Options for nonpolar solvation free energy calculation with mm_pbsa.pl

Table1: Parameters provided in the literature:

$G_{pb\|gb}$ [1)]	SASA [2)]	G_{np} [3)]	Radii set	Ref. [4)]	Validation / determination procedure
IGB = 1, GB^{HTC}	LCPO	$0.005 \times SASA + 0.0$ [5)]	mbondi	[1] [7)]	GB simulation of 10 base pair DNA oligomer
		$0.0072 \times SASA + 0.0$ [6)]			GB simulation of 108 residue protein Thioredoxin
IGB = 2, $GB^{OBC\ I}$	Not given	$0.005 \times SASA + 0.0$	mbondi2, bondi [8)]	[2] [9)]	GB simulations of native proteins, (e.g. Thioredoxin, Protein-A, and Ubiquitin)
IGB = 5, $GB^{OBC\ II}$	Not given	$0.005 \times SASA + 0.0$	mbondi2, bondi [8)]	[2] [9)]	GB simulations of native proteins, (e.g. Thioredoxin, Protein-A, and Ubiquitin)
PBSA	PBSA [10)]	$0.0378 \times SASA - 0.5692 + G_{dispersion}$	R_{min}	[3]	Comparison of G_{np} of implicit solvent and TI calculations
PBSA Hybrid	Molsurf	$0.069 \times MSA + 0.0 + G_{vdW\ solute\text{-}solvent}$	bondi	[4] [11)]	Binding free energy calculation for H-Ras/C-Raf1 complex
PBSA	Shrake & Rupley [12)]	$0.0055 \times SASA + 0.92$	Parse	[5, 6] [13)]	Least-squares fit to a plot of experimental alkane transfer free energies versus accessible surface area

1) Procedure used for the calculation of the polar solvation free energy
2) Method used for the calculation of the solvent accessible surface area
3) Equation employed for the calculation of the nonpolar solvation free energy. SURFTEN and SURFOFF values are given in [kcal mol^{-1} $Å^{-2}$] and [kcal mol^{-1}], respectively. Studies in which the equation was applied for the calculation of the nonpolar solvation free energy are provided in superscript.
4) Publication in which the method / parameters are described
5) Cross reference to [5].
6) Cross reference to [7], but in this paper SURFTEN = 7 cal mol^{-1} $Å^{-2}$ is only cited as having been used in the "original GB/SA work". In this work [8], which describes the early GB model of Still et al., a "preliminary" SURFTEN parameter of 7.2 cal mol^{-1} $Å^{-2}$ is employed.
7) Reference for parameters of current AMBER implementation of IGB=1 and reference for mbondi radii.
8) For the thioredoxin system both mbondi2 and bondi parameters were tested.
9) Reference for current IGB=2 and IGB=5 implementations in AMBER and for mbond2 radii.
10) Solvent accessible volume, but not SASA calculated with PBSA [9] of Amber9.
11) Gohlke et al. 2004 can be used as reference for the calculation of G_{np}. However, the GB model applied for the computation of the polar solvation free energy, used to demonstrate good agreement with experimental binding free energies in conjunction with the specific nonpolar solvation free energy calculation method, is not available in AMBER11. SURFTEN value of 0.069 kcal mol^{-1} $Å^{-2}$ [10] is cited in Gohlke et al. 2004. Reference for the hybrid model: A. Metz, H. Gohlke, 2012, in preparation.
12) Modified Shrake & Rupley [11] vertex algorithm
13) SURFTEN and SURFOFF values of 0.005 ($\pm$ 0.0005) and 0.86 ($\pm$ 0.1), respectively, determined for different radii sets in original Parse radii publication [5]. A fit of experimental vacuum to water solvation free energies to surface area yielded SURFTEN and SURFOFF values of 0.0055 kcal mol^{-1} $Å^{-2}$ and 0.92 kcal mol^{-1}, respectively [6].

Table 2: Input parameters recommended for nonpolar solvation free energy calculations for protein systems

$G_{pb\|gb}$ [1]	Flags affecting nonpolar solvation energy calculation			Calculation of G_{np} [2]	Radii [3]	SURFTEN	SURFOFF
IGB = 1	MS=0|1	GBSA=1		$G_{np}=\gamma$ A + b	mbondi	0.00720	0.0000
IGB = 2	MS=0|1	GBSA=1|2		$G_{np}=\gamma$ A + b	mbondi2	0.00500	0.0000
IGB = 5	MS=0|1	GBSA=1|2		$G_{np}=\gamma$ A + b	mbondi2	0.00500	0.0000
PB	MS=0	INP=1	RADIOPT=0	$G_{np}=\gamma$ A + b	Parse	0.00542	0.9200
	MS=0	INP=2 [4]	RADIOPT=1	$G_{np}=\gamma$ A + b + $G_{disp.}$	R_{min}	0.03780	-0.5692
	MS=1	IVCAP > 0	RADIOPT=1	$G_{np}= G_{cavity} + E_{vdW}$	bondi	[5] 0.06900	[5] 0.0000

[1] Procedure used for the calculation of the polar solvation free energy

[2] Method employed for determination of the nonpolar solvation free energy

[3] Radii used for calculation of the nonpolar solvation free energy (G_{np}).

[4] Calculation procedure for INP=2 changed in mm_pbsa.pl of AMBER12 according to the recommendations of Dr. Luo.

New parameters: DECOMPOPT = 2 (σ decomposition scheme)
USE_RMIN = 1 (vdW R_{min} values)
USE_SAV = 1 (Molecular volume enclosed by SASA (SAV) used for estimation of G_{cavity})
SPROB = 0.557 (Solvent probe radius for SASA used for calculation of $G_{dispersion}$)
VPROB = 1.3 (Solvent probe radius for molecular volume used for computation of G_{cavity})
RHOW_EFFECT = 1.129 (Effective water density used for calculation of $G_{dispersion}$)
DPROB = 1.6 (Solvent probe radius for molecular surface used to define the dielectric boundary between solute and solvent)

Parameters up to AMBER11: DECOMPOPT = 1 (6/12 decomposition scheme)
USE_RMIN = 0 (vdW σ values)
USE_SAV = 0 (SASA used for estimation of G_{cavity})
SPROB = 1.6 (Solvent probe radius for SASA used for calculation of G_{cavity}, $G_{dispersion}$ and polar solvation free energy (DPROB = SPROB))

[5] These parameters should only be applied when calculations according to the hybrid model are conducted (IVCAP > 0) or when an analogous calculation procedure as in [4] is intended. The nonpolar solvation free energy is calculated as the sum of the cavity free energy $G_{cavity} = \gamma$ MSA + b (where MSA = molecular surface area) and the van der Waals interaction energy between solute and solvent atoms (E_{vdW}).

Literature

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