

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092275.D
 Acq On : 14 Jan 2017 10:34
 Operator : UM/SJ
 Sample : I1162-04
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-45-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	269	rBV	1492564	2507916	44.85%	5.484%
2	5.170	294	296	310	rBV	4568393	5070605	90.67%	11.087%
3	6.244	387	390	397	rBV	4902374	5592392	100.00%	12.228%
4	6.347	397	399	402	rVB	5032097	4700181	84.05%	10.277%
5	6.576	417	419	421	rBV	1211798	1229912	21.99%	2.689%
6	6.725	430	432	435	rBV	2845351	3677116	65.75%	8.040%
7	7.147	466	469	471	rBV	3071496	3068653	54.87%	6.710%
8	7.856	529	531	534	rBV	1151793	1479093	26.45%	3.234%
9	8.942	623	626	629	rBV	4596517	4479446	80.10%	9.795%
10	9.342	659	661	663	rBV	584402	493867	8.83%	1.080%
11	9.559	678	680	682	rBV	63731	58401	1.04%	0.128%
12	9.605	682	684	687	rBV	1597465	1822621	32.59%	3.985%
13	10.062	720	724	725	rBV	114738	127961	2.29%	0.280%
14	10.279	740	743	746	rBV	41773	58076	1.04%	0.127%
15	10.393	751	753	756	rBV2	1950478	2623800	46.92%	5.737%
16	10.531	763	765	769	rBV	143902	167808	3.00%	0.367%
17	10.976	802	804	805	rBV	106368	94416	1.69%	0.206%
18	11.091	811	814	816	rBV	1078990	1454142	26.00%	3.180%
19	11.639	860	862	866	rBV	89072	106652	1.91%	0.233%
20	12.508	936	938	941	rVB	65151	60280	1.08%	0.132%
21	12.668	950	952	955	rBV	3321474	3553584	63.54%	7.770%
22	13.605	1030	1034	1041	rBV	99321	255143	4.56%	0.558%
23	13.708	1041	1043	1046	rBV	1006127	1183833	21.17%	2.589%
24	14.565	1115	1118	1121	rBV	47936	58523	1.05%	0.128%
25	14.782	1135	1137	1140	rBV	37845	60446	1.08%	0.132%
26	15.068	1159	1162	1164	rBV	822580	934416	16.71%	2.043%
27	15.102	1164	1165	1169	rVB	66388	83540	1.49%	0.183%
28	15.468	1193	1197	1201	rBV	93492	164026	2.93%	0.359%
29	15.560	1201	1205	1208	rBV3	25991	64381	1.15%	0.141%
30	15.880	1230	1233	1238	rVB2	71727	120519	2.16%	0.264%
31	16.360	1270	1275	1278	rBV2	64616	152068	2.72%	0.333%
32	16.931	1321	1325	1330	rVB	55726	138443	2.48%	0.303%
33	17.594	1379	1383	1391	rBV2	29960	90765	1.62%	0.198%

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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

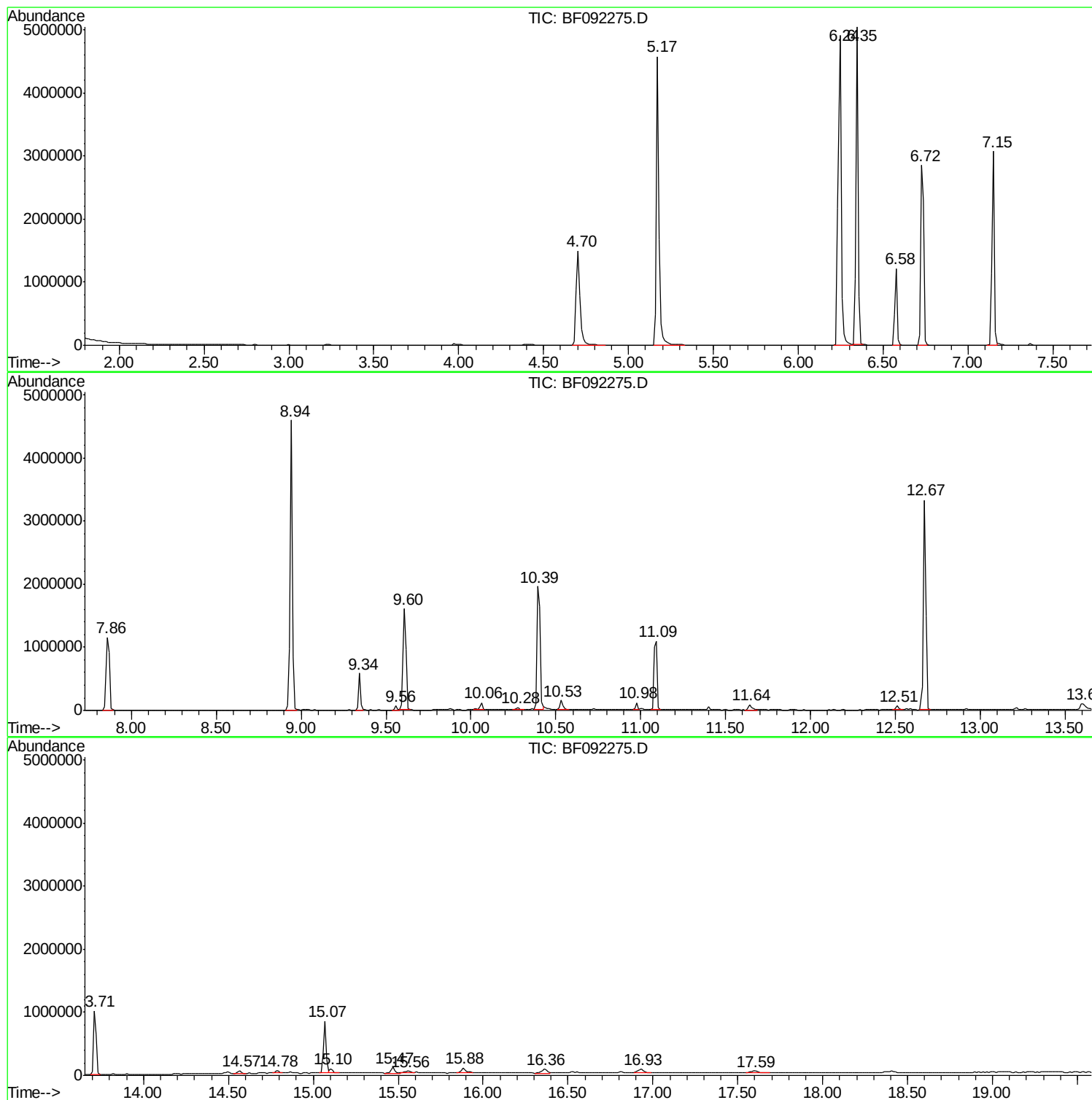
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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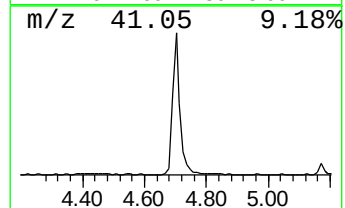
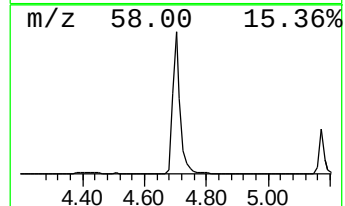
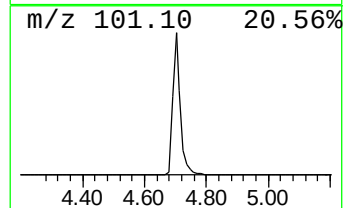
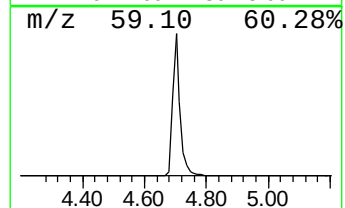
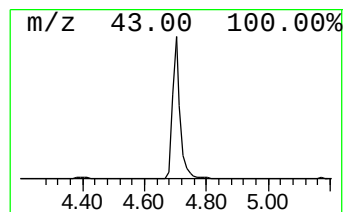
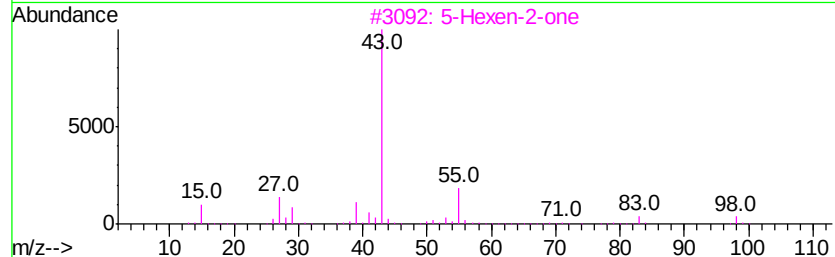
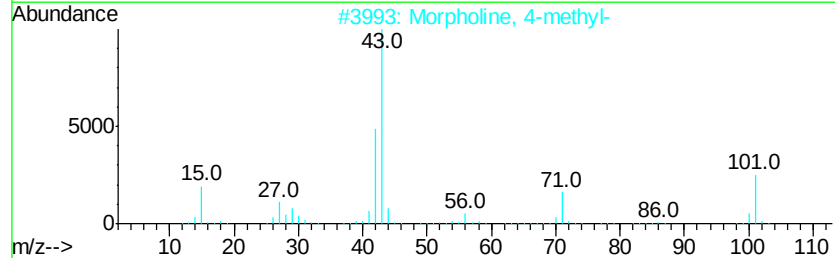
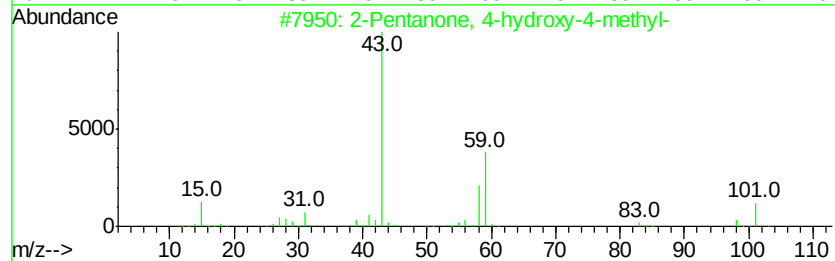
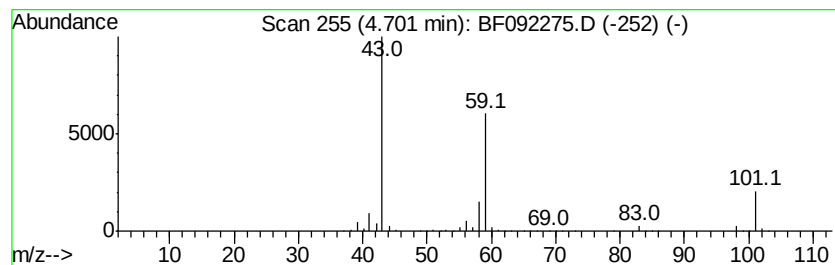
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	40.78 ng	2507920	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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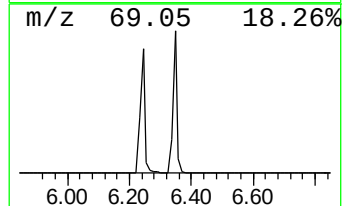
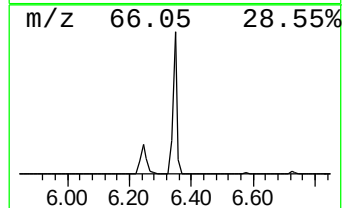
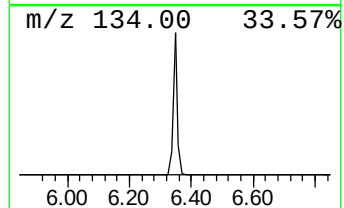
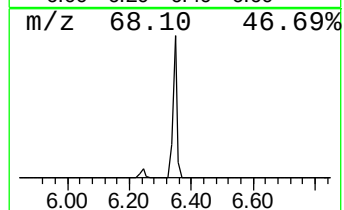
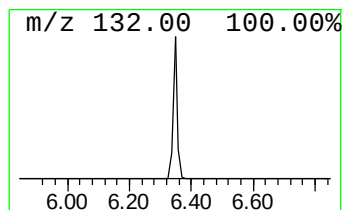
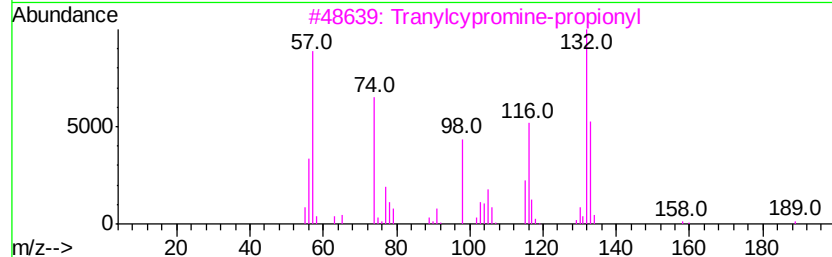
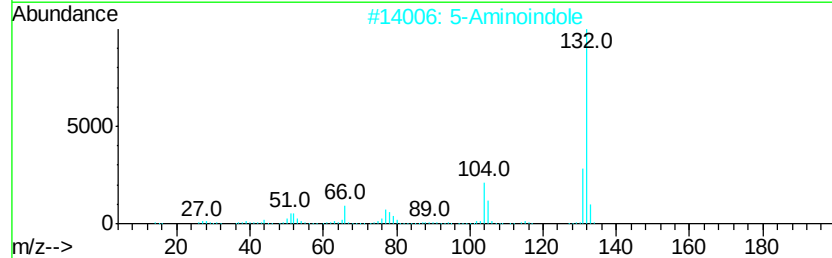
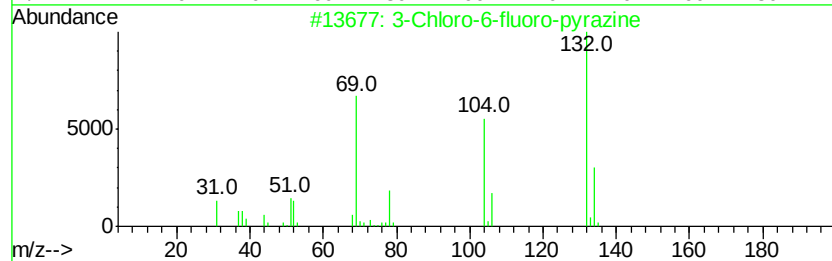
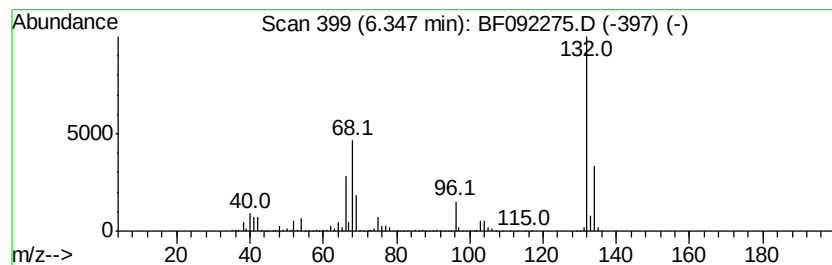
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	76.43 ng	4700180	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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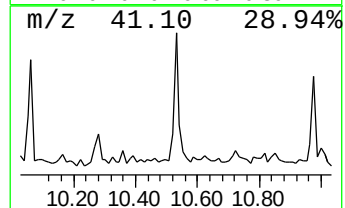
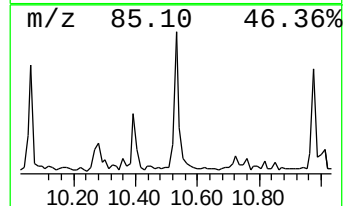
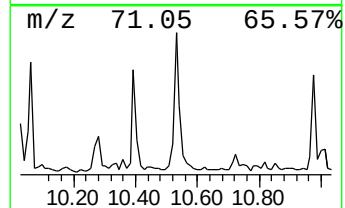
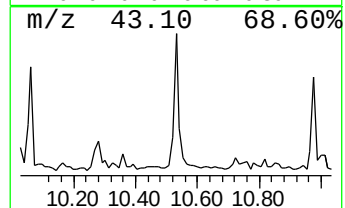
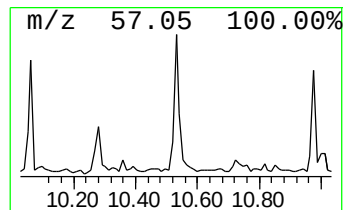
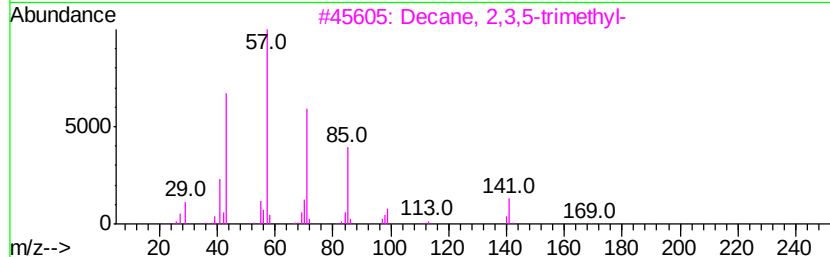
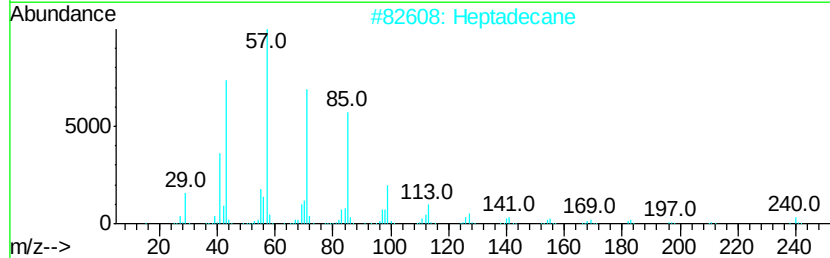
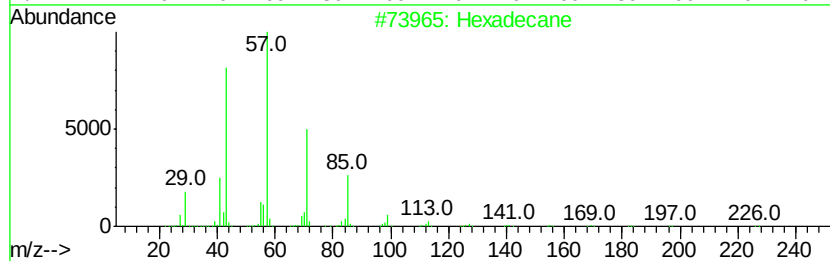
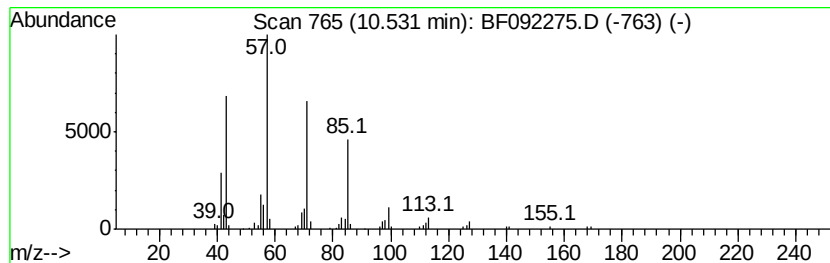
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.53	2.31 ng	167808	Phenanthrene-d10	11.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Eicosane	282	C20H42	000112-95-8	86



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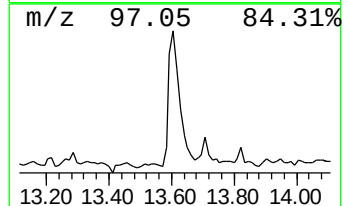
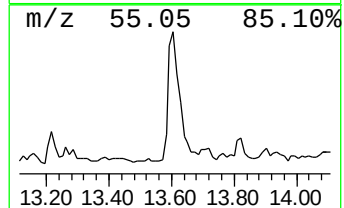
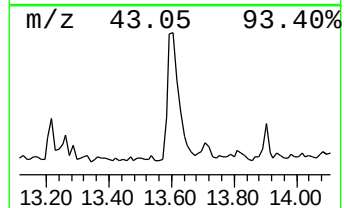
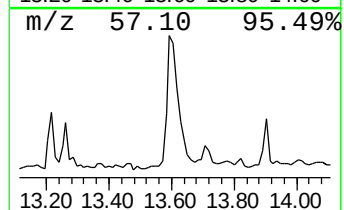
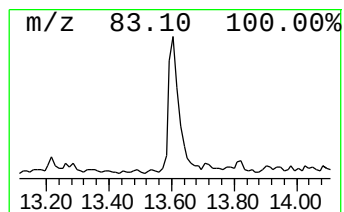
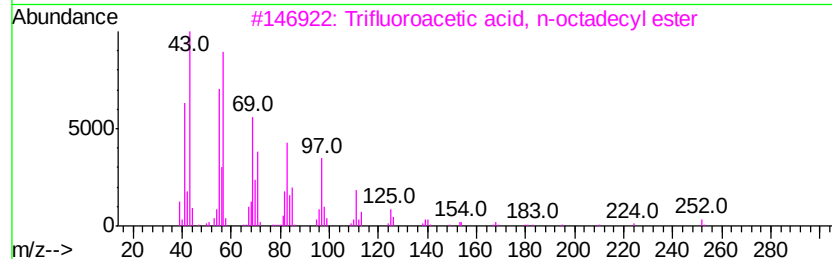
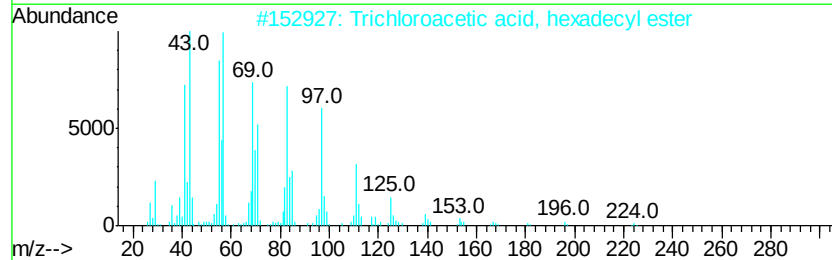
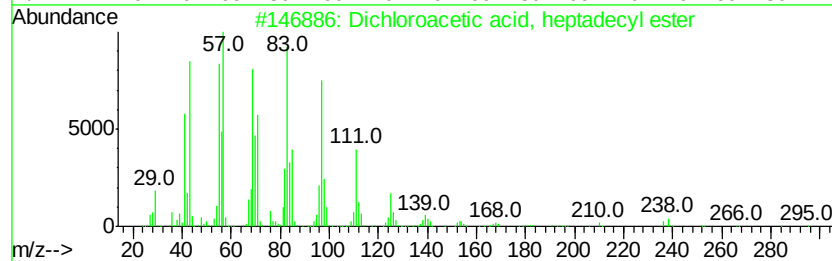
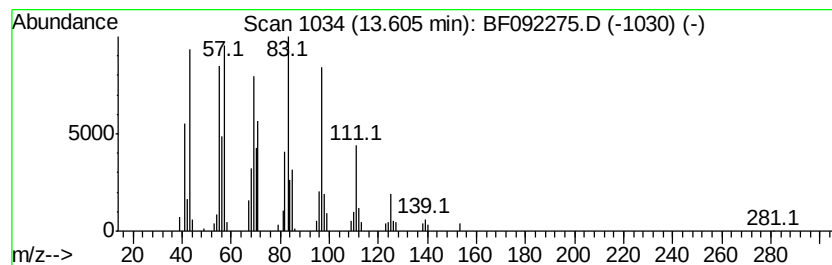
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	4.31 ng	255143	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trifluoroacetic acid, n-octadecyl ...	366	C20H37F3O2	079392-43-1	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		1-Nonadecene	266	C19H38	018435-45-5	90



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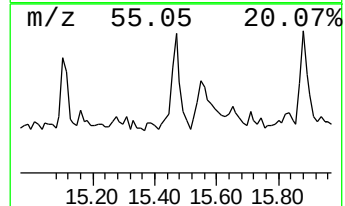
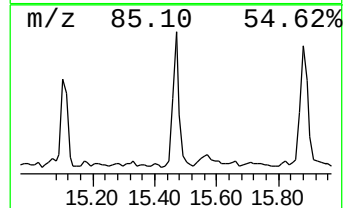
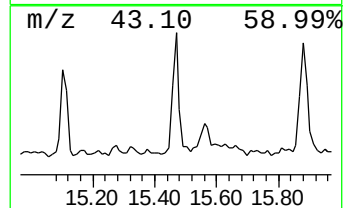
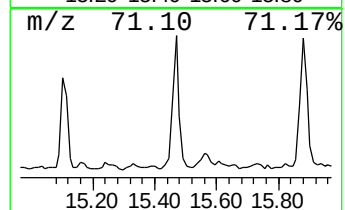
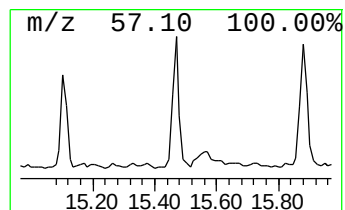
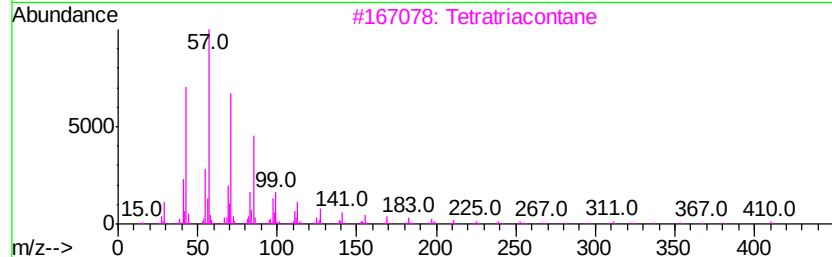
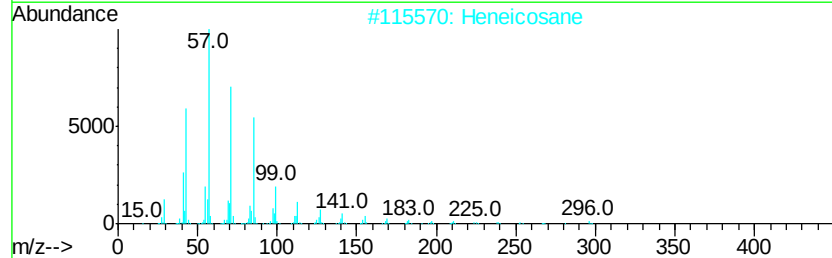
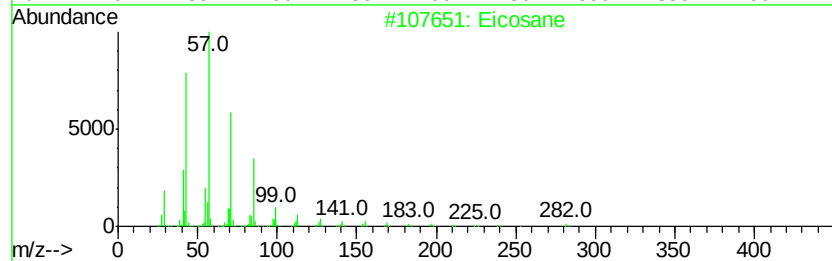
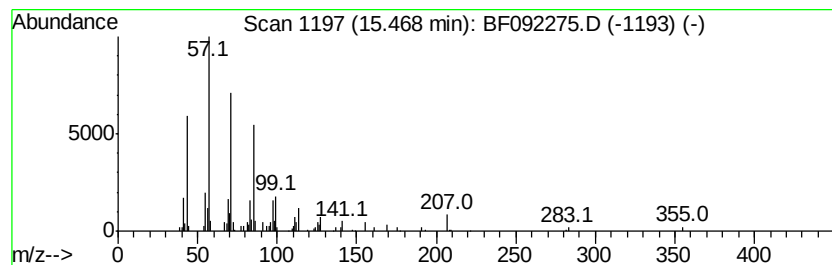
Instrument :
BNA_F
ClientSampleId :
SB-45-COMP

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 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.47	3.51 ng	164026	Perylene-d12		15.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratriacontane	479	C34H70	014167-59-0	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tetratetracontane	619	C44H90	007098-22-8	91



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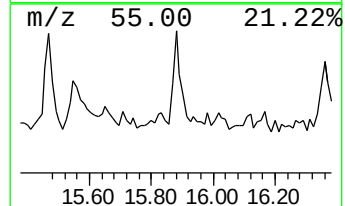
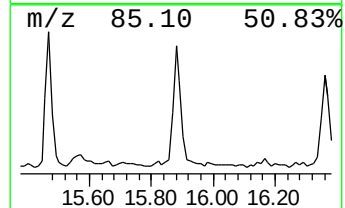
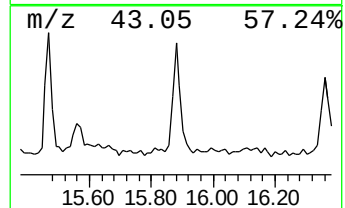
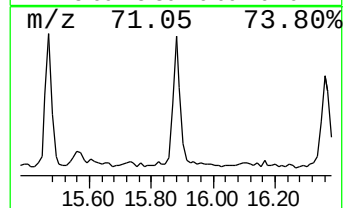
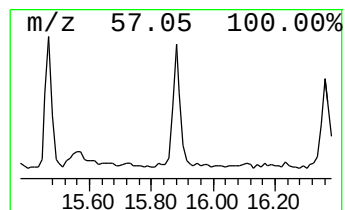
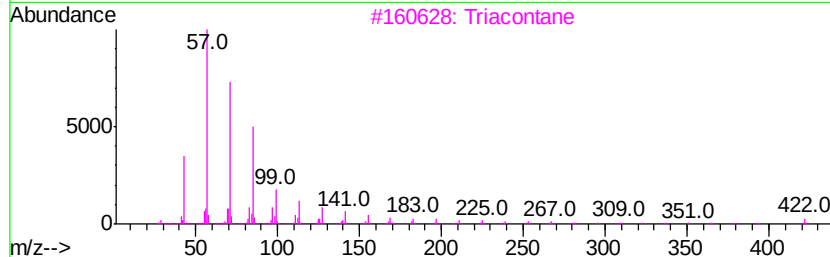
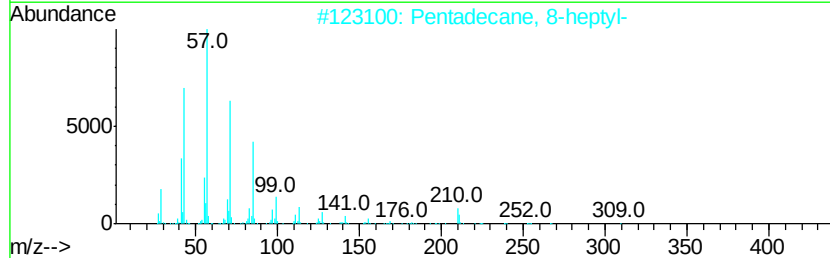
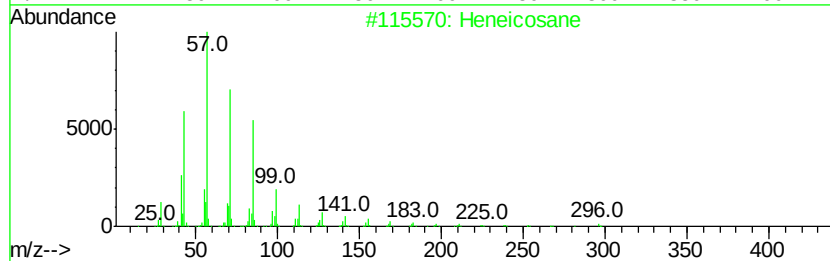
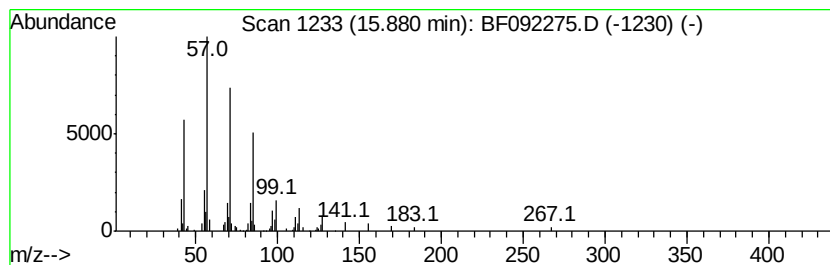
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BNA_F
ClientSampleId :
SB-45-COMP

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 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.88	2.58 ng	120519	Perylene-d12	15.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
3	Triacotane	422	C30H62	000638-68-6	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	Nonacosane	408	C29H60	000630-03-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092275.D
Acq On : 14 Jan 2017 10:34
Operator : UM/SJ
Sample : I1162-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-45-COMP

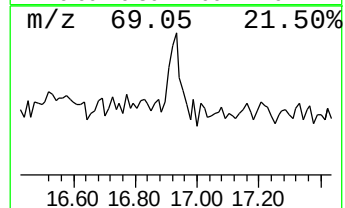
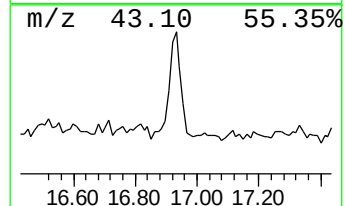
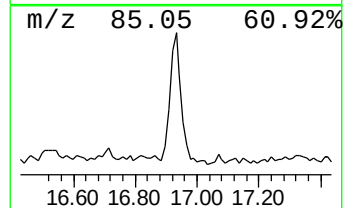
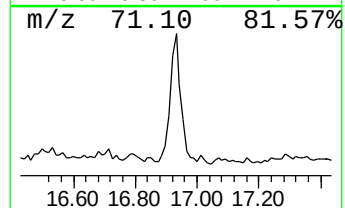
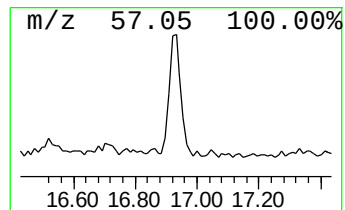
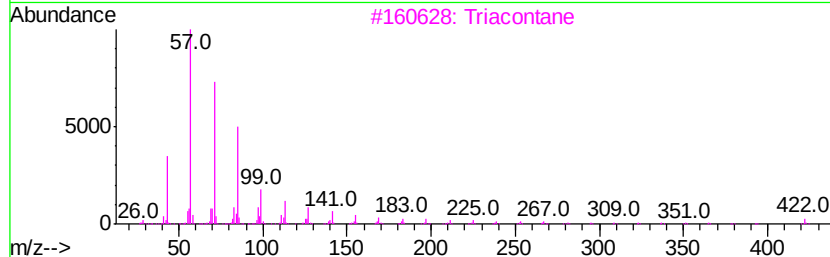
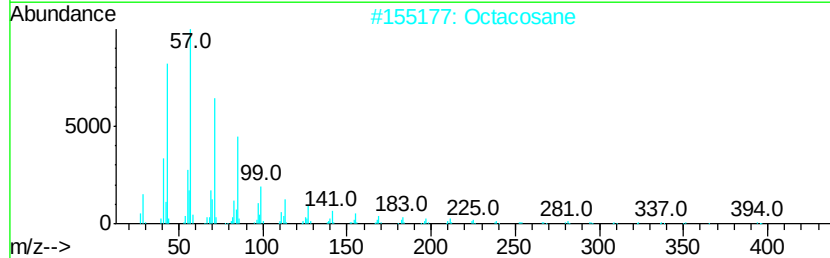
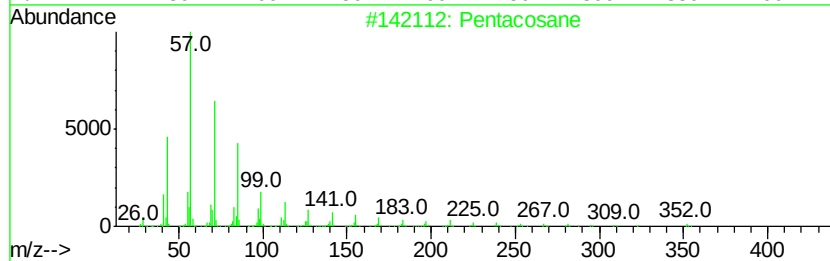
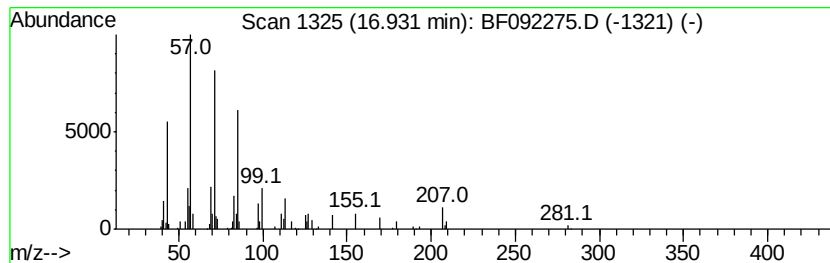
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	2.96 ng	138443	Perylene-d12	15.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	87
2	Octacosane		394	C28H58	000630-02-4	87
3	Triacontane		422	C30H62	000638-68-6	87
4	Tetratriacontane		479	C34H70	014167-59-0	86
5	Heneicosane		296	C21H44	000629-94-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092275.D
Acq On : 14 Jan 2017 10:34
Operator : UM/SJ
Sample : I1162-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-45-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	40.8	ng	2507920	1	6.58	1229910	20.0
unknown6.35	6.35	76.4	ng	4700180	1	6.58	1229910	20.0
Hexadecane	10.53	2.3	ng	167808	4	11.09	1454140	20.0
Dichloroacetic ac...	13.61	4.3	ng	255143	5	13.71	1183830	20.0
Eicosane	15.47	3.5	ng	164026	6	15.07	934416	20.0
Heneicosane	15.88	2.6	ng	120519	6	15.07	934416	20.0
Pentacosane	16.93	3.0	ng	138443	6	15.07	934416	20.0