

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
 Data File : BF092262.D
 Acq On : 14 Jan 2017 00:46
 Operator : UM/SJ
 Sample : I1031-09
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0025

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	3.970	188	191	201	rBV	48337	115917	2.50%	0.254%
2	4.701	252	255	267	rBV	1411055	2152355	46.45%	4.722%
3	5.170	293	296	312	rBV	4324364	4480932	96.70%	9.831%
4	6.244	387	390	392	rBV	3797419	4633939	100.00%	10.167%
5	6.347	397	399	401	rVB	4683406	4479054	96.66%	9.827%
6	6.576	416	419	421	rBV	1072306	1234261	26.64%	2.708%
7	6.724	430	432	435	rBV	2859647	3220969	69.51%	7.067%
8	7.147	466	469	471	rBV	2724237	2946516	63.59%	6.465%
9	7.285	480	481	487	rBV2	33269	58007	1.25%	0.127%
10	7.856	529	531	534	rBV	1506439	1623402	35.03%	3.562%
11	8.942	623	626	628	rBV	4297056	4297056	92.73%	9.428%
12	9.342	658	661	663	rBV	1171718	1031154	22.25%	2.262%
13	9.605	682	684	687	rVB	1566818	1612449	34.80%	3.538%
14	10.062	720	724	725	rBV	59908	75805	1.64%	0.166%
15	10.393	751	753	756	rBV2	2143139	2484409	53.61%	5.451%
16	10.531	763	765	771	rVB	103663	130673	2.82%	0.287%
17	10.976	802	804	805	rBV2	70158	69598	1.50%	0.153%
18	11.079	811	813	816	rBV	1200426	1607590	34.69%	3.527%
19	11.331	833	835	839	rVB	53402	67591	1.46%	0.148%
20	11.639	860	862	866	rBV2	224385	222801	4.81%	0.489%
21	12.291	917	919	921	rBV	72761	63050	1.36%	0.138%
22	12.508	936	938	941	rBV2	68572	99217	2.14%	0.218%
23	12.668	949	952	955	rBV	3128014	3393511	73.23%	7.446%
24	12.919	970	974	976	rBV3	25483	55853	1.21%	0.123%
25	13.582	1029	1032	1041	rBV	298245	461510	9.96%	1.013%
26	13.708	1041	1043	1046	rBV	1312830	1346774	29.06%	2.955%
27	14.211	1084	1087	1090	rBV	100781	171399	3.70%	0.376%
28	14.622	1120	1123	1126	rBV	131835	130731	2.82%	0.287%
29	14.702	1128	1130	1135	rBV	26391	52656	1.14%	0.116%
30	14.805	1135	1139	1145	rBV2	105871	310472	6.70%	0.681%
31	15.068	1159	1162	1164	rBV	686709	980404	21.16%	2.151%
32	15.102	1164	1165	1169	rVB	47090	53156	1.15%	0.117%
33	15.274	1177	1180	1185	rBV	39806	59638	1.29%	0.131%
34	15.468	1194	1197	1199	rBV	111904	178500	3.85%	0.392%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.514	1199	1201	1204	rVV2	39397	72715	1.57%	0.160%
36	15.880	1230	1233	1238	rVB2	37500	61293	1.32%	0.134%
37	16.120	1250	1254	1257	rBV3	27849	57702	1.25%	0.127%
38	16.303	1266	1270	1272	rBV3	28915	61167	1.32%	0.134%
39	16.360	1272	1275	1276	rVV	49161	97983	2.11%	0.215%
40	16.405	1276	1279	1285	rVV	308564	671514	14.49%	1.473%
41	16.497	1285	1287	1289	rVV2	45948	101237	2.18%	0.222%
42	16.531	1289	1290	1297	rVB	67821	118122	2.55%	0.259%
43	16.668	1299	1302	1305	rVB3	34489	66494	1.43%	0.146%
44	16.760	1306	1310	1315	rBV5	51526	136051	2.94%	0.299%
45	17.068	1334	1337	1341	rVB5	28758	64566	1.39%	0.142%
46	17.274	1351	1355	1358	rBV5	19348	48686	1.05%	0.107%
47	17.583	1379	1382	1386	rVB3	23653	58948	1.27%	0.129%
48	18.417	1449	1455	1462	rVB10	13493	60051	1.30%	0.132%

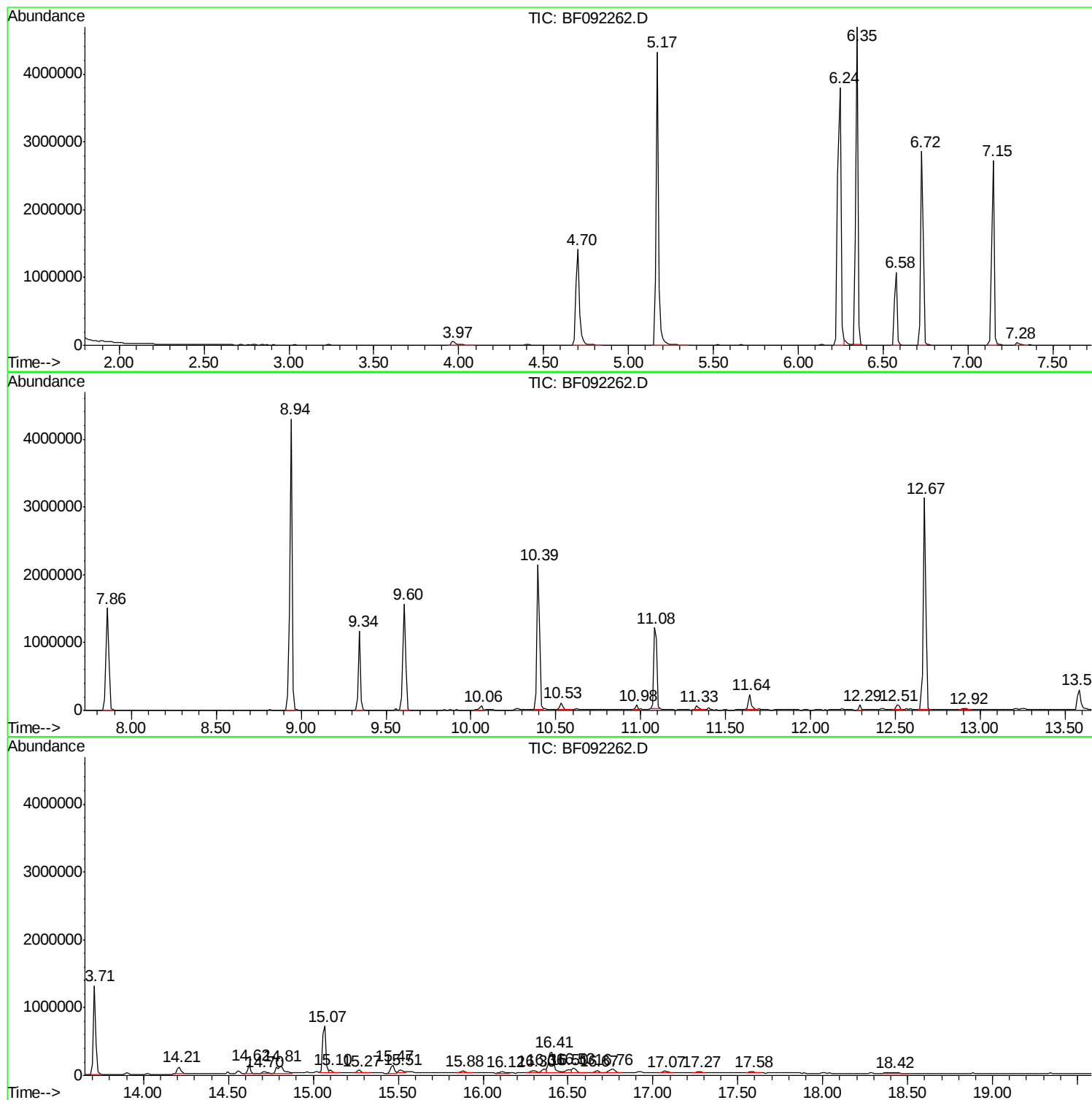
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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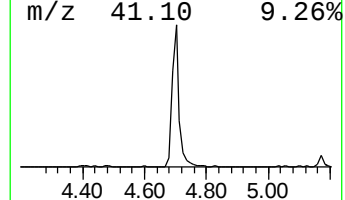
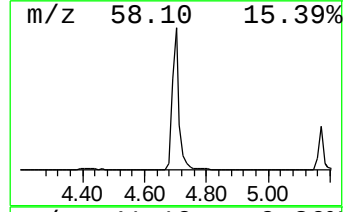
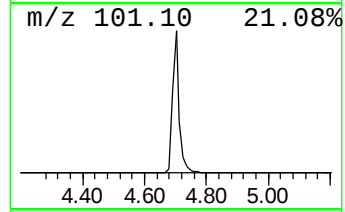
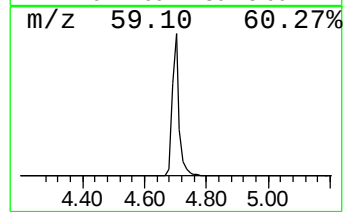
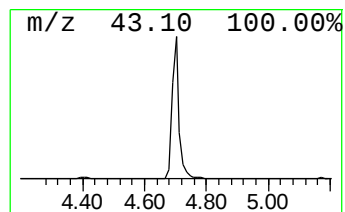
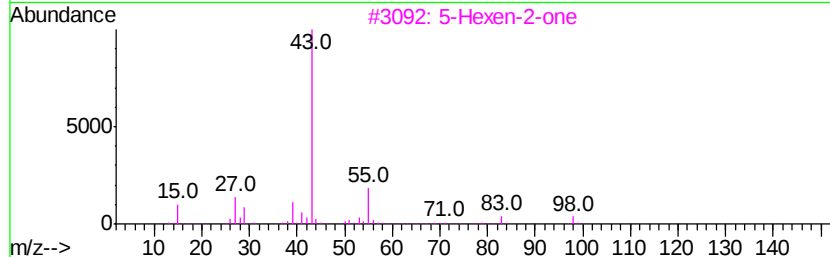
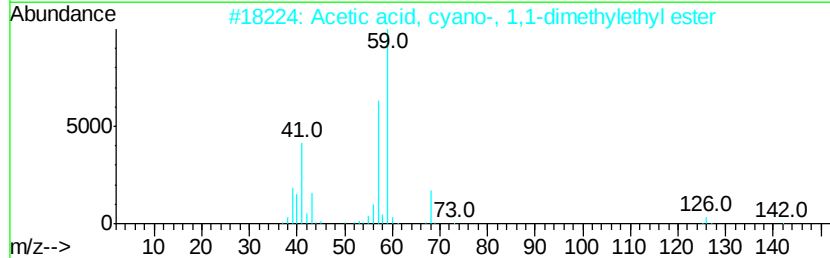
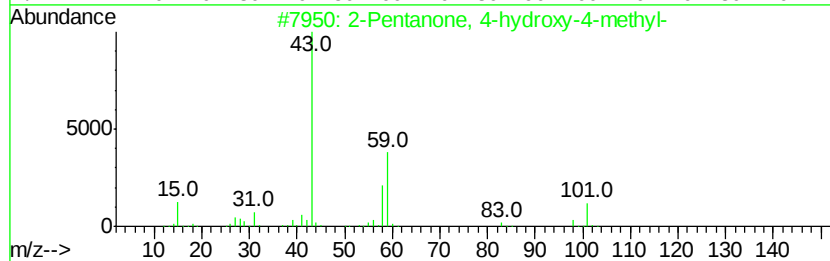
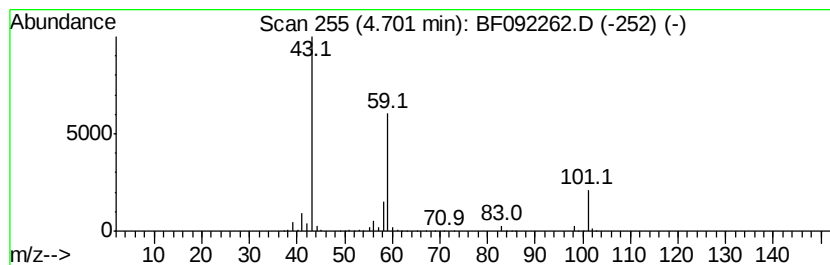
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	34.88 ng	2152360	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	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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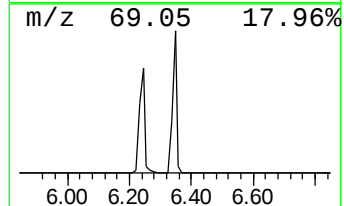
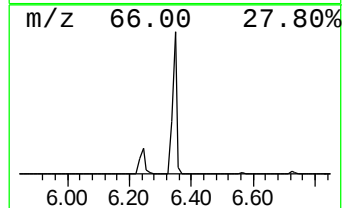
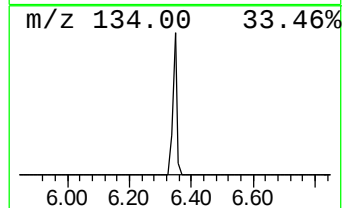
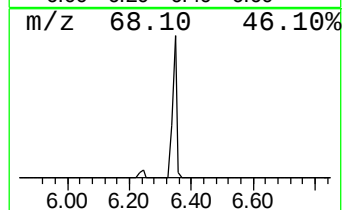
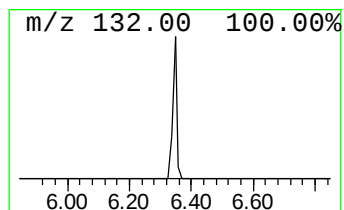
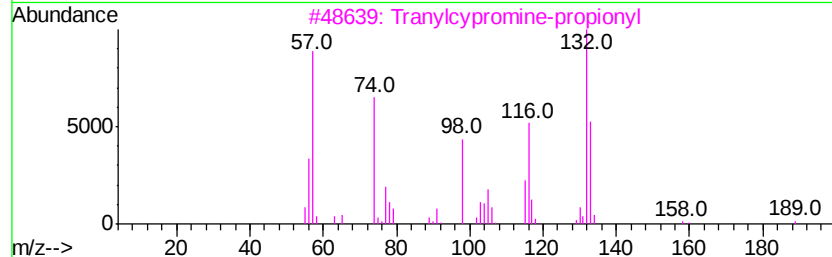
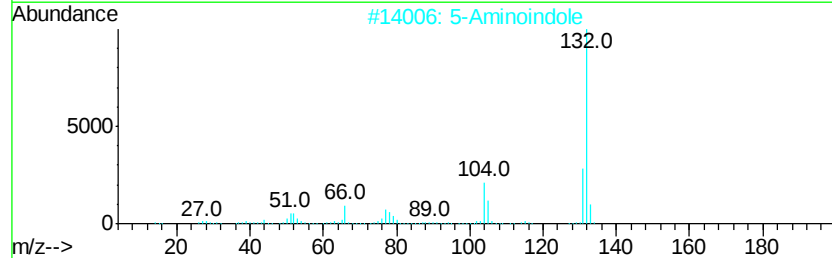
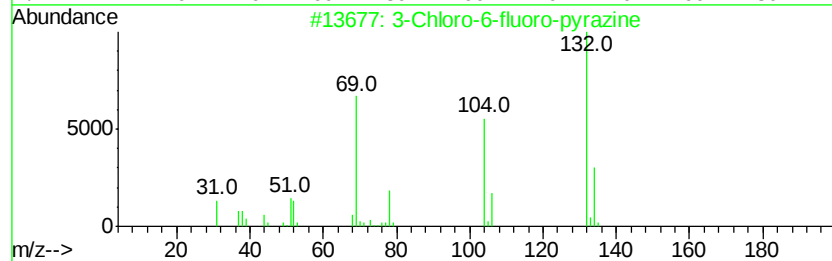
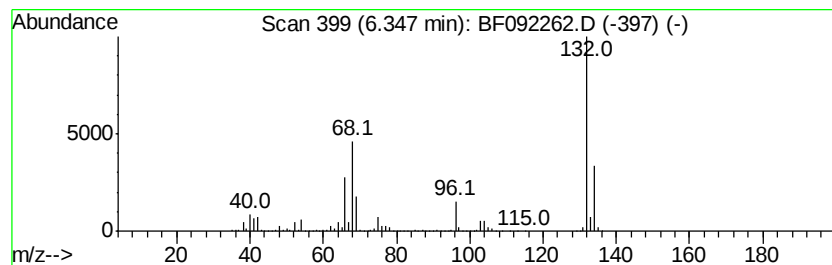
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	72.58 ng	4479050	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	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			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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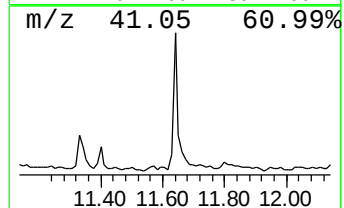
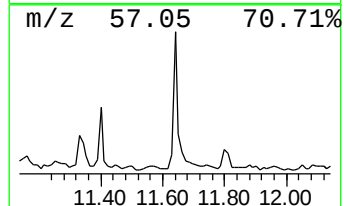
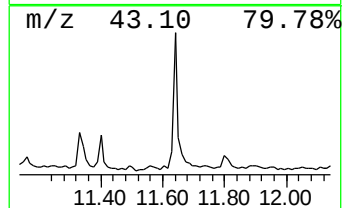
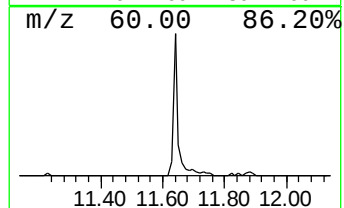
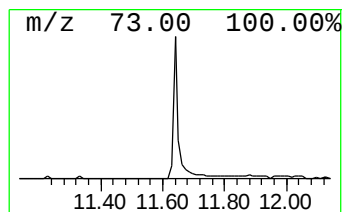
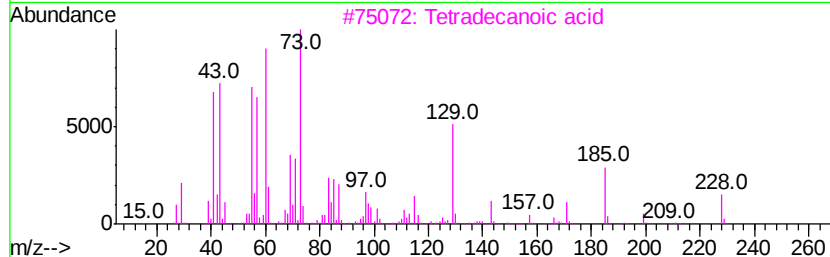
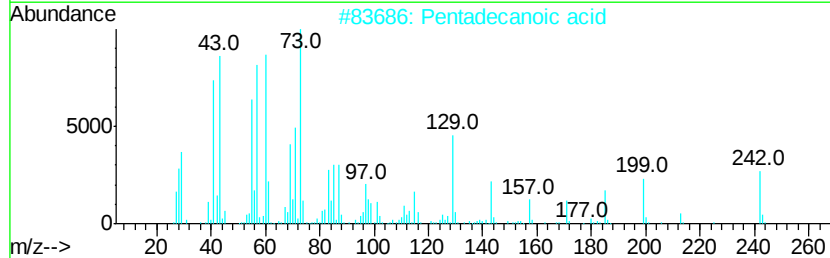
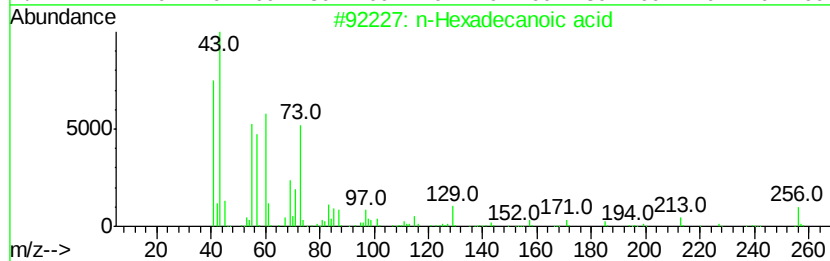
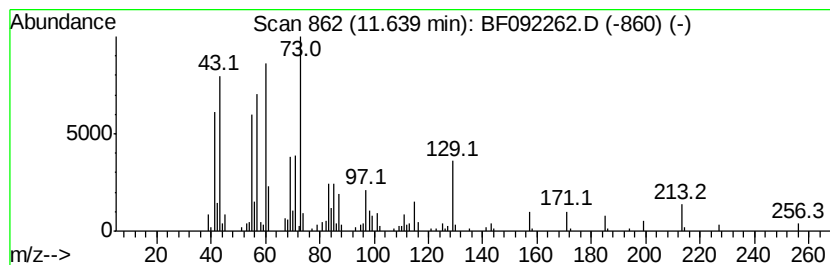
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	2.77 ng	222801	Phenanthrene-d10	11.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	18



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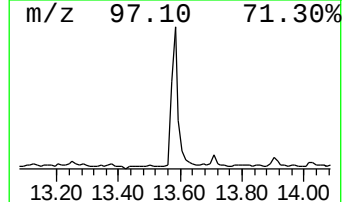
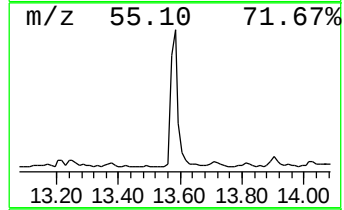
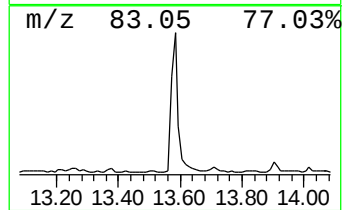
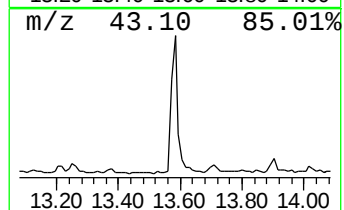
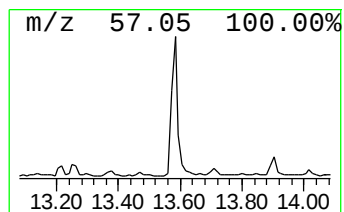
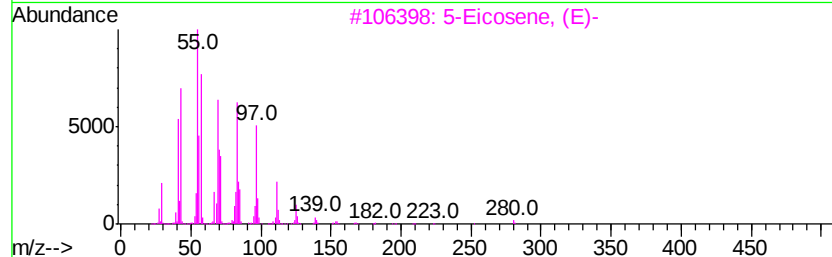
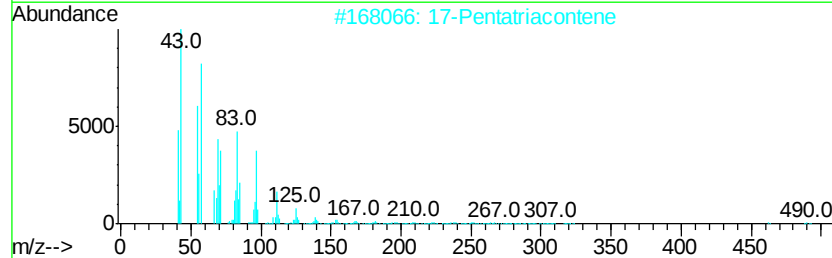
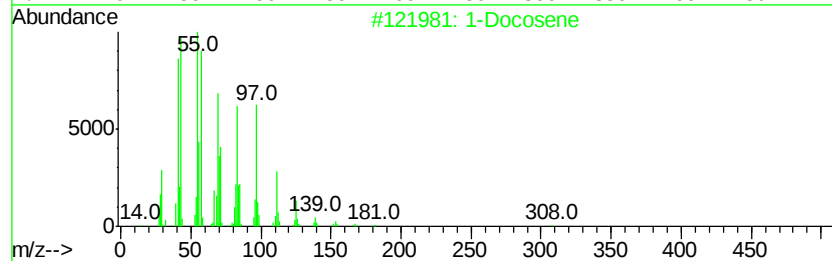
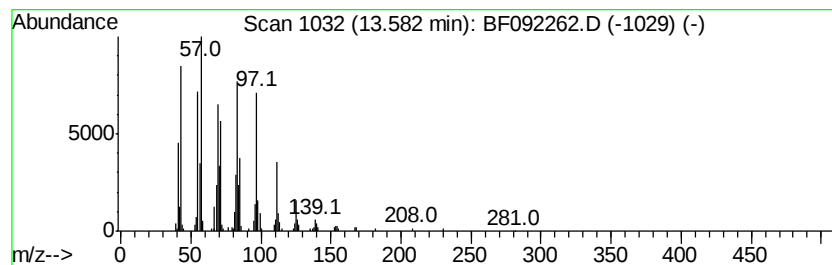
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	6.85 ng	461510	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	90
2	17-Pentatriacontene		491	C35H70	006971-40-0	87
3	5-Eicosene, (E)-		280	C20H40	074685-30-6	87
4	1-Octadecanol		270	C18H38O	000112-92-5	87
5	1-Nonadecene		266	C19H38	018435-45-5	83



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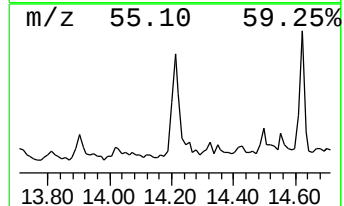
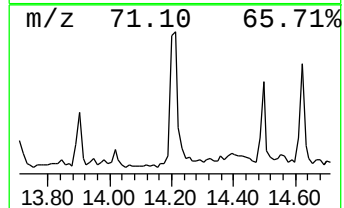
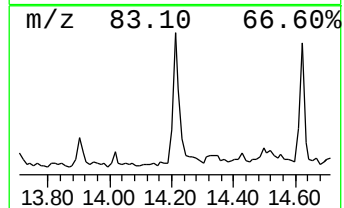
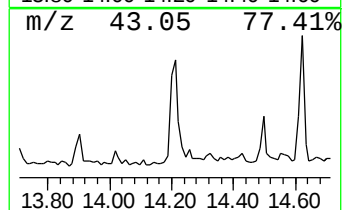
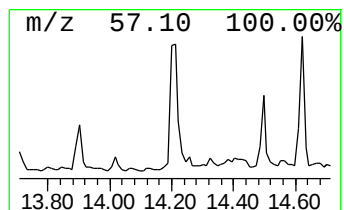
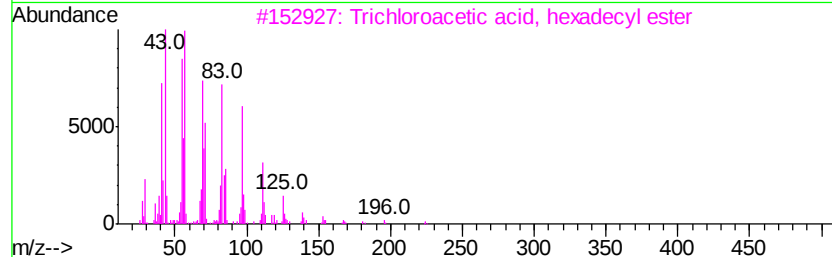
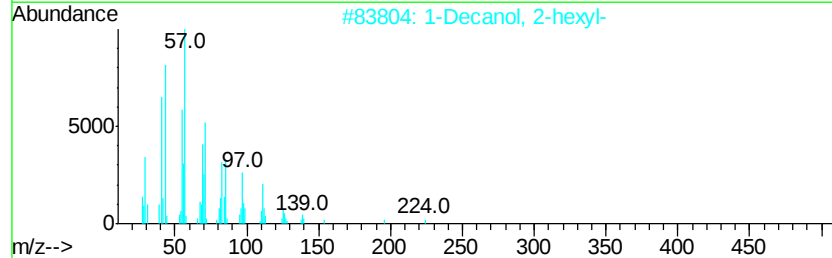
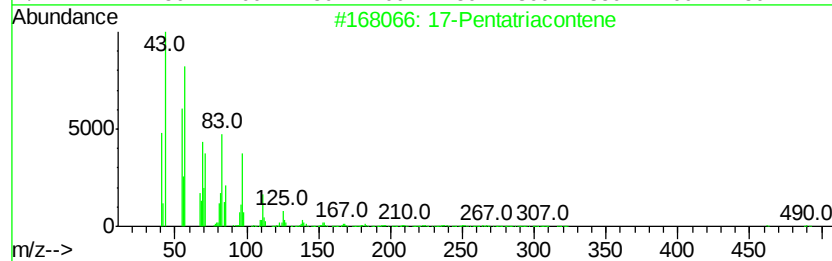
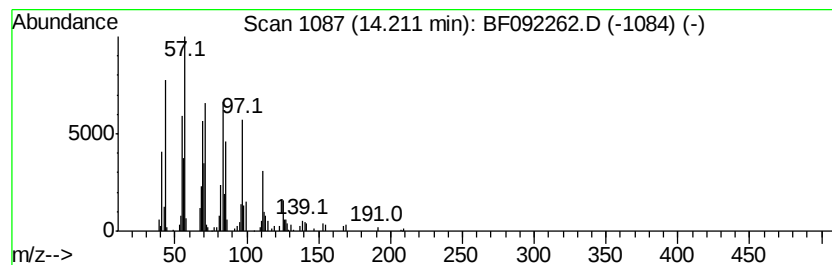
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17-Pentatriacontene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.55 ng	171399	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	83
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	72
4		2-Hexyl-1-octanol	214	C14H30O	019780-79-1	72
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092262.D
Acq On : 14 Jan 2017 00:46
Operator : UM/SJ
Sample : I1031-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

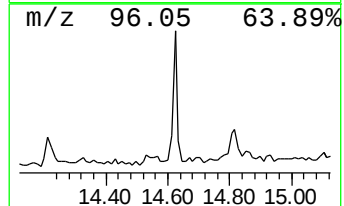
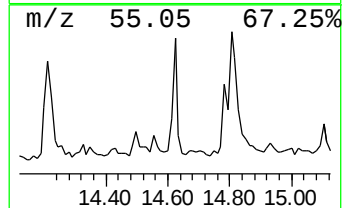
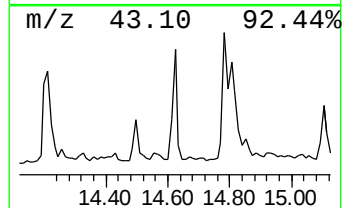
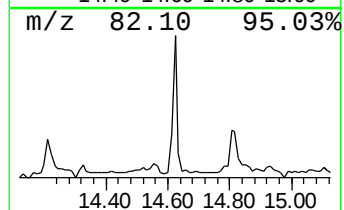
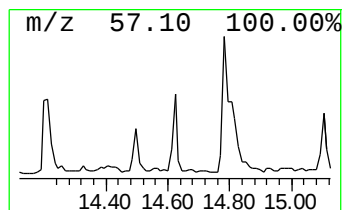
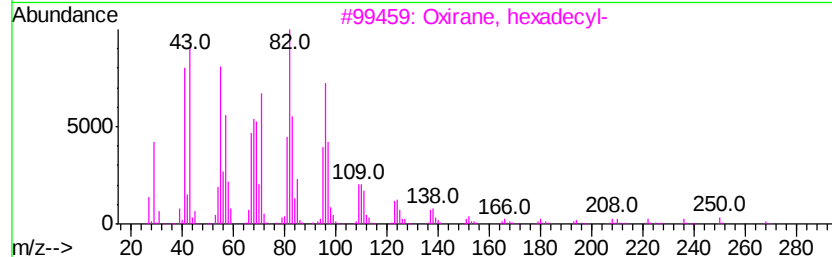
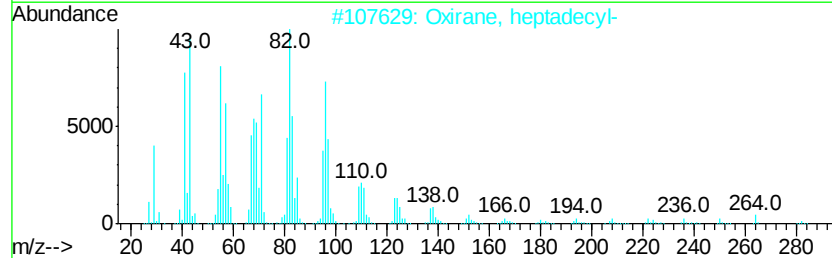
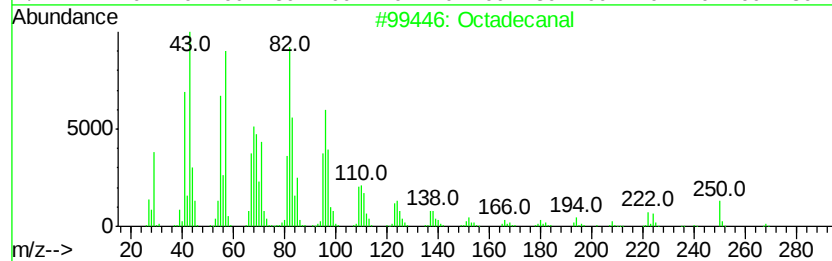
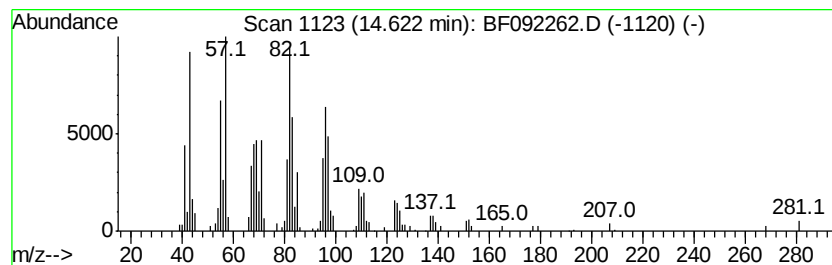
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.62	2.67 ng	130731	Perylene-d12		15.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	1,19-Eicosadiene	278	C20H38	014811-95-1	74
5	16-Heptadecenal	252	C17H32O	1000144-57-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
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ClientSampleId :
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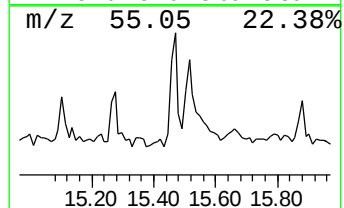
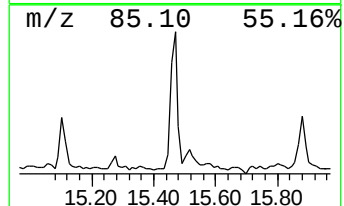
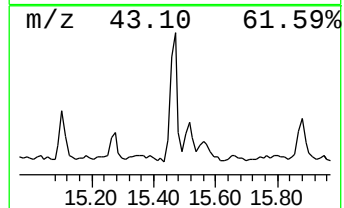
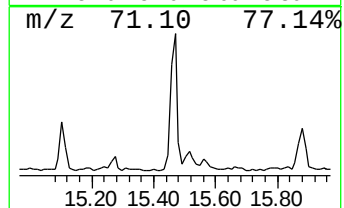
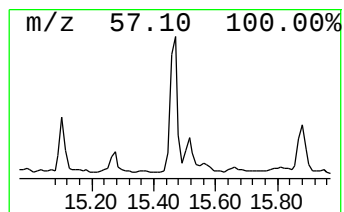
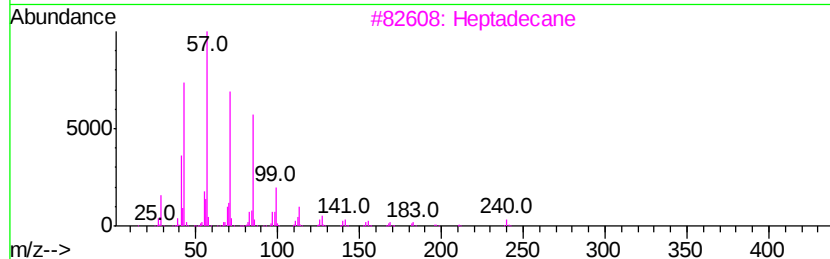
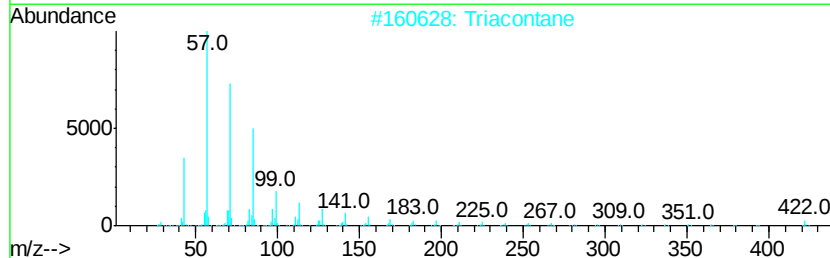
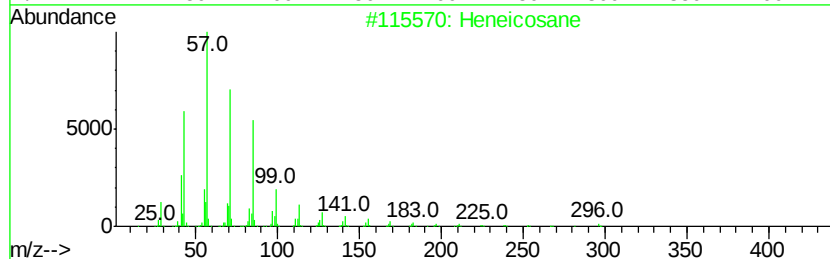
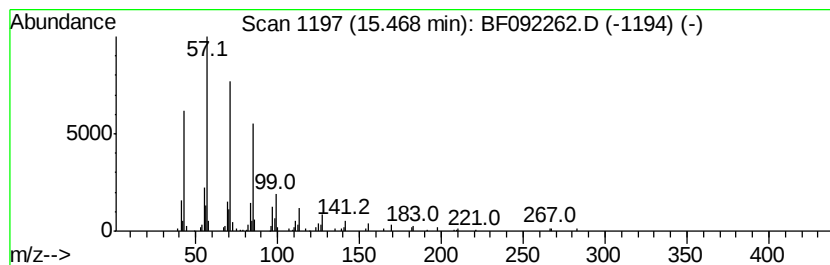
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	3.64 ng	178500	Perylene-d12	15.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacontane		422	C30H62	000638-68-6	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
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Sample : I1031-09
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ClientSampleId :
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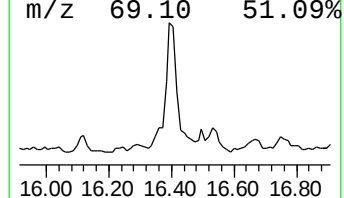
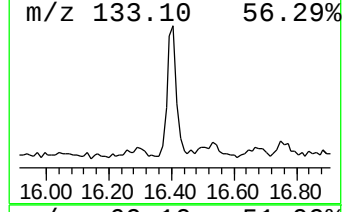
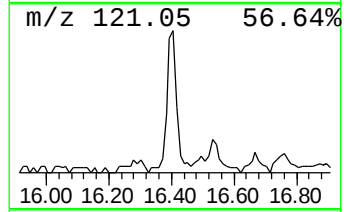
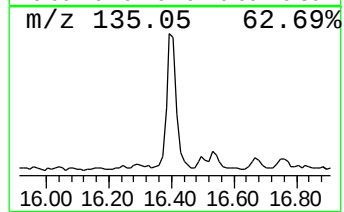
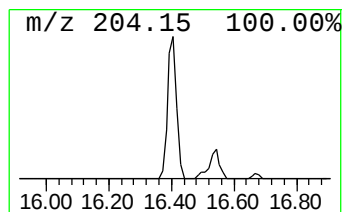
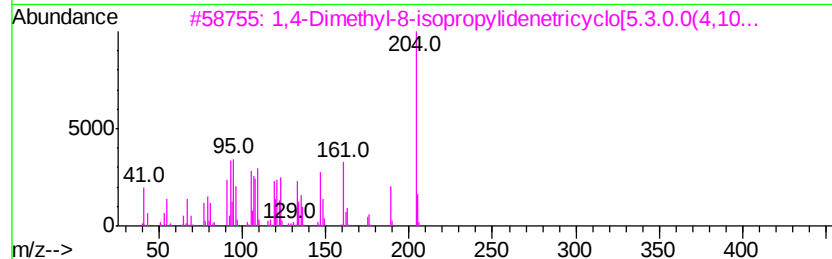
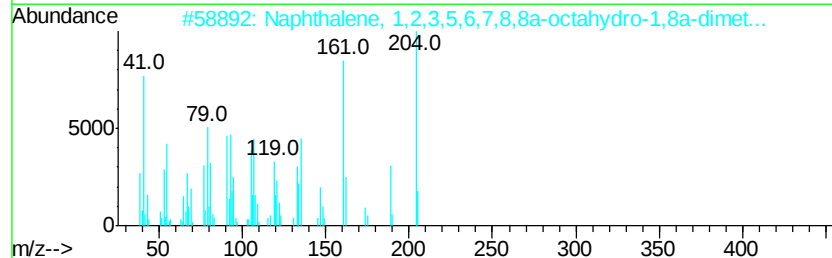
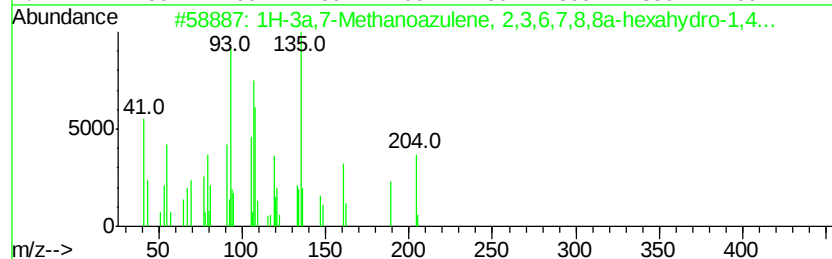
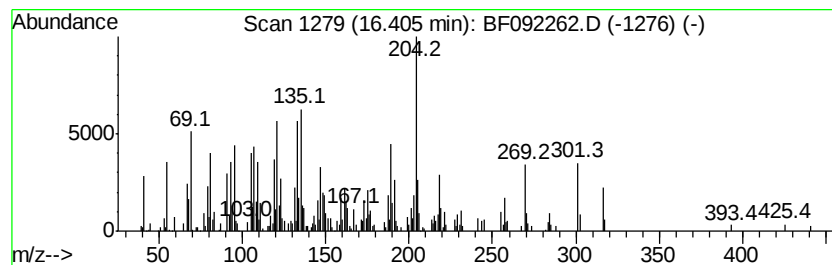
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	13.70 ng	671514	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	53
2		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	50
3		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	49
4		Guaia-3,9-diene	204	C15H24	000489-83-8	47
5		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
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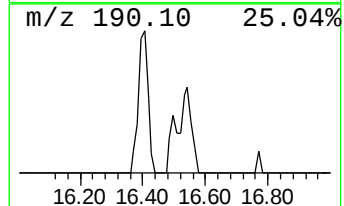
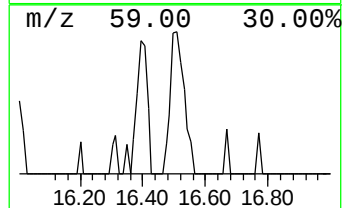
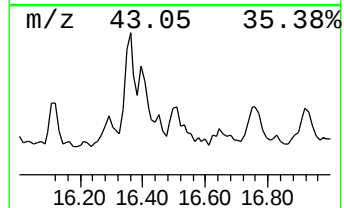
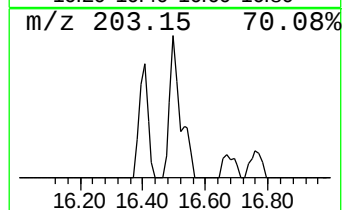
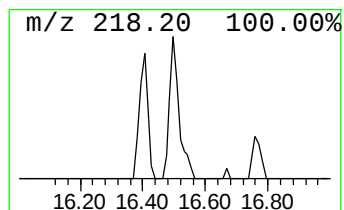
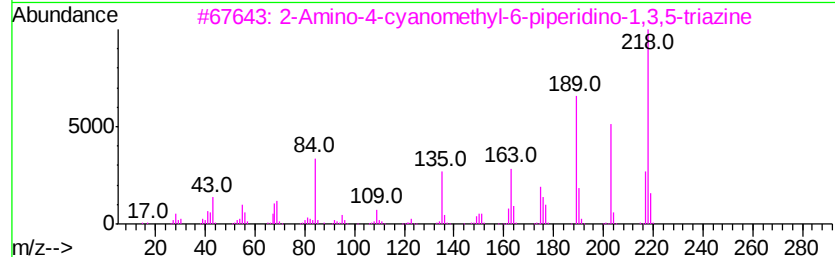
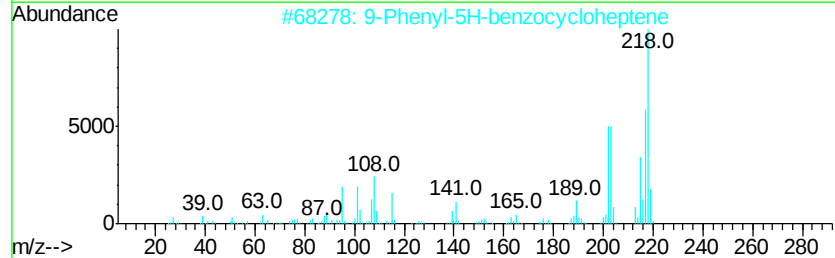
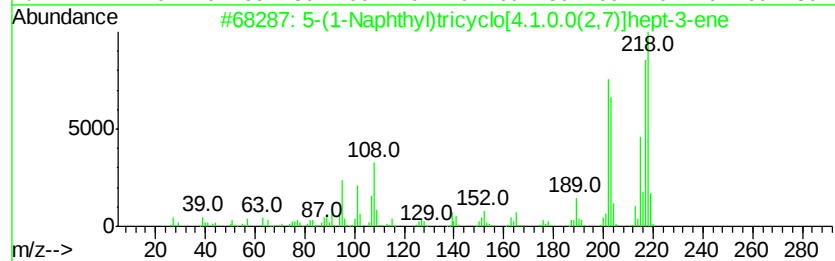
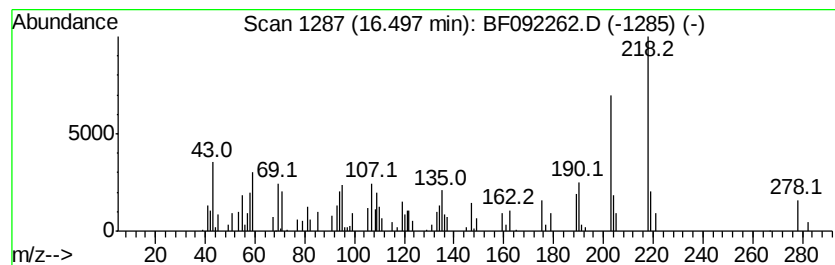
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 5-(1-Naphthyl)tricyclo[4.1.... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.07 ng	101237	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...]	218	C17H14	107729-05-5	53
2		9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	50
3		2-Amino-4-cyanomethyl-6-piperidin...	218	C10H14N6	1000241-05-9	47
4		6,7,8,9-Tetrahydrodibenzo[b,d]fu...	260	C15H16O4	1000196-34-3	47
5		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

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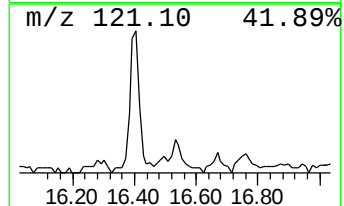
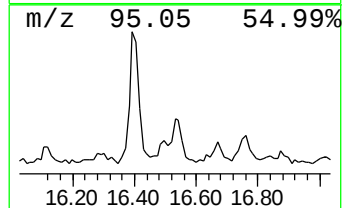
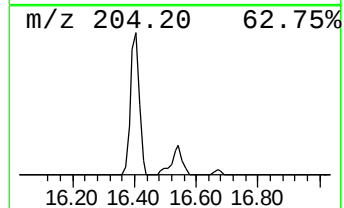
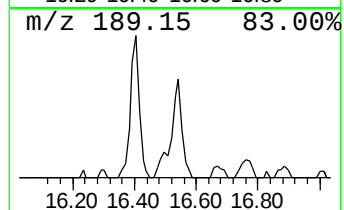
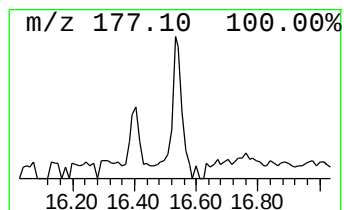
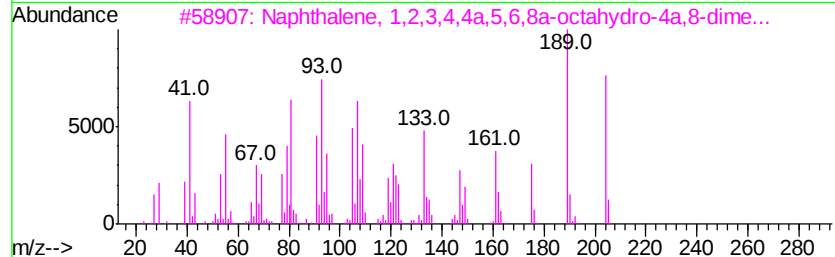
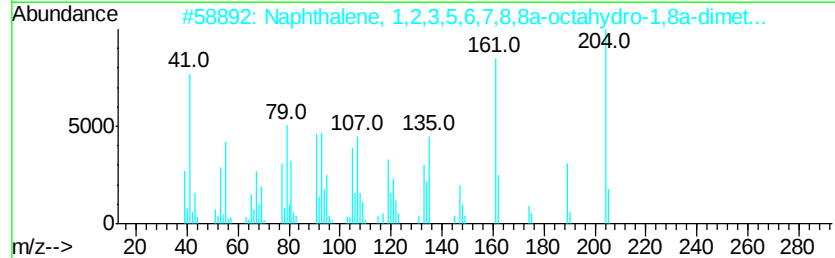
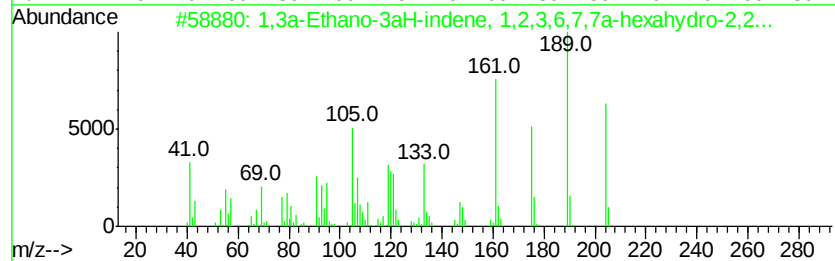
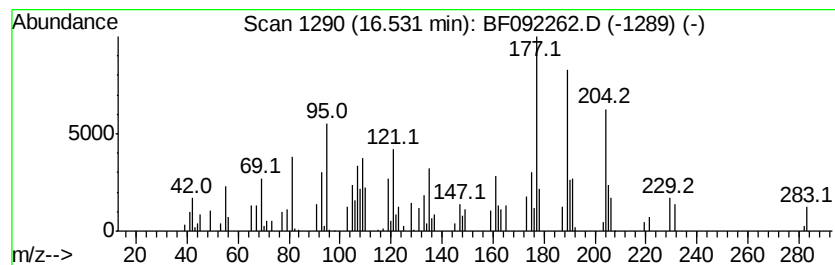
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,3a-Ethano-3aH-indene, 1,2... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.41 ng	118122	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	50
2		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	41
3		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	38
4		1,2-Dicarbadodecaborane(12), 1-[...	234	C6H20B10S	062906-36-9	30
5		3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
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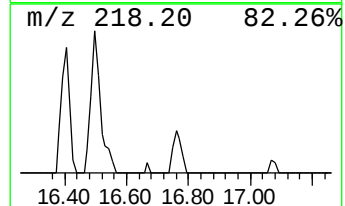
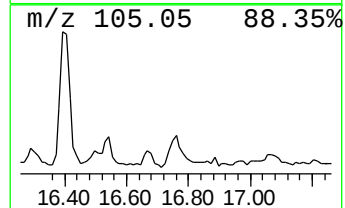
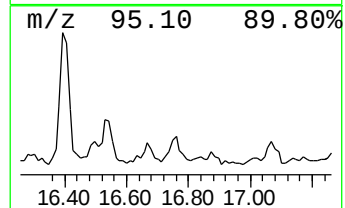
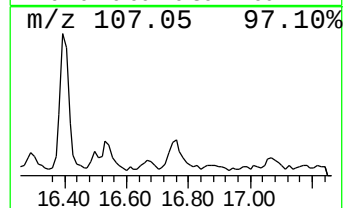
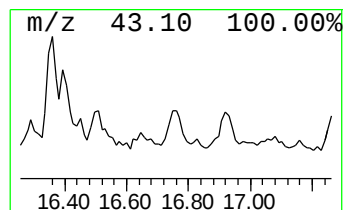
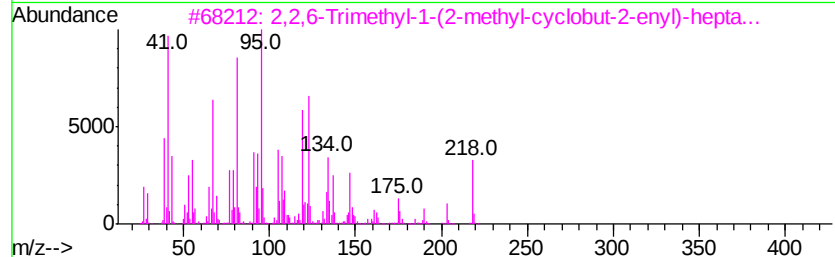
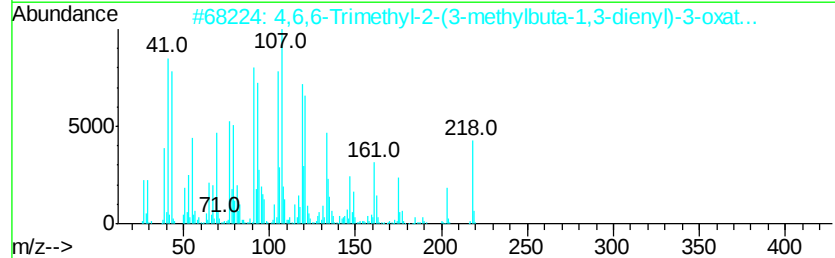
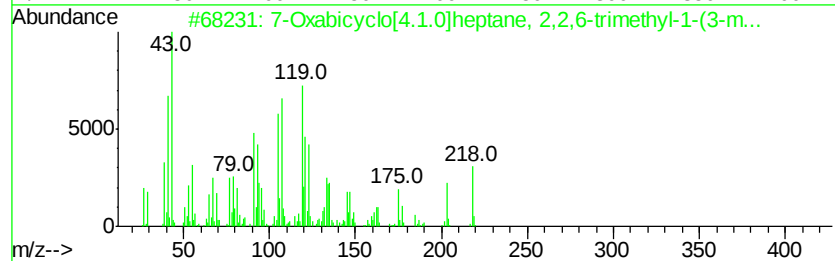
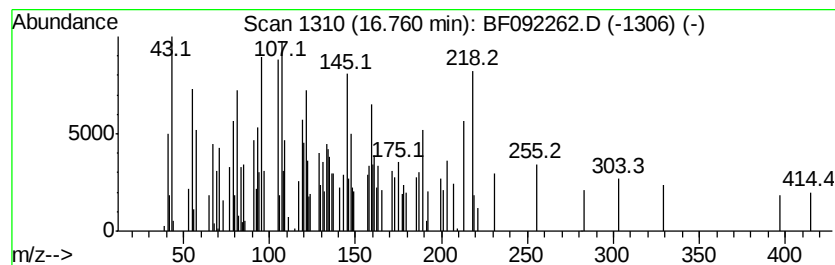
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.76 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	2.78 ng	136051	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	42
2		4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	40
3		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
4		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38
5		Acetic acid, 3-hydroxy-6-isoprop...	278	C17H26O3	1000185-44-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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	34.9	ng	2152360	1	6.58	1234260	20.0
unknown6.35	6.35	72.6	ng	4479050	1	6.58	1234260	20.0
n-Hexadecanoic acid	11.64	2.8	ng	222801	4	11.08	1607590	20.0
1-Docosene	13.58	6.8	ng	461510	5	13.71	1346770	20.0
17-Pentatriacontene	14.21	2.5	ng	171399	5	13.71	1346770	20.0
Octadecanal	14.62	2.7	ng	130731	6	15.07	980404	20.0
Heneicosane	15.47	3.6	ng	178500	6	15.07	980404	20.0
1H-3a,7-Methanoaz...	16.41	13.7	ng	671514	6	15.07	980404	20.0
5-(1-Naphthyl)tri...	16.50	2.1	ng	101237	6	15.07	980404	20.0
1,3a-Ethano-3aH-i...	16.53	2.4	ng	118122	6	15.07	980404	20.0
unknown16.76	16.76	2.8	ng	136051	6	15.07	980404	20.0