-30-6 83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
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Acq On : 7 Jul 2016 7:13
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Misc :
ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
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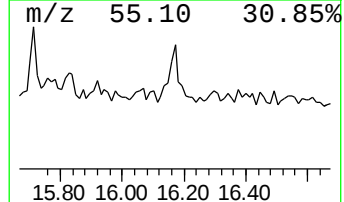
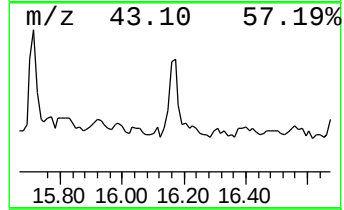
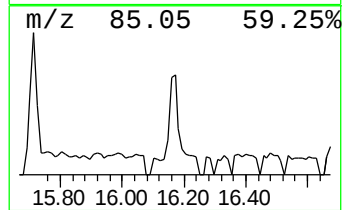
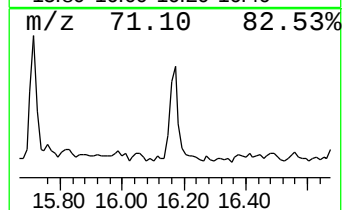
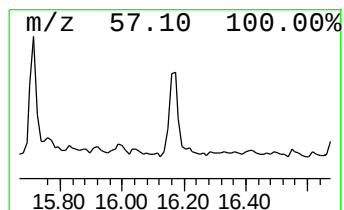
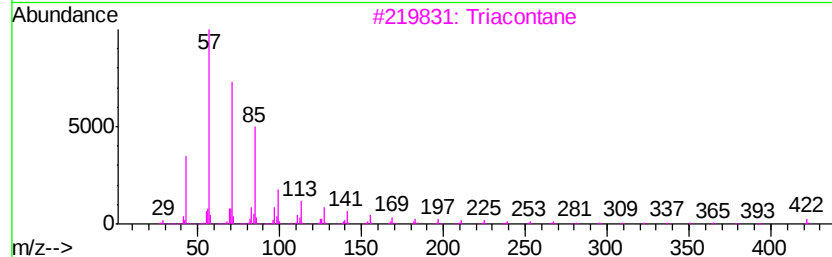
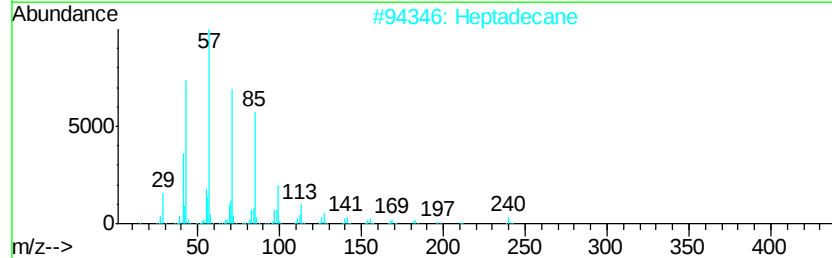
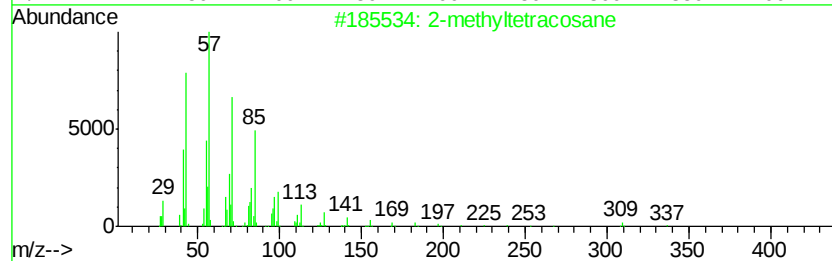
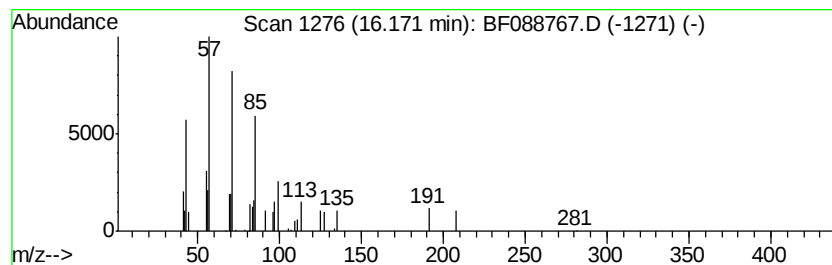
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 2-methyltetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.02 ng	49224	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyltetracosane	352	C25H52	1000376-72-6	72
2			Heptadecane	240	C17H36	000629-78-7	64
3			Triacontane	422	C30H62	000638-68-6	64
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	59
5			Tetracosane	338	C24H50	000646-31-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088767.D
Acq On : 7 Jul 2016 7:13
Operator : UM/SJ
Sample : H3870-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	4.91	4.8	ng	133799	1	6.75	553326	20.0
unknown6.51	6.51	85.1	ng	2353850	1	6.75	553326	20.0
Heptacosane	11.14	3.0	ng	99558	4	11.26	657443	20.0
Octadecane	11.56	2.9	ng	94073	4	11.26	657443	20.0
unknown12.67	12.67	11.4	ng	304433	5	13.89	535794	20.0
Heptadecyl acetate	12.75	2.1	ng	55393	5	13.89	535794	20.0
Butyl myristate	13.38	7.1	ng	189755	5	13.89	535794	20.0
1-Heneicosanol	13.75	4.7	ng	125728	5	13.89	535794	20.0
2-methyltetracosane	16.17	2.0	ng	49224	6	15.27	487228	20.0