

SUPPLEMENTARY INFORMATION

A critical assessment of pharmaceutical photodegradation in aquatic environments:

Defining our current understanding and identifying knowledge gaps

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Table S1A-G: Complete list of rubric-evaluated studies (120 total studies) and their respective lab/field scores, organized by compound class, in alphabetical order. Means and standard errors for lab/field scores can be plotted for a given compound to produce scoring plots.

Table S1A: Antibiotics

| Antibiotic | Data Type and Source | | Score | | | | | |
|------------------------|----------------------|---------------------|--------------|--------|----------|----------------|-------|-------|
| | Lab/Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total | |
| Antimicrobial | | | | | | | | |
| Triclocarban | Lab | Ding, 2013 | 13 | 14 | 8 | -- | 35 | |
| | | Guerard, 2009 | 11 | 10 | 18 | -- | 39 | |
| | | <i>Mean (SE)</i> | | | | | | 37(2) |
| Triclosan | Lab | Chen, 2010 | 9 | 11 | -- | -- | 20 | |
| | | Latch, 2005 | 15 | 8 | 13 | -- | 36 | |
| | | Sanchez-Prado, 2006 | 13 | 9 | 11 | -- | 33 | |
| | | Tixier, 2002 | 10 | 13 | 11 | -- | 34 | |
| | | <i>Mean (SE)</i> | | | | | | 31(4) |
| | | <i>Mean (SE)</i> | | | | | | 31(4) |
| | Field | Latch, 2005 | 16 | 8 | 7 | 3 | 34 | |
| | | Lindstrom, 2002 | 8 | 5 | 8 | 5 | 26 | |
| Tixier, 2002 | | 11 | 7 | 3 | 5 | 26 | | |
| <i>Mean (SE)</i> | | | | | | 29(3) | | |
| β-Lactam | | | | | | | | |
| Amoxicilin | Lab | Xu, 2011 | 13 | 8 | 14 | -- | 35 | |
| | | Zhao, 2013 | 12 | 10 | 14 | -- | 36 | |
| | | <i>Mean (SE)</i> | | | | | | 36(1) |
| Cephalosporin | | | | | | | | |
| Cefazolin | Lab | Wang, 2012 | 15 | 15 | 15 | -- | 45 | |
| | | <i>Mean (SE)</i> | | | | | | 45 |
| Cefazolin | Lab | Wang, 2012 | 15 | 15 | 15 | -- | 45 | |
| | | <i>Mean (SE)</i> | | | | | | 45 |
| Cephalexin | Lab | Wang, 2012 | 15 | 15 | 15 | -- | 45 | |
| | | <i>Mean (SE)</i> | | | | | | 45 |
| Cephapirin | Lab | Wang, 2012 | 15 | 15 | 15 | -- | 45 | |
| | | <i>Mean (SE)</i> | | | | | | 45 |
| Fluoroquinolone | | | | | | | | |
| Balofloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 | |
| | | <i>Mean (SE)</i> | | | | | | 53 |
| Ciprofloxacin | Lab | Babic, 2013 | 22 | 11 | 13 | -- | 46 | |
| | | Belden, 2007 | 15 | -- | 10 | -- | 25 | |
| | | Cardoza, 2005 | 18 | -- | 17 | -- | 35 | |
| | | Ge, 2010 | 16 | 19 | 18 | -- | 53 | |
| | | Lam, 2003 | 15 | 8 | 15 | -- | 38 | |
| | | Torniainen, 1996 | 16 | 10 | -- | -- | 26 | |
| | | Vasconcelos, 2009 | 13 | 10 | -- | -- | 23 | |
| | | Wei, 2013 | 12 | 18 | -- | -- | 30 | |
| | | <i>Mean (SE)</i> | | | | | | 35(4) |
| | | <i>Mean (SE)</i> | | | | | | 35(4) |
| | Field | Cardoza, 2005 | 18 | -- | 9 | 9 | 36 | |
| Sturini, 2012 | | 14 | -- | 7 | 4 | 25 | | |
| Turiel, 2005 | | 16 | 2 | 4 | 3 | 25 | | |
| <i>Mean (SE)</i> | | | | | | | 29(4) | |
| Danofloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 | |
| | | <i>Mean (SE)</i> | | | | | | 53 |
| | Field | Sturini, 2012 | 14 | -- | 7 | 4 | 25 | |

| | | | | | | | |
|--------------------|-------|-----------------------|----|----|-------|-------|-------|
| | | <i>Mean (SE)</i> | | | | | 25 |
| Difloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 |
| | | Prabhakaran, 2009 | 13 | 18 | 12 | -- | 43 |
| | | <i>Mean (SE)</i> | | | | | 48(5) |
| Enoxacin | Lab | Fasani, 1999 | 8 | 8 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| Enrofloxacin | Lab | Babic, 2013 | 22 | 11 | 13 | -- | 46 |
| | | Ge, 2010 | 16 | 19 | 18 | -- | 53 |
| | | Sturini, 2010 | 20 | -- | 11 | -- | 31 |
| | | Wammer, 2013 | 13 | 15 | 11 | -- | 39 |
| | | <i>Mean (SE)</i> | | | | | 42(5) |
| | Field | Schmitt-Kopplin, 1999 | 9 | 4 | 5 | 2 | 20 |
| | | Sturini, 2010 | 20 | -- | 6 | 2 | 28 |
| <i>Mean (SE)</i> | | | | | | 24(4) | |
| Flumequine | Lab | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| Gatifloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 |
| | | <i>Mean (SE)</i> | | | | | 53 |
| Levofloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 |
| | | Lam, 2005 | 17 | 10 | 11 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 46(8) |
| | Field | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | Sturini, 2012 | 14 | -- | 7 | 4 | 25 |
| <i>Mean (SE)</i> | | | | | 29(4) | | |
| Lomefloxacin | Lab | Fasani, 1999 | 8 | 8 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| Marbofloxacin | Lab | Sturini, 2010 | 20 | -- | 11 | -- | 31 |
| | | <i>Mean (SE)</i> | | | | | 31 |
| | Field | Sturini, 2010 | 20 | -- | 6 | 2 | 28 |
| | | <i>Mean (SE)</i> | | | | | 28 |
| Moxifloxacin | Field | Sturini, 2012 | 14 | -- | 7 | 4 | 25 |
| | | <i>Mean (SE)</i> | | | | | 25 |
| Norfloxacin | Lab | Babic, 2013 | 22 | 11 | 13 | -- | 46 |
| | | Fasani, 1999 | 8 | 8 | -- | -- | 16 |
| | | Wammer, 2013 | 13 | 15 | 11 | -- | 39 |
| | | <i>Mean (SE)</i> | | | | | 34(9) |
| Ofloxacin | Lab | Wammer, 2013 | 13 | 15 | 11 | -- | 39 |
| | | <i>Mean (SE)</i> | | | | | 39 |
| | Field | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| <i>Mean (SE)</i> | | | | | | 20 | |
| Orbifloxacin | Lab | Morimura, 1995 | 16 | 14 | -- | -- | 30 |
| | | <i>Mean (SE)</i> | | | | | 30 |
| Sarafloxacin | Lab | Ge, 2010 | 16 | 19 | 18 | -- | 53 |
| | | Prabhakaran, 2009 | 13 | 18 | 12 | -- | 43 |
| | | <i>Mean (SE)</i> | | | | | 48(5) |
| Sitafloxacin | Lab | Araki, 2002 | 11 | 12 | 3 | -- | 26 |
| | | <i>Mean (SE)</i> | | | | | 26 |
| Lincosamide | | | | | | | |
| Lincomycin | Lab | Calza, 2013 | 12 | -- | 5 | -- | 17 |
| | | <i>Mean (SE)</i> | | | | | 17 |
| Macrolide | | | | | | | |
| Azithromycin | Lab | Tong, 2011 | 16 | 7 | 9 | -- | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |

| | | | | | | | |
|-----------------------|-------|------------------|----|----|----|-------|-------|
| | Field | Tong, 2011 | 16 | -- | 5 | 3 | 24 |
| | | <i>Mean (SE)</i> | | | | | 24 |
| Clarithromycin | Lab | Calza, 2013 | 12 | -- | 5 | -- | 17 |
| | | Vione, 2009 | 15 | -- | 14 | -- | 29 |
| | | <i>Mean (SE)</i> | | | | | 23(6) |
| Roxithromycin | Lab | Vione, 2009 | 15 | -- | 14 | -- | 29 |
| | | <i>Mean (SE)</i> | | | | | 29 |
| Tylosin | Lab | Werner, 2007 | 10 | 9 | 9 | -- | 28 |
| | | <i>Mean (SE)</i> | | | | | 28 |
| Methoprim | | | | | | | |
| Ormetoprim | Lab | Guerard, 2012 | 12 | 6 | 19 | -- | 37 |
| | | <i>Mean (SE)</i> | | | | | 37 |
| | Field | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| Trimethoprim | Lab | Luo, 2012 | 9 | 9 | 16 | -- | 34 |
| | | Ryan, 2011 | 6 | 13 | 16 | -- | 35 |
| | | Sirtori, 2010 | 11 | 5 | 8 | -- | 24 |
| | | <i>Mean (SE)</i> | | | | | 31(4) |
| | Field | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | Ryan, 2011 | 6 | 13 | 16 | 2 | 37 |
| | | <i>Mean (SE)</i> | | | | 29(5) | |
| Nitrofuran | | | | | | | |
| Furaltadone | Lab | Edhlund, 2006 | 13 | 17 | 10 | -- | 40 |
| | | <i>Mean (SE)</i> | | | | | 40 |
| Furazolidone | Lab | Edhlund, 2006 | 13 | 17 | 10 | -- | 40 |
| | | <i>Mean (SE)</i> | | | | | 40 |
| | Field | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | 19 | |
| Nitrofurantoin | Lab | Edhlund, 2006 | 13 | 17 | 10 | -- | 40 |
| | | <i>Mean (SE)</i> | | | | | 40 |
| Nitroimidazole | | | | | | | |
| Metronidazole | Lab | Dantas, 2010 | 6 | 8 | -- | -- | 14 |
| | | <i>Mean (SE)</i> | | | | | 14 |
| | Field | Dantas, 2010 | 7 | 5 | -- | 2 | 14 |
| | | Wu, 2012 | 16 | 10 | -- | 4 | 30 |
| | | <i>Mean (SE)</i> | | | | 22(8) | |
| Quinolone | | | | | | | |
| Oxolinic acid | Field | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | Turiel, 2005 | 16 | 2 | 4 | 3 | 25 |
| | | <i>Mean (SE)</i> | | | | | 22(3) |
| Sulfonamide | | | | | | | |
| Sulfachloropyridazine | Lab | Boreen, 2005 | 12 | -- | 15 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2005 | 12 | 16 | -- | 2 | 30 |
| | | <i>Mean (SE)</i> | | | | 30 | |
| Sulfadiazine | Lab | Boreen, 2005 | 12 | -- | 15 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2005 | 12 | 16 | -- | 2 | 30 |
| | | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | 25(6) | |
| Sulfadimethoxine | Lab | Boreen, 2005 | 12 | -- | 15 | -- | 27 |
| | | Guerard, 2009 | 11 | 10 | 18 | -- | 39 |

| | | | | | | | |
|-------------------------|-------|--------------------|----|----|----|----|-------|
| | | <i>Mean (SE)</i> | | | | | 33(6) |
| | Field | Boreen, 2005 | 12 | 16 | -- | 2 | 30 |
| | | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | | 25(6) |
| Sulfamerazine | Lab | Boreen, 2005 | 12 | -- | 15 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2005 | 12 | 16 | -- | 2 | 30 |
| | | <i>Mean (SE)</i> | | | | | 30 |
| Sulfamethazine | Lab | Boreen, 2005 | 12 | -- | 15 | -- | 27 |
| | | Garcia-Galan, 2012 | 14 | 7 | 10 | -- | 31 |
| | | <i>Mean (SE)</i> | | | | | 29(2) |
| | Field | Boreen, 2005 | 12 | 16 | -- | 2 | 30 |
| | | <i>Mean (SE)</i> | | | | | 30 |
| Sulfamethizole | Lab | Boreen, 2004 | 14 | -- | 13 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2004 | 15 | 16 | -- | 2 | 33 |
| | | <i>Mean (SE)</i> | | | | | 33 |
| Sulfamethoxazole | Lab | Bonvin, 2013 | 22 | 19 | -- | -- | 41 |
| | | Boreen, 2004 | 14 | -- | 13 | -- | 27 |
| | | Jasper, 2013 | 15 | 9 | 24 | -- | 48 |
| | | Lam, 2005 | 17 | 10 | 11 | -- | 38 |
| | | Moore, 1994 | 7 | 11 | -- | -- | 18 |
| | | Niu, 2013 | 14 | 14 | 12 | -- | 40 |
| | | Ryan, 2011 | 6 | 13 | 16 | -- | 35 |
| | | Trovo, 2009 | 15 | 5 | 9 | -- | 29 |
| | | <i>Mean (SE)</i> | | | | | 35(3) |
| | Field | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| | | Boreen, 2004 | 15 | 16 | -- | 2 | 33 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | Moore, 1994 | 8 | 11 | -- | 3 | 22 |
| | | Ryan, 2011 | 6 | 13 | 16 | 2 | 37 |
| | | <i>Mean (SE)</i> | | | | | 29(3) |
| Sulfamethoxyypyridazine | Lab | Khaleel, 2013 | 9 | 7 | 7 | -- | 23 |
| | | <i>Mean (SE)</i> | | | | | 23 |
| Sulfamoxole | Lab | Boreen, 2004 | 14 | -- | 13 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2004 | 15 | 16 | -- | 2 | 33 |
| | | <i>Mean (SE)</i> | | | | | 33 |
| Sulfapyridine | Lab | Challis, 2013 | 13 | 18 | 13 | -- | 44 |
| | | Garcia-Galan, 2012 | 14 | 7 | 10 | -- | 31 |
| | | <i>Mean (SE)</i> | | | | | 38(7) |
| Sulfathiazole | Lab | Boreen, 2004 | 14 | -- | 13 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2004 | 15 | 16 | -- | 2 | 33 |
| | | <i>Mean (SE)</i> | | | | | 33 |
| Sulfisoxazole | Lab | Boreen, 2004 | 14 | -- | 13 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| | Field | Boreen, 2004 | 15 | 16 | -- | 2 | 33 |
| | | <i>Mean (SE)</i> | | | | | 33 |
| Sulfone | | | | | | | |
| Dapsone | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |

| | | | | | | | |
|---------------------|-------|------------------|----|----|----|----|-------|
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 18 |
| Tetracycline | | | | | | | |
| Oxytetracycline | Field | Lunestad, 1995 | 10 | -- | 4 | 5 | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| Tetracycline | Lab | Chen, 2008 | 10 | 11 | 11 | -- | 32 |
| | | Jiao, 2008 | 11 | 10 | 7 | -- | 28 |
| | | Oka, 1989 | 9 | 3 | -- | -- | 12 |
| | | Wammer, 2011 | 10 | -- | 11 | -- | 21 |
| | | Werner, 2006 | 11 | 22 | -- | -- | 33 |
| | | <i>Mean (SE)</i> | | | | | 25(4) |

Table S1B: Anti-psychotics

| Anti-psychotic Compound | Data Type and Source | | Score | | | | |
|--|----------------------|------------------|--------------|--------|----------|----------------|-------|
| | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total |
| Anti-depressant | | | | | | | |
| Chlorpromazine | Lab | Trautwein, 2012 | 10 | 10 | -- | -- | 20 |
| | | <i>Mean (SE)</i> | | | | | 20 |
| Anti-depressant - benzodiazepine | | | | | | | |
| Alprazolam | Lab | Calisto, 2011b | 16 | 11 | 11 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| Citalopram | Lab | Kwon, 2005 | 18 | 13 | 11 | -- | 42 |
| | | <i>Mean (SE)</i> | | | | | 42 |
| Diazepam | Lab | West, 2012 | 16 | 9 | 11 | -- | 36 |
| | | Calisto, 2011b | 16 | 11 | 11 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 37(1) |
| Lorazepam | Lab | Calisto, 2011b | 16 | 11 | 11 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| Midazolam | Lab | Andersin, 1995 | 14 | 5 | -- | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| Oxazepam | Lab | Calisto, 2011b | 16 | 11 | 11 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| Anti-depressant – reuptake inhibitors | | | | | | | |
| Bupropion | Lab | Santoke, 2012 | 8 | 2 | 7 | -- | 17 |
| | | <i>Mean (SE)</i> | | | | | 17 |
| Duloxetine | Lab | Santoke, 2012 | 8 | 2 | 7 | -- | 17 |
| | | <i>Mean (SE)</i> | | | | | 17 |
| Fluoxetine | Lab | Kwon, 2006 | 16 | 12 | 13 | -- | 41 |
| | | Lam, 2005 | 17 | 11 | 13 | -- | 41 |
| | | <i>Mean (SE)</i> | | | | | 41(0) |
| Paroxetine | Lab | Kwon, 2004 | 17 | 16 | 12 | -- | 45 |
| | | <i>Mean (SE)</i> | | | | | 45 |
| Sertraline | Field | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |
| Venlafaxine | Lab | Rua-Gomez, 2013 | 10 | 11 | 11 | -- | 32 |
| | | Santoke, 2012 | 8 | 2 | 7 | -- | 17 |
| | | <i>Mean (SE)</i> | | | | | 25(8) |
| | Field | Rua-Gomez, 2013 | 10 | 11 | 11 | 6 | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| Anti-epileptic | | | | | | | |
| Carbamazepine | Lab | Calisto, 2011a | 17 | 19 | -- | -- | 36 |
| | | Calza, 2013 | 12 | -- | 5 | -- | 17 |

| | | | | | | | |
|------------------|-------|------------------|----|----|----|----|-------|
| | | Chiron, 2006 | 10 | 5 | 14 | -- | 29 |
| | | Doll, 2003 | 19 | 11 | 11 | -- | 41 |
| | | Jasper, 2013 | 15 | 9 | 24 | -- | 48 |
| | | Lam, 2005 | 17 | 10 | 11 | -- | 38 |
| | | Matamoros, 2009 | 12 | 10 | 11 | -- | 33 |
| | | Peuravuori, 2009 | 12 | 5 | 13 | -- | 30 |
| | | <i>Mean (SE)</i> | | | | | |
| | Field | Andreozzi, 2002 | 13 | 4 | 6 | 9 | 32 |
| | | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | Matamoros, 2009 | 12 | -- | 11 | 4 | 27 |
| | | Yamamoto, 2009 | 13 | 6 | -- | 5 | 24 |
| <i>Mean (SE)</i> | | | | | | | 28(2) |
| Phenytoin | Lab | Chen, 2009 | 18 | -- | 19 | -- | 37 |
| | | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | |

Table S1C: β -blockers

| β -blocker | Data Type and Source | | Score | | | | |
|------------------|----------------------|------------------|-----------|--------------|--------|----------|----------------|
| | Compound | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight |
| Acebutolol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | |
| Alprenolol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | |
| Atenolol | Lab | Andrisano, 1999 | 9 | 11 | -- | -- | 20 |
| | | Chen, 2012 | 16 | 5 | 26 | -- | 47 |
| | | Jasper, 2013 | 15 | 9 | 24 | -- | 48 |
| | | Ji, 2012 | 17 | -- | 20 | -- | 37 |
| | | Liu, 2007 | 19 | 11 | -- | -- | 30 |
| | | Liu, 2009 | 18 | 6 | 12 | -- | 36 |
| | | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | Wang, 2012 | 13 | 8 | 17 | -- | 38 |
| | | Zeng, 2012 | 18 | -- | 13 | -- | 31 |
| | <i>Mean (SE)</i> | | | | | | 34(3) |
| Field | Yamamoto, 2009 | 13 | 7 | -- | 5 | 25 | |
| | <i>Mean (SE)</i> | | | | | | 25 |
| Bisoprolol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | |
| Metoprolol | Lab | Chen, 2012 | 16 | 5 | 26 | -- | 47 |
| | | Liu, 2007 | 19 | 11 | -- | -- | 30 |
| | | Liu, 2009 | 18 | 6 | 12 | -- | 36 |
| | | Peuravuori, 2009 | 12 | 5 | 13 | -- | 20 |
| | | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | Wang, 2012 | 13 | 8 | 17 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | |
| | Field | Fono, 2006 | 14 | 8 | 8 | 14 | 44 |
| Kunkel, 2012 | | 15 | -- | 8 | 8 | 31 | |
| <i>Mean (SE)</i> | | | | | | | 38(7) |
| Nadolol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |

| | | | | | | | |
|------------------|-------|------------------|----|----|----|-------|--------|
| | | Wang, 2012 | 13 | 8 | 17 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 29(10) |
| Pindolol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| Propranolol | Lab | Chen, 2009 | 18 | -- | 19 | -- | 37 |
| | | Dantas, 2010 | 6 | 8 | -- | -- | 14 |
| | | Jasper, 2013 | 15 | 9 | 24 | -- | 48 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Liu, 2007 | 19 | 11 | -- | -- | 30 |
| | | Liu, 2009 | 18 | 6 | 12 | -- | 36 |
| | | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | Robinson, 2007 | 15 | 10 | -- | -- | 25 |
| | | <i>Mean (SE)</i> | | | | | 31(4) |
| | Field | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| | | Dantas, 2010 | 7 | 5 | -- | 2 | 14 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Yamamoto, 2009 | 13 | 7 | -- | 5 | 25 |
| <i>Mean (SE)</i> | | | | | | 23(4) | |
| Sotalol | Lab | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| | Field | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | <i>Mean (SE)</i> | | | | | 31 |
| Timolol | Lab | Chen, 2013 | 14 | 5 | 24 | -- | 43 |
| | | Piram, 2008 | 11 | 4 | 4 | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | 31(12) |

Table S1D: Hormones

| Hormone | Data Type and Source | | Score | | | | |
|--------------------------------|----------------------|------------------|--------------|--------|----------|----------------|-------|
| Compound | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total |
| 17 α -ethinyl estradiol | Lab | Atkinson, 2011 | 8 | 8 | 9 | -- | 25 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Liu, 2003 | 7 | 7 | 5 | -- | 19 |
| | | Matamoros, 2009 | 12 | 10 | 11 | -- | 33 |
| | | Mazellier, 2008 | 11 | 8 | -- | -- | 19 |
| | | Whidbey, 2012 | 11 | 7 | 9 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27(3) |
| | Field | Matamoros, 2009 | 12 | -- | 11 | 4 | 27 |
| | | Zuo, 2013 | 14 | -- | 3 | 5 | 22 |
| <i>Mean (SE)</i> | | | | | | 25(3) | |
| 17 β -estradiol | Lab | Chowdhury, 2011 | 19 | 19 | 11 | -- | 49 |
| | | Leech, 2009 | 14 | 6 | 8 | -- | 28 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Mazellier, 2008 | 11 | 8 | -- | -- | 19 |
| | | Whidbey, 2012 | 11 | 7 | 9 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 33(5) |
| Equilenin | Lab | Whidbey, 2012 | 11 | 7 | 9 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| Equilin | Lab | Whidbey, 2012 | 11 | 7 | 9 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| Estriol | Lab | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | <i>Mean (SE)</i> | | | | | 40 |
| Estrone | Lab | Atkinson, 2011 | 8 | 8 | 9 | -- | 25 |

| | | | | | | | |
|------------|-----|------------------|----|----|----|----|-------|
| | | Caupos, 2011 | 18 | 5 | 13 | -- | 36 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Whidbey, 2012 | 11 | 7 | 9 | -- | 27 |
| | | <i>Mean (SE)</i> | | | | | 32(4) |
| Raloxifene | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| | | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 18 |

Table S1E: Lipid-lowering agents

| Lipid-lowering Compound | Data Type and Source | | Score | | | | |
|----------------------------|----------------------|------------------|--------------|--------|----------|----------------|-------|
| | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total |
| Fibrates | | | | | | | |
| Bezafibrate | Lab | Cermola, 2005 | 11 | 1 | 3 | -- | 15 |
| | | <i>Mean (SE)</i> | | | | | 15 |
| | Field | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Radke, 2010 | 13 | 11 | 13 | 7 | 44 |
| | <i>Mean (SE)</i> | | | | | 38(7) | |
| Clofibrac acid | Lab | Doll, 2003 | 19 | 11 | 11 | -- | 41 |
| | | Lam, 2003 | 15 | 8 | 15 | -- | 38 |
| | | <i>Mean (SE)</i> | | | | | 40(2) |
| | Field | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| | | Packer, 2003 | 17 | 10 | 14 | 3 | 44 |
| | | Radke, 2010 | 13 | 11 | 13 | 7 | 44 |
| | <i>Mean (SE)</i> | | | | | 36(8) | |
| Fenofibrate | Lab | Cermola, 2005 | 11 | 1 | 3 | -- | 15 |
| | | <i>Mean (SE)</i> | | | | | 15 |
| Fenofibrac acid | Lab | Cermola, 2005 | 11 | 1 | 3 | -- | 15 |
| | | <i>Mean (SE)</i> | | | | | 15 |
| Statins | | | | | | | |
| Atorvastatin | Lab | Lam, 2005 | 17 | 10 | 11 | -- | 38 |
| | | Razavi, 2011 | 6 | -- | 14 | -- | 20 |
| | | <i>Mean (SE)</i> | | | | | 29(9) |
| | Field | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |

Table S1F: Non-steroidal anti-inflammatory drugs (NSAIDs)

| NSAID Compound | Data Type and Source | | Score | | | | |
|-------------------|----------------------|------------------|--------------|--------|----------|----------------|-------|
| | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total |
| Diclofenac | Lab | Eriksson, 2010 | 8 | 7 | 5 | -- | 20 |
| | | Peuravuori, 2012 | 16 | 7 | 8 | -- | 31 |
| | | Zhang, 2011 | 12 | 5 | 14 | -- | 31 |
| | | <i>Mean (SE)</i> | | | | | 27(4) |
| | Field | Aguera, 2005 | 16 | 4 | 4 | 3 | 27 |
| | | Andreozzi, 2003 | 10 | 4 | 4 | 2 | 20 |
| | | Bartels, 2007 | 16 | 11 | 1 | 6 | 34 |
| | | Buser, 1998 | 15 | 4 | 3 | 7 | 29 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Lindstrom, 2002 | 8 | 5 | 8 | 5 | 26 |
| | Packer, 2003 | 17 | 10 | 14 | 3 | 44 | |

| | | | | | | | |
|----------------|-------|------------------|----|----|----|----|--------|
| | | Poiger, 2001 | 14 | 7 | 6 | 5 | 32 |
| | | Radke, 2010 | 13 | 11 | 13 | 7 | 44 |
| | | <i>Mean (SE)</i> | | | | | 32(3) |
| Ibuprofen | Lab | Jacobs, 2011 | 17 | 9 | 13 | -- | 39 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Matamoros, 2009 | 12 | 10 | 11 | -- | 33 |
| | | Packer, 2003 | 17 | 10 | 14 | 3 | 44 |
| | | Peuravuori, 2009 | 12 | 5 | 13 | -- | 20 |
| | | Vione, 2011 | 9 | 8 | 9 | -- | 26 |
| | | <i>Mean (SE)</i> | | | | | 34(4) |
| | Field | Fono, 2006 | 14 | 8 | 8 | 14 | 44 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Matamoros, 2009 | 12 | -- | 11 | 4 | 27 |
| Yamamoto, 2009 | | 13 | 7 | -- | 5 | 25 | |
| | | <i>Mean (SE)</i> | | | | | 32(4) |
| Indomethacin | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | Yamamoto, 2009 | 13 | 7 | -- | 5 | 25 |
| | | <i>Mean (SE)</i> | | | | | 22(4) |
| Ketoprofen | Lab | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | Matamoros, 2009 | 12 | 10 | 11 | -- | 33 |
| | | <i>Mean (SE)</i> | | | | | 37(4) |
| | Field | Matamoros, 2009 | 12 | -- | 11 | 4 | 27 |
| | | <i>Mean (SE)</i> | | | | | 27 |
| Mefenamic acid | Lab | Werner, 2005 | 12 | 10 | 15 | -- | 37 |
| | | <i>Mean (SE)</i> | | | | | 37 |
| | Field | Werner, 2005 | 13 | 10 | 11 | 2 | 36 |
| | | Yamamoto, 2009 | 13 | 7 | -- | 5 | 25 |
| | | <i>Mean (SE)</i> | | | | | 31(6) |
| Naproxen | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | Lin, 2005 | 14 | 15 | 11 | -- | 40 |
| | | <i>Mean (SE)</i> | | | | | 28(12) |
| | Field | Fono, 2006 | 14 | 8 | 8 | 14 | 44 |
| | | Kunkel, 2012 | 15 | -- | 8 | 8 | 31 |
| | | Packer, 2003 | 17 | 10 | 14 | 3 | 44 |
| | | Radke, 2010 | 13 | 11 | 13 | 7 | 44 |
| | | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 36(5) |
| Sulindac | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 18 |

Table S1G: Others

| Other Compound | Data Type and Source | | Score | | | | |
|-------------------------------|----------------------|------------------|--------------|--------|----------|----------------|-------|
| | Lab or Field | Reference | Experimental | Direct | Indirect | Field/Sunlight | Total |
| Analgesic | | | | | | | |
| Acetaminophen/ paracetamol | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | Peuravuori, 2012 | 7 | 10 | 9 | -- | 26 |
| | | <i>Mean (SE)</i> | | | | | 21(5) |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |

| | | | | | | | |
|--|-------|------------------|----|----|----|----|-------|
| | | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | Yamamoto, 2009 | 13 | 6 | -- | 5 | 24 |
| | | <i>Mean (SE)</i> | | | | | 25(4) |
| Antipyrine | Lab | Chen, 2009 | 18 | -- | 19 | -- | 37 |
| | | <i>Mean (SE)</i> | | | | | 37 |
| Salicylic acid | Lab | Gangwang, 2012 | 13 | 9 | 10 | -- | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |
| Tramadol | Lab | Rua-Gomez, 2013 | 10 | 11 | 11 | -- | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |
| | Field | Rua-Gomez, 2013 | 10 | 11 | 11 | 6 | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| β_2-adrenergic agonist | | | | | | | |
| Salbutamol | Lab | Dodson, 2011 | 7 | 12 | -- | -- | 19 |
| | | <i>Mean (SE)</i> | | | | | 19 |
| H₂-antagonist | | | | | | | |
| Cimetidine | Lab | Latch, 2003 | 12 | 11 | 19 | -- | 42 |
| | | <i>Mean (SE)</i> | | | | | 42 |
| | Field | Latch, 2003 | 12 | 11 | -- | 3 | 26 |
| | | <i>Mean (SE)</i> | | | | | 26 |
| Ranitidine | Lab | Latch, 2003 | 12 | 11 | 19 | -- | 42 |
| | | <i>Mean (SE)</i> | | | | | 42 |
| | Field | Latch, 2003 | 12 | 11 | -- | 3 | 26 |
| | | <i>Mean (SE)</i> | | | | | 26 |
| Anti-arrhythmic | | | | | | | |
| Amiodarone | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 18 |
| Lidocaine | Lab | Rua-Gomez, 2013 | 10 | 11 | 11 | -- | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |
| | Field | Rua-Gomez, 2013 | 10 | 11 | 11 | 6 | 38 |
| | | <i>Mean (SE)</i> | | | | | 38 |
| Mexiletine | Lab | Chen, 2009 | 18 | -- | 19 | -- | 37 |
| | | <i>Mean (SE)</i> | | | | | 37 |
| Anti-cancer | | | | | | | |
| Cyclophosphamide | Lab | Lin, 2013 | 18 | 14 | 12 | -- | 44 |
| | | <i>Mean (SE)</i> | | | | | 44 |
| 5-Fluorouracil | Lab | Lin, 2013 | 18 | 14 | 12 | -- | 44 |
| | | <i>Mean (SE)</i> | | | | | 44 |
| Anti-coagulant | | | | | | | |
| Warfarin | Lab | Peuravuori, 2009 | 12 | 5 | 13 | -- | 20 |
| | | <i>Mean (SE)</i> | | | | | 20 |
| Anti-histamine | | | | | | | |
| Diphenhydramine | Lab | Chen, 2009 | 18 | -- | 19 | -- | 37 |
| | | <i>Mean (SE)</i> | | | | | 37 |
| Anti-viral | | | | | | | |
| Oseltamivir ester | Lab | Goncalves, 2011 | 16 | 12 | 13 | -- | 41 |
| | | <i>Mean (SE)</i> | | | | | 41 |
| | Field | Goncalves, 2011 | 16 | 4 | 6 | 4 | 30 |
| | | <i>Mean (SE)</i> | | | | | 30 |
| Oseltamivir carboxylate | Lab | Goncalves, 2011 | 16 | 12 | 13 | -- | 41 |
| | | <i>Mean (SE)</i> | | | | | 41 |
| | Field | Goncalves, 2011 | 16 | 4 | 6 | 4 | 30 |

| | | | | | | | |
|-------------------------------|-------|------------------|----|----|----|----|-------|
| | | Bartels, 2008 | 15 | 8 | 11 | 6 | 40 |
| | | <i>Mean (SE)</i> | | | | | 35(5) |
| Glucocorticoid steroid | | | | | | | |
| Dexamethasone | Lab | Kawabata, 2013 | 12 | 4 | -- | -- | 16 |
| | | <i>Mean (SE)</i> | | | | | 16 |
| | Field | Kawabata, 2013 | 12 | 4 | -- | 2 | 18 |
| | | <i>Mean (SE)</i> | | | | | 18 |
| Vasodilator | | | | | | | |
| Ifenprodil | Field | Yamamoto, 2009 | 13 | 6 | -- | 5 | 24 |
| | | <i>Mean (SE)</i> | | | | | 24 |
| Stimulant | | | | | | | |
| Caffeine | Lab | Jacobs, 2012 | 10 | 6 | 14 | -- | 30 |
| | | <i>Mean (SE)</i> | | | | | 30 |
| | Field | Lam, 2004 | 14 | -- | 6 | 12 | 32 |
| | | <i>Mean (SE)</i> | | | | | 32 |

Table S2: Scoring rubric used as the weight-of-evidence tool to evaluate each study. The coloured dots beside the sections indicate that those sections apply. For example, a study done in the field (field/sun photolysis) is still evaluated on the experimental, direct photolysis, and indirect photolysis criteria, if applicable.

| Quality/relevance/extent of photolysis study | 0 (no) | 1 (yes) | 2 | 3 | 4 |
|--|------------------------------|--|--|---|---------------------------------------|
| Experimental | | | | | |
| Wavelength distribution of light source | $\lambda < 290$ nm | mono/polychromatic ($\lambda > 290$) | 290 – 800 nm (Xe lamp/sunlight) | | |
| Sample vessel | absorbs $\lambda > 290$ nm | absorbs $\lambda < 290$ nm | absorbs $\lambda < 290$ nm and reports material (glass, quartz etc.) =2; geometry =3; positioning, λ cut-off etc. =4 | | |
| Measured light flux – spectral radiometer/actinometer | no | once – before or after study | before and after; entire study | | |
| Triplicate irradiations | no | yes | | | |
| Number of time points | 2 or less | 3-4 | >5 | | |
| Study duration | <1 half life | ≥ 1 half life | | | |
| Dark control | No (= -2) | yes | | | |
| Temperature (°C) | not reported | 10 > temp > 40 | environmental temp. (25 ± 15) | multiple temp. including 25 °C | |
| Sampling (aliquot versus sacrificial) | 20 – 30% of sample vol. | 5-10% of sample vol. | <5% of sample vol./sacrificial sampling | | |
| Solvent carrier | any solvent | in H ₂ O | | | |
| Concentration of test chemical (absorbance) | not optically dilute (>0.05) | optically dilute (<0.05) | close to environ. conc. (i.e., ppb) | | |
| Photodegradation product (pp) identification (id) | no | yes | pp id – LC-UV+ standards; MS/(MS) | pp id – TOF, NMR | quantify pp loss/ produc.; pp pathway |
| Direct photolysis • | | | | | |
| Buffered nanopure H ₂ O | no | yes | | | |
| pH of sample | not reported | @ 1 pH: 5 > pH > 9 | @ 1 pH: 5 – 9 | @ 2 pH: 5 – 9 | @ 3 pH: 5 – 9 |
| Considered pKa of test compound | no | yes | single species (i.e., ≥ 2 pH from pKa) | | |
| UV-vis spectra of compound | no | yes – shown/ described | | | |
| Pseudo-1 st -order plot | C _t vs. time | C _t / C ₀ vs. time | ln[C _t / C ₀] vs. time | ln[C _t / C ₀] vs. time and reports k | |
| R ² -1 st -order decay curve; rate ± error (k, time ⁻¹); $\emptyset \pm$ error | no | k / $\emptyset \pm$ error: +1 if given; -1 if not | R ² < 0.8 | R ² < 0.9 | R ² > 0.9 |
| Quantum yield (\emptyset) | no | yes | calculations and formulas shown | | |
| Use \emptyset to estimate sunlight half-life | no | L _{λ} data (latitude-season) | compare estimation to environ. fate | | |
| Indirect photolysis • • | | | | | |
| Natural water (NW) or simulated NW (SNW) | | source of NW/ SNW reported | Species relevant to photolysis: DOC/cDOM, NO ₃ ² (1), Fe (1), DO (1), CO ₃ ⁻ (1) etc. (must have [DOC/cDOM] to score 4) | | |
| UV-vis spec of NW/SNW | no | yes | S _{λ} calc, reported, applied | | |
| R ² -1 st -order decay curve; rate ± error (k, time ⁻¹) | no | k ± error: +1 if given; -1 if not | R ² < 0.7 | 0.7 < R ² < 0.9 | R ² > 0.9 |
| Quenching/competition/ mechanism experiments | no | 1 species | 2 species | 3 species (i.e. OH, ¹ O ₂ , ³ DOM) | 4 species |
| Field/solar photolysis • • • | | | | | |
| Whole versus isolated system | | isolated in sample vessels | small microcosms (1-100 L) | med. microcosms (100-1000 L) | mesocosms (>1000 L) or real system |
| Diurnal cycle versus partial exposure | | partial exposure | full diurnal cycle | | |
| Compare measured flux to L _{λ} data | no | is the comparison valid (1), do they discuss any differences in flux (1), how well do they match (1) | | | |
| R ² -1 st -order decay curve; rate ± error (k, time ⁻¹) | no | k ± error: +1 if given; -1 if not | R ² < 0.7 | R ² < 0.8 | R ² > 0.8 |
| Consider depth/attenuation | no | yes | | | |
| Report weather conditions | no | yes | | | |
| Other processes considered as they relate to photolysis | no | sediment binding (1), biota binding (1), microbial degradation (1), plant uptake (1), hydrolysis (1), photo-toxicity (1), etc. | | | |

LC-UV=liquid chromatography (LC) – ultra-violet (UV) detection. MS=mass spectrometry. TOF=time of flight. NMR=nuclear magnetic resonance. DOC/cDOM=dissolved organic carbon/chromaphoric dissolved organic matter

Table S3A-B: Two examples of scored and evaluated studies showing the filled in rubric with scores and a brief description of the study. All scored studies included in this review were evaluated in an identical manner. See the comments following Table S3B for a demonstration of how lab, field, and total scores are derived for Table S1A-G. Individual scoring sheets for specific studies are available from the contact author upon request.

Table S3A: M. W. Lam and S. A. Mabury, *Aquatic Sciences*, 2005, **67**, 177-188

Keywords: atorvastatin, carbamazepine, levofloxacin, sulfamethoxazole, lab irradiations, direct and indirect photolysis, photo-products, quenching/competition mechanism experiments

| Quality/relevance/extent of photolysis study | | Score |
|--|--|-----------|
| Experimental | | 17 |
| Wavelength distribution of light source | Suntest CPS Photosimulator equipped with Xe lamp as the UV radiation source and glass filters restricting the transmission of wavelengths below 290 nm | 2 |
| Sample vessel | 10 mL quartz vessels | 1 |
| Measured light flux – spectral radiometer/actinometer | The lamp was set to maximum intensity 765 W/m ² on irradiation apparatus (Suntest). PNA/PYR used as actinometer | 2 |
| Triplicate irradiations | Yes | 1 |
| Number of time points | 5 time points | 2 |
| Study duration | To at least one half life | 1 |
| Dark control | Yes | 1 |
| Temperature (°C) | A cold water tray was used to maintain the internal temperature at 27 °C | 2 |
| Sampling (aliquot versus sacrificial) | Not reported | 0 |
| Solvent carrier | No, stocks were made up pure water | 1 |
| Concentration of test chemical (absorbance) | 10 µM (approximately >1 ppm) – not optically dilute or environmentally relevant | 0 |
| Photodegradation products (pp) | Yes. LC-MS/MS used to identify pp. Pathway proposed for some of the pp | 4 |
| Direct photolysis • | | 10 |
| Buffered nanopure H ₂ O | DI water | 1 |
| pH of sample | pH = 4, 7, 9 | 3 |
| Considered pKa of test compound | No | 0 |
| UV-vis spectra of compound | Yes | 1 |
| Pseudo-1 st -order decay plot | ln[C _t /C ₀] vs. time plotted for sulfamethoxazole. Rate constants/half lives reported for others | 3 |
| R ² -1 st -order decay curve; rate ± error (k, time ⁻¹); Ø ± error | R ² not reported. Errors in half lives given, not for quantum yields | 1 |
| Quantum yield (Ø) | Yes. Calculations for quantum yields not reported | 1 |
| Use Ø to estimate sunlight half-life | No | 0 |
| Indirect photolysis •• | | 11 |
| Natural water (NW) or simulated NW (SNW) | SNW – water spiked with different concentrations of DOM, nitrate, and carbonate according to the PhotoFate solutions. Differing concentrations (=1) | 4 |
| pH of sample | Not reported | 0 |
| UV-vis spec of NW/SNW | Spectra not shown but screening factors were calculated | 1 |
| Pseudo-1 st -order decay plot | Not given. Half lives of drugs are reported based on first order kinetics and plotted as a bar graph as a function of SNW solution | 3 |
| R ² -1 st -order decay curve; rate ± error (k, time ⁻¹) | R ² not reported. Errors in half lives given | 1 |
| Quenching experiments | 2-propanol used as OH-radical quencher | 1 |
| Other processes considered as they relate to photolysis | OH-radical second order rate constants determined through competition kinetics | 1 |
| Field/sun photolysis ••• | No | 0 |

Comments: This is a very good photochemical study examining the direct and indirect photolytic fate of four pharmaceuticals under simulated sunlight. They found that direct photolysis was the major photodegradation mechanism for some of the target compounds, while indirect photolysis more significantly enhanced degradation for others. Carbamazepine was the most persistent drug in all cases and saw a large enhancement in removal in SNW. Interestingly, some of the quantum yield determinations from this study did not agree with others in the literature, specifically Andreozzi et al. (2003) which determined quantum yields for some of the same compounds in sunlight.

Total (lab) score = 38 (17+10+11)

Table S3B: A. L. Boreen, W. A. Arnold and K. McNeill, *Environmental Science & Technology*, 2004, **38**, 3933-3940

Keywords: sulfamethoxazole, sulfisoxazole, sulfamethizole, sulfathiazole, sulfamoxole, lab and sunlight irradiations, direct and indirect photolysis, photo-products, quenching/competition mechanism experiments

| Quality/relevance/extent of photolysis study | | Score |
|--|---|--------------|
| Experimental | | 15/14 |
| Wavelength distribution of light source | Natural sunlight – 45° N (May 13, June 5, 9). (2 – for sunlight irradiations) Lab irradiations - turntable apparatus with 4x Pyrex-filtered 175 W medium-pressure Hg-vapor lamp (1 – for lab irradiations) | 2/1 |
| Sample vessel | Natural sunlight - uncapped quartz test tubes (o.d.=1.3 cm, i.d.=1.1 cm, 10 mL) – held at 45° to sunlight. Lab irradiations - uncapped borosilicate test tubes | 3 |
| Measured light flux – spectral radiometer/actinometer | PNA/PYR actinometer for sunlight. Not reported for lab irradiations. Frequency of measurement not reported. Sounds like they may have used L_{λ} data for sunlight experiments (mentioned in footnote of Table 2). | 1 |
| Triplicate irradiations | Not reported | 0 |
| Number of time points | Not reported but based on plots, looks like 6 | 2 |
| Study duration | Not reported. Based on plots between minutes to hours | 1 |
| Dark control | Yes | 1 |
| Temperature (°C) | Not reported | 0 |
| Sampling (aliquot versus sacrificial) | Aliquot, 500 μ L from 10 mL (5% v/v) for both experiments | 1 |
| Solvent carrier | No. Dissolved in water | 1 |
| Concentration of test chemical (absorbance) | 100 μ M (\approx 25 ppm) for both experiments – not optically dilute or environmentally relevant. | 0 |
| Photodegradation products (pp) | Yes. LC-UV and LC-MS/MS and authentic standards to confirm some products. Monitored formation of sulfanilic acid as a pp and breakdown of sulfa drugs. Proposed some cleavage sites for the formation of identified pp | 3 |
| Field/sun photolysis | Direct photolysis experiments done under natural sunlight | |
| Direct photolysis • | | 16 |
| Buffered nanopure H ₂ O | Yes, various buffers in DI water | 1 |
| pH of sample | Between 5 – 6 pH values between 2 – 10, depending on compound. Generally pH \approx 2, 4, 5, 7, 9, 10 | 4 |
| Considered pKa of test compound | Yes. The pK _{a1} and pK _{a2} were determined for all sulfa drugs using spectrophotometric titration techniques. Irradiations were done at each protonation state for all sulfa drugs | 2 |
| UV-vis spectra of compound | Yes, at multiple pH's | 1 |
| Pseudo-1 st -order decay plot | $\ln[C_t / C_0]$ vs. time and reports k | 3 |
| r ² -1 st -order decay curve; rate \pm error (k, time ⁻¹); $\emptyset \pm$ error | r ² not reported. k \pm error, $\emptyset \pm$ error reported | 2 |
| Quantum yield (\emptyset) | Yes, quantum yields given for all compounds at the various protonation states. Formula provided. | 2 |
| Use \emptyset to estimate sunlight half-life | Yes, direct photolysis half lives estimated for mid-spring, noon, 45° N and for “half light attenuation” (rate constant is halved). | 1 |
| Indirect photolysis • • | Indirect experiments done using laboratory irradiation techniques | 13 |
| Natural water (NW) or simulated NW (SNW) | NW - taken from Lake Josephine and Lake Superior, filtered. All important cations and anions analyzed (18 ions in total). DOC=2-6 mg/L | 4 |
| pH of sample | Josephine pH = 8.4; Superior pH = 8.3 | 2 |
| UV-vis spectra of compound | Yes, at multiple pH's | 1 |
| UV-vis spec of NW/SNW | Not provided | 0 |
| Pseudo-1 st -order decay plot | $\ln[C_t / C_0]$ vs. time. Rate constants not reported for indirect experiments | 2 |
| r ² -1 st -order decay curve; rate \pm error (k, time ⁻¹) | r ² not reported. k \pm error not reported | 0 |
| Quenching experiments | Yes, experiments were done to consider singlet oxygen (¹ O ₂) and hydroxyl radicals ([•] OH). Laser flash photolysis determined k _{tot} ¹ O ₂ (substrate can quench and react with ¹ O ₂). Steady state photolysis was used to determine k _{rxn} ¹ O ₂ (by comparison with FFA). Bimolecular hydroxyl radical rate constants for the sulfa drugs were also determined using Fenton's reagent (determining bimolecular rate constants =1) | 3 |
| Other processes considered as they relate to photolysis | Using the [•] OH radical and ¹ O ₂ rate constants, environmental half lives of each sulfa drug were estimated assuming environmental conc. of [•] OH radicals and ¹ O ₂ | 1 |

| Field/sun photolysis • • • | | 2 |
|---|---|---|
| Whole versus isolated system | Isolated system | 1 |
| Diurnal cycle versus partial exposure | Unclear, but based on data it seems like exposures were short, i.e. less than 1 day. Partial exposure | 1 |
| Compare measured flux to L_{λ} data | No, L_{λ} data was used | 0 |
| Consider depth/attenuation | No | 0 |
| Report weather conditions | No | 0 |

Comments: This is an excellent study looking at the photochemical fate of sulfa drugs in the environment. Natural sunlight was used for the direct photolysis experiments and lab irradiations were done for indirect photolysis and quenching experiment. Based on the many different photolysis mechanisms that were studied here, the authors determined that direct photolysis is the primary mechanism of photolysis in the environment. Singlet oxygen and OH-radicals may only play a role in nitrate and humic rich waters where the concentration of these species would be quite high.

Lab score = 27 (14+13)

Field score = 33 (15+16+2)

Total (lab/field) score = 46 (15+16+13+2)