Preliminary study of a 1,5-benzodiazepine-derivative labelled with indium-111 for CCK-2 receptors targeting.

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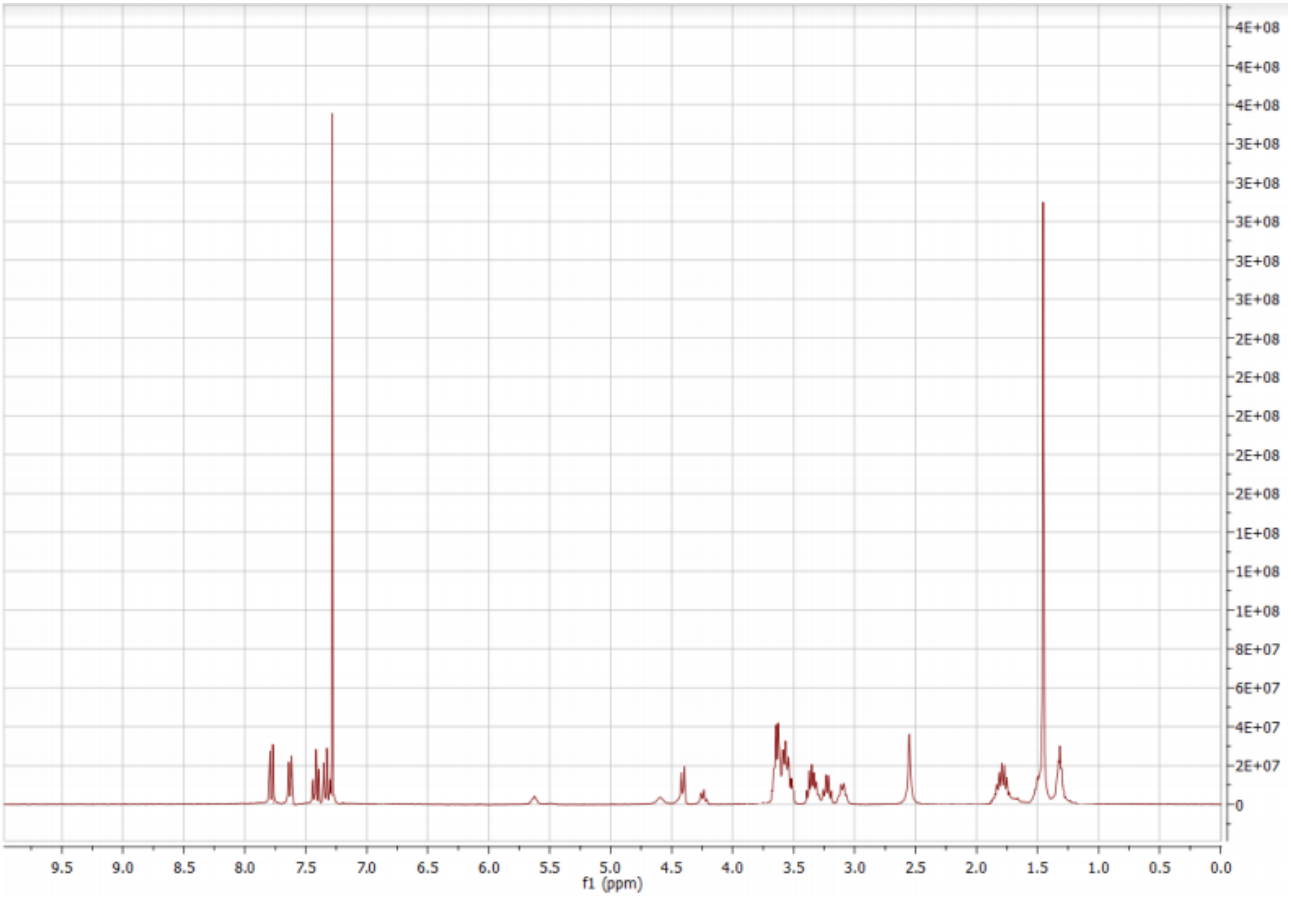

Figure S1. ^{1}H-NMR spectrum of **3** in $CDCl_3$ at 25 °C.

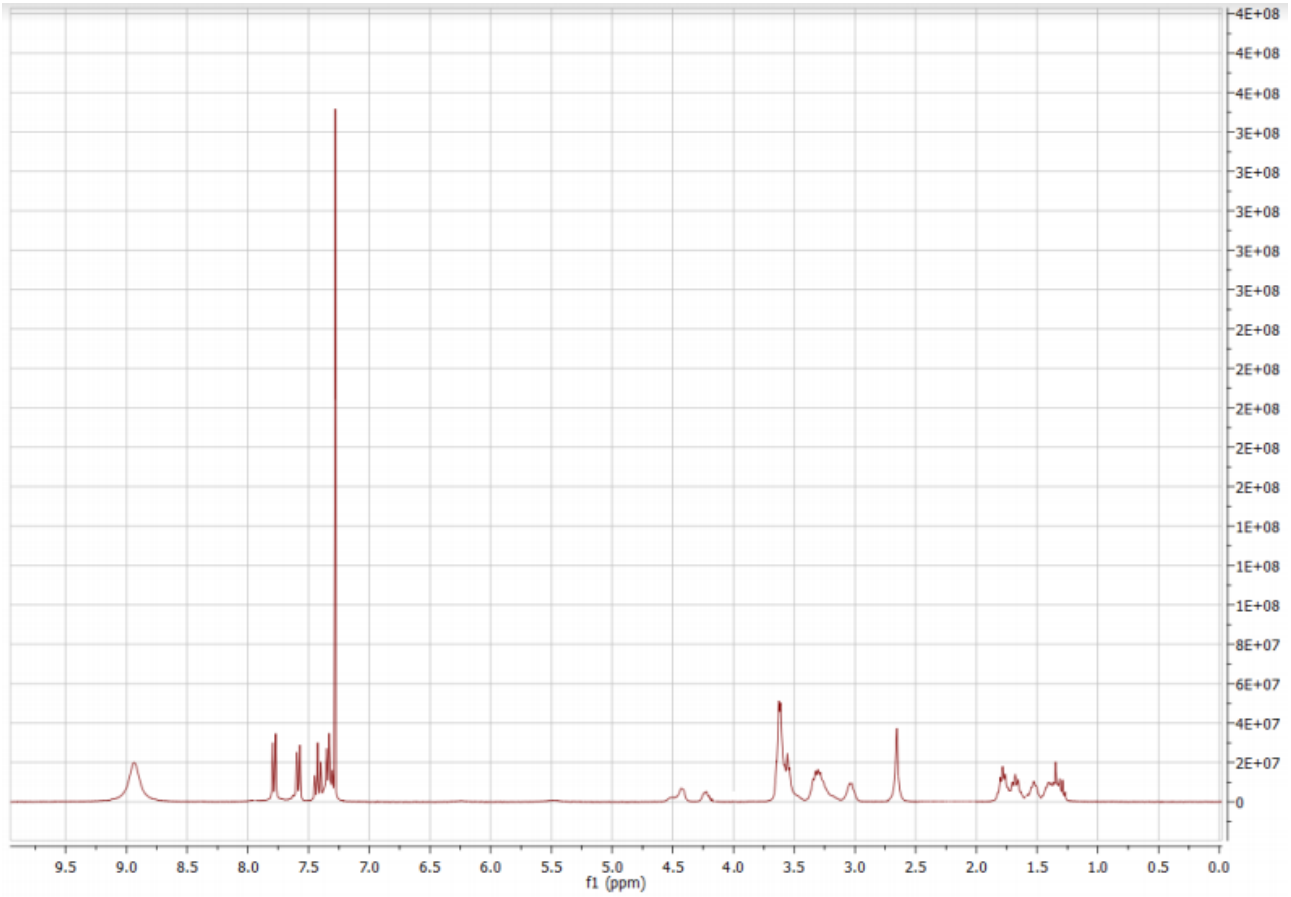

Figure S2. ^{1}H-NMR spectrum of **4** in $CDCl_3$ at 25 °C.

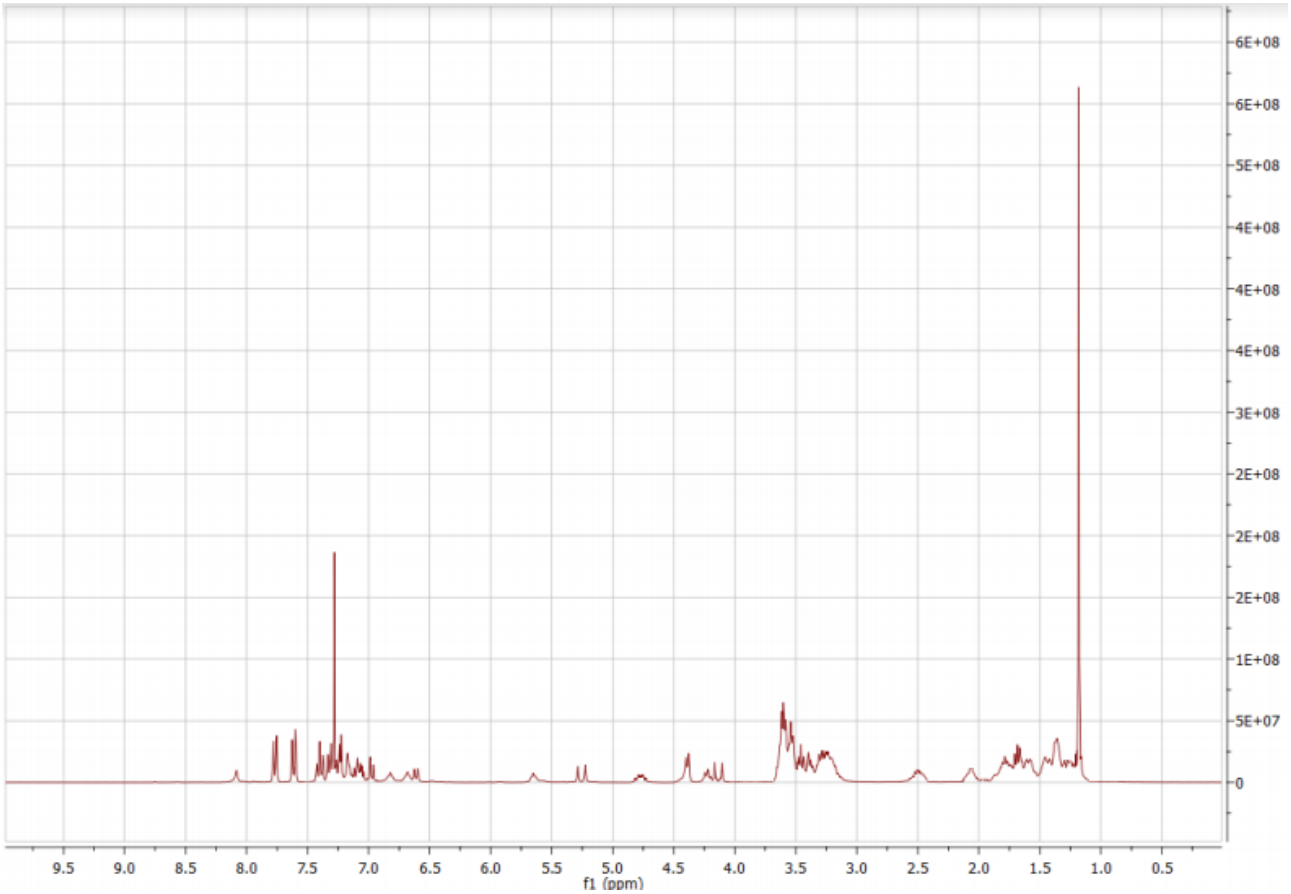

Figure S3. ^{1}H-NMR spectrum of **6** in $CDCl_3$ at 25 °C.

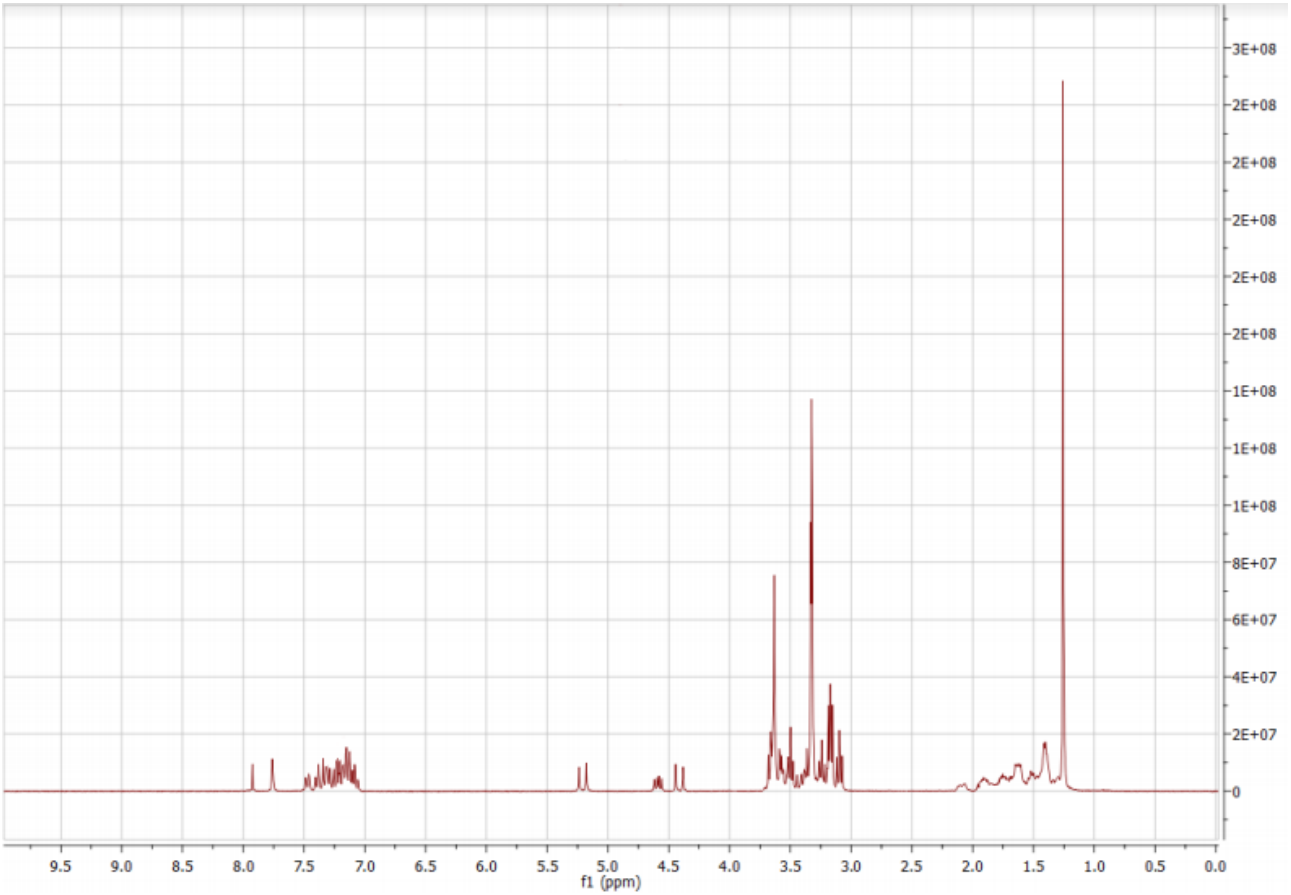

Figure S4. ^{1}H-NMR spectrum of **7** in $CDCl_3$ at 25 °C.

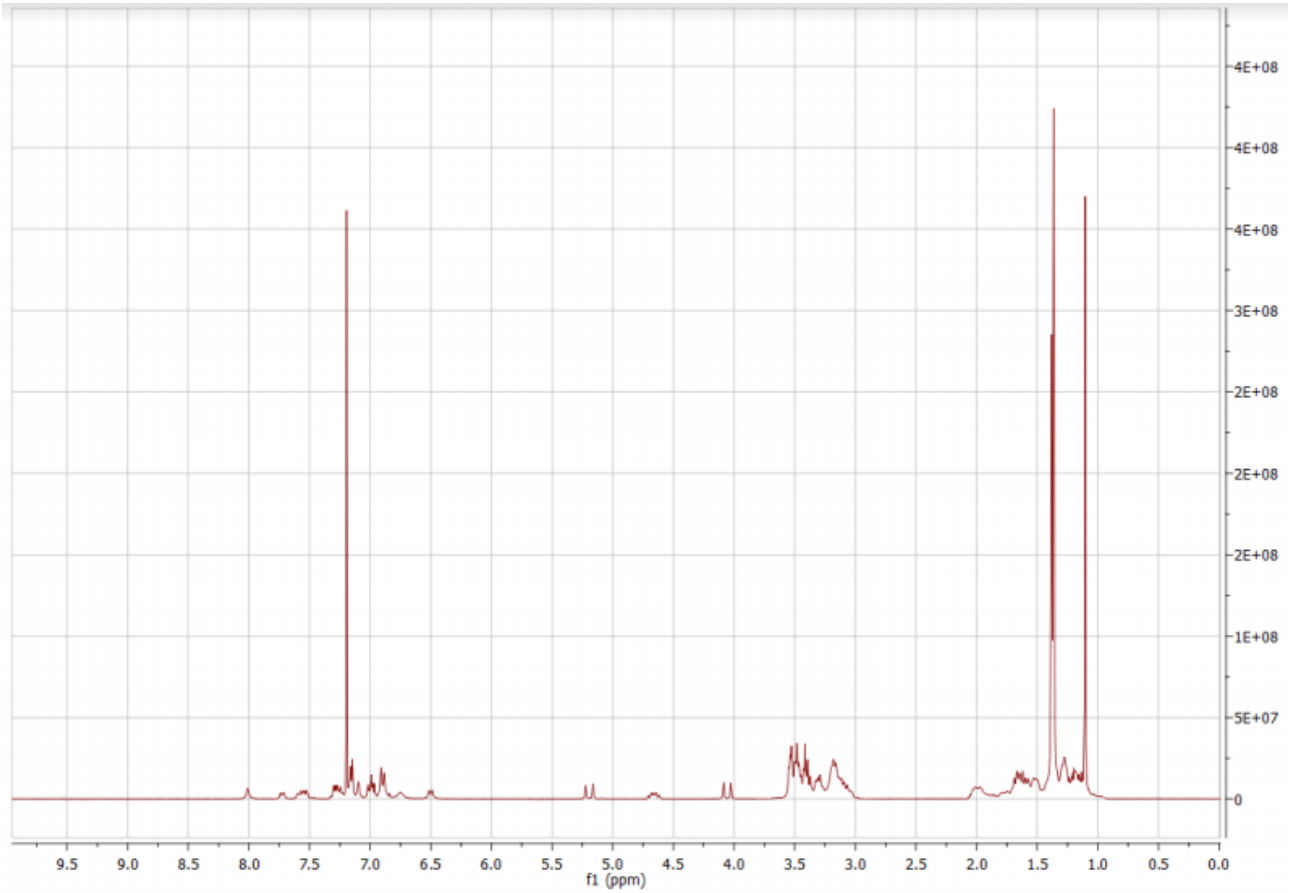

Figure S5. ^{1}H-NMR spectrum of **8** in $CDCl_3$ at 25 °C.

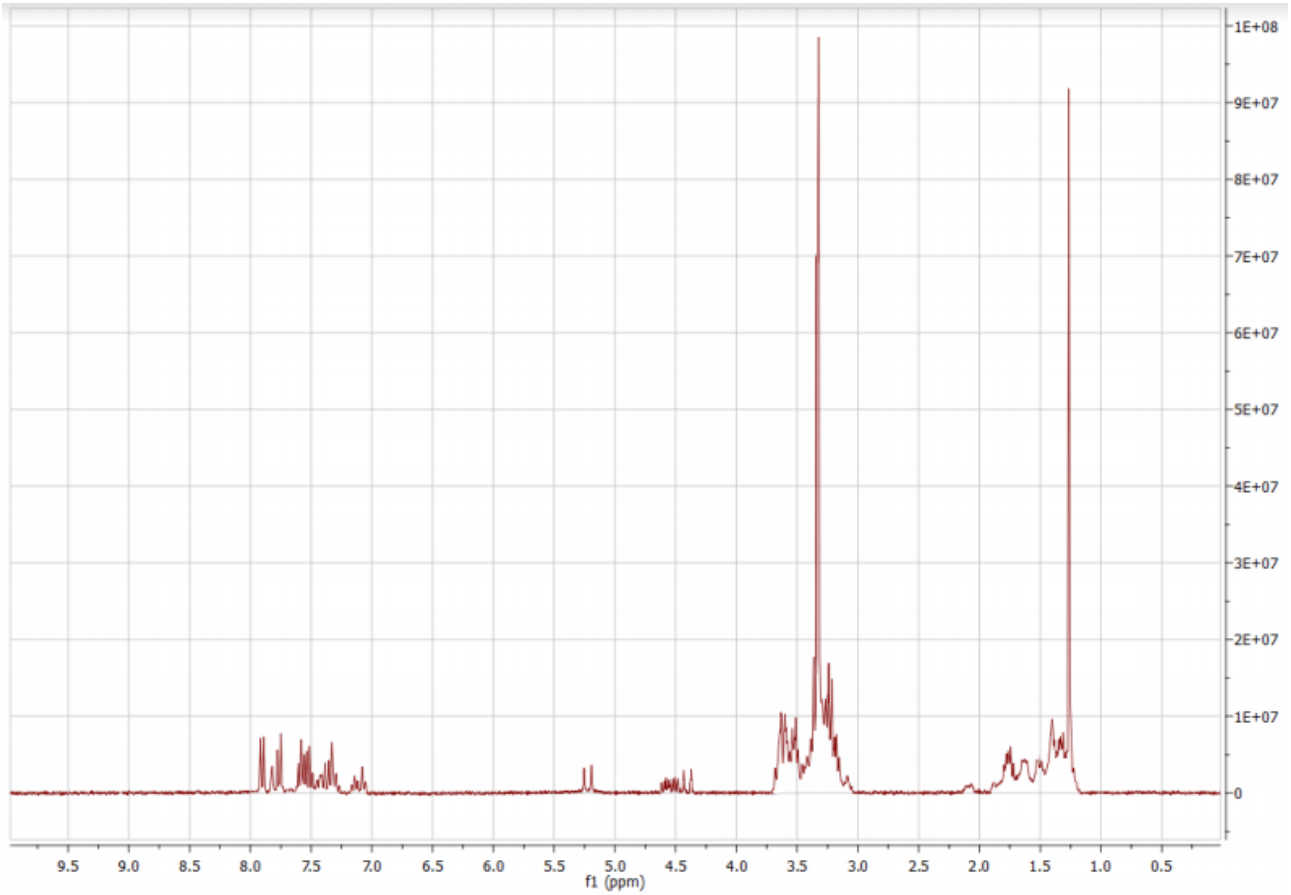

Figure S6. ^{1}H-NMR spectrum of **IP-001** in MeOD-d_4 at 25 °C.

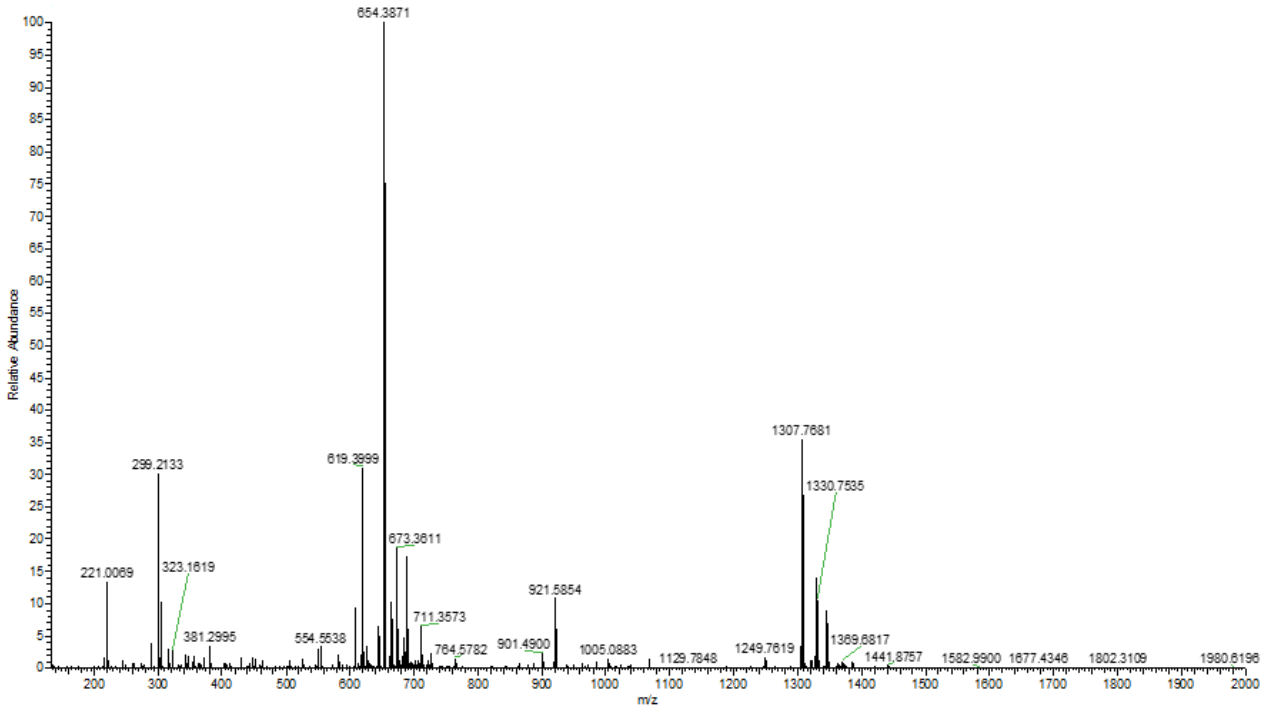

Figure S7. HRMS analysis of **IP-001.** m/z = 1307.76 [M+H$^+$]; m/z = 654.38 [M+2H$^+$]; m/z = 921.58 [M-DOTA]; m/z = 619.39 [M+H$^+$ of **7**, originating from fragmentation of **IP-001**].

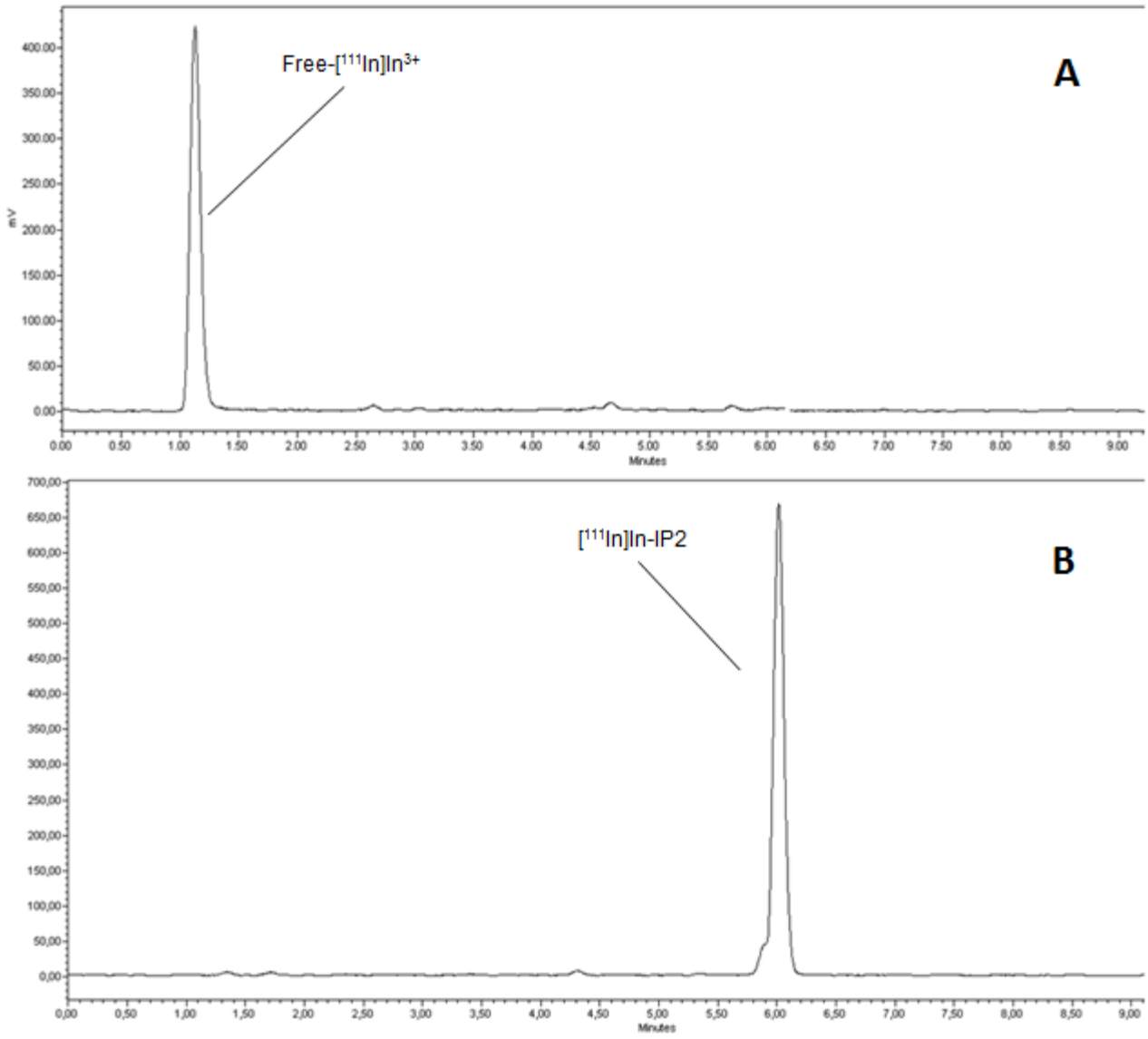

Figure S8. Representative RP-HPLC chromatograms of free [111 In]In3+ (**A**) and [111In]In-IP-001 (**B**). Rt: free-[111In]In3+ = 1.1 minutes; [111In]In-IP-001 = 6.0 minutes.

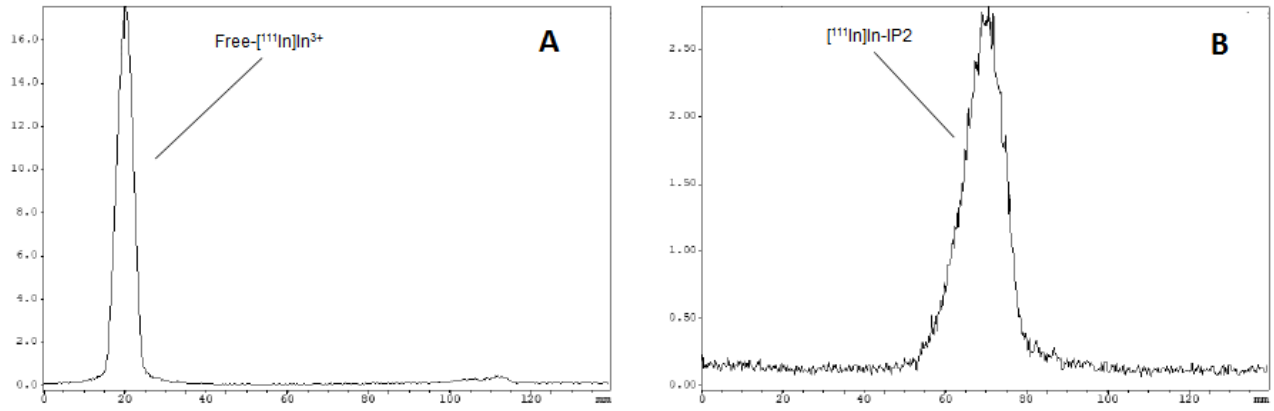

Figure S9. Representative radio-TLC chromatograms of free-[^{111}In]In^{3+} (**A**) and [^{111}In]In-IP-001 (**B**).

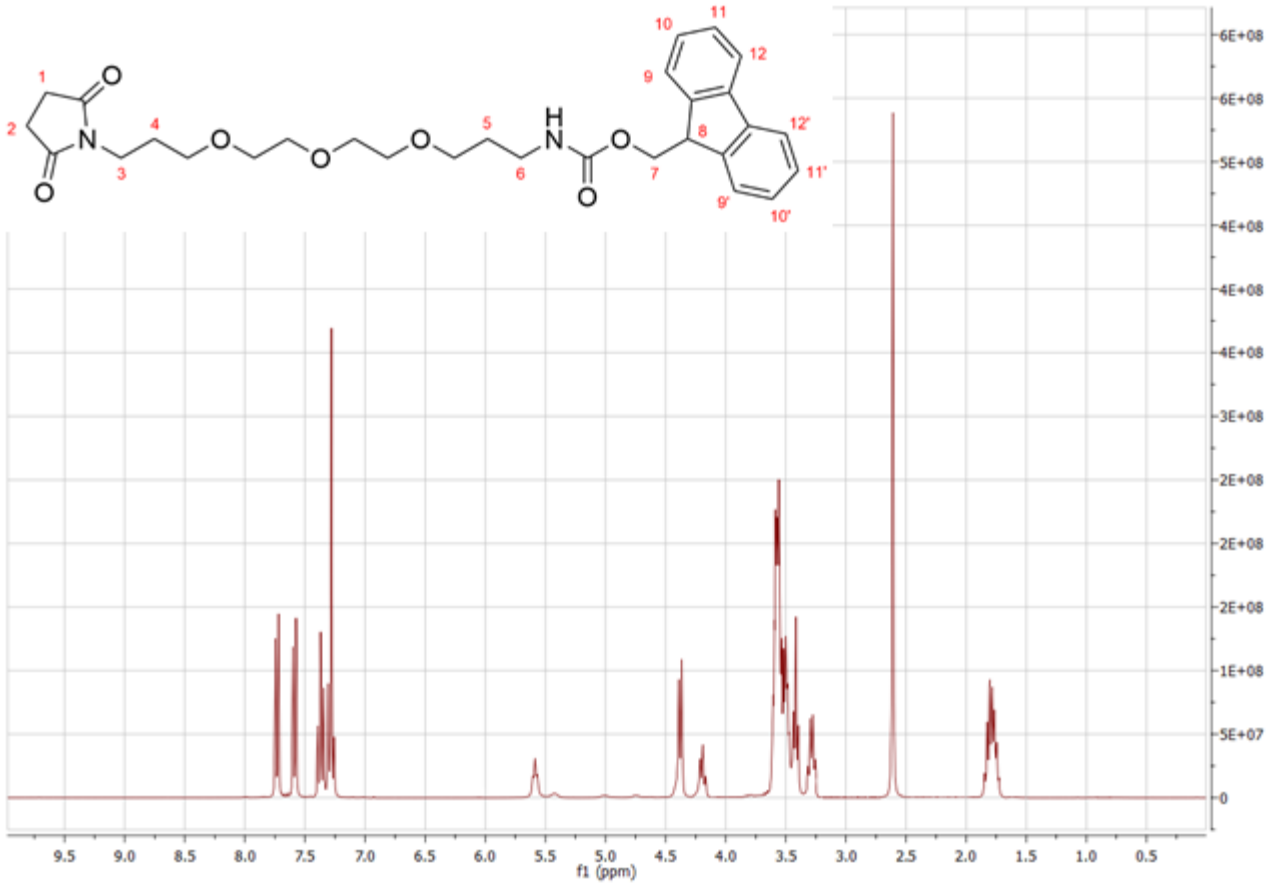

Figure S10. ^{1}H-NMR spectrum in $CDCl_3$ of the compound due to the cyclization of the succinyl- group of compound **2.** ^{1}H-NMR (400 MHz, $CDCl_3$) δ ppm 7.71 (d, *J*=7.4, 2H); 7.57 (d, *J*=7.4, 2H); 7.35 (t, *J*=7.3, 2H); 7.36 (t, *J*=7.3, 2H); 5.57 (t, *J*=5.4, 1H); 4.42-4.32 (m, 2H); 4.22-4.14 (m, 1H); 3.60-3.44 (m, 12H); 3.39 (t, *J*=6.4, 2H); 3.26 (q, *J*=6.2, 2H); 2.59 (s, 4H); 1.84-1.70 (m, 4H).