

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
 Data File : BF087859.D
 Acq On : 9 Jun 2016 18:26
 Operator : UM/SJ
 Sample : H3399-13DL 20X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-32DL

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-BF060716.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	1.884	24	26	72	rVB	1591680	4002249	100.00%	29.885%
2	5.404	332	334	336	rVB	177275	174500	4.36%	1.303%
3	6.444	423	425	427	rBV	189208	178122	4.45%	1.330%
4	6.581	434	437	439	rBV	234902	194037	4.85%	1.449%
5	6.822	456	458	460	rVB	684583	688485	17.20%	5.141%
6	6.970	469	471	473	rVB	174472	149234	3.73%	1.114%
7	7.382	505	507	509	rBV	86763	99418	2.48%	0.742%
8	8.102	568	570	573	rBV	920377	847498	21.18%	6.328%
9	9.176	662	664	666	rVB	295234	224566	5.61%	1.677%
10	9.850	721	723	725	rBV	1064725	927772	23.18%	6.928%
11	10.628	789	791	794	rVB2	79711	94121	2.35%	0.703%
12	11.325	850	852	856	rBV2	631953	817074	20.42%	6.101%
13	12.536	956	958	960	rBV	123146	109012	2.72%	0.814%
14	12.765	974	978	979	rBV	74228	107775	2.69%	0.805%
15	12.902	989	990	993	rVB2	113947	140620	3.51%	1.050%
16	13.394	1030	1033	1035	rBV	1595382	1648023	41.18%	12.306%
17	13.691	1058	1059	1061	rVV	40911	51429	1.29%	0.384%
18	13.736	1061	1063	1065	rVV	82916	81789	2.04%	0.611%
19	13.954	1079	1082	1086	rBV	959296	918367	22.95%	6.857%
20	14.159	1097	1100	1104	rBV2	43246	60069	1.50%	0.449%
21	14.319	1111	1114	1115	rBV	97357	102760	2.57%	0.767%
22	14.354	1115	1117	1119	rVB	56779	53383	1.33%	0.399%
23	14.559	1133	1135	1137	rBV	222341	187608	4.69%	1.401%
24	14.731	1148	1150	1153	rVB	32103	41125	1.03%	0.307%
25	14.811	1153	1157	1159	rBV2	24722	53500	1.34%	0.399%
26	14.902	1163	1165	1168	rVB	89178	110011	2.75%	0.821%
27	14.959	1168	1170	1176	rBV	88880	136540	3.41%	1.020%
28	15.188	1187	1190	1193	rBV	113424	221532	5.54%	1.654%
29	15.302	1197	1200	1202	rBV2	37833	54271	1.36%	0.405%
30	15.359	1202	1205	1208	rBV	524700	652273	16.30%	4.871%
31	15.622	1223	1228	1231	rBV	30299	79456	1.99%	0.593%
32	15.977	1256	1259	1262	rBV	80532	131503	3.29%	0.982%
33	17.028	1347	1351	1356	rVB	21507	54126	1.35%	0.404%

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Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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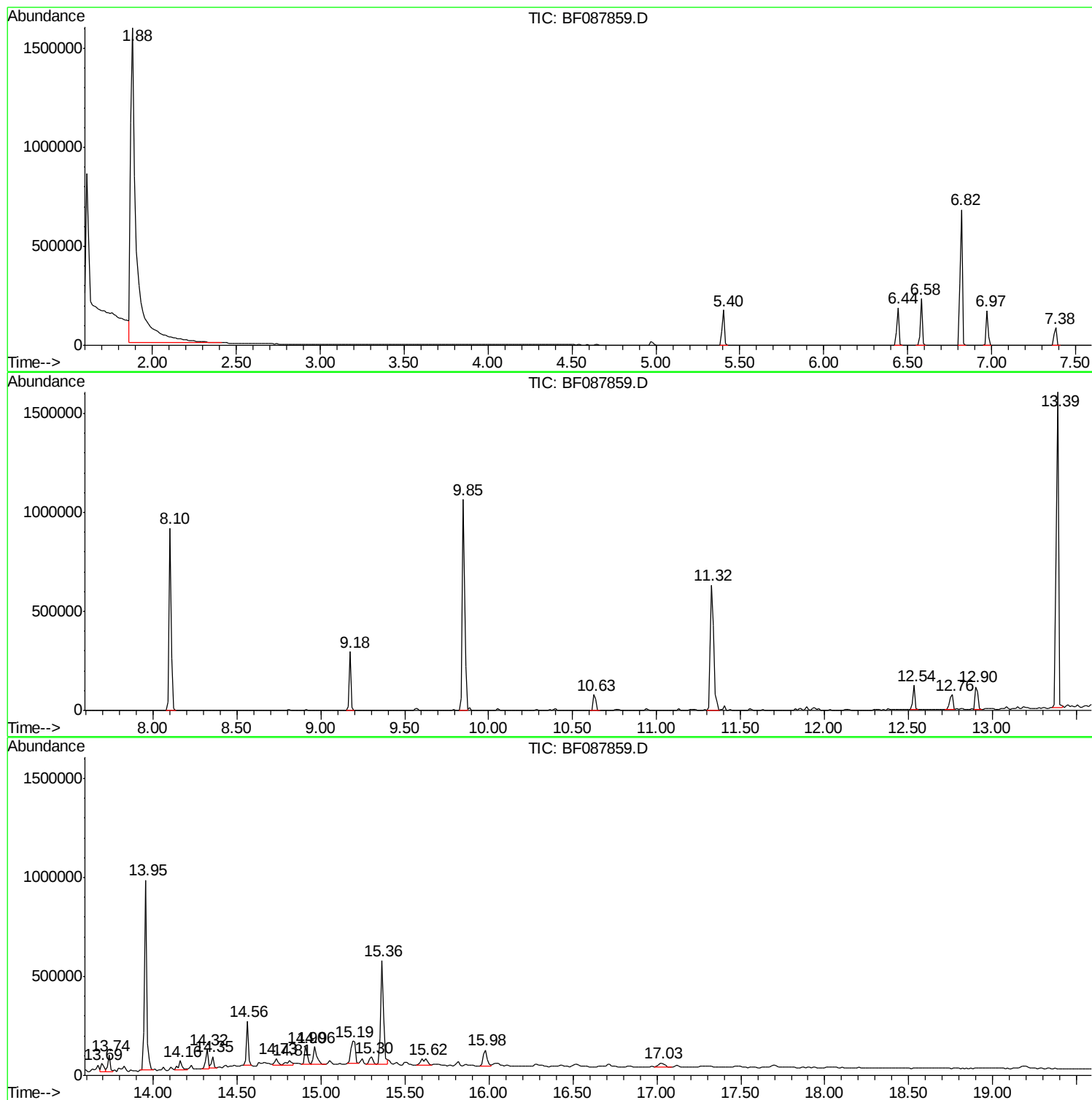
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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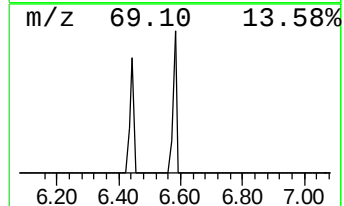
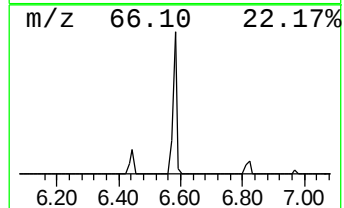
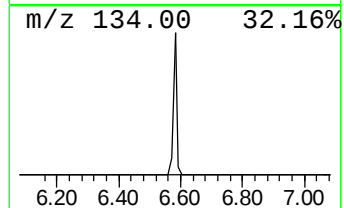
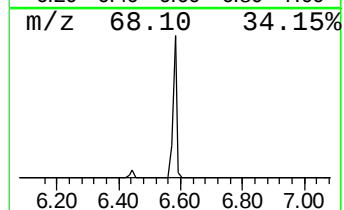
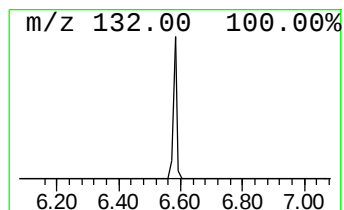
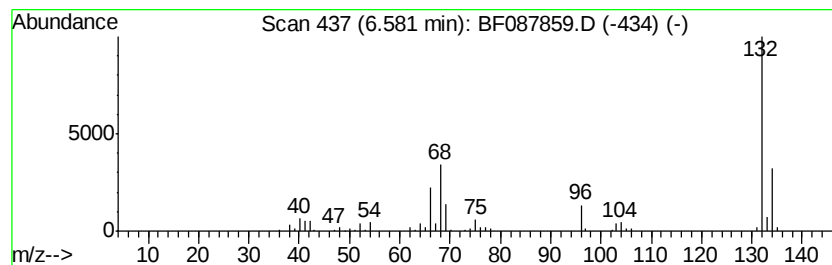
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	5.64 ng	194037	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Xenon	132	Xe	007440-63-3	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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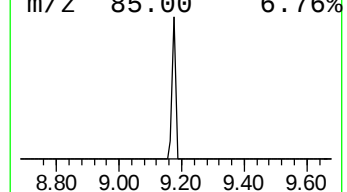
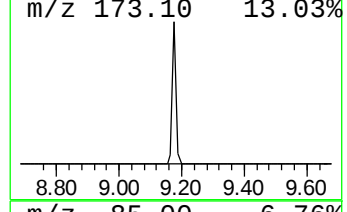
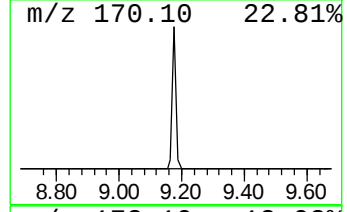
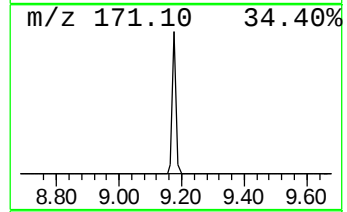
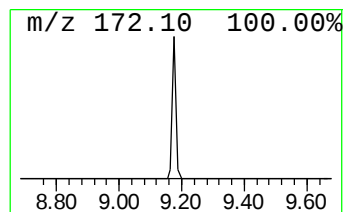
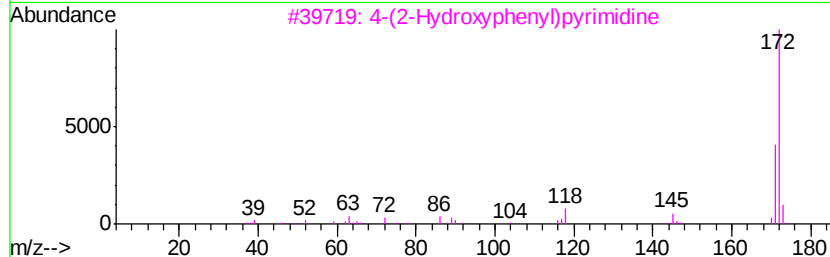
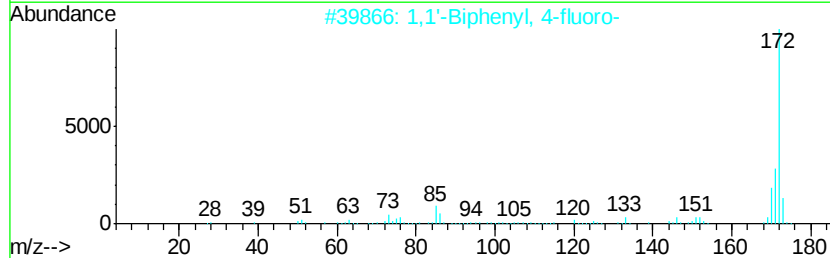
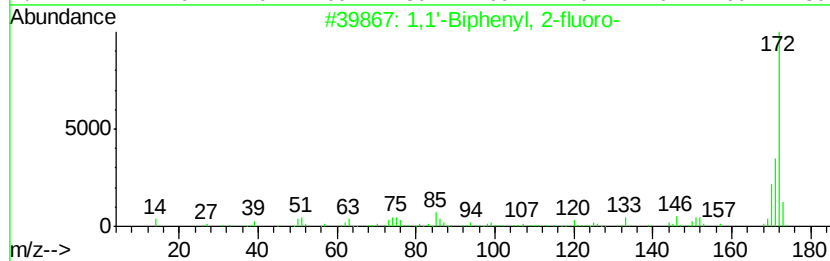
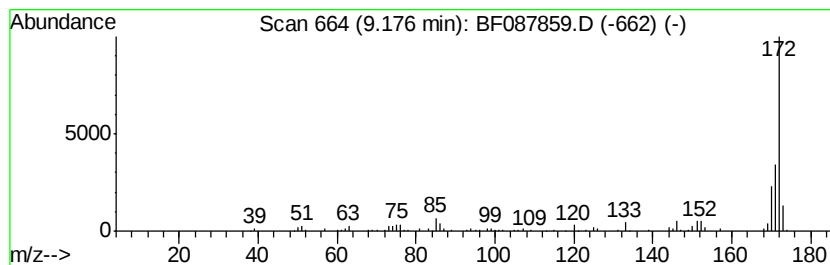
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Peak Number 4 1,1'-Biphenyl, 2-fluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.18	4.84 ng	224566	Acenaphthene-d10	9.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	96
2	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	93
3	4-(2-Hydroxyphenyl)pyrimidine	172	C10H8N2O	068535-55-7	58
4	2,2'-Oxydipyridine	172	C10H8N2O	053258-94-9	58
5	4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	42



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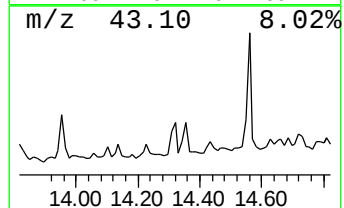
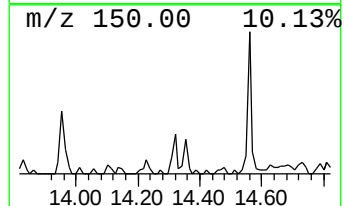
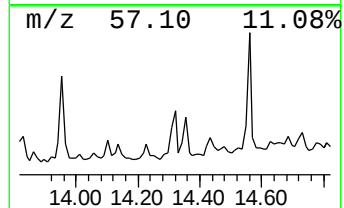
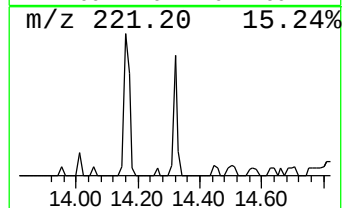
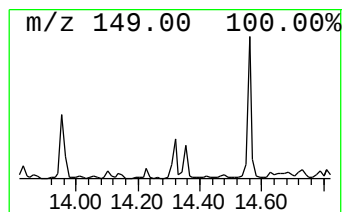
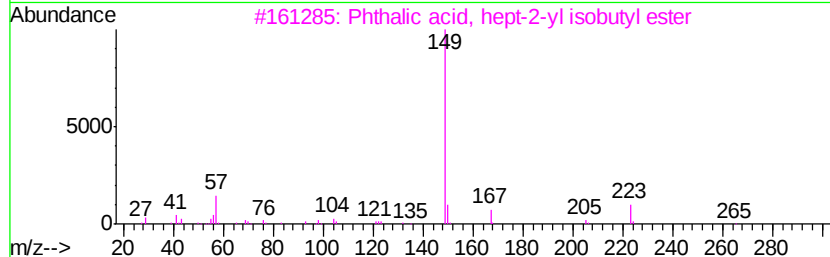
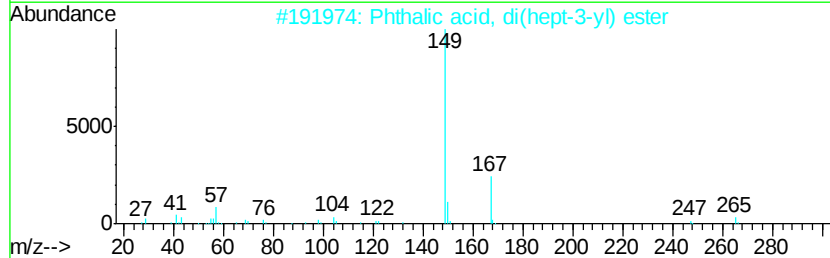
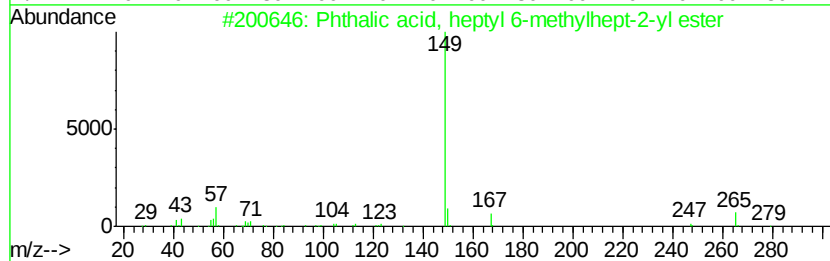
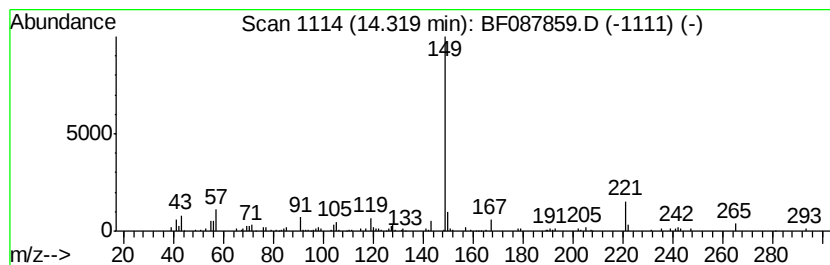
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Phthalic acid, heptyl 6-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.24 ng	102760	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, heptyl 6-methylhe...	376	C23H36O4	1000377-96-1	72
2		Phthalic acid, di(hept-3-yl) ester	362	C22H34O4	1000357-00-0	64
3		Phthalic acid, hept-2-yl isobutyl...	320	C19H28O4	1000356-97-0	64
4		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	64
5		Phthalic acid, isobutyl 2-pentyl...	292	C17H24O4	1000315-48-6	59



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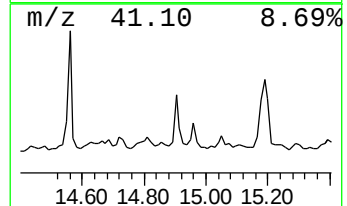
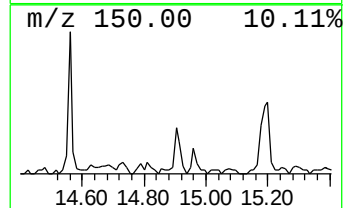
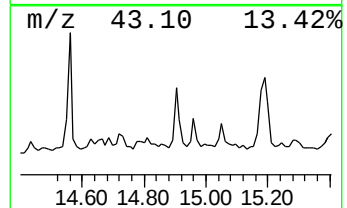
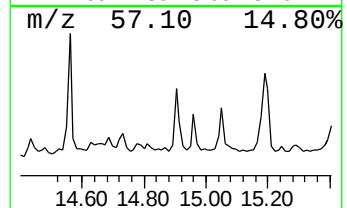
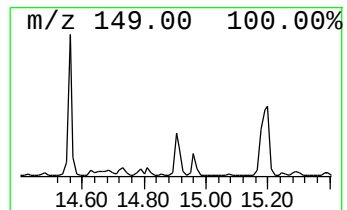
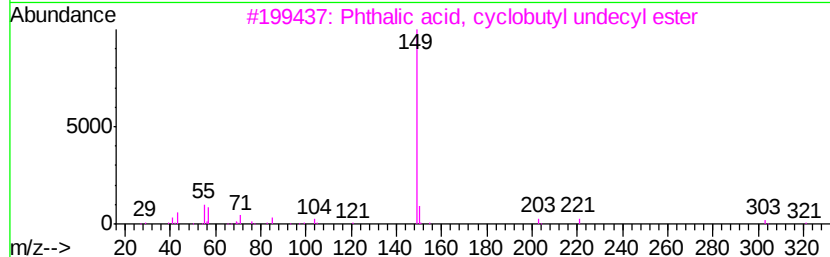
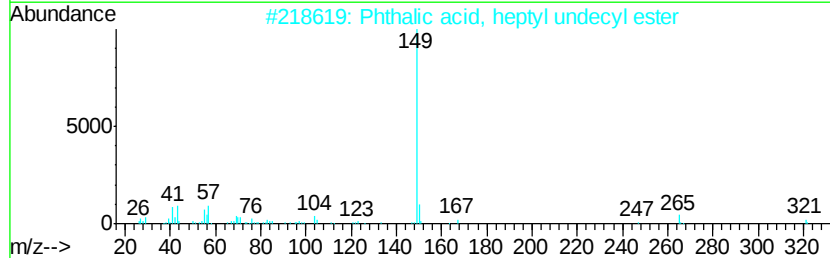
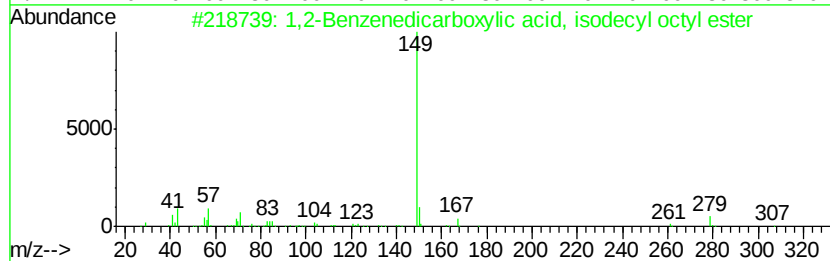
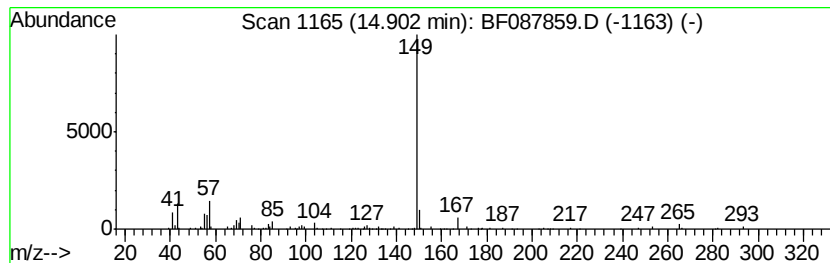
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.37 ng	110011	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	78
2		Phthalic acid, heptyl undecyl ester	418	C26H42O4	1000308-94-0	72
3		Phthalic acid, cyclobutyl undecyl...	374	C23H34O4	1000314-90-6	72
4		Phthalic acid, octadecyl pent-4-...	486	C31H50O4	1000360-47-7	72
5		Phthalic acid, dodecyl 2-fluorop...	428	C26H33FO4	1000356-15-1	72



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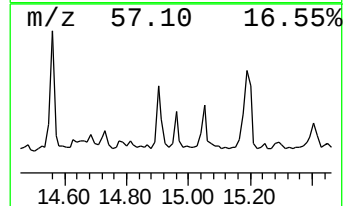
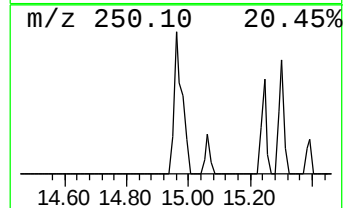
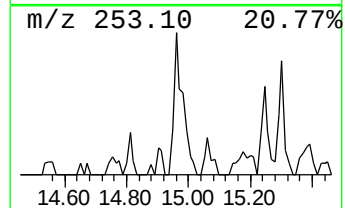
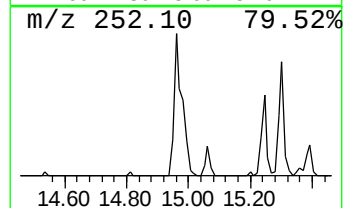
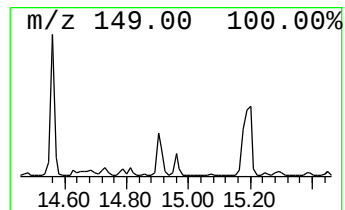
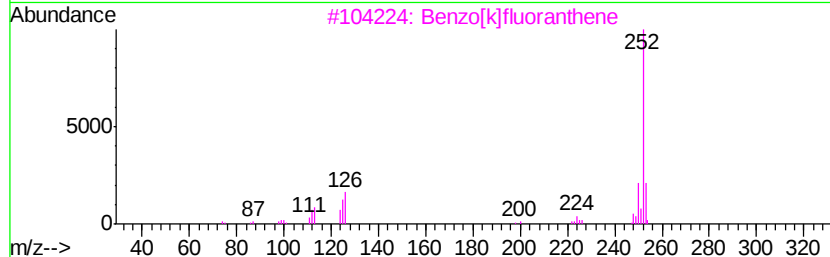
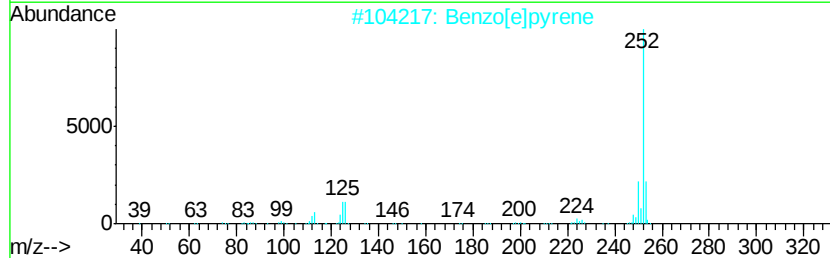
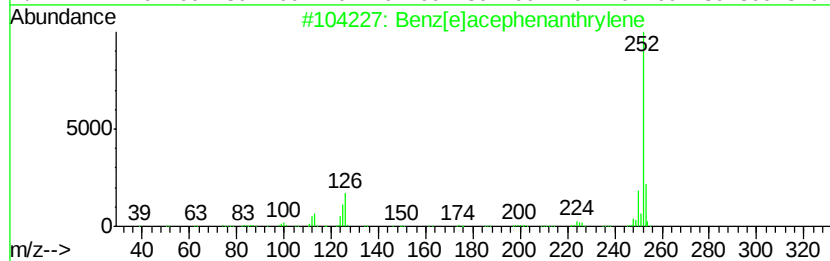
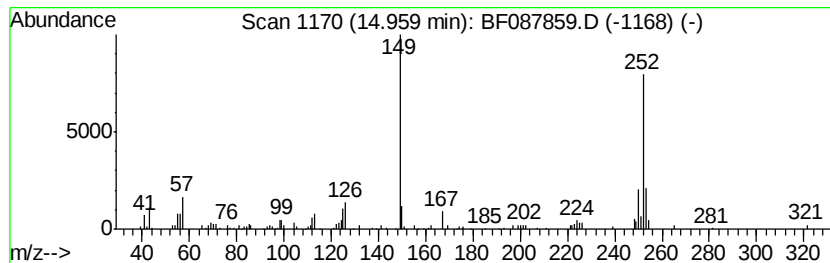
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Benz[e]acephenanthrylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.96	4.19 ng	136540	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[elacephenanthrylene	252	C20H12	000205-99-2	89
2	Benzo[elpyrene	252	C20H12	000192-97-2	86
3	Benzo[klfluoranthene	252	C20H12	000207-08-9	83
4	Benzo[alpyrene	252	C20H12	000050-32-8	50
5	Perylene	252	C20H12	000198-55-0	46



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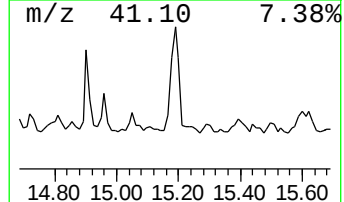
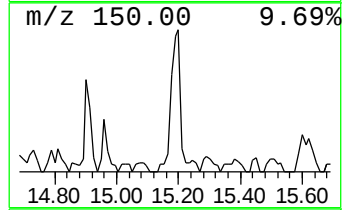
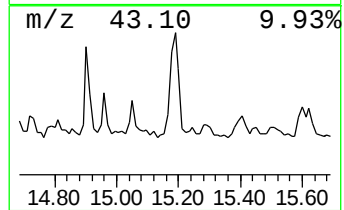
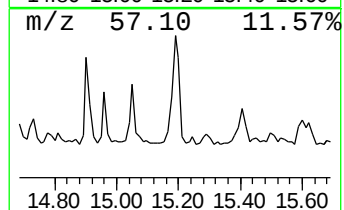
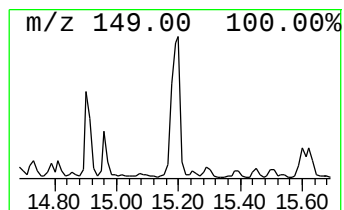
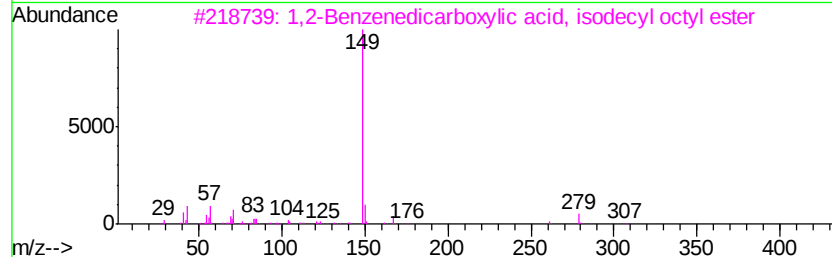
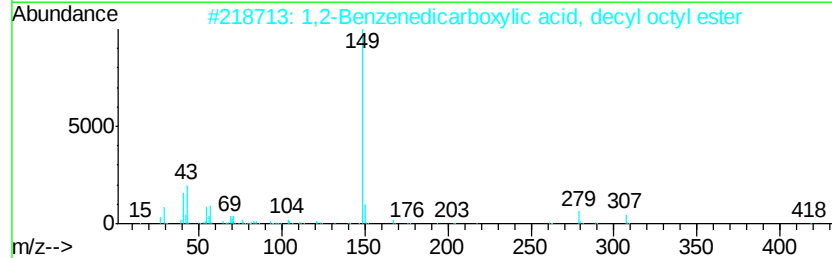
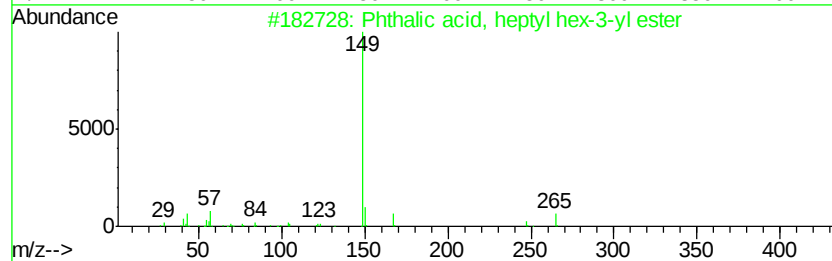
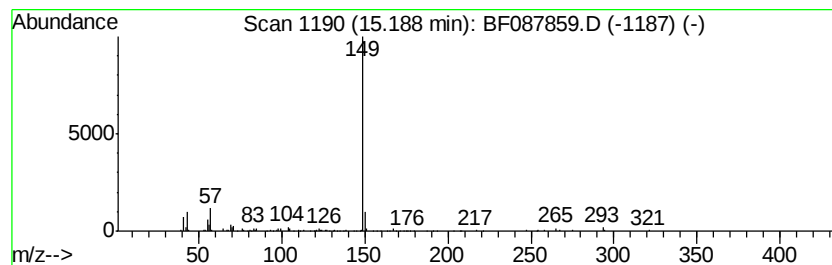
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Phthalic acid, heptyl hex-3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	6.79 ng	221532	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, heptyl hex-3-yl e...	348	C21H32O4	1000356-95-8	80
2		1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	72
3		1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	72
4		Phthalic acid, 4-methylpent-2-yl...	362	C22H34O4	1000356-87-8	72
5		Phthalic acid, heptyl 6-methylhe...	376	C23H36O4	1000377-96-1	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087859.D
Acq On : 9 Jun 2016 18:26
Operator : UM/SJ
Sample : H3399-13DL 20X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32DL

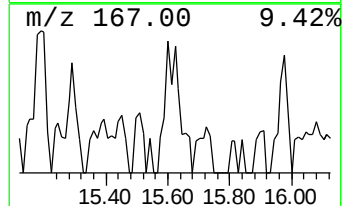
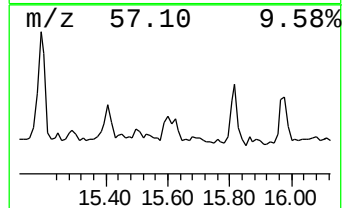
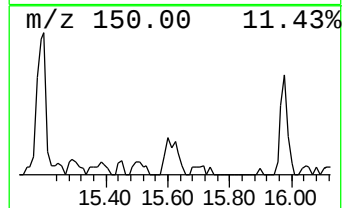
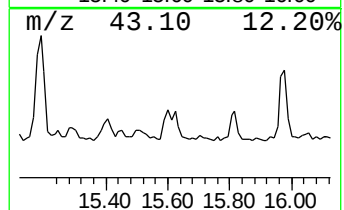
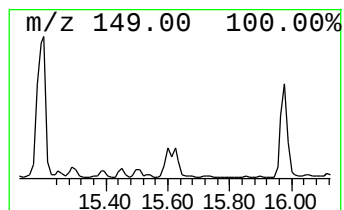
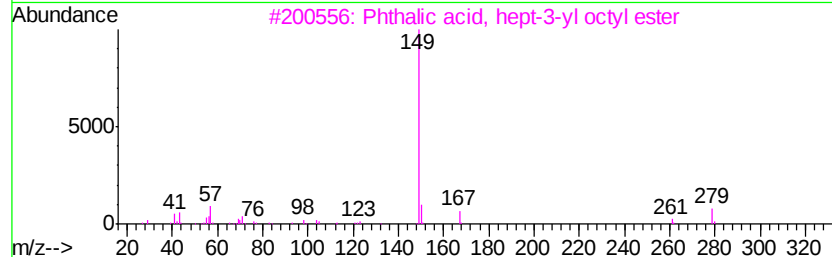
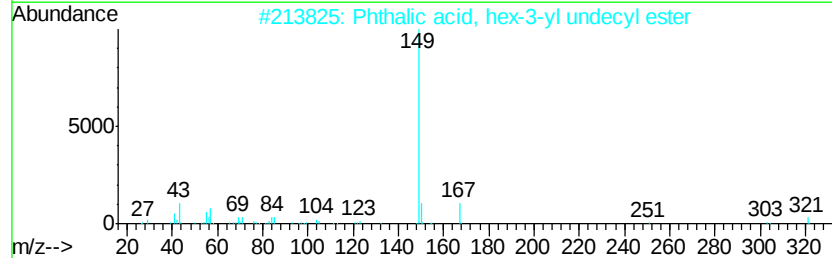
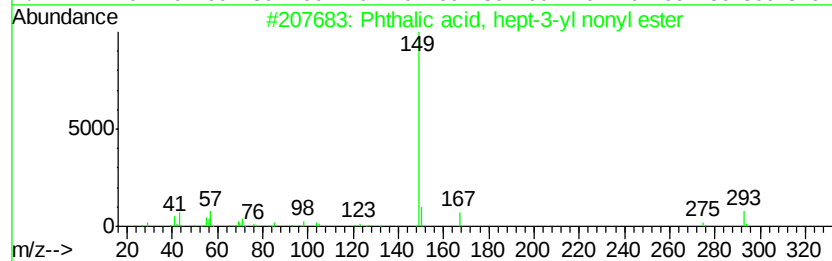
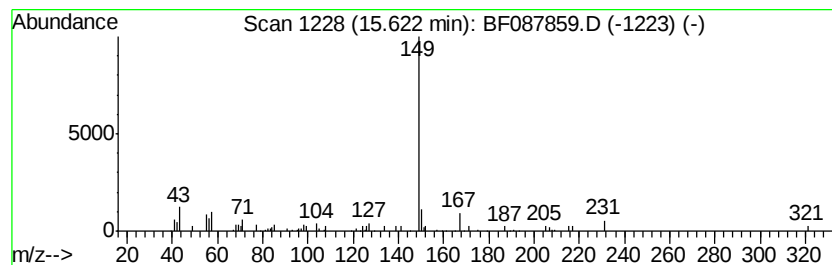
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Phthalic acid, hept-3-yl no... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.44 ng	79456	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
2		Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	80
3		Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	80
4		Phthalic acid, decyl 2-methylpen...	390	C24H38O4	1000356-91-5	72
5		Phthalic acid, dec-2-yl isobutyl...	362	C22H34O4	1000356-93-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087859.D
Acq On : 9 Jun 2016 18:26
Operator : UM/SJ
Sample : H3399-13DL 20X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32DL

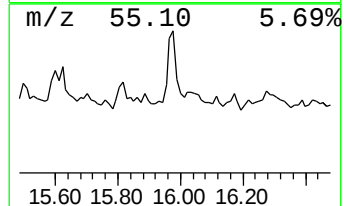
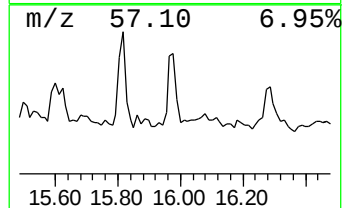
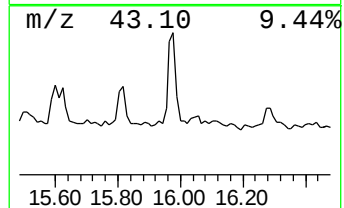
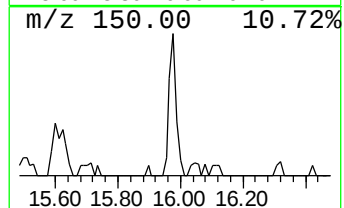
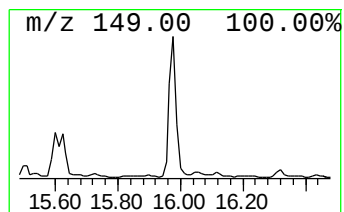
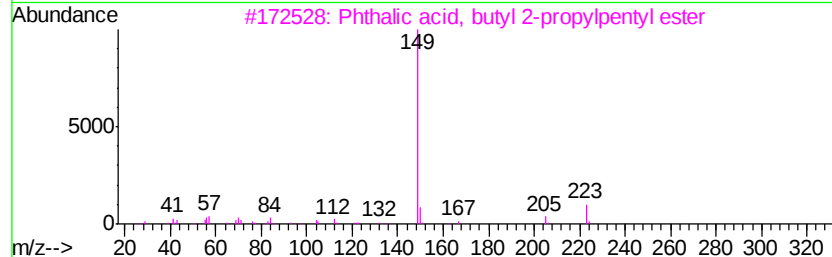
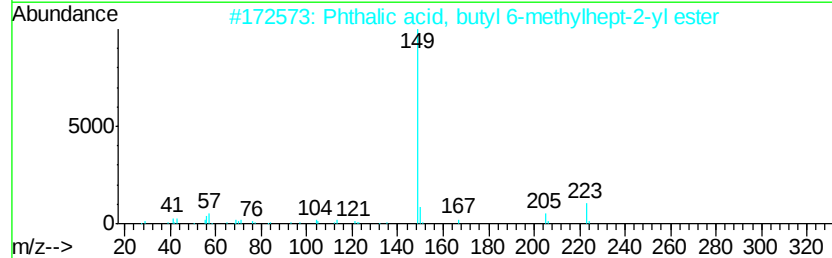
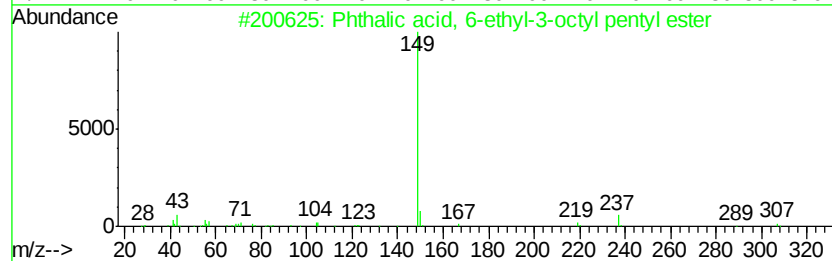
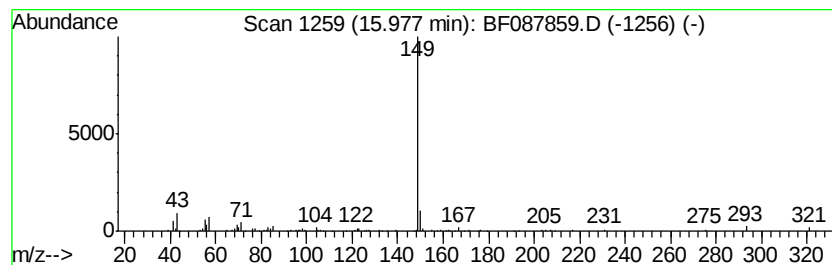
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Phthalic acid, 6-ethyl-3-oc... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	4.03 ng	131503	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 6-ethyl-3-octyl p...	376	C23H36O4	1000315-17-5	78
2		Phthalic acid, butyl 6-methylhept...	334	C20H30O4	1000377-95-8	78
3		Phthalic acid, butyl 2-propylpent...	334	C20H30O4	1000377-92-0	78
4		Phthalic acid, hept-4-yl nonyl e...	390	C24H38O4	1000356-79-0	78
5		Phthalic acid, decyl hept-3-yl e...	404	C25H40O4	1000356-99-4	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
Data File : BF087859.D
Acq On : 9 Jun 2016 18:26
Operator : UM/SJ
Sample : H3399-13DL 20X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32DL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.58	6.58	5.6 ng		194037	1	6.82	688485	20.0
1,1'-Biphenyl, 2-...	9.18	4.8 ng		224566	3	9.85	927772	20.0
Phthalic acid, he...	14.32	2.2 ng		102760	5	13.95	918367	20.0
1,2-Benzenedicarb...	14.90	3.4 ng		110011	6	15.36	652273	20.0
Benz[e]acephenant...	14.96	4.2 ng		136540	6	15.36	652273	20.0
Phthalic acid, he...	15.19	6.8 ng		221532	6	15.36	652273	20.0
Phthalic acid, he...	15.62	2.4 ng		79456	6	15.36	652273	20.0
Phthalic acid, 6-...	15.98	4.0 ng		131503	6	15.36	652273	20.0