Supporting Information

Structure-activity relationship studies on a series of 3α -[bis(4-fluorophenyl)methoxy]tropanes and 3α -[bis(4-fluorophenyl)methylamino]tropanes as novel atypical dopamine transporter (DAT) inhibitors for the treatment of cocaine use disorders

Mu-Fa Zou,[†] Jianjing Cao,[†] Ara M. Abramyan,[†] Theresa Kopajtic,[‡] Claudio Zanettini,[†]
Daryl A. Guthrie,[†] Rana Rais,[&] Barbara S. Slusher,[&] Lei Shi,[†] Claus J. Loland,[§]
Amy Hauck Newman^{†*}

[†]Molecular Targets and Medications Discovery Branch, National Institute on Drug

Abuse - Intramural Research Program, National Institutes of Health, 333 Cassell Drive,

Baltimore, Maryland 21224, United States

[‡]Psychobiology Section, Molecular Neuropsychiatry Research Branch, National Institute on Drug Abuse - Intramural Research Program, National Institutes of Health, 251 Bayview Blvd., Baltimore, Maryland 21224, United States

[&]Department of Neurology, Johns Hopkins Drug Discovery, The Johns Hopkins
University School of Medicine, 855 N. Wolfe Street, Baltimore, MD 21205, United
States

§Molecular Neuropharmacology and Genetics Laboratory, Department of
Neuroscience and Pharmacology, Faculty of Health and Medical Sciences, University of
Copenhagen, DK-2200 Copenhagen, Denmark

Supporting information Contents:

I. Table S1. Microanalysis data ... S3

Table S1: Microanalysis data

compd	fomula	Theory			Found		
		С	Н	N	С	Н	N
10a	$C_{24}H_{30}F_2N_2O \cdot 2C_2H_2O_4 \cdot 2.5H_2O$	53.76	6.28	4.48	53.48	5.87	4.25
10b	$C_{24}H_{31}F_2N_3\cdot 3C_2H_2O_4\cdot 3H_2O$	49.79	5.99	5.81	49.92	5.97	5.83
10c	$C_{27}H_{34}F_2N_2O \cdot 2C_2H_2O_4 \cdot 1.25H_2O$	57.89	6.35	4.36	57.95	6.09	4.33
10d	$C_{27}H_{35}F_2N_3\cdot 3C_2H_2O_4\cdot 1.5H_2O$	53.80	6.02	5.70	53.95	5.82	5.63
10e	$C_{25}H_{33}F_2N_3 \cdot 3C_2H_2O_4 \cdot 0.5H_2O \cdot 0.5i$ -PrOH	54.01	6.14	5.81	53.87	6.13	5.60
12a	$C_{27}H_{31}F_2NO_3$	71.19	6.86	3.07	71.36	6.79	2.95
12b	$C_{33}H_{34}F_2N_2O_3$	72.77	6.29	5.14	72.63	6.33	5.20
12c	$C_{28}H_{36}F_2N_2O_3$	69.11	7.46	5.76	68.89	7.53	5.84
13a	$C_{25}H_{30}F_2N_2O_3$	67.55	6.80	6.30	67.78	6.64	6.45
15	$C_{26}H_{32}F_2N_2O$	73.21	7.56	6.57	72.95	7.63	6.69
19a	$C_{30}H_{28}F_2N_2O_2$	74.06	5.80	5.76	73.90	5.84	5.86
S-(+)-	$C_{30}H_{28}F_2N_2O_2$	74.06	5.80	5.76	73.82	5.87	5.95
19a							
19b	$C_{31}H_{30}F_2N_2O_2$	74.38	6.04	5.60	74.47	5.93	5.54
19c	$C_{30}H_{27}ClF_2N_2O_2$	69.16	5.22	5.38	68.83	5.30	5.51
19d	$C_{30}H_{27}F_3N_2O_2$	71.42	5.39	5.55	71.58	5.26	5.37