*Supplementary Materials*

# On Some Origins of Tautomeric Preferences in Neutral Creatinine in Vacuo: Search for Analogies and Differences in Cyclic Azoles and Azines

**Ewa Daniela Raczyńska**

Department of Chemistry, Warsaw University of Life Sciences (SGGW)
ul. Nowoursynowska 159c, 02-776 Warszawa, Poland
ewa_raczyńska@sggw.edu.pl; Tel.: +48-22-59-37623

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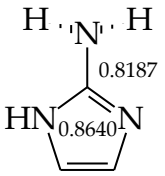
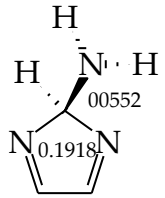



**2AIm-16/36** (0.00)

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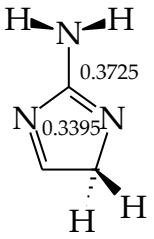


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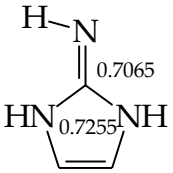


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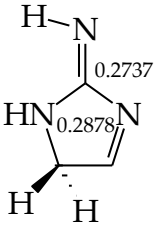


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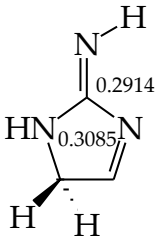


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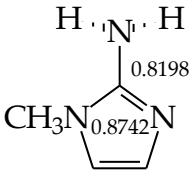


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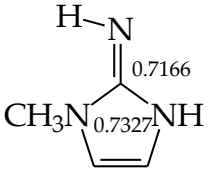


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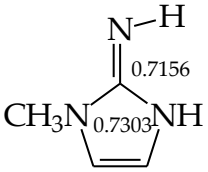


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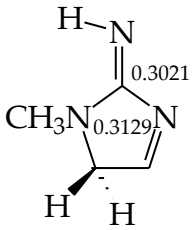
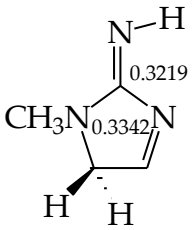
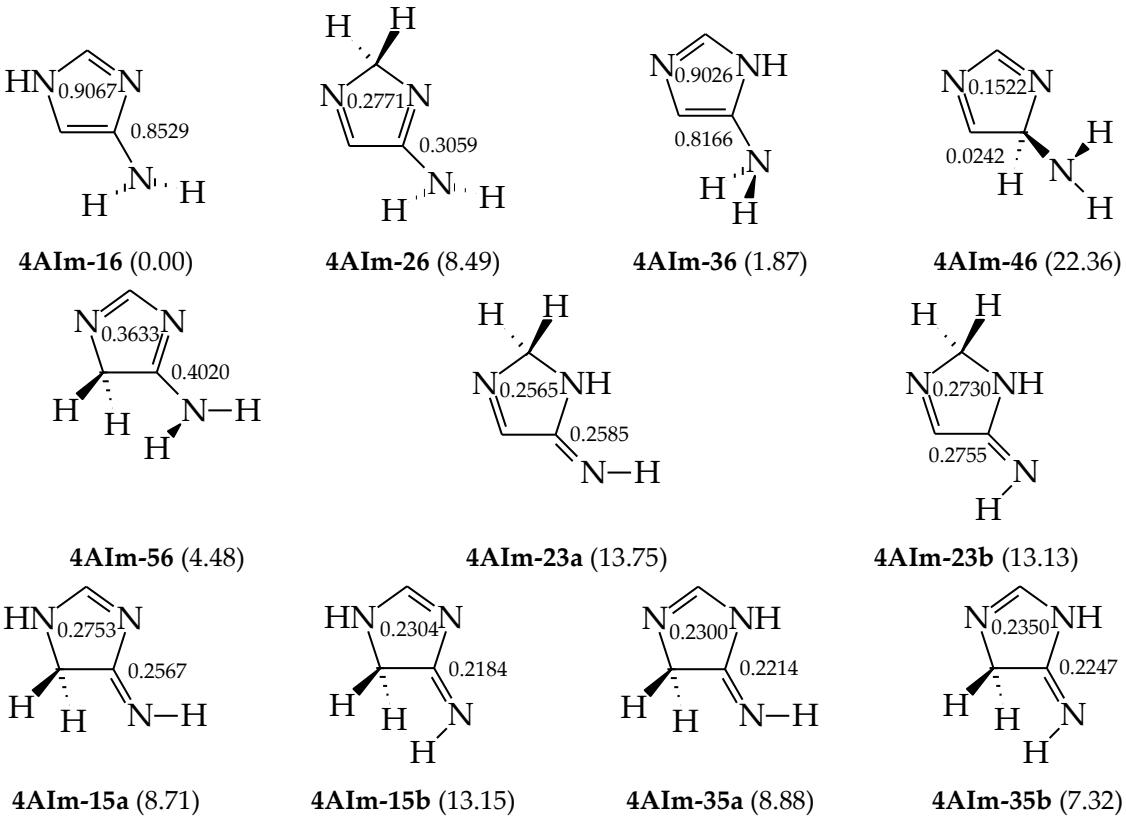



**2A1MIm-5a** (16.88)




**2A1MIm-5b** (11.99)

**Figure S1.** Structures for tautomers-rotamers of 2-amino-imidazole (**2AIm**) and its 1-methyl derivative (**2A1MIm**), their HOMEDs and $\Delta G$s estimated at the DFT(B3LYP)/6-311+G(d,p) level. HOMED5s included in the ring. HOMED6s for isomers of **2AIm** and **2A1MIm** placed near formula. $\Delta G$s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation.

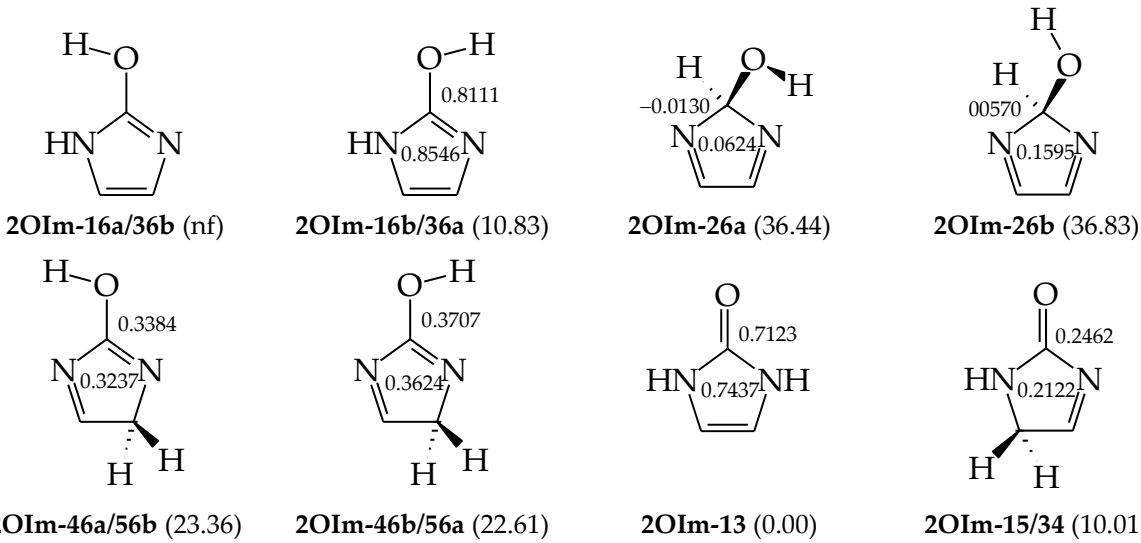



**4AIm-16** (0.00) **4AIm-26** (8.49) **4AIm-36** (1.87) **4AIm-46** (22.36)

**4AIm-56** (4.48) **4AIm-23a** (13.75) **4AIm-23b** (13.13)

**4AIm-15a** (8.71) **4AIm-15b** (13.15) **4AIm-35a** (8.88) **4AIm-35b** (7.32)

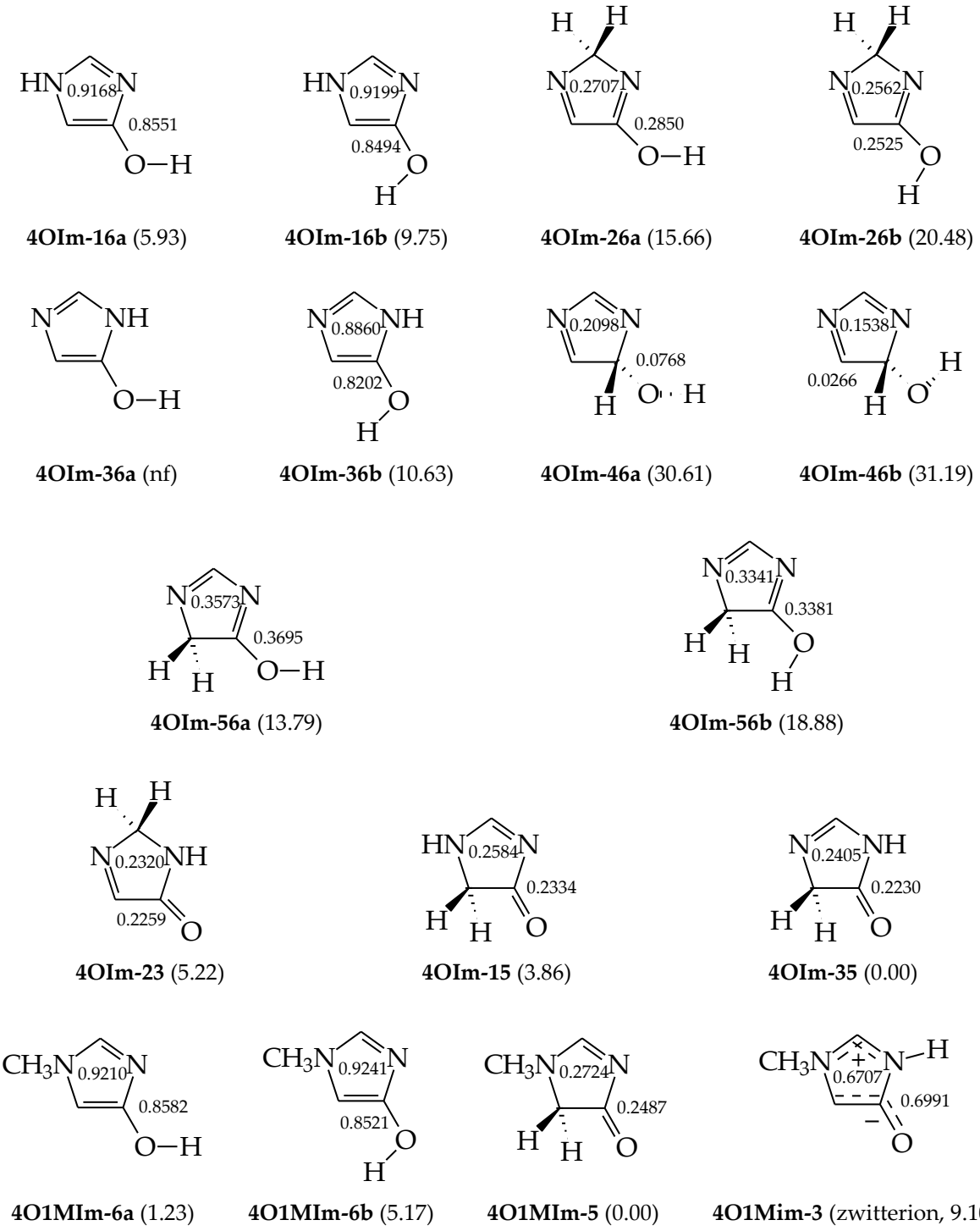
**Figure S2.** Structures for tautomers-rotamers of 4-amino-imidazole (**4AIm**), their HOMEDs and Δ*G*s estimated at the DFT(B3LYP)/6-311+G(d,p) level. HOMED5s included in the ring, and HOMED6s placed near formula. Δ*G*s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation.




**2OIm-16a/36b** (nf) **2OIm-16b/36a** (10.83) **2OIm-26a** (36.44) **2OIm-26b** (36.83)

**2OIm-46a/56b** (23.36) **2OIm-46b/56a** (22.61) **2OIm-13** (0.00) **2OIm-15/34** (10.01)

**Figure S3.** Structures for tautomers-rotamers of 2-hydroxy-imidazole (**2OIm**), their HOMEDs and Δ*G*s estimated at the DFT(B3LYP)/6-311+G(d,p) level (nf – structure not found). HOMED5s included in the ring, and HOMED6s placed near formula. Δ*G*s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation.




**4OIm-16a** (5.93) **4OIm-16b** (9.75) **4OIm-26a** (15.66) **4OIm-26b** (20.48)

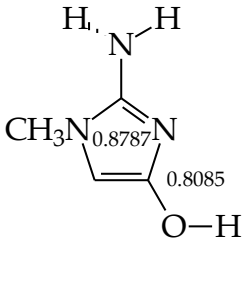
**4OIm-36a** (nf) **4OIm-36b** (10.63) **4OIm-46a** (30.61) **4OIm-46b** (31.19)

**4OIm-56a** (13.79) **4OIm-56b** (18.88)

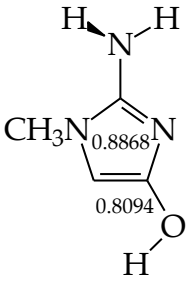
**4OIm-23** (5.22) **4OIm-15** (3.86) **4OIm-35** (0.00)

**4O1MIm-6a** (1.23) **4O1MIm-6b** (5.17) **4O1MIm-5** (0.00) **4O1Mim-3** (zwitterion, 9.10)

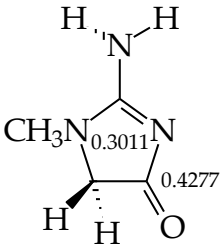
**Figure S4.** Structures for tautomers-rotamers of 4-hydroxy-imidazole (**4OIm**) and its 1-methyl derivative (**4O1MIm**), their HOMEDs and Δ*G*s (in kcal mol$^{-1}$) estimated at the DFT(B3LYP)/6-311+G(d,p) level (nf – structure not found). HOMED5s included in the ring. HOMED6s for isomers of **4OIm** and **4O1MIm** placed near formula. Δ*G*s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation.



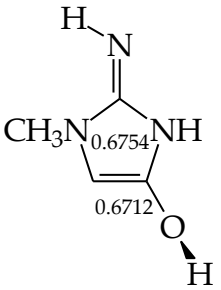

**Crea-67a** (11.89)



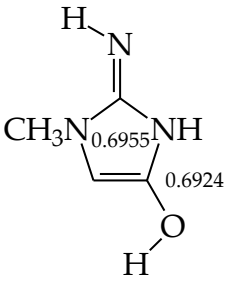

**Crea-67b** (15.35)



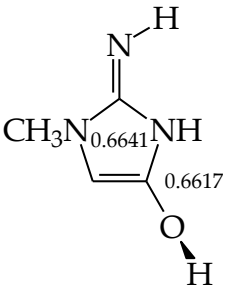

**Crea-56** (1.97)




**Crea-37aa** (26.71)




**Crea-37ab** (25.87)

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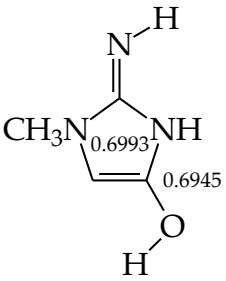


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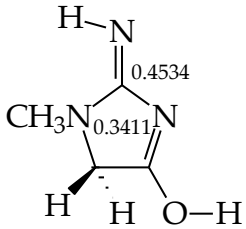
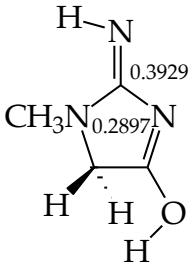
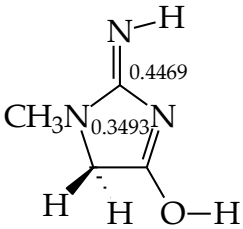


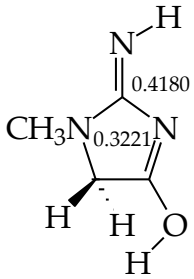

**Crea-57aa** (18.57)



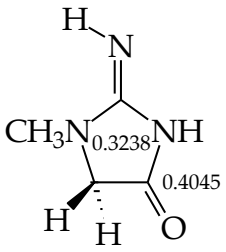

**Crea-57ab** (24.87)



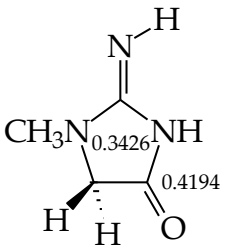

**Crea-57ba** (14.05)



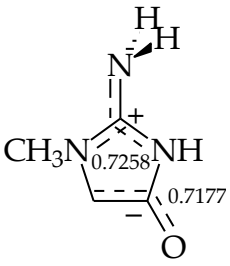

**Crea-57bb** (19.69)




**Crea-35a** (0.39)



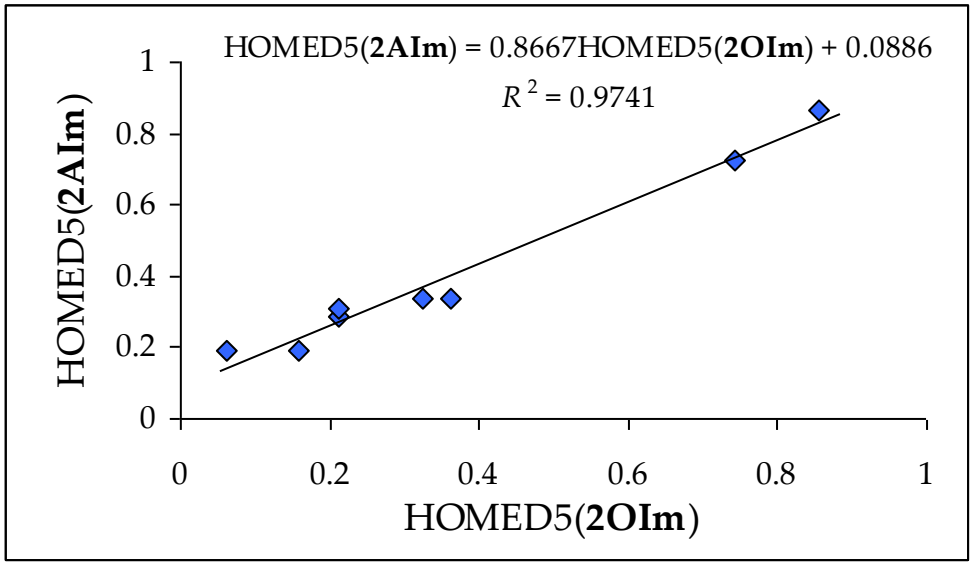

**Crea-35b** (0.00)




**Crea-36** (zwitterion, 21.93)

**Figure S5.** Structures for isomers of creatinine (**Crea**), their HOMEDs and Δ*G*s estimated for at the DFT(B3LYP)/6-311+G(d,p) level. HOMED5s included in the ring, and HOMED7s placed near formula. Δ*G*s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation.

(a) **2AIm** vs **2OIm**




(b) **4AIm** vs **4OIm**

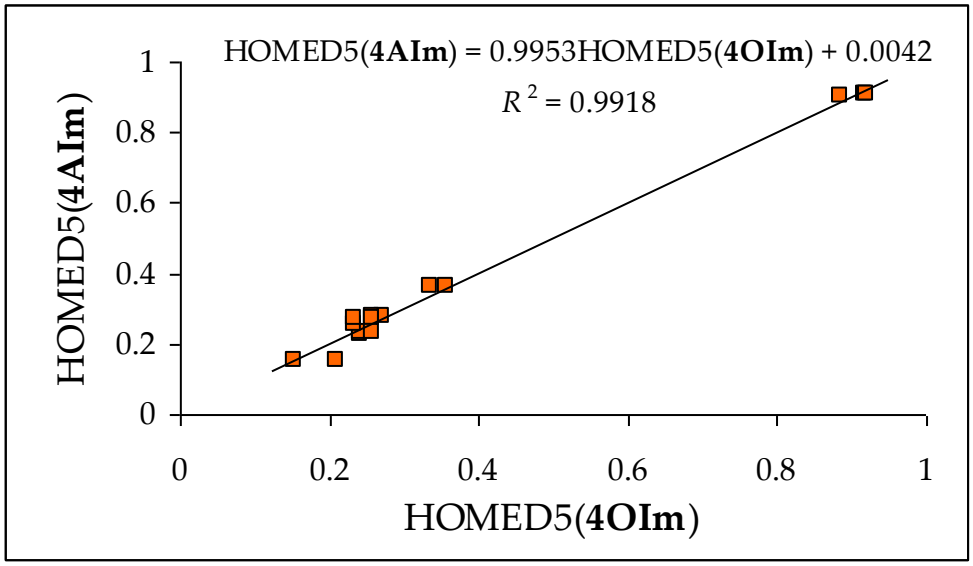
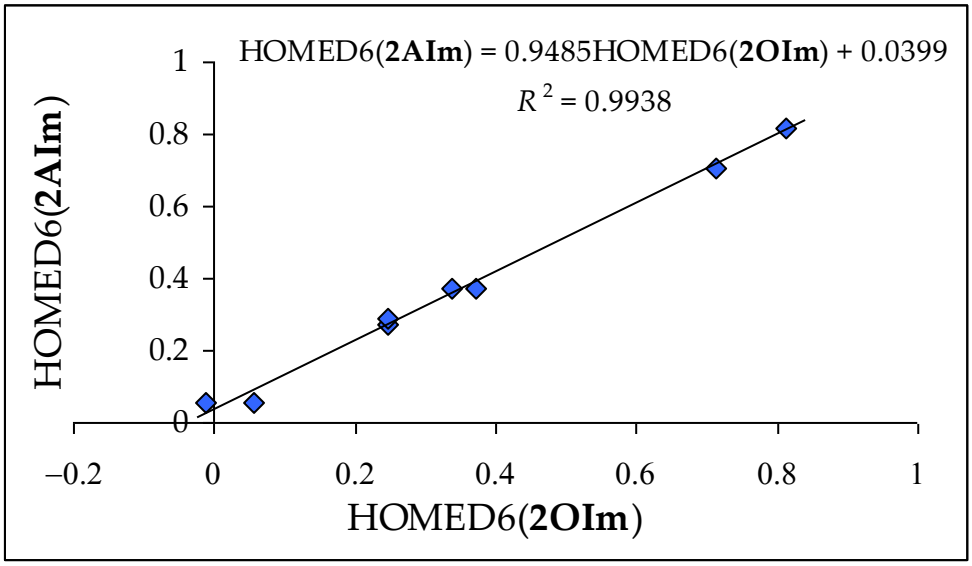



**Figure S6.** Linear trends between HOMED5s estimated for tautomers-rotamers of mono-amino and mono-hydroxy imidazoles: (a) **2AIm** vs **2OIm**, and (b) **4AIm** vs **4OIm**). HOMED5s refer to electron delocalization in the five-membered ring.

(a) **2AIm** vs **2OIm**




(b) **4AIm** vs **4OIm**

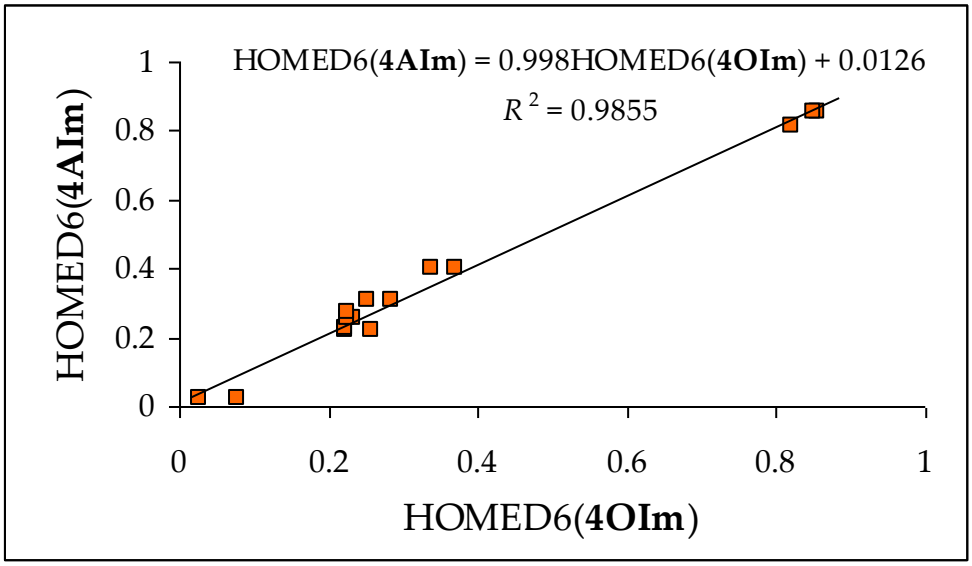
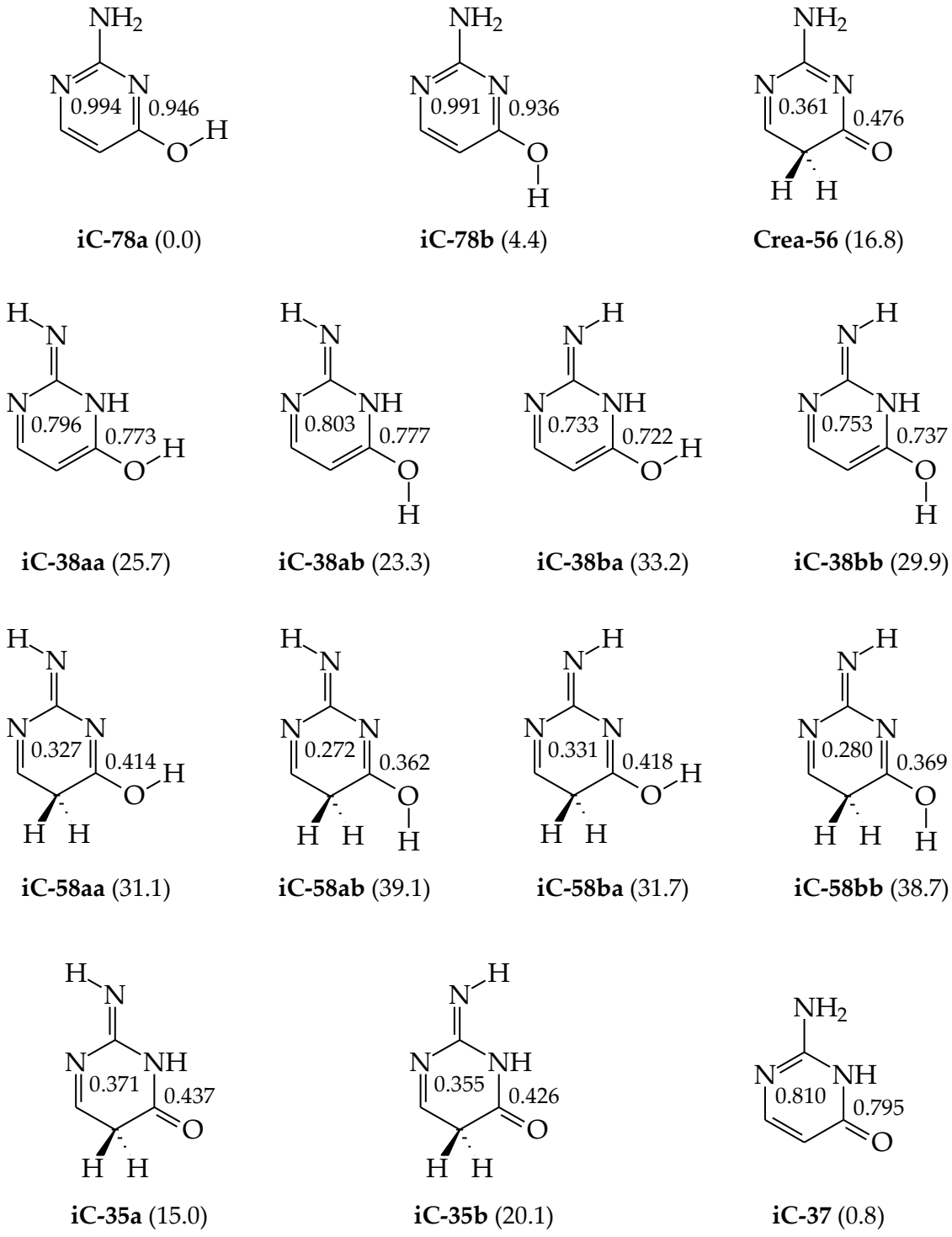



**Figure S7.** Linear trends between HOMED6s estimated for tautomers-rotamers of mono-amino and mono-hydroxy imidazoles: (a) **2AIm** vs **2OIm**, and (b) **4AIm** vs **4OIm**. HOMED6 refer to electron delocalization in the entire isomer-molecule.




**iC-78a** (0.0) **iC-78b** (4.4) **Crea-56** (16.8)

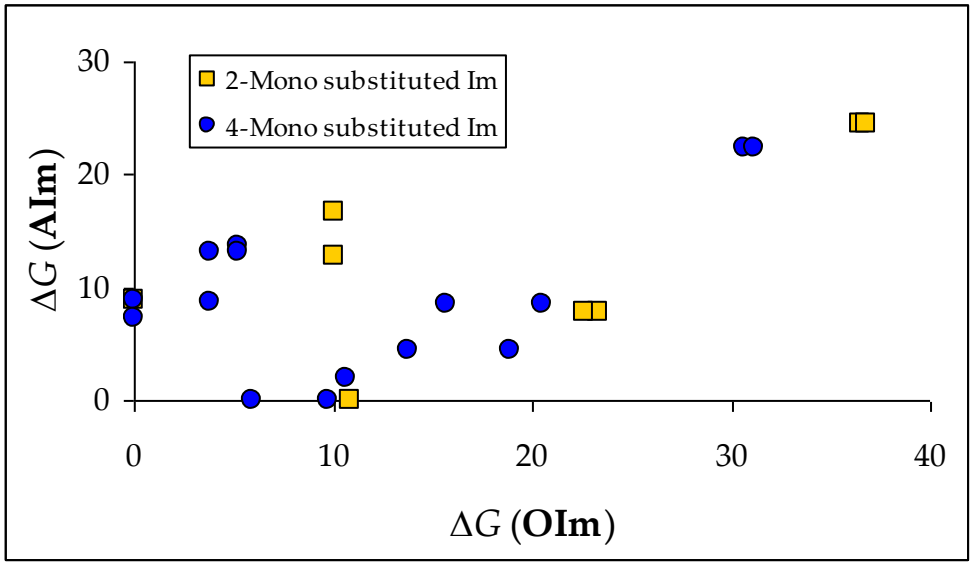
**iC-38aa** (25.7) **iC-38ab** (23.3) **iC-38ba** (33.2) **iC-38bb** (29.9)

**iC-58aa** (31.1) **iC-58ab** (39.1) **iC-58ba** (31.7) **iC-58bb** (38.7)

**iC-35a** (15.0) **iC-35b** (20.1) **iC-37** (0.8)

**Figure S8.** Structures for selected isomers of isocytosine (**iC**), analogous to those of creatinine given in Fig. S5, their HOMEDs and Δ*G*s estimated at the DFT(B3LYP)/6-311+G(d,p) level. HOMED6s included in the ring, and HOMED8s placed near formula. Δ*G*s (in kcal mol$^{-1}$) given in parentheses after isomer abbreviation. Data taken from refs [33,34].

(a) $\Delta G$(**AIm**) vs $\Delta G$(**OIm**)




(b) HOMED7(**XIm**) vs $\Delta G$(**XIm**)

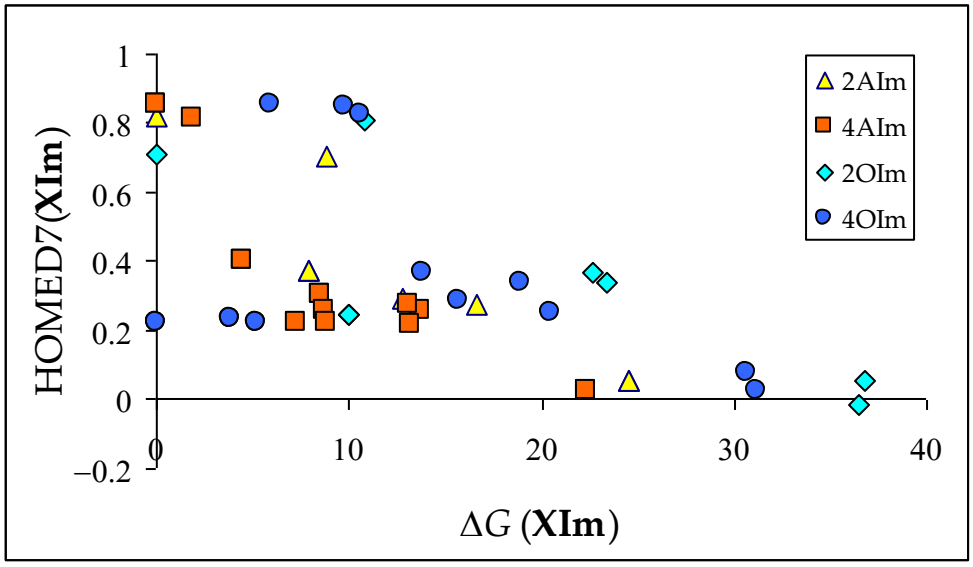



**Figure S9.** Scatter plots (a) between $\Delta G$s (in kcal mol$^{-1}$) for isomers of mono-amino (**AIm**) and mono-hydroxy imidazoles (**OIm**), and also (b) between HOMEDs and $\Delta G$s for isomers of mono-substituted imidazoles (**2AIm**, **4AIm**, **2OIm**, and **4OIm**). Data taken from Figs S1-S4.

**Table S1.** Comparison of structural and thermochemical parameters estimated at the DFT-level for tautomers-rotamers of mono-substituted imidazoles in the gas phase.

| Isomer | HOMED5 | HOMED6 | Δ(*E* + ZPE)[a] | Δ*H*[a] | *T*Δ*S*[a] | Δ*G*[a] | *K* | $x_i$[b] |
|---|---|---|---|---|---|---|---|---|
| **2AIm-16/36** | 0.8640 | 0.8187 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **100** |
| **2AIm-26** | 0.1918 | 0.0552 | 24.59 | 24.49 | −0.08 | 24.57 | $1{\cdot}10^{-20}$ | $1{\cdot}10^{-18}$ |
| **2AIm-46/56** | 0.3395 | 0.3725 | 7.83 | 7.78 | −0.12 | 7.89 | $2{\cdot}10^{-6}$ | $2{\cdot}10^{-4}$ |
| **2AIm-13** | 0.7255 | 0.7065 | 9.12 | 9.30 | 0.43 | 8.87 | $3{\cdot}10^{-7}$ | $3{\cdot}10^{-5}$ |
| **2AIm-15a/34b** | 0.2878 | 0.2737 | 16.66 | 16.53 | −0.14 | 16.67 | $6{\cdot}10^{-13}$ | $6{\cdot}10^{-11}$ |
| **2AIm-15b/34a** | 0.3085 | 0.2914 | 12.78 | 12.66 | −0.08 | 12.74 | $5{\cdot}10^{-10}$ | $5{\cdot}10^{-8}$ |
| **4AIm-16** | 0.9067 | 0.8529 | 0.00 | 0.00 | 0.00 | 0.00 | 1.0 | **95.84** |
| **4AIm-26** | 0.2771 | 0.3059 | 8.41 | 8.30 | −0.19 | 8.49 | $6{\cdot}10^{-7}$ | $6{\cdot}10^{-5}$ |
| **4AIm-36** | 0.9026 | 0.8166 | 2.52 | 2.63 | 0.76 | 1.87 | 0.04 | **4.10** |
| **4AIm-46** | 0.1522 | 0.0242 | 22.36 | 22.23 | −0.13 | 22.36 | $4{\cdot}10^{-17}$ | $4{\cdot}10^{-15}$ |
| **4AIm-56** | 0.3633 | 0.4020 | 4.72 | 4.83 | 0.35 | 4.48 | $5{\cdot}10^{-4}$ | **0.05** |
| **4AIm-23a** | 0.2565 | 0.2585 | 13.87 | 13.81 | 0.05 | 13.75 | $8{\cdot}10^{-11}$ | $8{\cdot}10^{-9}$ |
| **4AIm-23b** | 0.2730 | 0.2755 | 13.47 | 13.47 | 0.34 | 13.13 | $2{\cdot}10^{-10}$ | $2{\cdot}10^{-8}$ |
| **4AIm-15a** | 0.2753 | 0.2567 | 8.81 | 8.73 | 0.01 | 8.71 | $4{\cdot}10^{-7}$ | $4{\cdot}10^{-5}$ |
| **4AIm-15b** | 0.2304 | 0.2184 | 13.18 | 13.04 | −0.11 | 13.15 | $2{\cdot}10^{-10}$ | $2{\cdot}10^{-8}$ |
| **4AIm-35a** | 0.2300 | 0.2214 | 9.02 | 8.95 | 0.08 | 8.88 | $3{\cdot}10^{-7}$ | $3{\cdot}10^{-5}$ |
| **4AIm-35b** | 0.2350 | 0.2247 | 7.41 | 7.29 | −0.04 | 7.32 | $4{\cdot}10^{-6}$ | $4{\cdot}10^{-4}$ |
| **2OIm-16a/36b** | [c] | [c] | [c] | [c] | [c] | [c] | [c] | [c] |
| **2OIm-16b/36a** | 0.8546 | 0.8111 | 10.75 | 10.70 | −0.12 | 10.83 | $1{\cdot}10^{-8}$ | $1{\cdot}10^{-6}$ |
| **2OIm-26a** | 0.0624 | −0.0130 | 36.56 | 36.57 | 0.13 | 36.44 | $2{\cdot}10^{-27}$ | $2{\cdot}10^{-25}$ |
| **2OIm-26b** | 0.1595 | 0.0570 | 39.94 | 36.94 | 0.12 | 36.83 | $1{\cdot}10^{-27}$ | $1{\cdot}10^{-25}$ |
| **2OIm-46a/56b** | 0.3237 | 0.3384 | 23.29 | 23.17 | −0.19 | 23.36 | $8{\cdot}10^{-18}$ | $8{\cdot}10^{-16}$ |
| **2OIm-46b/56a** | 0.3624 | 0.3707 | 22.51 | 23.35 | −0.26 | 22.61 | $3{\cdot}10^{-17}$ | $3{\cdot}10^{-15}$ |
| **2OIm-13** | 0.7437 | 0.7123 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **100** |
| **2OIm-15/34** | 0.2122 | 0.2462 | 10.39 | 10.45 | 0.45 | 10.01 | $5{\cdot}10^{-8}$ | $5\cdot10^{-6}$ |
| **4OIm-16a** | 0.9168 | 0.8551 | 5.80 | 5.84 | −0.08 | 5.93 | $4{\cdot}10^{-5}$ | $4{\cdot}10^{-3}$ |
| **4OIm-16b** | 0.9199 | 0.8494 | 9.74 | 9.89 | 0.13 | 9.75 | $7{\cdot}10^{-8}$ | $7{\cdot}10^{-6}$ |
| **4OIm-26a** | 0.2707 | 0.2850 | 15.50 | 15.41 | −0.25 | 15.66 | $3{\cdot}10^{-12}$ | $3{\cdot}10^{-10}$ |
| **4OIm-26b** | 0.2562 | 0.2525 | 20.42 | 20.44 | −0.05 | 20.48 | $1{\cdot}10^{-15}$ | $1{\cdot}10^{-13}$ |
| **4OIm-36a** | [c] | [c] | [c] | [c] | [c] | [c] | [c] | [c] |
| **4AOm-36b** | 0.8860 | 0.8202 | 10.74 | 10.94 | 0.31 | 10.63 | $2{\cdot}10^{-8}$ | $2{\cdot}10^{-6}$ |
| **4OIm-46a** | 0.2098 | 0.0768 | 30.70 | 30.81 | 0.19 | 30.61 | $4{\cdot}10^{-23}$ | $4{\cdot}10^{-21}$ |
| **4OIm-46b** | 0.1538 | 0.0266 | 31.30 | 31.42 | 0.23 | 31.19 | $1{\cdot}10^{-23}$ | $1{\cdot}10^{-21}$ |
| **4OIm-56a** | 0.3573 | 0.3695 | 13.64 | 13.56 | −0.23 | 13.79 | $8{\cdot}10^{-11}$ | $8{\cdot}10^{-9}$ |
| **4OIm-56b** | 0.3341 | 0.3381 | 18.80 | 18.80 | −0.08 | 18.88 | $1{\cdot}10^{-14}$ | $1{\cdot}10^{-12}$ |
| **4OIm-23** | 0.2320 | 0.2259 | 5.28 | 5.33 | 0.11 | 5.22 | $1{\cdot}10^{-4}$ | **0.01** |
| **4OIm-15** | 0.2584 | 0.2334 | 4.55 | 4.84 | 0.98 | 3.86 | $0.01_5$ | **0.15** |
| **4OIm-35** | 0.2405 | 0.2230 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **99.84** |

[a] In kcal $mol^{-1}$. [b] Percentage contents. [c] Not Found.

**Table S2.** Comparison of structural and thermochemical parameters estimated at the DFT-level for isomers of 1-methyl-imidazoles in the gas phase.

| Isomer | HOMED5 | HOMED6 | $\Delta(E + ZPE)^a$ | $\Delta H^a$ | $T\Delta S^a$ | $\Delta G^a$ | $K$ | $x_i{}^b$ |
|---|---|---|---|---|---|---|---|---|
| **2A1MIm-6** | 0.8742 | 0.8198 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **100** |
| **2A1MIm-3a** | 0.7327 | 07166 | 8.77 | 8.92 | 0.57 | 8.35 | $8{\cdot}10^{-7}$ | $8{\cdot}10^{-5}$ |
| **2A1MIm-3b** | 0.7303 | 07156 | 8.34 | 8.55 | 0.77 | 7.78 | $2{\cdot}10^{-6}$ | $2{\cdot}10^{-4}$ |
| **2A1MIm-5a** | 0.3129 | 0.3021 | 16.95 | 16.84 | −0.04 | 16.88 | $4{\cdot}10^{-13}$ | $4{\cdot}10^{-11}$ |
| **2A1MIm-5b** | 0.3342 | 0.3219 | 12.21 | 12.14 | 0.15 | 11.99 | $2{\cdot}10^{-9}$ | $2{\cdot}10^{-7}$ |
| **4O1MIm-6a** | 0.9210 | 0.8582 | 0.92 | 0.93 | −0.31 | 1.23 | $0.12_{4795}$ | **11.09** |
| **4O1MIm-6b** | 0.9241 | 0.8521 | 4.96 | 5.05 | −0.12 | 5.17 | $2{\cdot}10^{-4}$ | **0.02** |
| **4O1MIm-5** | 0.2724 | 0.2487 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **88.89** |
| **4O1MIm-3** (zwitterion) | 0.6707 | 0.6991 | 10.30 | 8.70 | −0.39 | 9.10 | $2{\cdot}10^{-7}$ | $2{\cdot}10^{-5}$ |

[a] In kcal mol$^{-1}$. [b] Percentage contents.

**Table S3.** Comparison of structural and thermochemical parameters estimated at the DFT-level for isomers of creatinine in the gas phase.

| Isomer | HOMED5 | HOMED7 | $\Delta(E + ZPE)^a$ | $\Delta H^a$ | $T\Delta S^a$ | $\Delta G^a$ | $K$ | $x_i{}^b$ |
|---|---|---|---|---|---|---|---|---|
| **Crea-67a** | 0.8787 | 0.8085 | 11.70 | 11.90 | 0.01 | 11.89 | $2{\cdot}10^{-9}$ | $1{\cdot}10^{-7}$ |
| **Crea-67b** | 0.8868 | 0.8094 | 15.25 | 15.52 | 0.16 | 15.35 | $6{\cdot}10^{-12}$ | $4{\cdot}10^{-10}$ |
| **Crea-56** | 0.3011 | 0.4277 | 1.77 | 1.79 | −0.17 | 1.97 | $0.03_{6222}$ | **2.33** |
| **Crea-37aa** | 0.6754 | 0.6712 | 26.72 | 26.99 | 0.28 | 26.71 | $3{\cdot}10^{-20}$ | $2{\cdot}10^{-18}$ |
| **Crea-37ab** | 0.6955 | 0.6924 | 26.06 | 26.45 | 0.58 | 25.87 | $1{\cdot}10^{-19}$ | $7{\cdot}10^{-18}$ |
| **Crea-37ba** | 0.6641 | 0.6617 | 26.36 | 26.65 | 0.42 | 26.23 | $6{\cdot}10^{-20}$ | $3{\cdot}10^{-18}$ |
| **Crea-37bb** | 0.6993 | 0.6945 | 25.63 | 26.12 | 0.95 | 25.17 | $4{\cdot}10^{-19}$ | $2{\cdot}10^{-17}$ |
| **Crea-57aa** | 0.3411 | 0.4534 | 18.24 | 18.10 | −0.47 | 18.57 | $2{\cdot}10^{-14}$ | $2{\cdot}10^{-12}$ |
| **Crea-57ab** | 0.2897 | 0.3929 | 24.58 | 24.53 | −0.34 | 24.87 | $6{\cdot}10^{-19}$ | $4{\cdot}10^{-17}$ |
| **Crea-57ba** | 0.3493 | 0.4469 | 13.79 | 13.68 | −0.37 | 14.05 | $5{\cdot}10^{-11}$ | $3{\cdot}10^{-9}$ |
| **Crea-57bb** | 0.3221 | 0.4180 | 19.43 | 19.40 | −0.29 | 19.69 | $4{\cdot}10^{-15}$ | $2{\cdot}10^{-13}$ |
| **Crea-35a** | 0.3238 | 0.4045 | 0.21 | 0.13 | −0.26 | 0.39 | $0.51_{6953}$ | **33.3** |
| **Crea-35b** | 0.3426 | 0.4194 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | **64.4** |
| **Crea-36** (zwitterion) | 0.7258 | 0.7177 | 21.87 | 22.10 | 0.17 | 21.93 | $8{\cdot}10^{-17}$ | $5{\cdot}10^{-15}$ |

[a] In kcal mol$^{-1}$. [b] Percentage contents.

**Table S4.** Comparison of relative energetic parameters (in kcal mol$^{-1}$) for creatinine isomers calculated in this work at DFT level with the literature data.

| Isomer | B3LYP(1)[a] | | B2[b] | B3LYP(2)[c] | | MP2[c] | | M062X[c] | |
|---|---|---|---|---|---|---|---|---|---|
| | Δ*E* | Δ*G* | Δ*E* | Δ*E* | Δ*G* | Δ*E* | Δ*G* | Δ*E* | Δ*G* |
| **Crea-67a** | 11.7 | 11.9 | 10.8 | 11.0 | 10.8 | 7.0 | 5.9 | 8.5 | 7.8 |
| **Crea-67b** | 15.2 | 15.4 | 14.2 | 14.1 | 13.8 | 10.6 | 9.4 | 12.4 | 11.9 |
| **Crea-56** | 1.8 | 2.0 | 1.8 | 1.5 | 1.4 | 1.6 | 1.7 | 1.7 | 1.6 |
| **Crea-37aa** | 26.7 | 26.7 | 27.0 | 24.4 | 24.3 | 25.0 | 24.8 | 24.3 | 23.9 |
| **Crea-37ab** | 26.1 | 25.9 | 26.3 | 23.9 | 23.1 | 24.6 | 24.5 | 23.8 | 23.0 |
| **Crea-37ba** | 26.4 | 26.2 | 26.8 | [d] | [d] | [d] | [d] | [d] | [d] |
| **Crea-37bb** | 25.6 | 25.2 | 26.2 | [d] | [d] | [d] | [d] | [d] | [d] |
| **Crea-57aa** | 18.2 | 18.6 | 17.4 | 17.2 | 17.4 | 15.9 | 16.3 | 16.5 | 16.8 |
| **Crea-57ab** | 24.6 | 24.9 | 23.4 | 22.5 | 22.7 | 22.1 | 22.2 | 22.6 | 22.7 |
| **Crea-57ba** | 13.8 | 14.0 | 13.3 | [d] | [d] | [d] | [d] | [d] | [d] |
| **Crea-57bb** | 19.4 | 19.7 | 18.7 | [d] | [d] | [d] | [d] | [d] | [d] |
| **Crea-35a** | 0.2 | 0.4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **Crea-35b** | 0.0 | 0.0 | 0.1 | [d] | [d] | [d] | [d] | [d] | [d] |
| **Crea-36** (zwitterion) | 21.9 | 21.9 | [d] | 21.3 | 20.6 | 19.5 | 17.5 | 22.9 | 22.7 |

[a] This work, B3LYP(1): B3LYP/6-311+G(d,p). [b] B2: B2PLYP−D3/maug-cc-pVTZ-dH, data from ref. [14], [c] B3LYP(2): B3LYP/6-311++G(3df, 3pd), data from ref. [13]. [d] MP2/6-311++G(d, p), data from ref. [13]. [e] M062X/6-311++G(d, p), data from ref. [13]. [d] Lack of data.

**Table S5.** Comparison of thermochemical parameters estimated in this work at the DFT, G2 and G2(MP2) levels of theory for selected isomers of 4-hydroxy-imidazole in the gas phase.

| Isomer | Method | Δ*E*[a] | Δ*H*[a] | *T*Δ*S*[a] | Δ*G*[a] | *K* | $x_i$[b] |
|---|---|---|---|---|---|---|---|
| **4OIm-16a** | DFT[c] | 5.80 | 5.84 | −0.08 | 5.93 | $4.52 \cdot 10^{-5}$ | $4 \cdot 10^{-3}$ |
| | G2 | 5.20 | 5.23 | −0.11 | 5.34 | $1.22 \cdot 10^{-4}$ | 0.01 |
| | G2(MP2) | 4.92 | 4.96 | −0.11 | 5.07 | $1.92 \cdot 10^{-4}$ | 0.02 |
| **4OIm-15** | DFT[c] | 4.55 | 4.84 | 0.98 | 3.86 | $0.01_5$ | 0.15 |
| | G2 | 5.28 | 5.36 | 0.14 | 5.22 | $1.50 \cdot 10^{-4}$ | 0.02 |
| | G2(MP2) | 5.24 | 5.31 | 0.14 | 5.17 | $1.62 \cdot 10^{-4}$ | 0.02 |
| **4OIm-35** | DFT[c] | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 99.84 |
| | G2 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 99.97 |
| | G2(MP2) | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 99.96 |

[a] In kcal mol$^{-1}$. [b] Percentage contents. [c] DFT(B3LYP)/6-311+G(d,p).