APPENDIX

Appendix I. Characterization of Sulfoxides

(a) Methylphenylsulfoxide: Isolated as light yellow solid; mp 28-29ºC; ν (KBr)/cm^{-1} 1045;

^{1}H NMR (400MHz; $CDCl_3$, δ): 2.74(s, 3H); 7.30-7.35(m, 1H); 7.42-7.50(m, 2H); 7.62-7.69(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 43.83; 121.54; 128.43; 130.75; 145.32

(b) Methyl-p-tolylsulfoxide: Isolated as pale yellow liquid; mp 42-45 ºC; ν (KBr)/cm^{-1} 1035

^{1}H NMR (400MHz; $CDCl_3$, δ): 7.45 (d, 2H), 7.35 (d, 2H), 2.72 (s, 3H), 2.41 (s, 3H)

^{3}C NMR (100.5MHz; $CDCl_3$, δ): 142.59, 141.56, 129.93, 123.59, 44.21, 21.42

(c) Dibutylsulfoxide: Isolated as white solid; mp 32-33ºC; ν (KBr)/cm^{-1} 1060;

^{1}H NMR (400MHz; $CDCl_3$, δ): 0.95(t, 6H, J=7.42Hz); 1.37-1.47(m, 4H); 1.67-1.72(m, 4H); 2.62-2.69(m, 4H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 13.64; 22.15; 24.51; 51.81.

(d) Dibenzothiophene sulfoxide: Isolated as white solid; mp 188-189ºC; ν (KBr)/cm^{-1} 1042;

^{1}H NMR (400MHz; $CDCl_3$, δ): 7.54-7.60(m, 2H); 7.72-7.76(m, 2H); 7.92-7.97(m, 4H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 123.44; 124.14; 126.36; 129.83; 132.57; 143.37

(e) Dimethylsulfoxide: Isolated as liquid; ν (KBr)/cm^{-1} 1054;

^{1}H NMR (400MHz; $CDCl_3$, δ): 2.53(s, 6H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 40.39.

(f) 2-(Phenylsulfinyl)ethanol: Isolated as light brown solid; mp 42-43ºC; ν (KBr)/cm^{-1} 1039;

^{1}H NMR (400MHz; $CDCl_3$, δ): 2.44(s, 1H); 3.11(t, 2H, J=5.21Hz); 3.77(t, 2H, J=5.24Hz); 7.26-7.89(m, 1H); 7.48-7.47(m, 2H); 7.61-7.88(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 56.18; 60.92; 125.47; 130.04; 131.23; 144.57.

(g) Dihexylsulfoxide: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1043;

^{1}H NMR (400MHz; $CDCl_3$, δ): 0.96 (t, 6H, J= 7.65 Hz), 1.22-1.40 (m, 12H), 1.67 (m, 4H), 2.70 (t, 4H, J=6.71Hz)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 13.53, 21.93, 32.84, 27.64, 28.43, 52.64.

(h) Allylphenylsulfoxide: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1041;

^{1}H NMR (400MHz; $CDCl_3$, δ): 3.42(dt, 2H, J=7.12, 1.12Hz); 5.01(dq, 1H, J=1.44, 17.11Hz); 5.16(dq, 1H, J=1.12, 10.23Hz); 5.43(ddt, 1H, J=7.11, 10.23, 17.11 Hz), 7.26-7.31(m, 1H); 7.36-7.40(m, 2H); 7.61-7.64(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 60.36; 117.93; 124.72; 125.09; 129.07; 131.34; 142.15.

(i) Ethylphenylsulfoxide: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1050;

^{1}H NMR (400MHz; $CDCl_3$, δ): 1.23(t, 3H, J=6.61Hz); 2.68-2.78(q, 1H, J=6.62Hz); 2.92(q, 1H, J=6.62Hz) 7.13-7.47(m, 3H); 7.49-7.83(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 10.18, 47.12, 125.40, 129.81, 131.37, 145.81

(j) Diphenyl sulfoxide: Isolated as white solid; mp 70 ^{o}C; ν (KBr)/cm^{-1} 1041;

^{1}H NMR(400MHz; $CDCl_3$, δ): 7.63-7.68(m, 4H), 7.43-7.50(m, 6H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 144.68, 129.57, 128.03, 123.70.

(k) 4-Methoxyphenyl methyl sulfoxide: Colorless solid; mp 42-43 ^{o}C; ν (KBr)/cm^{-1} 1043;

^{1}H NMR(400MHz; $CDCl_3$, δ): 7.60-7.54 (m, 2H), 7.05-6.99 (m, 2H), 3.76 (s, 3H), 2.69 (s, 3H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 44.12, 54.90, 117.10, 124.64, 136.8, 162.91.

(l) Phenylvinylsulfoxide: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1053;

^{1}H NMR (400MHz; $CDCl_3$, δ): 5.93(d, 1H, J=10.13Hz); 6.25(d, 1H, J=15.89Hz); 6.56-6.70(m, 1H); 7.27-7.37(m, 1H); 7.44-7.54(m, 2H); 7.62-7.69(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 120.49; 124.51; 129.36; 131.14; 142.98; 143.41

(m) Benzylphenylsulfoxide: Isolated as white solid; mp 120 ^{o}C; ν (KBr)/cm^{-1} 1034;

^{1}H NMR (400MHz; $CDCl_3$, δ): 3.88(s, 2H), 6.94-7.11(m, 5H), 7.16-7.36(m, 3H), 7.40-7.54(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 63.43, 124.11, 128.14, 128.24, 128.47, 128.86, 130.25, 130.81, 142.60.

Appendix II. Characterization of Sulfones

(a) Methylphenylsulfone: Isolated as white solid; mp 85-86^{o}C; ν (KBr)/cm^{-1} 1322, 1166;

^{1}H NMR (400MHz; $CDCl_3$, δ): 3.01(s, 3H); 7.53-7.59(m, 1H); 7.62-7.71(m, 2H); 7.79-7.95(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 44.73; 126.33; 128.57; 132.91; 137.54.

(b) Methyl-p-tolylsulfone: Isolated as white solid; mp 86-87°C; ν (KBr)/cm^{-1} 1294, 1145

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.83 (d, 2H), 7.36 (d, 2H), 3.03 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 144.70, 137.63, 129.56, 127.38, 44.33, 22.44.

(c) Dibutylsulfone: Isolated as white solid; mp 42-43°C; ν (KBr)/cm^{-1} 1341, 1134;

^{1}H NMR (400MHz; $CDCl_3$, δ): 0.97 (t, 6H, J=7.39Hz); 1.39-1.52(m, 4H); 1.79-1.87(m, 4H); 2.87-2.92(m, 4H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 13.51; 21.69; 23.97; 52.51.

(d) Dibenzothiophene sulfone: Isolated as white solid; mp 231-232°C; ν (KBr)/cm^{-1} 1361, 1166;

^{1}H NMR (400MHz; $CDCl_3$, δ): 7.52-7.55(m, 2H); 7.61-7.68(m, 2H); 7.78-7.84(m, 4H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 120.14; 121.81; 130.06; 130.93; 133.78; 137.62.

(e) Dimethylsulfone: Isolated as white solid; mp 236-237°C; ν (KBr)/cm^{-1} 1312, 1135;

^{1}H NMR (400MHz; $CDCl_3$, δ): 3.25(s, 6H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 44.53.

(f) 2-(Phenylsulfonyl)ethanol: Isolated as white solid; mp 96-97°C; ν (KBr)/cm^{-1} 1335, 1152;

^{1}H NMR (400MHz; $CDCl_3$, δ): 2.48(s, 1H); 3.23(t, 2H, J=5.46Hz); 3.95(t, 2H, J=5.26Hz); 7.44-7.53(m, 1H); 7.57-7.67(m, 2H); 7.86-7.95(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 57.35; 61.56; 128.92; 129.58; 134.06; 140.71.

(g) Dihexylsulfone: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1323, 1161;

^{1}H NMR (400MHz; $CDCl_3$, δ): 0.95 (t, 6H, J= 7.66 Hz), 1.24-1.40 (m, 12H), 1.92 (m, 4H), 3.36 (t, 4H, J=6.71Hz)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 13.46, 21.75, 32.62, 27.91, 26.44, 53.72.

(h) Allylphenylsulfone: Isolated as pale yellow liquid; ν (KBr)/cm^{-1} 1317, 1142;

^{1}H NMR (400MHz; $CDCl_3$, δ): 3.91(dt, 2H, J= 7.19, 1.22Hz); 5.05(dq, 1H, J= 1.49, 17.21Hz); 5.18(dq,1H, J= 1.22, 10.32Hz); 5.63(ddt, 1H, J= 7.19, 10.31, 17.21Hz); 7.37-7.44(m, 1H); 7.62-7.69(m, 2H); 7.91-7.94(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 60.53; 117.41; 124.44; 128.88; 129.13; 133.72; 137.26.

(i) Ethylphenylsulfone: Isolated as white solid; mp > 260 ºC; ν (KBr)/cm^{-1} 1322, 1152;

^{1}H NMR (400MHz; $CDCl_3$, δ): 1.31(t, 3H, J=7.11Hz); 3.07(q, 2H, J=7.12Hz); 7.58(m, 3H); 7.96(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 7.24, 50.18, 127.75, 128.90, 133.77, 138.11.

(j) Diphenyl sulfone: Isolated as pale yellow solid; mp 128ºC; ν (KBr)/cm^{-1} 1313, 1154;

^{1}H NMR (400MHz; $CDCl_3$, δ): 7.91-7.95(m, 4H),7.44-7.54(m, 6H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 141.68, 133.12, 129.21, 127.64.

(k) 4-Methoxyphenyl methyl sulfone: Colourless solid; mp 118-119 ºC; ν(KBr)/cm^{-1} 1318, 1146;

^{1}H NMR (400MHz; $CDCl_3$, δ): 2.88 (s, 3H), 3.78 (s, 3H), 6.99 (d, 2H, J=8.7), 7.80 (d,J=8.7, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 44.41, 55.70, 114.21, 129.63, 131.14, 164.28.

(l) Phenylvinylsulfone: Isolated as white solid; mp 63-64ºC; ν (KBr)/cm^{-1} 1364, 1161;

^{1}H NMR (400MHz; $CDCl_3$, δ): 6.11(d, 1H, J=9.60Hz); 6.43(d, 1H, J=16.42Hz); 6.64-6.78(m, 1H); 7.44-7.51(m, 1H); 7.56-7.68(m, 2H); 7.87-7.93(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 127.85; 129.33; 133.77; 138.51; 139.70

(m) Benzylphenylsulfone: Isolated as white solid; mp 143 ºC; ν (KBr)/cm^{-1} 1327, 1159;

^{1}H NMR (400MHz; $CDCl_3$, δ): 4.41(s, 2H), 7.05-7.14(m, 5H), 7.3-7.41(1m, 3H), 7.65-7.72(m, 2H)

^{13}C NMR (100.5MHz; $CDCl_3$, δ): 62.53, 128.32, 128.39, 128.47, 128.64, 130.52, 133.41, 137.39

Splitting patterns are designated as s (singlet), d (dublet), t (triplet), dt (double triplet), ddt (double-double triplet), q (quartet), dq (double quartet), m (multiplet).

Appendix III. Identification of styrene oxidation products

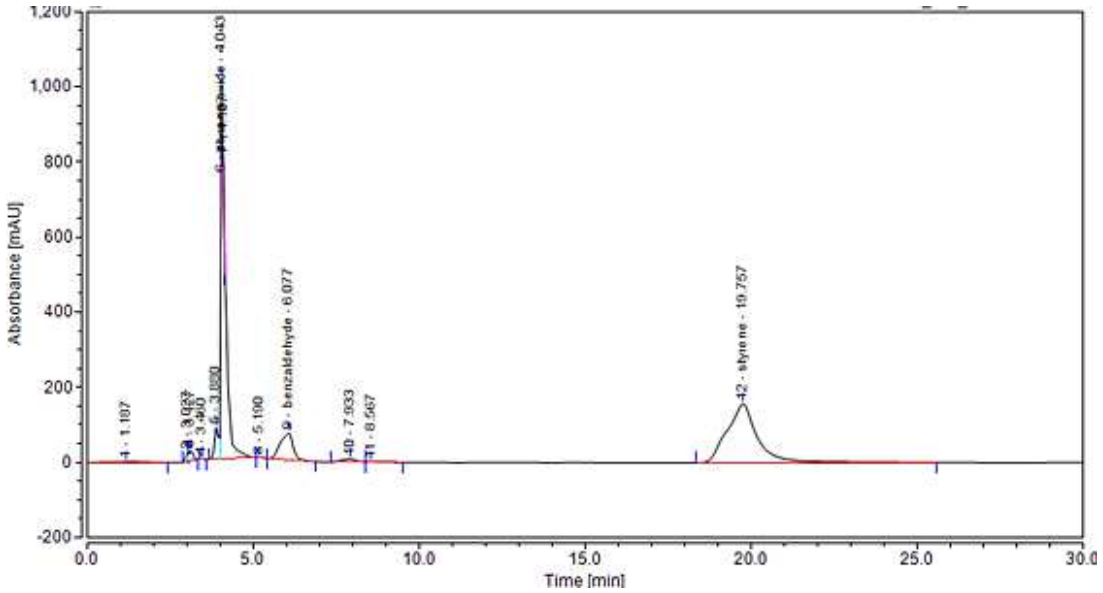

Fig. 1A A typical chromatogram of styrene oxidation highlighting resolution of all the components

Appendix IV. Identification of 5-hydroxyfurfural oxidation products

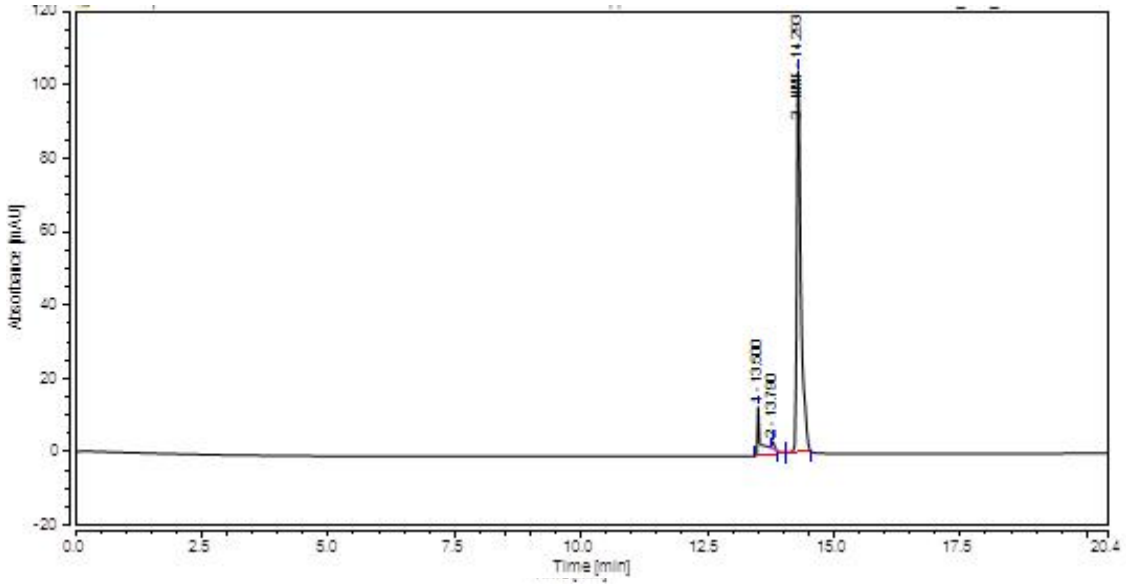

Fig. 2A HPLC chromatogram of HMF in water.

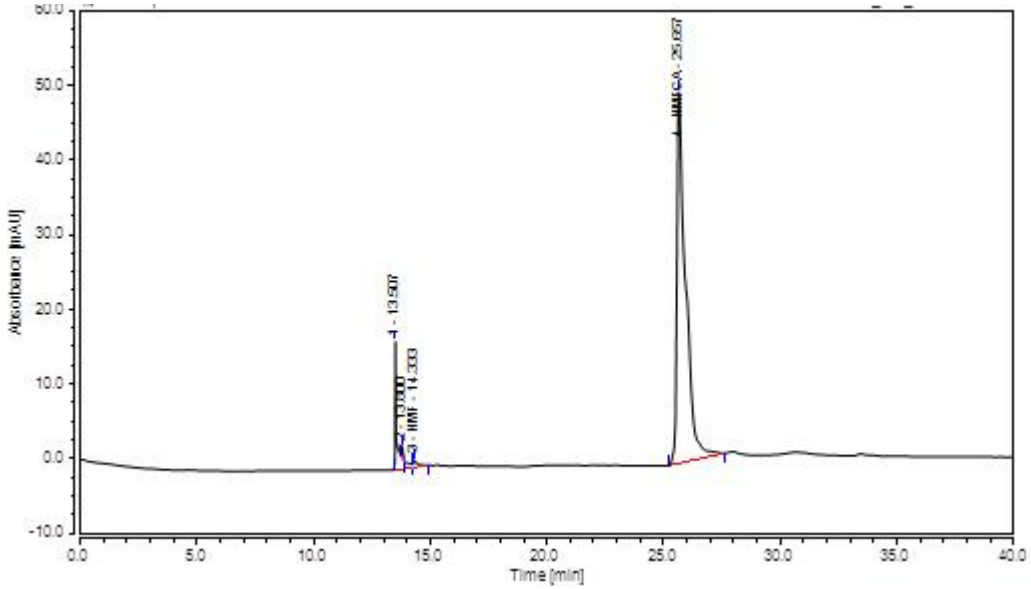

Fig. 3A HPLC chromatogram of the diluted reaction mixture (0.1 mL of the reaction mixture diluted to 10 mL with distilled water) at 30 minutes of reaction time.