

Partitioning behavior of petrodiesel/biodiesel blends in water — Supporting Information

Mohamad H. Yassine[†], Shuyun Wu[†], Makram T. Suidan^{‡}, and Albert D. Venosa[§]*

[†]Department of Environmental Engineering, School of Energy, Environmental, Biological, and Medical Engineering, University of Cincinnati, Ohio 45221

[‡] Faculty of Engineering and Architecture, American University of Beirut, P.O. Box 11-0236 Riad El-Solh, Beirut, Lebanon 1107 2020

[§]U.S. Environmental Protection Agency, 26 W. Martin Luther King Drive, Cincinnati, OH 45268

*Corresponding author e-mail: msuidan@aub.uc.edu.lb

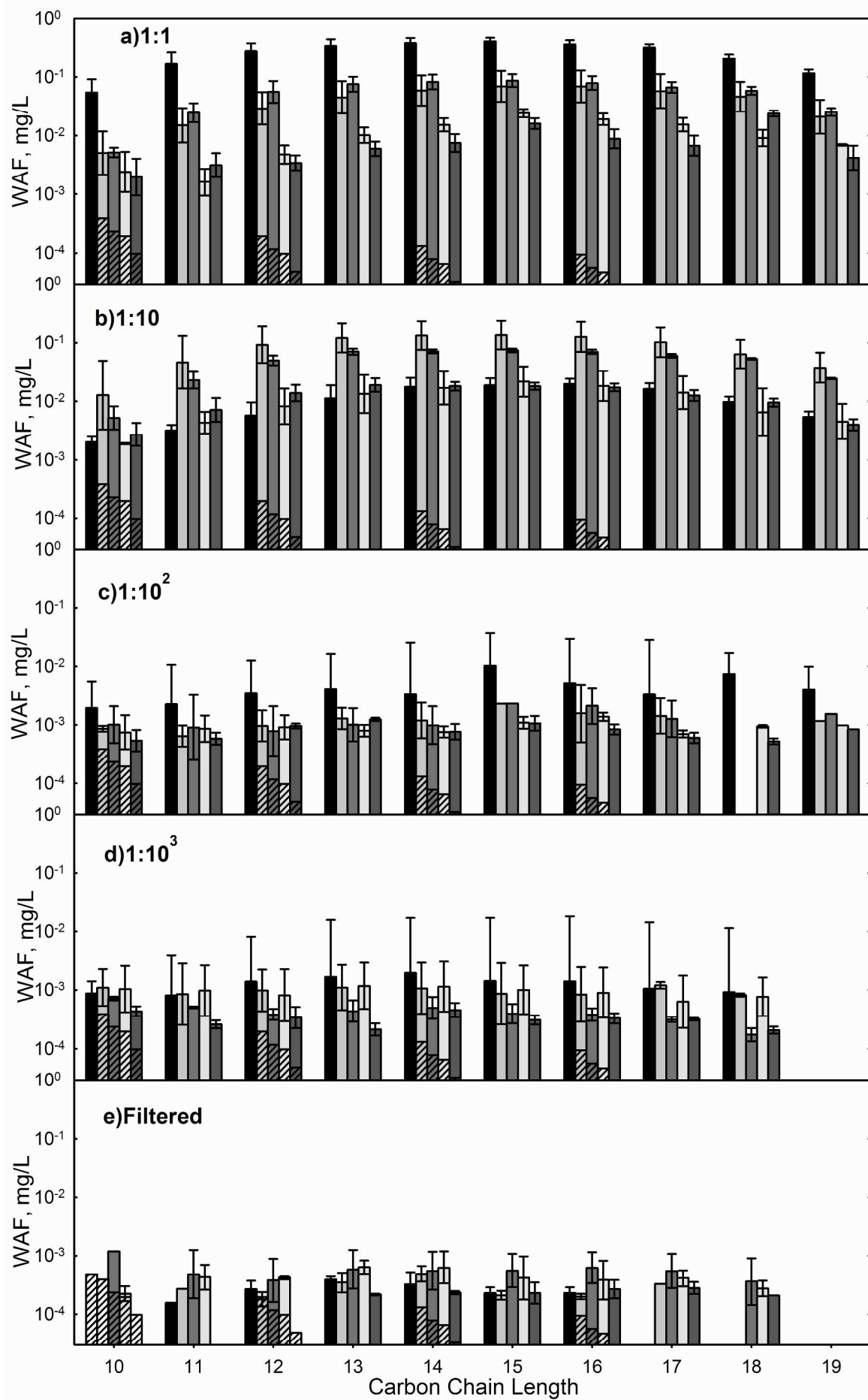


Figure S1. n-alkanes WAF concentrations in B0 (■), B20 (▨), B40 (▩), B60 (▤), B80 (▥), and $S_{aq,WAF}^{sat}$ is n-alkanes concentrations calculated by Equation 1 using solubilities reported by Franks¹ (▧)) at dilution levels: (a) 1:10⁰, (b) 1:10¹, (c) 1:10², (d) 1:10³, (e) and 1:10³ filtered. Means and standard deviations are calculated geometrically (n = 3). Error bars are ± 1 geometric standard deviation. Not shown data were below detection limits.

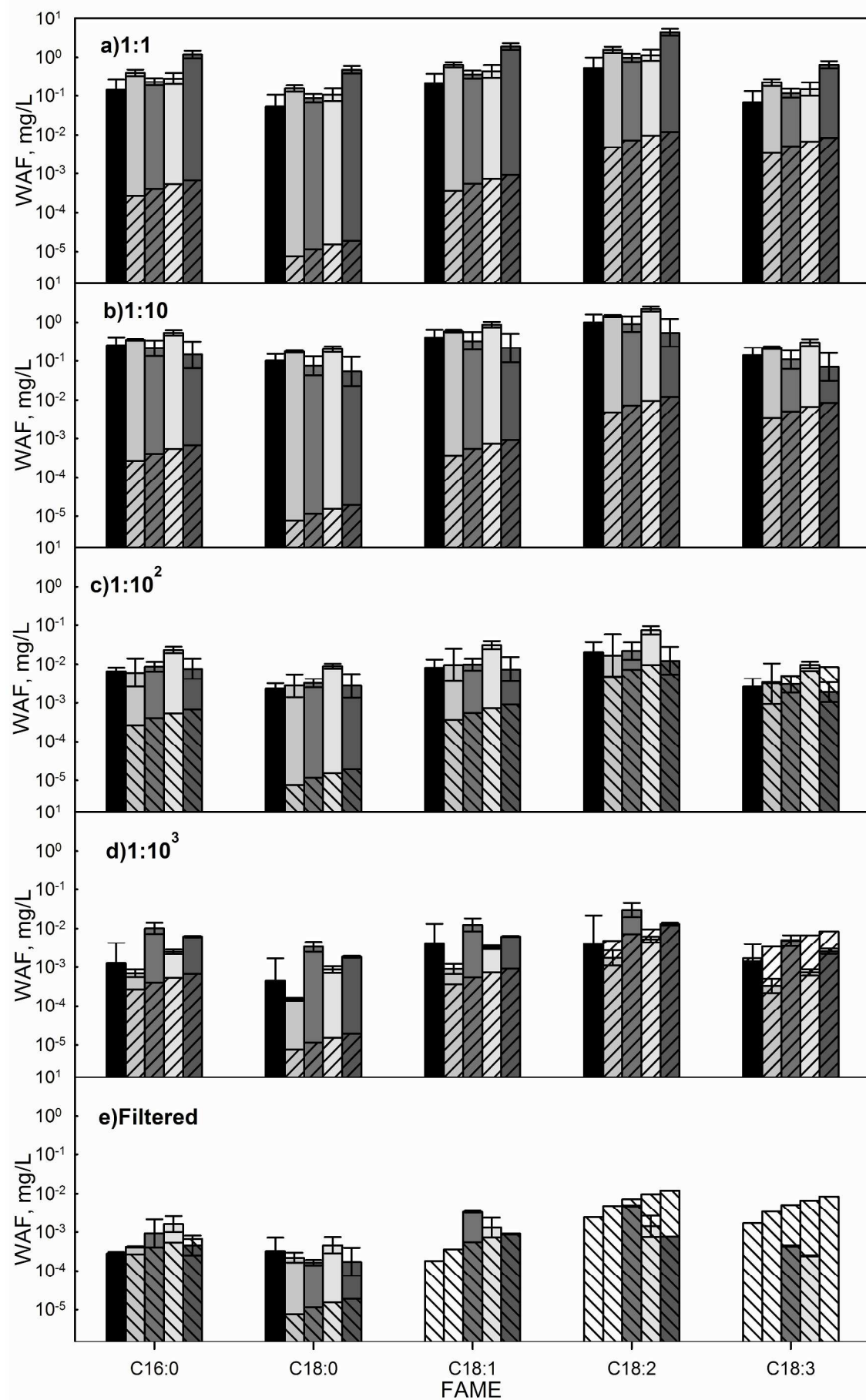


Figure S2. FAMES WAF concentrations in B20 (■), B40 (▤), B60 (▥), B80 (▦), B100 (▧), and $S_{aq,WAF}^{sat}$ is FAMES concentrations calculated by Equation 1 using solubilities reported by Krop et al.² (▨) at dilution levels: (a) 1:10⁰, (b) 1:10¹, (c) 1:10², (d) 1:10³, (e) and 1:10³ filtered. Means and standard deviations are calculated geometrically (n=3). Error bars are ± 1 geometric standard deviation. Not shown data were below detection limits.

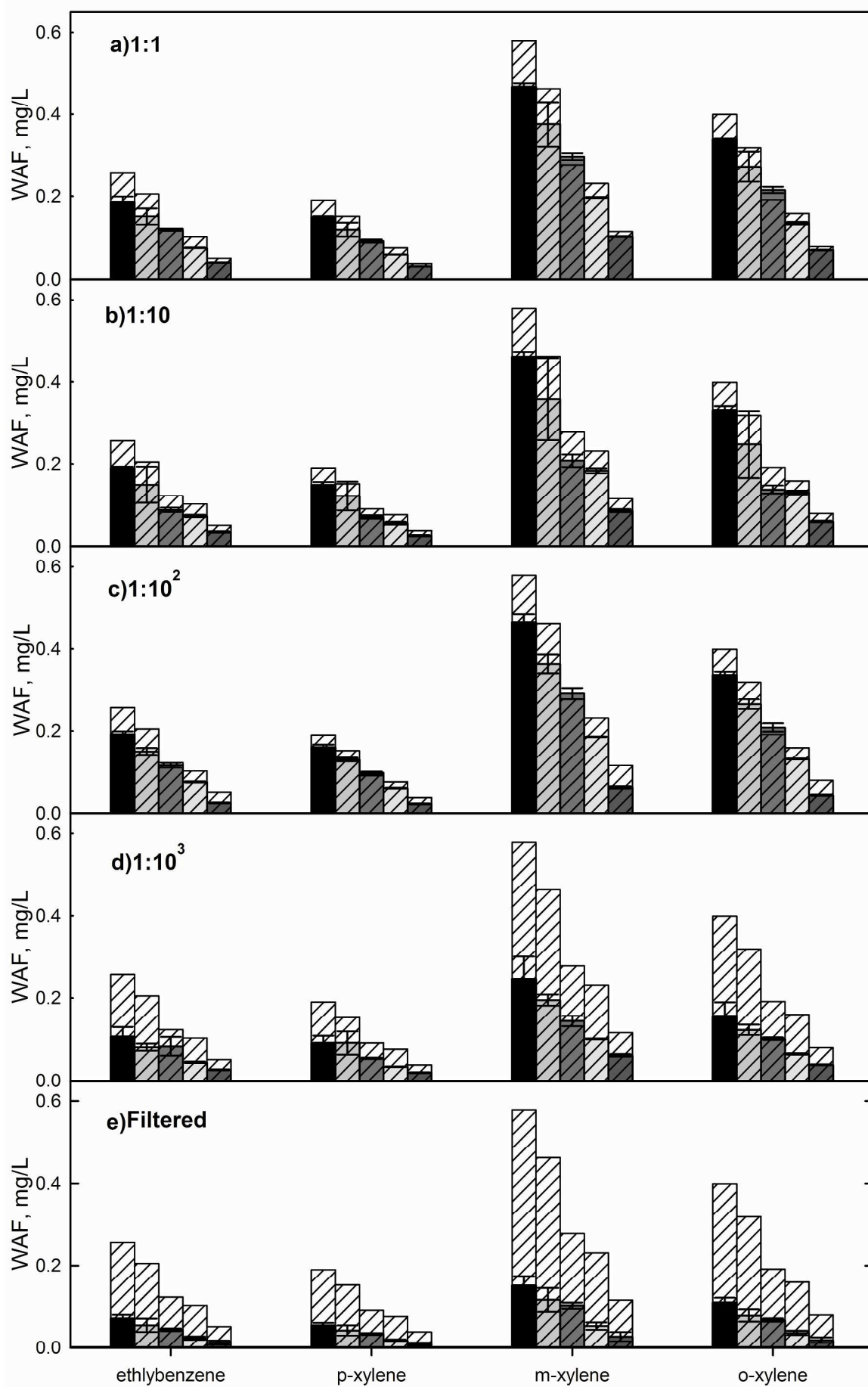


Figure S 3 Target aromatic compounds WAF concentrations in B0 (■), B20 (▤), B40 (▥), B60 (▦), B80 (▧), and $S_{aq,WAF}^{sat}$ is aromatic compounds concentrations calculated by Equation 1 using solubilities reported by Sanemasa et al.³ (▨) at dilution levels: (a) 1:10⁰, (b) 1:10¹, (c) 1:10², (d) 1:10³, (e) and 1:10³ filtered. Means and standard deviations are calculated arithmetically (n=3). Error bars are ± 1 arithmetic standard deviation.

Table S1. Reported aqueous solubility of pure selected hydrocarbons in deionized water at room temperature (22 ± 1 °C)

Compound	Pure solubility @ room temperature (µg/L)	Reference
<u>n-alkanes</u>		
C10	26	1
C16	6	1
<u>FAMEs</u>		
C16:0	4	2
C18:0	0.3	2
C18:1	4.39	2
C18:2	21	2
C18:3	91.85	2
<u>mono-aromatic</u>		
benzene	1,780,000 (or 1.78g/L)	4
toluene	563,000	5
ethylbenzene	187,000	6
p-xylene	153,000	6
m-xylene	159,000	6
o-xylene	212,000	6

PAHs		
Naphthalene	30,618	7
Fluorene	1,685	8
phenanthrene	994	8

References

1. Franks, F., Solute-Water Interactions and the Solubility Behaviour of Long-chain Paraffin Hydrocarbons. *Nature* **1966**, 210, (5031), 87-88.
2. Krop, H. B.; van Velzen, M. J. M.; Parsons, J. R.; Govers, H. A. J., n-Octanol-water partition coefficients, aqueous solubilities and Henry's law constants of fatty acid esters. *Chemosphere* **1997**, 34, (1), 107-119.
3. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H., Solubility measurements of benzene and the alkylbenzenes in water by making use of solute vapor. *Bulletin of the Chemical Society of Japan* **1982**, 55, (4), 1054-1062.
4. Goral, M., IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater - Revised and updated. Part 2. Benzene with water and heavy water. *Journal of physical and chemical reference data* **2005**, 34, (2), 477-552.
5. Goral, M., IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater-revised and updated. Part 5. C7 hydrocarbons with water and heavy water. *Journal of physical and chemical reference data* **2005**, 34, (3), 1399-1487.
6. Goral, M., IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater - Revised and updated. Part 6. C8H8-C8H 10 hydrocarbons with water. *Journal of physical and chemical reference data* **2005**, 34, (3), 1489-1553.
7. Goral, M., IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater - Revised and updated. Part 9. C10 hydrocarbons with water. *Journal of physical and chemical reference data* **2006**, 35, (1), 93-151.
8. Goral, M., IUPAC-NIST solubility data series. 81. Hydrocarbons with water and seawater - Revised and updated. Part 11. C13-C36 hydrocarbons with water. *Journal of physical and chemical reference data* **2006**, 35, (2), 687-784.