Supporting Information

Four-Component Synthesis of 9*H*-Pyrimido[4,5-*b*]indoles Using Ammonium Iodide as the Nitrogen Source

Yufeng Chen [1], Ruitong Yang [1], Fuhong Xiao [1,*], Tong Li [1], Guojiang Mao [2] and Guo-Jun Deng [1,*]

[1] Key Laboratory of Environmentally Friendly Chemistry and Application of Ministry of Education, Hunan Province Key Laboratory of Green Organic Synthesis and Application, College of Chemistry, Xiangtan University, Xiangtan 411105, China

[2] School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, 453007, P. R. China

* Correspondence: Fuhong Xiao: fhxiao@xtu.edu.cn; Guo-jun Deng: gjdeng@xtu.edu.cn.

^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra of Products

^{1}H NMR and ^{13}C NMR of compound 3aa

^{1}H NMR and ^{13}C NMR of compound 3ba

^{1}H NMR and ^{13}C NMR of compound 3ca

^{1}H NMR and ^{13}C NMR of compound 3da

^{1}H NMR and ^{13}C NMR of compound 3ea

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3fa

160.622
159.201
157.144
156.866
150.271
138.561
135.885
130.796
129.069
128.313
120.244
120.140
115.889
115.635
113.494
113.402
112.756
112.711
108.083
107.836
NH
N
N
F
160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108 10
f1 (ppm)

-121.907
NH
N
N
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR and ^{13}C NMR of compound 3ga

^{1}H NMR and ^{13}C NMR of compound 3ha

^{1}H NMR and ^{13}C NMR of compound 3ia

^{1}H NMR and ^{13}C NMR of compound 3ja

^{1}H NMR and ^{13}C NMR of compound 3ka

^{1}H NMR and ^{13}C NMR of compound 3la

^{1}H NMR and ^{13}C NMR of compound 3ma

^{1}H NMR and ^{13}C NMR of compound 3na

^{1}H NMR and ^{13}C NMR of compound 3ab

^{1}H NMR and ^{13}C NMR of compound 3ac

^{1}H NMR and ^{13}C NMR of compound 3ad

^{1}H NMR and ^{13}C NMR of compound 3ae

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3af

-111.505
NH
N
N
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR and ^{13}C NMR of compound 3ag

^{1}H NMR and ^{13}C NMR of compound 3ah

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3ai

130.965
130.649
130.330
130.018
128.823
128.426
126.137
126.097
126.056
126.020
123.432
122.304
121.651
120.731
119.332
NH
N
N
F
F
F
131.5
130.5
129.5
128.5
127.5
126.5
125.5
124.5
123.5
122.5
121.5
120.5
119.5
118.5
f1 (ppm)

-61.072
NH
N
N
F
F
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3aj

130.170
128.230
124.388
122.153
121.835
121.573
121.365
119.400
119.284
116.732
113.024
112.365
NH
N
N
O
F
F
F
133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 110
f1 (ppm)

-51.853
NH
N
N
O
F
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR and ^{13}C NMR of compound 3ak

^{1}H NMR and ^{13}C NMR of compound 3al

^{1}H NMR and ^{13}C NMR of compound 3am

^{1}H NMR and ^{13}C NMR of compound 3an

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3ao

127.058
124.494
123.096
122.241
121.946
121.631
119.940
119.399
119.367
116.850
113.364
112.404
NH
N
N
O
F
F
F
127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112
f1 (ppm)

-56.638
NH
N
N
O
F
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR and ^{13}C NMR of compound 3ap

^{1}H NMR and ^{13}C NMR of compound 3aq

^{1}H NMR and ^{13}C NMR of compound 3ar

^{1}H NMR and ^{13}C NMR of compound 3as

^{1}H NMR, ^{13}C NMR and ^{19}F NMR of compound 3at

162.096
159.579
158.733
158.690
156.126
149.316
139.442
132.477
132.456
131.981
131.897
128.282
127.740
127.643
124.813
124.777
122.251
121.544
119.235
117.282
117.060
112.575
112.355
NH
N
N
F
72 168 164 160 156 152 148 144 140 136 132 128 124 120 116 112 108
f1 (ppm)

-114.385
NH
N
N
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR and ^{13}C NMR of compound 3au

^{1}H NMR and ^{13}C NMR of compound 3av

^{1}H NMR and ^{13}C NMR of compound 3aw

^{1}H NMR and ^{13}C NMR of compound 3ax

^{1}H NMR and ^{13}C NMR of compound 3ay

^{1}H NMR and ^{13}C NMR of compound 3az