pharmaceutics

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Article

Acylation of Oleanolic Acid Oximes Effectively Improves Cytotoxic Activity in In Vitro Studies

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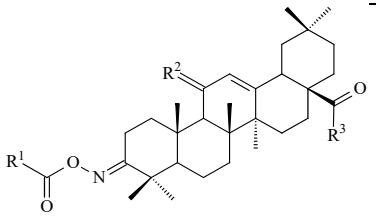
Supplementary Materials SM.S1. The detailed results of SAR analysis

Table S1. Predicted activity of oleanolic acid (**1**) its oximes (**2** – **4**) and their acylderivatives (**5a – 5g**, **6a – 6g** and **7a - 7g**) determined by the PASS method.
Legend: ***P_a*** *– probability of activity;* ***P_i*** *– probability of inactivity;* ***inh.*** *– inhibitor;* ***stim.*** *– stimulator;* ***antag.***– *antagonist,* ***TF NF*** *– transcription factor,* ***Membr.*** *– membrane*

1.000 – 0.950	0.949 – 0.900	0.899 – 0.850	0.849 – 0.800	0.799 – 0.750	0.749 – 0.700	< 0.700

Compound structure				P_a factor (and P_i factor) for $P_a \geq 0.700$									
													
Comp. No.	**R^1**	**R^2**	**R^3**	**Antineoplastic**	**Apoptosis agonist**	**Caspase 3 stim.**	**Caspase 8 stim.**	**Hepatoprotectant**	**Insulin promoter**	**Membr. integrity antag.**	**Oxidoreductase inhib.**	**TF NF kappa B stim.**	**TF stim.**
2	**H**	**H_2**	**OMe**	0.824 (0.009)	0.855 (0.005)	0.952 (0.003)	0.745 (0.003)	0.747 (0.005)	0.776 (0.004)	0.797 (0.007)	< 0.700	0.896 (0.002)	0.896 (0.002)
5a	**CH_3-**			0.730 (0.021)	0.769 (0.010)	0.777 (0.007)	0.761 (0.002)	0.757 (0.005)	0.743 (0.005)	0.813 (0.006)	< 0.700	0.886 (0.002)	0.886 (0.002)
5b	**Cl-CH_2-**			0.809 (0.011)	0.747 (0.011)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.732 (0.012)	0.873 (0.002)	0.873 (0.002)

5c	**CH_3-CH_2-**			< 0.700	0.720 (0.013)	0.712 (0.010)	0.738 (0.003)	0.727 (0.006)	0.751 (0.004)	0.792 (0.007)	< 0.700	0.878 (0.002)	0.878 (0.002)
5d	**C_6H_5-**			< 0.700	0.809 (0.008)	0.774 (0.007)	0.715 (0.003)	0.716 (0.007)	0.775 (0.004)	0.777 (0.008)	< 0.700	0.884 (0.002)	0.884 (0.002)
5e	**2-NO_2-C_6H_4-**			< 0.700	0.748 (0.011)	0.739 (0.009)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.848 (0.002)	0.848 (0.002)
5f	**4-NO_2-C_6H_4-**			< 0.700	0.801 (0.008)	0.794 (0.006)	0.716 (0.003)	0.775 (0.005)	< 0.700	0.764 (0.009)	< 0.700	0.867 (0.002)	0.867 (0.002)
5g	**2,4-di-NO_2-C_6H_3-**			< 0.700	0.762 (0.010)	0.762 (0.008)	< 0.700	0.737 (0.006)	< 0.700	< 0.700	< 0.700	0.834 (0.002)	0.834 (0.002)
3	**H**			0.828 (0.009)	0.858 (0.005)	0.885 (0.004)	< 0.700	0.742 (0.006)	< 0.700	< 0.700	< 0.700	0.883 (0.002)	0.883 (0.002)
6a	**CH_3-**			0.741 (0.020)	0.781 (0.009)	< 0.700	< 0.700	0.752 (0.005)	< 0.700	< 0.700	0.735 (0.012)	0.872 (0.002)	0.872 (0.002)
6b	**Cl-CH_2-**			0.814 (0.010)	0.758 (0.010)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.804 (0.006)	0.858 (0.002)	0.858 (0.002)
6c	**CH_3-CH_2-**	**O**	**OMe**	< 0.700	0.733 (0.012)	< 0.700	< 0.700	0.720 (0.007)	< 0.700	< 0.700	< 0.700	0.864 (0.002)	0.864 (0.002)
6d	**C_6H_5-**			0.706 (0.025)	0.815 (0.007)	< 0.700	< 0.700	0.709 (0.007)	< 0.700	< 0.700	0.715 (0.014)	0.870 (0.002)	0.870 (0.002)
6e	**2-NO_2-C_6H_4-**			< 0.700	0.758 (0.010)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.766 (0.009)	0.832 (0.002)	0.832 (0.002)
6f	**4-NO_2-C_6H_4-**			0.703 (0.026)	0.811 (0.007)	< 0.700	< 0.700	0.768 (0.005)	< 0.700	< 0.700	0.733 (0.012)	0.857 (0.002)	0.857 (0.002)
6g	**2,4-di-NO_2-C_6H_3-**			0.706 (0.025)	0.776 (0.009)	< 0.700	< 0.700	0.728 (0.006)	< 0.700	< 0.700	0.751 (0.010)	0.823 (0.002)	0.823 (0.002)
4	**H**			0.819 (0.010)	0.795 (0.008)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.819 (0.002)	0.819 (0.002)
7a	**CH_3-**			0.724 (0.022)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.802 (0.003)	0.802 (0.003)
7b	**Cl-CH_2-**			0.798 (0.012)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.785 (0.003)	0.785 (0.003)
7c	**CH_3-CH_2-**			< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.793 (0.003)	0.793 (0.003)
7d	**C_6H_5-**	**H_2**	**Mor**	< 0.700	0.710 (0.014)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.797 (0.003)	0.797 (0.003)
7e	**2-NO_2-C_6H_4-**			< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.755 (0.003)	0.755 (0.003)
7f	**4-NO_2-C_6H_4-**			< 0.700	0.710 (0.014)	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.781 (0.003)	0.781 (0.003)
7g	**2,4-di-NO_2-C_6H_3-**			< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	< 0.700	0.745 (0.004)	0.745 (0.004)