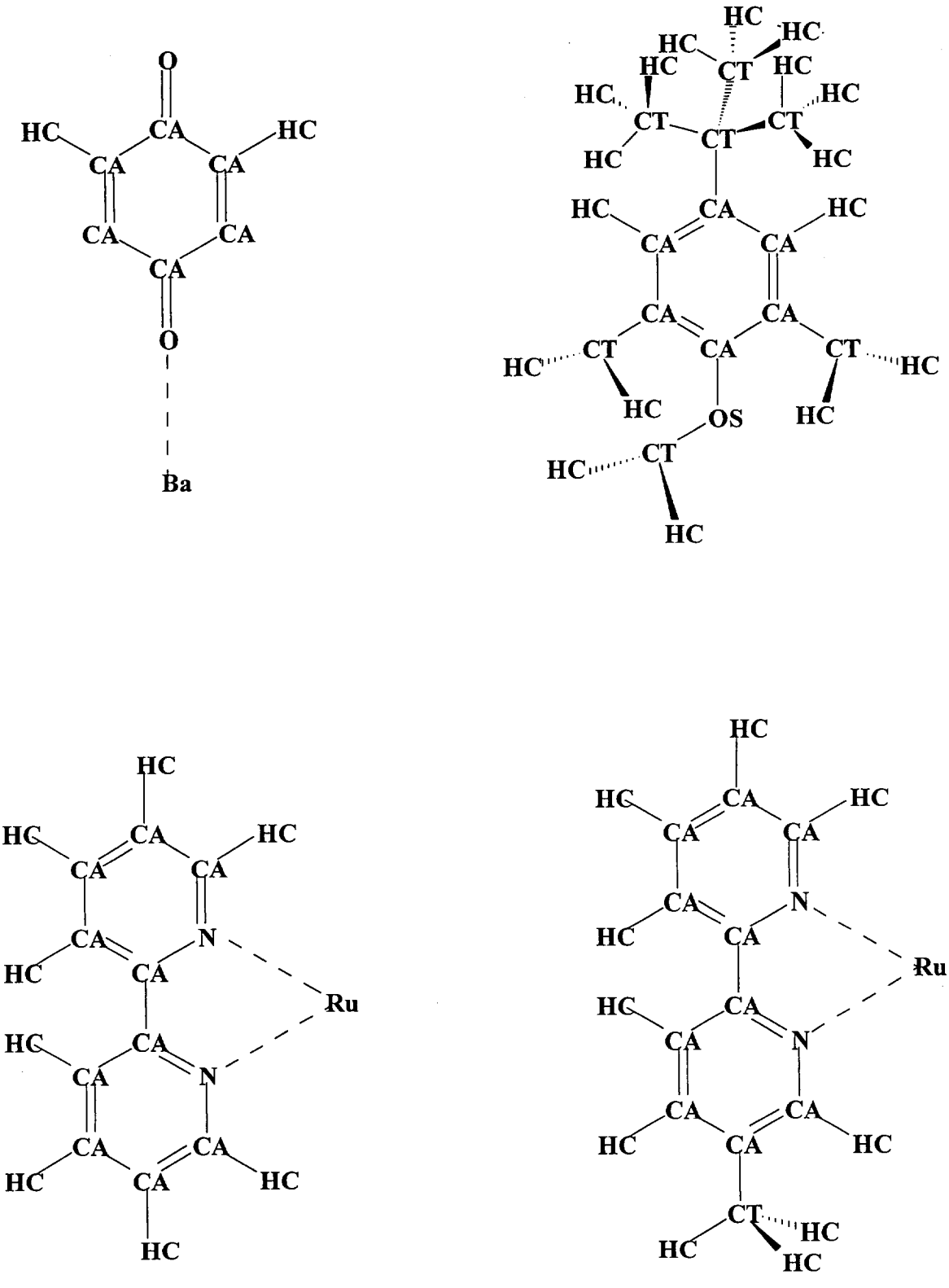

Figure S1. Atom types used in the AMBER calculations on the quinone, anisole (*top*), $Ru^{II}bpy_{(C)}$ and $Ru^{II}bpy_{(A)}$ fragments (*bottom*) of **Ru(Q)** and **Ru_2(Q)**.

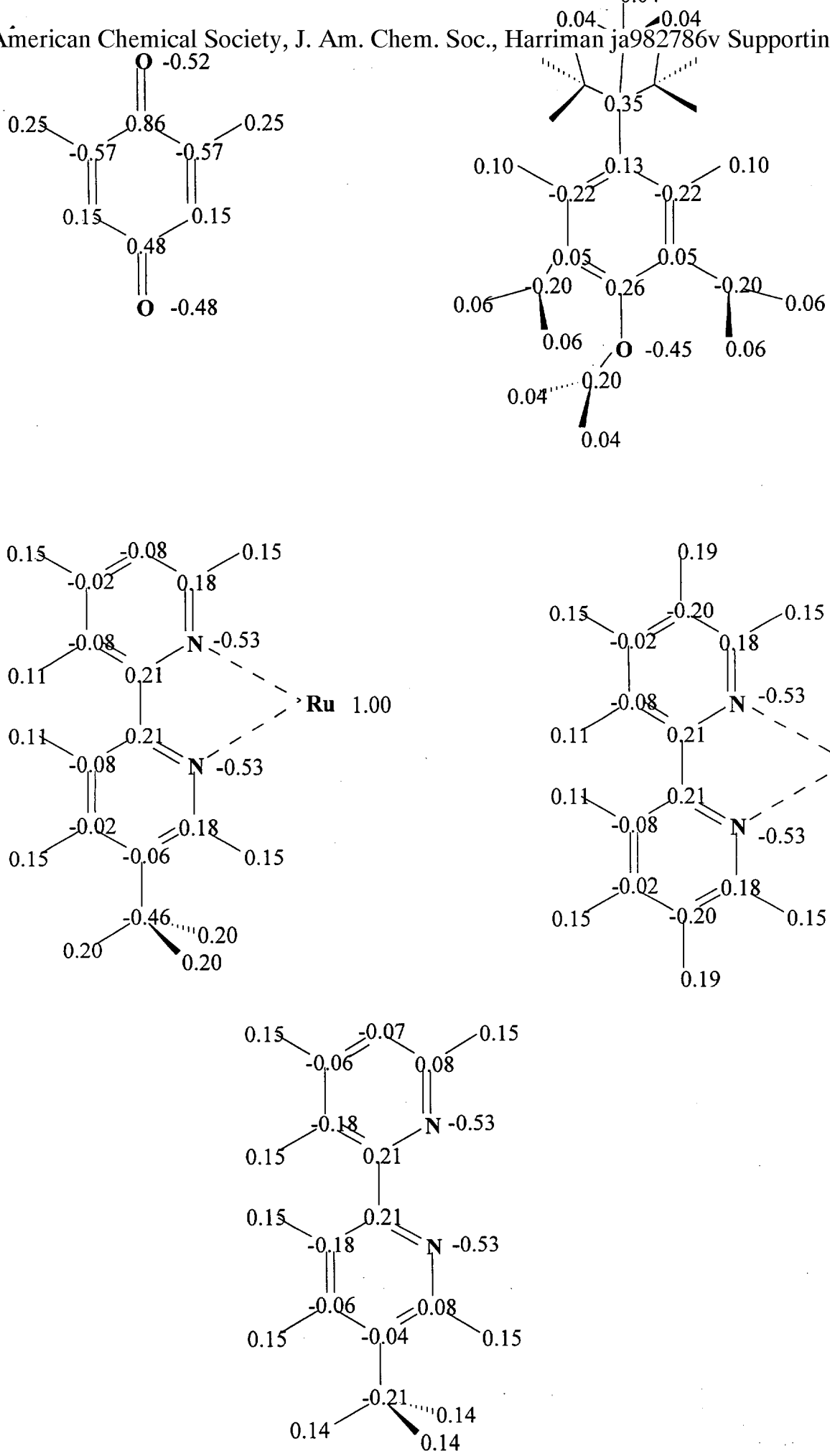

Figure S2 Atomic charges on fragments of uncomplexed **Ru(Q)** and **Ru(QH)**; quinones and anisoles (top), $Ru^{II}bpy_{(3)}$ and $Ru^{III}bpy_{(3)}$

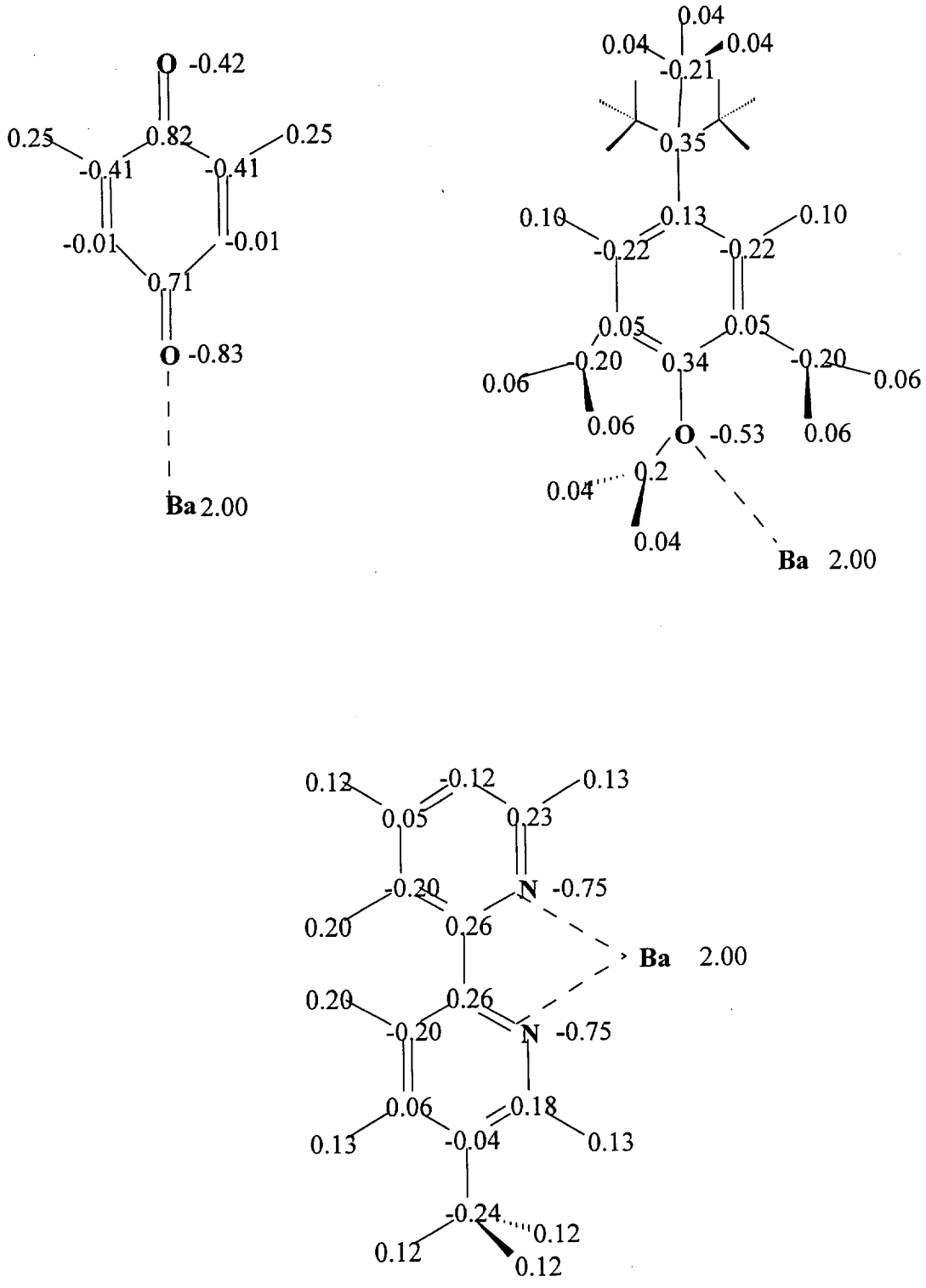

Figure S3. Atomic charges on fragments of $Ba(ClO_4)_2$ complexes of **Ru(Q)** and **Ru_2(Q)**: quinones and anisoles (*top*), $bpy_{(A')}$ (*bottom*) . The charges of $Ru^{II}bpy_{(C)}$ and $bpy_{(A')}$ residues are the same as in the uncomplexed ligands (Figure S2). See Figure 1 for definition of residues.

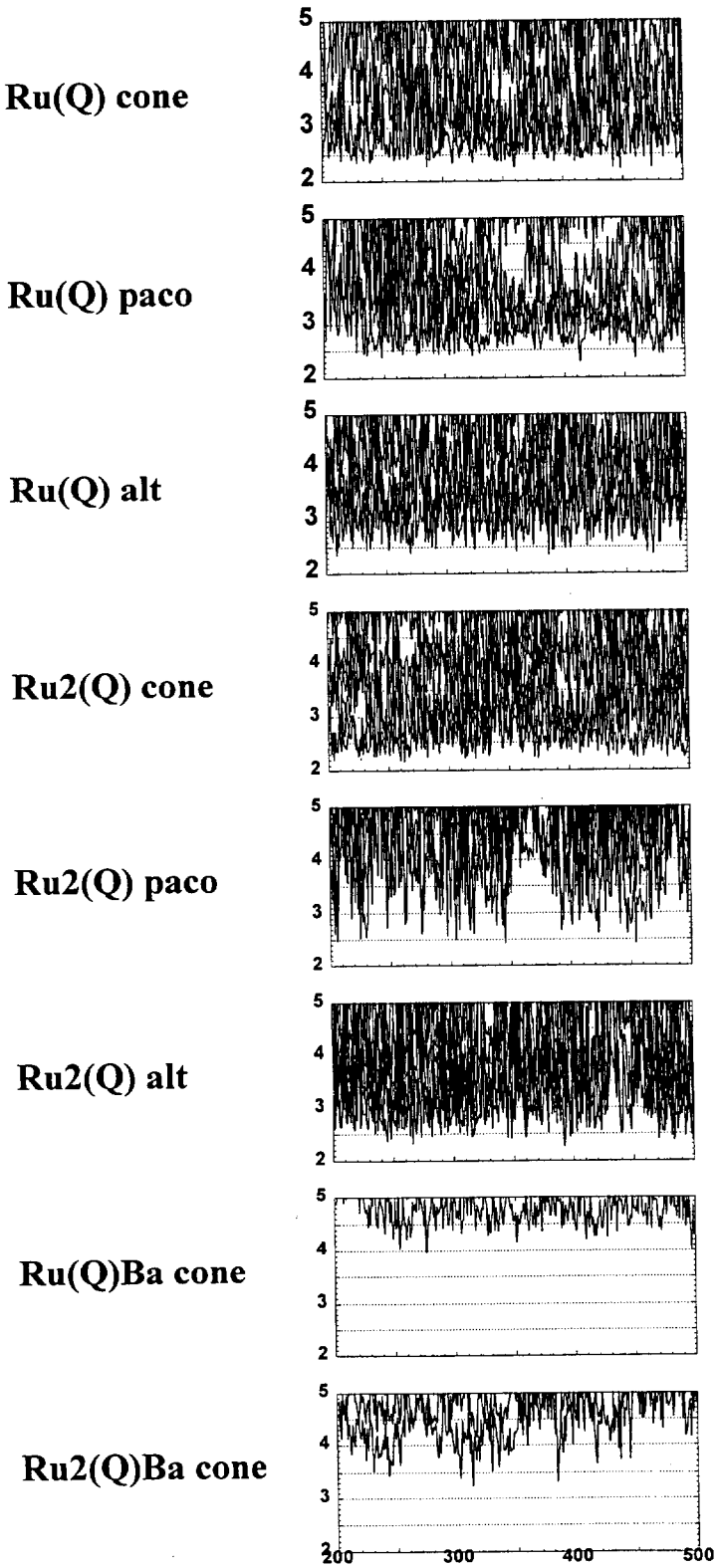

Figure S4. Time evolution (200-500 ps) of the shortest distances (< 5 Å) between H_{pyr} protons of $Ru(Bpy)_3$ and O_Q quinolic oxygens. From top to bottm: **Ru(Q)**$_{-cone}$, **Ru(Q)**$_{-paco}$, **Ru(Q)**$_{-1,3alt}$, **Ru$_2$(Q)**$_{-cone}$, **Ru$_2$(Q)**$_{-paco}$, **Ru$_2$(Q)**$_{-1,3alt}$, and the $Ba(ClO_4)_2$ cone complexes of **Ru(Q)**, **Ru$_2$(Q)**

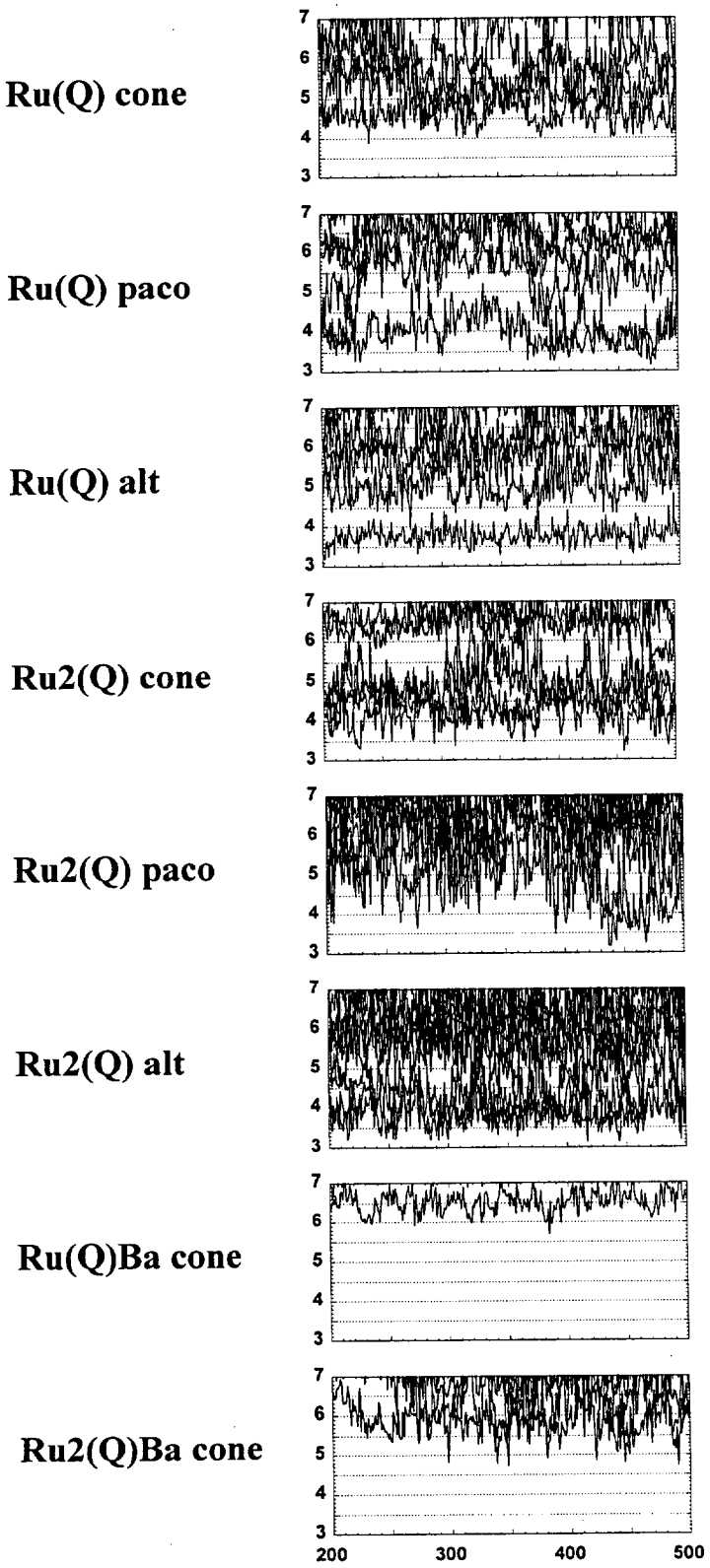

Figure S5. Time evolution (200-500 ps) of the shortest distances (< 7 Å) between the center-of-mass of bipyridines of $Ru(Bip)_3$ and the center-of-mass of quinolic carbonyles: From top to bottom: uncomplexed **Ru(Q)** cone, paco, 1,3-alt, **Ru2(Q)** cone, paco, 1,3-alt and the $Ba(ClO_4)_2$

Ligand	α_A	$\alpha_{A'}$	$\omega_{AA'}$	$\omega_{QQ'}$
Ru(Q) cone	195 ± 10	190 ± 15	50 ± 10	50± 10
Ru(Q) paco	170 ± 20	175 ± 15	25 ± 15	140 ± 15
Ru(Q) 1,3-alt	145 ± 15	180 ± 15	20 ± 5	30 ±10
Ru_2(Q) cone	-95 ± 15	-60 ± 15	105 ± 15	15 ± 10
Ru_2(Q) paco	175 ± 15	110 ± 30	6 ± 4	120 ± 15
Ru_2(Q) 1,3-alt	145 ± 15	160 ± 20	10 ± 8	20 ± 15
Ru(Q) Ba cone	60 ± 10	180 ± 10	30 ± 10	80 ± 10
Ru_2(Q) Ba cone	80 ± 15	80 ± 15	20 ± 10	100 ± 20

Table S1. Average angles and fluctuations (±) of the **Ru(Q)** and **Ru_2(Q)** ligands and of their Ba^{2+} complexes. Orientation of the pendent pyridine chains (α_A and $\alpha_{A'}$) and angles between opposite anisoles ($\omega_{AA'}$) or opposite quinones ($\omega_{QQ'}$). Averages are performed during the last 200 ps of the dynamics.