SUPPORTING INFORMATION

MOLECULAR RECOGNITION-BASED CATALYSIS IN NUCLEOPHILIC AROMATIC SUBSTITUTION: A MECHANISTIC STUDY

Nuno Basilio,[†] Luis García-Río,*[,†] Ángeles Peña-Gallego[†] and Moisés Pérez-Lorenzo*[,‡]

Center for Research in Biological Chemistry and Molecular Materials (CIQUS), University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, and Department of Physical Chemistry, University of Vigo, 36310 Vigo, Spain.

Corresponding author email: moisespl@uvigo.es

INDEX

S_NAr reaction of 1-chloro-2,4-dinitrobenzene

S_NAr reaction of 1-fluoro-4-nitrobenzene

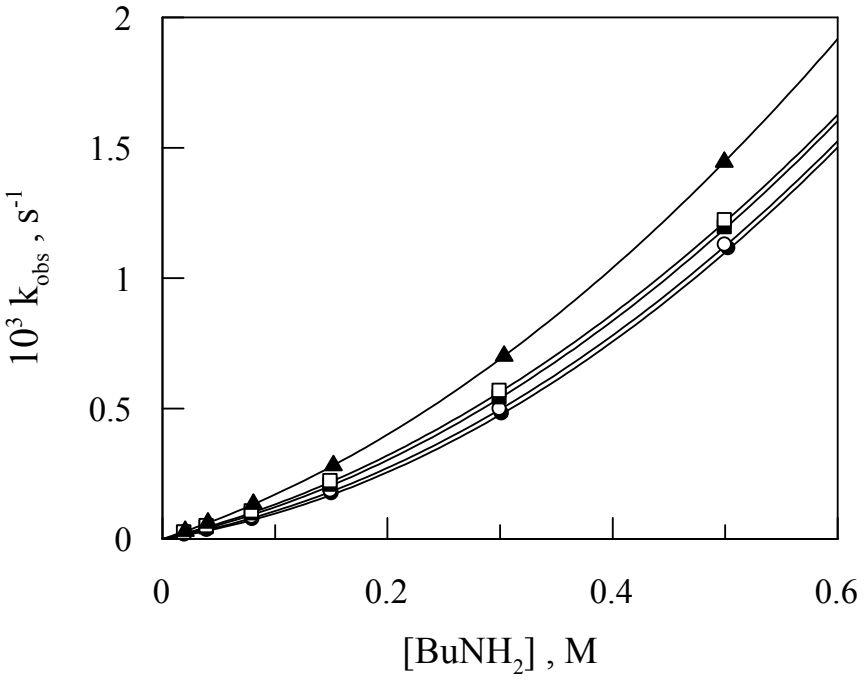

Figure S-1. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G2]=0M; (○) [G2]=0.10M; (■) [G2]=0.20M; (□) [G2]=0.30M and (▲) [G2]=0.51M.

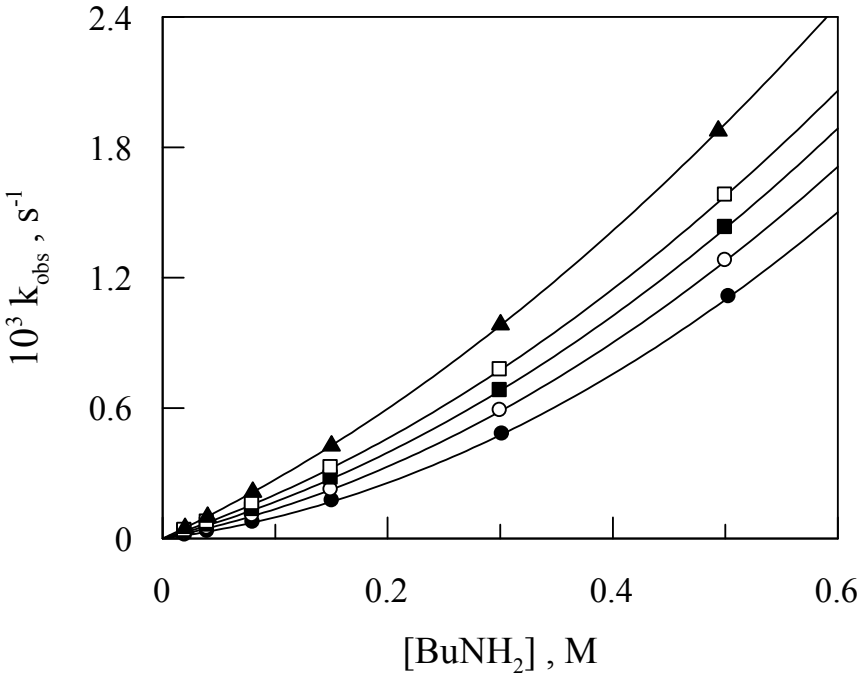

Figure S-2. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G3]=0M; (○) [G3]=0.10M; (■) [G3]=0.21M; (□) [G3]=0.31M and (▲) [G3]=0.52M.

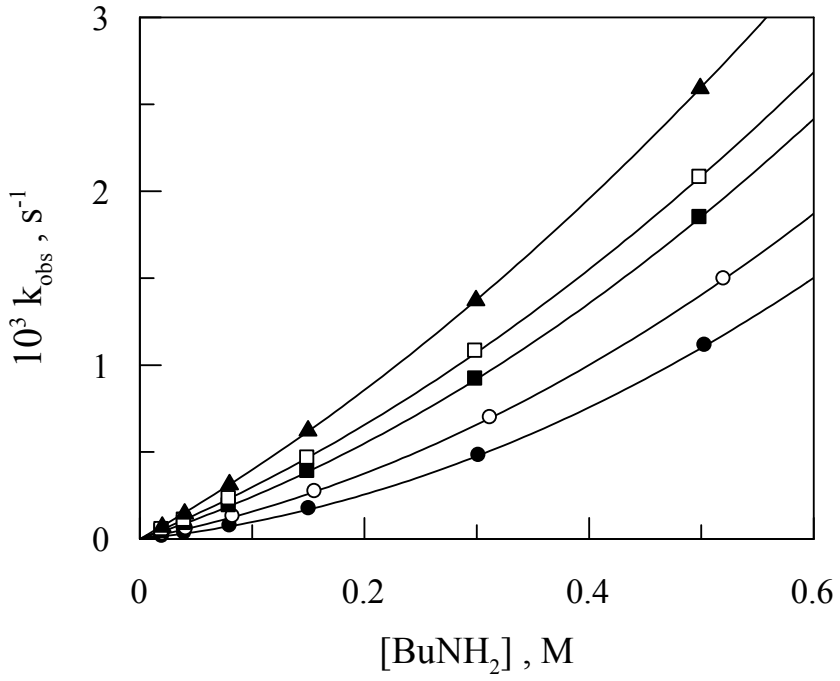

Figure S-3. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G5]=0M; (○) [G5]=0.10M; (■) [G5]=0.26M; (□) [G5]=0.35M and (▲) [G5]=0.56M.

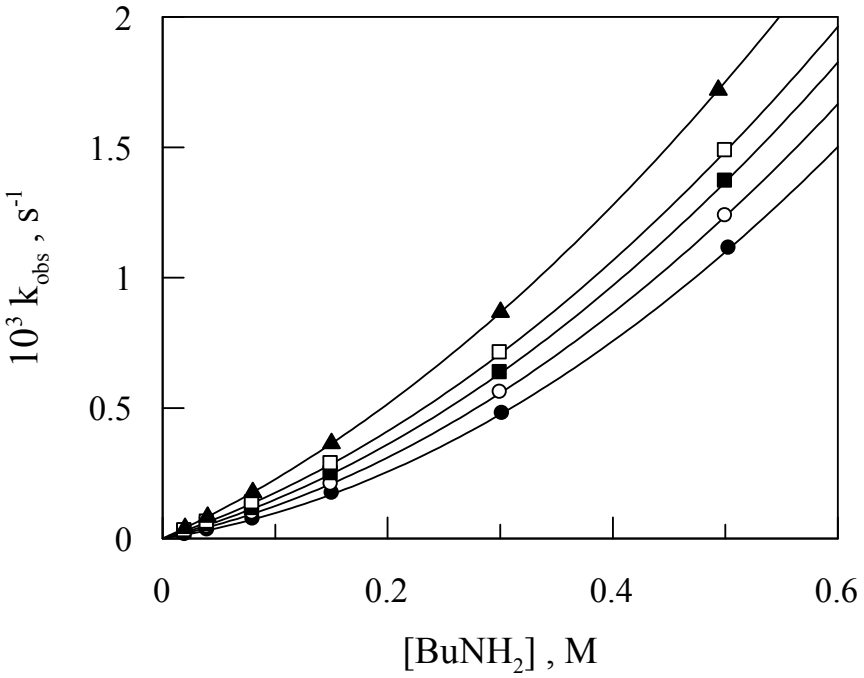

Figure S-4. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [12C4]=0M; (○) [12C4]=0.11M; (■) [12C4]=0.22M; (□) [12C4]=0.33M and (▲) [12C4]=0.55M.

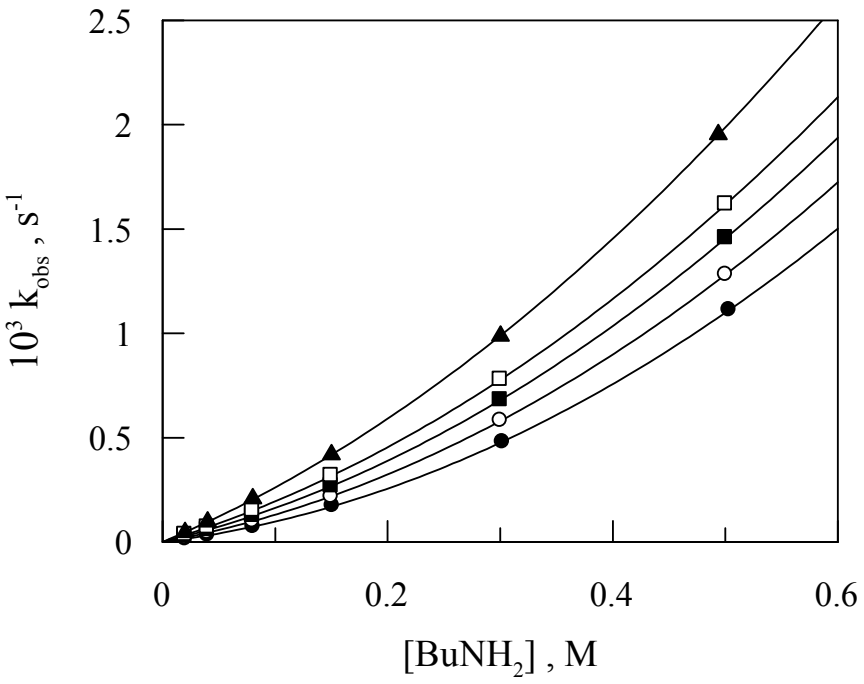

Figure S-5. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [15C5]=0M; (○) [15C5]=0.10M; (■) [15C5]=0.20M; (□) [15C5]=0.31M and (▲) [15C5]=0.51M.

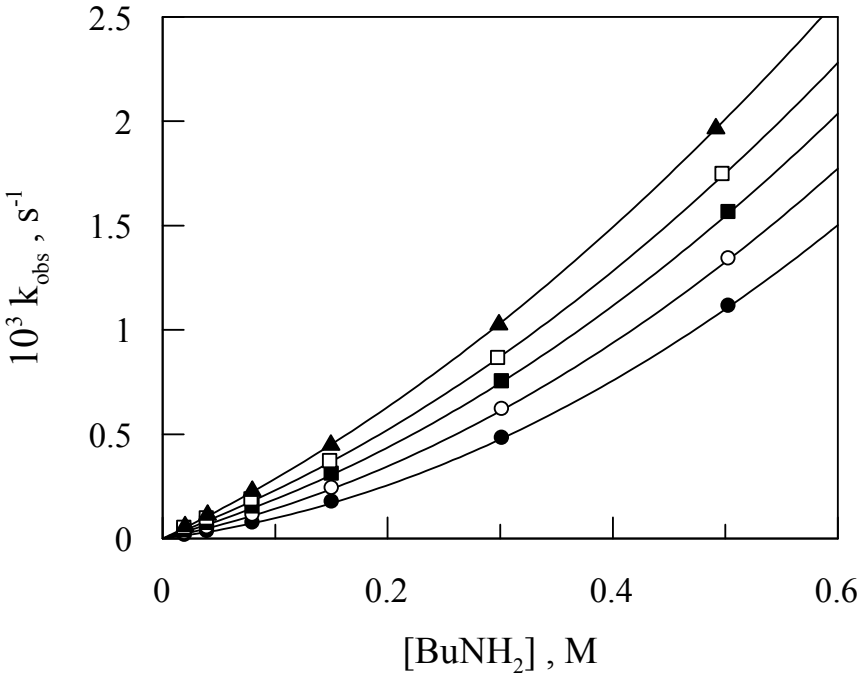

Figure S-6. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [18C6]=0M; (○) [18C6]=0.10M; (■) [18C6]=0.25M; (□) [18C6]=0.35M and (▲) [18C6]=0.50M.

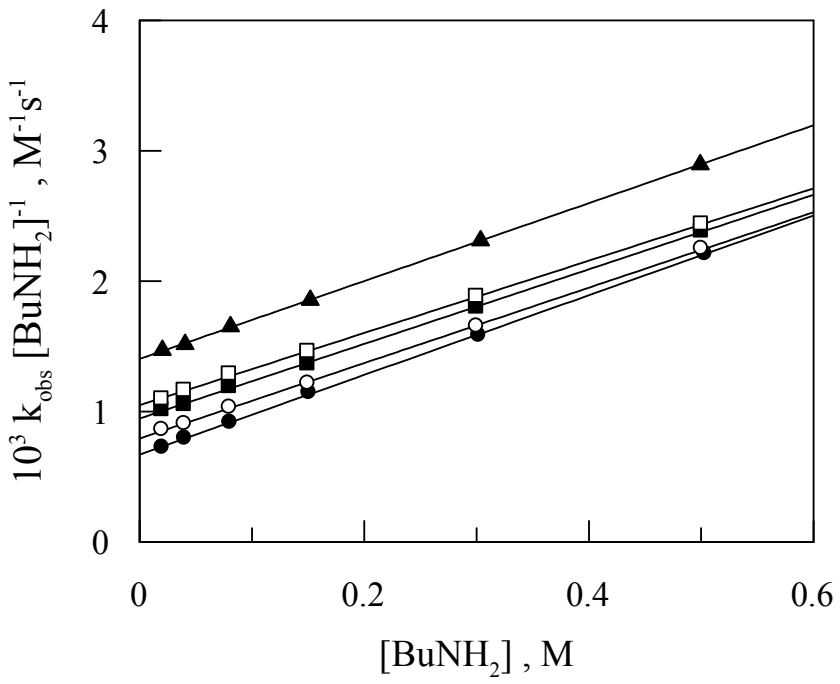

Figure S-7. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G2]=0M; (○) [G2]=0.10M; (■) [G2]=0.20M; (□) [G2]=0.31M and (▲) [G2]=0.51M.

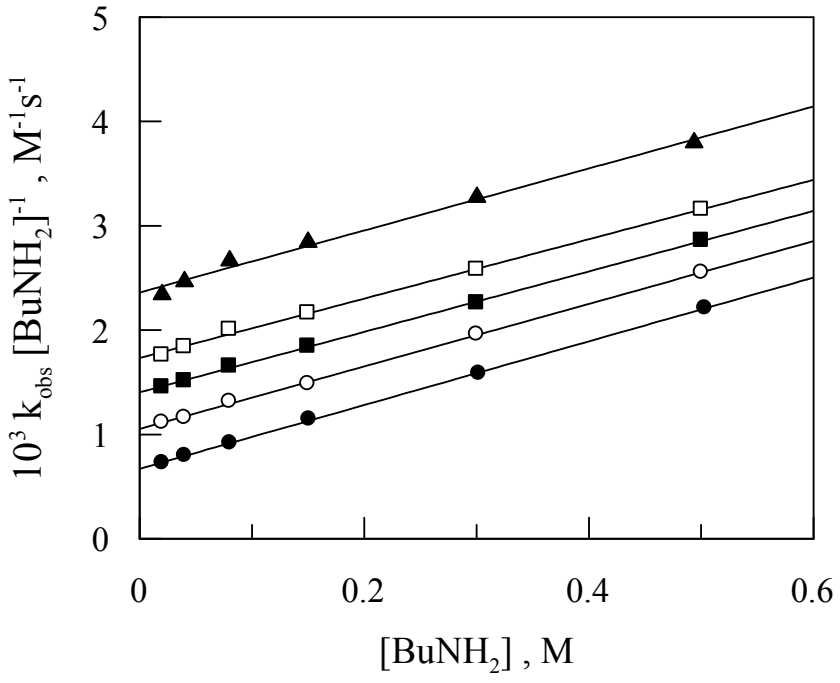

Figure S-8. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G3]=0M; (○) [G3]=0.10M; (■) [G3]=0.21M; (□) [G3]=0.31M and (▲) [G3]=0.52M.

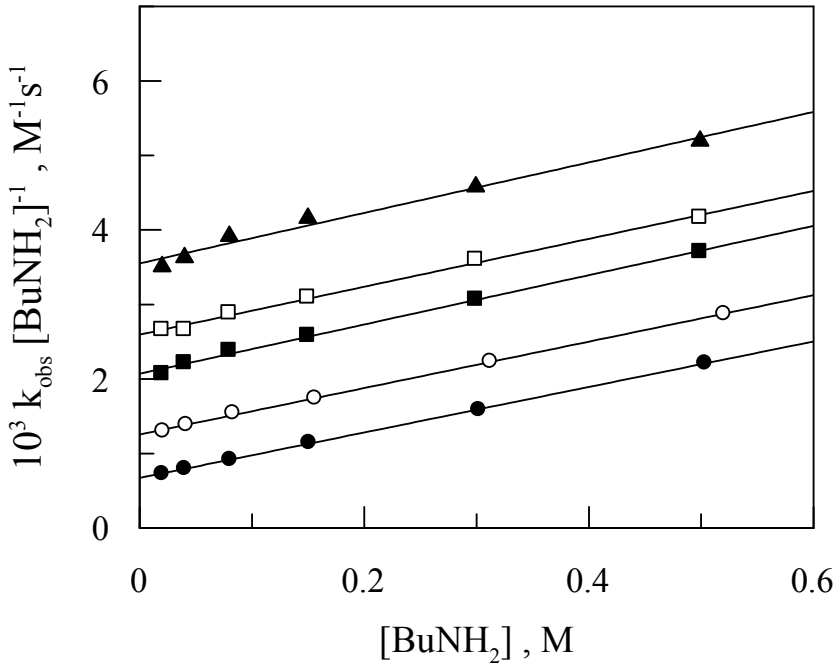

Figure S-9. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [G5]=0M; (○) [G5]=0.10M; (■) [G5]=0.26M; (□) [G5]=0.35M and (▲) [G5]=0.56M.

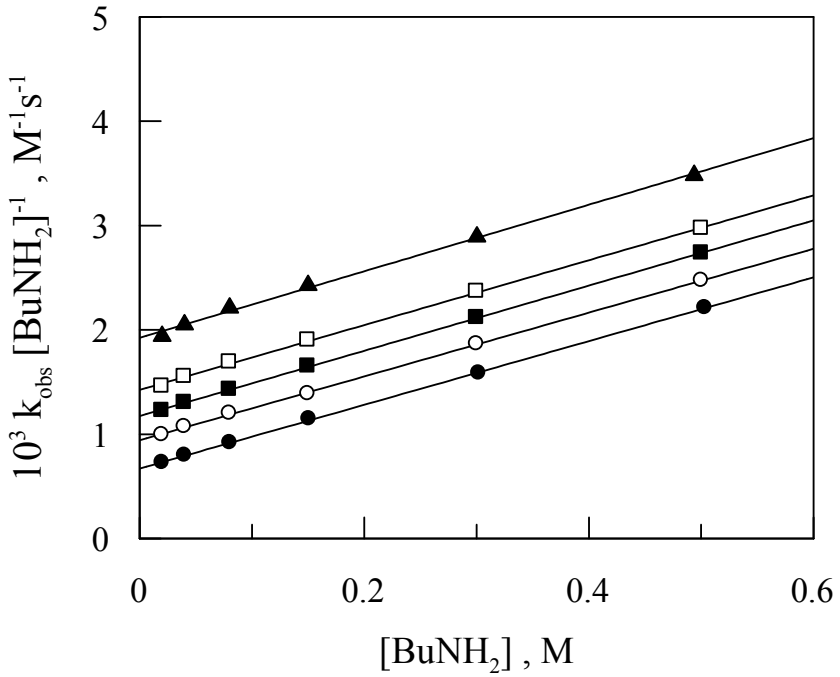

Figure S-10. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [12C4]=0M; (○) [12C4]=0.11M; (■) [12C4]=0.22M; (□) [12C4]=0.33M and (▲) [12C4]=0.55M.

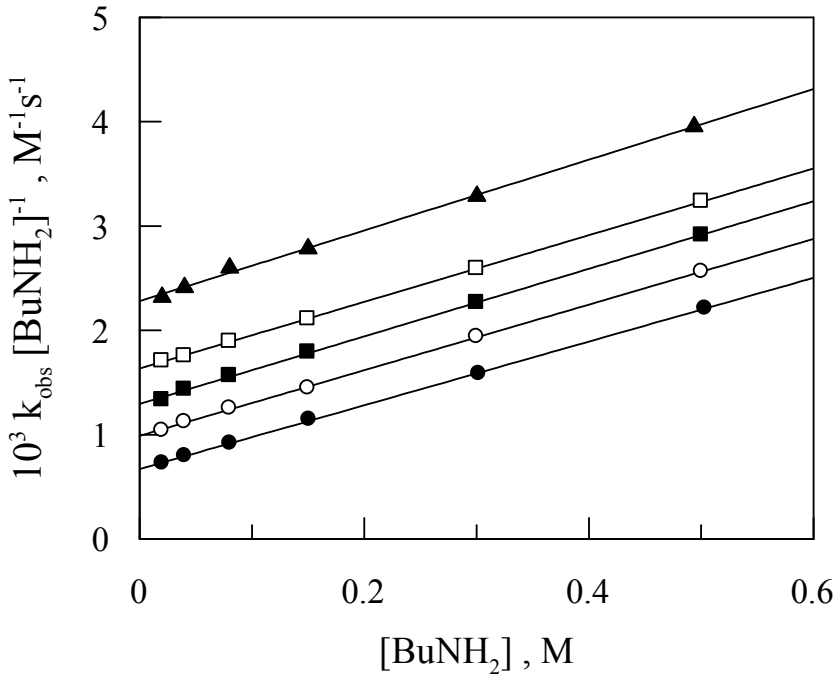

Figure S-11. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [15C5]=0M; (○) [15C5]=0.10M; (■) [15C5]=0.20M; (□) [15C5]=0.31M and (▲) [15C5]=0.51M.

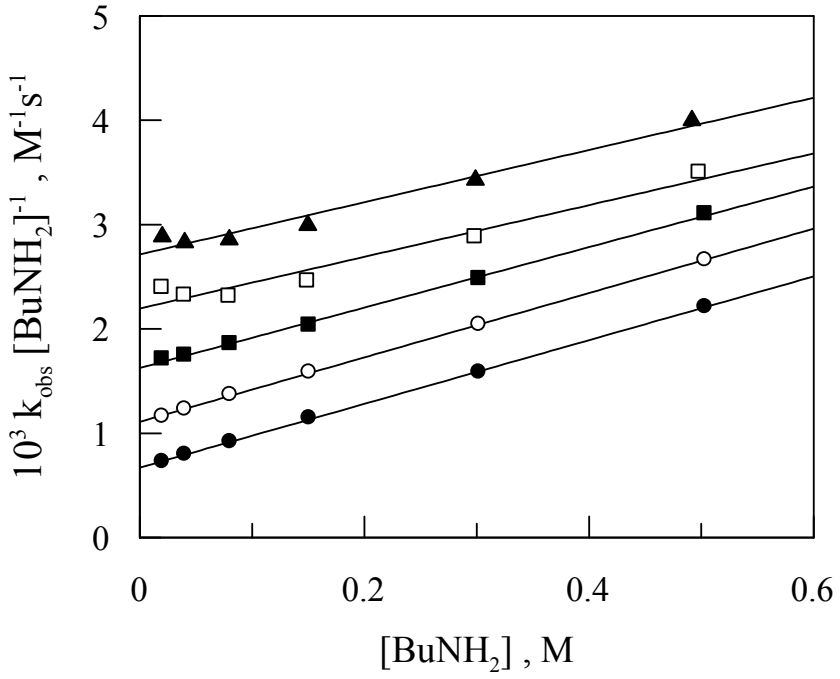

Figure S-12. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. T=25.0ºC. [CDNB]=1.4×10^{-4}M. (●) [18C6]=0M; (○) [18C6]=0.10M; (■) [18C6]=0.25M; (□) [18C6]=0.35M and (▲) [18C6]=0.50M.

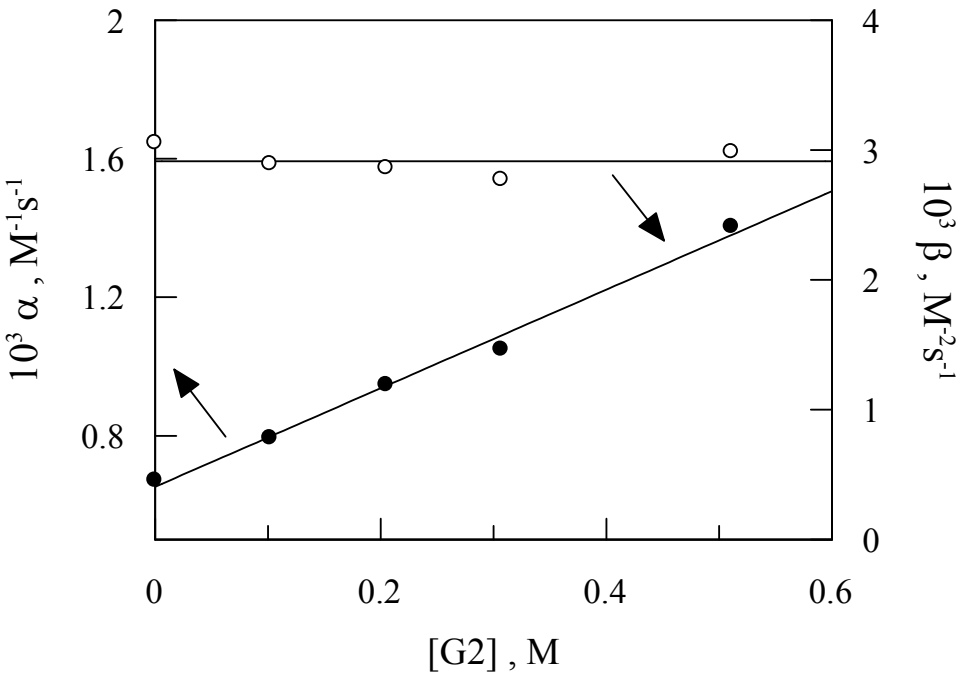

Figure S-13. Influence of G2 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

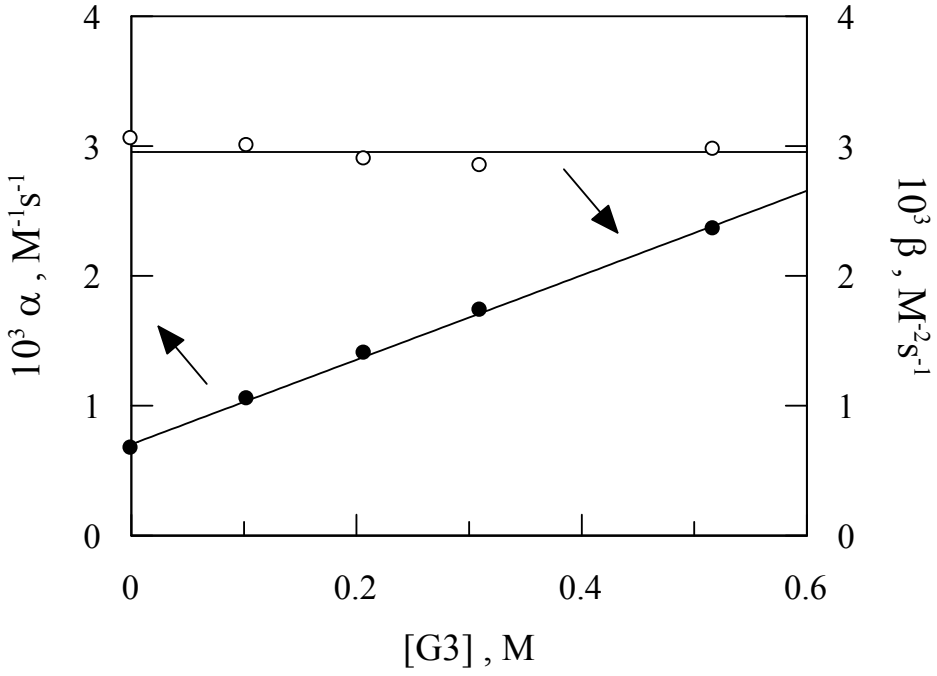

Figure S-14. Influence of G3 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

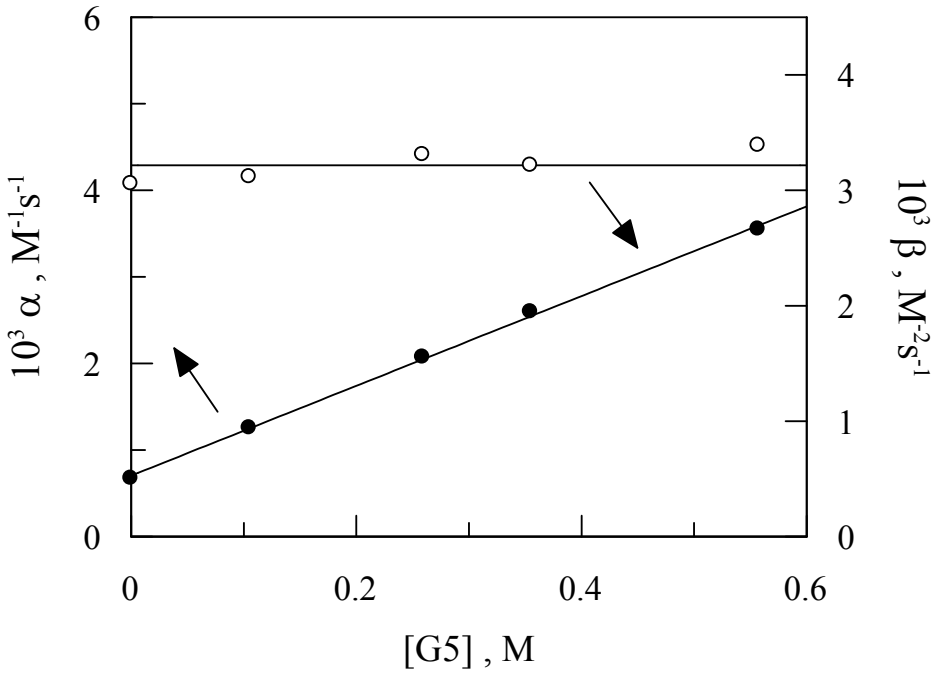

Figure S-15. Influence of G5 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

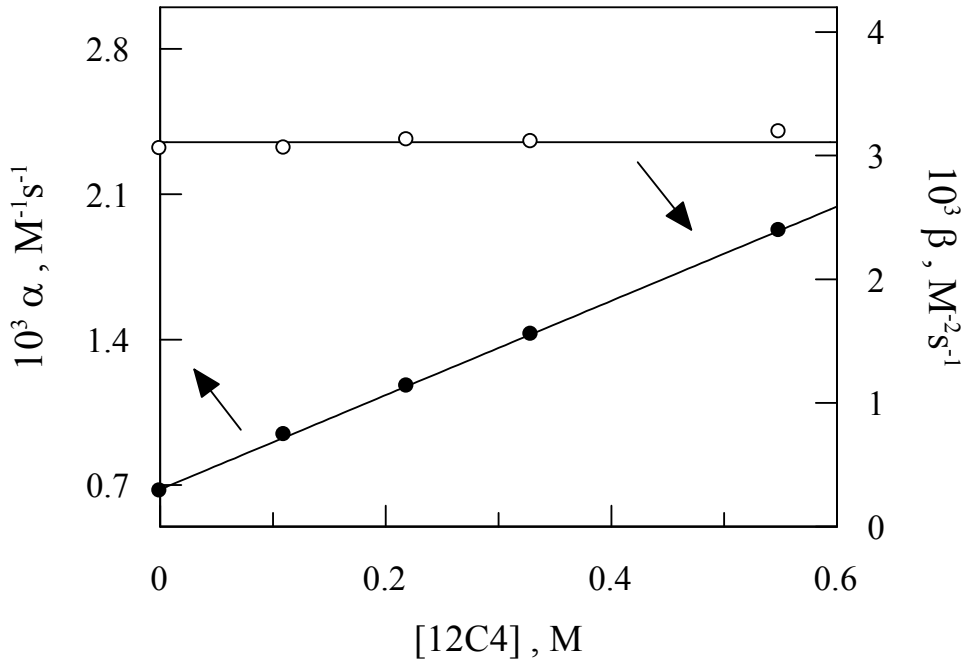

Figure S-16. Influence of 12C4 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

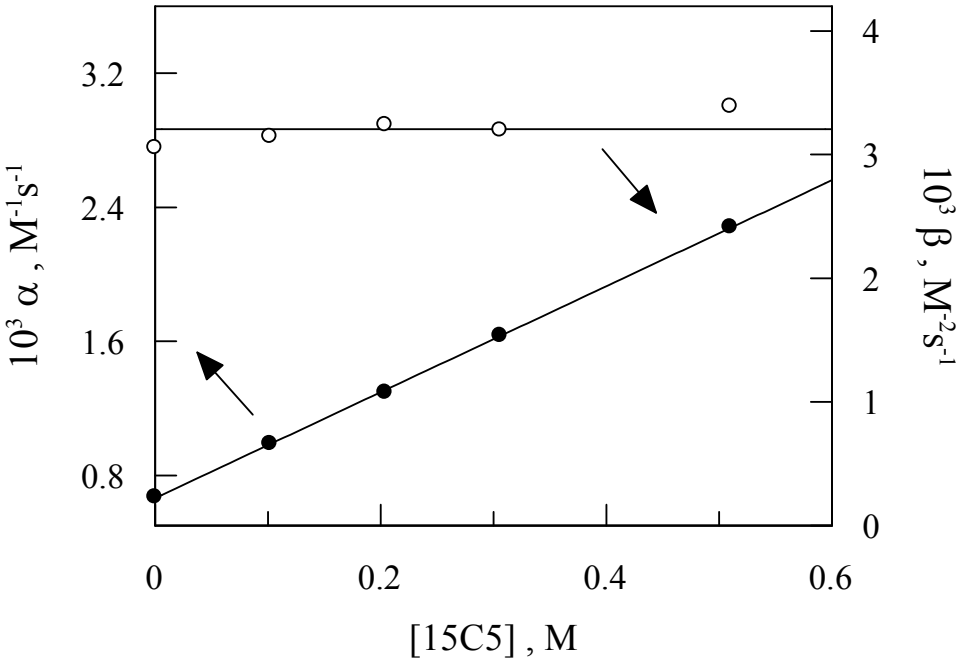

Figure S-17. Influence of 15C5 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

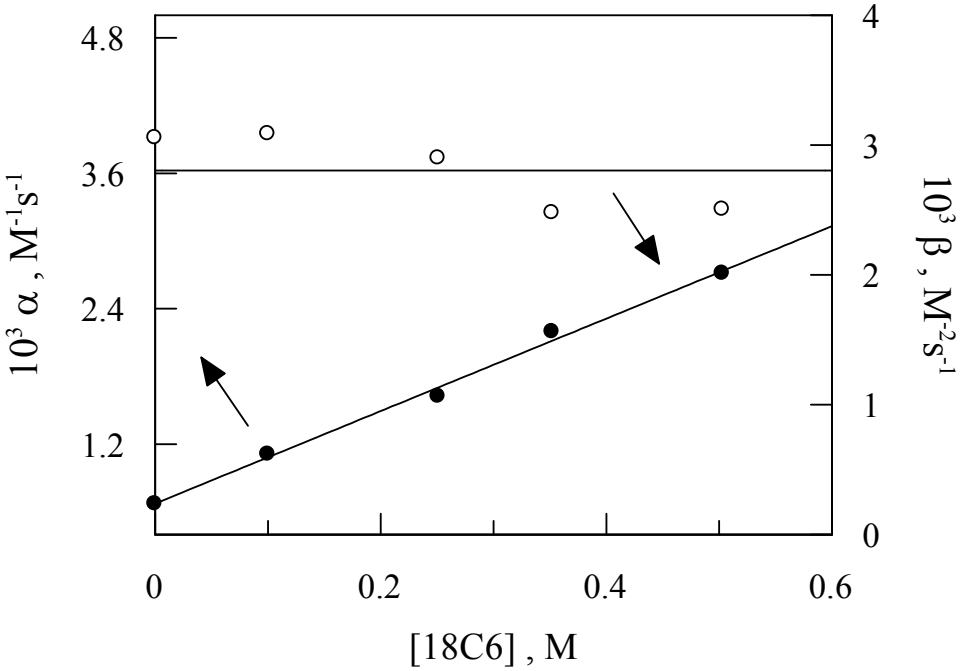

Figure S-18. Influence of 18C6 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-chloro-2,4-dinitrobenzene. (●) α and (○) β.

Table S-1. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the absence of polyethers. T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.01×10^{-2}	1.46×10^{-5}
4.03×10^{-2}	3.20×10^{-5}
8.06×10^{-2}	7.38×10^{-5}
1.51×10^{-1}	1.73×10^{-4}
3.02×10^{-1}	4.79×10^{-4}
5.03×10^{-1}	1.11×10^{-3}

Table S-2. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G2]=0.10M; T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	1.72×10^{-5}
4.00×10^{-2}	3.63×10^{-5}
8.01×10^{-2}	8.26×10^{-5}
1.50×10^{-1}	1.83×10^{-4}
3.00×10^{-1}	4.96×10^{-4}
5.00×10^{-1}	1.13×10^{-3}

Table S-3. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G2]=0.20M; T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.03×10^{-5}
4.00×10^{-2}	4.21×10^{-5}
8.01×10^{-2}	9.53×10^{-5}
1.50×10^{-1}	2.05×10^{-4}
3.00×10^{-1}	5.41×10^{-4}
5.00×10^{-1}	1.19×10^{-3}

Table S-4. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G2]=0.31M; T=25.0ºC.

[$BuNH_2$] , M	**[$BuNH_2$] , M**
2.00×10^{-2}	2.19×10^{-5}
4.00×10^{-2}	4.64×10^{-5}
8.01×10^{-2}	1.03×10^{-4}
1.50×10^{-1}	2.19×10^{-4}
3.00×10^{-1}	5.65×10^{-4}
5.01×10^{-1}	1.22×10^{-3}

Table S-5. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G2]=0.51M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.02×10^{-2}	2.97×10^{-5}
4.05×10^{-2}	6.14×10^{-5}
8.09×10^{-2}	1.34×10^{-4}
1.52×10^{-1}	2.82×10^{-4}
3.04×10^{-1}	7.01×10^{-4}
4.99×10^{-1}	1.44×10^{-3}

Table S-6. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G3]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.23×10^{-5}
4.00×10^{-2}	4.65×10^{-5}
8.01×10^{-2}	1.05×10^{-4}
1.50×10^{-1}	2.23×10^{-4}
3.00×10^{-1}	5.88×10^{-4}
5.00×10^{-1}	1.28×10^{-3}

Table S-7. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G3]=0.21M; T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.91×10^{-5}
4.00×10^{-2}	6.05×10^{-5}
8.01×10^{-2}	1.32×10^{-4}
1.50×10^{-1}	2.77×10^{-4}
3.00×10^{-1}	6.79×10^{-4}
5.00×10^{-1}	1.43×10^{-3}

Table S-8. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G3]=0.31M; T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	3.52×10^{-5}
4.00×10^{-2}	7.37×10^{-5}
8.01×10^{-2}	1.61×10^{-4}
1.50×10^{-1}	3.25×10^{-4}
3.00×10^{-1}	7.75×10^{-4}
5.00×10^{-1}	1.58×10^{-3}

Table S-9. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G3]=0.52M; T=25.0ºC.

[BuNH$_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	4.69×10^{-5}
4.00×10^{-2}	9.87×10^{-5}
8.01×10^{-2}	2.13×10^{-4}
1.50×10^{-1}	4.27×10^{-4}
3.00×10^{-1}	9.83×10^{-4}
4.94×10^{-1}	1.88×10^{-3}

Table S-10. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G4]=0.11M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.56×10^{-5}
3.99×10^{-2}	5.43×10^{-5}
7.98×10^{-2}	1.19×10^{-4}
1.50×10^{-1}	2.46×10^{-4}
2.99×10^{-1}	6.46×10^{-4}
4.99×10^{-1}	1.37×10^{-3}

Table S-11. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G4]=0.25M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	3.72×10^{-5}
3.99×10^{-2}	8.09×10^{-5}
7.98×10^{-2}	1.75×10^{-4}
1.50×10^{-1}	3.54×10^{-4}
2.99×10^{-1}	8.47×10^{-4}
4.99×10^{-1}	1.71×10^{-3}

Table S-12. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G4]=0.35M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	4.69×10^{-5}
3.99×10^{-2}	9.74×10^{-5}
7.98×10^{-2}	2.09×10^{-4}
1.50×10^{-1}	4.28×10^{-4}
2.99×10^{-1}	9.85×10^{-4}
4.99×10^{-1}	1.92×10^{-3}

Table S-13. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G4]=0.55M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	6.53×10^{-5}
3.99×10^{-2}	1.36×10^{-4}
7.98×10^{-2}	2.84×10^{-4}
1.50×10^{-1}	5.56×10^{-4}
2.99×10^{-1}	1.24×10^{-3}
4.99×10^{-1}	2.36×10^{-3}

Table S-14. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G5]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.08×10^{-2}	2.70×10^{-5}
4.16×10^{-2}	5.76×10^{-5}
8.33×10^{-2}	1.28×10^{-4}
1.56×10^{-1}	2.72×10^{-4}
3.12×10^{-1}	6.97×10^{-4}
5.20×10^{-1}	1.49×10^{-3}

Table S-15. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G5]=0.26M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	4.13×10^{-5}
3.99×10^{-2}	8.84×10^{-5}
7.98×10^{-2}	1.90×10^{-4}
1.50×10^{-1}	3.86×10^{-4}
2.99×10^{-1}	9.18×10^{-4}
4.99×10^{-1}	1.85×10^{-3}

Table S-16. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G5]=0.35M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	5.31×10^{-5}
3.99×10^{-2}	1.06×10^{-4}
7.98×10^{-2}	2.30×10^{-4}
1.50×10^{-1}	4.63×10^{-4}
2.99×10^{-1}	1.08×10^{-3}
4.99×10^{-1}	2.08×10^{-3}

Table S-17. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G5]=0.56M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	7.00×10^{-5}
3.99×10^{-2}	1.45×10^{-4}
7.98×10^{-2}	3.12×10^{-4}
1.50×10^{-1}	6.23×10^{-4}
2.99×10^{-1}	1.37×10^{-3}
4.99×10^{-1}	2.59×10^{-3}

Table S-18. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [G5]=0.26M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	4.13×10^{-5}
3.99×10^{-2}	8.84×10^{-5}
7.98×10^{-2}	1.90×10^{-4}
1.50×10^{-1}	3.86×10^{-4}
2.99×10^{-1}	9.18×10^{-4}
4.99×10^{-1}	1.85×10^{-3}

Table S-19. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [12C4]=0.11M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	1.99×10^{-5}
4.00×10^{-2}	4.28×10^{-5}
8.01×10^{-2}	9.61×10^{-5}
1.50×10^{-1}	2.08×10^{-4}
3.00×10^{-1}	5.60×10^{-4}
5.00×10^{-1}	1.24×10^{-3}

Table S-20. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [12C4]=0.22M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.45×10^{-5}
4.00×10^{-2}	5.21×10^{-5}
8.01×10^{-2}	1.14×10^{-4}
1.50×10^{-1}	2.48×10^{-4}
3.00×10^{-1}	6.35×10^{-4}
5.00×10^{-1}	1.37×10^{-3}

Table S-21. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [12C4]=0.33M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.92×10^{-5}
4.00×10^{-2}	6.21×10^{-5}
8.01×10^{-2}	1.35×10^{-4}
1.50×10^{-1}	2.85×10^{-4}
3.00×10^{-1}	7.11×10^{-4}
5.00×10^{-1}	1.49×10^{-3}

Table S-22. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [12C4]=0.55M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	3.88×10^{-5}
4.00×10^{-2}	8.21×10^{-5}
8.01×10^{-2}	1.77×10^{-4}
1.50×10^{-1}	3.64×10^{-4}
3.00×10^{-1}	8.69×10^{-4}
4.94×10^{-1}	1.72×10^{-3}

Table S-23. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [15C5]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.08×10^{-5}
4.00×10^{-2}	4.49×10^{-5}
8.01×10^{-2}	1.00×10^{-4}
1.50×10^{-1}	2.17×10^{-4}
3.00×10^{-1}	5.82×10^{-4}
5.00×10^{-1}	1.28×10^{-3}

Table S-24. Influence of *n*-butylamine concentration on k_{obs} for he CDNB S_NAr in the presence of polyethers. [15C5]=0.20M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	2.67×10^{-5}
4.00×10^{-2}	5.74×10^{-5}
8.01×10^{-2}	1.25×10^{-4}
1.50×10^{-1}	2.69×10^{-4}
3.00×10^{-1}	6.80×10^{-4}
5.00×10^{-1}	1.46×10^{-3}

Table S-25. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [15C5]=0.31M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	3.41×10^{-5}
4.00×10^{-2}	7.03×10^{-5}
8.01×10^{-2}	1.52×10^{-4}
1.50×10^{-1}	3.17×10^{-4}
3.00×10^{-1}	7.78×10^{-4}
5.00×10^{-1}	1.62×10^{-3}

Table S-26. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [15C5]=0.51M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.00×10^{-2}	4.64×10^{-5}
4.00×10^{-2}	9.65×10^{-5}
8.01×10^{-2}	2.08×10^{-4}
1.50×10^{-1}	4.18×10^{-4}
3.00×10^{-1}	9.87×10^{-4}
4.94×10^{-1}	1.95×10^{-3}

Table S-27. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [18C6]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.01×10^{-2}	2.34×10^{-5}
4.03×10^{-2}	4.95×10^{-5}
8.06×10^{-2}	1.10×10^{-4}
1.51×10^{-1}	2.39×10^{-4}
3.02×10^{-1}	6.17×10^{-4}
5.03×10^{-1}	1.34×10^{-3}

Table S-28. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [18C6]=0.25M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
2.01×10^{-2}	3.44×10^{-5}
4.03×10^{-2}	7.03×10^{-5}
8.06×10^{-2}	1.50×10^{-4}
1.51×10^{-1}	3.07×10^{-4}
3.02×10^{-1}	7.50×10^{-4}
5.03×10^{-1}	1.56×10^{-3}

Table S-29. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [18C6]=0.35M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
1.99×10^{-2}	4.77×10^{-5}
3.99×10^{-2}	9.25×10^{-5}
7.97×10^{-2}	1.84×10^{-4}
1.49×10^{-1}	3.67×10^{-4}
2.99×10^{-1}	8.62×10^{-4}
4.98×10^{-1}	1.74×10^{-3}

Table S-30. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [18C6]=0.50M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
1.99×10^{-2}	5.75×10^{-5}
3.99×10^{-2}	1.13×10^{-4}
7.97×10^{-2}	2.28×10^{-4}
1.49×10^{-1}	4.48×10^{-4}
2.99×10^{-1}	1.02×10^{-3}
4.92×10^{-1}	1.97×10^{-3}

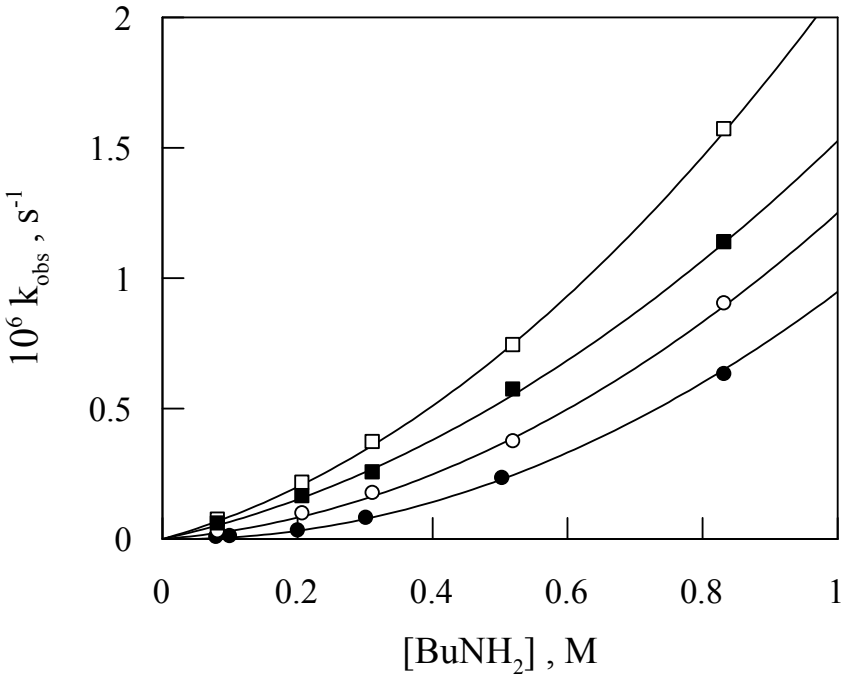

Figure S-19. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [G4]=0M; (○) [G4]=0.10M; (■) [G4]=0.20M and (□) [G4]=0.30M.

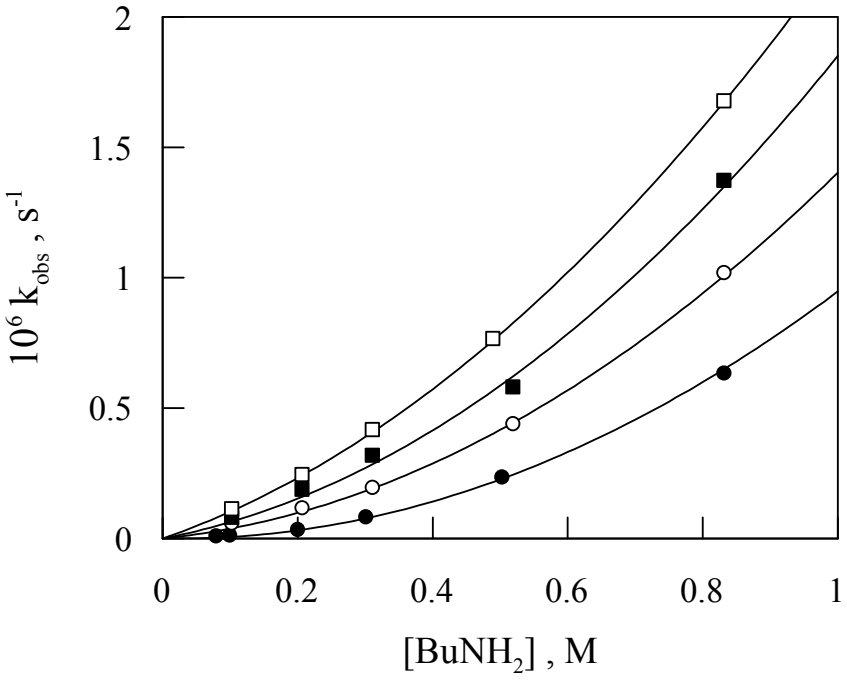

Figure S-20. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [G5]=0M; (○) [G5]=0.10M; (■) [G5]=0.20M and (□) [G5]=0.30M.

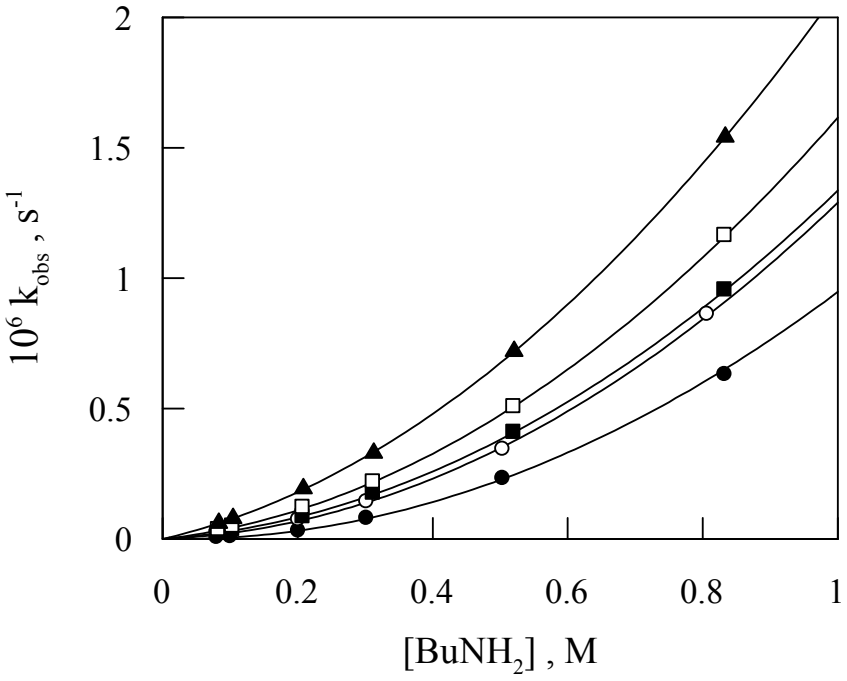

Figure S-21. Influence of *n*-butylamine concentration on k_{obs} for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [18C6]=0M; (○) [18C6]=0.10M; (■) [18C6]=0.20M; (□) [18C6]=0.30M and (▲) [18C6]=0.51M.

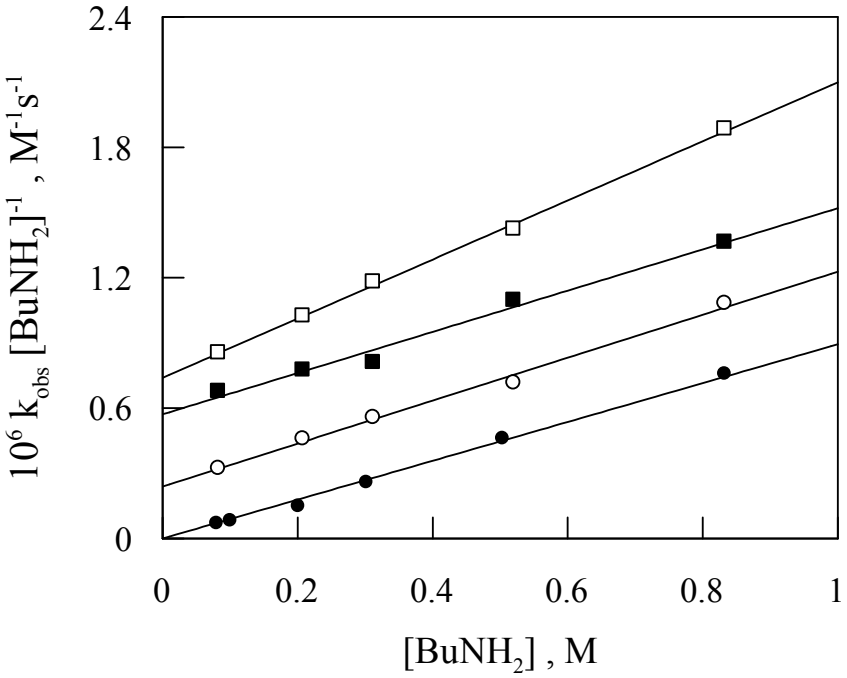

Figure S-22. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [G4]=0M; (○) [G4]=0.10M; (■) [G4]=0.20M and (□) [G4]=0.30M.

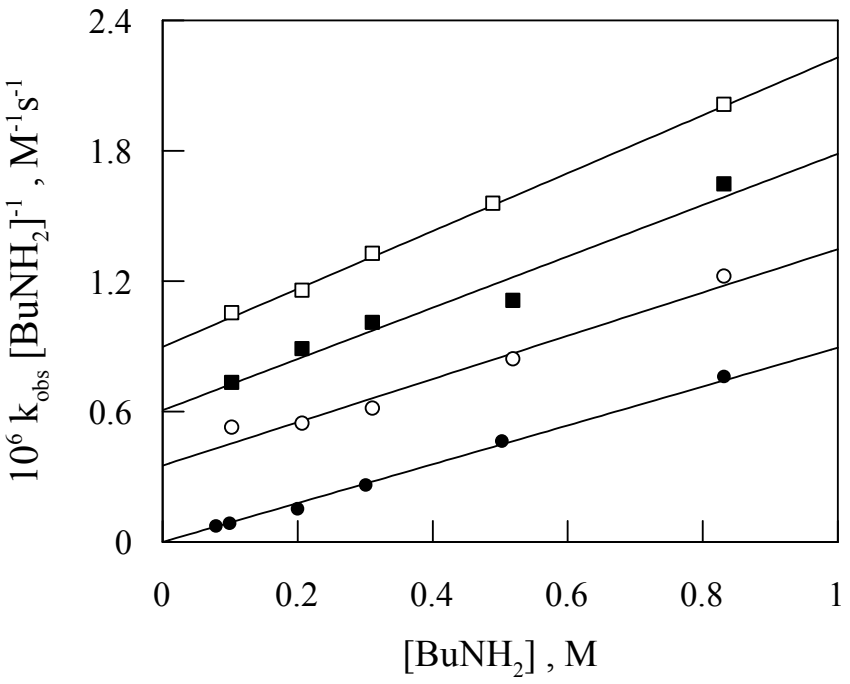

Figure S-23. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [G5]=0M; (○) [G5]=0.10M; (■) [G5]=0.20M and (□) [G5]=0.30M.

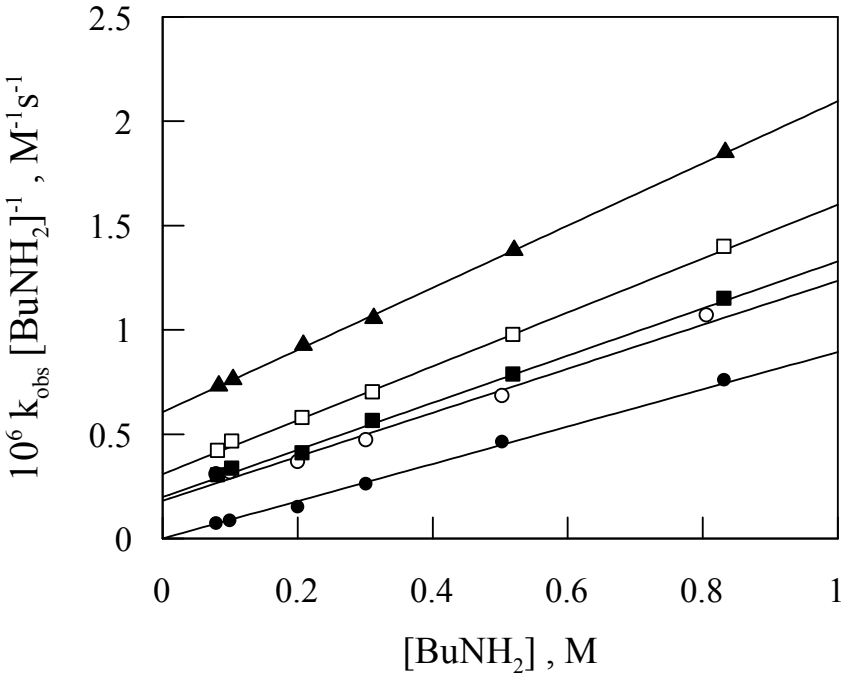

Figure S-24. Influence of *n*-butylamine concentration on $k_{obs}/[BuNH_2]$ (Equation [2]) for the S_NAr reaction of 1-fluoro-4-nitrobenzene. T=25ºC. [FNB]=1.5×10^{-4}M. (●) [18C6]=0M; (○) [18C6]=0.10M; (■) [18C6]=0.20M; (□) [18C6]=0.30M and (▲) [18C6]=0.51M.

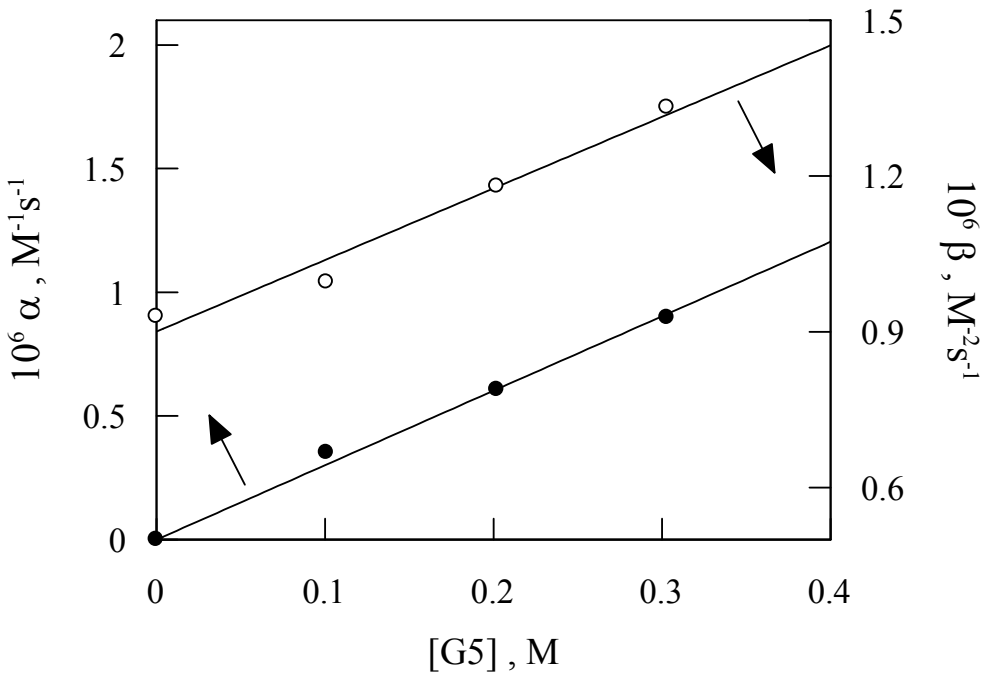

Figure S-25. Influence of G5 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-fluoro-4-nitrobenzene. (●) α and (○) β.

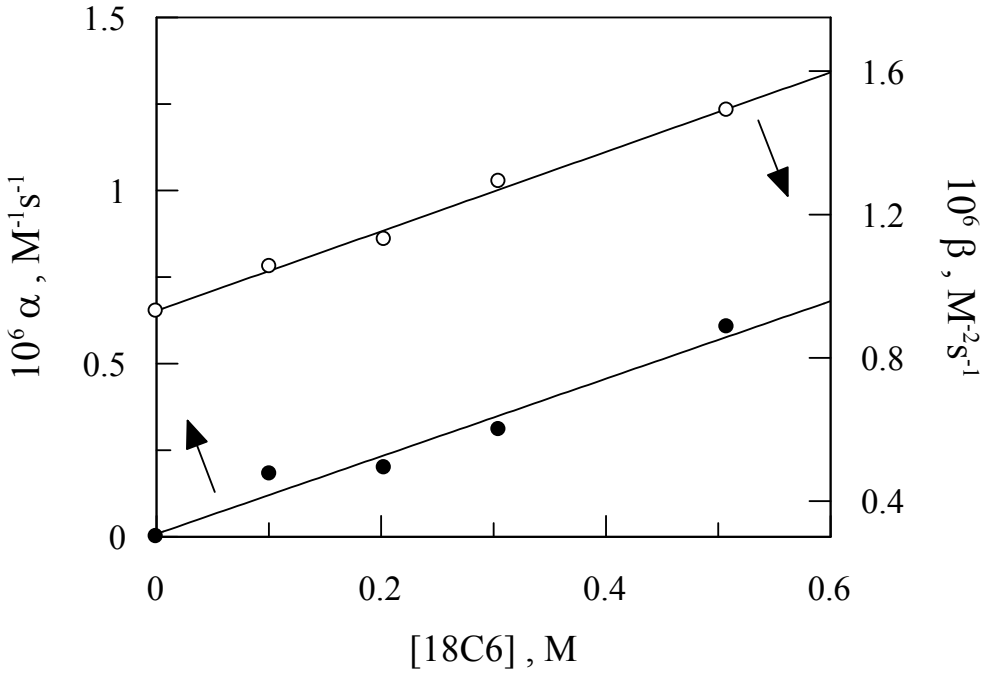

Figure S-26. Influence of 18C6 concentration on α and β terms (Equation 2) for the S_NAr reaction of 1-fluoro-4-nitrobenzene. (●) α and (○) β.

Table S-31. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the absence of polyethers. T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.07×10^{-2}	5.48×10^{-9}
1.01×10^{-1}	8.13×10^{-9}
2.02×10^{-1}	2.96×10^{-8}
3.03×10^{-1}	7.77×10^{-8}
5.04×10^{-1}	2.31×10^{-7}
8.33×10^{-1}	6.29×10^{-7}

Table S-32. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G4]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	2.68×10^{-8}
2.08×10^{-1}	9.54×10^{-8}
3.12×10^{-1}	1.74×10^{-7}
5.21×10^{-1}	3.72×10^{-7}
8.33×10^{-1}	9.01×10^{-7}

Table S-33. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G4]=0.20M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	5.63×10^{-8}
2.08×10^{-1}	1.61×10^{-7}
3.12×10^{-1}	2.53×10^{-7}
5.21×10^{-1}	5.70×10^{-7}
8.33×10^{-1}	1.13×10^{-6}

Table S-34. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G4]=0.30M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	7.11×10^{-8}
2.08×10^{-1}	2.13×10^{-7}
3.12×10^{-1}	3.69×10^{-7}
5.21×10^{-1}	7.41×10^{-7}
8.33×10^{-1}	1.57×10^{-6}

Table S-35. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G5]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
1.04×10^{-1}	5.44×10^{-8}
2.08×10^{-1}	1.13×10^{-7}
3.12×10^{-1}	1.91×10^{-7}
5.21×10^{-1}	4.36×10^{-7}
8.33×10^{-1}	1.02×10^{-6}

Table S-36. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G5]=0.20M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
1.04×10^{-1}	7.59×10^{-8}
2.08×10^{-1}	1.84×10^{-7}
3.12×10^{-1}	3.14×10^{-7}
5.21×10^{-1}	5.76×10^{-7}
8.33×10^{-1}	1.37×10^{-6}

Table S-37. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G5]=0.30M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
1.04×10^{-1}	1.09×10^{-7}
2.08×10^{-1}	2.40×10^{-7}
3.12×10^{-1}	4.13×10^{-7}
4.91×10^{-1}	7.62×10^{-7}
8.33×10^{-1}	1.67×10^{-6}

Table S-38. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [18C6]=0.10M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.07×10^{-2}	2.45×10^{-8}
1.01×10^{-1}	3.16×10^{-8}
2.02×10^{-1}	7.34×10^{-8}
3.03×10^{-1}	1.41×10^{-7}
5.04×10^{-1}	3.43×10^{-7}
8.07×10^{-1}	8.61×10^{-7}

Table S-39. Influence of *n*-butylamine concentration on k_{obs} for the CDNB S_NAr in the presence of polyethers. [18C6]=0.20M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	2.49×10^{-8}
1.04×10^{-1}	3.45×10^{-8}
2.08×10^{-1}	8.42×10^{-8}
3.12×10^{-1}	1.75×10^{-7}
5.21×10^{-1}	4.07×10^{-7}
8.33×10^{-1}	9.54×10^{-7}

Table S-40. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [G5]=0.30M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	3.47×10^{-8}
1.04×10^{-1}	4.80×10^{-8}
2.08×10^{-1}	1.20×10^{-7}
3.12×10^{-1}	2.18×10^{-7}
5.21×10^{-1}	5.06×10^{-7}
8.33×10^{-1}	1.16×10^{-6}

Table S-41. Influence of *n*-butylamine concentration on k_{obs} for the FNB S_NAr in the presence of polyethers. [18C6]=0.51M; T=25.0ºC.

[$BuNH_2$] , M	**k_{obs} , s^{-1}**
8.33×10^{-2}	6.10×10^{-8}
1.04×10^{-1}	7.94×10^{-8}
2.08×10^{-1}	1.93×10^{-7}
3.12×10^{-1}	3.30×10^{-7}
5.21×10^{-1}	7.20×10^{-7}
8.33×10^{-1}	1.54×10^{-6}