SUPPLEMENTARY DATA

Deazapurine nucleoside analogues for the treatment of *Trichomonas vaginalis*

Manal J. Natto[1,*], Fabian Hulpia[2,*], Eric R. Kalkman[1], Susan Bailie[1], Amani Alhejeli[1], Yukiko Miyamoto[3], Lars Eckmann[3,4], Serge Van Calenbergh[2] and Harry P. de Koning[1,**]

1. Institute of Infection, Immunity and Inflammation, College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow, UK
2. Laboratory for Medicinal Chemistry, Campus Heymans (FFW), Ghent University, Ottergemsesteenweg 460, B-9000 Gent, Belgium
3. Department of Medicine, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093, USA
4. Center for Discovery and Innovation in Parasitic Diseases, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093, USA

[*], These authors contributed equally

[**], to whom correspondence should be addressed: Harry.de-Koning@glasgow.ac.uk

List of supplementary tables and figures

Table S1. Hits found in primary screening assay with the Enamine library.
Cells indicated with a red box show compounds confirmed as hits in the secondary screen; however, both compounds were later dismissed as pan-assay interference compounds.

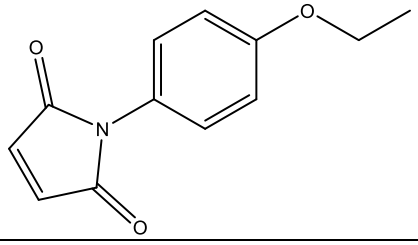
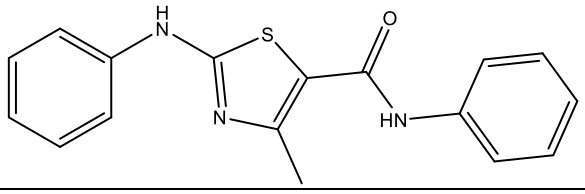
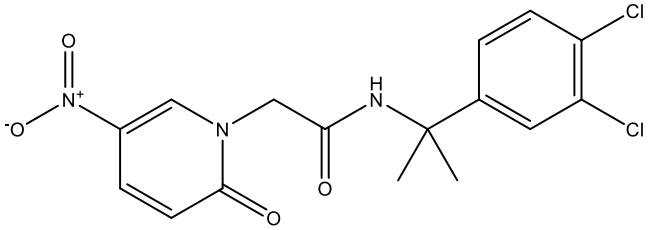
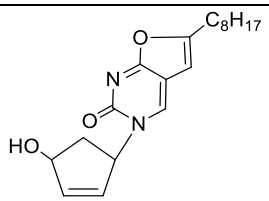
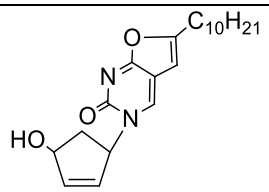
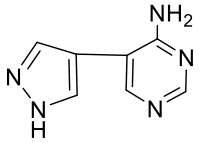
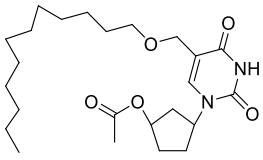
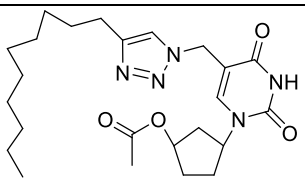
Plate	Hit ID	Structure
4	T0514-5155	1-(2-phenylethyl)-2,5-dihydro-1H-pyrrole-2,5-dione
9	T0514-5112	1-(2,5-dimethylphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0514-5117	1-(3,5-dichlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0514-5182	1-[(4-chlorophenyl)methyl]-2,5-dihydro-1H-pyrrole-2,5-dione
	T0514-5185	1-(3,4-dichlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0514-5236	1-(2,4-dimethoxyphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0514-5280	1-(2,5-dimethoxyphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0515-0096	1-(2,4,5-trichlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0515-0129	1-(4-phenoxyphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0519-1011	1-(2,3-dimethylphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0515-0127	1-(2,6-dimethylphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0515-0141	1-(2-bromophenyl)-2, : E7 - T0515-01415-dihydro-1H-pyrrole-2,5-dione
	T0400-1184	1-(2-chlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0400-1180	1-(4-iodophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0515-0227	1-(2-methoxyphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0400-2175	1-(4-methoxyphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0400-1196	1-(4-bromophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0400-2167	1-(2,5-dichlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
	T0516-9981	
	T0516-9354	1-(2-bromo-4-methyl-phenyl)-pyrrole-2,5-dione
11	T6162496	1-[2-(3,4-dimethoxyphenyl)ethyl]-2,5-dihydro-1H-pyrrole-2,5-dione
	T5416617	
12	T6935022	'N-[2-(3,4-dichlorophenyl)propan-2-yl]-2-(5-nitro-2-oxo-1,2-dihydropyridin-1-yl)acetamide 
15	T0514-5246	1-(4-chlorophenyl)-2,5-dihydro-1H-pyrrole-2,5-dione

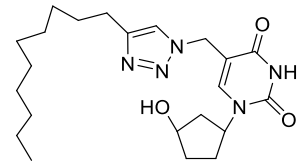
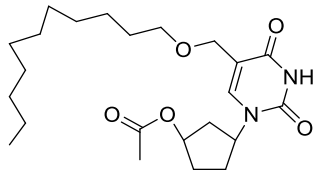
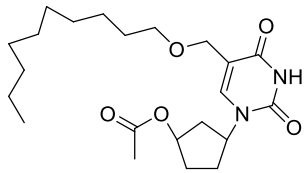
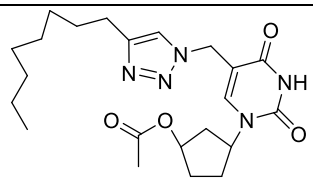
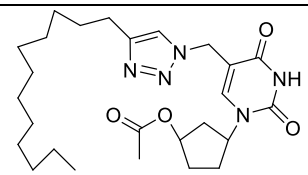
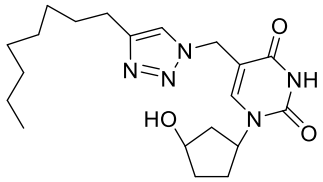
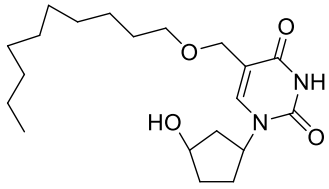
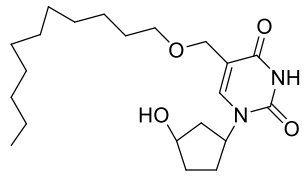
Table S2. EC_{50} values for aminosteroid compounds from *Holarrhena* (mean ± SD of three repeats).

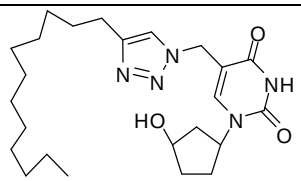
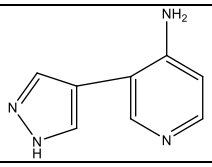
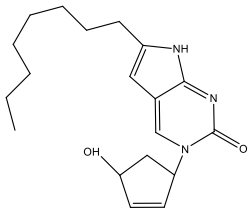
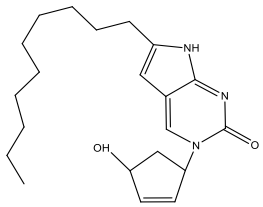
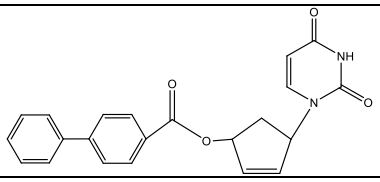
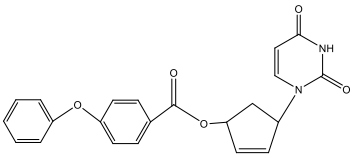
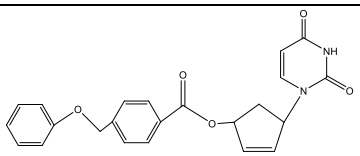
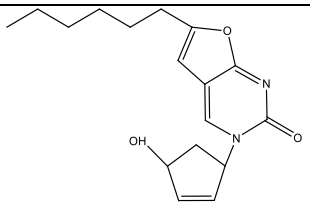
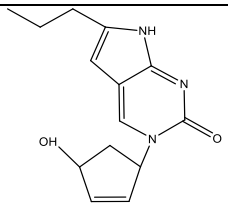
Compound	EC_{50} (μM), mean ± SD
β-holaphyllamine	28.64 ± 0.002
α-Holaphyllamine	26.85 ± 0.004
β-Dihydroholaphyllamine	43.72 ± 0.006
α-Dihydroholaphyllamine	43.29 ± 0.000
N-Methylholaphyllamine	14.49 ± 0.001
Isoconessimine	16.76 ± 0.002
Conessimine	>200 ± 0.001
Holarrhetine	85.19 ± 0.006
Holarrhesine	21.11 ± 0.008
Conessine	39.8 ± 0.003

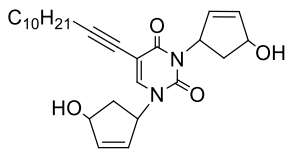
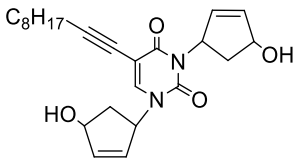
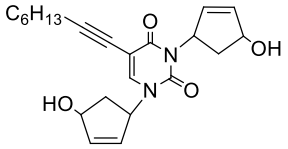
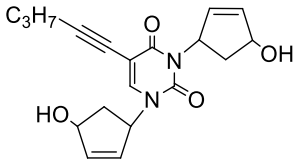
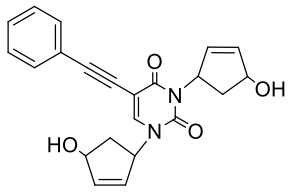
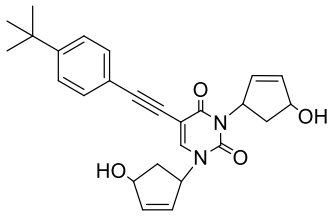
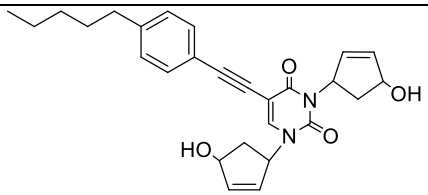
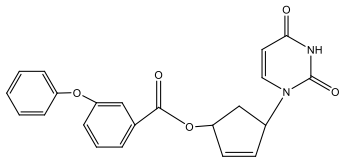
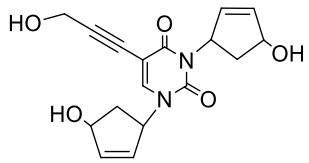
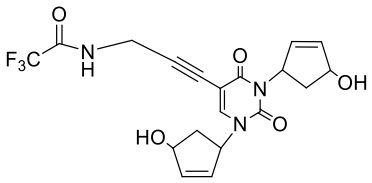
Table S3. EC_{50} values for 5'-norcarbocyclic uridine analogues (mean ± SD of three repeats).

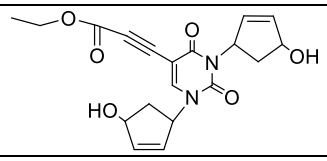
Compound	EC_{50} (μM), mean ± SD	Compound	EC_{50} (μM), mean ± SD
LN-111	46.95 ± 0.009	LN-121	70.22 ± 0.063
LN-112	68.11 ± 0.078	LN-122	52.84 ± 0.007
LN-113	54.76 ± 0.069	LN-123	36.85 ± 0.179
LN-124	120.23 ± 0.071	LN-125	84.76 ± 0.004
LN-74	101.42 ± 0.004	LN-126	69.22 ± 0.054
LN-98	84.52 ± 0.001	LN-78	59.37 ± 0.008
LN-1	46.11 ± 0.009	LN-79	65.81 ± 0.376
LN-2	73.60 ± 0.057	LN-80	36.28 ± 0.008
LN-114	69.65 ± 0.060	LN-85	193.77 ± 0.298
LN-115	78.48 ± 0.064	LN-86	105.49 ± 0.081
LN-101	63.28 ± 0.002	LN-87	52.95 ± 0.007
LN-103	81.19 ± 0.087	LN-88	45.37 ± 0.039
LN-127	53.75 ± 0.740	LN-92	82.36 ± 0.370
LN-117	48.94 ± 0.046	LN-93	79.44 ± 0.947
LN-118	31.99 ± 0.005	LN-94	82.79 ± 0.176
LN-119	54.05 ± 0.002	LN-95	58.04 ± 0.046
LN-120	73.45 ± 0.075		

	LN-1	M.w. = 330.42
	LN-2	M.w. = 358.47
	LN-74	MW = 161,18
	LN-78	MW = 436,58
	LN-79	MW = 459,58

	LN-80	MW = 417,55
	LN-85	M.w. = 422. 56
	LN-86	M.w. = 408. 53
	LN-87	M.w. = 431.53
	LN-8	M.w. = 487.63
	LN-92	M.w. = 389.49
	LN-93	M.w. = 366.49
	LN-94	M.w. = 380.52

	LN-95	M.w. = 445.60
	LN-98	M.w. = 160.18
	LN-101	M.w.= 329
	LN-103	M.w.= 357.24
	LN-111	M.w. =374.39
	LN-112	M.w. =390.39
	LN-113	M.w. =404.42
	LN-114	M.w. =302.37
	LN-115	M.w. =259.30

	LN-117	M.w. =440.58
	LN-118	M.w. =412.52
	LN-119	M.w. =384.47
	LN-120	M.w. =342.39
	LN-121	M.w. =376.41
	LN-122	M.w. =432.51
	LN-123	M.w. =446.54
	LN-124	M.w. =390.39
	LN-125	M.w. =330.34
	LN-126	M.w. =425.36

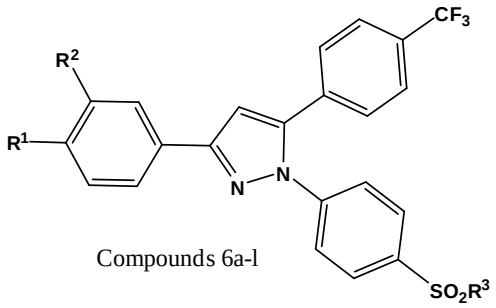
	LN-127	M.w. =372.37

Reference: Khandazhinskaya AL, Matyugina ES, Solyev PN, Wilkinson M, Buckheit KW, Buckheit RW Jr, Chernousova LN, Smirnova TG, Andreevskaya SN, Alzahrani KJ, Natto MJ, Kochetkov SN, de Koning HP, Seley-Radtke KL (2019) Investigation of 5'-Norcarbocyclic Nucleoside Analogues as Antiprotozoal and Antibacterial Agents. Molecules 24, 3433 doi: 10.3390/molecules24193433

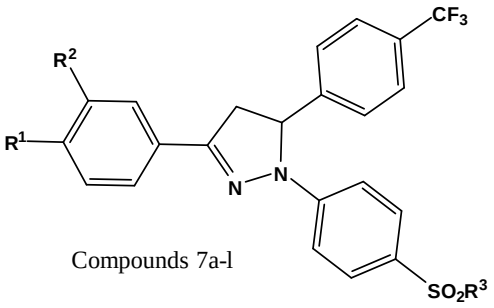
Table S4. EC_{50} values for KJZ-series compounds: pyrazolines/pyrazoles; coumarines and bicouoraines; triarylpyrazolines (mean ± SD of three repeats).
For structures see Tables S5-S7.

Compound	EC_{50} (μM), mean ± SD	Compound	EC_{50} (μM), mean ± SD
KJZ01	50.76 ± 0.002	KJZ25	47.74 ± 0.007
KJZ02	40.00 ± 0.002	KJZ26	35.37 ± 0.001
KJZ03	34.32 ± 0.019	KJZ27	33.17 ± 0.093
KJZ04	57.57 ± 0.023	KJZ28	35.53 ± 0.586
KJZ05	36.98 ± 0.269	KJZ29	43.45 ± 0.009
KJZ06	21.82 ± 0.002	KJZ30	101.57 ± 0.048
KJZ07	48.68 ± 0.005	KJZ31	51.13 ± 0.038
KJZ08	21.87 ± 0.004	KJZ32	10.75 ± 0.869
KJZ09	21.14 ± 0.008	KJZ33	79.19 ± 0.047
KJZ10	54.94 ± 0.065	KJZ34	39.74 ± 0.914
KJZ11	39.19 ± 0.368	KJZ35	12.28 ± 0.179
KJZ12	33.12 ± 0.016	KJZ36	76.30 ± 0.550
KJZ13	27.48 ± 0.006	KJZ37	53.99 ± 0.081
KJZ14	33.03 ± 0.140	KJZ38	61.96 ± 0.886
KJZ15	63.33 ± 0.031	KJZ39	59.29 ± 0.009
KJZ16	24.95 ± 0.135	KJZ40	45.94 ± 0.056
KJZ17	27.16 ± 0.033	KJZ41	28.57 ± 0.001
KJZ18	22.16 ± 0.958	KJZ42	57.29 ± 1.019
KJZ19	37.64 ± 0.068	KJZ43	132.37 ± 0.005
KJZ20	27.32 ± 0.001	KJZ44	119.78 ± 0.095
KJZ21	6.96 ± 0.012	KJZ45	15.65 ± 0.064
KJZ22	47.27 ± 0.004	KJZ46	19.37 ± 0.009
KJZ23	17.02 ± 0.041	KJZ47	27.49 ± 0.033
KJZ24	26.58 ± 0.083	KJZ48	74.74 ± 0.071

Table S5. Structures of pyrazolines/pyrazoles compounds KJZ01-KJZ20



Compounds 6a-l



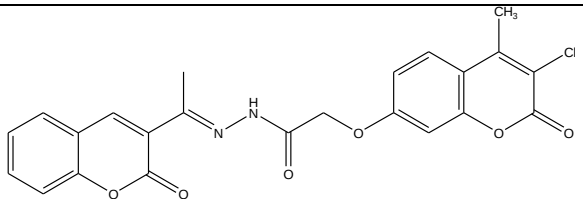
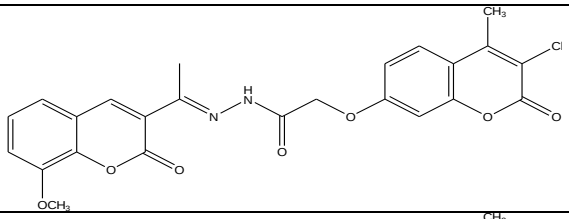
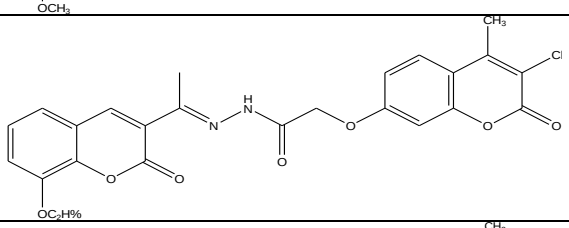
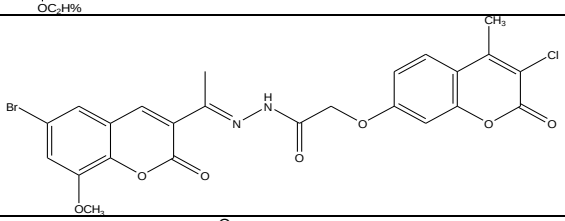
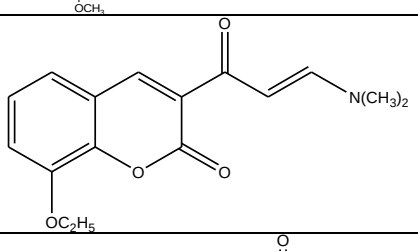
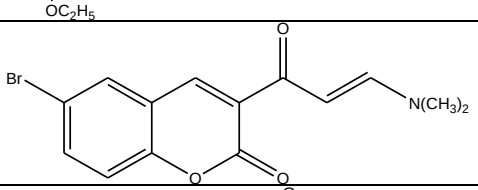
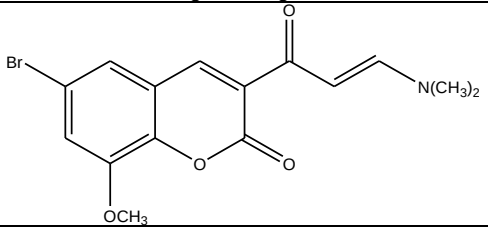
Compounds 7a-l

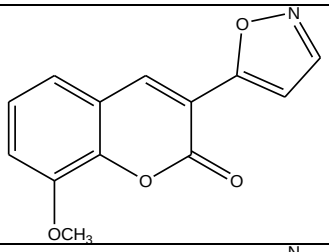
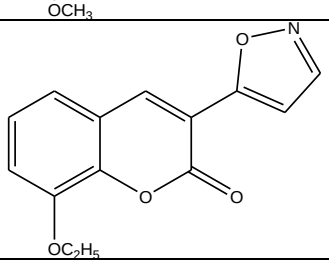
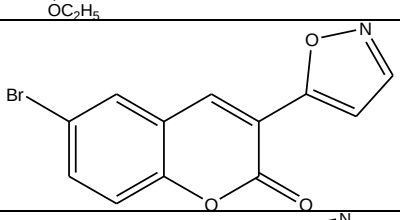
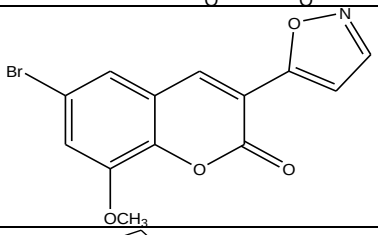
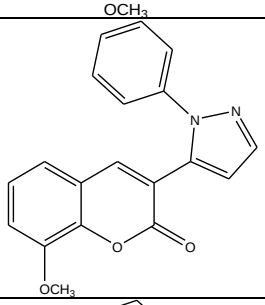
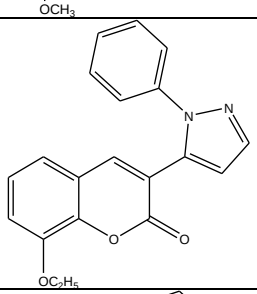
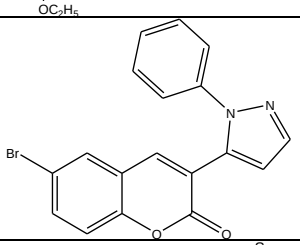
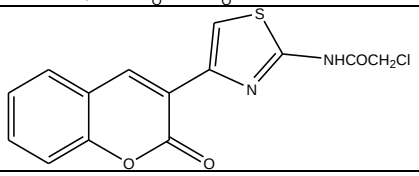
R^1 = OH, CH_3, OCH_3, OCH_2CH_3, F; R^2 = H, F; R^3 = CH_3, NH_2

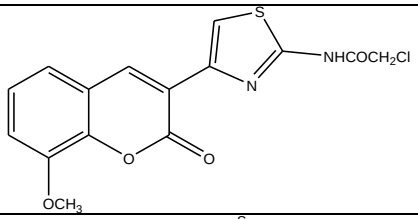
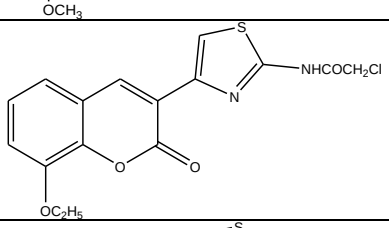
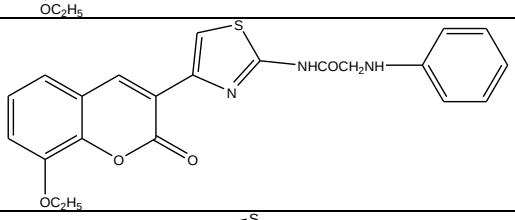
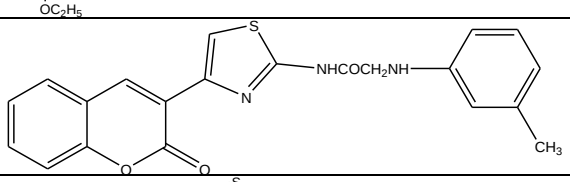
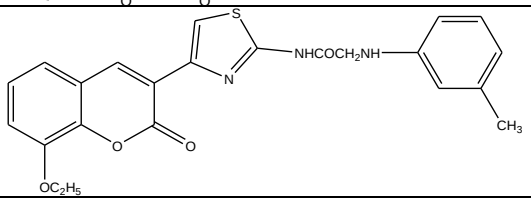
Compound	R^1	R^2	R^3	**Compound**	R^1	R^2	R^3
KJZ01	F	H	CH_3	KJZ11	F	F	CH_3
KJZ02	CH_3	H	CH_3	KJZ12	CH_3	H	CH_3
KJZ03	OH	H	CH_3	KJZ13	OH	H	CH_3
KJZ04	OCH_3	H	CH_3	KJZ14	OCH_3	H	CH_3
KJZ05	F	H	NH_2	KJZ15	OC_2H_5	H	CH_3
KJZ06	F	F	NH_2	KJZ16	F	F	NH_2
KJZ07	CH_3	H	NH_2	KJZ17	CH_3	H	NH_2
KJZ08	OH	H	NH_2	KJZ18	OH	H	NH_2
KJZ09	OC_2H_5	H	NH_2	KJZ19	OCH_3	H	NH_2
KJZ10	F	H	CH_3	KJZ20	OC_2H_5	H	NH_2

Reference: Abdellatif KRA, Elshemy HAH, Azoz AA (2015) 1-(4-Methane(amino)sulfonylphenyl)-3-(4-substituted-phenyl)-5-(4-trifluoromethylphenyl)-1H-2-pyrazolines/pyrazoles as potential anti-inflammatory agents. Bioorg Chem 63, 13-23.

Table S6. List of coumarine and bicoumarine-type compounds.

Code	Structure	Paper	Code in paper
KJZ21		**DPC**	**5a**
KJZ22		**DPC**	**5b**
KJZ23		**DPC**	**5c**
KJZ24		**DPC**	**5d**
KJZ25		**LDDD**	**5b**
KJZ26		**LDDD**	**5c**
KJZ27		**LDDD**	**5d**

KJZ28		**LDDD**	**6a**
KJZ29		**LDDD**	**6b**
KJZ30		**LDDD**	**6c**
KJZ31		**LDDD**	**6d**
KJZ32		**LDDD**	**7a**
KJZ33		**LDDD**	**7b**
KJZ34		**LDDD**	**7c**
KJZ35		**LDDD**	**3a**

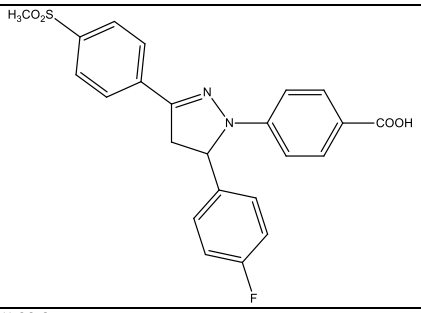
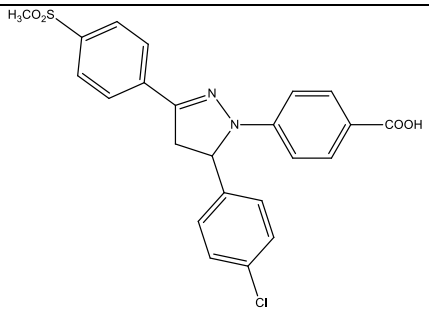
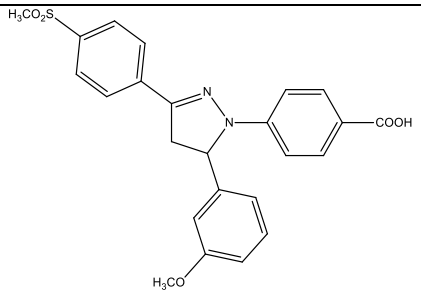
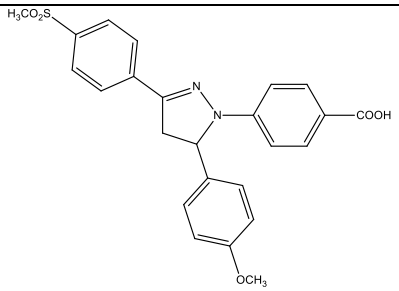
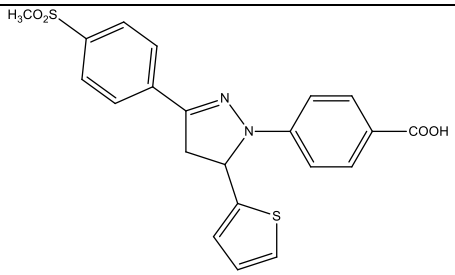
KJZ36		**LDDD**	**3b**
KJZ37		**LDDD**	**3c**
KJZ38		**LDDD**	**4c**
KJZ39		**LDDD**	**4d**
KJZ40		**LDDD**	**4e**

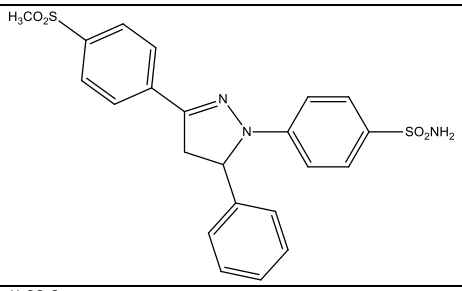
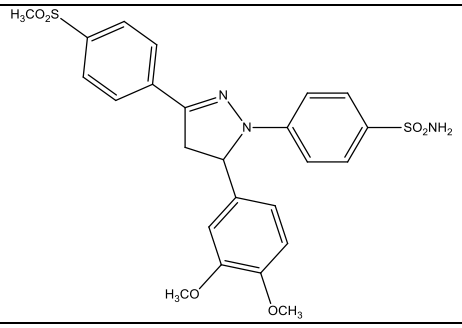
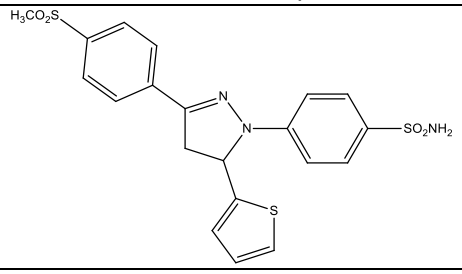
References:

DPC = Abdelatif KRA, Abdelgawad MA, Elshemy HAH, Kahk NM (2016) Design and synthesis of certain novel bicoumarin derivatives as anticancer agents. Der Pharm Chem 8(3), 13-19

LDDD = Abdelatif KRA, Abdelgawad MA, Elshemy HAH, Kahk NM, El Amir DM (2017) Design, Synthesis, Antioxidant and Anticancer Activity of New Coumarin Derivatives Linked with Thiazole, Isoxazole or Pyrazole Moiety. Letters in Drug Design & Discovery, 14 (7), 773-781

Table S7. List of triarylpyrazoline compounds KJZ41-KJZ-48.

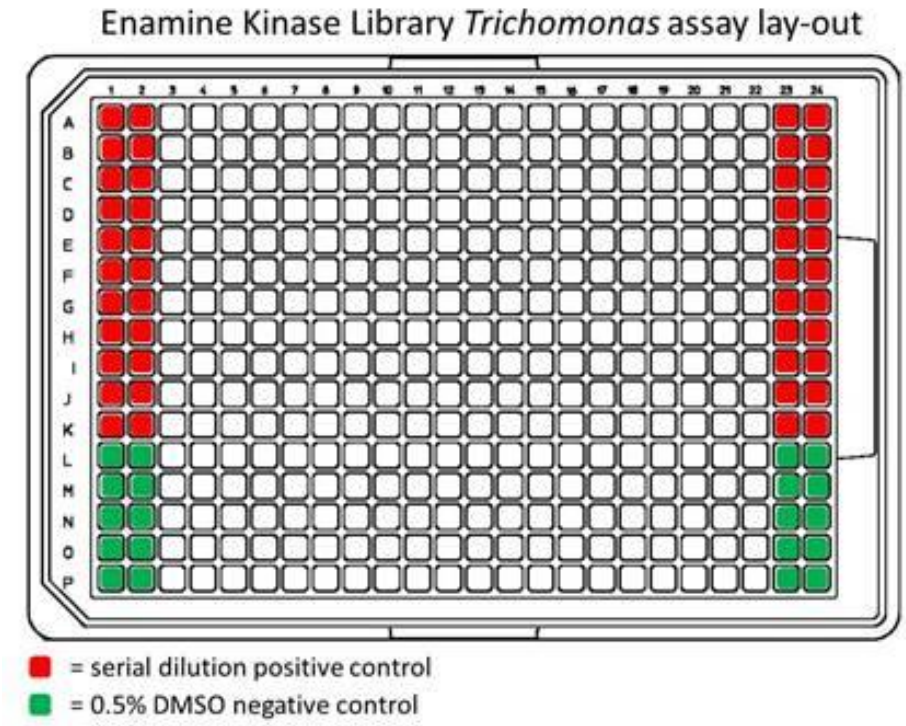
Compound no	structure	**Code in paper**
KJZ41		7b
KJZ42		6b
KJZ43		5b
KJZ44		4b
KJZ45		8b

KJZ46		1a
KJZ47		2a
KJZ48		8a

Reference: Abdellatif KR, Abdelgawad MA, Labib MB, Zidan TH (2015a) Synthesis, cyclooxygenase inhibition, anti-inflammatory evaluation and ulcerogenic liability of novel triarylpyrazoline derivatives as selective COX-2 inhibitors. Bioorg Med Chem Lett 25(24):5787-5791. doi: 10.1016/j.bmcl.2015.10.047

Figure S1. (A) Primary *T. vaginalis* assay layout using 384-well plates. Eleven serial dilutions of metronidazole (positive control) were applied top-down in columns 1, 2, 23 and 24 (red), leaving 20 cells free for 5% DMSO controls (green). **(B)** Follow-up assay layout. Each plate contained each compound twice (serial diluted 10 μM down), and the total in triplicate (making six assay plates), with four serial dilution controls (in red), 24 DMSO controls (green) and eight medium controls (yellow).

(A)



(B)

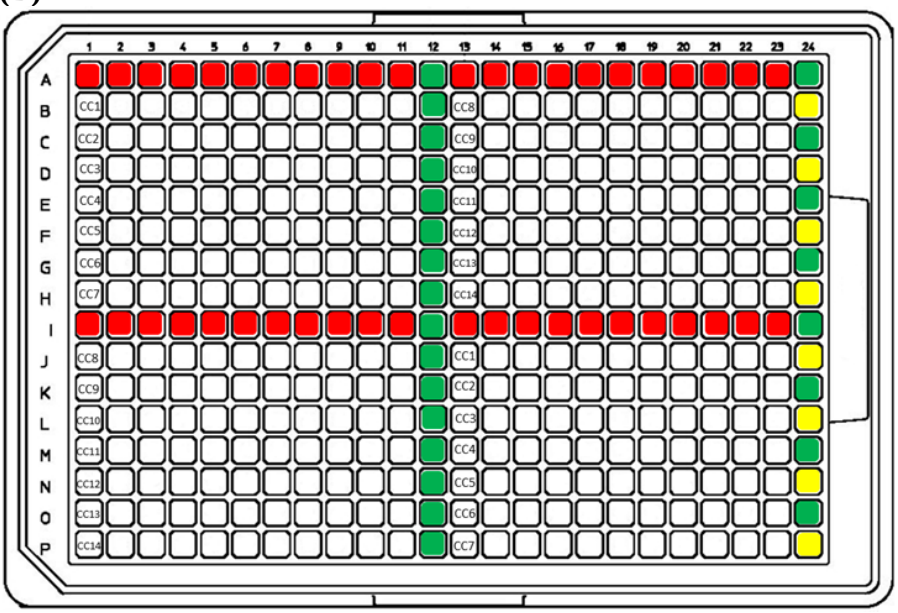
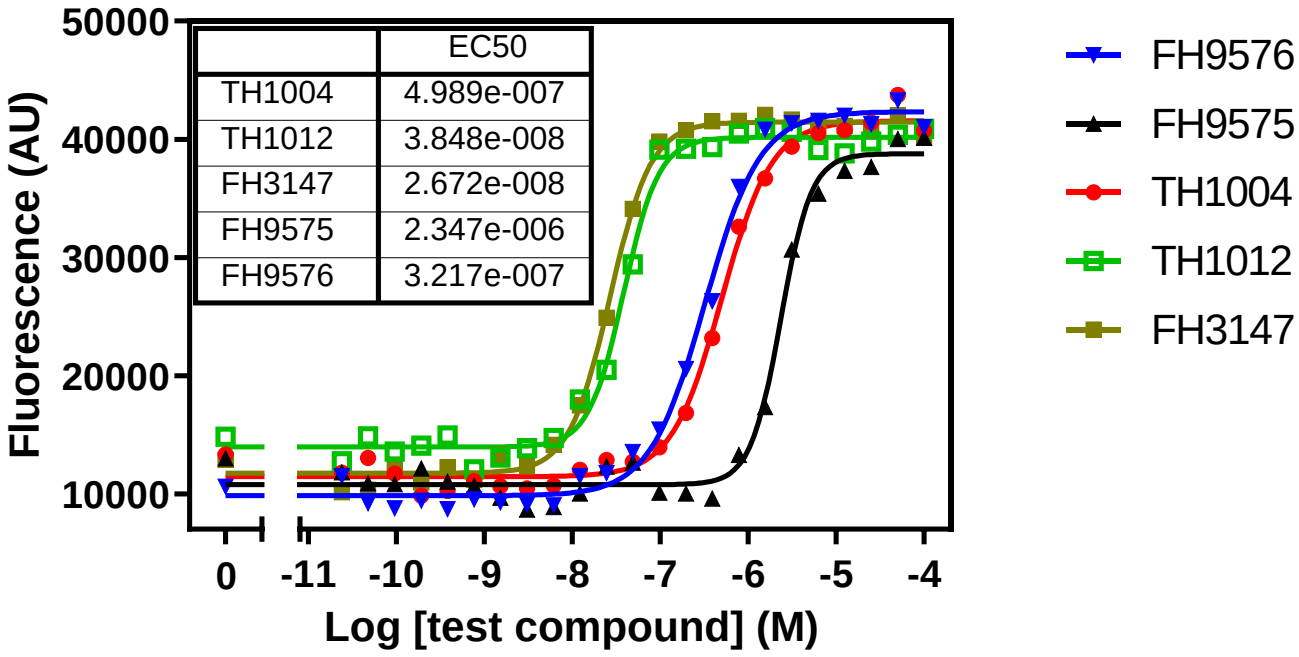


Figure S2. Representative examples of fluorescence readouts. **(A)** The sigmoidal curves for TH1004, TH1012, FH3147, FH9575 and FH9576 using the resorufin assay. **(B)** Sigmoidal curves for metronidazole (positive control).

(A)



(B)

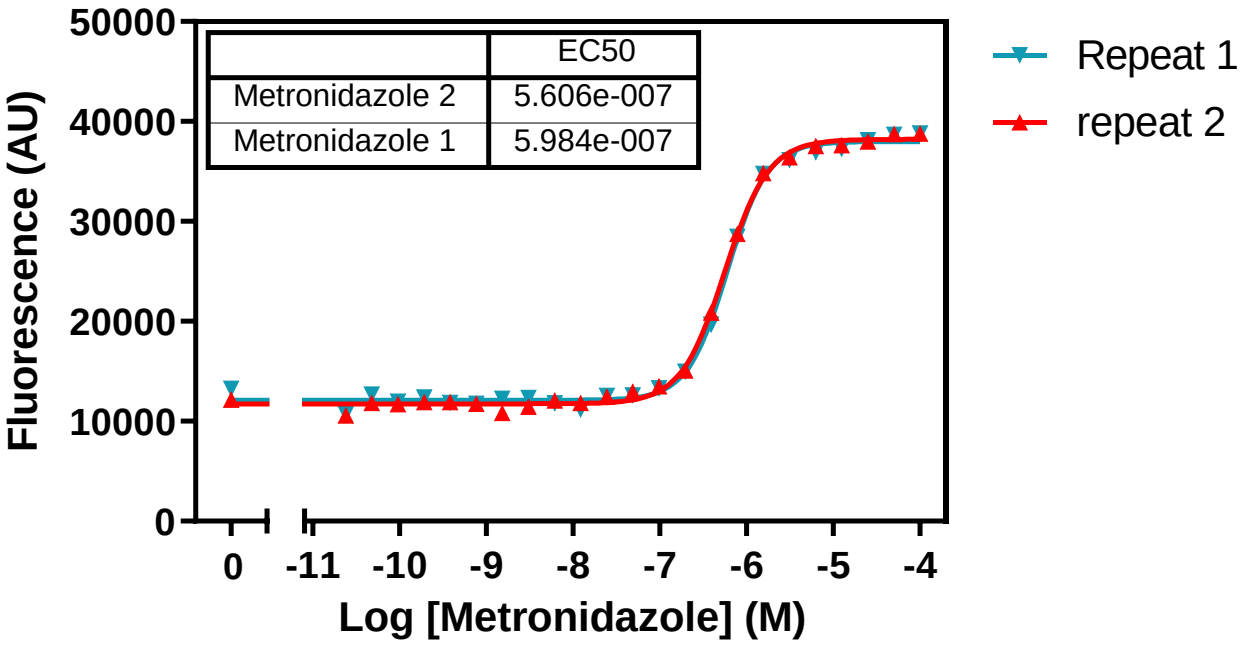


Figure S3. Correlation between the EC_{50} values of the six ribofuranoses depicted in Figure 4 and the EC_{50}s of the corresponding 3'-deoxy and 2'-deoxy analogs. An F-test showed that the two slopes were significantly non-zero, and runs tests showed the lines did not significantly deviate from linearity. The two slopes were significantly different from each other by F-test (P = 0.0090). Analysis by GraphPad Prism 9.0.

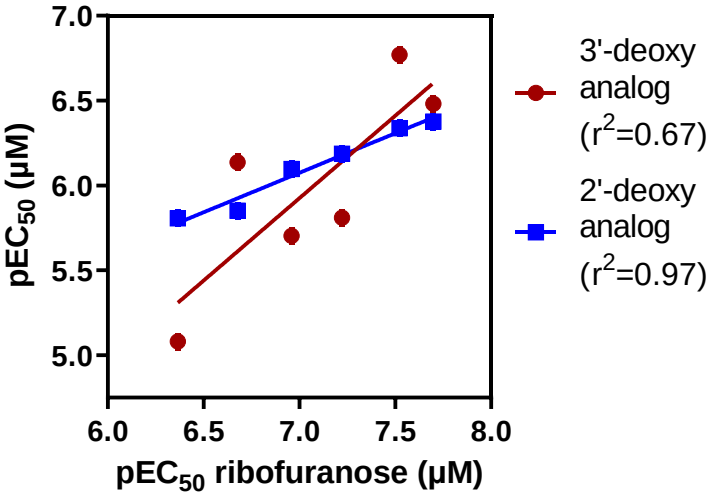
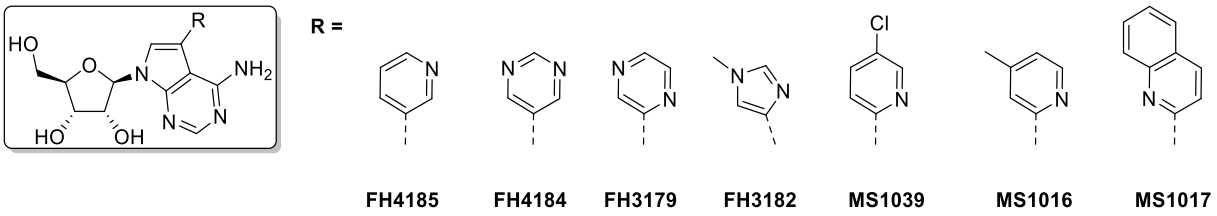


Figure S4. Structures of azaheterocycle 7-substituted derivatives



References for previously published compounds:

Compound	Reference
TH1004	[1]
TH1011	[1]
TH1012	[1]
FH3147	[1]
TH1013	[1]
FH4185	[1]
FH4184	[1]
FH3179	[1]
FH3182	[1]
FH7435	[1]
MS1001	[1]
FH8459	[1]
FH8460	[1]
FH8461	[1]
MS1016	[1]
MS1017	[1]
FH8494	[2]
FH8512	[2]
FH8513	[2]
FH5319	[3]
FH9526	[4]
MS1039	[1]
FH9574	[2]
FH9575	[2]
FH9577	[2]
FH9576	[2]
FH9582	[2]
FH9581	[2]
FH9610	[4]
FH9611	[4]
FH9613	[4]
FH10639	[2]
FH10640	[2]
FH10641	[2]
FH10642	[2]
FH10644	[2]
FH10645	[2]
FH10647	[2]
FH10648	[2]
FH10649	[2]
FH10653	[2]
FH10667	[2]
FH10669	[2]
FH10680	[2]
FH10681	[2]
FH10682	[2]

FH10683	[2]
FH8480	[2]
FH8481	[2]

Literature compounds

FH11708	[7]

New compounds (**29** analogues – experimental data below)

FH11709
FH11710
FH11711
FH11712
FH11713
FH11707
FH11706
FH11705
FH11703
FH11704
FH11702
FH10714
FH10715
FH13817
FH13820
FH13821
FH13823
FH13824
FH13825
FH13826
FH13827
FH13828
FH13829
FH13830
FH13832
FH13833
FH13834
FH13835
FH13822

General experimental

All reagents and solvents, obtained from standard commercial sources were at least of analytical grade, and were used as received. Nucleoside analogues **TH1003**[5] and **FH10678**[6] were prepared exactly as described in literature. Reactions were carried out under a nitrogen atmosphere. Analytical TLC was performed precoated F254 aluminum plates (Machery-

Nagel®) and visualized by UV followed by staining with basic aq. $KMnO_4$ spray. Column chromatography was performed using Machery-Nagel 60 M silica (40-63 µm) or on a Reveleris X2 (Grace/Büchi) automated Flash unit employing pre-packed silica or RP-silica (C18, Büchi) columns. Exact mass measurements were performed on a Waters Time of Flight (ToF) mass spectrometer equipped with electrospray (ESI) and modular Lockspray™ interface. Samples were infused in a MeCN/water (1:1) + 0.1 % formic acid mixture at 100 µL/min. NMR spectra were recorded on a Varian Mercury 300 MHz spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants are given in Hz. Spectra were referenced to the residual solvent peak. In ^{19}F-NMR, signals were referenced to $CDCl_3$ or DMSO-d_6 lock resonance frequency (IUPAC referencing: $CFCl_3$ set to 0 ppm). Melting points were determined on a Büchi-545 apparatus and are uncorrected. Purity was assessed by means of analytical LC-MS. A Waters AutoPurification system (equipped with ACQUITY QDa (mass; 100 – 1000 amu)) and 2998 Photodiode Array (220 – 400 nm)) was employed. Analytical column: Waters Cortecs® C18 (2.7 µm 100 x 4.6mm) column. A default, linear gradient of HCOOH in H_2O (0.2 %, v/v) / MeCN at a flow rate of 1.44 mL/min ranging from 95:05 to 00:100 in 6.5 minutes, was employed for LC analysis. All final compounds had purity > 95 %, (UV signal integration).

General procedure for Suzuki coupling reaction

TH1003 or **FH10678** (1 eq.), boronic acid (1.5 eq.), Na_2CO_3 (9 eq.) (Cs_2CO_3, 9 eq. for 2'-deoxynucleosides), $Pd(OAc)_2$ (0.05 eq.) and TPPTS (0.15 eq.) were weight and added to a 10 mL flask. The flask was evacuated and backfilled with nitrogen, a procedure repeated three times in total. Then, MeCN/water mixture (1/2 ratio, 6 mL/mmol starting material (SM)) was added. The resulting suspension mixture was then vigorously stirred at ambient temperature (~5 min), and then heated to reflux (for 2'-deoxynucleosides: 75 °C). The reaction was monitored LC/MS (~10 min to 3 h). Upon completion or stalled progression of the reaction,

the mixture was allowed to cool to ambient temperature. Then, the mixture was neutralized employing a 0.5 M aq. HCl solution (pH ~ 7). Then, the solvent was removed *in vacuo*. Then, the residue was resuspended in MeOH and evaporated, which was repeated three times. Next, the residue was adsorbed onto Celite® (from MeOH) and eluted with 20 % MeOH/DCM over a short pad of silica gel (~ 5 cm). The obtained liquid was evaporated and purified by column chromatography (MeOH/DCM gradient, as indicated for each individual compound). Alternatively, after cooling to ambient temperature, the mixture was immediately evaporated till dryness, re-dissolved in DMSO (2 mL) and water (8 mL) and purified by RP-flash chromatography (C18 column, Büchi) by the gradient indicated for each compound.

4-Amino-5-(4-ethylphenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11702) **FH11702** was prepared according to the general procedure for Suzuki coupling (reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11702** as a white solid (0.048 g, 0.13 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 37 %. Melting point: 117 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 1.23 (t, *J* = 7.5 Hz, 3H, CH_3), 2.66 (q, *J* = 7.5 Hz, 2H, CH_2), 3.53 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5’’), 3.63 (ddd, *J* = 12.0, 5.1, 4.2 Hz, 1H, H-5’), 3.90 (q, *J* = 3.6 Hz, 1H, H-4’), 4.08 – 4.13 (m, 1H, H-3’), 4.43 – 4.48 (m, 1H, H-2’), 5.10 (d, *J* = 4.8 Hz, 1H, OH-3’), 5.18 (dd, *J* = 6.0, 5.1 Hz, 1H, OH-5’), 5.31 (d, *J* = 6.3 Hz, 1H, OH-2’), 6.11 (d, *J* = 6.3 Hz, 1H, H-1’), 6.11 (br. s, 2H, NH_2), 7.31 – 7.34 (m, 2H, H_{Phe}), 7.38 – 7.41 (m, 2H, H_{Phe}), 7.50 (s, 1H, H-6), 8.14 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 15.6 (CH_3), 27.8 (CH_2), 61.7 (C-5’), 70.6 (C-3’), 73.8 (C-2’), 85.1 (C-4’), 87.0 (C-1’), 100.6 (C-4a), 116.2 (C-5), 120.9 (C-6), 128.38 ($2C_{Phe}$), 128.41 ($2C_{Phe}$), 131.8 (C_{Phe}) 142.5 (C_{Phe}), 150.7 (C-7a), 151.6 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{19}H_{23}N_4O_4$ ($[M+H]^+$): 371.1714, found: 371.1710.

4-Amino-5-(3-chloro-4-methylphenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11703) FH11703 was prepared according to the general procedure for Suzuki coupling

(reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11703** as a white solid (0.049 g, 0.13 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 36 %. Melting point: 135 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.38 (s, 3H, CH_3), 3.53 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5’’), 3.63 (ddd, *J* = 12.0, 5.1, 4.2 Hz, 1H, H-5’), 3.90 (q, *J* = 3.9 Hz, 1H, H-4’), 4.08 – 4.13 (m, 1H, H-3’), 4.42 – 4.48 (m, 1H, H-3’), 5.11 (d, *J* = 4.8 Hz, 1H, OH-3’), 5.16 (dd, *J* = 6.0, 5.1 Hz, 1H, OH-5’), 5.31 (d, *J* = 6.3 Hz, 1H, OH-2’), 6.11 (d, *J* = 6.3 Hz, 1H, H-1’), 6.21 (br. s, 2H, NH_2), 7.33 (dd, *J* = 7.5, 1.8 Hz, 1H, H-6$_{Phe}$), 7.45 (d, *J* = 7.8 Hz, 1H, H-5$_{Phe}$), 7.50 (d, *J* = 1.8 Hz, 1H, H-2$_{Phe}$), 7.59 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 19.3 (CH_3), 61.6 (C-5’), 70.6 (C-3’), 73.8 (C-2’), 85.1 (C-4’), 89.0 (C-1’), 100.3 (C-4a), 114.9 (C-5), 121.5 (C-6), 127.1 (C$_{Phe}$), 128.4 (C$_{Phe}$), 131.6 (C$_{Phe}$), 133.6 (C$_{Phe}$), 133.7 (C$_{Phe}$), 133.9 (C$_{Phe}$), 151.0 (C-7a), 151.8 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{20}ClN_4O_4$ ([M+H]$^+$): 391.1168, found: 391.1195.

4-Amino-5-(4-trifluoromethylphenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11704) FH11704 was prepared according to the general procedure for Suzuki coupling (reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11704** as a white solid (0.052 g, 0.13 mmol). Column chromatography: 1 → 9 % MeOH / DCM. Yield = 36 %. Melting point: 154 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.54 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5’’), 3.64 (ddd, *J* = 12.0, 5.1, 4.2 Hz, 1H, H-5’), 3.91 (q, *J* = 3.6 Hz, 1H, H-4’), 4.09 – 4.14 (m, 1H, H-3’), 4.46 (q, *J* = 6.0 Hz, 1H, H-2’), 5.12 (d, *J* = 4.8 Hz, 1H, OH-3’), 5.17 (dd, *J* = 6.3, 5.1 Hz, 1H, OH-5’), 6.13 (d, *J* = 6.3 Hz, 1H, H-1’), 6.30 (br. s, 2H, NH_2), 7.67 – 7.69 (m, 2H, H$_{Phe}$), 7.69 (s, 1H, H-6), 7.81 – 7.83 (m, 2H, H$_{Phe}$), 8.17 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -60.7. ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.6 (C-5’), 70.6 (C-3’), 73.8 (C-2’), 85.2 (C-4’), 87.1 (C-1’), 100.1 (C-4a), 115.1 (C-5), 122.3 (C-6), 124.5 (q, *J* = 270.0 Hz, 1C, CF_3), 125.7 (q, *J* = 3.8 Hz, 2C, C-3$_{Phe}$, C-5$_{Phe}$), 126.9 (q, *J* = 32.3 Hz, 1C, C-4$_{Phe}$),

128.8 (2C, C-2$_{Phe}$, C-6$_{Phe}$), 138.6 (C-1$_{Phe}$), 151.3 (C-7a), 151.9 (C-2), 157.4 (C-4). HRMS (ESI): calculated for $C_{18}H_{28}F_3N_4O_4$ ($[M+H]^+$): 411.1275, found: 411.1271.

4-Amino-5-(3-methyl-4-chlorophenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11705) FH11705 was prepared according to the general procedure for Suzuki coupling (reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11705** as a white solid (0.053 g, 0.14 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 39 %. Melting point: 134 °C / 235 °C. ^{1}H NMR (300 MHz, DMSO-d$_6$) δ: 2.39 (s, 3H, CH_3), 3.53 (ddd, *J* = 12.0, 6.3, 4.2 Hz, 1H, H-5''), 3.63 (ddd, *J* = 12.0, 4.5, 3.9 Hz, 1H, H-5'), 3.90 (q, *J* = 3.6 Hz, 1H, H-4'), 4.08 – 4.12 (m, 1H, H-3'), 4.44 (q, *J* = 6.0 Hz, 1H, H-2'), 5.12 (d, *J* = 4.8 Hz, 1H, OH-3'), 5.16 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.32 (d, *J* = 6.3 Hz, 1H, OH-2'), 6.11 (d, *J* = 6.0 Hz, 1H, H-1'), 6.19 (br. s, 2H, NH_2), 7.29 (dd, *J* = 8.7, 2.1 Hz, 1H, H-6$_{Phe}$), 7.45 (d, *J* = 1.8 Hz, 1H, H-2$_{Phe}$), 7.50 (d, *J* = 8.4 Hz, 1H, H-5$_{Phe}$), 7.56 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ: 19.7 (CH3), 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.3 (C-4a), 115.2 (C-5), 121.3 (C-6), 127.5 (C$_{Phe}$), 129.3 (C$_{Phe}$), 131.1 (C$_{Phe}$), 131.8 (C$_{Phe}$), 133.4 (C$_{Phe}$), 135.9 (C$_{Phe}$), 151.0 (C-7a), 151.7 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{20}ClN_4O_4$ ($[M+H]^+$): 391.1168, found: 391.1167.

4-Amino-5-(3,4-difluorophenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11706) FH11706 was prepared according to the general procedure for Suzuki coupling (reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11706** as a white solid (0.058 g, 0.15 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 44 %. Melting point: 130 °C / 210 °C. ^{1}H NMR (300 MHz, DMSO-d$_6$) δ: 3.53 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5''), 3.63 (ddd, *J* = 11.7, 5.1, 4.2 Hz, 1H, H-5'), 3.90 (q, *J* = 3.6 Hz, 1H, H-4'), 4.08 – 4.13 (m, 1H, H-3'), 4.44 (q, *J* = 5.7 Hz, 1H, H-2'), 5.11 (d, *J* = 4.8 Hz, 1H, OH-3'), 5.16 (dd, *J* = 6.0, 5.1 Hz, 1H, OH-5'), 5.31 (d, *J* = 6.3 Hz, 1H, OH-2'), 6.11 (d, *J* = 6.0 Hz, 1H, H-1'), 6.29 (br. s, 2H, NH_2), 7.25 – 7.30 (m, 1H, H$_{Phe}$), 7.44 – 7.57 (m, 2H, H$_{Phe}$), 7.59 (s,

1H, H-6), 8.15 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -138.27 - -138.12 (m, 1F), 142.00 – 141.86 (m, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.6 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.2 (C-4a), 114.5 (C-5), 117.3 – 117.9 (m, 2C, C_{Phe}), 121.7 (C-6), 125.13 (dd, *J* = 6.0, 3.8 Hz, 1C, C_{Phe}), 131.9 – 132.0 (m, 1C, C_{Phe}), 149.5 (dd, *J* = 246.8, 12.8 Hz, 1C, C_{Phe}), 148.7 (dd, *J* = 243.0, 12.8 Hz, 1C, C_{Phe}), 151.0 (C-7a), 151.8 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{17}H_{17}F_2N_4O_4$ ($[M+H]^+$): 379.1212, found: 379.1207.

4-Amino-5-(3-chloro-4-fluorophenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11707) FH11707 was prepared according to the general procedure for Suzuki coupling (reaction time: 0.5 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH11707** as a white solid (0.052 g, 0.13 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 38 %. Melting point: 135 °C / 172 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5''), 3.63 (ddd, *J* = 12.0, 4.8, 4.2 Hz, 1H, H-5'), 3.90 (q, *J* = 3.6 Hz, 1H, H-4'), 4.08 – 4.13 (m, 1H, H-3'), 4.44 (q, *J* = 6.0 Hz, 1H, H-2'), 5.11 (d, *J* = 4.5 Hz, 1H, OH-3'), 5.15 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.31 (d, *J* = 6.3 Hz, 1H, OH-2'), 6.11 (d, *J* = 6.3 Hz, 1H, H-1'), 6.29 (br. s, 2H, NH_2), 7.43 (ddd, *J* = 8.7, 5.1, 2.1 Hz, 1H, H-6_{Phe}), 7.48 (dd, *J* = 18.0, 8.7 Hz, 1H, H-5_{Phe}), 7.61 (s, 1H, H-6), 7.63 (dd, *J* = 7.2, 2.1 Hz, 1H, H-2_{Phe}), 8.15 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -119.76 – -119.83 (m, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.6 (C-5'), 70.5 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.2 (C-4a), 114.2 (C-5), 117.2 (d, *J* = 21.0 Hz, 1C, C-5_{Phe}), 119.7 (d, *J* = 18.8 Hz, 1C, C-3_{Phe}), 121.8 (C-6), 128.9 (d, *J* = 6.8 Hz, 1C, C-6_{Phe}), 130.2 (C-2_{Phe}), 132.2 (d, *J* = 3.8 Hz, 1C, C-1_{Phe}), 151.0 (C-7a), 156.4 (d, *J* = 245.3 Hz, 1C, C-4_{Phe}), 151.8 (C-2), 157.4 (C-4). HRMS (ESI): calculated for $C_{17}H_{17}ClFN_4O_4$ ($[M+H]^+$): 395.0917, found: 395.0930.

4-Amino-5-(3-fluoro-4-chlorophenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH10714) FH10714 was prepared according to the general procedure for Suzuki coupling

(reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH10714** as a white solid (0.055 g, 0.14 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 40 %. Melting point: 117 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (ddd, *J* = 12.0, 6.0, 4.2 Hz, 1H, H-5''), 3.60 – 3.67 (m, 1H, H-5'), 3.90 (q, *J* = 3.6 Hz, 1H, H-4'), 4.09 – 4.13 (m, 1H, H-3'), 4.41 – 4.47 (m, 1H, H-2'), 5.12 (d, *J* = 4.5 Hz, 1H, OH-3'), 5.16 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.32 (d, *J* = 6.0 Hz, 1H, OH-2'), 6.11 (d, *J* = 6.0 Hz, 1H, H-1'), 6.35 (br. s, 2H, NH_2), 7.31 (dd, *J* = 8.4, 1.5 Hz, 1H, H-6$_{Phe}$), 7.46 (dd, *J* = 10.5, 2.1 Hz, 1H, H-2$_{Phe}$), 7.65 (s, 1H, H-6), 7.63 – 7.69 (m, 1H, H-5$_{Phe}$), 8.16 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -115.89 - -115.96 (m, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.6 (C-5'), 70.5 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.1 (C-4a), 114.4 (d, *J* = 2.3 Hz, 1C, C-5), 116.5 (d, *J* = 21.8 Hz, 1C, C-2$_{Phe}$), 117.6 (d, *J* = 17.3 Hz, 1C, C-4$_{Phe}$), 122.1 (C-6), 125.5 (d, *J* = 3.8 Hz, 1C, C$_{Phe}$), 130.9 (C-6$_{Phe}$), 135.6 (d, *J* = 7.5 Hz, 1C, C$_{Phe}$), 151.1 (C-7a), 151.8 (C-2), 157.4 (C-4), 157.4 (d, *J* = 230.3 Hz, 1C, C-3$_{Phe}$). HRMS (ESI): calculated for $C_{17}H_{17}ClFN_4O_4$ ($[M+H]^+$): 395.0917, found: 395.0927.

4-Amino-5-(4-trifluoromethoxyphenyl)-N7-(β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH10715) FH10715 was prepared according to the general procedure for Suzuki coupling (reaction time: 1 h). **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH10715** as a white solid (0.054 g, 0.13 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 36 %. Melting point: 140 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (ddd, *J* = 12.0, 6.3, 3.9 Hz, 1H, H-5''), 3.63 (ddd, *J* = 12.0, 5.1, 4.2 Hz, 1H, H-5'), 3.91 (q, *J* = 3.6 Hz, 1H, H-4'), 4.08 – 4.13 (m, 1H, H-3'), 4.42 – 4.48 (m, 1H, H-2'), 5.11 (d, *J* = 4.5 Hz, 1H, OH-3'), 5.16 (dd, *J* = 6.0, 5.1 Hz, 1H, OH-5'), 5.32 (d, *J* = 6.3 Hz, 1H, OH-2'), 6.12 (d, *J* = 6.3 Hz, 1H, H-1'), 6.22 (br. s, 2H, NH_2), 7.45 – 7.48 (m, 2H, H$_{Phe}$), 7.56 – 7.60 (m, 2H, H$_{Phe}$), 7.60 (s, 1H, H-6), 8.16 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -56.72. ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.3 (C-4a),

115.0 (C-5), 120.2 (q, *J* = 255.7 Hz, 1C, CF_3), 121.5 (2C, C_{Phe}), 121.7 (C-6), 130.1 (2C, C_{Phe}), 133.8 (C-1_{Phe}), 147.2 (C-4_{Phe}), 151.0 (C-7a), 151.8 (C-2), 157.4 (C-4).HRMS (ESI): calculated for $C_{18}H_{18}F_3N_4O_5$ ($[M+H]^+$): 427.1224, found: 427.1232.

4-Amino-5-(phenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11708)[7] **FH11708** was prepared according to the general procedure for Suzuki coupling (reaction time: 10 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11708** as a white solid (0.084 g, 0.26 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 74 %. Melting point: 106 °C / 200 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.20 (ddd, *J* = 13.2, 6.0, 2.7 Hz, 1H, H-2''), 2.57 (ddd, *J* = 13.2, 8.1, 6.0 Hz, 1H, H-2'), 3.47 – 3.62 (m, 2H, H-5', H-5''), 3.82 – 3.86 (m, 1H, H-4'), 4.34 – 4.39 (m, 1H, H-3'), 5.05 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.26 (d, *J* = 3.9 Hz, 1H, OH-3'), 6.11 (br. s, 2H, NH_2), 6.59 (dd, *J* = 8.1, 6.3 Hz, 1H, H-1'), 7.34 – 7.41 (m, 1H, H_{Phe}), 7.48 – 7.49 (m, 4H, H_{Phe}), 7.53 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 39.7 (C-2'), 62.0 (C-5'), 71.1 (C-3'), 82.9 (C-1'), 87.4 (C-4'), 100.4 (C-4a), 116.4 (C-5), 120.7 (C-6), 126.9 (C-1_{Phe}), 128.5 (2 C_{Phe}), 129.0 (2 C_{Phe}), 134.5 (C-4_{Phe}), 150.4 (C-7a), 151.7 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{17}H_{19}N_4O_3$ ($[M+H]^+$): 327.1452, found: 327.1445. Spectral data are in accordance with literature values.[7]

4-Amino-5-(4-methylphenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11709) FH11709 was prepared according to the general procedure for Suzuki coupling (reaction time: 5 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11709** as a white solid (0.092 g, 0.27 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 78 %. Melting point: 112 °C / 205 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.19 (ddd, *J* = 13.2, 6.3, 2.7 Hz, 1H, H-2''), 2.36 (s, 3H, CH_3), 2.57 (ddd, *J* = 13.2, 8.1, 5.4 Hz, 1H, H-2'), 3.47 – 3.61 (m, 2H, H-5'', H-5'), 3.81 – 3.85 (m, 1H, H-4'), 4.32 – 4.39 (m, 1H, H-3'), 5.05 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.26 (d, *J* = 3.6 Hz, 1H, OH-3'), 6.09 (br. s, 2H, NH_2), 6.58 (dd, *J* = 8.4, 6.3 Hz, 1H, H-1'), 7.28 – 7.30 (m, 2H, H_{Phe}), 7.35 – 7.38 (m, 2H, H_{Phe}), 7.47 (s, 1H, H-6), 8.14

(s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 20.7 (CH_3), 39.7 (C-2'), 62.0 (C-5'), 71.1 (C-3'), 82.9 (C-1'), 87.3 (C-4'), 100.4 (C-4a), 116.3 (C-5), 120.3 (C-6), 128.4 ($2C_{Phe}$), 129.5 ($2C_{Phe}$), 131.5 (C_{Phe}), 136.1 (C_{Phe}), 150.4 (C-7a), 151.6 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{21}N_4O_3$ ($[M+H]^+$): 341.1608, found: 341.1609.

4-Amino-5-(4-methoxyphenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11710) FH11710 was prepared according to the general procedure for Suzuki coupling (reaction time: 5 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11710** as a white solid (0.089 g, 0.25 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 72 %. Melting point: 96 °C / 165 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.19 (ddd, *J* = 13.2, 6.0, 2.4 Hz, 1H, H-2''), 2.56 (ddd, *J* = 13.2, 8.4, 5.7 Hz, 1H, H-2'), 3.47 – 3.61 (m, 2H, H-5', H-5''), 3.80 (s, 3H, OCH_3), 3.82 – 3.85 (m, 1H, H-4'), 4.33 – 4.38 (m, 1H, H-3'), 5.05 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.25 (d, *J* = 4.2 Hz, 1H, OH-2'), 6.08 (br. s, 2H, NH_2), 6.58 (dd, *J* = 8.4, 6.0 Hz, 1H, H-1'), 7.03 – 7.07 (m, 2H, H_{Phe}), 7.36 – 7.41 (m, 2H, H_{Phe}), 7.43 (s, 1H, H-6), 8.13 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 39.7 (C-2'), 55.2 (OCH_3), 62.0 (C-5'), 71.1 (C-3'), 82.9 (C-1'), 87.3 (C-4'), 100.6 (C-4a), 114.4 (C-5), 116.0 (C-6), 120.1 ($2C_{Phe}$), 126.6 (CPhe), 129.7 ($2C_{Phe}$), 150.2 (C-7a), 151.6 (C-2), 157.3 (C-4), 158.4 ($C\text{-}4_{Phe}$). HRMS (ESI): calculated for $C_{17}H_{19}N_4O_3$ ($[M+H]^+$): 357.1557, found: 357.1537.

4-Amino-5-(4-chlorophenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11711) FH11711 was prepared according to the general procedure for Suzuki coupling (reaction time: 5 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11711** as a white solid (0.10 g, 0.28 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 80 %. Melting point: 120 °C / 220 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.20 (ddd, *J* = 13.2, 6.0, 2.7 Hz, 1H, H-2''), 2.56 (ddd, *J* = 13.2, 8.1, 5.7 Hz, 1H, H-5'), 3.47 – 3.62 (m, 2H, H-5', H-5''), 3.82 – 3.85 (m, 1H, H-4'), 4.34 – 4.39 (m, 1H, H-3'), 5.04 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.26 (d, *J* = 4.2 Hz, 1H, OH-3'), 6.20 (br. s, 1H, NH_2), 6.59 (dd, *J* = 8.1, 6.0 Hz, 1H, H-1'),

7.46 – 7.54 (m, 4H, H_{Phe}), 7.56 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 39.7 (C-2'), 62.0 (C-5'), 71.0 (C-3'), 82.9 (C-1'), 87.4 (C-4'), 100.2 (C-4a), 115.2 (C-5), 121.0 (C-6), 128.8 ($2C_{Phe}$), 130.1 ($2C_{Phe}$), 131.5 (C_{Phe}), 133.3 (C_{Phe}), 150.6 (C-7a), 151.8 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{17}H_{19}N_4O_3$ ($[M+H]^+$): 361.1062, found: 361.1078.

4-Amino-5-(4-fluorophenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11712) FH11712 was prepared according to the general procedure for Suzuki coupling (reaction time: 5 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11712** as a white solid (0.096 g, 0.28 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 81 %. Melting point: 115 °C / 215 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.19 (ddd, *J* = 13.2, 6.3, 2.7 Hz, 1H, H-2''), 2.56 (ddd, *J* = 13.2, 8.4, 6.0 Hz, 1H, H-2'), 3.47 – 3.62 (m, 2H, H-5', H-5''), 3.81 – 3.85 (m, 1H, H-4'), 4.33 – 4.38 (m, 1H, H-3'), 5.02 (dd, *J* = 6.0, 5.1 Hz, 1H, OH-5'), 5.26 (d, *J* = 4.2 Hz, 1H, OH-3'), 6.14 (br. s, 2H, NH_2), 6.58 (dd, *J* = 8.4, 6.0 Hz, 1H, H-1'), 7.27 – 7.34 (m, 2H, H_{Phe}), 7.46 – 7.51 (m, 2H, H_{Phe}), 7.51 (s, 1H, H-6), 8.14 (s, 1H, H-2). ^{19}F-NMR (282 MHz, DMSO-d_6) δ: -116.08 - -115.98 (m, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 39.7 (C-2'), 62.0 (C-5'), 71.0 (C-3'), 82.9 (C-1'), 87.4 (C-2'), 100.4 (C-4a), 115.3 (C-5), 115.7 (d, *J* = 21.8 Hz, 2C, C-3 & $C\text{-}5_{Phe}$), 120.7 (C-6), 130.4 (d, *J* = 7.5 Hz, 2C, C-2 & $C\text{-}6_{Phe}$), 130.8 (d, *J* = 3.0 Hz, 1C, C_{Phe}), 150.4 (C-7a), 151.7 (C-2), 157.3 (C-4), 161.4 (d, *J* = 241.5 Hz, 1C, $C\text{-}4_{Phe}$). HRMS (ESI): calculated for $C_{17}H_{17}FN_4O_3$ ($[M+H]^+$): 345.1357, found: 345.1352.

4-Amino-5-(3,4-dichlorophenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH11713) FH11713 was prepared according to the general procedure for Suzuki coupling (reaction time: 10 min). **FH10678** (0.13 g, 0.35 mmol) gave rise to **FH11713** as a white solid (0.10 g, 0.35 mmol). Column chromatography: 1 → 9 % MeOH/DCM. Yield = 75 %. Melting point: 135 °C / 185 °C. ^{1}H NMR (300 MHz, DMSO-d_6)

δ: 2.20 (ddd, *J* = 13.2, 6.0, 3.0 Hz, 1H, H-2''), 2.56 (ddd, *J* = 13.2, 8.1, 5.7 Hz, 1H, H-2'), 3.47 – 3.62 (m, 2H, H-5', H-5''), 3.81 – 3.85 (m, 1H, H-4'), 4.34 – 4.39 (m, 1H, H-3'), 5.03 (t, *J* = 5.7 Hz, 1H, OH-5'), 5.26 (d, *J* = 4.2 Hz, 1H, OH-3'), 6.30 (br. s, 2H, NH_2), 6.58 (dd, *J* = 8.1, 6.0 Hz, 1H, H-1'), 7.43 (dd, *J* = 8.1, 2.1 Hz, 1H, H-6_{Phe}), 7.65 (s, 1H, H-6), 7.70 (d, *J* = 8.4 Hz, 1H, H-5_{Phe}), 7.70 (d, *J* = 2.1 Hz, 1H, H-2_{Phe}), 8.16 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 39.6 (C-2'), 61.9 (C-5'), 71.0 (C-3'), 82.9 (C-1'), 87.4 (C-4'), 99.9 (C-4a), 114.2 (C-5), 121.7 (C-6), 128.5 (C_{Phe}), 129.1 (C_{Phe}), 130.0 (C_{Phe}), 130.8 (C_{Phe}), 131.3 (C_{Phe}), 135.1 (C_{Phe}), 150.8 (C-7a), 151.9 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{17}H_{17}Cl_2N_4O_3$ ($[M+H]^+$): 395.0672, found: 395.0680.

4-Amino-5-(3-methylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13817) Compound **FH13817** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH13817** (0.087 g, 0.24 mmol) as a tan solid in 67 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 170 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.38 (s, 3H, CH_3), 3.53 (dd, *J* = 12.0, 4.1 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.11 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.6 Hz, 1H, H-2'), 5.19 (br. s, 3H, OH-2', OH-3', OH-5'), 6.12 (br. s, 2H, NH_2), 6.12 (d, *J* = 6.2 Hz, 1H, H-1'), 7.18 – 7.20 (m, 1H, H_{Phe}), 7.25 – 7.20 (m, 2H, H_{Phe}), 7.35 – 7.40 (m, 1H, H_{Phe}), 7.52 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 21.1 (CH_3), 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.5 (C-4a), 116.4 (C-5), 121.0 (C-6), 125.5 (C_{Phe}), 127.6 (C_{Phe}), 128.9 (C_{Phe}), 129.1 (C_{Phe}), 134.4 (C_{Phe}), 138.2 (C_{Phe}), 150.8 (C-7a), 151.7 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{21}N_4O_4$ ($[M+H]^+$): 357.1557, found: 357.1561.

4-Amino-5-(3,4-dimethylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13820)[8] Compound **FH13820** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH13820** (0.083 g, 0.23 mmol) as

a tan solid in 64 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.27 (s, 3H, CH_3), 2.28 (s, 3H, CH_3), 3.52 (d, *J* = 12.0, 4.1 Hz, 1H, H-5''), 3.63 (dd, *J* = 11.7, 3.5 Hz, 1H, H-5'), 3.88 (q, *J* = 3.5 Hz, 1H, H-4'), 4.08 (dd, *J* = 5.3, 3.5 Hz, 1H, H-3'), 4.43 (t, *J* = 5.6 Hz, 1H, H-2'), 5.39 (br. s, 5H, NH_2, OH-2', OH-3', OH-5'), 6.09 (d, *J* = 6.2 Hz, 1H, H-1'), 7.16 – 7.19 (m, 1H, H_{Phe}), 7.23 – 7.26 (m, 2H, H_{Phe}), 7.45 (s, 1H, H-6), 8.13 (s, 1H, H-2). Spectral data are in accordance with literature values.[8]

4-Amino-5-(2-methylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13821) Compound **FH13821** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.12 g, 0.35 mmol) gave rise to **FH13821** (0.084 g, 0.24 mmol) as a tan solid in 67 % yield. Purification: RP column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 200 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.21 (s, 3H, CH_3), 3.53 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.90 (q, *J* = 3.5 Hz, 1H, H-4'), 4.10 (dd, *J* = 4.8, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.3 Hz, 1H, H-2'), 5.33 (br. s, 5H, NH_2, OH-2', OH-3', OH-5'), 6.09 (d, *J* = 6.2 Hz, 1H, H-1'), 7.27 – 7.38 (m, 4H, H_{Phe}), 7.42 (s, 1H, H-6), 8.13 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 20.0 (CH_3), 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.4 (C-1'), 101.9 (C-4a), 114.3 (C-5), 121.0 (C-6), 126.0 (C_{Phe}), 127.8 (C_{Phe}), 130.3 (C_{Phe}), 130.6 (C_{Phe}), 133.6 (C_{Phe}), 136.7 (C_{Phe}), 150.1 (C-7a), 151.7 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{21}N_4O_4$ ($[M+H]^+$): 357.1557, found: 357.1551.

4-Amino-5-(3-chloro-4-methylphenyl)-N7-(2'-deoxy-β-D-ribofuranosyl)-pyrrolo[2,3-*d*]pyrimidine (FH13822) Compound **FH13822** was prepared according to the general procedure for Suzuki coupling. **FH10678** (0.15 g, 0.40 mmol) gave rise to **FH13822** (0.035 g, 0.092 mmol) as a tan solid in 23 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 188-191 °C. ^{1}H NMR

(300 MHz, DMSO-d_6) δ: 2.18 (ddd, *J* = 13.2, 6.2, 2.6 Hz, 1H, H-2''), 2.37 (s, 3H, CH_3), 2.52 – 2.61 (m, 1H, H-2'), 3.50 (dd, *J* = 11.7, 4.4 Hz, 1H, H-5''), 3.58 (dd, *J* = 11.7, 4.6 Hz, 1H, H-5'), 3.81 – 3.85 (m, 1H, H-4'), 4.34 – 4.38 (m, 1H, H-3'), 5.68 (br. s, 4H, NH_2, OH-3', OH-5'), 6.56 (dd, *J* = 8.2, 6.2 Hz, 1H, H-1'), 7.35 (dd, *J* = 7.6, 1.8 Hz, 1H, H-6_{Phe}), 7.43 (d, *J* = 7.9 Hz, 1H, H-5_{Phe}), 7.55 (s, 2H, H-6, H-2_{Phe}), 8.11 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 19.3 (CH_3), 40.1 (C-2'), 61.9 (C-5'), 71.0 (C-3'), 83.0 (C-1'), 87.3 (C-4'), 100.2 (C-4a), 115.0 (C-5), 120.9 (C-6), 127.0 (C-6_{Phe}), 128.4 (C-1_{Phe}), 131.5 (C-5_{Phe}), 133.5 (C_{Phe}), 133.6 (C_{Phe}), 134.1 (C_{Phe}), 150.5 (C-7a), 151.7 (C-2), 157.5 (C-4). HRMS (ESI): calculated for $C_{18}H_{20}ClN_4O_3$ ($[M+H]^+$): 375.1218, found: 375.1204.

4-Amino-5-(2-fluoro-4-chlorophenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13823) Compound **FH13823** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13823** (0.083 g, 0.21 mmol) as a tan solid in 70 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 168-170 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.63 (dd, *J* = 12.0, 3.5 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.09 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.6 Hz, 1H, H-2'), 5.20 (br. s, 5H, NH_2, OH-2', OH-3', OH-5'), 6.11 (d, *J* = 6.2 Hz, 1H, H-1'), 6.22 (br. s, 2H, NH_2), 7.38 (dd, *J* = 8.5, 2.1 Hz, 1H, H-5_{Phe}), 7.43 (t, *J* = 8.2 Hz, 1H, H-6_{Phe}), 7.54 (dd, *J* = 10.3, 2.1 Hz, 1H, H-3_{Phe}), 7.58 (s, 1H, H-6), 8.14 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -112.7 (dd, *J* = 9.6, 7.2 Hz, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.2 (C-4'), 87.2 (C-1'), 101.2 (C-4a), 107.1 (C-5), 116.7 (d, *J* = 26.5 Hz, 1C, C-3_{Phe}), 121.0 (d, *J* = 15.0 Hz, 1C, C-1_{Phe}), 122.6 (d, *J* = 2.3 Hz, 1C, C-6), 125.0 (d, *J* = 3.5 Hz, 1C, C-5_{Phe}), 132.5 (d, *J* = 10.4 Hz, 1C, C-4_{Phe}), 132.9 (d, *J* = 3.5 Hz, 1C, C-6_{Phe}), 150.7 (C-7a), 151.8 (C-2), 157.4 (C-4), 159.4 (d, *J* = 247.6 Hz, 1C, C-F). HRMS (ESI): calculated for $C_{17}H_{17}ClFN_4O_4$ ($[M+H]^+$): 395.0917, found: 395.0923.

4-Amino-5-(2-fluoro-4-methylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13824) Compound **FH13824** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13824** (0,075 g, 0.200 mmol) as a tan solid in 67 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 138-140 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.38 (s, 3H, CH_3), 3.53 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.63 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.09 (dd, *J* = 5.3, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.3 Hz, 1H, H-2'), 5.19 (br. s, 3H, OH-2', OH-3', OH-5'), 6.03 (br. s, 2H, NH_2), 6.10 (d, *J* = 6.4 Hz, 1H, H-1'), 7.11 – 7.15 (m, 1H, H-5$_{Phe}$), 7.18 (d, *J* = 10.8 Hz, 1H, H-3$_{Phe}$), 7.31 (t, *J* = 7.9 Hz, 1H, H-6$_{Phe}$), 7.52 (s, 1H, H-6), 8.14 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -116.3 (dd, *J* = 10.8, 8.5 Hz, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 20.6 (CH3), 61.7 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.2 (C-1'), 101.5 (C-4a), 108.5 (C-5), 122.1 (C-6), 116.5 (d, *J* = 21.9 Hz, 1C, C-3$_{Phe}$), 118.7 (d, *J* = 15.0 Hz, 1C, C-1$_{Phe}$), 125.5 (d, *J* = 2.3 Hz, 1C, C-5$_{Phe}$), 131.5 (d, *J* = 2.3 Hz, 1C, C-6$_{Phe}$), 139.6 (d, *J* = 8.1 Hz, 1C, C-4$_{Phe}$), 150.5 (C-7a), 151.7 (C-2), 157.3 (C-4), 159.2 (d, *J* = 244.2 Hz, 1C, C-2$_{Phe}$). HRMS (ESI): calculated for $C_{18}H_{20}FN_4O_4$ ($[M+H]^+$): 375.1463, found: 375.1466.

4-Amino-5-(3-chloro-4-trifluoromethylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13825) Compound **FH13825** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13825** (0.080 g, 0,18 mmol) as a tan solid in 60 % yield. Purification: RP column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 152-154 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.54 (dd, *J* = 12.0, 4.1 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.12 (dd, *J* = 5.0, 3.5 Hz, 1H, H-3'), 4.45 (t, *J* = 5.6 Hz, 1H, H-2'), 5.15 (br. s, 3H, OH-2', OH-3', OH-5'), 6.13 (d, *J* = 6.2 Hz, 1H, H-1'), 6.45 (br. s, 2H, NH_2), 7.57 – 7.60 (m, 1H, H-6$_{Phe}$), 7.78 (s, 1H, H-2$_{Phe}$), 7.79 (s, 1H, H-6), 7.91 (d, *J* = 8.5 Hz,

1H, H-5$_{Phe}$), 8.18 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -60.6. ^{13}C NMR (75 MHz, DMSO-d$_6$) δ: 61.6 (C-5'), 70.5 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 99.9 (C-4a), 113.9 (C-5), 123.1 (C-6), 123.2 (q, *J* = 273.0 Hz, 1C, CF_3), 124.1 (q, *J* = 31.1 Hz, 1C, C-4$_{Phe}$), 127.0 (C-6$_{Phe}$), 128.2 (q, *J* = 4.6 Hz, 1C, C-5$_{Phe}$), 130.5 (C-2$_{Phe}$), 131.0 (C-3$_{Phe}$), 140.4 (C-1$_{Phe}$), 151.1 (C-7a), 152.0 (C-2), 157.5 (C-4). HRMS (ESI): calculated for $C_{18}H_{17}ClF_3N_4O_4$ ([M+H]$^+$): 445.0885, found: 445.0889.

4-Amino-5-(3-fluorophenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13826) Compound **FH13826** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13826** 0.068 g, 0.19 mmol) as a tan solid in 63 % yield. Purification: RP column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 128 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.91 (q, *J* = 3.8 Hz, 1H, H-4'), 4.11 (dd, *J* = 4.7, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.3 Hz, 1H, H-2'), 5.21 (br. s, 3H, OH-2', OH-3', OH-5'), 6.12 (d, *J* = 6.2 Hz, 1H, H-1'), 6.24 (br. s, 2H, NH_2), 7.15 – 7.22 (m, 1H, H$_{Phe}$), 7.26 – 7.32 (m, 2H, H$_{Phe}$), 7.48 – 7.56 (m, 1H, H$_{Phe}$), 7.63 (s, 1H, H-6), 8.16 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -112.7 - -112.6 (m, 1F). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ: 61.6 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.2 (C-4a), 113.5 (d, *J* = 20.7 Hz, 1C, C$_{Phe}$), 114.9 (C-4a), 115.2 (d, *J* = 2.3 Hz, 1C, C$_{Phe}$), 121.8 (C-6), 124.4 (d, *J* = 2.3 Hz, 1C, C$_{Phe}$), 130.9 (d, *J* = 9.2 Hz, 1C, C$_{Phe}$), 136.8 (d, *J* = 8.1 Hz, 1C, C-1$_{Phe}$), 151.0 (C-7a), 151.8 (C-2), 157.3 (C-4), 162.2 (d, *J* = 243.0 Hz, 1C, C-F). HRMS (ESI): calculated for $C_{17}H_{18}FN_4O_4$ ([M+H]$^+$): 361.1307, found: 361.1302.

4-Amino-5-(3-trifluoromethyl-4-chlorophenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13827) Compound **FH13827** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13827** (0.052 g, 0.12 mmol) as a tan solid in 39 % yield. Purification: RP column, 2.5 min 0 % MeCN/water;

then: in 14.5 min to 70 % MeCN/water. Melting point: 180 – 182 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (dd, *J* = 12.0, 4.1 Hz, 1H, H-5’’), 3.64 (dd, *J* = 12.0, 4.1 Hz, 1H, H-5’), 3.90 (q, *J* = 3.8 Hz, 1H, H-4’), 4.11 (dd, *J* = 5.0, 3.5 Hz, 1H, H-3’), 4.46 (t, *J* = Hz, 1H, H-2’), 5.21 (br. s, 3H, OH-2’, OH-3’, OH-5’), 6.13 (d, *J* = 6.2 Hz, 1H, H-1’), 6.40 (br. s, 2H, NH_2), 7.73 (s, 1H, H-6), 7.73 (dd, *J* = 8.2, 2.0 Hz, 1H, H-6$_{Phe}$), 7.79 (d, *J* = 8.2 Hz, 1H, H-5$_{Phe}$), 7.86 (d, *J* = 1.8 Hz, 1H, H-1), 8.17 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -61.2. ^{13}C NMR (75 MHz, DMSO-d$_6$) δ: 61.6 (C-5’), 70.5 (C-3’), 73.7 (C-2’), 85.1 (C-4’), 87.0 (C-1’), 100.0 (C-4a), 114.1 (C-5), 122.4 (C-6), 122.9 (q, *J* = 273.0 Hz, 1C, CF_3), 126.8 (q, *J* = 31.1 Hz, 1C, C-4$_{Phe}$), 127.2 (q, *J* = 4.6 Hz, 1C, C-5$_{Phe}$), 131.9 (C$_{Phe}$), 133.5 (C$_{Phe}$), 134.0 (C-1$_{Phe}$), 151.3 (C-7a), 151.9 (C-2), 157.5 (C-4). One carbon (C-3$_{Phe}$) could not be detected. HRMS (ESI): calculated for $C_{18}H_{17}ClF_3N_4O_4$ ([M+H]$^+$): 445.0885, found: 445.0889.

4-Amino-5-(4-cyanophenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13828)

Compound **FH13828** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13828** (0.072 g, 0.20 mmol) as a tan solid in 65 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 235 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.54 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5’’), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5’), 3.91 (q, *J* = 3.5 Hz, 1H, H-4’), 4.12 (dd, *J* = 4.7, 3.5 Hz, 1H, H-3’), 4.45 (t, *J* = 5.6 Hz, 1H, H-2’), 5.21 (br. s, 3H, OH-2’, OH-3’, OH-5’), 6.13 (d, *J* = 6.2 Hz, 1H, H-1’), 6.34 (br. s, 2H, NH_2), 7.64 – 7.66 (m, 2H, H$_{Phe}$), 7.73 (s, 1H, H-6), 7.90 – 7.93 (m, 2H, H$_{Phe}$), 8.18 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d$_6$) δ: 61.6 (C-5’), 70.5 (C-3’), 73.8 (C-2’), 85.2 (C-4’), 87.1 (C-1’), 100.0 (C-4a), 108.8 (C-1$_{Phe}$), 115.1 (C-5), 119.1 (CN), 122.7 (C-6), 128.9 (2C$_{Phe}$), 132.7 (2C$_{Phe}$), 139.4 (C-4$_{Phe}$), 151.4 (C-7a), 151.9 (C-2), 157.4 (C-4). HRMS (ESI): calculated for $C_{18}H_{18}N_5O_4$ ([M+H]$^+$): 368.1353, found: 368.1355.

4-Amino-5-(3-fluoro-4-methylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13829) Compound **FH13829** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13829** (0.075 g, 0.20 mmol) as a tan solid in 67 % yield. Purification: RP column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 138 – 141 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.28 (d, *J* = 1.5 Hz, 3H, CH_3), 3.53 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.90 (q, *J* = 3.5 Hz, 1H, H-4'), 4.11 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.45 (t, *J* = 5.9 Hz, 1H, H-2'), 5.20 (br. s, 3H, OH-2', OH-3', OH-5'), 6.11 (d, *J* = 6.2 Hz, 1H, H-1'), 6.20 (br. s, 2H, NH_2), 7.18 – 7.24 (m, 2H, H_{Phe}), 7.38 (t, *J* = 8.2 Hz, 1H, H-1_{Phe}), 7.57 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{19}F NMR (282 MHz, DMSO-d_6) δ: -117.0 (dd, *J* = 8.4, 2.4 Hz, 1F). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 13.9 (CH_3), 61.6 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.0 (C-1'), 100.3 (C-4a), 114.8 (d, *J* = 21.9 Hz, 1C, C-2_{Phe}), 115.2 (d, *J* = 2.3 Hz, 1C, C-6_{Phe}), 121.4 (C-6), 122.5 (d, *J* = 17.3 Hz, 1C, C-4_{Phe}), 124.1 (d, *J* = 3.5 Hz, 1C, C-5_{Phe}), 132.0 (d, *J* = 5.8 Hz, 1C, C-5_{Phe}), 134.1 (d, *J* = 7.9 Hz, 1C, C-1_{Phe}), 150.9 (C-7a), 151.7 (C-2), 157.3 (C-4), 160.8 (d, *J* = 243.0 Hz, 1C, C-3_{Phe}). HRMS (ESI): calculated for $C_{18}H_{20}FN_4O_4$ ($[M+H]^+$): 375.1463, found: 375.1425.

4-Amino-5-(3-chloro-5-methylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13830) Compound **FH13830** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13830** (0.069 g, 0.18 mmol) as a tan solid in 59 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 209 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 2.37 (s, 3H, CH_3), 3.53 (dd, *J* = 12.0, 4.1 Hz, 1H, H-5''), 3.64 (dd, *J* = 11.7, 3.8 Hz, 1H, H-5'), 3.90 (q, *J* = 3.8 Hz, 1H, H-4'), 4.11 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.44 (t, *J* = 5.6 Hz, 1H, H-2'), 5.21 (br. s, 3H, OH-2', OH-3', OH-5'), 6.13 (d, *J* = 6.2 Hz, 1H, H-1'), 6.23 (br. s, 2H, NH_2), 7.25 – 7.31 (m, 3H, H_{Phe}), 7.61 (s, 1H, H-6), 8.15 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-

d_6) δ: 20.8 (CH3), 61.6 (C-5'), 70.5 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 86.9 (C-1'), 100.2 (C-4a), 115.1 (C-5), 121.7 (C-6), 125.0 (C_{Phe}), 127.0 (C_{Phe}), 127.7 (C_{Phe}), 133.2 (C_{Phe}), 136.2 (C_{Phe}), 140.5 (C_{Phe}), 151.0 (C-7a), 151.8 (C-2), 157.3 (C-4). HRMS (ESI): calculated for $C_{18}H_{20}ClN_4O_4$ ($[M+H]^+$): 391.1168, found: 391.1163.

4-Amino-5-(4-carboxamido-phenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13832) Compound **FH13832** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13832** (0.074 g, 0.19 mmol) as a tan solid in 64 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 188 – 191 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.54 (dd, *J* = 11.4, 3.2 Hz, 1H, H-5''), 3.65 (dd, *J* = 11.7, 3.5 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.12 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.46 (t, *J* = 5.6 Hz, 1H, H-2'), 5.18 (br. s, 3H, OH-2', OH-3', OH-5'), 6.13 (d, *J* = 6.2 Hz, 1H, H-1'), 6.23 (br. s, 2H, NH_2), 7.37 (br. s, 1H, NH_2), 7.53 – 7.56 (m, 2H, H_{Phe}), 7.64 (s, 1H, H-6), 7.97 – 8.00 (m, 2H, H_{Phe}), 8.01 (br. s, 1H, NH_2), 8.17 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.6 (C-5'), 70.6 (C-3'), 73.8 (C-2'), 85.1 (C-4'), 87.1 (C-1'), 100.3 (C-4a), 115.7 (C-5), 121.8 (C-6), 128.0 ($2C_{Phe}$), 128.2 ($2C_{Phe}$), 132.3 (C_{Phe}), 137.3 (C_{Phe}), 151.1 (C-7a), 151.8 (C-2), 157.4 (C-4), 167.6 (C=O). HRMS (ESI): calculated for $C_{18}H_{20}N_5O_5$ ($[M+H]^+$): 386.1459, found: 386.1465.

4-Amino-5-(4-hydroxyphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13833) Compound **FH13833** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.104 g, 0.300 mmol) gave rise to **FH13833** (0.10 g, 0.29 mmol) as a tan solid in 97 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 170-173 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.52 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5''), 3.62 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.90 (q, *J* = 3.5 Hz, 1H, H-4'), 4.09 (dd, *J* = 5.0, 3.2 Hz, 1H, H-3'), 4.44 (t, *J* = 5.6 Hz, 1H, H-2'), 6.09 (d, *J* = 6.2 Hz, 1H, H-1'), 6.09 (br. s, 5H, NH_2, OH-2', OH-3', OH-5'), 6.76 – 6.81 (m, 2H, H_{Phe}),

7.16 – 7.20 (m, 2H, H_{Phe}), 7.34 (s, 1H, H-6), 8.10 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.8 (C-5'), 70.7 (C-3'), 73.7 (C-2'), 85.0 (C-4'), 87.0 (C-1'), 100.9 (C-4a), 116.4 ($2C_{Phe}$), 116.8 (C_{Phe}), 119.9 (C-6), 129.6 ($2C_{Phe}$), 150.4 (C-7a), 151.5 (C-2), 157.3 (C-4). $1C_{Phe}$ could not be observed. HRMS (ESI): calculated for $C_{17}H_{19}N_4O_5$ ($[M+H]^+$): 359.1350, found: 359.1360.

4-Amino-5-(4-methylsulfonylphenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13834) Compound **FH13834** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13834** (0.10 g, 0.24 mmol) as a tan solid in 79 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 215 °C (decomposed). ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.24 (s, 3H, CH_3), 3.54 (dd, J = 12.0, 3.8 Hz, 1H, H-5''), 3.64 (dd, *J* = 12.0, 3.5 Hz, 1H, H-5'), 3.92 (q, *J* = 3.2 Hz, 1H, H-4'), 4.12 (dd, *J* = 4.7, 3.5 Hz, 1H, H-3'), 4.46 (t, *J* = 5.6 Hz, 1H, H-2'), 5.21 (br. s, 3H, OH-2', OH-3', OH-5'), 6.14 (d, *J* = 5.9 Hz, 1H, H-1'), 6.35 (br. s, 2H, NH_2), 7.70 – 7.73 (m, 2H, H_{Phe}), 7.73 (s, 1H, H-6), 7.98 – 8.01 (m, 2H, H_{Phe}), 8.18 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 43.7 (CH3), 61.6 (C-5'), 70.6 (C-3'), 73.9 (C-2'), 85.2 (C-4'), 87.1 (C-1'), 100.0 (C-4a), 115.0 (C-5), 122.6 (C-6), 127.6 ($2C_{Phe}$), 128.8 ($2C_{Phe}$), 138.5 (C_{Phe}), 139.7 (C_{Phe}), 151.4 (C-7a), 151.9 (C-2), 157.4 (C-4). HRMS (ESI): calculated for $C_{18}H_{21}N_4O_6S$ ($[M+H]^+$): 421.1176, found: 421.1171.

4-Amino-5-(2-chlorophenyl)-N7-β-D-ribofuranosyl-pyrrolo[2,3-*d*]pyrimidine (FH13835) Compound **FH13835** was prepared according to the general procedure for Suzuki coupling. **TH1003** (0.10 g, 0.30 mmol) gave rise to **FH13835** (0.069 g, 0.18 mmol) as a tan solid in 61 % yield. Purification: RP (C18) column, 2.5 min 0 % MeCN/water; then: in 14.5 min to 70 % MeCN/water. Melting point: 140 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ: 3.53 (dd, J = 12.0, 3.8 Hz, 1H, H-5''), 3.63 (dd, *J* = 12.0, 3.8 Hz, 1H, H-5'), 3.91 (q, *J* = 3.5 Hz, 1H, H-4'), 4.10 (dd, *J* = 4.7, 3.2 Hz, 1H, H-3'), 4.46 (t, *J* = 5.6 Hz, 1H, H-2'), 5.22 (br. s, 3H, OH-2', OH-3',

OH-5'), 5.91 (br. s, 2H, NH_2), 6.10 (d, *J* = 6.2 Hz, 1H, H-1'), 7.42 – 7.46 (m, 3H, H_{Phe}), 7.53 (s, 1H, H-6), 7.59 – 7.63 (m, 1H, H_{Phe}), 8.14 (s, 1H, H-2). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 61.7 (C-5'), 70.6 (C-3'), 73.9 (C-2'), 85.1 (C-4'), 87.4 (C-1'), 101.8 (C-4a), 112.4 (C-5), 122.1 (C-6), 127.4 (C_{Phe}), 129.5 (C_{Phe}), 129.8 (C_{Phe}), 132.5 (C_{Phe}), 132.9 (C_{Phe}), 133.1 (C_{Phe}), 150.2 (C-7a), 151.7 (C-2), 157.2 (C-4). HRMS (ESI): calculated for $C_{17}H_{18}ClN_4O_4$ ($[M+H]^+$): 377.1011, found: 377.1011.

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