Supporting Information

Identification, Synthesis, and Characterisation of new Glycogen Phosphorylase Inhibitors binding to the Allosteric AMP Site.

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Table of content:

Data collection details for co-crystallazation of GPb and **4a** and **4j** (Table S1).

Analytical data for all the tested compounds (Table S2)

Table S1

Statistics of data and refinement		
	Compound **4a**	Compound **4j**
Space group	P43212	P43212
Unit cell parameters	a= b=127.3 c=115.1 Å	a= b=127.3 c=115.1 Å
Completeness (20-2.40 Å)	97.5%	98.9% (20.0-2.17 Å)
Completeness (2.44-2.40 Å)	95.8%	97.5% (2.21-2.17 Å)
Multiplicity (20-2.40 Å)	6.0	4.8
Rmerge (20-2.40 Å)	12.1%	11.1% (20.0-2.17 Å)
Rmerge (2.44-2.40 Å)	44.8%	43.4%(2.21-2.17 Å)
<I/σ(I)> (20-2.40 Å)	11.3	10.3 (20.0-2.17 Å)
<I/σ(I)> (2.36-2.32 Å)	2.8	2.8 (2.21-2.17 Å)
Unique reflections	36575	49838
R-factor[1]	21%	21%
R-free[2]	29%	28%

[1]R-factors were calculated using all data from 6 to 2.40 Å.

Crystallographic R-factor = $\sum_{(hkl)} \big| |Fo| - |Fc| \big| \Big/ \sum_{(hkl)} |Fo|$

[2]Rfree= $\sum_{(hkl)\varepsilon T} \big| |Fo| - |Fc| \big| \Big/ \sum_{(hkl)\varepsilon T} |Fo|$ where T is a test set containing a random 5% of the observations omitted from the refinement process.

Table S2 – Analytical data for the tested compounds

Compd	HPLC-purity	MS-data m/z (RI %)	NMR-data	Combustion analysis	
				Calc.	Anal.
4a		423 (MH^+) (10 %) 405 (MH^+- H_2O) (100 %)	OK	59.72 % C 3.34 % H 6.63 % N	59.65 % C 3.28 % H 6.48 % N
4b		412 (MH^+) (3 %) 396 (MH^+-H_2O) (40 %) 394 (MH^+- H_2O) (100 %)	OK	61.24 % C 3.43 % H 3.40 %	60,81 % C 3,56 % H 3,25 % N
4c	98 %	430 (M + Na) (7 %) 408 (MH^+) (30 %) 390 (MH^+- H_2O) (100 %)	OK		
4d	96 %	442 (M + Na) (20 %) 420 (MH^+) (5 %) 402 (MH^+- H_2O) (100 %)	OK		
4e	97.4 %	400 (M + Na) (15 %) 378 (MH^+) (5 %) 360 (MH^+- H_2O) (100 %)	OK		
4f	97.1 %	444 (M + Na) (14 %) 422 (MH^+) (5 %) 404 (MH^+- H_2O) (100 %)	OK		
4g	98 %	470 (M + Na) (10 %) 468 (M + Na) (16 %) 448 (MH^+) (5 %) 446 (MH^+) (7 %) 430 (MH^+- H_2O) (64 %) 428 (MH^+- H_2O) (100 %)	OK		
4h	96 %	414 (MH^+) (8 %) 412 (MH^+) (22 %) 396 (MH^+- H_2O) (37 %) 394 (MH^+- H_2O) (100 %)	OK		
4i	96 %	414 (M + Na) (20 %) 392 (MH^+) (40 %) 374 (MH^+- H_2O) (100 %)	OK		
4j		604 (M + NH_4^+) (100 %) 587 (MH^+) (15 %) 569 (MH^+- H_2O) (40 %)	OK	54.47 % C 3.50 % H 9.08 % (1.7 mol water)	54.28 % C 3.33 % H 9.19 %
4k	100 %	542 (MH^+) (50 %) 524 (MH^+- H_2O) (100 %)	OK		
4l	100 %	668 (MH^+) (60 %) 650 (MH^+- H_2O) (100 %)	OK		
4m	100 %	601 (MH^+) (20 %) 583 (MH^+- H_2O) (100 %)	OK		
4n	100 %	437 (MH^+) (10 %) 419 (MH^+- H_2O) (100 %)	OK		
4o	98 %	441 (MH^+) (20 %) 423 (MH^+- H_2O) (100 %)	OK		
4p	100 %	503 (MH^+) (8 %) 501 (MH^+) (8 %) 485 (MH^+- H_2O) (100 %) 483 (MH^+- H_2O) (100 %)	OK		
4q	98 %	491 (MH^+) (35 %) 473 (MH^+- H_2O) (100 %)	OK		
4r	98 %	480 (MH^+) (20 %) 462 (MH^+- H_2O) (100 %)	OK		
4s	100 %	481 (MH^+) (10 %) 463 (MH^+- H_2O) (100 %)	OK		

Compd	HPLC-purity	MS-data m/z (RI %)	NMR-data	Combustion analysis	
				Calc.	Anal.
4t	100 %	448 (MH^+) (8 %) 430 (MH^+ - H_2O) (100 %)	OK		
4u	98 %	437 (MH^+) (34 %) 419 (MH^+ - H_2O) (100 %)	OK		