

Table S3. Notation for the substitution scores considered.

Our notation	Petrokovski, 1996	Panchenko, 2003	Mittelman <i>et al.</i> , 2003	Marti-Renom <i>et al.</i> , 2004	Edgar & Sjölander, 2004	Wang & Dunbrack, 2004	Edgar, 2004b	Ohlson <i>et al.</i> , 2004	First proposed
<i>Euclid-f</i>					euclidf				
<i>Euclid-g</i>	d				euclidp				
<i>Euclid-q</i>				S ⁽³⁾					
<i>Euclid-r</i>									
<i>Euclid-s</i>									
<i>dot-f</i>			Dot Product2		fdotf				
<i>dot-g</i>	p		Dot Product	S ⁽¹⁾	pdotp	DotPFreq		DP	Rychlewski <i>et al.</i> , 2000
<i>dot-q</i>					mdotm	DotOdds			
<i>dot-r</i>					prc				
<i>dot-s</i>					correlf				
<i>ldot-g</i>					correlp		LAMA		
<i>ldot-r</i>					rankf	CORREL			
<i>ldot-gr</i>					rankp				
<i>corr-f</i>			Corr Coef1F						
<i>corr-g</i>	r		Score function 3	S ⁽²⁾					
<i>corr-q</i>			Corr Coef1						
<i>corr-r</i>			Corr Coef2						
<i>corr-s</i>									
<i>rank-f</i>									
<i>rank-g</i>	rho								
<i>rank-q</i>									
<i>rank-r</i>									
<i>aS-f</i>			Sum of Pairs2		aI		PSF		Bacon & Anderson, 1986
<i>aS-q</i>			Sum of Pairs			CrossProduct			
<i>laQ-f</i>					la	LogAverage			
<i>laQ-q</i>							LE		
<i>laR-f</i>							LA		
<i>laR-q</i>							log_aver		von Öhsen & Zimmer, 2001
<i>sre-q</i>					re				Sjölander, 1998
<i>JS-f</i>					yldf				
<i>JS-q</i>					yld				
<i>YL-f</i>					ylf				
<i>YL-q</i>					yl				
<i>sdot-fs</i>			Prof_Sim		JensenShannon	YL			
<i>comp-fs</i>			Picasso3						
<i>sdot-cs</i>						LogOddsMultin			
<i>comp-cs</i>									
<i>sdot-qs</i>			Score function 2						
<i>BLID</i>			Compass2						
			Compass1						
			Picasso3Q						