Supplementary Material for PCCP

Computational Comparison of the Stacking Interactions between the Aromatic Amino Acids and the Natural or (Cationic) Methylated Nucleobases

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Electronic Supplementary Information

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Gas-Phase Optimal MP2/6-31G*(0.25) Stacking Interaction (ΔE, kJ mol^{-1}) between the Amino Acids and Nucleobases as Determined by Varying R_1 (Å), α (deg.), and R_2 (X-displacement (Å), Y-displacement (Å))[ab]

Adenine[c]								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
A:HIS	3.3	–24.3	120	–27.0	–2.7	0, –0.5	–27.2	–0.2
A:HIS_f	3.3	–18.1	180	–28.3	–10.2	0, –1.0	–29.7	–1.4
A:PHE	3.4	–24.3	0	–24.3	—	0, 0	–24.3	—
A:TYR	3.4	–24.4	180	–29.3	–4.9	0, –0.5	–30.7	–1.4
A:TYR_f	3.4	–26.3	330	–28.1	–1.8	0, 0.5	–28.9	–0.8
A:TRP	3.5	–25.5	240	–30.5	–5.0	–0.5, –1.0	–35.0	–4.5
A:TRP_f	3.5	–26.9	300	–29.8	–2.9	–0.5, –1.0	–32.0	–2.2

1-methyladenine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
1MeA:HIS	3.3	–37.1	300	–48.9	–11.8	0, –0.5	–49.8	–0.9
1MeA:HIS_f	3.1	–51.0	0	–51.0	—	0, 0	–51.0	—
1MeA:PHE	3.3	–45.8	30	–45.9	–0.1	0, 0	–45.9	—
1MeA:TYR	3.3	–51.4	330	–54.0	–2.6	0, 0	–54.0	—
1MeA:TYR_f	3.4	–42.9	270	–52.9	–10.0	0.5, 0	–53.3	–0.4
1MeA:TRP	3.4	–66.2	0	–66.2	—	0.5, 0.5	–70.2	–4.0
1MeA:TRP_f	3.4	–52.4	270	–66.7	–14.3	1.0, –0.5	–69.6	–2.9

3-methyladenine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
3MeA:HIS	3.3	–32.9	180	–52.3	–19.4	–0.5, 0	–52.7	–0.4
3MeA:HIS_f	3.3	–38.1	240	–51.7	–13.6	0, 0	–51.7	—
3MeA:PHE	3.3	–47.2	0	–47.2	—	0, –0.5	–48.6	–1.4
3MeA:TYR	3.3	–51.6	240	–53.6	–2.0	–0.5, –0.5	–55.0	–1.4
3MeA:TYR_f	3.3	–52.0	180	–52.5	–0.5	0, –0.5	–53.9	–1.4
3MeA:TRP	3.4	–62.1	270	–68.5	–6.4	0.5, 0	–69.7	–1.2
3MeA:TRP_f	3.4	–64.3	120	–69.9	–5.6	–0.5, –0.5	–71.5	–1.6

7-methyladenine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
7MeA:HIS	3.2	–59.3	30	–61.9	–2.6	0, 0	–61.9	—
7MeA:HIS_f	3.3	–30.2	120	–57.8	–27.6	0, 0	–57.8	—
7MeA:PHE	3.3	–50.4	30	–50.9	–0.5	–0.5, 0	–51.0	–0.1
7MeA:TYR	3.4	–45.1	180	–57.8	–12.7	–0.5, –0.5	–58.8	–1.0
7MeA:TYR_f	3.3	–56.2	30	–58.5	–2.3	–0.5, 0.5	–59.5	–1.0
7MeA:TRP	3.4	–55.9	240	–72.2	–16.3	0, 1.0	–74.7	–2.5
7MeA:TRP_f	3.4	–70.8	300	–72.9	–2.1	0.5, 0.5	–71.3	–1.6

Guanine[c]								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
G:HIS	3.4	–10.5	150	–29.7	–19.2	–0.5, 0	–31.4	–1.7
G:HIS$_f$	3.3	–23.0	300	–32.4	–9.4	1.5, 1.0	–35.3	–2.9
G:PHE	3.4	–24.5	0	–24.5	—	–0.5, 0	–25.3	–0.8
G:TYR	3.4	–28.4	330	–33.4	–5.0	0, 0	–33.4	—
G:TYR$_f$	3.4	–20.3	120	–29.8	–9.5	1.0, 0.5	–32.8	–3.0
G:TRP	3.4	–36.7	0	–36.7	—	0.5, 0.5	–42.5	–5.8
G:TRP$_f$	3.4	–25.8	90	–39.0	–13.2	–1.0, –1.0	–42.4	–3.4

3-methylguanine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
3MeG:HIS	3.4	–20.5	180	–60.8	–40.3	–0.5, 0	–61.5	–0.7
3MeG:HIS$_f$	3.3	–45.5	270	–62.0	–16.5	–0.5, 0.5	–63.9	–1.9
3MeG:PHE	3.3	–49.8	0	–49.8	—	0, –0.5	–51.0	–1.2
3MeG:TYR	3.3	–59.8	330	–62.2	–2.4	0, 0	–62.2	—
3MeG:TYR$_f$	3.3	–47.6	120	–57.5	–9.9	0.5, 0.5	–60.6	–3.1
3MeG:TRP	3.4	–76.3	330	–78.5	–2.2	0.5, 0	–79.7	–1.2
3MeG:TRP$_f$	3.3	–64.9	90	–82.3	–17.4	0.5, 0	–84.7	–2.4

7-methylguanine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
7MeG:HIS	3.3	–39.9	90	–47.5	–7.6	–0.5, 0.5	–49.8	–2.3
7MeG:HIS$_f$	3.3	–29.4	120	–46.3	–16.9	0, –0.5	–46.6	–0.3
7MeG:PHE	3.3	–45.4	30	–45.9	–0.5	–0.5, 0	–48.0	–2.1
7MeG:TYR	3.3	–42.7	300	–54.0	–11.3	0, 0.5	–55.9	–1.9
7MeG:TYR$_f$	3.3	–45.4	270	–53.3	–7.9	0, 0	–53.3	—
7MeG:TRP	3.4	–58.1	180	–64.6	–6.5	0.5, 0.5	–66.8	–2.2
7MeG:TRP$_f$	3.4	–61.6	60	–66.8	–5.2	0.5, 0.5	–69.8	–3.0

O6-methylguanine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
O6MeG:HIS	3.3	–38.5	240	–45.3	–6.8	–0.5, 0	–47.5	–2.2
O6MeG:HIS$_f$	3.3	–43.2	330	–45.6	–2.4	–0.5, 0	–47.3	–1.7
O6MeG:PHE	3.3	–45.5	0	–45.5	—	–0.5, 0	–45.8	–0.3
O6MeG:TYR	3.4	–45.3	300	–50.1	–4.8	0, 0.5	–52.2	–2.1
O6MeG:TYR$_f$	3.3	–46.1	240	–51.4	–5.3	0, 0	–51.4	—
O6MeG:TRP	3.4	–62.8	30	–63.8	–1.0	–1.0, –0.5	–67.2	–3.4
O6MeG:TRP$_f$	3.4	–56.4	270	–62.7	–6.3	–0.5, –1.0	–65.3	–2.6

Cytosine[c]								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
C:HIS	3.4	–24.5	0	–24.5	—	–1.5, 0	–26.0	–1.5
C:HIS$_f$	3.5	–7.9	150	–24.2	–16.3	–0.5, –1.5	–26.9	–2.7
C:PHE	3.5	–15.1	0	–15.1	—	–1.5, 0	–18.4	–3.3
C:TYR	3.6	–14.1	180	–21.7	–7.6	–1.5, 0	–22.7	–1.0
C:TYR$_f$	3.5	–18.3	330	–20.6	–2.3	–1.0, –1.0	–24.2	–3.6
C:TRP	3.4	–18.5	180	–27.9	–9.4	–1.0, 0	–32.9	–5.0
C:TRP$_f$	3.5	–23.6	300	–28.2	–4.6	–1.0, –0.5	–33.4	–5.2

3-methylcytosine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
3MeC:HIS	3.3	–44.7	330	–45.9	–1.2	1.0, –1.0	–52.1	–6.2
3MeC:HIS$_f$	3.3	–41.6	90	–44.3	–2.7	1.0, –1.0	–48.2	–3.9
3MeC:PHE	3.4	–42.7	30	–43.0	–0.3	0, 0.5	–43.3	–0.3
3MeC:TYR	3.4	–43.7	180	–50.5	–6.8	0.5, 0	–51.3	–0.8
3MeC:TYR$_f$	3.4	–42.8	270	–48.4	–5.6	–1.0, 0	–50.2	–1.8
3MeC:TRP	3.4	–57.9	180	–64.1	–6.2	1.0, 1.0	–69.4	–5.3
3MeC:TRP$_f$	3.4	–55.7	270	–66.2	–10.5	–0.5, –0.5	–70.5	–4.3

O2-methylcytosine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
O2MeC:HIS	3.3	–35.0	30	–35.5	–0.5	0.5, 0.5	–38.9	–3.4
O2MeC:HIS$_f$	3.4	–27.0	180	–35.2	–8.2	0.5, 0.5	–38.2	–3.0
O2MeC:PHE	3.4	–36.7	0	–36.7	—	–1.0, –1.5	–38.5	–1.8
O2MeC:TYR	3.4	–36.9	150	–42.9	–6.0	0, 0	–42.9	—
O2MeC:TYR$_f$	3.4	–40.2	120	–42.7	–2.5	0, 0	–42.7	—
O2MeC:TRP	3.4	–53.1	240	–54.8	–1.7	–0.5, –0.5	–57.6	–2.8
O2MeC:TRP$_f$	3.4	–53.3	270	–56.5	–3.2	–0.5, –0.5	–59.9	–3.4

Thymine[c]								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
T:HIS	3.4	–18.8	120	–25.5	–6.7	–1.0, 0	–26.8	–1.3
T:HIS$_f$	3.5	–11.5	180	–24.3	–12.8	–1.0, 0	–25.0	–0.7
T:PHE	3.5	–20.6	30	–20.8	–0.2	–1.0, –0.5	–22.4	–1.6
T:TYR	3.6	–18.5	180	–24.6	–6.1	–0.5, –0.5	–25.5	–0.9
T:TYR$_f$	3.5	–20.5	120	–25.8	–5.3	0.5, 0	–26.1	–0.3
T:TRP	3.3	–33.4	180	–36.4	–3.0	0, 0	–36.4	—
T:TRP$_f$	3.4	–31.0	30	–36.0	–5.0	0, 0	–36.0	—

O2-methylthymine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
O2MeT:HIS	3.4	–27.4	120	–46.5	–19.1	1.0, 0.5	–54.1	–7.6
O2MeT:HIS$_f$	3.4	–34.1	270	–49.1	–15.0	0.5, 0.5	–54.7	–5.6
O2MeT:PHE	3.4	–44.8	30	–45.0	–0.2	–1.0, 0.5	–48.9	–3.9
O2MeT:TYR	3.4	–44.5	30	–50.7	–6.2	1.0, 0.5	–53.1	–2.4
O2MeT:TYR$_f$	3.4	–43.4	240	–55.0	–11.6	0.5, 0	–55.6	–0.6
O2MeT:TRP	3.2	–77.3	0	–77.3	—	–0.5, 0	–77.4	–0.1
O2MeT:TRP$_f$	3.4	–65.3	330	–74.7	–9.4	0, 0	–74.7	—

O4-methylthymine								
Dimer	R_1	ΔE	α	ΔE	Δ(α–R_1)	R_2	ΔE	Δ(R_2–α)
O4MeT:HIS	3.3	–40.7	300	–45.4	–4.7	1.0, 0	–51.9	–6.5
O4MeT:HIS$_f$	3.3	–45.4	0	–45.4	—	–1.0, –0.5	–47.8	–2.4
O4MeT:PHE	3.4	–46.7	0	–46.7	—	1.0, 0	–49.4	–2.7
O4MeT:TYR	3.4	–49.7	120	–53.8	–4.1	0.5, 0	–54.5	–0.7
O4MeT:TYR$_f$	3.5	–42.8	300	–53.6	–10.8	–0.5, –0.5	–53.9	–0.3
O4MeT:TRP	3.3	–74.2	180	–76.4	–2.2	0, –0.5	–77.7	–1.3
O4MeT:TRP$_f$	3.3	–64.1	240	–71.8	–7.7	0, –0.5	–77.2	–5.4