

Supporting Information

Relationship between urinary *N*-desmethyl-acetamidiprid and typical symptoms including neurological findings: A prevalence case-control study

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S3 Table. Physicochemical characteristics of neonicotinoid insecticides.

| | | | | Solubility (g/L) | | |
|---------------------|-----------|---|-----------------------|-------------------------|----------------|----------------|
| | MW | pK_a of conjugate acid | pK_a | Water (pH 7) | Octanol | Acetone |
| Thiamethoxam | 291.7 | N/A | N/A | 4.1 | 0.62 | 48 |
| Clothianidin | 249.7 | N/A | 11.1 | 0.327 | 1.64 | 15.2 |
| Acetamiprid | 222.7 | 0.7 | N/A | 2.95 | 18.5 | >200 |
| Imidacloprid | 255.7 | 1.56 | 11.1 | 0.48 | 0.78 | 47 |
| Thiacloprid | 252.7 | N/A | N/A | 0.185 | 3.36 | 64 |
| Nitenpyram | 270.7 | 3.1 | 11.5 | 840 | 192 | 290 |
| Dinotefuran | 202.2 | N/A | 12.6 | 40 | - | 58 |
| Sulfoxaflor | 277.3 | N/A | N/A | 0.568 | 1.66 | 217 |

Note: pK_a stands for the acid dissociation constant of the molecule (M) or the conjugated acid (MH⁺). N/A stands for not available. Although pK_a of conjugated acid are not known for thiamethoxam, clothianidin or thiacloprid, they theoretically exist because pseudo-molecule ions [MH⁺] of those NN are monitored in the positive mode by electrospray ionization mass spectrometry.

Reference:

US Environmental Protection Agency (USEPA) Factsheet-Acetamiprid. 2002.

National Pesticide Information Center. 1.800.858.7378. Imidacloprid Technical Fact Sheet A Rule by the US Environmental Protection Agency (USEPA) on 03/02/2012.

Thiamethoxam; Pesticide Tolerance. Fed Regist 78:18512-18513

US Environmental Protection Agency (USEPA) Factsheet-clothianidin.2003.

US Environmental Protection Agency (USEPA) Factsheet-thiacloprid. 2003.

US Environmental Protection Agency (USEPA) Factsheet-dinotefuran. 2004.