



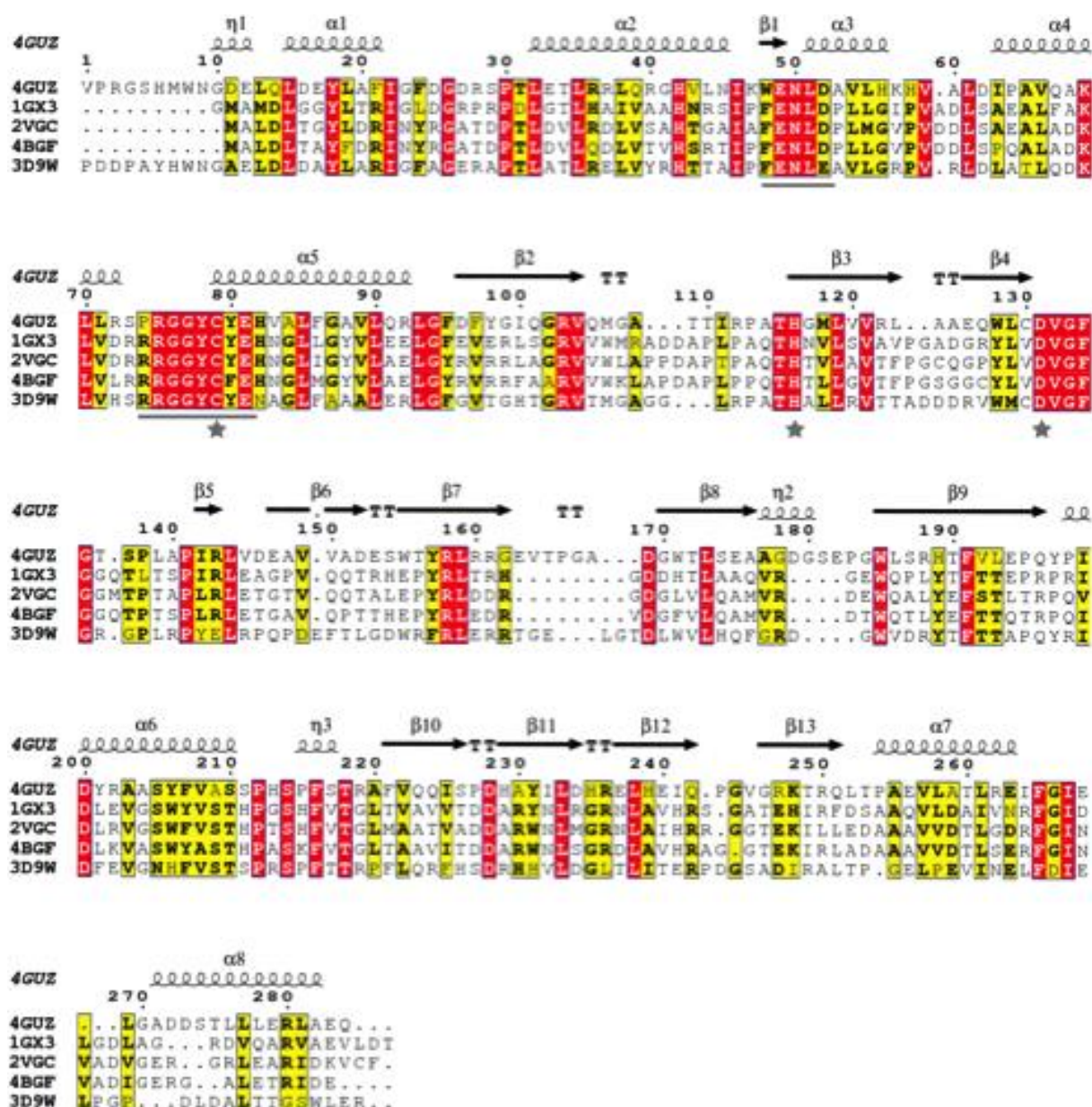
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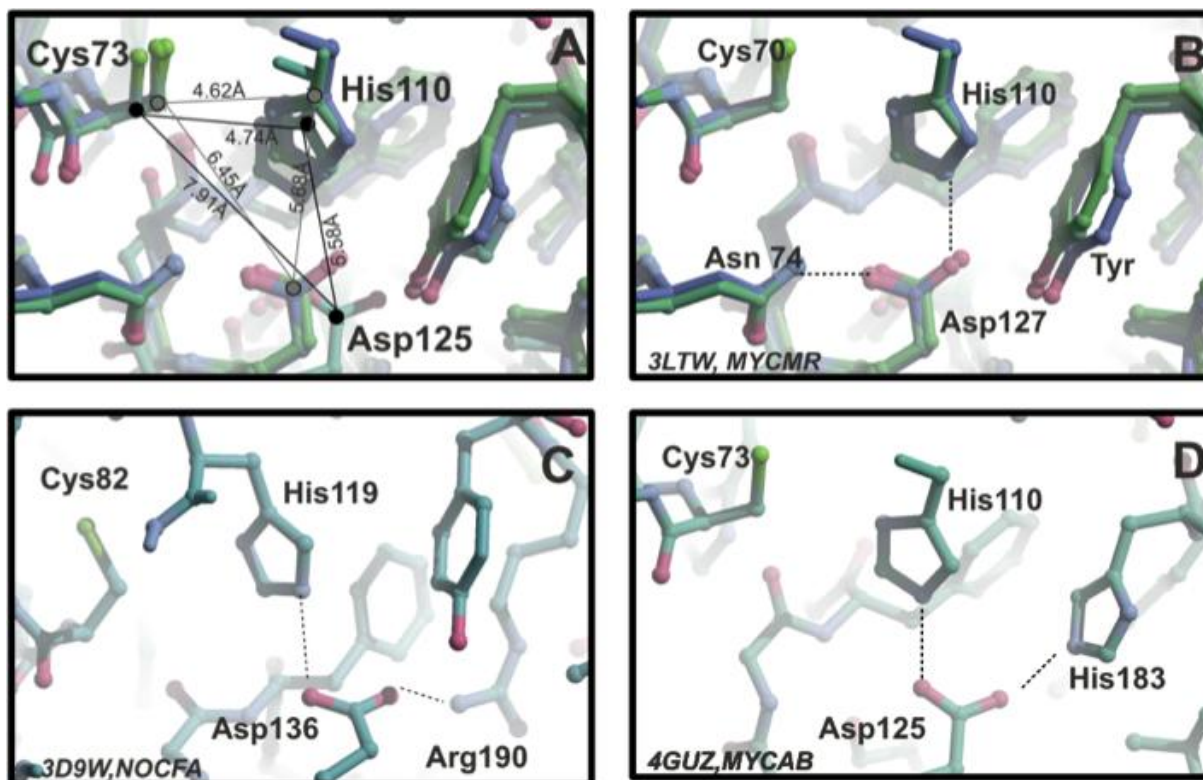
**Supporting information for article:**

**Structural and functional characterization of an arylamine *N*-acetyltransferase from the pathogen *Mycobacterium abscessus*: differences from other mycobacterial isoforms and implications for selective inhibition**

**Angélique Cocaign, Xavier Kubiak, Ximing Xu, Guillaume Garnier, Inès Li de la Sierra-Gallay, Linh Chi-Bui, Julien Dairou, Florent Busi, Areej Abuhammad, Ahmed Haouz, Jean-Marie Dupret, Jean-Louis Herrmann and Fernando Rodrigues-Lima**



**Figure S1. Structural alignment of (MYCAB)NAT1 with crystallized mycobacterial NATs.** Structures of (MYCAB)NAT1, (MYCSM)NAT1, (MYCMR)NAT1, (MYCTB)NAT1 and (NOCFA)NAT1 (4GUZ, 1W6F, 3LTW, 4BGF and 3D9W PDB entries, respectively) were aligned using 3D-COFFEE algorithm. They are shown according to their relative similarity. Catalytic triad residues are indicated by a star and the two conserved motifs are underlined. Secondary structure diagram of (MYCAB)NAT1 is shown on top of the alignment.



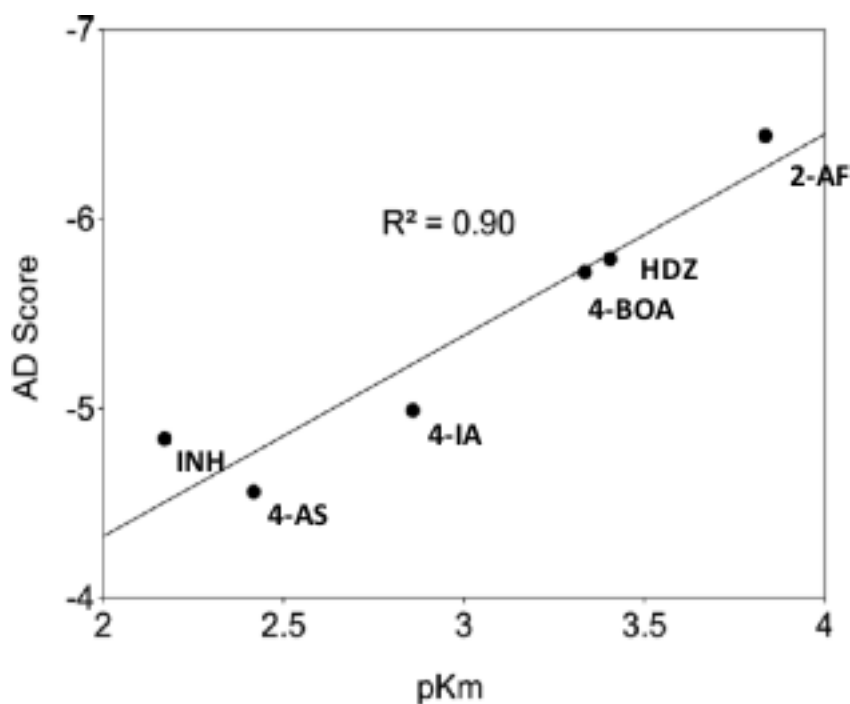
**Figure S2. Analysis of catalytic triad structural features of mycobacterial NATs**

**A.** Superposition of MYCAB(NAT1) with (MYCSM)NAT1, (MYCMR)NAT1 and (MYCTB)NAT1 (4GUZ, 1W6F, 3LTW and 4BGF PDB entries, respectively). The inter-atomic distances for the MYCAB(NAT1) (average distances for the others mycobacterial enzymes) are indicated.

**B.** Hydrogen bonds of catalytic Asp residue in (MYCSM)NAT1, (MYCMR)NAT1 and (MYCTB)NAT1 (1W6F, 3LTW and 4BGF PDB entries, respectively).

**C.** Hydrogen bonds of catalytic Asp125 residue from *N. farcinica* (NOCFA)NAT1 (3D9W).

**D.** Hydrogen bonds of catalytic Asp125 in NAT from *M. abscessus* (MYCAB)NAT1 (4GUZ).



**Figure S3 : Correlation between  $K_m^{app}$  and predicted binding energy of substrate docking models.** 2AF : 2-aminofluorene; 4-BOA : 4-butoxyaniline; 4IA : 4-iodoaniline; HDZ : hydralazine; 4AS : 4-aminosalicylate; INH : Isoniazid.

**Table S1 : R.m.s.d. values (Ca carbon) for structurally characterized NAT enzymes compared with (MYCAB)NAT1**

NAT isoform	PDB ID	r.m.s.d. values (Å)
(NOCFA)NAT1	3D9W	1.020
(MYCTB)NAT1	4BGF	1.639
(MYCMR)NAT1	2VFC	1.684
(RHILO)NAT1	2BSZ	1.772
(MYCSM)NAT1	1GX3	1.793
(SALTY)NAT1	1E2T	2.061
(BACAN)NAT1	3LNB	2.557
(BACCR)NAT3	4DMO	2.880
(HUMAN)NAT2	2PFR	3.555
(HUMAN)NAT1	2PQT	3.975