

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
 Data File : BF091645.D
 Acq On : 15 Dec 2016 23:00
 Operator : UM/SJ
 Sample : H5940-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS05-0-2IN

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-BF120916.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	4.967	248	252	261	rBV	1607346	2554593	36.00%	3.813%
2	5.390	286	289	292	rBV	4790794	6194921	87.30%	9.247%
3	5.493	293	298	301	rVV	40441	84083	1.18%	0.126%
4	6.053	345	347	349	rBV	159659	136275	1.92%	0.203%
5	6.430	377	380	383	rVB	5254960	6399782	90.19%	9.553%
6	6.487	383	385	387	rVB	163329	185788	2.62%	0.277%
7	6.556	388	391	393	rBV	6305719	6205783	87.45%	9.263%
8	6.784	408	411	413	rBV	1652805	1381799	19.47%	2.063%
9	6.944	422	425	427	rBV	5202667	5179963	73.00%	7.732%
10	7.356	457	461	463	rBV	4997295	6078620	85.66%	9.073%
11	7.470	466	471	473	rBV	298048	458686	6.46%	0.685%
12	8.064	521	523	526	rBV	1691617	2191703	30.89%	3.271%
13	9.150	615	618	620	rBV	7698045	7096039	100.00%	10.592%
14	9.550	650	653	655	rBV	2332582	2577382	36.32%	3.847%
15	9.825	674	677	679	rBV	2784249	2636789	37.16%	3.936%
16	10.259	714	715	719	rVB2	131418	187179	2.64%	0.279%
17	10.488	731	735	738	rBV	71302	140344	1.98%	0.209%
18	10.613	743	746	748	rBV	4086689	4261567	60.06%	6.361%
19	10.739	755	757	761	rBV	222645	297547	4.19%	0.444%
20	10.933	772	774	778	rBV2	34148	77464	1.09%	0.116%
21	11.185	794	796	797	rBV	159886	140976	1.99%	0.210%
22	11.299	804	806	809	rBV	1678644	1736886	24.48%	2.593%
23	11.368	809	812	816	rVB4	31868	73890	1.04%	0.110%
24	11.539	824	827	831	rBV	191267	194026	2.73%	0.290%
25	11.836	851	853	858	rBV2	80227	127772	1.80%	0.191%
26	12.511	910	912	914	rBV	116655	107556	1.52%	0.161%
27	12.739	929	932	933	rBV	85845	109499	1.54%	0.163%
28	12.888	942	945	948	rBV	4724903	4841001	68.22%	7.226%
29	13.368	983	987	989	rVB	77233	91564	1.29%	0.137%
30	13.791	1021	1024	1028	rBV	228788	296434	4.18%	0.442%
31	13.939	1034	1037	1039	rBV	1423039	1789762	25.22%	2.671%
32	14.419	1077	1079	1082	rBV2	98143	123560	1.74%	0.184%
33	14.717	1101	1105	1110	rVB3	49679	118685	1.67%	0.177%
34	14.854	1115	1117	1119	rBV	210328	216441	3.05%	0.323%

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SS05-0-2IN

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	14.945	1123	1125	1129	rVB	53926	113822	1.60%	0.170%
36	15.059	1130	1135	1138	rBV3	195378	500168	7.05%	0.747%
37	15.345	1157	1160	1163	rBV	926052	1250662	17.62%	1.867%
38	15.574	1178	1180	1183	rVB	129361	173621	2.45%	0.259%
39	15.791	1197	1199	1201	rVB	103525	140679	1.98%	0.210%
40	16.008	1216	1218	1223	rVB4	37614	84175	1.19%	0.126%
41	16.260	1238	1240	1246	rVB2	42643	100993	1.42%	0.151%
42	16.534	1261	1264	1267	rBV2	39598	84557	1.19%	0.126%
43	17.243	1322	1326	1330	rBV5	56840	134417	1.89%	0.201%
44	17.688	1362	1365	1370	rVB7	40224	117824	1.66%	0.176%

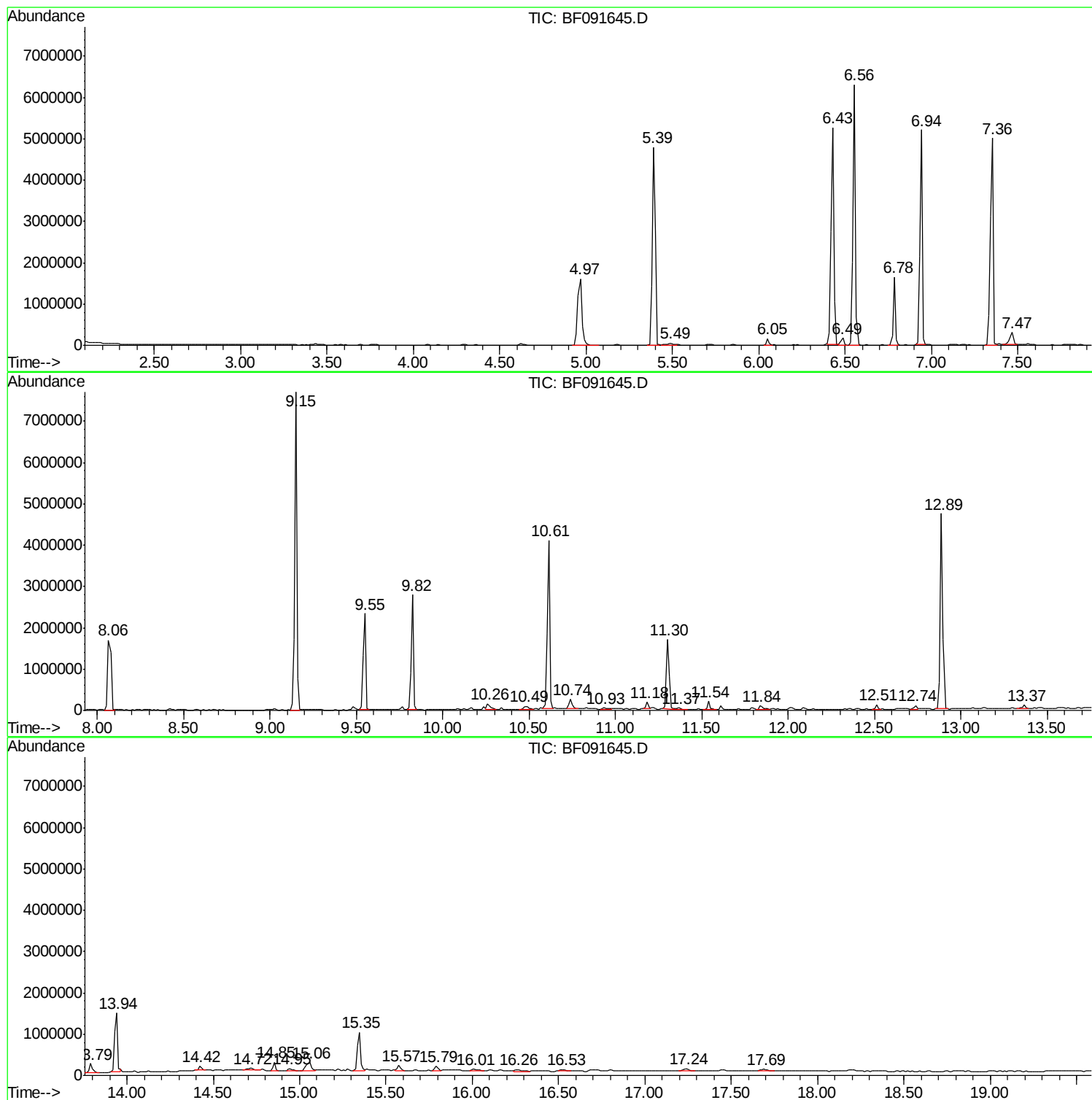
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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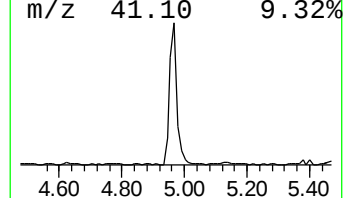
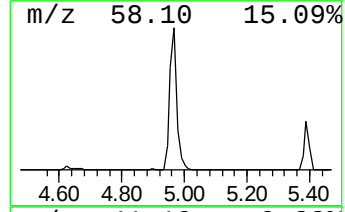
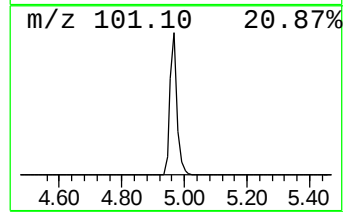
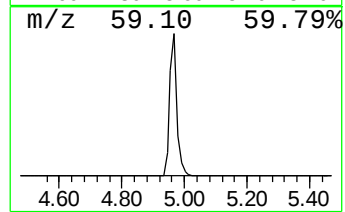
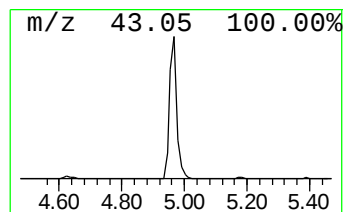
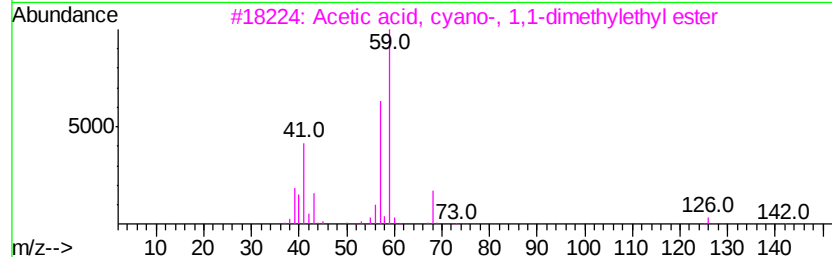
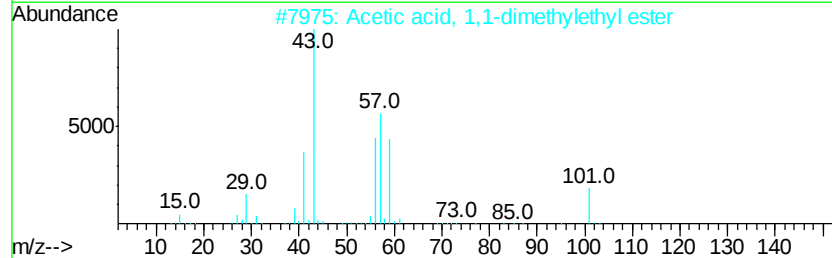
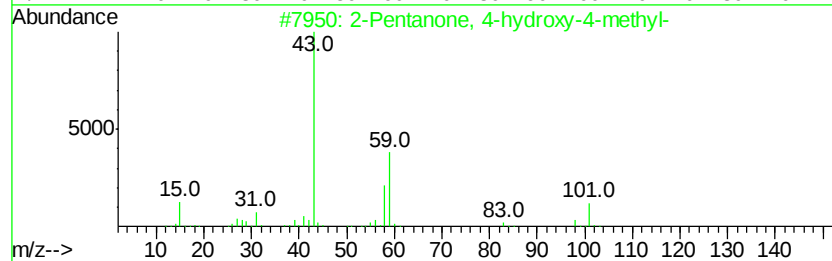
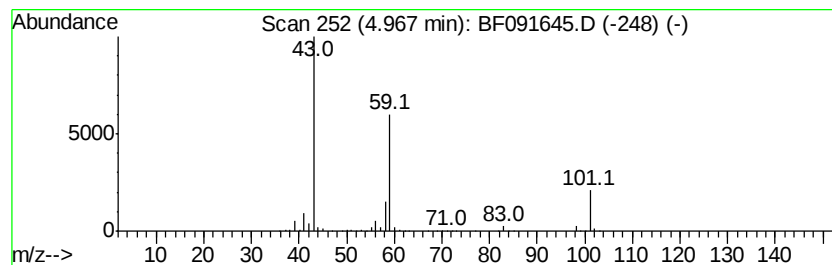
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.97	36.97 ng	2554590	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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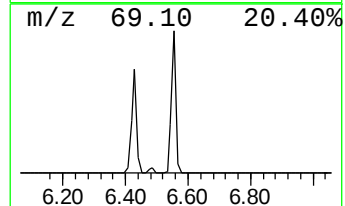
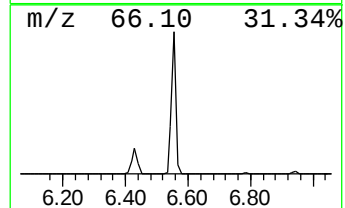
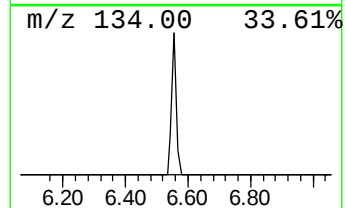
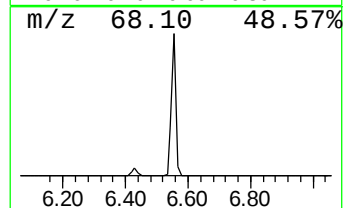
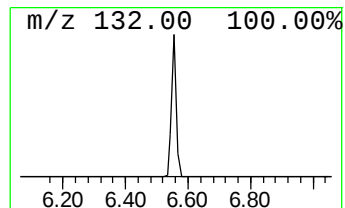
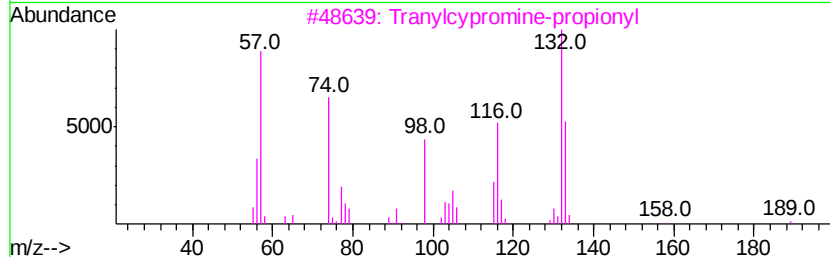
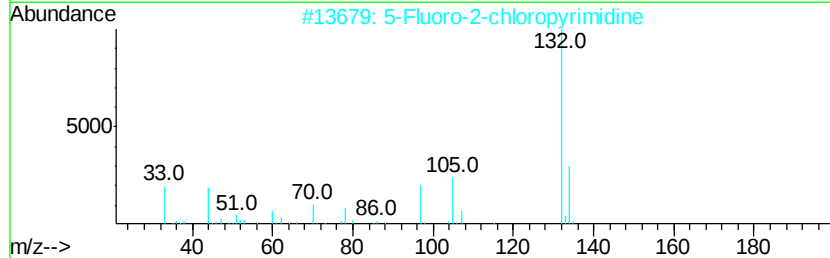
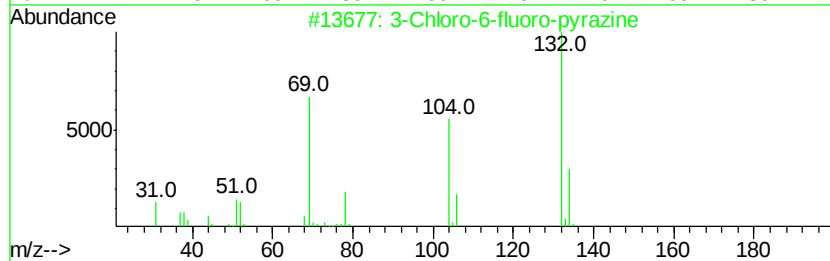
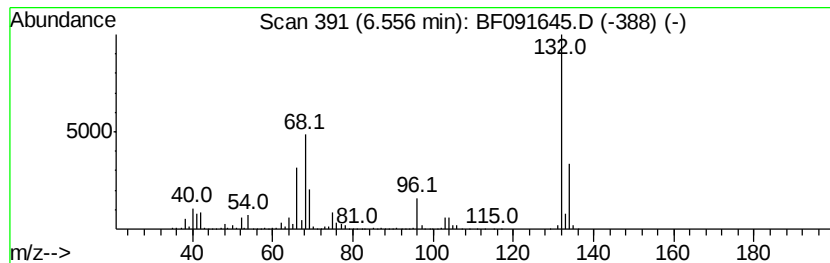
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	89.82 ng	6205780	1,4-Dichlorobenzene-d4	6.78

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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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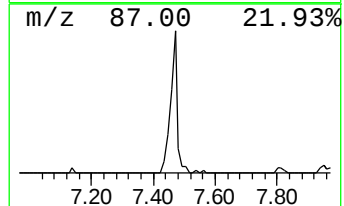
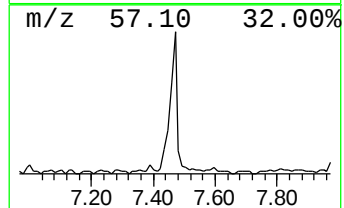
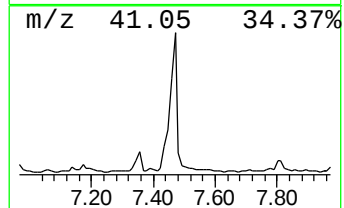
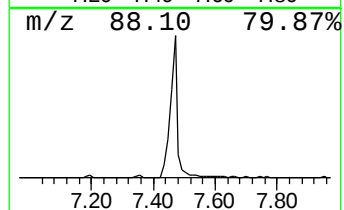
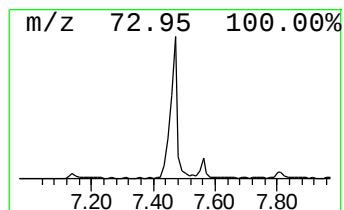
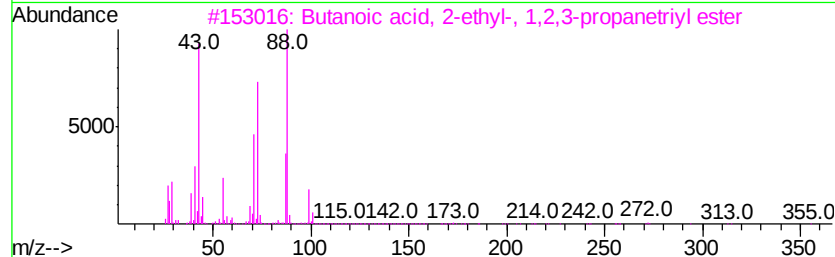
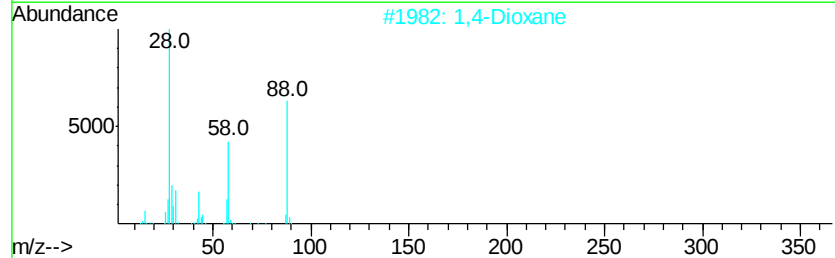
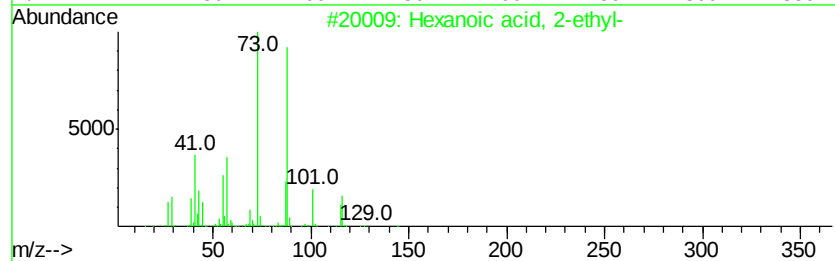
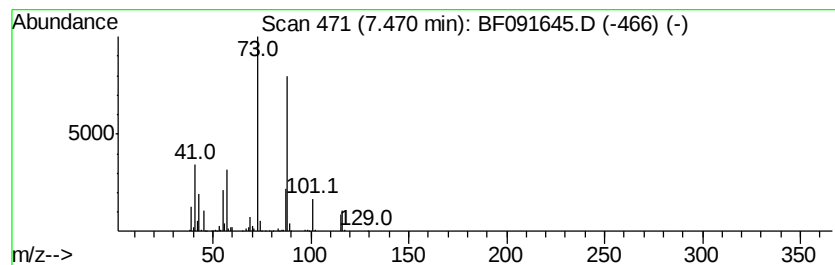
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	4.19 ng	458686	Naphthalene-d8	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		1,4-Dioxane	88	C4H8O2	000123-91-1	43
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	38



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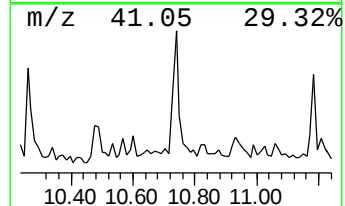
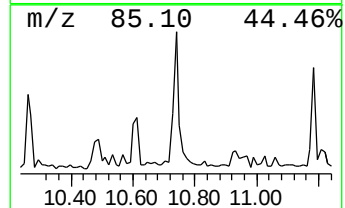
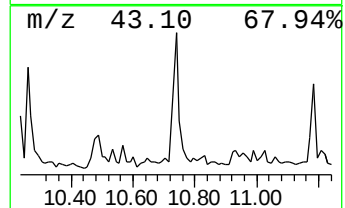
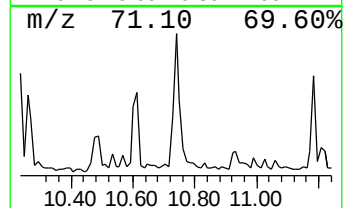
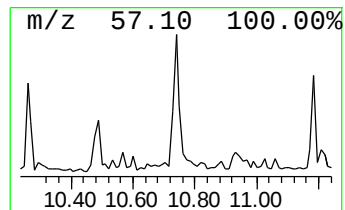
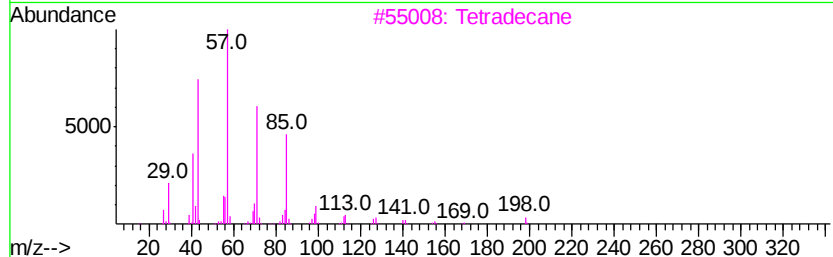
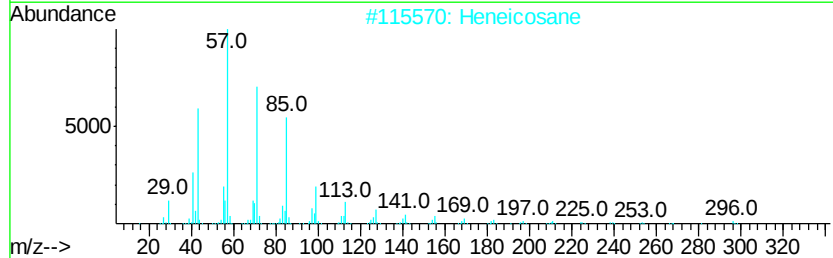
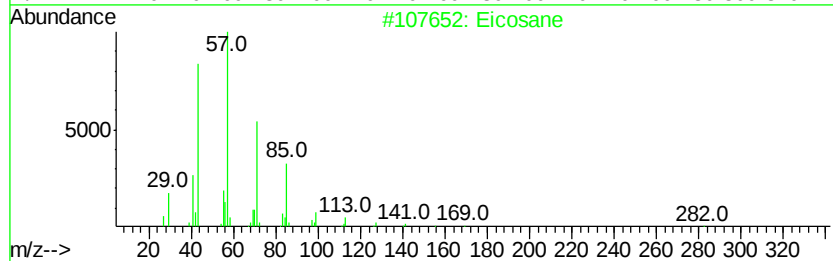
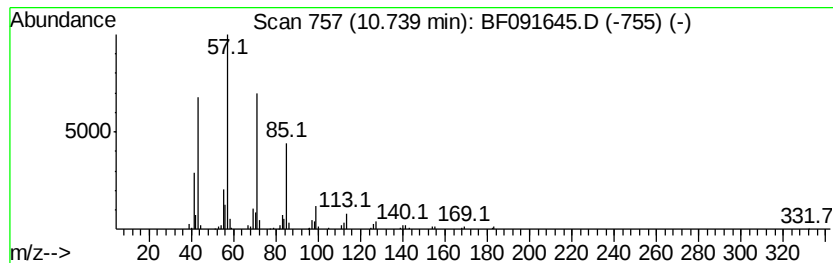
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.74	3.43 ng	297547	Phenanthrene-d10	11.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Tetradecane		198	C14H30	000629-59-4	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Heptadecane		240	C17H36	000629-78-7	87



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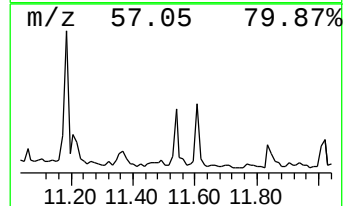
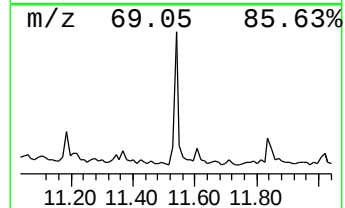
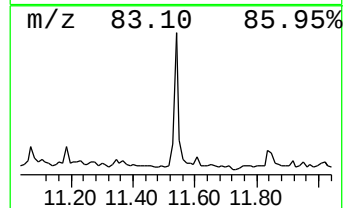
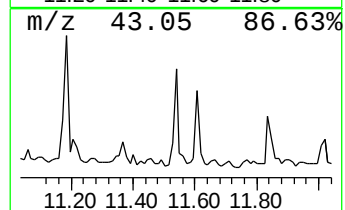
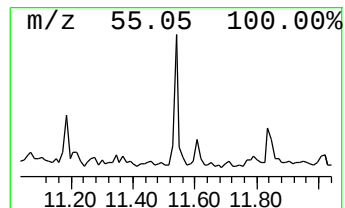
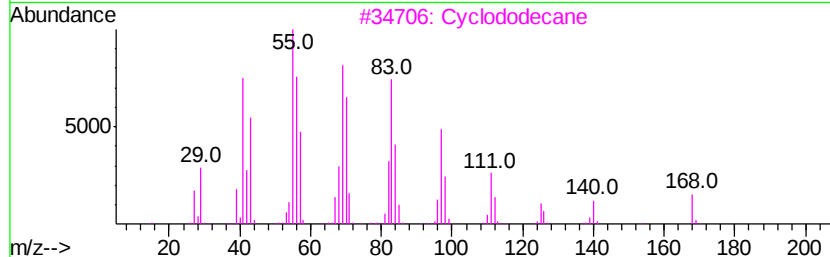
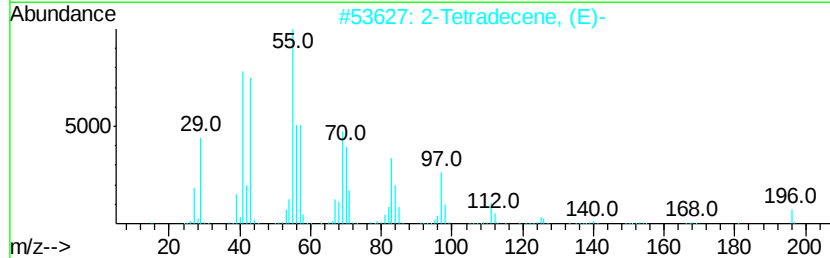
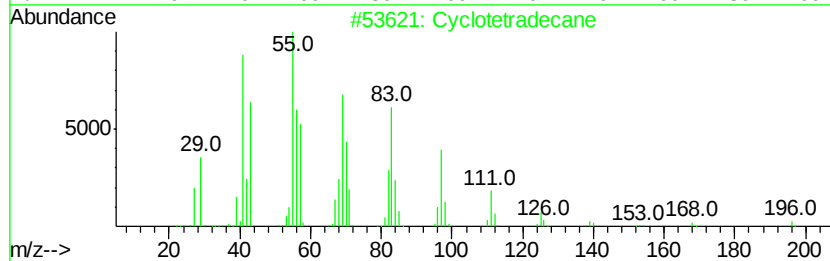
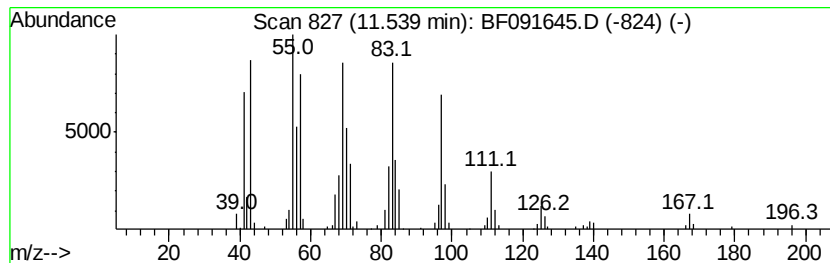
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.23 ng	194026	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetradecane	196	C14H28	000295-17-0	98
2		2-Tetradecene, (E)-	196	C14H28	035953-53-8	96
3		Cyclododecane	168	C12H24	000294-62-2	94
4		1-Octadecene	252	C18H36	000112-88-9	93
5		1-Tetradecene	196	C14H28	001120-36-1	92



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091645.D
Acq On : 15 Dec 2016 23:00
Operator : UM/SJ
Sample : H5940-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

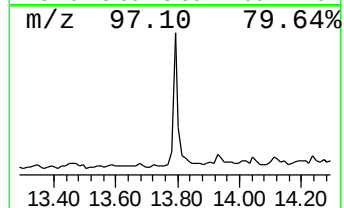
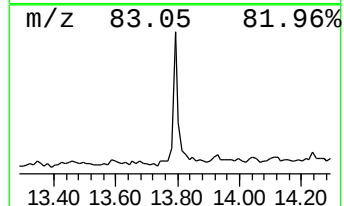
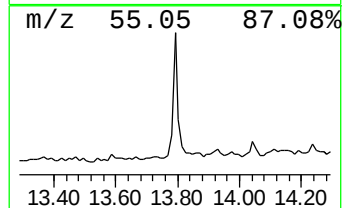
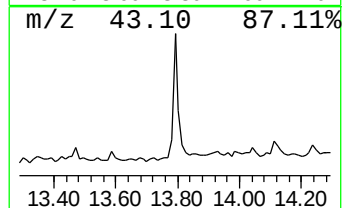
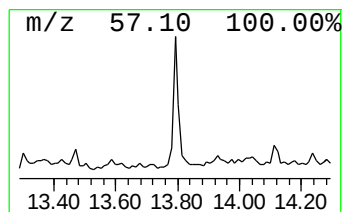
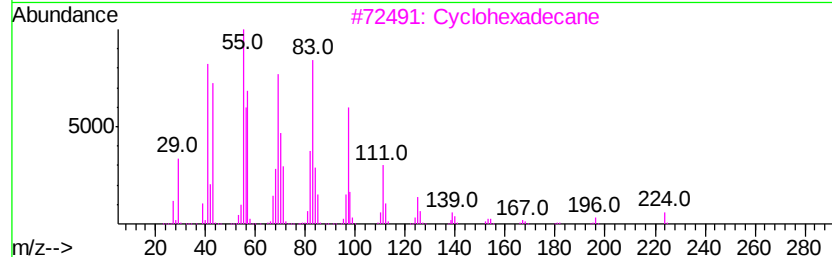
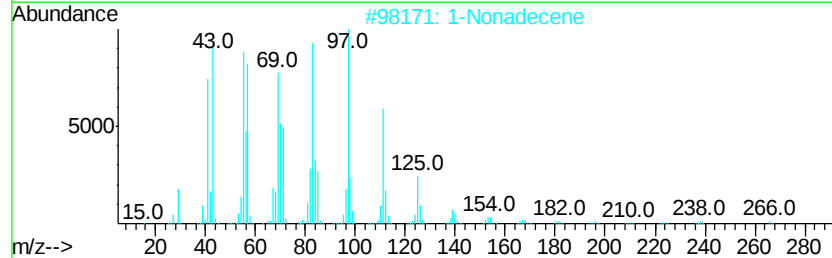
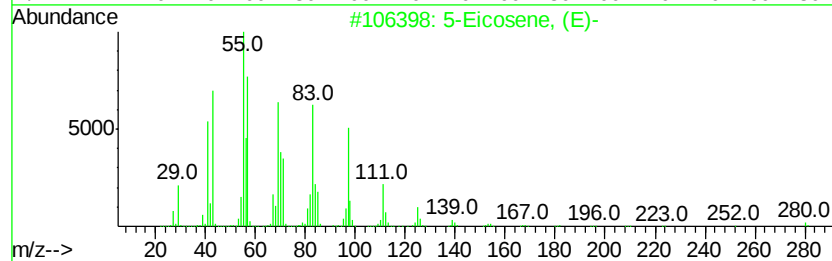
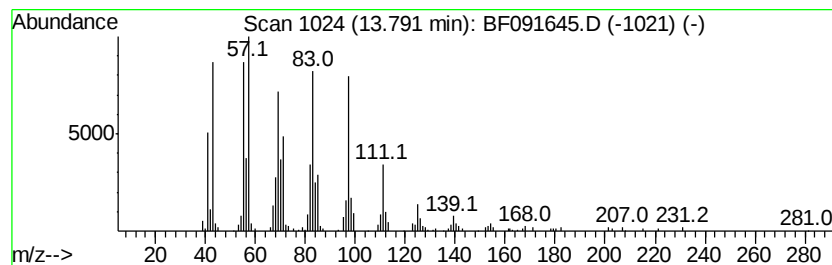
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	3.31 ng	296434	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	Cvclohexadecane	224	C16H32	000295-65-8	83
4	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	81
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
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Acq On : 15 Dec 2016 23:00
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ClientSampleId :
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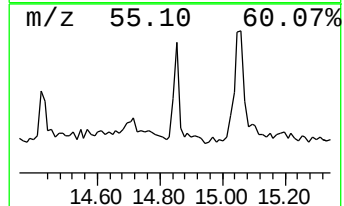
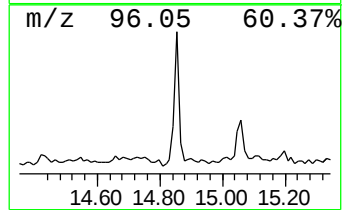
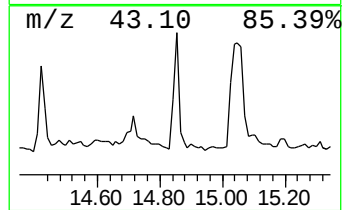
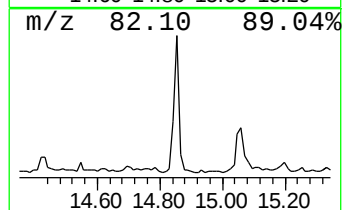
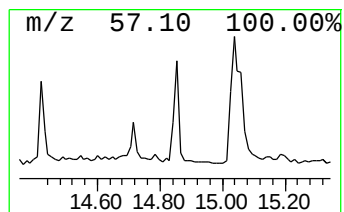
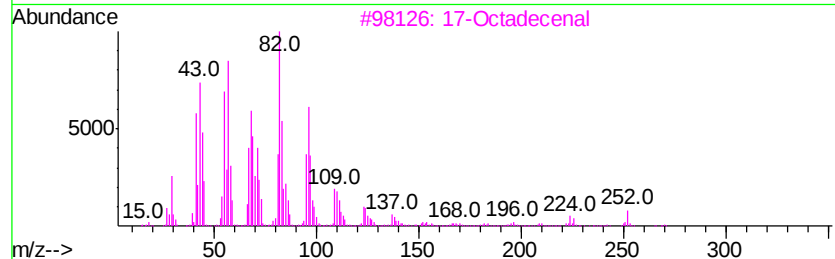
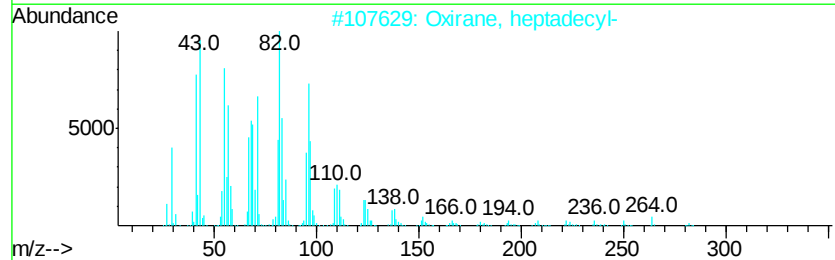
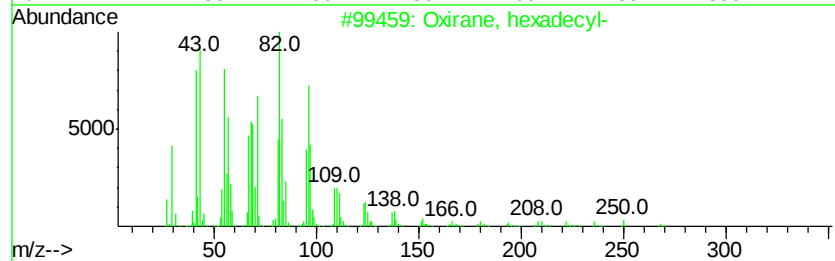
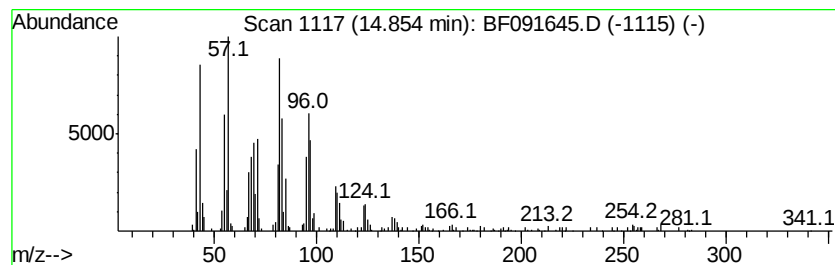
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	3.46 ng	216441	Perylene-d12	15.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91	
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91	
3	17-Octadecenal	266	C18H34O	056554-86-0	90	
4	Octadecanal	268	C18H36O	000638-66-4	87	
5	Tetradecanal	212	C14H28O	000124-25-4	86	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
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Acq On : 15 Dec 2016 23:00
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ALS Vial : 19 Sample Multiplier: 1

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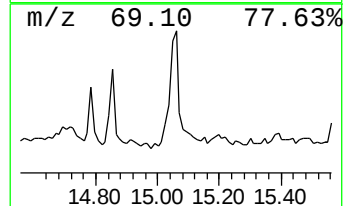
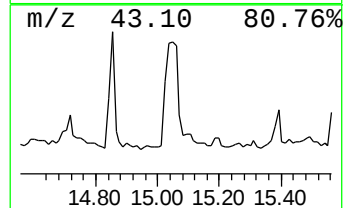
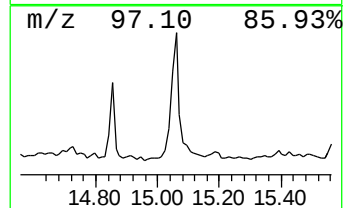
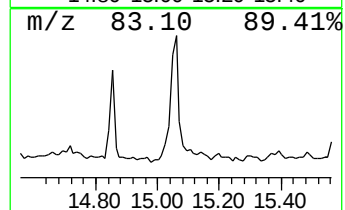
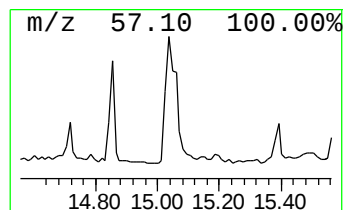
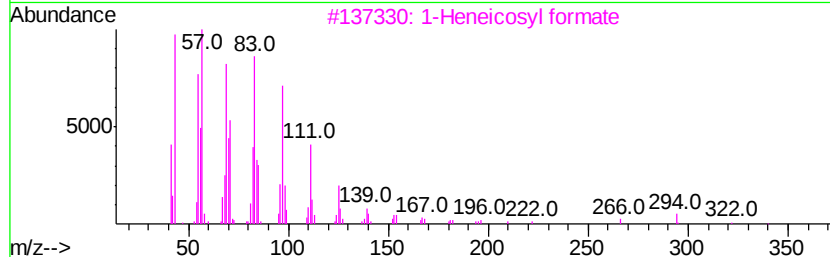
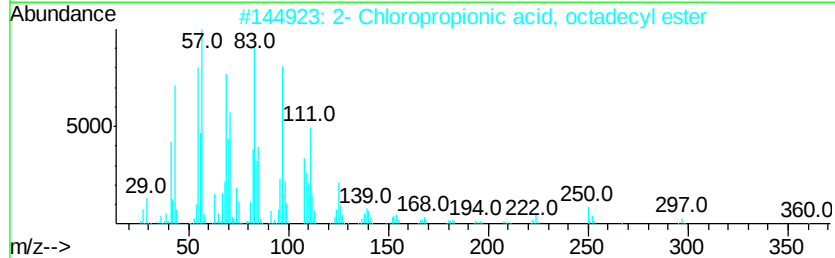
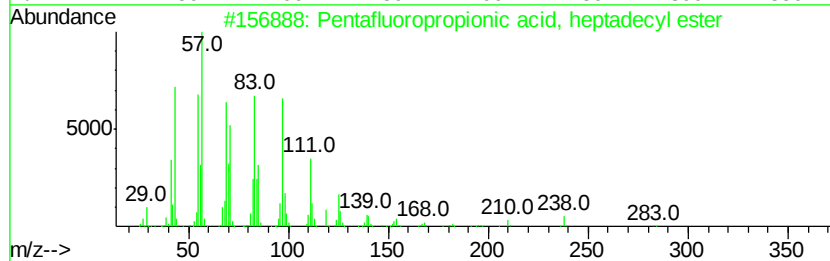
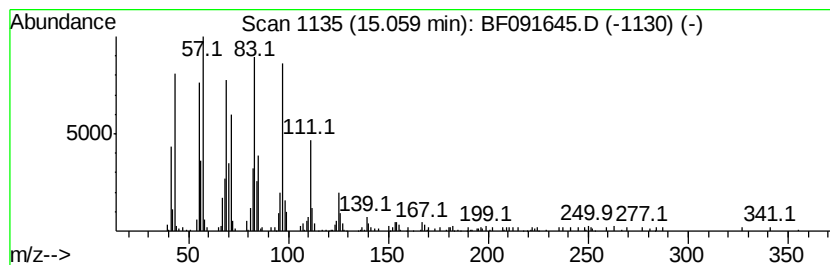
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	8.00 ng	500168	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	81
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	81
5		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81



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Acq On : 15 Dec 2016 23:00
Operator : UM/SJ
Sample : H5940-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

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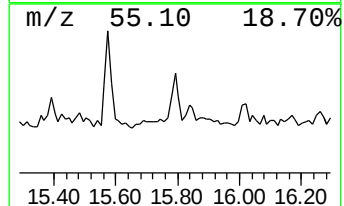
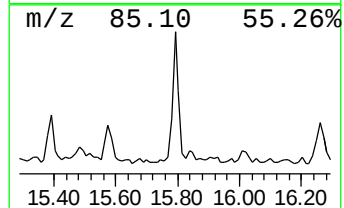
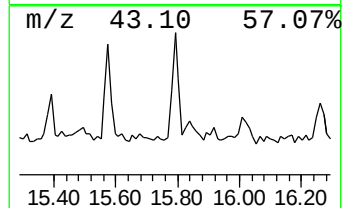
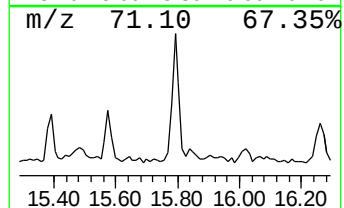
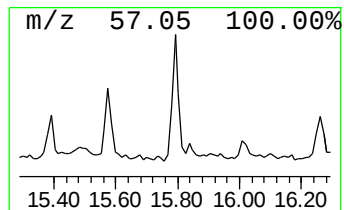
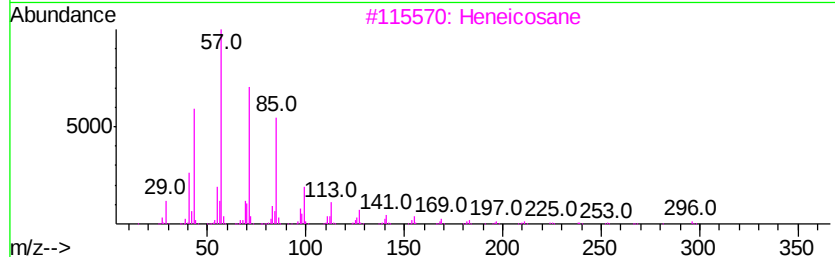
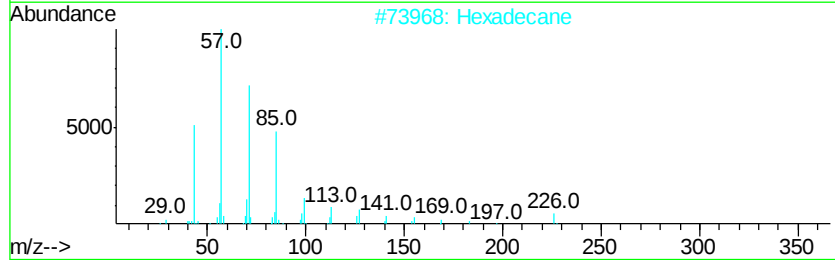
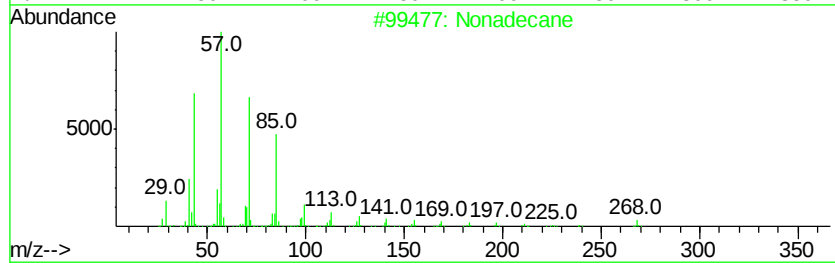
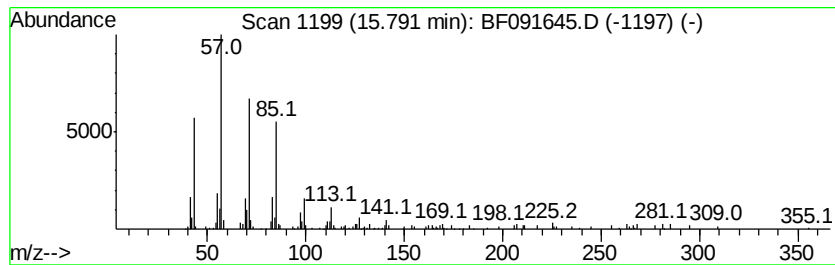
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.25 ng	140679	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Hexadecane	226	C16H34	000544-76-3	93
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5			Tetradecane	198	C14H30	000629-59-4	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
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ALS Vial : 19 Sample Multiplier: 1

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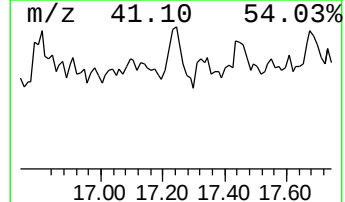
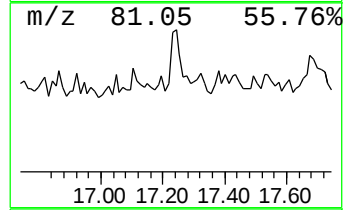
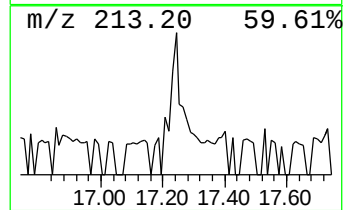
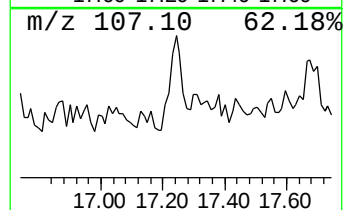
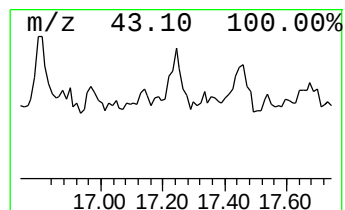
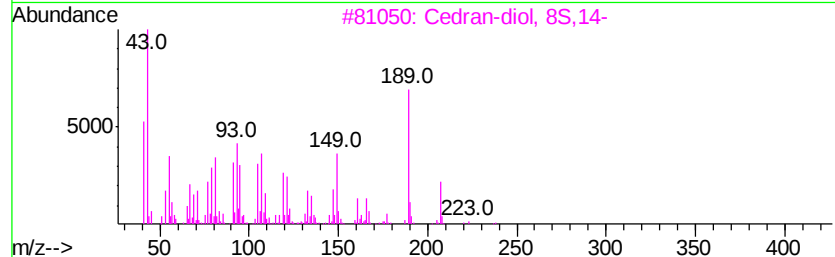
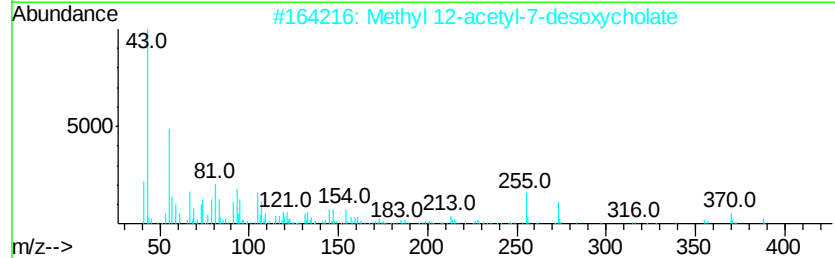
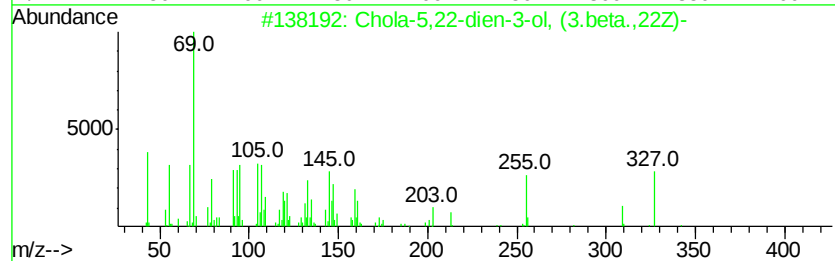
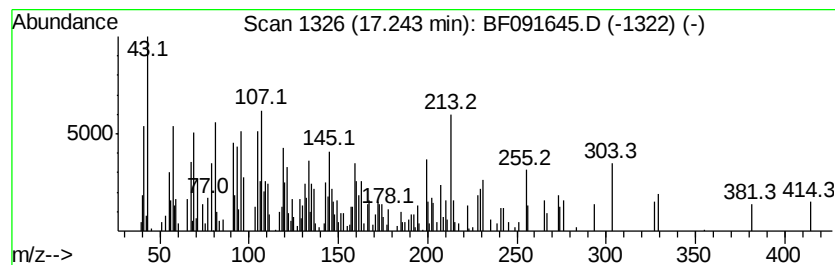
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.24 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	2.15 ng	134417	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chola-5,22-dien-3-ol, (3.beta.,2...	342	C24H38O	057597-14-5	43
2		Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	37
3		Cedran-diol, 8S,14-	238	C15H26O2	062600-05-9	25
4		14-Oxatricyclo[9..2.1.0(1,10)]te...	262	C18H30O	1000193-06-8	10
5		6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	10



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.56	6.56	89.8	ng	6205780	1	6.78	1381800	20.0
Hexanoic acid, 2-...	7.47	4.2	ng	458686	2	8.06	2191700	20.0
Eicosane	10.74	3.4	ng	297547	4	11.30	1736890	20.0
Cyclotetradecane	11.54	2.2	ng	194026	4	11.30	1736890	20.0
5-Eicosene, (E)-	13.79	3.3	ng	296434	5	13.94	1789760	20.0
Oxirane, hexadecyl-	14.85	3.5	ng	216441	6	15.35	1250660	20.0
Pentafluoropropio...	15.06	8.0	ng	500168	6	15.35	1250660	20.0
Nonadecane	15.79	2.3	ng	140679	6	15.35	1250660	20.0
unknown17.24	17.24	2.1	ng	134417	6	15.35	1250660	20.0