Supporting Information

Thiophene-Anthranilamides as Highly Potent and Orally Available Factor Xa Inhibitors

Bin Ye,* Damian O. Arnaiz, Yuo-Ling Chou, Brian D. Griedel, Rushad Karanjawala, Wheeseong Lee, Michael M. Morrissey, Karna L. Sacchi, Steven T. Sakata, Kenneth J. Shaw, Shung C. Wu, Zuchun Zhao, Marc Adler, Sarah Cheeseman, William P. Dole, Janice Ewing, Richard Fitch, Dao Lentz, Amy Liang, David Light, John Morser, Joseph Post, Galina Rumennik, Babu Subramanyam, Mark E. Sullivan, Ron Vergona, Janette Walters, Yi-Xin Wang, Kathy A. White, Marc Whitlow and Monica J. Kochanny*

Combustion Analysis for Newly Synthesized Target Compounds

Compound	Formula	C calcd	C found	H calcd	H found	N calcd	N found
3a	$C_{23}H_{22}Cl_3N_5O_2S$ 3.0 $C_2HF_3O_2$	39.54	39.62	2.86	2.70	7.95	8.11
3b	$C_{24}H_{23}Cl_3N_4O_3S$ 0.4 CH_2Cl_2	51.08	51.17	4.29	4.32	9.23	9.40
3c	$C_{24}H_{24}Cl_3N_4O_3S$ 3.4 $C_2HF_3O_2$ 0.5 H_2O	38.31	38.10	2.96	2.93	7.25	7.13
10a	$C_{19}H_{15}Cl_3N_4O_3S$	46.98	47.05	3.11	2.94	11.5	11.29
10b	$C_{20}H_{17}Cl_3N_4O_3S$	48.06	48.20	3.43	3.73	11.20	11.05
10c	$C_{21}H_{19}Cl_3N_4O_3S$ 1.25 $C_2HF_3O_2$ 0.5 H_2O	42.42	42.35	3.22	3.11	8.42	8.24
10d	$C_{22}H_{21}Cl_3N_4O_3S$	50.06	50.01	4.01	3.94	10.61	10.59
10e	$C_{22}H_{21}Cl_3N_4O_3S$ 0.05 CH_2Cl_2	49.77	49.9	4.00	4.01	10.53	10.51
10f	$C_{24}H_{23}Cl_3N_4O_3S$ 1.2 H_2O	49.02	48.80	4.54	4.14	9.94	9.75
10g	$C_{23}H_{21}Cl_3N_4O_3S$ 0.4 $C_4H_8O_2$	49.99	49.92	4.12	3.78	9.47	9.49
10h	$C_{23}H_{21}Cl_3N_4O_3S$ 0.1 CH_2Cl_2	50.6	50.33	3.9	4.02	10.22	10.15
10i	$C_{24}H_{23}Cl_3N_4O_4S$ 0.22 CH_2Cl_2 0.5 H_2O	48.68	48.84	4.12	3.93	9.38	9.11
10j	$C_{22}H_{21}Cl_3N_4O_3S$ 0.3 $C_4H_8O_2$	48.86	48.60	4.13	4.05	9.82	9.59
10k	$C_{23}H_{23}Cl_3N_4O_4S$ 2.45 $C_2HF_3O_2$	40.15	40.05	3.09	3.13	6.74	6.60
10l	$C_{23}H_{23}Cl_3N_4O_4S$ 2.1 $C_2HF_3O_2$ 1.0 H_2O	40.07	40.17	3.35	3.33	6.87	6.81
10m	$C_{24}H_{25}Cl_3N_4O_4S$ 2.7 $C_2HF_3O_2$	40.14	40.21	3.17	3.20	6.37	6.40
10n	$C_{23}H_{23}Cl_3N_4O_5S$ 0.5 $C_2HF_3O_2$	47.39	47.18	4.15	3.96	9.61	9.30
10o	$C_{25}H_{28}Cl_3N_5O_3S$	51.33	51.17	4.82	4.75	11.97	11.78
10p	$C_{26}H_{28}Cl_3N_5O_3S$ 1.0 H_2O	50.78	50.97	4.92	4.60	11.38	11.11
12a	$C_{21}H_{19}Cl_3N_4O_5S_2$ 0.42 $C_4H_8O_2$	44.37	44.14	3.67	3.73	9.12	9.03

Compound	Formula	C calcd	C found	H calcd	H found	N calcd	N found
12b	$C_{21}H_{18}Cl_3N_4O_4S$ 2.0 $C_2HF_3O_2$ 1.0 H_2O	38.06	38.78	2.81	2.49	8.88	8.60
12c	$C_{23}H_{22}Cl_3N_5O_4S$ 0.5 H_2O 0.19 CH_2Cl_2	46.73	46.68	3.95	3.78	11.75	11.45
12d	$C_{23}H_{22}Cl_3N_5O_5S$ 1.2 $C_2HF_3O_2$	42.16	41.90	3.23	3.50	9.68	9.99
12e	$C_{27}H_{29}Cl_3N_6O_4S$ 3.3 $C_2HF_3O_2$	39.67	39.60	3.30	3.46	8.26	8.15
12f	$C_{24}H_{22}Cl_3N_5O_6S$ 0.9 $C_2HF_3O_2$ 0.5 H_2O	42.65	42.34	3.32	3.02	9.64	9.32
13a	$C_{23}H_{20}Cl_3N_5O_4S$ 0.2 CH_2Cl_2	47.48	47.60	3.69	3.73	11.93	11.64
13b	$C_{24}H_{22}Cl_3N_5O_4S$ 2.15 $C_2HF_3O_2$	41.05	41.04	2.94	2.93	8.46	8.53
13c	$C_{24}H_{19}Cl_3F_3N_5O_4S$ 0.1 $C_4H_8O_2$	44.98	44.74	3.08	3.0	10.71	10.44
13d	$C_{26}H_{26}Cl_3N_5O_4S$ 2.0 $C_2HF_3O_2$	42.95	43.26	3.36	3.48	8.35	8.61
13e	$C_{25}H_{24}Cl_3N_5O_5S$ 2.9 $C_2HF_3O_2$	39.20	39.15	2.87	2.99	7.42	7.64
13f	$C_{24}H_{22}Cl_3N_5O_4S$ 0.9 $C_2HF_3O_2$ 0.8 H_2O	44.72	44.29	3.53	3.28	10.01	10.31
13g	$C_{25}H_{24}Cl_3N_5O_4S$ 0.3 H_2O	49.85	49.51	4.11	3.99	11.62	11.56
13h	$C_{24}H_{22}Cl_3N_5O_4S$ 1.8 $C_2HF_3O_2$ 0.5 H_2O	41.59	41.36	3.13	2.96	8.78	8.70
13i	$C_{23}H_{18}Cl_3N_5O_5S$ 0.4 CH_2Cl_2 0.3 $C_4H_8O_2$	45.93	46.07	3.32	3.14	10.89	10.90
13j	$C_{23}H_{20}Cl_3N_5O_4S_2$ 0.05 $C_4H_8O_2$	46.92	47.20	3.54	3.76	11.79	11.40
13k	$C_{23}H_{18}Cl_3N_5O_4S$ 1.0 $C_2HF_3O_2$ 1.0 H_2O	42.96	43.06	3.03	2.97	10.02	9.86
13l	$C_{24}H_{22}Cl_3N_5O_3S$ 1.65$C_2HF_3O_2$	43.37	43.6	3.29	3.21	9.26	9.02

Compound	Formula	C calcd	C found	H calcd	H found	N calcd	N found
17a	$C_{22}H_{18}Cl_3N_5O_4S$ 1.6$C_2HF_3O_2$ 0.5H_2O	40.56	40.48	2.78	2.79	9.38	9.43
17b	$C_{22}H_{18}Cl_3N_5O_3S$ 2.3 $C_2HF_3O_2$	38.35	38.37	2.46	2.39	8.41	8.47
17c	$C_{22}H_{18}Cl_3N_6O_3S$ 1.8 $C_2HF_3O_2$ 1.7 H_2O	38.94	38.61	3.09	2.73	10.64	10.69
17d	$C_{22}H_{17}Cl_3N_6O_4S$ 0.25 $C_2HF_3O_2$	45.25	45.32	2.94	2.92	14.1	14.09
17e	$C_{23}H_{20}Cl_3N_5O_3S_2$ 3.5 $C_2HF_3O_2$ 2.0 H_2O	35.32	35.35	2.71	2.4	6.86	6.65
17f	$C_{23}H_{20}Cl_3N_5O_3S$ 1.7 $C_2HF_3O_2$ 0.5 H_2O	41.96	42.16	3.03	3.01	9.26	9.26
17g	$C_{22}H_{18}Cl_3N_5O_3S$ 1.6 $C_2HF_3O_2$	41.96	42.01	2.74	2.8	9.71	9.71
17h	$C_{22}H_{20}Cl_3N_5O_3S$ 0.5 H_2O 1.9 $C_2HF_3O_2$	40.43	40.72	3.01	3.17	9.14	9.2
17i	$C_{21}H_{19}Cl_3N_6O_3S$ 1.5 $C_2HF_3O_2$	40.44	40.50	2.90	3.12	11.79	11.83
17j	$C_{22}H_{16}Cl_3N_5O_3S$ 2.0 $C_2HF_3O_2$	40.83	41.06	2.37	2.53	9.16	9.16
17k	$C_{23}H_{18}Cl_3N_5O_3S$ 1.7 $C_2HF_3O_2$	42.58	42.84	2.67	2.58	9.4	9.46
17l	$C_{22}H_{17}Cl_3N_6O_3S$ 0.4 CH_2Cl_2	45.93	45.96	3.06	3.06	14.35	14.47
17m	$C_{23}H_{19}Cl_3N_6O_3S$ 0.1 C_6H_{14} 1.2 H_2O	47.55	47.73	3.86	3.9	14.1	14.26
17n	$C_{24}H_{21}Cl_3N_6O_3S$ 1.6 $C_2HF_3O_2$	42.86	42.67	2.99	3.0	11.02	11.21
17o	$C_{25}H_{23}Cl_3N_6O_3S$ 0.1CH_2Cl_2 0.5H_2O	49.31	49.29	3.99	3.95	13.74	13.70
17p	$C_{23}H_{19}Cl_3N_6O_3S$ 0.05 C_6H_{14} 0.8 H_2O	47.87	47.56	3.67	3.65	14.38	14.22