Supplementary information for:

## Chlorantraniliprole

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**Materials and Methods.** All air or moisture sensitive reactions were conducted in flame-dried glassware, capped with a rubber septum and stirred with Teflon-coated magnetic stir bars under an atmosphere of nitrogen. All liquid reagents and solvents were transferred via syringe using standard Schlenk technique. Tetrahydrofuran (THF) was degassed and dried by passage over a column of activated alumina. All other solvents and reagents were used as received. Melting points were measured on a Buchi melting point apparatus and were corrected using vanillin (mp 80-81 °C) as a standard. <sup>1</sup>H and <sup>13</sup>C NMR shifts ( $\delta$ ) are reported in ppm relative to the residual solvent signal (DMSO-d<sub>6</sub>:  $\delta = 2.50$  for <sup>1</sup>H NMR spectra and  $\delta = 39.5$  ppm for <sup>13</sup>C NMR spectra). Data for <sup>1</sup>H spectra are reported as follows: chemical shifts (multiplicity, coupling, integration). Abbreviations are as follows: s = singlet, d=doublet, dd = doublet of doublets. IR spectra were recorded on a Nicolet MAGNA-IR 850 spectrometer as thin films on NaCl plates and are reported in frequency of absorption (cm<sup>-1</sup>). High-resolution mass spectral data were obtained from the University of California, Berkeley Mass Spectral Facility, on a VG Prospec Micromass spectrometer for EI.

## **Spectral Data**

Desmethyl-Chlo



<sup>1</sup>H NMR (500 MHz, dimethylsulfoxide- $d_6$ ) δ 10.30 (s, 1H), 8.50 (dd, J = 4.8, 1.3 Hz, 1H), 8.17 (d, J = 8.0, 1.5 Hz, 1H), 7.77 (s, 1H), 7.61 (dd, J = 8.0, 4.5 Hz, 1H), 7.51 (s, 1H), 7.47 (d, J = 2.0 Hz, 1H), 7.40 (d, J = 2.0 Hz, 1H), 7.37 (s, 1H), 2.14 (s, 3H)



<sup>13</sup>C NMR (125 MHz, dimethylsulfoxide-*d*<sub>6</sub>) δ 167.6, 155.7, 148.3, 147.2, 139.5, 139.3,
138.9, 135.6, 131.6, 131.3, 130.9, 127.7, 126.8, 126.6, 125.5, 110.7, 17.7

Supplementary information for:

Structure of Three Candidate Anthranilic Diamide Radioligands Reported Without Synthesis Procedures or Specific Activities



- Cordova, D., Benner, E. A., Sacher, M. D., Rauh, J. J., Sopa, J. S., Lahm, G. P., Selby, T. P., Stevenson, T. M., Flexner, L., Gutteridge, S., Rhoades, D. F., Wu, L., Smith, R. M., and Tao, Y. (2006) *Pestic. Biochem. Physiol.* 84, 196-214.
- (2) Lahm, G.P., Cordova, D., Barry, J.D., Andaloro, J.T., Annan, B., Marcon, P.C., Portillo, H.E., Stevenson, T.M., and Selby, T.P. (2012) Anthranilic Diamide Insecticides: Chlorantraniliprole and Cyantraniliprole. In *Modern Crop Protection Compounds* 2<sup>nd</sup> edition (Kramer, W., Schirmer, U., Jeschke, P., and Witschel, M., Eds.) 1-3, pp 1409-1425, *Wiley-VCH Verlag*, Weinheim, Germany.
- (3) Gnamm, C., Jeanguenat, A., Dutton, A. C., Grimm, C., Kloer, D. P., and Crossthwaite, A. J. (2012) *Bioorg. Med. Chem. Lett.* 22, 3800-3806.