

## Spectroscopic data for Cu/TEMPO lab unknowns

### Unknown A

Molecular mass: 138.18 g/mol

Elemental composition: 69.53 % C; 7.31 % H; 23.16 % O

$^1\text{H-NMR}$ :  $\delta$  2.58 (s, 1H); 3.75 (s, 3H); 4.53 (s, 2H); 6.83 (d, 2H); 7.23 (d, 2H).

$^{13}\text{C-NMR}$ :  $\delta$  55.32; 64.83; 114.20; 128.48; 133.73; 159.50

EI-MS:  $m/z$  138 (100%); 107 (26%)

### Unknown B

Molecular mass: 122.18 g/mol

Elemental composition: 78.64% C; 8.27% H; 13.09% O

$^1\text{H-NMR}$ :  $\delta$  2.31 (s, 3H); 2.35 (s, 1H); 4.55 (s, 2H); 7.10 (d, 2H); 7.21 (d, 2H).

$^{13}\text{C-NMR}$ :  $\delta$  21.09; 64.58; 127.12; 129.01; 136.89; 138.04

EI-MS:  $m/z$  122 (87%); 107 (100%), 91 (53%)

### Unknown C

Molecular mass: 150.24 g/mol

Elemental composition: 79.94 % C; 9.41 % H; 10.65 % O

$^1\text{H-NMR}$ :  $\delta$  1.23 (d, 6H); 2.28 (s, 1H); 2.89 (sept, 1H); 4.57 (s, 2H); 7.18 (d, 2H); 7.26 (d, 2H)

$^{13}\text{C-NMR}$ :  $\delta$  24.04; 34.02; 64.92; 126.56; 127.24; 138.44; 148.28

EI-MS:  $m/z$  150 (49%); 135 (100%); 119 (31%)

### Unknown D

Molecular mass: 142.64 g/mol

Elemental composition: 58.95 % C; 4.97 % H; 11.23 % O, 24.85 % X (X= halogen)

$^1\text{H-NMR}$ :  $\delta$  2.70 (s, 1H); 4.50 (s, 2H); 7.29 (d, 2H); 7.21 (d, 2H).

$^{13}\text{C-NMR}$ :  $\delta$  64.13; 128.23; 128.63; 133.22; 139.12

EI-MS:  $m/z$  144 (23%); 142 (70%) 107 (100%)