Supporting Information

Semiconductors as Heterogeneous Visible Light Photoredox Catalysts in Combined Dual Metal Catalyzed C-H Functionalizations

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1 General information

All commercially available chemicals were used as provided by the suppliers without further treatment. All solvents were dried and distilled under argon prior to use. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Macherey-Nagel ALUGRAM Xtra SIL G/UV254 aluminum plates with F-254 indicator, visualized by UV irradiation. Macherey-Nagel silica gel 60 (particle size 0.063 – 0.2 mm) was used for column chromatography. Solvent mixtures are understood as volume/volume. An 11 W fluorescent bulb, warm white, was used for irradiation with light. All reactions concerning the scope were repeated at least twice.

1H NMR, 13C NMR and 19F NMR spectra were recorded on VNMRS-400, VNMRS-600 or Mercury 300 spectrometer in CDCl3. Chemical shifts (δ) are reported in ppm and multiplicities are indicated: s (singlet), d (doublet), dd (doublet of doublet, t (triplet), dt (doublet of triplet), td (triplet of doublet), q, (quartet), quint (quintet) m (multiplet); coupling constants (J) are in Hertz (Hz). Mass spectra (MS-EI: 70 eV were conducted on a Finnigan MET SSQ 7000 system, LCMS spectra on a LTQ Orbitrap XL spectrometer and HRMS spectra on a Thermo Scientific LTQ Orbitrap XL spectrometer. IR spectra (ATR) were recorded on a Perkin Elmer spectrometer and wave numbers are given in reciprocal centimeters (cm⁻¹). Starting materials were synthesized according to literature-known procedures, products compared to literature known compounds.1,3

2 General procedure for the Ru-catalyzed ortho-selective olefination of diaryl ether

The respective diaryl ether (1 equiv.) and acrylate (2 equiv.), Ru-catalyst (5 mol%), AgSbF6 (0.2 equiv.) and photoredox catalyst (10 mol% or 1 equiv.) were dissolved in DMA (0.1 M). A 4 mL vial equipped with a Teflon-coated magnetic stirring bar served as reaction vessel. The mixture was irradiated by an 11 W lamp (distance ca. 3 cm) after placing it on an aluminium block heated at 120 °C. The reaction was quenched with 2 mL of 10% aqueous LiCl solution, after complete consumption of substrate (followed by TLC). The aqueous layer was then extracted with DCM (5x20 mL) and the combined organic layer dried.
over MgSO4. After removal of solvents, the crude product was purified by flash column chromatography (SiO2, n-pentane/EtOAc 5:1 -> 1:1).

**Butyl** (**E**)-(3)-**3**-(**3**-methoxy-2-(pyridin-2-yloxy)phenyl)acrylate 2a

According to general procedure and starting from 2-(2-methoxyphenoxy)pyridine (40 mg, 0.20 mmol) the product was obtained as brown oil (50 mg, 0.17 mmol, 84%).

1H-NMR (600 MHz; CDCl3): 8.08 (dt, J = 4.9, 0.9 Hz, 1H), 7.82 (d, J = 16.1 Hz, 1H), 7.68 (dd, J = 8.3, 7.2, 1H), 7.28 (dd, J = 8.0, 1.2 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H), 7.02-6.98 (m, 2H), 6.95 (dd, J = 7.1, 5.0 Hz, 1H), 6.45 (d, J = 16.1 Hz, 1H), 4.13 (t, J = 6.7 Hz, 2H), 3.72 (s, 3H), 1.62 (dd, J = 9.9, 5.2 Hz, 2H), 1.37 (t, J = 7.5 Hz, 2H), 0.91 (t, J = 7.4 Hz, 3H).

13C-NMR (151 MHz; CDCl3): 166.9, 152.4, 147.4, 141.5, 139.3, 138.7, 129.2, 125.8, 120.2, 119.1, 118.2, 114.0, 110.5, 64.3, 56.1, 30.7, 19.1, 13.7.

**Butyl** (**2E**)-(3)-**3**-(**3**-methoxy-5-(prop-1-en-1-yl)-2-(pyridin-2-yloxy)phenyl)acrylate 2b, mixture of isomers

According to general procedure and starting from 2-(2-methoxyphenoxy)pyridine (40 mg, 0.20 mmol) the product was obtained as brown oil (50 mg, 0.17 mmol, 84%; mixture of isomers).

1H-NMR (600 MHz; CDCl3): 8.10-8.08 (m, 1H), 7.79 (d, J = 16.1 Hz, 1H), 7.68-7.66 (m, 1H), 7.20 (d, J = 1.7 Hz, 2H), 6.99-6.97 (m, 3H), 6.94 (ddd, J = 7.1, 5.0, 0.8 Hz, 2H), 6.47 (s, 1H), 6.40-6.37 (m, 2H), 6.23 (t, J = 11.1 Hz, 1H), 4.14 (d, J = 6.7 Hz, 2H), 3.73 (s, 3H), 1.90 (dd, J = 6.6, 1.6 Hz, 4H), 1.62 (t, J = 7.5 Hz, 2H), 1.38 (t, J = 7.5 Hz, 2H), 0.92 (t, J = 7.4 Hz, 3H); 13C-NMR (151 MHz; CDCl3): 166.9, 152.3, 147.5, 139.3, 138.9, 135.9, 130.2, 128.9, 126.5, 120.1, 118.2, 116.9, 111.2, 110.4, 110.1, 83.5, 64.3, 56.0, 30.7, 19.1, 18.5, 13.7.

**Methyl** (**E**)-(3)-**3**-(**3**-methoxy-2-(pyridin-2-yloxy)phenyl)acrylate 2c

According to general procedure and starting from 2-(o-tolylxyloxy)pyridine (40 mg, 0.20 mmol) the product was obtained as colourless solid (36 mg, 0.13 mmol, 63%); mp: 108-110 °C.

1H-NMR (400 MHz; CDCl3): 8.06 (dd, J = 5.0, 1.4 Hz, 1H), 7.82 (d, J = 16.2 Hz, 1H), 7.66 (ddd, J = 8.3, 7.2, 1.9 Hz, 1H), 7.25 (dd, J = 7.8, 1.5 Hz, 1H), 7.19 (t, J = 8.0 Hz, 1H), 7.00-6.91 (m, 3H), 6.44 (d, J = 16.1 Hz, 1H), 3.71 (s, 3H), 3.69 (s, 3H); 13C-NMR (101 MHz; CDCl3): 167.2, 163.3, 152.4, 147.4, 141.5, 139.3, 139.0, 129.1, 125.8, 119.8, 119.2, 118.2, 114.1, 110.4, 56.0, 51.6; MS (ESI): m/z (%) = 396.1 (85), 286.1 ([M+H]+, 40), 254.1 (28), 210.1 (20), 196.1 (100); HRMS (ESI) for C16H16O4N: calculated for [M+H]+ 286.10730, found 286.10738; IR (ATR): ν = 3395, 3039, 2981, 2943, 1704, 1637, 1577, 1463, 1428, 1266, 1179, 1071, 994, 880, 770, 734.

**Ethyl** (**E**)-(3)-**3**-(**3**-methoxy-2-(pyridin-2-yloxy)phenyl)acrylate 2d
According to general procedure and starting from 2-(o-tolyloxy)pyridine (40 mg, 0.20 mmol) the product was obtained as brown oil (39 mg, 0.13 mmol, 65%).

$^1$H-NMR (400 MHz; CDCl$_3$): 8.07 (dd, $J = 4.9, 1.4$ Hz, 1H), 7.82 (d, $J = 16.1$ Hz, 1H), 7.66 (m, $J = 1.7$ Hz, 1H), 7.26 (dd, $J = 8.2, 1.5$ Hz, 1H), 7.19 (t, $J = 8.0$ Hz, 1H), 7.00-6.96 (m, 2H), 6.93 (dd, $J = 6.8, 5.4$ Hz, 1H), 6.44 (d, $J = 16.1$ Hz, 1H), 4.17 (q, $J = 7.1$ Hz, 2H), 3.69 (s, 3H), 1.25 (t, $J = 7.1$ Hz, 3H);

$^{13}$C-NMR (101 MHz; CDCl$_3$): 166.8, 163.3, 152.4, 147.4, 141.5, 139.3, 138.8, 129.2, 125.8, 120.2, 119.2, 118.2, 114.0, 110.4, 60.4, 56.0, 14.2.

2,2,3,3,3-pentafluoropropyl (E)-3-(3-methoxy-2-(pyridin-2-ylaxylo)phenyl)acrylate 2e

According to general procedure and starting from 2-(o-tolyloxy)pyridine (40 mg, 0.20 mmol) the product was obtained as colourless oil (55 mg, 0.11 mmol, 55%), mp: 120-122 °C

$^1$H-NMR (400 MHz; CDCl$_3$): 8.06 (dd, $J = 4.9, 1.4$ Hz, 1H), 7.91 (d, $J = 16.2$ Hz, 1H), 7.70-7.66 (m, 1H), 7.28 (dd, $J = 7.9, 1.1$ Hz, 1H), 7.22 (t, $J = 8.1$ Hz, 1H), 7.05-6.98 (m, 2H), 6.94 (dd, $J = 6.7, 5.3$ Hz, 1H), 6.47 (d, $J = 16.1$ Hz, 1H), 4.57 (t, $J = 12.8$ Hz, 2H), 3.71 (s, 3H);

$^{19}$F-NMR (376 MHz; CDCl$_3$): -83.9, -123.4 (t, $J = 12.9$ Hz); MS (ESI): $m/z$ (%) = 396.1 (85), 286.1 ([M+H]$^+$, 40), 254.1 (28), 210.1 (20), 196.1 (100); HRMS (ESI) for C$_{18}$H$_{15}$O$_4$N$_5$F$_5$: calculated for [M+H]$^+$ 404.09125, found 404.09158; IR (ATR): v = 3395, 3039, 2981, 2943, 1704, 1637, 1577, 1463, 1428, 1266, 1179, 994, 880, 770, 734.

3 General procedure for the Pd-catalysed indole synthesis

In a 4 mL vial equipped with a Teflon-coated magnetic stirring bar, the appropriate N-aryl enamide (1 equiv.), Pd(OAc)$_2$ (10 mol%), K$_2$CO$_3$ (3 equiv.) and photoredox catalyst (10 mol%, 1 equiv.) were dissolved in DMF (0.1 M) and the reaction mixture placed in front of an 11 W household lamp (distance ca. 3 cm) on an aluminium block heated at 120 °C. After complete consumption of starting material (followed by TLC), the reaction was quenched with 2 mL of 10% aqueous LiCl solution, the aqueous layer extracted with DCM (5x20 mL) and the combined organic layer dried over MgSO$_4$. After removal of solvents, the crude product was purified by flash column chromatography (SiO$_2$, n-pentane/EtOAc 5:1 → 1:1).

Methyl 2-methyl-1H-indole-3-carboxylate 4a

According to general procedure and starting from methyl (Z)-3-(phenylamino)but-2-enooate (38 mg, 0.20 mmol) the product was obtained as colorless solid (32 mg, 0.17 mmol, 85%).

$^1$H-NMR (600 MHz; CDCl$_3$): 8.43 (s, 1H), 8.09 (d, $J = 7.7$ Hz, 1H), 7.30 (d, $J = 7.4$ Hz, 1H), 7.21 (ddd, $J = 11.1, 7.6, 1.3$ Hz, 2H), 3.94 (s, 3H), 2.74 (s, 3H); $^{13}$C-NMR (101 MHz; CDCl$_3$): 166.5, 144.0, 134.4, 127.1, 122.4, 121.7, 121.2, 110.5, 104.5, 50.8, 14.2.
Methyl 5-methoxy-2-methyl-1H-indole-3-carboxylate 4b

According to general procedure and starting from methyl (Z)-3-((4-methoxyphenyl)amino)but-2-enoate (44 mg, 0.20 mmol) the product was obtained as colorless solid (36 mg, 0.16 mmol, 82%).

$^1$H-NMR (600 MHz; CDCl$_3$): 8.32 (s, 1H), 7.60 (d, $J = 2.5$ Hz, 1H), 7.18 (d, $J = 8.8$ Hz, 1H), 6.83 (dd, $J = 8.7, 2.5$ Hz, 1H), 3.93 (d, $J = 11.6$ Hz, 3H), 3.88 (s, 3H), 2.71 (s, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 166.5, 155.6, 144.1, 129.3, 128.1, 112.1, 111.1, 104.3, 103.4, 55.8, 50.8, 14.5.

Methyl 2,5-dimethyl-1H-indole-3-carboxylate 4c

According to general procedure and starting from methyl (Z)-3-(p-tolylamino)but-2-enoate (41 mg, 0.20 mmol) the product was obtained as colorless solid (28 mg, 0.14 mmol, 69%).

$^1$H-NMR (600 MHz; CDCl$_3$): 8.32 (s, 1H), 7.88 (s, 1H), 7.18 (d, $J = 8.2$ Hz, 1H), 7.01 (dd, $J = 8.2, 1.0$ Hz, 1H), 3.93 (s, 3H), 2.72 (s, 3H), 2.47 (d, $J = 6.7$ Hz, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 166.5, 143.9, 132.7, 131.1, 127.3, 123.8, 121.0, 110.1, 104.0, 50.7, 21.6, 14.3.

Methyl 5-chloro-2-methyl-1H-indole-3-carboxylate 4d

According to general procedure and starting from methyl (Z)-3-((4-chlorophenyl)amino)but-2-enoate (45 mg, 0.20 mmol) the product was obtained as yellow solid (37 mg, 0.17 mmol, 83%).

$^1$H-NMR (600 MHz; CDCl$_3$): 8.62 (s, 1H), 8.05 (d, $J = 2.0$ Hz, 1H), 7.20 (d, $J = 8.5$ Hz, 1H), 7.14 (dd, $J = 8.5, 2.0$ Hz, 1H), 3.93 (s, 3H), 2.73 (d, $J = 7.3$ Hz, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 166.0, 145.3, 132.8, 128.2, 127.5, 122.6, 120.9, 111.5, 104.3, 50.9, 14.2.

Methyl 2,7-dimethyl-1H-indole-3-carboxylate 4e

According to general procedure and starting from methyl (Z)-3-((o-tolylamino)but-2-enoate (44 mg, 0.20 mmol) the product was obtained as colorless solid (29 mg, 0.14 mmol, 71%).

$^1$H-NMR (400 MHz; CDCl$_3$): 8.33 (s, 1H), 7.93 (d, $J = 8.0$ Hz, 1H), 7.13 (t, $J = 7.6$ Hz, 1H), 6.99 (d, $J = 7.2$ Hz, 1H), 3.98 (s, 3H), 2.76 (s, 3H), 2.48 (s, 3H);

$^{13}$C-NMR (101 MHz; CDCl$_3$): 166.5, 143.9, 133.9, 126.5, 123.0, 121.1, 119.5, 118.8, 104.2, 50.5, 16.2, 14.2.
Methyl 7-chloro-2-methyl-1H-indole-3-carboxylate 4f

According to general procedure and starting from methyl (Z)-3-((2-chlorophenyl)amino)but-2-enoate 1h (45 mg, 0.20 mmol) the product was obtained as yellow solid (27 mg, 0.12 mmol, 60%).

$^1$H-NMR (400 MHz; CDCl$_3$): 8.36 (s, 1H), 8.10-8.08 (m, 1H), 7.30 (dd, $J = 7.0$, 1.2 Hz, 1H), 7.23-7.18 (m, 2H), 3.96-3.93 (m, 3H), 2.78 (s, 3H); $^{13}$C-NMR (101 MHz; CDCl$_3$): 166.4, 143.9, 134.4, 127.1, 122.4, 121.7, 121.3, 110.4, 104.6, 50.7, 14.2

Tert-butyl 2-methyl-1H-indole-3-carboxylate 4g

According to general procedure and starting from tert-butyl (Z)-3-(phenylamino)but-2-enoate 1n (47 mg, 0.20 mmol) the product was obtained as colorless solid (37 mg, 0.16 mmol, 80%).

$^1$H-NMR (600 MHz; CDCl$_3$): 8.32 (s, 1H), 8.08 (d, $J = 7.5$ Hz, 1H), 7.27 (dd, $J = 8.6$, 7.7 Hz, 1H), 7.21-7.15 (m, 2H), 2.73 (s, 3H), 1.66 (s, 9H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 165.4, 143.3, 134.4, 127.2, 122.1, 121.47, 121.27, 110.3, 106.0, 79.8, 28.7, 14.2

4 General procedure for the Rh-catalysed ortho olefination

A 4 mL vial was equipped with the corresponding Weinreb amide (1 equiv.), [RhCp*Cl$_2$(1.0/2.5 mol%) and photoredox catalyst (10 mol%, 1 equiv.) and a teflon-coated magnetic stirring bar. After addition of AgSbF$_6$ (5/10 mol%) in chlorobenzene (0.01 mM) the corresponding electrophile (2 equiv.) was added and the reaction mixture placed in a preheated aluminum block (100 °C, actual vial temperature ~80 °C) under light irradiation from ca. 3 cm distance. After the indicated time, the reaction mixture was directly absorbed on SiO$_2$ and the product purified by flash column chromatography.

Butyl (E)-3-(2-(methoxy(methyl)carbamoyl)phenyl)acrylate 6a

Starting from N-methoxy-N-methylbenzamide (33 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 5:1) 49 mg (0.17 mmol, 84% yield).

$^1$H-NMR (600 MHz; CDCl$_3$): 7.72 (d, $J = 15.9$ Hz, 1H), 7.66-7.64 (m, 1H), 7.43-7.37 (m, 3H), 6.42 (d, $J = 15.9$ Hz, 1H), 4.18 (t, $J = 6.7$ Hz, 2H), 3.39-3.35 (m, 6H), 1.68-1.65 (m, 2H), 1.42 (q, $J = 7.5$ Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 3H); $^1$H-$^{13}$C-NMR (151 MHz; CDCl$_3$): 166.5, 141.3, 136.0, 131.7, 130.5, 129.6, 128.11, 127.98, 127.2, 120.4, 83.5, 64.5, 61.1, 30.7, 19.2, 13.7.
Butyl (E)-3-(2-(methoxy(methyl)carbamoyl)-5-methylphenyl)acrylate 6b

Starting from N-methoxy-N,4-dimethylbenzamide (36 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 5:1) 39 mg (0.13 mmol, 64% yield).

$^1$H-NMR (600 MHz; CDCl$_3$): 7.71 (d, $J = 15.9$ Hz, 1H), 7.45 (s, 1H), 7.27 (d, $J = 7.8$ Hz, 1H), 7.21-7.20 (m, 1H), 6.40 (d, $J = 15.9$ Hz, 1H), 4.18 (t, $J = 6.7$ Hz, 2H), 3.42-3.33 (m, 6H), 2.38 (s, 3H), 1.68-1.63 (m, 2H), 1.41 (dq, $J = 15.0$, 7.5 Hz, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 166.6, 141.4, 139.6, 133.2, 131.6, 130.4, 127.2, 126.9, 120.2, 83.5, 64.4, 61.1, 30.7, 21.3, 19.2, 13.7

Butyl (E)-3-(5-(tert-butyl)-2-(methoxy(methyl)carbamoyl)phenyl)acrylate 6c

Starting from 4-(tert-butyl)-N-methoxy-N-methylbenzamide (44 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 5:1) 46 mg (0.13 mmol, 66% yield).

$^1$H-NMR (600 MHz; CDCl$_3$): 7.74 (d, $J = 15.9$ Hz, 1H), 7.63 (d, $J = 1.7$ Hz, 1H), 7.43 (dd, $J = 8.1$, 1.8 Hz, 1H), 7.31 (d, $J = 8.1$ Hz, 1H), 6.42 (d, $J = 15.9$ Hz, 1H), 4.18 (t, $J = 6.7$ Hz, 2H), 3.41 (s, 6H), 1.66 (dd, $J = 14.8$, 7.0 Hz, 2H), 1.42 (dd, $J = 15.0$, 7.5 Hz, 2H), 1.33 (s, 9H), 0.95 (t, $J = 7.4$ Hz, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 166.7, 153.1, 152.7, 141.9, 133.1, 131.3, 127.0, 123.3, 120.0, 64.4, 61.1, 34.8, 31.1, 30.7, 19.2, 13.7.

Butyl (E)-3-(2-(dimethylcarbamoyl)-5-methoxyphenyl)acrylate 6d

Starting from 4-methoxy-N,N-dimethylbenzamide (36 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 1:1) 44 mg (0.14 mmol, 72% yield).

$^1$H-NMR (600 MHz; CDCl$_3$): 7.63 (d, $J = 15.9$ Hz, 1H), 7.26 (s, 1H), 7.11 (d, $J = 2.5$ Hz, 1H), 6.94 (dd, $J = 8.5$, 2.5 Hz, 1H), 6.40 (d, $J = 15.9$ Hz, 1H), 4.18 (t, $J = 6.7$ Hz, 2H), 3.84 (s, 3H), 3.13 (s, 3H), 2.79 (s, 3H), 1.67 (t, $J = 7.5$ Hz, 2H), 1.42 (dd, $J = 15.0$, 7.5 Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 3H); $^{13}$C-NMR (151 MHz; CDCl$_3$): 170.2, 166.5, 160.0, 141.0, 132.7, 130.0, 128.5, 120.8, 116.2, 111.2, 64.5, 55.4, 38.8, 35.0, 30.7, 19.2, 13.7.

Butyl (E)-3-(2-(piperidin-1-carbonyl)phenyl)acrylate 6e

Starting from phenyl (piperidin-1-yl)methanone (38 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 10:1) 45 mg (0.14 mmol, 71% yield).

$^1$H-NMR (400 MHz; CDCl$_3$): 7.69 (d, $J = 16.0$ Hz, 1H), 7.26 (s, 1H), 6.42 (d, $J = 16.0$ Hz, 1H), 3.69 (s, 2H), 3.32 (s, 2H), 1.66 (s, 7H), 1.49 (s, 2H), 1.42 (d, $J = 7.5$ Hz, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); $^{13}$C-NMR (101 MHz; CDCl$_3$): 170.2, 141.0, 136.5, 130.2, 129.3, 128.3, 126.74, 126.70, 126.51, 120.5, 64.4, 48.1, 42.6, 30.7, 25.6, 24.6, 19.2, 13.7.
**Butyl (E)-3-(2-(morpholin-4-carbonyl)phenyl)acrylate 4f**

Starting from morpholin(phenyl)methanone (38 mg, 0.2 mmol) the product was isolated as colorless oil after flash chromatography (n-pentane/ethyl acetate 10:1) 43 mg (0.14 mmol, 68% yield).

**1H-NMR (600 MHz; CDCl₃):** 7.69 (d, J = 16.0 Hz, 1H), 7.64-7.63 (m, 1H), 7.41-7.39 (m, 2H), 7.29-7.28 (m, 1H), 6.42 (d, J = 16.0 Hz, 1H), 4.18 (s, 2H), 3.76 (d, J = 5.0 Hz, 2H), 3.53 (t, J = 4.6 Hz, 2H), 3.15 (t, J = 4.7 Hz, 2H), 1.68-1.64 (m, 2H), 1.41 (q, J = 7.5 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H); **13C-NMR (151 MHz; CDCl₃):** 172.7, 168.6, 140.6, 136.4, 130.3, 129.5, 126.7, 126.1, 121.0, 66.8, 64.6, 47.4, 42.2, 30.7, 19.1, 13.7

**Solid State UV-Vis Reflectance spectra**
References:


Pulse Sequence: ss2mull
Spectrometer Freq.: 599.86 MHz
Solvent: CDCl3
Temperature: 293.15 K
Spectral Width: 27.06 ppm
Number of Scans: 4
Relaxation Delay: 1.000 s