

Table 4. Non-substrate ligands of L-PGDS/ β -trace

Ligand	Affinities Kd	Binding ratio	Methods*	Ref
Retinoids <i>All-trans- or 9-cis-retinoic acid</i> <i>All-trans- or 13-cis-retinal</i> <i>All-trans-retinoic acid</i> <i>All-trans-retinoic acid,</i>	70-80 nM	1:1	TFQ, CD NMR SAXS	Tanaka et al., 1997 Shimamoto et al., 2007 Inoue et al., 2009
Thyroids L-thyroxine 3-3',5'-Triiodo-L-thyronine 3-3',5'-Triiodo-L-thyronine	660 nM 820 nM 2.6 μ M		TFQ, SPR	Beuckmann et al., 1999
Heme and its degradation products Biliverdin Bilirubin Bilirubin, biliverdin Biliverdin Biliverdin in human CSF Heme	33 nM 37 nM conjugates	1:1	TFQ, SPR SAXS SAXS, NMR NMR NMR	Beuckmann et al., 1999 Inoue et al., 2009 Miyamoto et al., 2009 Inui et al., 2014 Phillips et al., 2020
Amyloid β (Aβ) peptides A β (1-40), A β (1-42) A β (1-40), A β (25-35)	18-50 nM	1:1 1:1	SPR NMR, SAXS	Kanekiyo et al., 2007 Kannaian et al., 2019
Lipids and fatty acids GM1 and GM2 gangliosides Oleic acid & palmitoleic acid Oleic acid Palmitoleic acid Synthetic FABP inhibitor SBFI-26	65-210 nM Ki=1.8 μ M Ki=3.7 μ M Ki=3.0 μ M	1:(1+1)	SPR X-ray crystallography Displacement of DAUDA binding, TFQ	Mohri et al., 2006a Zhou et al., 2010 Elmes et al., 2018
Poorly water-soluble drugs Diazepam, NBQX Telmisartan Anti-cancer drug SN-38 Telmisartan and imatinib Cannabinoid receptor 2 antagonists AM630 WIN55212-2	 60 μ M 0.4-40 μ M N.D. N.D.	1:3 1:3 1:2	ITC ITC ITC Docking simulation	Fukuhara et al., 2012 Mizoguchi et al., 2015 Nakatsuji et al., 2015 Teraoka et al., 2017 Yeh et al., 2019
Cannabinoid metabolites, synthetic cannabinoids Cannabidiol Δ^9 -tetrahydrocannabinol (THC) 11-hydroxy- Δ^9 -tetrahydrocannabinol (11-OH-THC) 11-nor-9-carboxy- Δ^9 -tetrahydrocannabinol (THC-COOH) Synthetic FABP inhibitor SBFI-26	Ki=78 μ M Ki=175 μ M Ki=61 μ M Ki=7.8 μ M 3.0 μ M		Displacement of DAUDA binding, TFQ	Elmes et al., 2018
Anticholinergic drugs Chlorpheniramine Trazodone	4.3 - 5.7 μ M 5.3 - 6.5 μ M	1:3 1:3.4	TFQ, ITC, NMR	Low et al., 2020

Nicotinamide coenzymes NADPH, NADP+, and NADH	47-370 μ M	1:1	ITC, NMR	Qin et al., 2015
Substrate analog and product U-46619 PGD ₂ PGE ₂ PGF _{2a}	0.53 and 7.91 μ M 0.31 and 44.3 μ M 25.8 μ M 2.52 and 137.4 μ M	1:2 1:2 1:1 1:2	ITC, NMR	Shimamoto et al., 2021

*TFQ: tryptophan fluorescence quenching, SAXS: Small angle X-ray scattering, SPR: Surface plasmon resonance,

ITC: Isothermal titration calorimetry, DAUDA: 11-(dansylamino)undecanoic acid.