

Supplementary Information to:

Conformational Flexibility of C8-Phenoxy-guanine Adducts in Deoxydinucleoside Monophosphates

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TABLE S1: Values of Backbone Torsional Angles (deg.) in Deoxydinucleoside Monophosphates containing Natural dG^a

Containing Natural ds											
	Cytosine		Thymine		Guanine		Adenine		Average		Exp ^b
	5'	3'	5'	3'	5'	3'	5'	3'	5'	3'	
<i>anti</i>											
χ5'	242.1	227.8	244.8	218.9	253.5	253.5	251.9	256.2	248.1	239.1	— ^c
χ3'	237.8	287.1	218.1	280.1	265.3	265.3	270.8	266.8	248.0	274.8	— ^c
γ5'	48.1	50.9	49.8	50.6	49.7	49.7	46.6	49.8	48.6	50.2	48 ± 11
δ5'	146.4	144.9	148.2	137.2	149.0	149.0	146.8	149.7	147.6	145.2	128 ± 13
ε5'	189.6	202.9	186.4	199.5	188.4	188.4	195.7	187.6	190.0	194.6	184 ± 11
ζ	275.7	283.5	276.9	277.8	277.0	277.0	277.8	277.7	276.9	279.0	265 ± 10
α	295.7	291.6	295.7	297.5	297.1	297.1	290.5	296.6	294.8	295.7	298 ± 15
β3'	165.9	173.6	164.1	174.3	166.2	166.2	171.1	166.8	166.8	170.2	176 ± 9
γ3'	55.4	51.7	56.6	58.6	53.1	53.1	46.7	51.6	52.9	53.7	48 ± 11
δ3'	112.3	148.0	86.6	152.8	137.1	137.1	137.1	138.3	118.3	144.0	128 ± 13
ε3'	188.1	176.4	193.4	176.2	180.5	180.5	180.9	180.5	185.7	178.4	184 ± 11
<i>syn</i>											
χ5'	76.2	224.0	88.0	225.3	88.5	239.7	86.7	236.8	84.9	231.5	
χ3'	239.8	78.1	253.3	78.8	263.9	66.5	261.4	65.2	254.6	72.2	
γ5'	45.7	48.3	48.8	48.1	49.2	48.4	49.8	48.5	48.4	48.3	
δ5'	138.2	138.3	139.3	140.5	142.9	141.9	143.1	142.2	140.9	140.7	
ε5'	165.0	201.1	158.5	199.1	159.4	179.8	149.0	182.4	158.0	190.6	
ζ	265.2	282.9	265.9	282.3	266.3	268.6	268.7	272.5	266.5	276.6	
α	298.1	294.9	303.1	295.2	301.2	306.9	304.4	306.5	301.7	300.9	
β3'	185.9	173.0	180.2	172.3	179.6	171.0	185.5	167.8	182.8	171.0	
γ3'	60.4	50.9	62.5	51.2	65.5	55.0	60.0	55.9	62.1	53.3	
δ3'	143.7	143.6	146.9	143.4	152.8	136.5	151.4	133.8	148.7	139.3	
ε3'	176.5	176.4	176.5	176.4	174.2	179.1	175.6	179.8	175.7	177.9	

^a M06-2X/6-31G(d,p) optimized geometries. All angles are defined in Figure 2. ^b Taken from Reference 85. ^c Average value for purine nucleobases is 258 ± 14° and 241 ± 8° for pyrimidines.

TABLE S2: Values of Backbone Torsional Angles (deg.) in Deoxydinucleoside Monophosphates containing the o-PhOH-dG adduct.^a

	Cytosine		Thymine		Guanine		Adenine		Average	
	5'	3'	5'	3'	5'	3'	5'	3'	5'	3'
<i>anti</i>										
$\chi 5'$	241.6	222.4	238.0	236.2	254.3	260.6	245.3	262.7	244.8	245.5
$\chi 3'$	252.0	257.2	244.1	256.7	256.5	245.8	267.5	248.6	255.0	252.1
$\gamma 5'$	54.1	51.5	55.1	51.2	55.0	49.4	52.4	52.4	54.1	51.1
$\delta 5'$	87.9	145.8	87.4	147.4	87.5	150.6	81.0	152.5	85.95	149.1
$\epsilon 5'$	166.2	215.0	154.5	207.6	162.3	191.1	170.8	191.1	163.4	201.2
ζ	274.7	290.6	275.3	281.6	273.6	275.1	266.0	276.5	272.4	280.9
α	311.8	276.1	318.6	284.3	315.2	293.8	310.5	293.6	314.0	287.0
$\beta 3'$	168.5	159.6	167.3	159.8	164.7	160.6	169.7	159.5	167.6	159.9
$\gamma 3'$	56.9	52.7	61.0	53.9	58.1	57.5	60.9	57.8	59.2	55.5
$\delta 3'$	139.9	92.1	142.1	91.5	145.9	90.7	152.6	91.6	145.1	91.5
$\epsilon 3'$	178.8	194.9	178.0	193.5	176.7	193.7	174.5	193.7	177.0	193.9
<i>syn</i>										
$\chi 5'$	84.0	225.1	94.3	220.9	97.3	225.9	68.9	228.3	86.1	225.1
$\chi 3'$	250.4	89.8	241.1	89.9	271.1	90.9	279.5	92.8	260.5	90.9
$\gamma 5'$	47.5	48.6	48.5	47.9	50.0	48.0	45.9	48.3	48.0	48.2
$\delta 5'$	139.1	140.7	140.3	140.9	145.0	143.7	134.3	144.2	139.7	142.4
$\epsilon 5'$	174.4	199.6	169.8	199.5	165.9	199.8	179.2	198.6	172.3	199.4
ζ	270.9	284.2	266.4	283.7	263.8	283.5	265.2	284.5	266.6	284.0
α	301.1	292.2	303.2	292.4	303.1	291.8	308.2	290.6	303.9	291.8
$\beta 3'$	168.9	172.9	171.5	171.5	178.3	172.4	164.1	173.6	170.7	172.6
$\gamma 3'$	65.5	50.1	68.2	50.8	64.4	50.1	67.1	50.2	66.3	50.3
$\delta 3'$	138.3	145.8	140.6	145.3	153.9	146.3	153.9	146.9	146.7	146.1
$\epsilon 3'$	177.5	175.8	177.4	175.8	175.6	176.0	175.1	175.7	176.4	175.8

^a M06-2X/6-31G(d,p) optimized geometries. All angles are defined in Figure 2.

TABLE S3: Values of Backbone Torsional Angles (deg.) in Deoxydinucleoside Monophosphates containing the *p*-PhOH-dG adduct.^a

	Cytosine		Thymine		Guanine		Adenine		Average	
	5'	3'	5'	3'	5'	3'	5'	3'	5'	3'
<i>anti</i>										
$\chi 5'$	246.1	227.3	241.5	234.0	247.0	232.9	248.1	240.1	245.7	233.6
$\chi 3'$	247.8	261.2	245.7	264.0	261.1	263.3	248.0	280.7	250.7	267.3
$\gamma 5'$	55.5	50.6	54.8	52.5	55.2	51.5	45.2	51.7	52.7	51.6
$\delta 5'$	86.1	144.0	86.6	150.0	85.5	149.8	137.6	150.6	99.0	148.6
$\epsilon 5'$	160.4	219.8	153.4	207.7	167.4	214.6	187.0	199.9	167.1	210.5
ζ	276.2	289.3	275.5	287.3	273.0	295.2	225.2	284.6	262.5	289.1
α	313.1	279.0	316.6	283.7	315.2	275.6	304.5	290.1	312.4	282.1
$\beta 3'$	166.7	158.0	167.1	163.2	165.1	163.2	177.6	168.1	169.1	163.1
$\gamma 3'$	57.8	51.6	61.2	52.4	61.5	51.7	53.0	52.6	58.4	52.1
$\delta 3'$	136.4	90.0	142.1	89.5	151.3	89.7	151.3	140.8	145.3	102.5
$\epsilon 3'$	179.3	193.3	177.7	194.6	175.2	193.9	176.0	178.5	177.1	190.1
<i>syn</i>										
$\chi 5'$	91.4	224.1	93.9	220.3	89.6	228.5	88.3	232.4	90.8	226.3
$\chi 3'$	236.2	82.2	242.7	86.5	264.3	87.4	251.2	95.5	248.6	87.9
$\gamma 5'$	47.8	49.6	48.4	48.5	48.5	48.0	47.5	50.1	48.1	49.1
$\delta 5'$	142.2	142.7	139.8	140.8	140.7	143.9	141.0	147.9	140.9	143.8
$\epsilon 5'$	170.9	195.6	169.1	199.2	170.5	198.8	169.4	204.1	170.0	199.4
ζ	257.5	285.0	257.0	283.0	258.8	283.7	250.4	293.7	255.9	286.4
α	300.7	295.3	305.3	292.6	305.0	292.2	305.7	284.2	304.2	291.1
$\beta 3'$	175.1	173.9	171.5	171.3	170.6	173.1	172.2	169.9	172.4	172.1
$\gamma 3'$	61.6	49.7	63.7	51.4	65.7	50.4	60.8	54.4	63.0	51.5
$\delta 3'$	140.7	144.2	142.9	144.1	151.5	145.1	148.2	146.4	145.8	145.0
$\epsilon 3'$	176.5	175.0	176.1	176.2	175.9	175.8	176.1	175.3	176.2	175.6

^a M06-2X/6-31G(d,p) optimized geometries. All angles are defined in Figure 2.