

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
 Data File : BF092903.D
 Acq On : 11 Feb 2017 00:29
 Operator : SJ/MA
 Sample : I1777-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38-SB-02-0-2

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-BF013017.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	259	262	271	rBV	1379724	1923940	36.76%	4.232%
2	5.504	296	299	301	rBV	3798362	4272502	81.64%	9.399%
3	6.533	386	389	392	rBV	3288767	4059688	77.57%	8.930%
4	6.670	398	401	403	rBV	3391650	4434006	84.73%	9.754%
5	6.899	418	421	423	rBV	766095	1047074	20.01%	2.303%
6	7.047	432	434	437	rBV	2757462	3224110	61.61%	7.092%
7	7.459	467	470	472	rBV	2017611	2895144	55.32%	6.369%
8	8.179	531	533	536	rBV	1335634	1441773	27.55%	3.172%
9	9.265	624	628	630	rBV	4405039	5233265	100.00%	11.512%
10	9.333	632	634	643	rVB3	30679	75851	1.45%	0.167%
11	9.653	660	662	664	rBV	823693	710091	13.57%	1.562%
12	9.871	677	681	683	rBV	65136	114696	2.19%	0.252%
13	9.939	684	687	689	rBV	1787883	1773216	33.88%	3.901%
14	10.362	723	724	726	rVB	181397	147900	2.83%	0.325%
15	10.579	740	743	747	rBV	56397	97270	1.86%	0.214%
16	10.728	753	756	758	rBV	2377594	2500477	47.78%	5.501%
17	10.831	764	765	770	rVB	158999	257443	4.92%	0.566%
18	11.025	780	782	787	rBV	32649	62000	1.18%	0.136%
19	11.288	802	805	806	rBV	92049	129999	2.48%	0.286%
20	11.425	814	817	819	rBV	1222387	1721086	32.89%	3.786%
21	11.711	840	842	844	rBV	62636	55099	1.05%	0.121%
22	12.031	868	870	874	rVB2	40137	65444	1.25%	0.144%
23	12.625	920	922	925	rVB	246540	265896	5.08%	0.585%
24	12.854	938	942	945	rBV	246738	333617	6.37%	0.734%
25	13.002	952	955	958	rBV	2968664	4005106	76.53%	8.810%
26	13.185	968	971	973	rBV	35890	60730	1.16%	0.134%
27	13.894	1032	1033	1038	rVB2	147235	220414	4.21%	0.485%
28	14.054	1044	1047	1054	rVB	1246829	1527120	29.18%	3.359%
29	14.214	1059	1061	1065	rBV3	21017	55037	1.05%	0.121%
30	14.522	1085	1088	1090	rBV3	42151	77635	1.48%	0.171%
31	14.820	1112	1114	1119	rVB	53092	89153	1.70%	0.196%
32	14.900	1119	1121	1123	rBV	120191	141985	2.71%	0.312%
33	15.082	1134	1137	1141	rBV	134230	256451	4.90%	0.564%
34	15.151	1141	1143	1145	rVB	76788	81869	1.56%	0.180%

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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-BF013017.M
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35	15.380	1161	1163	1166	rVB	86328	107918	2.06%	0.237%
36	15.437	1166	1168	1171	rVV	104449	138955	2.66%	0.306%
37	15.505	1171	1174	1184	rVB	744356	1141698	21.82%	2.511%
38	15.940	1209	1212	1216	rBV	84834	157751	3.01%	0.347%
39	16.431	1252	1255	1260	rBV	69609	133785	2.56%	0.294%
40	16.934	1295	1299	1302	rVV2	48470	98276	1.88%	0.216%
41	17.003	1302	1305	1309	rVB	47619	100992	1.93%	0.222%
42	17.357	1333	1336	1340	rBV	38835	76456	1.46%	0.168%
43	17.688	1361	1365	1370	rVB	33389	86714	1.66%	0.191%
44	18.489	1432	1435	1440	rVB5	21344	59344	1.13%	0.131%

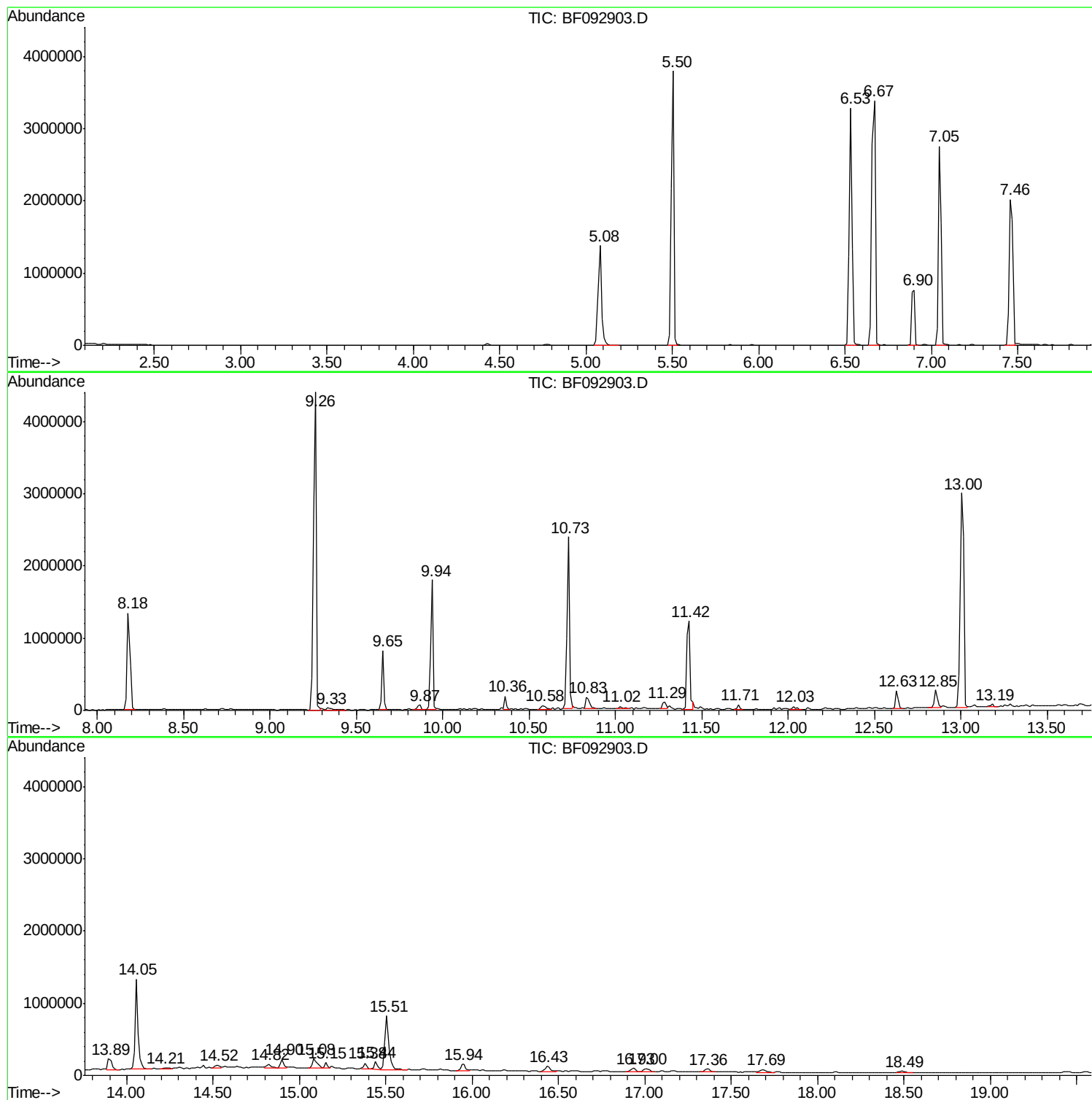
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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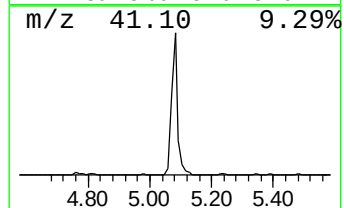
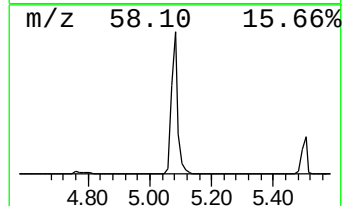
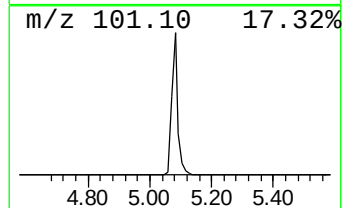
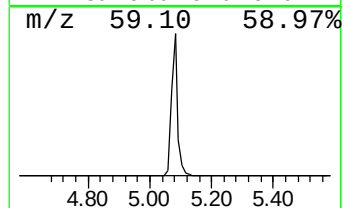
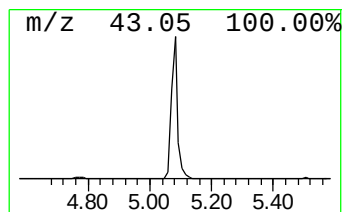
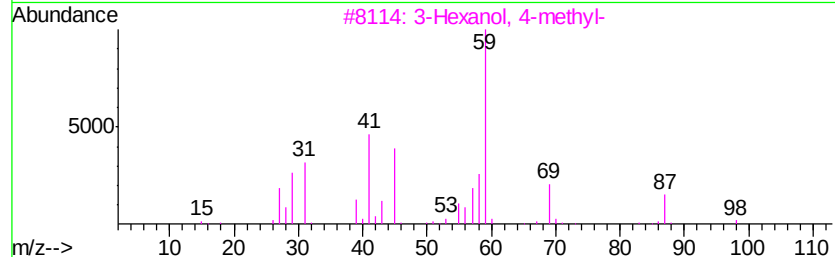
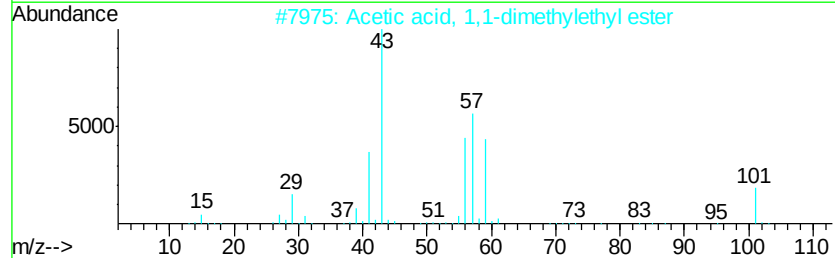
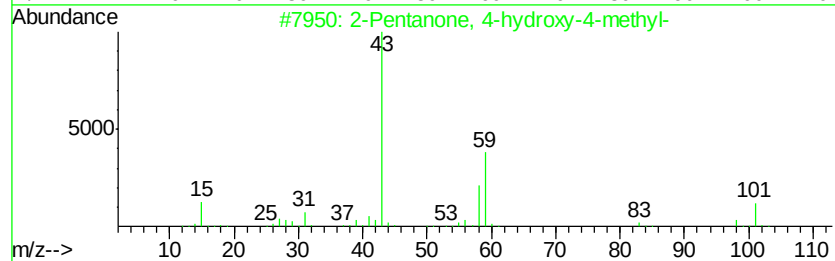
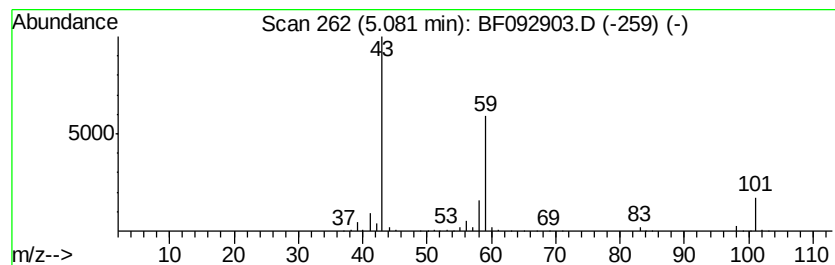
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.08	36.75 ng	1923940	1,4-Dichlorobenzene-d4	6.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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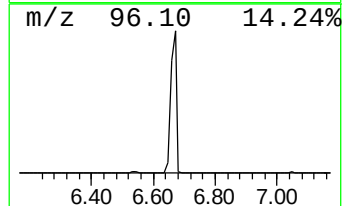
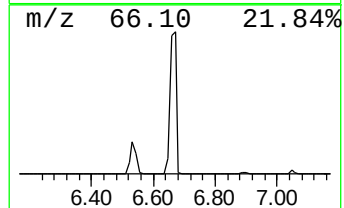
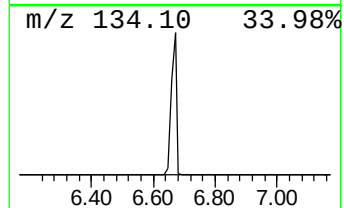
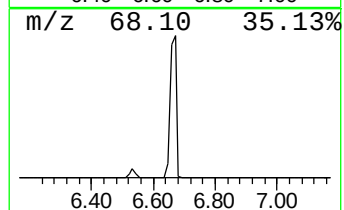
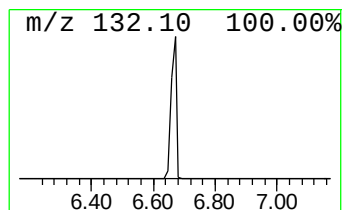
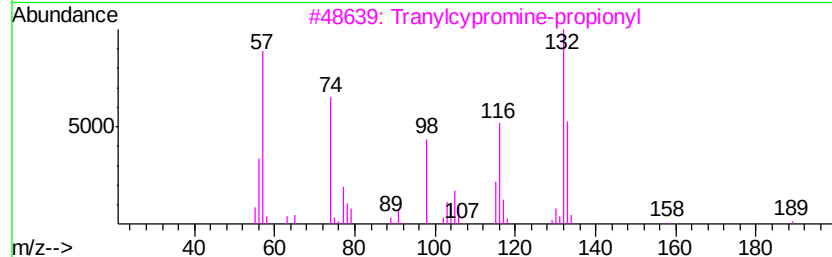
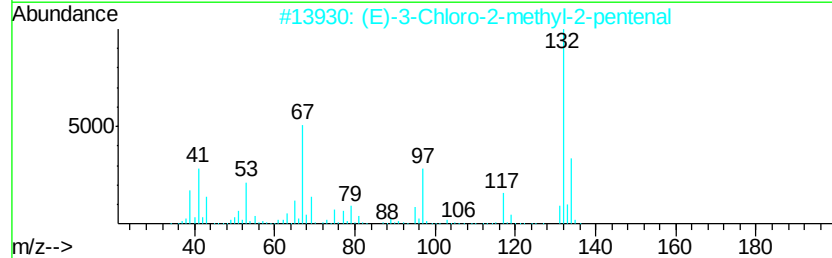
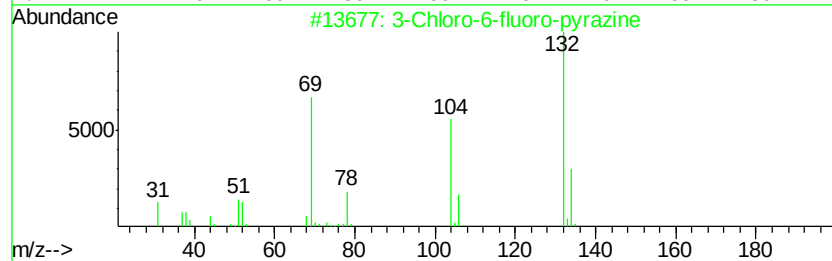
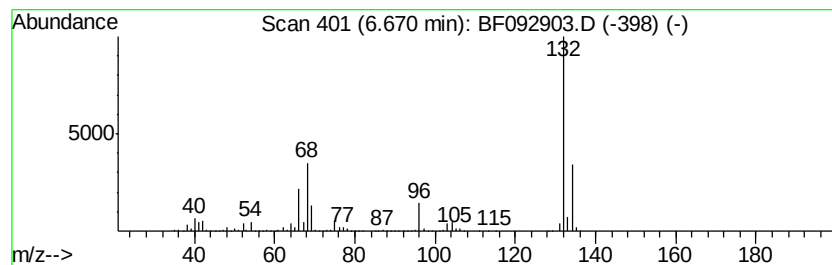
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	84.69 ng	4434010	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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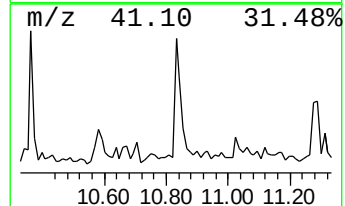
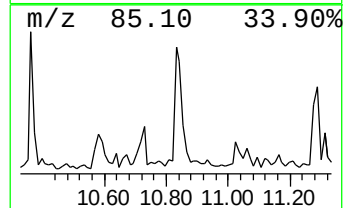
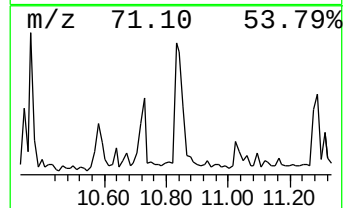
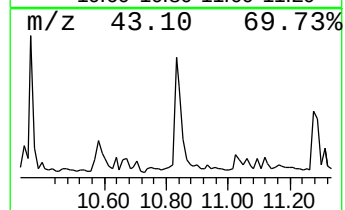
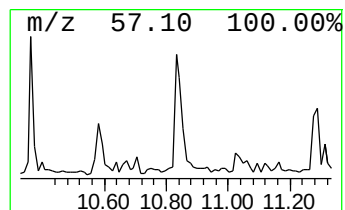
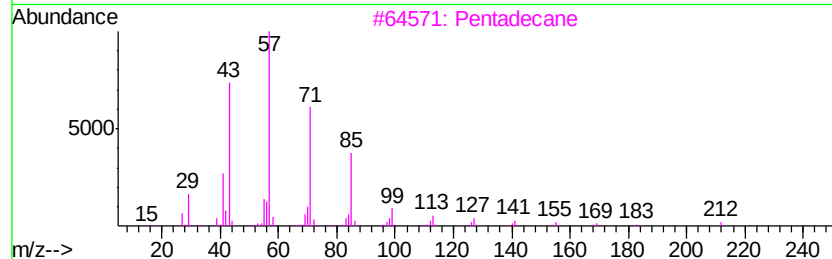
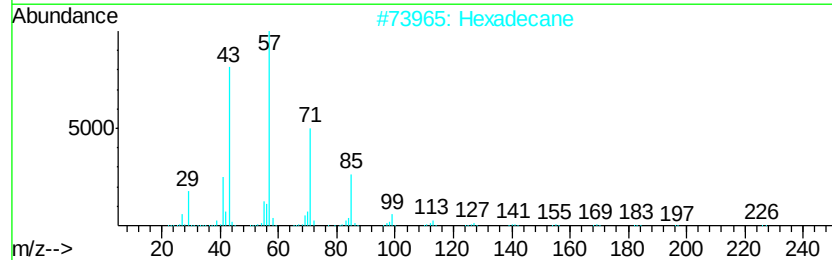
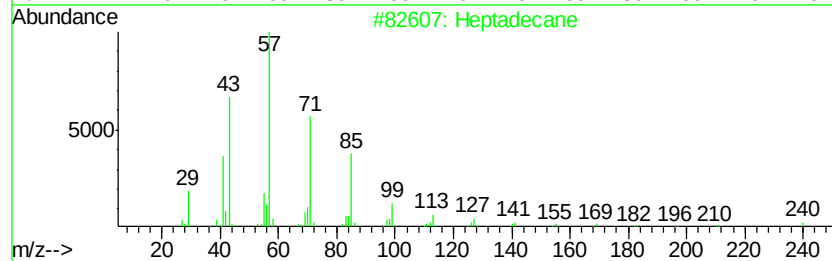
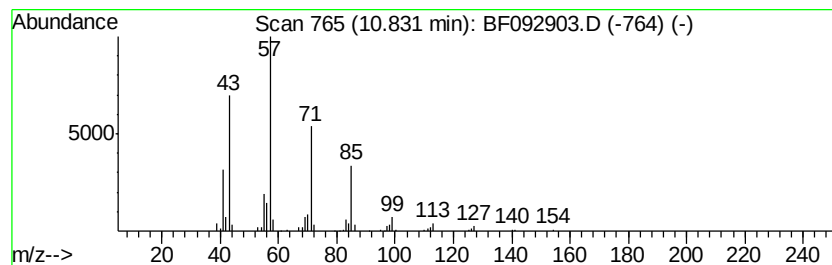
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.83	2.99 ng	257443	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Pentadecane		212	C15H32	000629-62-9	78
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	72
5	Pentadecane, 7-methyl-		226	C16H34	006165-40-8	72



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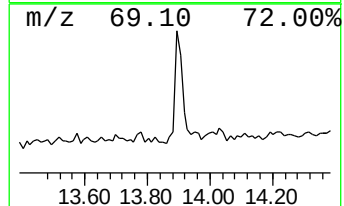
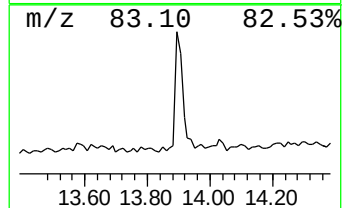
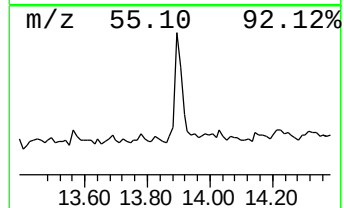
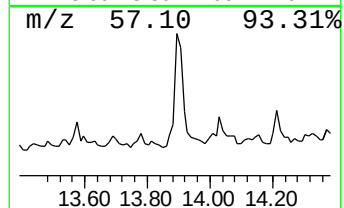
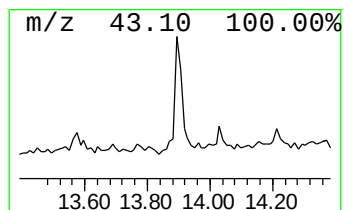
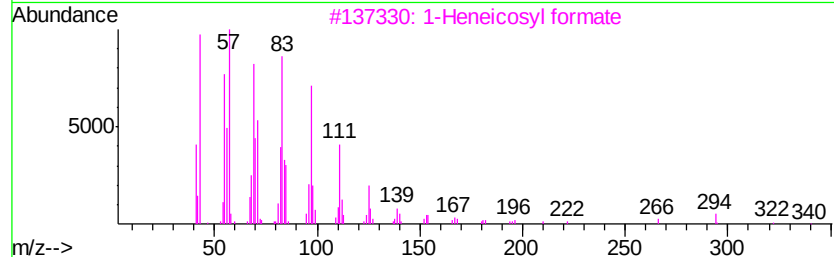
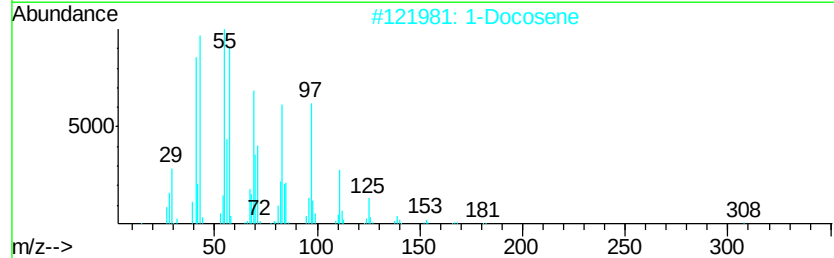
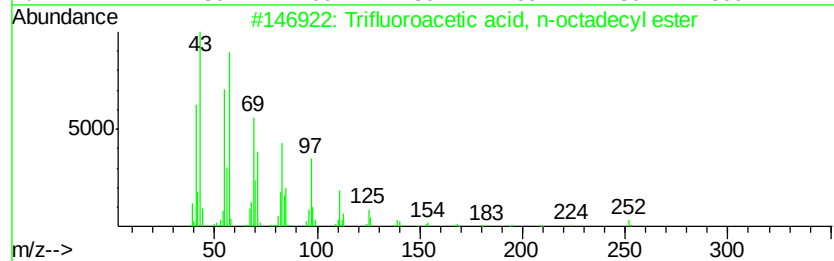
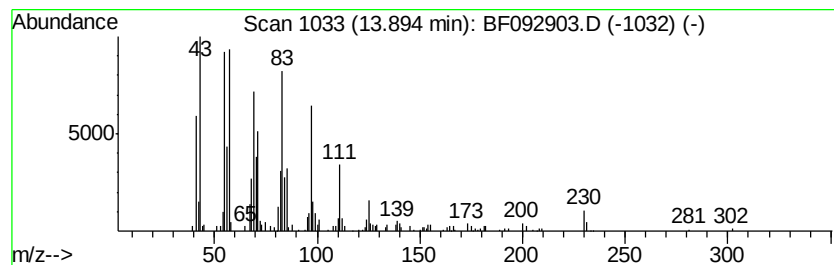
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetic acid, n-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.89 ng	220414	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	87



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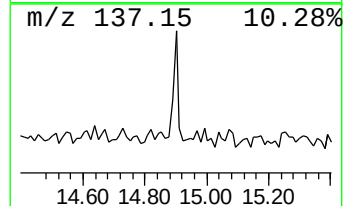
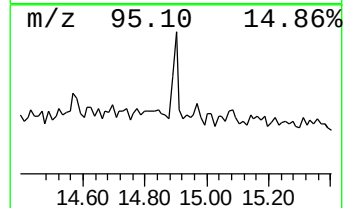
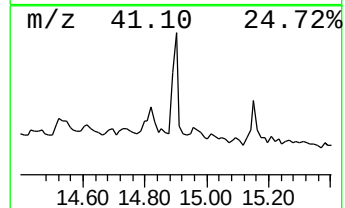
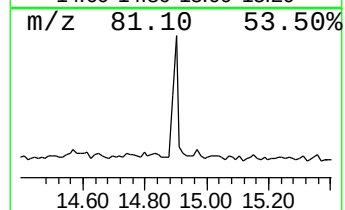
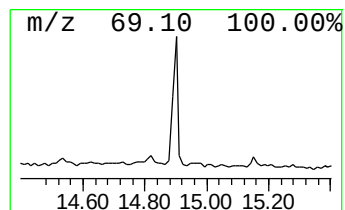
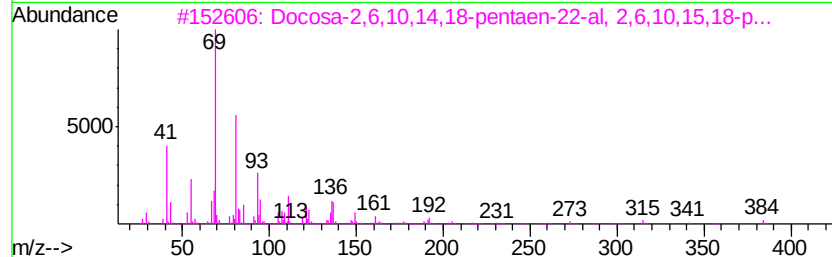
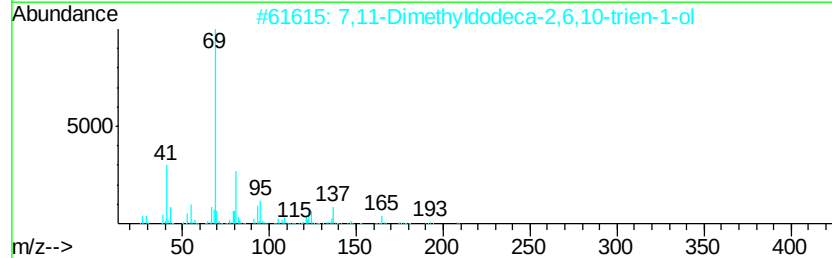
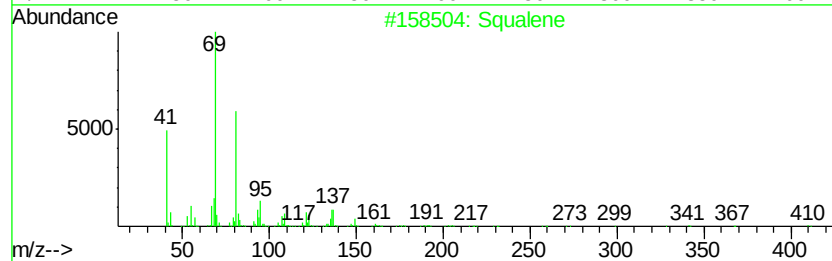
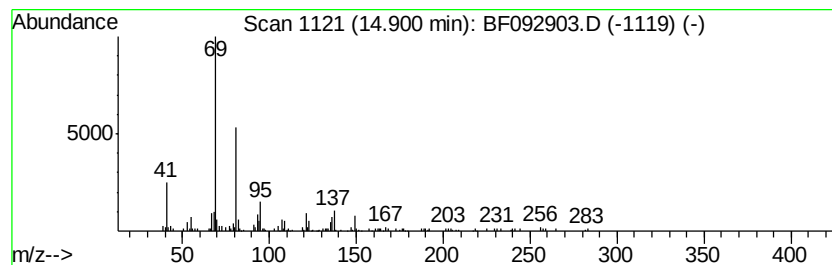
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Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.49 ng	141985	Perylene-d12	15.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 87
2	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H24O	125529-10-4 64
3	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...		264 C17H28O2	004128-17-0 53
5	1,5-Heptadiene, 3,4-dimethyl-		124 C9H16	1000061-77-9 52



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Data File : BF092903.D
Acq On : 11 Feb 2017 00:29
Operator : SJ/MA
Sample : I1777-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-02-0-2

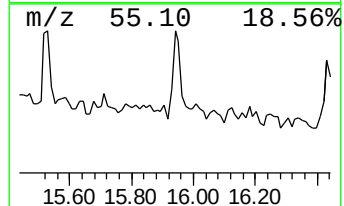
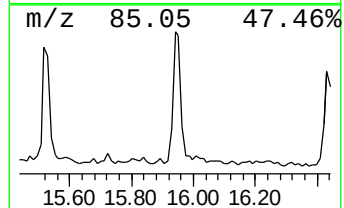
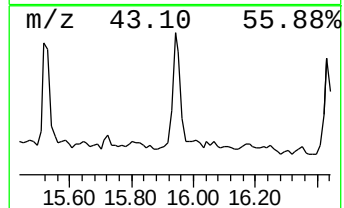
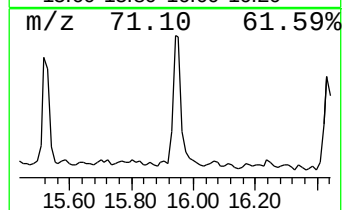
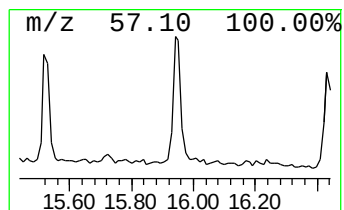
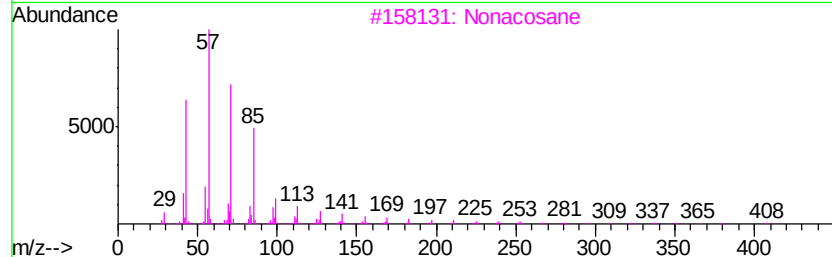
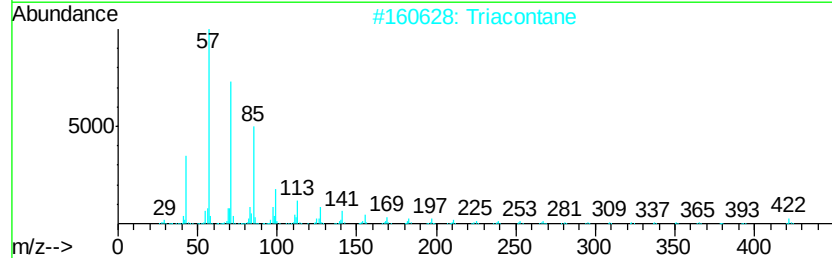
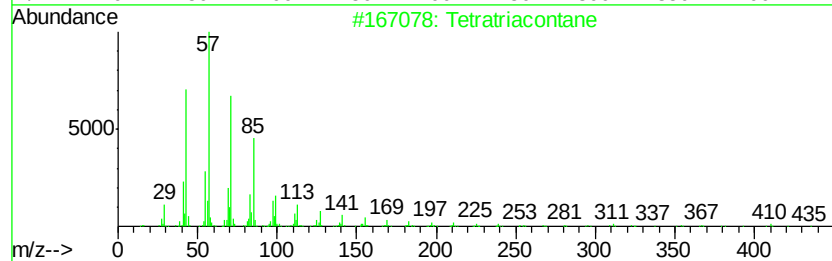
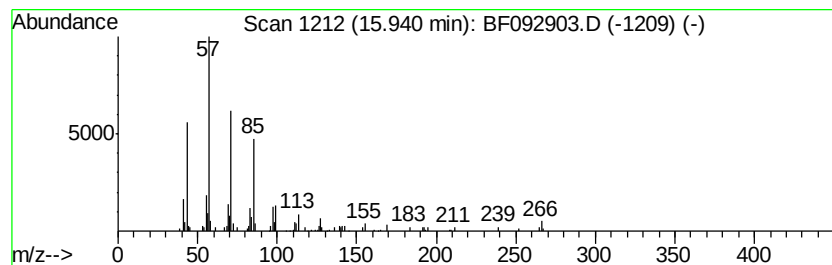
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.76 ng	157751	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontane	479	C34H70	014167-59-0	90
2		Triacontane	422	C30H62	000638-68-6	87
3		Nonacosane	408	C29H60	000630-03-5	87
4		Octacosane	394	C28H58	000630-02-4	86
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092903.D
Acq On : 11 Feb 2017 00:29
Operator : SJ/MA
Sample : I1777-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-02-0-2

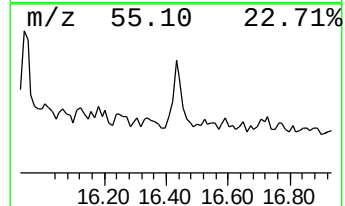
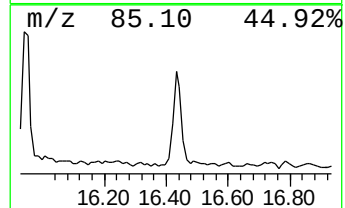
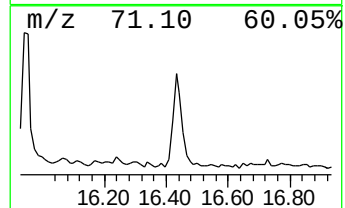
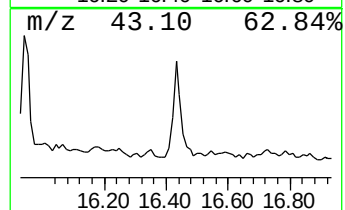
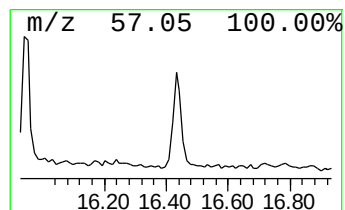
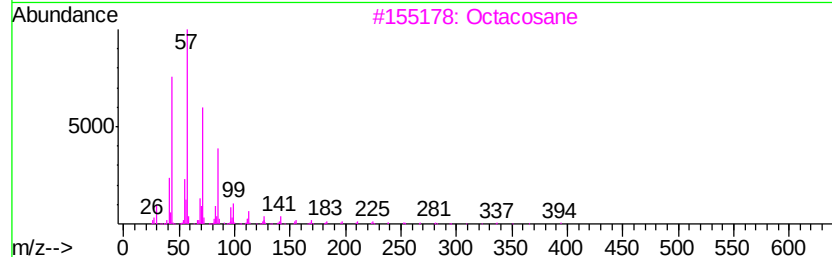
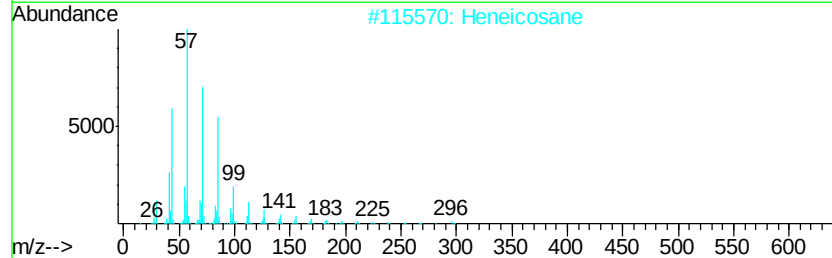
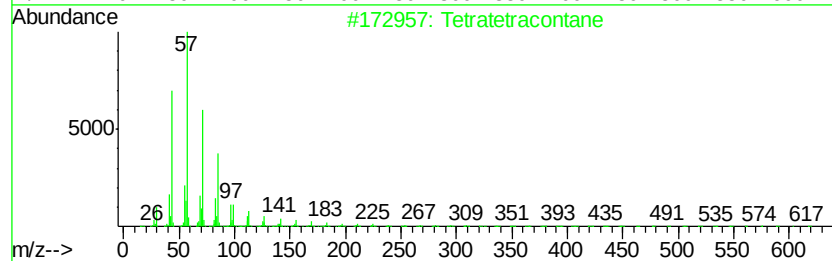
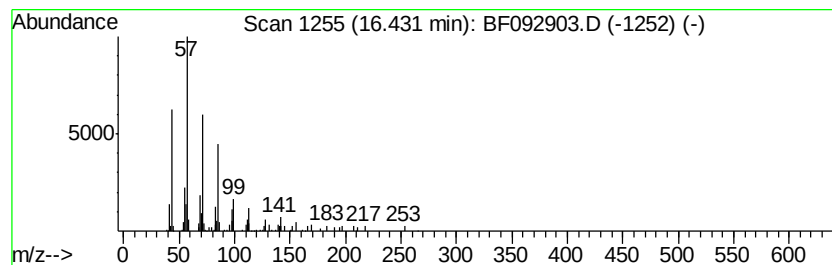
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.34 ng	133785	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092903.D
Acq On : 11 Feb 2017 00:29
Operator : SJ/MA
Sample : I1777-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-02-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	36.8	ng	1923940	1	6.90	1047070	20.0
unknown6.67	6.67	84.7	ng	4434010	1	6.90	1047070	20.0
Heptadecane	10.83	3.0	ng	257443	4	11.43	1721090	20.0
Trifluoroacetic a...	13.89	2.9	ng	220414	5	14.05	1527120	20.0
Squalene	14.90	2.5	ng	141985	6	15.51	1141700	20.0
Tetratriacontane	15.94	2.8	ng	157751	6	15.51	1141700	20.0
Tetratetracontane	16.43	2.3	ng	133785	6	15.51	1141700	20.0