Supplementary Material

Screening of scaffolds for the design of G-quadruplex ligands

Joana Figueiredo[1], David Peitinho[2], Maria Paula Cabral Campello[2], Maria Cristina Oliveira[2], António Paulo[2], Jean-Louis Mergny,[3,4] Carla Cruz[1*]

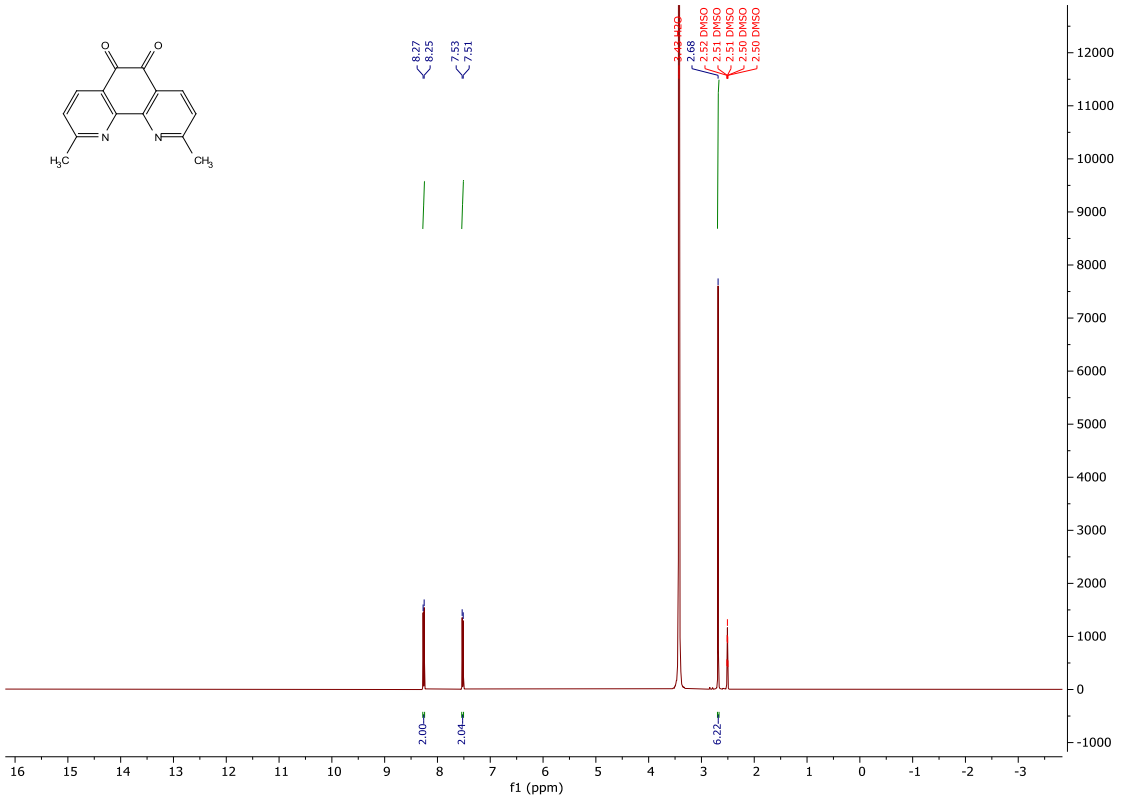
[1]Centro de Investigação em Ciências da Saúde, Universidade da Beira Interior, Av. Infante D. Henrique, Covilhã, Portugal

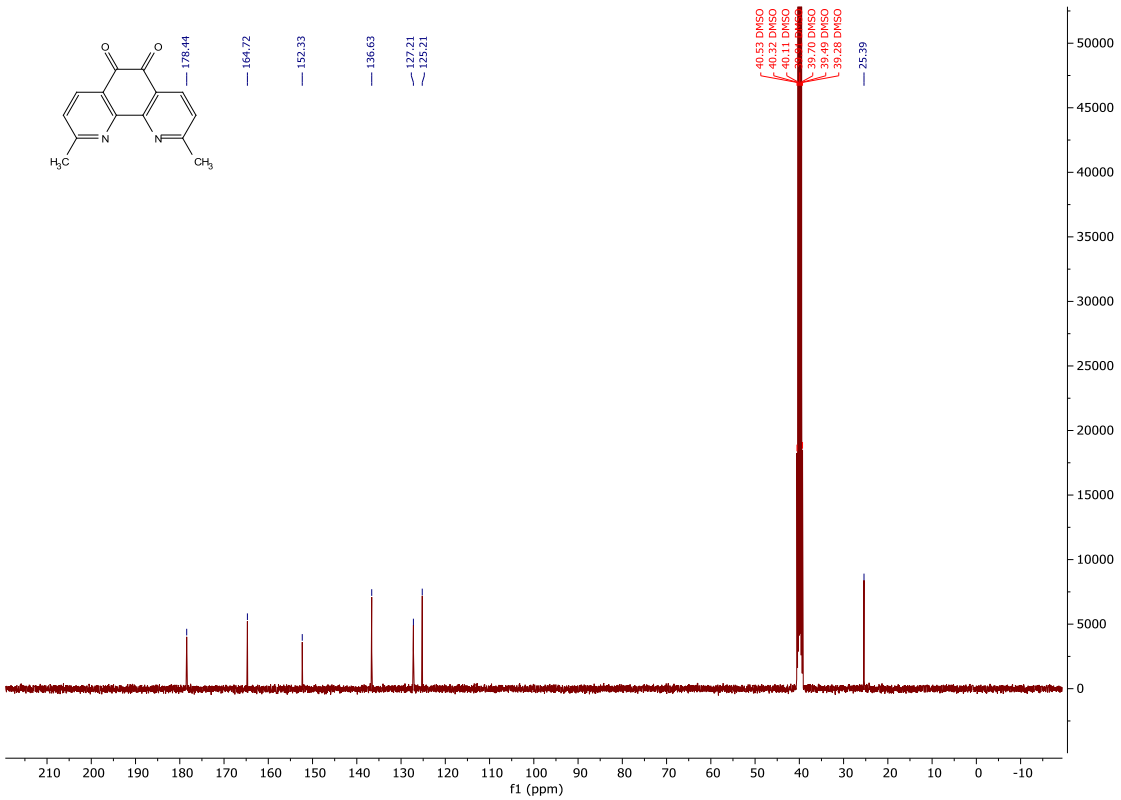
[2] Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, Universidade de Lisboa, Estrada Nacional 10 (km 139,7), 2695-066 Bobadela LRS, Portugal.

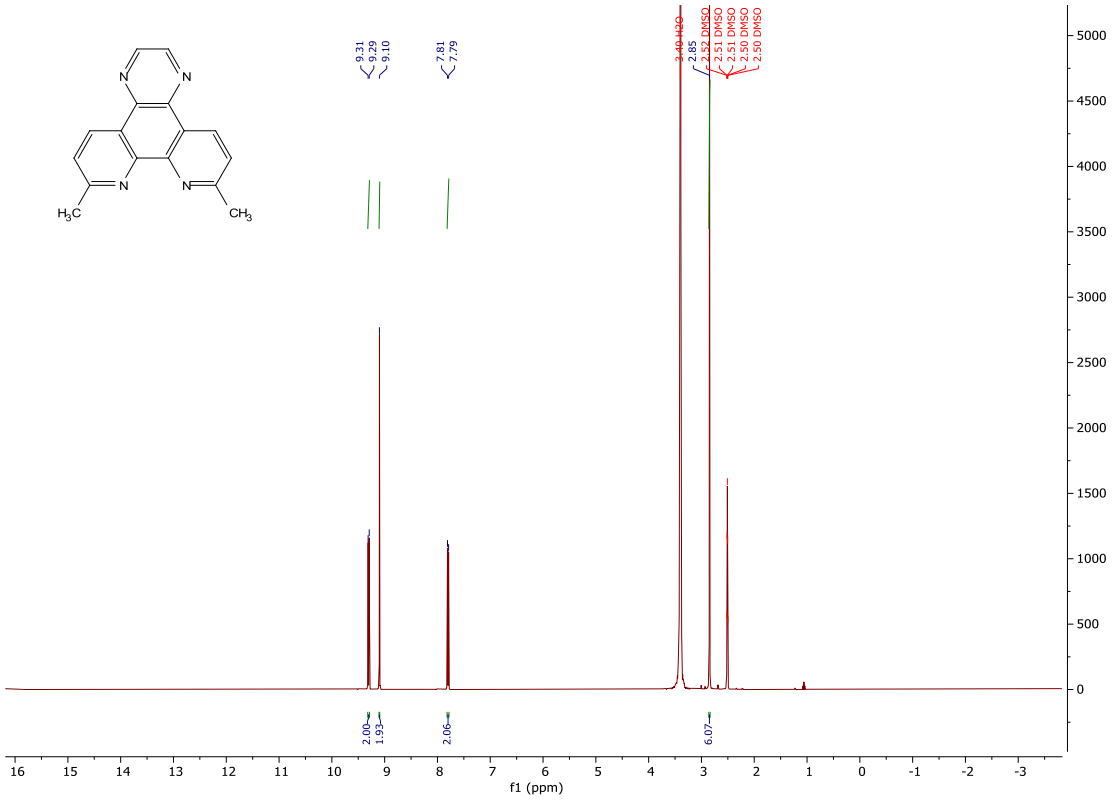
[3] Institute of Biophysics of the CAS, v.v.i., Královopolská 135, 612 65 Brno, Czech Republic

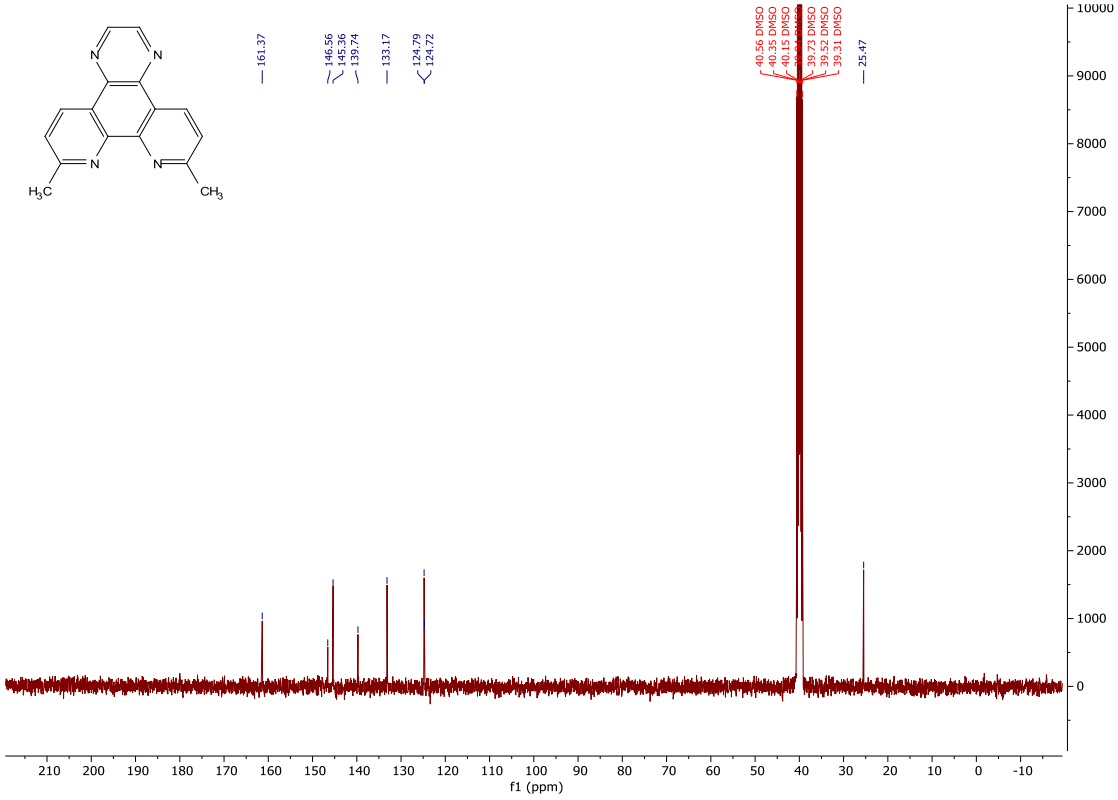
[4] Laboratoire d'Optique et Biosciences, Ecole Polytechnique, CNRS, INSERM, Institut Polytechnique de Paris, 91128 Palaiseau, France

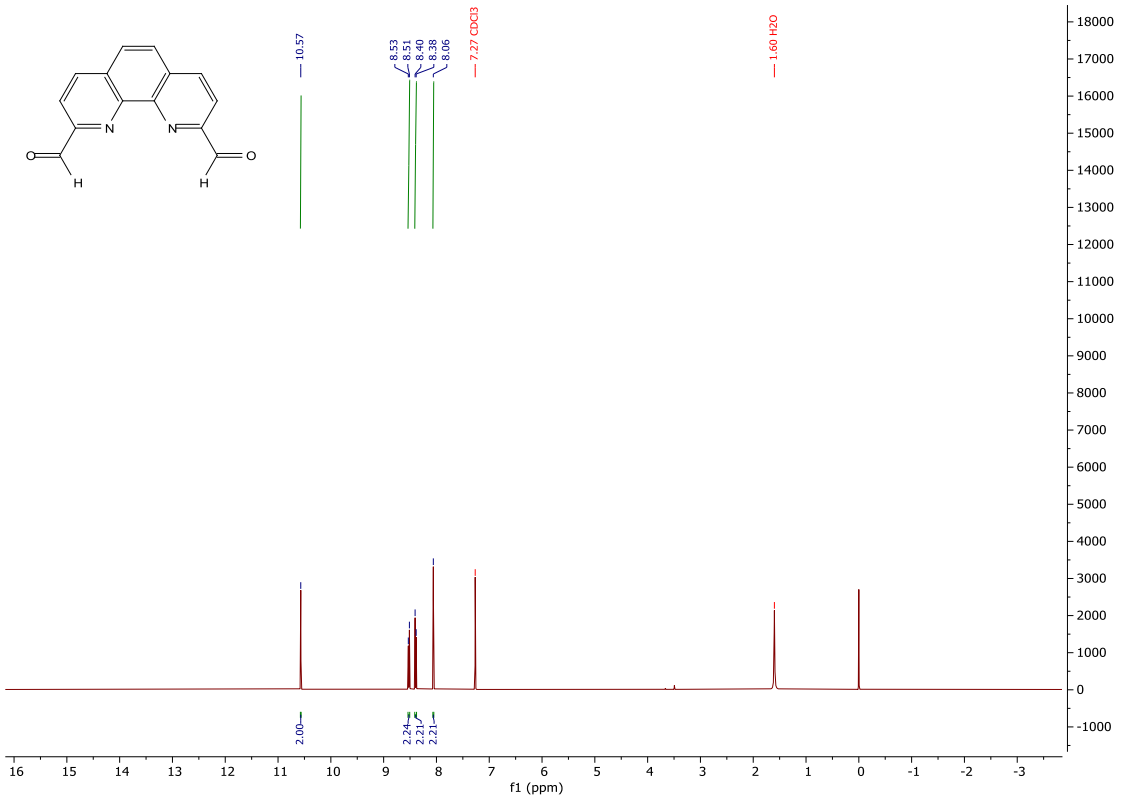
[*]Correspondence: carlacruz@fcsaude.ubi.pt;

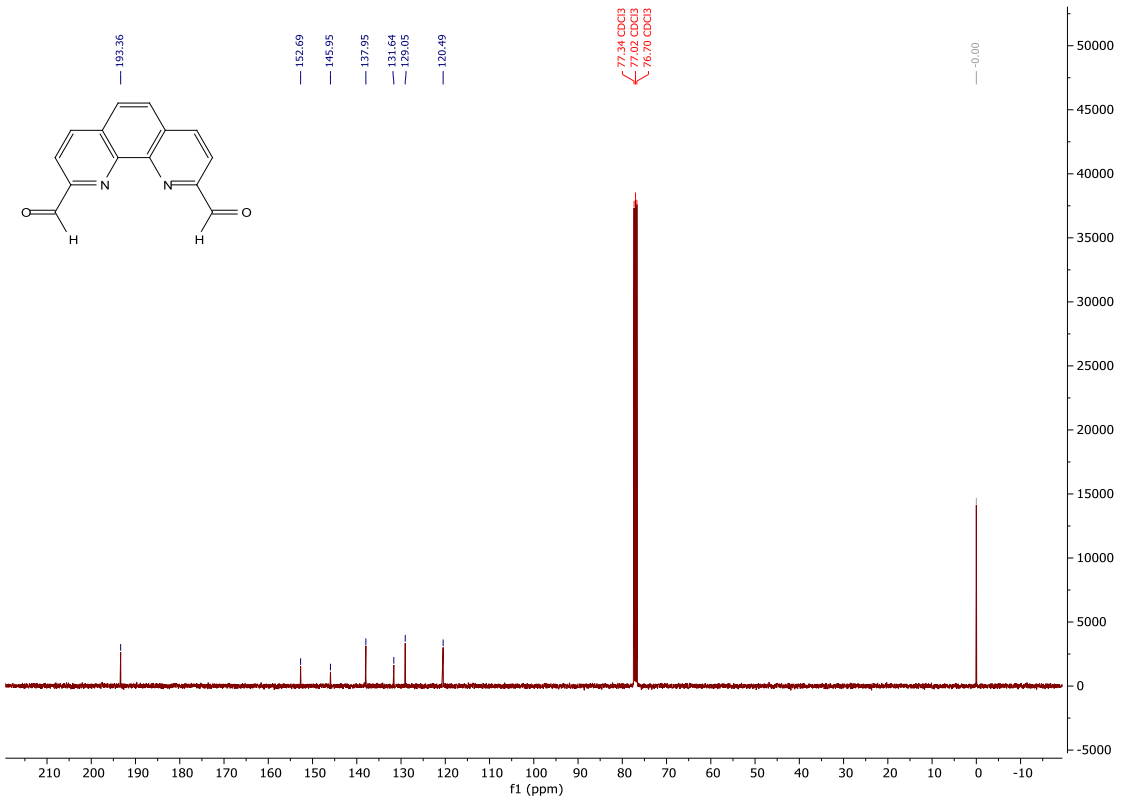

8.27
8.25
7.53
7.51
3.43 H2O
2.68
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.00
2.04
6.22
f1 (ppm)

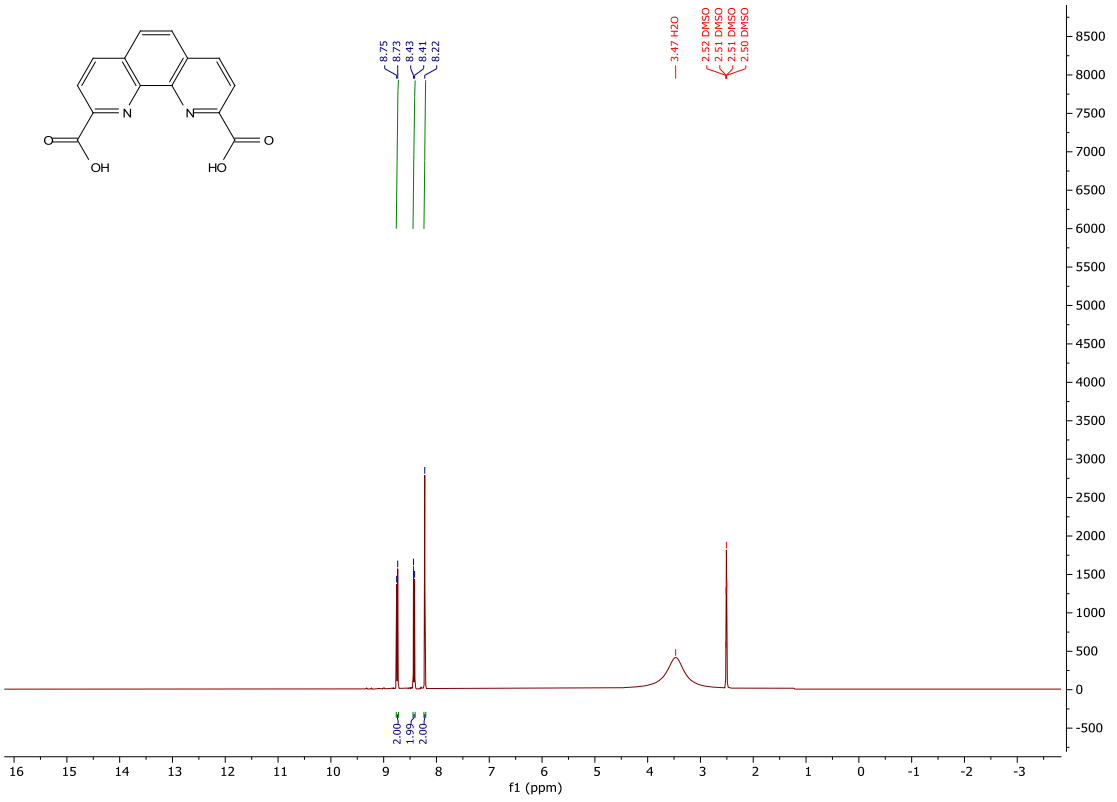

178.44
164.72
152.33
136.63
127.21
125.21
40.53 DMSO
40.32 DMSO
40.11 DMSO
39.90 DMSO
39.70 DMSO
39.49 DMSO
39.28 DMSO
25.39
f1 (ppm)

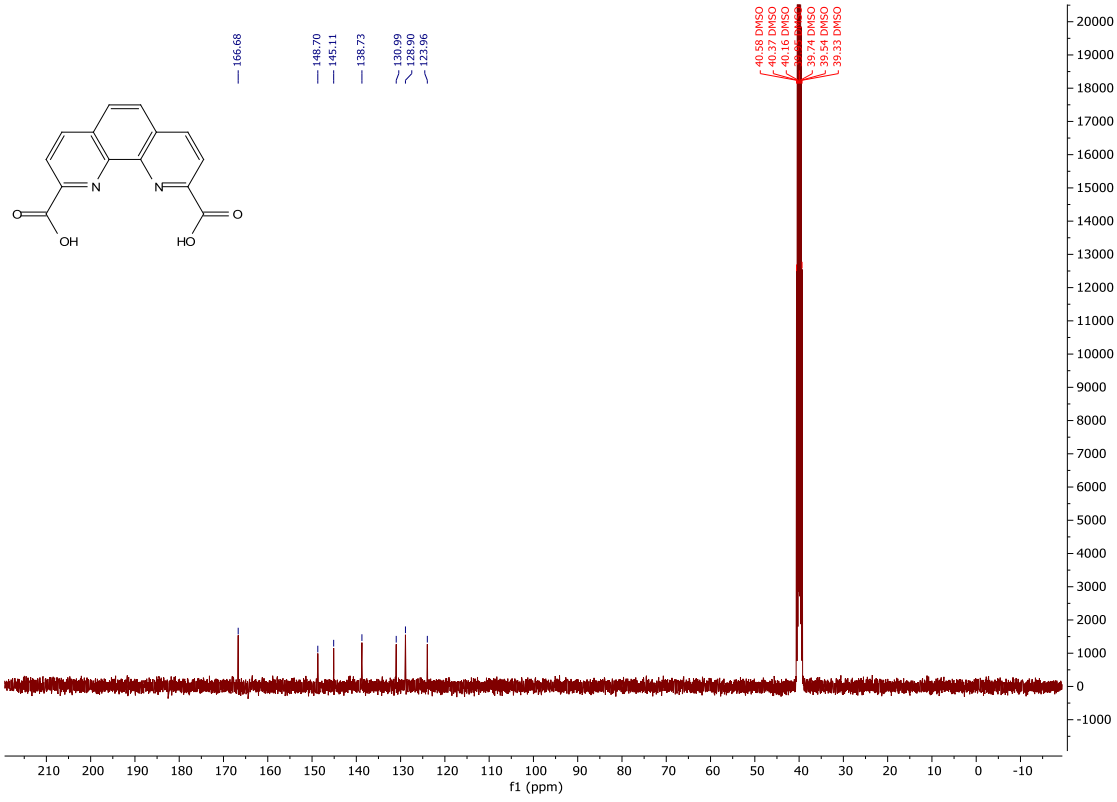

9.31
9.29
9.10
7.81
7.79
3.40 H2O
2.85
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.00
1.93
2.06
6.07
f1 (ppm)

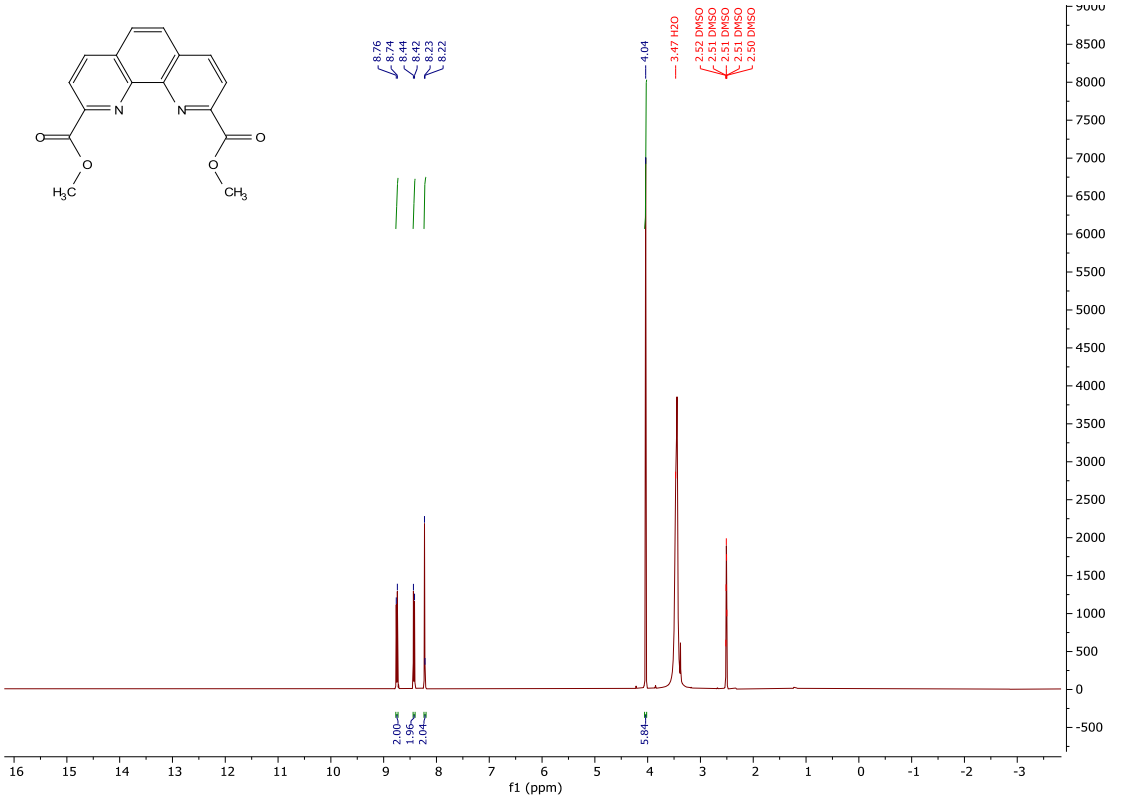

161.37
146.56
145.36
139.74
133.17
124.79
124.72
40.56 DMSO
40.35 DMSO
40.15 DMSO
39.73 DMSO
39.52 DMSO
39.31 DMSO
25.47
f1 (ppm)

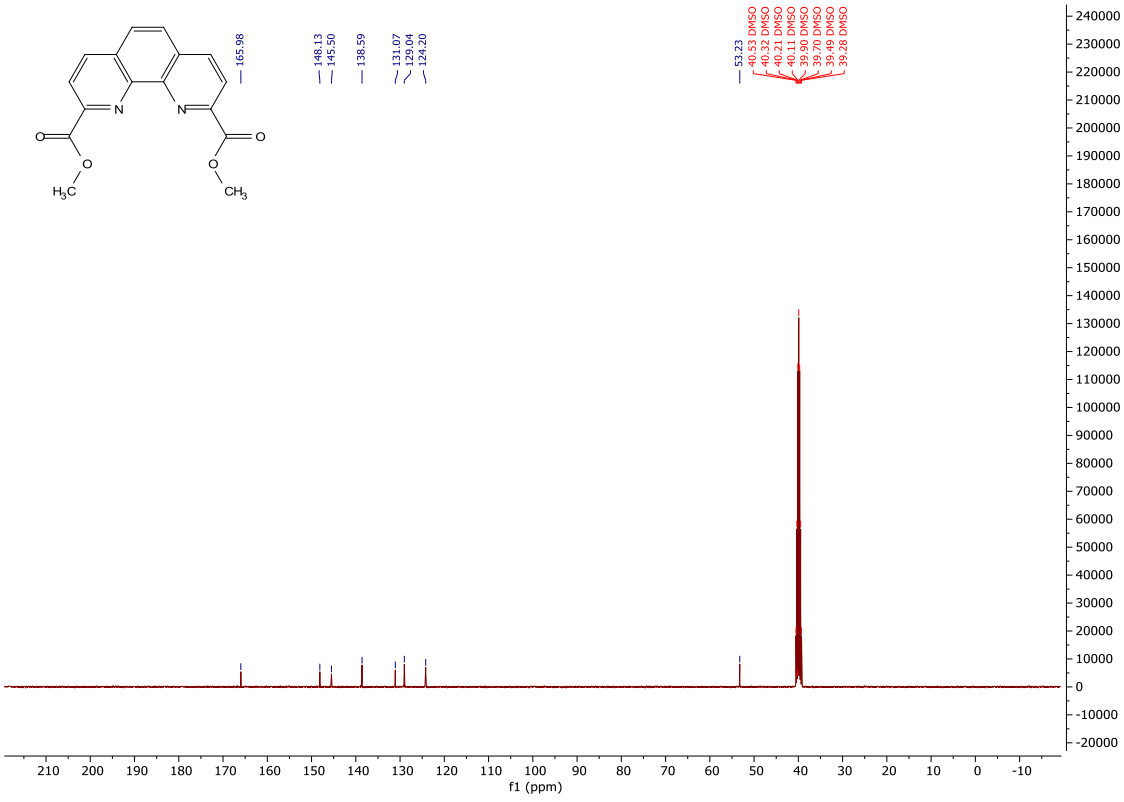

10.57
8.53
8.51
8.40
8.38
8.06
7.27 CDCl3
1.60 H2O
2.00
2.24
2.21
2.21
f1 (ppm)

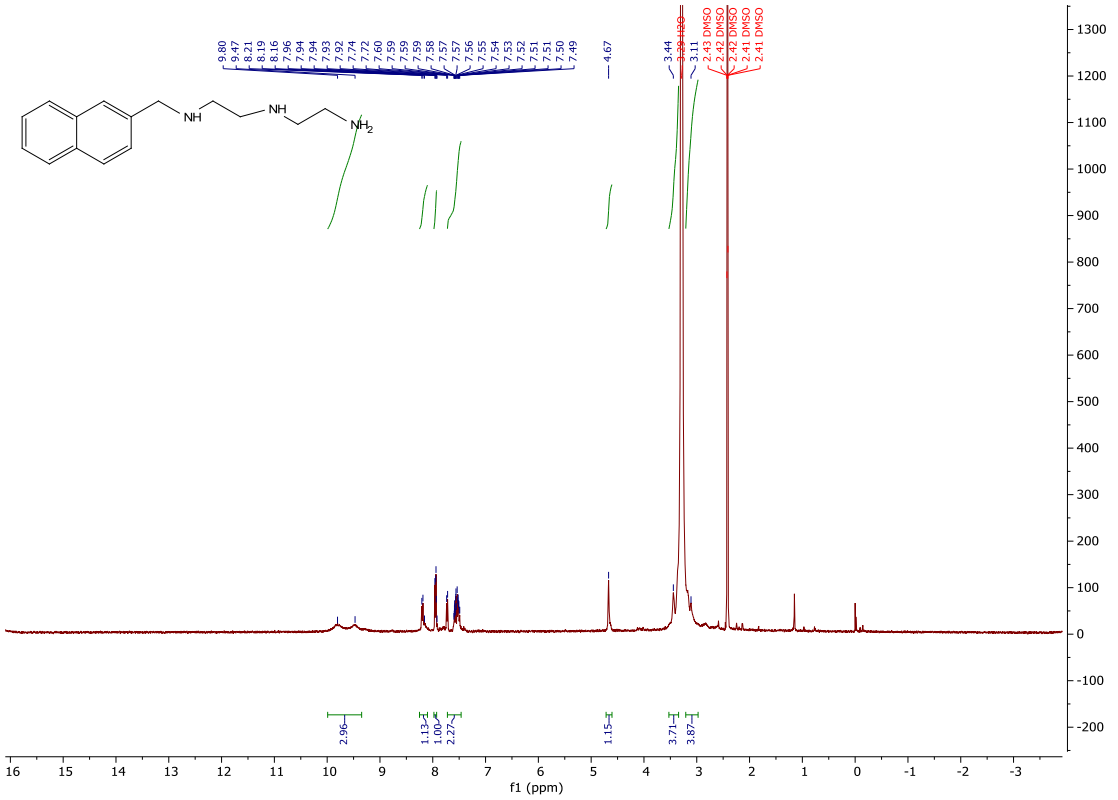

193.36
152.69
145.95
137.95
131.64
129.05
120.49
77.34 CDCl3
77.02 CDCl3
76.70 CDCl3
-0.00
f1 (ppm)

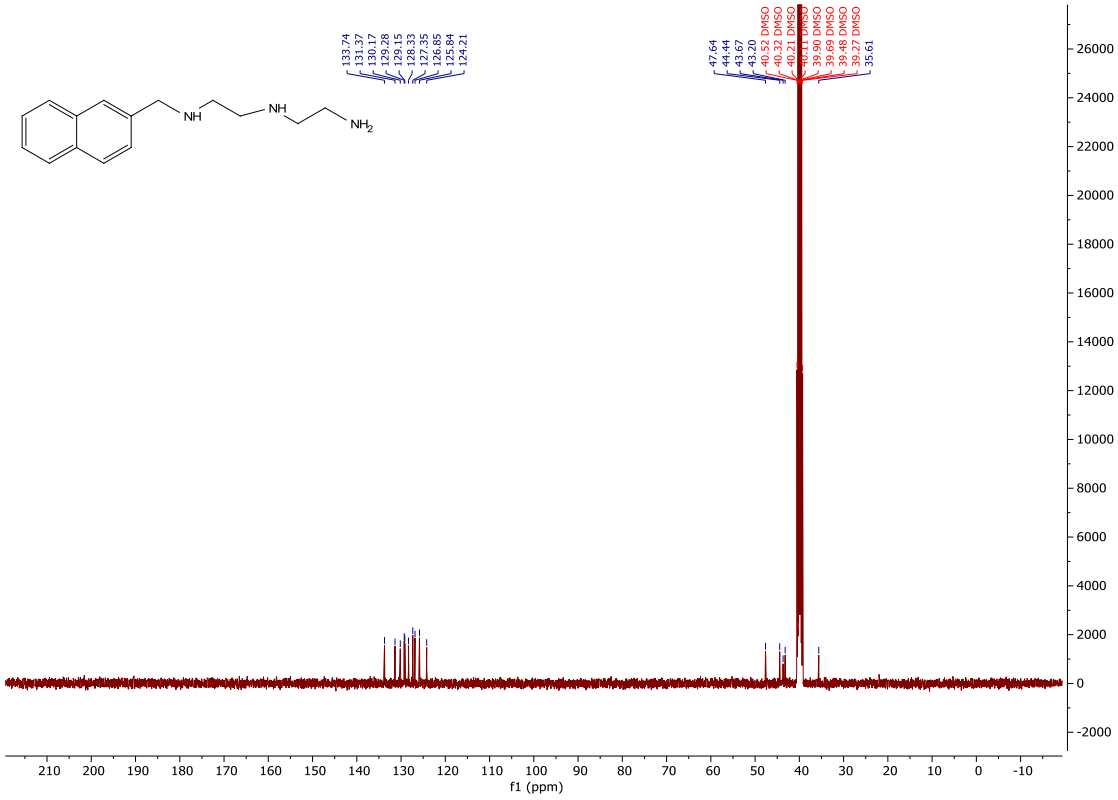

8.75
8.73
8.43
8.41
8.22
3.47 H2O
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.00
1.99
2.00
f1 (ppm)


166.68
148.70
145.11
138.73
130.99
128.90
123.96
40.58 DMSO
40.37 DMSO
40.16 DMSO
39.95 DMSO
39.74 DMSO
39.54 DMSO
39.33 DMSO
f1 (ppm)


8.76
8.74
8.44
8.42
8.23
8.22
4.04
3.47 H2O
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.00
1.96
2.04
5.84
f1 (ppm)


165.98
148.13
145.50
138.59
131.07
129.04
124.20
53.23
40.53 DMSO
40.32 DMSO
40.21 DMSO
40.11 DMSO
39.90 DMSO
39.70 DMSO
39.49 DMSO
39.28 DMSO
f1 (ppm)


9.80
9.47
8.21
8.19
8.16
7.96
7.94
7.94
7.93
7.92
7.74
7.72
7.60
7.59
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.54
7.53
7.52
7.51
7.51
7.50
7.49
4.67
3.44
3.38 H2O
3.11
2.43 DMSO
2.42 DMSO
2.42 DMSO
2.41 DMSO
2.41 DMSO
NH
NH
NH2
2.96
1.13
1.00
2.27
1.15
3.71
3.87
f1 (ppm)


133.74
131.37
130.17
129.28
129.15
128.33
127.35
126.85
125.84
124.21
47.64
44.44
43.67
43.20
40.52 DMSO
40.32 DMSO
40.21 DMSO
40.11 DMSO
39.90 DMSO
39.69 DMSO
39.48 DMSO
39.27 DMSO
35.61
NH
NH
NH2
f1 (ppm)

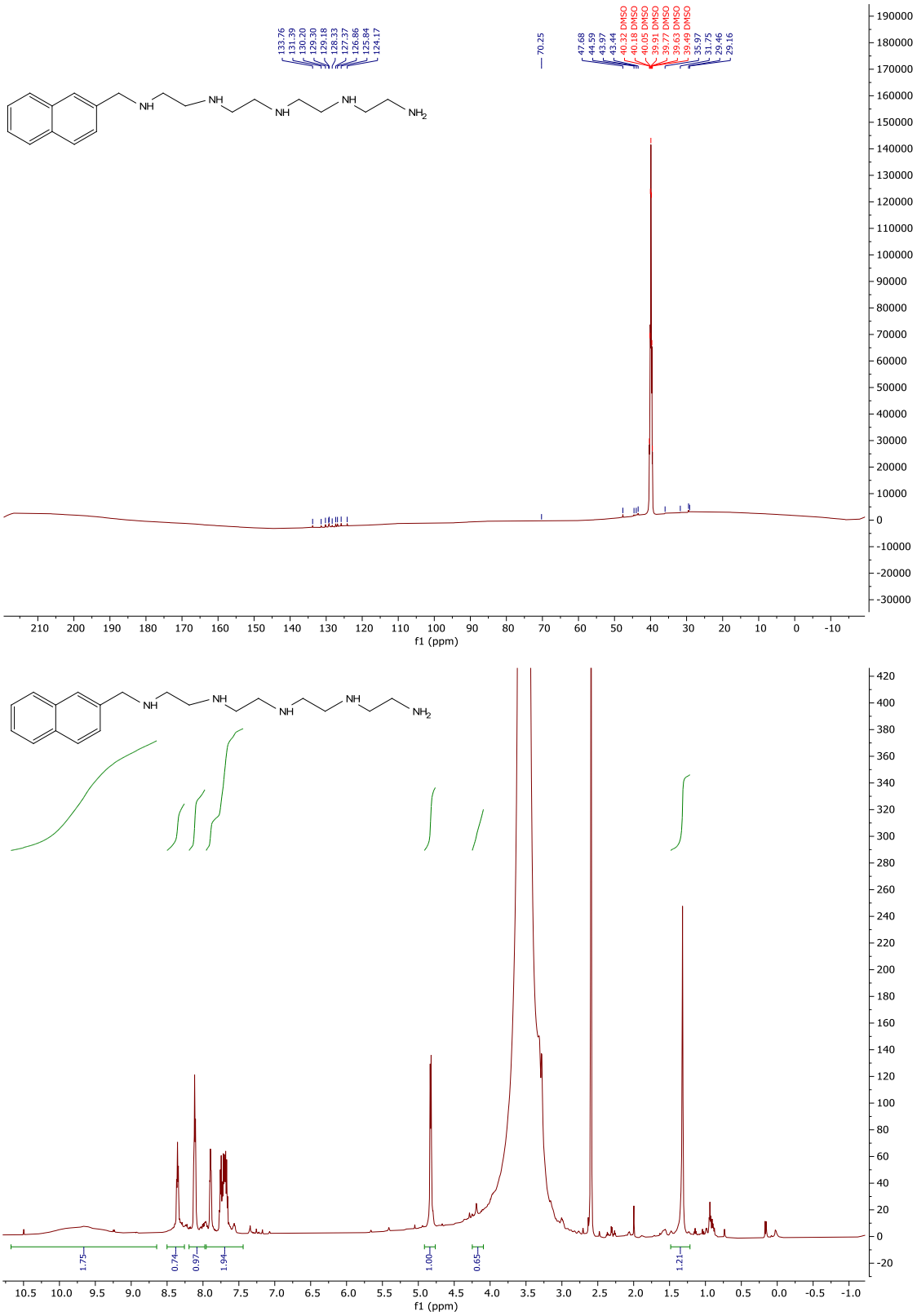


Figure S1. ^{1}H NMR and ^{13}C NMR spectra of synthetized compounds

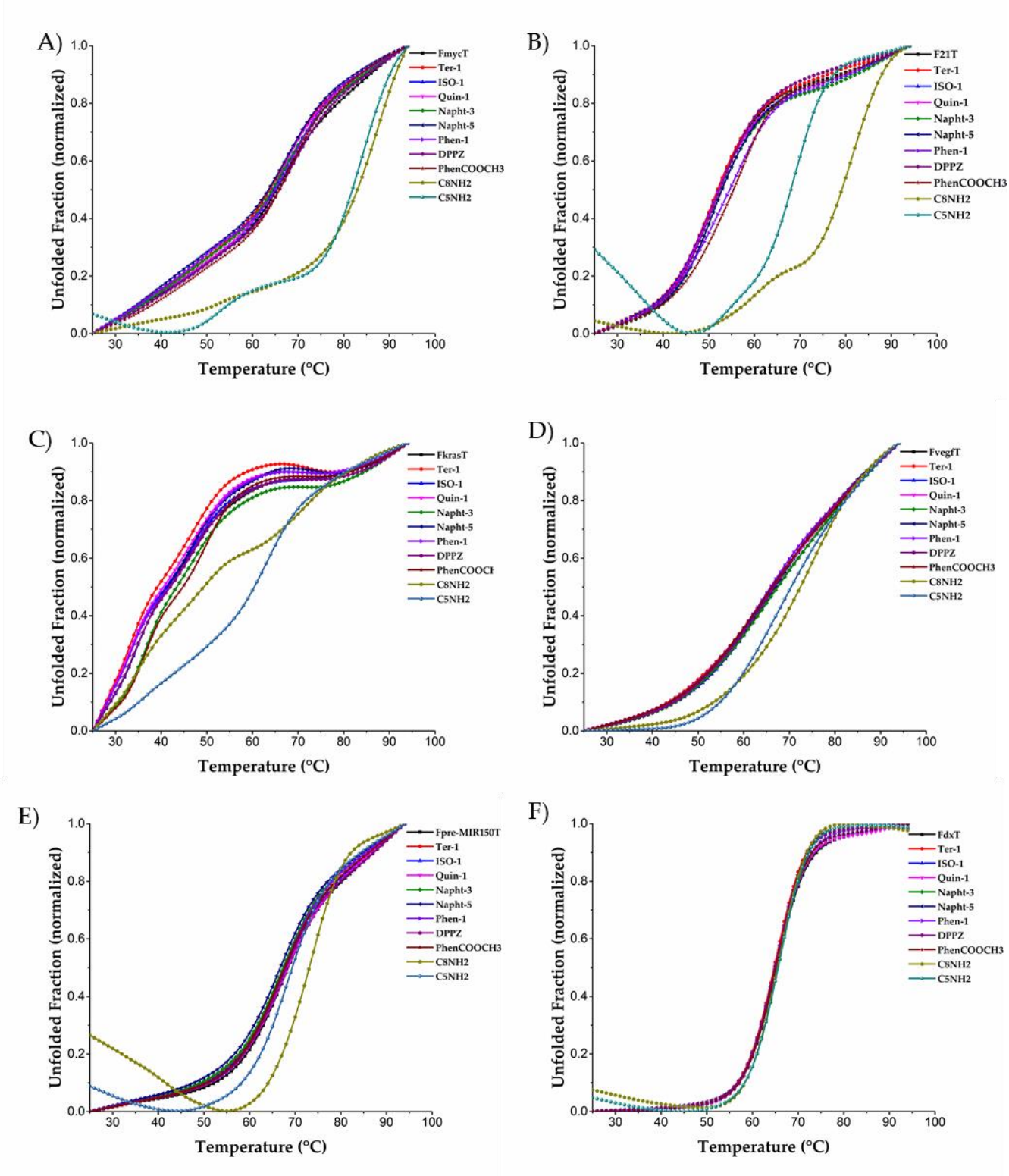


Figure S2. Normalized FRET melting curves of (A) FmycT, (B) F21T, (C) FkrasT, (D) FvegfT, (E) Fpre-MIR150T and (F) FdxT in the presence and absence of ligands. The buffer used was 10 mM lithium cacodylate, pH 7.2. FmycT, F21T and FkrasT was supplemented with 10 mM KCl and 90 mM LiCl, FvegfT and Fpre-MIR150T with 1 mM KCl and 99 mM LiCl and FdxT with 100 mM KCl.