Supporting Information

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Discovery of new capsaicin and dihydrocapsaicin derivatives as histone deacetylase inhibitors and molecular docking studies

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Figure S1: IR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-ena-mide (1) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (2)



Figure S2: ¹H NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6enamide (1) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (2)



Figure S3: ¹³C NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6enamide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)



Figure S4: IR spectrum of (E)-N-(4-(tert-butyldimethylsilyloxy)-3-methoxybenzyl)-8-
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Figure S5: 1 H NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-8-
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Figure S6: 13 C NMR spectrum of (E)-N-(4-(tert-butyldimethylsilyloxy)-3-methoxy-benzyl)-8-
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methoxybenzyl)-8-methylnonanamide (4)



Figure S7: IR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-5hydroxy-8-methylnon-6-enamide (**5**)



Figure S8: ¹H NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5hydroxy-8-methylnon-6-enamide (**5**)



Figure S9: ¹³C NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5hydroxy-8-methylnon-6-enamide (**5**)



Figure S10: Mass spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)



Figure S11: IR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6enamide (**6**)



Figure S12: ¹H NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)



Figure S13: ¹³C NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)



Figure S14: Mass spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)



Figure S15: IR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7)



Figure S16:¹H NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9oxononan-4-yl acetate (7)



Figure S17: ¹³C NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9oxononan-4-yl acetate (7)



Figure S18: Mass spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7)



Figure S19: IR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S20: ¹H NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S21: ¹³C NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S22: IR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4 dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S23: ¹H NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S24: ¹³C NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)



Figure S25: Mass spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)