

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
 Data File : BF104889.D
 Acq On : 27 Apr 2018 18:51
 Operator : JU/SJ
 Sample : J2522-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

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-BF040618.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

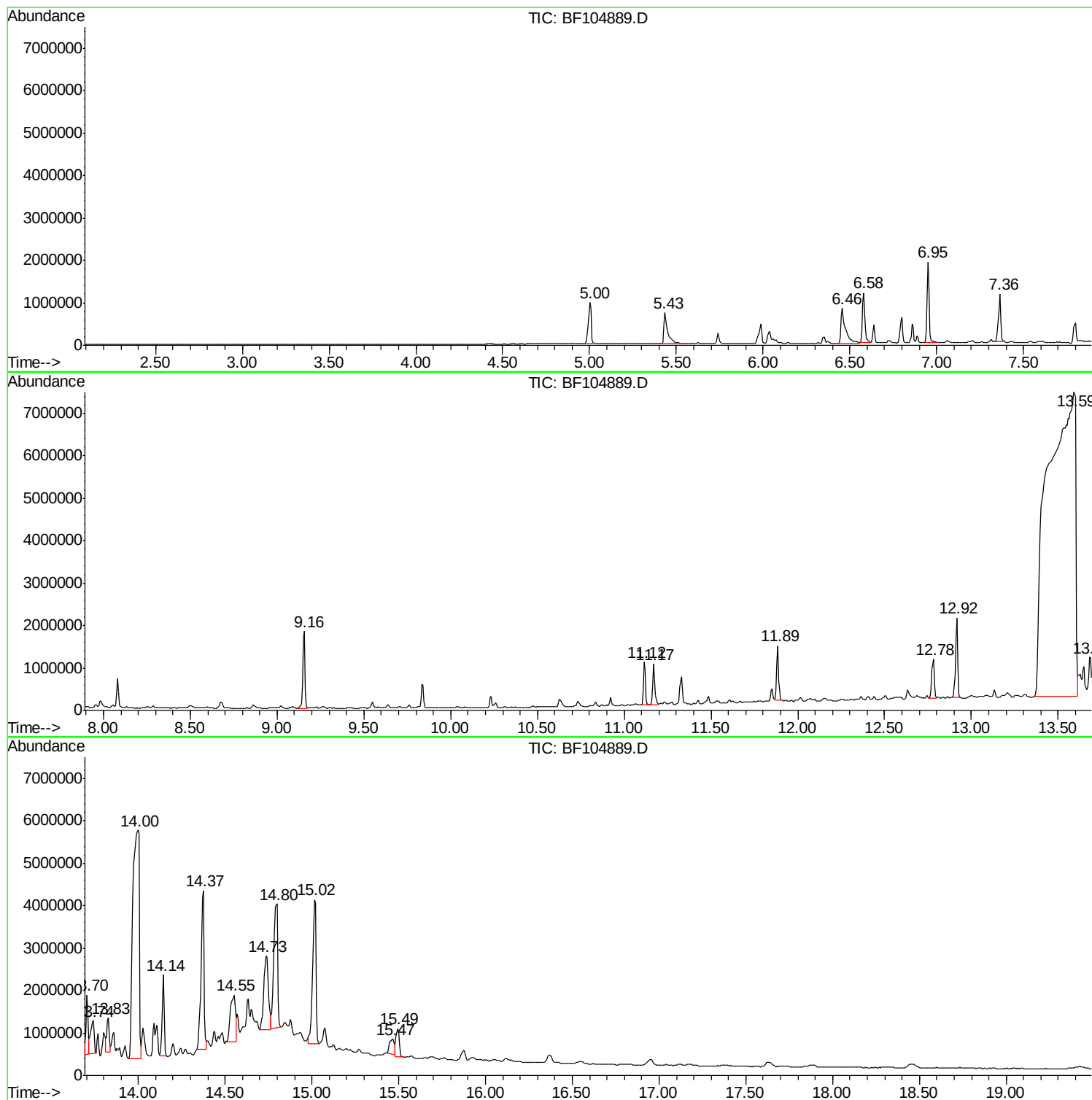
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	490	496	499	rBV	967870	1205683	1.60%	0.933%
2	5.434	566	569	585	rBV	727557	1142219	1.52%	0.884%
3	6.457	739	743	760	rBV	822490	1436371	1.91%	1.111%
4	6.581	760	764	770	rVV	1176843	1257588	1.67%	0.973%
5	6.951	823	827	836	rBV	1903677	1738151	2.31%	1.345%
6	7.363	892	897	900	rBV	1131661	971754	1.29%	0.752%
7	9.157	1195	1202	1205	rBV	1811162	1644777	2.19%	1.272%
8	11.116	1532	1535	1540	rBV	1017949	846255	1.12%	0.655%
9	11.169	1540	1544	1549	rBV	969954	900155	1.20%	0.696%
10	11.886	1663	1666	1669	rVB	1277538	1017286	1.35%	0.787%
11	12.780	1814	1818	1821	rBV	914321	753193	1.00%	0.583%
12	12.915	1837	1841	1844	rBV	1873027	1629798	2.17%	1.261%
13	13.592	1917	1956	1959	rBV2	7158769	75236116	100.00%	58.201%
14	13.686	1968	1972	1973	rVV2	761220	756627	1.01%	0.585%
15	13.704	1973	1975	1977	rVV	1398528	1188422	1.58%	0.919%
16	13.739	1977	1981	1984	rVB2	773118	1058579	1.41%	0.819%
17	13.827	1993	1996	1998	rVV2	798340	849872	1.13%	0.657%
18	13.998	2016	2025	2028	rBV2	5383078	13548590	18.01%	10.481%
19	14.145	2046	2050	2053	rVB	1907280	1695129	2.25%	1.311%
20	14.374	2083	2089	2092	rBV	3747909	4614521	6.13%	3.570%
21	14.551	2112	2119	2121	rBV2	1093987	2125178	2.82%	1.644%
22	14.733	2144	2150	2155	rBV3	1734979	3084618	4.10%	2.386%
23	14.798	2155	2161	2165	rVB	2912115	4089820	5.44%	3.164%
24	15.015	2192	2198	2203	rVB	3393050	4955014	6.59%	3.833%
25	15.468	2269	2275	2277	rBV2	339249	756217	1.01%	0.585%
26	15.492	2277	2279	2285	rVB	676858	768439	1.02%	0.594%

Sum of corrected areas: 129270372

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



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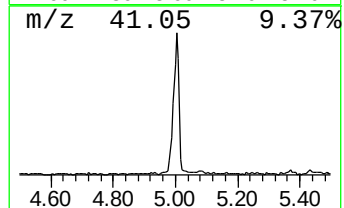
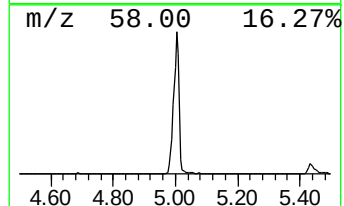
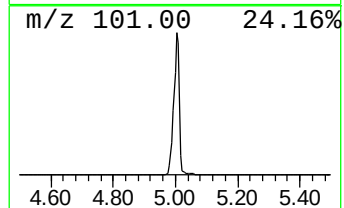
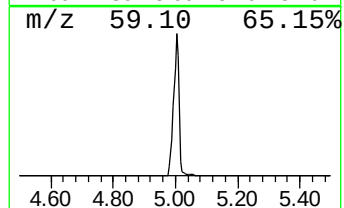
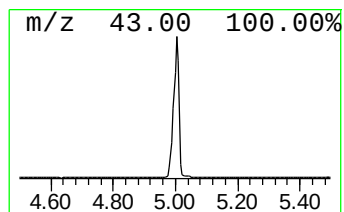
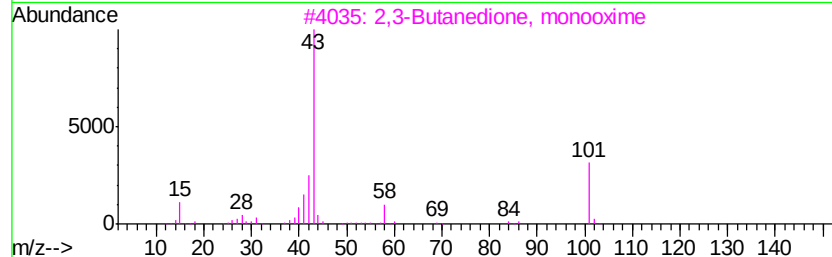
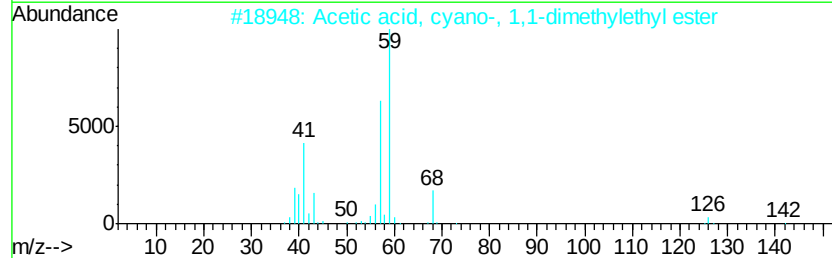
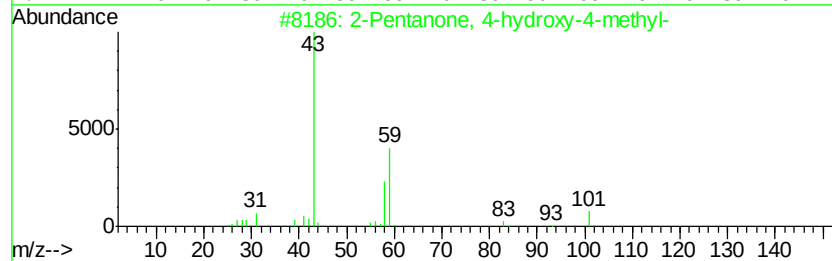
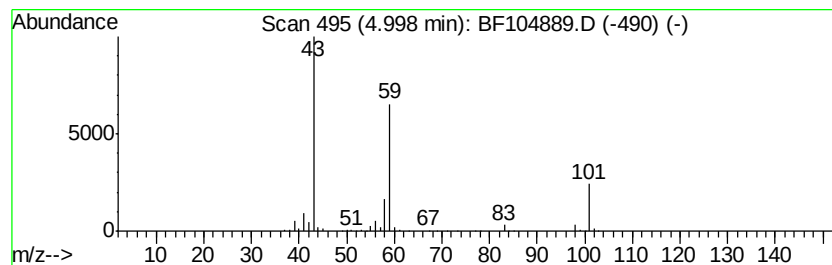
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	13.87 ng	1205680	1,4-Dichlorobenzene-d4	6.80

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	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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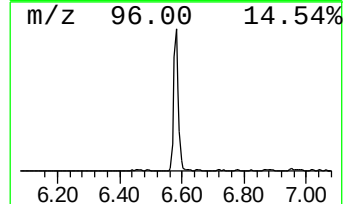
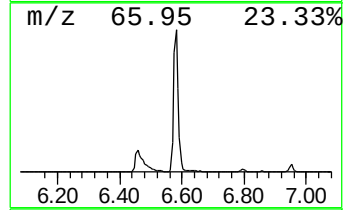
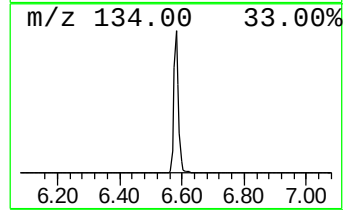
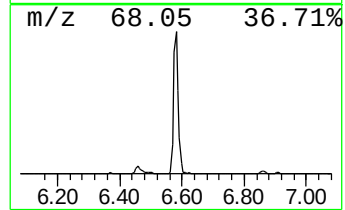
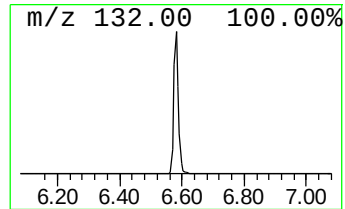
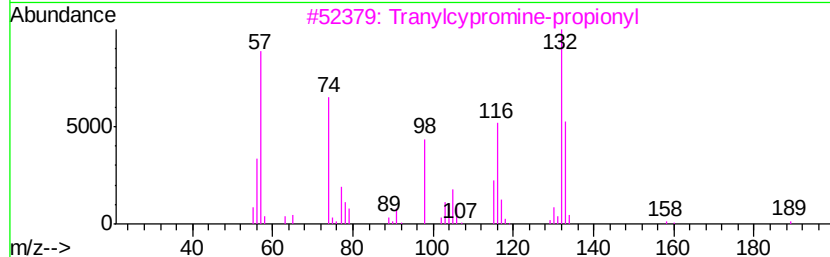
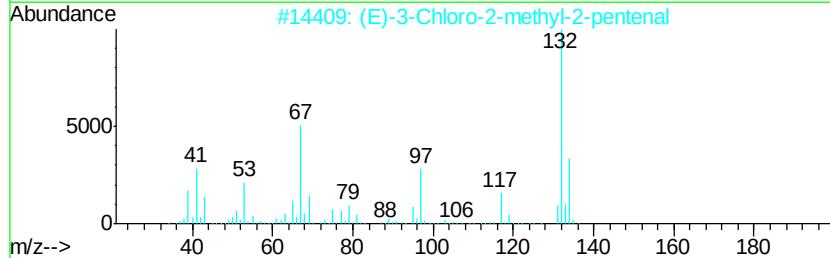
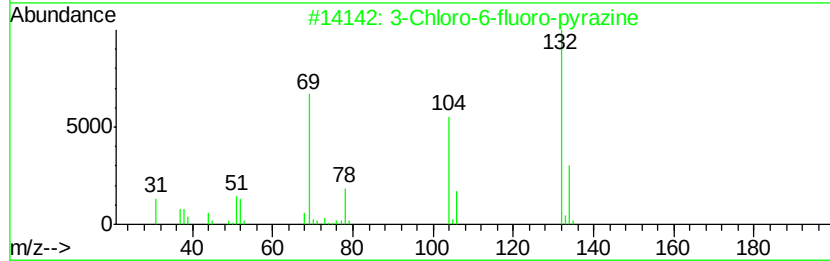
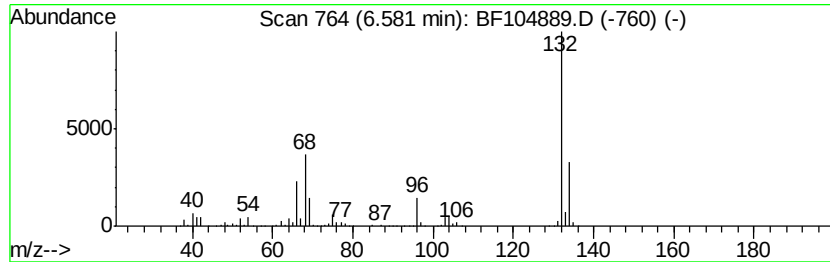
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Peak Number 2 unknown6.58 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	14.47 ng	1257590	1,4-Dichlorobenzene-d4	6.80

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10



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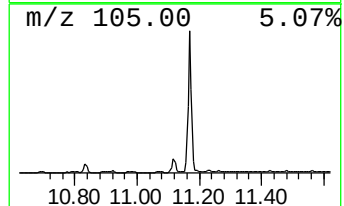
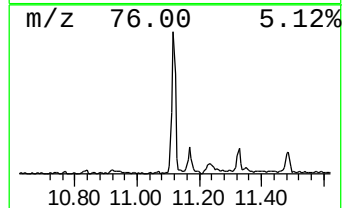
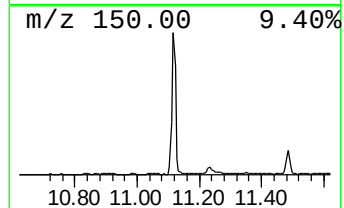
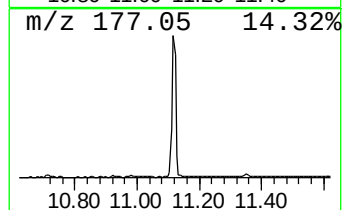
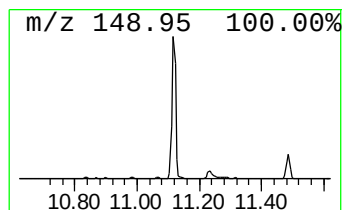
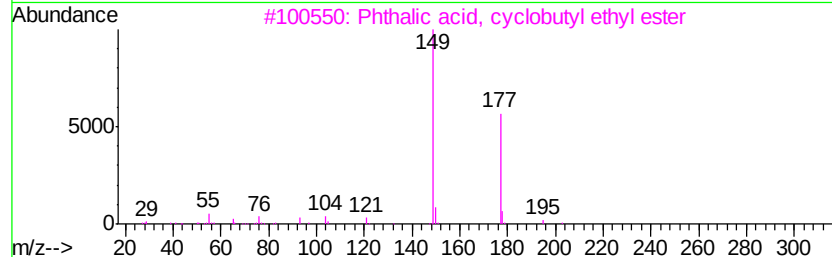
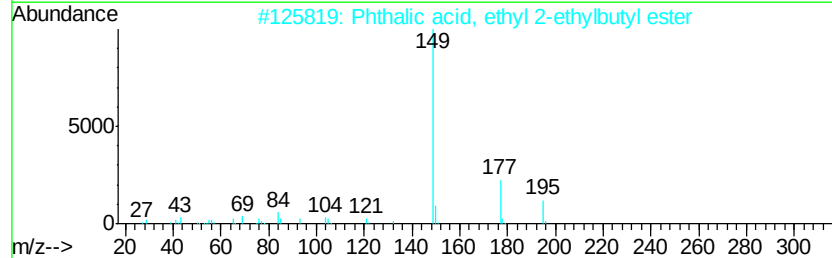
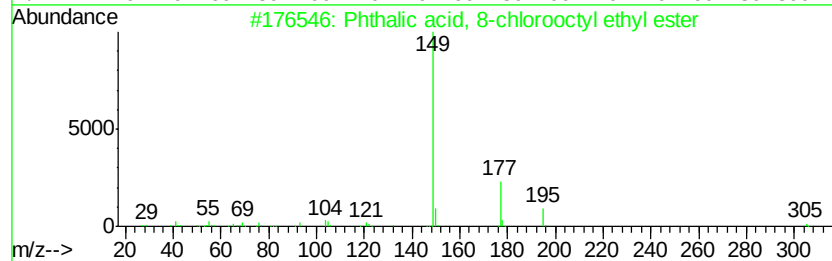
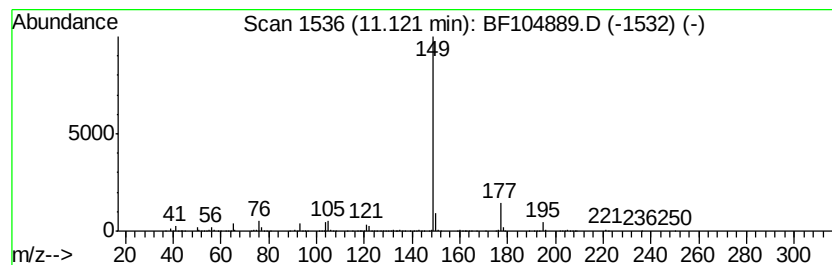
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Peak Number 3 Phthalic acid, 8-chloroocty... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	18.80 ng	846255	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 8-chlorooctyl eth...	340	C18H25ClO4	1000356-85-6	90
2		Phthalic acid, ethyl 2-ethylbuty...	278	C16H22O4	1000356-88-7	83
3		Phthalic acid, cyclobutyl ethyl ...	248	C14H16O4	1000315-41-1	83
4		Phthalic acid, 5-methylhex-2-yl ...	292	C17H24O4	1000371-09-3	83
5		Phthalic acid, ethyl pentyl ester	264	C15H20O4	1000308-93-6	83



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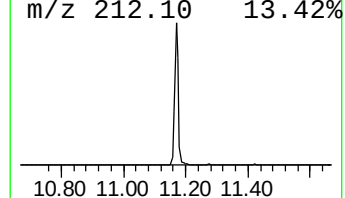
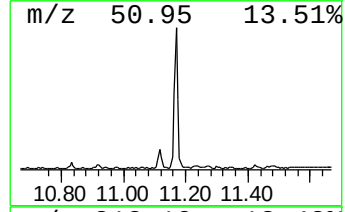
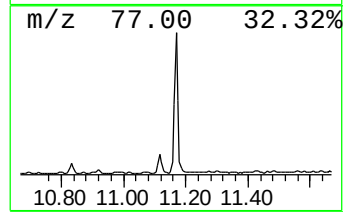
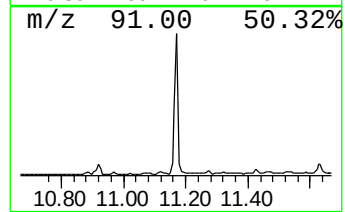
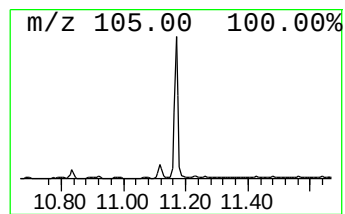
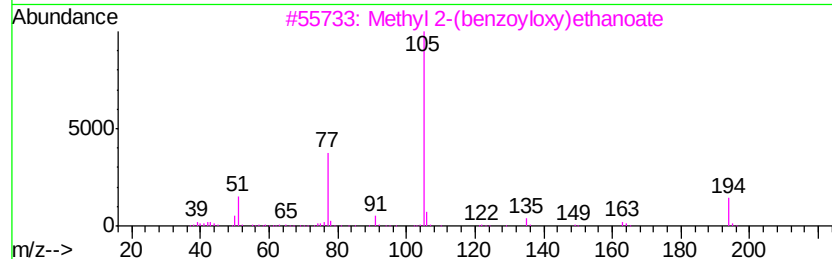
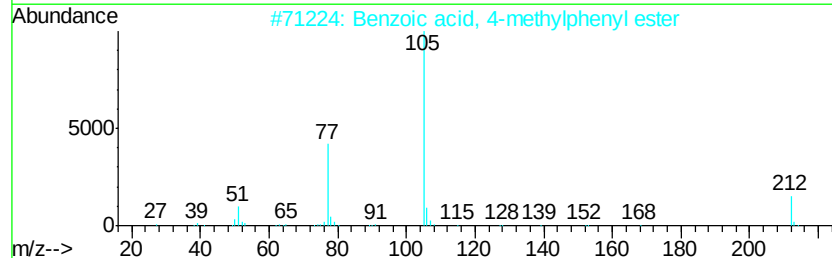
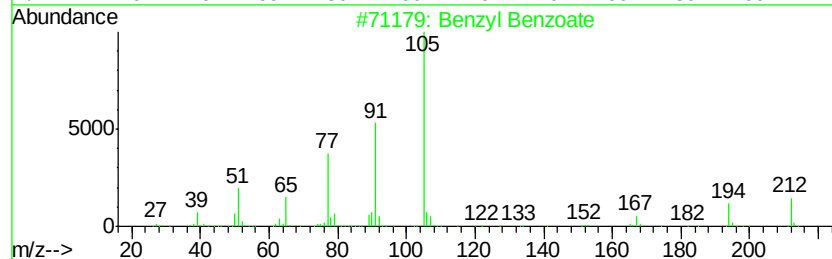
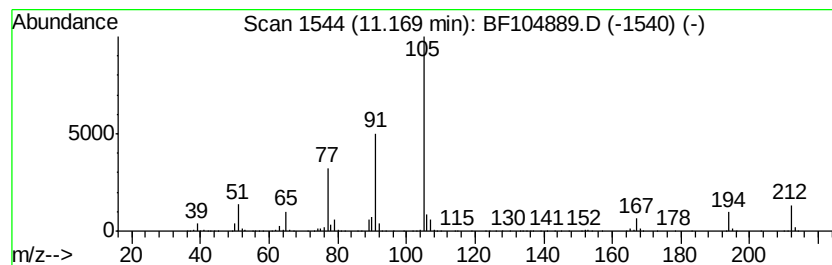
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Peak Number 4 Benzyl Benzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	20.00 ng	900155	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzyl Benzoate	212	C14H12O2	000120-51-4	98
2		Benzoic acid, 4-methylphenyl ester	212	C14H12O2	000614-34-6	60
3		Methyl 2-(benzoyloxy)ethanoate	194	C10H10O4	1000326-74-4	53
4		Benzoic acid, 3-methylphenyl ester	212	C14H12O2	1000357-80-0	49
5		Benzoic acid, 2-methylphenyl ester	212	C14H12O2	000617-02-7	49



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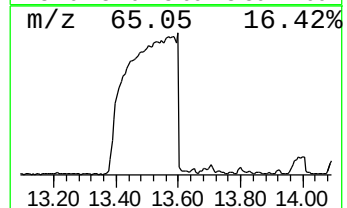
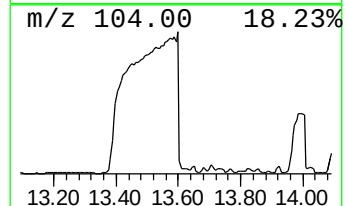
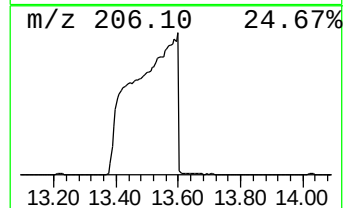
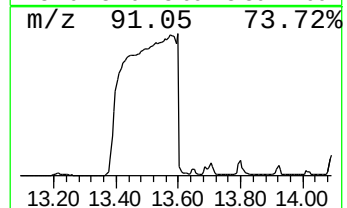
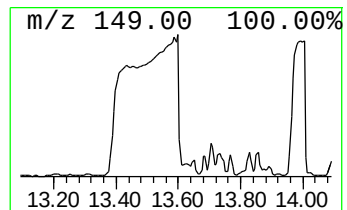
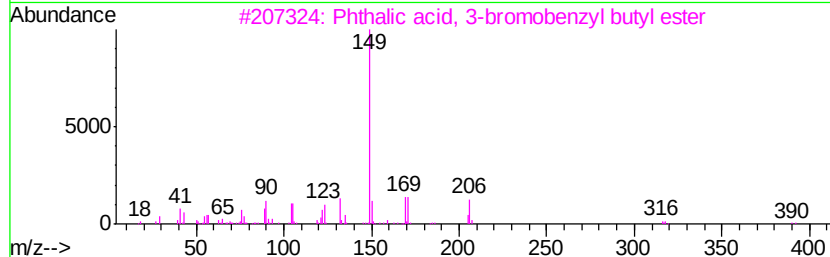
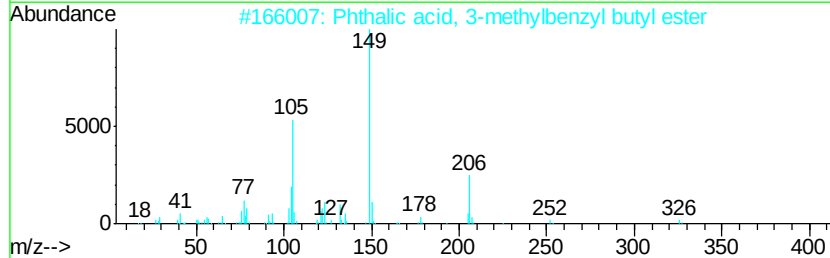
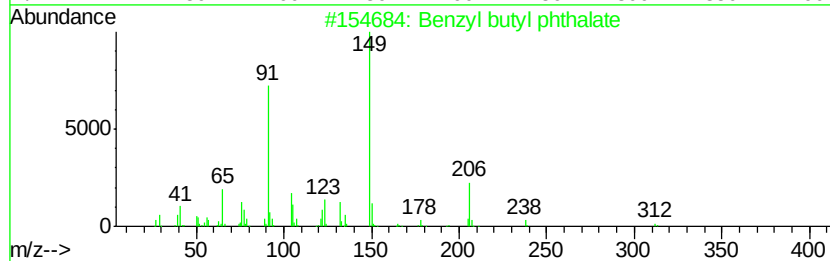
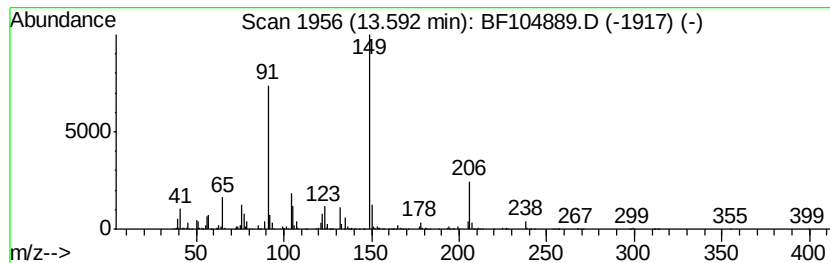
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Peak Number 5 Benzyl butyl phthalate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	111.06 ng	75236100	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzyl butyl phthalate	312	C19H20O4	000085-68-7	94
2		Phthalic acid, 3-methylbenzyl bu...	326	C20H22O4	1000371-10-6	72
3		Phthalic acid, 3-bromobenzyl but...	390	C19H19BrO4	1000371-05-3	59
4		Oxazolidine, 3-phenyl-	149	C9H11NO	020503-92-8	52
5		Phthalic acid, 1-(3-bromophenyl)...	446	C23H27BrO4	1000377-88-0	50



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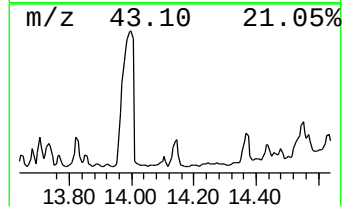
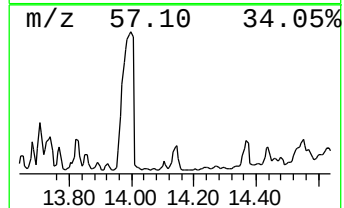
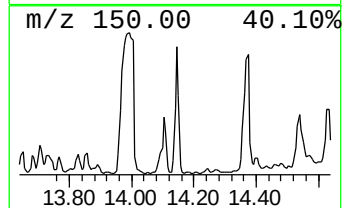
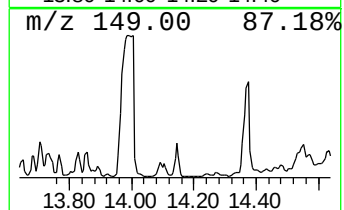
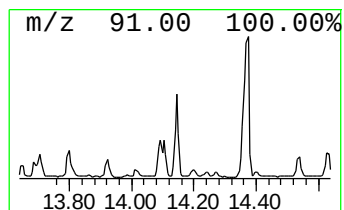
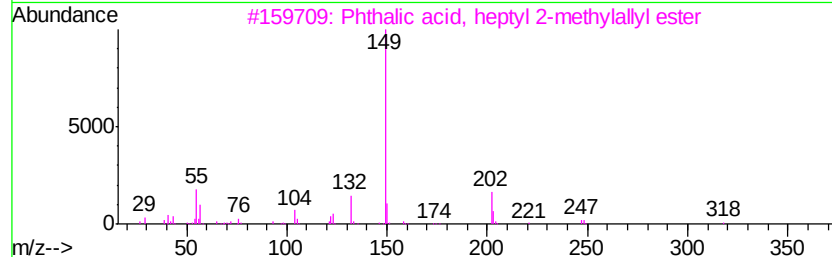
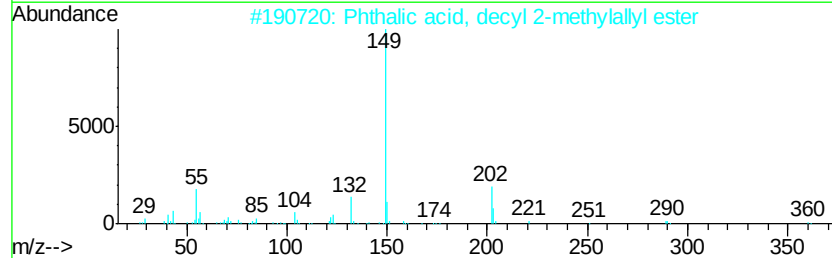
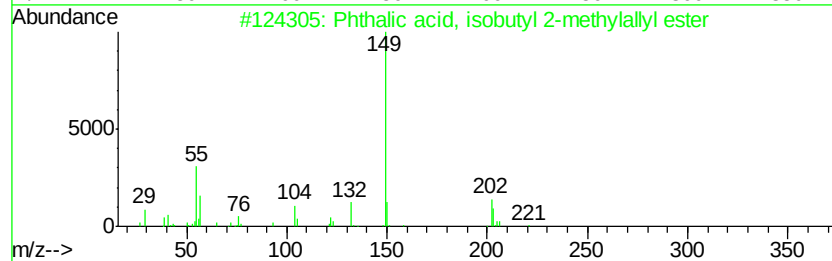
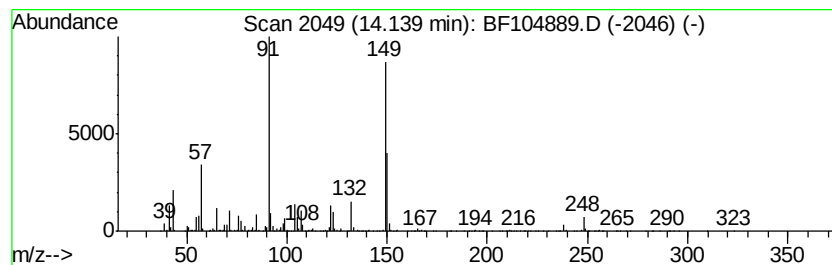
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.14 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.50 ng	1695130	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phthalic acid, isobutyl 2-methyl...	276	C16H20O4	1000315-82-3	47
2		Phthalic acid, decyl 2-methylal...	360	C22H32O4	1000315-83-0	47
3		Phthalic acid, heptyl 2-methylal...	318	C19H26O4	1000315-82-7	47
4		Phthalic acid, isobutyl 3-methyl...	290	C17H22O4	1000315-45-0	47
5		1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	43



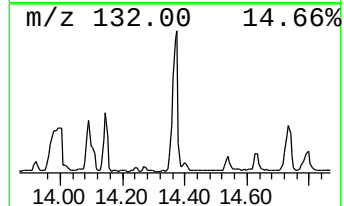
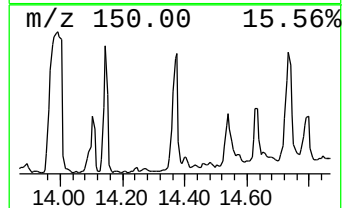
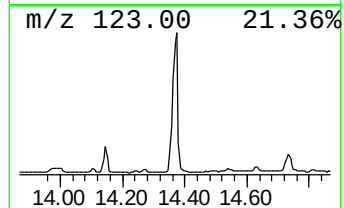
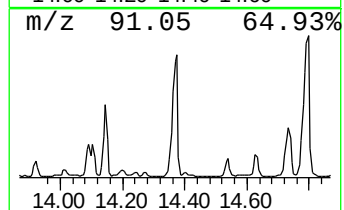
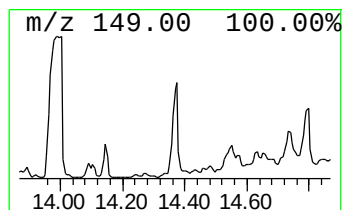
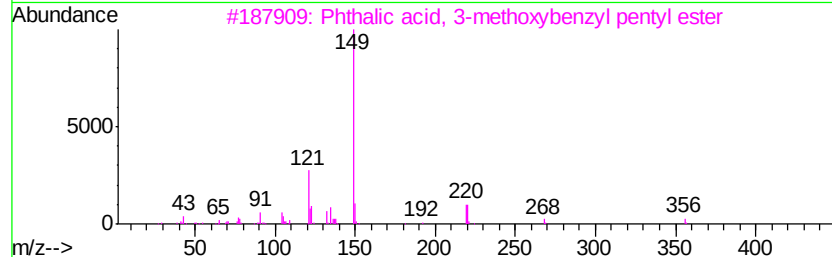
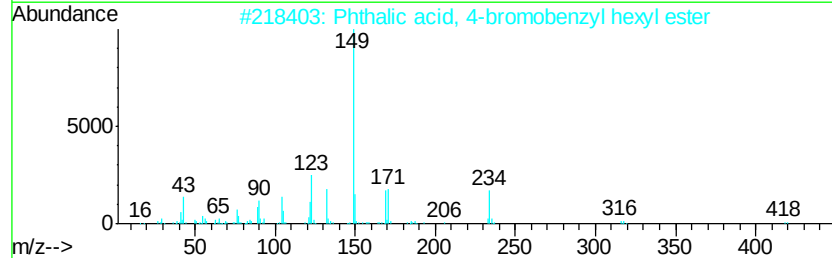
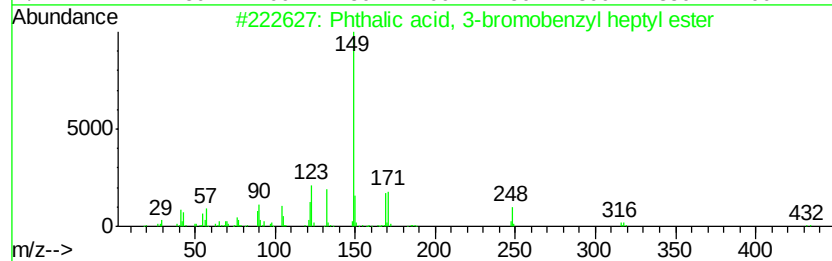
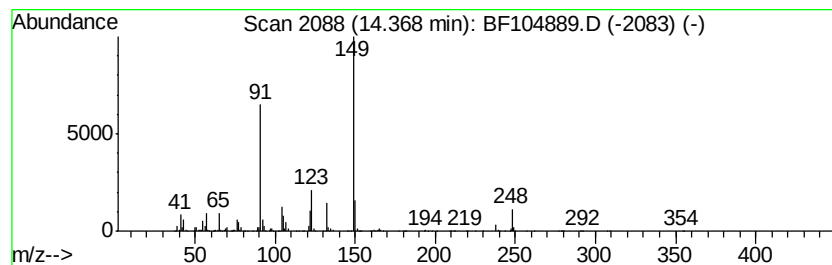
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Data File : BF104889.D
Acq On : 27 Apr 2018 18:51
Operator : JU/SJ
Sample : J2522-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phthalic acid, 3-bromobenzy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.37	6.81 ng	4614520	Chrysene-d12	14.03		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 3-bromobenzyl hep...	432	C22H25BrO4	1000371-05-0	90	
2	Phthalic acid, 4-bromobenzyl hex...	418	C21H23BrO4	1000371-05-9	72	
3	Phthalic acid, 3-methoxybenzyl p...	356	C21H24O5	1000377-97-8	64	
4	Phthalic acid, 2-methylallyl non...	346	C21H30O4	1000315-82-9	59	
5	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	53	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
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Acq On : 27 Apr 2018 18:51
Operator : JU/SJ
Sample : J2522-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

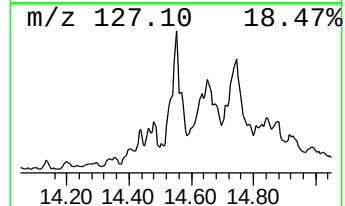
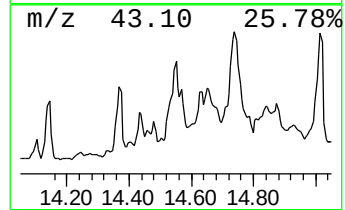
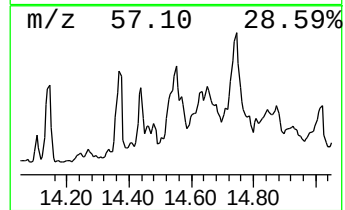
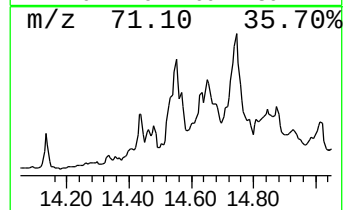
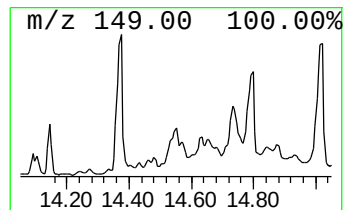
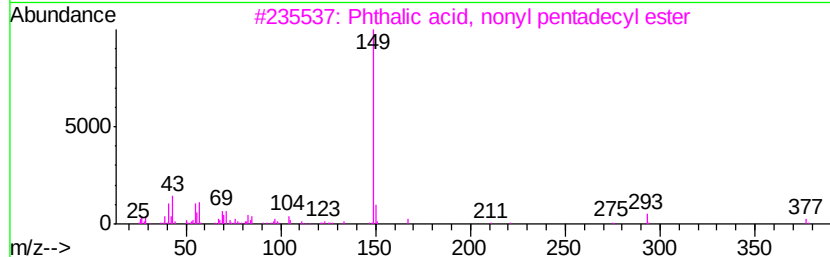
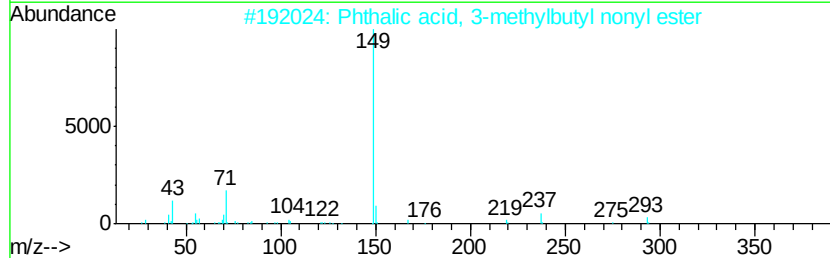
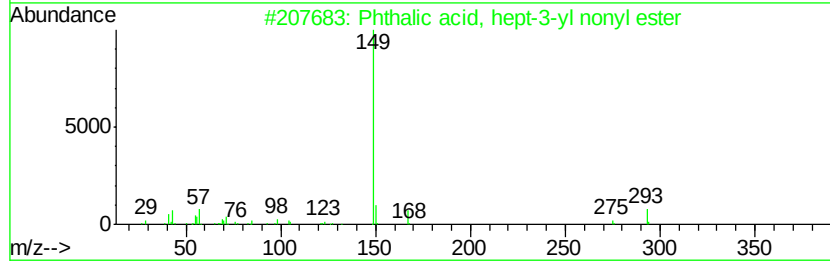
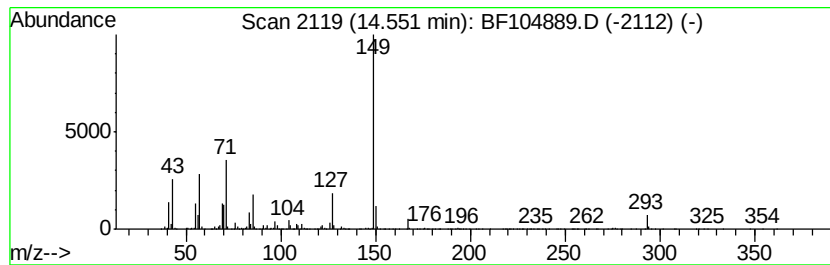
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, hept-3-yl no... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	3.14 ng	2125180	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	64
2		Phthalic acid, 3-methylbutyl non...	362	C22H34O4	1000356-81-0	64
3		Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	59
4		Phthalic acid, 2-fluorophenyl he...	484	C30H41FO4	1000356-50-1	59
5		Phthalic acid, 3-fluorophenyl he...	484	C30H41FO4	1000356-66-4	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
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Operator : JU/SJ
Sample : J2522-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

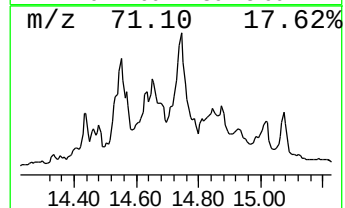
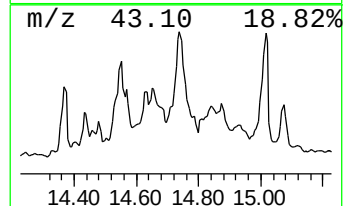
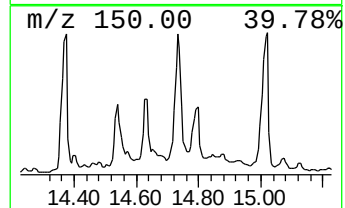
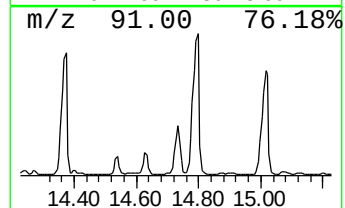
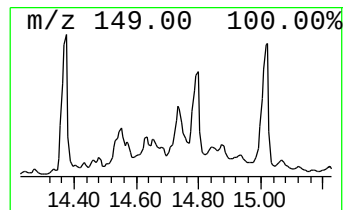
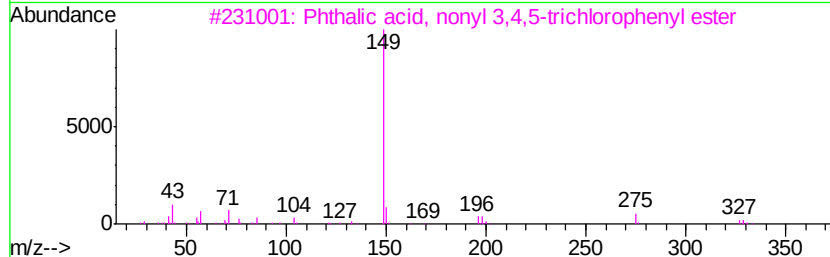
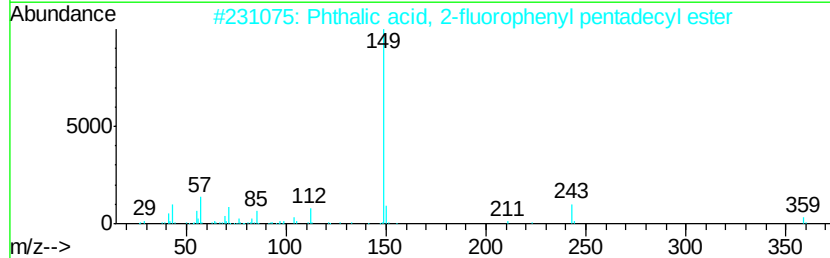
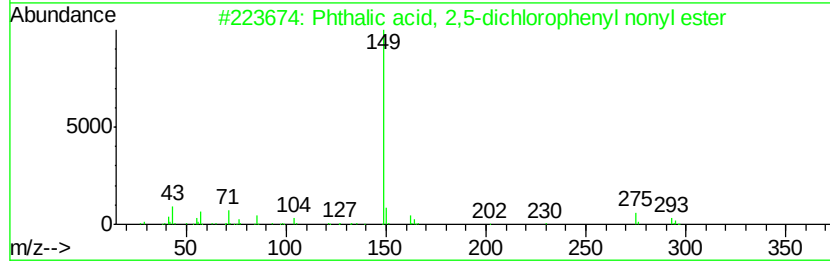
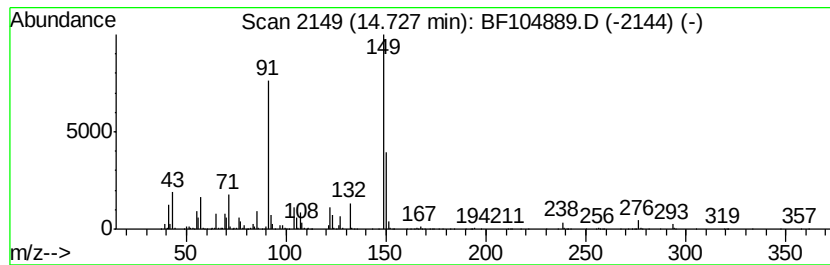
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.73 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.55 ng	3084620	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2,5-dichloropheny...	436	C23H26Cl2O4	1000356-84-4	47
2		Phthalic acid, 2-fluorophenyl pe...	470	C29H39FO4	1000356-50-2	47
3		Phthalic acid, nonyl 3,4,5-trich...	470	C23H25Cl3O4	1000357-07-2	47
4		2-(Nonyloxycarbonyl)benzoic acid	292	C17H24O4	1000373-89-9	47
5		Phthalic acid, heptyl 2-methylal...	318	C19H26O4	1000315-82-7	47



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Sample : J2522-03
Misc :
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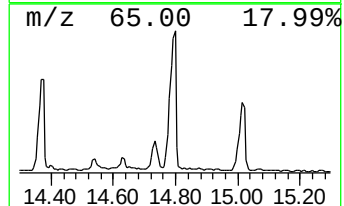
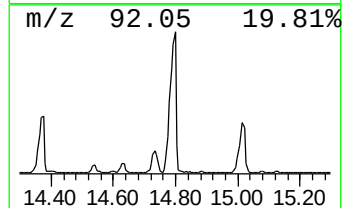
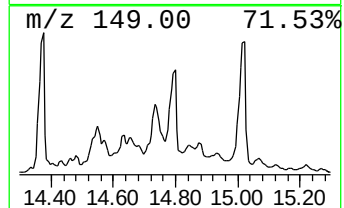
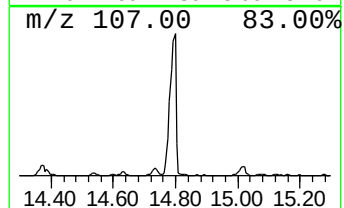
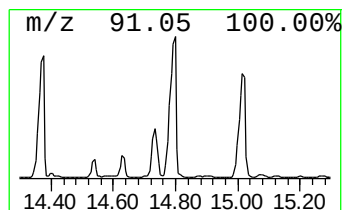
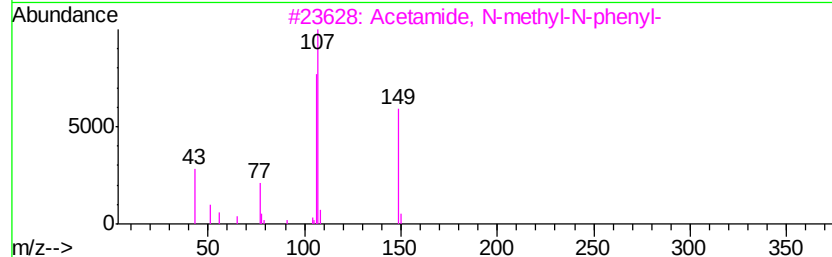
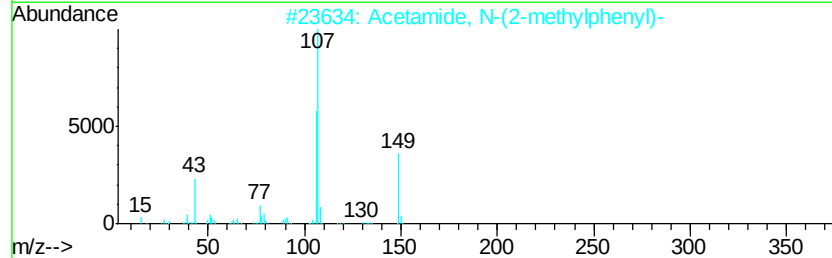
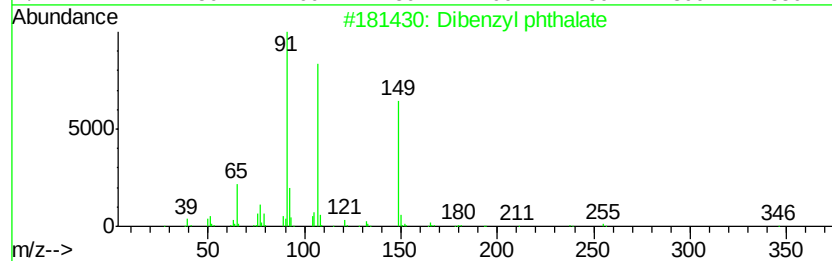
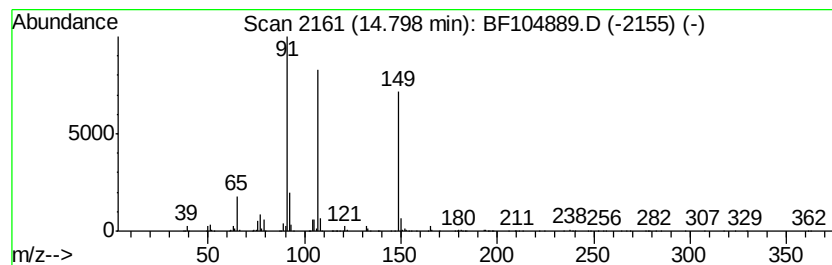
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dibenzyl phthalate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	108.17 ng	4089820	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzyl phthalate	346	C22H18O4	000523-31-9	91
2		Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	53
3		Acetamide, N-methyl-N-phenyl-	149	C9H11NO	000579-10-2	50
4		1,4-Dimethyl-pyridinium chloride	143	C7H10ClN	1000145-43-8	43
5		2-Carbamoyl-4,6-dimethylpyridine	150	C8H10N2O	072693-02-8	35



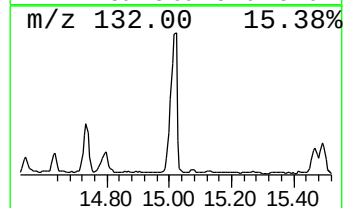
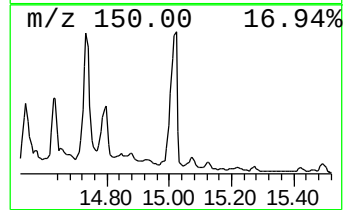
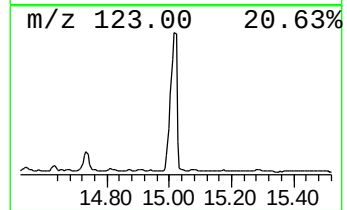
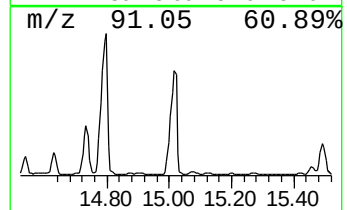
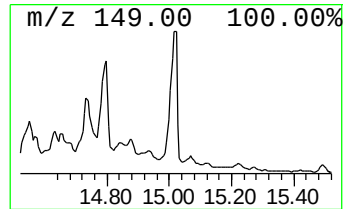
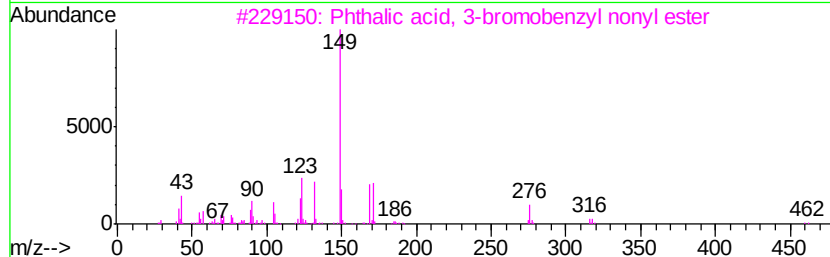
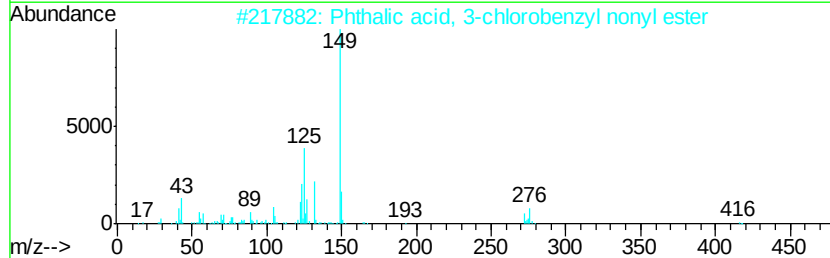
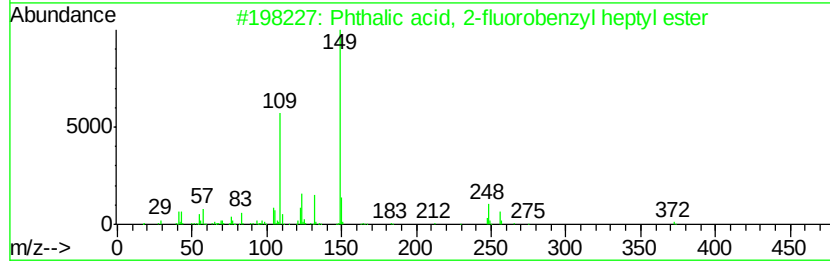
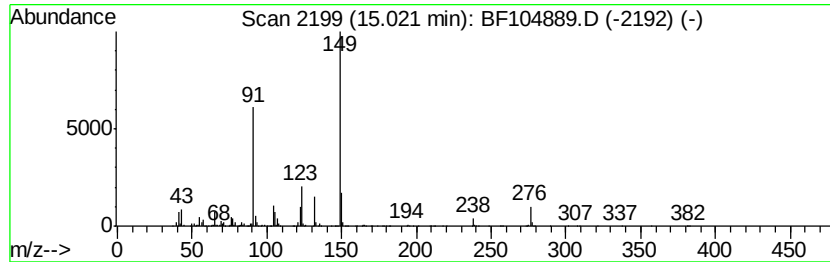
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Acq On : 27 Apr 2018 18:51
Operator : JU/SJ
Sample : J2522-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phthalic acid, 2-fluorobenz... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.02	131.05 ng	4955010	Perylene-d12	15.47		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 2-fluorobenzyl he...	372	C22H25F04	1000371-06-8	86	
2	Phthalic acid, 3-chlorobenzyl no...	416	C24H29Cl04	1000371-15-1	78	
3	Phthalic acid, 3-bromobenzyl non...	460	C24H29Br04	1000371-04-8	78	
4	Phthalic acid, 4-bromobenzyl non...	460	C24H29Br04	1000371-07-6	78	
5	Phthalic acid, 2-fluorobenzyl he...	358	C21H23F04	1000371-06-9	72	



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.58	6.58	14.5	ng	1257590	1	6.80	1738150	20.0
Phthalic acid, 8-...	11.12	18.8	ng	846255	4	11.33	900155	20.0
Benzyl Benzoate	11.17	20.0	ng	900155	4	11.33	900155	20.0
Benzyl butyl phth...	13.59	111.1	ng	75236100	5	14.03	13548600	20.0
unknown14.14	14.14	2.5	ng	1695130	5	14.03	13548600	20.0
Phthalic acid, 3-...	14.37	6.8	ng	4614520	5	14.03	13548600	20.0
Phthalic acid, he...	14.55	3.1	ng	2125180	5	14.03	13548600	20.0
unknown14.73	14.73	4.5	ng	3084620	5	14.03	13548600	20.0
Dibenzyl phthalate	14.80	108.2	ng	4089820	6	15.47	756217	20.0
Phthalic acid, 2-...	15.02	131.1	ng	4955010	6	15.47	756217	20.0