Supplementary Materials

N-Directed Pd-Catalyzed Photoredox-Mediated C-H Arylation for Accessing Phenyl-Extended Analogues of Biginelli/Suzuki-Derived Ethyl 4-Methyl-2,6-Diphenylpyrimidine-5-Carboxylates

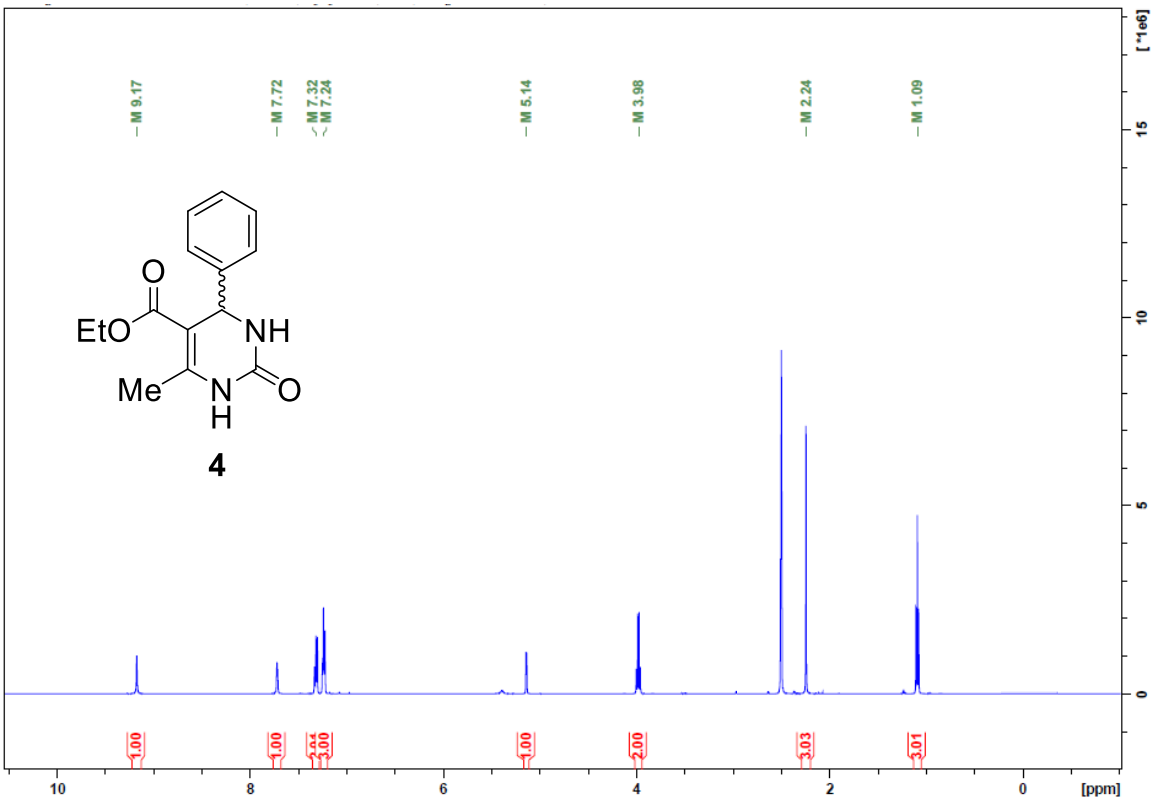
Savvas N. Georgiades,* Persefoni G. Nicolaou, Nikos Panagiotou

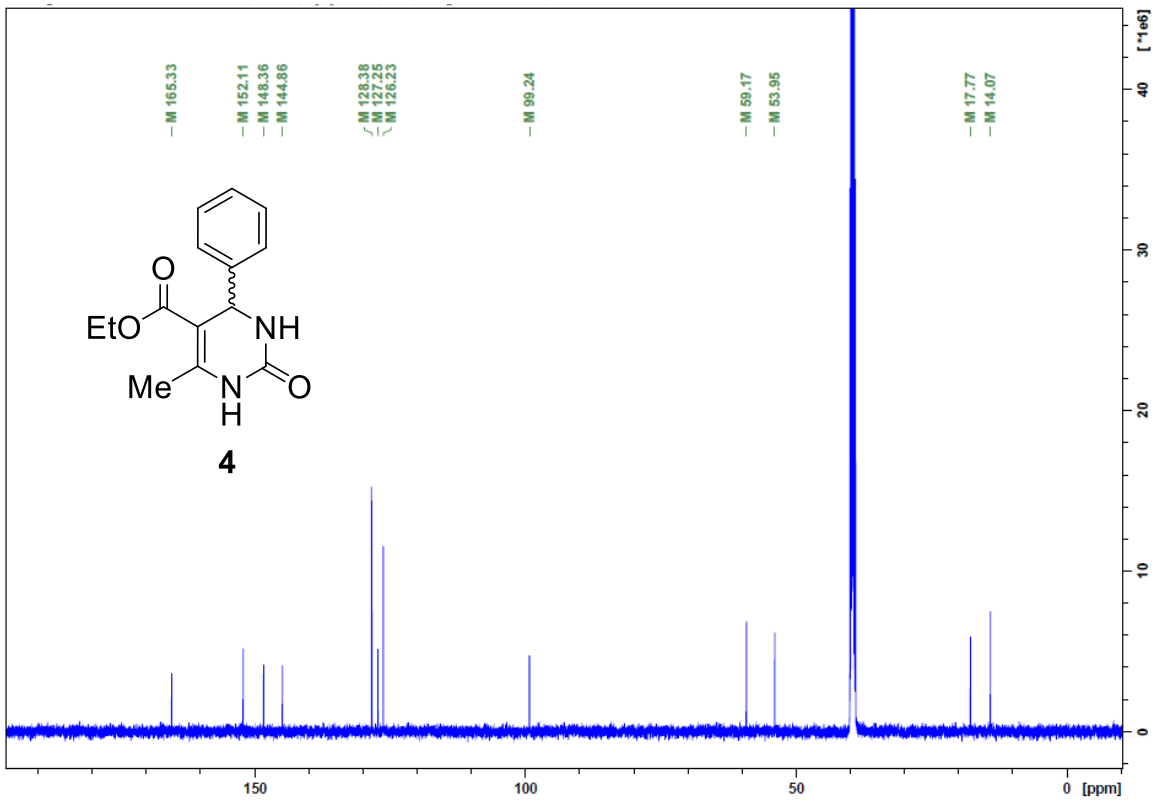
Department of Chemistry, University of Cyprus

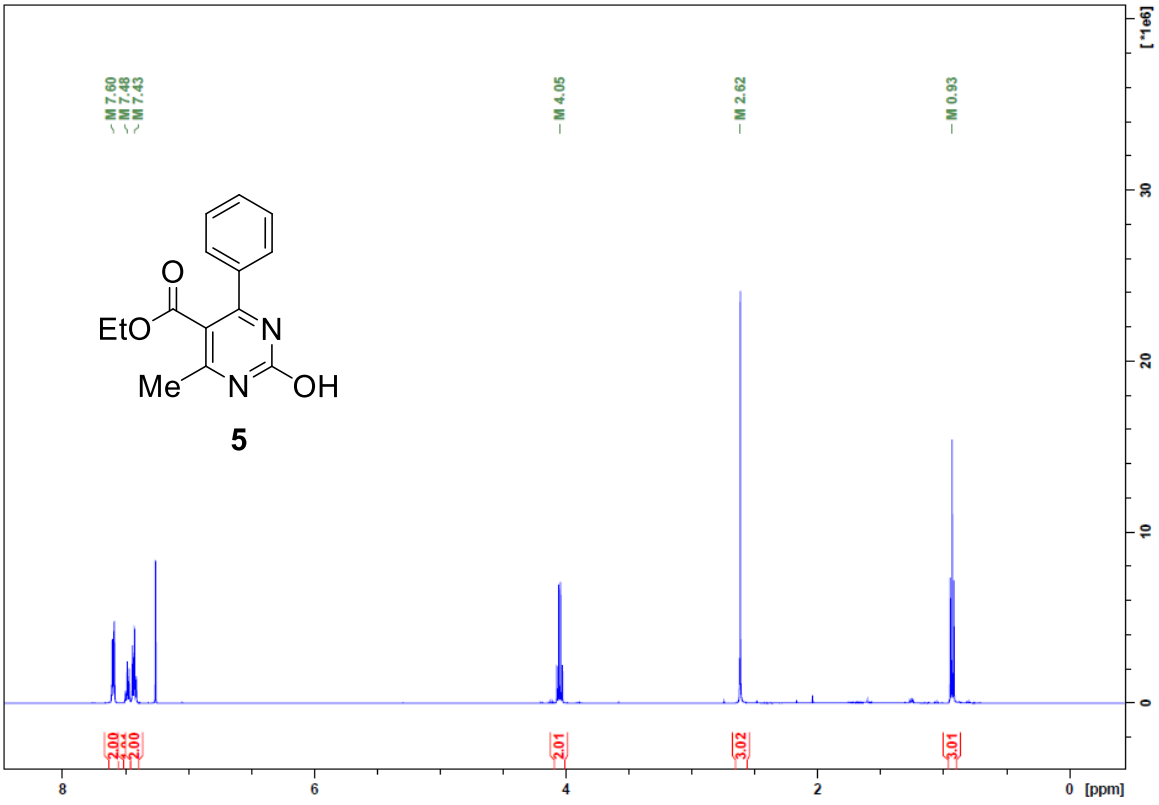
E-mail: georgiades.savvas@ucy.ac.cy

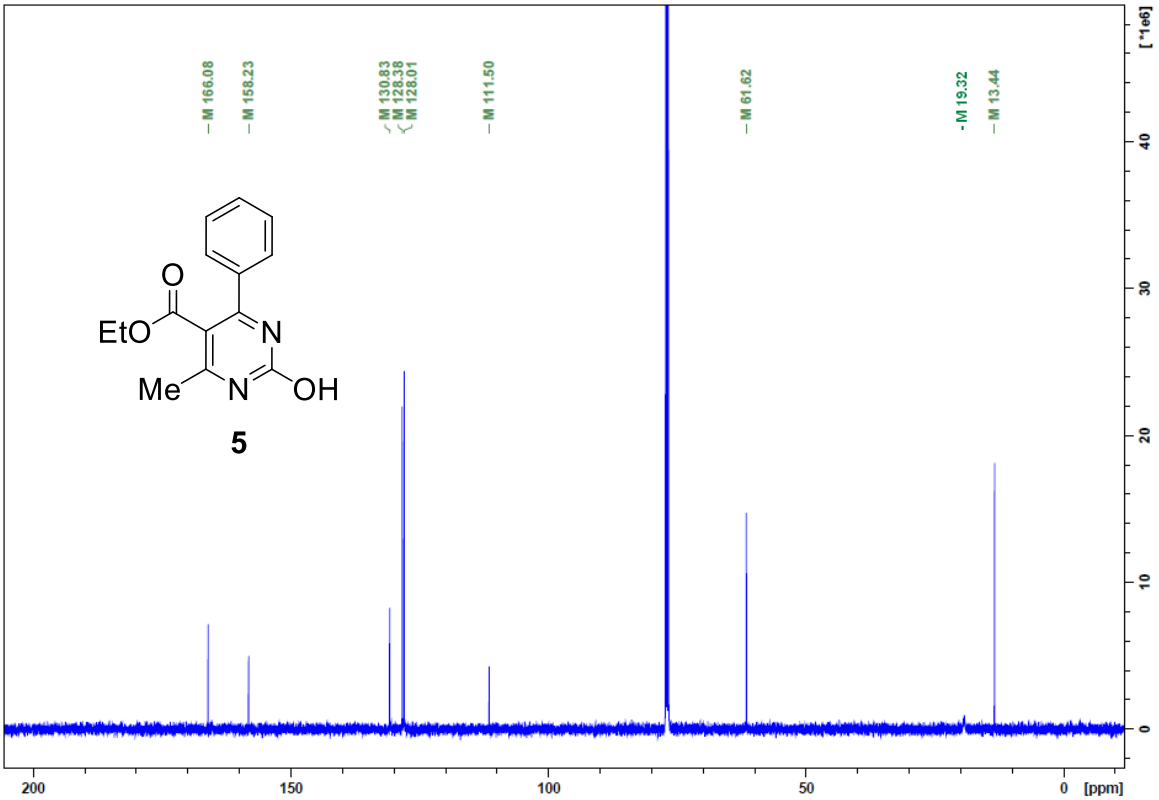
Table of Contents:

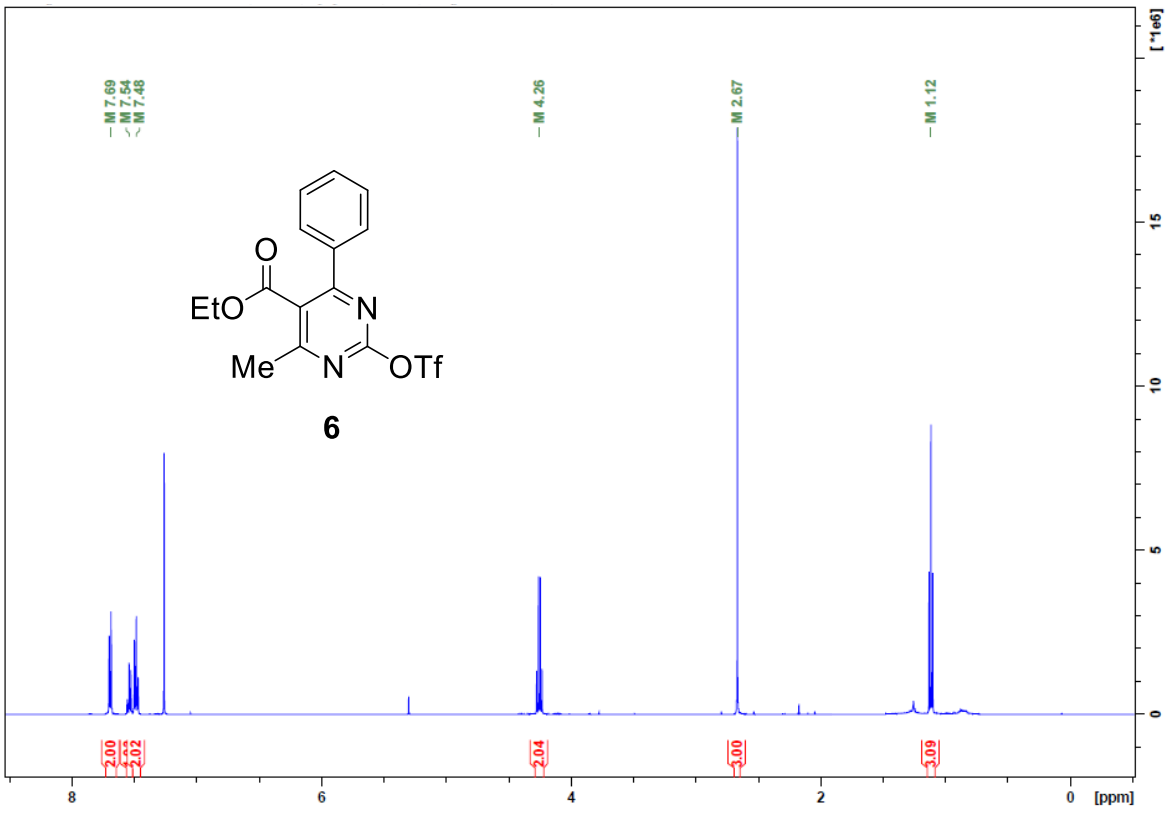
^{1}H NMR and ^{13}C NMR Spectra of Isolated Products

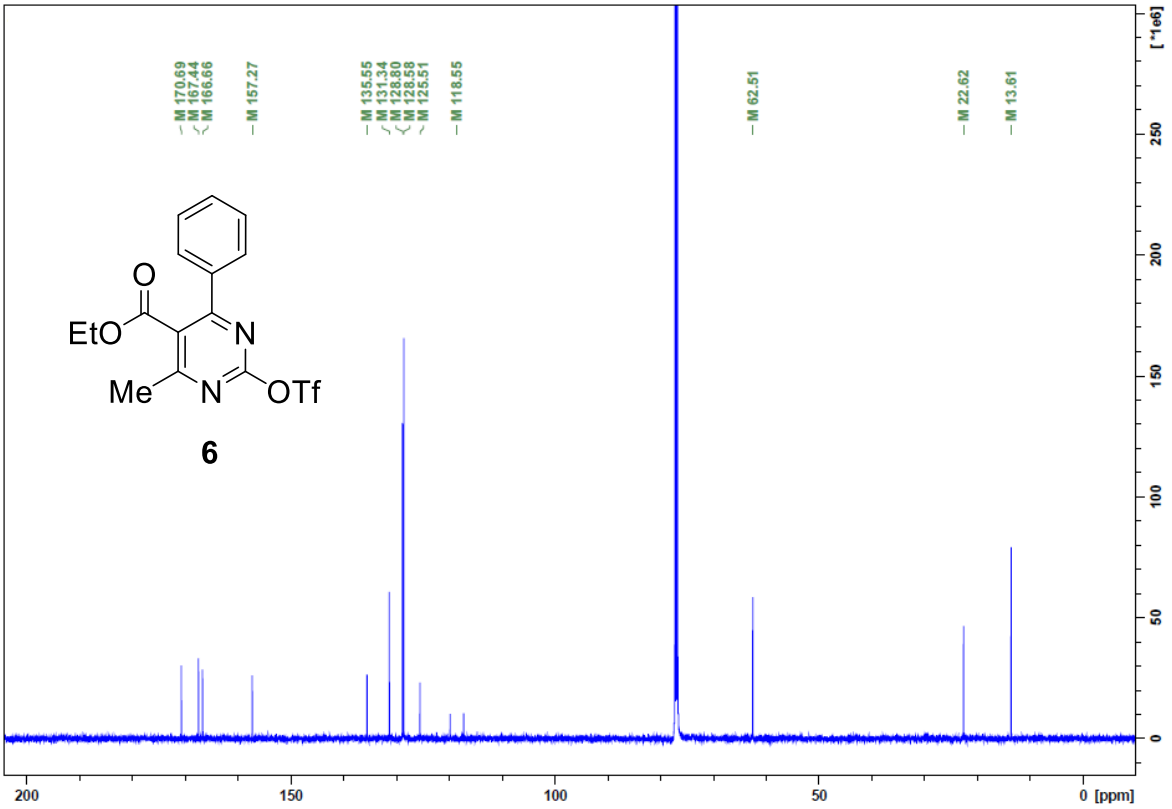


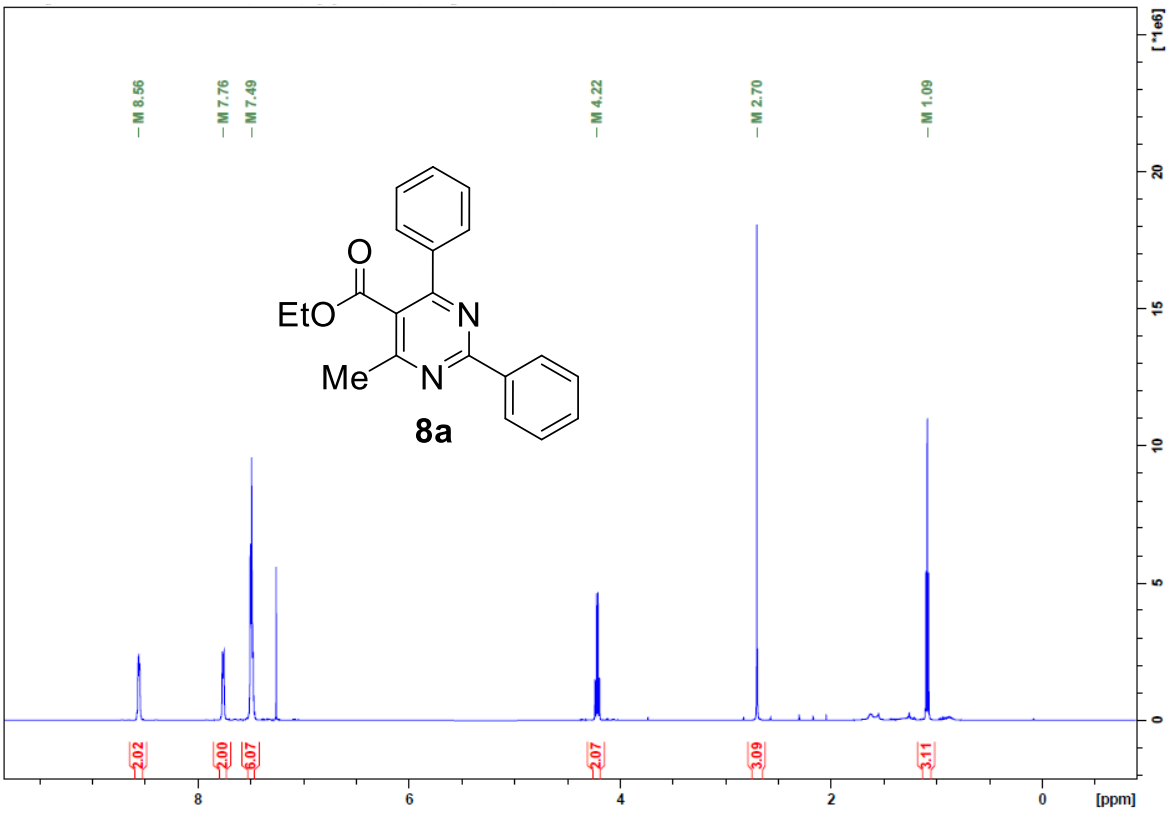


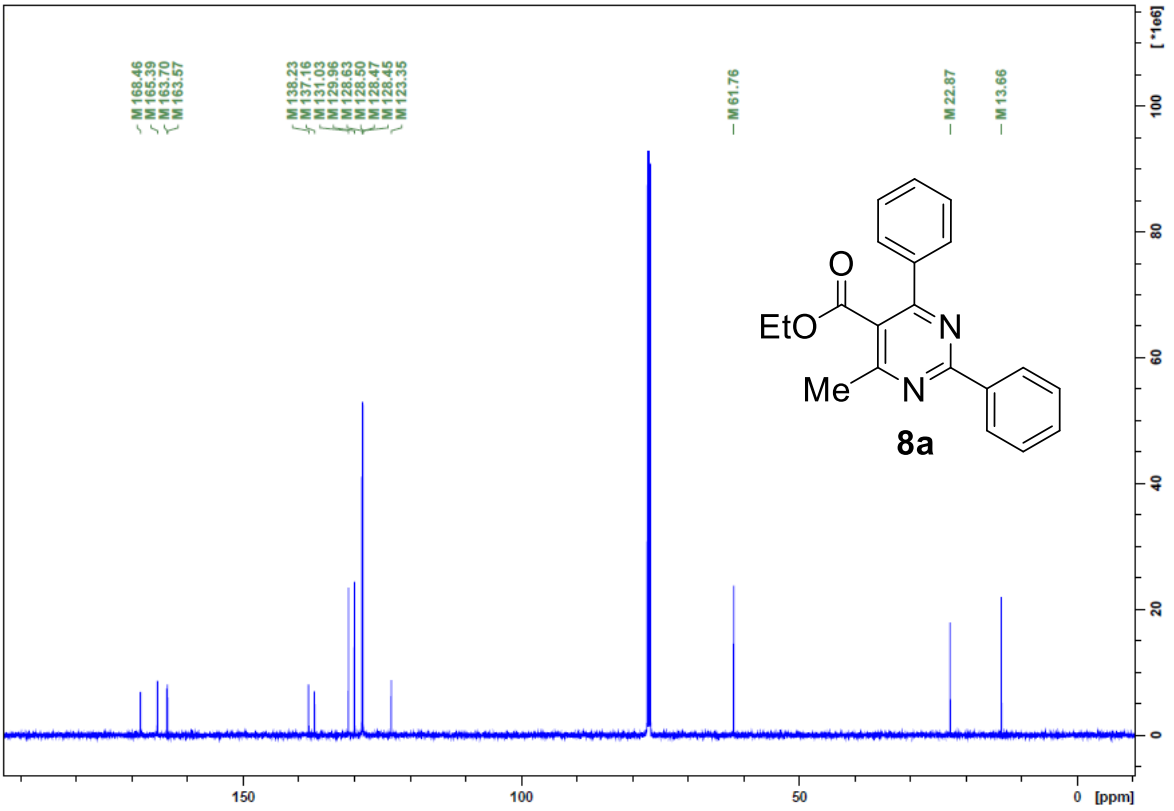

M 7.60
M 7.48
M 7.43
M 4.05
M 2.62
M 0.93
O
EtO
N
Me
N
OH
5
2.00
4.44
2.00
2.01
3.02
3.01
8
6
4
2
0 [ppm]
[*1e6]
0
10
20
30

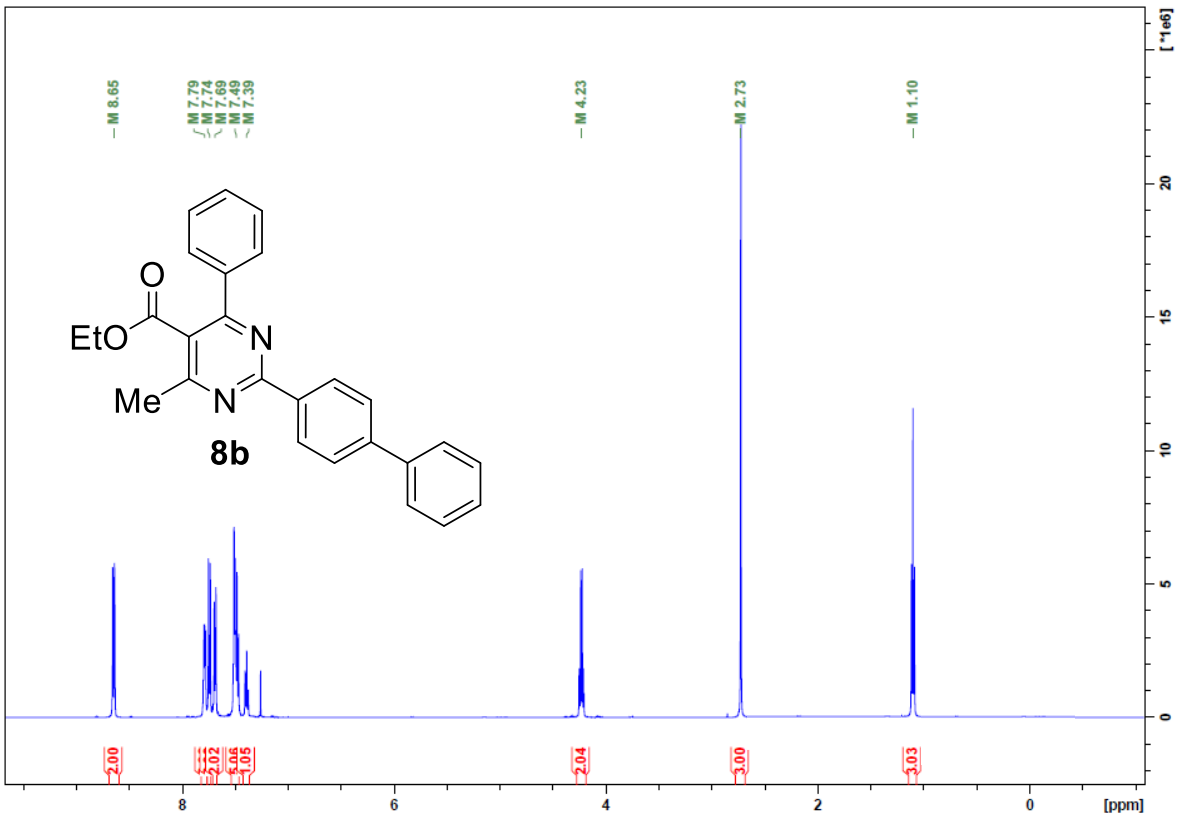

M 166.08
M 158.23
M 130.83
M 128.38
M 128.01
M 111.50
M 61.62
M 19.32
M 13.44
O
EtO
N
Me
N
OH
5
200
150
100
50
0 [ppm]
[*1e6]
0
10
20
30
40

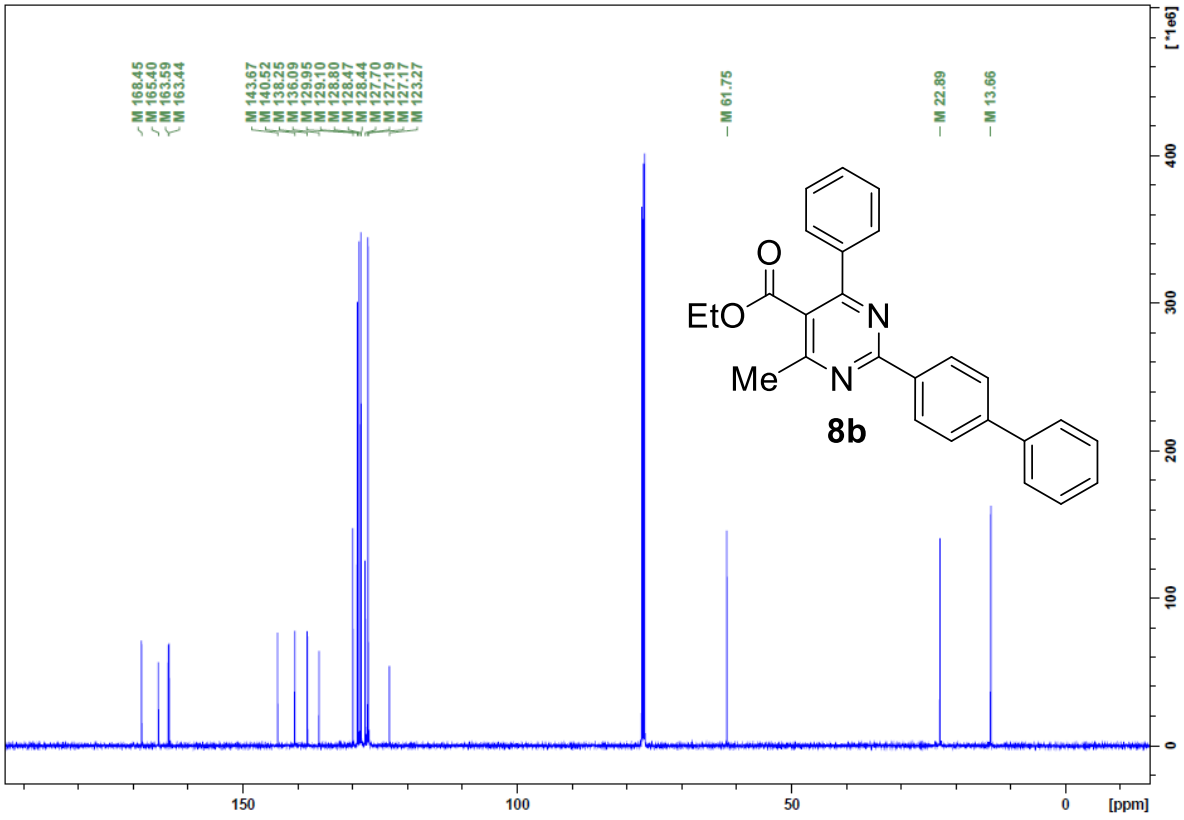

M 7.69
M 7.54
M 7.48
M 4.26
M 2.67
M 1.12
O
EtO
N
Me
N
OTf
6
2.00
2.04
5.00
3.09
8
6
4
2
0
[ppm]
[*1e6]

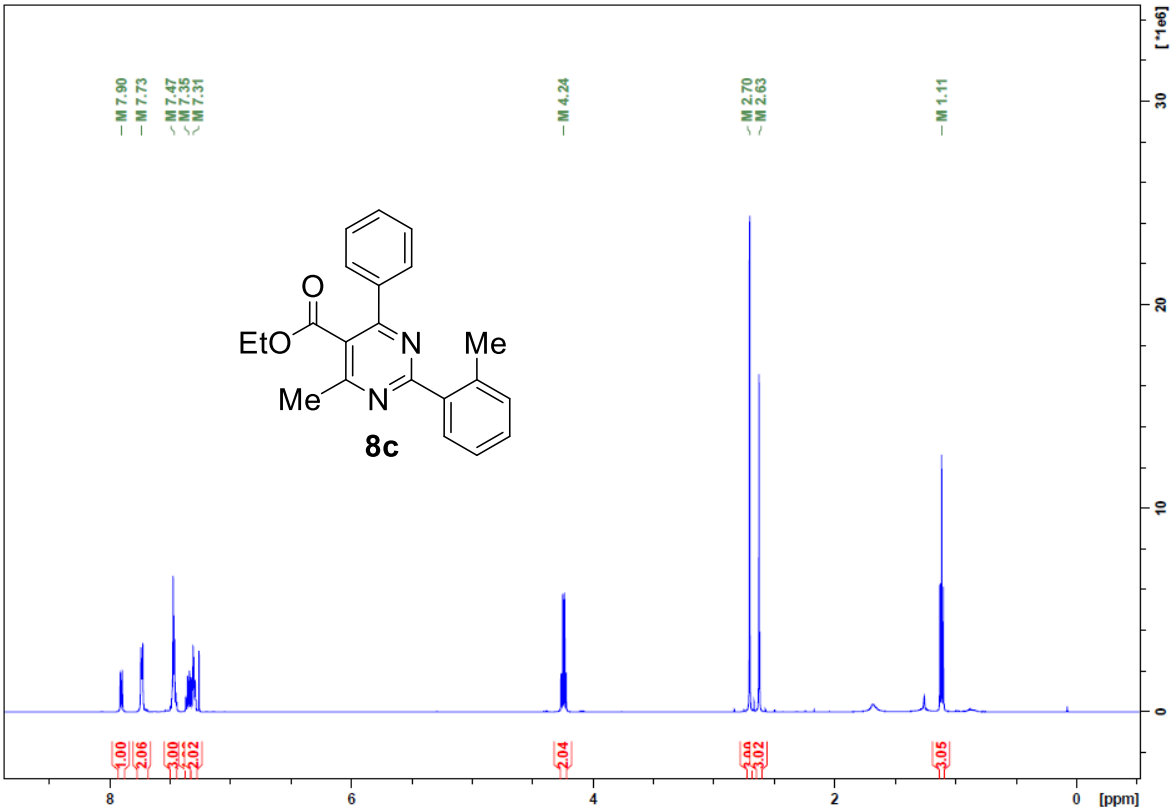

M 170.69
M 167.44
M 166.66
M 157.27
M 135.55
M 131.34
M 128.80
M 128.58
M 125.51
M 118.55
M 62.51
M 22.62
M 13.61
O
EtO
N
Me
N
OTf
6
200
150
100
50
0 [ppm]
[*1e6]

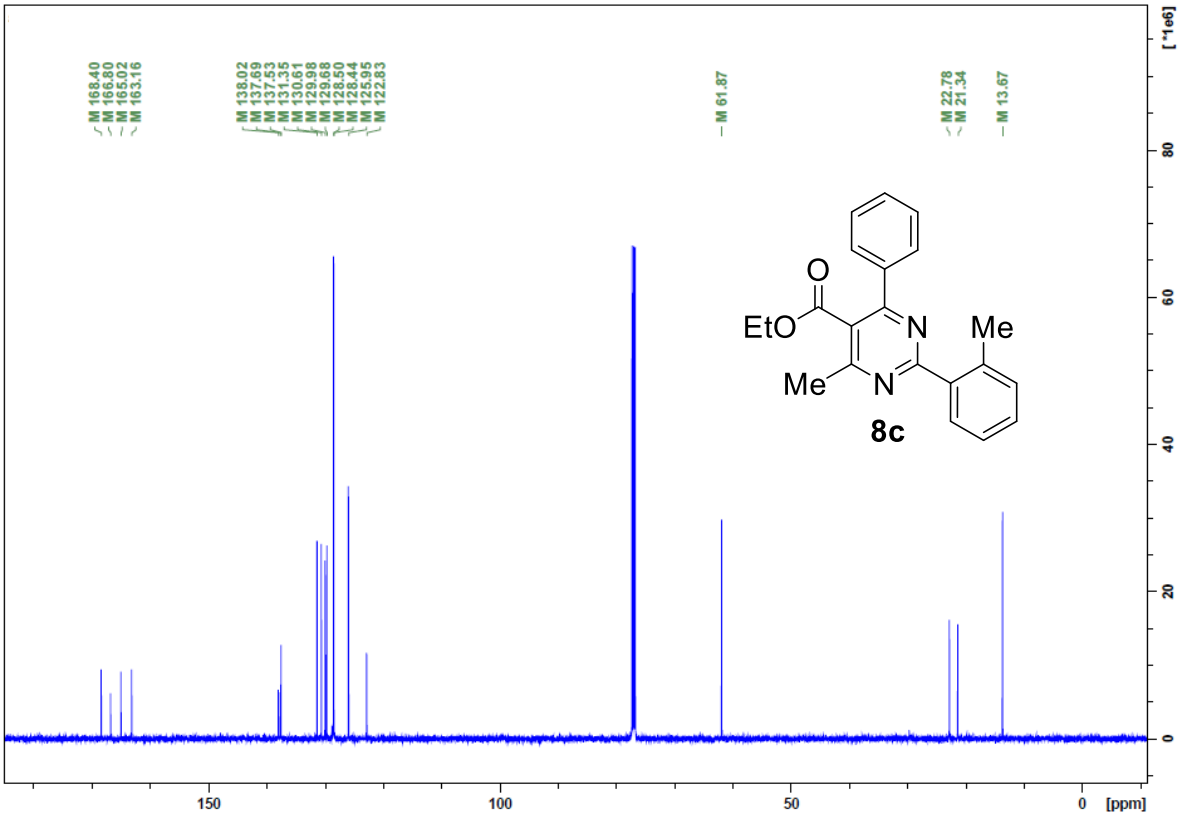

M 8.56
M 7.76
M 7.49
M 4.22
M 2.70
M 1.09
O
EtO
N
Me
N
8a
2.02
2.00
6.07
2.07
3.09
3.11
8
6
4
2
0
[ppm]
[*1e6]

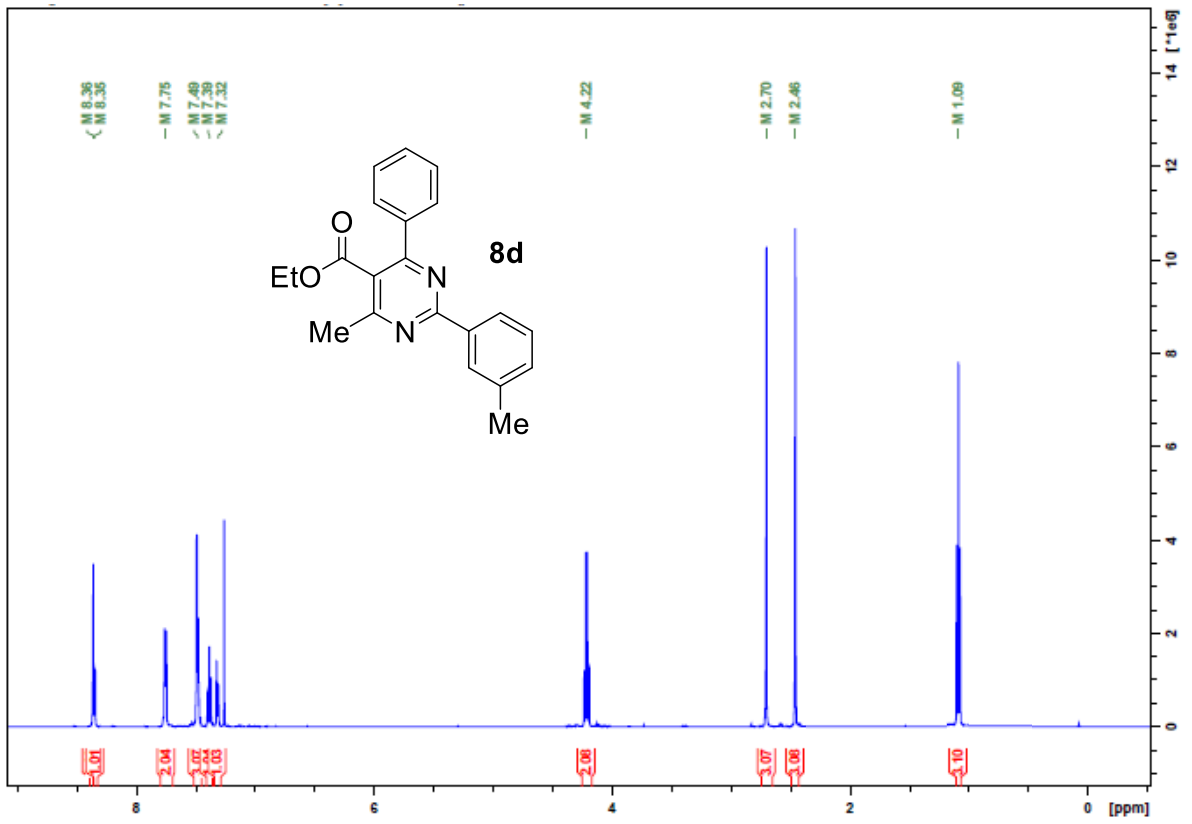

M 168.46
M 165.39
M 163.70
M 163.57
M 138.23
M 137.16
M 131.03
M 129.96
M 128.63
M 128.50
M 128.47
M 128.45
M 123.35
M 61.76
M 22.87
M 13.66
O
EtO
N
Me
N
8a
150
100
50
0
[ppm]
[*1e6]

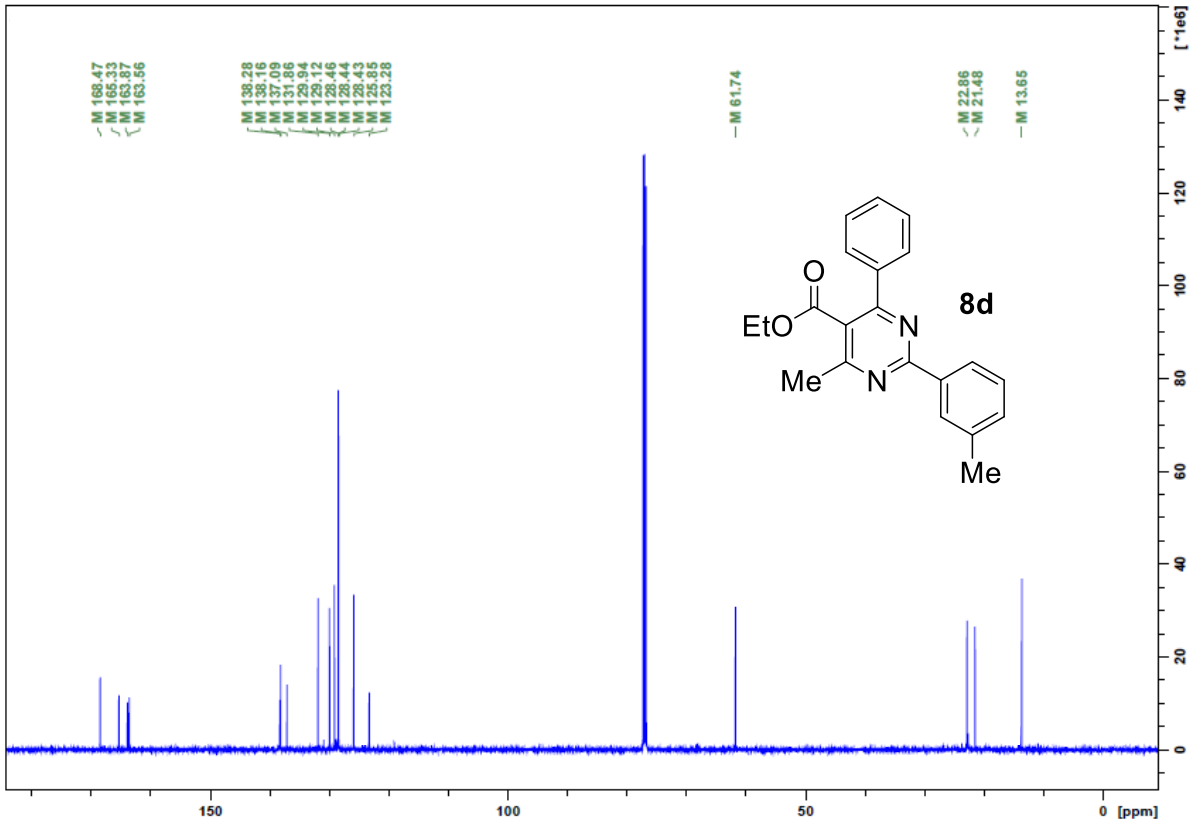

M 8.65
M 7.79
M 7.74
M 7.69
M 7.49
M 7.39
M 4.23
M 2.73
M 1.10
O
EtO
N
Me
N
8b
2.00
2.02
1.05
2.04
3.00
3.03
8
6
4
2
0
[ppm]
[*1e6]

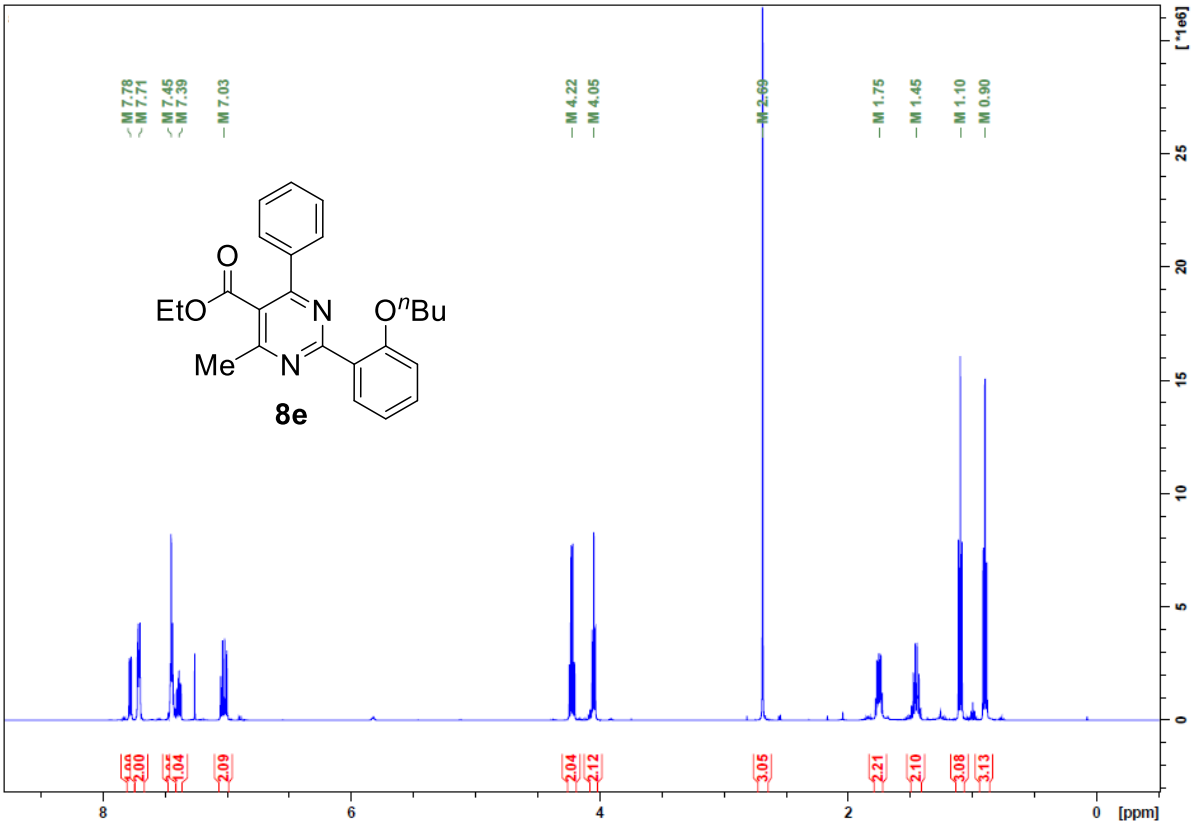

M 168.45
M 165.40
M 163.59
M 163.44
M 143.67
M 140.52
M 138.25
M 136.09
M 129.95
M 129.10
M 128.80
M 128.47
M 128.44
M 127.70
M 127.19
M 127.17
M 123.27
M 61.75
M 22.89
M 13.66
O
EtO
N
Me
N
8b
150
100
50
0
[ppm]
[*1e6]

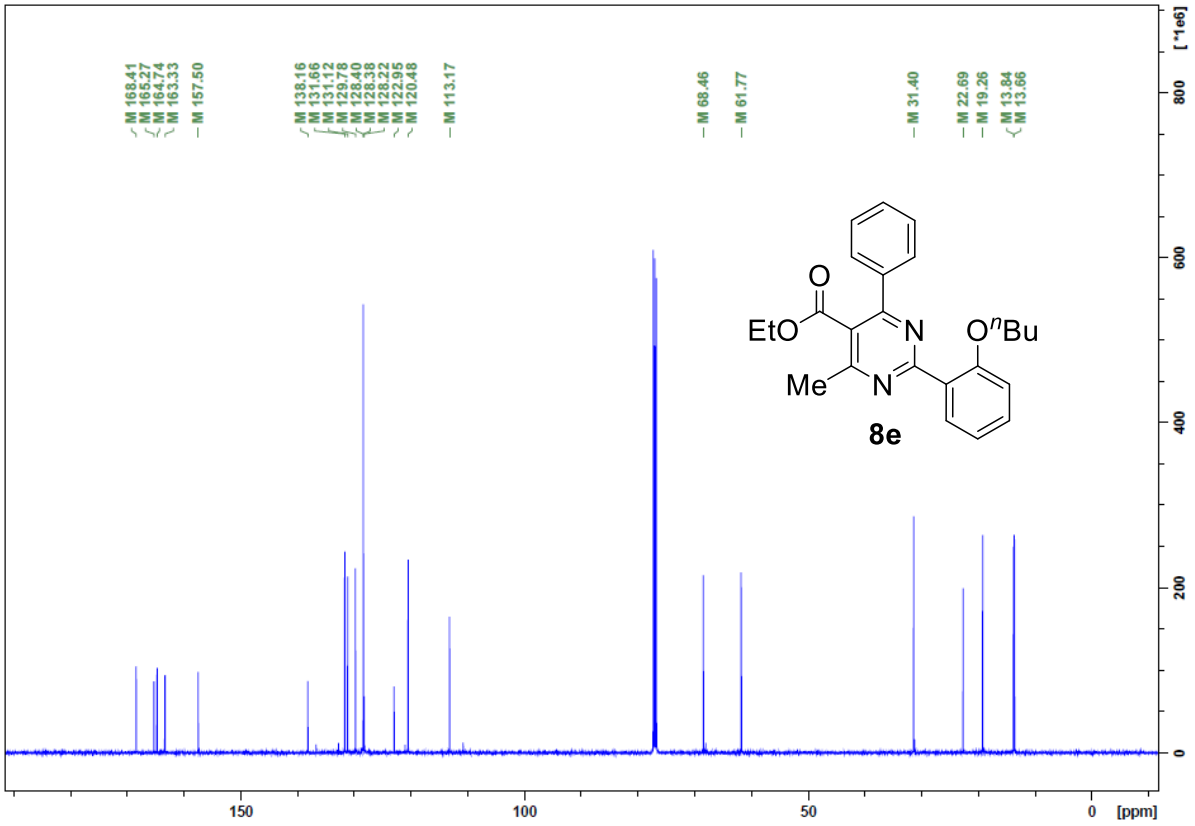

M 7.90
M 7.73
M 7.47
M 7.35
M 7.31
M 4.24
M 2.70
M 2.63
M 1.11
O
EtO
N
Me
Me
N
8c
[*1e6]
30
20
10
0
8
6
4
2
0
[ppm]

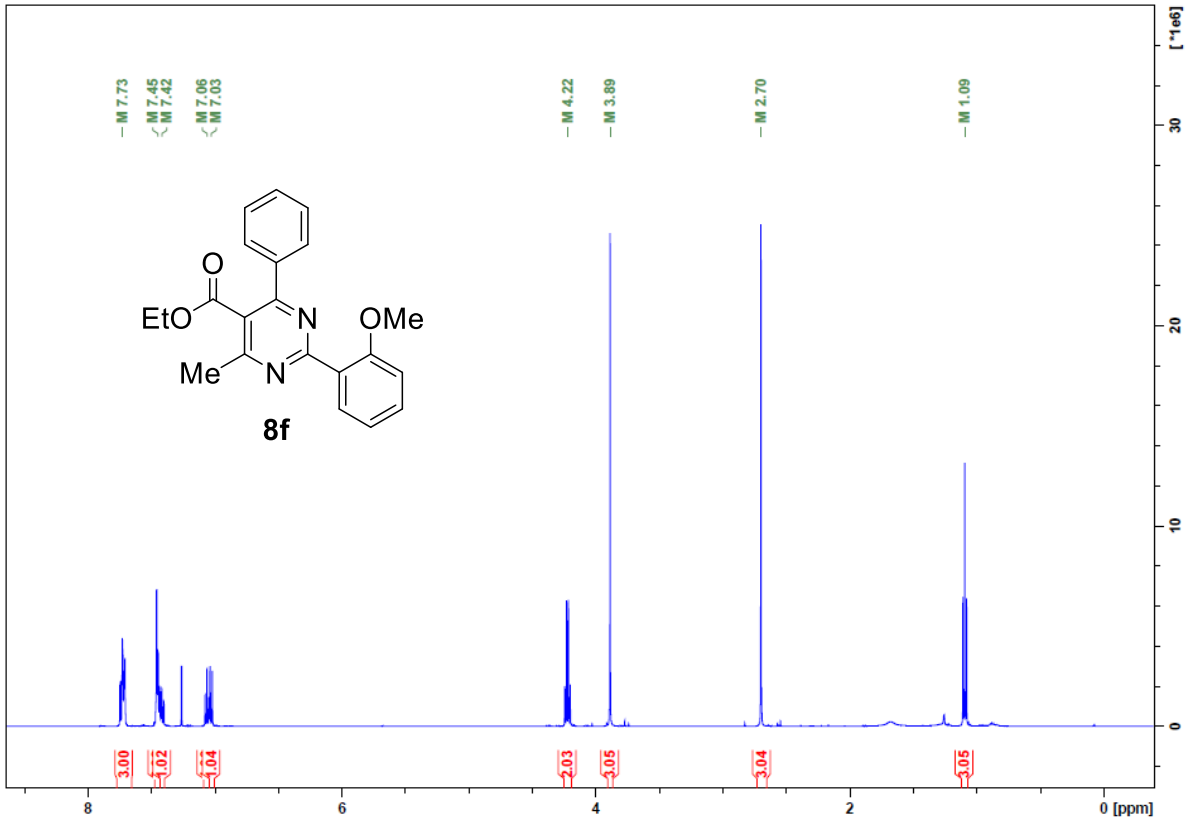

M 168.40
M 166.80
M 165.02
M 163.16
M 138.02
M 137.69
M 137.53
M 131.35
M 130.61
M 129.98
M 129.68
M 128.50
M 128.44
M 125.95
M 122.83
M 61.87
M 22.78
M 21.34
M 13.67
O
EtO
N
Me
Me
N
8c
[*1e6]
80
60
40
20
0
150
100
50
0
[ppm]

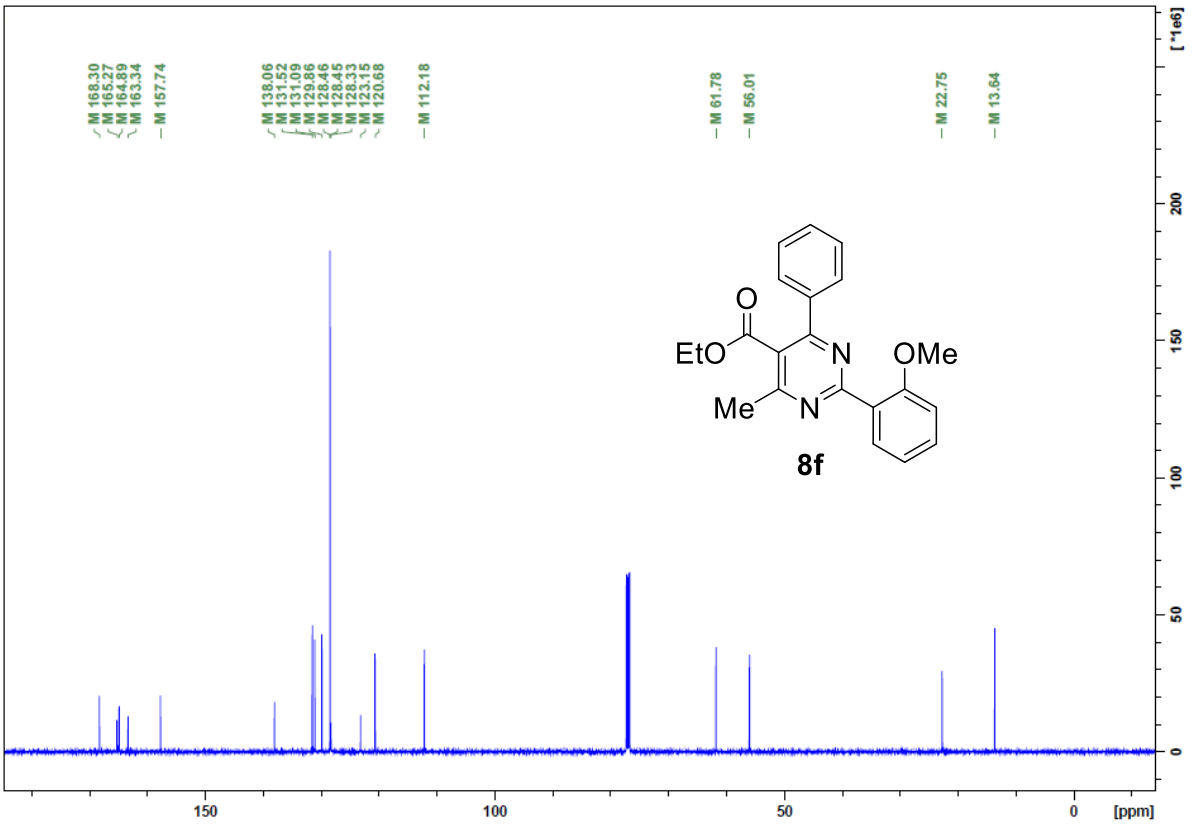

M 8.36
M 8.35
M 7.75
M 7.49
M 7.39
M 7.32
M 4.22
M 2.70
M 2.46
M 1.09
8d
O
EtO
N
Me
N
Me
2.01
2.04
1.07
2.24
1.03
2.06
3.07
3.06
3.10
8
6
4
2
0
[ppm]
[*1e6]

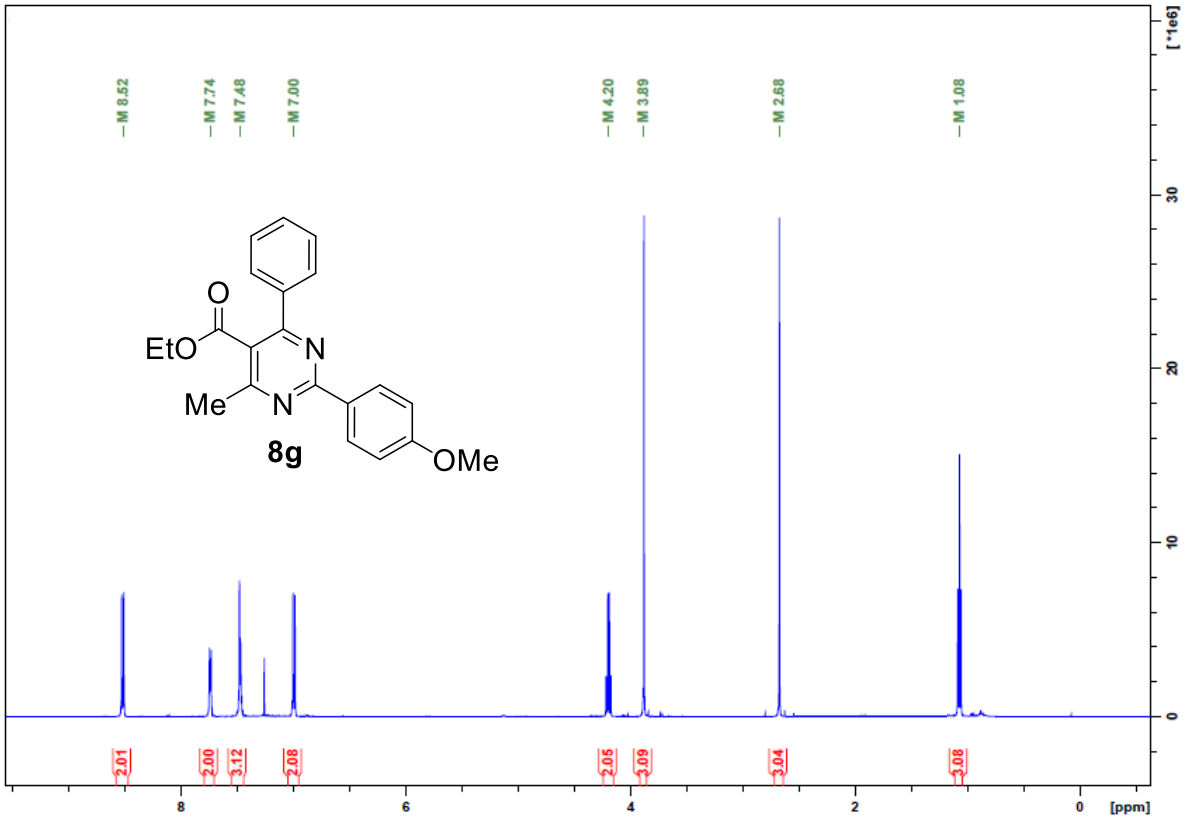

M 168.47
M 165.33
M 163.87
M 163.56
M 138.28
M 138.16
M 137.09
M 131.86
M 129.94
M 129.12
M 128.46
M 128.44
M 128.43
M 125.85
M 123.28
M 61.74
M 22.86
M 21.48
M 13.65
8d
O
EtO
N
Me
N
Me
150
100
50
0
[ppm]
[*1e6]

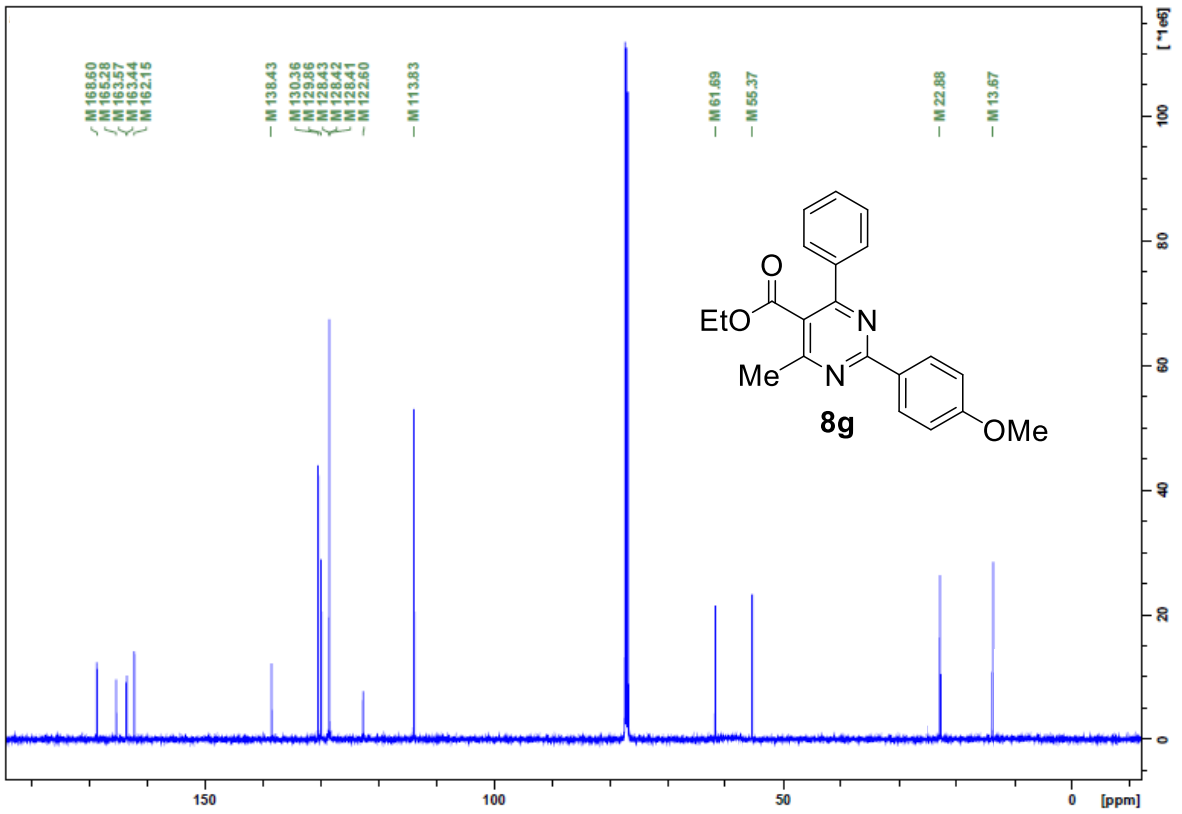

M 7.78
M 7.71
M 7.45
M 7.39
M 7.03
M 4.22
M 4.05
M 2.69
M 1.75
M 1.45
M 1.10
M 0.90
O
EtO
N
O^{n}Bu
Me
N
8e
2.00
1.04
2.09
2.04
2.12
3.05
2.21
2.10
3.08
3.13
8
6
4
2
0
[ppm]
[*1e6]

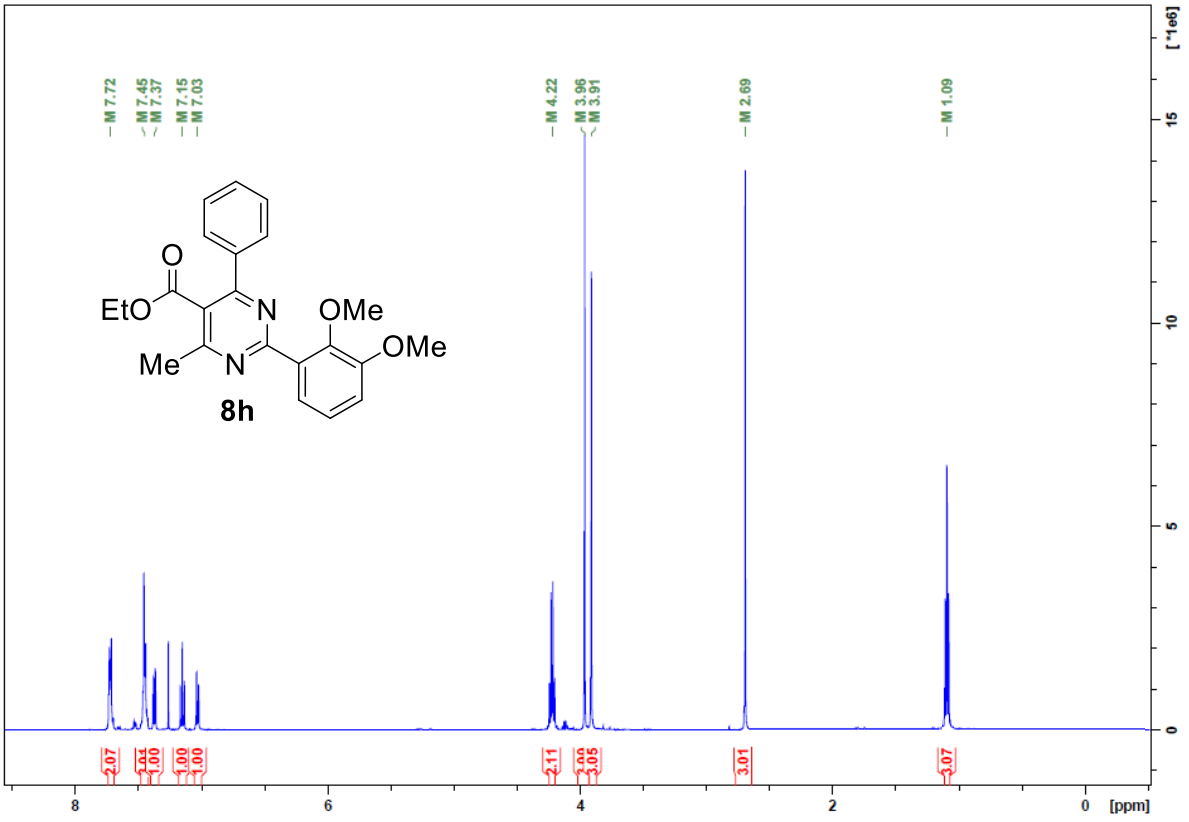

M 168.41
M 165.27
M 164.74
M 163.33
M 157.50
M 138.16
M 131.66
M 131.12
M 129.78
M 128.40
M 128.33
M 122.22
M 122.95
M 120.48
M 113.17
M 68.46
M 61.77
M 31.40
M 22.69
M 19.26
M 13.84
M 13.66
O
EtO
N
O^{n}Bu
Me
N
8e
150
100
50
0
[ppm]
[*1e6]

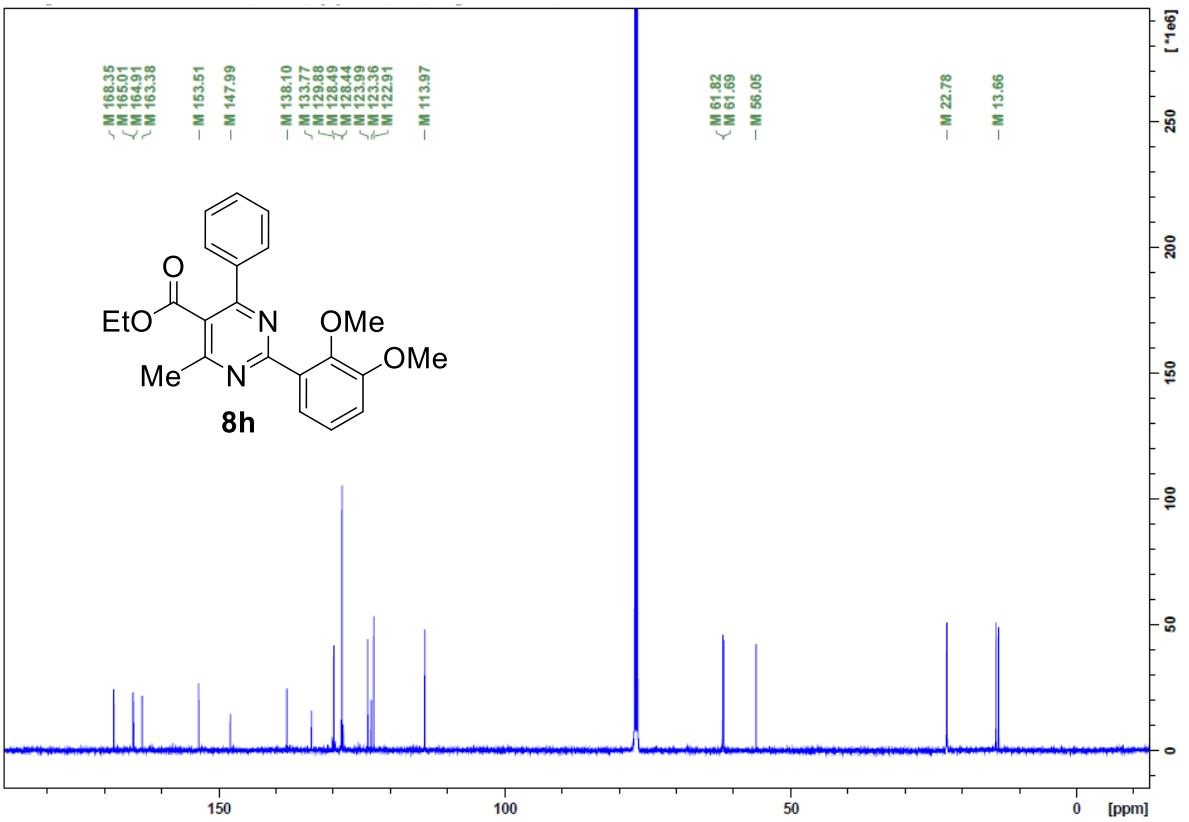

M 7.73
M 7.45
M 7.42
M 7.06
M 7.03
M 4.22
M 3.89
M 2.70
M 1.09
O
EtO
N
OMe
Me
N
8f
3.00
1.02
1.04
2.03
3.05
3.04
3.05
8
6
4
2
0 [ppm]
[*1e6]
30
20
10
0

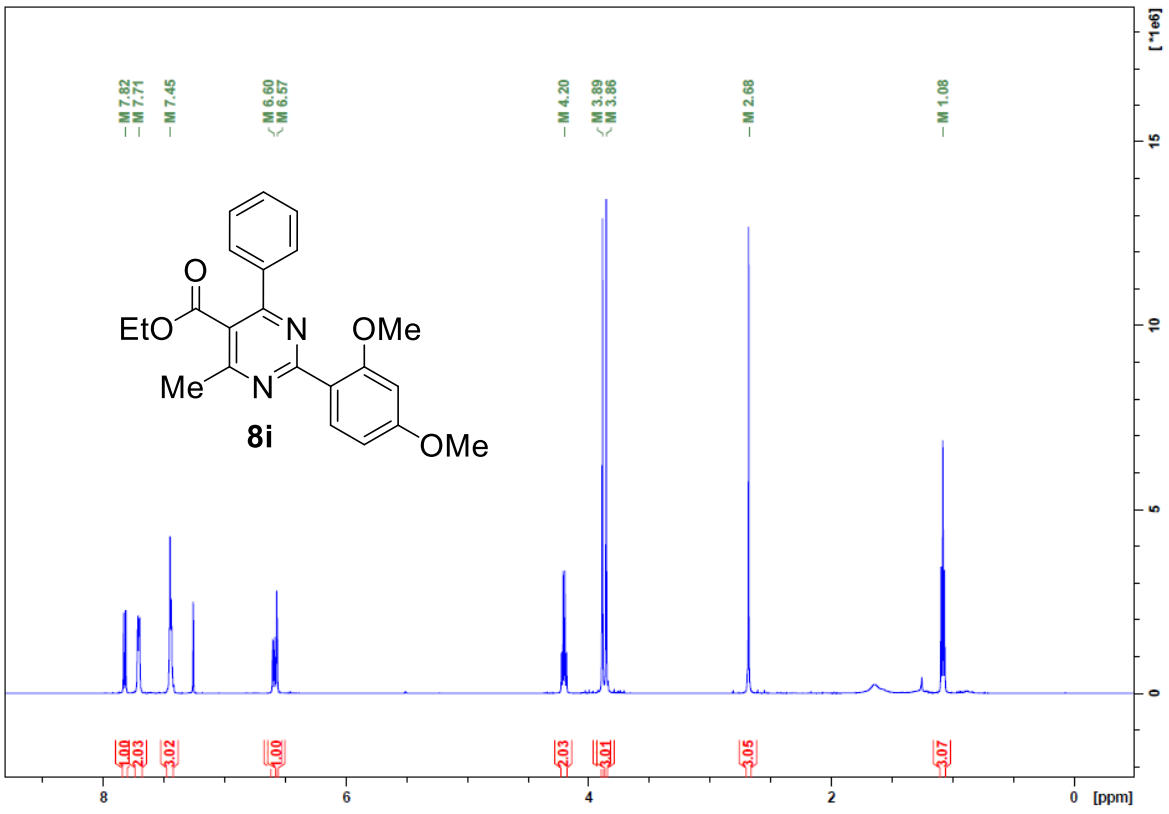

M 168.30
M 165.27
M 164.89
M 163.34
M 157.74
M 138.06
M 131.52
M 131.09
M 129.86
M 128.46
M 128.45
M 128.33
M 123.15
M 120.68
M 112.18
M 61.78
M 56.01
M 22.75
M 13.64
O
EtO
N
OMe
Me
N
8f
150
100
50
0
[ppm]
[*1e6]
200
150
100
50
0

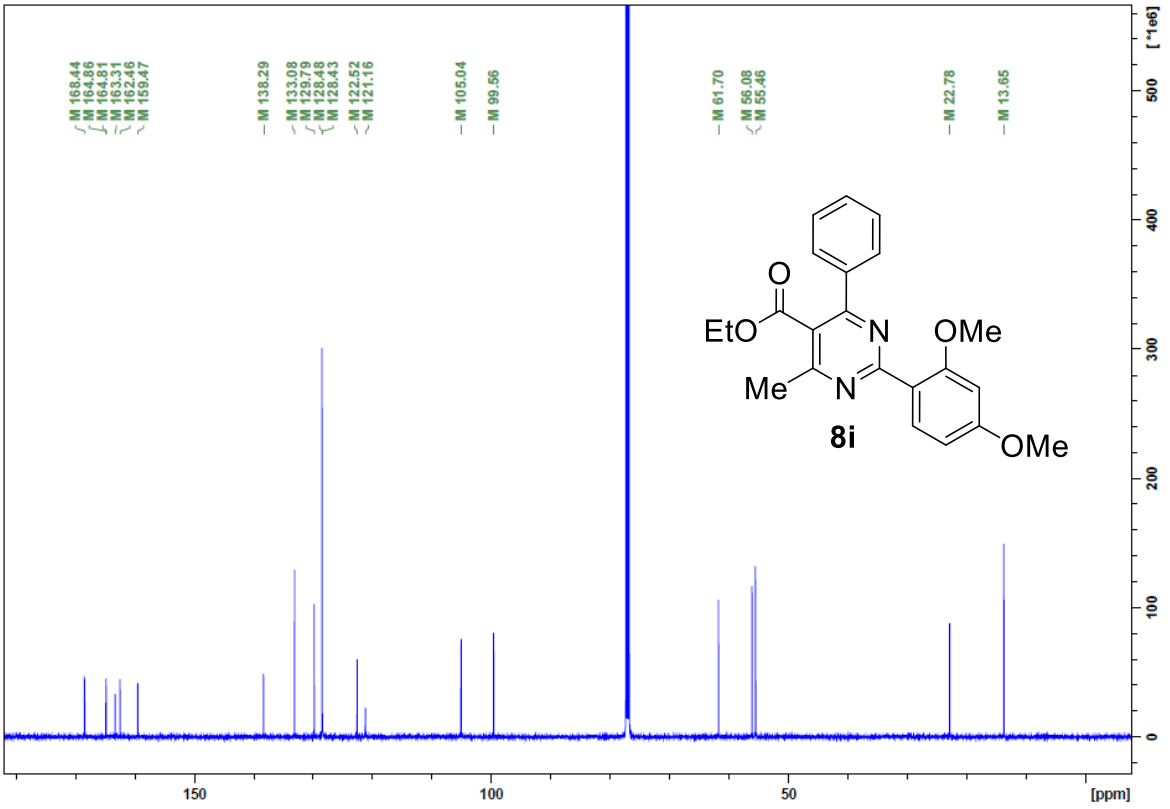

M 8.52
M 7.74
M 7.48
M 7.00
M 4.20
M 3.89
M 2.68
M 1.08
O
EtO
N
Me
N
8g
OMe
2.01
2.00
3.12
2.08
2.05
3.09
3.04
3.08
8
6
4
2
0
[ppm]
[*1e6]

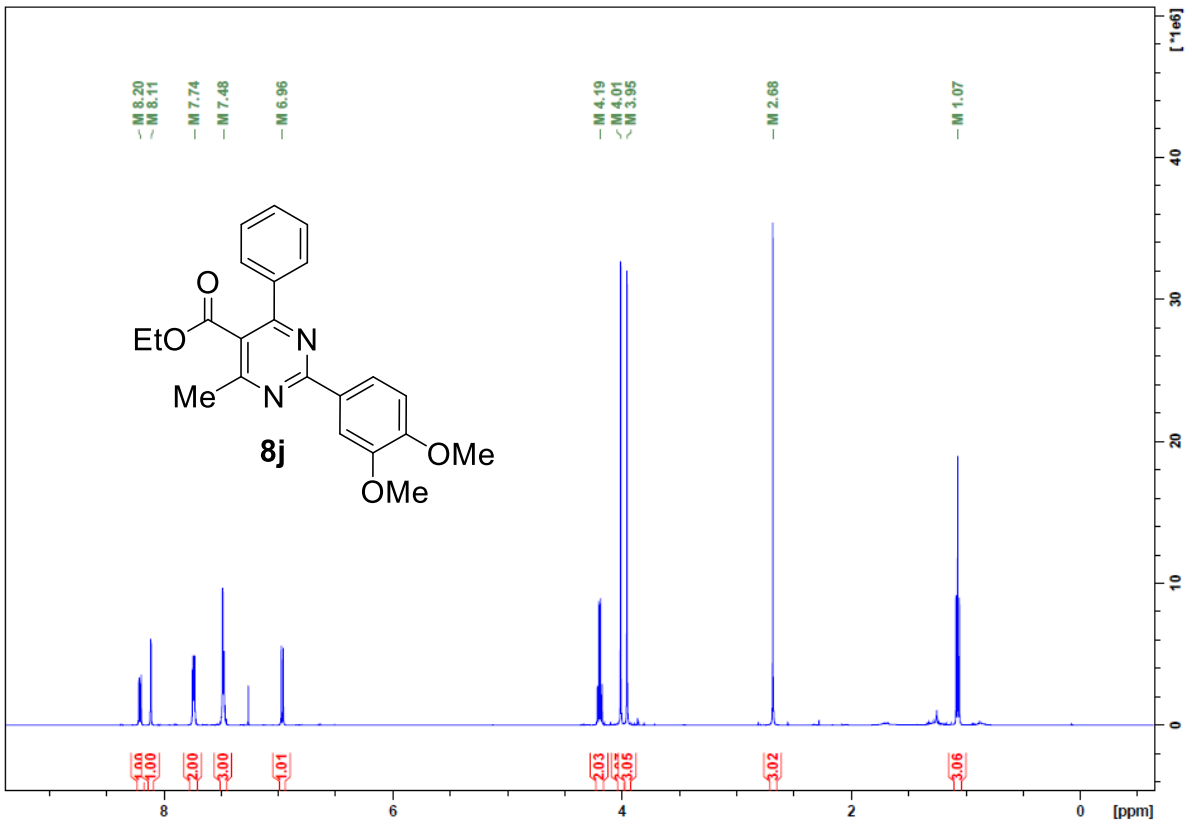

M 168.60
M 165.28
M 163.57
M 163.44
M 162.15
M 138.43
M 130.36
M 129.86
M 128.43
M 128.42
M 128.41
M 122.60
M 113.83
M 61.69
M 55.37
M 22.88
M 13.67
O
EtO
N
Me
N
8g
OMe
150
100
50
0
[ppm]
[*1e6]

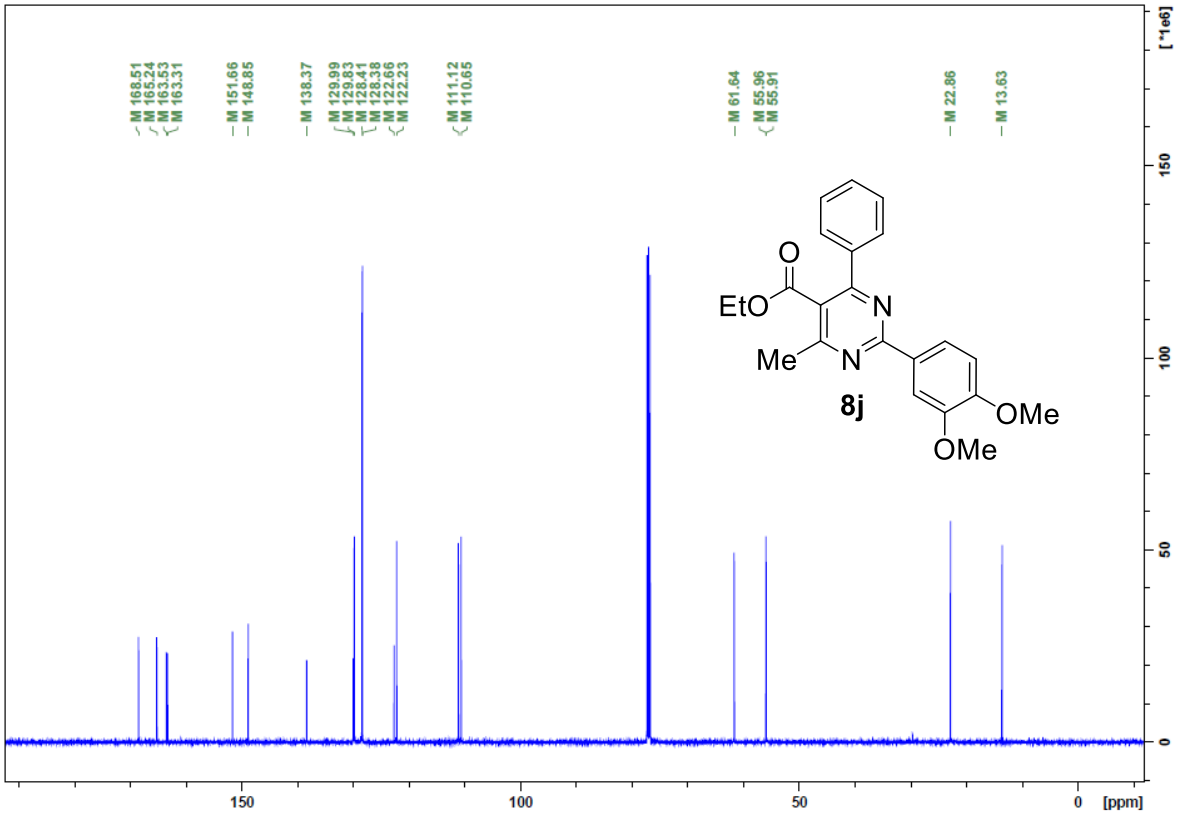

M 7.72
M 7.45
M 7.37
M 7.15
M 7.03
M 4.22
M 3.96
M 3.91
M 2.69
M 1.09
O
EtO
N
OMe
OMe
Me
N
8h
2.07
2.11
3.01
3.07
8
6
4
2
0
[ppm]
[*1e6]

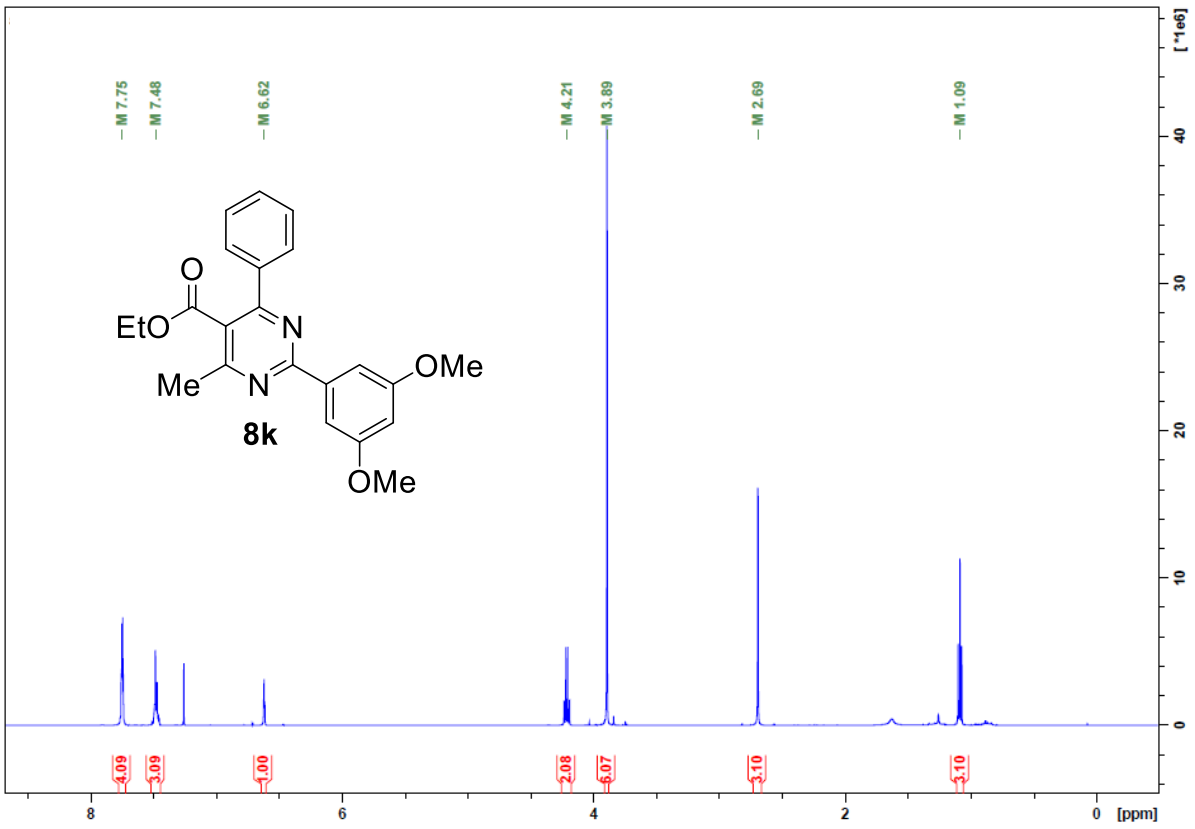

M 168.35
M 165.01
M 164.91
M 163.38
M 153.51
M 147.99
M 138.10
M 133.77
M 129.88
M 128.49
M 128.44
M 123.99
M 123.36
M 122.91
M 113.97
M 61.82
M 61.69
M 56.05
M 22.78
M 13.66
O
EtO
N
OMe
OMe
Me
N
8h
150
100
50
0
[ppm]
[*1e6]

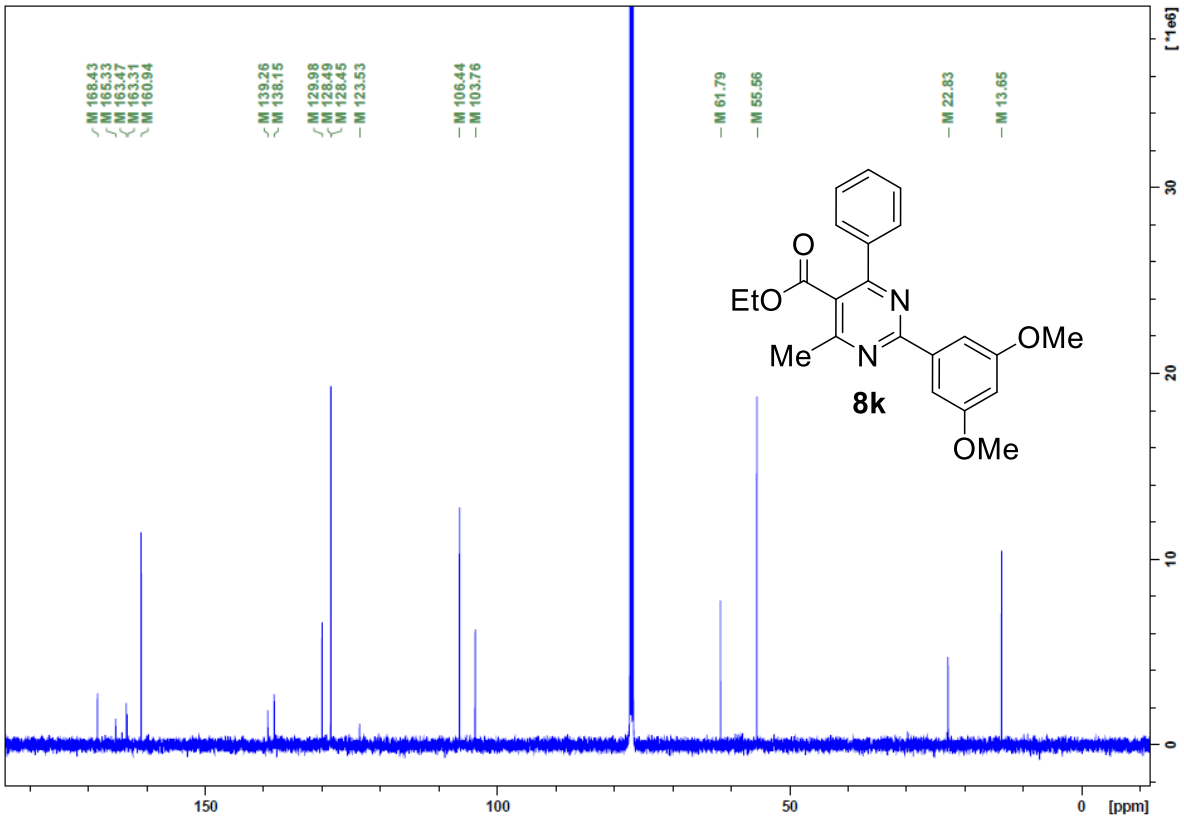

M 7.82
M 7.71
M 7.45
M 6.60
M 6.57
M 4.20
M 3.89
M 3.86
M 2.68
M 1.08
O
EtO
N
OMe
Me
N
OMe
8i
1.00
2.03
3.02
1.00
2.03
5.01
3.05
3.07
8
6
4
2
0
[ppm]
[*1e6]

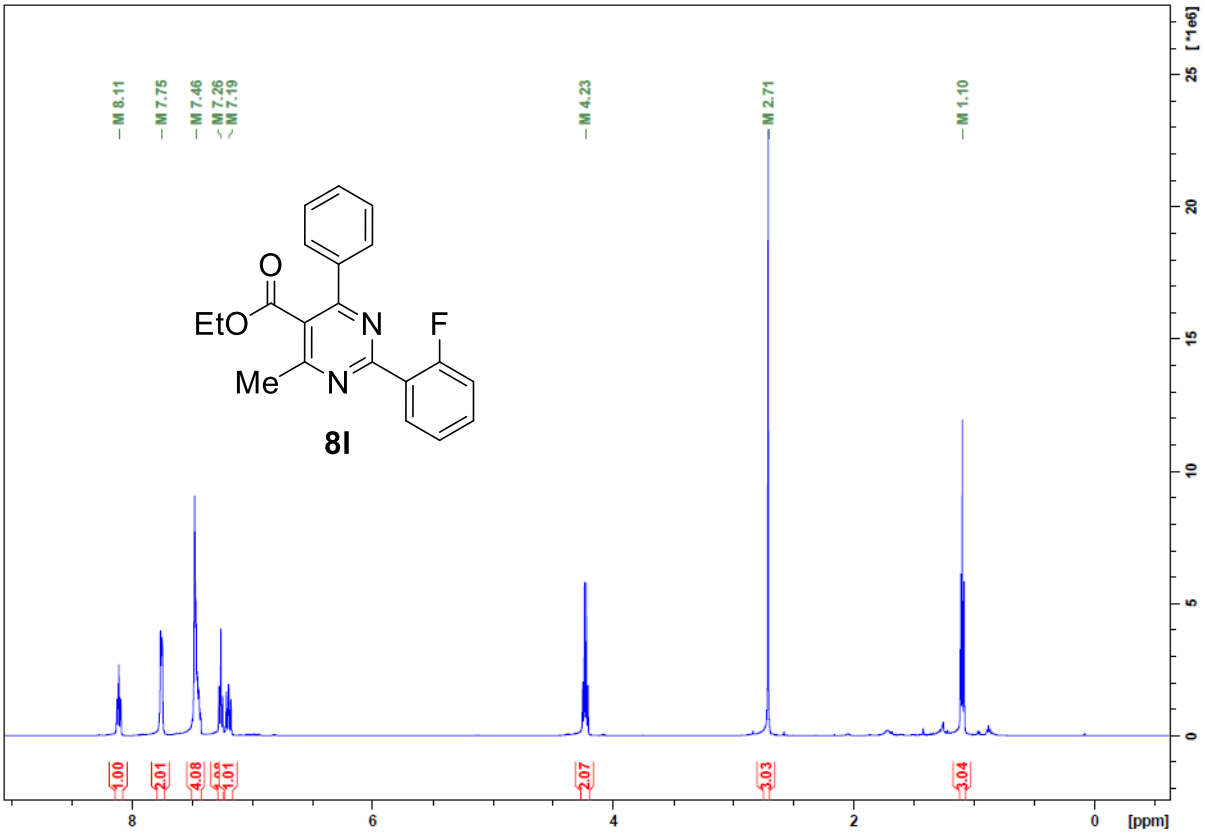

M 168.44
M 164.86
M 164.81
M 163.31
M 162.46
M 159.47
M 138.29
M 133.08
M 129.79
M 128.48
M 128.43
M 122.52
M 121.16
M 105.04
M 99.56
M 61.70
M 56.08
M 55.46
M 22.78
M 13.65
O
EtO
N
OMe
Me
N
8i
OMe
150
100
50
[ppm]
[*1e6]

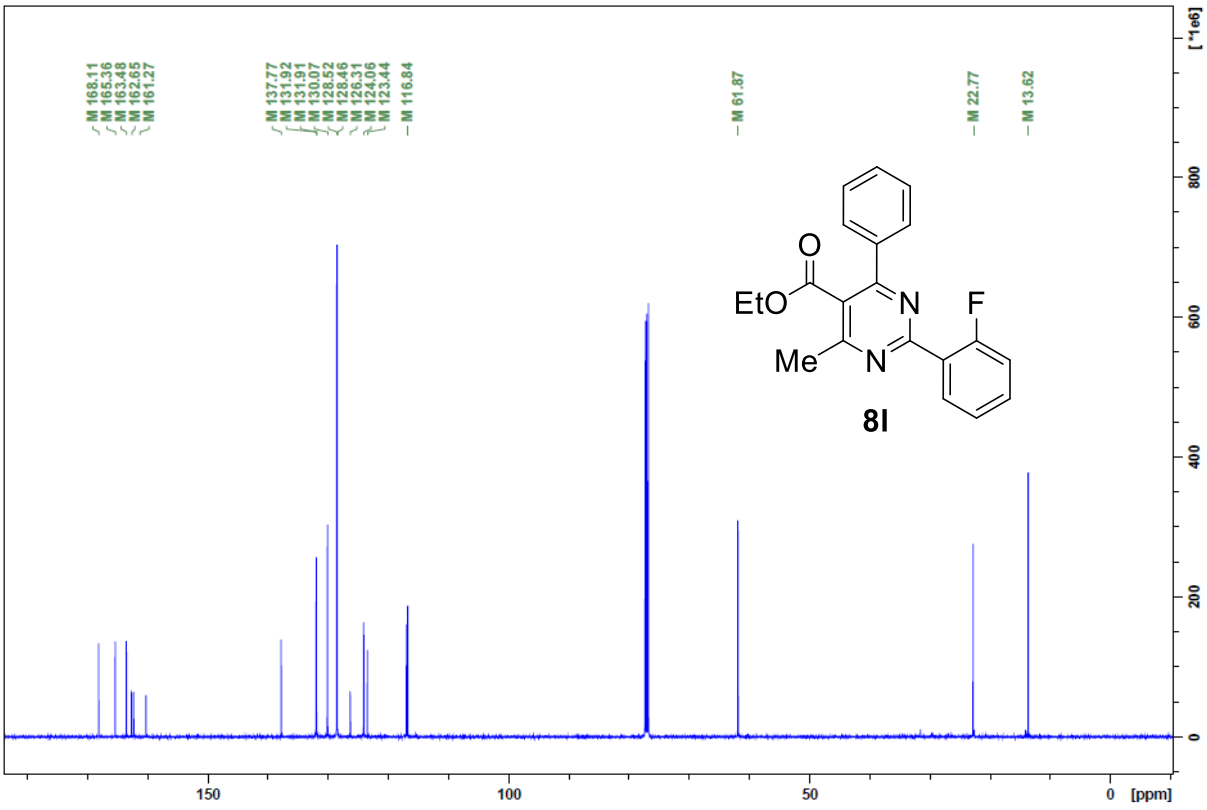

M 8.20
M 8.11
M 7.74
M 7.48
M 6.96
M 4.19
M 4.01
M 3.95
M 2.68
M 1.07
EtO
Me
8j
OMe
OMe
[ppm]

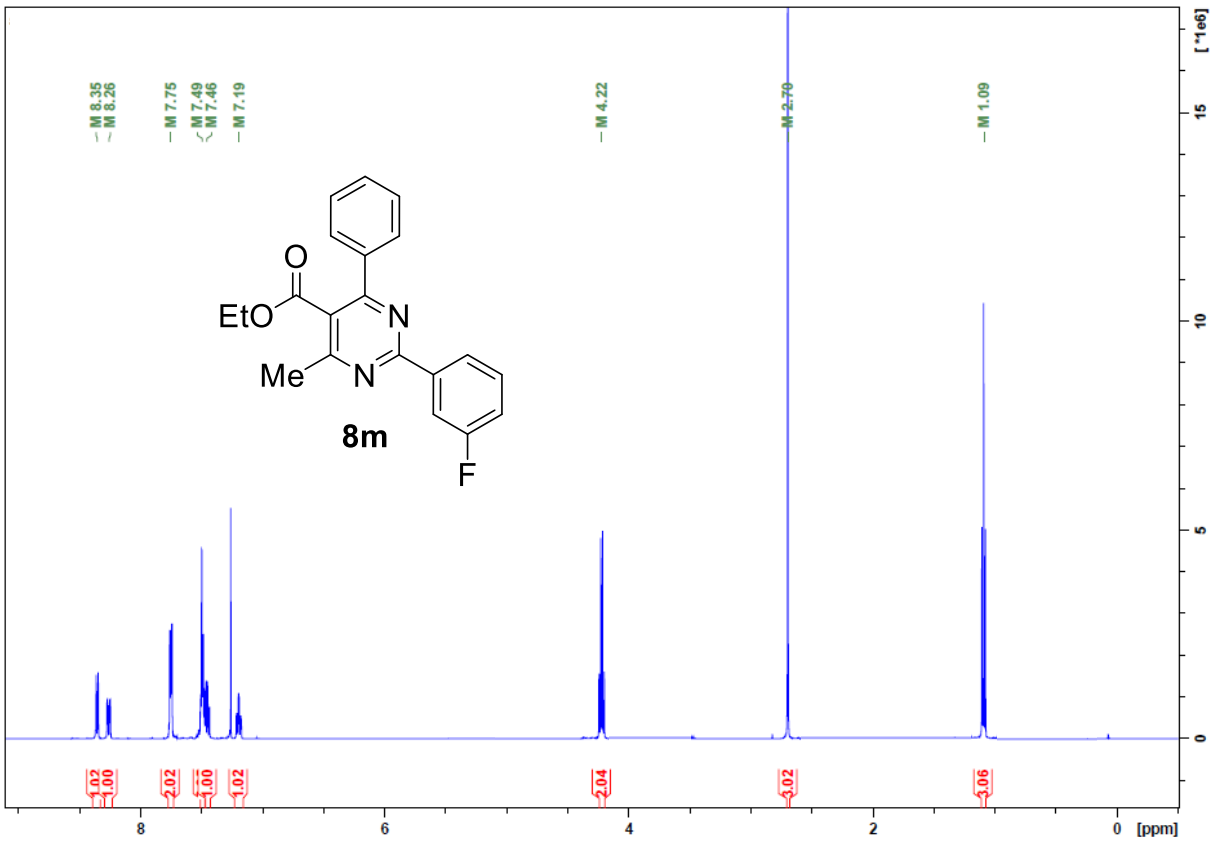

M 168.51
M 165.24
M 163.53
M 163.31
M 151.66
M 148.85
M 138.37
M 129.99
M 129.83
M 128.41
M 128.38
M 122.66
M 122.23
M 111.12
M 110.65
M 61.64
M 55.96
M 55.91
M 22.86
M 13.63
EtO
Me
8j
OMe
OMe
[ppm]

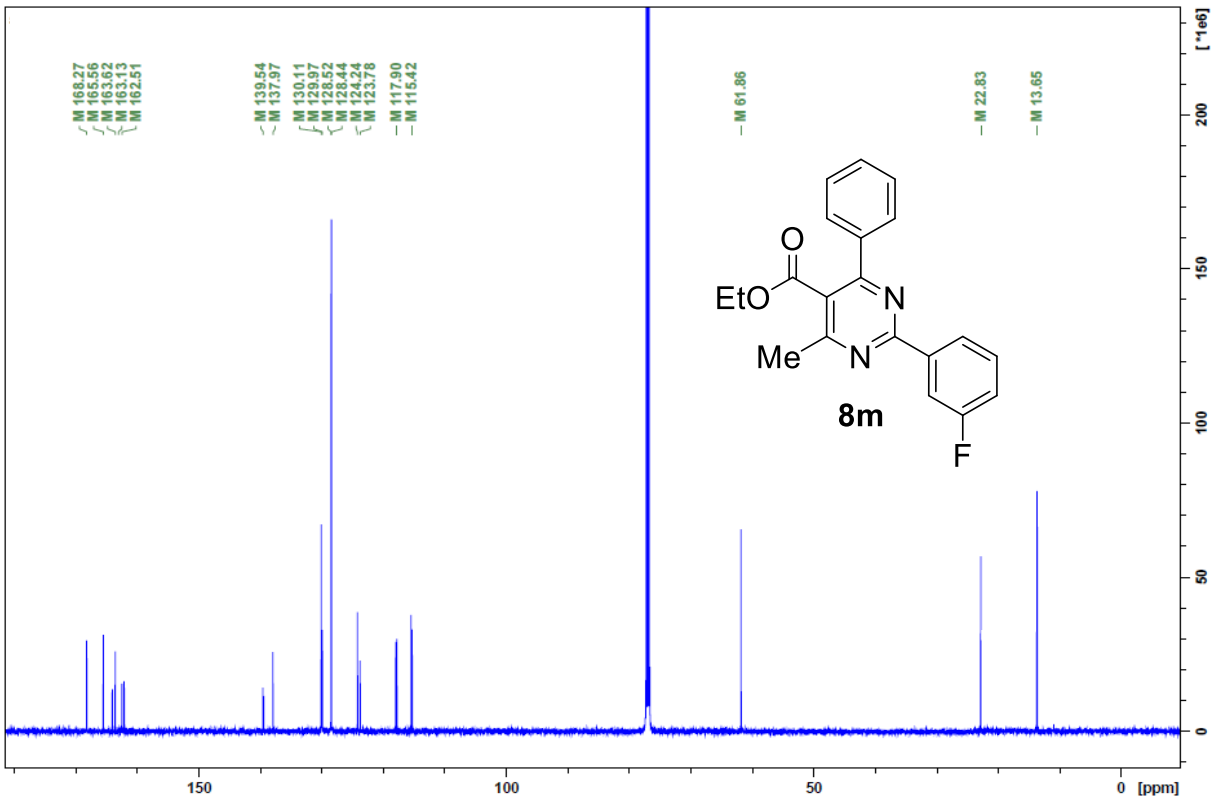

M 7.75
M 7.48
M 6.62
M 4.21
M 3.89
M 2.69
M 1.09
O
EtO
N
Me
N
OMe
OMe
8k
4.09
3.09
1.00
2.08
6.07
3.10
5.10
8
6
4
2
0
[ppm]
[*1e6]

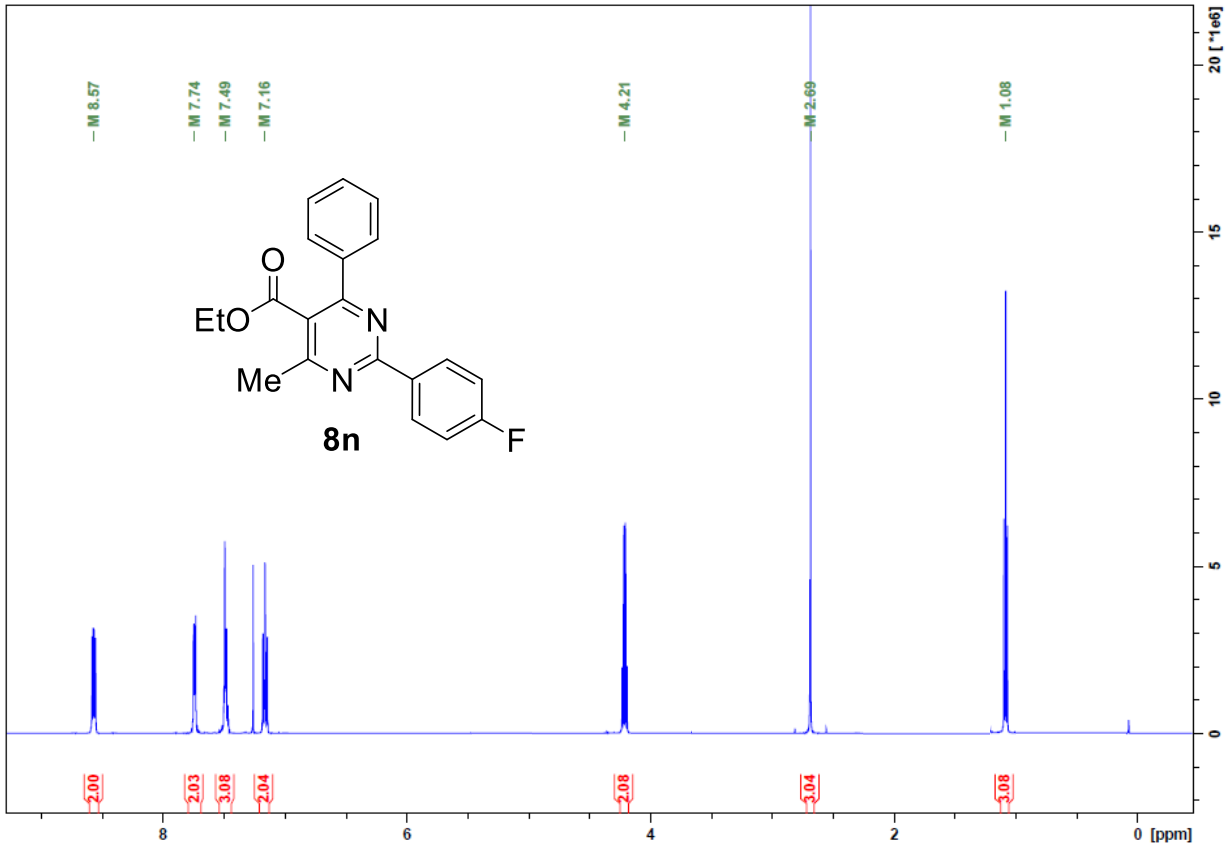

M 168.43
M 165.33
M 163.47
M 163.31
M 160.94
M 139.26
M 138.15
M 129.98
M 128.49
M 128.45
M 123.53
M 106.44
M 103.76
M 61.79
M 55.56
M 22.83
M 13.65
O
EtO
N
Me
N
OMe
OMe
8k
150
100
50
0
[ppm]
[*1e6]

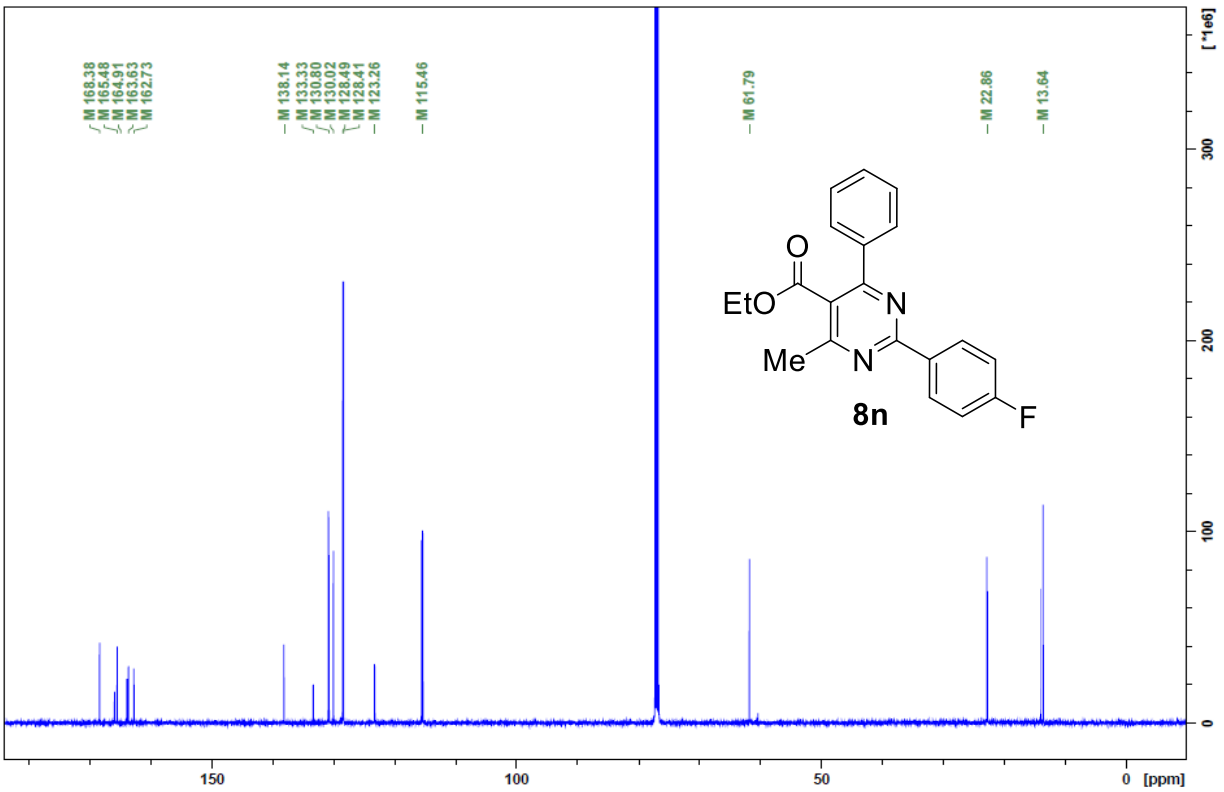

M 8.11
M 7.75
M 7.46
M 7.26
M 7.19
M 4.23
M 2.71
M 1.10
O
EtO
N
F
Me
N
8I
1.00
2.01
4.08
1.01
2.07
3.03
3.04
8
6
4
2
0
[ppm]
[*1e6]

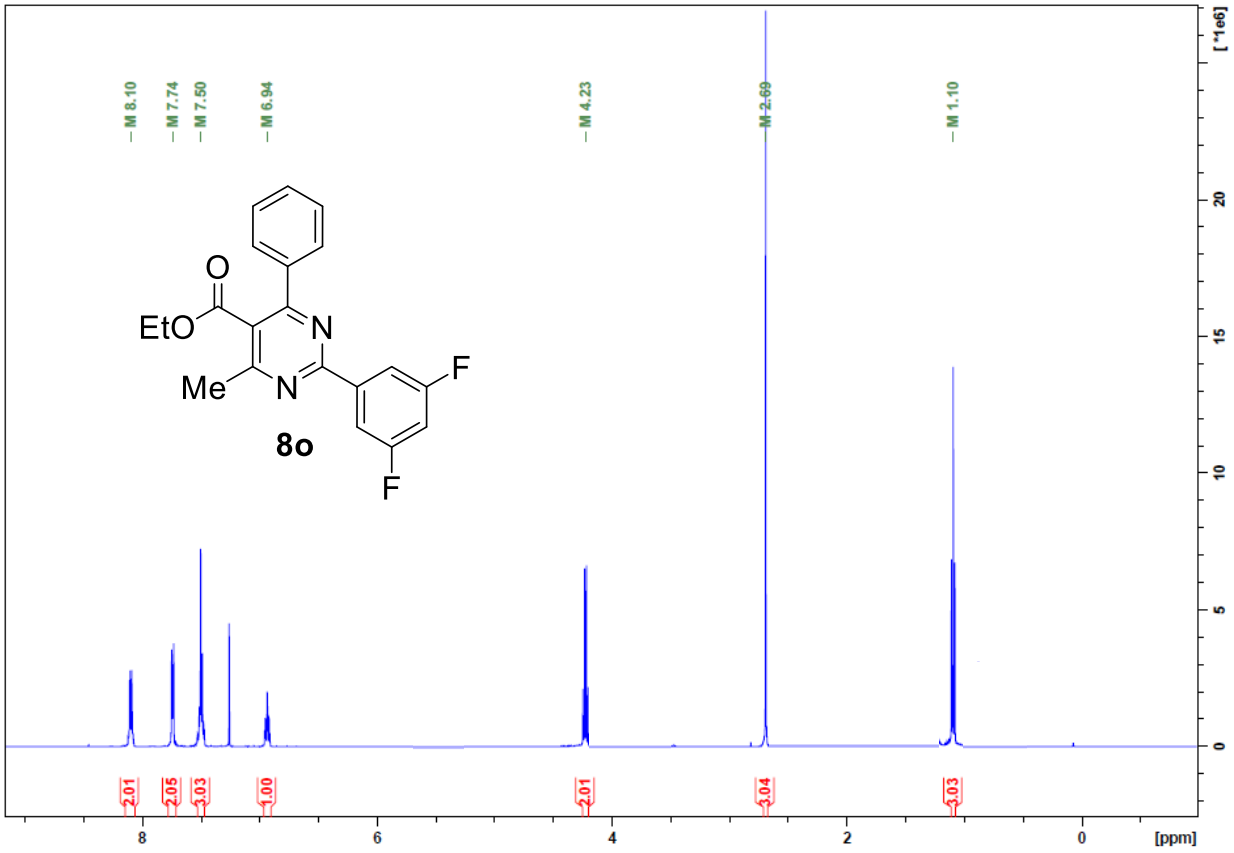

M 168.11
M 165.36
M 163.48
M 162.65
M 161.27
M 137.77
M 131.92
M 131.91
M 130.07
M 128.52
M 128.46
M 126.31
M 124.06
M 123.44
M 116.84
M 61.87
M 22.77
M 13.62
O
EtO
N
F
Me
N
8I
150
100
50
0
[ppm]
[*1e6]

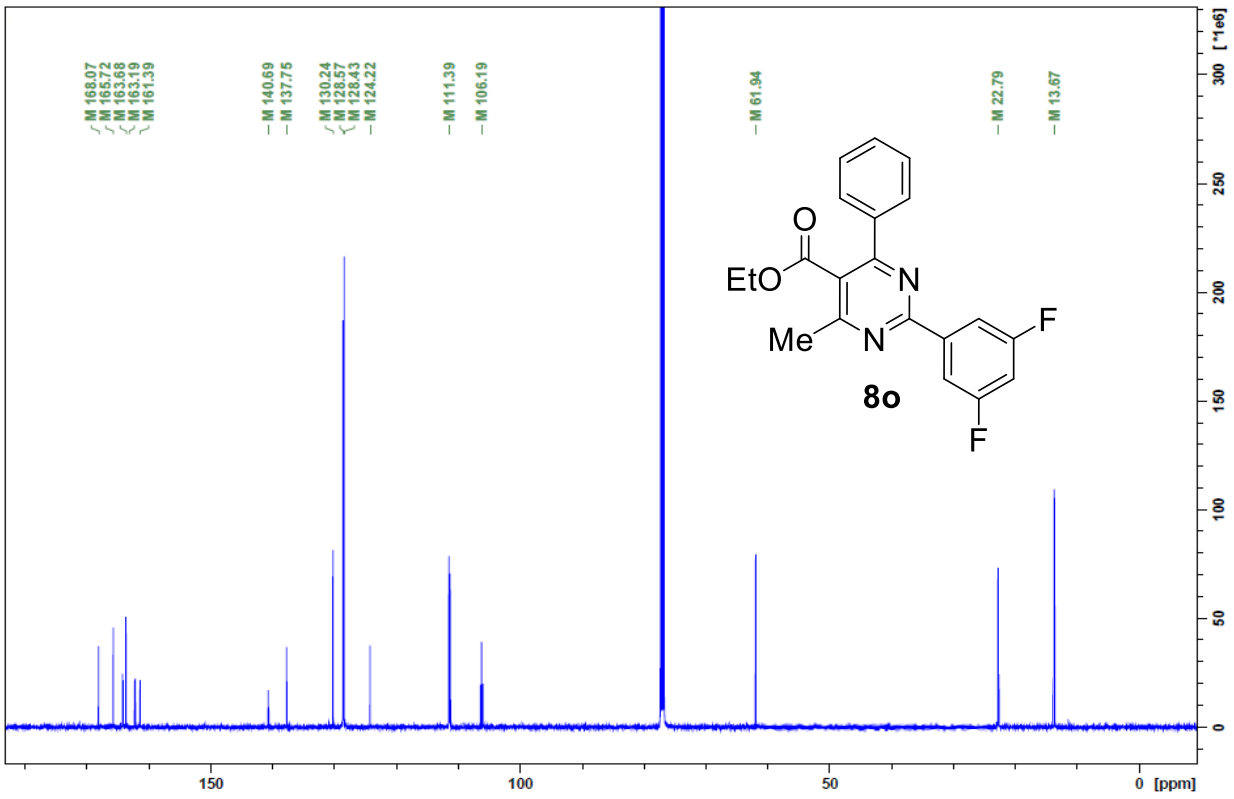

M 8.35
M 8.26
M 7.75
M 7.49
M 7.46
M 7.19
M 4.22
M 2.70
M 1.09
O
EtO
N
Me
N
8m
F
1.02
1.00
2.02
1.00
1.02
2.04
6.02
3.06
8
6
4
2
0 [ppm]
[*1e6]
15
10
5
0

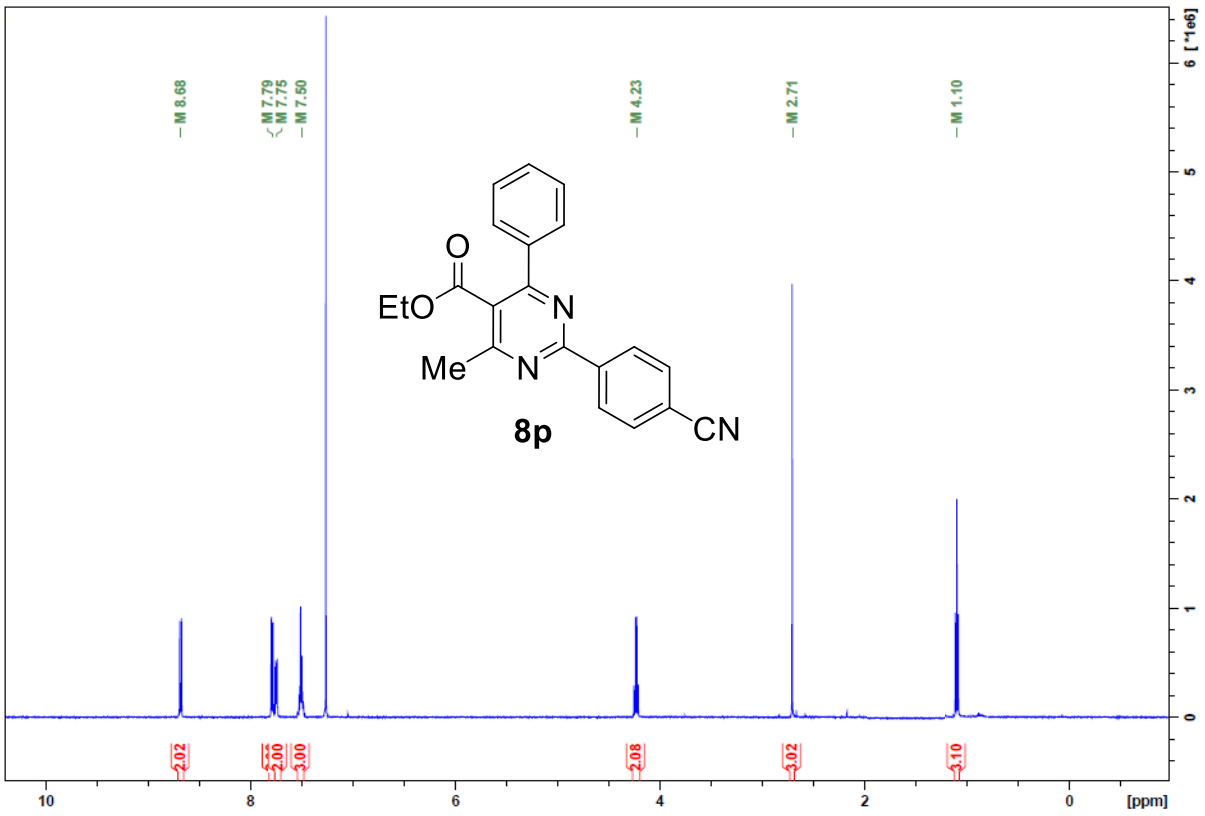

M 168.27
M 165.56
M 163.62
M 163.13
M 162.51
M 139.54
M 137.97
M 130.11
M 129.97
M 128.52
M 128.44
M 124.24
M 123.78
M 117.90
M 115.42
M 61.86
M 22.83
M 13.65
O
EtO
N
Me
N
8m
F
150
100
50
0 [ppm]
[*1e6]
200
150
100
50
0

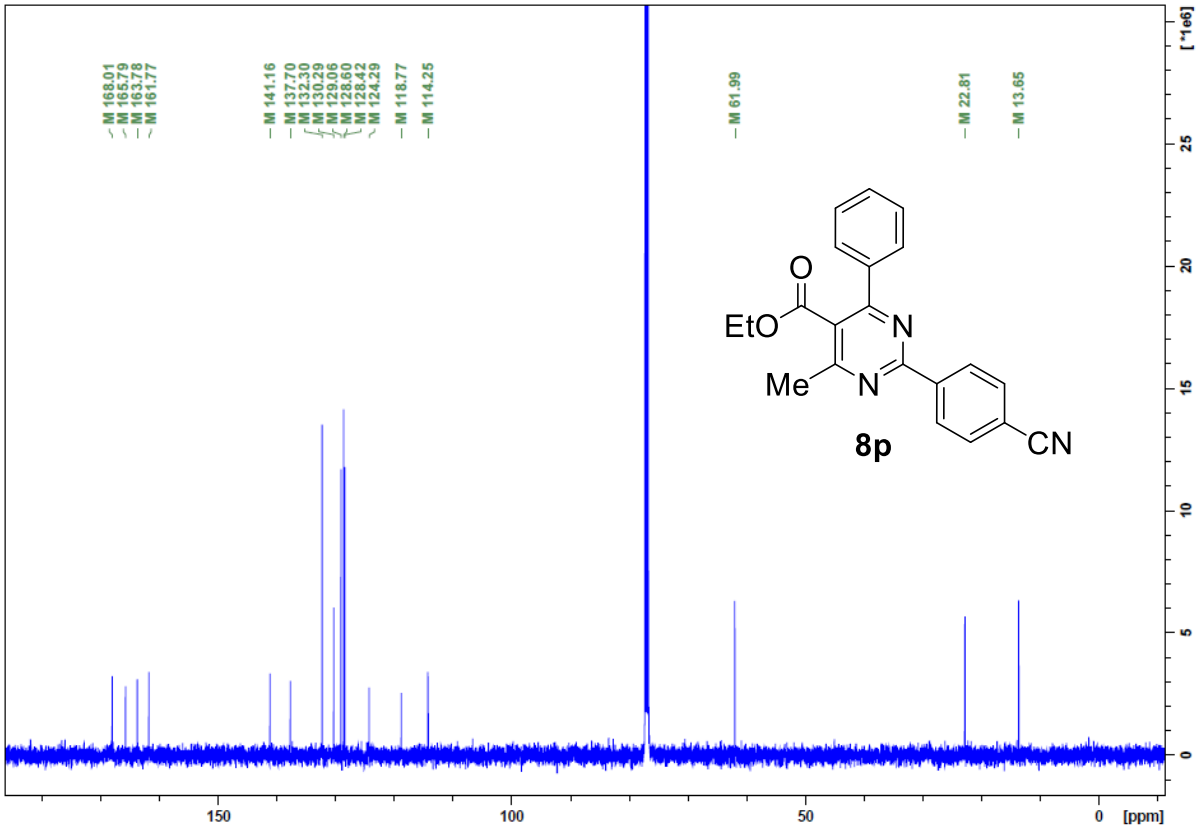

M 8.57
M 7.74
M 7.49
M 7.16
M 4.21
M 2.69
M 1.08
O
EtO
N
Me
N
F
8n
2.00
2.03
3.08
2.04
2.06
3.04
3.08
8
6
4
2
0 [ppm]
20 [*1e6]
15
10
5
0

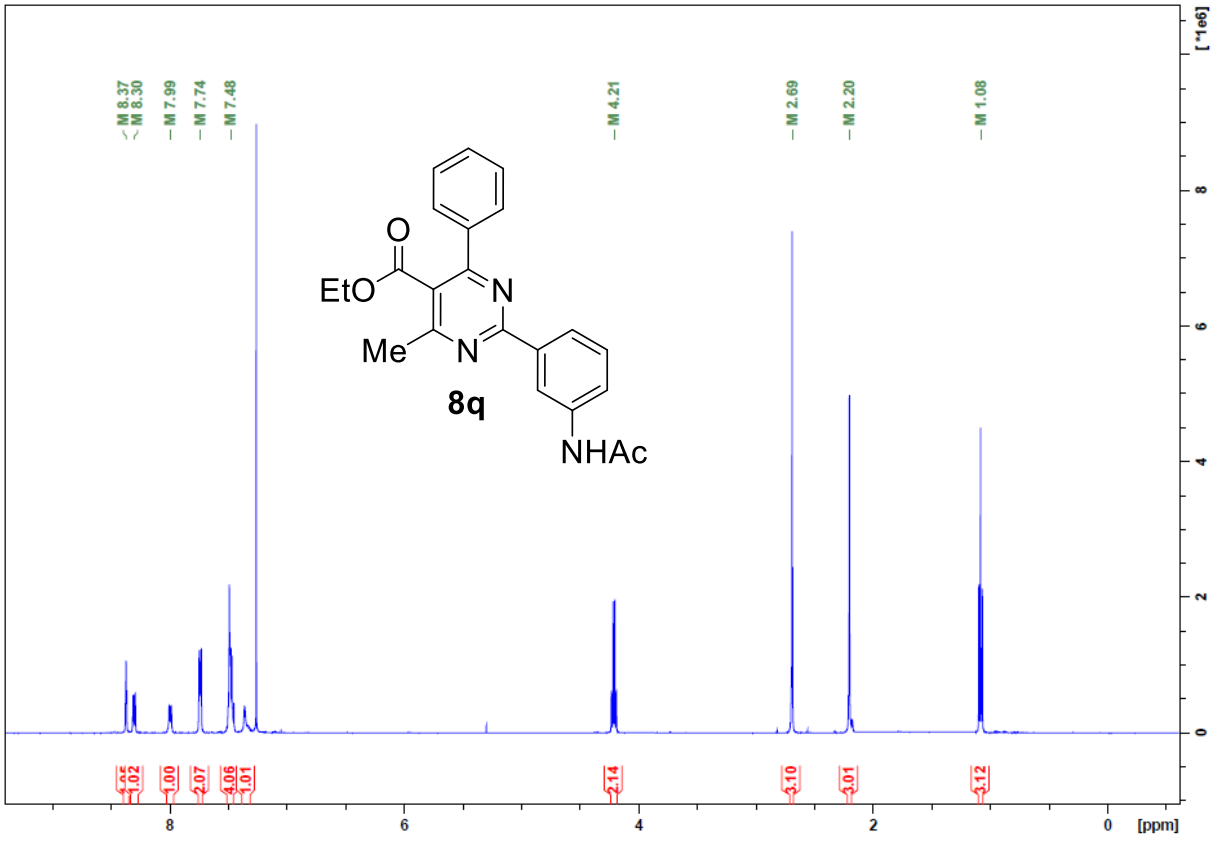

M 168.38
M 165.48
M 164.91
M 163.53
M 162.73
M 138.14
M 133.33
M 130.80
M 130.02
M 128.49
M 128.41
M 123.26
M 115.46
M 61.79
M 22.86
M 13.64
O
EtO
N
Me
N
F
8n
150
100
50
0 [ppm]
[*1e6]
300
200
100
0

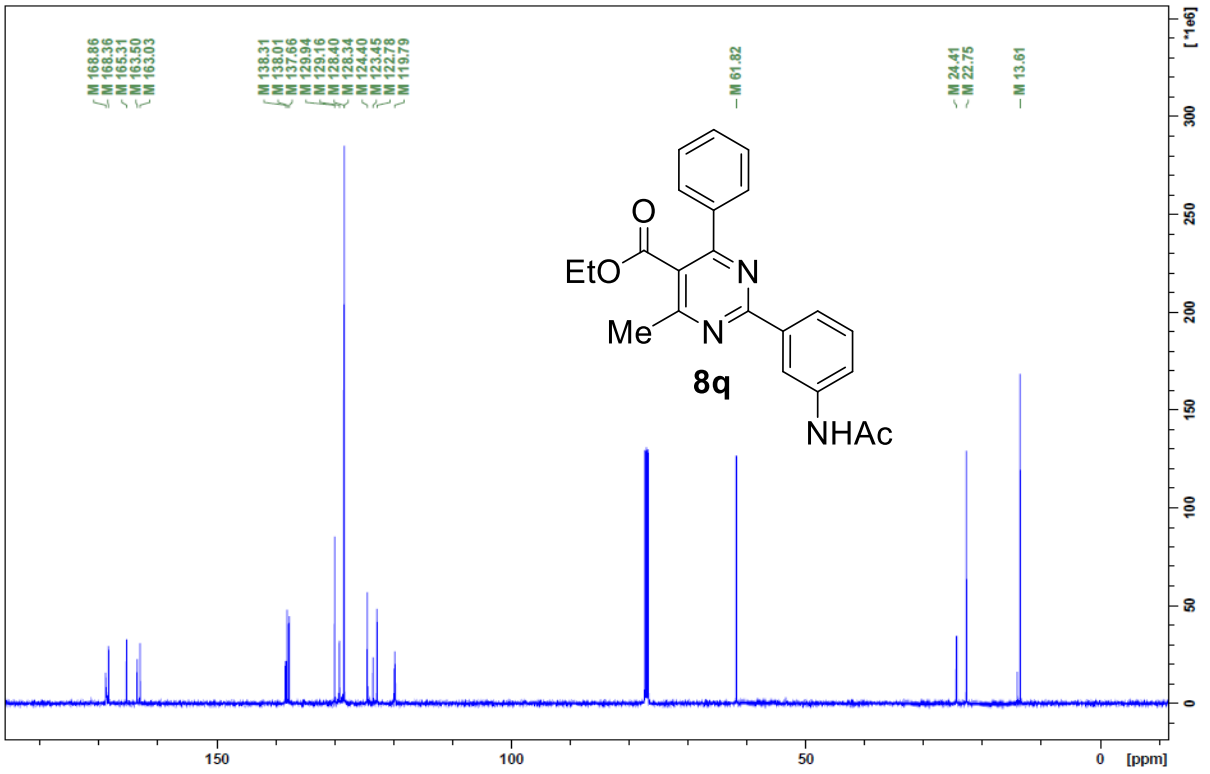

M 8.10
M 7.74
M 7.50
M 6.94
M 4.23
M 2.69
M 1.10
EtO
O
N
Me
N
F
F
8o
2.01
2.05
3.03
1.00
2.01
3.04
3.03
[*1e6]
[ppm]

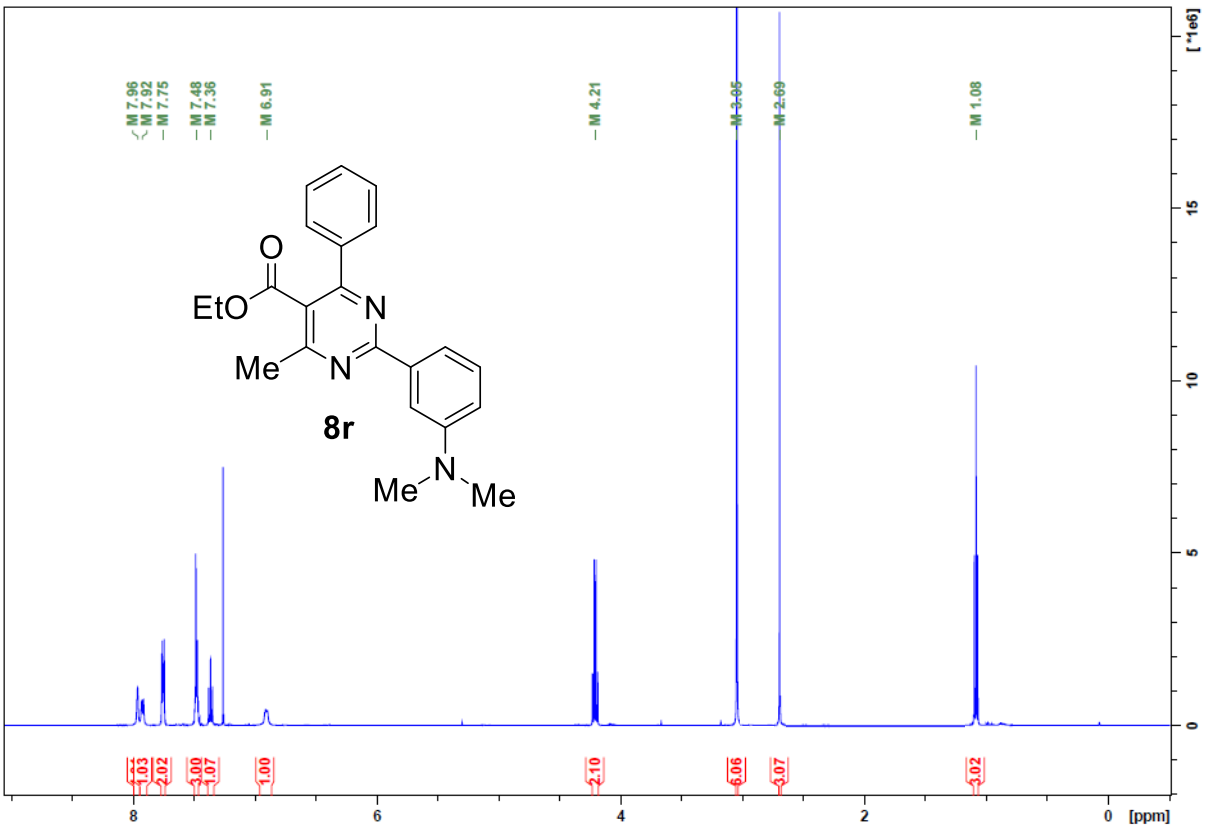

M 168.07
M 165.72
M 163.68
M 163.19
M 161.39
M 140.69
M 137.75
M 130.24
M 128.57
M 128.43
M 124.22
M 111.39
M 106.19
M 61.94
M 22.79
M 13.67
EtO
O
N
Me
N
F
F
8o
[*1e6]
[ppm]

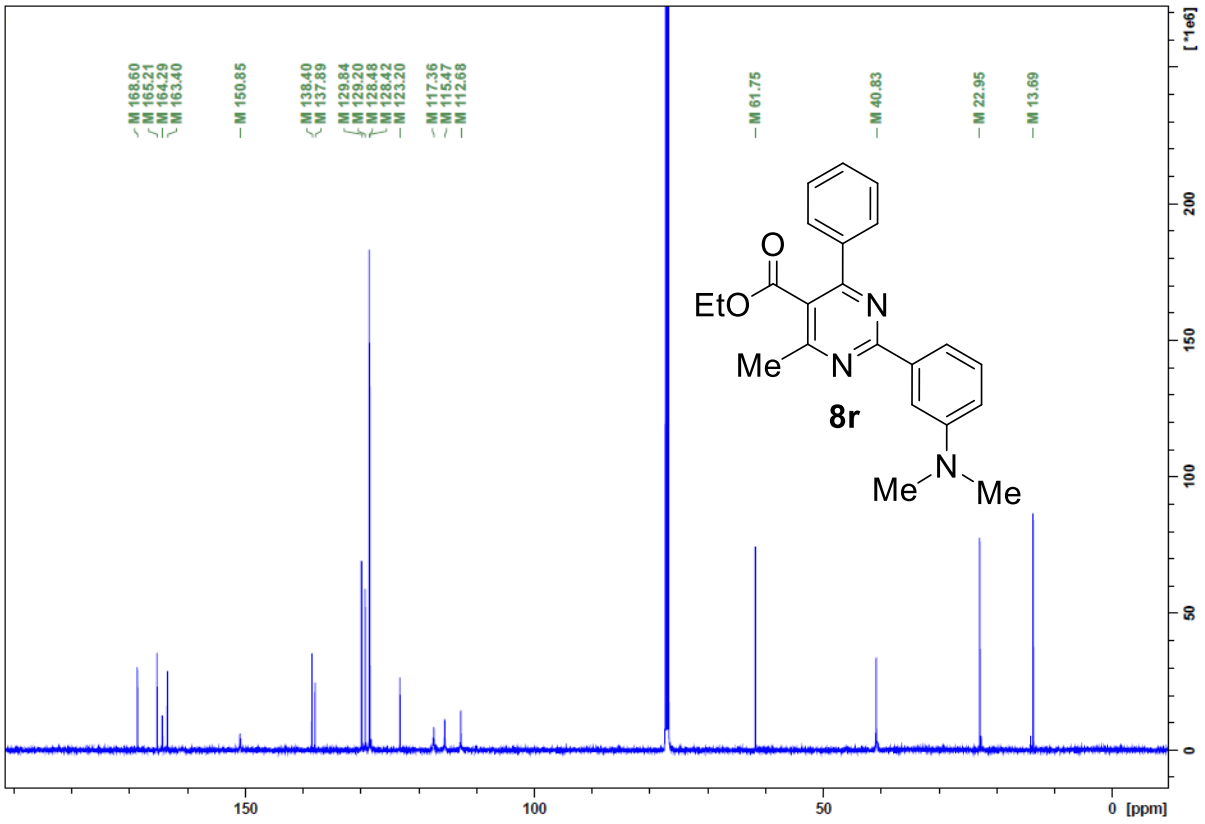

M 8.68
M 7.79
M 7.75
M 7.50
M 4.23
M 2.71
M 1.10
O
EtO
N
Me
N
CN
8p
2.02
2.00
3.00
2.08
3.02
3.10
10
8
6
4
2
0
[ppm]
[*1e6]

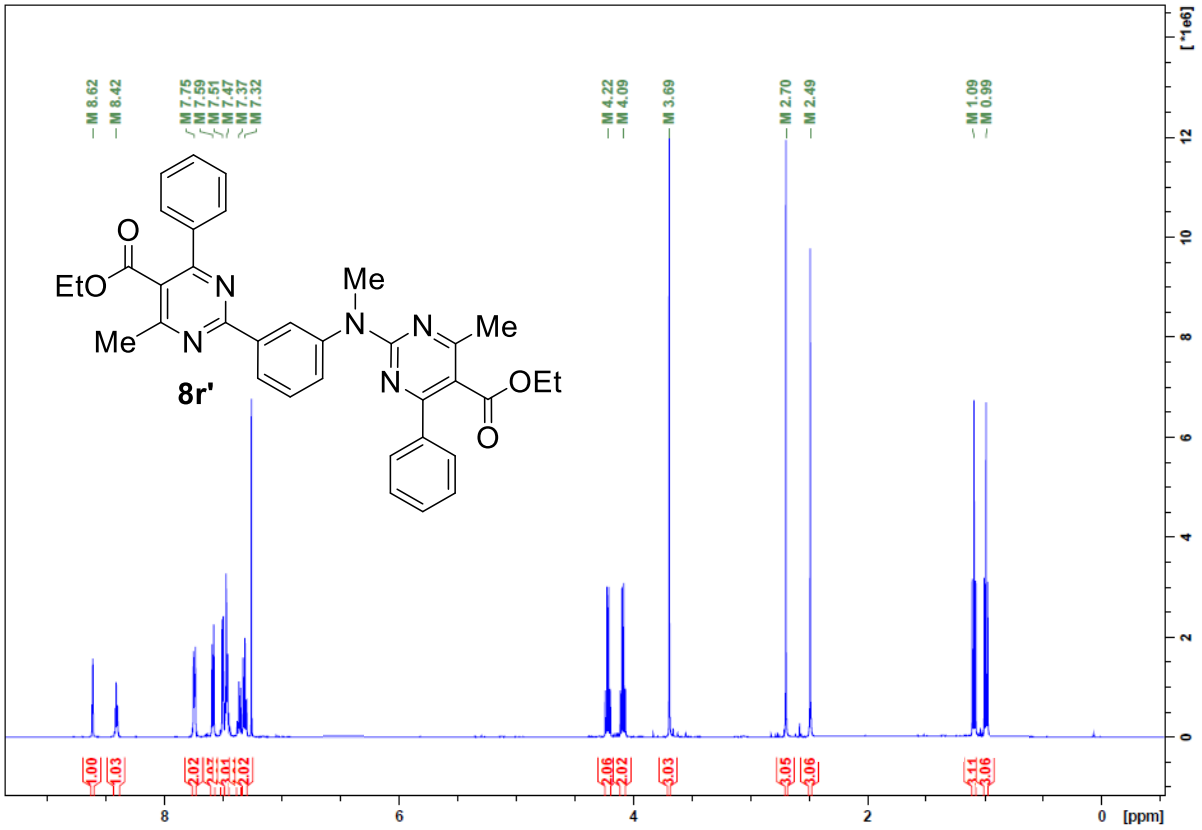

M 168.01
M 165.79
M 163.78
M 161.77
M 141.16
M 137.70
M 132.30
M 130.29
M 129.06
M 128.60
M 128.42
M 124.29
M 118.77
M 114.25
M 61.99
M 22.81
M 13.65
O
EtO
N
Me
N
CN
8p
150
100
50
0
[ppm]
[*1e6]

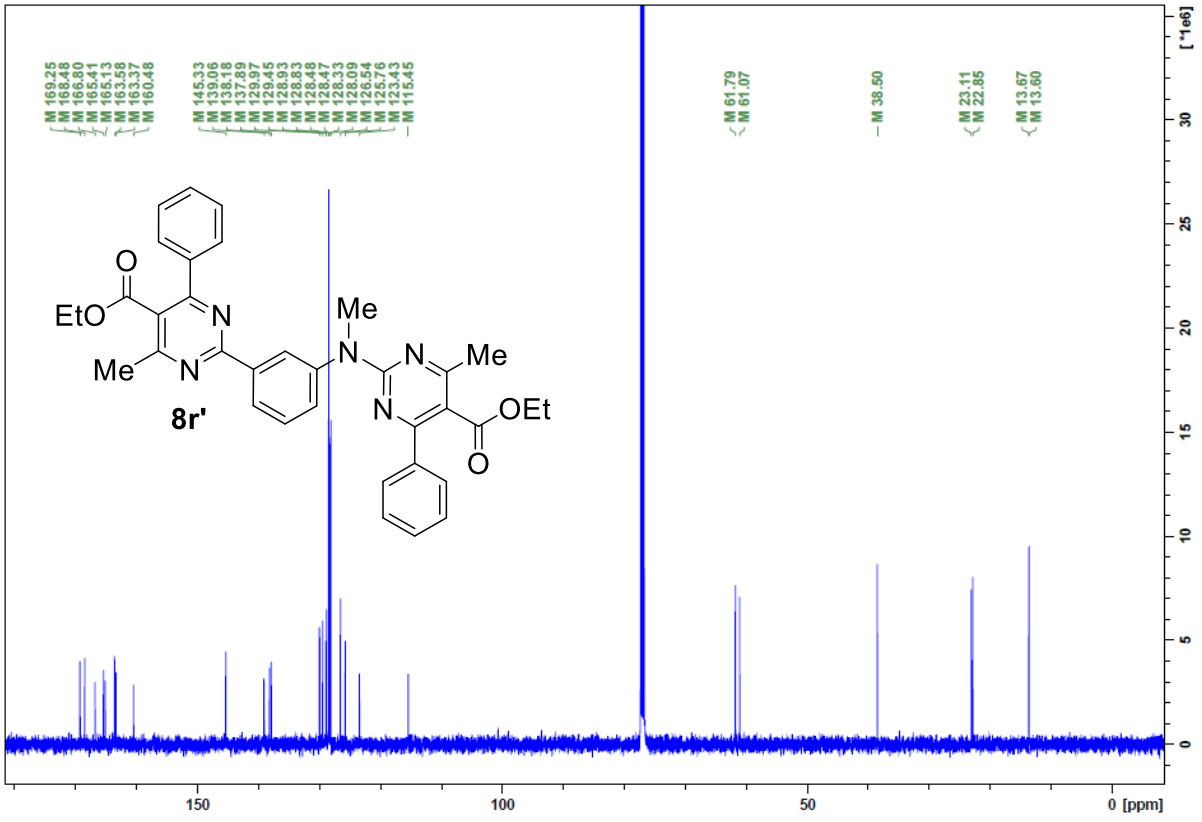

M 8.37
M 8.30
M 7.99
M 7.74
M 7.48
M 4.21
M 2.69
M 2.20
M 1.08
O
EtO
N
Me
N
8q
NHAc
[*1e6]
[ppm]

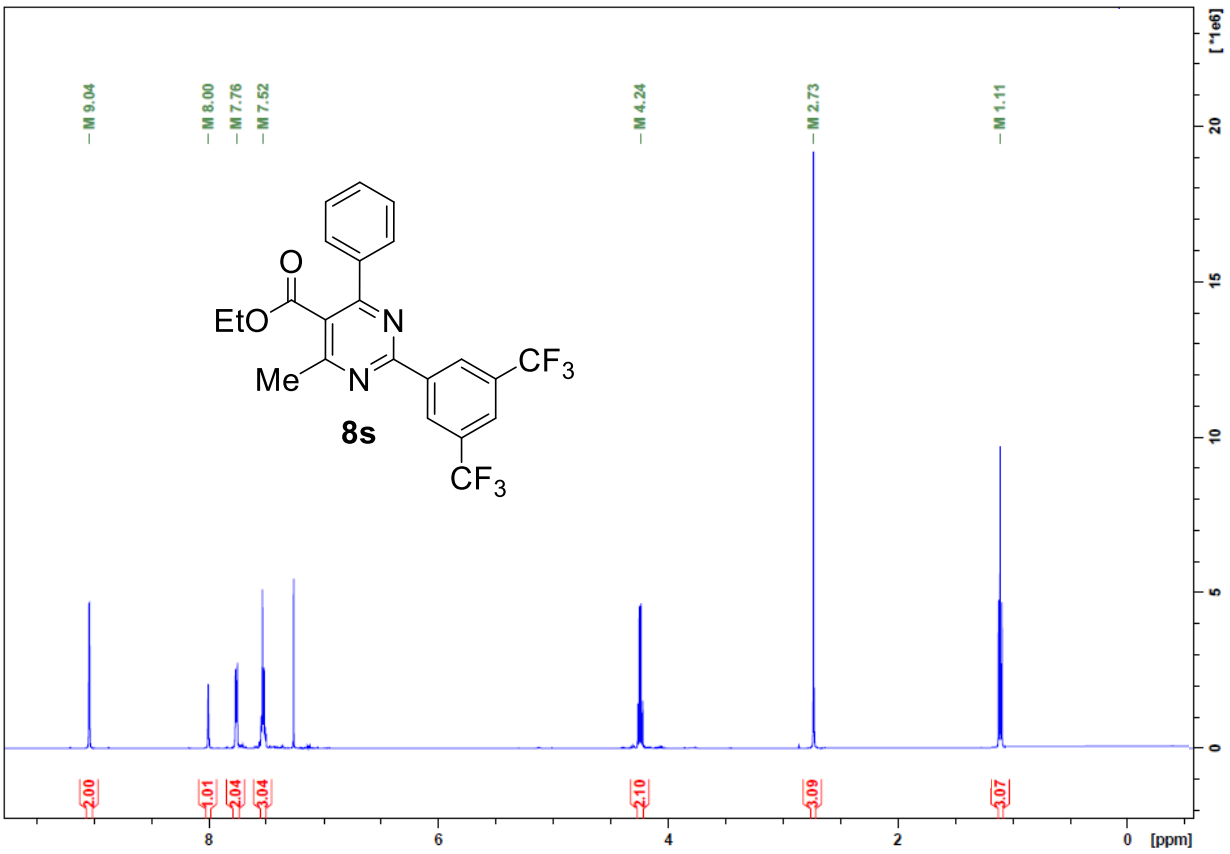

M 168.86
M 168.36
M 165.31
M 163.50
M 163.03
M 138.31
M 138.01
M 137.66
M 129.94
M 129.16
M 128.40
M 128.34
M 124.40
M 123.45
M 122.78
M 119.79
M 61.82
M 24.41
M 22.75
M 13.61
O
EtO
N
Me
N
8q
NHAc
[*1e6]
[ppm]

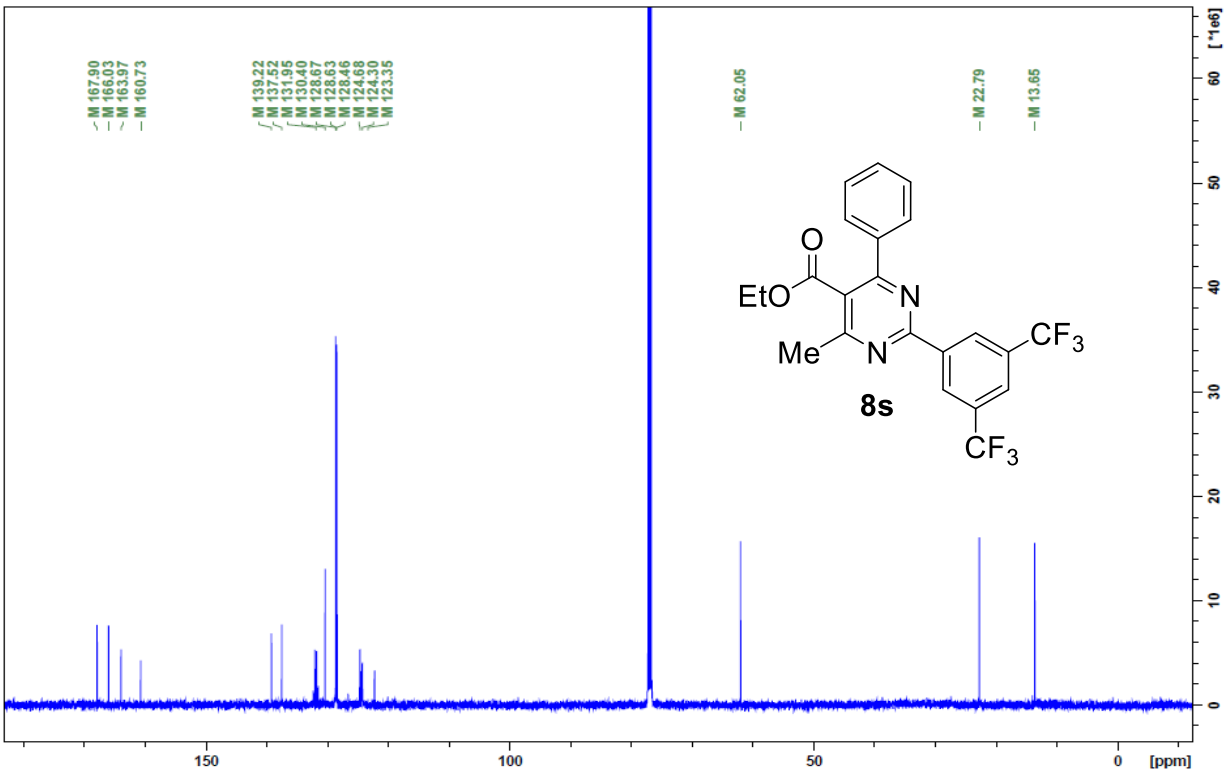

M 7.96
M 7.92
M 7.75
M 7.48
M 7.36
M 6.91
M 4.21
M 2.85
M 2.69
M 1.08
O
EtO
N
Me
N
8r
N
Me
Me
[*1e6]
15
10
5
0
1.03
2.02
3.00
1.07
1.00
2.10
6.06
5.07
3.02
8
6
4
2
0
[ppm]

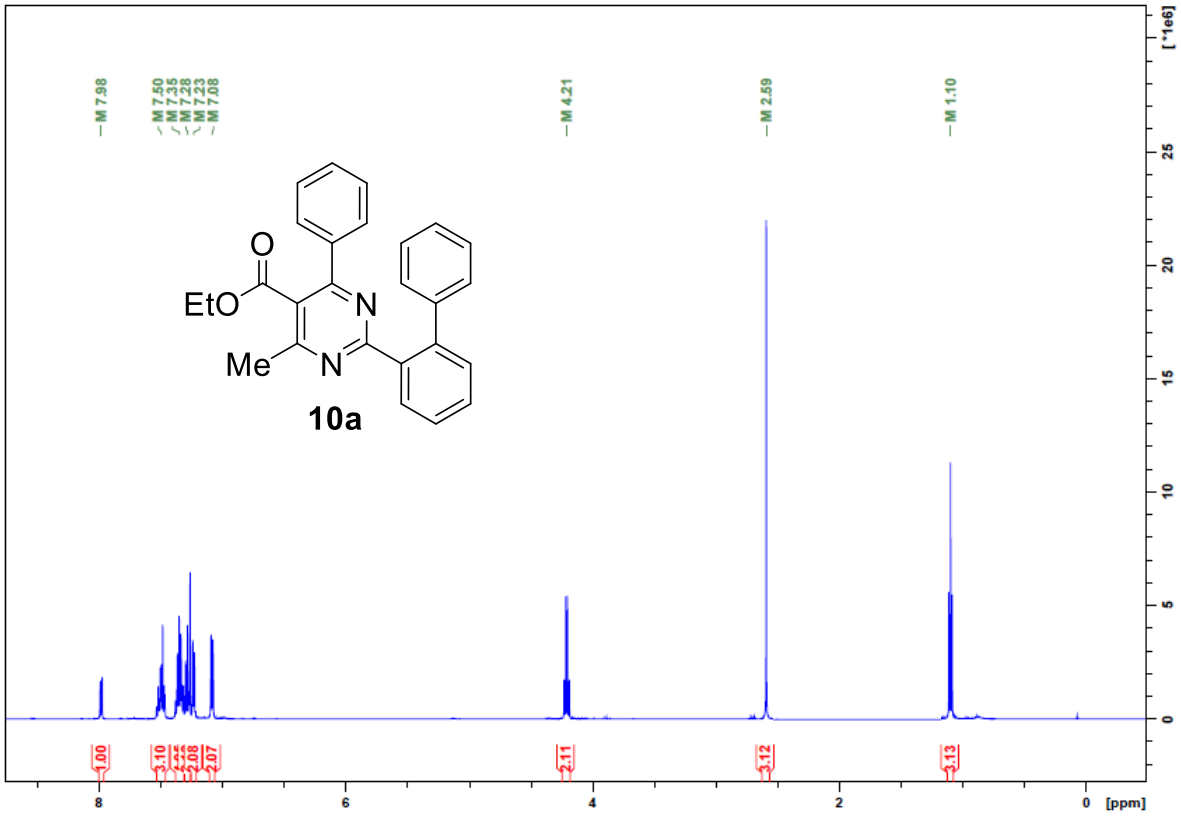

M 168.60
M 165.21
M 164.29
M 163.40
M 150.85
M 138.40
M 137.89
M 129.84
M 129.20
M 128.48
M 128.42
M 123.20
M 117.36
M 115.47
M 112.68
M 61.75
M 40.83
M 22.95
M 13.69
O
EtO
N
Me
N
8r
N
Me
Me
[*1e6]
200
150
100
50
0
150
100
50
0
[ppm]

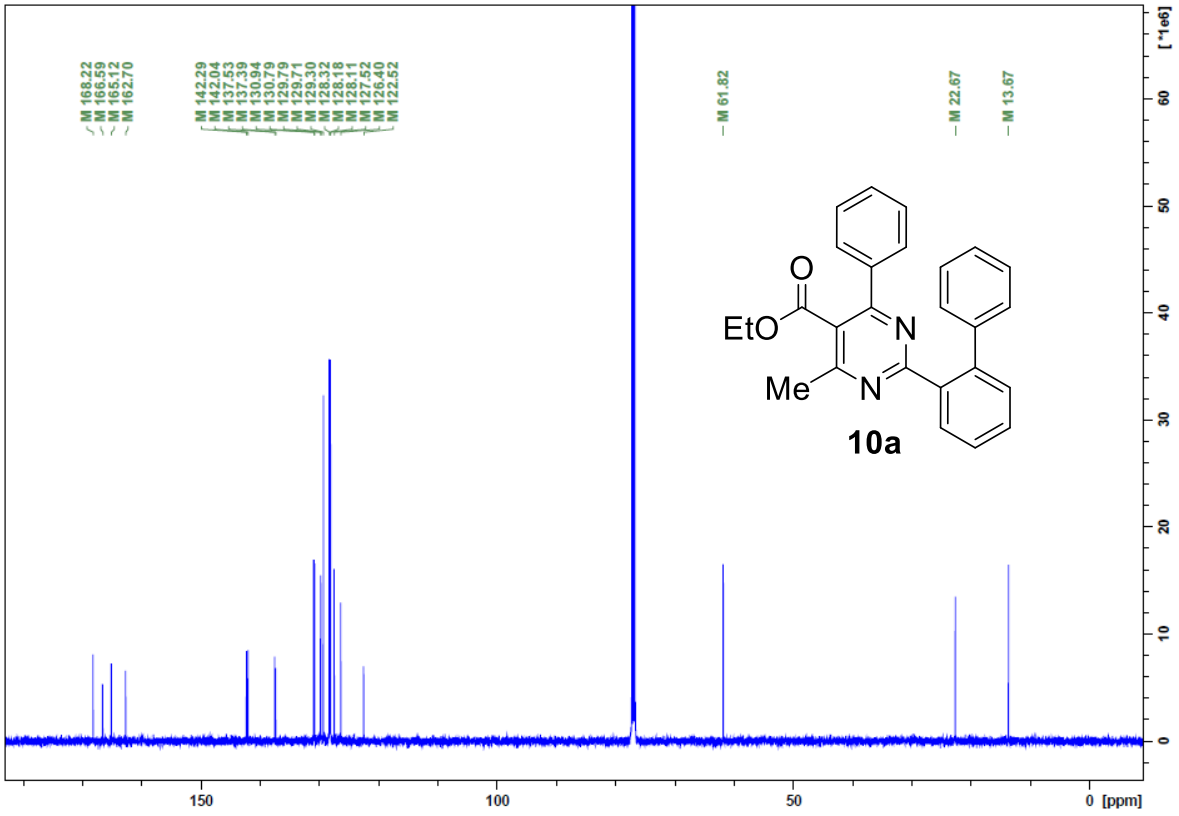

M 8.62
M 8.42
M 7.75
M 7.59
M 7.51
M 7.47
M 7.37
M 7.32
M 4.22
M 4.09
M 3.69
M 2.70
M 2.49
M 1.09
M 0.99
EtO
Me
Me
OEt
8r'
[*1e6]
[ppm]

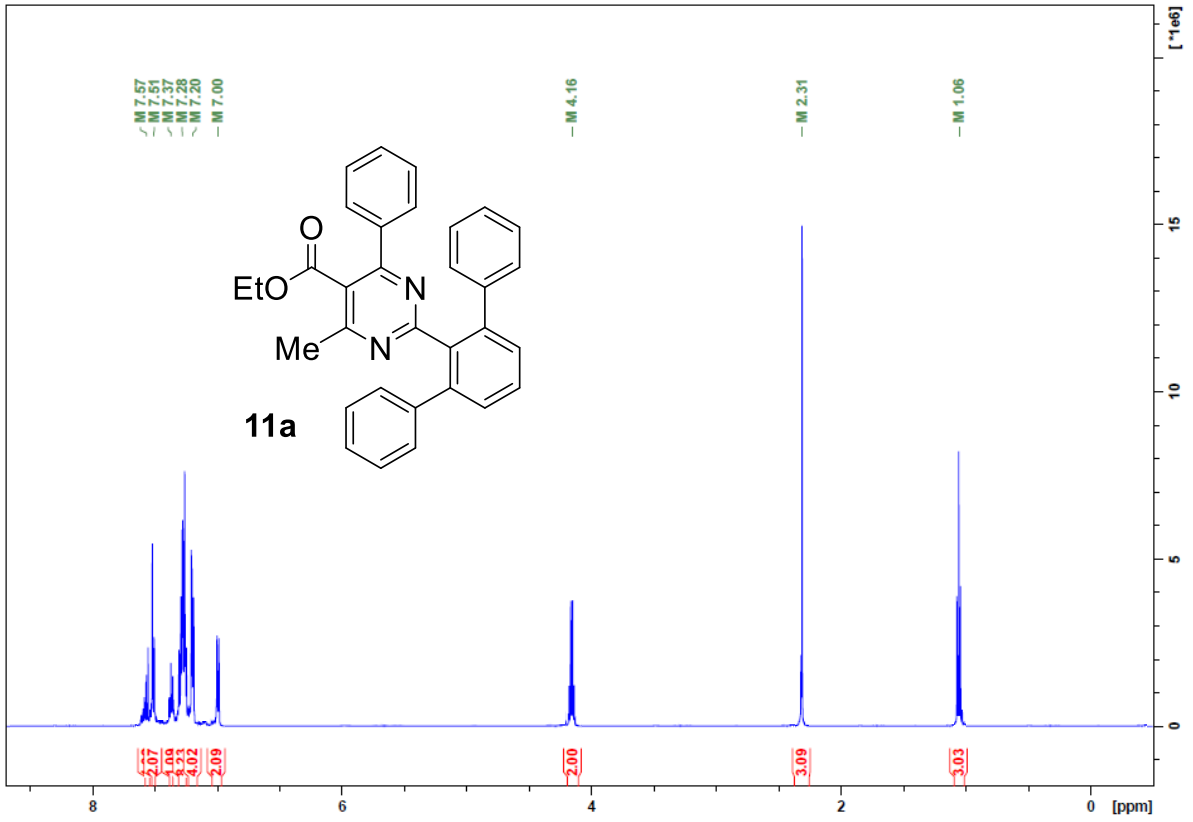

M 169.25
M 168.48
M 168.40
M 165.41
M 165.13
M 163.58
M 163.37
M 160.48
M 145.33
M 139.06
M 138.18
M 137.89
M 129.97
M 129.45
M 128.93
M 128.83
M 128.48
M 128.47
M 128.33
M 128.09
M 126.54
M 125.76
M 123.43
M 115.45
M 61.79
M 61.07
M 38.50
M 23.11
M 22.85
M 13.67
M 13.60
EtO
Me
Me
OEt
8r'
[*1e6]
[ppm]

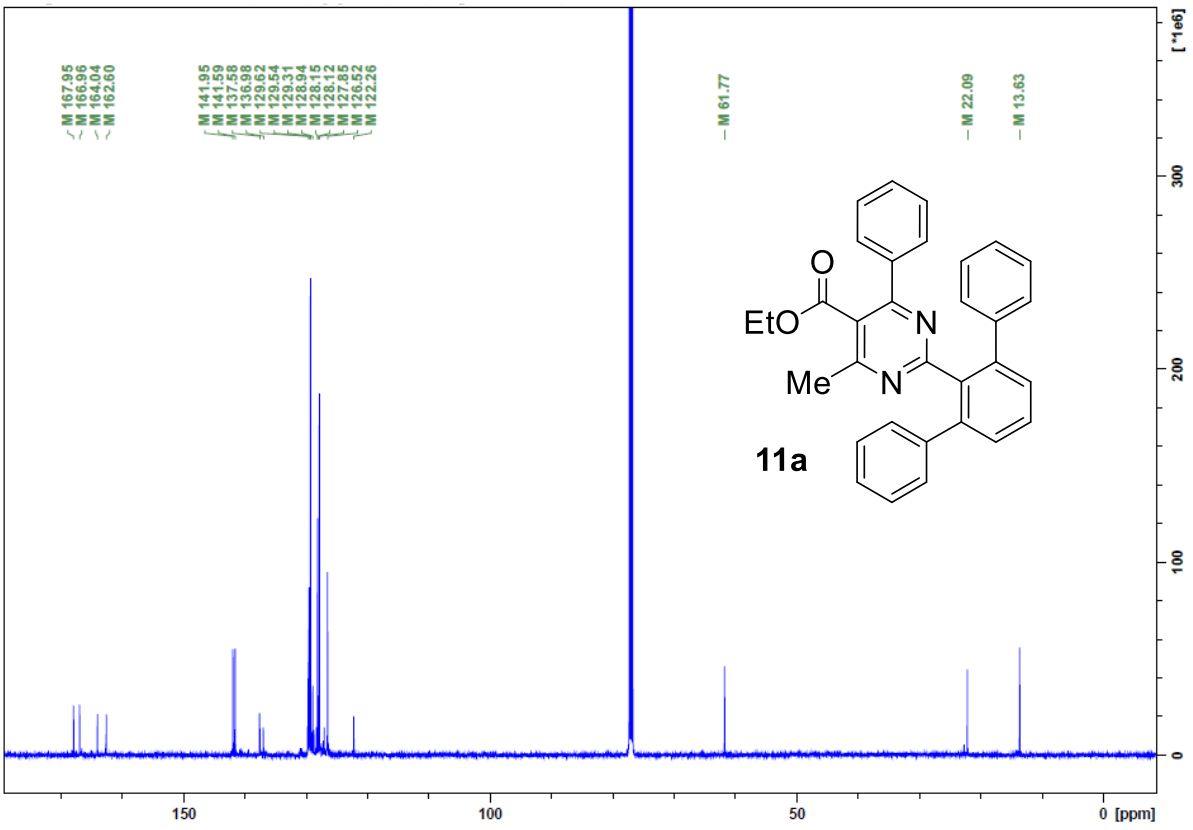

M 9.04
M 8.00
M 7.76
M 7.52
M 4.24
M 2.73
M 1.11
O
EtO
N
Me
N
CF3
CF3
8s
2.00
1.01
2.04
3.04
2.10
3.09
3.07
8
6
4
2
0
[ppm]
[*1e6]

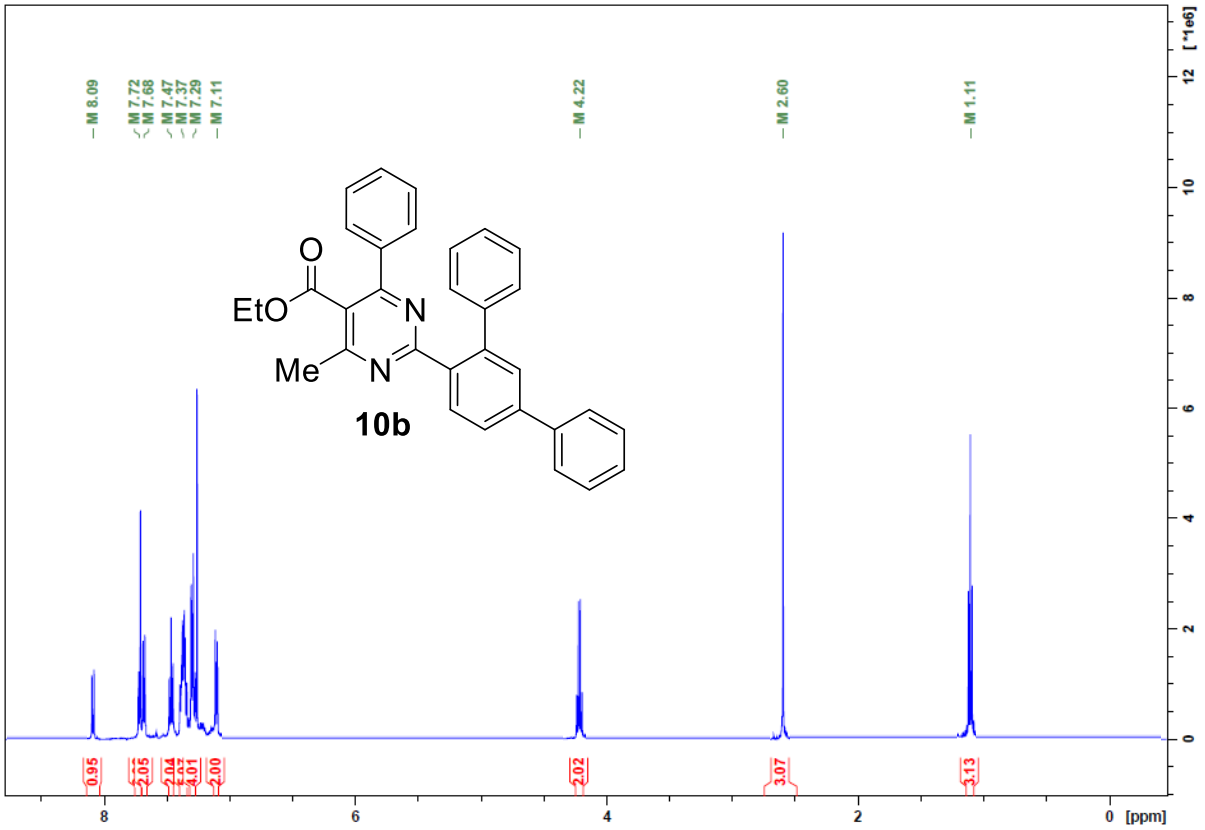

M 167.90
M 165.03
M 163.97
M 160.73
M 139.22
M 137.52
M 131.95
M 130.40
M 128.67
M 128.63
M 128.46
M 124.68
M 124.30
M 123.35
M 62.05
M 22.79
M 13.65
O
EtO
N
Me
N
CF3
CF3
8s
150
100
50
0
[ppm]
[*1e6]

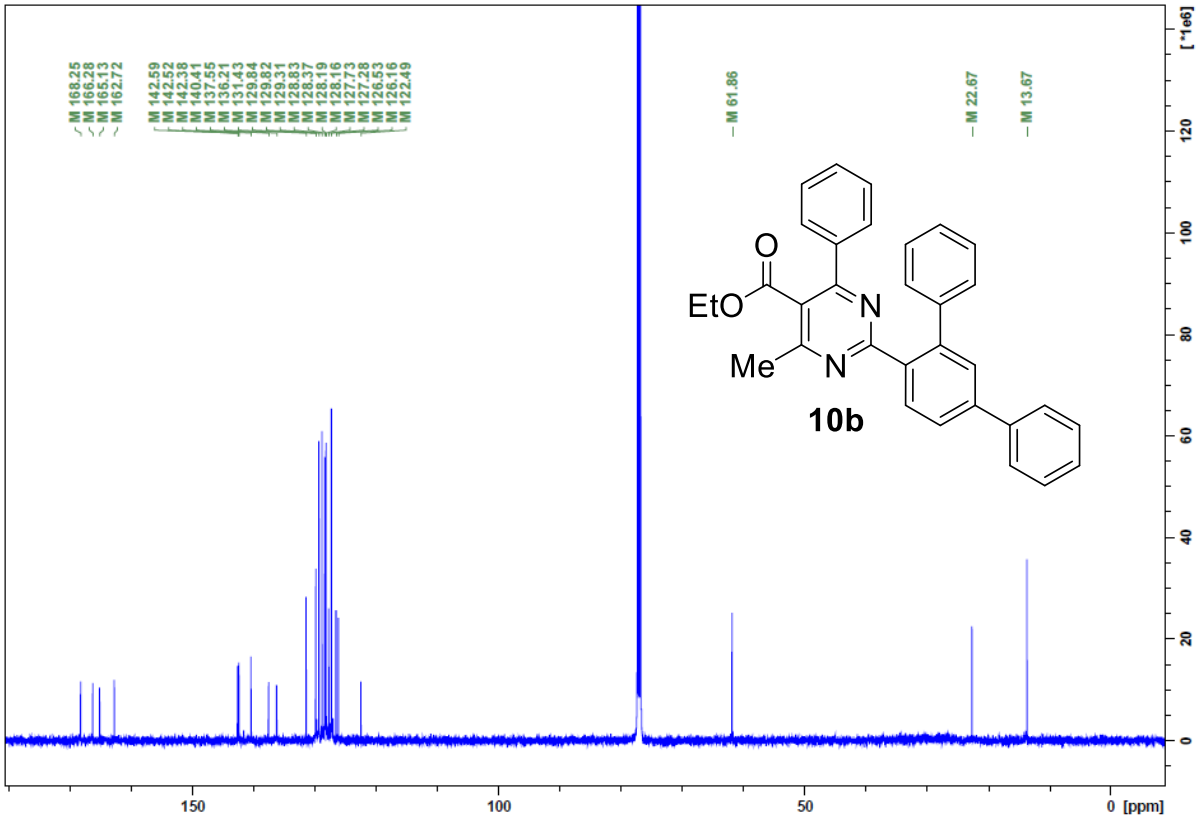

M 7.98
M 7.50
M 7.35
M 7.28
M 7.23
M 7.08
M 4.21
M 2.59
M 1.10
O
EtO
N
Me
N
10a
1.00
3.10
2.11
3.12
3.13
8
6
4
2
0
[ppm]
[*1e6]

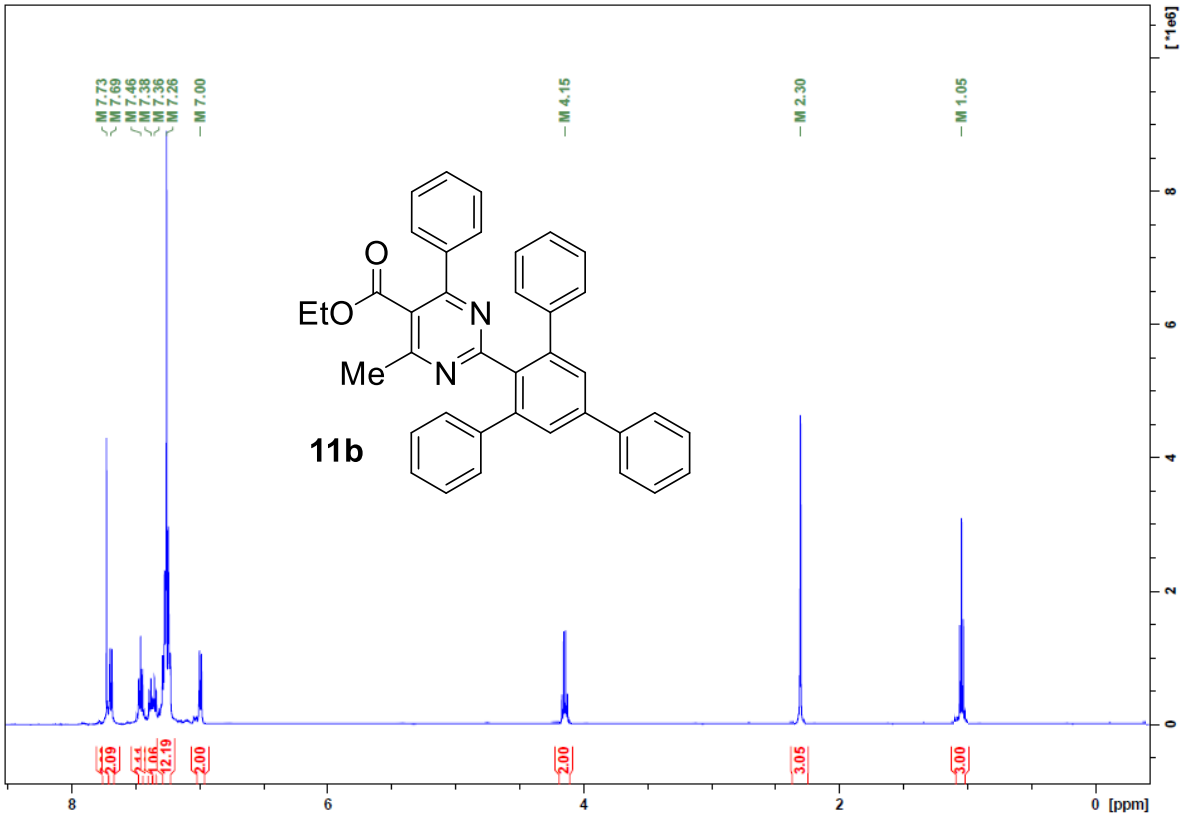

M 168.22
M 166.59
M 165.12
M 162.70
M 142.29
M 142.04
M 137.53
M 137.39
M 130.94
M 130.79
M 129.79
M 129.71
M 129.30
M 128.32
M 128.18
M 128.11
M 127.52
M 126.40
M 122.52
M 61.82
M 22.67
M 13.67
O
EtO
N
Me
N
10a
150
100
50
0
[ppm]
[*1e6]

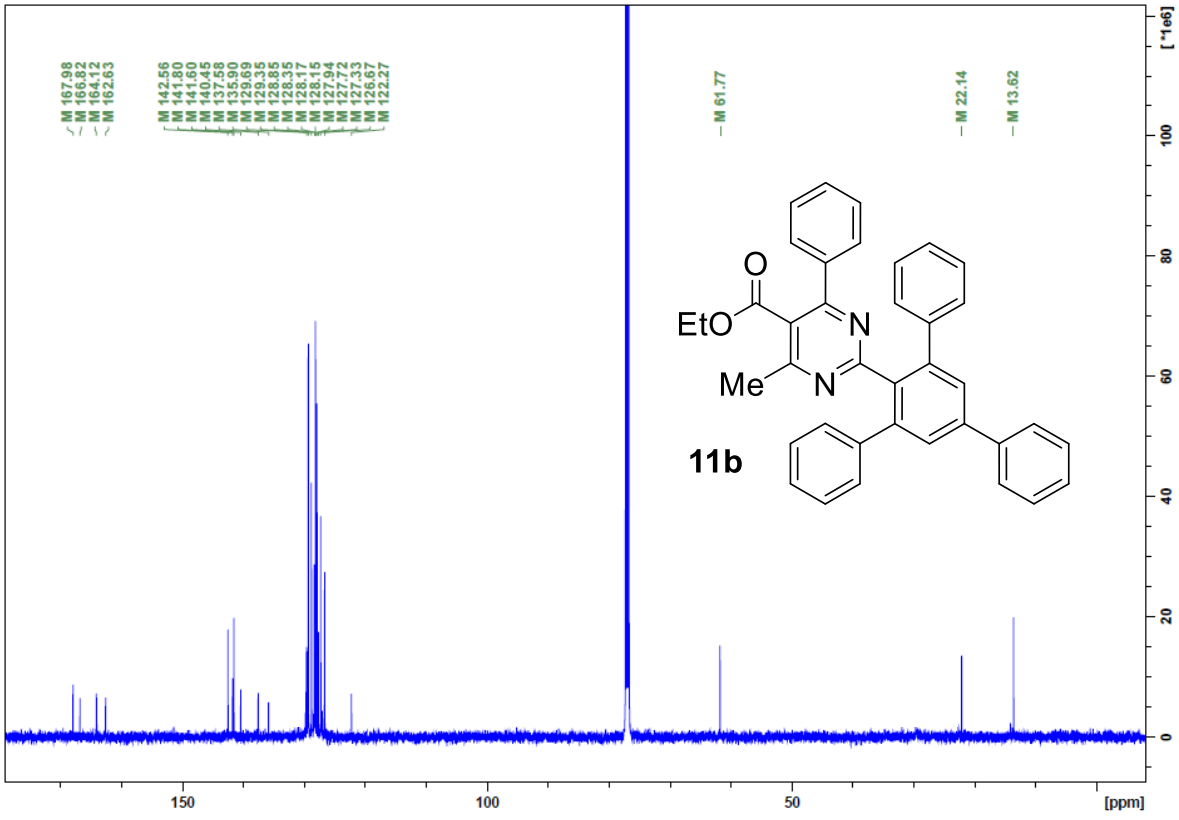

M 7.57
M 7.51
M 7.37
M 7.28
M 7.20
M 7.00
M 4.16
M 2.31
M 1.06
O
EtO
N
Me
N
11a
[*1e6]
15
10
5
0
2.07
1.09
8.33
4.02
2.09
2.00
3.09
3.03
8
6
4
2
0 [ppm]

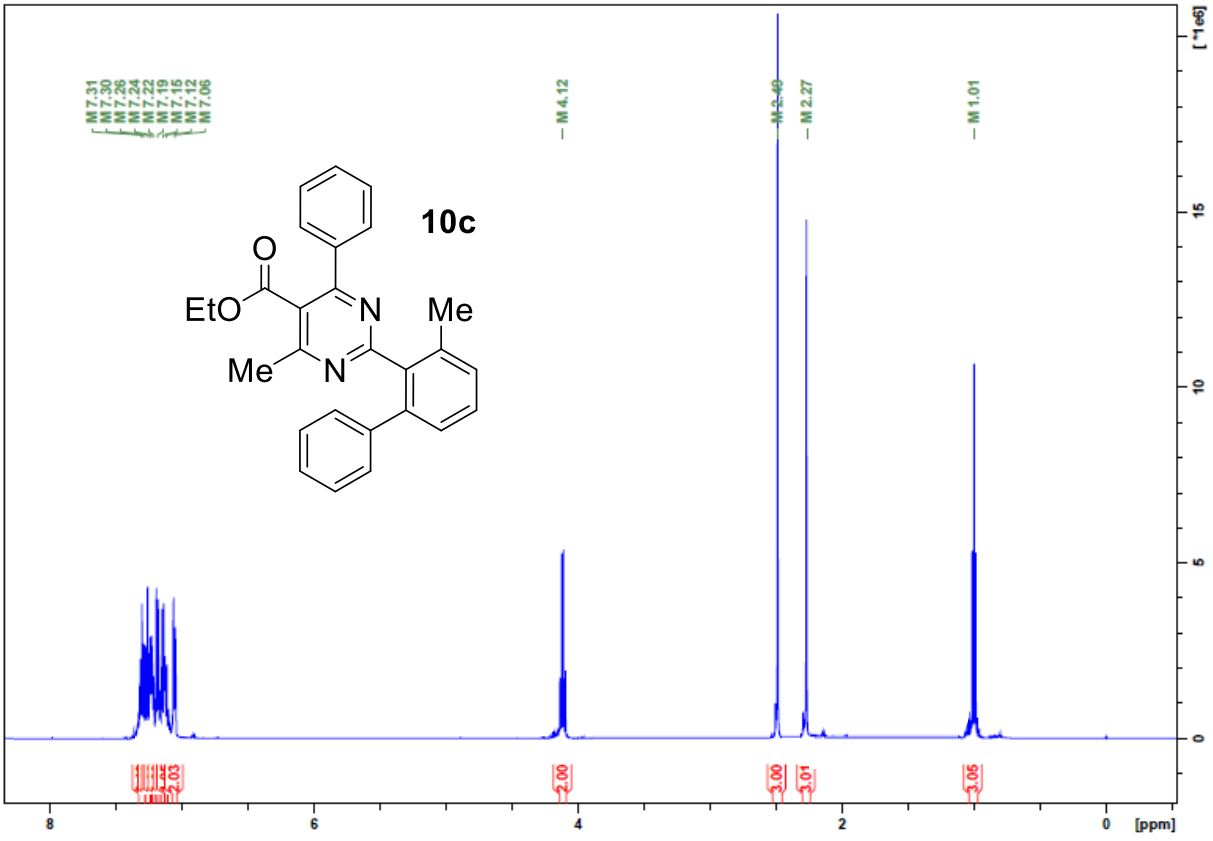

M 167.95
M 166.96
M 164.04
M 162.60
M 141.95
M 141.59
M 137.58
M 136.98
M 129.62
M 129.54
M 129.31
M 128.94
M 128.15
M 128.12
M 127.85
M 126.52
M 122.26
M 61.77
M 22.09
M 13.63
O
EtO
N
Me
N
11a
[*1e6]
300
200
100
0
150
100
50
0 [ppm]

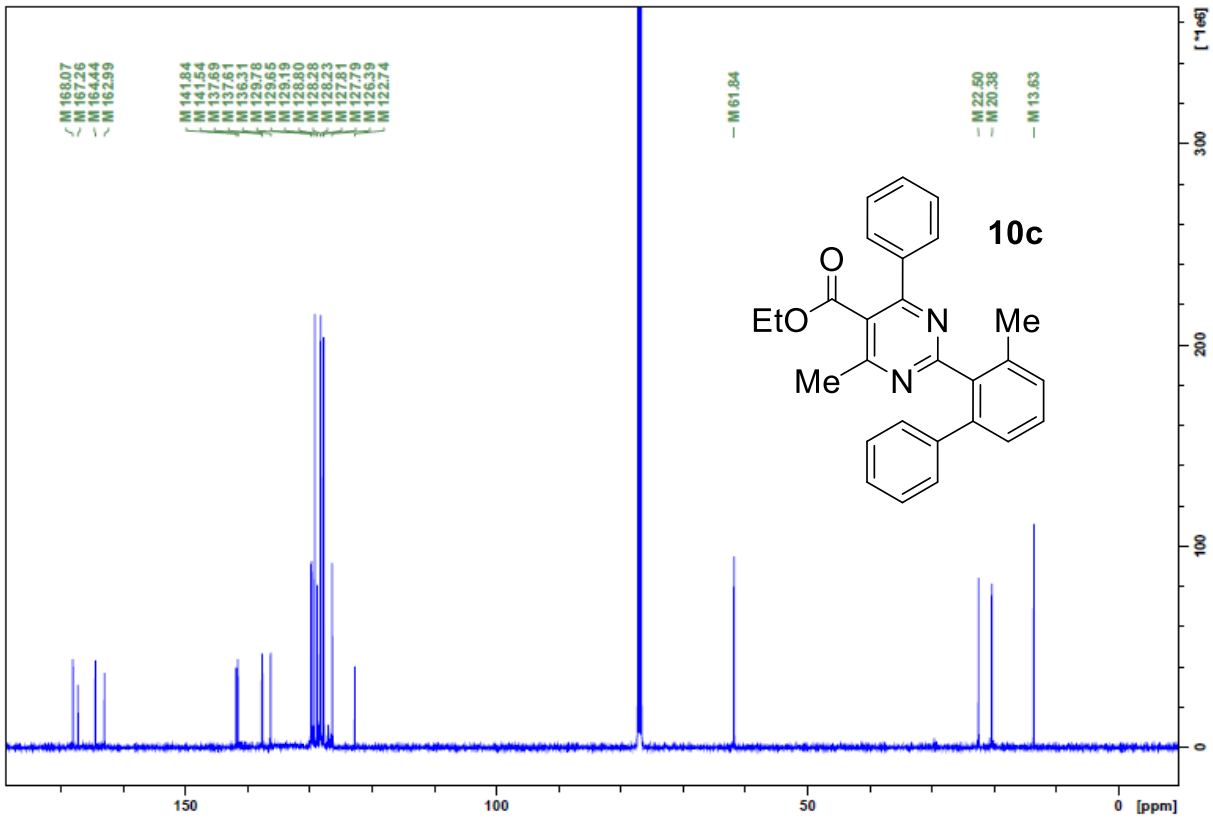

M 8.09
M 7.72
M 7.68
M 7.47
M 7.37
M 7.29
M 7.11
M 4.22
M 2.60
M 1.11
O
EtO
N
Me
N
10b
0.95
2.05
2.04
4.01
2.00
2.02
3.07
3.13
8
6
4
2
0 [ppm]
[*1e6]

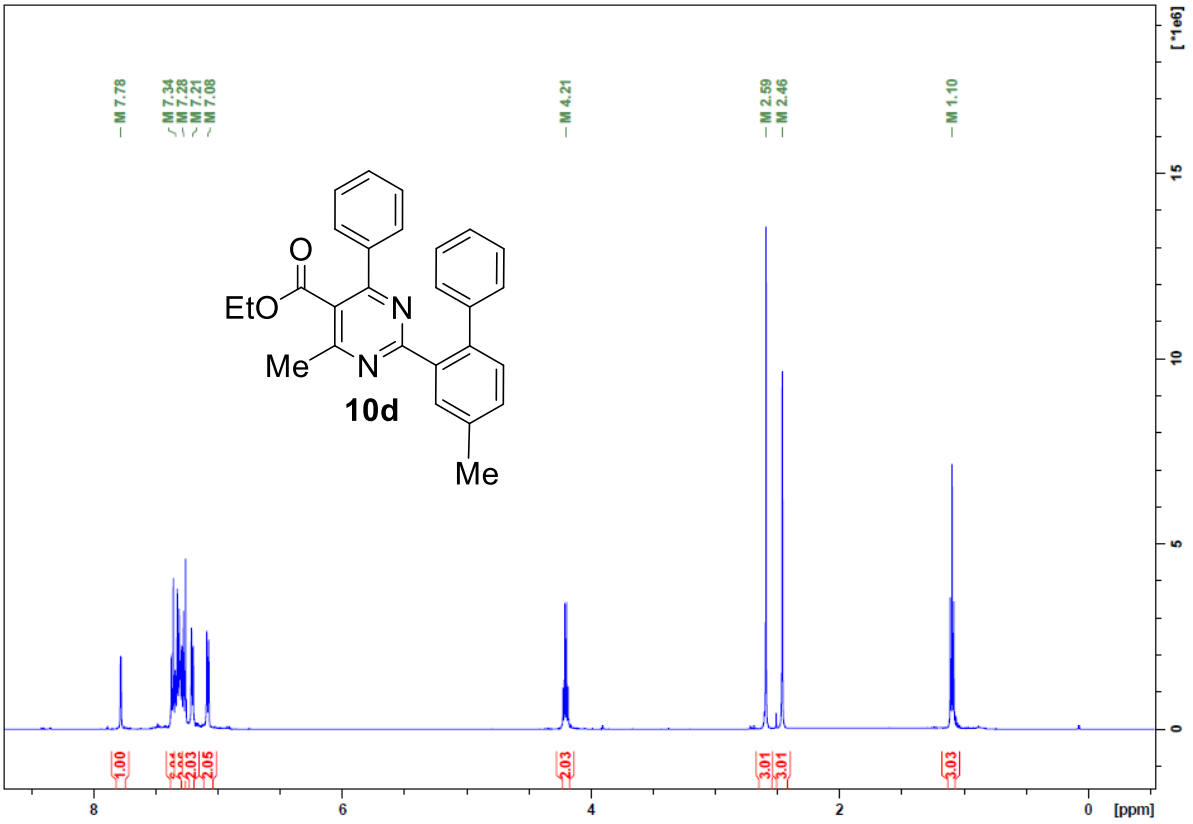

M 168.25
M 166.28
M 165.13
M 162.72
M 142.59
M 142.52
M 142.38
M 140.41
M 137.55
M 136.21
M 131.43
M 129.84
M 129.82
M 129.31
M 128.83
M 128.37
M 128.19
M 128.16
M 127.73
M 127.28
M 126.53
M 126.16
M 122.49
M 61.86
M 22.67
M 13.67
O
EtO
N
Me
N
10b
150
100
50
0 [ppm]
[*1e6]

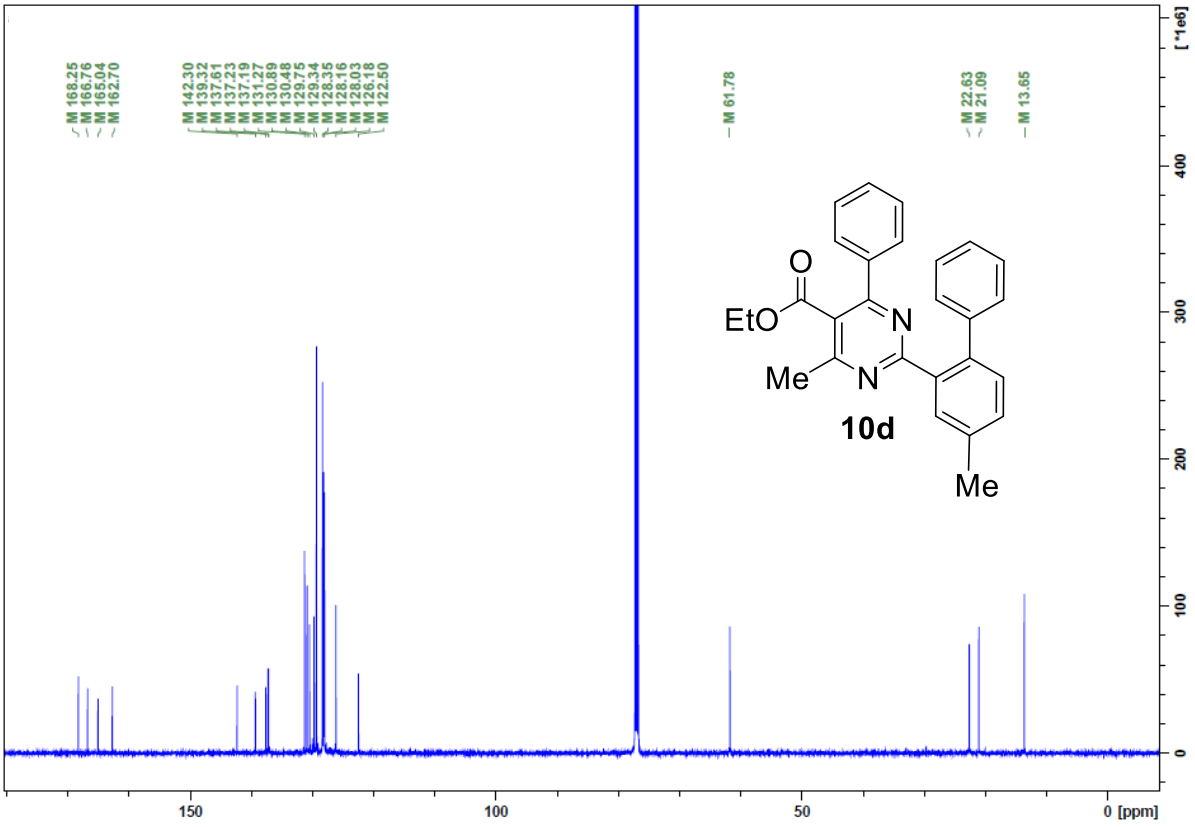

M 7.73
M 7.69
M 7.46
M 7.38
M 7.36
M 7.26
M 7.00
M 4.15
M 2.30
M 1.05
O
EtO
N
Me
N
11b
[*1e6]
8
6
4
2
0 [ppm]

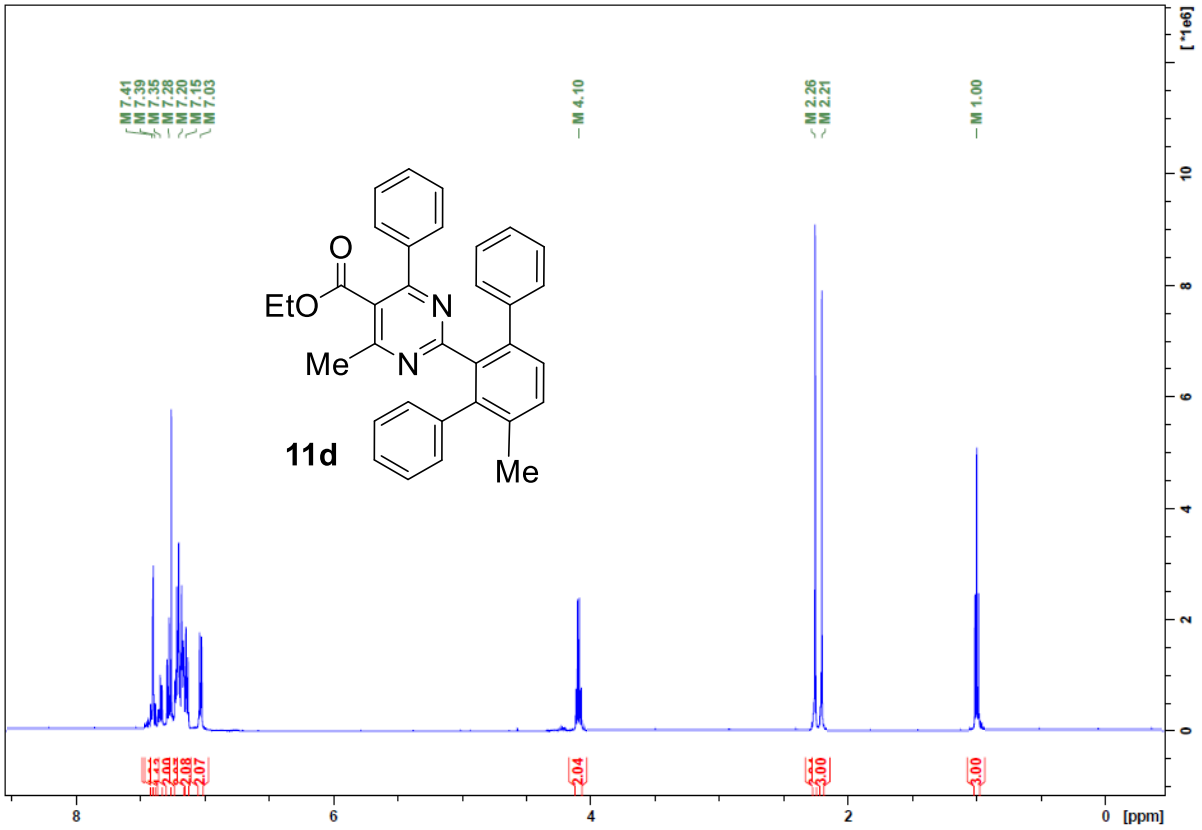

M 167.98
M 166.82
M 164.12
M 162.63
M 142.56
M 141.80
M 141.60
M 140.45
M 137.58
M 135.90
M 129.69
M 129.35
M 128.85
M 128.35
M 128.17
M 128.15
M 127.94
M 127.72
M 127.33
M 126.67
M 122.27
M 61.77
M 22.14
M 13.62
O
EtO
N
Me
N
11b
[*1e6]
150
100
50
[ppm]

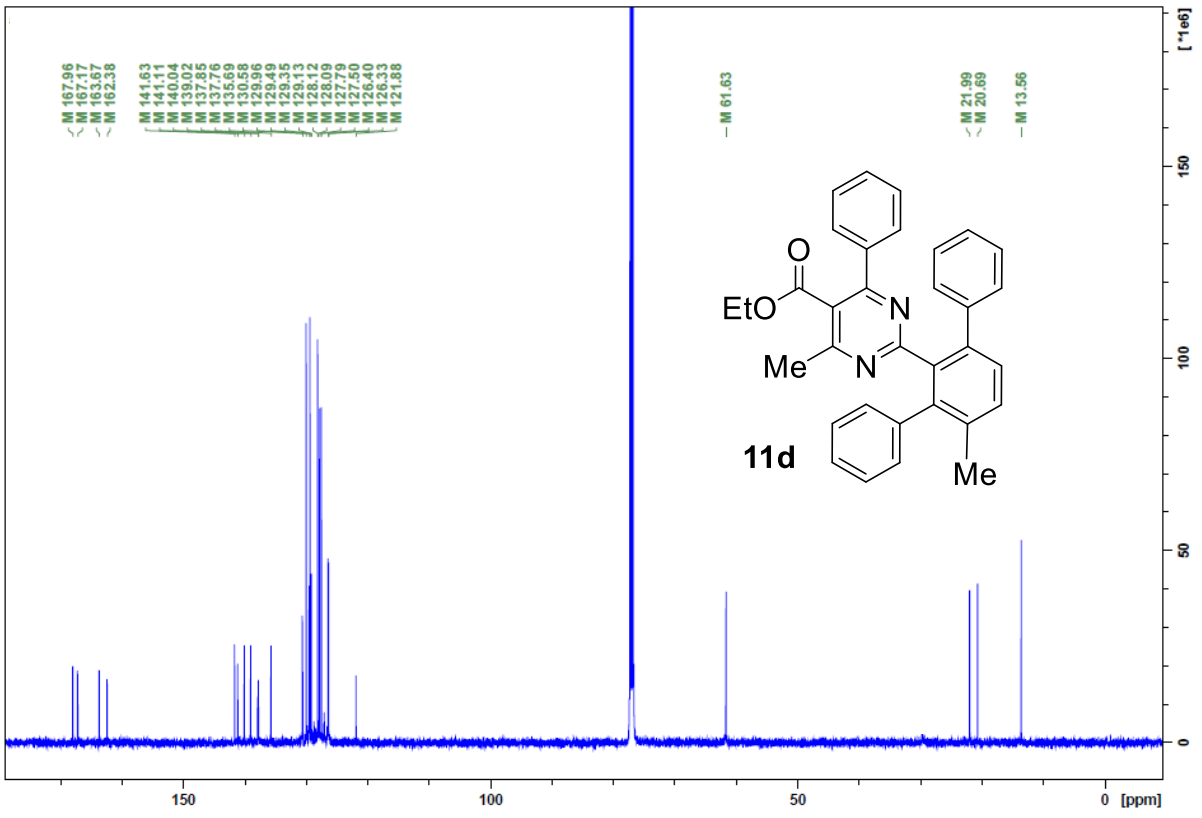

10c
O
EtO
N
Me
Me
N
M 7.31
M 7.30
M 7.26
M 7.24
M 7.22
M 7.19
M 7.15
M 7.12
M 7.06
M 4.12
M 2.49
M 2.27
M 1.01
2.03
2.00
3.00
3.01
3.05
8
6
4
2
0
[ppm]
[*1e6]

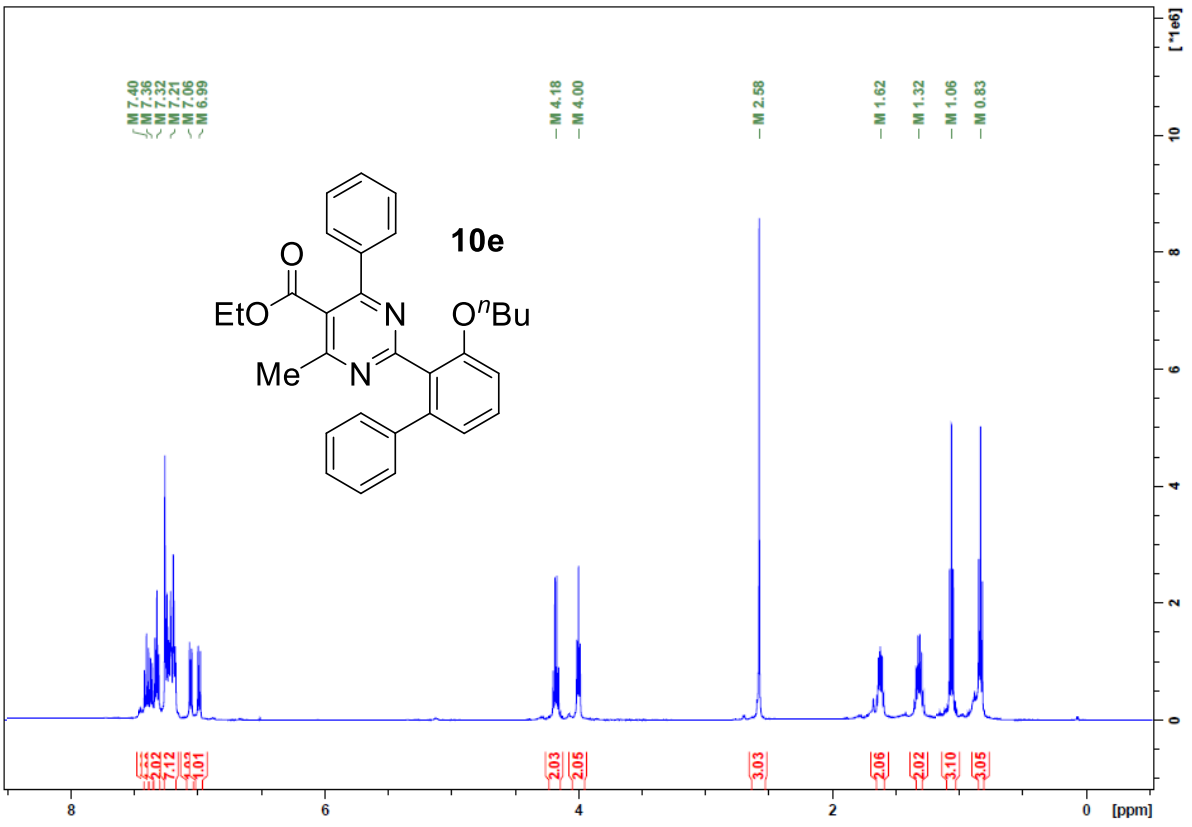

10c
O
EtO
N
Me
Me
N
M 168.07
M 167.26
M 164.44
M 162.99
M 141.84
M 141.54
M 137.69
M 137.51
M 136.31
M 129.78
M 129.65
M 129.19
M 128.80
M 128.28
M 128.23
M 127.81
M 127.79
M 126.39
M 122.74
M 61.84
M 22.50
M 20.38
M 13.63
150
100
50
0
[ppm]
[*1e6]

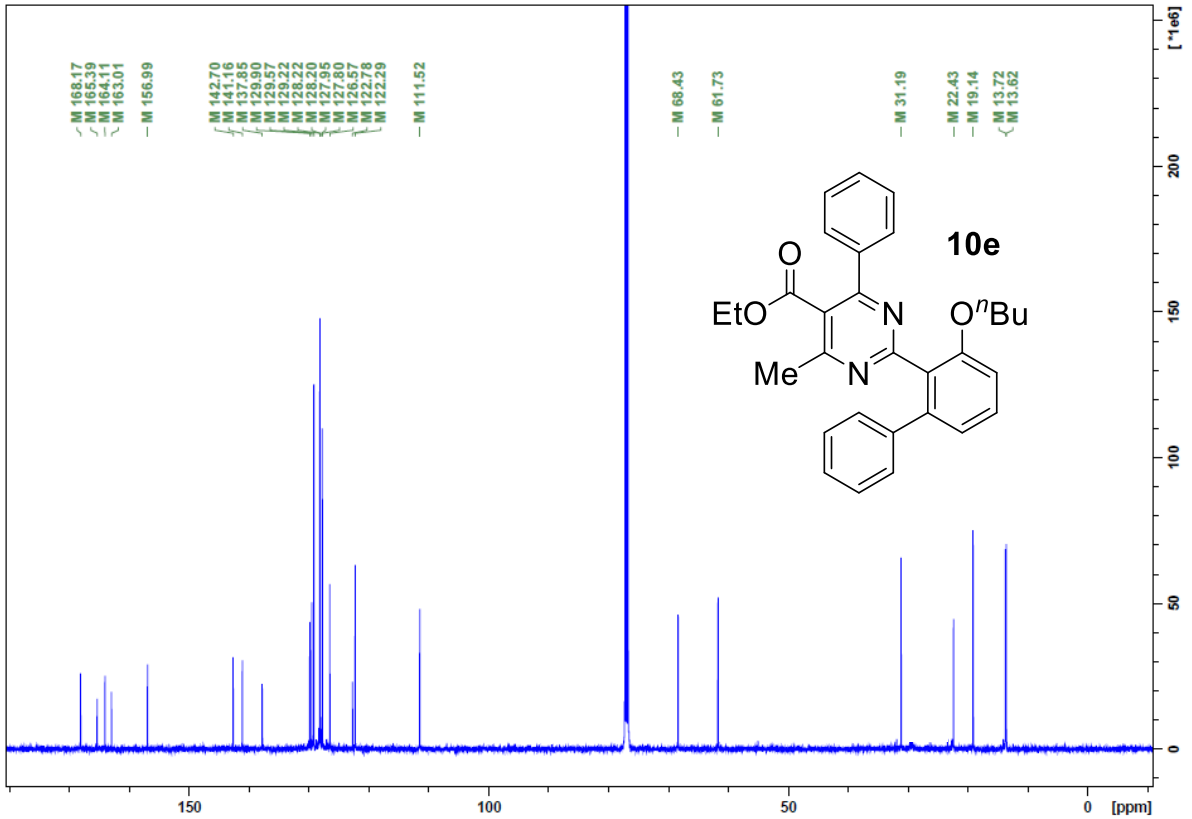

M 7.78
M 7.34
M 7.28
M 7.21
M 7.08
M 4.21
M 2.59
M 2.46
M 1.10
O
EtO
N
Me
N
10d
Me
1.00
2.03
2.05
2.03
3.01
3.01
3.03
8
6
4
2
0
[ppm]
[*1e6]

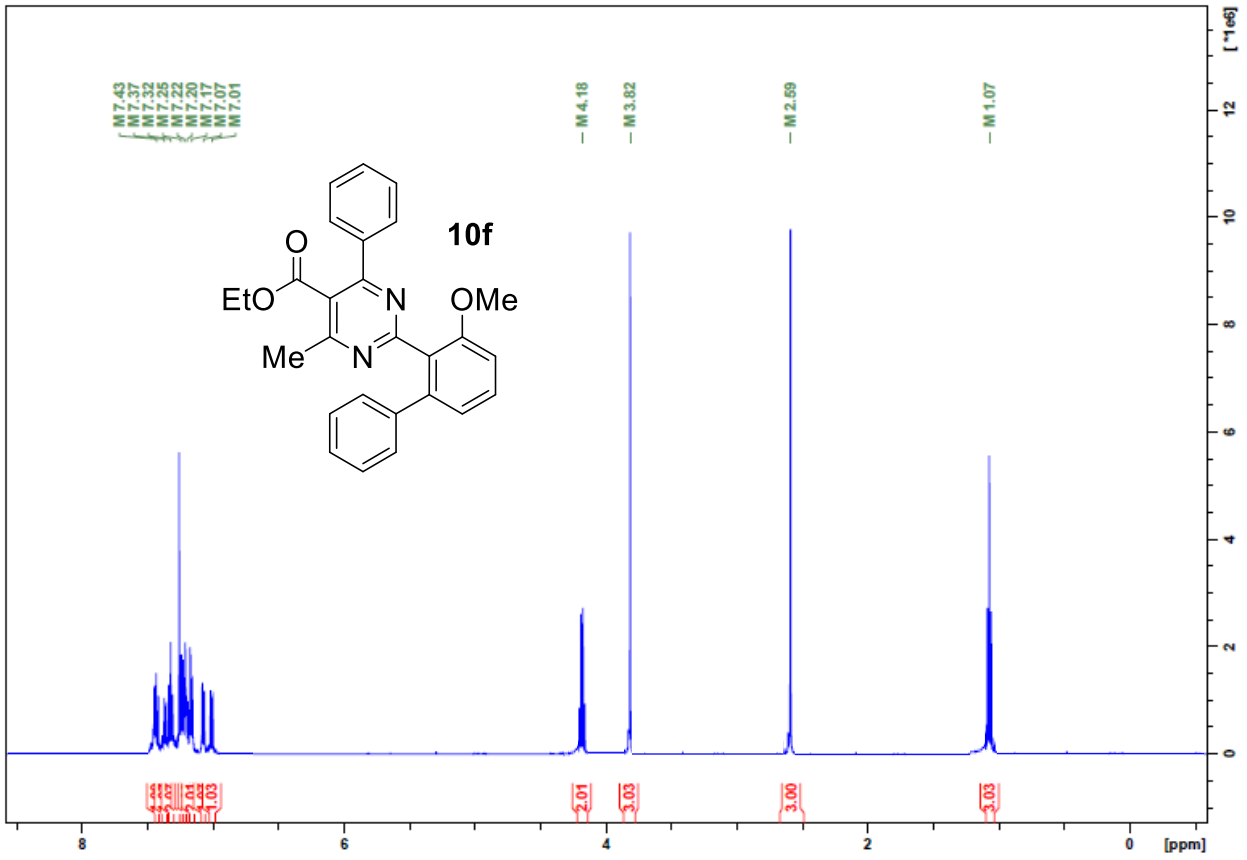

M 168.25
M 166.76
M 165.04
M 162.70
M 142.30
M 139.32
M 137.61
M 137.23
M 137.19
M 131.27
M 130.89
M 130.48
M 129.75
M 129.34
M 128.35
M 128.16
M 128.03
M 126.18
M 122.50
M 61.78
M 22.63
M 21.09
M 13.65
O
EtO
N
Me
N
10d
Me
150
100
50
0 [ppm]
[*1e6]

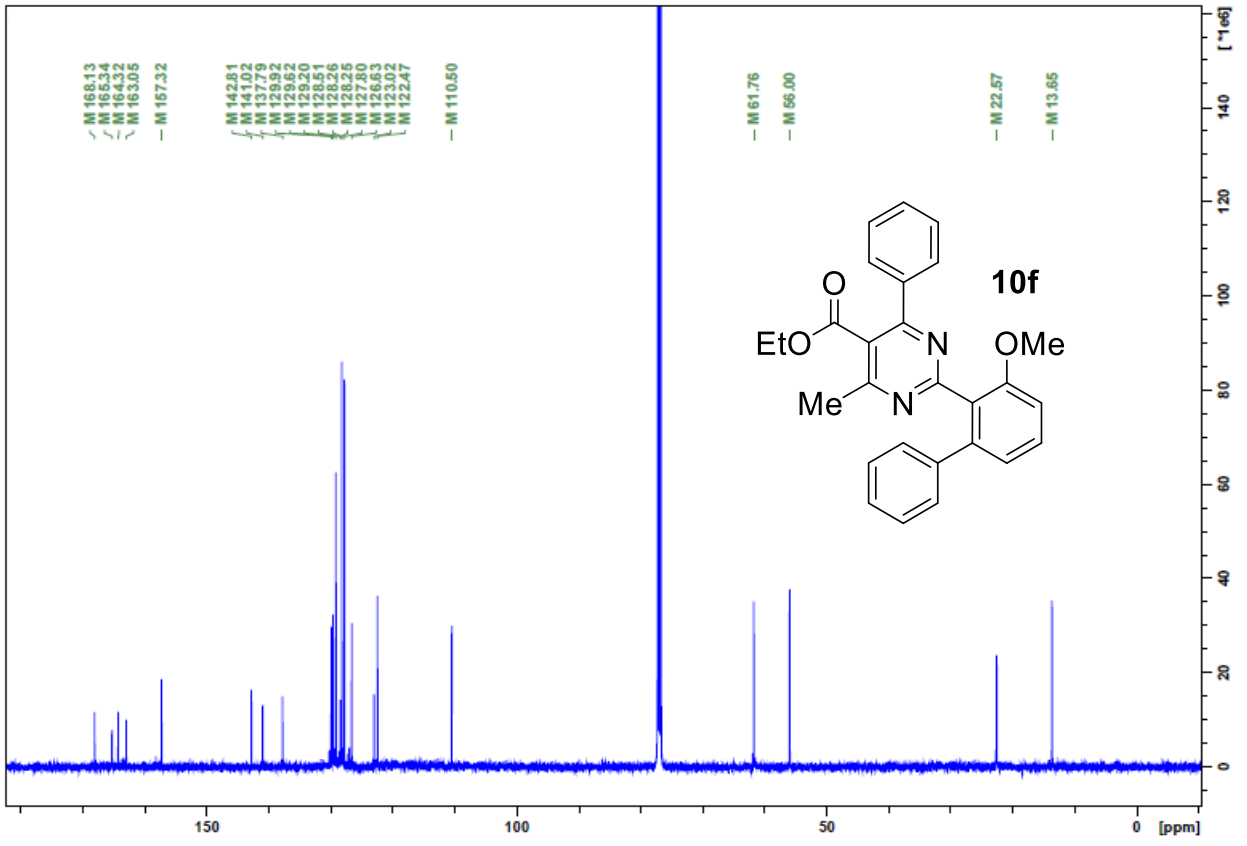

M 7.41
M 7.39
M 7.35
M 7.28
M 7.20
M 7.15
M 7.03
M 4.10
M 2.26
M 2.21
M 1.00
O
EtO
N
Me
N
11d
Me
2.04
2.01
3.00
3.00
[*1e6]
8
6
4
2
0 [ppm]

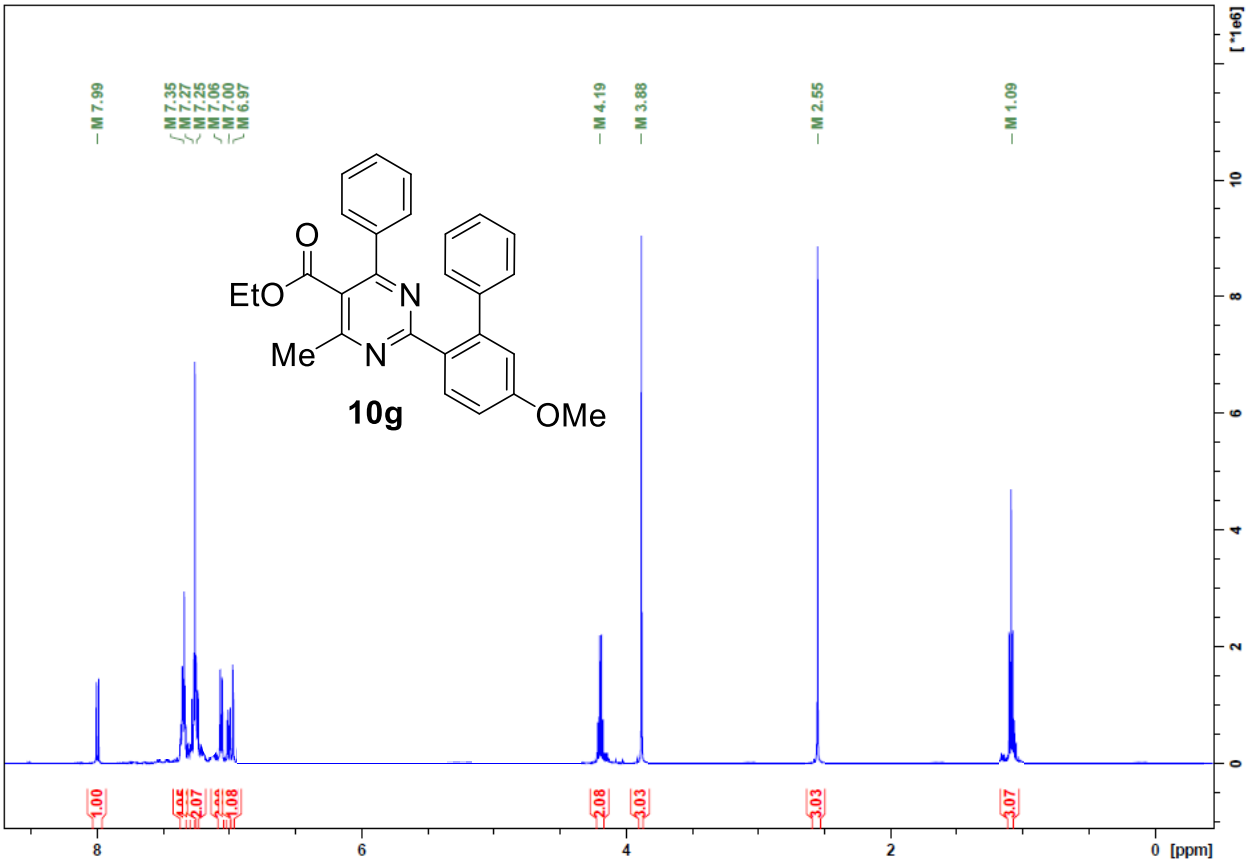

M 167.96
M 167.17
M 163.87
M 162.38
M 141.63
M 141.11
M 140.04
M 139.02
M 137.85
M 137.76
M 135.69
M 130.58
M 129.96
M 129.49
M 129.35
M 129.13
M 128.12
M 128.09
M 127.79
M 127.50
M 126.40
M 126.33
M 121.88
M 61.63
M 21.99
M 20.69
M 13.56
O
EtO
N
Me
N
11d
Me
[*1e6]
150
100
50
0 [ppm]

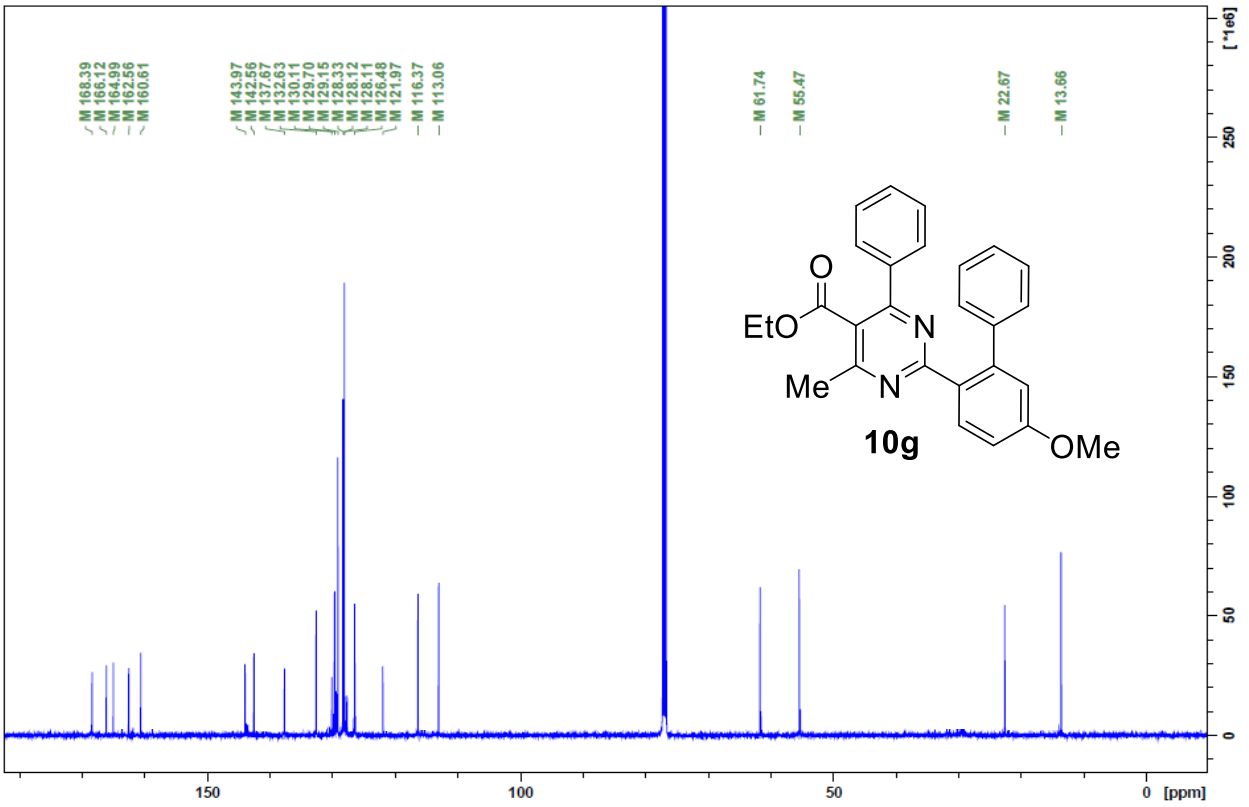

M 7.40
M 7.36
M 7.32
M 7.21
M 7.06
M 6.99
M 4.18
M 4.00
M 2.58
M 1.62
M 1.32
M 1.06
M 0.83
10e
EtO
O
N
O^{n}Bu
Me
N
2.03
2.05
3.03
2.06
2.02
3.10
3.05
[ppm]

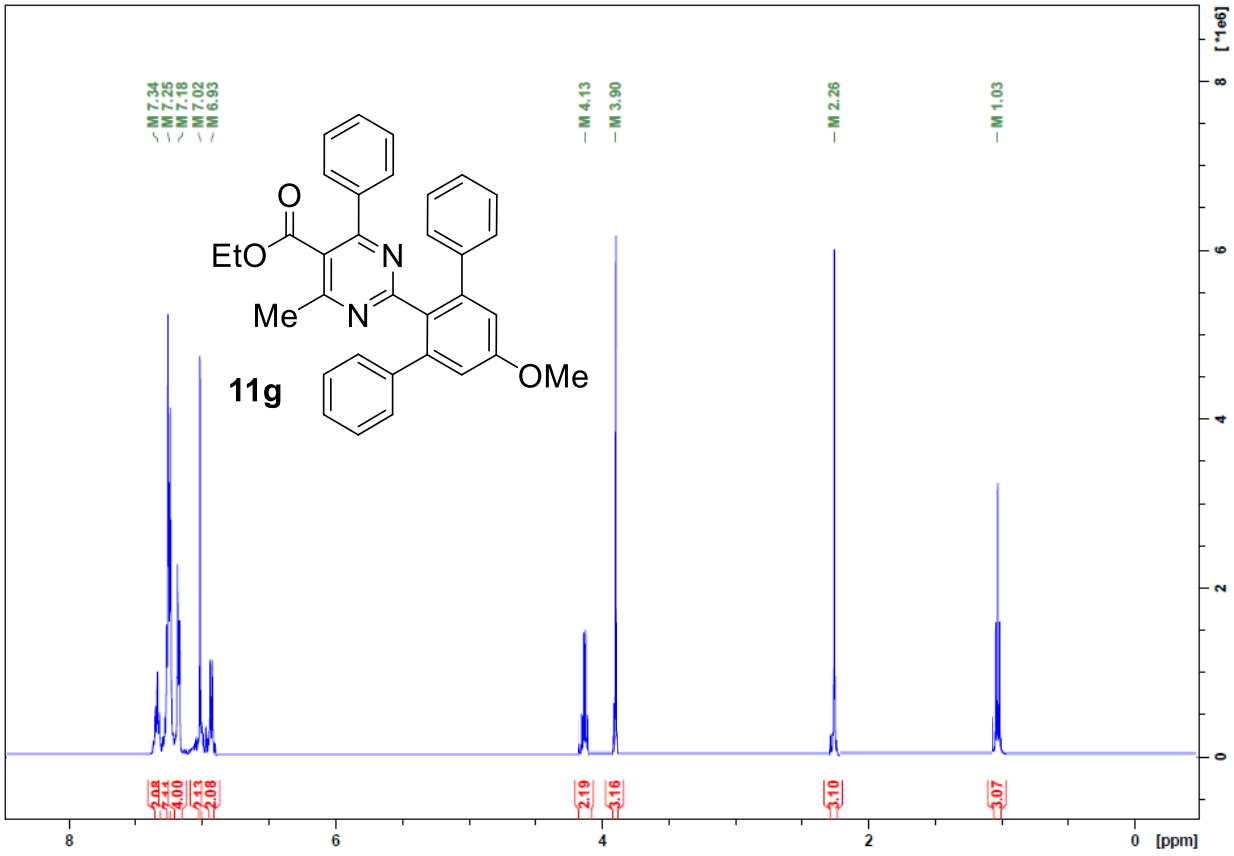

M 168.17
M 165.39
M 164.11
M 163.01
M 156.99
M 142.70
M 141.16
M 137.85
M 129.90
M 129.57
M 129.22
M 128.20
M 127.85
M 127.80
M 126.57
M 122.78
M 122.29
M 111.52
M 68.43
M 61.73
M 31.19
M 22.43
M 19.14
M 13.72
M 13.62
10e
EtO
O
N
O^{n}Bu
Me
N
[ppm]

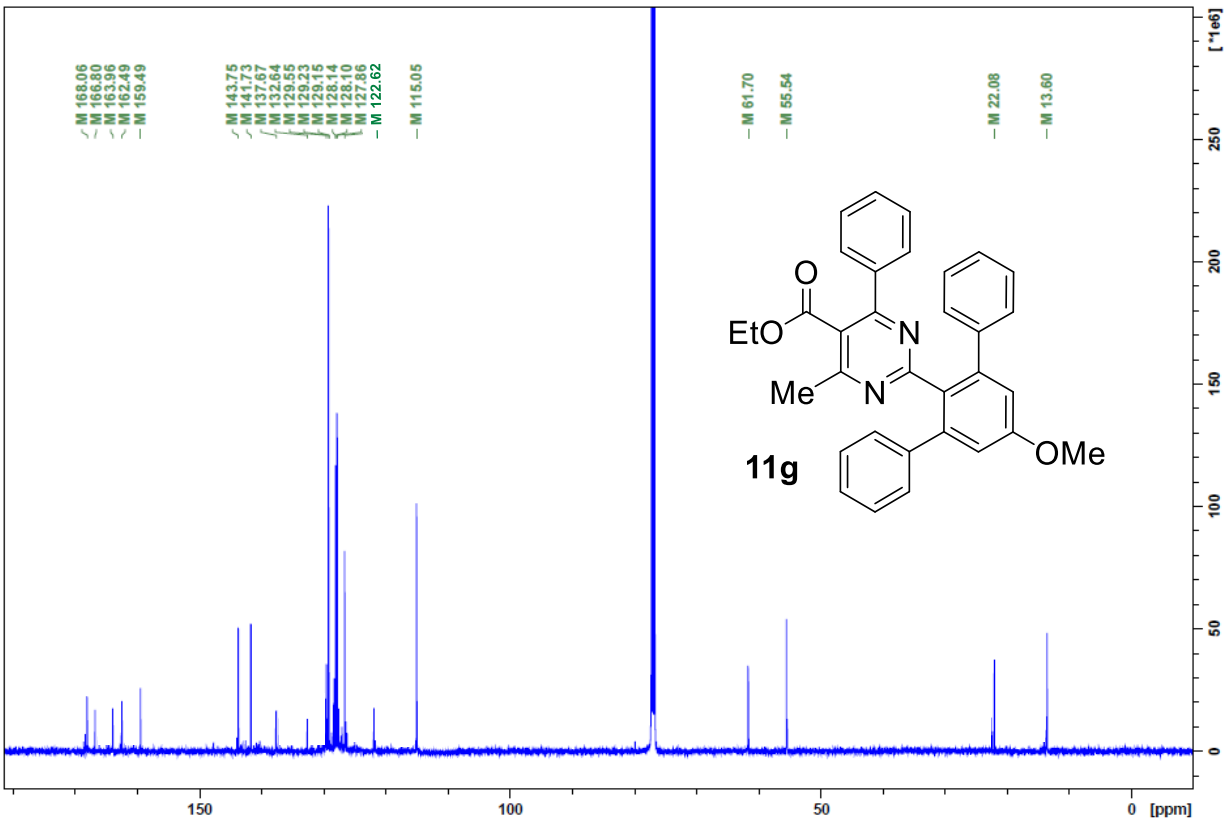

M 7.43
M 7.37
M 7.32
M 7.25
M 7.22
M 7.20
M 7.17
M 7.07
M 7.01
M 4.18
M 3.82
M 2.59
M 1.07
10f
O
EtO
N
OMe
Me
N
2.01
3.03
3.00
3.03
[*1e6]
[ppm]

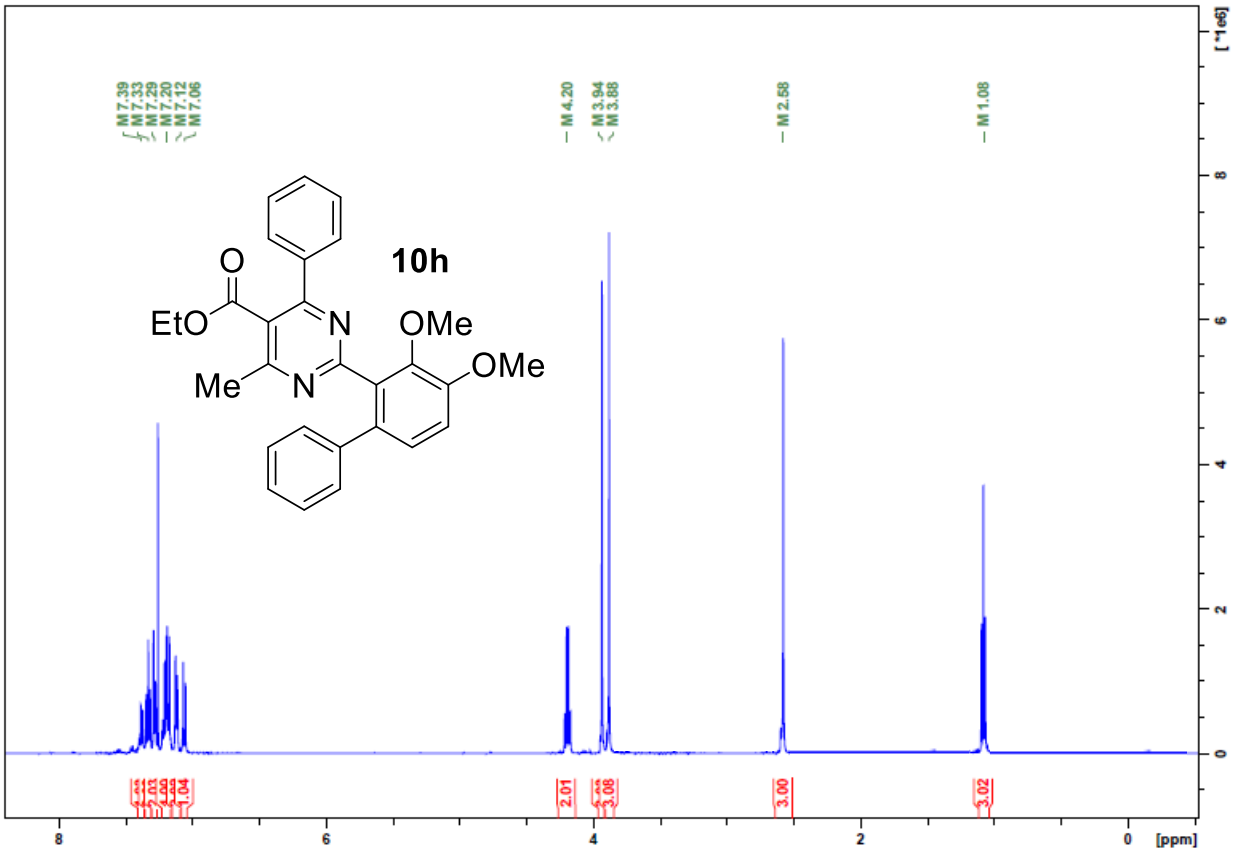

M 168.13
M 165.34
M 164.32
M 163.05
M 157.32
M 142.81
M 141.02
M 137.79
M 129.92
M 129.62
M 129.20
M 128.51
M 128.26
M 128.25
M 127.80
M 126.63
M 123.02
M 122.47
M 110.50
M 61.76
M 56.00
M 22.57
M 13.65
10f
O
EtO
N
OMe
Me
N
[*1e6]
[ppm]

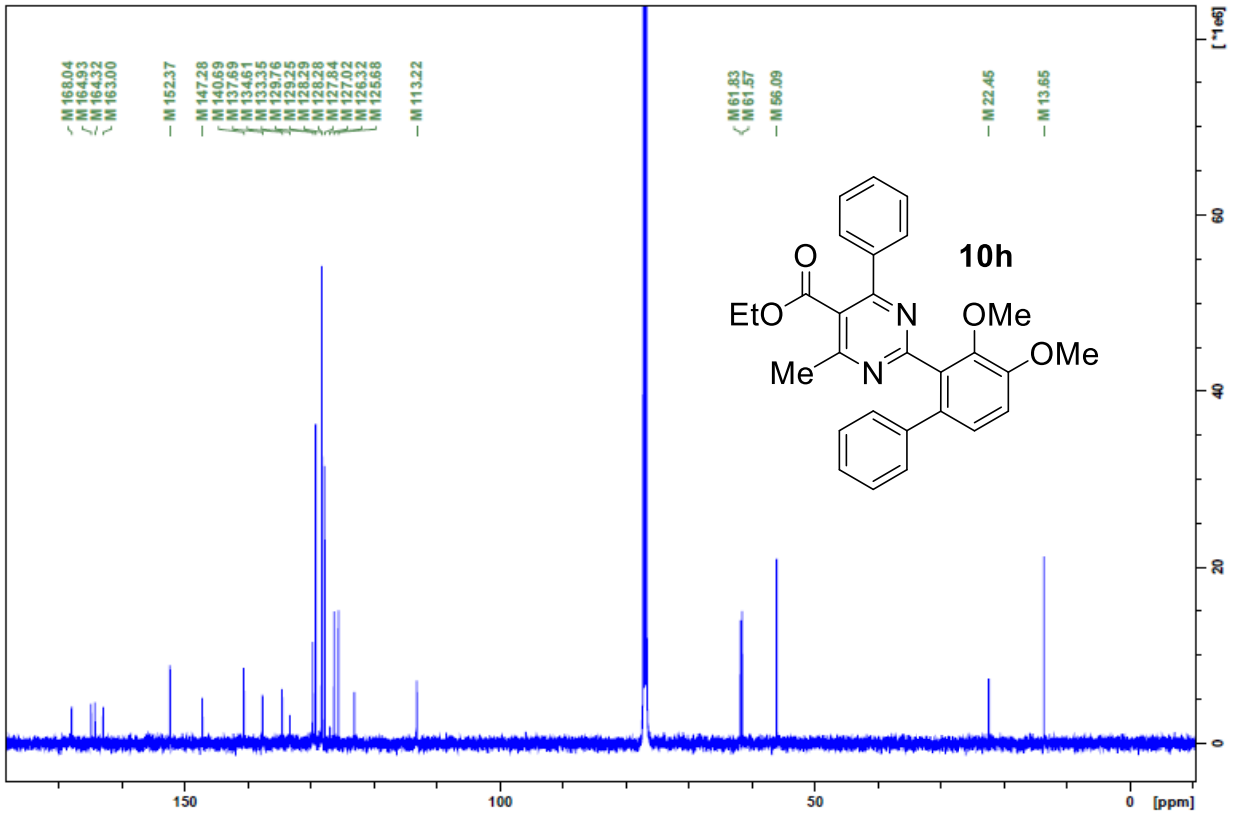

M 7.99
M 7.35
M 7.27
M 7.25
M 7.06
M 7.00
M 6.97
M 4.19
M 3.88
M 2.55
M 1.09
EtO
O
N
Me
N
OMe
10g
1.00
2.07
1.08
2.08
3.03
3.03
3.07
8
6
4
2
0 [ppm]
[*1e6]

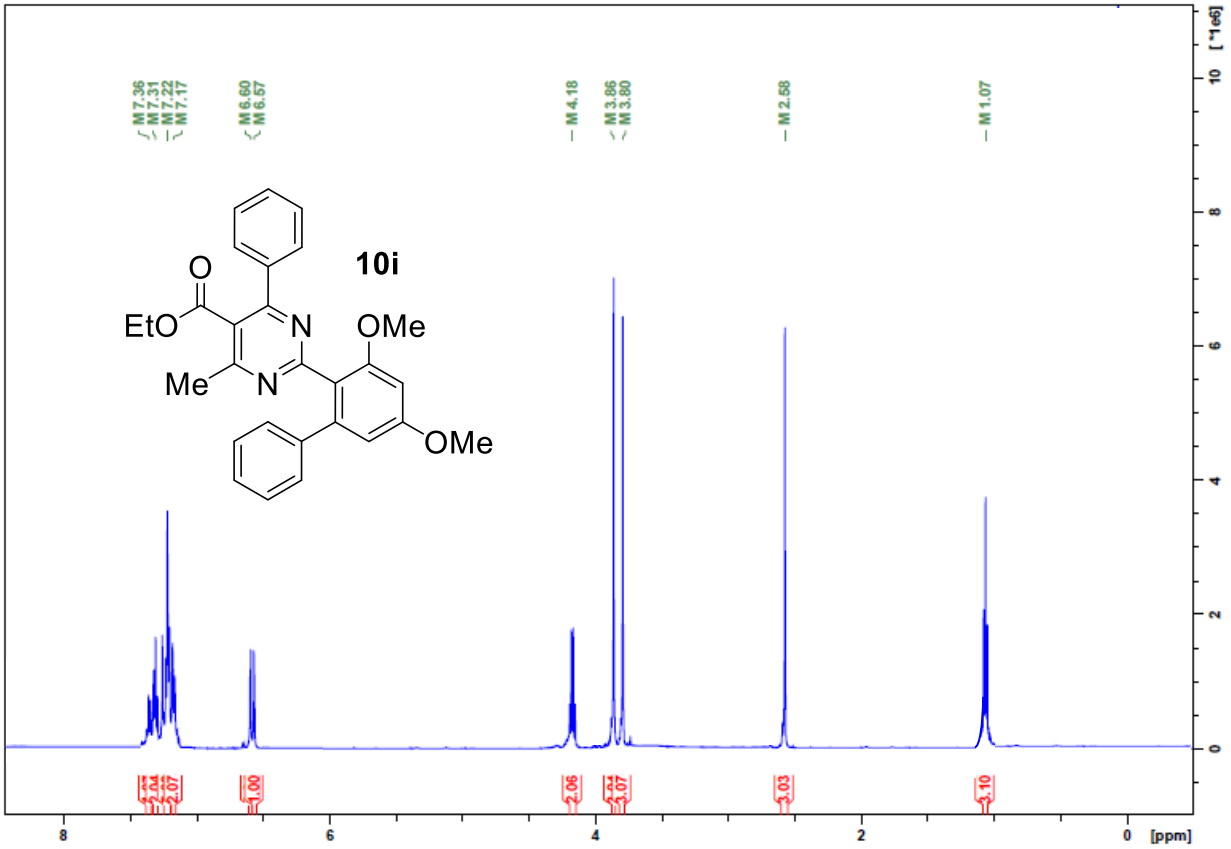

M 168.39
M 166.12
M 164.99
M 162.56
M 160.61
M 143.97
M 142.56
M 137.67
M 132.63
M 130.11
M 129.70
M 129.15
M 128.33
M 128.12
M 128.11
M 126.48
M 121.97
M 116.37
M 113.06
M 61.74
M 55.47
M 22.67
M 13.66
EtO
O
N
Me
N
OMe
10g
150
100
50
0 [ppm]
[*1e6]

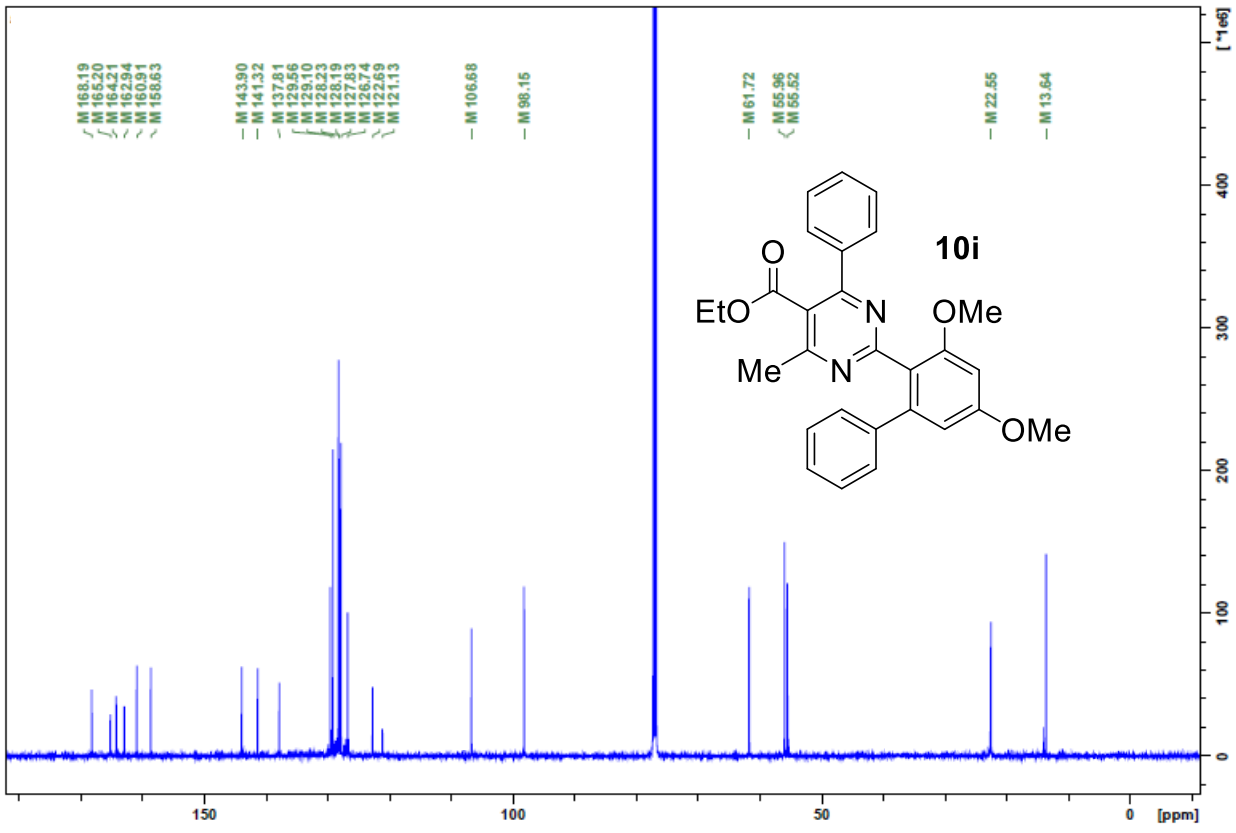

M 7.34
M 7.25
M 7.18
M 7.02
M 6.93
M 4.13
M 3.90
M 2.26
M 1.03
EtO
Me
N
N
O
OMe
11g
2.19
3.16
3.10
3.07
8
6
4
2
0
[ppm]
[*1e6]

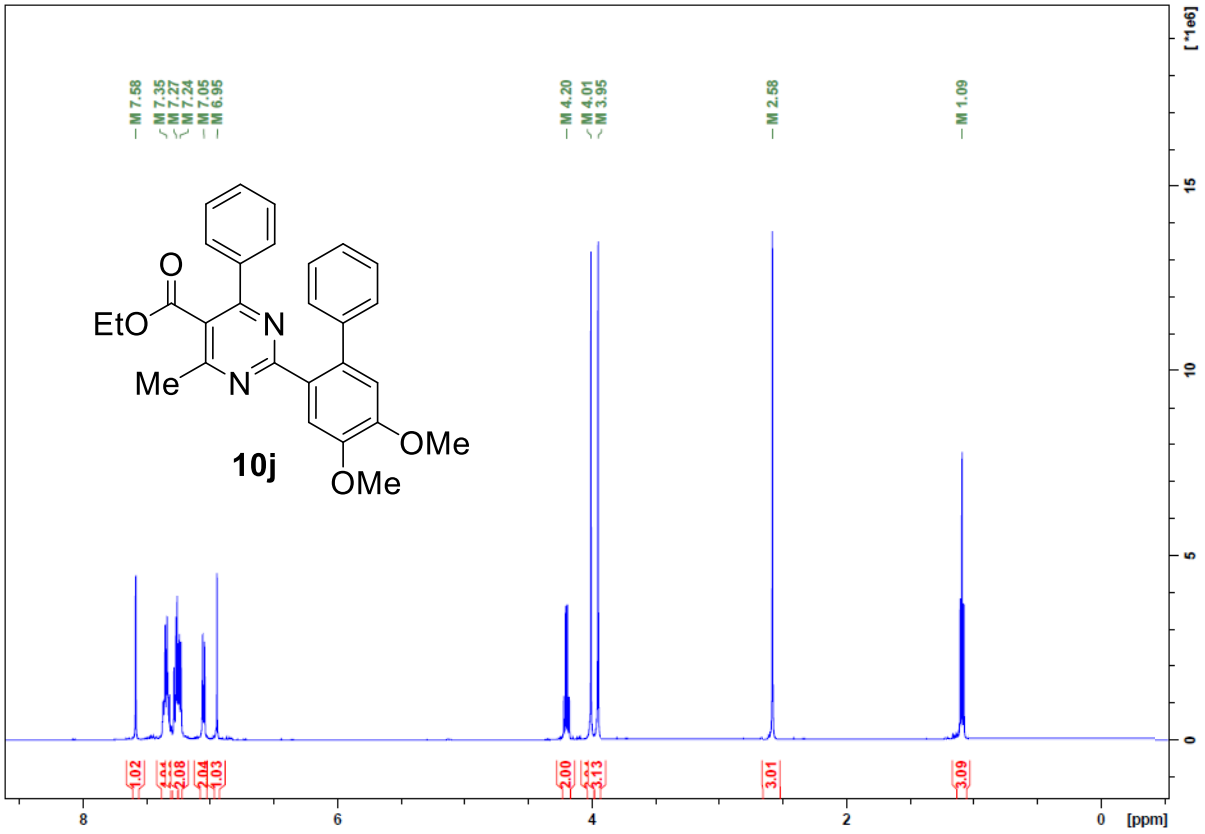

M 168.06
M 166.80
M 163.96
M 162.49
M 159.49
M 143.75
M 141.73
M 137.67
M 132.64
M 129.55
M 129.23
M 128.15
M 128.14
M 125.10
M 127.86
M 122.62
M 115.05
M 61.70
M 55.54
M 22.08
M 13.60
EtO
Me
N
N
O
OMe
11g
150
100
50
0
[ppm]
[*1e6]

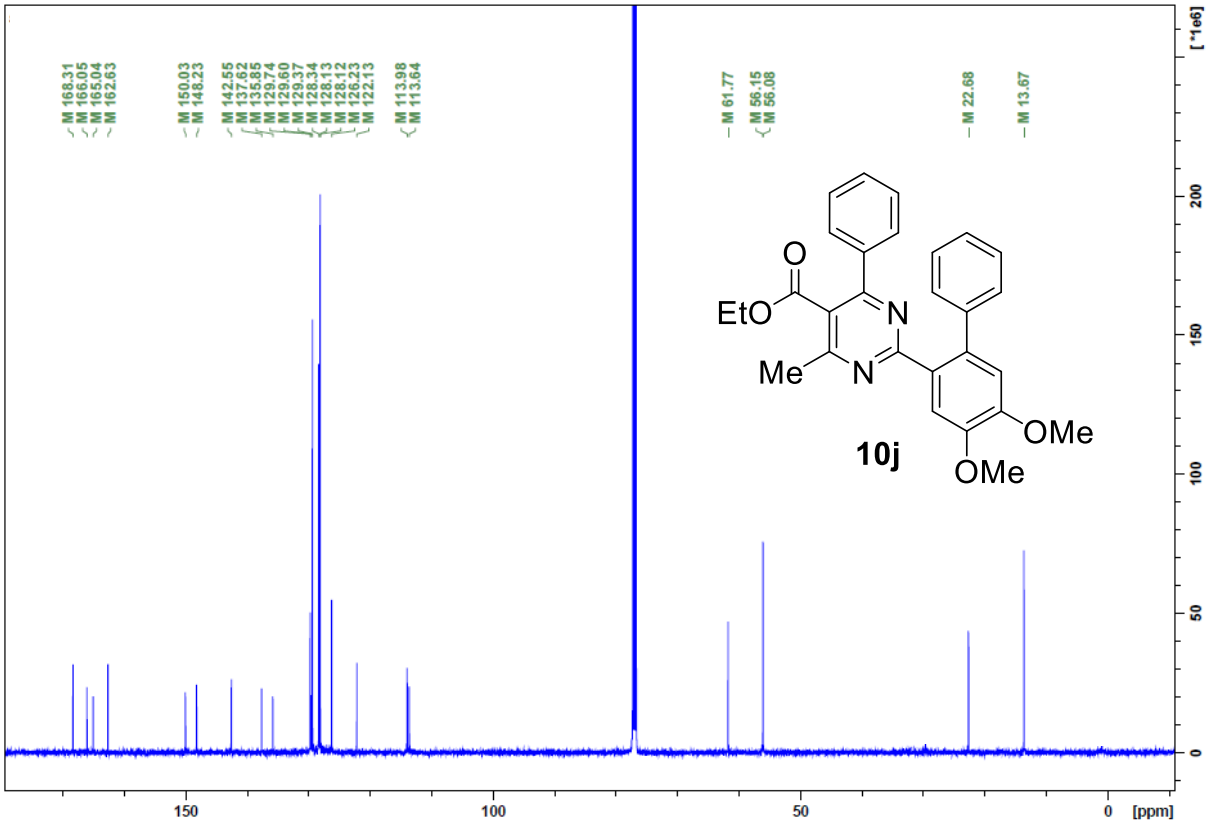

M 7.39
M 7.33
M 7.29
M 7.20
M 7.12
M 7.06
M 4.20
M 3.94
M 3.88
M 2.58
M 1.08
10h
O
EtO
N
OMe
Me
N
OMe
2.01
3.08
3.00
3.02
8
6
4
2
0
[ppm]
[*1e6]

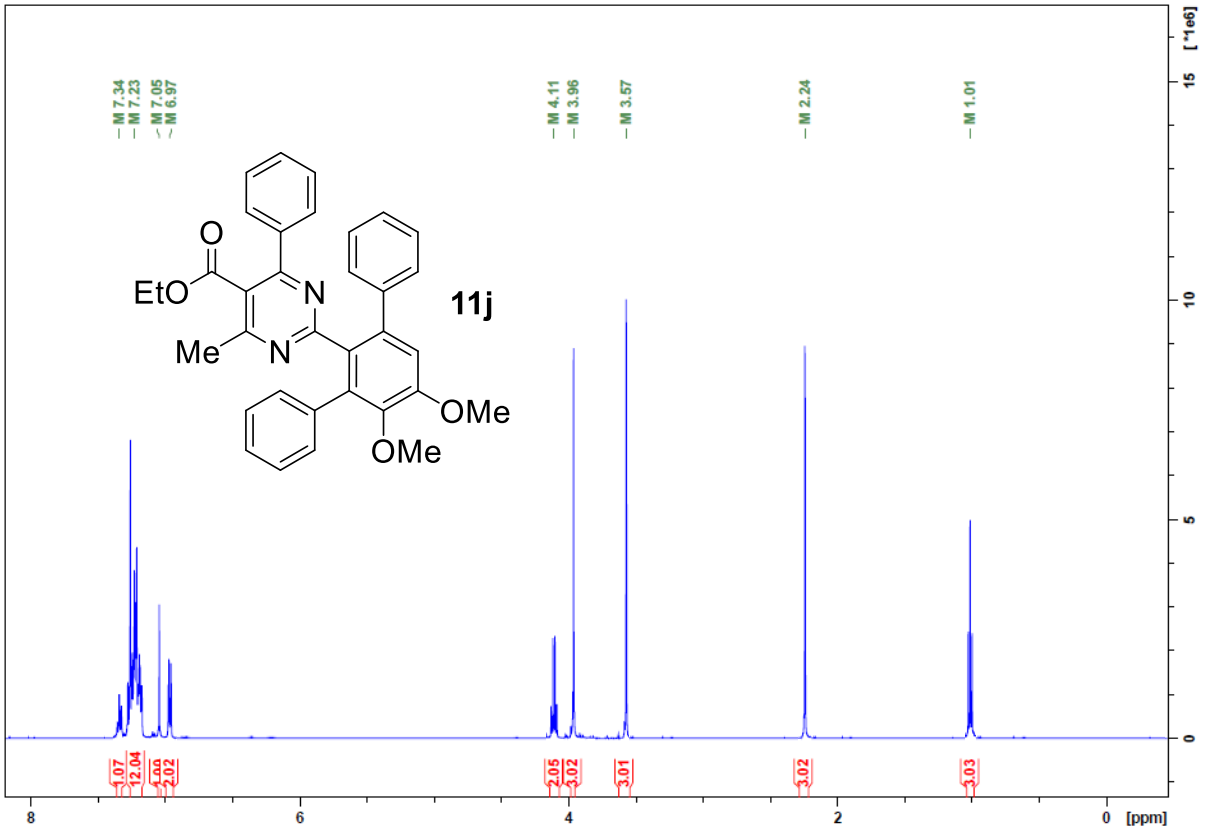

M 168.04
M 164.93
M 164.32
M 163.00
M 152.37
M 147.28
M 140.69
M 137.69
M 134.61
M 133.35
M 129.76
M 129.25
M 128.29
M 128.28
M 127.84
M 127.02
M 126.32
M 125.68
M 113.22
M 61.83
M 61.57
M 56.09
M 22.45
M 13.55
10h
O
EtO
N
OMe
Me
N
OMe
150
100
50
0
[ppm]
[*1e6]

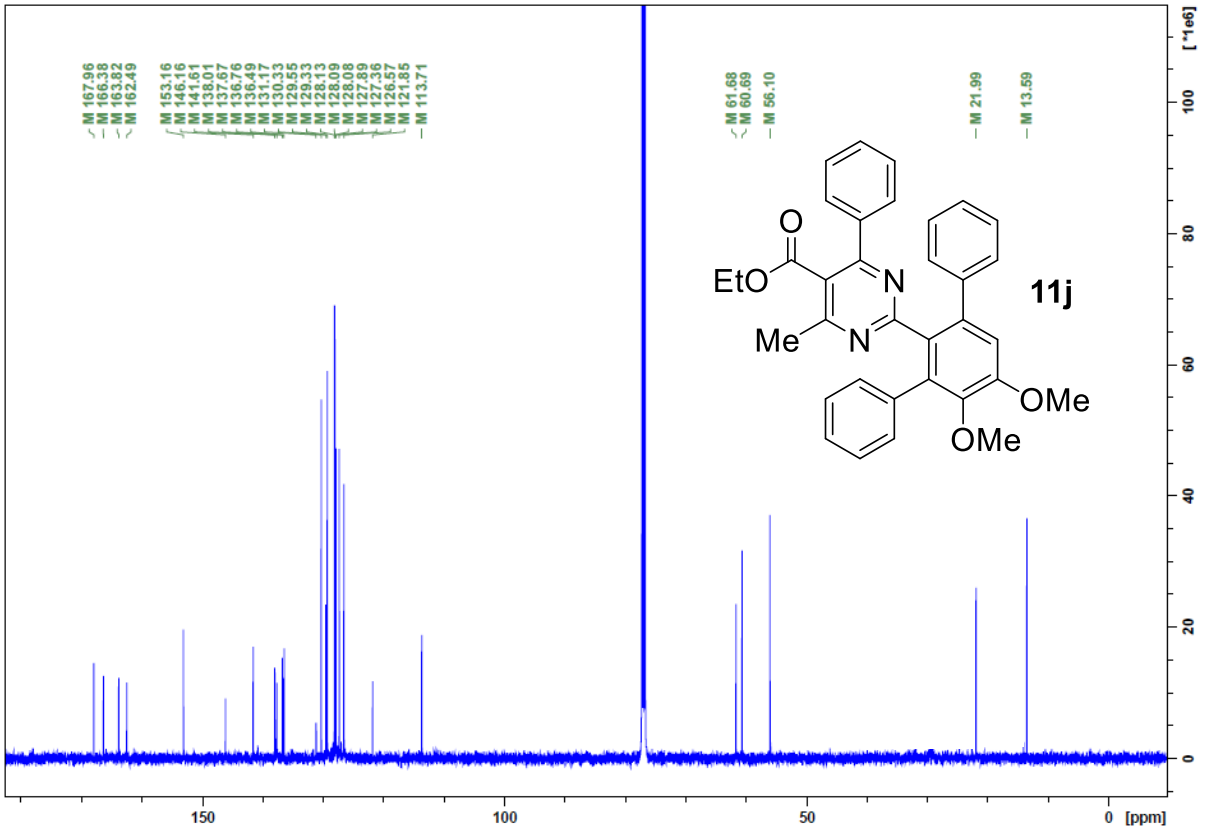

M 7.36
M 7.31
M 7.22
M 7.17
M 6.60
M 6.57
M 4.18
M 3.86
M 3.80
M 2.58
M 1.07
10i
O
EtO
N
OMe
Me
N
OMe
2.33
2.44
2.07
1.00
2.06
3.07
3.03
3.10
8
6
4
2
0
[ppm]
[*1e6]

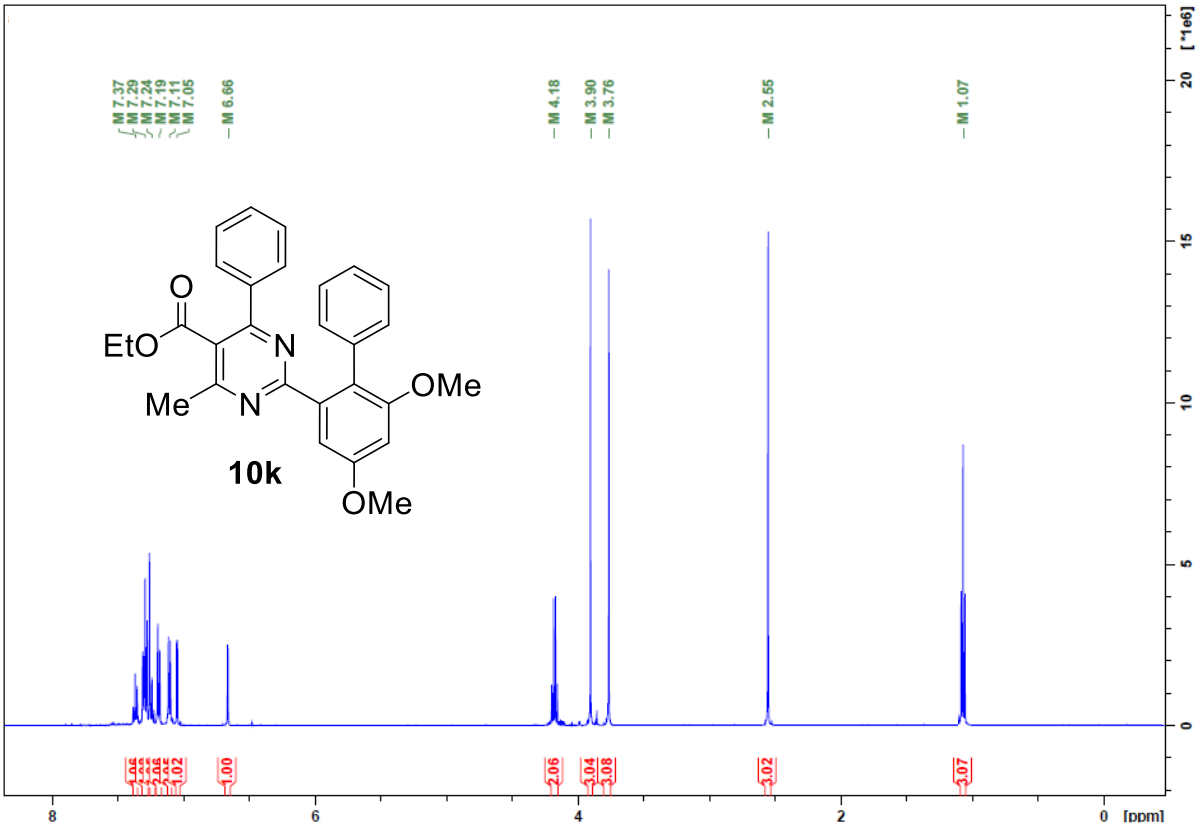

M 168.19
M 165.20
M 164.21
M 162.94
M 160.91
M 158.63
M 143.90
M 141.32
M 137.81
M 129.56
M 129.10
M 128.23
M 128.19
M 127.83
M 127.74
M 126.74
M 122.69
M 121.13
M 106.68
M 98.15
M 61.72
M 55.96
M 55.52
M 22.55
M 13.64
10i
O
EtO
N
OMe
Me
N
OMe
150
100
50
0
[ppm]
[*1e6]

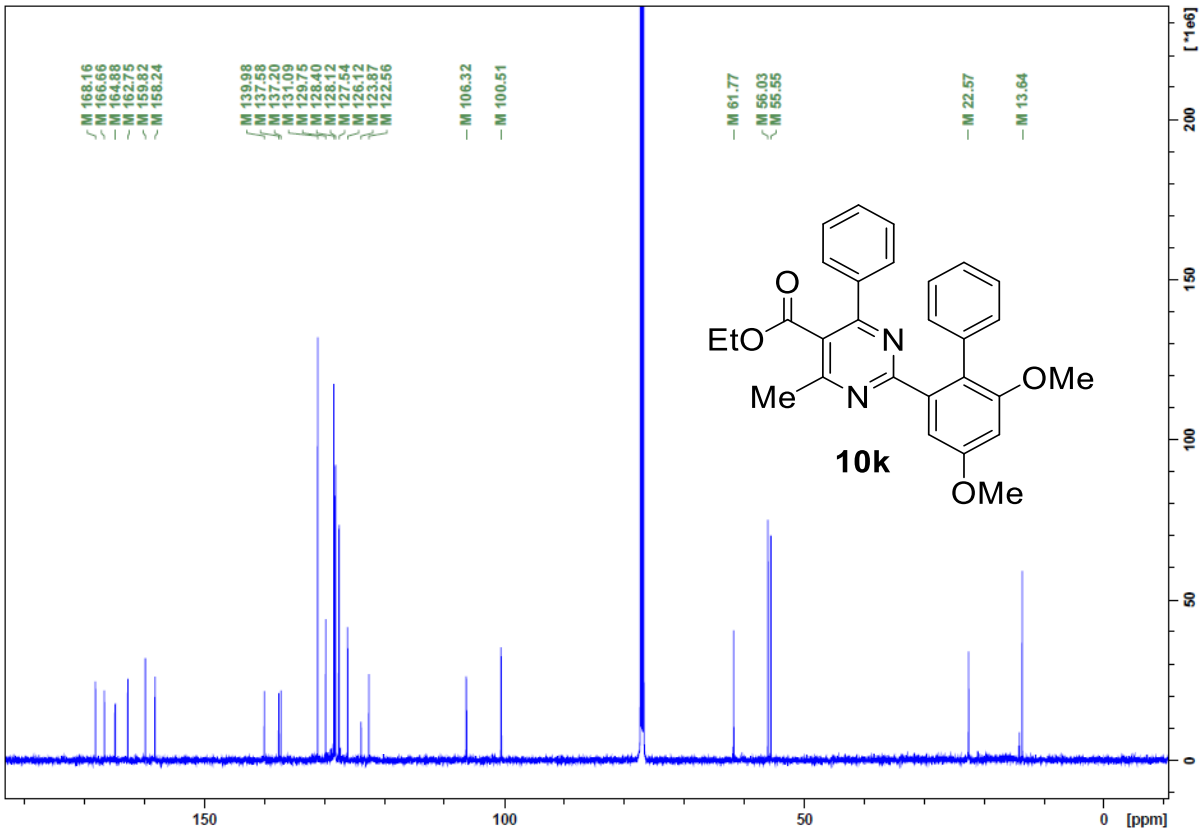

M 7.58
M 7.35
M 7.27
M 7.24
M 7.05
M 6.95
M 4.20
M 4.01
M 3.95
M 2.58
M 1.09
O
EtO
N
Me
N
OMe
OMe
10j
1.02
2.08
2.04
1.03
2.00
3.01
3.09
[*1e6]
15
10
5
0
8
6
4
2
0
[ppm]

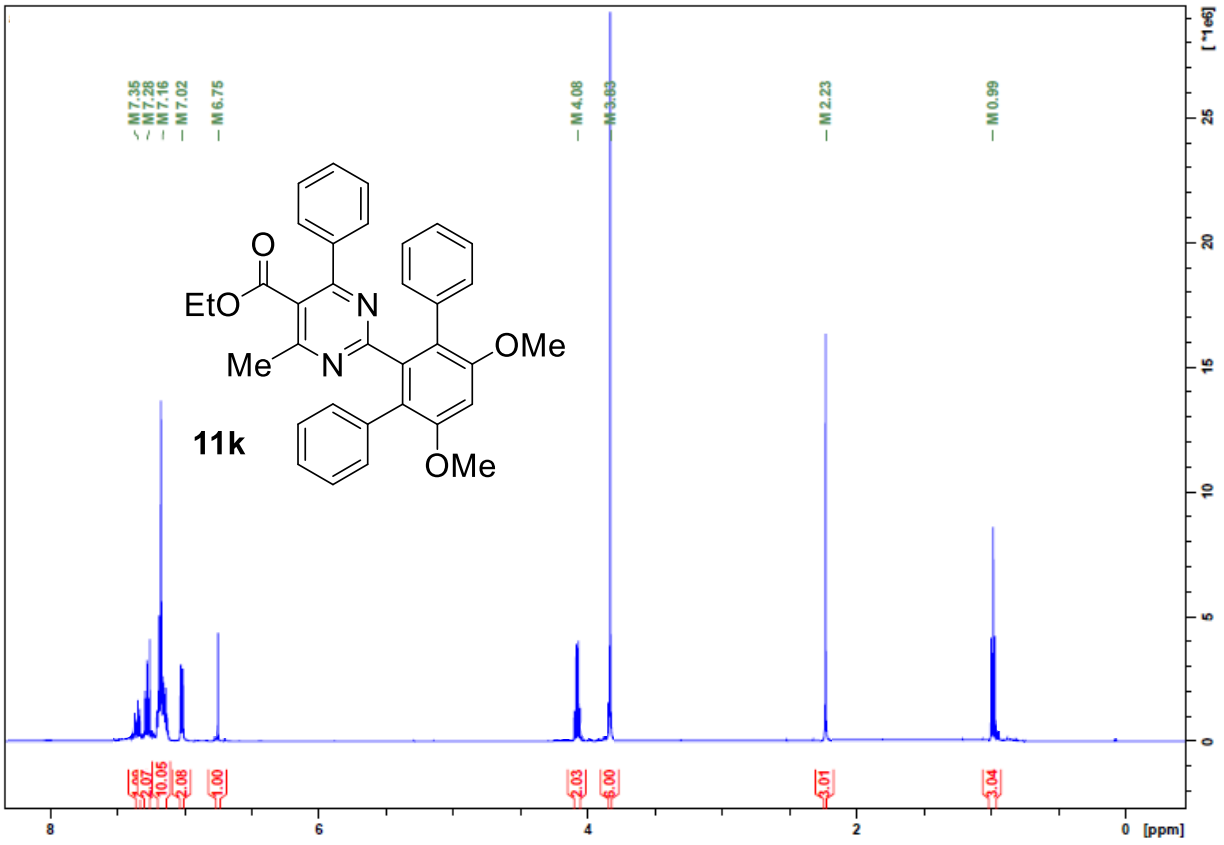

M 168.31
M 166.05
M 165.04
M 162.63
M 150.03
M 148.23
M 142.55
M 137.62
M 135.85
M 129.74
M 129.60
M 129.37
M 128.34
M 128.13
M 128.12
M 126.23
M 122.13
M 113.98
M 113.64
M 61.77
M 56.15
M 56.08
M 22.68
M 13.67
O
EtO
N
Me
N
OMe
OMe
10j
[*1e6]
200
150
100
50
0
150
100
50
0
[ppm]

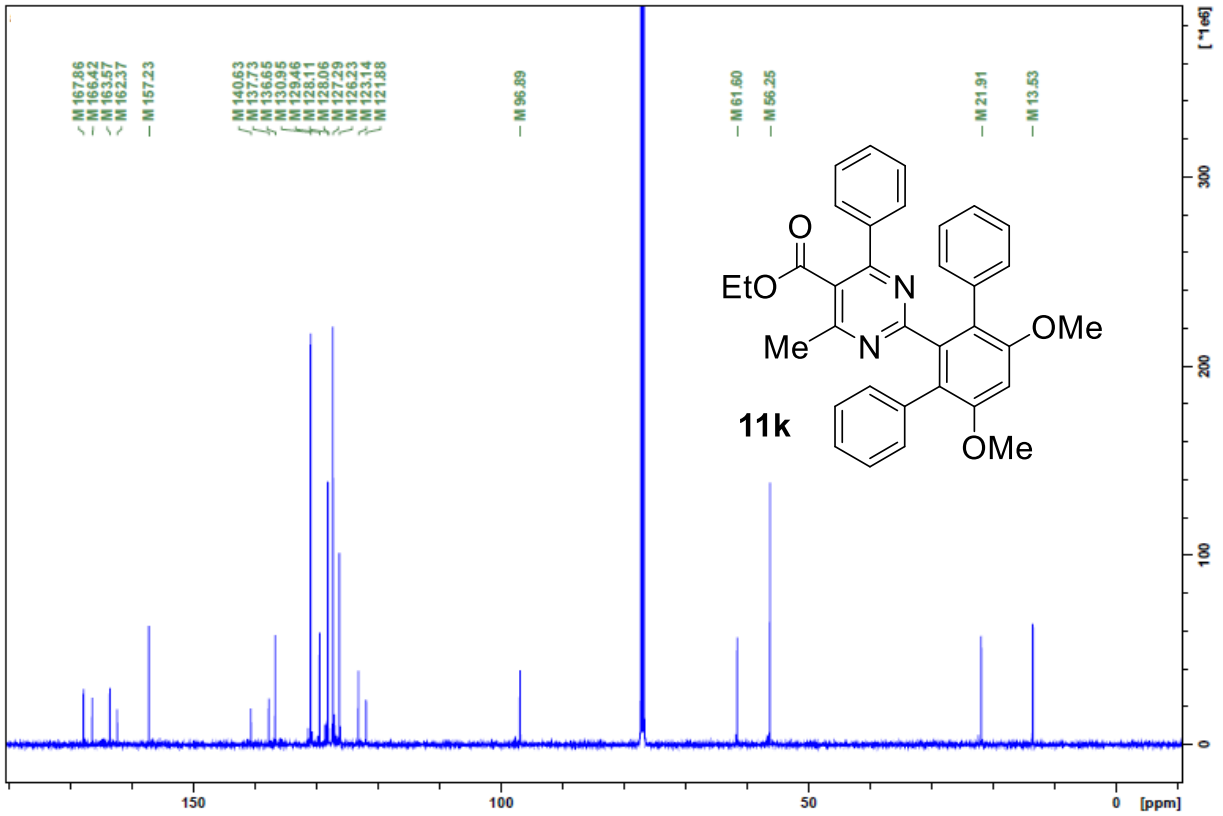

M 7.34
M 7.23
M 7.05
M 6.97
M 4.11
M 3.96
M 3.57
M 2.24
M 1.01
O
EtO
N
Me
N
11j
OMe
OMe
1.07
12.04
1.06
2.02
2.05
3.02
3.01
3.02
3.03
8
6
4
2
0 [ppm]
[*1e6]
15
10
5
0

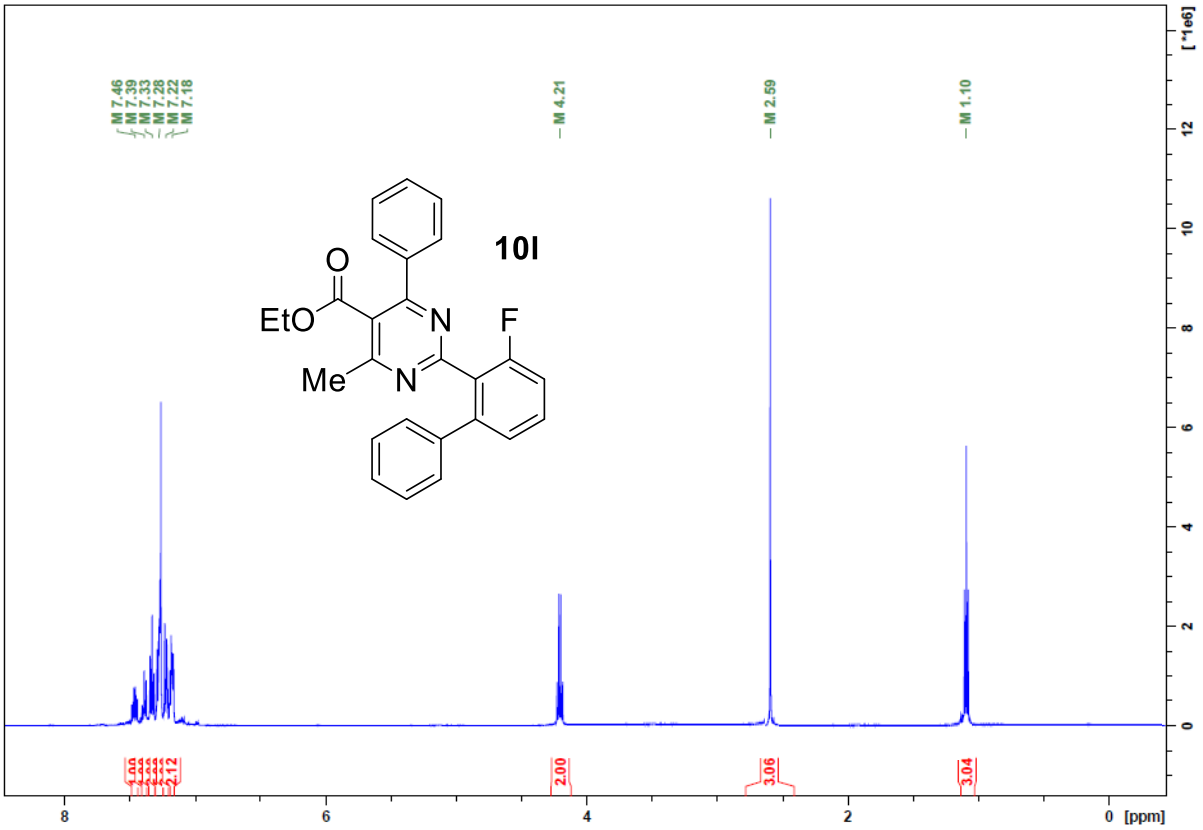

M 167.96
M 166.38
M 163.82
M 162.49
M 153.16
M 146.16
M 141.61
M 138.01
M 137.67
M 136.76
M 136.49
M 131.17
M 130.33
M 129.55
M 129.33
M 128.13
M 128.09
M 128.08
M 127.89
M 127.36
M 126.57
M 121.85
M 113.71
M 61.68
M 60.69
M 56.10
M 21.99
M 13.59
O
EtO
N
Me
N
11j
OMe
OMe
150
100
50
0 [ppm]
[*1e6]
100
80
60
40
20
0

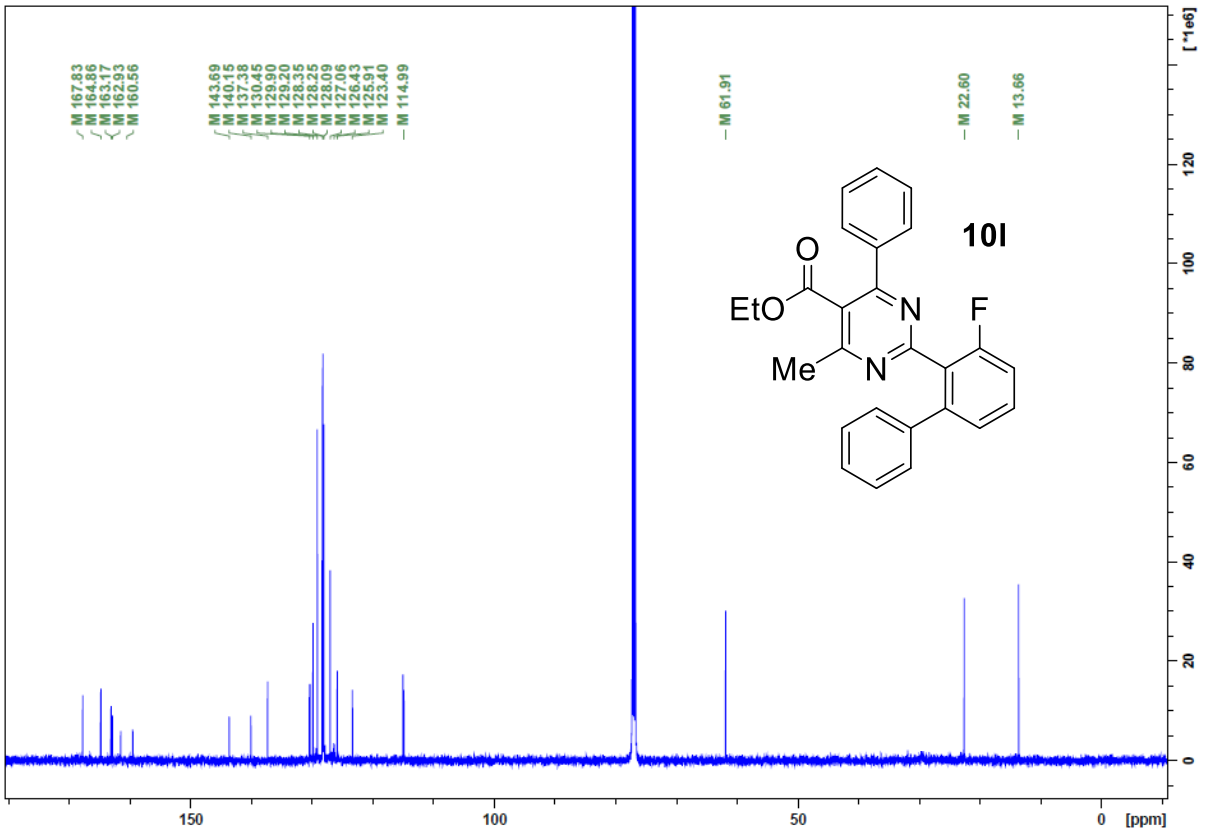

M 7.37
M 7.29
M 7.24
M 7.19
M 7.11
M 7.05
M 6.66
M 4.18
M 3.90
M 3.76
M 2.55
M 1.07
O
EtO
N
Me
N
OMe
OMe
10k
[*1e6]
20
15
10
5
0
8
6
4
2
0
[ppm]

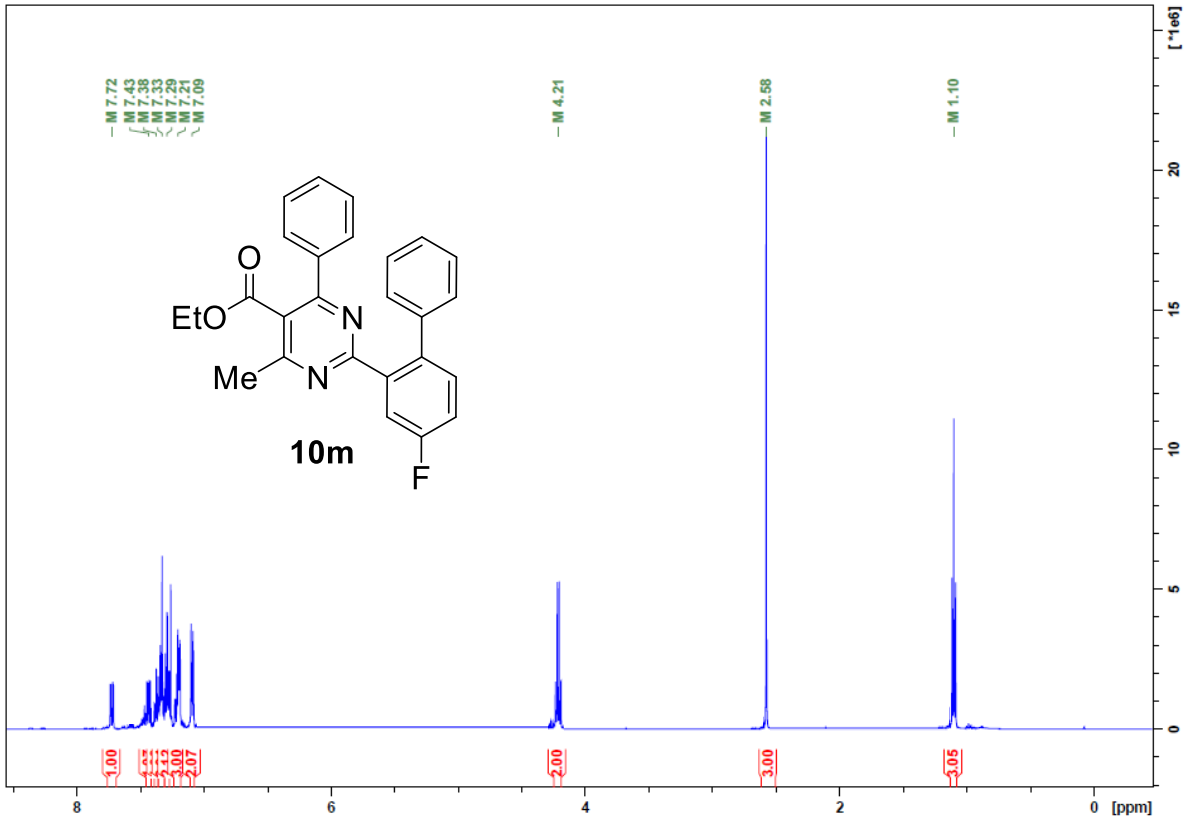

M 168.16
M 166.66
M 164.88
M 162.75
M 159.82
M 158.24
M 139.98
M 137.58
M 137.20
M 131.09
M 129.75
M 128.40
M 128.12
M 127.54
M 126.12
M 123.87
M 122.56
M 106.32
M 100.51
M 61.77
M 56.03
M 55.55
M 22.57
M 13.64
O
EtO
N
Me
N
OMe
OMe
10k
[*1e6]
200
150
100
50
0
150
100
50
0
[ppm]

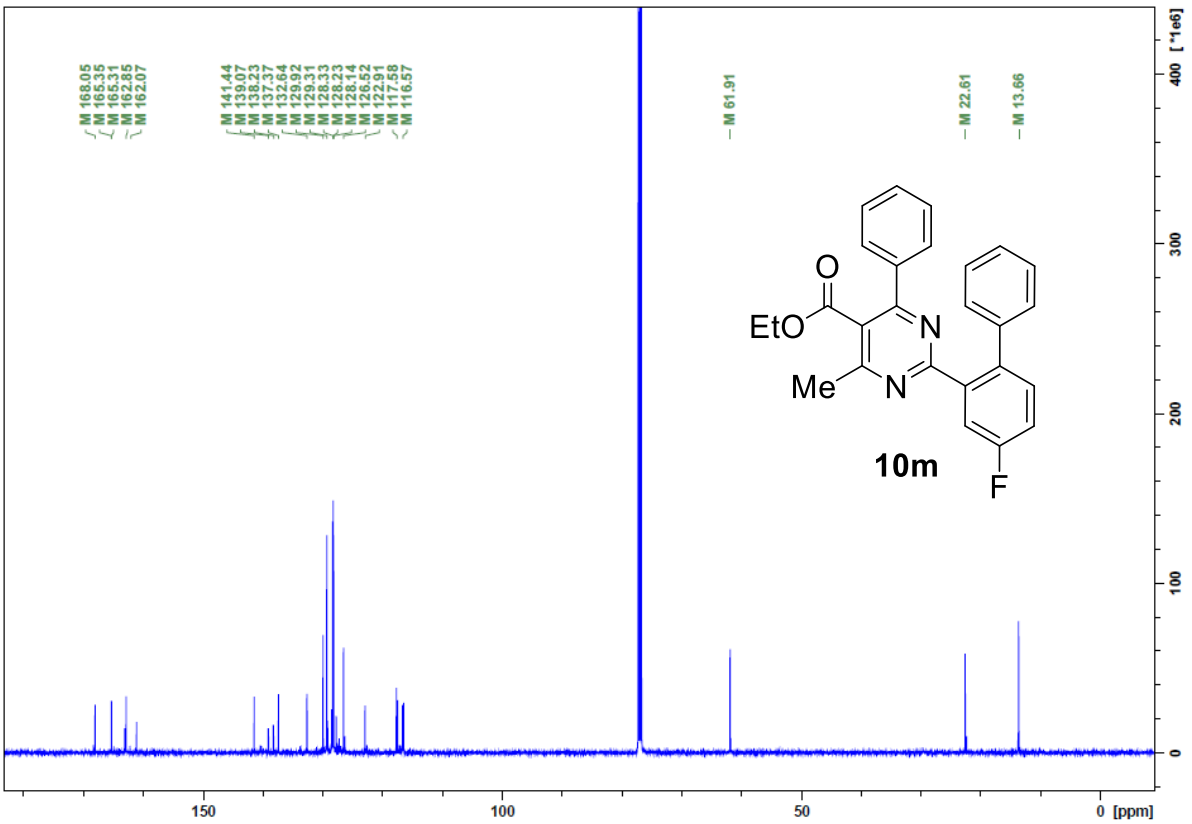

M 7.35
M 7.28
M 7.16
M 7.02
M 6.75
M 4.08
M 3.83
M 2.23
M 0.99
O
EtO
N
Me
N
OMe
OMe
11k
2.06
2.07
10.05
2.08
1.00
2.03
6.00
3.01
3.04
8
6
4
2
0
[ppm]
[*1e6]

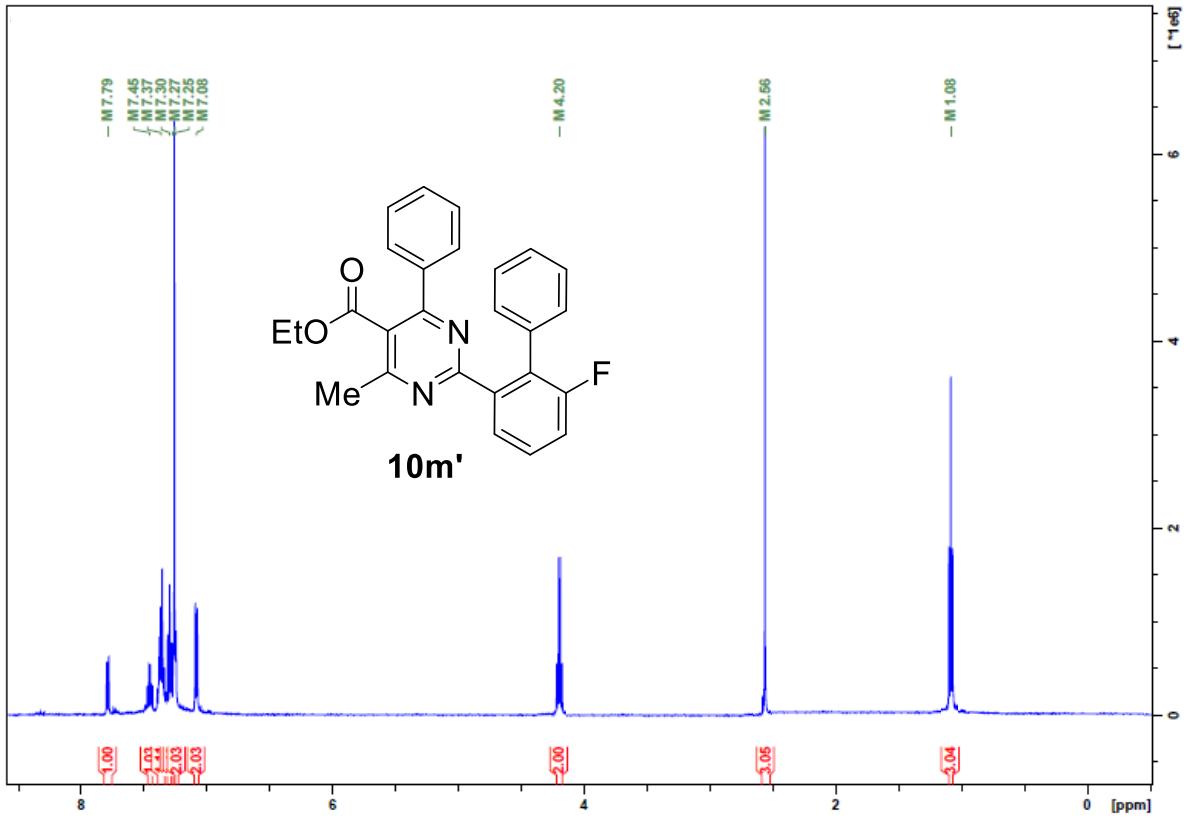

M 167.86
M 166.42
M 163.57
M 162.37
M 157.23
M 140.63
M 137.73
M 136.65
M 130.95
M 129.46
M 128.11
M 128.06
M 127.29
M 126.23
M 123.14
M 121.88
M 96.89
M 61.60
M 56.25
M 21.91
M 13.53
O
EtO
N
Me
N
OMe
OMe
11k
150
100
50
0
[ppm]
[*1e6]

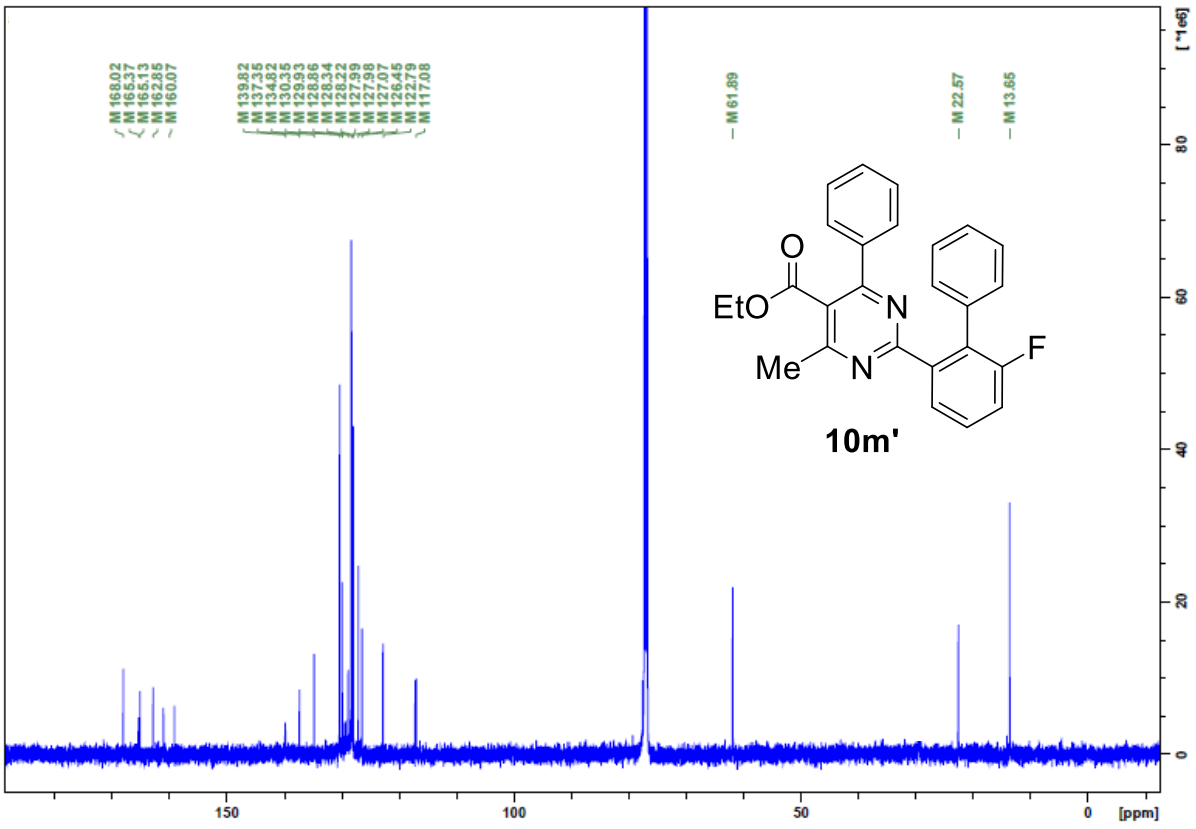

M 7.46
M 7.39
M 7.33
M 7.28
M 7.22
M 7.18
M 4.21
M 2.59
M 1.10
10l
O
EtO
N
F
Me
N
2.00
3.06
3.04
8
6
4
2
0 [ppm]
[*1e6]

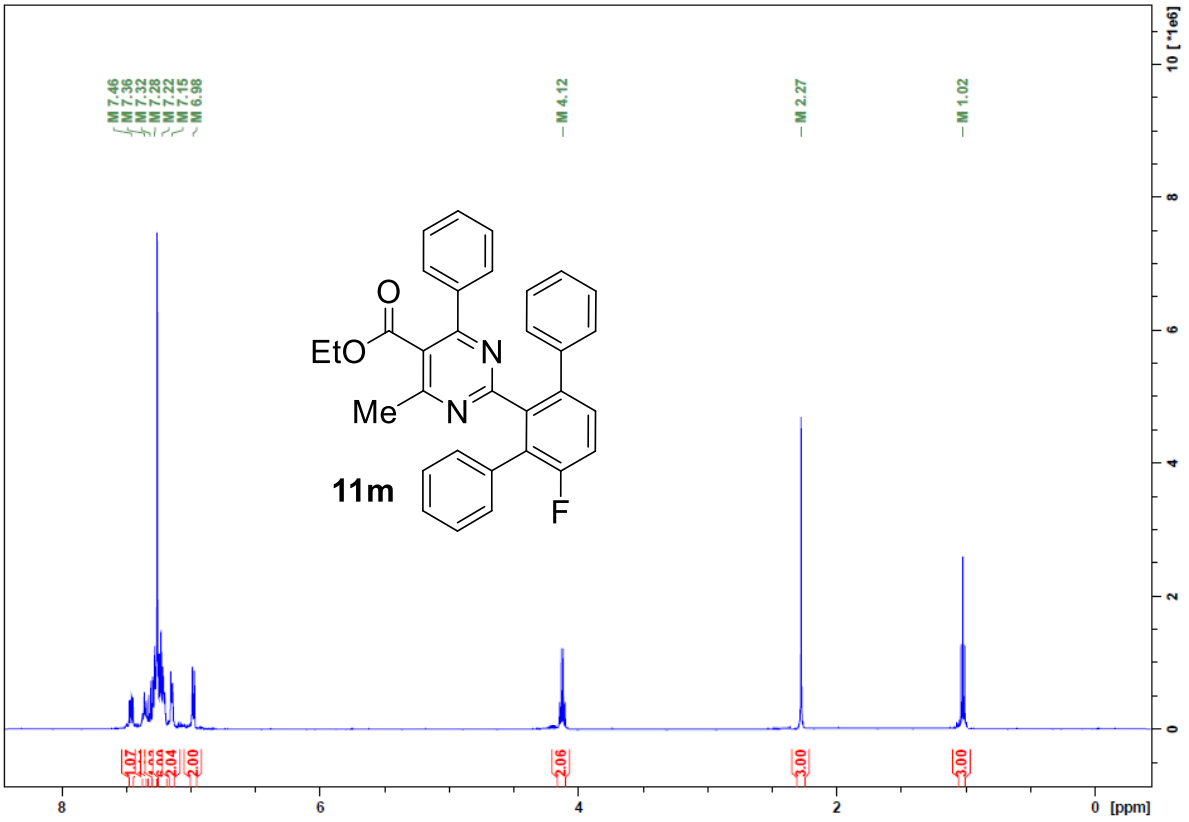

M 167.83
M 164.86
M 163.17
M 162.93
M 160.56
M 143.69
M 140.15
M 137.38
M 130.45
M 129.90
M 129.20
M 128.35
M 128.25
M 128.09
M 127.06
M 126.43
M 125.91
M 123.40
M 114.99
M 61.91
M 22.60
M 13.66
10l
O
EtO
N
F
Me
N
150
100
50
0 [ppm]
[*1e6]

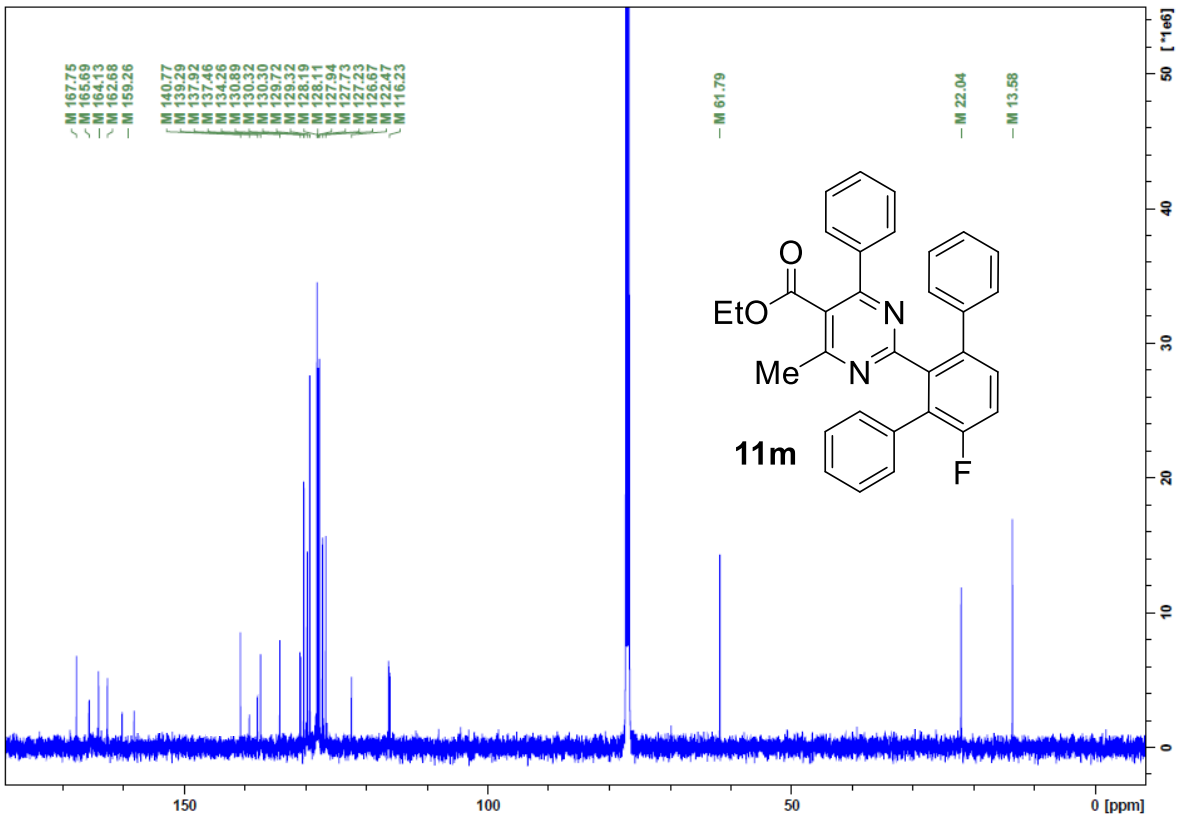

M 7.72
M 7.43
M 7.38
M 7.33
M 7.29
M 7.21
M 7.09
M 4.21
M 2.58
M 1.10
O
EtO
N
Me
N
10m
F
1.00
2.00
3.00
3.05
8
6
4
2
0 [ppm]
[*1e6]

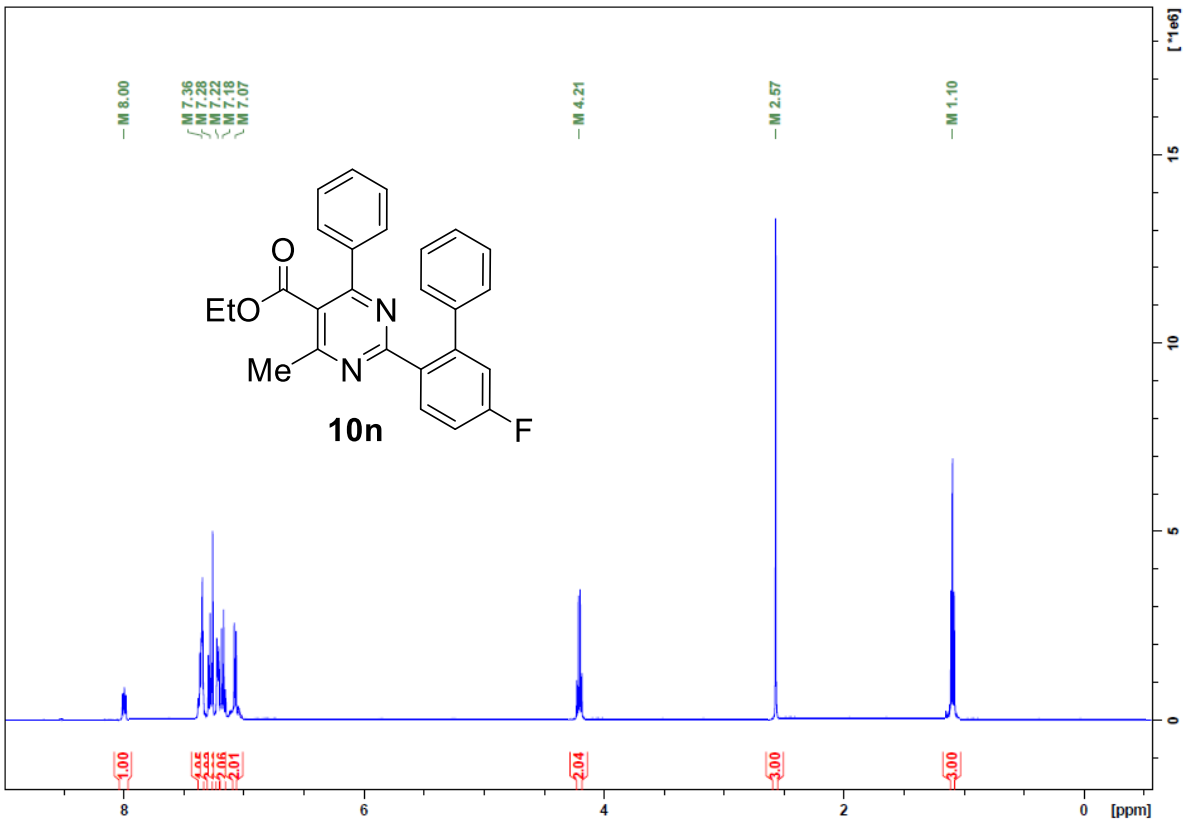

M 168.05
M 165.35
M 165.31
M 162.85
M 162.07
M 141.44
M 139.07
M 138.21
M 137.37
M 132.64
M 129.92
M 129.31
M 128.33
M 128.23
M 128.14
M 126.52
M 122.91
M 117.58
M 116.57
M 61.91
M 22.61
M 13.66
O
EtO
N
Me
N
10m
F
150
100
50
0 [ppm]
[*1e6]

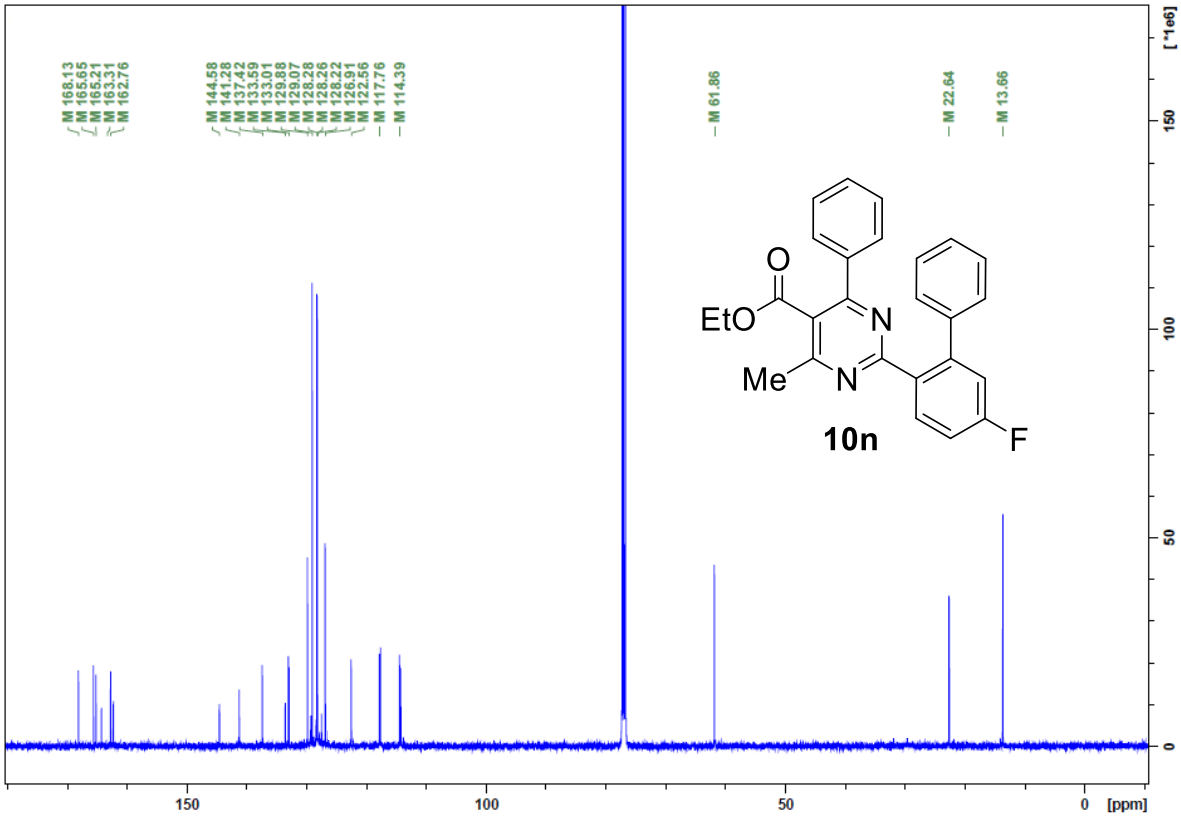

M 7.79
M 7.45
M 7.37
M 7.30
M 7.27
M 7.25
M 7.08
M 4.20
M 2.66
M 1.08
O
EtO
N
Me
N
F
10m'
1.00
2.00
3.05
3.04
8
6
4
2
0
[ppm]
[*1e6]

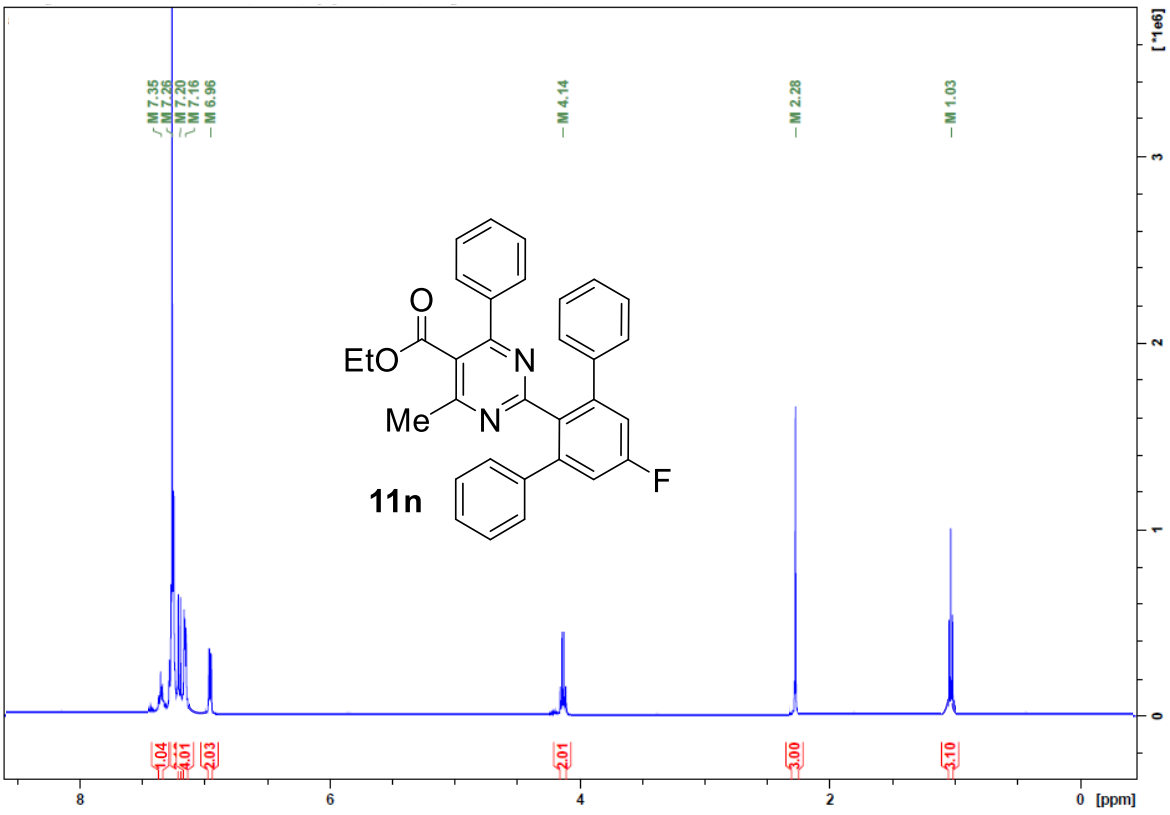

M 168.02
M 165.37
M 165.13
M 162.85
M 160.07
M 139.82
M 137.35
M 134.82
M 130.35
M 129.93
M 128.86
M 128.34
M 128.22
M 127.99
M 127.98
M 127.07
M 126.45
M 122.79
M 117.08
M 61.89
M 22.57
M 13.65
O
EtO
N
Me
N
F
10m'
150
100
50
0
[ppm]
[*1e6]

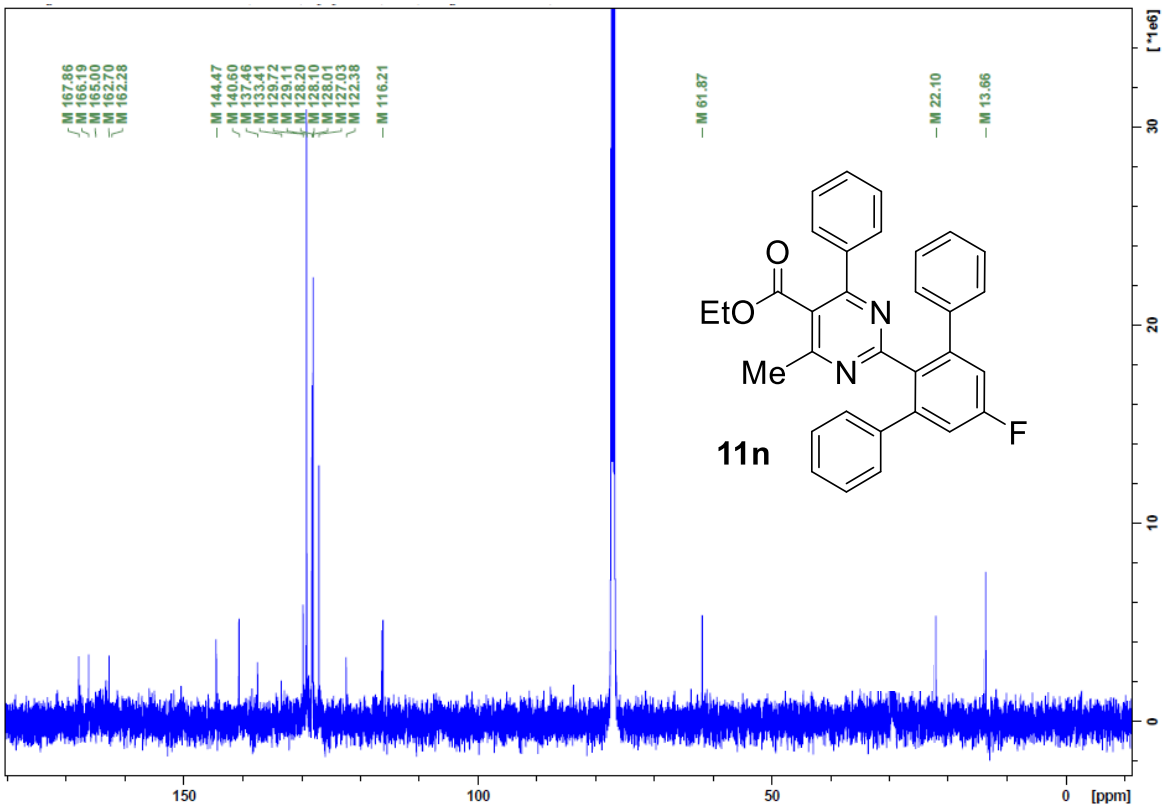

M 7.46
M 7.36
M 7.32
M 7.28
M 7.22
M 7.15
M 6.98
M 4.12
M 2.27
M 1.02
O
EtO
N
Me
N
11m
F
10 [*1e6]
8
6
4
2
0 [ppm]

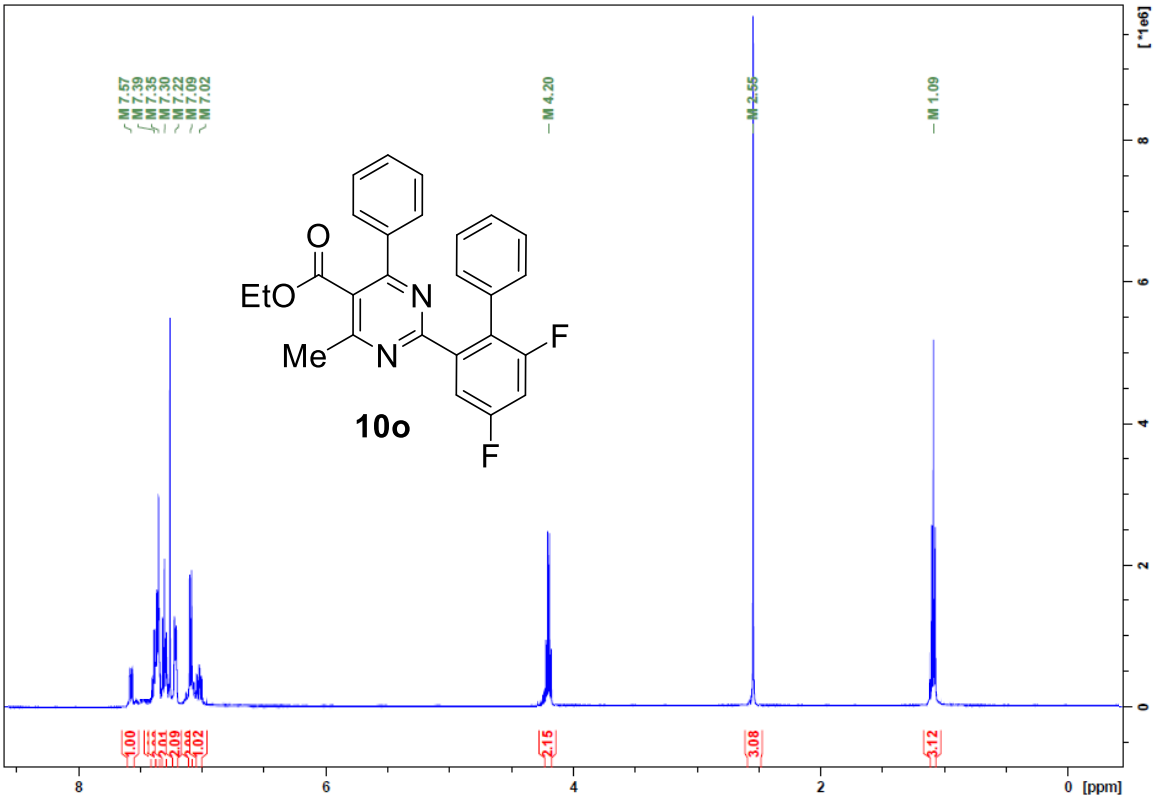

M 167.75
M 165.69
M 164.13
M 162.68
M 159.26
M 140.77
M 139.29
M 137.92
M 137.46
M 134.26
M 130.89
M 130.32
M 130.30
M 129.72
M 129.32
M 128.19
M 128.11
M 127.94
M 127.73
M 127.23
M 126.67
M 122.47
M 116.23
M 61.79
M 22.04
M 13.58
O
EtO
N
Me
N
11m
F
50 [*1e6]
40
30
20
10
0
150
100
50
0 [ppm]

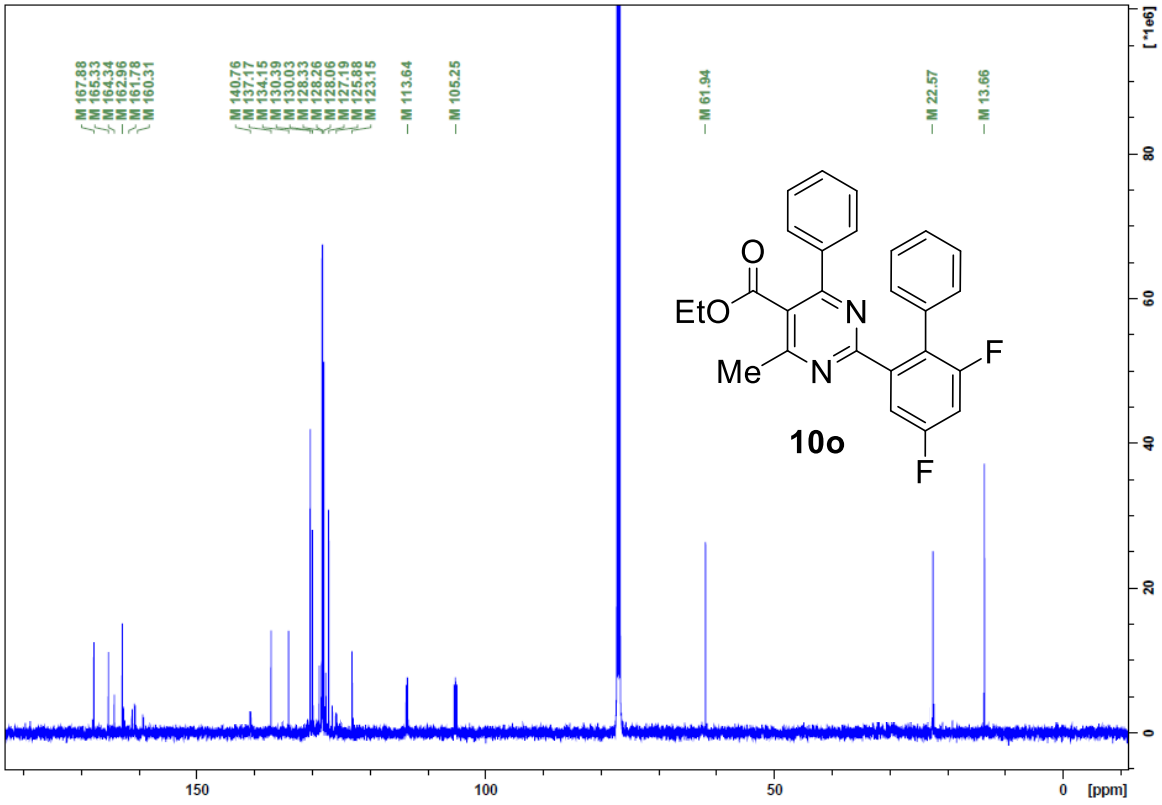

M 8.00
M 7.36
M 7.28
M 7.22
M 7.18
M 7.07
M 4.21
M 2.57
M 1.10
O
EtO
N
Me
N
F
10n
[*1e6]
15
10
5
0
1.00
4.25
2.06
2.01
2.04
3.00
3.00
8
6
4
2
0
[ppm]

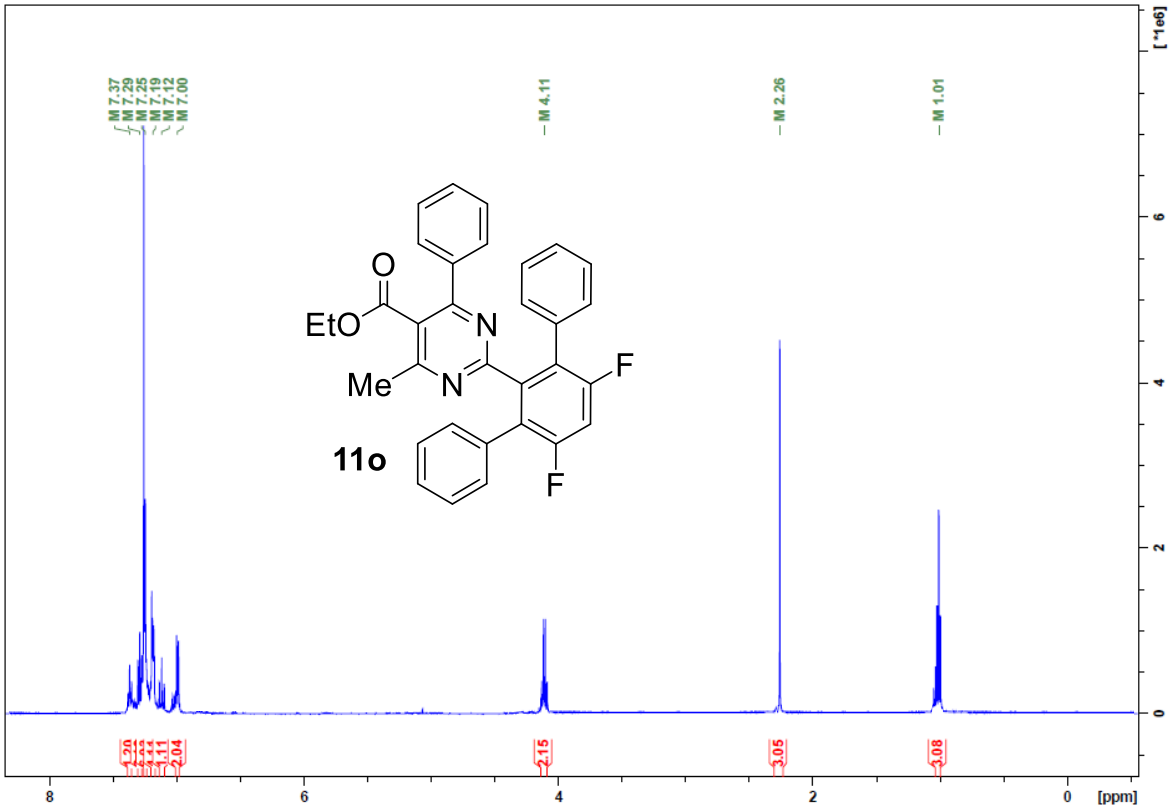

M 168.13
M 165.65
M 165.21
M 163.31
M 162.76
M 144.58
M 141.28
M 137.42
M 133.59
M 133.01
M 129.88
M 129.07
M 128.28
M 128.22
M 126.91
M 122.56
M 117.76
M 114.39
M 61.86
M 22.64
M 13.66
O
EtO
N
Me
N
F
10n
[*1e6]
150
100
50
0
150
100
50
0
[ppm]

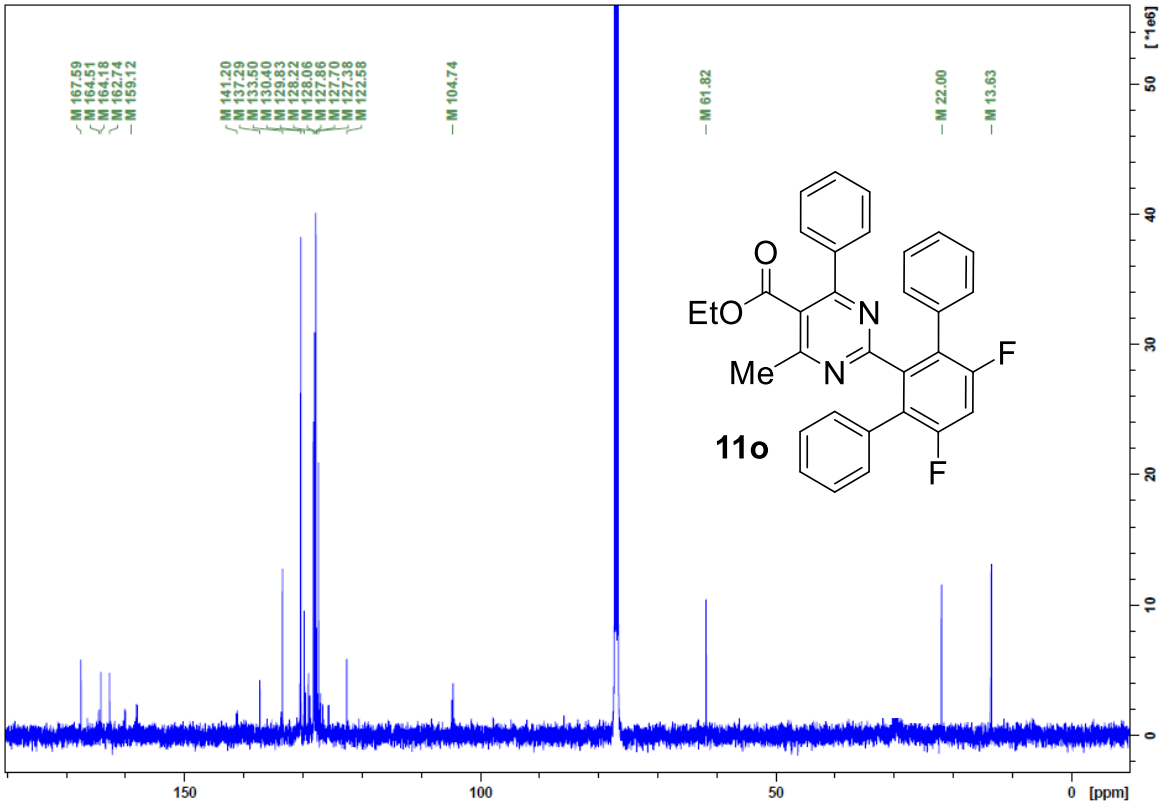

M 7.35
M 7.26
M 7.20
M 7.16
M 6.96
M 4.14
M 2.28
M 1.03
1.04
1.01
2.03
2.01
3.00
3.10
O
EtO
N
Me
N
F
11n
[*1e6]
8
6
4
2
0 [ppm]

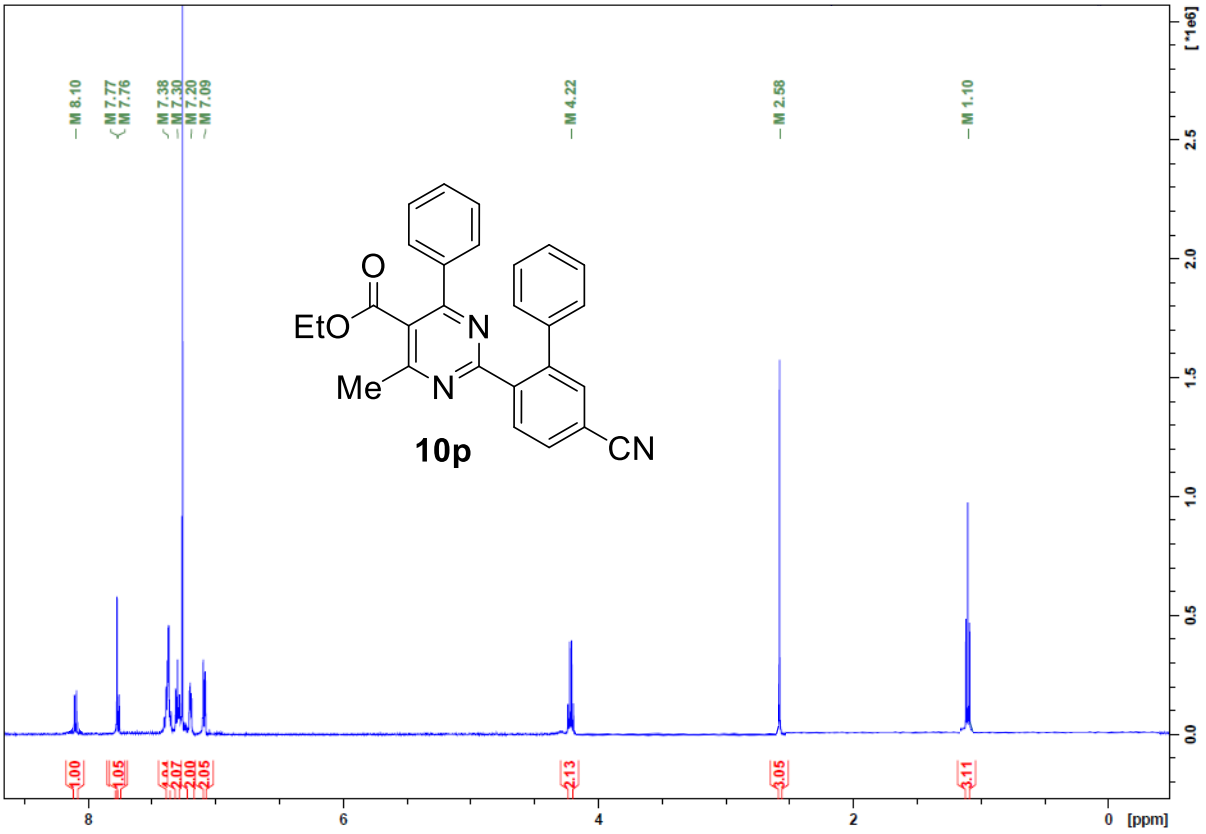

M 167.86
M 166.19
M 165.00
M 162.70
M 162.28
M 144.47
M 140.60
M 137.46
M 133.41
M 129.72
M 128.71
M 128.20
M 128.10
M 128.01
M 127.03
M 122.38
M 116.21
M 61.87
M 22.10
M 13.66
O
EtO
N
Me
N
F
11n
[*1e6]
150
100
50
0 [ppm]

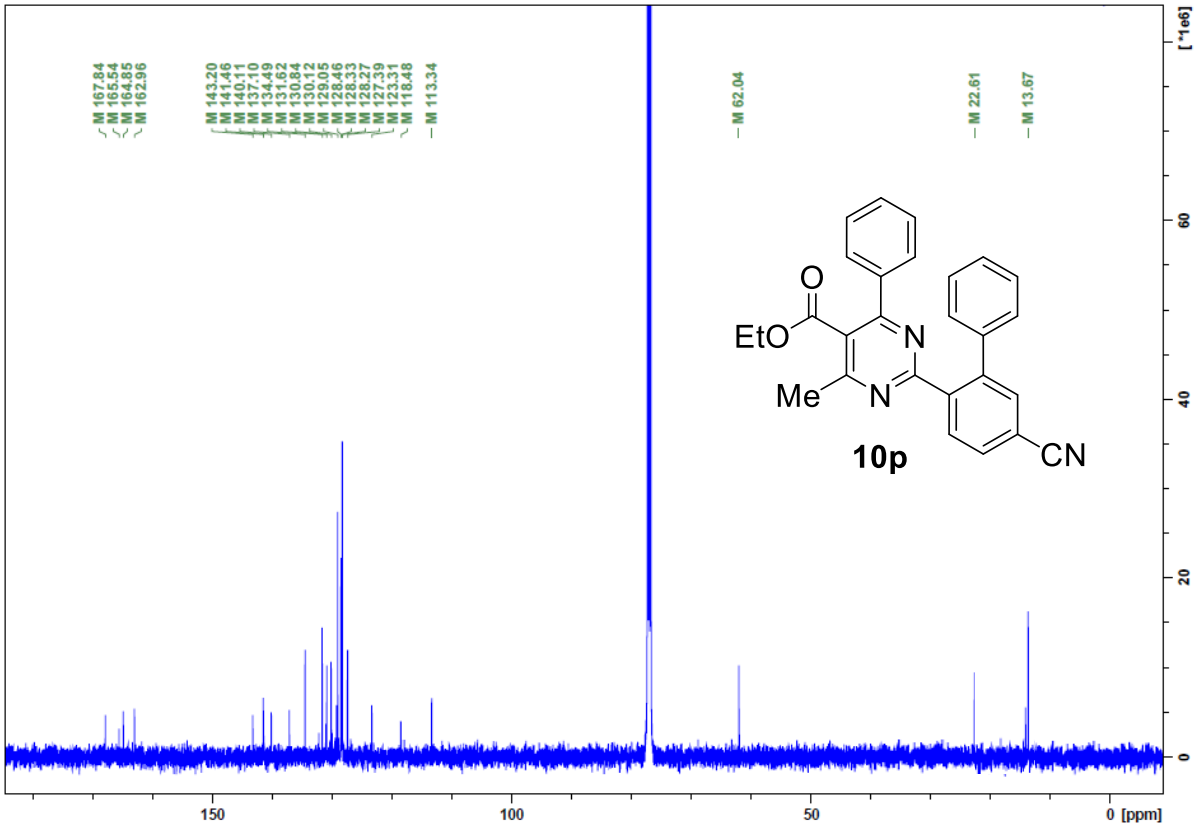

M 7.57
M 7.39
M 7.35
M 7.30
M 7.22
M 7.09
M 7.02
M 4.20
M 2.55
M 1.09
O
EtO
N
Me
N
F
F
10o
1.00
2.15
3.08
3.12
8
6
4
2
0 [ppm]
[*1e6]

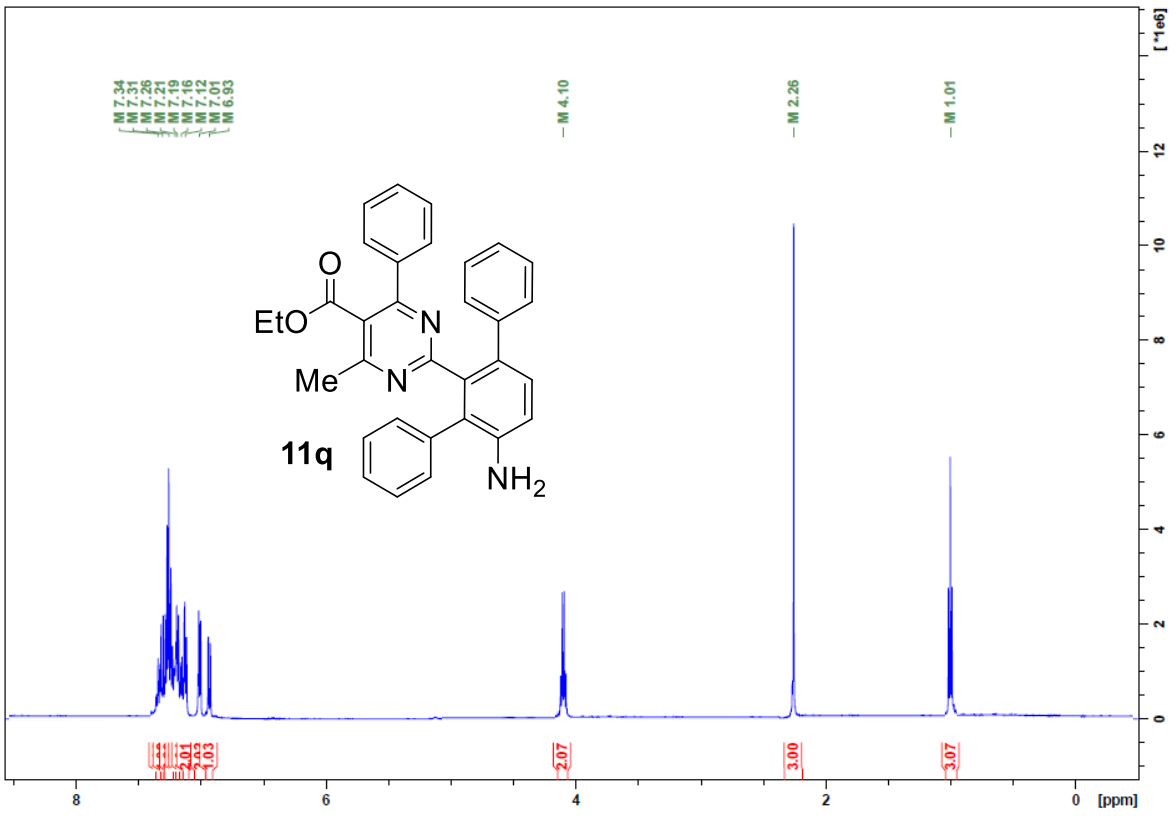

M 167.88
M 165.33
M 164.34
M 162.96
M 161.78
M 160.31
M 140.76
M 137.17
M 134.15
M 130.39
M 130.03
M 128.33
M 128.26
M 128.06
M 127.19
M 125.88
M 123.15
M 113.64
M 105.25
M 61.94
M 22.57
M 13.66
O
EtO
N
Me
N
F
F
10o
150
100
50
0 [ppm]
[*1e6]

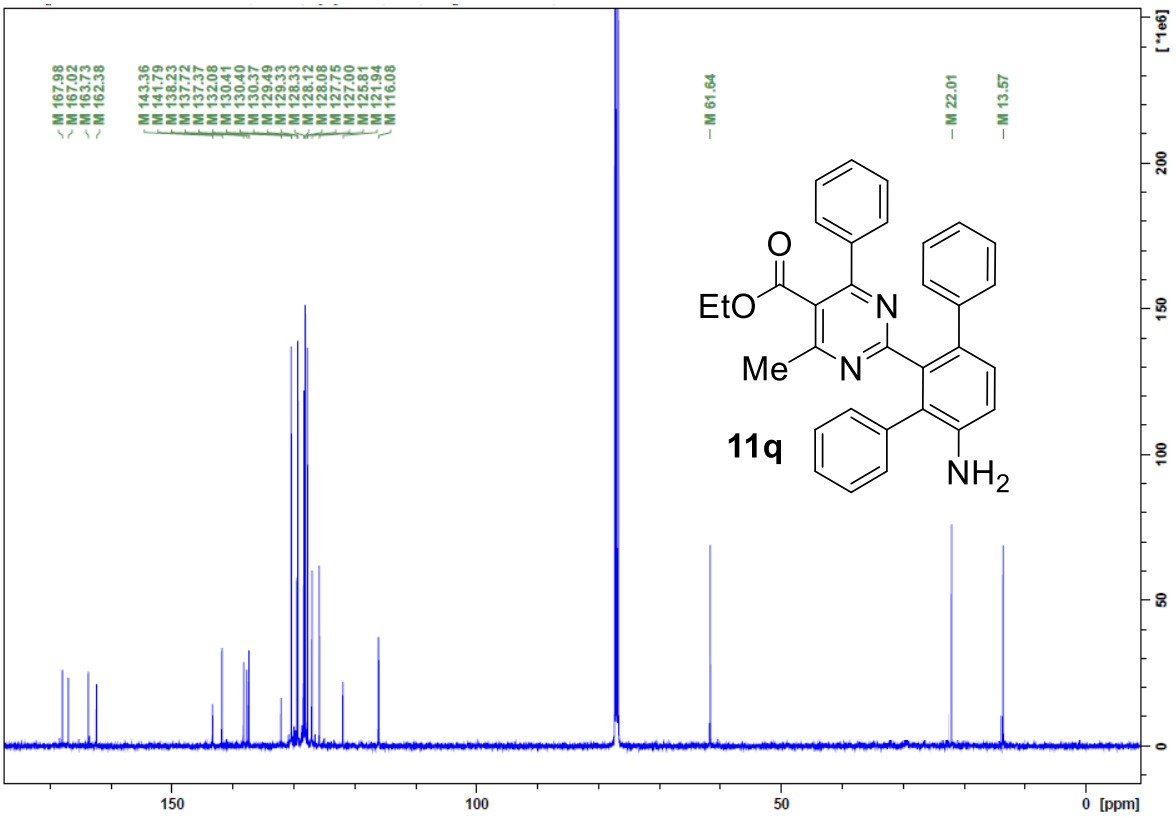

M 7.37
M 7.29
M 7.25
M 7.19
M 7.12
M 7.00
M 4.11
M 2.26
M 1.01
O
EtO
N
Me
N
F
F
11o
[*1e6]
8
6
4
2
0
[ppm]

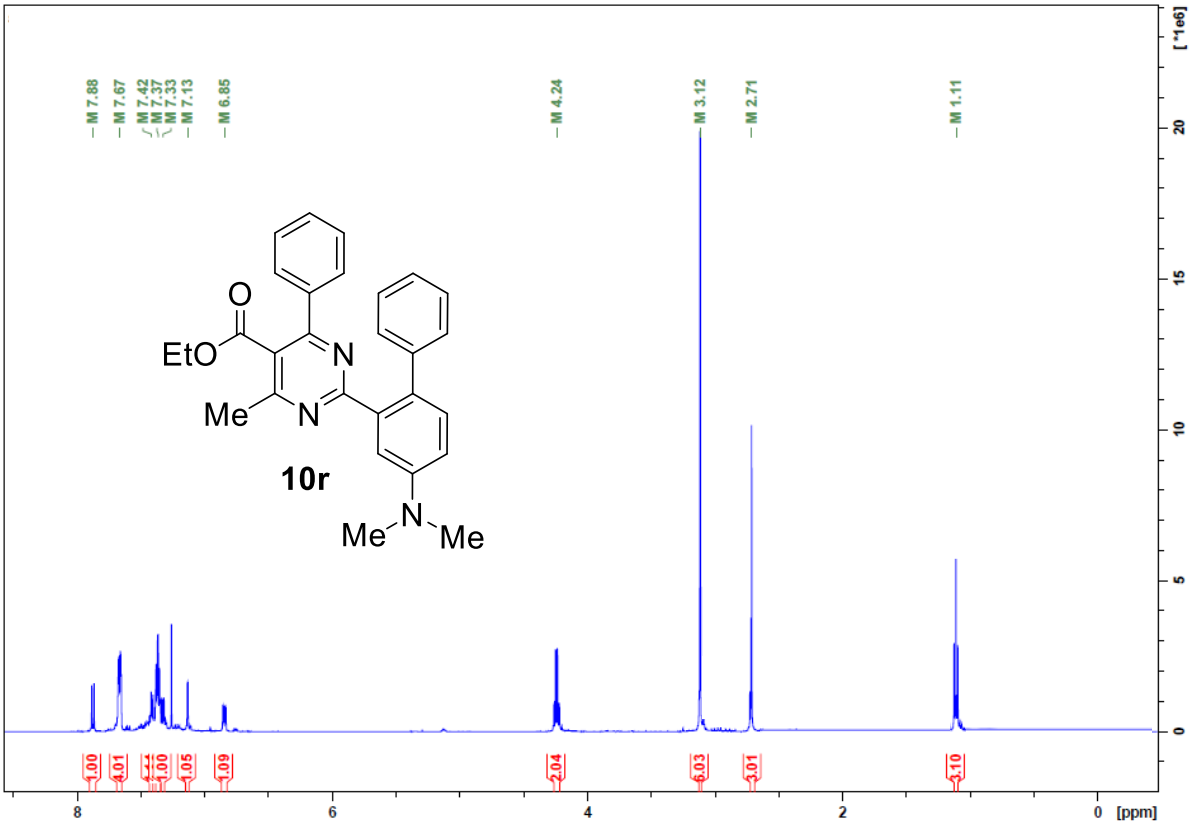

M 167.59
M 164.51
M 164.18
M 162.74
M 159.12
M 141.20
M 137.29
M 133.50
M 130.40
M 129.83
M 128.22
M 128.06
M 127.86
M 127.70
M 127.38
M 122.58
M 104.74
M 61.82
M 22.00
M 13.63
O
EtO
N
Me
N
F
F
11o
[*1e6]
150
100
50
0
[ppm]

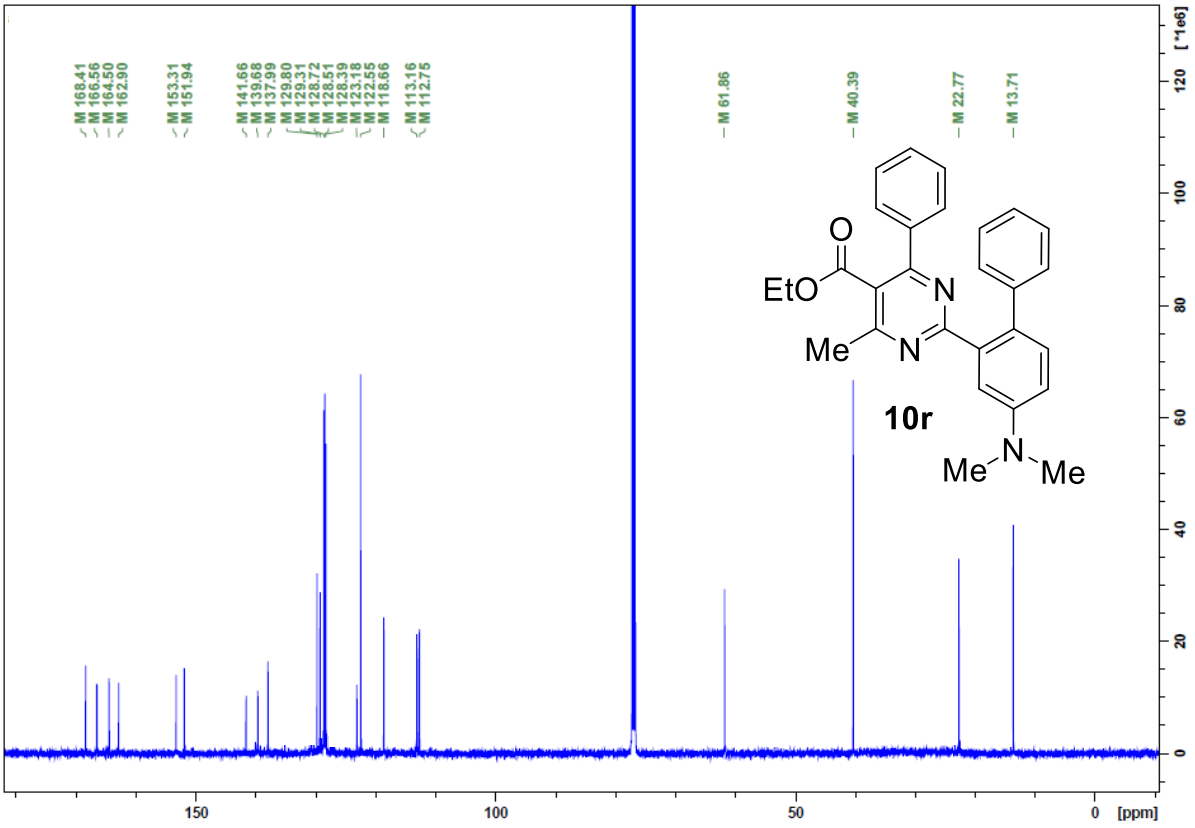

M 8.10
M 7.77
M 7.76
M 7.38
M 7.30
M 7.20
M 7.09
M 4.22
M 2.68
M 1.10
1.00
1.05
4.04
2.07
2.00
2.05
2.13
3.05
3.11
8
6
4
2
0 [ppm]
[*1e6]
2.5
2.0
1.5
1.0
0.5
0.0
O
EtO
N
Me
N
CN
10p


M 167.84
M 165.54
M 164.85
M 162.96
M 143.20
M 141.46
M 140.11
M 137.10
M 134.49
M 131.62
M 130.84
M 130.12
M 129.05
M 128.46
M 128.33
M 128.27
M 127.39
M 123.31
M 118.48
M 113.34
M 62.04
M 22.61
M 13.67
150
100
50
0 [ppm]
[*1e6]
60
40
20
0
O
EtO
N
Me
N
CN
10p

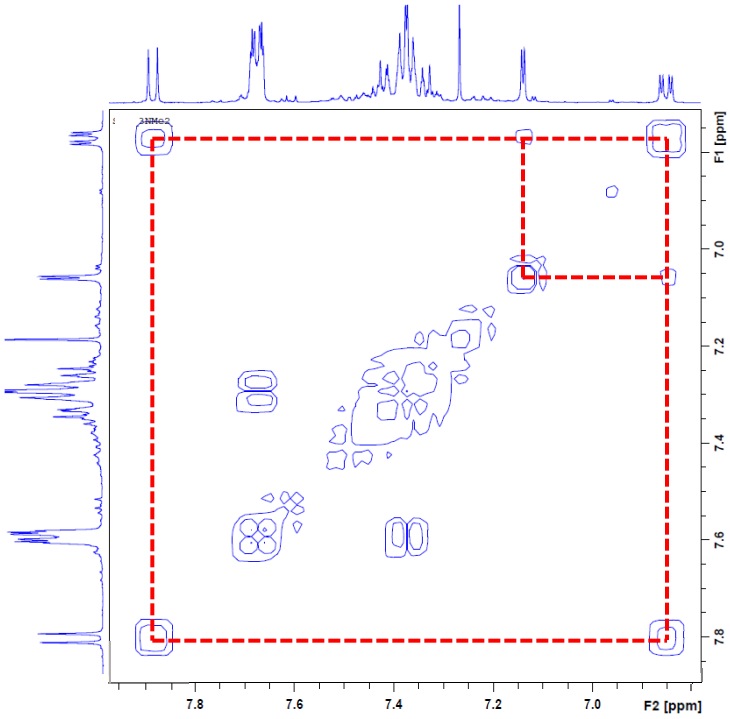

M 7.34
M 7.31
M 7.26
M 7.21
M 7.19
M 7.16
M 7.12
M 7.01
M 6.93
M 4.10
M 2.26
M 1.01
O
EtO
N
Me
N
11q
NH2
2.07
3.00
3.07
[*1e6]
[ppm]


M 167.98
M 167.02
M 163.73
M 162.38
M 143.36
M 141.79
M 138.23
M 137.72
M 137.37
M 132.08
M 130.41
M 130.40
M 130.37
M 129.49
M 129.33
M 128.33
M 128.12
M 128.08
M 127.75
M 127.00
M 125.81
M 121.94
M 116.08
M 61.64
M 22.01
M 13.57
O
EtO
N
Me
N
11q
NH2
[*1e6]
[ppm]

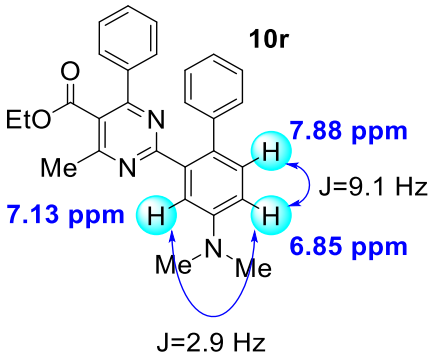

M 7.88
M 7.67
M 7.42
M 7.37
M 7.33
M 7.13
M 6.85
M 4.24
M 3.12
M 2.71
M 1.11
O
EtO
N
Me
N
10r
Me
N
Me
1.00
4.01
4.11
1.00
1.05
1.09
2.04
6.03
3.01
5.10
8
6
4
2
0
[ppm]
[*1e6]

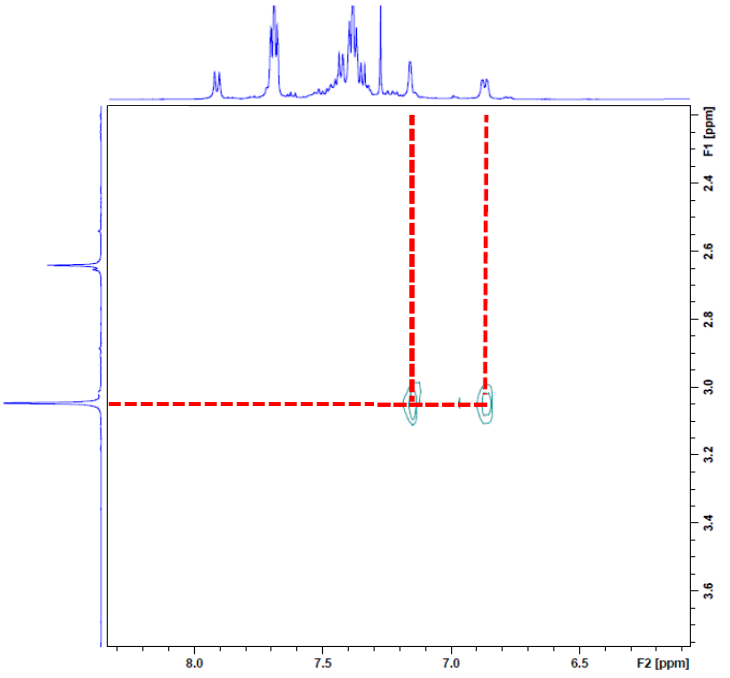

M 168.41
M 166.56
M 164.50
M 162.90
M 153.31
M 151.94
M 141.66
M 139.68
M 137.99
M 129.80
M 129.31
M 128.72
M 128.51
M 123.39
M 122.18
M 122.05
M 116.66
M 113.16
M 112.75
M 61.86
M 40.39
M 22.77
M 13.71
O
EtO
N
Me
N
10r
Me
N
Me
150
100
50
0
[ppm]
[*1e6]

^{1}H – ^{1}H COSY and NOESY NMR Spectra of Compound 10r

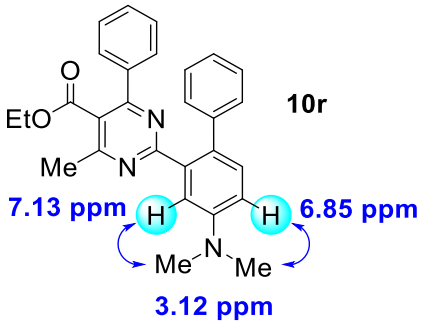


COSY Relay





NOESY Relay



Single Crystal X-ray Crystallography Procedures

Single crystal X-ray diffraction data were collected on an Oxford-Diffraction Supernova diffractometer, equipped with a CCD area detector utilizing Cu-Ka (λ=1.54184 Å) radiation. Suitable crystals were attached to glass fibers using paratone-N oil and transferred to a goniostat where they were cooled for data collection. Empirical absorption corrections (multi-scan based on symmetry-related measurements) were applied using CrysAlis RED software.[1] The structures were solved by direct methods with SHELXT[2] and refined on F2 using full-matrix least squares with SHELXL-2014/7.[2] Software packages used: CrysAlis CCD for data collection;[1] CrysAlis RED for cell refinement and data reduction;[1] WINGX for geometric calculations;[3] DIAMOND[4] and MERCURY[5] for molecular graphics. The non-H atoms were treated anisotropically, whereas the H atoms were placed in calculated, ideal positions and refined as riding on their respective carbon atoms. Unit cell parameters and structure solution and refinement data for compound **10a** are listed in Table S1.

[1] Oxford Diffraction, CrysAlis CCD and CrysAlis RED, Oxford Diffraction Ltd, Abingdon, Oxford, England, 2008.
[2] G. M. Sheldrick, SHELXL-2014/7, Program for Refinement of Crystal Structures, University of Göttingen, Germany, 2014.
[3] L. J. Farrugia, WinGX suite for small-molecule single-crystal crystallography, *J. Appl. Crystallogr.* **1999**, *32*, 837-838.
[4] Diamond - Crystal and Molecular Structure Visualization Crystal Impact - K. Brandenburg & H. Putz, GbR, Rathausgasse 30, D-53111, Bonn, Germany.
[5] Mercury CSD 2.0 - new features for the visualization and investigation of crystal structures, C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek, P. A. Wood, *J. Appl. Crystallogr.* **2008**, *41*, 466-470.

Crystallographic Data of Compound 10a

Table S1. Crystal data and structure refinement for compound **10a** at 108.15(10) K.

Empirical formula	C26 H22 N2 O2
Formula weight	394.45
Temperature	108.15(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 2_1/c
Unit cell dimensions	a = 10.1280(3) Å, α = 90°
	b = 18.8434(4) Å, β = 111.420(3)°
	c = 11.5758(3) Å, γ = 90°
Volume	2056.6(1) $Å^3$
Z	4
Density (calculated)	1.274 g/cm^3
Absorption coefficient	0.643 mm^{-1}
F(000)	832
Crystal size	0.1 x 0.09 x 0.01 mm^3
θ range for data collection	4.690 to 66.992°
Index ranges	-11<=h<=12, -22<=k<=22, -13<=l<=13
Reflections collected	12573
Independent reflections	3667 [R_{int} = 0.0259]
Completeness to θ = 66.992°	100%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3667 / 0 / 271
Goodness-of-fit	1.013
Final R indices [I > 2σ(I)]	R_{obs} = 0.0416, wR_{obs} = 0.1123

R indices [all data]	R_{all} = 0.0472, wR_{all} = 0.1165
Largest diff. peak and hole	0.406 and -0.420 e·Å^{-3}

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0676P)^2+0.8373P]$, where $P=(Fo^2+2Fc^2)/3$

Table S2. Bond lengths [Å] for compound **10a** at 108.15(10) K with estimated standard deviations in parentheses.

Label*	Distances
C(2)-N(3)	1.3325(19)
C(2)-N(1)	1.3462(19)
C(2)-C(17)	1.490(2)
C(4)-N(3)	1.3428(19)
C(4)-C(5)	1.402(2)
C(4)-C(7)	1.486(2)
C(5)-C(6)	1.399(2)
C(5)-C(13)	1.496(2)
C(6)-N(1)	1.3375(19)
C(6)-C(16)	1.502(2)
C(7)-C(12)	1.391(2)
C(7)-C(8)	1.398(2)
C(8)-C(9)	1.386(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.388(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.387(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.389(2)

C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-O(1)	1.2034(18)
C(13)-O(2)	1.3313(18)
C(14)-O(2)	1.4679(18)
C(14)-C(15)	1.496(2)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(18)	1.399(2)
C(17)-C(22)	1.406(2)
C(18)-C(19)	1.385(2)
C(18)-H(18)	0.9300
C(19)-C(20)	1.390(2)
C(19)-H(19)	0.9300
C(20)-C(21)	1.384(2)
C(20)-H(20)	0.9300
C(21)-C(22)	1.402(2)
C(21)-H(21)	0.9300
C(22)-C(23)	1.491(2)
C(23)-C(28)	1.394(2)
C(23)-C(24)	1.397(2)

C(24)-C(25)	1.388(2)
C(24)-H(24)	0.9300
C(25)-C(26)	1.386(2)
C(25)-H(25)	0.9300
C(26)-C(27)	1.386(2)
C(26)-H(26)	0.9300
C(27)-C(28)	1.387(2)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300

* Atom numbering corresponds to the deposited crystal structure numbering.

Table S3. Bond angles [°] for compound **10a** at 108.15(10) K with estimated standard deviations in parentheses.

Label*	Angles
N(3)-C(2)-N(1)	126.28(13)
N(3)-C(2)-C(17)	117.33(13)
N(1)-C(2)-C(17)	116.33(13)
N(3)-C(4)-C(5)	120.85(13)
N(3)-C(4)-C(7)	115.68(12)
C(5)-C(4)-C(7)	123.46(13)
C(6)-C(5)-C(4)	117.37(13)
C(6)-C(5)-C(13)	119.02(13)
C(4)-C(5)-C(13)	123.61(13)
N(1)-C(6)-C(5)	121.59(13)
N(1)-C(6)-C(16)	116.43(13)
C(5)-C(6)-C(16)	121.93(13)
C(12)-C(7)-C(8)	119.28(14)

C(12)-C(7)-C(4)	122.22(13)
C(8)-C(7)-C(4)	118.50(13)
C(9)-C(8)-C(7)	119.97(15)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	120.52(16)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	119.68(15)
C(11)-C(10)-H(10)	120.2
C(9)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	120.13(16)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	120.43(15)
C(11)-C(12)-H(12)	119.8
C(7)-C(12)-H(12)	119.8
O(1)-C(13)-O(2)	125.19(14)
O(1)-C(13)-C(5)	123.07(13)
O(2)-C(13)-C(5)	111.73(12)
O(2)-C(14)-C(15)	110.07(14)
O(2)-C(14)-H(14A)	109.6
C(15)-C(14)-H(14A)	109.6
O(2)-C(14)-H(14B)	109.6
C(15)-C(14)-H(14B)	109.6
H(14A)-C(14)-H(14B)	108.2
C(14)-C(15)-H(15A)	109.5

C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(6)-C(16)-H(16A)	109.5
C(6)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(6)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(22)	119.55(13)
C(18)-C(17)-C(2)	117.20(13)
C(22)-C(17)-C(2)	123.14(13)
C(19)-C(18)-C(17)	121.10(14)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(18)-C(19)-C(20)	119.50(14)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(21)-C(20)-C(19)	120.01(14)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	121.34(14)
C(20)-C(21)-H(21)	119.3
C(22)-C(21)-H(21)	119.3
C(21)-C(22)-C(17)	118.48(13)

C(21)-C(22)-C(23)	118.37(13)
C(17)-C(22)-C(23)	123.12(13)
C(28)-C(23)-C(24)	119.07(14)
C(28)-C(23)-C(22)	120.43(13)
C(24)-C(23)-C(22)	120.41(13)
C(25)-C(24)-C(23)	120.26(14)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	120.11(15)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(25)-C(26)-C(27)	120.06(15)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(28)-C(27)-C(26)	119.96(15)
C(28)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0
C(27)-C(28)-C(23)	120.53(14)
C(27)-C(28)-H(28)	119.7
C(23)-C(28)-H(28)	119.7
C(6)-N(1)-C(2)	116.54(12)
C(2)-N(3)-C(4)	117.27(12)
C(13)-O(2)-C(14)	115.96(12)

* Atom numbering corresponds to the deposited crystal structure numbering.