

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090717\
 Data File : BF098326.D
 Acq On : 7 Sep 2017 21:05
 Operator : SJ/JU
 Sample : I5071-03 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G61A-0-1.5

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-BF081517.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	4.857	468	471	480	rBV	38458	43095	3.21%	0.325%
2	5.287	541	544	559	rBV	605661	570512	42.45%	4.308%
3	6.334	719	722	732	rBV	636101	606775	45.15%	4.582%
4	6.457	740	743	752	rVB	697321	593086	44.13%	4.479%
5	6.687	779	782	786	rBV	755607	649706	48.34%	4.906%
6	6.845	805	809	812	rBV	466449	430363	32.02%	3.250%
7	7.251	874	878	884	rBV	390162	320591	23.85%	2.421%
8	7.975	997	1001	1004	rBV	931555	804639	59.87%	6.076%
9	9.045	1180	1183	1187	rBV	713505	600118	44.65%	4.532%
10	9.445	1246	1251	1255	rVB	89772	67707	5.04%	0.511%
11	9.728	1294	1299	1302	rBV	838094	767279	57.09%	5.794%
12	10.510	1429	1432	1441	rBV	301347	270434	20.12%	2.042%
13	10.633	1450	1453	1459	rBV3	9085	15083	1.12%	0.114%
14	10.810	1480	1483	1487	rBV	164066	130038	9.68%	0.982%
15	11.075	1526	1528	1531	rBV3	19463	17929	1.33%	0.135%
16	11.210	1547	1551	1553	rBV	776878	704575	52.43%	5.321%
17	11.228	1553	1554	1557	rVB	38479	28796	2.14%	0.217%
18	11.316	1566	1569	1576	rVB4	30743	28724	2.14%	0.217%
19	11.375	1576	1579	1585	rBV	18471	22130	1.65%	0.167%
20	12.416	1753	1756	1760	rBV	69577	61365	4.57%	0.463%
21	12.645	1790	1795	1798	rBV	80314	81523	6.07%	0.616%
22	12.792	1816	1820	1823	rBV	500725	471620	35.09%	3.561%
23	12.886	1830	1836	1840	rBV2	16605	32329	2.41%	0.244%
24	13.080	1865	1869	1873	rBV3	13876	21998	1.64%	0.166%
25	13.269	1897	1901	1905	rBV	1523646	1343937	100.00%	10.149%
26	13.339	1910	1913	1915	rBV	17413	20451	1.52%	0.154%
27	13.386	1918	1921	1927	rBV	23385	25364	1.89%	0.192%
28	13.463	1931	1934	1937	rBV	41568	46383	3.45%	0.350%
29	13.569	1949	1952	1955	rBV	65768	61372	4.57%	0.463%
30	13.616	1957	1960	1963	rVB	176019	144068	10.72%	1.088%
31	13.692	1971	1973	1980	rBV5	41804	65769	4.89%	0.497%
32	13.763	1983	1985	1990	rVV	32883	30311	2.26%	0.229%
33	13.839	1993	1998	2001	rVV	923645	1044901	77.75%	7.891%
34	13.886	2004	2006	2010	rVB2	47693	53542	3.98%	0.404%

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 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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35	13.986	2020	2023	2026	rBV2	50602	57063	4.25%	0.431%
36	14.039	2029	2032	2035	rVB	344971	327420	24.36%	2.473%
37	14.110	2041	2044	2046	rBV	52953	46334	3.45%	0.350%
38	14.198	2055	2059	2062	rBV	348380	335304	24.95%	2.532%
39	14.233	2062	2065	2068	rVB	153280	130252	9.69%	0.984%
40	14.445	2097	2101	2106	rVB	418170	391950	29.16%	2.960%
41	14.510	2110	2112	2115	rBV	89150	97271	7.24%	0.735%
42	14.786	2156	2159	2164	rVB	208845	239347	17.81%	1.807%
43	14.839	2165	2168	2173	rBV2	114217	159268	11.85%	1.203%
44	15.074	2202	2208	2212	rBV	298737	441369	32.84%	3.333%
45	15.257	2234	2239	2246	rVB	409678	532752	39.64%	4.023%
46	15.468	2272	2275	2277	rBV2	66595	83199	6.19%	0.628%
47	15.839	2334	2338	2344	rBV	147910	224413	16.70%	1.695%

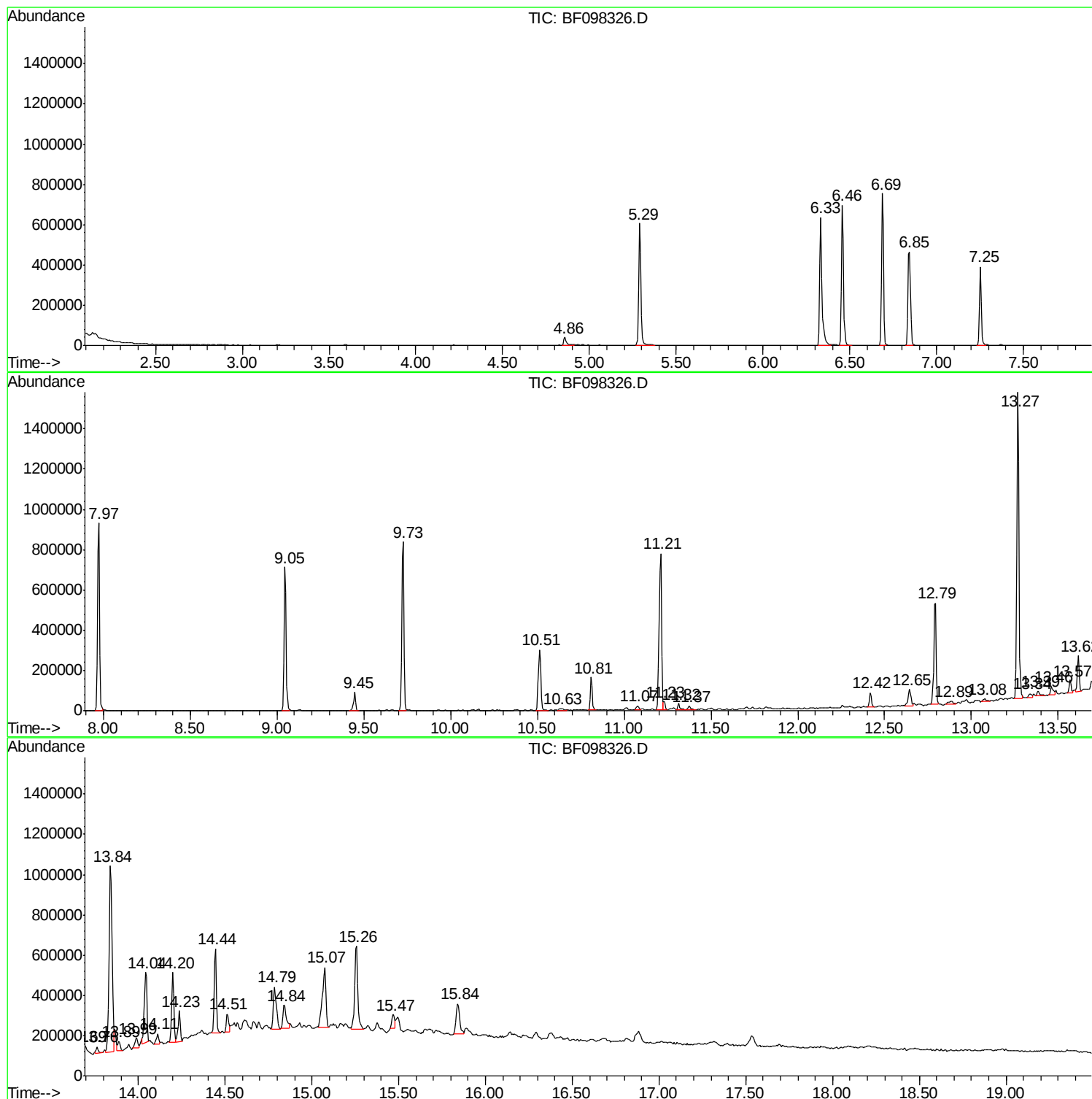
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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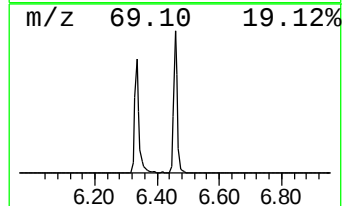
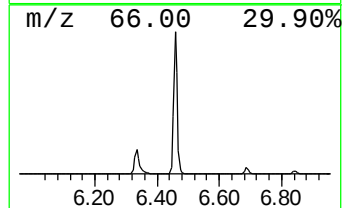
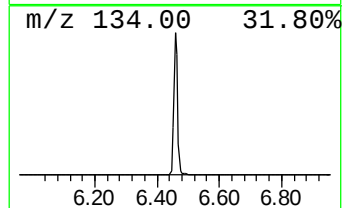
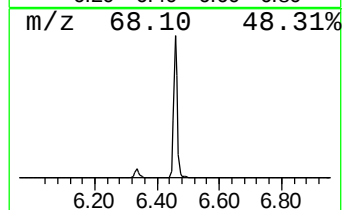
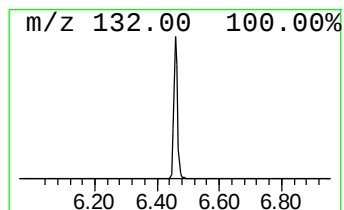
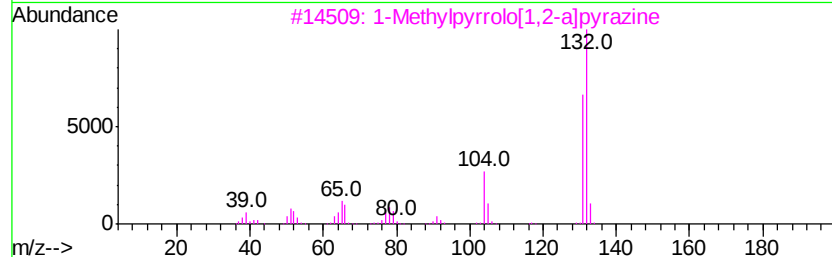
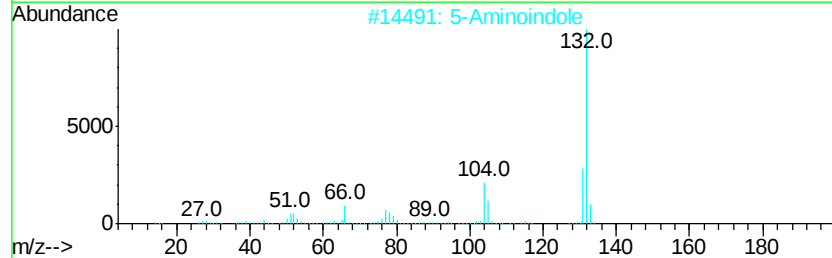
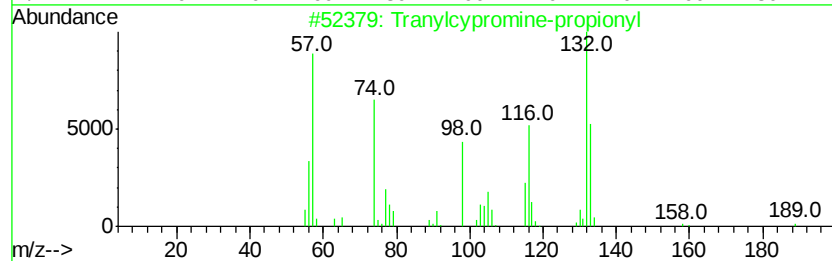
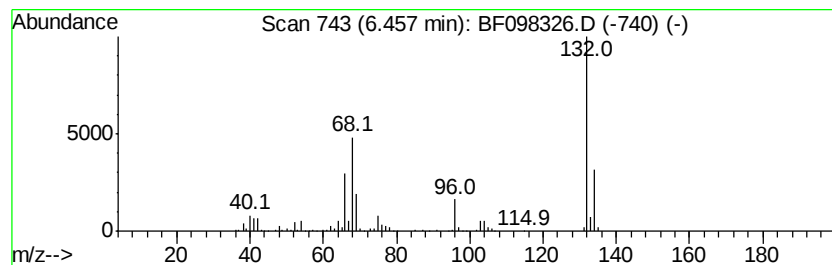
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	18.26 ng	593086	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		5-Aminoindole	132	C8H8N2	005192-03-0	10
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		Xenon	132	Xe	007440-63-3	9



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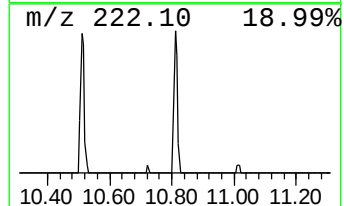
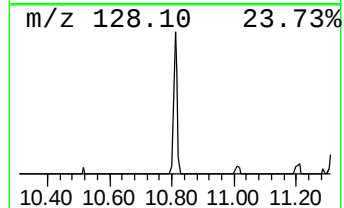
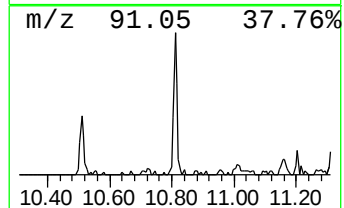
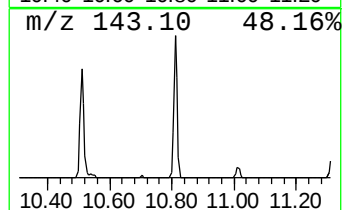
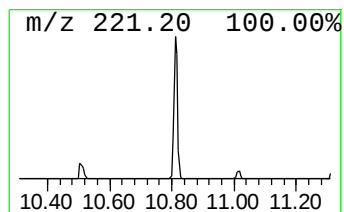
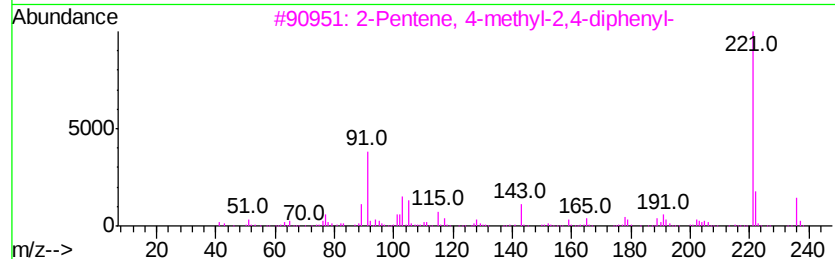
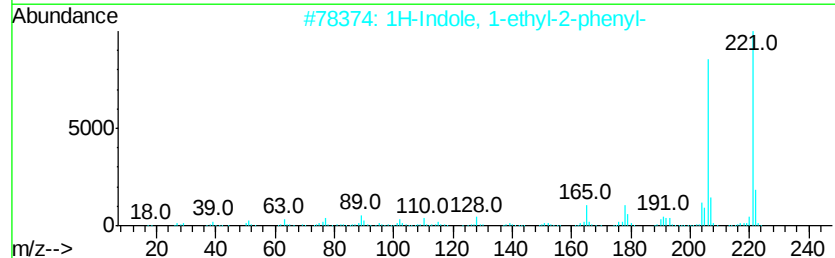
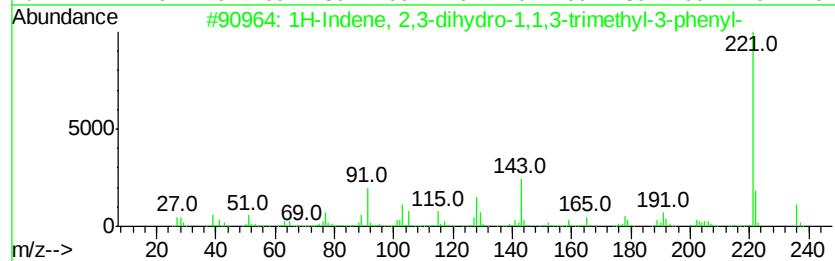
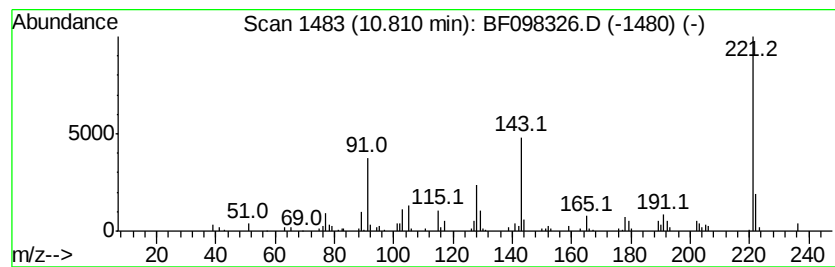
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	3.69 ng	130038	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	78
2		1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	38
3		2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	38
4		Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
5		Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	38



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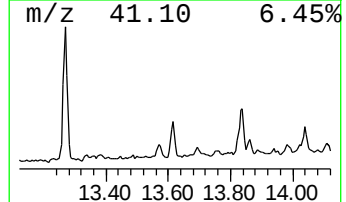
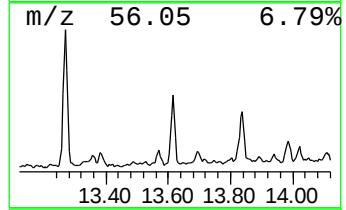
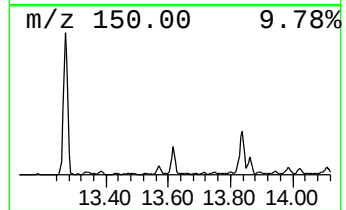
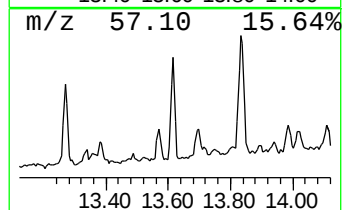
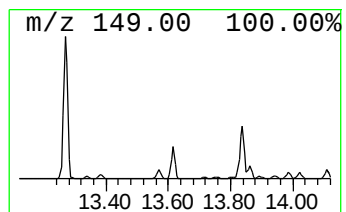
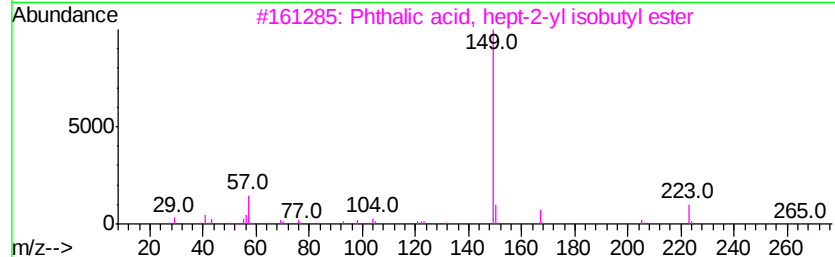
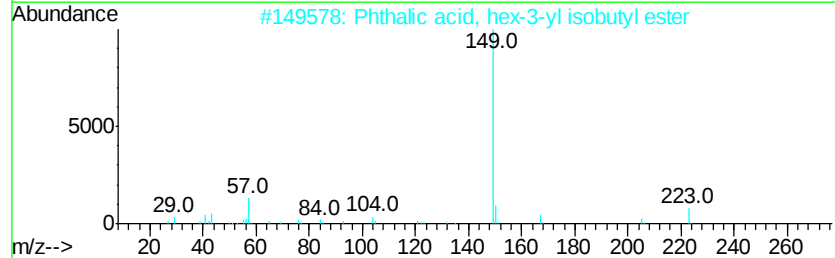
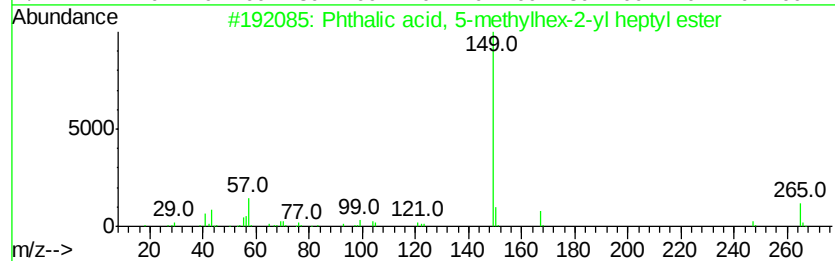
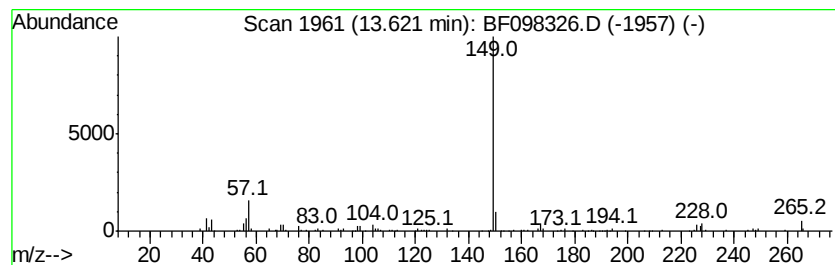
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phthalic acid, 5-methylhex-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.62	2.76 ng	144068	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 5-methylhex-2-yl ...	362	C22H34O4	1000371-08-7	90	
2	Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	86	
3	Phthalic acid, hept-2-yl isobutyl...	320	C19H28O4	1000356-97-0	80	
4	Phthalic acid, dec-2-yl isobutyl...	362	C22H34O4	1000356-93-8	78	
5	Phthalic acid, cyclohexyl isohex...	304	C18H24O4	1000315-34-0	72	



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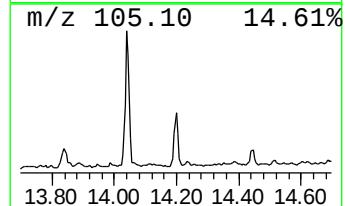
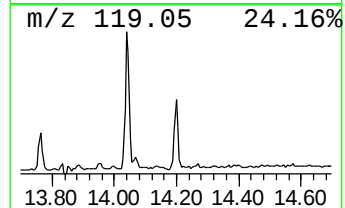
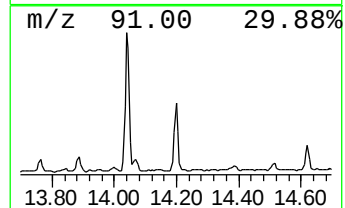
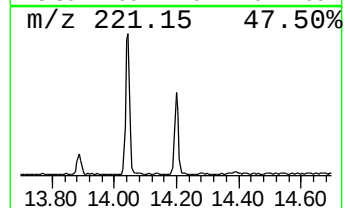
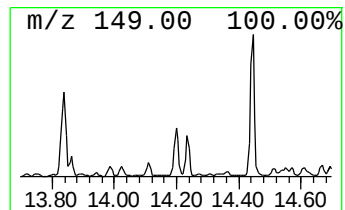
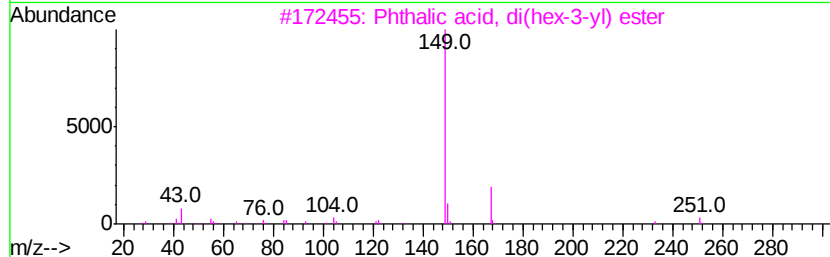
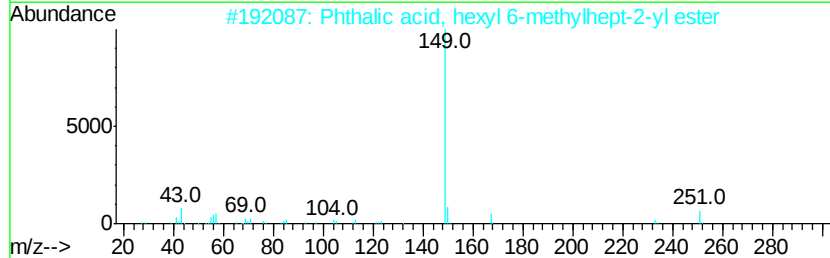
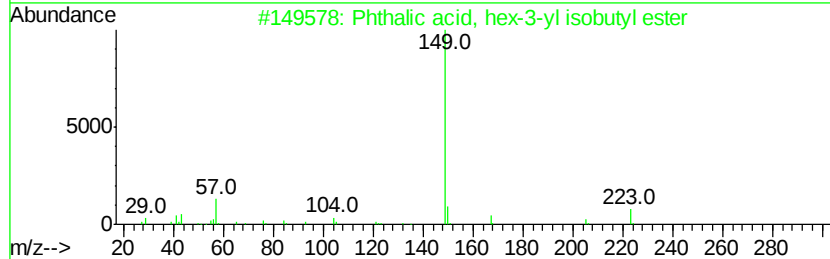
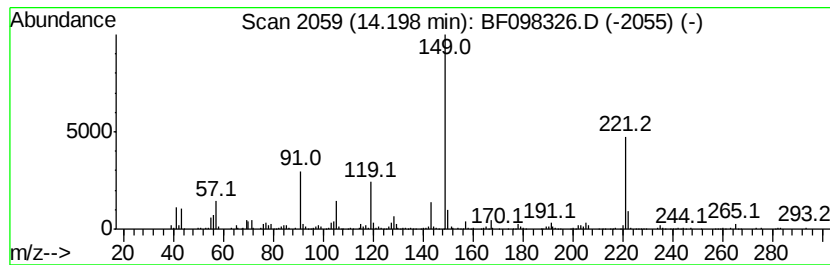
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.20 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	6.42 ng	335304	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	43
2		Phthalic acid, hexyl 6-methylhept...	362	C22H34O4	1000377-96-0	43
3		Phthalic acid, di(hex-3-yl) ester	334	C20H30O4	1000356-96-7	38
4		Phthalic acid, 4-methylhept-3-yl...	348	C21H32O4	1000377-94-0	38
5		Phthalic acid, 2-ethylcyclohexyl...	332	C20H28O4	1000315-36-3	38



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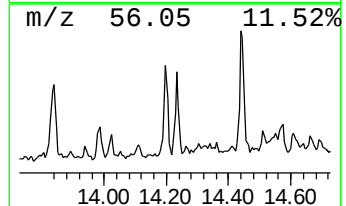
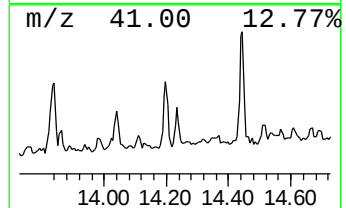
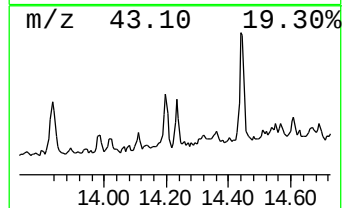
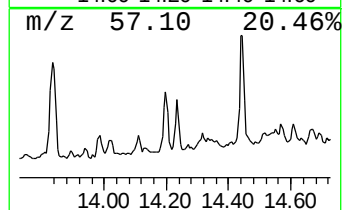
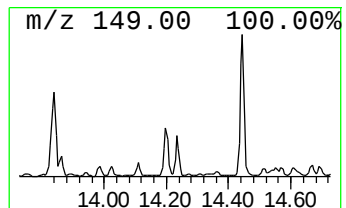
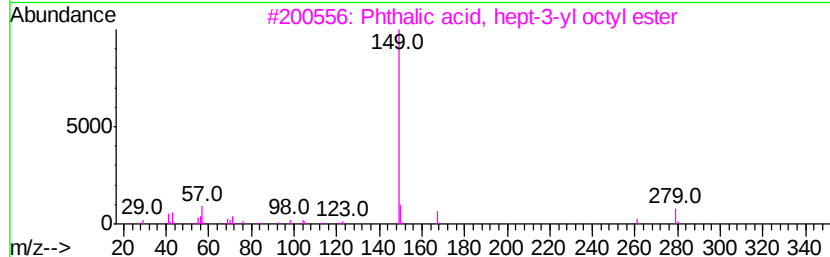
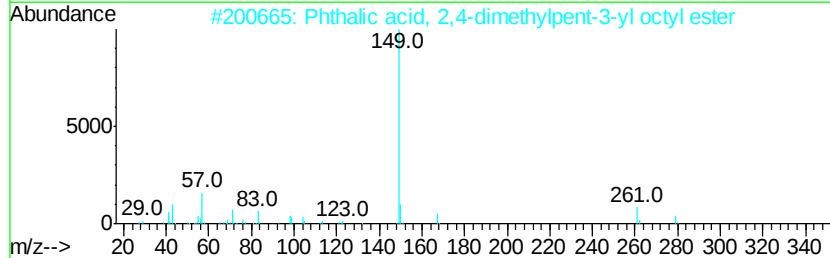
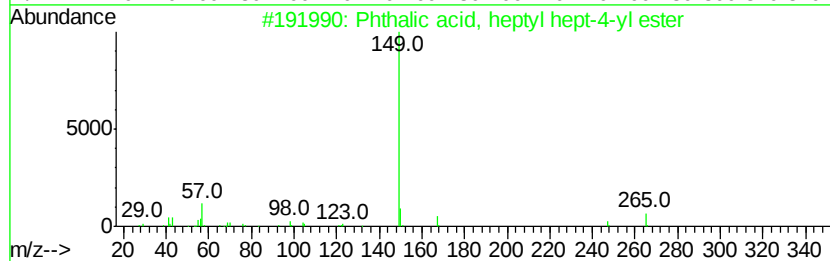
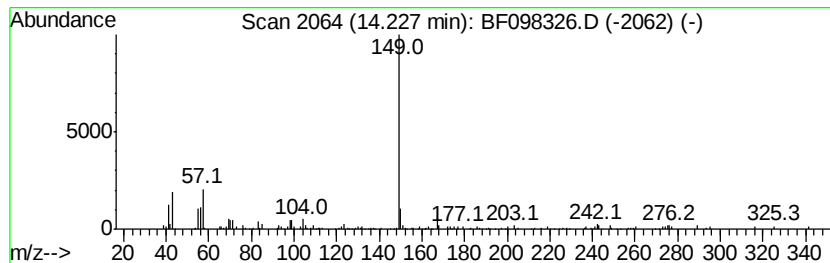
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phthalic acid, heptyl hept-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.49 ng	130252	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, heptyl hept-4-yl ...	362	C22H34O4	1000356-78-8	86
2		Phthalic acid, 2,4-dimethylpent-...	376	C23H36O4	1000356-84-7	83
3		Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	80
4		Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
5		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	80



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098326.D
Acq On : 7 Sep 2017 21:05
Operator : SJ/JU
Sample : I5071-03 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

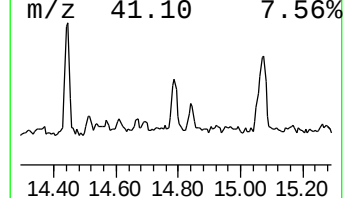
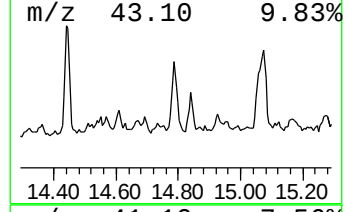
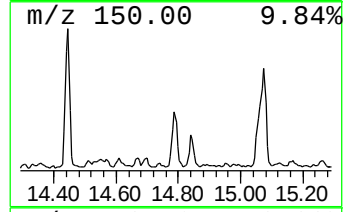
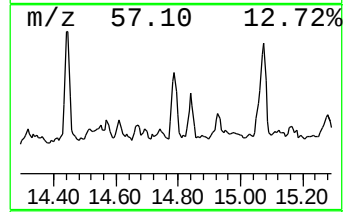
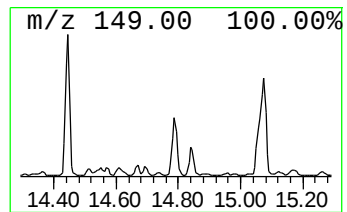
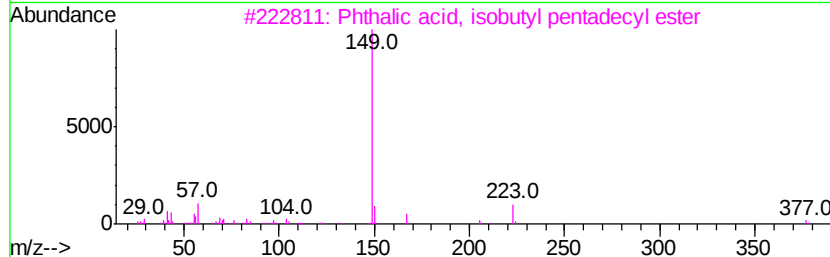
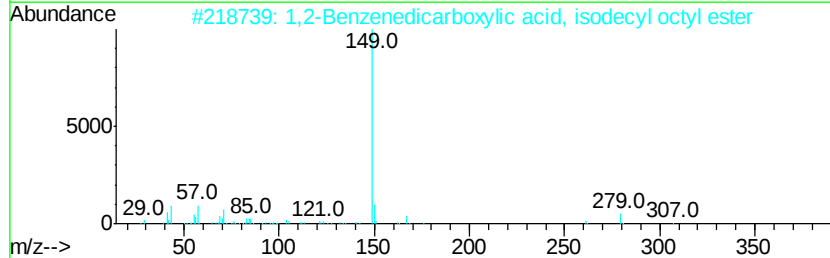
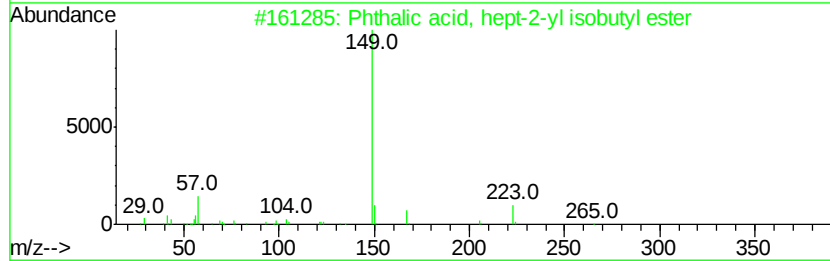
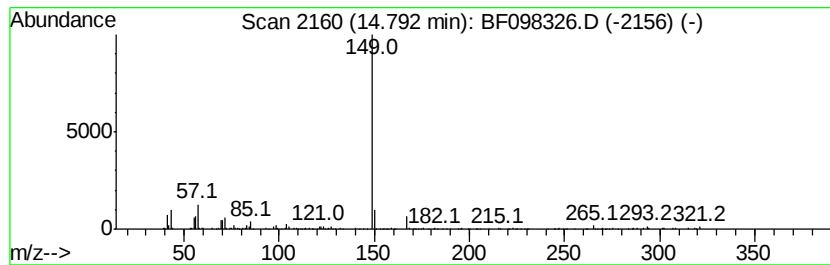
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ClientSampleId :
G61A-0-1.5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
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-2-yl is... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	8.99 ng	239347	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phthalic acid, hept-2-yl isobutyl...	320 C19H28O4	1000356-97-0	80
2	1,2-Benzenedicarboxylic acid, is...	418 C26H42O4	001330-96-7	80
3	Phthalic acid, isobutyl pentadec...	432 C27H44O4	1000309-07-3	72
4	1,2-Benzenedicarboxylic acid, di...	474 C30H50O4	003648-20-2	72
5	Phthalic acid, 2,5-dichloropheny...	478 C26H32Cl2O4	1000356-44-0	72



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098326.D
Acq On : 7 Sep 2017 21:05
Operator : SJ/JU
Sample : I5071-03 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
G61A-0-1.5

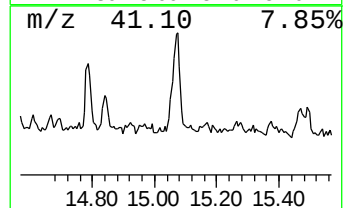
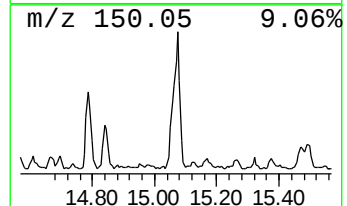
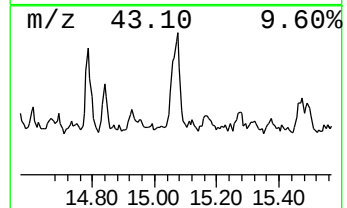
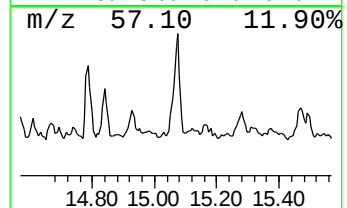
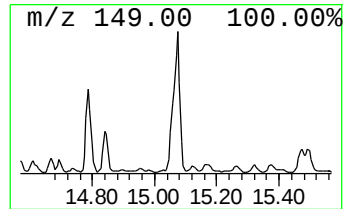
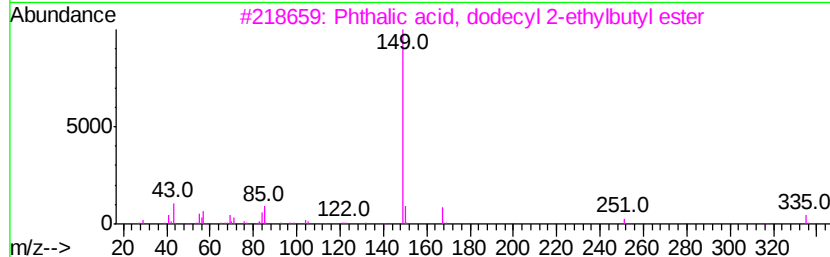
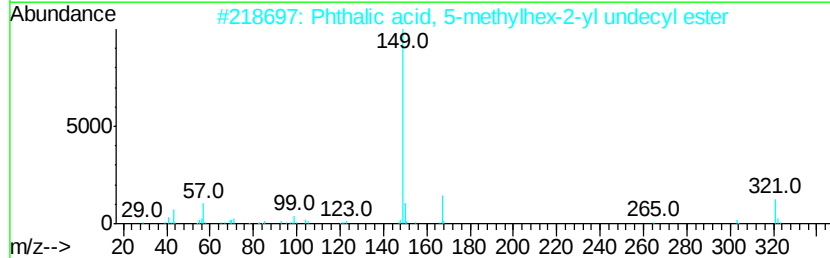
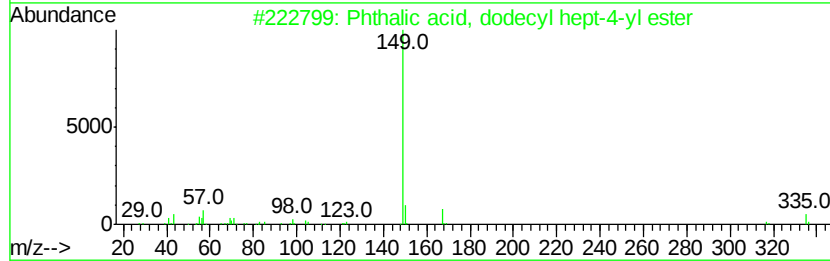
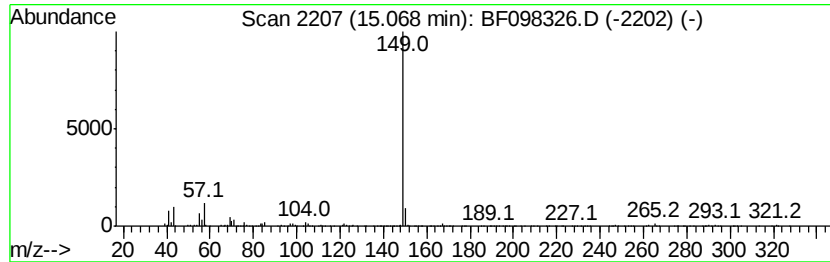
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phthalic acid, dodecyl hept... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	16.57 ng	441369	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, dodecyl hept-4-yl...	432	C27H44O4	1000356-79-3	72
2		Phthalic acid, 5-methylhex-2-yl ...	418	C26H42O4	1000371-08-3	72
3		Phthalic acid, dodecyl 2-ethylbu...	418	C26H42O4	1000356-89-7	72
4		Phthalic acid, heptyl hept-3-yl ...	362	C22H34O4	1000356-99-1	72
5		Phthalic acid, 2-propylphenyl tr...	466	C30H42O4	1000357-02-8	72



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098326.D
Acq On : 7 Sep 2017 21:05
Operator : SJ/JU
Sample : I5071-03 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
G61A-0-1.5

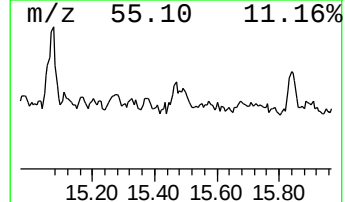
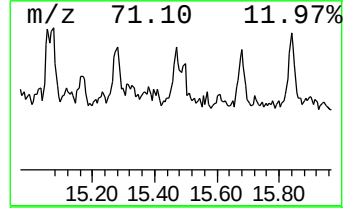
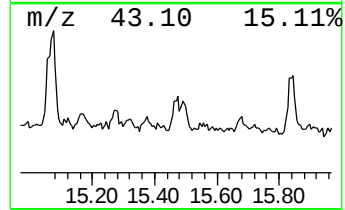
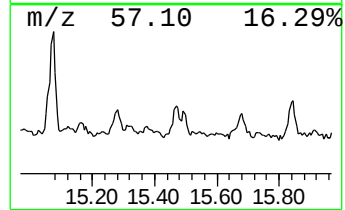
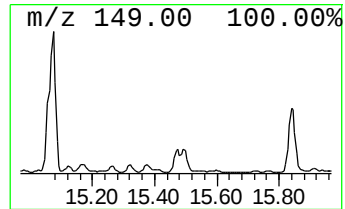
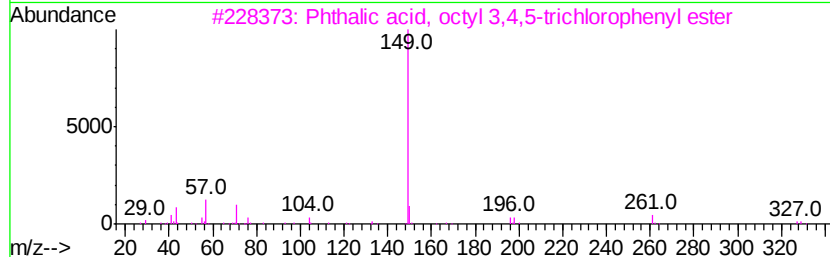
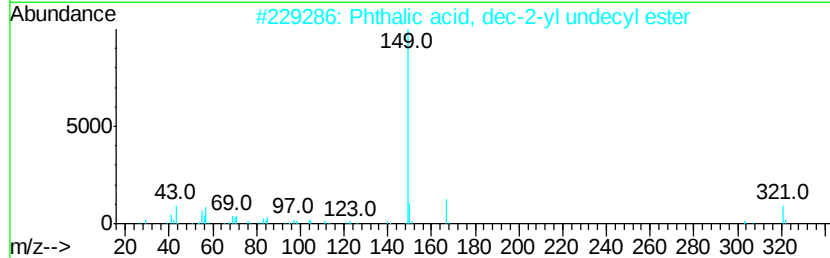
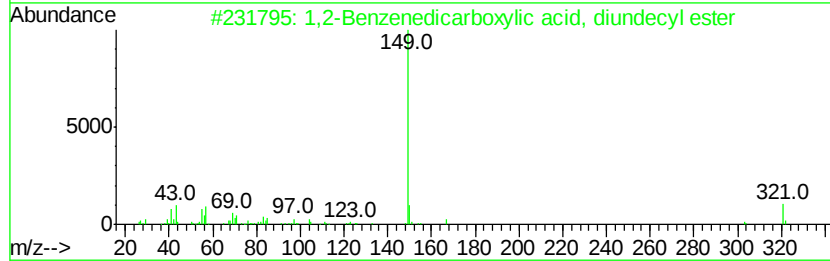
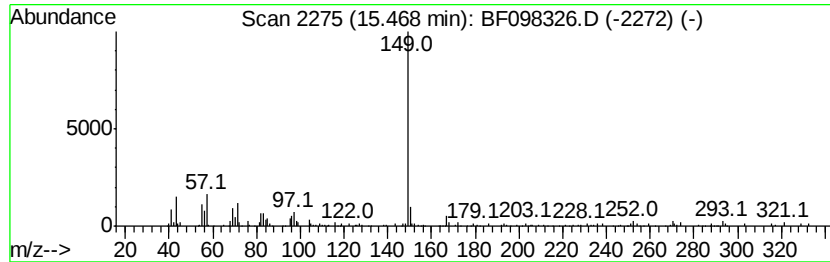
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	3.12 ng	83199	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	80
2			Phthalic acid, dec-2-yl undecyl ...	460	C29H48O4	1000356-94-6	72
3			Phthalic acid, octyl 3,4,5-trich...	456	C22H23Cl3O4	1000357-07-1	72
4			Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	72
5			Phthalic acid, heptyl tridec-2-y...	442	C28H42O4	1000315-44-0	64



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090717\
Data File : BF098326.D
Acq On : 7 Sep 2017 21:05
Operator : SJ/JU
Sample : I5071-03 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G61A-0-1.5

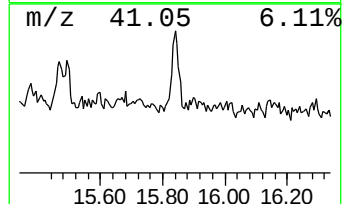
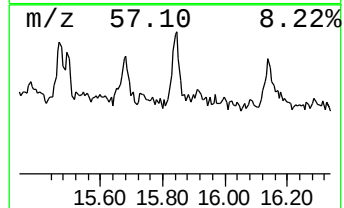
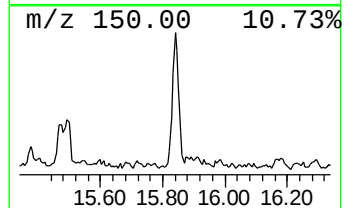
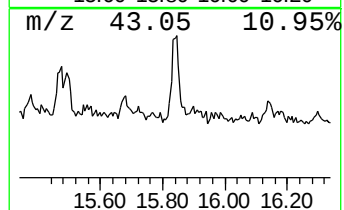
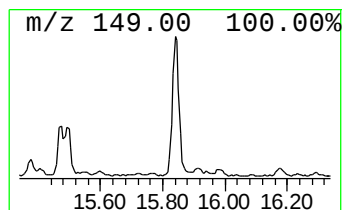
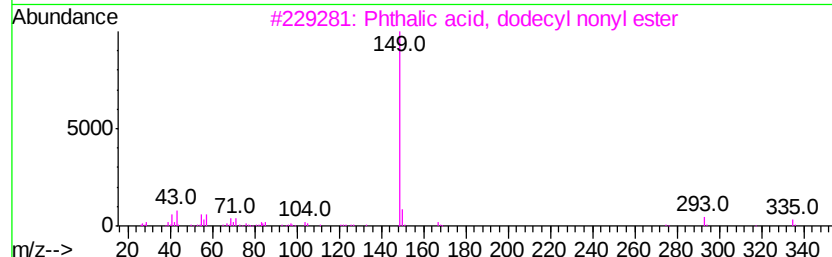
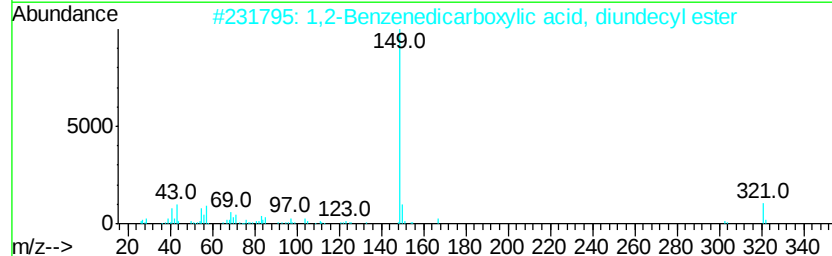
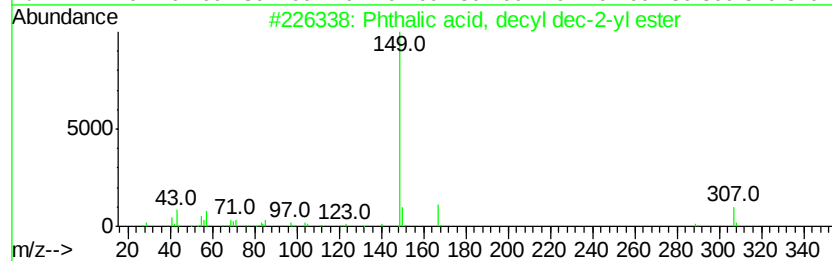
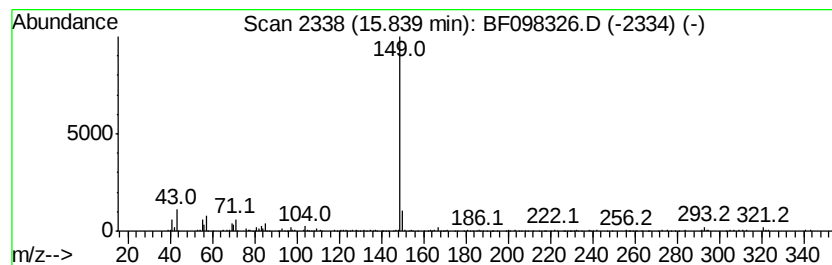
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phthalic acid, decyl dec-2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	8.42 ng	224413	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, decyl dec-2-yl ester	446	C28H46O4	1000356-94-5	80
2		1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	80
3		Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	80
4		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	72
5		Phthalic acid, decyl 3,4-dimethy...	410	C26H34O4	1000309-82-4	72



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090717\
Data File : BF098326.D
Acq On : 7 Sep 2017 21:05
Operator : SJ/JU
Sample : I5071-03 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G61A-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
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1H-Indene, 2,3-di...	10.81	3.7	ng	130038	4	11.21	704575	20.0
Phthalic acid, 5-...	13.62	2.8	ng	144068	5	13.85	1044900	20.0
unknown14.20	14.20	6.4	ng	335304	5	13.85	1044900	20.0
Phthalic acid, he...	14.23	2.5	ng	130252	5	13.85	1044900	20.0
Phthalic acid, he...	14.79	9.0	ng	239347	6	15.26	532752	20.0
Phthalic acid, do...	15.07	16.6	ng	441369	6	15.26	532752	20.0
1,2-Benzenedicarb...	15.47	3.1	ng	83199	6	15.26	532752	20.0
Phthalic acid, de...	15.84	8.4	ng	224413	6	15.26	532752	20.0