Table 1: Descriptors used for the development of dipeptide QSAR models.

	Descriptors	Class	Description
1	ATSm4	Auto correlation Descriptor Mass	ATS autocorrelation descriptor, weighted by scaled atomic mass (2D)
2	nHBint7	Electrotopological State Atom Type Descriptor	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 7 (2D)
3	nsOm	Electrotopological State Atom Type Descriptor	Count of atom-type E-State: -O- (2D)
4	minHBd	Electrotopological State Atom Type Descriptor	Minimum E-States for (strong) Hydrogen Bond donors (2D)
5	PetitjeanNumber	Petitjean Number Descriptor	Petitjean number (2D)
6	XLogP	XLogP Descriptor	XLog P (2D)
7	FP186	CDK Fingerprint	Fingerprint of length 1024 and search depth of 8
8	FP509	CDK Fingerprint	Fingerprint of length 1024 and search depth of 8
9	FP728	CDK Fingerprint	Fingerprint of length 1024 and search depth of 8
10	MACCSFP128	MACCS fingerprint	('*~[CH2]~*~*~*~[CH2]~*',0), # ACH2AAACH2A
11	PubchemFP690	Pubchem Fingerprint	O-C-C-C-C-C-O
12	PubchemFP699	Pubchem Fingerprint	O-C-C-C-C-C(C)-C

Table 2: Descriptors used for the development of tripeptide QSAR models.

	Descriptors	Class	Description
1	ETA_BetaP_s	Extended Topochemical Atom Descriptor	A measure of electronegative atom count of the molecule relative to molecular size (2D)
2	ExtFP58	Extended Fingerprint	Extends the Fingerprinter with additional bits describing ring features
3	ExtFP751	Extended Fingerprint	Extends the Fingerprinter with additional bits describing ring features
4	GraphFP173	CDK graph only fingerprint	Specialized version of the Fingerprinter which does not take bond orders into account
5	GraphFP353	CDK graph only fingerprint	Specialized version of the Fingerprinter which does not take bond orders into account
6	GraphFP598	CDK graph only fingerprint	Specialized version of the Fingerprinter which does not take bond orders into account
7	GraphFP833	CDK graph only fingerprint	Specialized version of the Fingerprinter which does not take bond orders into account
8	MACCSFP115	MACCS fingerprint	('[CH3]~*~[CH2]~*',0), # CH3ACH2A
9	PubchemFP17	Pubchem Fingerprint	>= 8 N
10	PubchemFP639	Pubchem Fingerprint	O-C-C-C-O
11	SubFP169	Substructure Fingerprint	Presence of SMARTS Patterns for Functional Group Classification by Christian Laggner
12	KRFP697	Klekota-Roth Fingerprint	Presence of chemical substructures
13	KRFP840	Klekota-Roth Fingerprint	Presence of chemical substructures
14	KRFP842	Klekota-Roth Fingerprint	Presence of chemical substructures
15	KRFP4125	Klekota-Roth Fingerprint	Presence of chemical substructures
16	KRFP4225	Klekota-Roth Fingerprint	Presence of chemical substructures
17	SubFPC100	Substructure Fingerprint Count	Count of SMARTS Patterns for Functional Group Classification by Christian Laggner
18	KRFPC483	KlekotaRoth Fingerprint Count	Count of chemical substructures
19	KRFPC3946	KlekotaRoth Fingerprint Count	Count of chemical substructures
20	KRFPC4125	KlekotaRoth Fingerprint Count	Count of chemical substructures