Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

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Developing novel non-hydroxamate histone deacetylase inhibitors: the chelidamic warhead

Electronic supplementary information

Contents:

Table S1. Chemical and physical data of compounds **4-7**

Compounds	n	Melting Point (°C)	Recrystallization Solvent	Yield (%)
4a	2	106-108	Cyclohexane	63.2
4b	3	190-192	Acetonitrile	70.4
4c	4	160-162	Benzene/Acetonitrile	72.8
4d	5	159-161	Benzene/Acetonitrile	72.5
5a	2	228-230	Acetonitrile/methanol	87.5
5b	3	232-234	Acetonitrile/methanol	93.2
5c	4	224-226	Acetonitrile/methanol	89.0
5d	5	222-224	Acetonitrile/methanol	85.7
6a	2	182-184	Benzene/Acetonitrile	70.3
6b	3	169-171	Benzene	72.0
6c	4	146-148	Benzene	64.5
6d	5	133-135	Cyclohexane/Benzene	68.
6e	6	114-116	Cyclohexane/Benzene	59.6
6f	7	130-132	Cyclohexane/Benzene	66.8
6g	8	125-127	Cyclohexane/Benzene	67.4
6h	-	212-214	Acetonitrile/methanol	92
6i	-	169-171	acetonitrile	97
7	-	118-120	Cyclohexane/Benzene	65.7

Table S2. Chemical and physical data of compounds **9**, **13**, **14**

Compounds	n	Melting Point (°C)	Recrystallization solvent	Yield (%)
9a	2	122-124	cyclohexane/benzene	68.5
9b	3	79-81	cyclohexane	70.7
9c	4	82-84	cyclohexane	74.3
9d	5	80-82	cyclohexane	73.8
9e	6	94-95	cyclohexane	72.3
9f	7	71-73	cyclohexane	80.2
9g	8	89-91	cyclohexane	84.7
13		191-192	acetonitrile/methanol	73
14		161-163	acetonitrile	77

Table S3. Analytical results for compounds **4-7**

cpd	MW	% calcd				% found			
		C	H	N	S	C	H	N	S
4a	441.46	57.13	4.34	9.52	7.26	56.92	4.21	9.77	7.35
4b	455.48	58.01	4.65	9.23	7.04	57.88	4.45	9.52	7.18
4c	469.51	58.84	4.94	8.95	6.83	59.03	5.09	8.72	6.74
4d	483.54	59.61	5.21	8.69	6.63	59.77	5.36	8.49	6.52
5a	413.40	55.20	3.66	10.16	7.76	55.44	3.78	9.94	7.62
5b	427.43	56.20	4.01	9.83	7.50	56.01	3.87	9.99	7.63
5c	441.46	57.13	4.34	9.52	7.26	56.89	4.19	9.69	7.35
5d	455.48	58.01	4.65	9.23	7.04	58.26	4.77	9.11	6.89
6a	464.47	64.65	5.21	6.03		64.88	5.32	5.84	
6b	478.49	65.26	5.48	5.85		65.44	5.59	5.62	
6c	492.52	65.84	5.73	5.69		65.69	5.60	5.84	
6d	506.55	66.39	5.97	5.53		66.54	6.11	5.39	
6e	520.57	66.91	6.20	5.38		67.14	6.32	5.12	
6f	534.60	67.40	6.41	5.24		67.22	6.30	5.52	
6g	548.63	67.87	6.61	5.11		67.98	6.73	4.86	
6h	420.41	65.71	4.79	6.66		65.96	4.87	6.46	
6i	434.44	66.35	5.10	6.45		66.54	5.28	6.27	
7	386.40	62.17	5.74	7.25		62.45	5.82	7.01	

Figure S1. Effects of compounds **4b, 5-7** (50 μM, 24 h) on acetylation levels of histone H3 and α–tubulin, in U937 leukemia cells. Western blot analysis were performed with specific antibodies. ERKs were used for equal loading.

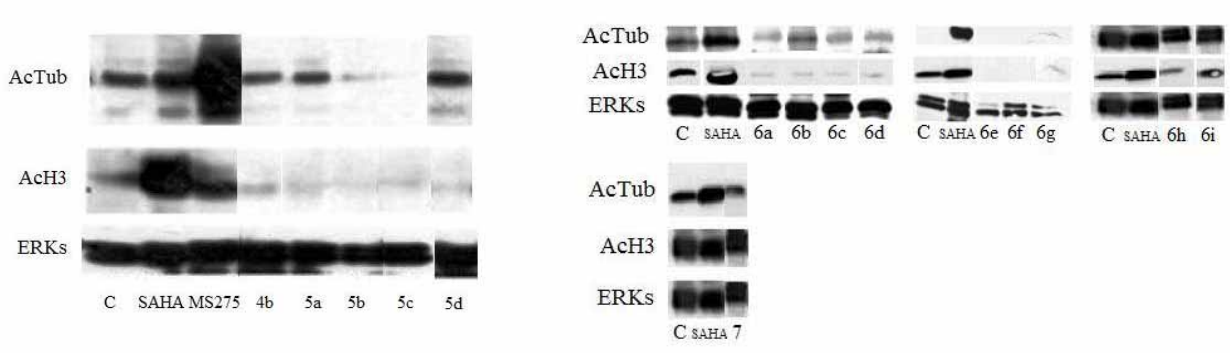

Figure S2. Apoptosis induction on U937 leukemia cells by compounds **4-7** at 50 μM for 30 h.

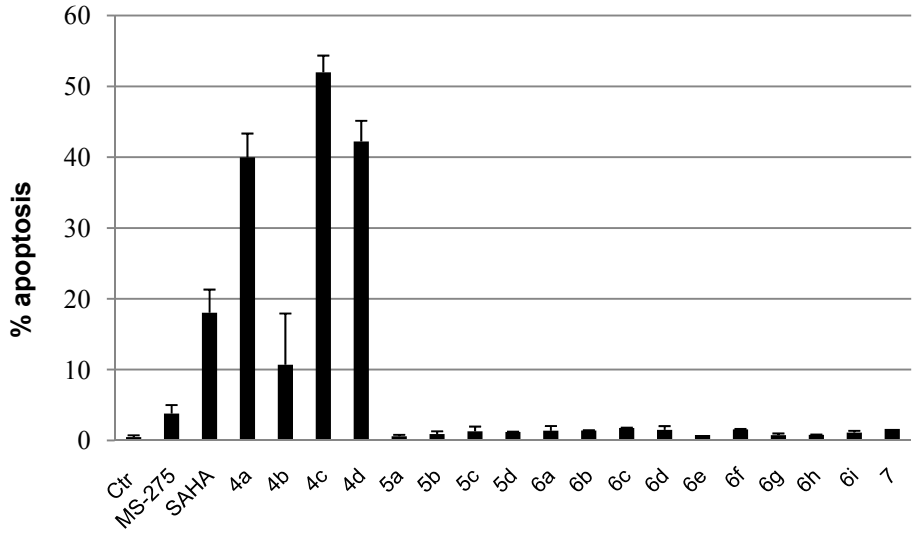

Figure S3. Cytodifferentiation activity (evaluated as % of CD11c positive/PI negative cells) given by compounds **4-7** at 50 μM for 30 h on U937 leukemia cells