

**(Supporting Information)**

Highly efficient and straightforward functionalization surface through  
thiol-ene click chemistry

Philippe Tingaut<sup>1</sup>, Roland Hauert and Tanja Zimmermann

*Swiss Federal Laboratories for Materials Testing and Research (EMPA), Überlandstrasse. 129*

*CH-8600 Dübendorf, Switzerland*

---

<sup>1</sup> To whom correspondence should be addressed. Tel: +41 44 823 4749. Fax: +41 44 823 4007. E-mail:

[Philippe.Tingaut@empa.ch](mailto:Philippe.Tingaut@empa.ch)

### **Kinetics profile of Figure 4 established with Infrared spectroscopy (FTIR-ATR).**

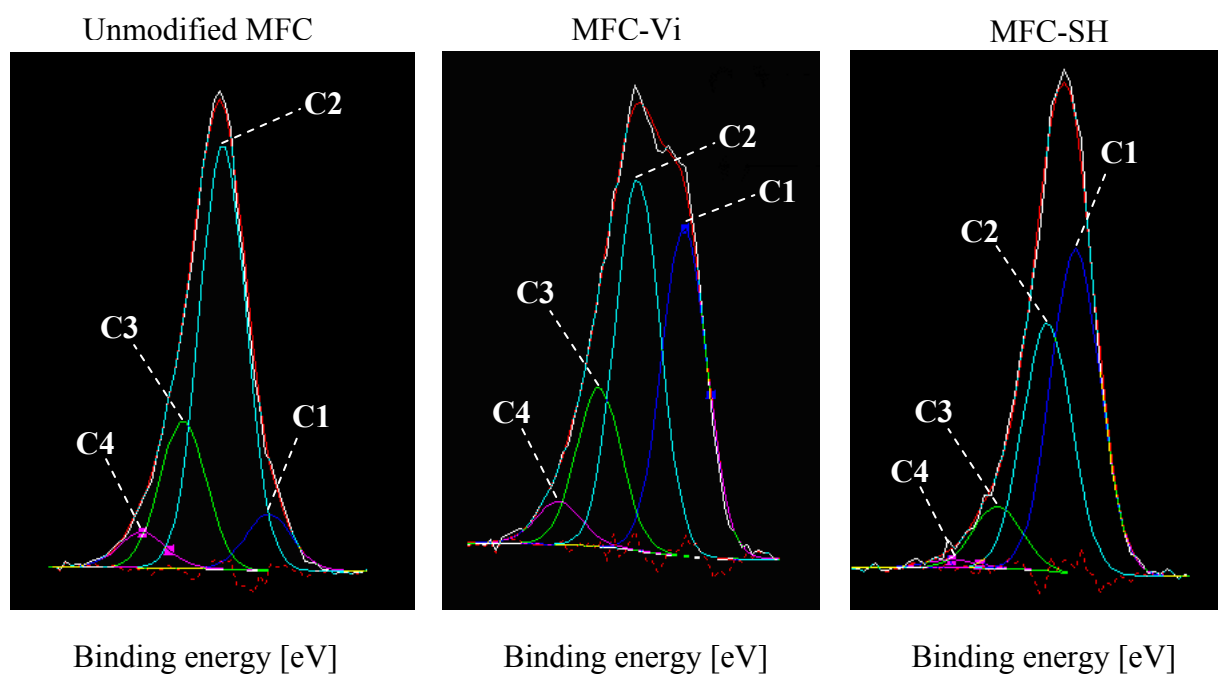
The kinetics profile was established using FTIR spectra of ene-functionalized cellulose films before (MFC-Vi) and after “click” derivatization (MFC-Vi-S<sub>x</sub>). Several peaks were of interests, namely the carbonyl peak at 1733 cm<sup>-1</sup>, the vinyl peaks at 1601 cm<sup>-1</sup> and 1409 cm<sup>-1</sup>, the C-H deformation band at 1436 cm<sup>-1</sup>, the C-O stretching vibration at 1276 cm<sup>-1</sup> and the band associated with the C-O and Si-O-Si stretching vibrations, at about 1001 cm<sup>-1</sup>.

Spectra were first normalized to the band at 1001 cm<sup>-1</sup>, and a linear baseline correction was then applied on all spectra using five points located at 3700, 2400, 1800, 1500, 1220 and 808 cm<sup>-1</sup>. In each spectrum, the peak heights at 1733 (I<sub>1733</sub>), 1601 (I<sub>1601</sub>), 1436 (I<sub>1436</sub>), 1409 (I<sub>1409</sub>), 1276 (I<sub>1276</sub>) and 1001 cm<sup>-1</sup> (I<sub>1001</sub>) were calculated using baselines constructed by extrapolating lines between 1800 and 1500 cm<sup>-1</sup> to calculate I<sub>1733</sub> and I<sub>1601</sub>, between 1500 and 1220 cm<sup>-1</sup> to calculate I<sub>1436</sub>, I<sub>1408</sub> and I<sub>1276</sub>, and between 1220 and 808 cm<sup>-1</sup> to calculate I<sub>1001</sub>. The kinetics of the reaction was determined by calculating the peak height ratios I<sub>1733</sub>/I<sub>1001</sub>, I<sub>1601</sub>/I<sub>1001</sub>, I<sub>1436</sub>/I<sub>1001</sub>, I<sub>1409</sub>/I<sub>1001</sub>, I<sub>1276</sub>/I<sub>1001</sub>, and plotting them against reaction time.

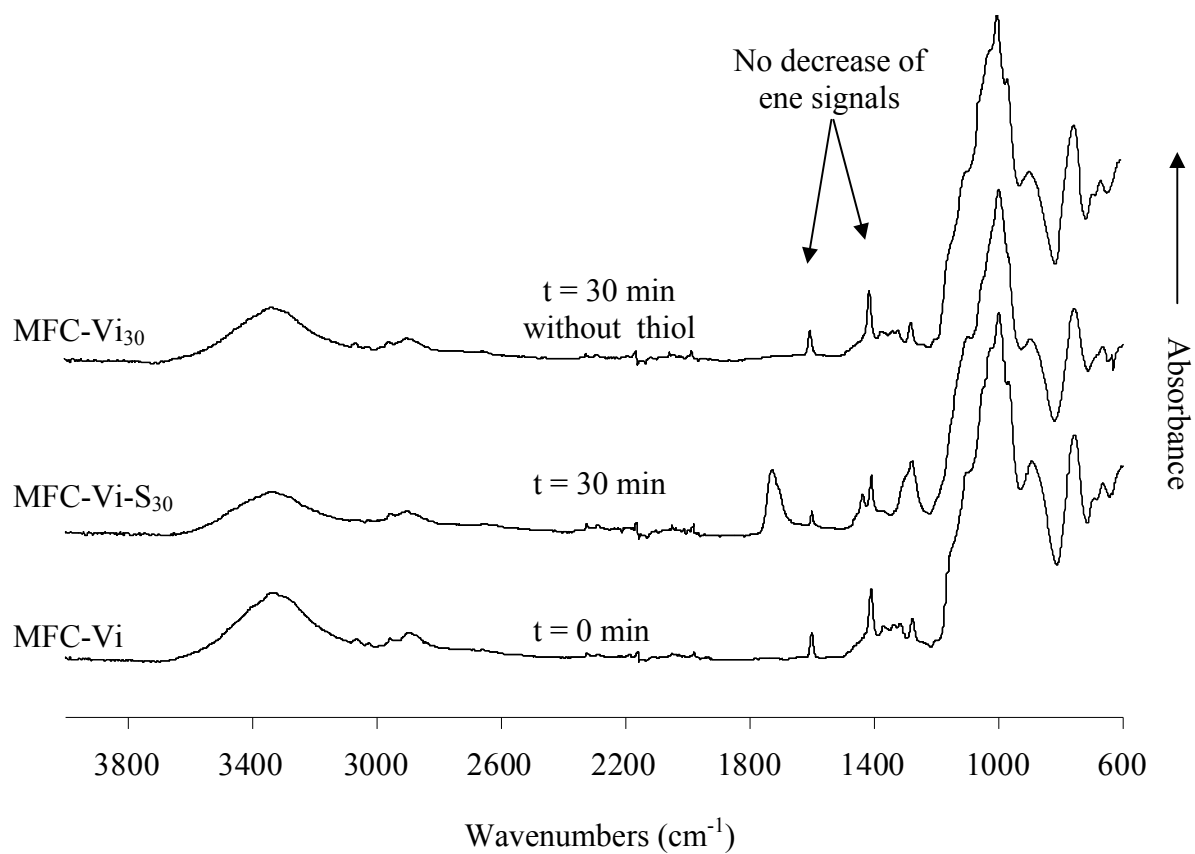
### **Kinetics profile of Figure 7 established with Infrared spectroscopy (FTIR-ATR).**

The kinetics profile was established using FTIR spectra of thiol-functionalized cellulose films before (MFC-SH) and after “click” derivatization (MFC-S-AlB<sub>x</sub>). Spectra were first normalized to the band at 1001 cm<sup>-1</sup>, and a linear baseline correction was then applied on all spectra using five points located at 3700, 2400, 1900, 1500, 1220 and 826 cm<sup>-1</sup>.

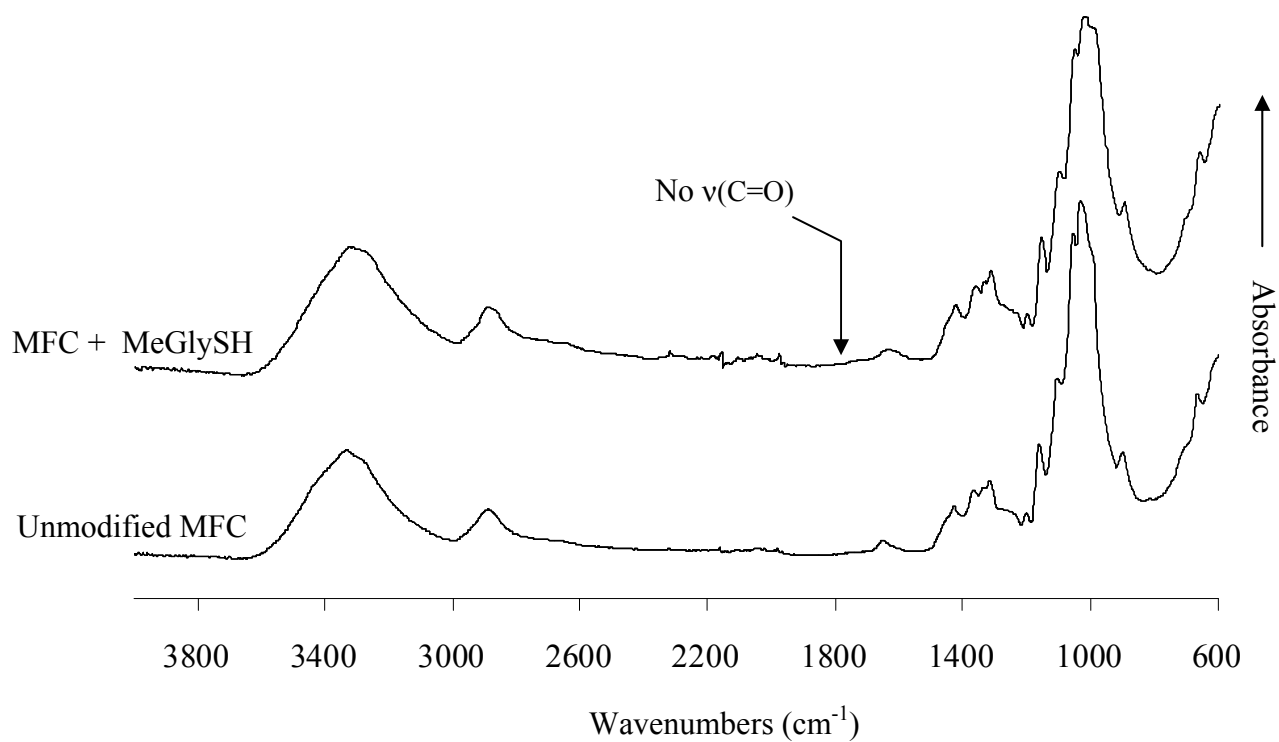
The peak heights ratio of 1730 to 996 cm<sup>-1</sup> vibrations (I<sub>1730</sub>/I<sub>996</sub>) in each spectrum was calculated using a baseline constructed by extrapolating two lines between the valleys at 1900 and 1500 cm<sup>-1</sup> and between the valleys at 1220 and 826 cm<sup>-1</sup>. The kinetics of the reaction was determined by plotting the ratio I<sub>1730</sub>/I<sub>996</sub> against reaction time.



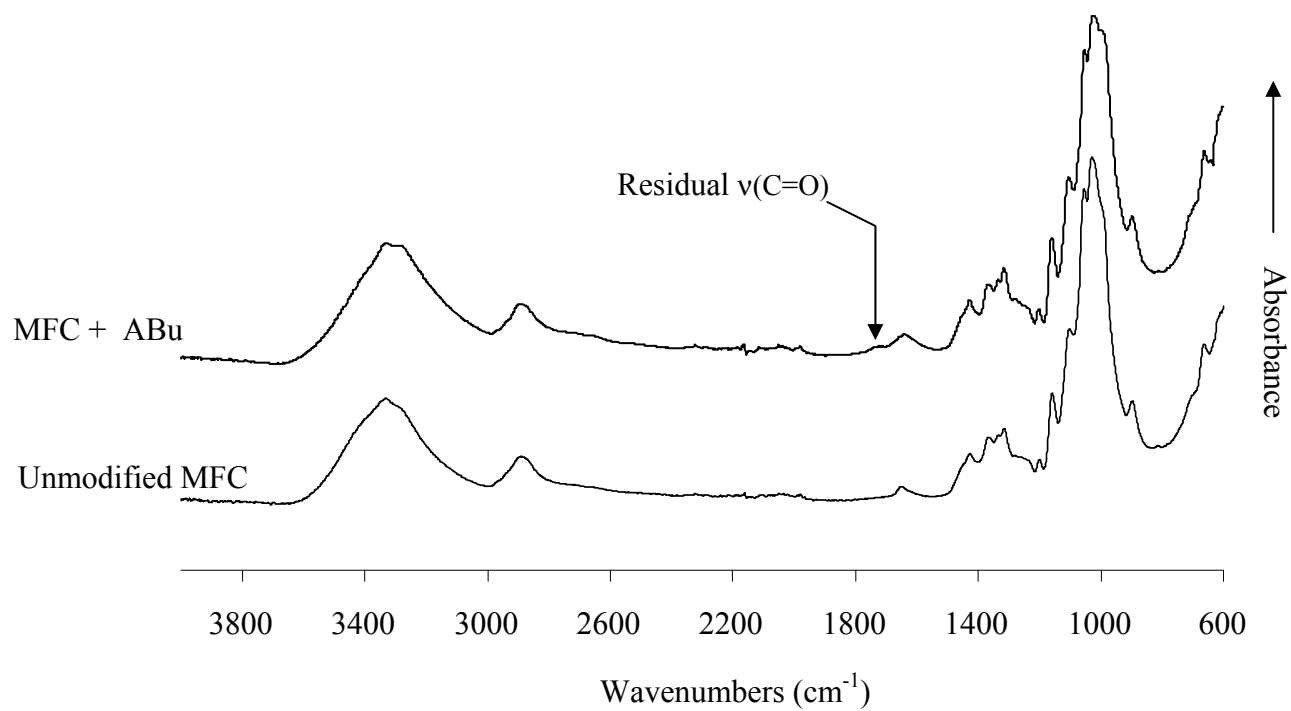
**Figure S1.** Deconvolution of  $C_{1s}$  high resolution signal of unmodified MFC, MFC-Vi and MFC-SH.



**Figure S2.** FTIR absorbance spectra of MFC-Vi ( $t = 0$  min), MFC-Vi-S<sub>30</sub> and MFC-Vi after 30 min reaction time without thiol (MFC-Vi<sub>30</sub>).



**Figure S3.** FTIR absorbance spectra of unmodified MFC and MFC reacted with MeGlySH for 30 min.

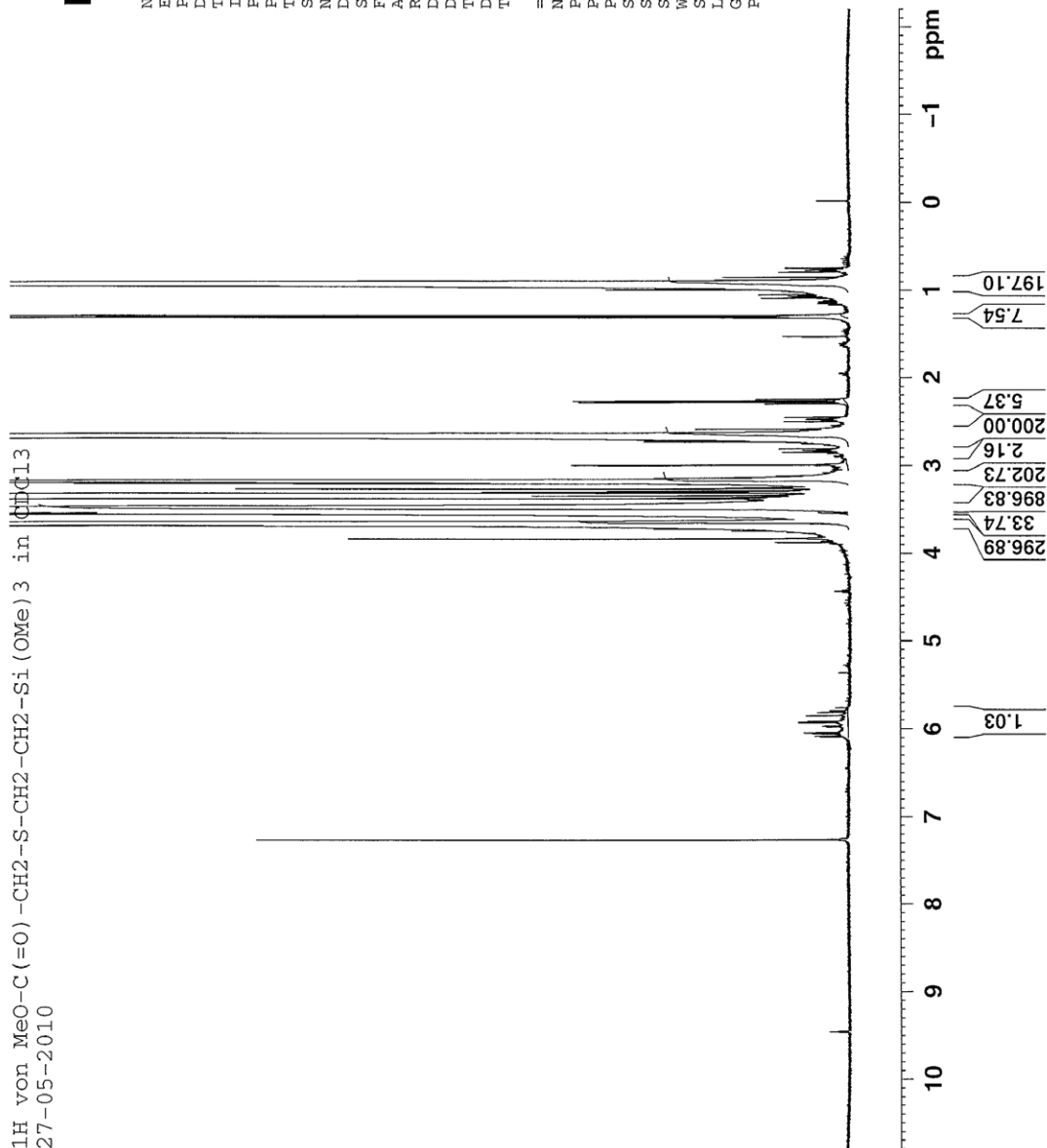


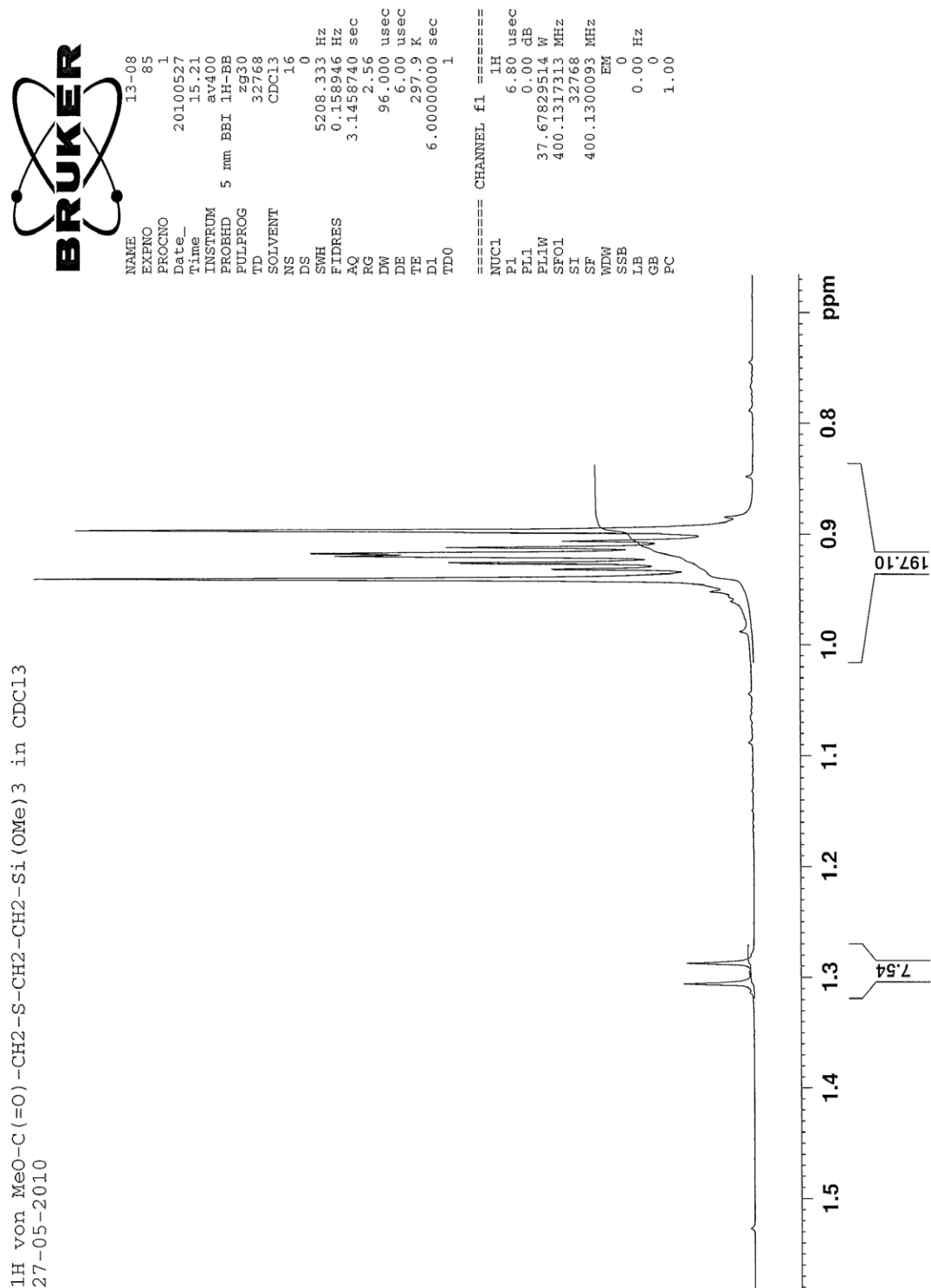
**Figure S4.** FTIR absorbance spectra of unmodified MFC and MFC reacted with **ABu** for 120 min.



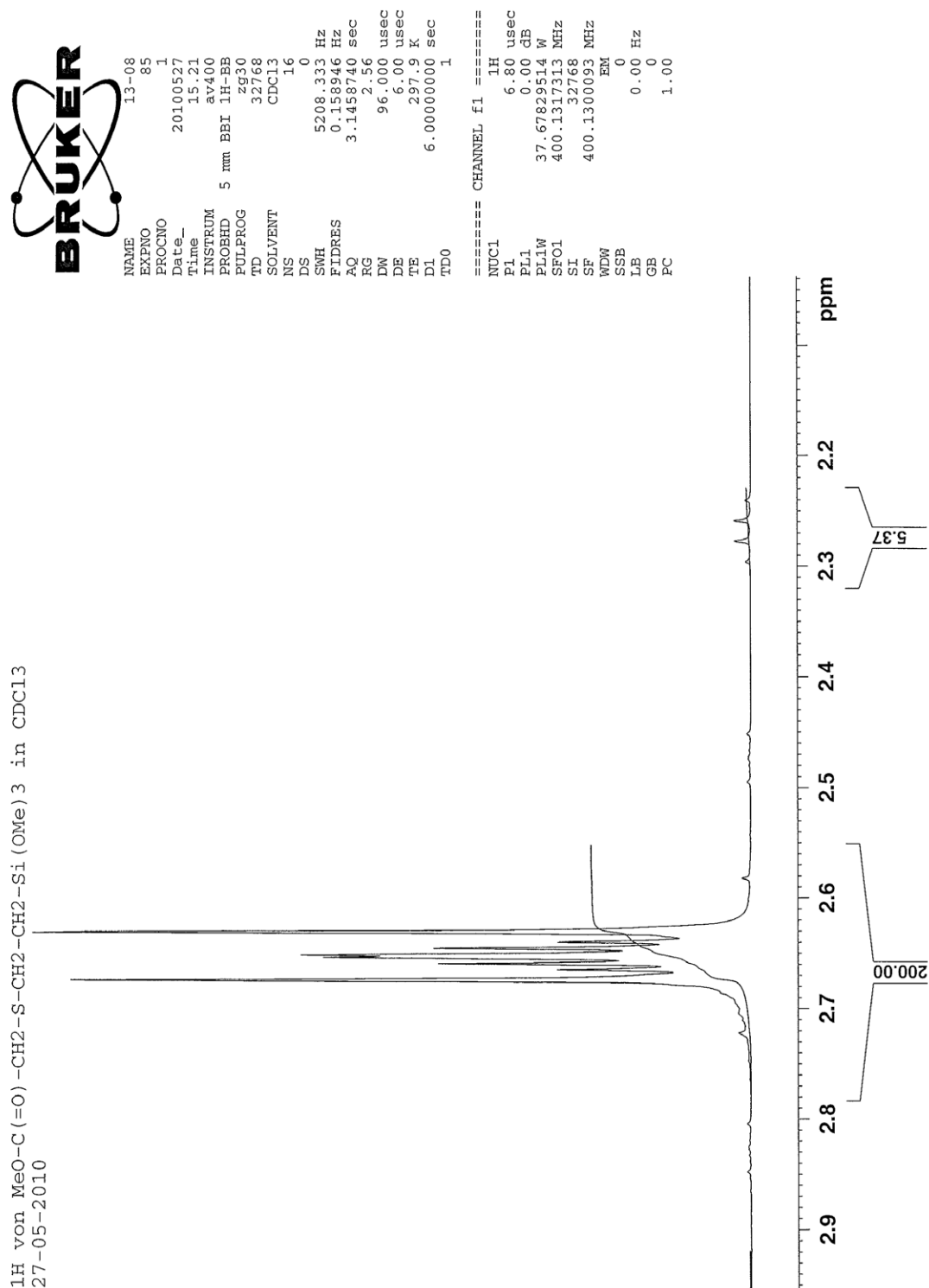
<sup>1</sup>H von MeO-C(=O)-CH<sub>2</sub>-S-CH<sub>2</sub>-CH<sub>2</sub>-Si(OMe)<sub>3</sub> in CDCl<sub>3</sub>  
27-05-2010

NAME 13-08  
EXPNO 85  
PROCNO 1  
Date\_ 20100527  
Time\_ 15.21  
INSTRUM 5 mm BBI 1H-BB  
PROBHD zg30  
PULPROG 32768  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 5208.333 Hz  
FIDRES 0.158946 Hz  
AQ 3.1458740 sec  
RG 2.56  
DM 96.000 usec  
DE 6.00 usec  
TE 297.9 K  
D1 6.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 6.80 usec  
PL1 0.00 dB  
PL1W 37.67829514 W  
SF01 400.1317313 MHz  
SI 32768  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00





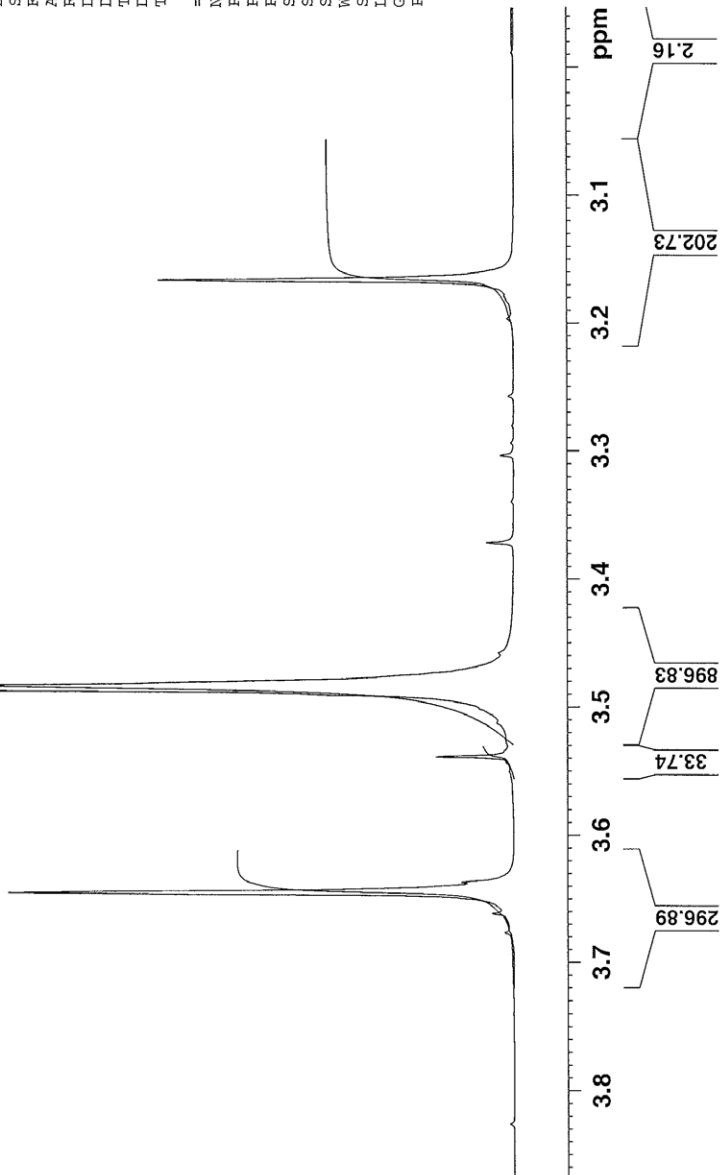


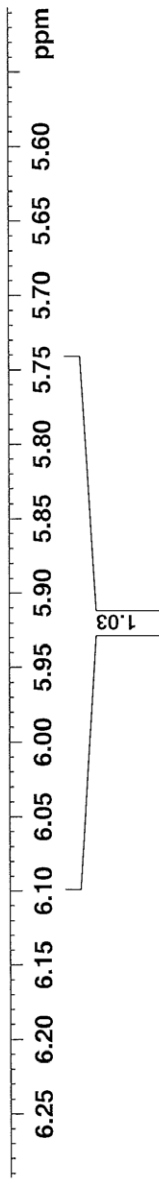
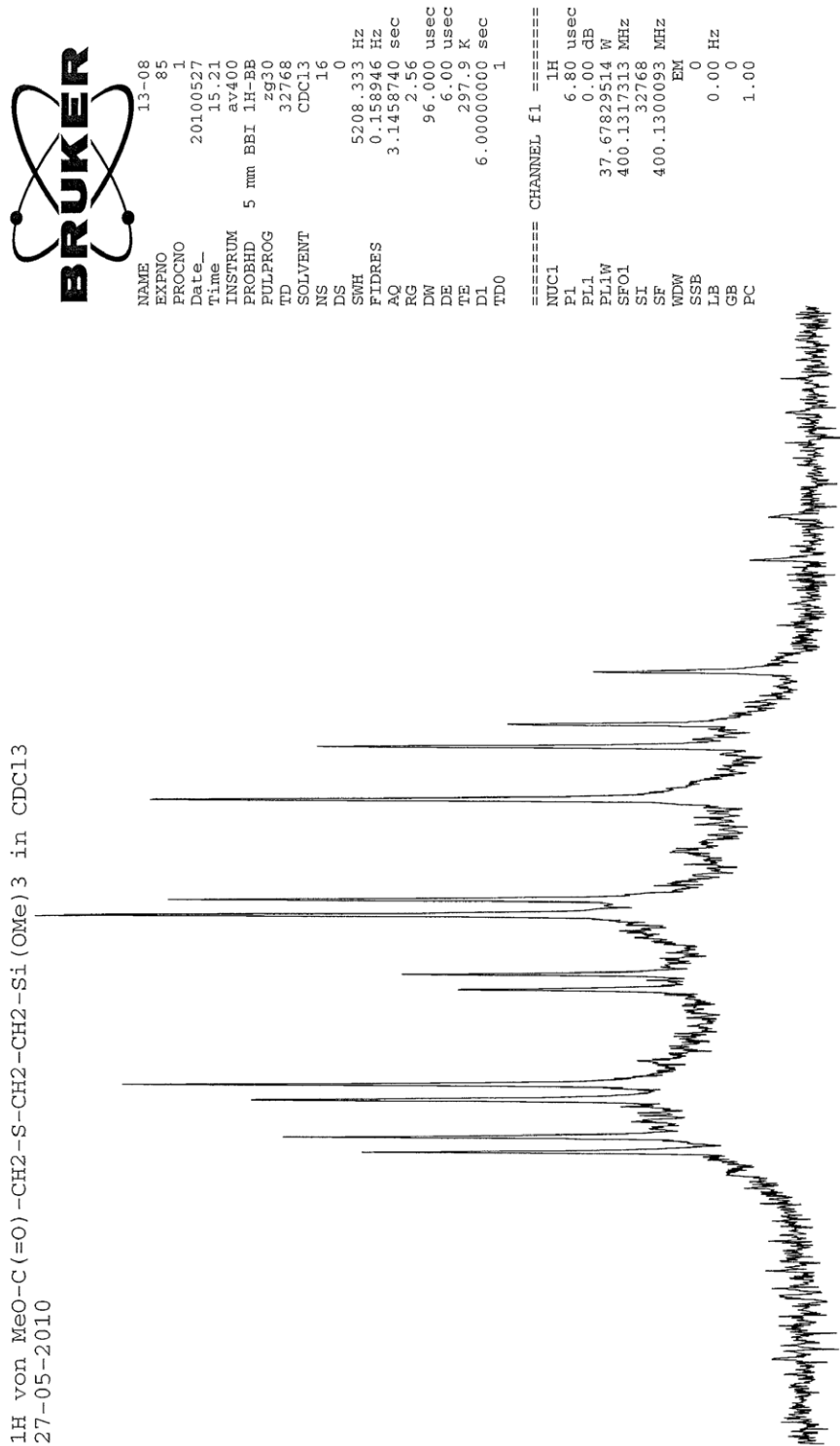


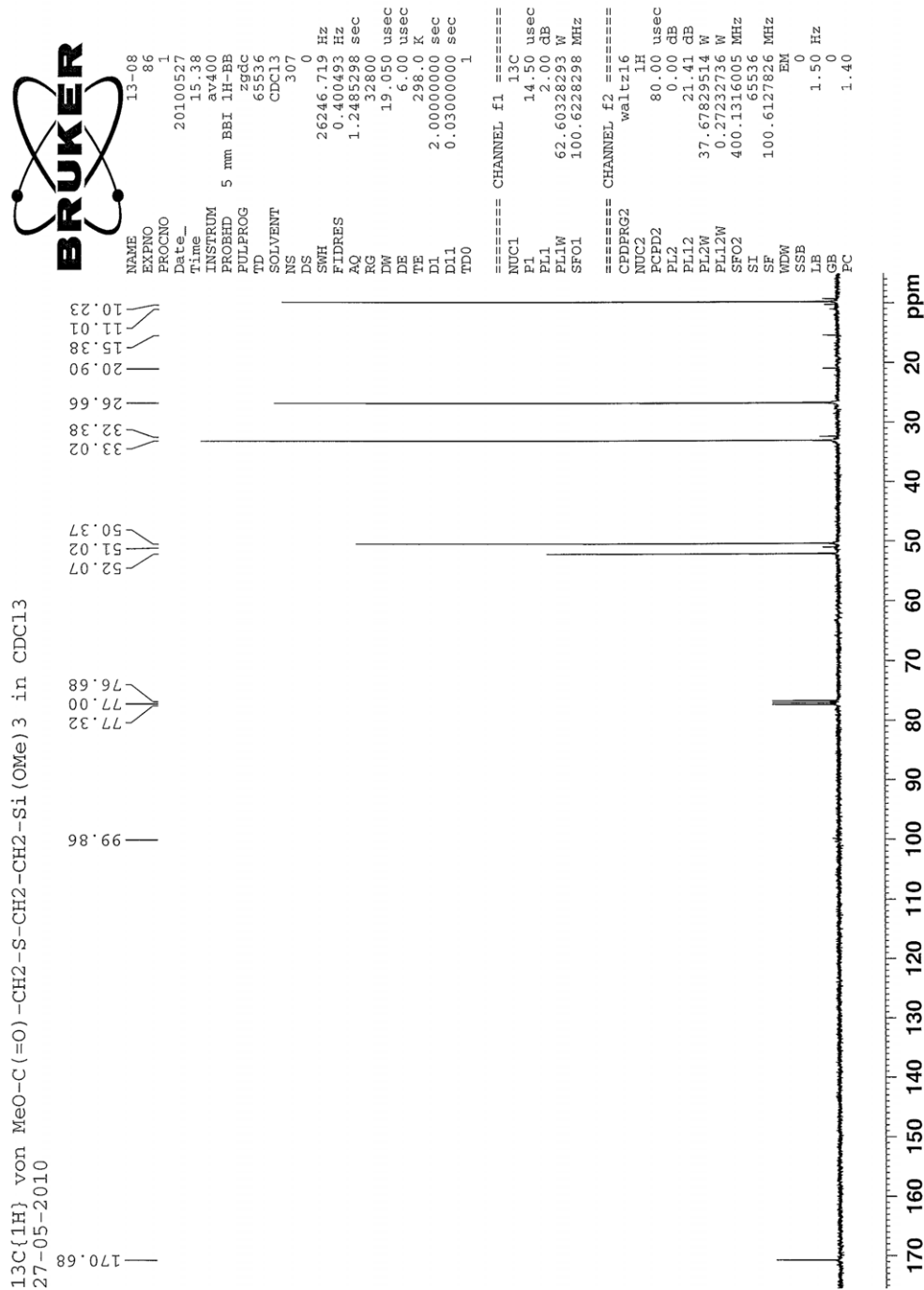
<sup>1</sup>H von MeO-C(=O)-CH<sub>2</sub>-S-CH<sub>2</sub>-CH<sub>2</sub>-Si(OMe)<sub>3</sub> in CDCl<sub>3</sub>  
27-05-2010



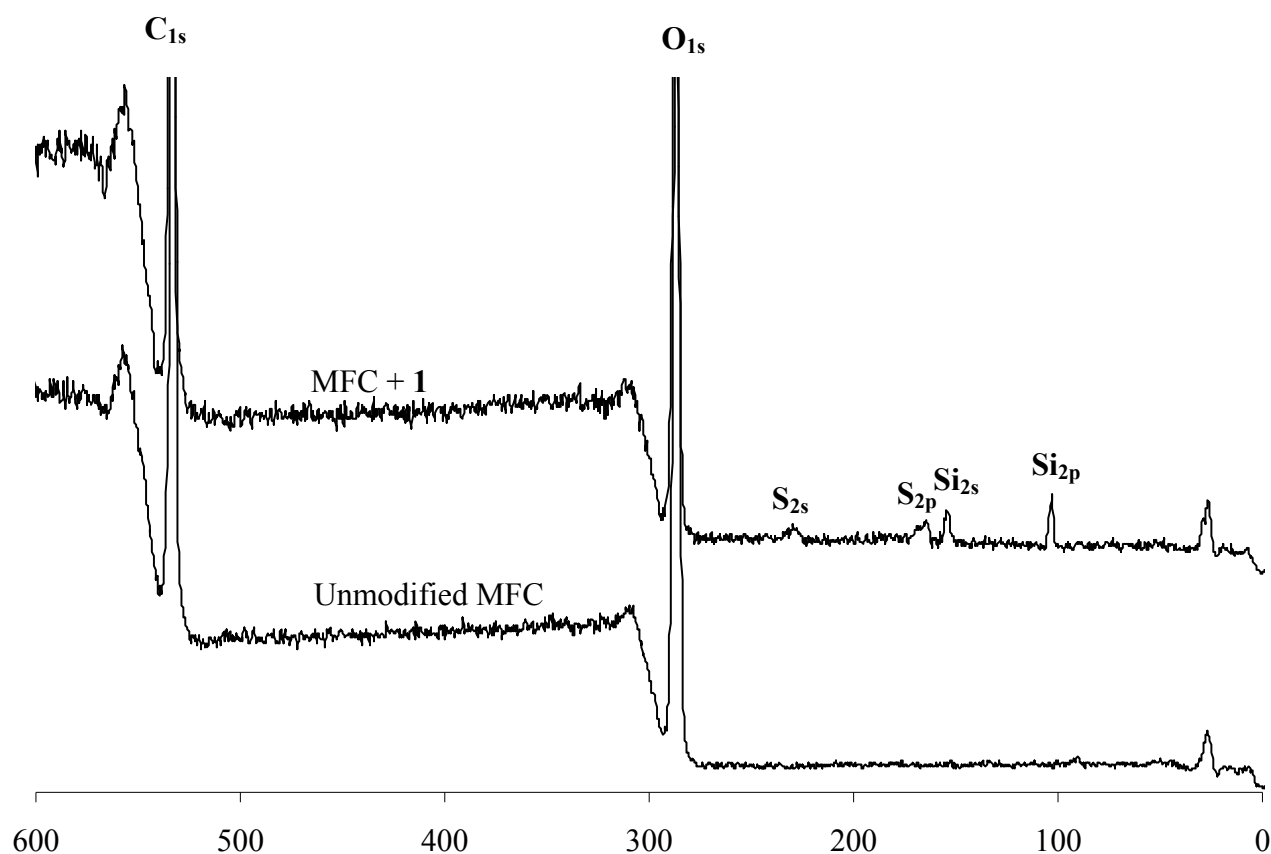
NAME 13-08  
EXPNO 85  
PROCNO 1  
Date\_ 20100527  
Time 15.21  
INSTRUM 5 mm BBI 1H-BB  
PROBHD av400  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 5208.333 Hz  
FIDRES 0.158946 Hz  
AQ 3.1458740 sec  
RG 2.56  
DW 96.000 usec  
DE 6.00 usec  
TE 297.9 K  
D1 6.0000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 <sup>1</sup>H  
P1 6.80 usec  
PL1 0.00 dB  
PL1W 37.67829514 W  
SFO1 400.1317313 MHz  
SI 32768  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00







**Figure S5.** <sup>1</sup>H and <sup>13</sup>C NMR spectra of **1**. The chemical shifts are in agreement with the literature.<sup>1</sup>



**Figure S6.** XPS low-resolution survey spectra of unmodified MFC and MFC modified with **1**.

1. Al-Hashimi, M.; Sullivan, A. C.; Wilson, J. R. H., Palladium ethylthioglycolate modified silica - a new heterogeneous catalyst for Suzuki and Heck cross-coupling reactions. *J. Mol. Catal. A-Chem.* **2007**, 273, (1-2), 298-302.