Supplementary material for
"Bridging QTAIM with vibrational spectroscopy: the energy of intramolecular hydrogen bonds in DNA-related biomolecules"

(T.Yu.Nikolaienko, L.A.Bulavin, D.M.Hovorun)

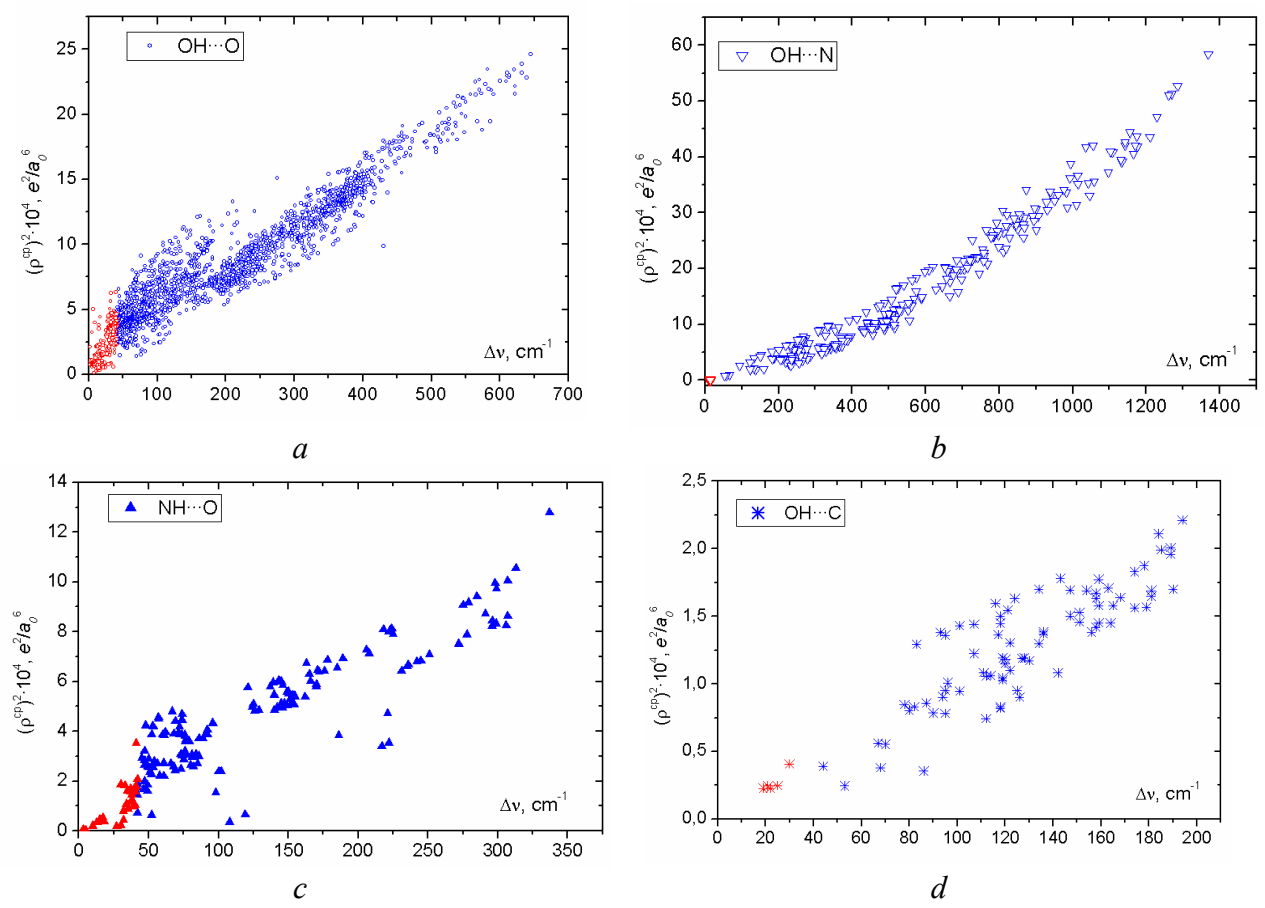

Figure SF1. Correlation between hydrogen bond proton donation group stretching frequency red-shift (Δν) and the square of the electron charge density at the bond critical point ($(\rho^{cp})^2$) on the bond path corresponding to hydrogen bond for OH···O (*a*), OH···N (*b*), NH···O (*c*) and OH···C (*d*) bonds. Red color denotes points with 0 cm^{-1} < Δν < 40 cm^{-1}. Linear regression correlation coefficients are: 0.956 (OH···O; $(\rho^{cp})^2 = 3.10 \cdot 10^{-6} \cdot \Delta\nu + 2.20 \cdot 10^{-4}$), 0.977 (OH···N; $(\rho^{cp})^2 = 4.05 \cdot 10^{-6} \cdot \Delta\nu - 6.50 \cdot 10^{-4}$), 0.913 (NH···O; $(\rho^{cp})^2 = 2.80 \cdot 10^{-6} \cdot \Delta\nu + 9.20 \cdot 10^{-5}$), 0.895 (OH···C; $(\rho^{cp})^2 = 1.01 \cdot 10^{-6} \cdot \Delta\nu - 3.54 \cdot 10^{-7}$).

Table S1. Cartesian coordinates (in Angstroms) of (3S,4R)-3,4,5-trihydroxypentanal conformer optimized at DFT B3LYP level of theory exhibiting the maximum red-shift (78 cm^{-1}) of non-hydrogen-bonded hydroxyl group O16–H19

DFT B3LYP/6-31G(d,p) using *ultrafine* grid and *tight* convergence criteria

Atom	x	y	z
O1	3.733056	0.137090	-0.304965
C2	2.667706	-0.225619	0.145543
H3	2.590631	-0.694098	1.148116
C4	1.350449	-0.089710	-0.591580
C5	0.224477	0.417882	0.336888
H6	1.081287	-1.089917	-0.961820
H7	1.507952	0.561829	-1.457728
C8	-1.063029	0.737487	-0.448002
H9	0.542810	1.363423	0.793606
O10	0.016578	-0.483490	1.411440
H11	-0.610966	-1.159899	1.103198
C12	-1.776684	-0.494038	-1.022362
H13	-0.792393	1.414874	-1.271517
O14	-1.961399	1.382224	0.466201
H15	-2.613713	1.873365	-0.051156
O16	-2.252362	-1.330071	0.031002
H17	-1.109232	-1.101816	-1.640254
H18	-2.609507	-0.166692	-1.665498
H19	-2.691369	-0.723111	0.650707

DFT B3LYP/cc-pVTZ using *ultrafine* grid and *tight* convergence criteria

Atom	x	y	z
O1	3.711832000	0.176862000	-0.307700000
C2	2.670550000	-0.246293000	0.127404000
H3	2.627914000	-0.766326000	1.102108000
C4	1.346916000	-0.117356000	-0.586991000
C5	0.233668000	0.384740000	0.352506000
H6	1.076963000	-1.113441000	-0.954515000
H7	1.488295000	0.539365000	-1.446788000
C8	-1.043375000	0.742687000	-0.423274000
H9	0.566478000	1.309888000	0.829472000
O10	0.014638000	-0.535993000	1.409767000
H11	-0.644201000	-1.180851000	1.114957000
C12	-1.781551000	-0.453414000	-1.027179000
H13	-0.753243000	1.421189000	-1.232706000
O14	-1.925744000	1.408429000	0.491005000
H15	-2.525356000	1.970015000	-0.009170000
O16	-2.288062000	-1.316933000	-0.011523000
H17	-1.123345000	-1.055791000	-1.652740000
H18	-2.598009000	-0.091415000	-1.663321000
H19	-2.774052000	-0.753742000	0.605513000

Table S2. Conformational parameters (deg.) of canonical ribo- and 2'-deoxyribonucleosides conformers containing intramolecular OH···O, NH···O, OH···N or OH···C hydrogen bonds with the highest energy

H-bond	$O_2'H\cdots O_2$	$O_5'H\cdots N_3$	$N_2H\cdots O_{5'}$	$O_5'H\cdots C_8$
Molecule name[a]	rC	rG	rG	rG
Conformer number[b]	**16**	**6**	**118**	**75**
Proper citation[b]	[R1]	[R2]	[R2]	[R2]
Conformational parameters[c] (deg.)				
β ($C_4'C_5'O_5'H$)	68.7	60.9	-49.7	85.7
γ ($C_3'C_4'C_5'O_5'$)	-75.4	46.5	-17.2	46.0
ε ($C_4'C_3'O_3'H$)	145.7	31.3	86.3	-163.3
χ ($O_4'C_1'N_1C_2$ in rC, $O_4'C_1'N_9C_4$ in rG)	-171.9	55.2	49.5	170.9
η ($C_3'C_2'O_2'H$)	151.3	22.7	73.4	40.3
P	163.9	168.2	356.0	234.0
ν_{max}	35.5	32.7	34.6	25.9

[a]: molecule names: rC – cytidine (IUPAC Name: 4-amino-1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2(1H)-one), rG – guanosine (IUPAC Name: 2-amino-9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,9-dihydro-6H-purin-6-one);
[b] conformer numbers according to the following papers:
rC: [R1] R.O. Zhurakivsky and D.M. Hovorun, *Physics of the Alive*, 2007, **15**(1), 92,
rG: [R2] R.O. Zhurakivsky and D.M. Hovorun, *Physics of the Alive*, 2007, **15**(2), 24;
[c] atom numbers are given in accordance with: W. Saenger, *Principles of nucleic acid structure*, Springer-Verlag, 1984; *P* and ν_{max} denote furanose ring pseudorotation phase angle and pseudorotation amplitude correspondingly.