

Data Path : Z:\HPCHEM1\BNA F\Data\BF012517\
 Data File : BF092465.D
 Acq On : 25 Jan 2017 9:57
 Operator : UM/SJ
 Sample : I1305-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 0024

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-BF012417.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	5.162	266	269	275	rVB	1469448	2005291	17.84%	0.708%
2	5.562	301	304	307	rBV	3317797	4010258	35.67%	1.416%
3	6.590	390	394	397	rBV	3158622	4353595	38.72%	1.537%
4	6.705	401	404	405	rVV	2353276	2107541	18.75%	0.744%
5	6.739	405	407	411	rVB2	3816050	7999540	71.15%	2.825%
6	6.990	425	429	431	rBV2	4750658	5662838	50.37%	2.000%
7	7.150	438	443	445	rBV2	5357755	9383246	83.46%	3.314%
8	7.230	446	450	451	rVV	5745512	8777540	78.07%	3.100%
9	7.253	451	452	455	rVV	1979369	2184369	19.43%	0.771%
10	7.379	459	463	466	rBV	4419294	6188532	55.05%	2.185%
11	7.493	470	473	475	rBV	4890187	5503436	48.95%	1.944%
12	7.562	475	479	481	rVB2	3081096	5896310	52.45%	2.082%
13	7.802	497	500	504	rBV	3309072	4258608	37.88%	1.504%
14	7.882	504	507	509	rBV	2844701	3172662	28.22%	1.120%
15	8.019	515	519	521	rVB	3094860	3905920	34.74%	1.379%
16	8.213	532	536	538	rBV	5093068	7510889	66.81%	2.652%
17	8.293	538	543	545	rVB2	3916386	6297992	56.02%	2.224%
18	8.408	550	553	555	rBV	2100645	2166482	19.27%	0.765%
19	8.990	600	604	606	rBV	6695014	9323633	82.93%	3.293%
20	9.082	610	612	614	rVB	154751	151959	1.35%	0.054%
21	9.265	624	628	629	rBV	4675004	6305539	56.09%	2.227%
22	9.299	629	631	633	rVV	5184325	5281165	46.97%	1.865%
23	9.345	633	635	638	rVV	3300313	4876472	43.38%	1.722%
24	9.482	645	647	651	rVB	165681	173212	1.54%	0.061%
25	9.768	666	672	673	rBV	3861718	6576449	58.50%	2.322%
26	9.825	673	677	679	rVB	4605242	6365798	56.62%	2.248%
27	9.962	686	689	691	rBV	142471	131403	1.17%	0.046%
28	10.031	692	695	697	rVB	1898145	1671340	14.87%	0.590%
29	10.133	700	704	707	rBV	1843242	2808080	24.98%	0.992%
30	10.248	709	714	716	rVB	5941604	10533411	93.69%	3.720%
31	10.465	729	733	735	rBV	275609	259692	2.31%	0.092%
32	10.579	739	743	746	rVV	5291579	6047971	53.80%	2.136%
33	10.682	749	752	756	rBV	71998	131263	1.17%	0.046%
34	10.819	761	764	767	rVV	2470827	2693095	23.95%	0.951%

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35	10.899	769	771	773	rVB	167752	143819	1.28%	0.051%
36	10.945	773	775	779	rBV	186507	312582	2.78%	0.110%
37	11.071	782	786	789	rBV2	4779177	6986262	62.14%	2.467%
38	11.334	805	809	811	rBV	3636294	5259681	46.78%	1.857%
39	11.391	811	814	815	rVV	177955	198475	1.77%	0.070%
40	11.414	815	816	819	rVB	117292	113103	1.01%	0.040%
41	11.551	823	828	830	rBV2	5365471	7616275	67.74%	2.690%
42	11.608	830	833	835	rVB	5277003	6222126	55.34%	2.197%
43	11.745	843	845	847	rBV	137088	131720	1.17%	0.047%
44	12.054	870	872	873	rBV	216301	303111	2.70%	0.107%
45	12.088	873	875	877	rVB	5142674	7906246	70.32%	2.792%
46	12.339	895	897	899	rVB	99166	114426	1.02%	0.040%
47	12.751	928	933	935	rBV	6746655	10699893	95.17%	3.779%
48	12.888	943	945	947	rVB	121644	159560	1.42%	0.056%
49	12.979	949	953	955	rVV	6477922	9880632	87.89%	3.489%
50	13.105	961	964	967	rVB	3890734	4249534	37.80%	1.501%
51	13.585	1003	1006	1008	rVB	4916831	4914208	43.71%	1.735%
52	13.997	1039	1042	1046	rBV2	632513	677663	6.03%	0.239%
53	14.145	1052	1055	1057	rBV	6716213	10059978	89.48%	3.553%
54	14.191	1057	1059	1062	rVB	4981545	7585423	67.47%	2.679%
55	14.637	1095	1098	1106	rBV3	265239	382037	3.40%	0.135%
56	14.762	1106	1109	1112	rBV	5567077	8861401	78.82%	3.129%
57	15.025	1129	1132	1136	rVB	93646	128914	1.15%	0.046%
58	15.220	1144	1149	1151	rBV	3822657	11242571	100.00%	3.970%
59	15.265	1151	1153	1155	rVB	4750521	6181588	54.98%	2.183%
60	15.597	1177	1182	1184	rBV	3587894	6195092	55.10%	2.188%
61	15.643	1184	1186	1188	rVB	825032	915824	8.15%	0.323%
62	16.123	1225	1228	1230	rBV	121783	218787	1.95%	0.077%
63	16.168	1230	1232	1237	rVB	121310	228349	2.03%	0.081%
64	17.174	1310	1320	1325	rBV2	2882828	9806973	87.23%	3.463%
65	17.254	1325	1327	1330	rVV	62165	144552	1.29%	0.051%
66	17.334	1331	1334	1341	rVB4	53039	164693	1.46%	0.058%
67	17.723	1364	1368	1371	rBV3	76535	190890	1.70%	0.067%
68	17.826	1374	1377	1383	rVB5	45621	125332	1.11%	0.044%
69	18.546	1436	1440	1449	rVB10	31608	133785	1.19%	0.047%

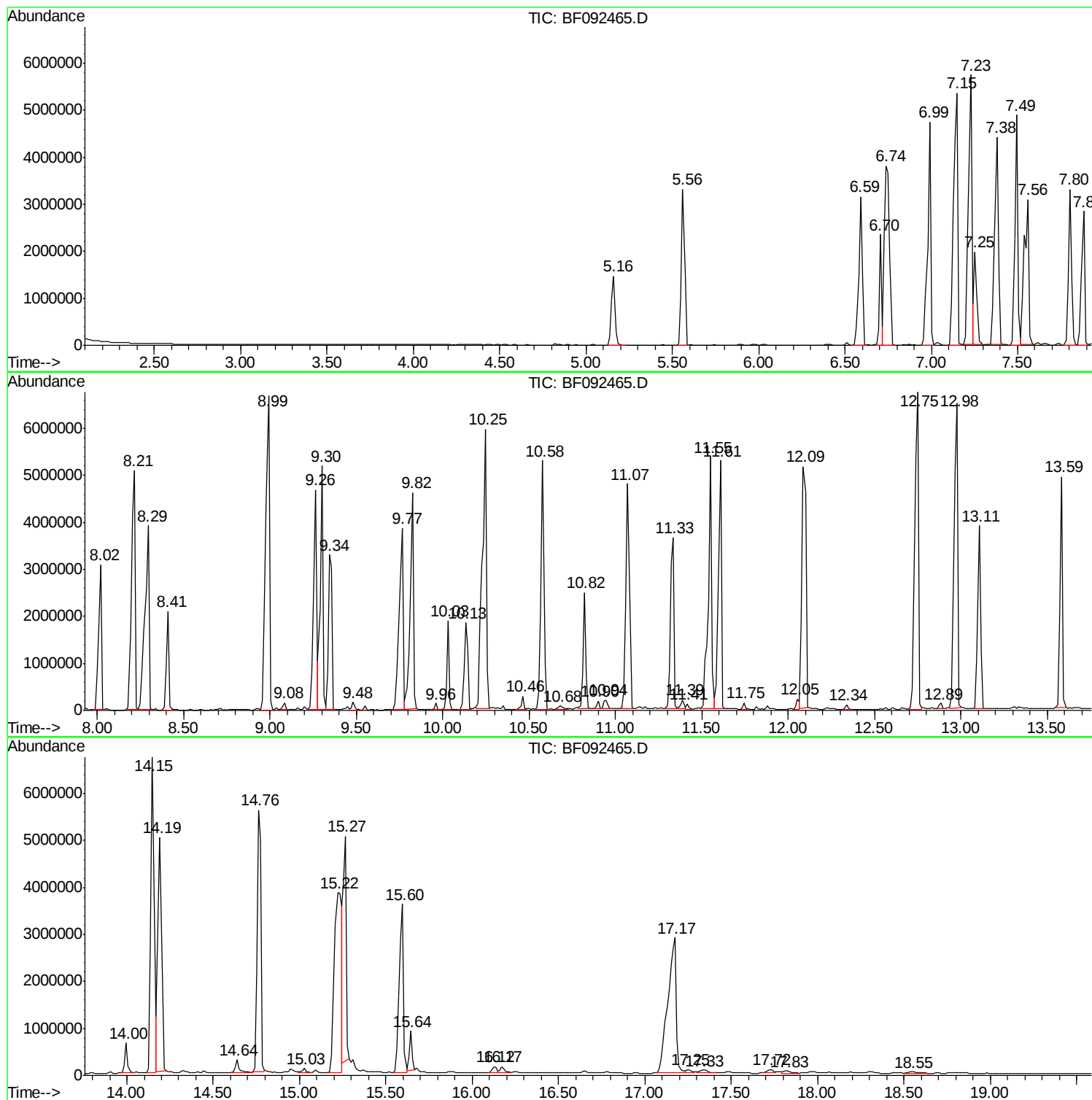
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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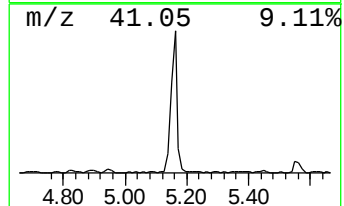
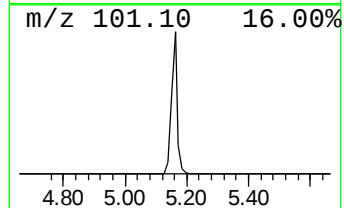
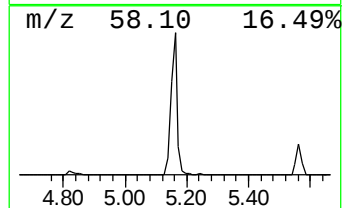
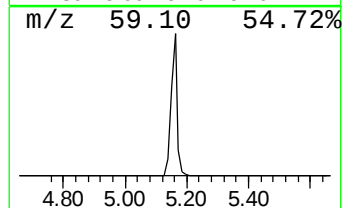
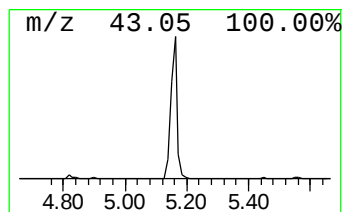
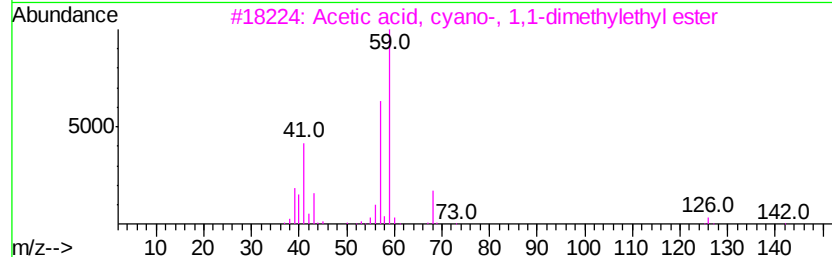
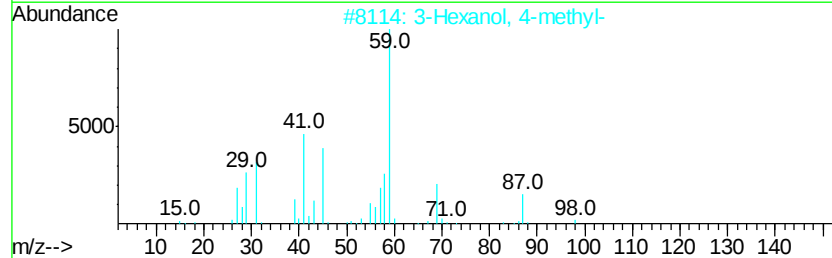
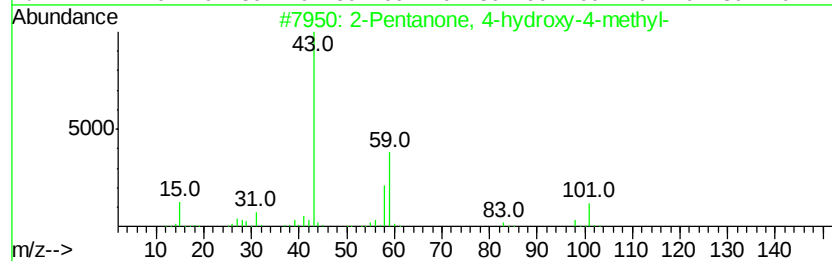
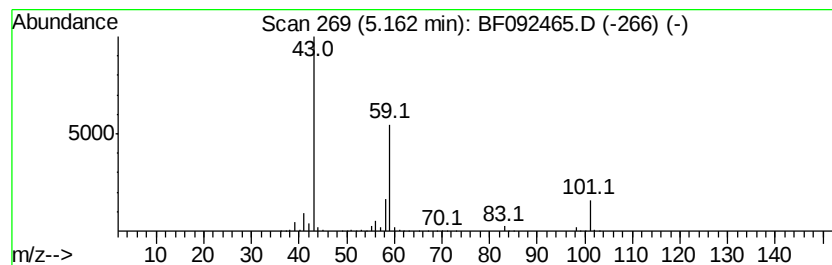
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	7.08 ng	2005290	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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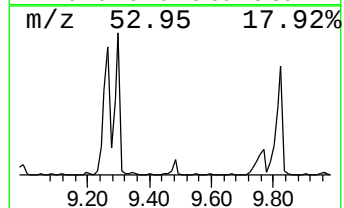
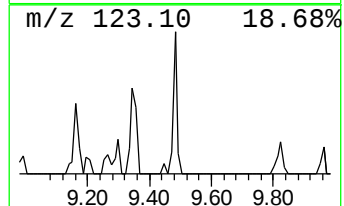
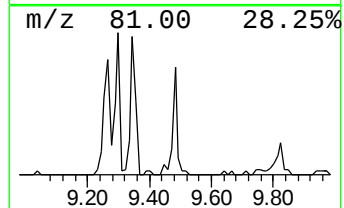
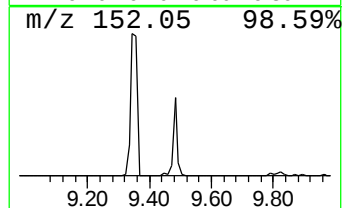
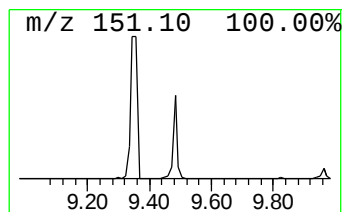
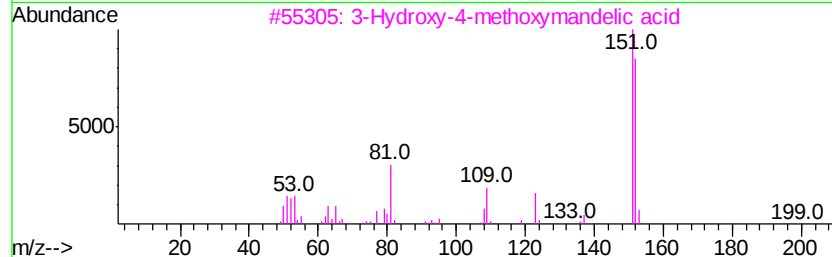
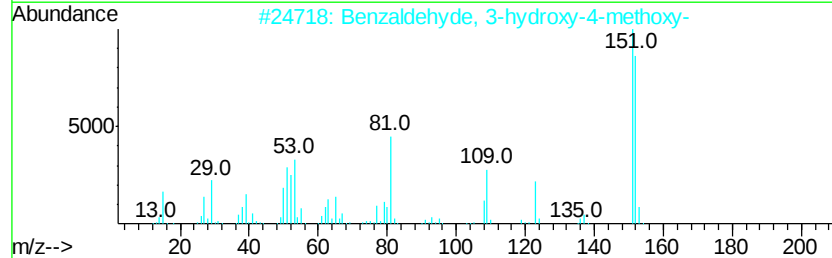
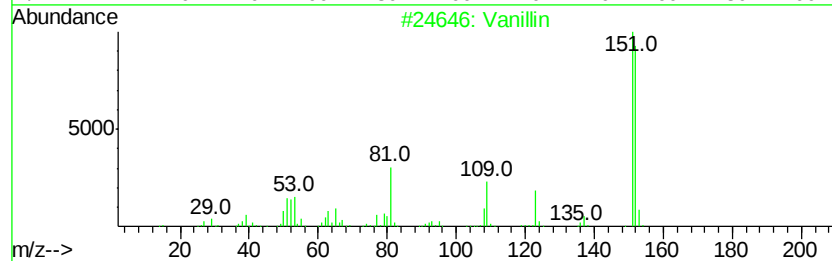
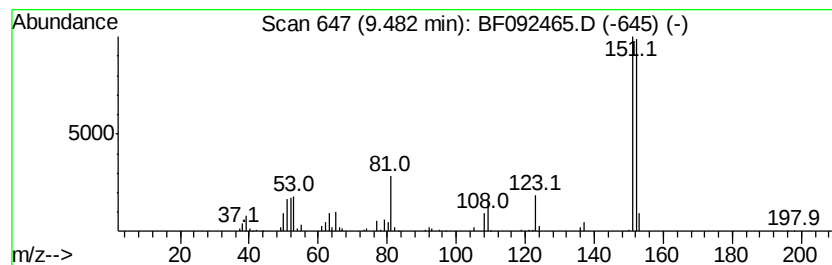
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 Vanillin Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	2.07 ng	173212	Acenaphthene-d10	10.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin		152	C8H8O3	000121-33-5	95
2	Benzaldehyde, 3-hydroxy-4-methoxy-		152	C8H8O3	000621-59-0	95
3	3-Hydroxy-4-methoxymandelic acid		198	C9H10O5	003695-24-7	91
4	4-Hydroxy-2-methoxybenzaldehyde		152	C8H8O3	018278-34-7	90
5	Benzaldehyde, 4-(methylthio)-		152	C8H8OS	003446-89-7	72



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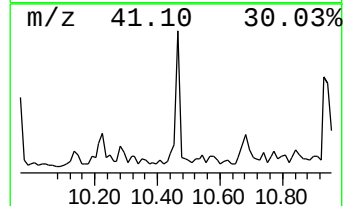
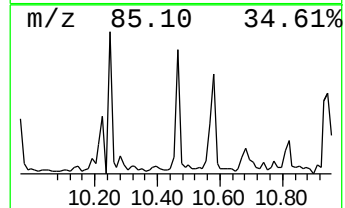
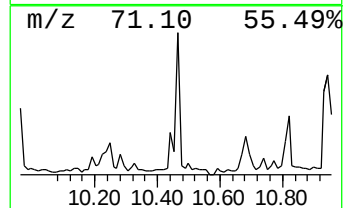
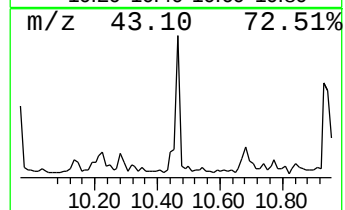
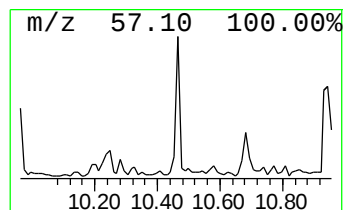
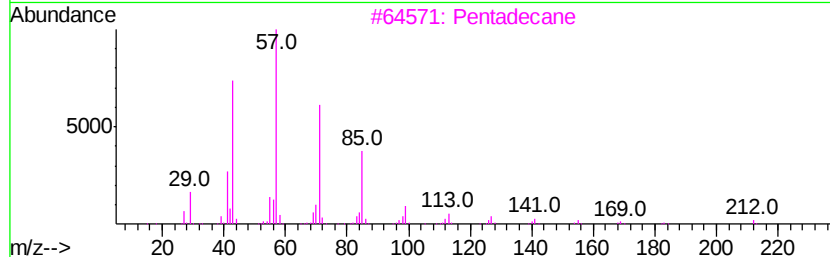
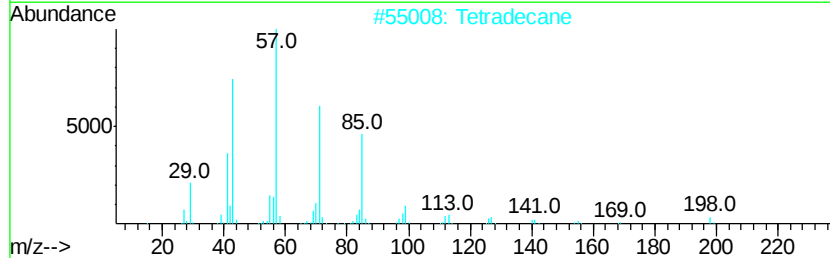
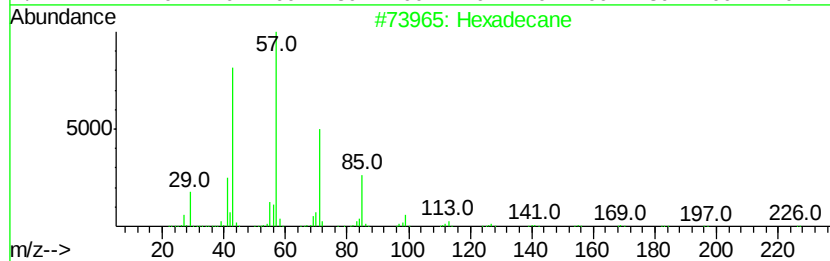
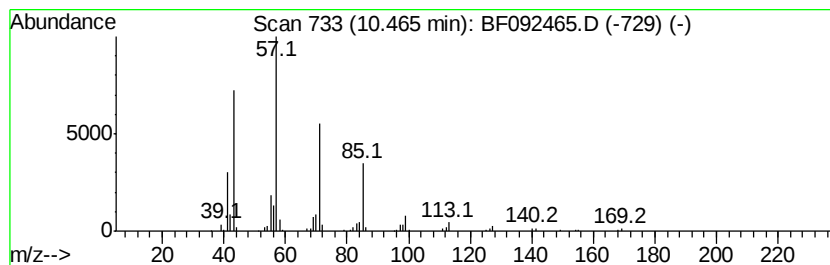
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.46	3.11 ng	259692	Acenaphthene-d10		10.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Tetradecane	198	C14H30	000629-59-4	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Eicosane	282	C20H42	000112-95-8	58



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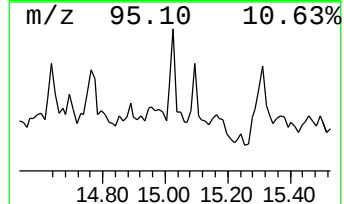
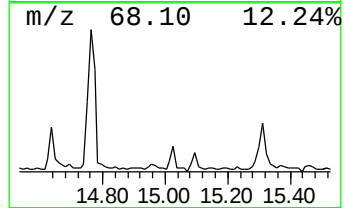
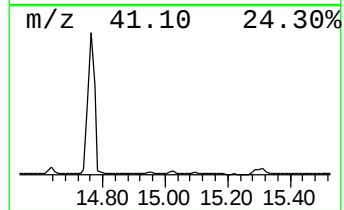
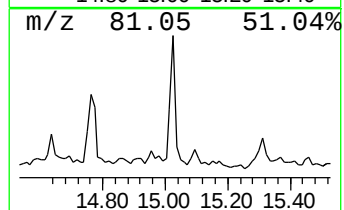
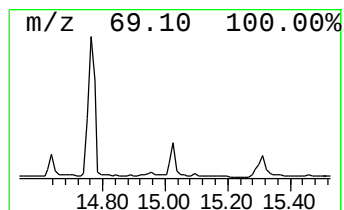
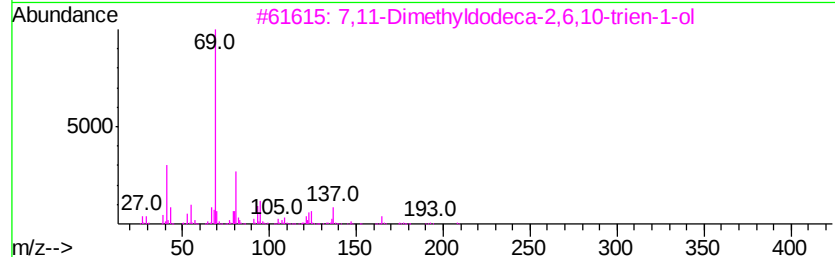
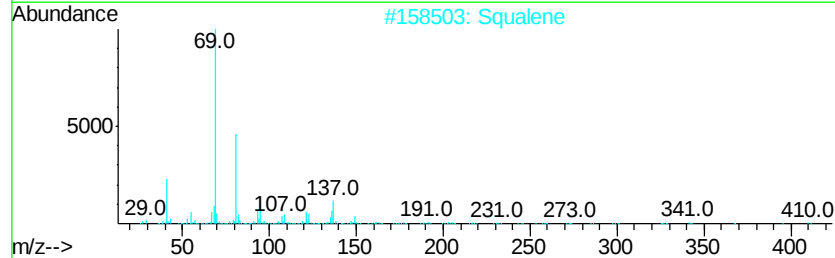
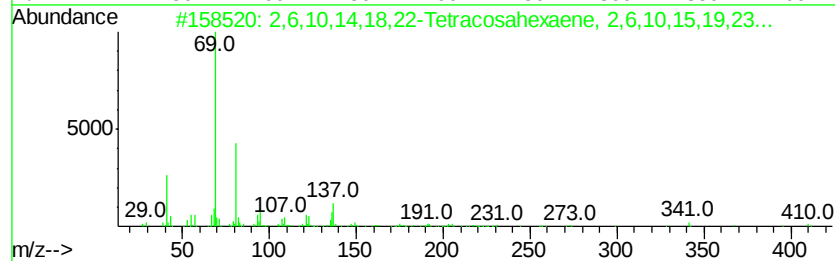
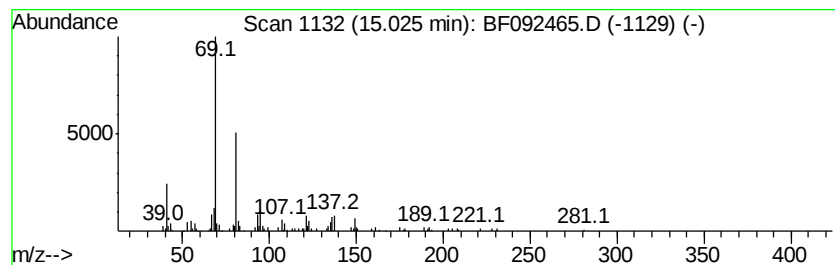
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.82 ng	128914	Perylene-d12	15.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87		
2	Squalene	410	C30H50	007683-64-9	86		
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24	125529-10-4	72		
4	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	72		
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59		



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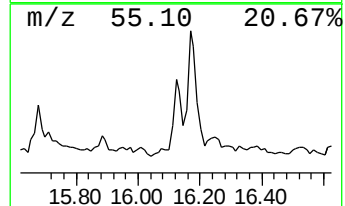
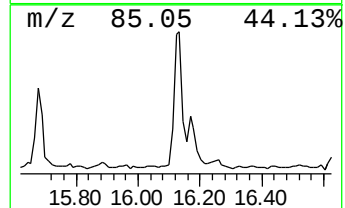
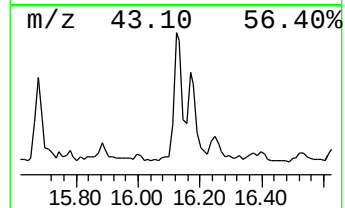
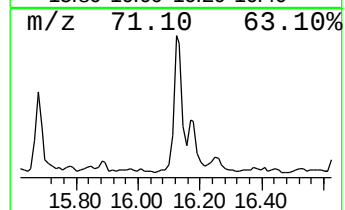
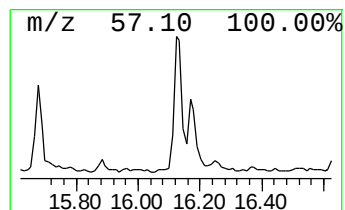
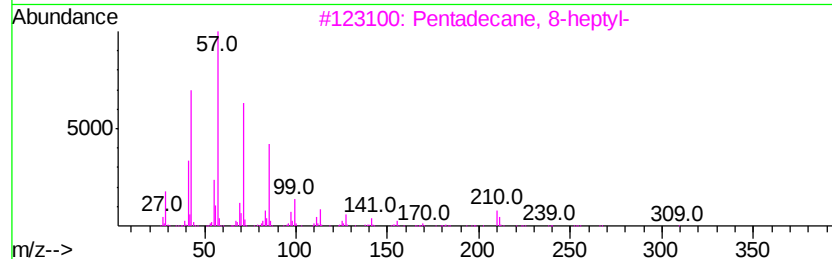
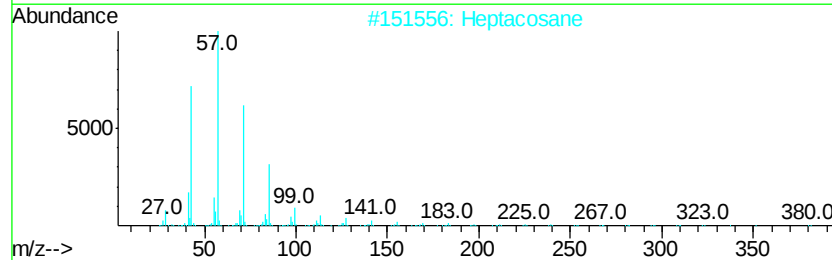
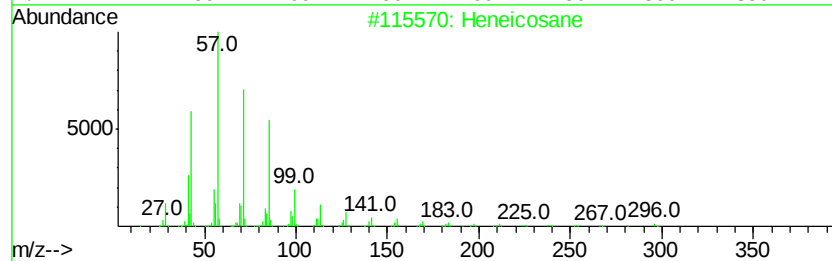
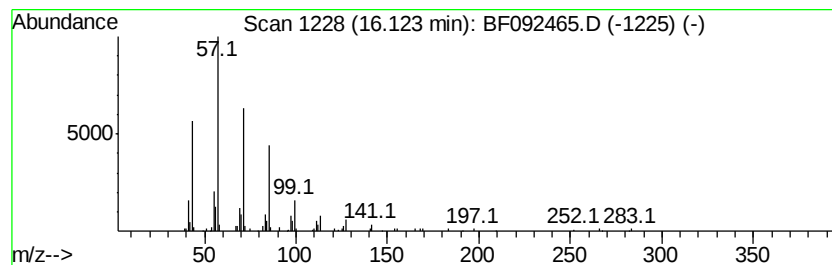
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	4.78 ng	218787	Perylene-d12	15.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptacosane		380	C27H56	000593-49-7	91
3	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	90
4	Nonadecane		268	C19H40	000629-92-5	90
5	Hexadecane		226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA_F\Data\BF012517\
Data File : BF092465.D
Acq On : 25 Jan 2017 9:57
Operator : UM/SJ
Sample : I1305-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

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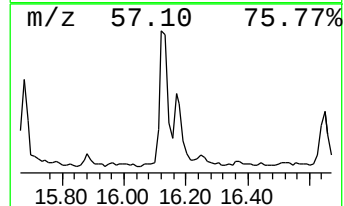
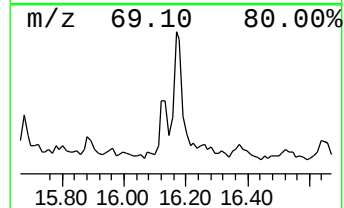
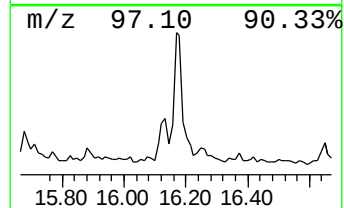
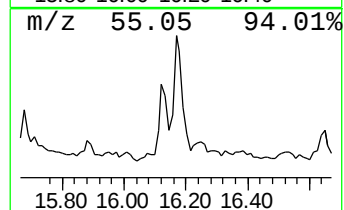
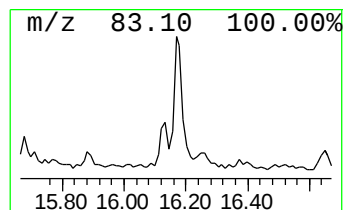
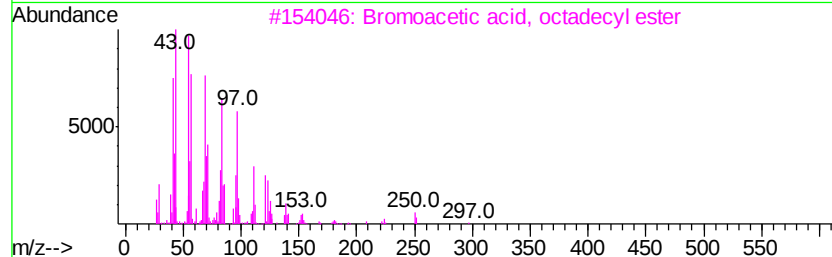
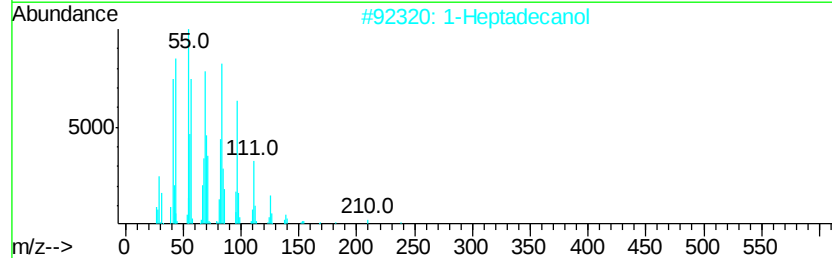
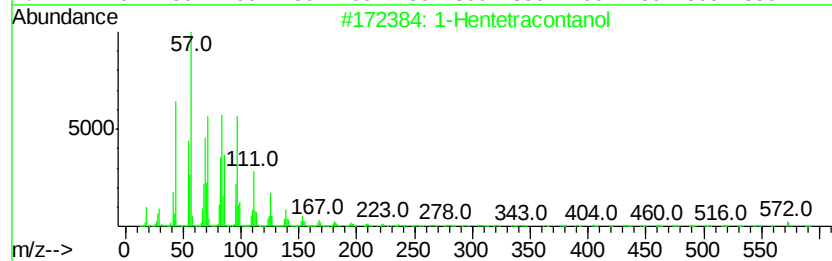
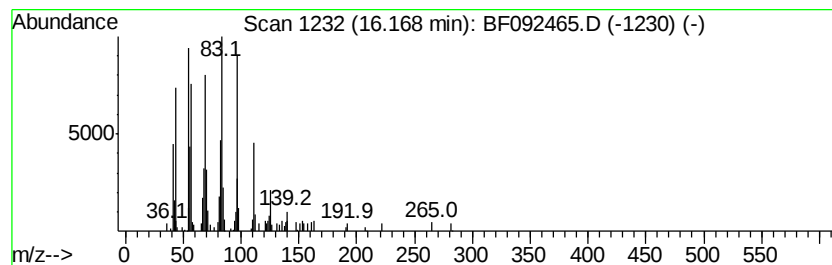
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hentetracontanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	4.99 ng	228349	Perylene-d12	15.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol		593	C41H84O	040710-42-7	64
2	1-Heptadecanol		256	C17H36O	001454-85-9	50
3	Bromoacetic acid, octadecyl ester		390	C20H39BrO2	018992-03-5	47
4	1-Hexadecanol		242	C16H34O	036653-82-4	47
5	Cyclopentane, (2-methylpropyl)-		126	C9H18	003788-32-7	43



Data Path : Z:\HPCHEM1\BNA F\Data\BF012517\
Data File : BF092465.D
Acq On : 25 Jan 2017 9:57
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Sample : I1305-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

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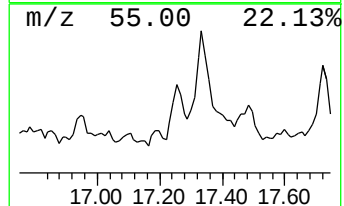
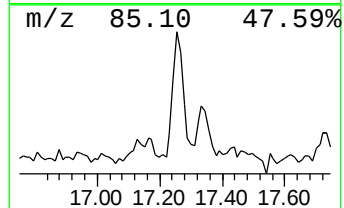
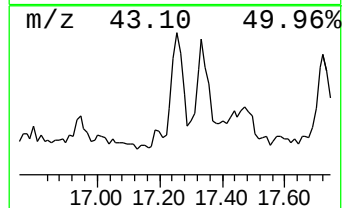
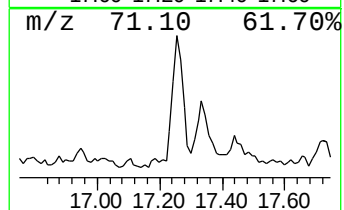
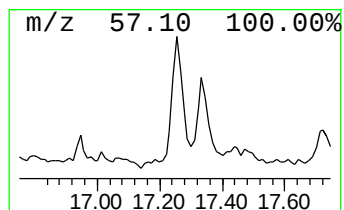
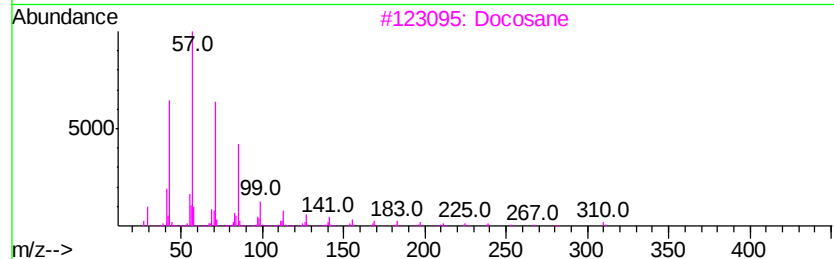
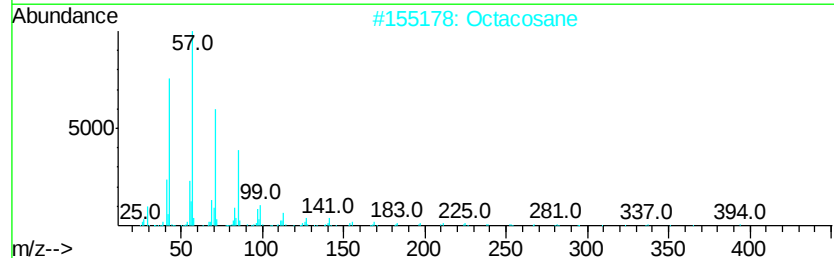
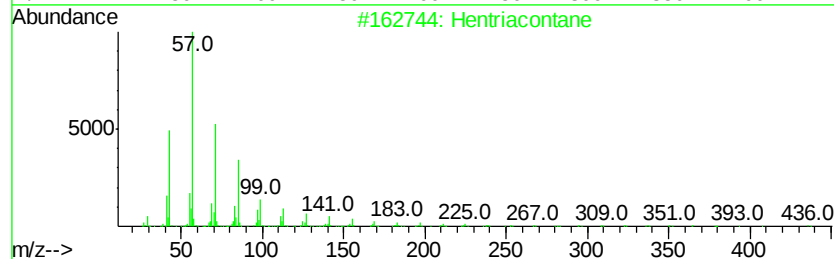
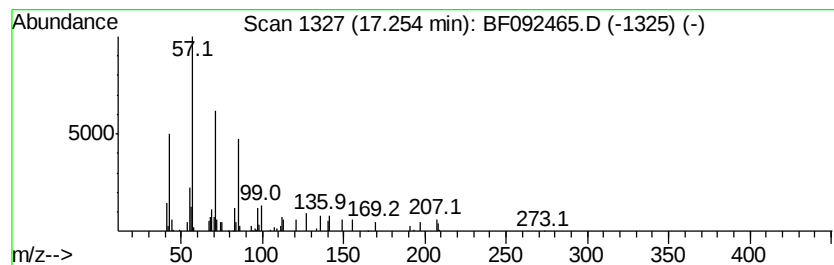
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.25	3.16 ng	144552	Perylene-d12	15.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	86
2	Octacosane		394	C28H58	000630-02-4	80
3	Docosane		310	C22H46	000629-97-0	72
4	Tetracosane		338	C24H50	000646-31-1	72
5	Pentacosane		352	C25H52	000629-99-2	64



Data Path : Z:\HPCHEM1\BNA_F\Data\BF012517\
Data File : BF092465.D
Acq On : 25 Jan 2017 9:57
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Misc :
ALS Vial : 3 Sample Multiplier: 1

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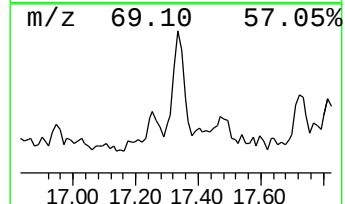
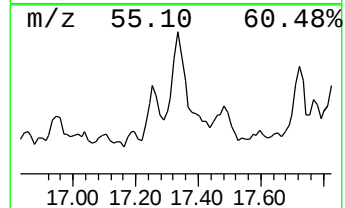
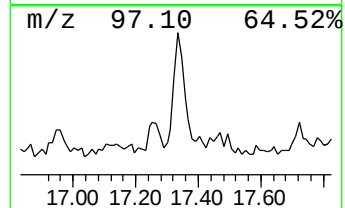
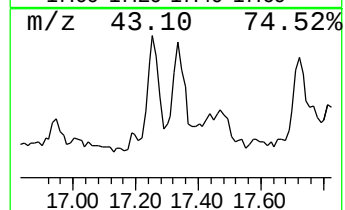
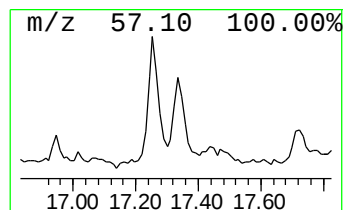
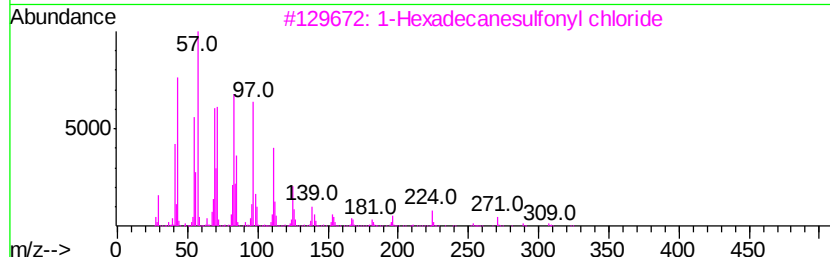
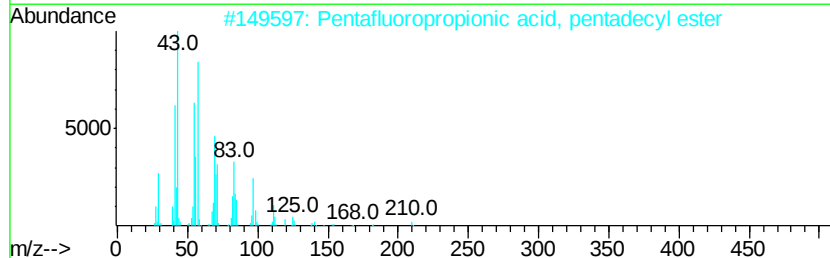
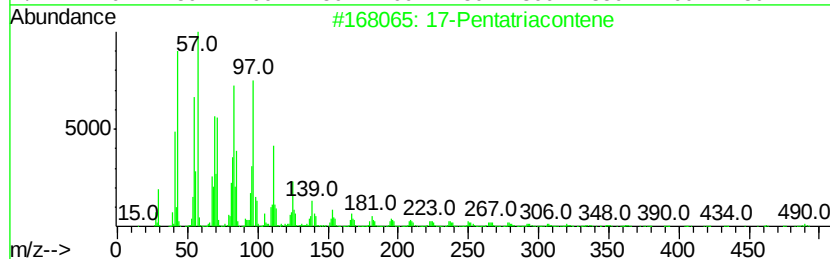
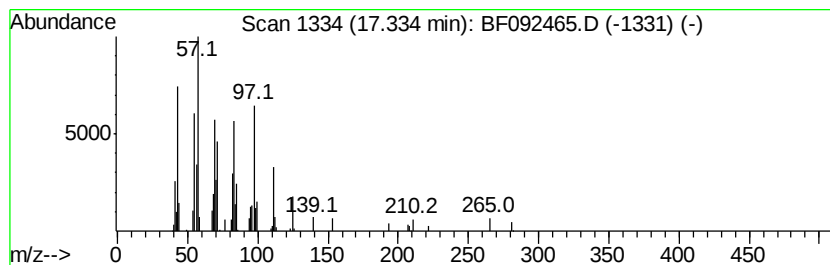
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	3.60 ng	164693	Perylene-d12	15.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene		491	C35H70	006971-40-0	86
2	Pentafluoropropionic acid, penta...		374	C18H31F5O2	1000280-07-5	80
3	1-Hexadecanesulfonyl chloride		324	C16H33ClO2S	038775-38-1	72
4	1-Tetracosanol		354	C24H50O	000506-51-4	58
5	1-Eicosanol		298	C20H42O	000629-96-9	58



Data Path : Z:\HPCHEM1\BNA F\Data\BF012517\
Data File : BF092465.D
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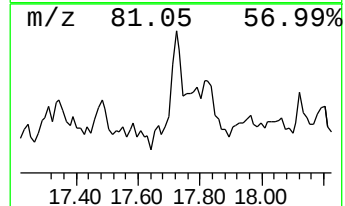
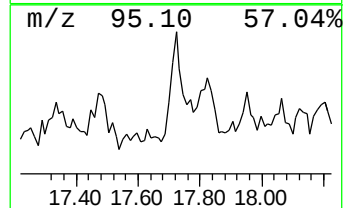
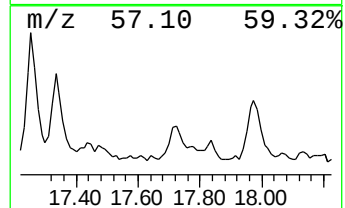
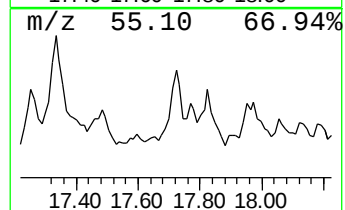
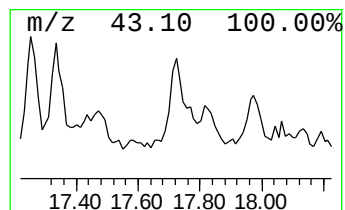
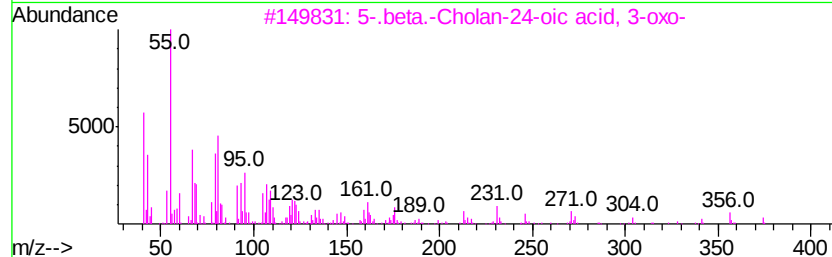
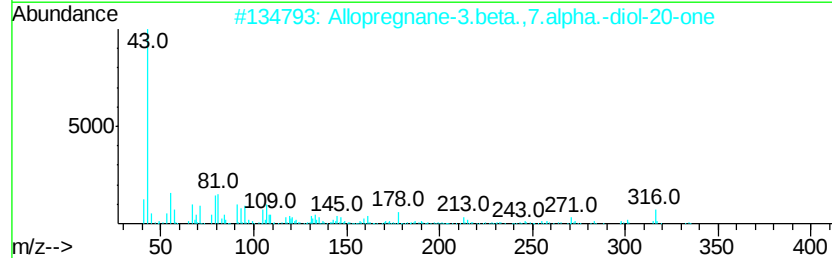
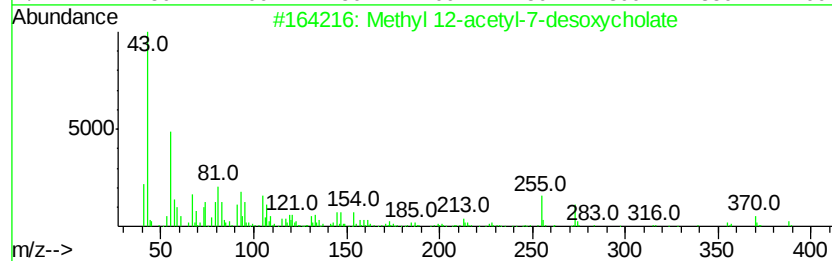
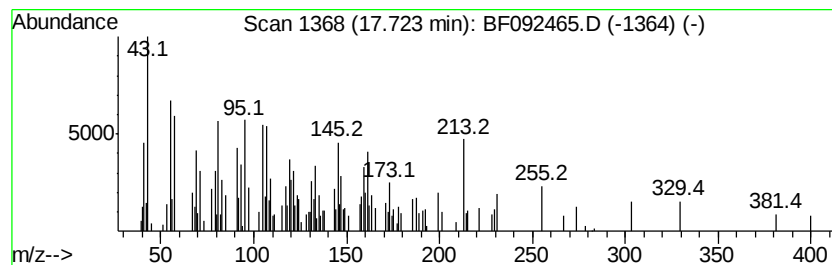
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	4.17 ng	190890	Perylene-d12	15.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	27
2		Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	25
3		5-.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	12
4		4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	12
5		1-[4-Hydroxymethyl-5-(2-mercapto...	272	C11H16N2O4S	128453-39-4	10



Data Path : Z:\HPCHEM1\BNA F\Data\BF012517\
Data File : BF092465.D
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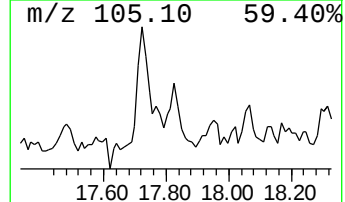
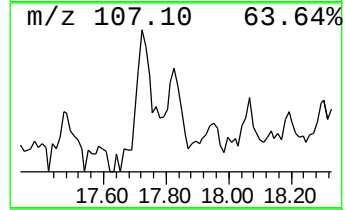
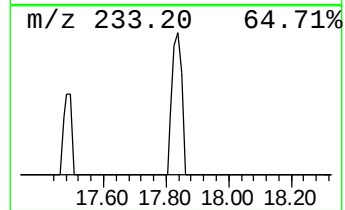
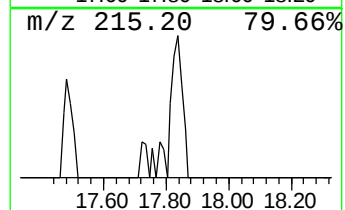
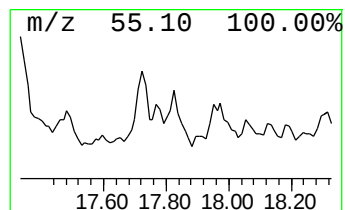
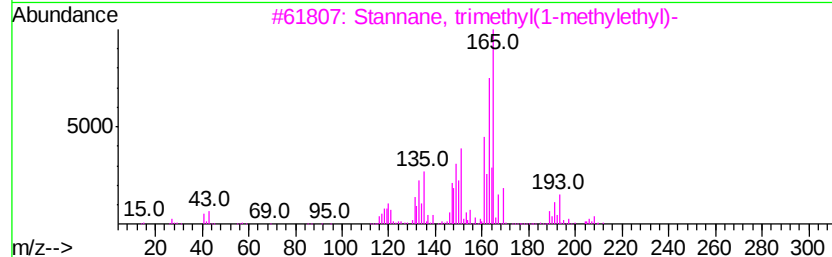
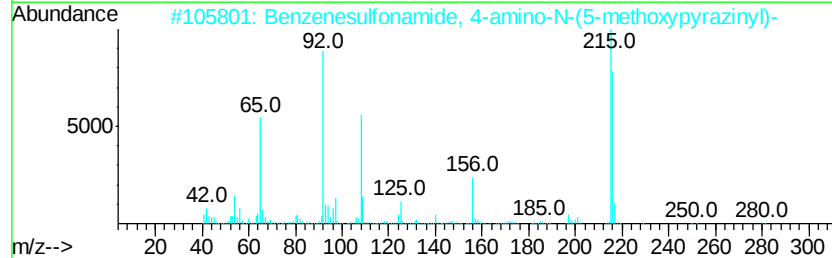
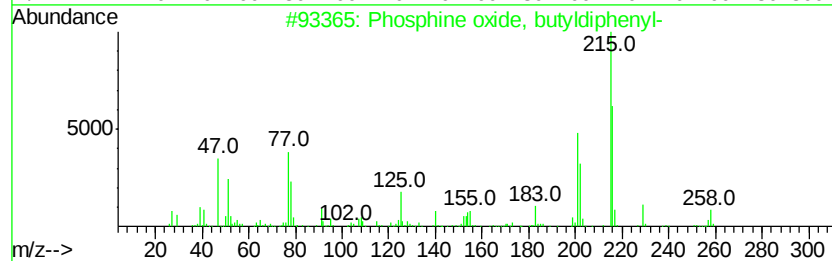
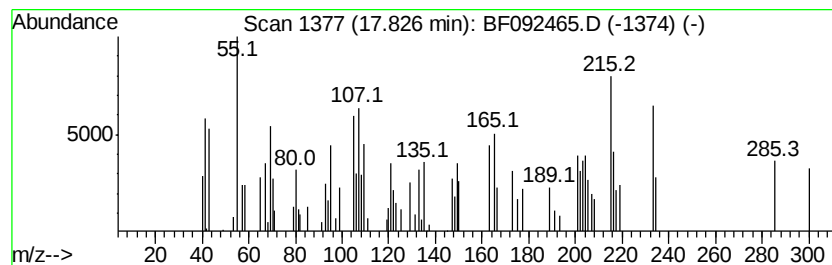
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.83 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	2.74 ng	125332	Perylene-d12	15.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosphine oxide, butyldiphenyl-	258	C16H19OP	004233-13-0	27
2		Benzenesulfonamide, 4-amino-N-(5-methoxypyrazinyl)-	280	C11H12N4O3S	003373-93-1	10
3		Stannane, trimethyl(1-methylethyl)-	208	C6H16Sn	003531-46-2	10
4		Phosphine oxide, heptyldiphenyl-	300	C19H25OP	079422-30-3	10
5		Cyclopent[e]-1,3-oxazine, octahydro-	216	C13H16N2O	1000138-92-2	10



Data Path : Z:\HPCHEM1\BNA F\Data\BF012517\
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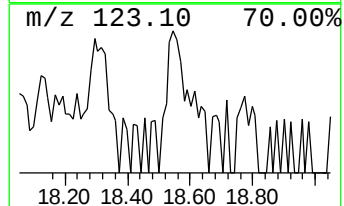
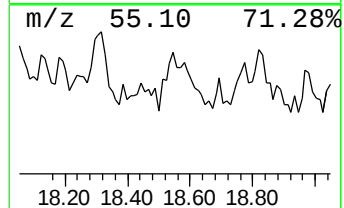
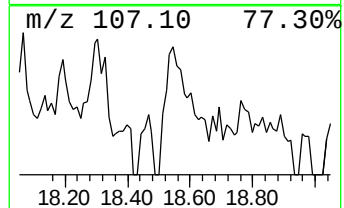
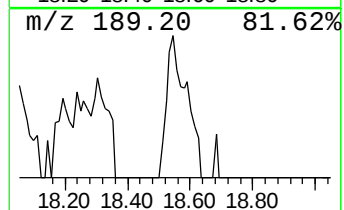
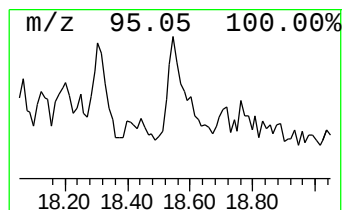
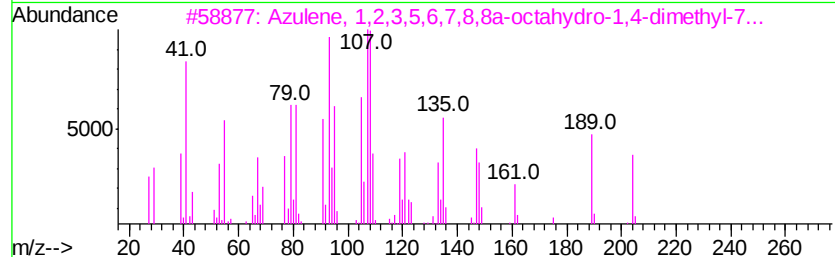
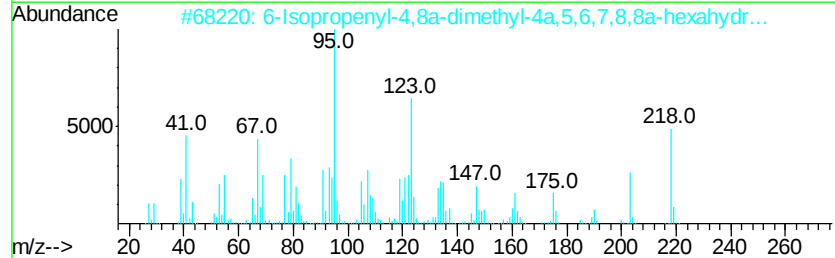
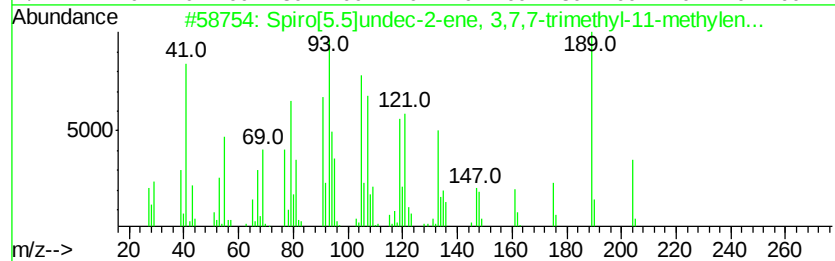
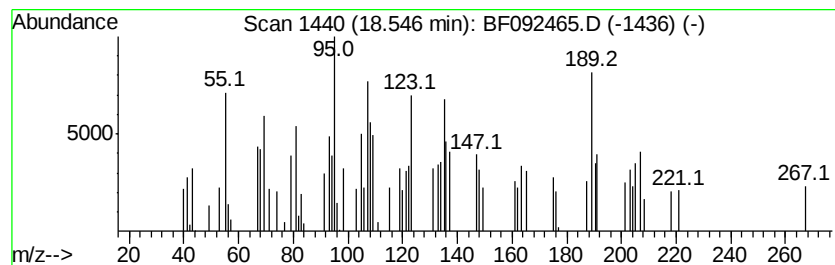
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown18.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.92 ng	133785	Perylene-d12	15.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Spiro[5.5]undec-2-ene, 3,7,7-tri...	204 C15H24	018431-82-8 30
2		6-Isopropenyl-4,8a-dimethyl-4a,5...	218 C15H220	086917-79-5 18
3		Azulene, 1,2,3,5,6,7,8,8a-octahv...	204 C15H24	003691-11-0 14
4		Azulene, 1,2,3,4,5,6,7,8-octahyd...	204 C15H24	003691-12-1 11
5		Sesquirosefuran	218 C15H220	039007-93-7 11



Data Path : Z:\HPCHEM1\BNA_F\Data\BF012517\
Data File : BF092465.D
Acq On : 25 Jan 2017 9:57
Operator : UM/SJ
Sample : I1305-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0024

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.16	7.1 ng		2005290	1	6.97	5662840	20.0
Vanillin	9.48	2.1 ng		173212	3	10.03	1671340	20.0
Hexadecane	10.46	3.1 ng		259692	3	10.03	1671340	20.0
2,6,10,14,18,22-T...	15.03	2.8 ng		128914	6	15.64	915824	20.0
Heneicosane	16.12	4.8 ng		218787	6	15.64	915824	20.0
1-Hentetracontanol	16.17	5.0 ng		228349	6	15.64	915824	20.0
Hentriacontane	17.25	3.2 ng		144552	6	15.64	915824	20.0
17-Pentatriacontene	17.33	3.6 ng		164693	6	15.64	915824	20.0
unknown17.72	17.72	4.2 ng		190890	6	15.64	915824	20.0
unknown17.83	17.83	2.7 ng		125332	6	15.64	915824	20.0
unknown18.55	18.55	2.9 ng		133785	6	15.64	915824	20.0