

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122216\
 Data File : BF091879.D
 Acq On : 22 Dec 2016 12:07
 Operator : UM/SJ
 Sample : H5943-01
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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	4.933	246	249	257	rBV	2350483	3961731	42.42%	4.838%
2	5.367	284	287	289	rBV	6547741	8953825	95.87%	10.934%
3	6.407	374	378	380	rBV	6308842	9337526	99.98%	11.403%
4	6.522	385	388	390	rBV	7405859	8084517	86.56%	9.873%
5	6.750	405	408	410	rBV	1206475	1633775	17.49%	1.995%
6	6.899	419	421	424	rVB	5129385	6429150	68.84%	7.851%
7	7.310	454	457	460	rBV	3822034	5593987	59.90%	6.831%
8	8.030	517	520	522	rBV	2293196	2232948	23.91%	2.727%
9	9.116	611	615	617	rBV	5996725	9339513	100.00%	11.405%
10	9.505	646	649	652	rBV	941452	879634	9.42%	1.074%
11	9.779	670	673	676	rBV	2603837	2589144	27.72%	3.162%
12	10.191	707	709	710	rBV	113547	151137	1.62%	0.185%
13	10.225	710	712	713	rVB	184737	206229	2.21%	0.252%
14	10.442	728	731	734	rBV	116532	156904	1.68%	0.192%
15	10.568	739	742	745	rBV2	3699841	5214508	55.83%	6.368%
16	10.693	751	753	758	rVB	309887	398533	4.27%	0.487%
17	11.139	790	792	793	rBV	193843	165393	1.77%	0.202%
18	11.265	800	803	805	rBV	2288352	2432495	26.05%	2.971%
19	11.802	848	850	855	rBV2	317548	446450	4.78%	0.545%
20	12.682	925	927	929	rVB	221443	212105	2.27%	0.259%
21	12.854	939	942	944	rBV	6855698	7416844	79.41%	9.057%
22	13.379	986	988	990	rBV2	142188	186057	1.99%	0.227%
23	13.757	1018	1021	1029	rBV	339757	482433	5.17%	0.589%
24	13.894	1030	1033	1035	rBV	2271119	2124441	22.75%	2.594%
25	14.374	1071	1075	1081	rBV2	52210	125048	1.34%	0.153%
26	14.671	1097	1101	1103	rBV2	85808	139448	1.49%	0.170%
27	14.740	1105	1107	1110	rVB	275511	257970	2.76%	0.315%
28	14.980	1126	1128	1131	rBV	90779	106546	1.14%	0.130%
29	15.288	1152	1155	1157	rBV	1303324	1672026	17.90%	2.042%
30	15.334	1157	1159	1162	rVB	100823	154973	1.66%	0.189%
31	15.723	1190	1193	1196	rBV	112197	176187	1.89%	0.215%
32	16.180	1230	1233	1241	rVB	116984	205948	2.21%	0.252%
33	16.717	1276	1280	1284	rBV	76381	162056	1.74%	0.198%
34	17.346	1331	1335	1340	rVB	59423	155734	1.67%	0.190%

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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	18.089	1395	1400	1404	rBV	37548	101890	1.09%	0.124%
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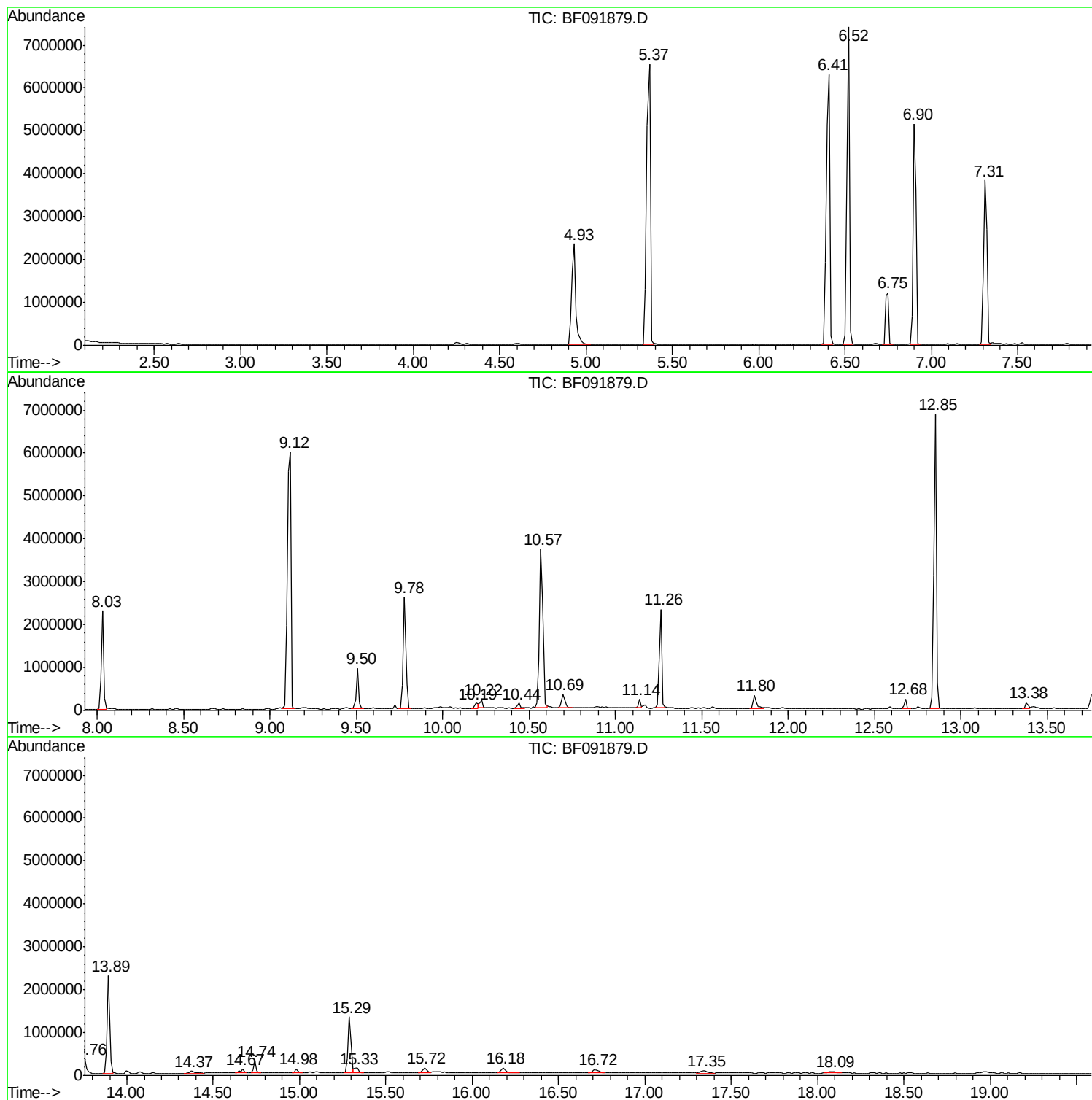
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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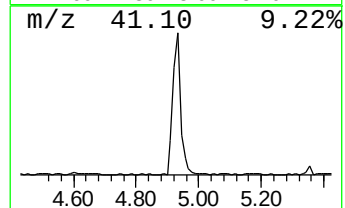
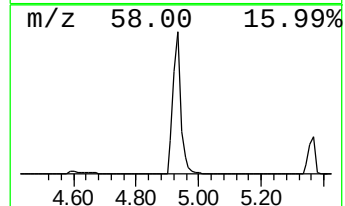
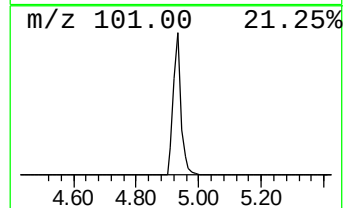
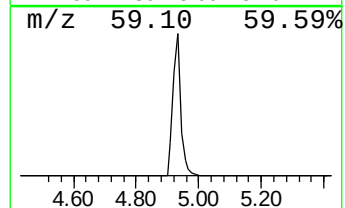
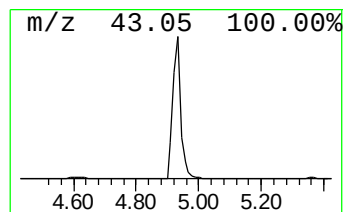
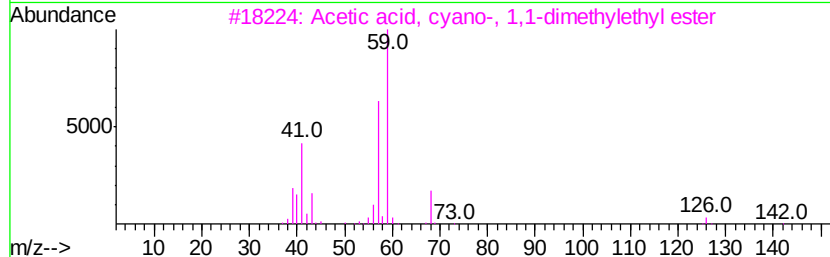
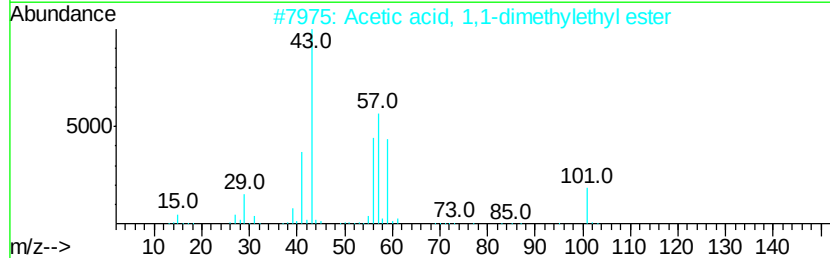
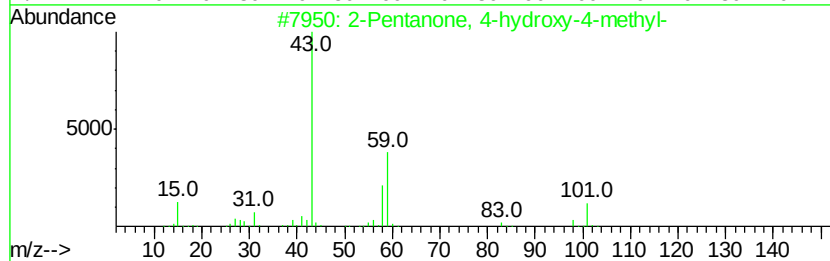
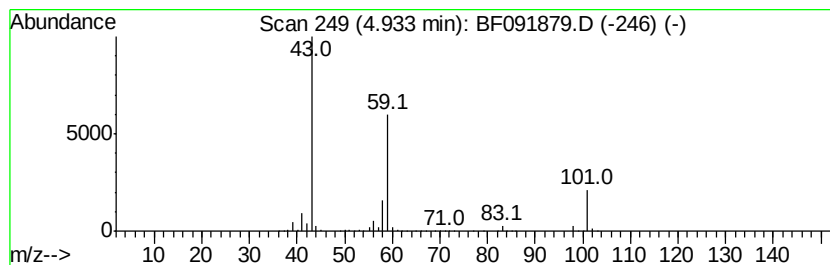
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	48.50 ng	3961730	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	72
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	23
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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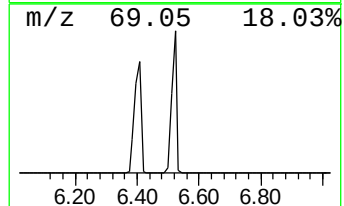
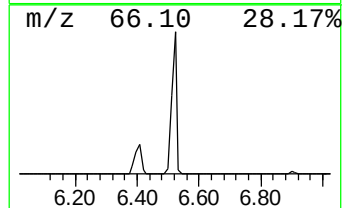
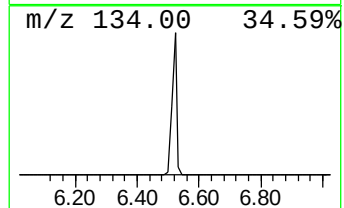
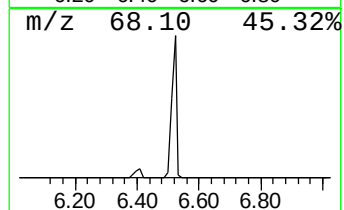
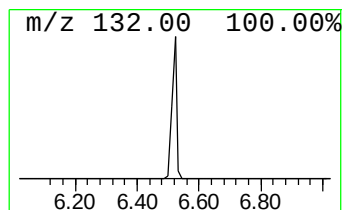
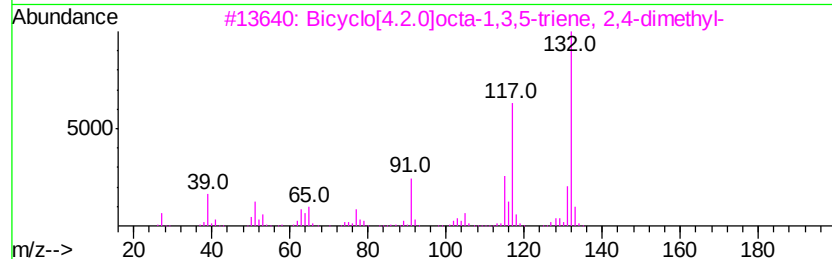
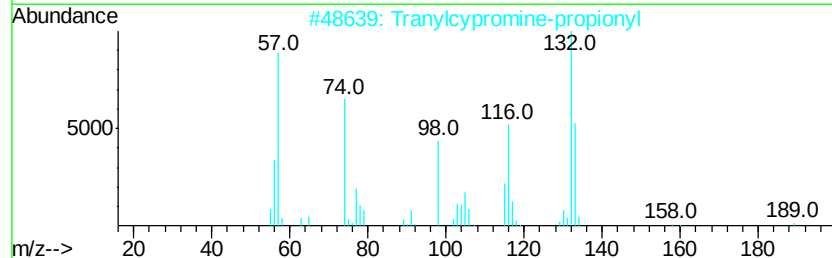
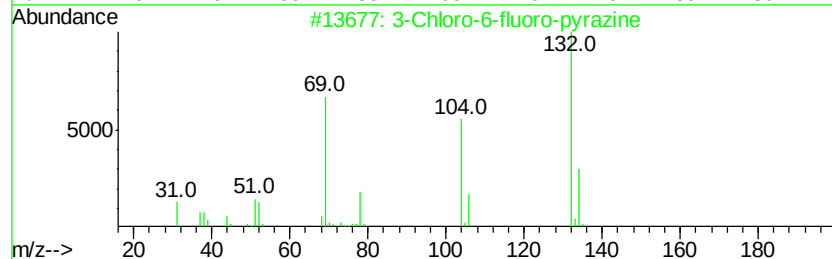
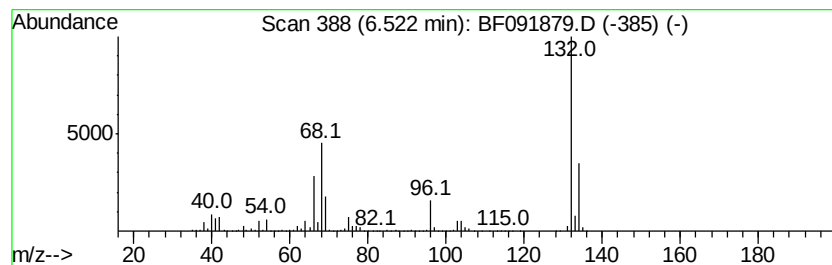
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	98.97 ng	8084520	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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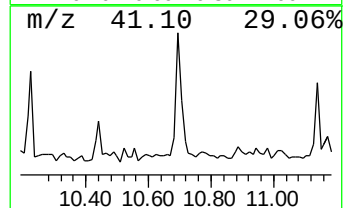
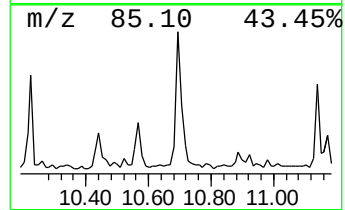
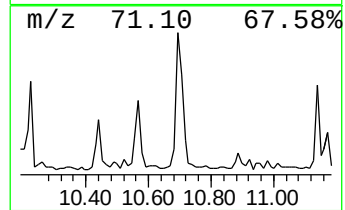
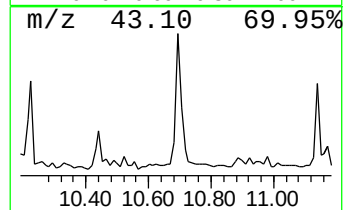
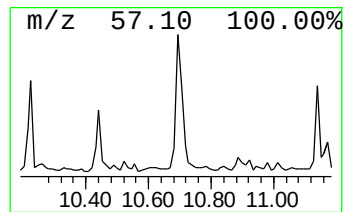
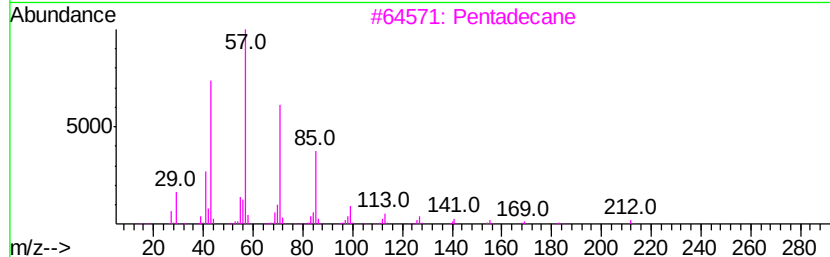
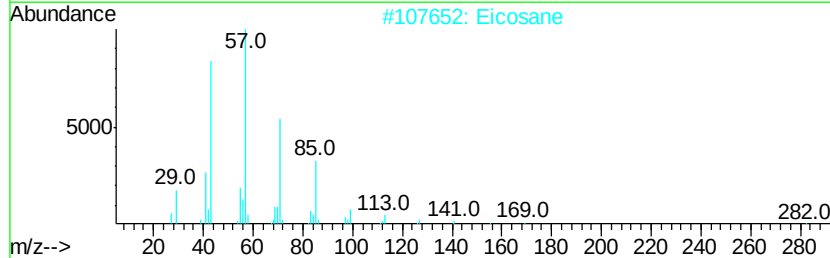
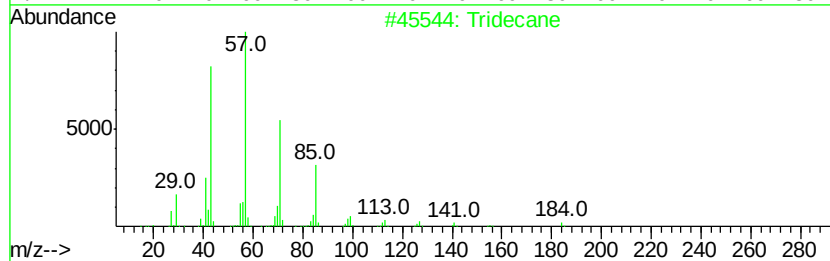
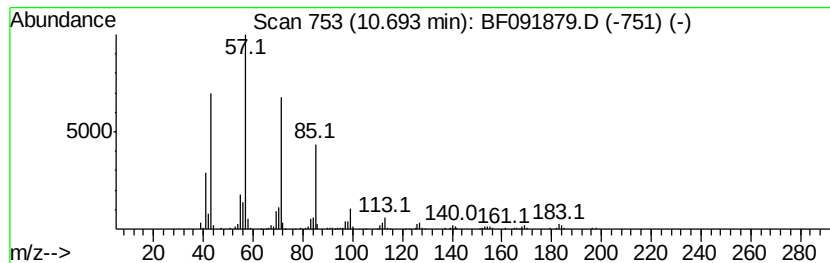
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.69	3.28 ng	398533	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Eicosane	282	C20H42	000112-95-8	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetradecane	198	C14H30	000629-59-4	86



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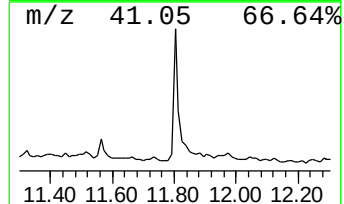
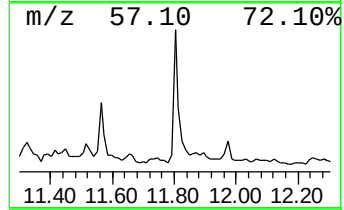
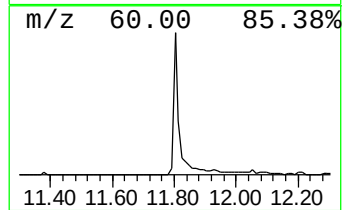
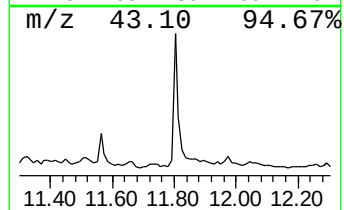
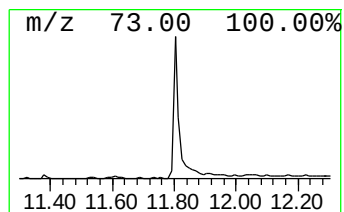
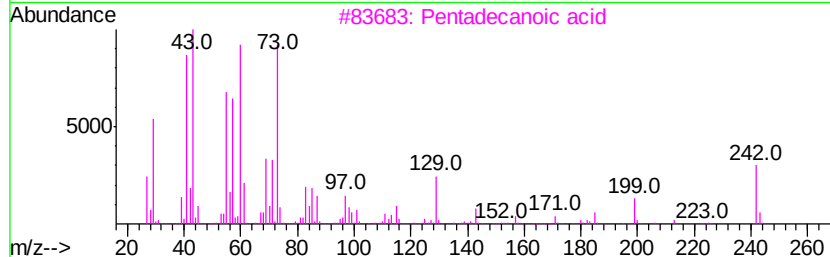
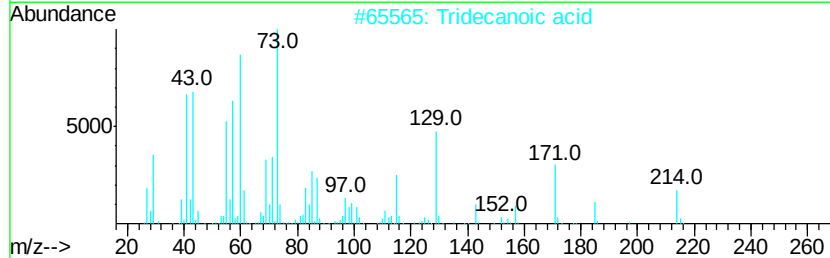
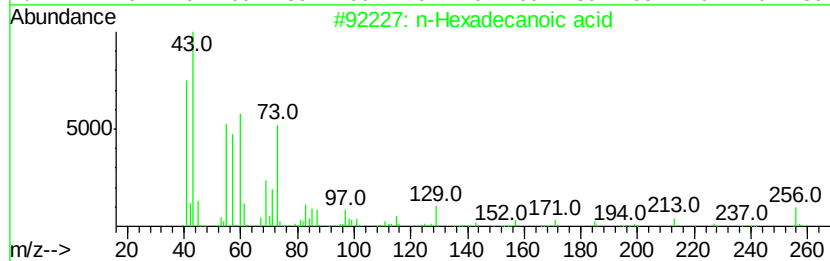
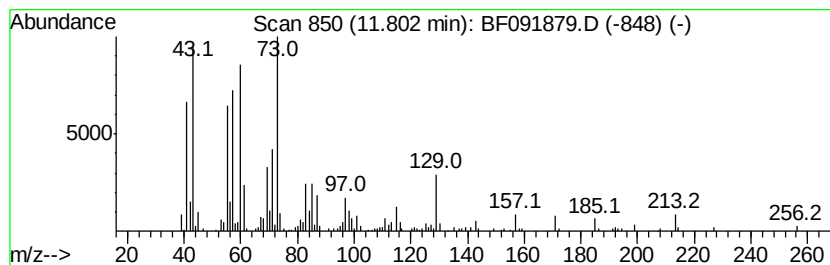
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.80	3.67 ng	446450	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47



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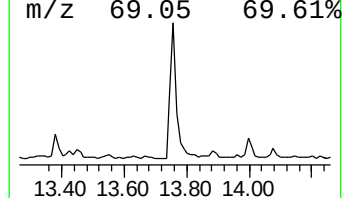
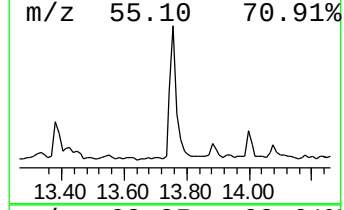
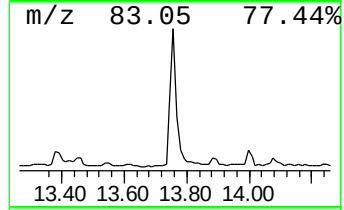
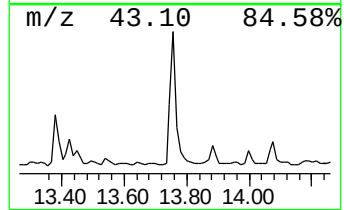
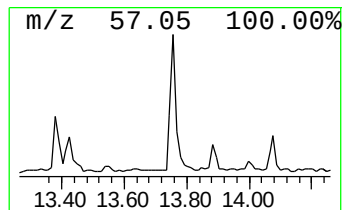
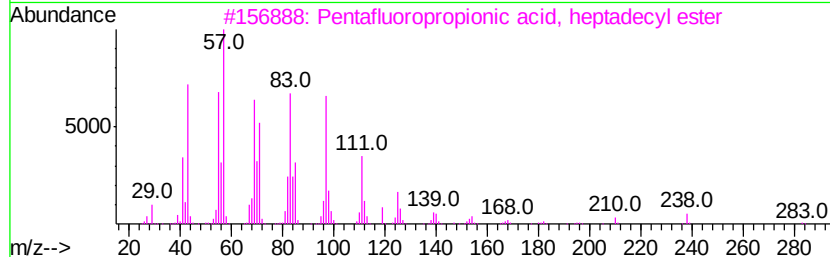
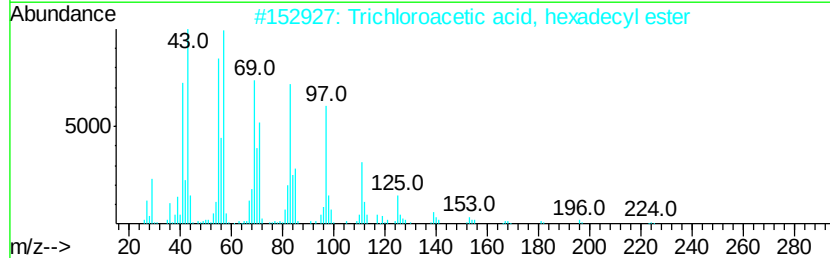
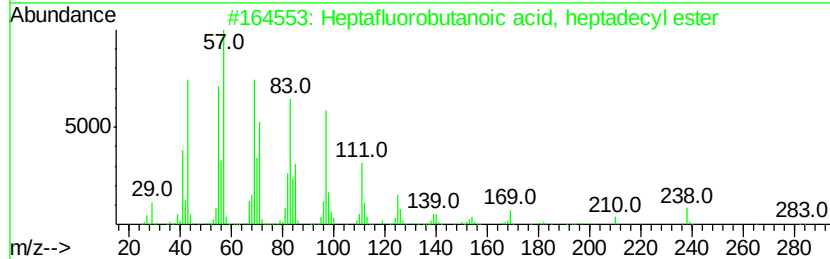
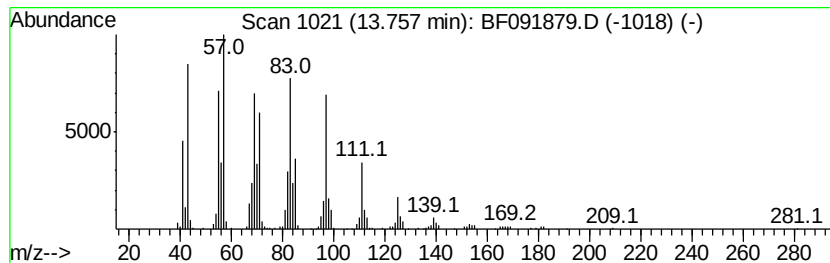
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.54 ng	482433	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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ALS Vial : 49 Sample Multiplier: 1

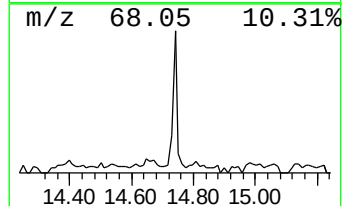
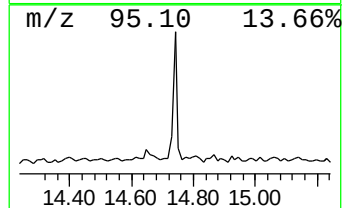
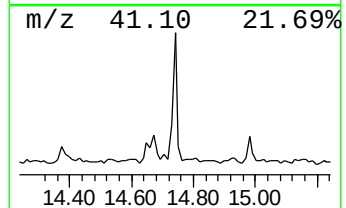
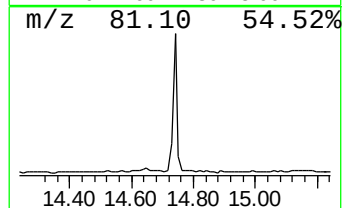
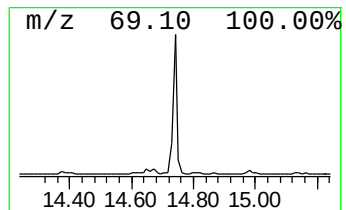
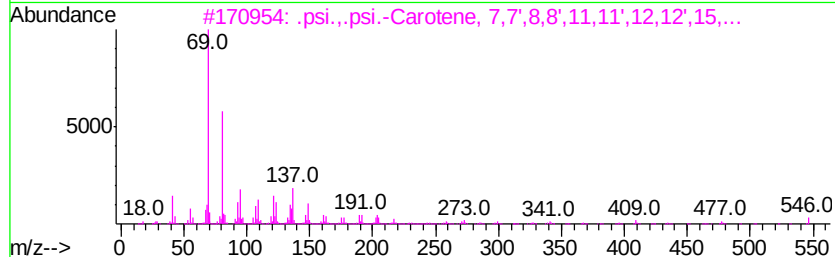
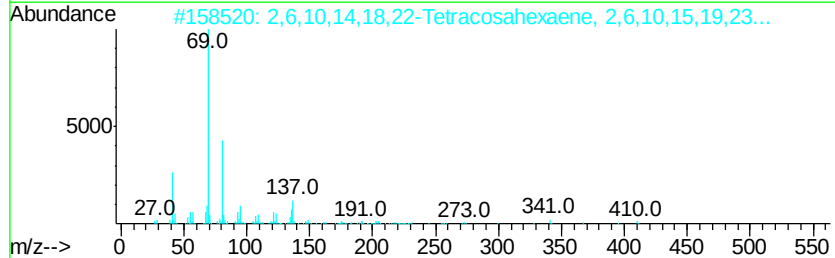
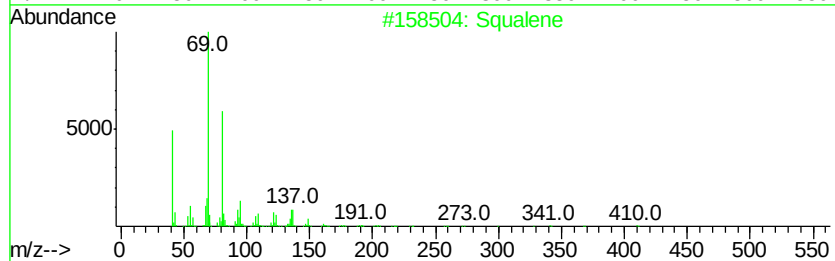
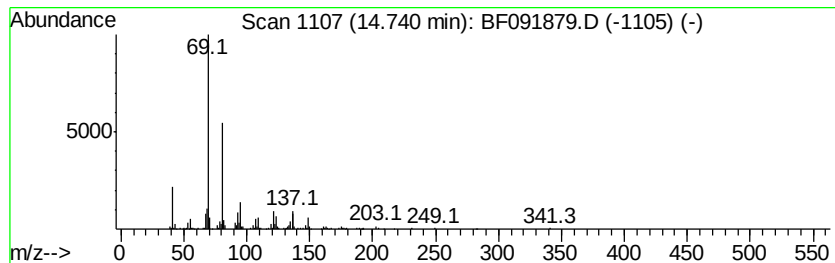
Instrument :
BNA_F
ClientSampleId :
MW-1

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 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.74	3.09 ng	257970	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122216\
Data File : BF091879.D
Acq On : 22 Dec 2016 12:07
Operator : UM/SJ
Sample : H5943-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

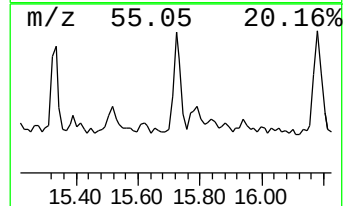
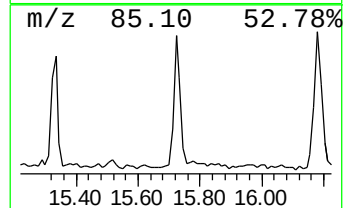
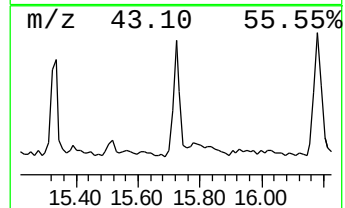
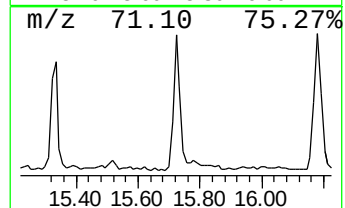
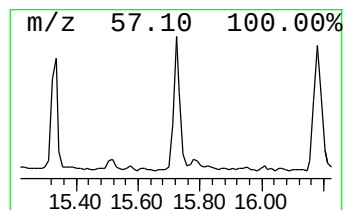
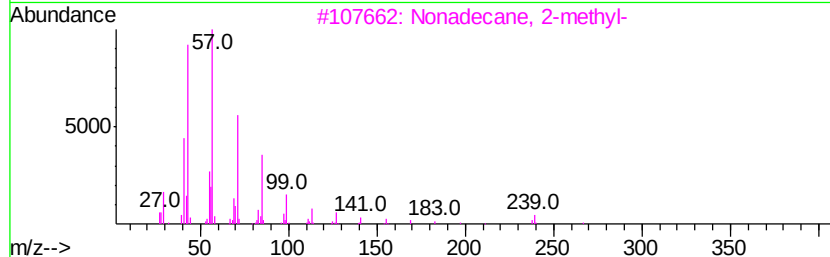
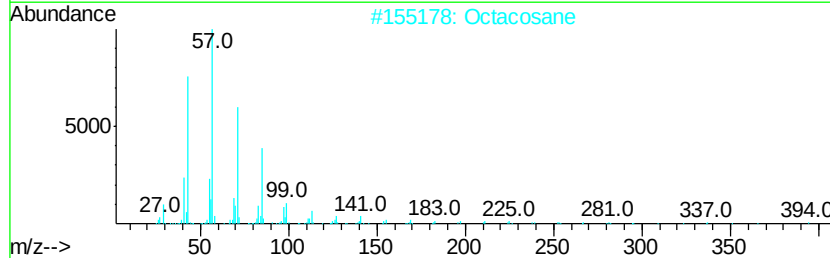
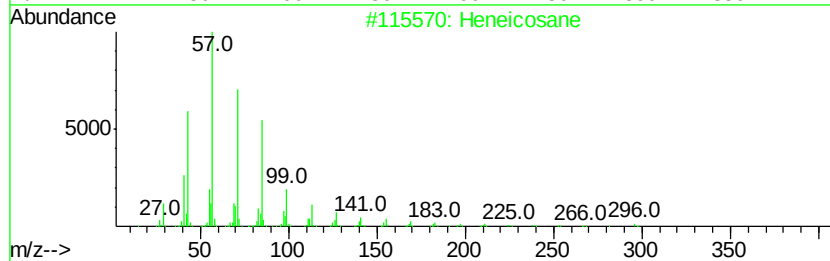
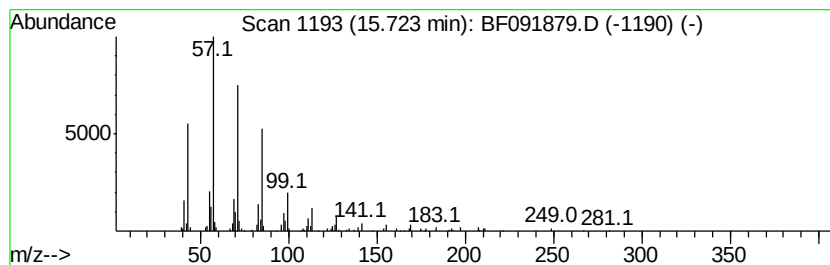
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.11 ng	176187	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	90
3	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	90
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
5	Tetracosane		338	C24H50	000646-31-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122216\
Data File : BF091879.D
Acq On : 22 Dec 2016 12:07
Operator : UM/SJ
Sample : H5943-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

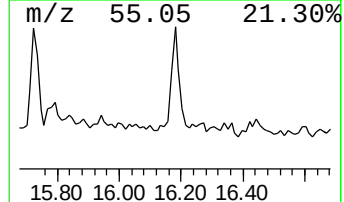
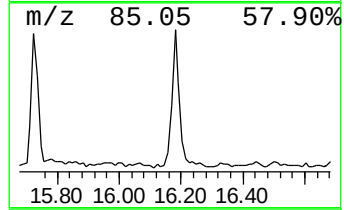
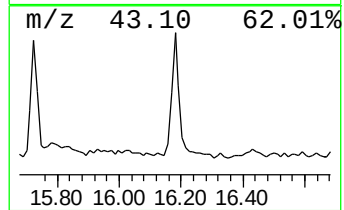
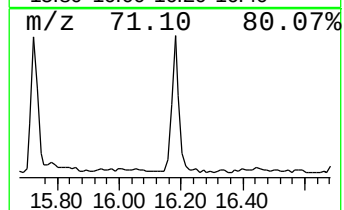
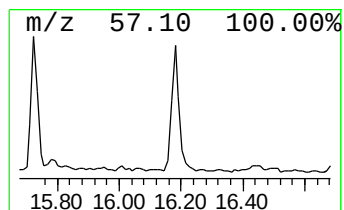
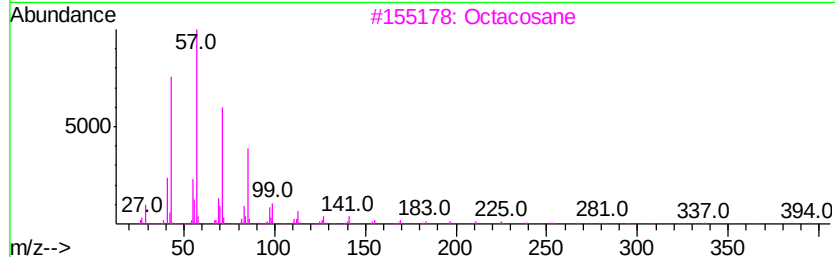
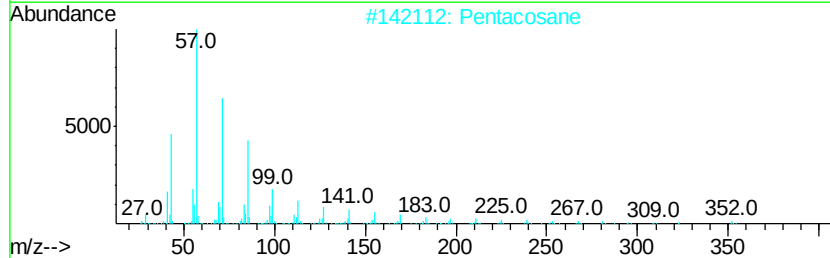
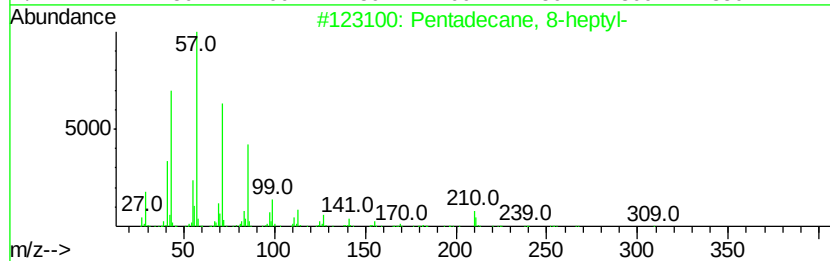
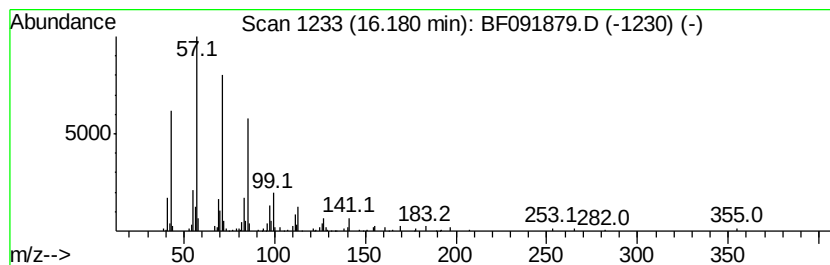
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.46 ng	205948	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
2		Pentacosane	352	C25H52	000629-99-2	90
3		Octacosane	394	C28H58	000630-02-4	87
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122216\
Data File : BF091879.D
Acq On : 22 Dec 2016 12:07
Operator : UM/SJ
Sample : H5943-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

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...	4.93	48.5	ng	3961730	1	6.75	1633780	20.0
unknown6.52	6.52	99.0	ng	8084520	1	6.75	1633780	20.0
Tridecane	10.69	3.3	ng	398533	4	11.27	2432500	20.0
n-Hexadecanoic acid	11.80	3.7	ng	446450	4	11.27	2432500	20.0
Heptafluorobutano...	13.76	4.5	ng	482433	5	13.89	2124440	20.0
Squalene	14.74	3.1	ng	257970	6	15.29	1672030	20.0
Heneicosane	15.72	2.1	ng	176187	6	15.29	1672030	20.0
Pentadecane, 8-he...	16.18	2.5	ng	205948	6	15.29	1672030	20.0