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Reconstructive methodology in the synthesis of 2-aminopurine

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**ELECTRONIC SUPPLEMENTARY INFORMATION**

**(ESI)**

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1. Spectra of compounds





**Figure S1**. 1H NMR (400 MHz, DMSO-d6) and 13C NMR (100 MHz, DMSO-d6) spectra of tetrazolo[1,5-*a*]pyrimidin-7-amine **3**





**Figure S2**. 1H NMR (400 MHz, DMSO-d6) and 13C NMR (100 MHz, DMSO-d6) spectra of 6-nitrotetrazolo[1,5-*a*]pyrimidin-7-amine **4**





**Figure S3**. 1H NMR (400 MHz, DMSO-d6) and 13C NMR (100 MHz, DMSO-d6) spectra of **5**





**Figure S4**. 1H NMR (400 MHz, DMSO-d6) and 13C NMR (151 MHz, DMF-d7) spectra of pyrimidine-2,4,5-triamine **6**



**Figure S5**. IR spectra of tetrazolo[1,5-*a*]pyrimidin-7-amine **3**



**Figure S6**. IR spectra of 6-nitrotetrazolo[1,5-*a*]pyrimidin-7-amine **4**



**Figure S7**. IR spectra of 5-nitropyrimidine-2,4-diamine **5**



**Figure S8**. IR spectra of pyrimidine-2,4,5-triamine **6**

### 2. Crystallography

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **D-H** | **d(D-H)** | **d(H..A)** | **<DHA** | **d(D..A)** | **A** |
| N1A-H1A | 0.86(3) | 2.26(3) | 163(2) | 3.093(4) | Cl1 [2-x, 1-y, 1-z] |
| N2A-H2AA | 0.95(4) | 1.87(4) | 176(2) | 2.814(4) | O00H [2-x, 1-y, 1-z] |
| N2A-H2AB | 0.85(4) | 2.43(4) | 159(2) | 3.237(4) | Cl2 [x, y+1, z-1] |
| N4A-H4AA | 0.95(4) | 2.48(4) | 146(2) | 3.312(4) | Cl2 [1-x, -y, 1-z] |
| N4A-H4AA | 0.95(4) | 2.02(4) | 122(2) | 2.658(4) | O1A |
| N4A-H4AB | 0.80(4) | 2.28(4) | 167(2) | 3.064(4) | N3A [1-x, 1-y, -z] |
| N1-H1 | 0.81(3) | 2.38(3) | 154(2) | 3.129(4) | Cl2 |
| N1-H1 | 0.81(3) | 2.58(3) | 124(2) | 3.100(4) | O1A [1-x, -y, 1-z] |
| N2-H2A | 0.87(4) | 2.33(4) | 166(2) | 3.176(4) | Cl1 [x+1, y, z] |
| N2-H2B | 0.92(4) | 2.38(4) | 151(2) | 3.212(4) | Cl2 |
| N4-H4A | 0.82(3) | 2.57(3) | 146(2)  | 3.287(4) | Cl1 [1-x, 1-y, 1-z] |
| N4-H4A | 0.82(3) | 2.12(3) | 125(2) | 2.684(4) | O1 |
| N4-H4B | 0.85(3) | 2.22(3) | 169(2) | 3.064(4) | N3 [2-x, 1-y, 1-z] |
| C6-H6 | 0.930 | 2.414 | 125.3 | 3.047(4) | O1A [1-x, -y, 1-z] |
| C6A-H6A | 0.930 | 2.390 | 163.4 | 3.292(4) | O1 [x+1, y, z] |

 **Table S1.** Hydrogen bonds with H..A < r(A) + 2.000 Å and <DHA > 110o.