

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092281.D
 Acq On : 14 Jan 2017 13:23
 Operator : UM/SJ
 Sample : I1162-16
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-09-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-BF122116.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	4.701	252	255	267	rBV	1461441	2344700	45.80%	5.297%
2	5.170	293	296	313	rBV	4341647	4791246	93.59%	10.825%
3	6.244	387	390	392	rBV	4566085	5119481	100.00%	11.566%
4	6.347	397	399	402	rVB	5152910	4817595	94.10%	10.884%
5	6.576	417	419	421	rBV	1306387	1321790	25.82%	2.986%
6	6.724	430	432	435	rBV	3036816	3866743	75.53%	8.736%
7	7.147	466	469	471	rBV	3191141	3171454	61.95%	7.165%
8	7.856	529	531	534	rBV	1126007	1425738	27.85%	3.221%
9	8.942	623	626	629	rBV	4196992	3919840	76.57%	8.856%
10	9.342	659	661	664	rBV	615831	529633	10.35%	1.197%
11	9.559	678	680	682	rBV	63009	58486	1.14%	0.132%
12	9.605	682	684	687	rBV	1342147	1565523	30.58%	3.537%
13	10.062	715	724	725	rBV	145915	188810	3.69%	0.427%
14	10.279	740	743	744	rBV	49764	59799	1.17%	0.135%
15	10.393	751	753	756	rBV2	1567866	2228899	43.54%	5.036%
16	10.530	763	765	769	rBV	146695	171142	3.34%	0.387%
17	10.976	802	804	805	rBV	113024	98741	1.93%	0.223%
18	11.091	811	814	816	rBV	1095102	1306751	25.53%	2.952%
19	11.399	839	841	844	rVB	58078	54653	1.07%	0.123%
20	11.639	861	862	866	rBV2	70231	92200	1.80%	0.208%
21	12.291	917	919	921	rBV	120797	110501	2.16%	0.250%
22	12.508	936	938	941	rBV2	147254	207393	4.05%	0.469%
23	12.588	941	945	947	rVB2	56364	71729	1.40%	0.162%
24	12.668	950	952	955	rVB	2932664	3037293	59.33%	6.862%
25	13.216	997	1000	1001	rBV	52566	53008	1.04%	0.120%
26	13.605	1030	1034	1041	rBV2	75333	209712	4.10%	0.474%
27	13.708	1041	1043	1046	rBV	994020	1241062	24.24%	2.804%
28	14.199	1082	1086	1088	rBV2	25515	53673	1.05%	0.121%
29	14.565	1116	1118	1120	rBV2	52458	72120	1.41%	0.163%
30	14.702	1128	1130	1134	rBV	70457	143623	2.81%	0.324%
31	14.794	1135	1138	1140	rVV2	50775	78939	1.54%	0.178%
32	14.965	1150	1153	1156	rVB	50726	57193	1.12%	0.129%
33	15.022	1156	1158	1160	rBV	48732	77276	1.51%	0.175%
34	15.068	1160	1162	1164	rVV	838424	960911	18.77%	2.171%

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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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.102	1164	1165	1169	rVB	69816	91242	1.78%	0.206%
36	15.468	1194	1197	1201	rVB	72349	105491	2.06%	0.238%
37	15.880	1230	1233	1238	rVB2	86275	160195	3.13%	0.362%
38	16.360	1272	1275	1281	rVB	56288	117024	2.29%	0.264%
39	16.931	1322	1325	1328	rVB	51464	105238	2.06%	0.238%
40	17.594	1379	1383	1390	rVB2	33910	95445	1.86%	0.216%
41	18.394	1450	1453	1462	rVB3	22294	79684	1.56%	0.180%

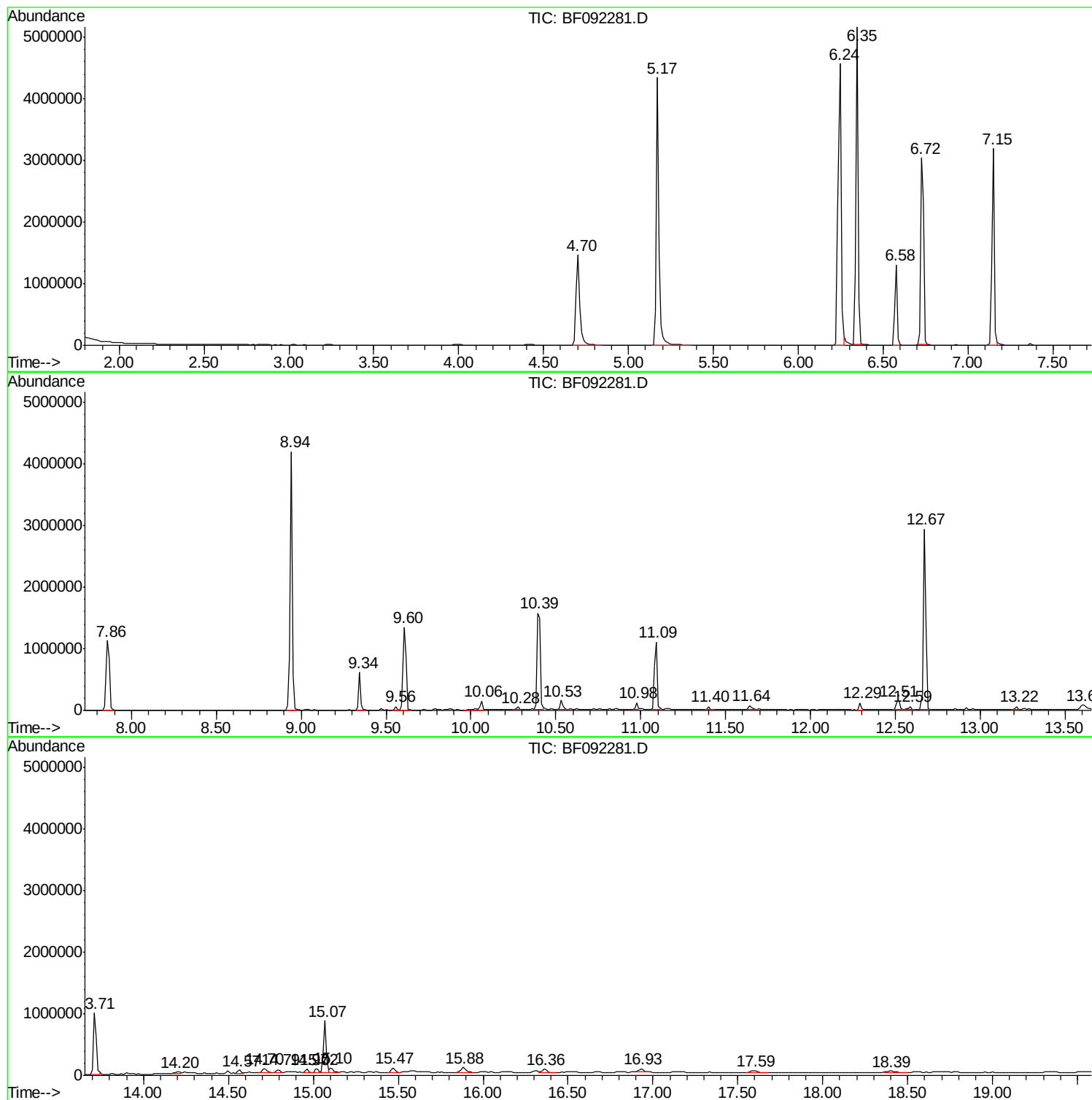
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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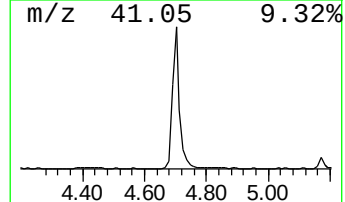
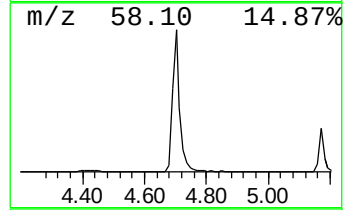
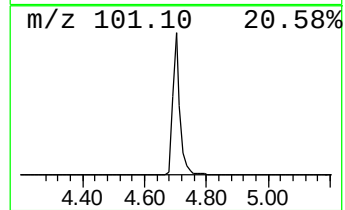
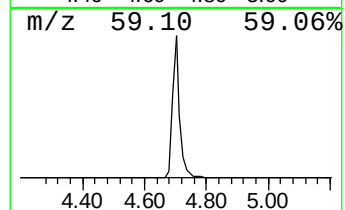
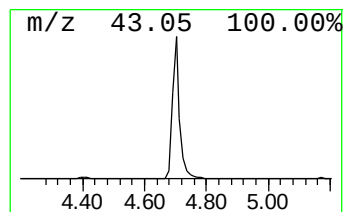
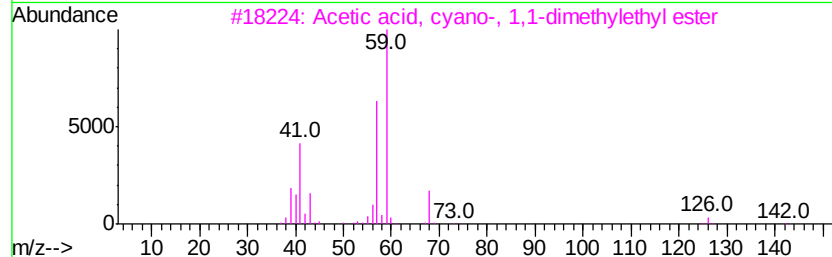
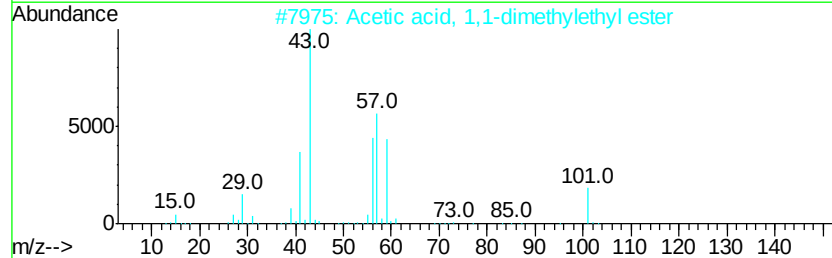
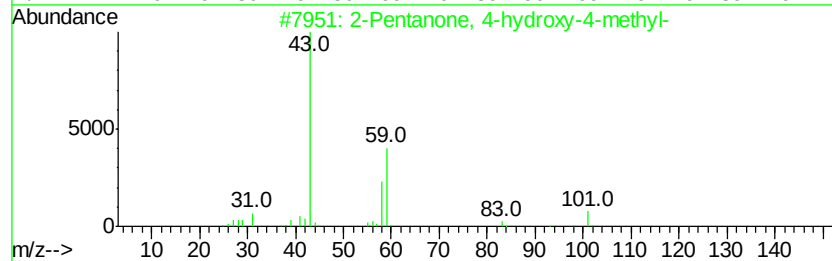
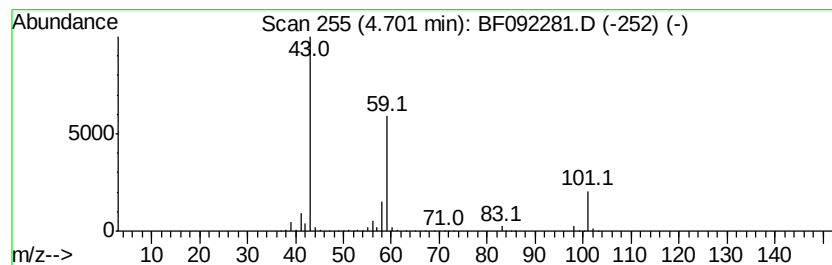
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.70	35.48 ng	2344700	1,4-Dichlorobenzene-d4	6.58

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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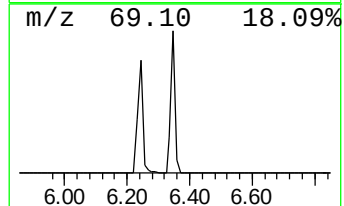
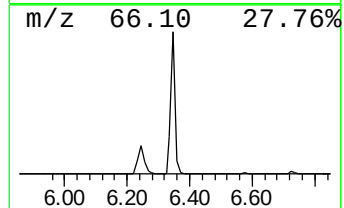
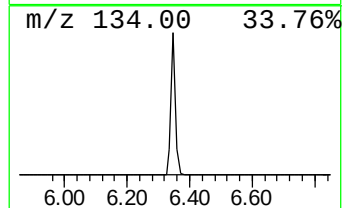
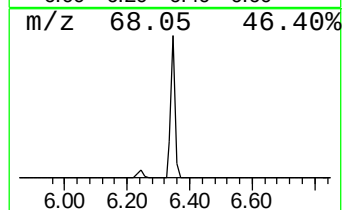
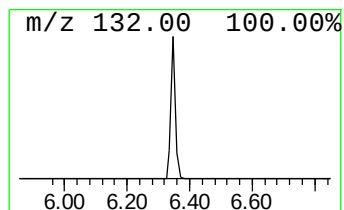
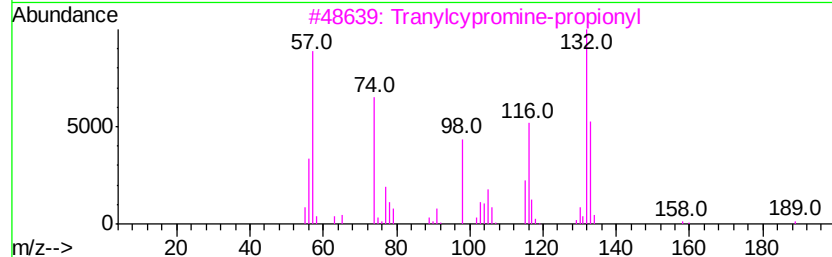
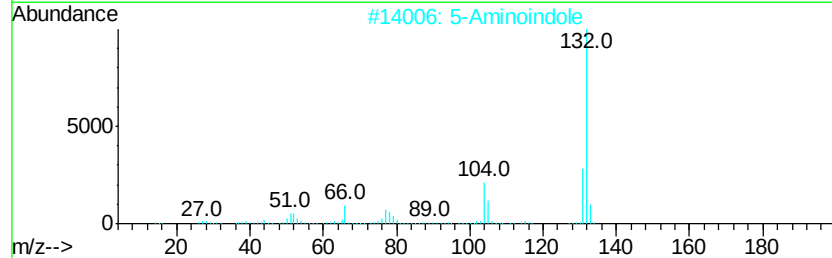
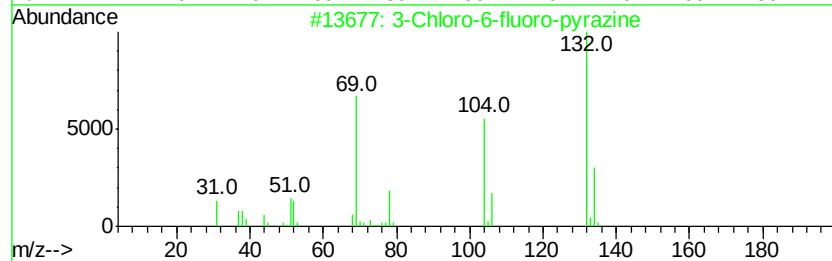
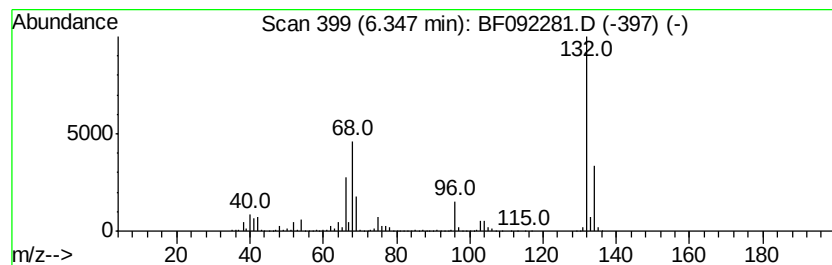
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	72.90 ng	4817600	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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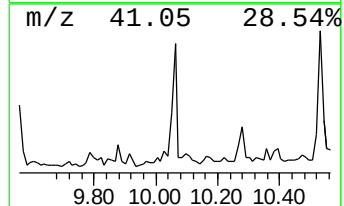
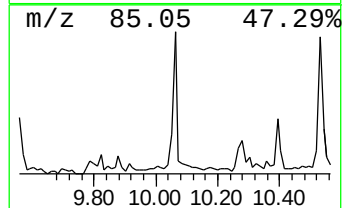
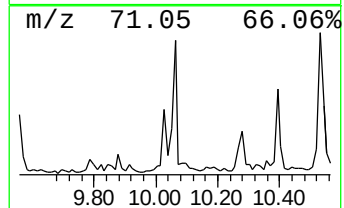
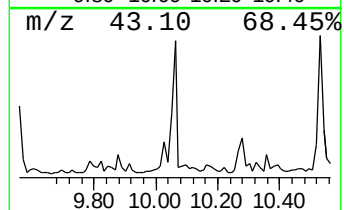
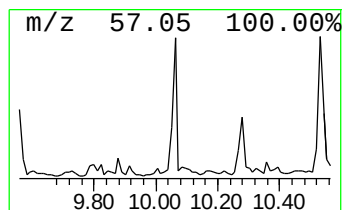
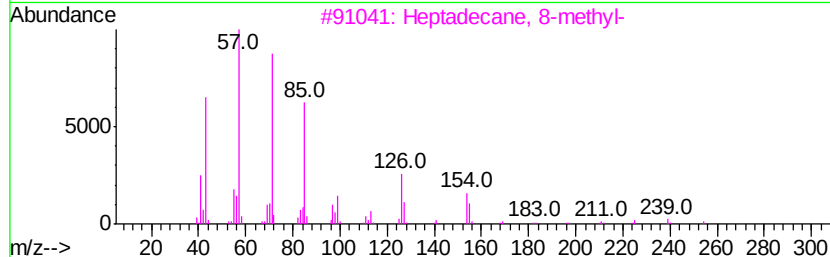
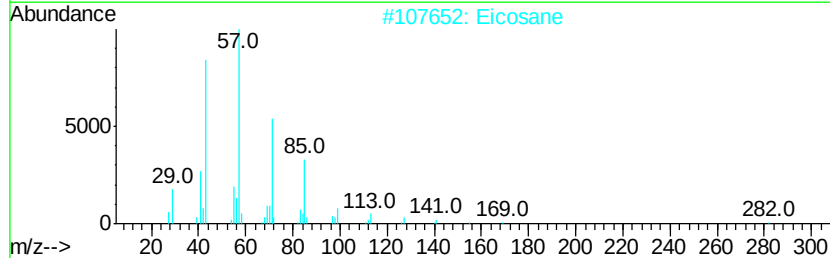
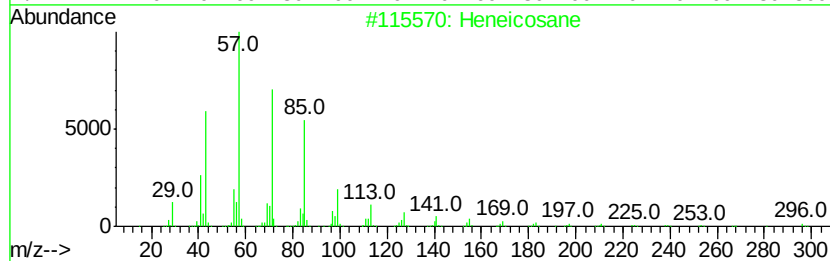
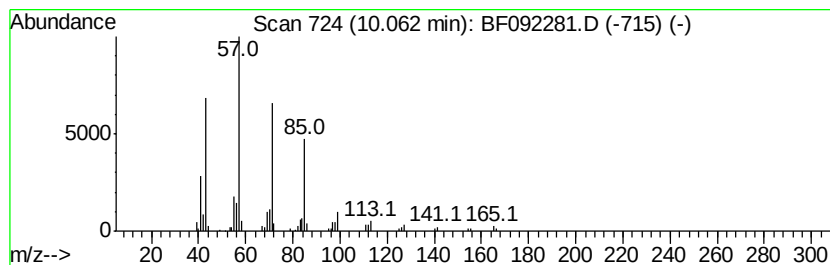
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	2.41 ng	188810	Acenaphthene-d10	9.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Heptadecane, 8-methyl-		254	C18H38	013287-23-5	90
4	Heptadecane		240	C17H36	000629-78-7	86
5	Tetradecane		198	C14H30	000629-59-4	86



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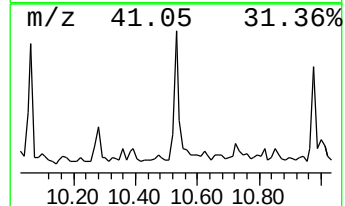
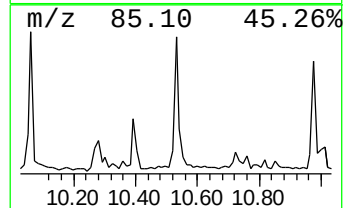
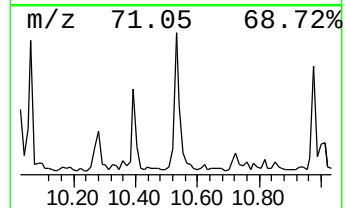
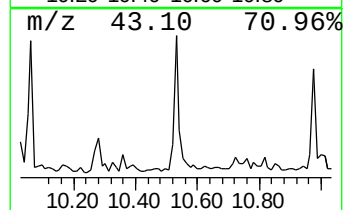
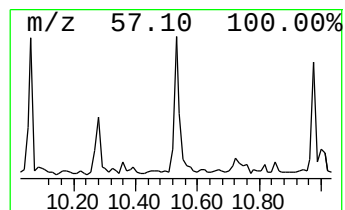
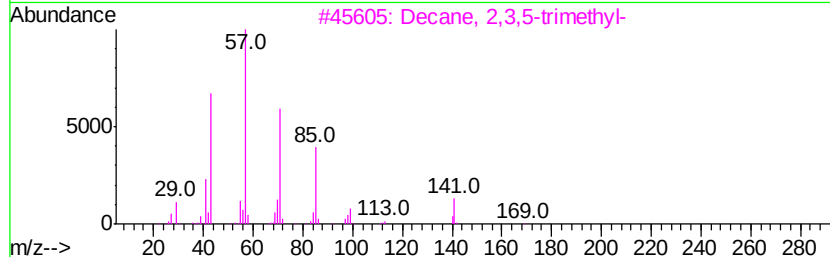
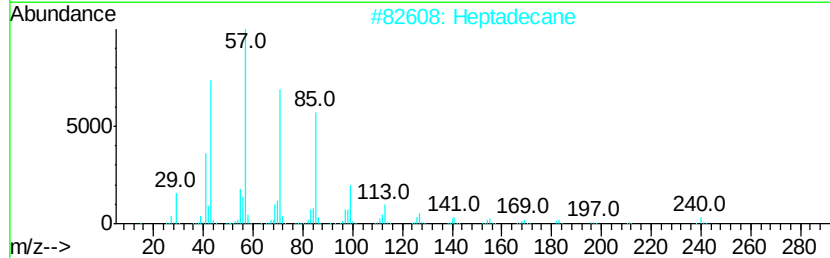
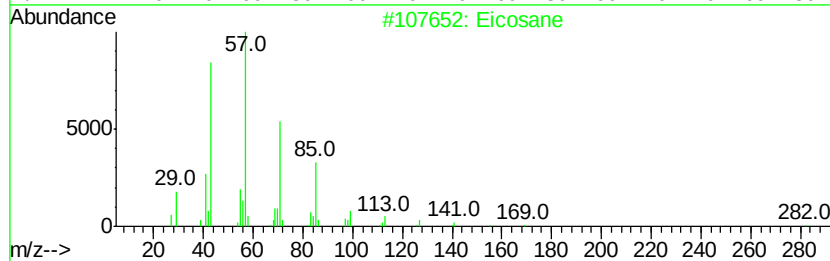
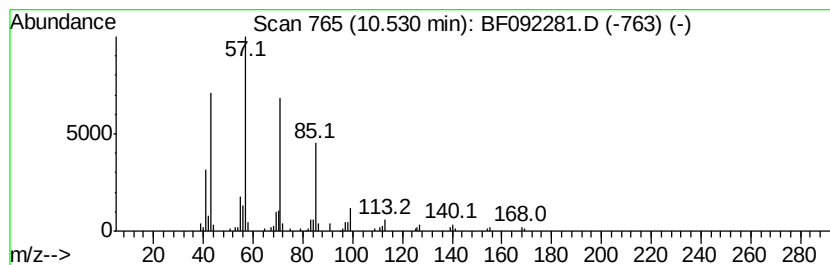
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.53	2.62 ng	171142	Phenanthrene-d10		11.09
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	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptacosane	380	C27H56	000593-49-7	86



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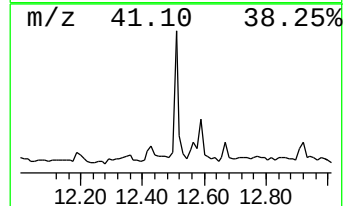
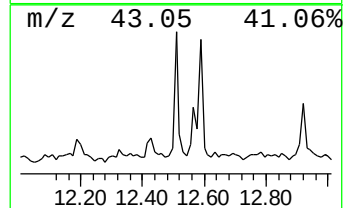
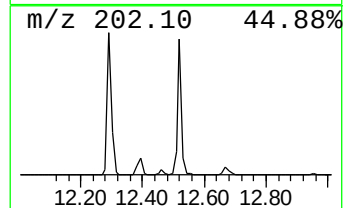
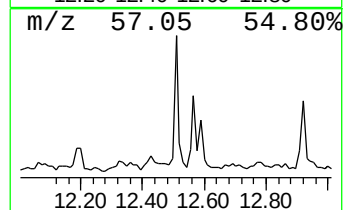
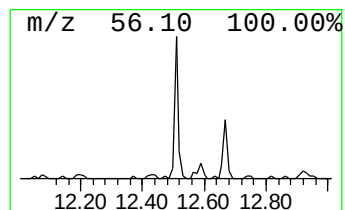
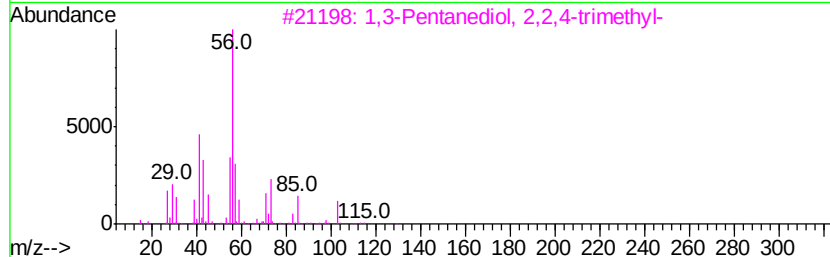
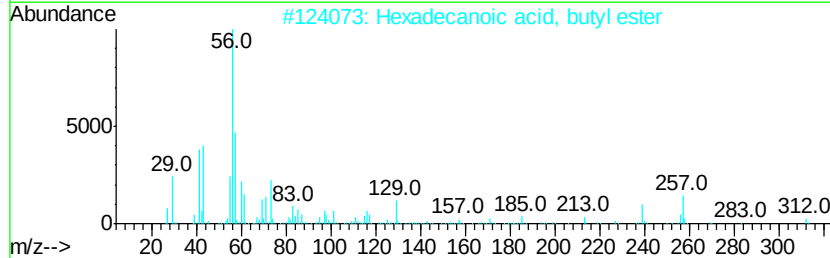
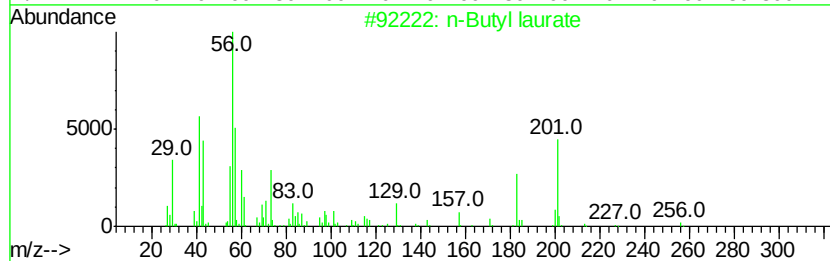
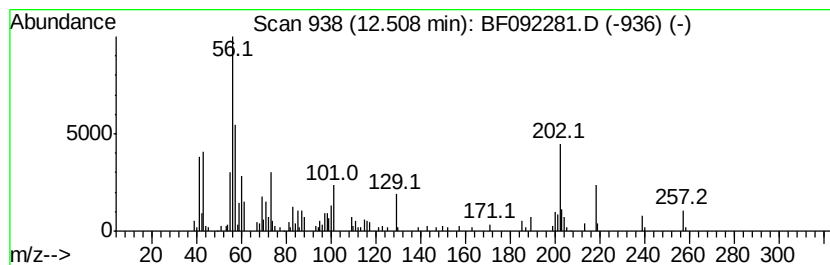
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.51 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.51	3.34 ng	207393	Chrysene-d12	13.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl laurate	256	C16H32O2	000106-18-3	49
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	45
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	27
4	Dodecanoic acid, 1-methylpropyl ...	256	C16H32O2	006937-42-4	22
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
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Acq On : 14 Jan 2017 13:23
Operator : UM/SJ
Sample : I1162-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-09-COMP

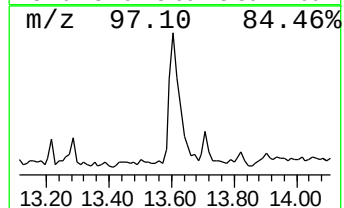
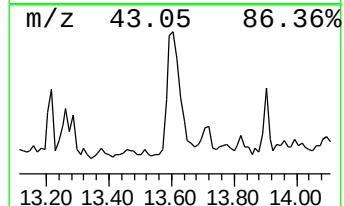
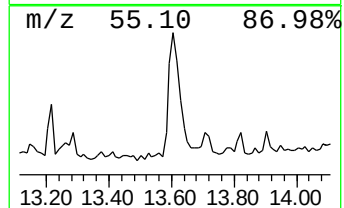
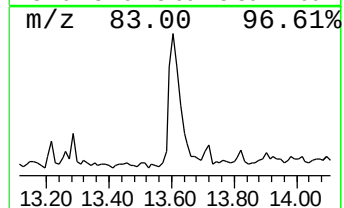
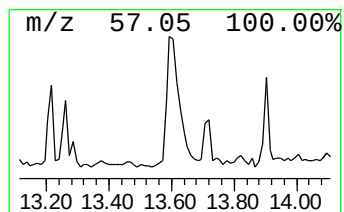
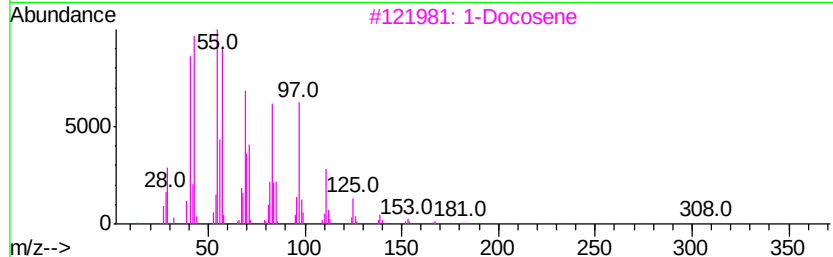
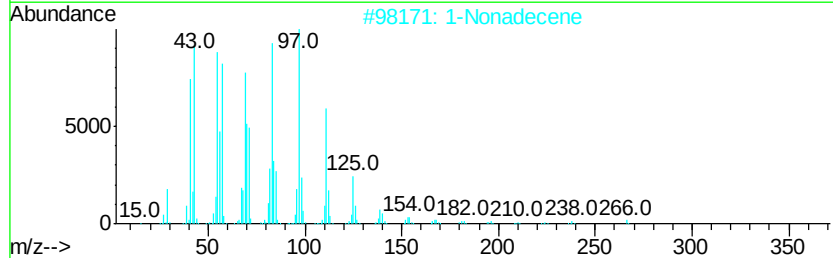
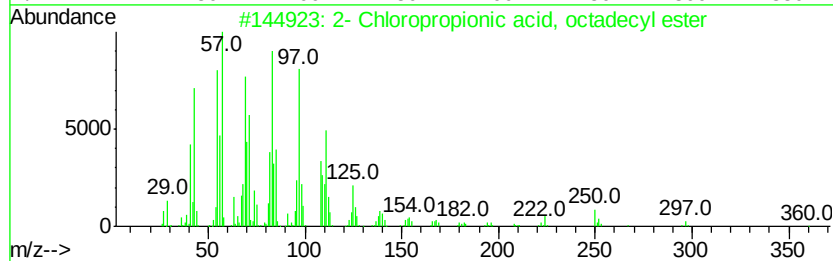
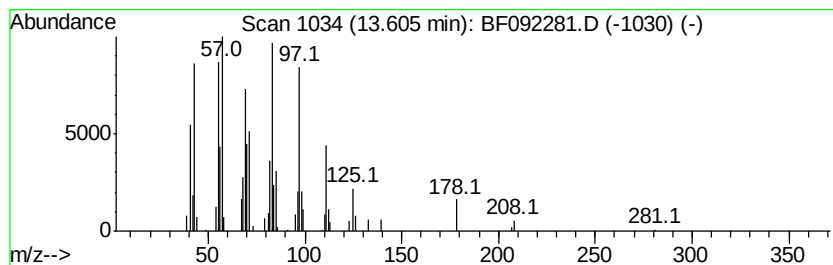
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	3.38 ng	209712	Chrysene-d12	13.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-		Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	1-		Nonadecene	266	C19H38	018435-45-5	91
3	1-		Docosene	308	C22H44	001599-67-3	91
4			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81



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Misc :
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Instrument :
BNA_F
ClientSampleId :
SB-09-COMP

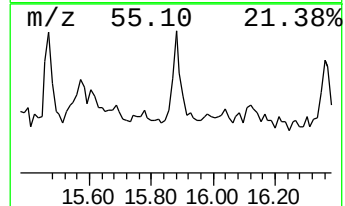
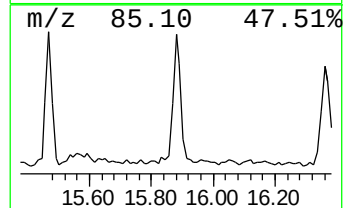
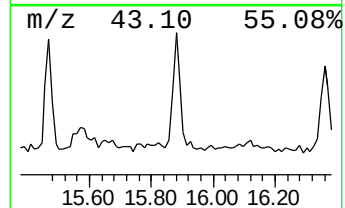
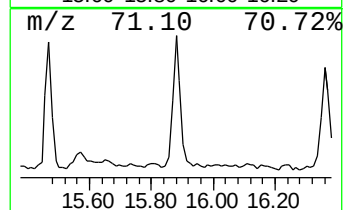
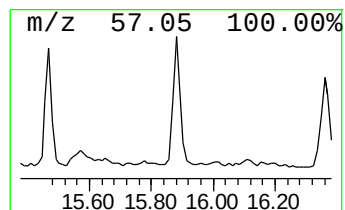
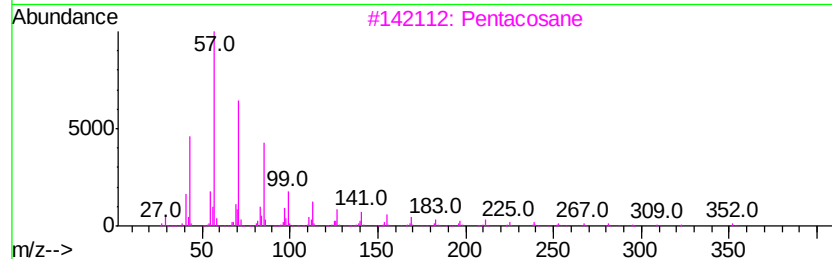
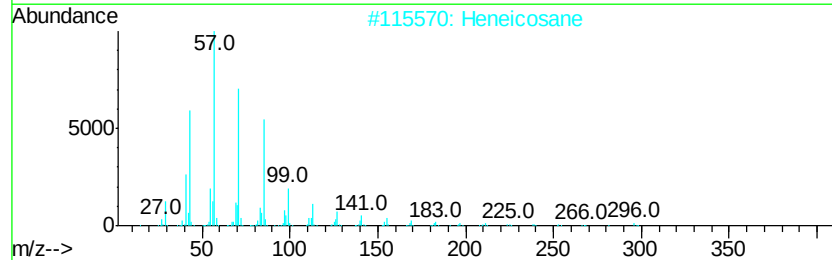
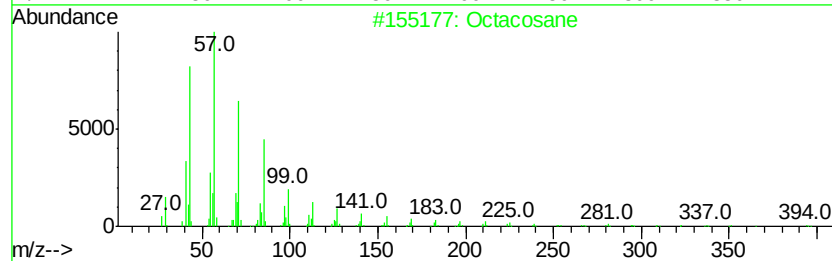
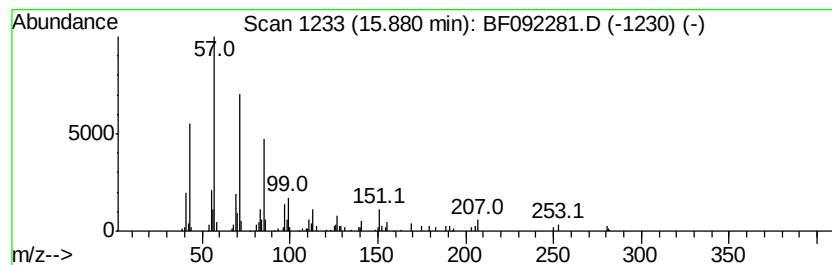
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.33 ng	160195	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Hentriacontane	437	C31H64	000630-04-6	83
5		Triacontane	422	C30H62	000638-68-6	83



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Acq On : 14 Jan 2017 13:23
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Sample : I1162-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

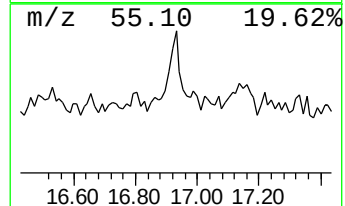
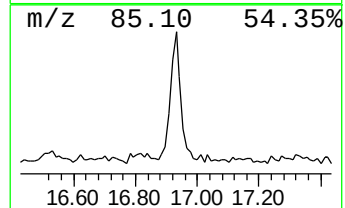
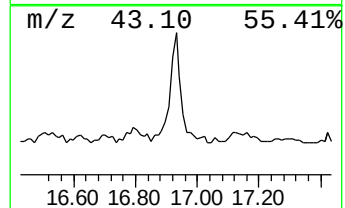
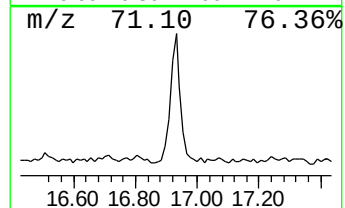
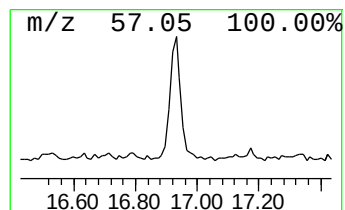
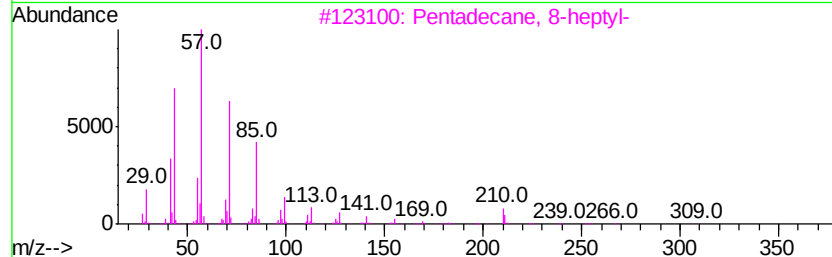
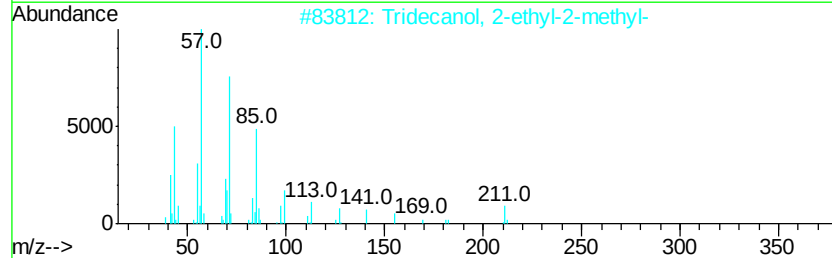
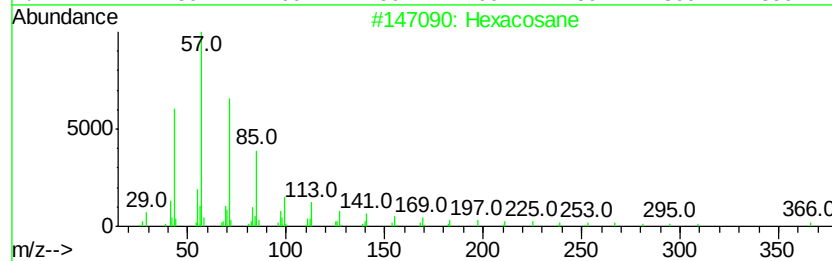
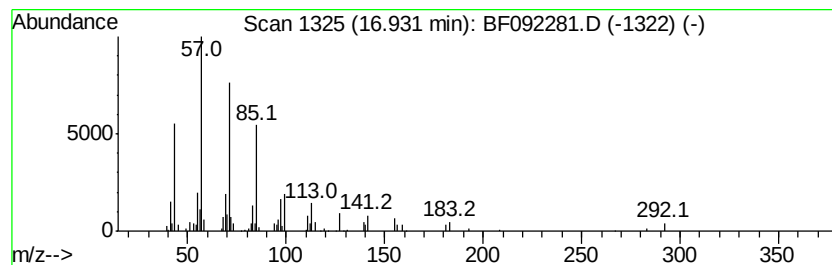
Instrument :
BNA_F
ClientSampleId :
SB-09-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	2.19 ng	105238	Perylene-d12	15.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane		366 C26H54	000630-01-3 91
2	Tridecanol, 2-ethyl-2-methyl-		242 C16H34O	1000115-66-1 86
3	Pentadecane, 8-heptyl-		310 C22H46	071005-15-7 86
4	Octadecane, 1-iodo-		380 C18H37I	000629-93-6 86
5	Pentacosane		352 C25H52	000629-99-2 86



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Operator : UM/SJ
Sample : I1162-16
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-09-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.70	35.5	ng	2344700	1	6.58	1321790	20.0
unknown6.35	6.35	72.9	ng	4817600	1	6.58	1321790	20.0
Heneicosane	10.06	2.4	ng	188810	3	9.60	1565520	20.0
Eicosane	10.53	2.6	ng	171142	4	11.09	1306750	20.0
unknown12.51	12.51	3.3	ng	207393	5	13.71	1241060	20.0
2- Chloropropioni...	13.61	3.4	ng	209712	5	13.71	1241060	20.0
Octacosane	15.88	3.3	ng	160195	6	15.07	960911	20.0
Hexacosane	16.93	2.2	ng	105238	6	15.07	960911	20.0