


BIOPRINT® PROFILE

FULL PROFILE

 Ref. **P22**

BIOPRINT® IN VITRO PHARMACOLOGY PROFILE

 Ref. **P22-p**

Suggested testing: 10 µM (n=2)

 3 weeks

The **BioPrint® profile** includes the assays used to explore the properties of about 2,450 BioPrint® compounds, establishing individual Pharma-ADME fingerprints for each compound.






The BioPrint® profile is mainly based on target diversity and includes today 105 binding assays (GPCRs, nuclear and other receptors, ion channels and transporters), 33 enzyme assays (including 10 kinases, 9 proteases and 5 PDEs), as well as 19 ADME-Tox assays (Solubility, Absorption, Metabolism and CYP-mediated drug-drug interaction). More than 70% are human targets.

The 157 assays of this profile represent a rationalized panel from a larger assay collection in the database, selected for highest information content.

→ **BioPrint® services – Drug profile interpretation & Target profile design** – are now part of our custom offer. For further information, please contact us at customresearch@cerep.com.

GPCRs

Family	Assay	Ref.
ADENOSINE	 A ₁ - agonist radioligand	 0442
	A _{2A} - agonist radioligand	 0004
	A _{2B} - antagonist radioligand	 0005
	A ₃ - agonist radioligand	 0006
ADRENERGIC	alpha _{1A} - antagonist radioligand	 2338
	alpha _{1B} - antagonist radioligand	 1633
	alpha _{2A} - antagonist radioligand	 0013
	alpha _{2B} - antagonist radioligand	 1344
	alpha _{2C} - antagonist radioligand	 0016
	beta ₁ - agonist radioligand	 0018
	beta ₂ - agonist radioligand	 0020
ANGIOTENSIN-II	beta ₃ - antagonist radioligand	 0227
	AT ₁ - antagonist radioligand	 0024
	AT ₂ - agonist radioligand	 0026
APELIN	APJ (apelin) - agonist radioligand	 2154
BOMBESIN	BB ₃ - agonist radioligand	 0472
BRADYKININ	B ₂ - agonist radioligand	 0033
CANNABINOID	CB ₁ - agonist radioligand	 0036
	CB ₂ - agonist radioligand	 0037
CHEMOKINES	CCR2 - agonist radioligand	 0362
	CXCR4 - agonist radioligand	 1022
CHOLECYSTOKININ	CCK ₁ (CCK _A) - agonist radioligand	 0039
	CCK ₂ (CCK _B) - agonist radioligand	 0041
CORTICOTROPIN RELEASING FACTOR	CRF1 - agonist radioligand	 1467
DOPAMINE	D ₁ - antagonist radioligand	 0044
	D _{2S} - agonist radioligand	 1322
	D ₃ - antagonist radioligand	 0048
ENDOTHELIN	ET _A - agonist radioligand	 0054
	ET _B - agonist radioligand	 0056
GABA	GABA _{B(1b)} - antagonist radioligand	 0885
GLUCAGON	glucagon - agonist radioligand	 1407
HISTAMINE	H ₁ - antagonist radioligand	 0870
	H ₂ - antagonist radioligand	 1208
	H ₃ - agonist radioligand	 1332
	H ₄ - agonist radioligand	 1384
LEUKOTRIENES	BLT ₁ (LTB ₄) - agonist radioligand	 1209
	CysLT ₁ (LTD ₄) - agonist radioligand	 0086
MELANIN CONCENTRATING HORMONE	MCH1 - agonist radioligand	 1115
MELANOCORTIN	MC ₁ - agonist radioligand	0644
	MC ₃ - agonist radioligand	 0447
	MC ₄ - agonist radioligand	 0420
MELATONIN	MT ₁ (ML _{1A}) - agonist radioligand	 1538

 Profile changed as compared to 2010  assay developed in 2010  new assay conditions  human  standard turnaround time

Anticipating clinical effects from *in vitro* data

GPCRs (cont'd)

Family	Assay	Ref.
MOTILIN	motilin - agonist radioligand	0470
MUSCARINIC	M ₁ - antagonist radioligand	0091
	M ₂ - antagonist radioligand	0093
	M ₃ - antagonist radioligand	0095
	M ₄ - antagonist radioligand	0096
NEUROKININ	NK ₁ - agonist radioligand	0100
	NK ₂ - agonist radioligand	0102
NEUROPEPTIDE Y	Y ₁ - agonist radioligand	0106
OPIOID AND OPIOID-LIKE	delta ₂ (DOP) - agonist radioligand	0114
	kappa (KOP) - agonist radioligand	1971
	mu (MOP) - agonist radioligand	0118
	☑ NOP (ORL1) - agonist radioligand	0358
PLATELET ACTIVATING FACTOR	PAF - agonist radioligand	0915
PROSTANOID	EP ₂ - agonist radioligand	1955
	FP - agonist radioligand	1979
	IP (PGI ₂) - agonist radioligand	2230
SEROTONIN	5-HT _{1A} - agonist radioligand	0131
	5-HT _{1B} - antagonist radioligand	0132
	5-HT _{1D} - agonist radioligand	1974
	5-HT _{2A} - agonist radioligand	0471
	5-HT _{2B} - agonist radioligand	1333
	5-HT _{2C} - agonist radioligand	1003
	5-HT _{4e} - antagonist radioligand	0501
	5-HT ₆ - agonist radioligand	0142
SOMATOSTATIN	5-HT ₇ - agonist radioligand	0144
	sst ₁ - agonist radioligand	1940
	sst ₄ - agonist radioligand	0482
UROTENSIN-II	UT - agonist radioligand	1386
VASOACTIVE INTESTINAL PEPTIDE	VPAC ₁ (VIP ₁) - agonist radioligand	0157
VASOPRESSIN	V _{1a} - agonist radioligand	0159
	V ₂ - agonist radioligand	0497

NUCLEAR RECEPTORS

Family	Assay	Ref.
STEROID NUCLEAR RECEPTORS	AR - agonist radioligand	0933
	ER α - agonist fluoligand	0484
	GR - agonist radioligand	0469
NON-STEROID NUCLEAR RECEPTORS	LXR β - agonist radioligand	2047
	PPAR γ - agonist radioligand	0641
	TR (TH) - agonist radioligand	0156





OTHER RECEPTORS

Family	Assay	Ref.
CYTOKINES	TNF- α - agonist radioligand	0076
GABA	GABA _{A1} (α 1, β 2, γ 2) - agonist radioligand	3051
	BZD (central) - agonist radioligand	0028
	Cl ⁻ channel (GABA-gated) - antagonist radioligand	0170
GLUTAMATE	AMPA - agonist radioligand	0064
	kainate - agonist radioligand	0065
	NMDA - antagonist radioligand	0066
	PCP - antagonist radioligand	0124
	glycine (strychnine-insensitive) - antagonist radioligand	0068
IMIDAZOLINE	I ₁ - agonist radioligand	0642
MELATONIN	MT ₃ (ML ₂) - agonist radioligand	0088
NICOTINIC	N muscle-type - antagonist radioligand	0936
	☑ N neuronal (α 4 β 2) - agonist radioligand	3029
SEROTONIN	5-HT ₃ - antagonist radioligand	0411
SIGMA	sigma (non-selective) - agonist radioligand	0146











ION CHANNELS

Family	Assay	Ref.
Ca ²⁺ CHANNELS	Ca ²⁺ -L (dihydropyridine site) - antagonist radioligand	0161
	Ca ²⁺ -L (diltiazem site) (benzothiazepines) - antagonist radioligand	0162
	☑ Ca ²⁺ -L (verapamil site) (phenylalkylamine) - antagonist radioligand	0163
	Ca ²⁺ - N - antagonist radioligand	0164
K ⁺ CHANNELS	SK _{Ca} - antagonist radioligand	0167
Na ⁺ CHANNELS	Na ⁺ site 2 - antagonist radioligand	0169


















TRANSPORTERS

Family	Assay	Ref.
CHOLINE	choline transporter (CHT1) - antagonist radioligand	1552 
DOPAMINE	dopamine transporter - antagonist radioligand	0052 
GABA	GABA transporter - antagonist radioligand	0060
NOREPINEPHRINE	norepinephrine transporter - antagonist radioligand	0355 
SEROTONIN	5-HT transporter - antagonist radioligand	0439 

KINASES

Family/Sub-family	Assay	Ref.
PROTEIN-TYROSINE KINASES		
[RTK]	FLT-1 kinase (VEGFR1)	3068 
	IRK (InsR)	2898 
[CTK]	Abl kinase	3056 
	Fyn kinase	0212 
	lyn A kinase	0669 
	ZAP70 kinase	0705 
PROTEIN-SERINE/THREONINE KINASES		
[CMGC]	CDK2 (cycA)	2908 
	ERK ₂ (P42 ^{mapk})	2878 
	p38 α kinase	2881 
[CaMK]	CaMK2 α	3024 

OTHER ENZYMES

Family/Sub-family	Assay	Ref.
PROTEASES		
[Cysteine proteases]	caspase-3	0774 
	caspase-9	0675 
[Aspartic proteases]	BACE-1 (β -secretase)	0701 
[Metalloproteases]	☑ ACE	3441 
	ACE-2	1954 
	MMP-1	0510 
	MMP-2	0489 
	MMP-9	0491 
	neutral endopeptidase	0509 
PHOSPHODIESTERASES		
	PDE2A ₁	2426 
	PDE3B	2705 
	☑ PDE4D ₂	2434 
	PDE5 (non-selective)	0204 
	PDE6 (non-selective)	0478
NO SYNTHASES	☑ inducible NOS	3185
ARACHIDONIC ACID METABOLISM		
[Cyclooxygenases]	☑ COX ₁	0726 
	COX ₂	0727 
MONOAMINE & NEUROTRANSMITTER SYNTHESIS & METABOLISM		
	acetylcholinesterase	0363 
	COMT (catechol-O-methyl transferase)	0457
	MAO-A - antagonist radioligand	0443
TRANSDUCTION SIGNAL ENZYMES	guanylyl cyclase (activator effect)	3004 
ATPases	ATPase (Na ⁺ /K ⁺)	2009
MISCELLANEOUS ENZYMES	xanthine oxidase/superoxide O ²⁻ scavenging	0276

IN VITRO ADME

Family/Sub-family	Assay	Ref.
SOLUTION PROPERTIES		
[Aqueous solubility]	Aqueous solubility (PBS, pH 7.4)	0435
[Partition Coefficient (LogD)]	Partition coefficient (log D, n-octanol/PBS, pH 7.4)	0417
DRUG ABSORPTION/DRUG TRANSPORT		
[A-B/B-A permeability]	<input type="checkbox"/> A-B permeability (Caco-2, pH 6.5/7.4) <input type="checkbox"/> B-A permeability (Caco-2, pH 6.5/7.4)	3318 3320
[P-glycoprotein interactions]	<input type="checkbox"/> P-gp inhibition (Caco-2, [³ H]-digoxin substrate)	3349
DRUG METABOLISM		
[Metabolic Stability (2 time points)]	Metabolic stability (liver microsomes, human)	0416
DRUG-DRUG INTERACTIONS		
[CYP Inhibition - hrCYPs, drug probes]	CYP3A4 inhibition (recombinant, midazolam substrate)	1183
	CYP3A4 inhibition (recombinant, testosterone substrate)	0940
[CYP Inhibition - hrCYPs, fluorescent probes]	CYP1A2 inhibition (recombinant, CEC substrate)	0389
	CYP2B6 inhibition (recombinant, EFC substrate)	0415
	CYP2C8 inhibition (recombinant, DBF substrate)	1201
	CYP2C9 inhibition (recombinant, MFC substrate)	0412
	CYP2C19 inhibition (recombinant, CEC substrate)	0390
	CYP2D6 inhibition (recombinant, MFC substrate)	1338
	CYP2E1 inhibition (recombinant, EC substrate)	0414
	CYP3A4 inhibition (recombinant, BFC substrate)	0391
	CYP3A4 inhibition (recombinant, BzRes substrate)	0939
	CYP3A5 inhibition (recombinant, BFC substrate)	0786

IN VITRO TOXICITY

Family/Sub-family	Assay	Ref.
CYTOTOXICITY	Cell viability (HepG2)	0430

SAMPLE SIZE (including IC₅₀ follow-up studies)

Values are based on a molecular weight ≤500 g/mol and a typical testing concentration of 10 μM in duplicate (including a possible retest).

	SCREENING		SCREENING + FOLLOW UP with highest concentration at 10 μM ¹		SCREENING + FOLLOW UP with highest concentration at 100 μM ¹	
	WEIGHT (pre-weighed)	VOLUME (100% DMSO)	WEIGHT (pre-weighed)	VOLUME (100% DMSO)	WEIGHT (pre-weighed)	VOLUME (100% DMSO)
BIOPRINT® PROFILE						
Number of assays ▼	157	3.4 mg	475 μL@ 10 mM	6.8 mg	1350 μL@ 10 mM	inquire

¹ Assuming ~10% of test in IC₅₀. Usually, for 1 IC₅₀: 30 μL@ 10 mM and + 25 μL@ 10 mM by additional IC₅₀.



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