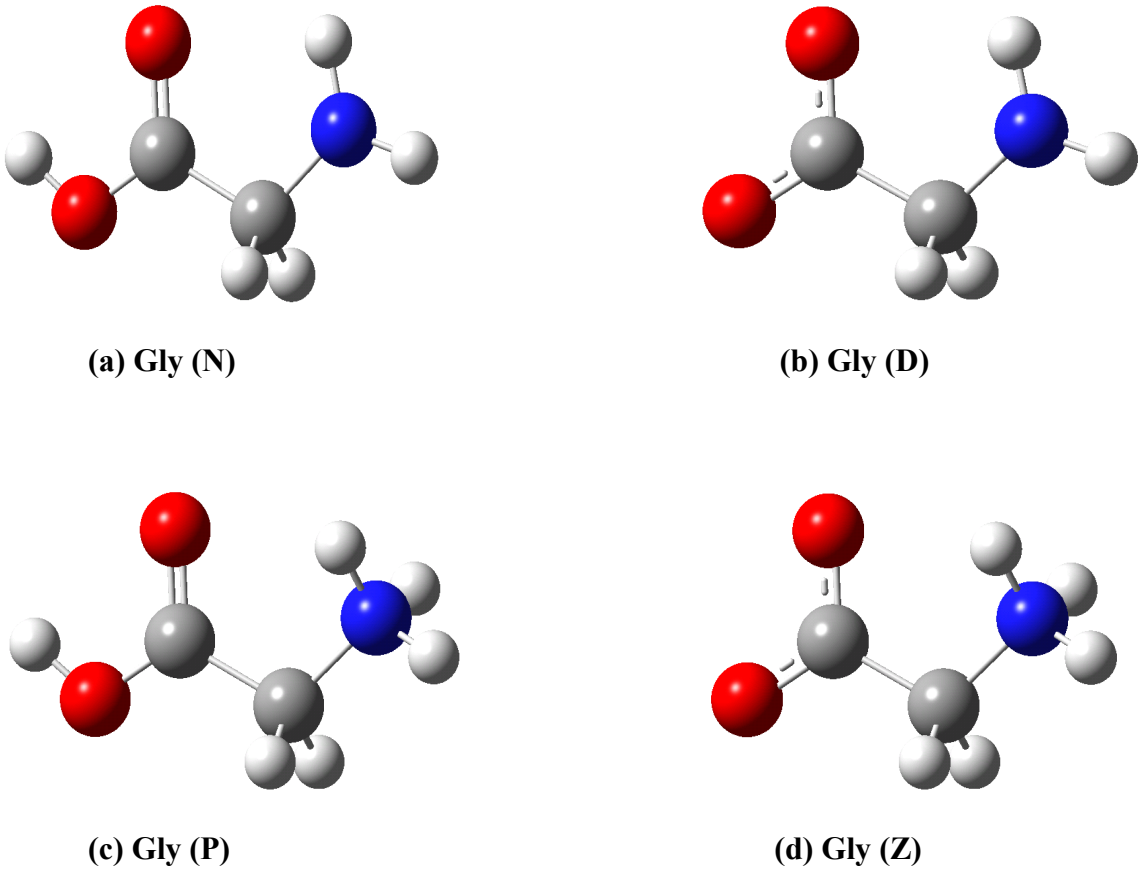
Supplementary information

Fig. S1

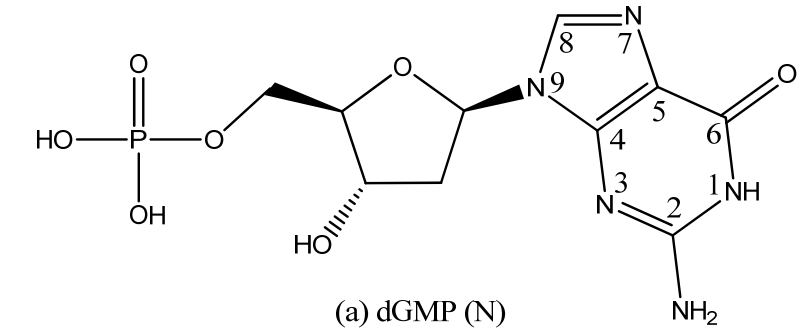


(a) Gly (N) **(b) Gly (D)**

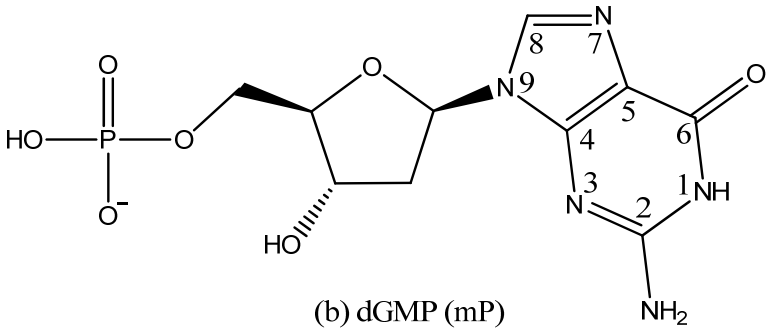
(c) Gly (P) **(d) Gly (Z)**

Figure S1: (a) Neutral Glycine, Gly (N); **(b)** Deprotonated Glycine, Gly (D); **(c)** Protonated Glycine, Gly (P); **(d)** Zwitteroinic Glycine, Gly (Z).

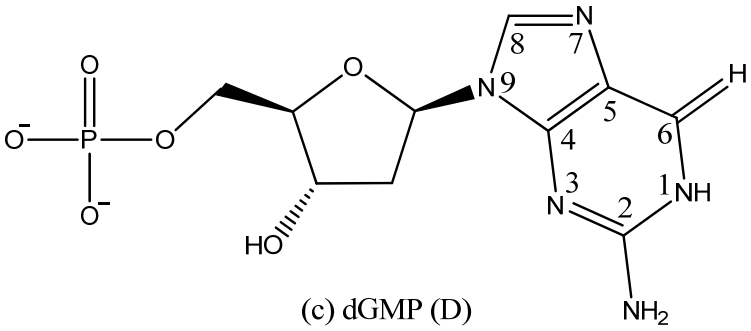
Fig. S2



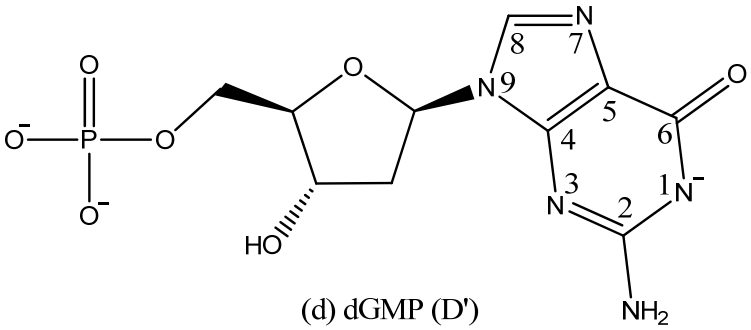
(a) dGMP (N)



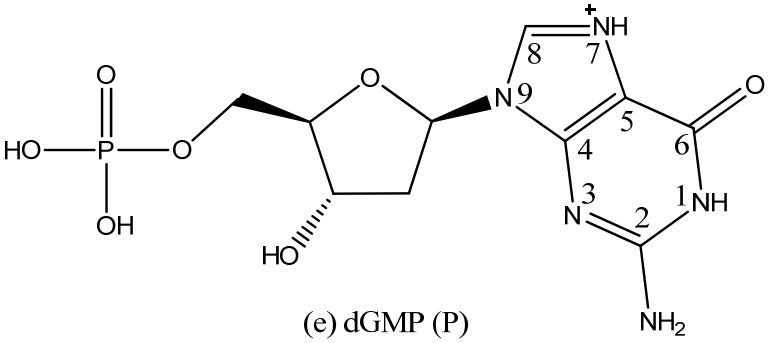
(b) dGMP (mP)



(c) dGMP (D)



(d) dGMP (D')



(e) dGMP (P)

Figure S2: Different protonic states of dGMP **(a)** Neutral, dGMP (N); **(b)** Monoprotonated, dGMP (mP); **(c)** Deprotonated, dGMP (D); **(d)** Deprotonation of the guanosine moiety at N1 site, dGMP (D´); **(e)** Protonation of the guanosine moiety at N7 site, dGMP (P).

Table S1. Calculated bond lengths (Å) for dGMP, (dGMP + 1Gly + 5W) and (dGMP + 2Gly + 5W) obtained using B3LYP method employing 6-311+G(d,p) basis set

Bond length	dGMP	dGMP+1Gly +5W	dGMP+2Gly +5W
O_{19}–C_{18}	1.213	1.232	1.253
C_{17}–C_{18}	1.437	1.425	1.413
N_{20}–C_{18}	1.440	1.411	1.394
N_{20}–C_{22}	1.368	1.378	1.380
N_{26}–C_{22}	1.308	1.335	1.337
C_{27}–N_{26}	1.356	1.353	1.348
C_{27}–C_{17}	1.392	1.393	1.396
C_{17}–N_{16}	1.379	1.384	1.382
N_{16}–C_{14}	1.304	1.304	1.302
C_{14}–N_{13}	1.390	1.382	1.387
N_{13}–C_{27}	1.375	1.382	1.381
C_{14}–H_{15}	1.078	1.076	1.076
N_{20}–H_{21}	1.012	1.022	1.026
C_{22}–N_{23}	1.376	1.338	1.333
N_{23}–H_{24}	1.009	1.020	1.021
N_{23}–H_{25}	1.009	1.021	1.022
N_{13}–C_{11}	1.446	1.460	1.467
C_{11}–O_{10}	1.426	1.424	1.421
O_{10}–C_{8}	1.433	1.437	1.437
C_{8}–C_{28}	1.544	1.539	1.536
C_{28}–C_{30}	1.529	1.531	1.533
C_{30}–H_{31}	1.092	1.090	1.088
C_{30}–H_{32}	1.091	1.091	1.091
C_{28}–O_{33}	1.430	1.432	1.430
O_{33}–H_{34}	0.962	0.963	0.963
C_{28}–H_{29}	1.094	1.094	1.094
C_{8}–C_{5}	1.516	1.519	1.519
C_{5}–H_{6}	1.091	1.092	1.092
C_{5}–H_{7}	1.094	1.095	1.095
C_{5}–O_{4}	1.451	1.452	1.450
O_{4}–P1	1.605	1.607	1.614
P_{1}–O_{3}	1.469	1.487	1.488
P_{1}–O_{35}	1.602	1.574	1.565
P_{1}–O_{2}	1.625	1.614	1.618
O_{35}–H_{36}	0.965	1.010	1.030
O_{2}–H_{37}	0.965	0.965	0.964