

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040216\
 Data File : BF085996.D
 Acq On : 2 Apr 2016 7:51
 Operator : UM/SJ
 Sample : H2055-03
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BH-3(5-10)

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-BF040216.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	4.967	250	252	262	rBV	48437	86174	2.61%	0.290%
2	5.367	285	287	290	rBV	1972853	2519982	76.31%	8.481%
3	6.419	376	379	381	rBV	2482176	2853780	86.42%	9.604%
4	6.545	387	390	392	rBV	2722681	2954842	89.48%	9.945%
5	6.773	408	410	416	rBV	671086	610466	18.49%	2.055%
6	6.922	421	423	426	rBV	1666015	2149553	65.10%	7.234%
7	7.345	457	460	462	rBV	1595770	1950240	59.06%	6.564%
8	8.053	520	522	525	rBV	820196	809325	24.51%	2.724%
9	9.128	614	616	619	rBV	2254526	3013931	91.27%	10.143%
10	9.528	649	651	654	rBV	389328	362860	10.99%	1.221%
11	9.745	667	670	672	rBV	56132	49297	1.49%	0.166%
12	9.802	673	675	678	rVV	686600	879418	26.63%	2.960%
13	10.236	712	713	715	rVB	58978	68489	2.07%	0.231%
14	10.453	729	732	736	rBV	25737	50612	1.53%	0.170%
15	10.602	742	745	747	rBV	1801474	2199948	66.62%	7.404%
16	10.716	753	755	761	rVB	86931	116400	3.53%	0.392%
17	11.162	792	794	795	rBV	41880	39835	1.21%	0.134%
18	11.288	803	805	808	rBV	1064661	952060	28.83%	3.204%
19	11.825	850	852	864	rBV	279962	334657	10.13%	1.126%
20	12.602	918	920	926	rVV2	82427	140957	4.27%	0.474%
21	12.694	926	928	931	rVB	70311	73335	2.22%	0.247%
22	12.877	941	944	946	rBV	3423052	3302112	100.00%	11.113%
23	13.357	980	986	988	rBV	152789	164216	4.97%	0.553%
24	13.402	988	990	991	rVB	50678	44457	1.35%	0.150%
25	13.780	1020	1023	1031	rBV	172252	397841	12.05%	1.339%
26	13.928	1034	1036	1038	rBV	866238	949174	28.74%	3.194%
27	14.431	1078	1080	1086	rVB3	15010	36769	1.11%	0.124%
28	14.751	1106	1108	1111	rBV	380245	357079	10.81%	1.202%
29	15.334	1156	1159	1165	rBV	568690	821264	24.87%	2.764%
30	15.837	1198	1203	1205	rBV5	12613	36447	1.10%	0.123%
31	16.465	1256	1258	1260	rVB2	39190	38083	1.15%	0.128%
32	16.557	1264	1266	1267	rBV2	45019	81563	2.47%	0.275%
33	16.603	1267	1270	1272	rVB4	23300	55024	1.67%	0.185%
34	16.786	1283	1286	1287	rBV3	47559	80976	2.45%	0.273%

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BH-3(5-10)

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-BF040216.M
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35	16.820	1287	1289	1290	rVV2	24930	47272	1.43%	0.159%
36	16.877	1292	1294	1296	rVV3	27063	62842	1.90%	0.211%
37	17.334	1330	1334	1337	rVB6	62254	179574	5.44%	0.604%
38	17.391	1337	1339	1342	rBV4	87666	152598	4.62%	0.514%
39	17.460	1342	1345	1348	rVV5	38030	115909	3.51%	0.390%
40	17.551	1351	1353	1355	rVB3	88905	134614	4.08%	0.453%
41	17.631	1357	1360	1361	rBV2	31261	53981	1.63%	0.182%
42	18.123	1398	1403	1405	rBV6	43460	143971	4.36%	0.485%
43	18.169	1405	1407	1409	rVV3	34903	71279	2.16%	0.240%
44	18.237	1412	1413	1416	rVV3	39024	57650	1.75%	0.194%
45	18.340	1420	1422	1424	rVV3	34203	53572	1.62%	0.180%
46	19.151	1491	1493	1496	rBV3	35358	58577	1.77%	0.197%

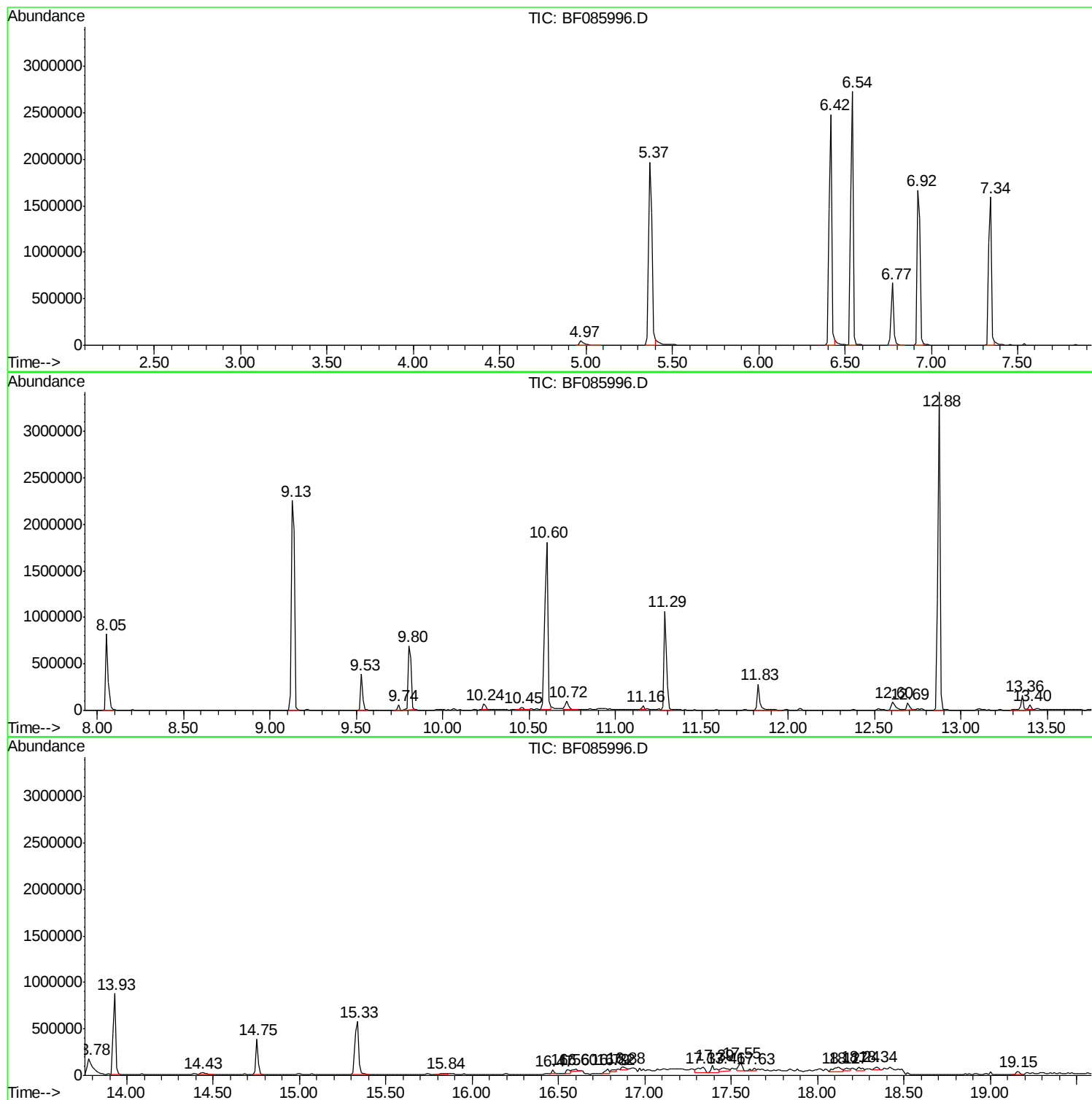
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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BH-3(5-10)

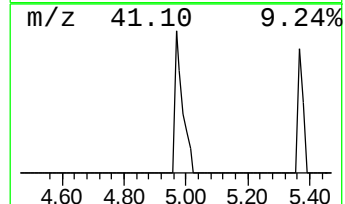
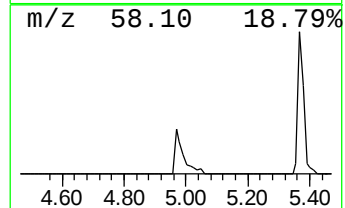
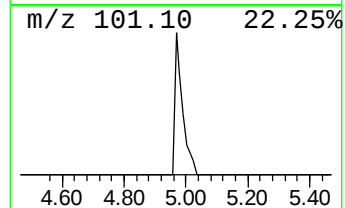
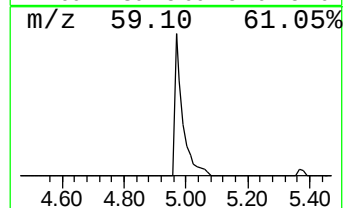
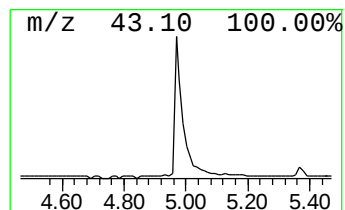
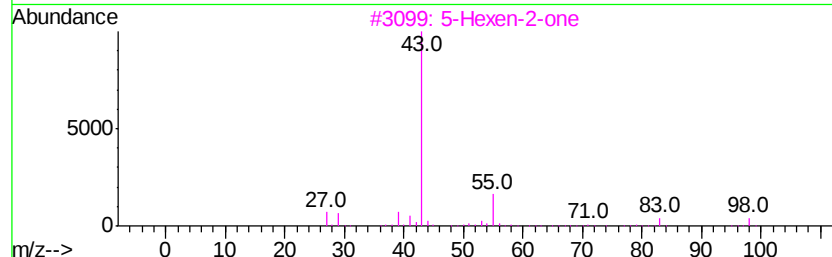
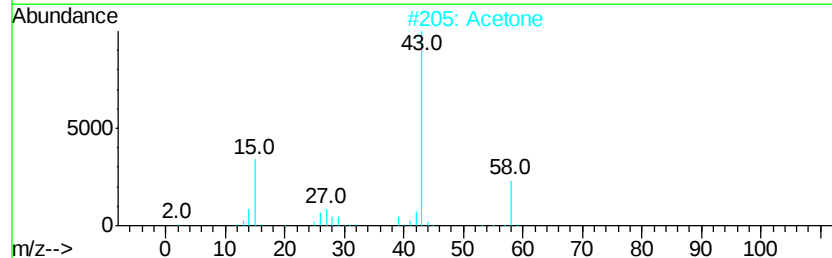
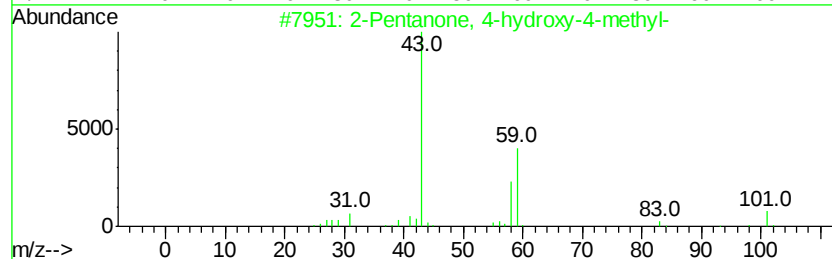
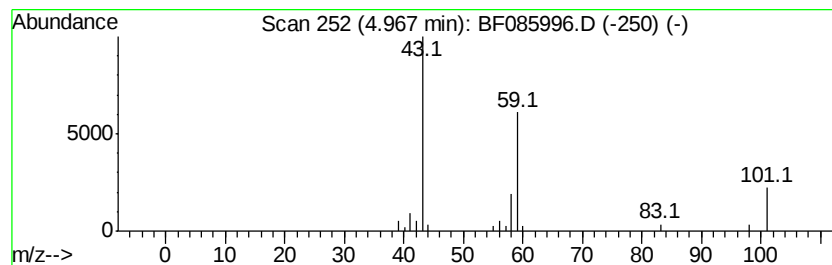
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.82 ng	86174	1,4-Dichlorobenzene-d4	6.77

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetone	58	C3H6O	000067-64-1	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9



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Instrument :
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ClientSampled :
BH-3(5-10)

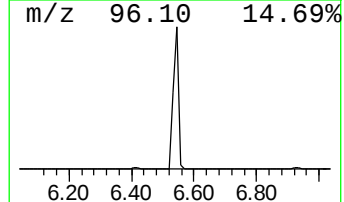
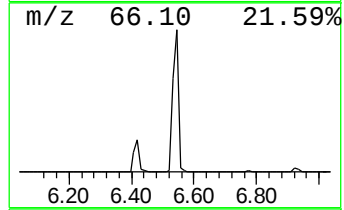
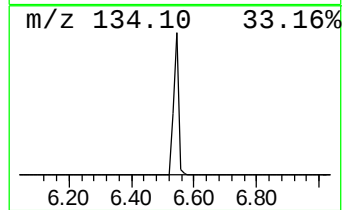
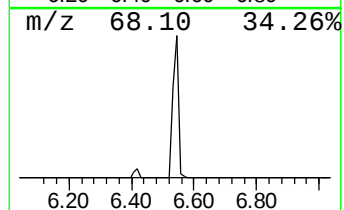
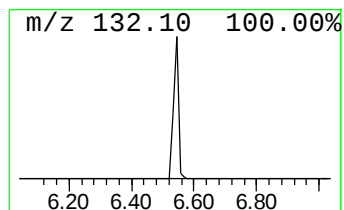
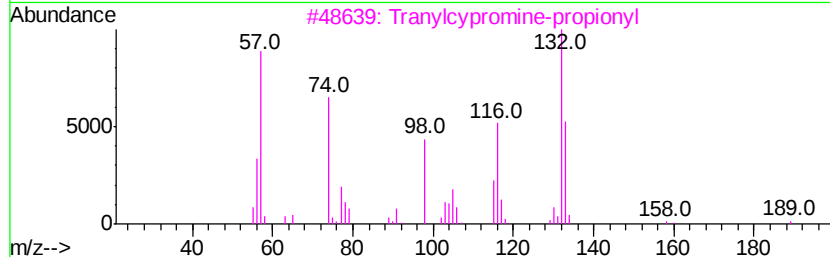
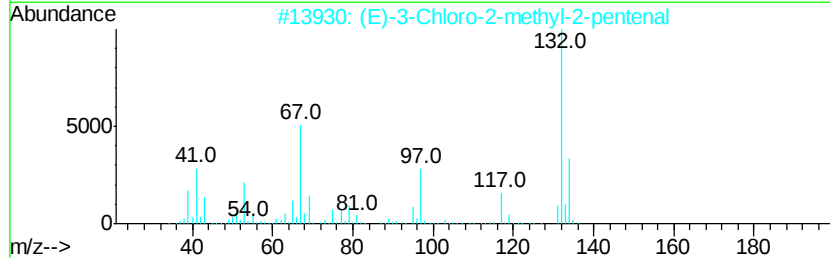
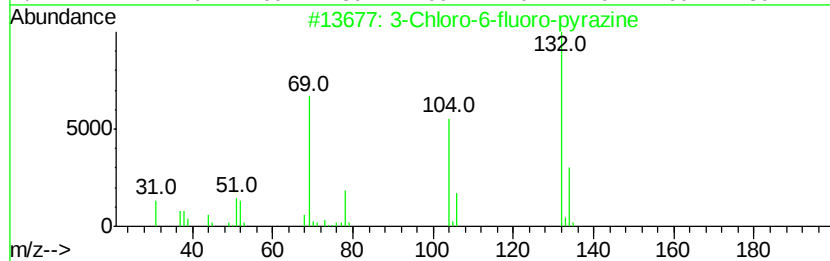
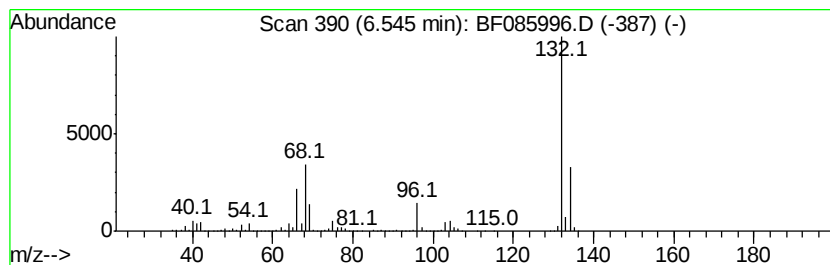
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	96.81 ng	2954840	1,4-Dichlorobenzene-d4	6.77

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	17
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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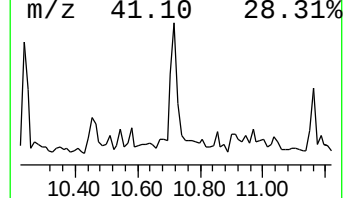
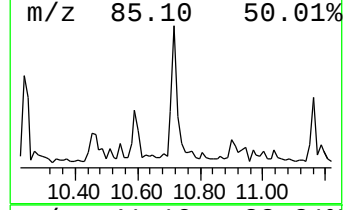
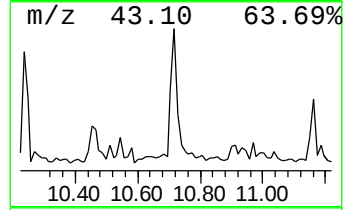
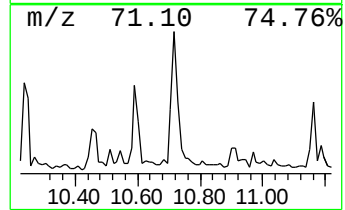
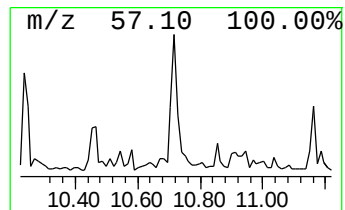
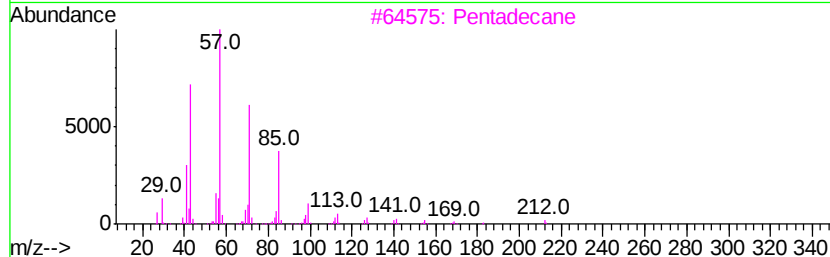
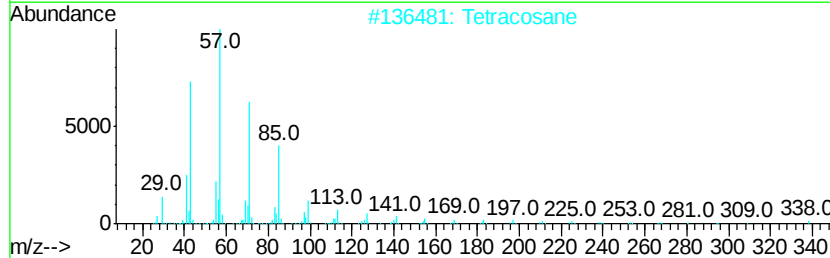
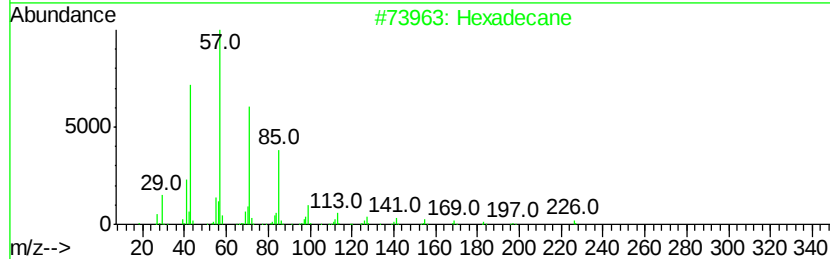
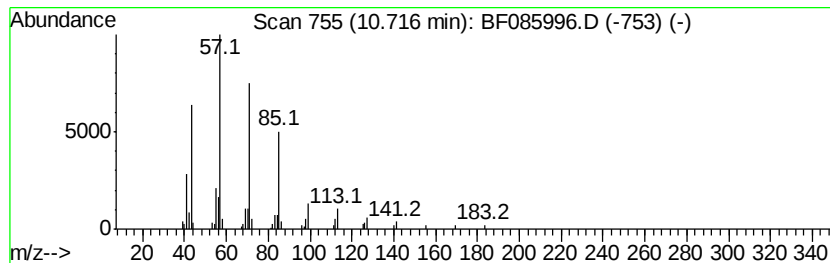
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.72	2.45 ng	116400	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octadecane	254	C18H38	000593-45-3	91



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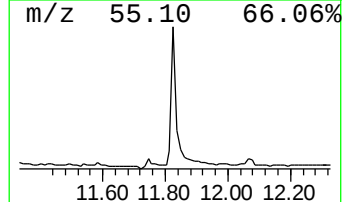
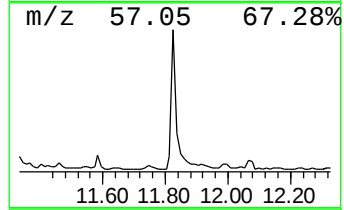
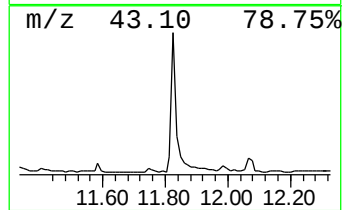
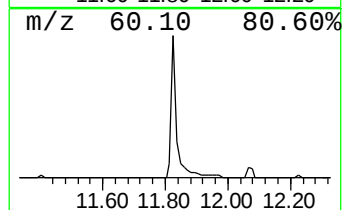
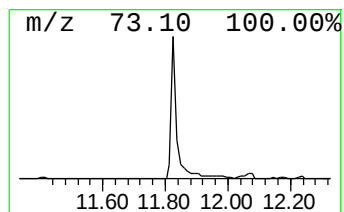
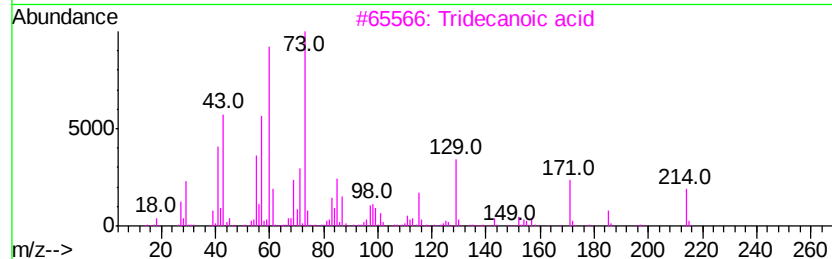
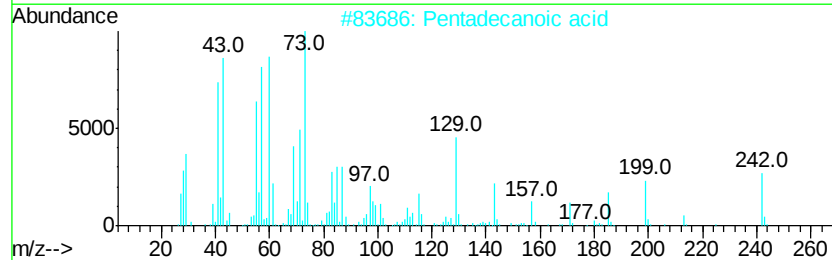
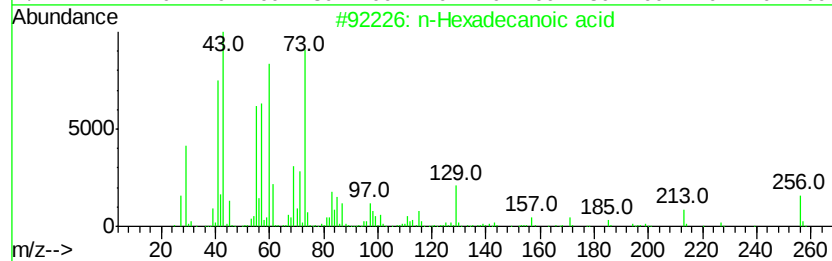
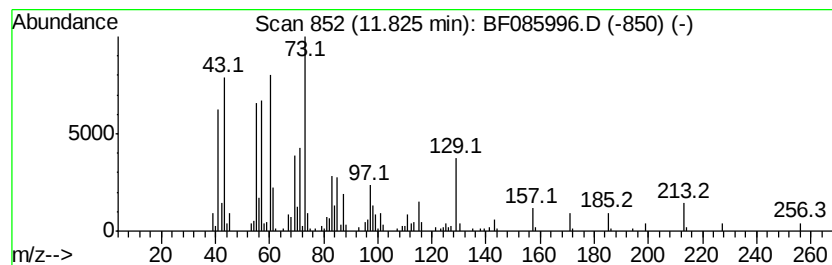
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	7.03 ng	334657	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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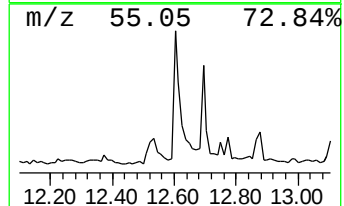
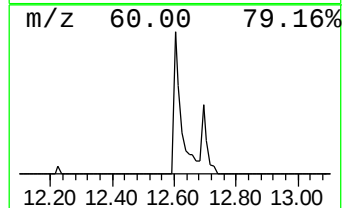
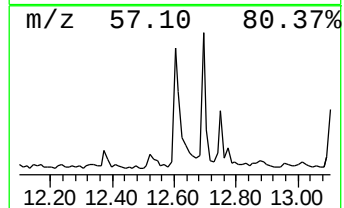
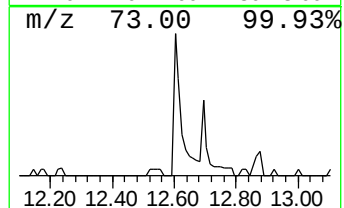
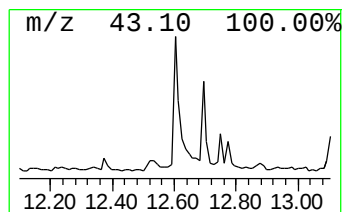
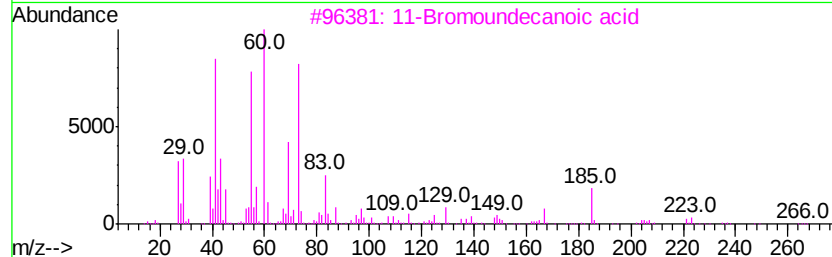
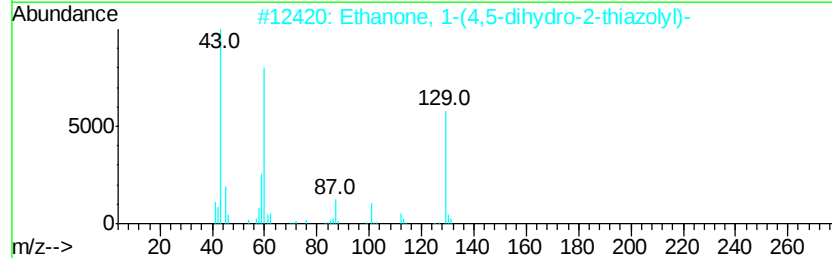
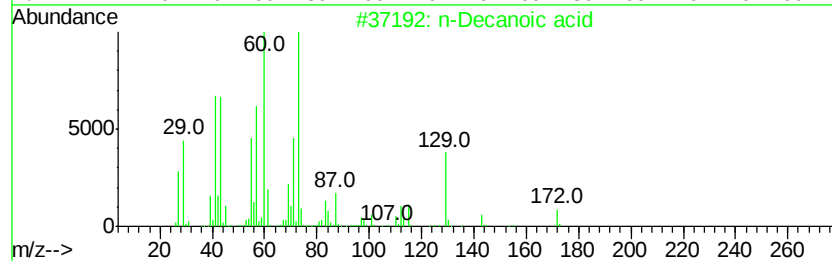
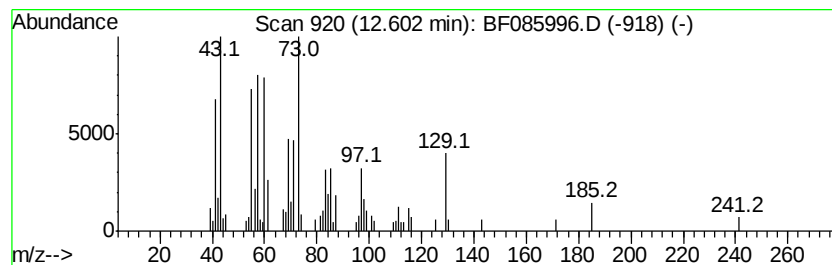
Instrument :
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BH-3(5-10)

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TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Decanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.60	2.96 ng	140957	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
4	17-Pentatriacontene	491	C35H70	006971-40-0	15
5	Tetratetracontane	619	C44H90	007098-22-8	14



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Acq On : 2 Apr 2016 7:51
Operator : UM/SJ
Sample : H2055-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
BH-3(5-10)

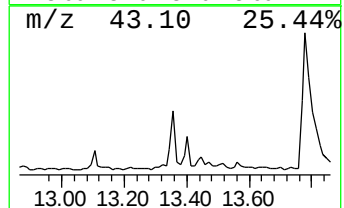
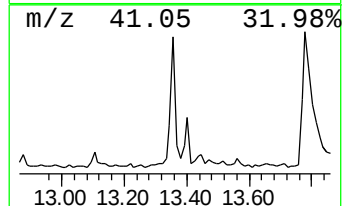
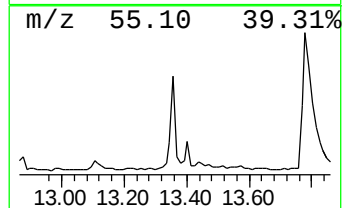
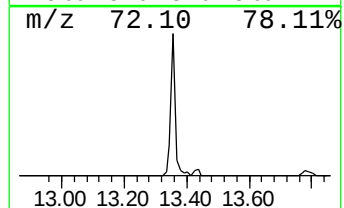
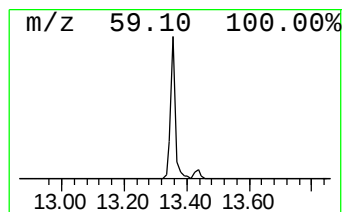
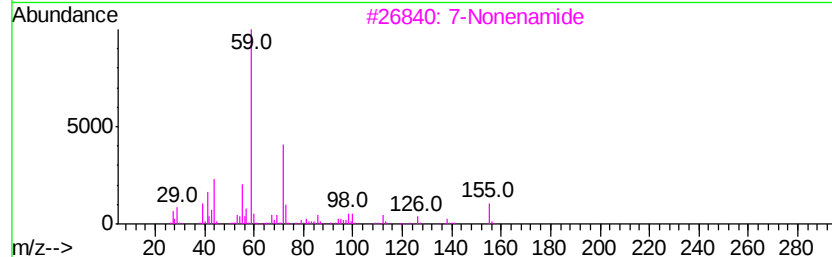
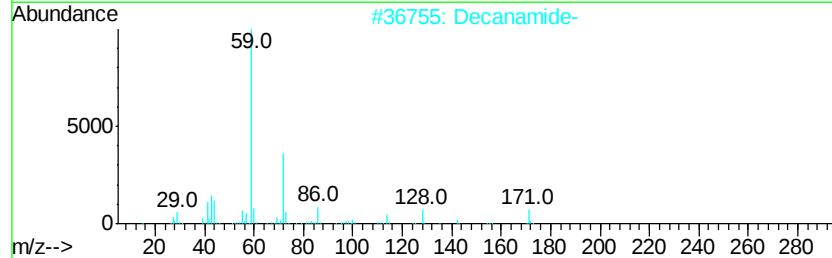
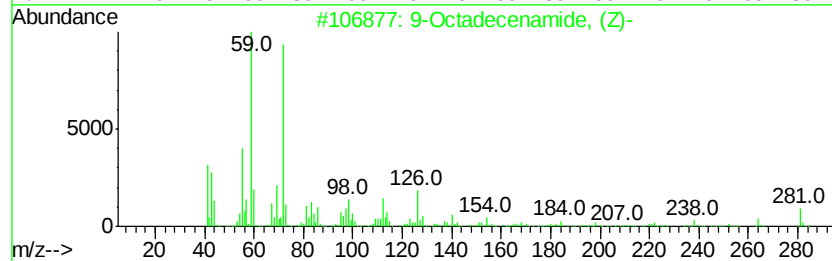
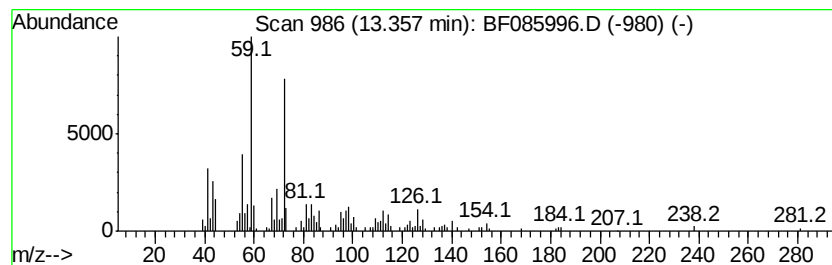
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	3.46 ng	164216	Chrysene-d12	13.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2		Decanamide-	171	C10H21NO	002319-29-1	59
3		7-Nonenamide	155	C9H17NO	090949-53-4	53
4		Tetradecanamide	227	C14H29NO	000638-58-4	43
5		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43



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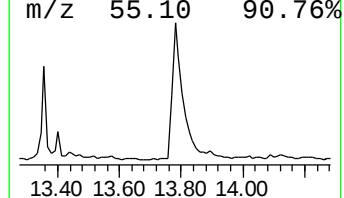
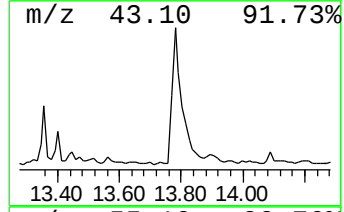
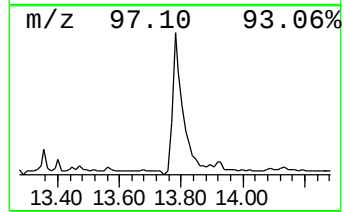
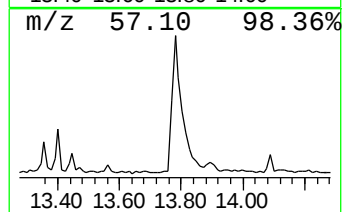
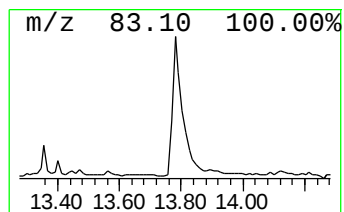
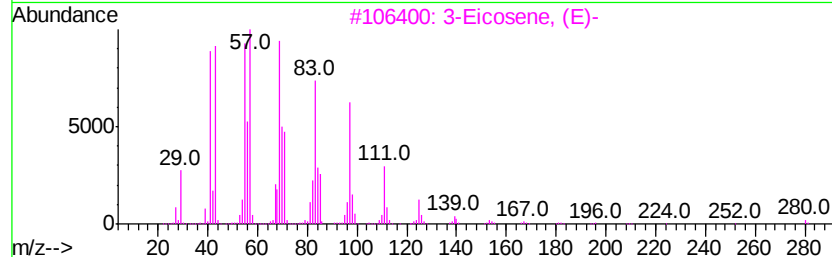
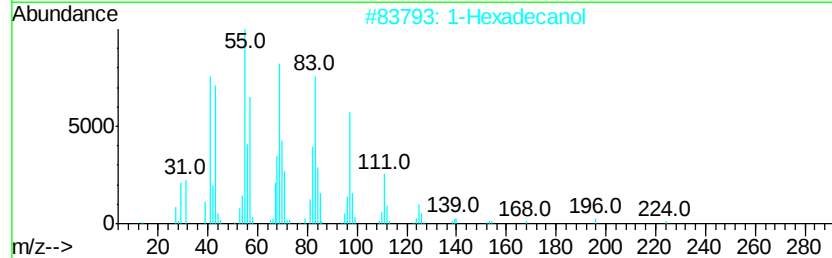
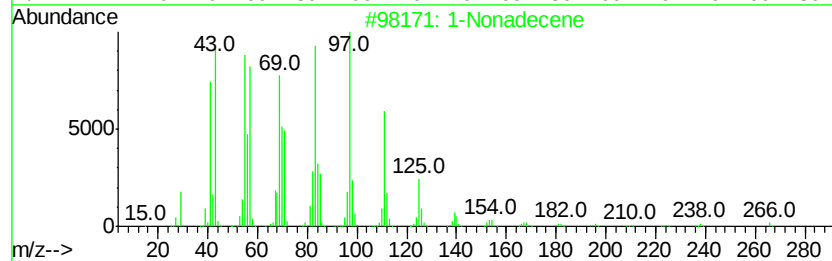
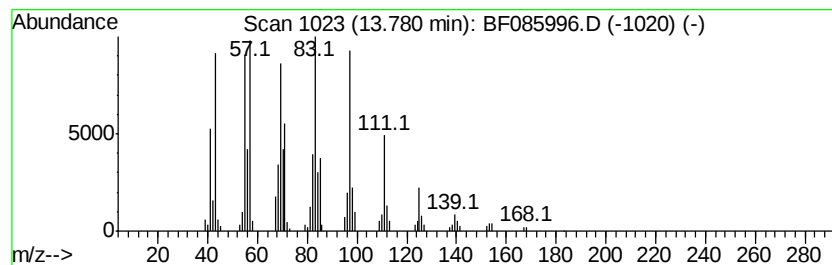
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	8.38 ng	397841	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
5	1-Tetracosanol	354	C24H50O	000506-51-4	87



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Sample : H2055-03
Misc :
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Instrument :
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ClientSampleId :
BH-3(5-10)

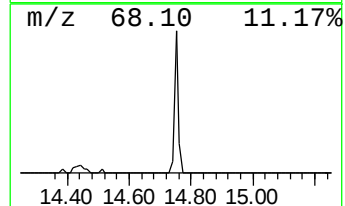
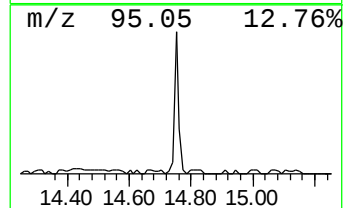
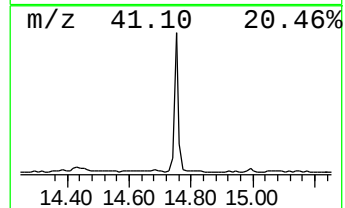
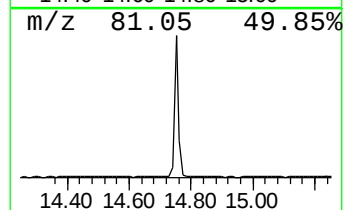
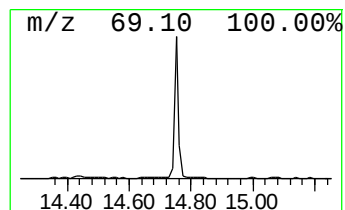
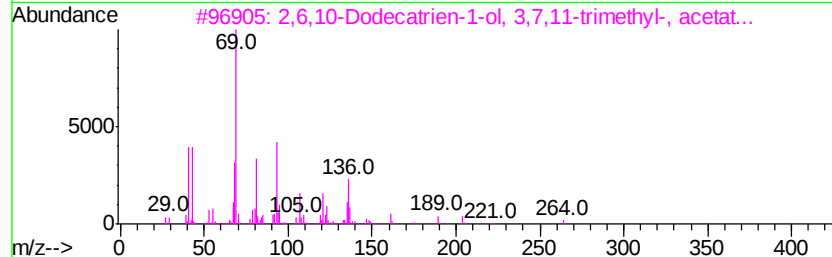
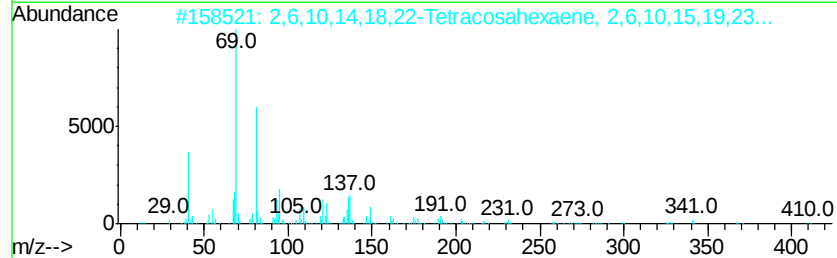
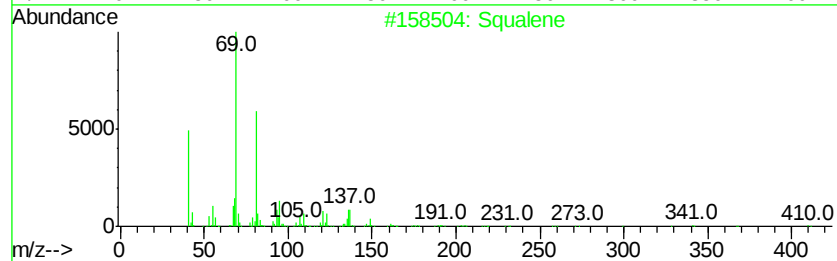
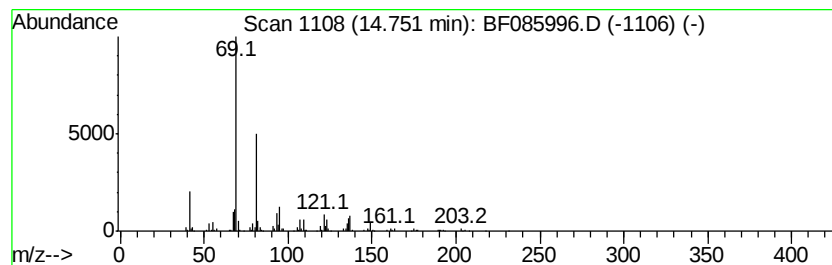
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	8.70 ng	357079	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59



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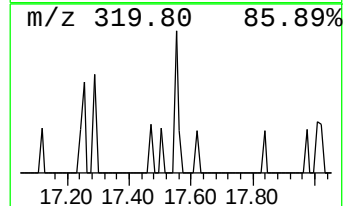
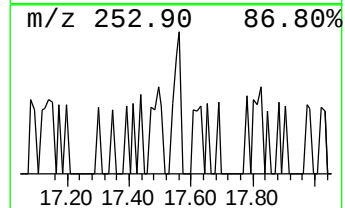
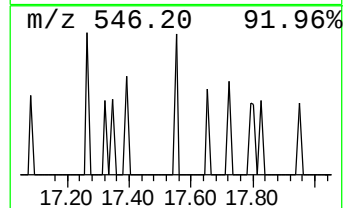
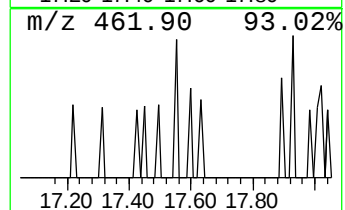
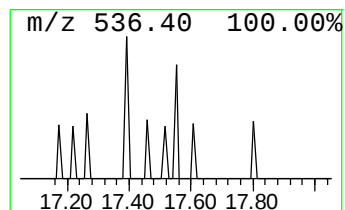
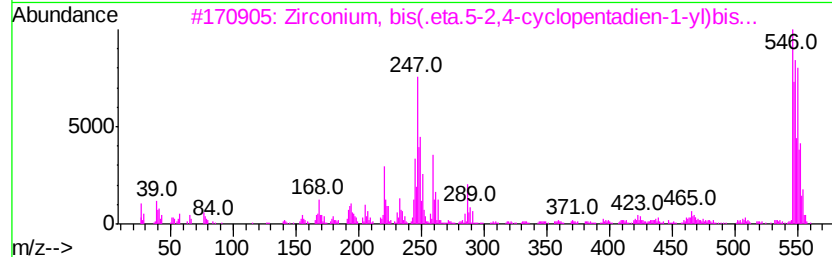
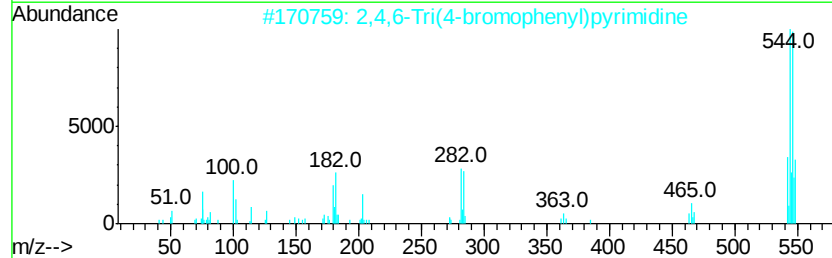
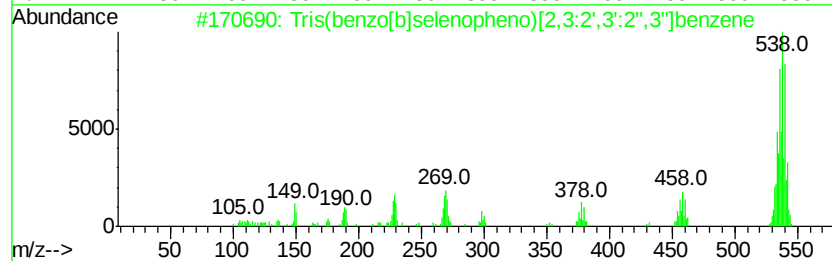
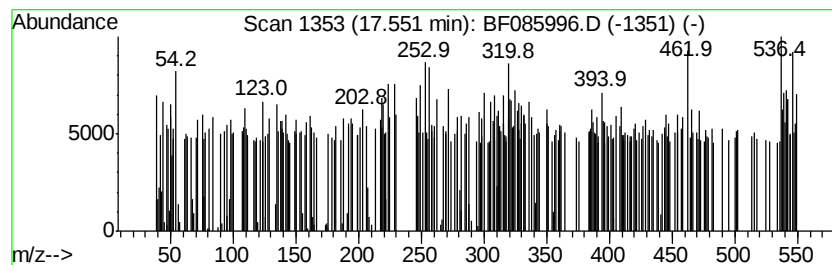
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.55 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.55	3.28 ng	134614	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	27
2		2,4,6-Tri(4-bromophenyl)pyrimidine	542	C22H13Br3N2	1000070-62-6	22
3		Zirconium, bis(.eta.5-2,4-cvclop...	546	C28H30Zr2	119144-91-1	11
4		Isoindole, 1-(hydrazinedicarboxy...	541	C26H31N5O8	1000152-41-0	11
5		Cyclodisilazane, hexaphenyl-	546	C36H30N2Si2	003284-07-9	10



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Sample : H2055-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BH-3(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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...	4.97	2.8	ng	86174	1	6.77	610466	20.0
unknown6.54	6.54	96.8	ng	2954840	1	6.77	610466	20.0
Hexadecane	10.72	2.5	ng	116400	4	11.29	952060	20.0
n-Hexadecanoic acid	11.83	7.0	ng	334657	4	11.29	952060	20.0
n-Decanoic acid	12.60	3.0	ng	140957	4	11.29	952060	20.0
9-Octadecenamide, ...	13.36	3.5	ng	164216	5	13.93	949174	20.0
1-Nonadecene	13.78	8.4	ng	397841	5	13.93	949174	20.0
Squalene	14.75	8.7	ng	357079	6	15.33	821264	20.0
unknown17.55	17.55	3.3	ng	134614	6	15.33	821264	20.0