## Supporting information for

## Addition of TMSCN to Chiral Ketimines Derived from Isatine. Synthesis of an Oxindole-based Peptidomimetic and of a Bioactive Spirohydantoine.

Alessandro Sacchetti, \*<sup>a</sup> Alessandra Silvani, \*<sup>b</sup> Francesco G. Gatti,<sup>a</sup> Giordano Lesma,<sup>b</sup> Tullio Pilati<sup>c</sup> and Beatrice Trucchi<sup>b</sup>

General	<b>S</b> 2
NMR spectra of compound 4	<b>S</b> 3
NMR spectra of compound 5	<b>S</b> 4
NMR spectra of compound 6	<b>S</b> 5
NMR spectra of compound <b>7a</b>	<b>S</b> 6
NMR spectra of compound 8a,b	<b>S</b> 7
NMR spectra of compound 9a,b	<b>S</b> 8
NMR spectra of compound 10a	<b>S</b> 9
NMR spectra of compound 10b	<b>S</b> 10
NMR spectra of compound 11a	S11
NMR spectra of compound 11b	S12
NMR spectra of compound 12	S13
NMR spectra of compound 14	<b>S</b> 14
NMR spectra of compound 15a	S15
NMR spectra of compound 16a	<b>S</b> 16
NMR spectra of compound 16b	S17
NMR spectra of compound 17	<b>S</b> 18
NMR spectra of compound 19	<b>S</b> 19
NMR spectra of compound 20a,b	S20
NMR spectra of compound <b>21a,b</b>	S21
NMR spectra of compound 3	S22
Crystallographic data for <b>10a</b>	S23

## **General methods**

All solvents were distilled and properly dried, when necessary, prior to use. All chemicals were purchased from commercial sources and used directly, unless indicated otherwise. All reactions were run under N<sub>2</sub>, unless otherwise indicated. All reactions were monitored by thin layer chromatography (TLC) on precoated silica gel 60 F<sub>254</sub>; spots were visualized with UV light ( $\lambda$ = 254 nm,  $\lambda$  = 365 nm) or by treatment with 1% aqueous alkaline KMnO<sub>4</sub> solution. Products were purified by flash chromatography on silica gel 60 (230-400 mesh). <sup>1</sup>H and <sup>13</sup>C NMR spectra were performed at room temperature on 300 and 400 MHz spectrometers. Chemical shifts ( $\delta$ ) are expressed in ppm relative to TMS at  $\delta$  = 0 ppm for <sup>1</sup>H NMR and relative to CDCl<sub>3</sub> at  $\delta$  = 77.16 ppm for <sup>13</sup>C NMR. High-resolution MS spectra were recorded with a FT-ICR (Fourier Transform Ion Ciclotron Resonance) instrument, equipped with an ESI source, or a standard MS instrument, equipped with an EI source.IR spectra were recorded using a FTIR instrument.





Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry This journal is C The Royal Society of Chemistry 2011



















 $^{1}$ H NMR and  $^{13}$ C NMR spectra of compound **12** 













<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **19** 





Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry This journal is The Royal Society of Chemistry 2011









Crystallographic data for 10a

 $2(C_{23}H_{32}N_3O_3Si)$ . $H_2O$ ,  $M_r = 869.21$ , monoclinic,  $P2_1$ , a = 16.4115(13), b = 8.1684(5), c = 17.6258(13) Å,  $\beta = 96.614(3)$ , V = 2347.1(3) Å<sup>3</sup>, Z = 2,  $D_c = 1.230$  gcm<sup>-3</sup>,  $\mu$ (Mo-K $\alpha$ )= 0.131 cm<sup>-1</sup>, F(000) =932, prism, 0.36x0.15x0.10 mm, Bruker APEX2000 diffractometer; 30501 data collected, 10530 unique,  $R_{\text{int}} = 0.0256$ , 9185 with  $I_0 > 2\sigma(I_0)$ . The structure was solved by direct method,<sup>1</sup> and refined anisotropically by matrix least-squares based on  $F^{2,2}$ . The asymmetric unit contains two independent molecules of 10a and a solvated water molecule; in one of the two molecules of 10a, the oxytrialkylsilane group is rotationally disordered and was refined by two equi-populated models restrained to have about the same geometry; H atoms were riding in calculated position. The final refinement was on 642 parameters and 187 restraints. The results for all reflections were  $R_1$ = 0.0467,  $wR_2$ = 0.0896, goodness-of-fit 1.028; residues on the final map were from -0.26 to 0.54 e.Å<sup>-</sup> <sup>3</sup>. The absolute configuration was established by anomalous dispersion [Flack parameters = 0.06(8)] and on the basis of the known R configuration on the phenylglycinol residue. The Supplementary crystallographic data were deposited as CCDC 816608. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K, e-mail deposit@ccdc.cam.ac.uk

1. M.C. Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna (2003). J. Appl. Cryst. 36,1103

2. Sheldrick, G. M. (2008). Acta Cryst., A64, 112-122.

