Spectral analysis of quinaldines

The products formed during photocatalytic synthesis were identified and their yields were determined by GC-MS. Structure of the products were confirmed by ^{1}H and ^{13}C NMR spectra.

6-Methoxy-2-methylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.71 (s, 3H), 3.91 (s, OCH_3), 7.22-7.94 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.03 (CH_3), 55.47 (OCH_3), 127.3, 142.5, 156.33, 157.14 (*ipso* carbons), 121.83-134.99 (aromatic carbons).

2,6-Dimethylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.5 (s, 3H), 2.72 (s, CH_3), 7.21-7.93 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.26, 21.44 (CH_3), 128.2, 135.4, 146.4, 157.9 (*ipso* carbons), 121.90-135.30 (aromatic carbons).

2,8-Dimethylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.84 (s, 3H), 2.78 (s, CH_3), 7.28-8.03 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.69, 17.97 (CH_3), 126.3, 136.53,147.0, 157.8 (*ipso* carbons), 121.61-136.24 (aromatic carbons).

2,7-Dimethylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.55 (s, 3H), 2.35 (s, CH_3), 7.03-7.90 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.2, 24.3 (CH_3), 124.5, 139.1,146.7, 158.7 (*ipso* carbons), 121.71-129.34 (aromatic carbons).

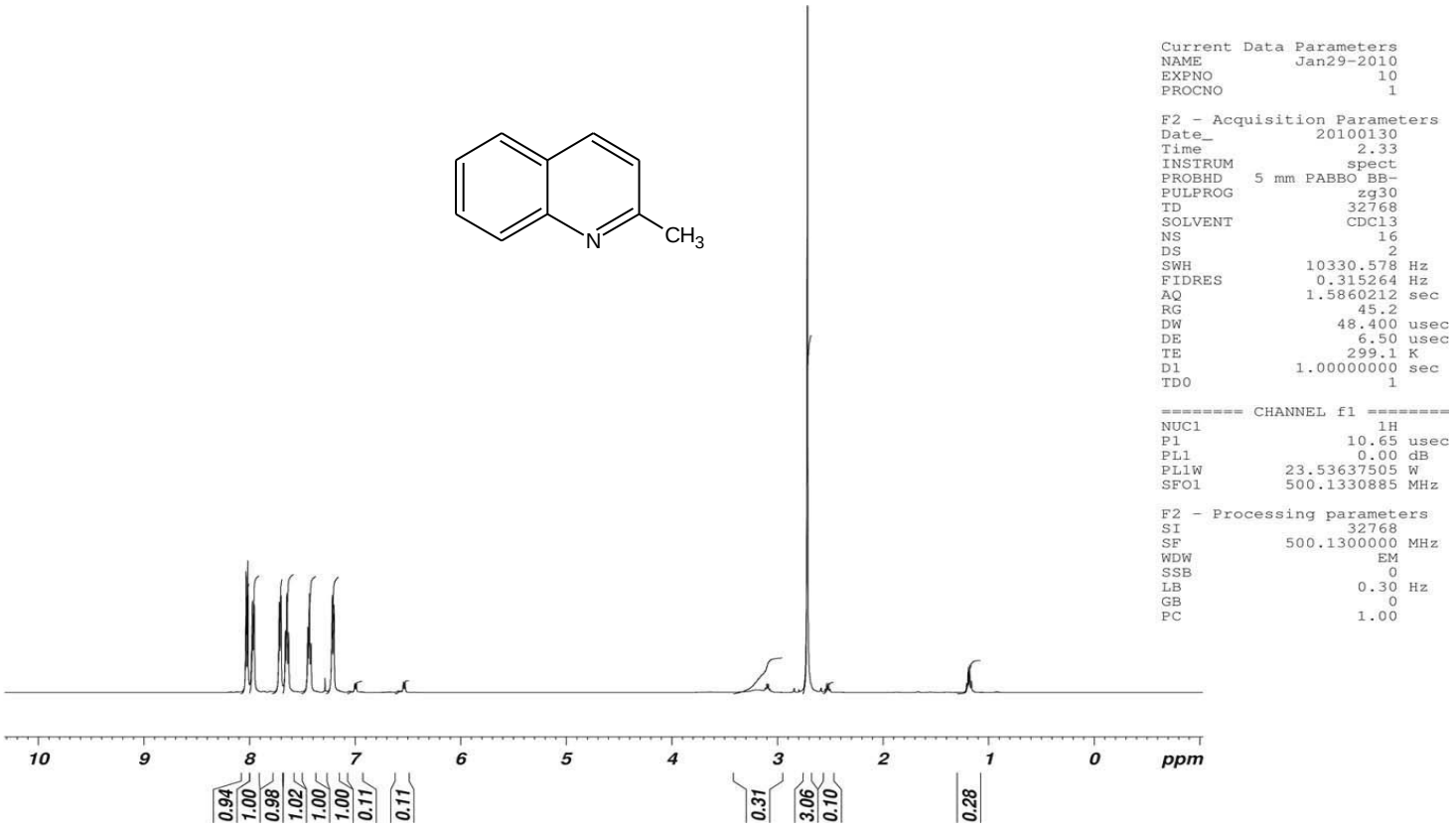
6-Ethoxyquinaldine. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.51 (s, 3H), 1.35 (t, CH_3), 3.99 (t, CH_2), 6.98-7.95 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.2 (CH_3), 14.8, $OCH_2\mathbf{C}H_3$, 64.8 ($O\mathbf{C}H_2CH_3$), 124.5, 139.1, 146.7, 158.7 (*ipso* carbons), 121.71-129.34 (aromatic carbons).

2,5,7-Trimethylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.55 (s, 3H), 2.35 (s, CH_3), 2.35 (s, CH_3), 7.08-8.05 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.2 (CH_3), 22.5 (CH_3), 24.6 (CH_3), 123.3, 139.7, 146.5, 158.0 (*ipso* carbons), 120.5-131.0 (aromatic carbons).

5,7-Dimethoxy-2-methylquinoline. ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.55 (s, 3H), 3.71 (s, OCH_3), 3.71 (s, OCH_3), 6.48-8.41 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 25.2 (CH_3), 55.9 (OCH_3), 56.3 (OCH_3), 147.6, 155.1, 159.0, 159.8 (*ipso* carbons), 110.1-129.0 (aromatic carbons).

Table 3.3.6. GC-MS spectral data of quinaldines

Run	Product	Retention time (min)	GC-MS (m/z)
1	2-Methylquinoline	10.8	143.0 (M^+) (128.0, 116.2, 100.0, 89.5, 75.1, 63.2, 50.1)
2	2,3-Dimethylindole	11.4	145.0 (130.3, 115.3, 103.4, 77.0, 67.1)
3	2,8-Dimethylquinoline	12.2	157.1 (142.0, 128.0, 115.3, 89.0, 77.0, 51.0)
4	2,7-Dimethylquinoline	12.3	157.0 (141.9, 115.0, 89.0, 63.0, 51.0)
5	2,6-Dimethylquinoline	12.0	157.0 (141.9, 115.0, 89.0, 63.0, 51.0)
6	6-Methoxy-2-methylquinoline	14.3	173.0 (158.1, 130.2, 103.1, 77.1, 63.1, 51.0)
7	5-Methoxy-2-methylquinoline	16.1	173.0 (158.1, 130.2, 103.1, 77.1, 63.1, 51.0)
8	7-Methoxy-2-methylquinoline	16.8	173.0 (158.1, 130.2, 103.1, 77.1, 63.1, 51.0)
9	2,5,7-Trimethylquinoline	14.5	171.0 (152.0, 115.0, 77.0, 63.0, 51.0)
10	2,5,6-Trimethylquinoline	13.9	171.0 (152.0, 115.0, 77.0, 63.0, 51.0)
10	5,7-Dimethoxy-2-methylquinoline	14.4	203.3 (181.2, 160.1, 117.0, 102.0)
11	6-Ethoxyquinaldine	14.8	187.0 (159.0, 130.0, 115.0, 103.0, 89.0, 77.0, 63.0, 51.0)
12	6-Chloro-2-methylquinoline	11.5	177.1 (142.1, 115.0, 77.3, 65.0, 51.0)
13	6-Fluoro-2-methylquinoline	10.5	160.0 (133.0, 126.0, 108,0, 99.0, 67.0, 57.0, 51.0)

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FIDRES          0.315264 Hz
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RG                  45.2
DW                48.400 usec
DE                 6.50 usec
TE                299.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
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P1                 10.65 usec
PL1                0.00 dB
PL1W        23.53637505 W
SFO1        500.1330885 MHz

F2 - Processing parameters
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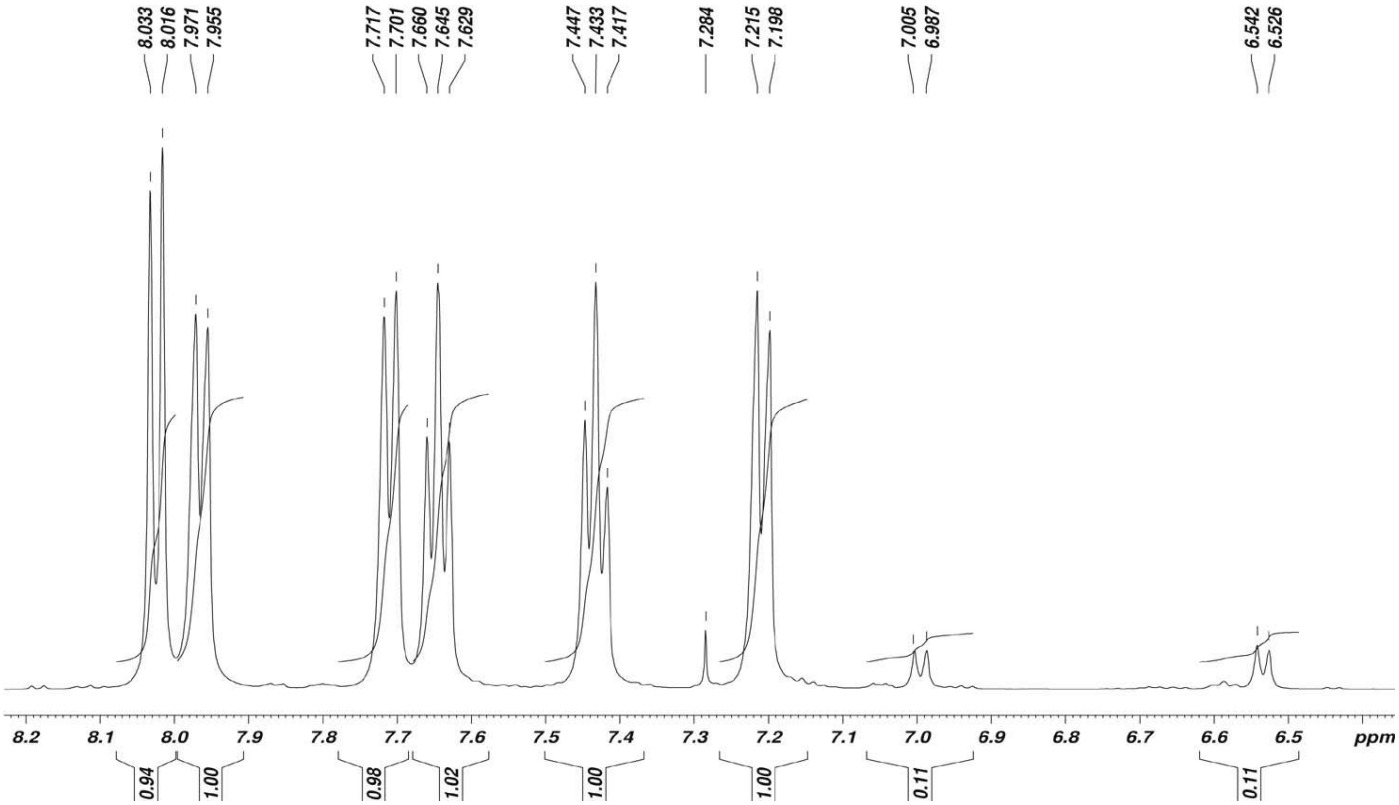
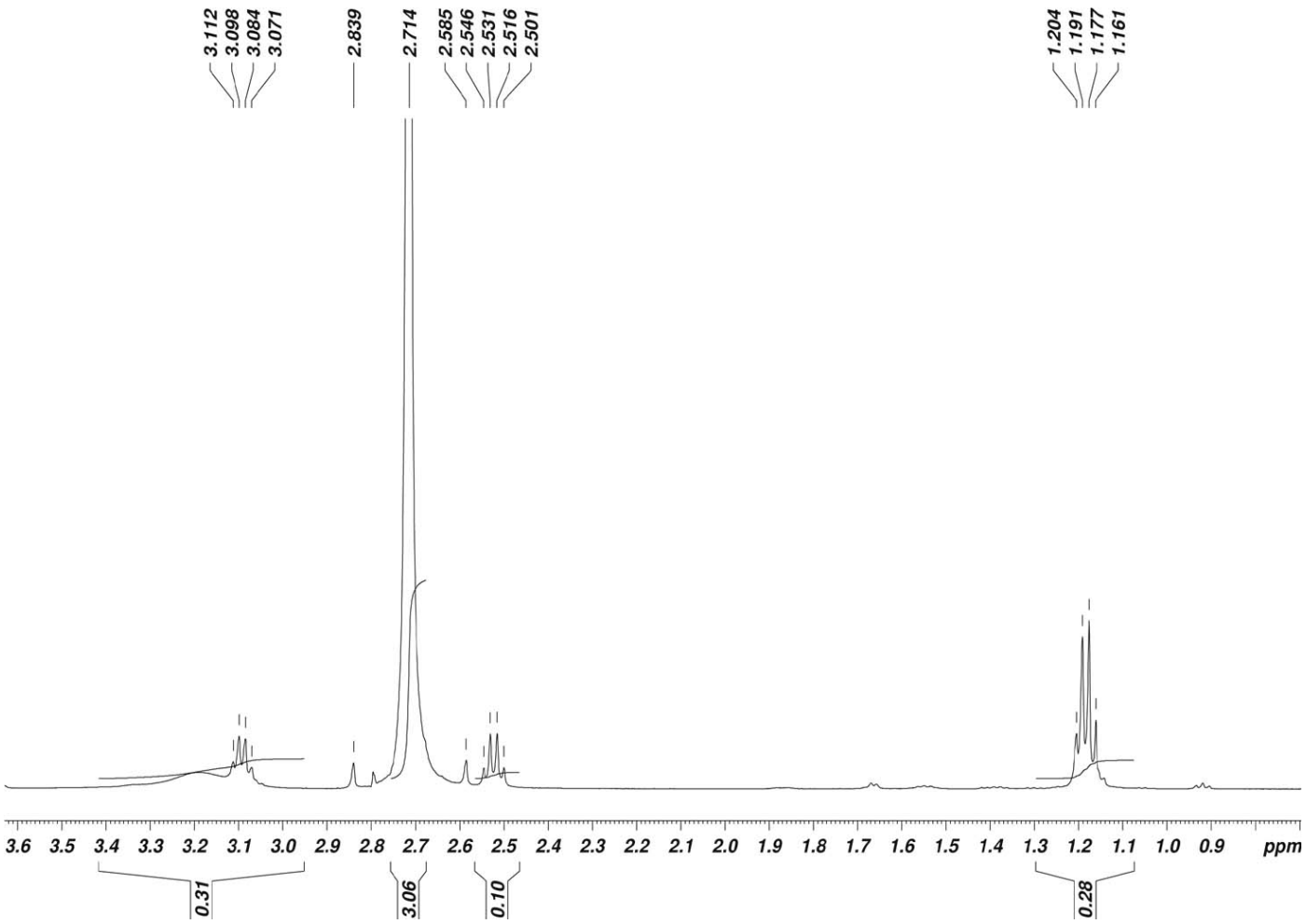
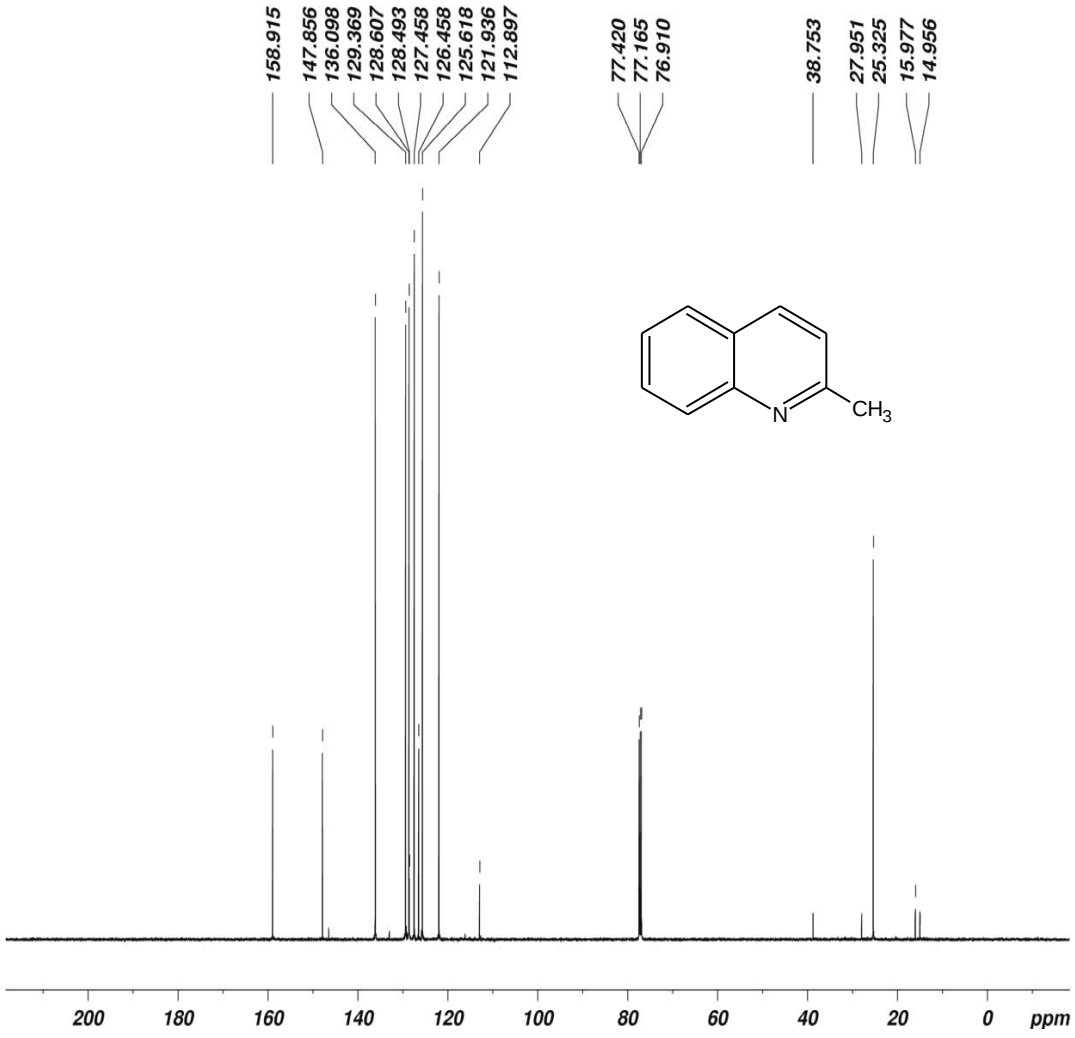
^{1}H NMR spectrum of quinaldine





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PROCNO                 1

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TD                 32768
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SWH           29761.904 Hz
FIDRES         0.908261 Hz
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RG                   203
DW               16.800 usec
DE                6.50 usec
TE                300.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.80 usec
PL1                 0.00 dB
PL1W        70.83519745 W
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.50 dB
PL13               17.50 dB
PL2W        23.53637505 W
PL12W        0.41854253 W
PL13W        0.41854253 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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^{13}C NMR spectrum of quinaldine