SUPPORTING INFORMATION
FOR

Guanylation reactions for the rational design of cancer therapeutic agents.

Almudena del Campo-Balguerías,[†,‡] Blanca Parra-Cadenas,[&] Cristina Nieto-Jimenez,[§] Iván Bravo,[†,§] Elisa Poyatos,[#] Pavel Gancarski,[#] Fernando Carrillo-Hermosilla,[†] Carlos Alonso-Moreno,[†,‡,] and Alberto Ocaña[§,]**

[†]Unidad nanoDrug, Facultad de Farmacia, Universidad de Castilla-La Mancha, 02008 Albacete, Spain.

[‡]Departamento Química Inorgánica, Orgánica y Bioquímica. ORCATS group. Facultad de Farmacia de Albacete-Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad de Castilla-La Mancha, 02008 Albacete, Spain

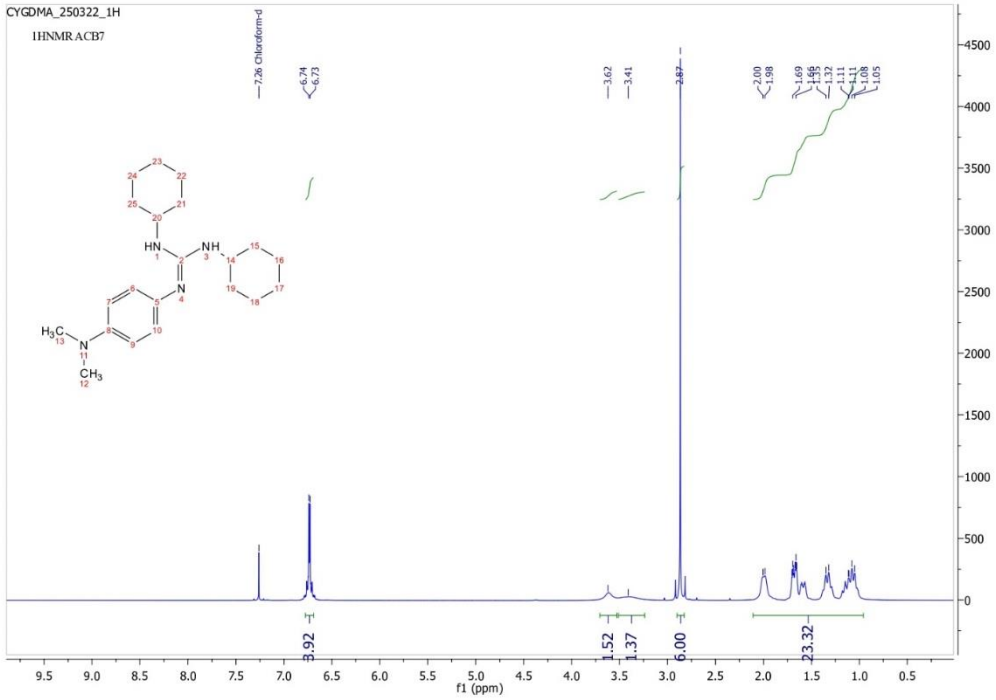
[&]Departamento de Química Inorgánica, Orgánica y Bioquímica. COMCAT group. Centro de Innovación en Química Avanzada (ORFEO−CINQA), Universidad de Castilla-La Mancha, E-13071 Ciudad Real, Spain.

[§]Experimental Therapeutics Unit, Hospital Clínico San Carlos, IdISSC, Fundación Jiménez Díaz, START. 28040 Madrid, Spain.

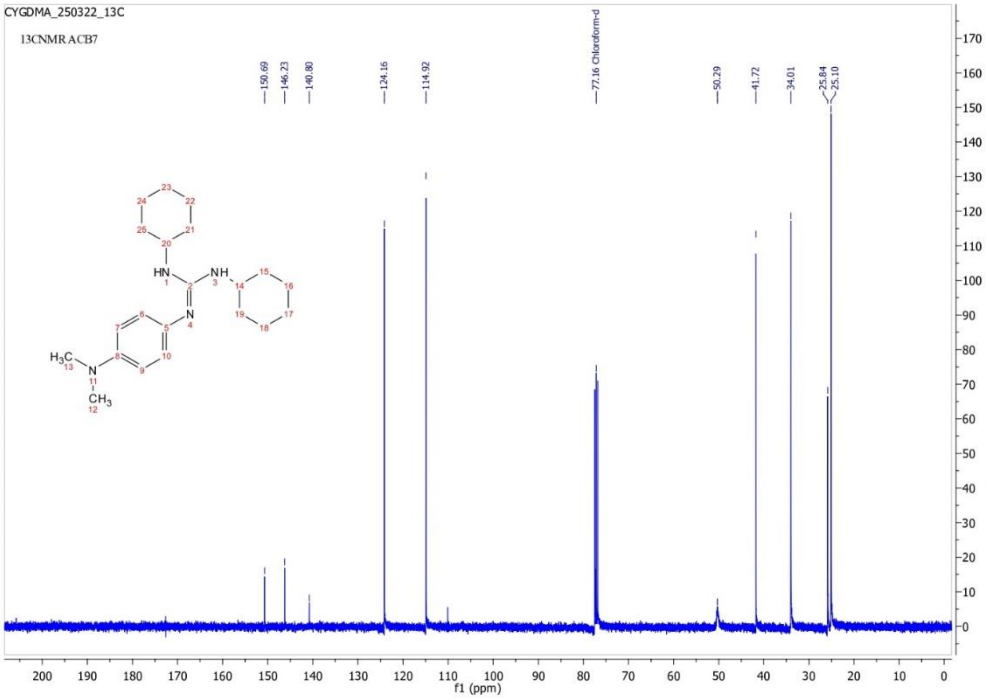
[§]Departamento Química-Física. Facultad de Farmacia de Albacete, FOTOAIR group, Universidad de Castilla-La Mancha, 02008 Albacete, Spain

[#]Cancerappy, Avda Ribera De Axpe, 28, 48950 Erandio, Bizkaia, Spain.

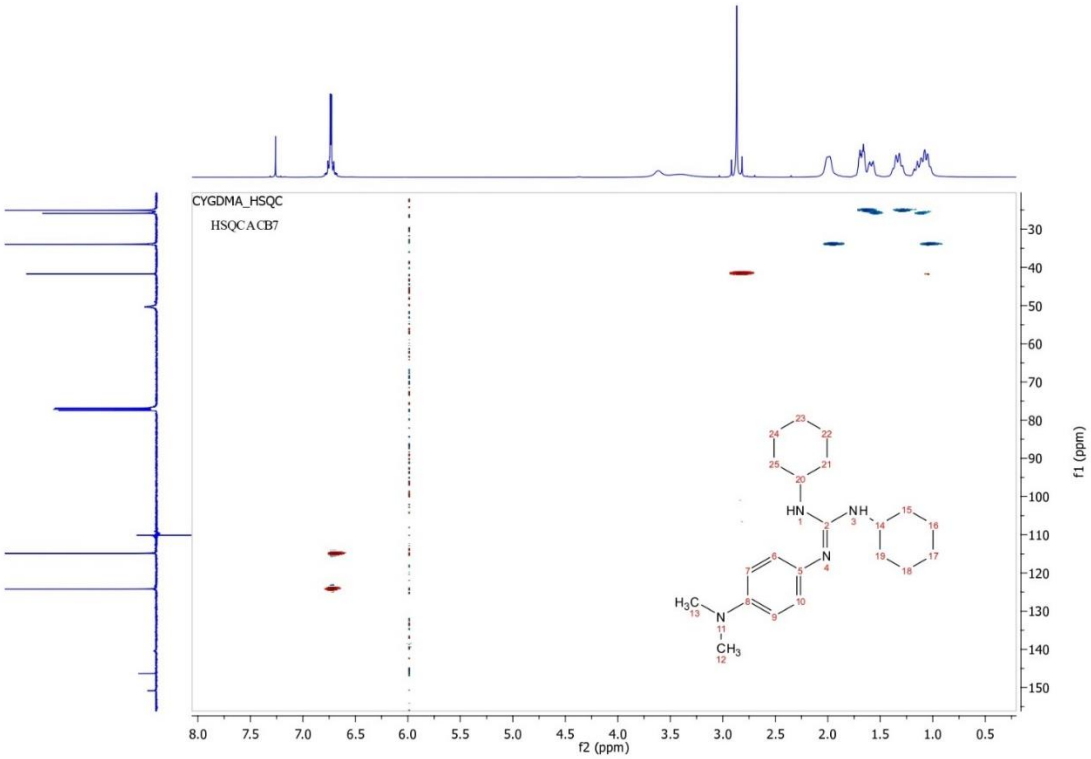
^{1}H-NMR of *ACB7* in $CDCl_3$.



^{13}C-NMR of *ACB7* in $CDCl_3$.



Multinuclear 2D (^{1}H-^{13}C HSQC) of *ACB7*



Multinuclear 2D (^{1}H-^{1}H COSY) of *ACB7*

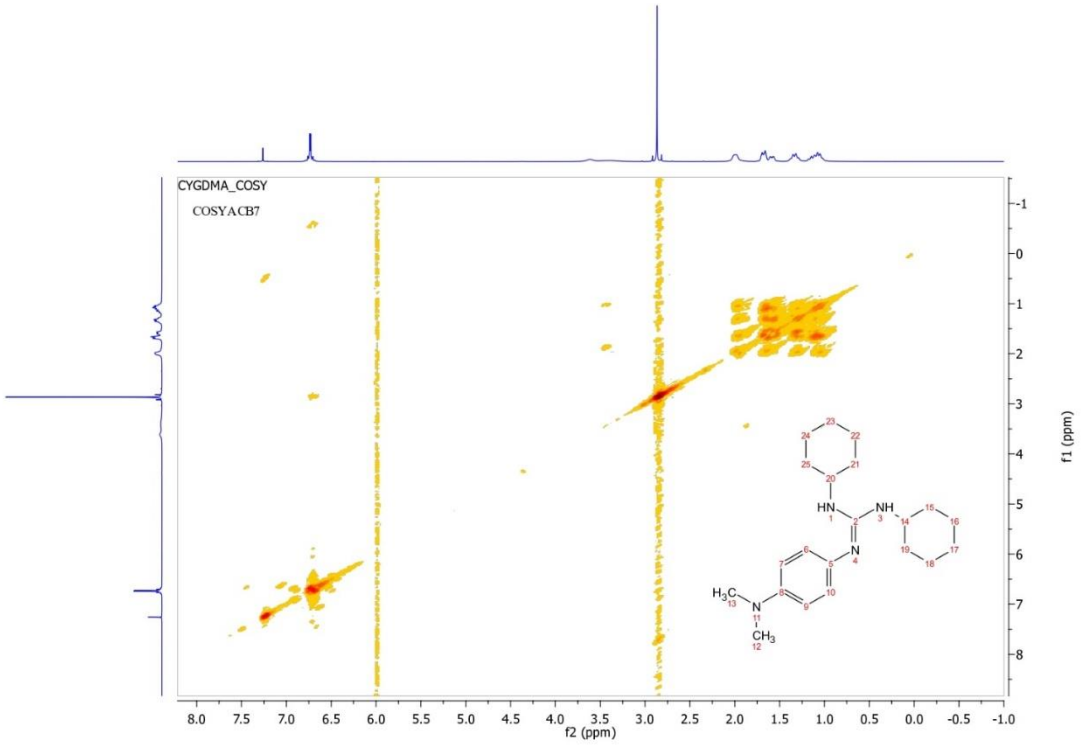
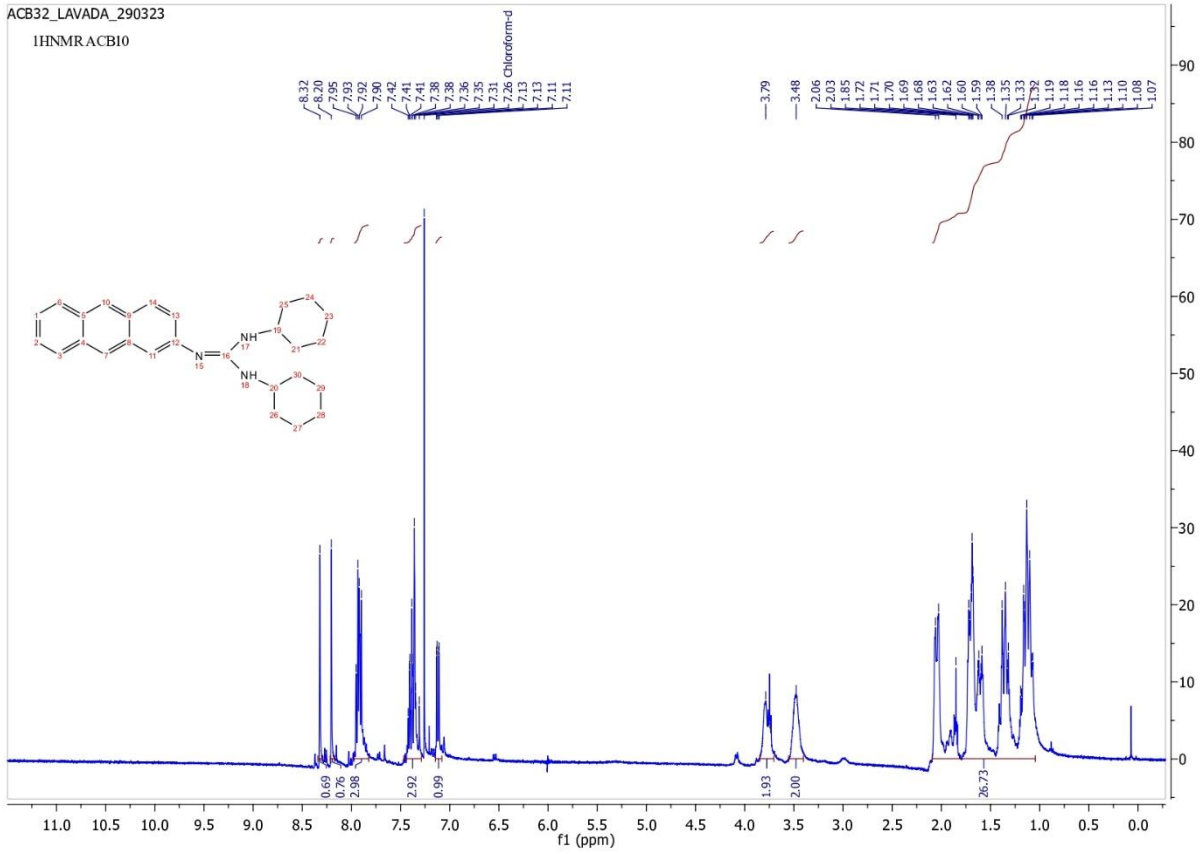
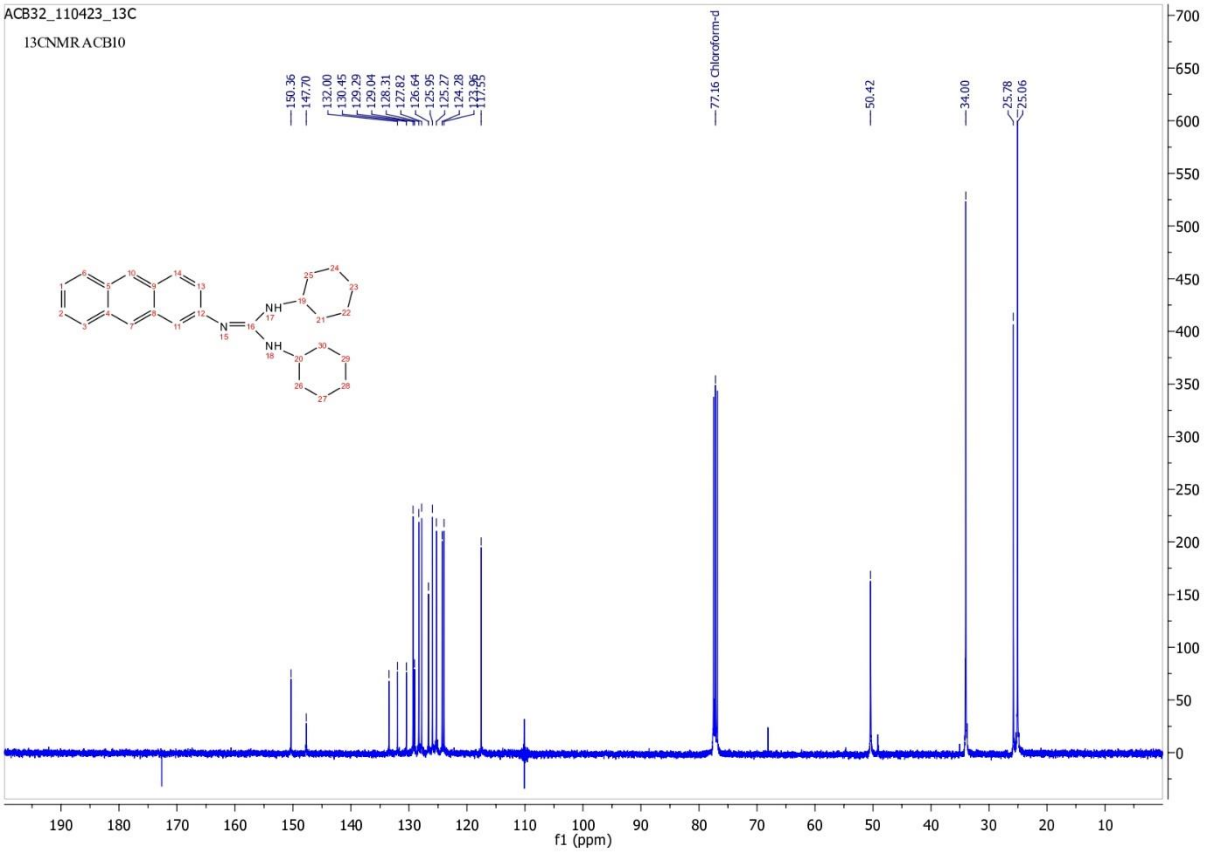


Figure S1. ^{1}H-NMR, ^{13}C-NMR, multinuclear 2D (^{1}H-^{13}C HSQC) and multinuclear 2D (^{1}H-^{1}H COSY) NMR spectra of *ACB7*

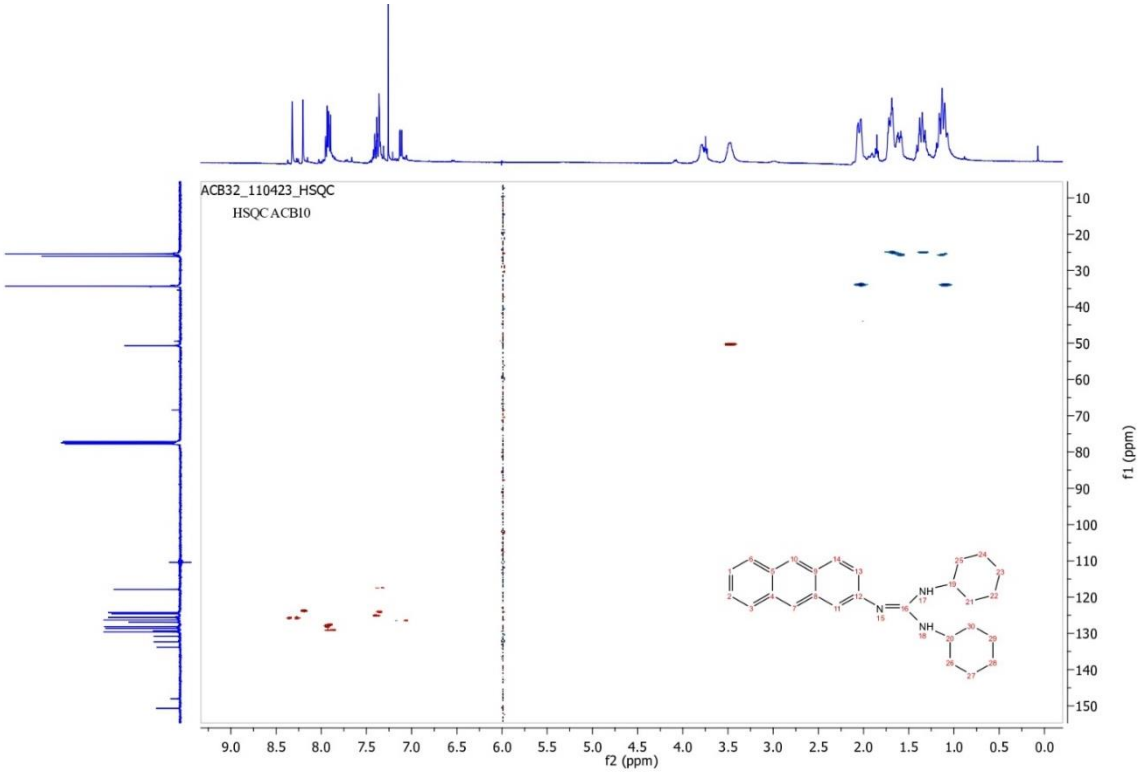
^{1}H-NMR of *ACB10* in $CDCl_3$.



^{13}C-NMR of *ACB10* in $CDCl_3$



Multinuclear 2D (^{1}H-^{13}C HSQC) of *ACB10*.



Multinuclear 2D (^{1}H-^{1}H COSY) of *ACB10*

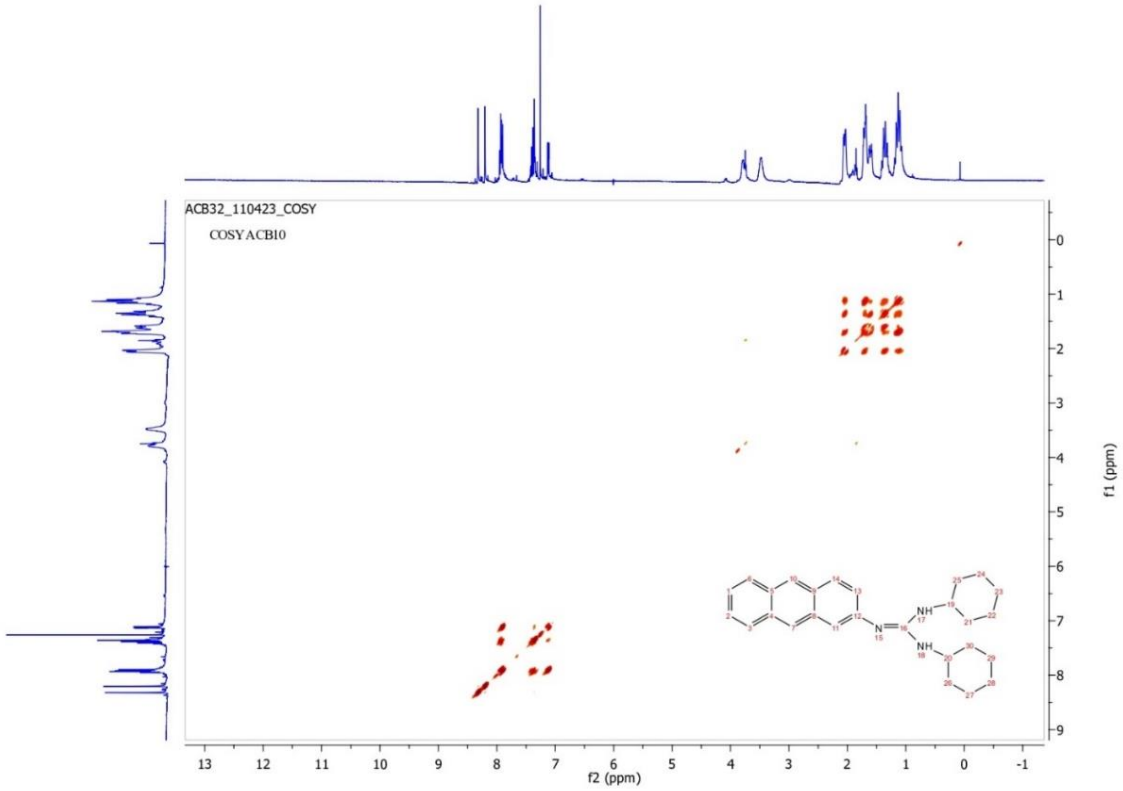


Figure S2. ^{1}H-NMR, ^{13}C-NMR, multinuclear 2D (^{1}H-^{13}C HSQC) and multinuclear 2D (^{1}H-^{1}H COSY) NMR spectra of *ACB10*.

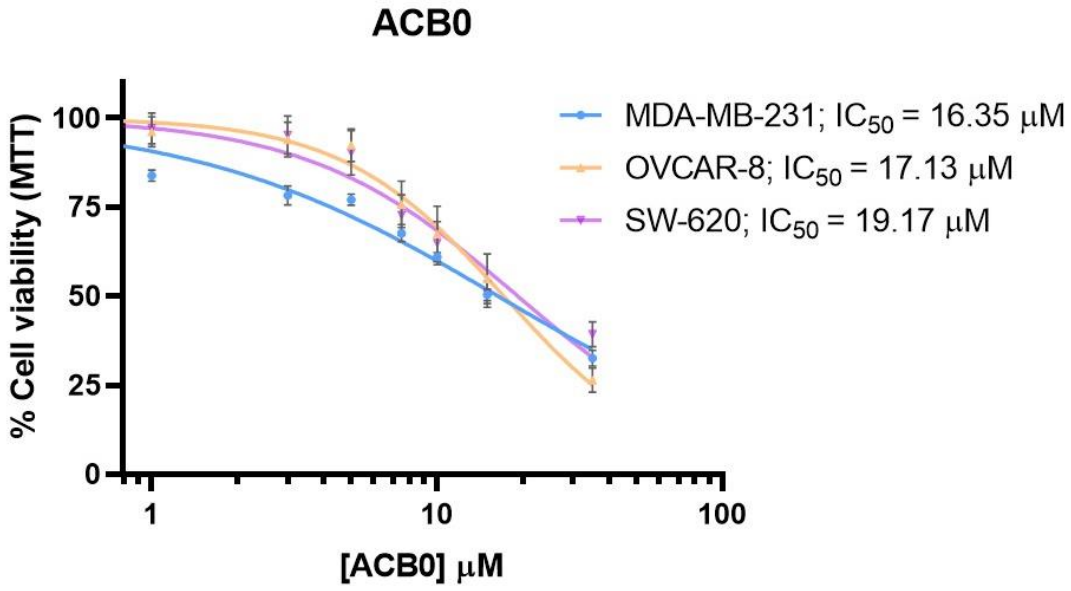


Figure S3. Antiproliferative effect induced by different concentrations of *ACB0* in the indicated cell lines at 72 h tested by MTT assay. Calculation of the concentrations IC50 based on a nonlinear regression curve fit (log(inhibitor) vs. normalized response-variable slope). The mean of three independent experiments (each in triplicate) is plotted together with the standard error (SEM).

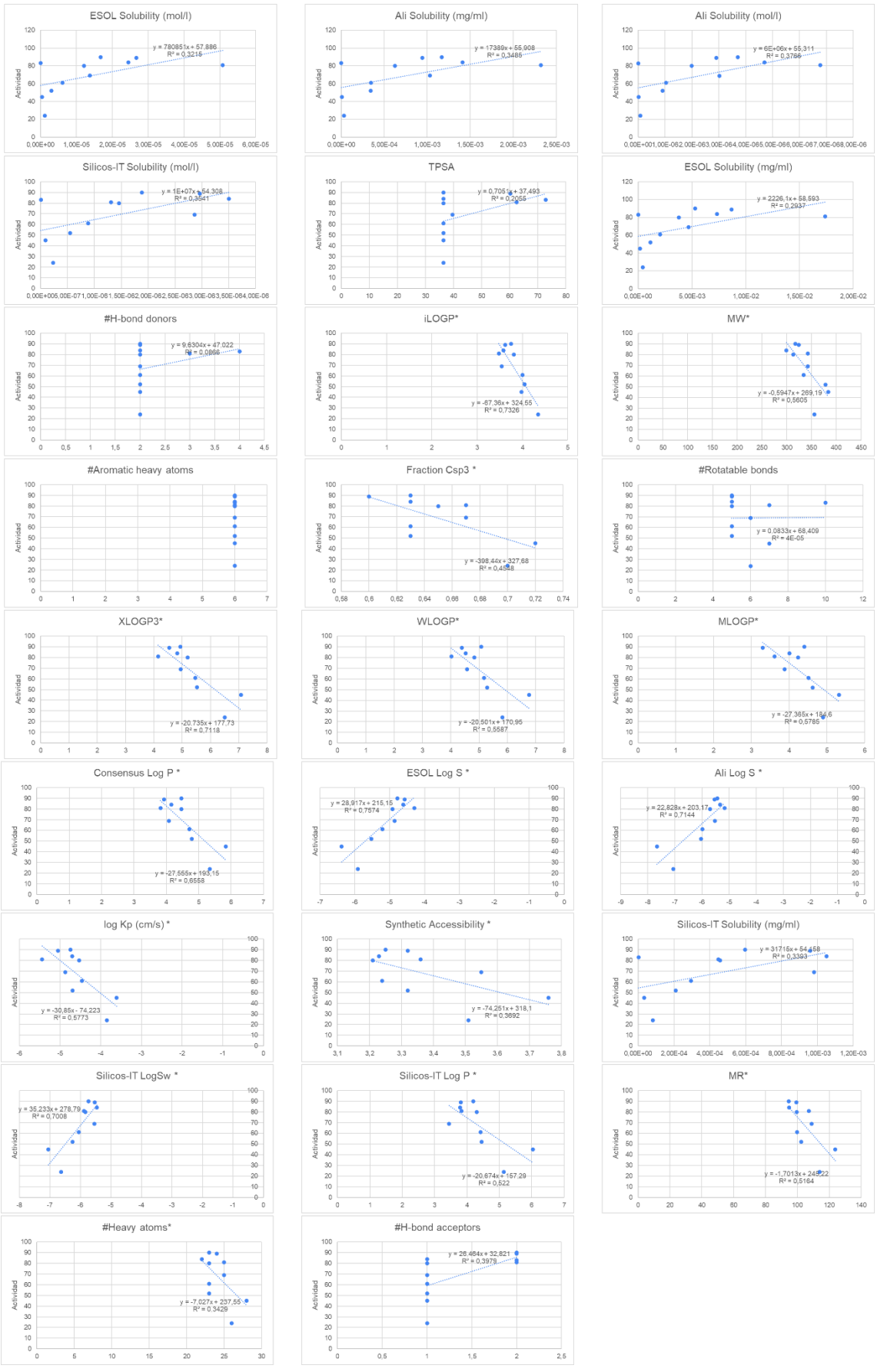


Figure S4: Correlations between ADME parameters.

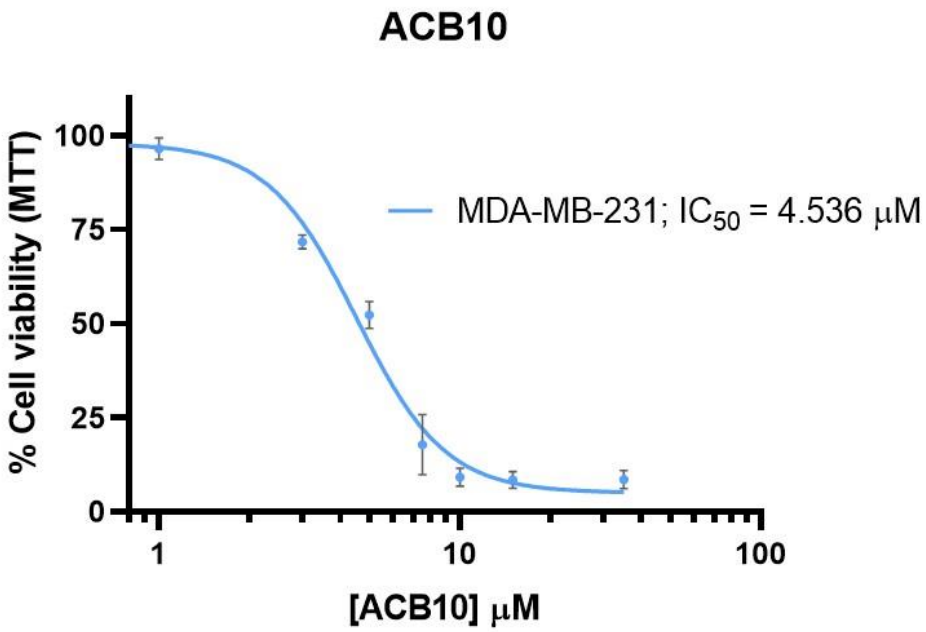


Figure S5: Antiproliferative effect induced by different concentrations of *ACB10* fluorescent guanidine in the MDA-MB-231 cell line at 72 h tested by MTT assay. The inhibitory concentration 50 (IC50) for MDA-MB-231 cell line is shown. Calculation of the concentrations IC50 based on a nonlinear regression curve fit (log(inhibitor) vs. response-variable slope). The mean of three independent experiments (each in triplicate) is plotted together with the standard error (SEM).