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Supplementary material

SUPPLEMENTARY MATERIAL TO

Simple and improved regioselective brominations of aromatic compounds using *N*-benzyl-*N*,*N*-dimethylanilinium peroxodisulfate in the presence of potassium bromide under mild reactions conditions

HASSAN GHASEMNEJAD-BOSRA[1]*, FARHAD RAMZANIAN-LEHMALI[2] and SOMAYE JAFARI[1]

[1]*Islamic Azad University – Babol Branch, School of Science, P.O. Box 755, Babol and* [2]*University of Payamenoor, Babol, Iran*

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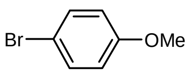
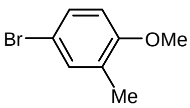
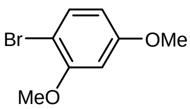
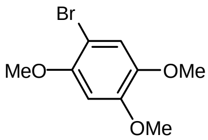
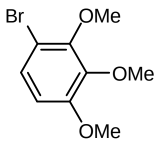
TABLE I-S. ^{1}H-NMR and ^{13}C-NMR spectral data of the products

Entry	Product	^{1}H-NMR, δ / ppm	^{13}CNMR, δ / ppm
1		3.70 (3H, *s*, –OCH_3), 6.57–6.61 (2H, *qq*, Ar), 7.19–7.23 (2H, *qq*, Ar)	55.15 (–OCH_3), 108.60 (C1), 111.90 (C3,5), 129.00 (C2,6), 156.91 (C4)
2		2.22 (3H, *s*, –CH_3), 3.72 (3H, *s*, –OCH_3), 6.63 (1H, *d*, Ar), 7.11 (1H, *d*, Ar), 7.23 (1H, *d*, Ar)	17.16 (–CH_3), 55.30 (–OCH_3), 103.03 (C1), 114.04 (C5), 128.86 (C3), 131.74 (C2), 133.25 (C6), 157.52 (C4)
3		3.70 (3H, *s*, –OCH_3), 3.83 (3H, *s*, –OCH_3), 6.45–6.50 (2H, *m*, Ar), 7.13 (1H, *dd*, Ar)	55.87(–OCH_3), 55.93(–OCH_3), 115.35 (C5), 116.27 (C2), 118.70 (C1), 125.66 (C6), 148.84 (C4), 149.78 (C3)
4		3.68 (3H, *s*, –OCH_3), 3.75 (3H, *s*, –OCH_3), 3.80 (3H, *s*, –OCH_3), 6.25 (1H, *s*, Ar), 6.87 (1H, *s*, Ar)	55.93 (–OCH_3), 56.52 (–OCH_3), 56.65 (–OCH_3), 100.46 (C3), 105.67 (C1), 117.06 (C6), 146.14 (C5), 150.26 (C4), 154.02 (C2)
5		3.65 (3H, *s*, –OCH_3), 3.77 (3H, *s*, –OCH_3), 3.95 (3H, *s*, –OCH_3), 6.24 (1H, *d*, Ar), 7.90 (1H, *d*, Ar)	57.03 (–OCH_3), 58.22 (–OCH_3), 60.68 (–OCH_3), 109.03 (C1), 111.56 (C4), 128.44 (C6), 139.54 (C3), 149.15 (C2), 152.43 (C4)

* Corresponding author. E-mail: h_ghasem2000@yahoo.com

TABLE I-S. Continued

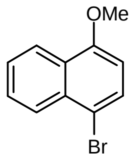
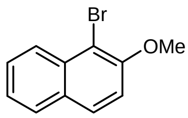
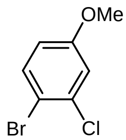
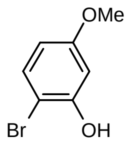
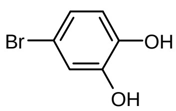
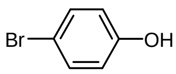
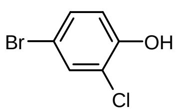
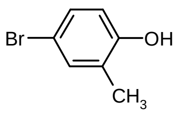
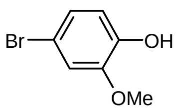
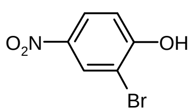
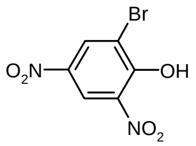
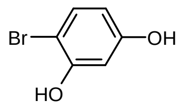
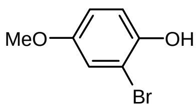
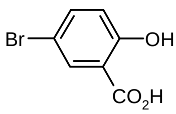
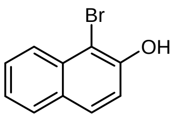
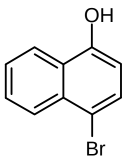
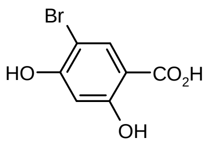
Entry	Product	^{1}H-NMR, δ / ppm	^{13}CNMR, δ / ppm
6		3.80 (3H, *s*, –OCH_3), 7.27 (1H, *d*, Ar), 7.41 (1H, *t*, Ar), 7.47 (1H, *d*, Ar), 7.58 (1H, *t*, Ar), 7.68–7.70 (2H, *m*, Ar)	55.22 (–OCH_3), 104.30 (C3), 113.00 (C1), 122.30 (C5), 125.70 (C6), 126.60 (C8), 127.40 (C10), 127.50 (C7), 129.30 (C2), 133.20 (C9), 155.00 (C4)
7		3.78 (3H, *s*, –OCH_3), 7.21 (1H, *d*, Ar), 7.40 (1H, *t*, Ar), 7.45 (1H, *d*, Ar), 7.58 (1H, *t*, Ar), 7.63–7.65 (2H, *m*, Ar)	56.80 (–OCH_3), 108.40 (C1), 113.40 (C3), 124.10 (C6), 125.80 (C8), 127.50 (C7), 127.80 (C5), 128.80 (C4), 129.60 (C9), 139.90 (C10), 153.60 (C2)
8		3.71 (3H, *s*, –OCH_3), 6.64 (1H, *dd*, Ar), 6.77 (1H, *m*, Ar), 7.35–7.37 (1H, *dd*, Ar)	55.76 (–OCH_3), 101.33 (C1), 103.07 (C3), 112.44 (C5), 134.63 (C6), 154.05 (C2), 157.68 (C4),
9		3.83 (3H, *s*, –OCH_3), 6.42–6.45 (1H, *qq*, Ar), 6.50 (1H, *m*, Ar), 7.09–7.11 (1H, *dd*, Ar)	55.70 (–OCH_3), 101.12 (C3), 103.28 (C5), 112.39 (C1), 133.97 (C2), 153.98 (C6), 157.58 (C4)
10		6.48 (1H, *d*, Ar), 6.70–6.72 (1H, *dd*, Ar), 7.07–7.10 (1H, *dd*, Ar)	113.51 (C4), 103.01 (C6), 117.63 (C3), 128.45 (C5), 141.33 (C1), 147.84 (C2)
11		6.89–6.92 (2H, *qq*, Ar), 7.23–7.26 (2H, *qq*, Ar)	107.20 (C4), 113.50 (C2,6), 128.90 (C3,5), 154.10 (C1)
12		6.94–6.96 (1H, *dd*, Ar), 7.20–7.21 (1H, *dd*, Ar), 7.27–7.29 (1H, *dd*, Ar)	112.40 (C4), 117.60 (C6), 120.80 (C2), 129.45 (C3), 131.30 (C5), 150.51 (C1)
13		2.21 (3H, *s*, –CH_3), 6.73 (1H, *m*, Ar), 7.09 (1H, *m*, Ar), 7.21 (1H, *m*, Ar)	17.45 (CH_3), 100.10 (C4), 117.18 (C6), 125.51 (C2), 130.19 (C3), 138.10 (C5), 152.20 (C1)
14		3.80 (3H, *s*, –CH_3), 6.88–6.90 (1H, *dd*, Ar), 6.97 (1H, *m*, Ar), 7.04–7.06 (1H, *dd*, Ar)	55.93 (OCH_3), 114.27 (C3), 116.96 (C4), 118.59 (C6), 125.60 (C5), 145.62 (C1), 148.53 (C2)
15		7.16–7.18 (1H, *dd*, Ar), 7.80–7.82 (1H, *dd*, Ar), 7.30 (1H, *d*, Ar)	107.04 (C2), 119.80 (C6), 122.91 (C5), 127.62 (C3), 142.04 (C4), 157.63 (C1)

TABLE I-S. Continued

Entry	Product	¹H-NMR, δ / ppm	¹³CNMR, δ / ppm
16		8.68 (1H, *d*, Ar), 8.82 (1H, *d*, Ar), 7.30 (1H, *d*, Ar)	104.26 (C2), 120.24 (C5), 134.21 (C3), 136.96 (C6), 141.62 (C4), 154.87 (C1)
17		6.47–6.49 (1H, *dd*, Ar), 6.70–6.73 (1H, *dd*, Ar), 7.30 (1H, *d*, Ar)	99.38 (C4), 104.08 (C2), 109.52 (C6), 133.60 (C5), 151.75 (C3), 155.28 (C3),
18		3.71 (3H, *s*, $-OCH_3$), 6.76 (1H, *m*, Ar), 6.91–6.93 (1H, *dd*, Ar), 6.98–7.01 (1H, *qq*, Ar)	55.34 (OCH_3),112.18 (C3), 113.98 (C2), 114.83 (C5), 118.15 (C6), 143.03 (C1), 155.71 (C4),
19		6.99–7.02 (1H, *dd*, Ar), 7.57–7.59 (1H, *dd*, Ar), 7.77–7.78 (1H, *dd*, Ar), 11.31 (1H, *s*, –COOH)	100.46 (C5), 112.38 (C1), 118.26 (C3), 132.81 (C4), 136.09 (C6), 157.86 (C2), 171.54 (CO_2H)
20		7.89 (1H, *d*, Ar), 7.29 (1H, *d*, Ar), 7.45 (1H, *t*, Ar), 7.58 (1H, *t*, Ar), 7.70–7.72 (2H, *m*, Ar)	106.00 (C1), 117.00 (C3), 124.00 (C6), 125.20 (C8), 127.70 (C7), 128.10 (C5), 129.20 (C4), 129.50 (C10), 132.10 (C9), 150.40 (C2)
21		7.95 (1H, *d*, Ar), 7.33 (1H, *d*, Ar), 7.46 (1H, *t*, Ar), 7.62 (1H, *t*, Ar), 7.75–7.78 (2H, *m*, Ar)	109.10 (C3), 113.43 (C1), 121.30 (C5), 125.50 (C10), 126.00 (C6), 127.00 (C8), 127.80 (C7), 129.30 (C2), 132.70(C9), 151.10 (C4)
22		6.46 (1H, *s*, Ar), 7.75 (1H, *s*, Ar)	98.53 (C5), 104.28 (C3), 105.50 (C1), 137.44 (C6), 153.28 (C4), 158.23 (C2), 171.52 (CO_2H),