**Figure SI-1**. Representation of the tautomers considered for benzoadenine and adenine.

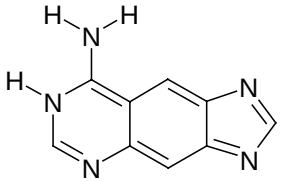
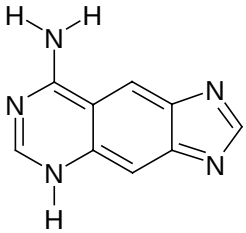
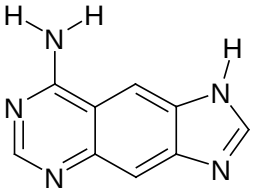
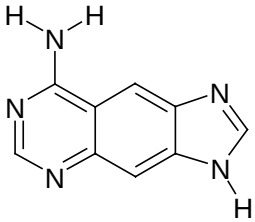
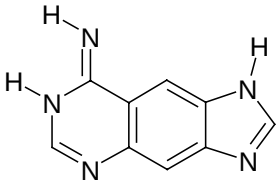
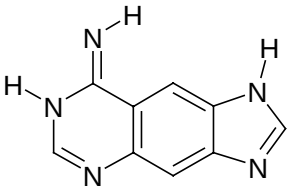
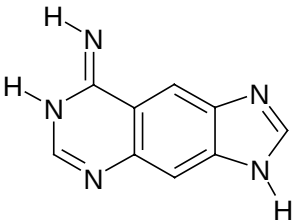
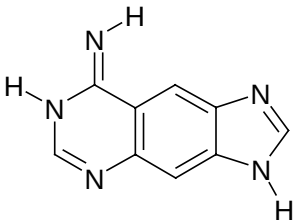
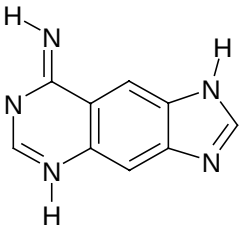
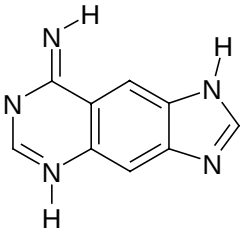
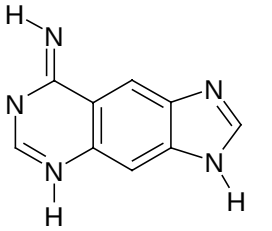
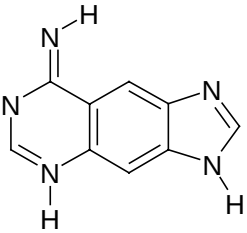
| Benzoadenine | | |
|---|---|---|
|  |  |  |
| A1 | A3 | A7 |
|  |  |  |
| A9 | I17c | I17t |
|  |  |  |
| I19c | I19t | I37c |
|  |  |  |
| I37t | I39c | I39t |

**Figure SI-1** (continued).

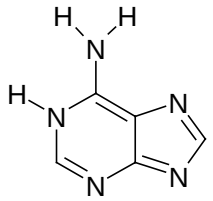
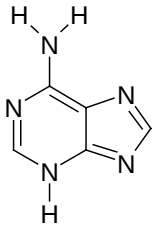
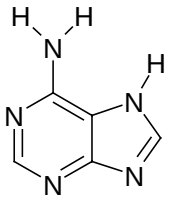
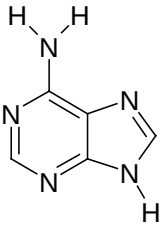
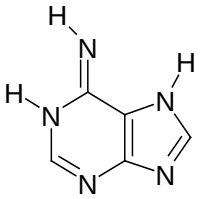
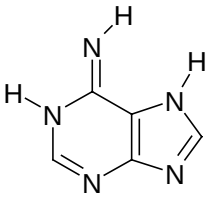
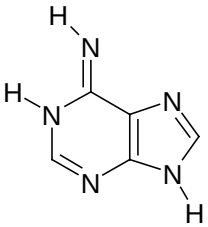
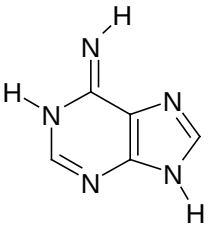
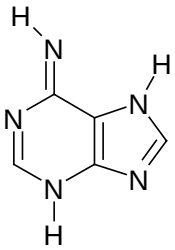
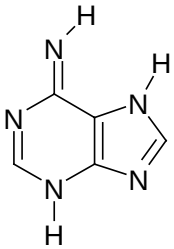
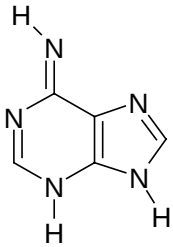
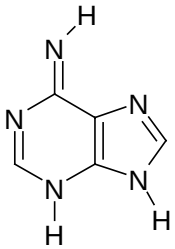
| Adenine | | |
|---|---|---|
|  |  |  |
| A1 | A3 | A7 |
|  |  |  |
| A9 | I17c | I17t |
|  |  |  |
| I19c | I19t | I37c |
|  |  |  |
| I37t | I39c | I39t |

**Figure SI-2**. Representation of the tautomers considered for benzothymine and thymine.

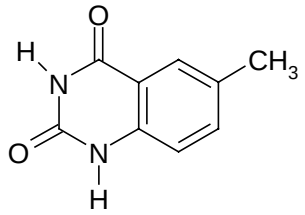
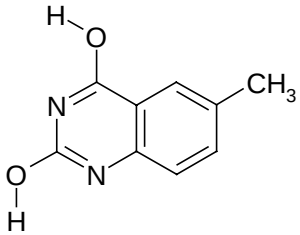
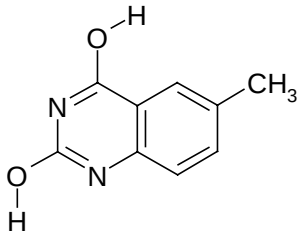
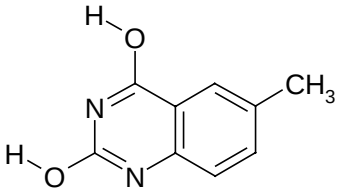
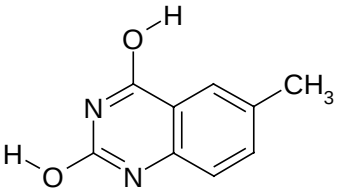
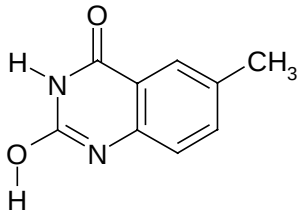
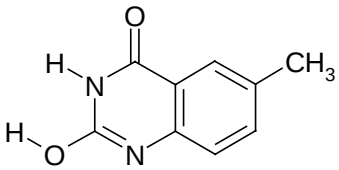
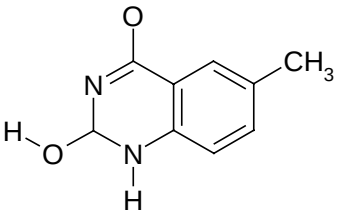
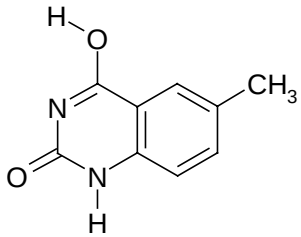
| Benzothymine | | |
|---|---|---|
|  |  |  |
| OO13 | EcEc | EcEt |
|  |  |  |
| EtEc | EtEt | EcO3 |
|  |  |  |
| EtO3 | EtO1 | OEc1 |

**Figure SI-2** (continued).

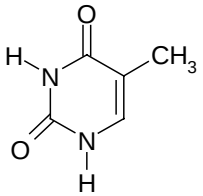
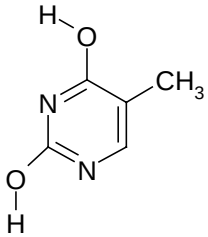
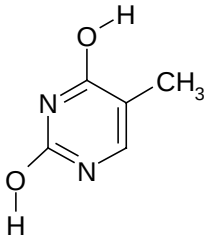
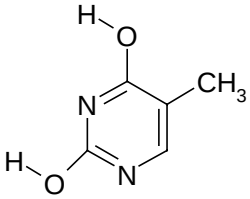
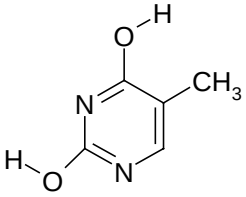
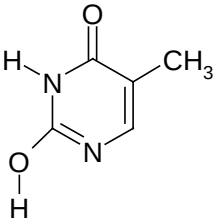
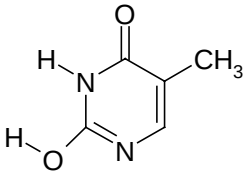
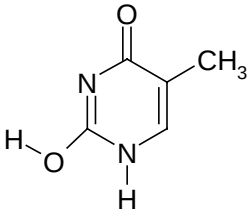
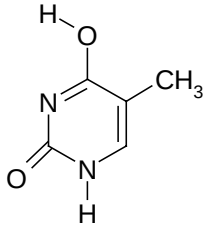
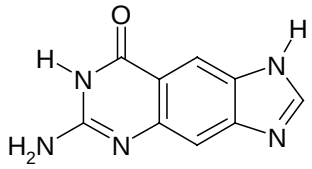
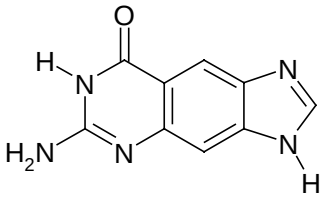
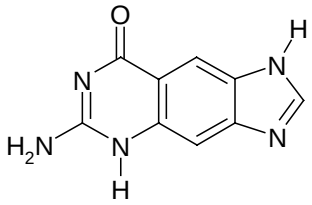
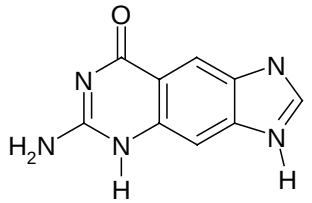
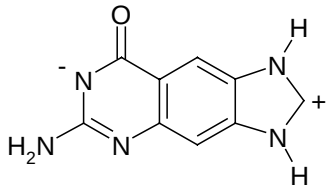
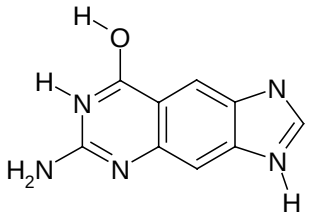
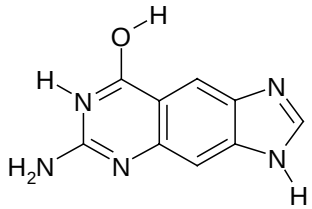
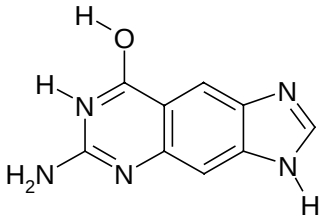
| Thymine | | |
|---|---|---|
|  |  |  |
| OO13 | EcEc | EcEt |
|  |  |  |
| EtEc | EtEt | EcO3 |
|  |  |  |
| EtO3 | EtO1 | OEc1 |

**Figure SI-3**. Representation of the tautomers considered for benzoguanine and guanine.

| Benzoguanine | | |
|---|---|---|
|  |  |  |
| AO17 | AO19 | AO37 |
|  |  |  |
| AO39 | AO79 | AEc9 |
|  |  | |
| AEt9 | AEc7 | |

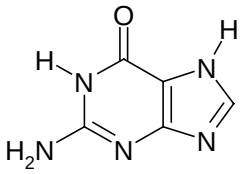
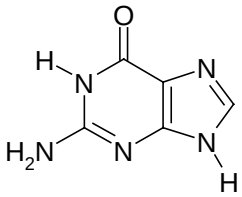
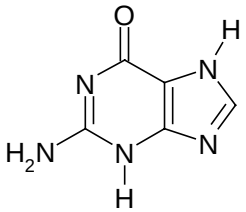
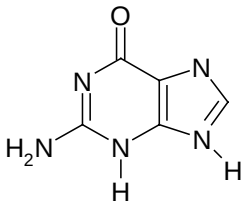
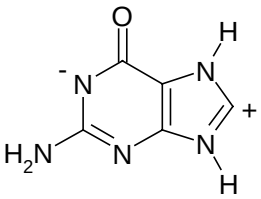
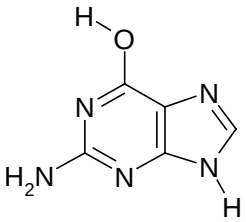
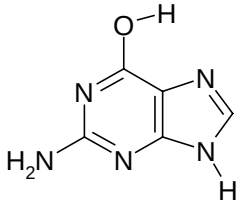
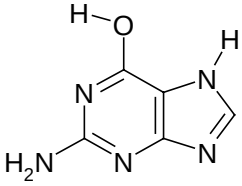
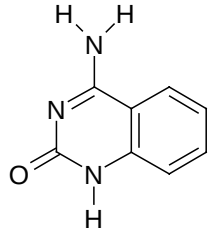
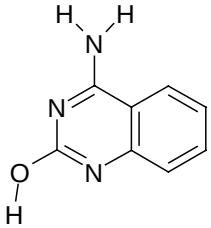
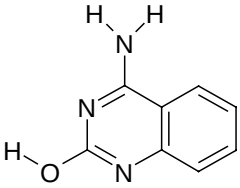
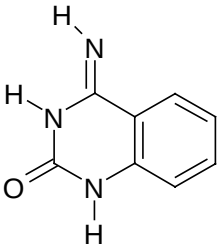
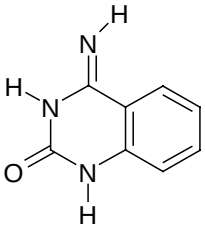
| Guanine | | |
|---|---|---|
|  |  |  |
| AO17 | AO19 | AO37 |
|  |  |  |
| AO39 | AO79 | AEc9 |
|  |  | |
| AEt9 | AEc7 | |

**Figure SI-4**. Representation of the tautomers considered for benzocytosine and cytosine.

| Benzocytosine | | |
|---|---|---|
|  |  |  |
| OA1 | EcA | EtA |
|  |  | |
| OIc3 | OIt3 | |

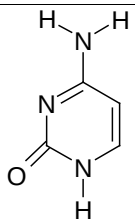
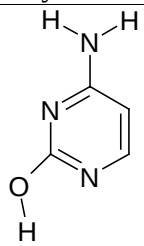
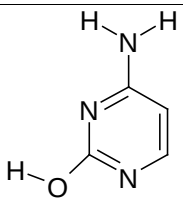
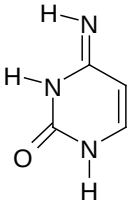
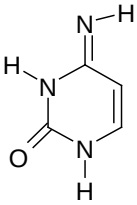
| Cytosine | | |
|---|---|---|
|  |  |  |
| OA1 | EcA | EtA |
|  |  | |
| OIc3 | OIt3 | |

**Figure SI-5**. MIP maps corresponding to the interaction of a positively (top) and negatively (bottom) charged oxygen-like probe with adenine (left) and benzoadenine (rigth). Values of the isoenergy contours are given in kcal/mol.

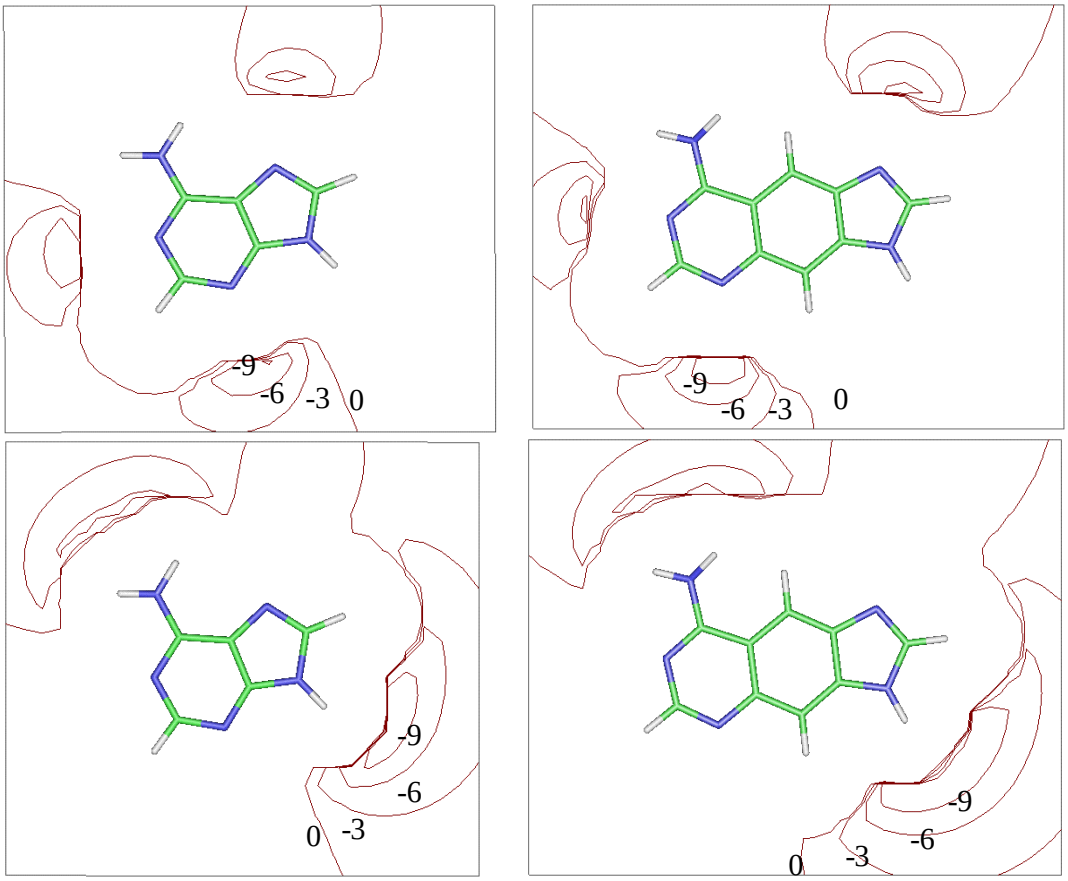


**Figure SI-6**. MIP maps corresponding to the interaction of a positively (top) and negatively (bottom) charged oxygen-like probe with thymine (left) and benzothymine (rigth). Values of the isoenergy contours are given in kcal/mol.

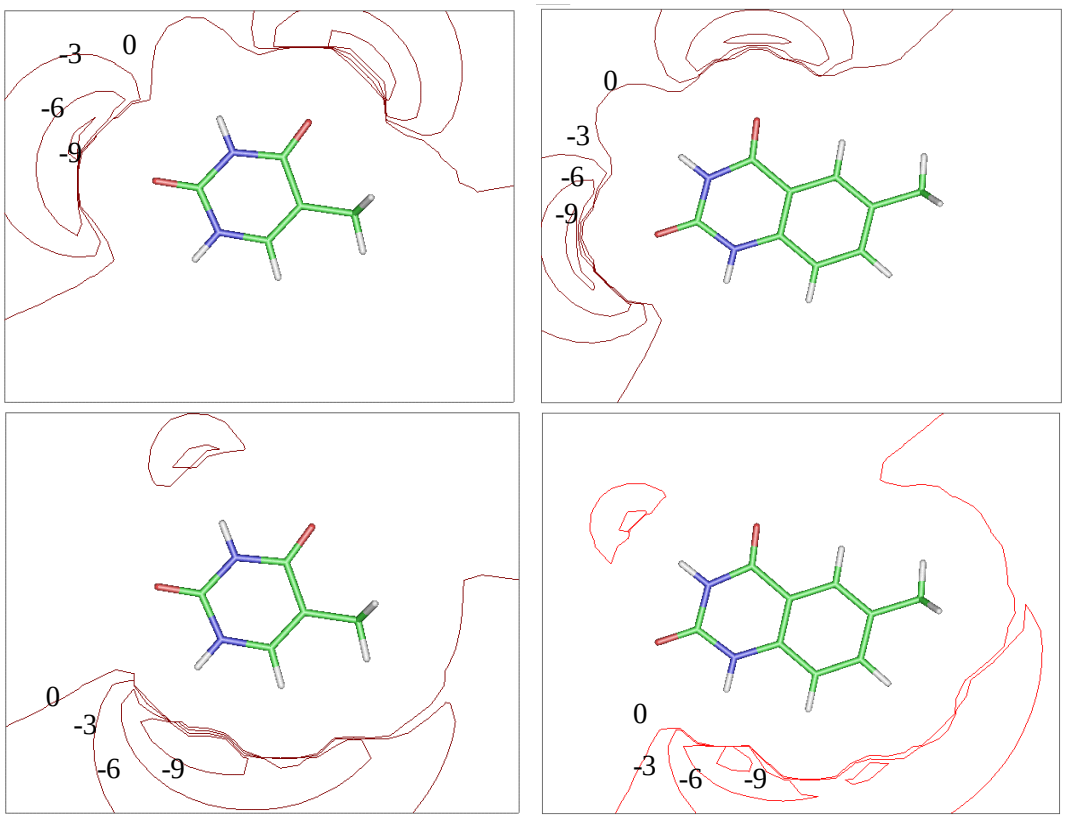
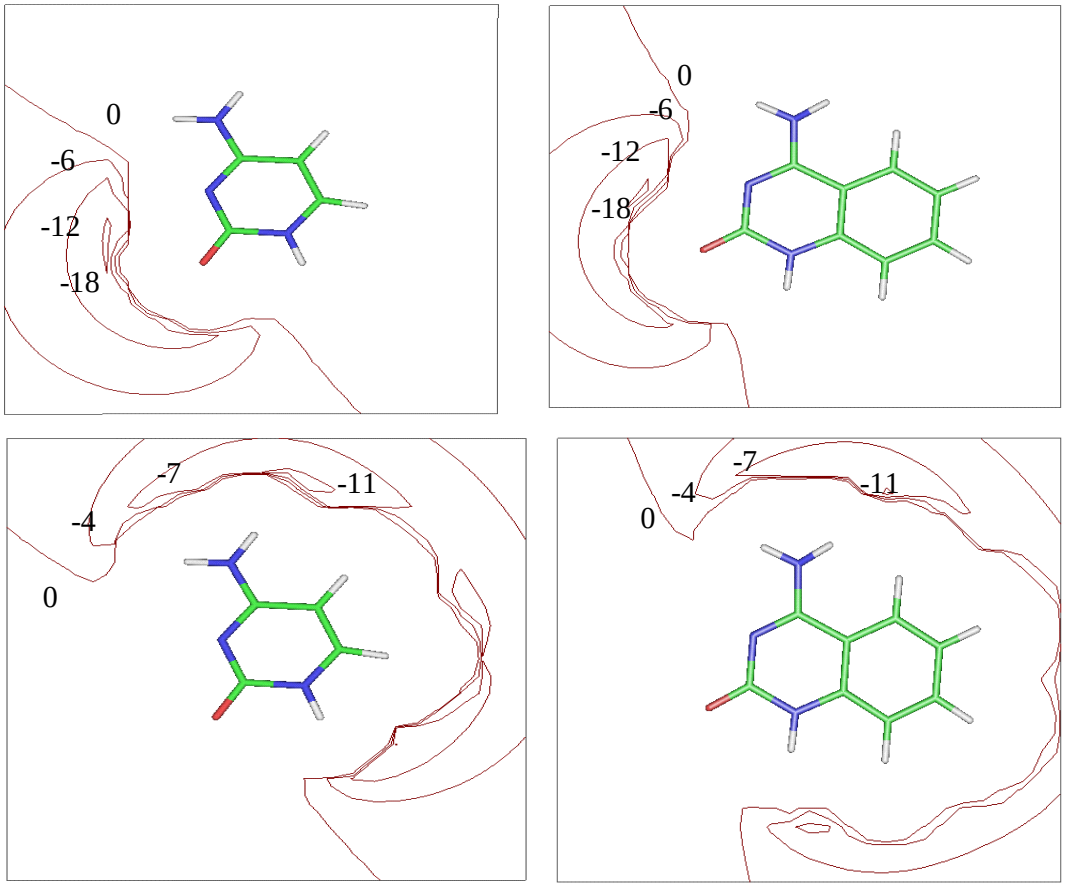



**Figure SI-7**. MIP maps corresponding to the interaction of a positively (top) and negatively (bottom) charged oxygen-like probe with cytosine (left) and benzocytosine (rigth). Values of the isoenergy contours are given in kcal/mol.