Supporting Information

New insights into the design of inhibitors of human *S*-adenosylmethionine decarboxylase: Studies of adenine C^8 substitution in structural analogues of AdoMetDC

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Purity as Evidenced by Elemental Analyses of the Target compounds

Compound	Empirical Formula	Calculated, %				Found, %			
		C	H	N	S	C	H	N	S
5	$C_{13}H_{21}N_7O_4.1.0\ H_2SO_4.0.\ 5C_2H_5OH.1.0H_2O$	35.14	5.90	20.49		34.91	6.06	20.69	
12a	$C_{14}H_{23}N_7O_4.2.2H_2SO_4.0.1C_2H_5OH.0.5H_2O$	29.26	5.01	16.82		29.48	5.21	16.47	
12b	$C_{14}H_{24}N_8O_4.2.1H_2SO_4.0.3C_2H_5OH.0.2H_2O$	29.63	5.17	18.93	11.37	29.43	5.20	19.05	11.13
12c	$C_{19}H_{25}N_7O_4.2.0H_2SO_4.3H_2O$	34.28	5.29	14.72	9.63	34.21	5.34	14.59	9.59
14a	$C_{16}H_{28}N_8O_4.0.4H_2SO_4.0.2C_2H_5OH.0.9H_2O$	42.71	6.95	24.30	2.78	42.53	6.84	24.16	2.56
14b	$C_{21}H_{29}N_7O_4.1.75H_2SO_4.0.05C_2H_5OH.2.4H_2O$	38.36	5.73	14.84	8.49	38.23	5.74	14.78	8.59
14c	$C_{15}H_{25}N_7O_5.1.9H_2SO_4.0.1C_2H_5OH.2H_2O$	29.91	5.51	16.06	9.98	30.03	5.49	16.14	9.74
14d	$C_{16}H_{27}N_7O_4.1.9H_2SO_4.0.4C_2H_5OH$	34.42	5.70	16.71		34.56	5.67	16.70	
14e	$C_{17}H_{29}N_7O_4.1.9H_2SO_4.0.2C_2H_5OH$	35.36	5.79	16.58		35.49	5.87	16.61	
14f	$C_{15}H_{25}N_7O_4.2.0H_2SO_4.0.3C_2H_5OH.1.5H_2O$	30.99	5.65	16.22	10.61	31.02	5.40	16.30	10.49
17c	$C_{16}H_{24}N_6O_5.0.5CHCl_3.0.3CH_3OH$	49.59	6.19	21.22		49.72	6.29	21.17	
17d	$C_{15}H_{23}N_7O_4.1.5H_2SO_4.0.8H_2O$	34.19	5.27	18.60	9.12	34.34	5.03	18.45	9.12
17e	$C_{16}H_{25}N_7O_4.1.1H_2SO_4.1.05H_2O$	37.96	5.83	19.36	6.95	37.64	5.84	19.43	6.81
17f	$C_{14}H_{21}N_7O_4.1.45H_2SO_4.0.2C_2H_5OH.1.3H_2O$	32.55	5.18	18.92	8.97	32.35	5.24	18.87	8.80
17j	$C_{14}H_{21}N_7O_4.1.9H_2SO_4.1.6H_2O$	29.68	4.98	17.31	10.75	29.54	4.68	17.05	10.64
17k	$C_{15}H_{24}N_8O_4.2.0\ H_2SO_4.2.7H_2O$	28.81	5.38	17.92	10.25	28.93	5.30	17.66	10.19
17l	$C_{14}H_{22}N_8O_4.2.0\ H_2SO_4.2.0H_2O$	28.09	5.05	18.72	10.71	27.81	5.14	19.10	10.51
17m	$C_{14}H_{22}N_8O_4.0.2\ CH_3OH.\ 0.4H_2O$	44.88	6.25	29.48		44.91	6.17	29.44	
18a	$C_{15}H_{26}N_8O_3.2.4H_2SO_4.0.2C_2H_5OH$	30.27	5.27	18.34		30.25	5.28	18.54	
18b	$C_{20}H_{27}N_7O_3.2.2H_2SO_4.0.1C_2H_5OH.2.5H_2O$	28.45	1.36	4.74		28.75	1.38	4.79	
18d	$C_{14}H_{23}N_7O_3.2.0H_2SO_4.0.25C_2H_5OH.0.7H_2O$	31.23	5.40	17.58		31.21	5.49	17.48	
18e	$C_{13}H_{21}N_7O_3.0.25CHCl_3.0.5H_2O$	47.80	7.24	27.09		47.76	7.13	27.03	
18f	$C_{14}H_{23}N_7O_3.0.5\ CH_3OH.\ 0.3H_2O$	48.53	7.19	27.32		48.73	7.17	27.09	
19a	$C_{15}H_{26}N_8O_3.2.4H_2SO_4.0.2C_2H_5OH$	35.73	5.49	14.44		35.92	5.39	14.49	
19b	$C_{20}H_{27}N_7O_3.1.7H_2SO_4.0.05C_2H_5OH.3.3H_2O$	37.32	5.82	15.15	8.67	37.29	5.79	15.18	8.40
19c	$C_{13}H_{21}N_7O_3.0.05\ CH_3OH.0.1H_2O$	47.97	6.60	30.00		47.70	6.86	29.95	
19d	$C_{14}H_{23}N_7O_3.0.4\ CH_3OH.\ 0.7H_2O$	43.93	6.19	27.06		44.15	6.27	27.18	
21c	$C_{15}H_{25}N_7O_3.2.0H_2SO_4.2.5H_2O$	30.40	5.78	16.54	10.52	30.55	5.85	16.19	10.82
21d	$C_{16}H_{27}N_7O_3.2.5H_2SO_4.2.5H_2O$	29.72	5.61	15.16		29.86	5.57	14.81	
22a	$C_{14}H_{23}N_9O_3.0.05CHCl_3.3.5H_2O$	38.84	6.97	29.01		38.54	6.65	29.25	
22c	$C_{14}H_{22}N_8O_4.1.2C_2H_5OH.0.2\ CH_3OH$	46.58	7.06	26.18		46.93	7.22	26.43	

Compound	Empirical Formula	Calculated, %				Found, %			
		C	H	N	S	C	H	N	S
23a	$C_{13}H_{20}N_6O_3.0.35CHCl_3.0.5C_2H_5OH$	45.43	6.14	22.95		45.54	5.85	22.79	
23b	$C_{12}H_{18}N_6O_3.0.35\ CH_3OH$	48.55	6.40	27.50		48.80	6.40	27.23	
25b	$C_{13}H_{20}ClN_5O_3S.2H_2O$	39.24	6.07	17.60		39.35	5.97	17.55	
25d	$C_{12}H_{18}ClN_5O_3S.1.5H_2O.0.1C_2H_5OH$	38.96	5.80	18.32	8.44	38.98	5.68	18.29	8.57