Synthesis and Evaluation of Synthetic Retinoid Derivatives as Inducers of Stem Cell Differentiation

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SUPPLEMENTARY INFORMATION

X-ray crystallography.

Single-crystal diffraction experiments were carried out on Bruker 3-circle diffractometers with CCD area detectors SMART 1K (**2a**, **6**, **7b**) 6K (**1**, **7a**) and APEX ProteumM (**3**), using graphite-monochromated radiation from a sealed tube or (for **3**) a 60W microfocus Bede Microsource with glass polycapillary optics. Crystals were cooled using Cryostream (Oxford Cryosystems) open-flow N_2 cryostats. For **1** data were corrected for absorption by semi-empirical method based on Laue equivalents[S1] (transmission factors T=0.376 to 0.455), for **6** by numerical integration based on crystal face-indexing (T=0.588 to 0.727). The structures were solved by direct methods and refined by full-matrix least squares against F^2 of all data, using SHELXTL software.[S2] Non-hydrogen atoms were refined in anisotropic and H atoms in isotopic approximation (methyl groups in **1** and all H atoms in **7a** were treated in "riding" model). Absolute structures of **1** and **2a** were determined from

anomalous dispersion by refining the Flack coefficient (x=−0.013(6) and 0.10(9), respectively).[S3] Full crystallographic data is available in CIF format (CCDC deposition numbers ??????−??????).

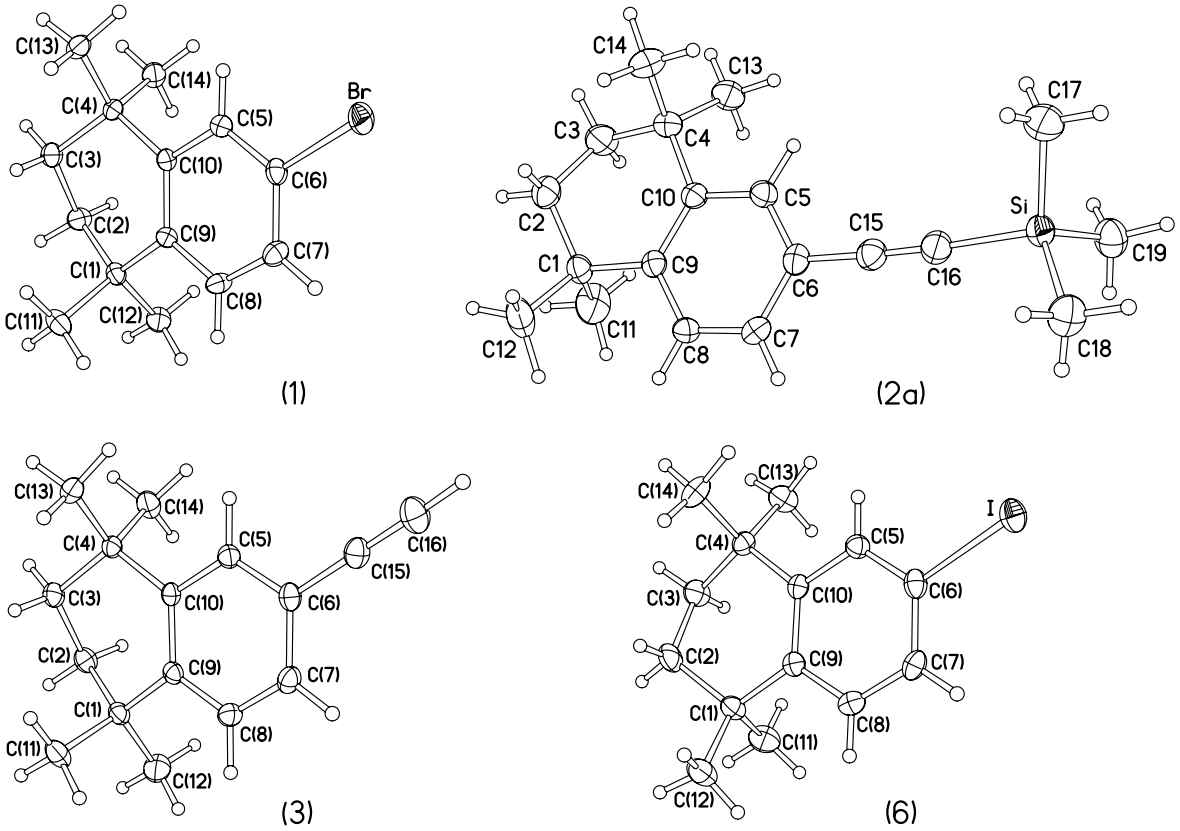

Figure S1. X-ray molecular structures of **1**, **2a**, **3** and **6**. Thermal ellipsoids are drawn at the 50% probability level. Selected bond distances (Å): C(6)-Br 1.904(1) [**1**], C(6)-I 2.104(2) [**6**], Si-C(16) 1.8374(15), C(6)-C(15) 1.443(2) [**2a**] and 1.4442(14) [**3**], C(15)-C(16) 1.200(2) [**2a**] and 1.1789(16) [**3**]

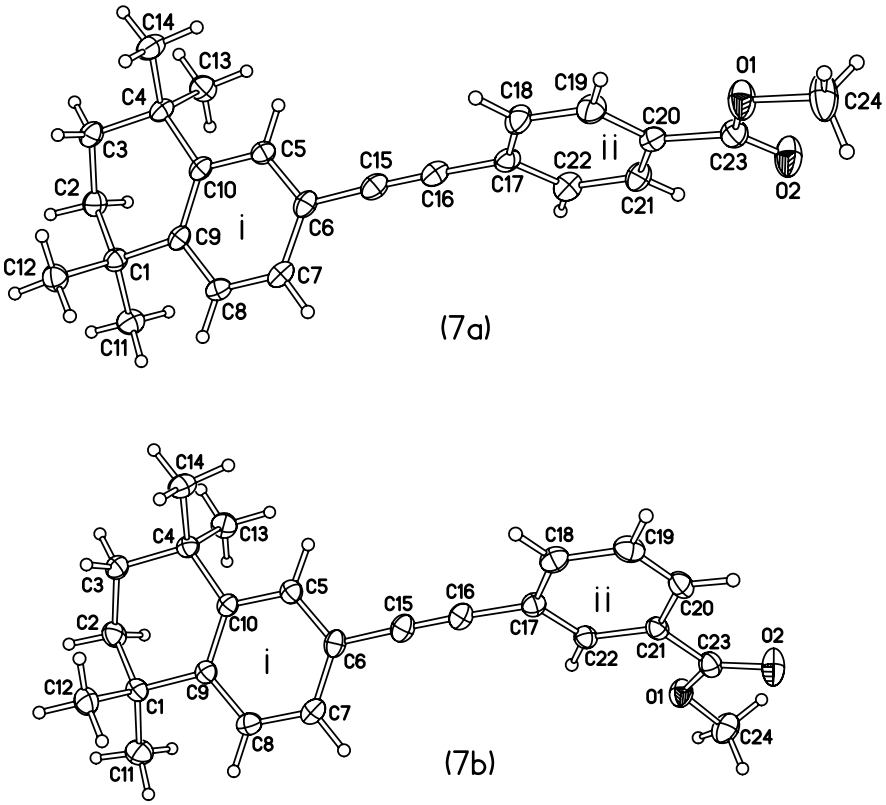

Figure 2. X-ray molecular structures of **7a** and **7b**. Thermal ellipsoids are drawn at the 50% probability level. Interplanar angles (°) between rings *i* and *ii* equal 69.3 [**7a**] and 56.7 [**7b**], between ring ii and methoxycarbonyl group 6.4 [**7a**] and 9.6 [**7b**]; Torsion angle C(7)-C(6)···C(17)-C(22) 66.2(2) [**7a**] and 55.3(2) [**7b**].

References

S1. G. M. Sheldrick, *SADABS*, version 2.10; Bruker-Nonius AXS, Madison, Wisconsin, U.S.A., **2003**.

S2. G. M. Sheldrick, *SHELXTL*, version 6.14; Bruker-Nonius AXS, Madison, Wisconsin, U.S.A., **2003**.

S3. (a) H. D. Flack, *Acta Crystallogr. Sect. A,* **1983**, *39*, 876-881; (b) H. D.Flack and G. Bernardinelli, *J. Appl. Cryst*., **2000**, *33,* 1143-1148.