Supporting Information

# Solvatochromic sensitivity of BODIPY probes: a new tool for selecting fluorophores and polarity mapping

**Felix Y. Telegin [1] (ORCID 0000-0002-8626-2583), Viktoria S. Karpova [2] (ORCID 0000-0001-8979-3593), Anna O. Makshanova [3] (ORCID: 0000-0001-5708-2682), Roman G. Astrakhantsev [4] (ORCID 0000-0001-9880-2826), Yuriy S. Marfin [1*] (ORCID 0000-0002-1620-7175)**

[1]G.A. Krestov Institute of Solution Chemistry of the RAS, 1, Akademicheskaya str., Ivanovo, 153045, Russia; ymarfin@gmail.com
[2]Ivanovo State University of Chemistry and Technology, 7, Sheremetevsky Ave, Ivanovo 153000, Russia;
[3]Mendeleev University of Chemical Technology of Russia, 9, p. 33, Miusskaya square, Moscow, 125047, Russia;
[4]National Research University Higher School of Economics, 20, Myasnitskaya str., Moscow, 101000, Russia

## Phenomenological approach for quantifying the solvatochromism of the fluorescent probes

The relationships between spectral parameters of absorption and emission are often used for the analysis of the solvatochromic effects and estimation of the dipole moments of the fluorophores in the ground and excited state. A general theory for analysis of the solvent effect was presented in [1,2] and reviewed in [3–5] for different variants of the approaches of Lippert-Mataga, Bilot-Kawski, Bakhshiev, Liptay [4,6–8] as well as their similarities in special cases. The general approach based on the assumptions that the polarisability of the molecules is isotropic is expressed in the following way:

$$\nu_{Abs} - \nu_{Em} = m_f\, f(\varepsilon, n) + \Delta^o \qquad (1)$$

$$\nu_{Abs} + \nu_{Em} = -m_\varphi\, \varphi(\varepsilon, n) + \Sigma^o \qquad (2)$$

with the following solvent functions and parameters

$$m_f = \frac{2\left(\mu_e - \mu_g\right)^2}{hca^3}; \quad m_\varphi = \frac{2(\mu_e^2 - \mu_g^2)}{hca^3} \qquad (3)$$

A detailed theory for solvent effect assuming polarisability of the fluorophore was developed by Liptay [8,9] and Marsh [10] whose results were applied in [11]. In the case of a spherical Onsager cavity, Liptay's equations are expressed in the following way (according to Kawski's notations)

$$f(\varepsilon, n) = \frac{\frac{\varepsilon-1}{2\varepsilon+1} - \frac{n^2-1}{2n^2+1}}{\left(1-\frac{2\alpha}{a^3}\frac{\varepsilon-1}{2\varepsilon+1}\right)\left(1-\frac{2\alpha}{a^3}\frac{n^2-1}{2n^2+1}\right)} \qquad (4)$$

$$\varphi(\varepsilon) = \frac{\frac{\varepsilon-1}{2\varepsilon+1}}{1-\frac{2\alpha}{a^3}\frac{\varepsilon-1}{2\varepsilon+1}} \qquad (5)$$

$h$ is Plank's constant; $c$ is the speed of light; $\mu_g$ *and* $\mu_e$ are the vectors of dipole moments in the ground and excited states; $\varepsilon$ and $n$ are relative dielectric constant and refractive index of solvent; $\alpha$ and $a$ are the mean isotropic polarisability of the solute and the Onsager cavity radius in a homogeneous dielectric, respectively.

A simple semiempirical approach provided in our recent publications [12,13] is useful for gaining new insight into quantifying the solvatochromism of fluorophores in a high range of their polarity sensitivity.

Functions $f(\varepsilon, n)$ and $\varphi(\varepsilon)$ in Eqs (1) and (2) are based on the physicochemical parameters of the solvents determined experimentally. Numerous attempts of exploring the above mentioned theoretical approach expressed by Eqs (1) and (2) helped to discover an approximate linear relationship between spectral functions $(\nu_{Abs} - \nu_{Em})$ and $(\nu_{Abs} + \nu_{Em})$ used for quantifying the solvatochromism of fluorophores. This point has an empirical background based on an assumption regarding the linear relationship between solvent functions $f(\varepsilon, n)$ and $\varphi(\varepsilon)$:

$$f(\varepsilon, n) = P\varphi(\varepsilon) + Q \qquad (6)$$

$$P, Q - const$$

Correlations of Liptay's functions $f(\varepsilon, n)$ and $\varphi(\varepsilon)$ for a dataset of 251 solvents [14] are demonstrating linear regression coefficient $P$ approximately equal to 1.02 ($R^2$=0.94-0.98) invariant to changes of polarisability $\alpha/a^3$ in the range 0-0.5. Therefore, the regression coefficient $P$ in Eq (7) could be approximated by unity, i.e. $P \approx 1$.

Correlations of Bilot-Kawski functions $f(\varepsilon, n)$ and $\varphi(\varepsilon, n)$ [1,2] exhibit much worse linear correlation for the total dataset [14], i.e. $R^2$=0.78, although in case of limited sets of solvents applied in certain studies higher correlations could be found.

A combination of Eqs (1), (2), and (6) yields a desirable linear relationship (7) between absorption and emission wavenumbers of fluorophore:

$$\nu_{Abs} - \nu_{Em} = -P\frac{m_f}{m_\varphi}(\nu_{Abs} + \nu_{Em}) + \left(P\Sigma^0\frac{m_f}{m_\varphi} + Qm_f + \Delta^0\right) \qquad (7)$$

where expressions $P\frac{m_f}{m_\varphi}$ and $\left(P\Sigma^0\frac{m_f}{m_\varphi} + Qm_f + \Delta^0\right)$ are the constants.

The above Eq (7) for the Stokes shift $\nu_{Abs} - \nu_{Em}$ as well as correspondent equations for absorption and emission wavenumbers $\nu_{Abs}$ and $\nu_{Em}$ could be written shortly:

$$\nu_{Abs} - \nu_{Em} = -A(\nu_{Abs} + \nu_{Em}) + B \quad (8)$$

$$\nu_{Abs} = \frac{1-A}{2}(\nu_{Abs} + \nu_{Em}) + \frac{B}{2} \quad (9)$$

$$\nu_{Em} = \frac{1+A}{2}(\nu_{Abs} + \nu_{Em}) - \frac{B}{2} \quad (10)$$

$$A = \frac{m_f}{m_\varphi} = \frac{(\mu_e - \mu_g)^2}{\mu_e^2 - \mu_g^2} \quad (11)$$

$$B = \Sigma^0 \frac{m_f}{m_\varphi} + Q m_f + \Delta^0 \quad (12)$$

Noteworthy that expression (11) is written in a more general form than in the previous research [12,13]. It helps to use dipole moments in vector form with no additional assumptions because the square of a vector function has a scalar value.

**Table S1.** List of dyes selected for the dataset

1998 Lopez-Arbeloa-PM567 [15]
1999 Lopez-Arbeloa(177)-PM546 [16]
2004 Banuelos Prieto(29)-PAr1Ac [17]
2004 Banuelos-Prieto(5503)-PM597 [18]
2004 Lopez-Arbeloa-PM650 [19]
2004 Shen-3d [20]
2004 Shen-4a [20]
2004 Shen-4b [20]
2004 Shen-4c [20]
2004 Shen-4e [20]
2004 Shen-4f [20]
2006 Baruah-1 [21]
2006 Qin(190)-1 [22]
2008 Qin-1 [23]
2009 Cieslik-Boczula-2CN [24]
2009 Cieslik-Boczula-4CN [24]
2009 Qin(11731)-1 [25]
2010 Chaudhuri-1b [26]
2010 Filarowski-1 [27]
2010 Filarowski-2 [27]
2010 Filarowski-3 [27]
2010 Leen(2016)-1 [28]
2010 Leen(2016)-2 [28]
2010 Leen(2016)-3 [28]
2011 Banuelos(3437)-BTAA [29]
2012 Boens(9621)-1 [30]
2012 Boens(9621)-2 [30]
2012 Boens(9621)-3 [30]
2012 Boens(9621)-4 [30]
2012 Boens(9621)-5 [30]
2012 Boens(9621)-6 [30]
2012 Yin-1 [31]
2012 Zhao-OH [32]
2013 Er-BDC-9 [33]
2013 Nano-TX(6) [34]
2013 Yang-TPA-BDP1 [35]
2013 Yang-TPA-BDP2 [35]
2013 Yang-TPA-BDP3 [35]
2014 Boens-10 [36]
2014 Boens-6 [36]
2014 Boens-8 [36]
2015 Caltagirone-Py-BODIPY [37]
2015 Feng-1 [38]
2015 Filarowski-A [39]
2015 Jiao-3 [40]
2015 Jiao-4 [40]
2015 Jiao -5 [40]
2015 Jiao-1 [40]
2015 Jiao-2 [40]
2015 Thorat-Dye 2 [41]
2015 Thorat-Dye 3 [41]
2015 Thorat-Dye 4 [41]
2015 Waddell-1 [42]
2015 Waddell-2 [42]
2015 Waddell-3 [42]
2015 Waddell-4 [42]

2015 Waddell-5 [42]
2015 Waddell-6 [42]
2016 Bacalum-1 [43]
2016 Gupta-1 [44]
2016 Marfin(1975)-2 [45]
2016 Marfin(1975)-3 [45]
2016 Marfin(1975)-4 [45]
2016 Marfin(1975)-5 [45]
2016 Orte-2-Ethyn [46]
2016 Orte-2-Ph [46]
2016 Orte-3-Ethyn [46]
2016 Orte-3-Ph [46]
2016 Orte-3-Styryl [46]
2016 Orte-8-Ethyn [46]
2016 Orte-8-Ph [46]
2016 Qin-1 [47]
2016 Telore-7 [48]
2016 Telore-7a [48]
2016 Vu-2 [49]
2016 Vu-3 [49]
2016 Zhu(35627)-BP-2 [50]
2017 Petrushenko(488)-1 [51]
2017 Sadak-15 [52]
2017 Suhina-1 [53]
2017 Thorat-Dye 1 [54]
2017 Thorat-Dye 2 [54]
2017 Zhang(2447)-Ph-TMBDP [55]
2018 Leen-BODIPY [56]
2018 Mallah-Bn-OH-BDY [57]
2018 Ordonez-Hernandez-mVP1 [58]
2018 Ordonez-Hernandez-mVP2 [58]
2018 Ordonez-Hernandez-mVP3 [58]
2018 Ripoll-2 [59]
2018 Ripoll-4 [59]
2018 Ripoll-6 [59]
2019 Ali-10 [60]
2019 Ali-12 [60]
2019 Ali-14 [60]
2019 Ali-16 [60]
2019 Ali-19 [60]
2019 Ali-2 [60]
2019 Ali-20 [60]
2019 Ali-21 [60]
2019 Ali-23 [60]
2019 Ali-6 [60]
2019 Ali-9 [60]
2019 Antina-2,2-CH2-bis(BODIPY) [61]
2019 Antina-2,3-CH2-bis(BODIPY) [61]
2019 Antina-3,3-CH2-bis(BODIPY) [61]
2019 Bai-NJ1060 [62]
2019 Guseva-BODIPY 1 [63]
2019 Kawakami-BFBODIPY-DMP-DMAS [64]
2019 Sevinc-TPy-BDP [65]
2019 Zhang(148)-BDP [66]
2020 Gonzalez-Vera-2 [67]
2020 Gonzalez-Vera-3 [67]
2020 Shen-BODIPY-DT [68]
2021 Vysnauskas-BODIPY2 [69]
2021 Vysnauskas-BODIPY3 [69]

**Table S2.** List of dyes selected for comparison of duplicates

1999 Lopez Arbeloa(315)-PM546 [70]
1999 Lopez Arbeloa(315)-PM567 [70]
2002 Costela-PM567 [71]
2007 Rohand-2 [72]
2008 Costela-PM567 [73]
2009 Arroyo-1 [74]
2009 Costela-PM597 [75]
2011 Banuelos(677)-BDP [76]
2011 Banuelos(7261)-8-PAB [77]
2011 Banuelos(7261)-BDP [77]
2012 Duran-Sampedro-15 [78]
2012 Osorio-Martinez-1 [79]
2012 Zhang(11215)-1a [80]
2013 Duran-Sampedro-PM546 [81]
2013 Duran-Sampedro-PM567 [81]
2013 Duran-Sampedro-PM650 [81]
2013 Esnal(2691)-9 [82]
2013 Esnal(4134)-3 [83]
2013 Flores-Rizo-BODIPY [84]
2013 Flores-Rizo-BODIPY 7 [84]
2014 Choi-2 [85]
2014 Liu(5471)-B1 [86]
2018 Filatov(8016)-13 [87]
2018 Prasannan-Phenyl-BODIPY [88]
2018 Zhang(13)-BDP [89]
2019 Belmonte-Vazquez-22 [90]
2019 Hu(139)-1 [91]
2019 Hu(15944)-1 [92]
2019 Mallah(122)-Bn-BDY [93]
2019 Mallah(126)-Bn-BPY [94]
2019 Mallah(126)-Bn-OH-BDY [94]
2019 Zhang(286)-BDP [95]
2020 Berezin-3 [96]

**Table S3.** Solvents used in solvatochromic studies and their frequency of occurance in a dataset of 115 BODIPYs

| Solvent, IUPAC name / Occurrence in a dataset | | Solvent, IUPAC name / Occurrence in a dataset | |
|---|---|---|---|
| acetonitrile | 104 | water | 7 |
| methanol | 100 | pyridine | 7 |
| ethyl acetate | 99 | 2-methylpropan-2-ol | 6 |
| oxolane | 92 | 1-methylpyrrolidin-2-one | 6 |
| toluene | 88 | 2-methylbutane | 6 |
| trichloromethane | 86 | 2-(propan-2-yloxy)propane | 6 |
| 1,4-dioxane | 77 | heptane | 5 |
| propan-2-one | 74 | 1-(2,2-dimethylpropoxy)-2,2-dimethylpropane | 5 |
| dichloromethane | 68 | 1,4-xylene | 4 |
| methanesulfinylmethane | 67 | 2,2,4-trimethylpentane | 4 |
| ethoxyethane | 66 | methyl formate | 4 |
| cyclohexane | 66 | methyl acetate | 4 |
| N,N-dimethylformamide | 60 | 2-methoxy-2-methylpropane | 3 |
| ethanol | 57 | 1,1,1-trichloroethane | 3 |
| butan-1-ol | 53 | phenylmethanol | 3 |
| propan-2-ol | 47 | cyclohexanol | 3 |
| hexane | 43 | 2-methylpropan-1-ol | 3 |
| 1-butoxybutane | 42 | butan-2-one | 3 |
| octan-1-ol | 40 | 2-chloroethan-1-ol | 3 |
| pentan-1-ol | 30 | pentan-2-one | 3 |
| tetrachloromethane | 27 | propane-1,2,3-triol | 2 |
| chlorobenzene | 27 | 2-phenoxyethan-1-ol | 2 |
| cyclohexanone | 22 | undecan-1-ol | 2 |
| butanenitrile | 21 | benzonitrile | 1 |
| propan-1-ol | 18 | 2-methyloxolane | 1 |
| benzene | 15 | 3-methylbutan-2-one | 1 |
| ethane-1,2-diol | 14 | 1,2-dibromoethane | 1 |
| decan-1-ol | 14 | 1,2-dichlorobenzene | 1 |
| hexan-1-ol | 12 | 2-methoxyethan-1-ol | 1 |
| 1,2-dichloroethane | 12 | 2-methylheptane | 1 |
| butyl acetate | 11 | pyrrolidin-2-one | 1 |
| pentane | 9 | formamide | 1 |
| propanenitrile | 8 | N-methylformamide | 1 |
| acetic acid | 8 | dimethylarsinate | 1 |
| 2,2,2-trifluoroethan-1-ol | 8 | 2-[(2-hydroxyethyl)amino]ethan-1-ol | 1 |
| methylcyclohexane | 7 | | |

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