Clicking Azides and Alkynes with Poly(pyrazolyl)borate-Copper(I) Catalysts: An Experimental and Computational Study

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Supplementary material
AB3
scic_uv_0661 78 (0.840) Cm (67:86) 1: TOF MS ES+ 7.20e3

![Chemical Structure](image_url)
fa128, sin disolve, volumen escaso
proton MeOH /opt/ptopspin PAUS 1
AB4

scic_uv_0662 87 (0.938) Cm (74:87)

1: TOF MS ES+

2.00e4

251.1299
GaLa-N₃ + Ph-C=CH, Tris, CuCl, EtOH/H₂O.1/1, 24h, TA
$^{13}$C, GaLa-N3 + Ph-C=CH, CuCl, Tris, H2O/EtOh
N3-(CH2)2-N3  +  Ph-C=CH,  CuCl,  Ligand, EtOH/H2O:1/1 TA, 24h

ppm
1.0  2.0  3.0  4.0  5.0  6.0  7.0  8.0  9.0
7.863
7.838
7.758
7.280
4.433
4.409
4.385
1.980
1.978
1.960
1.959
1.937
1.354
1.347
1.270
AB5  
scic_uv_0663 50 (0.537) Cm (50:60)  
1: TOF MS ES+  
4.56e3  

457.3088  
458.3122  

m/z  
%

100  

0  

200 400 600 800 1000 1200  
m/z
Gal-CH$_2$-OCH$_2$-C=CH(2,4eq) + N$_3$-(CH$_2$)$_{12}$-N$_3$, CuCl, Ligand Tris, H$_2$O/EtOH:1/1
