

Supplementary Material

The reactivity of Oxone towards 4,6-di(cycloamino)-1,3-phenylenediamines: synthesis of spirocyclic oxetane ring-fused imidazobenzimidazoles

Darren Conboy and Fawaz Aldabbagh

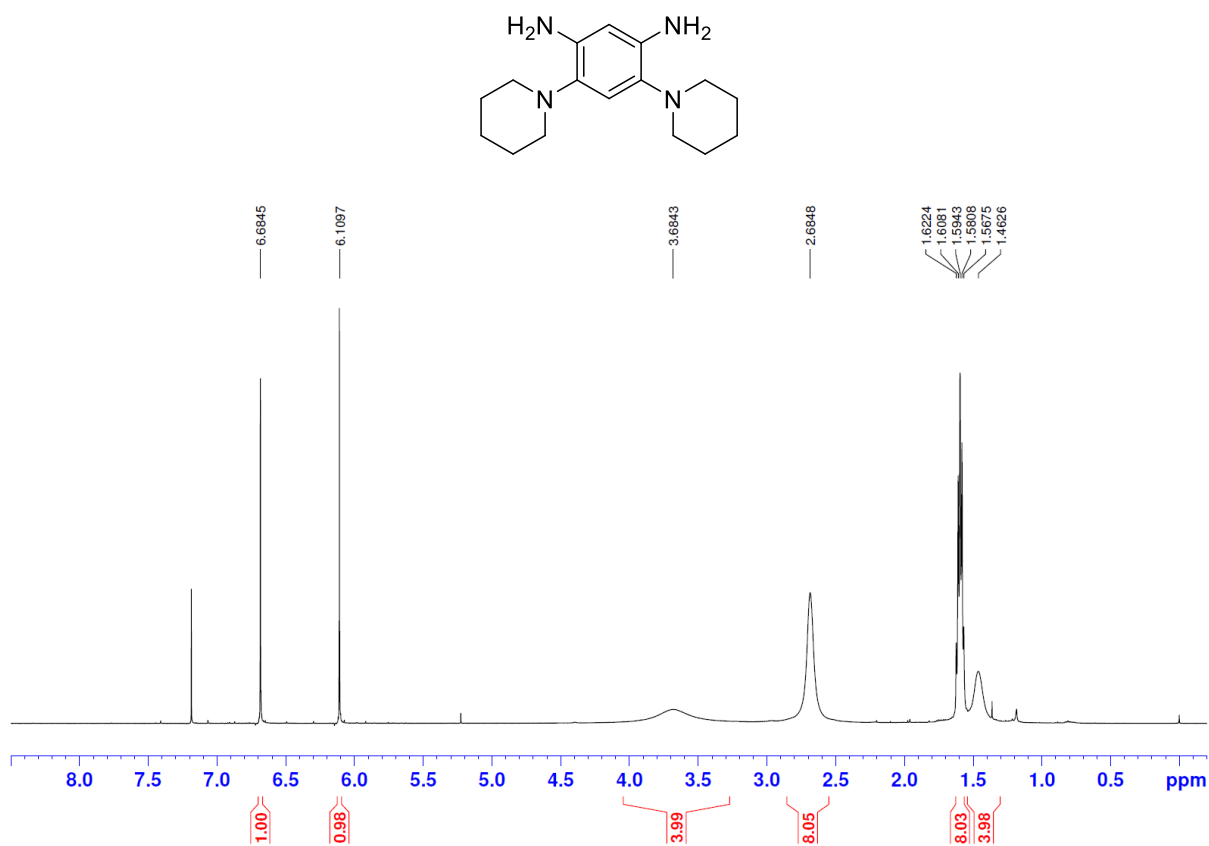
*Department of Pharmacy, School of Life Sciences, Pharmacy and Chemistry, Kingston University, Penrhyn Road,
Kingston upon Thames, KT1 2EE, U.K.*

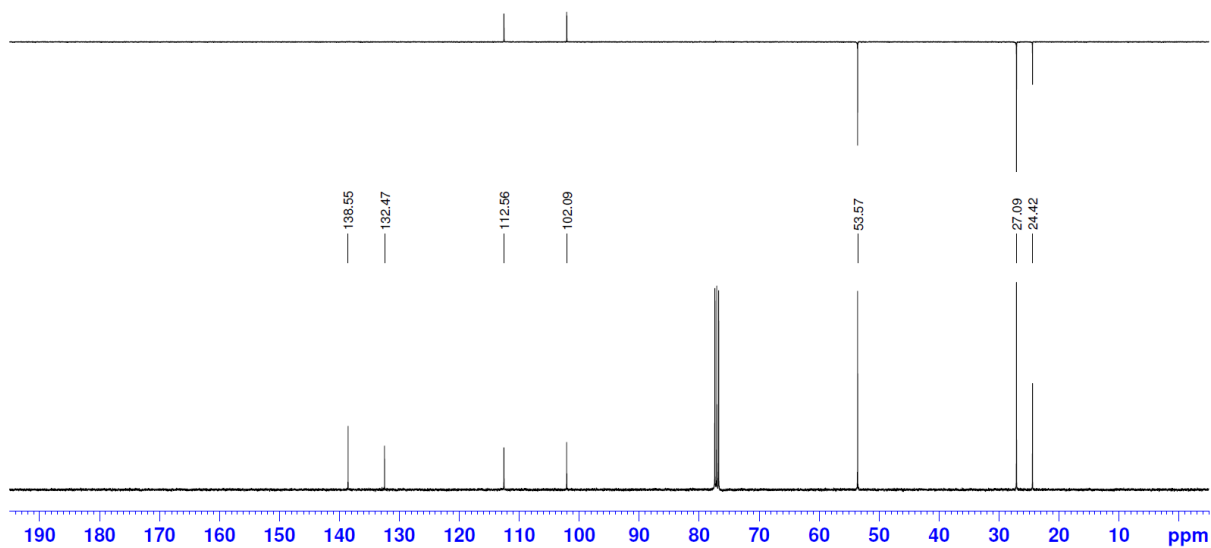
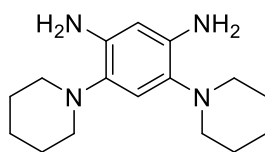
Email: f.aldabbagh@kingston.ac.uk

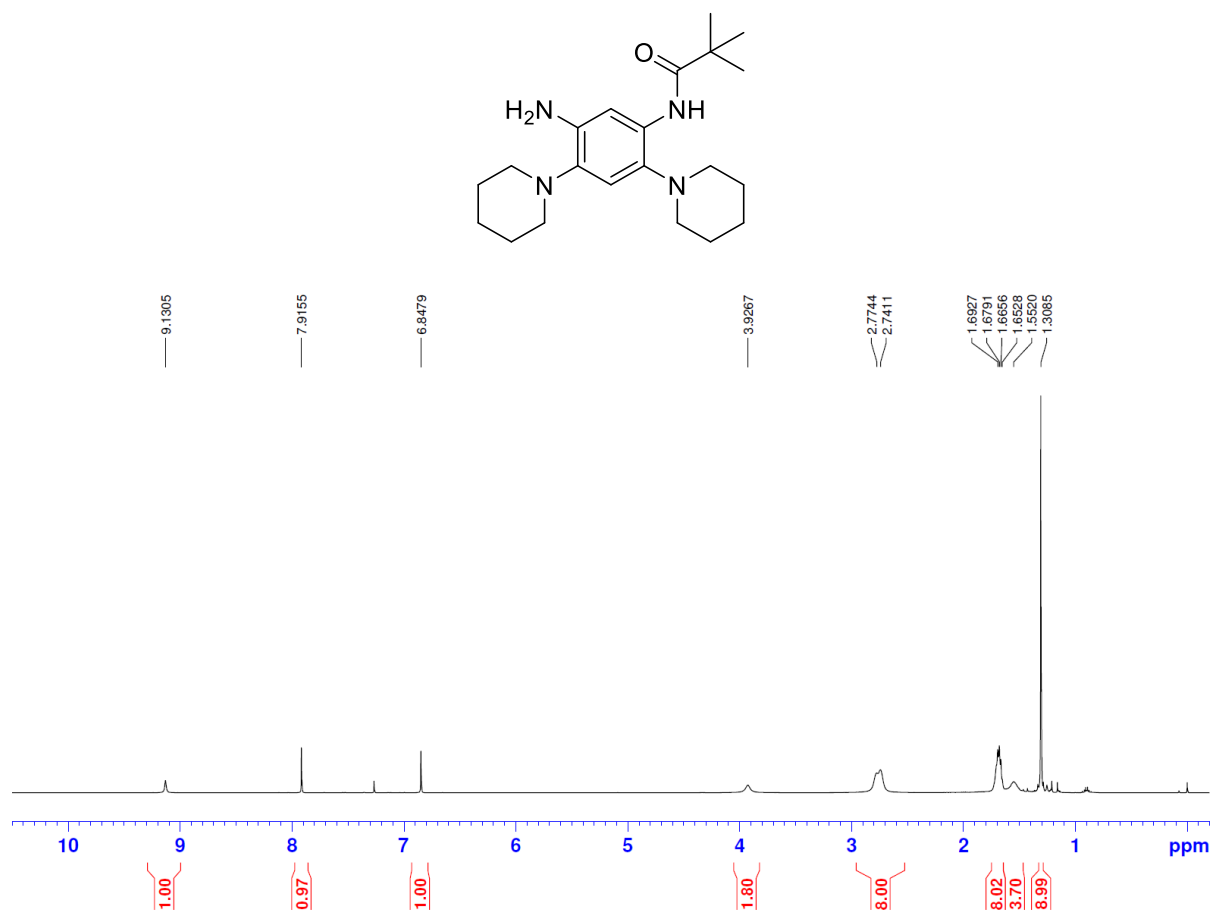
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NMR Spectra

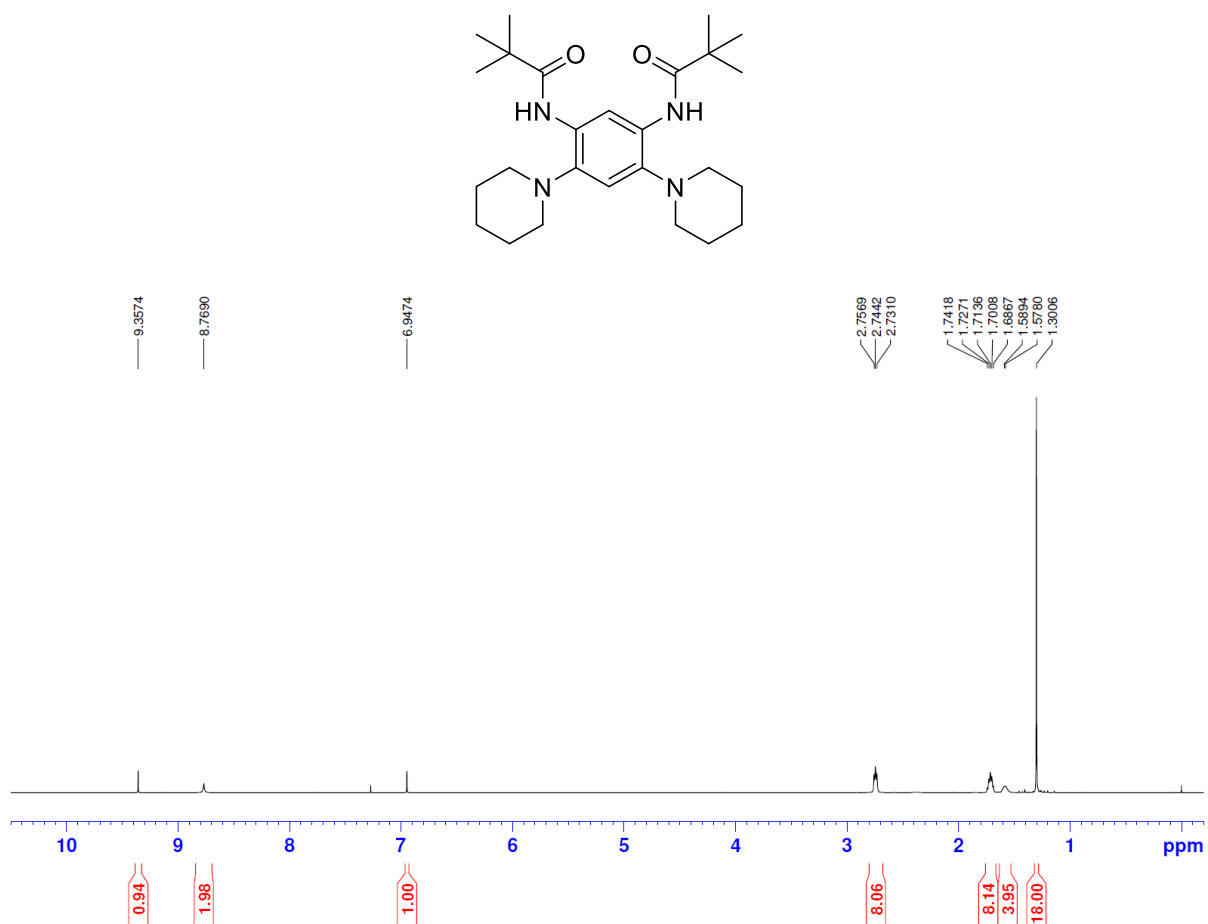
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Compound 11	S6
Compound 12	S8
Compound 13	S10
Compound 14	S12
Compound 18	S13
Compound 17	S14
Compound 19	S15
Compound 22	S17
Compound 20	S19
Compound 23	S21
Compound 21	S23
Compound 24	S25
Compound 4	S27
Compound 5	S29

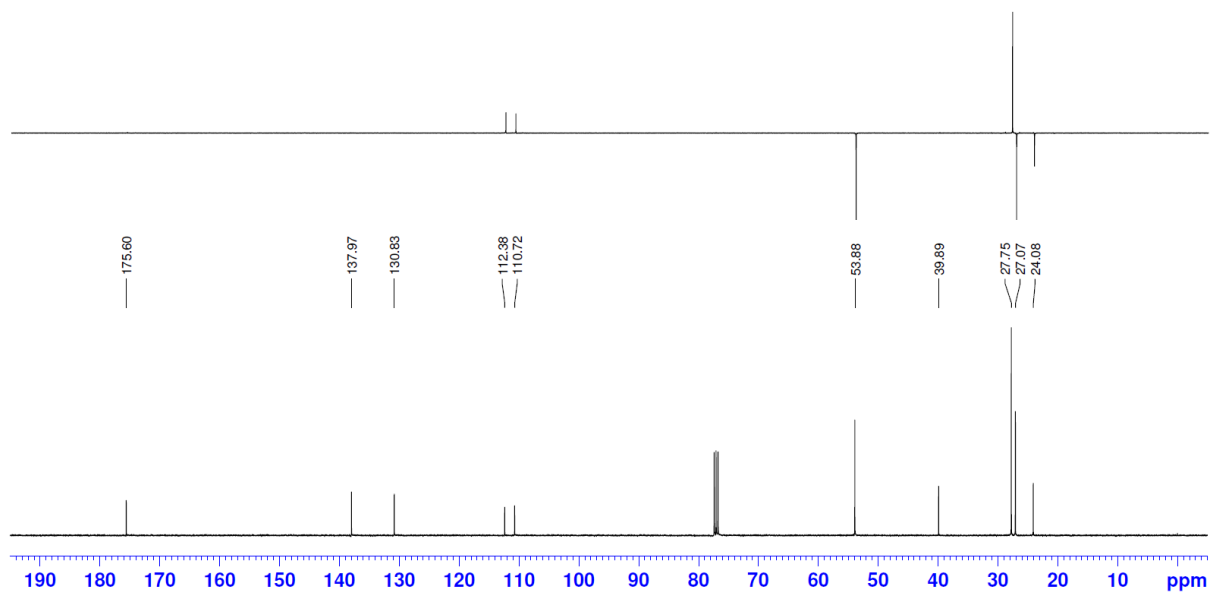
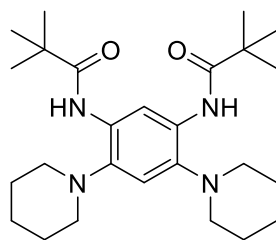
^1H NMR (400 MHz) of 4,6-di(piperidin-1-yl)benzene-1,3-diamine (6) in CDCl_3 

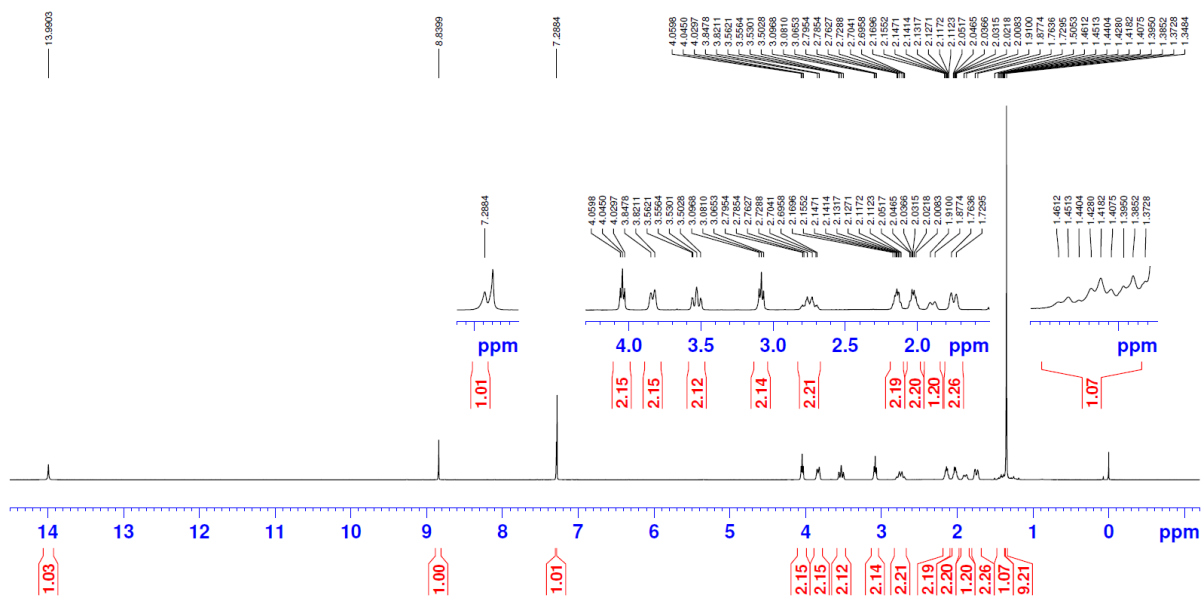
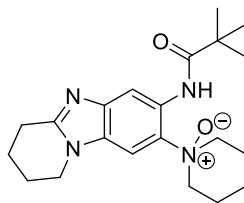
^{13}C NMR (100 MHz) of 4,6-di(piperidin-1-yl)benzene-1,3-diamine (6) in CDCl_3 

^1H NMR (400 MHz) of *N*-[5-amino-2,4-di(piperidin-1-yl)phenyl]-2,2-dimethylpropanamide (10) in CDCl_3 

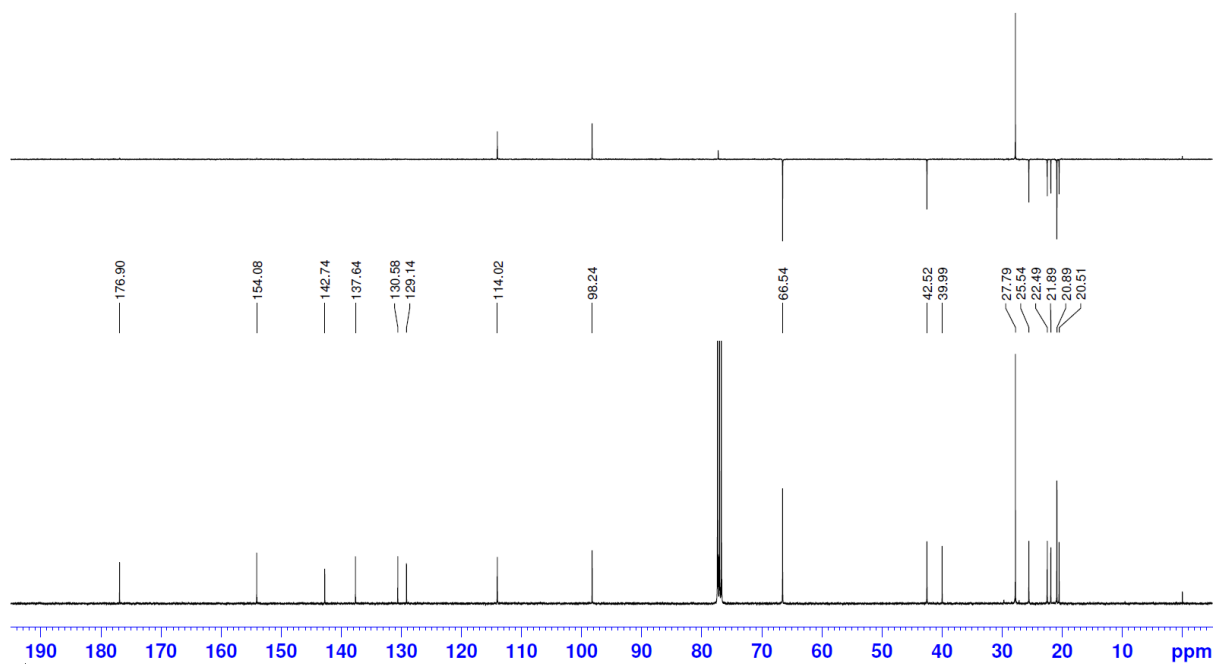
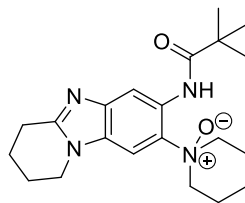
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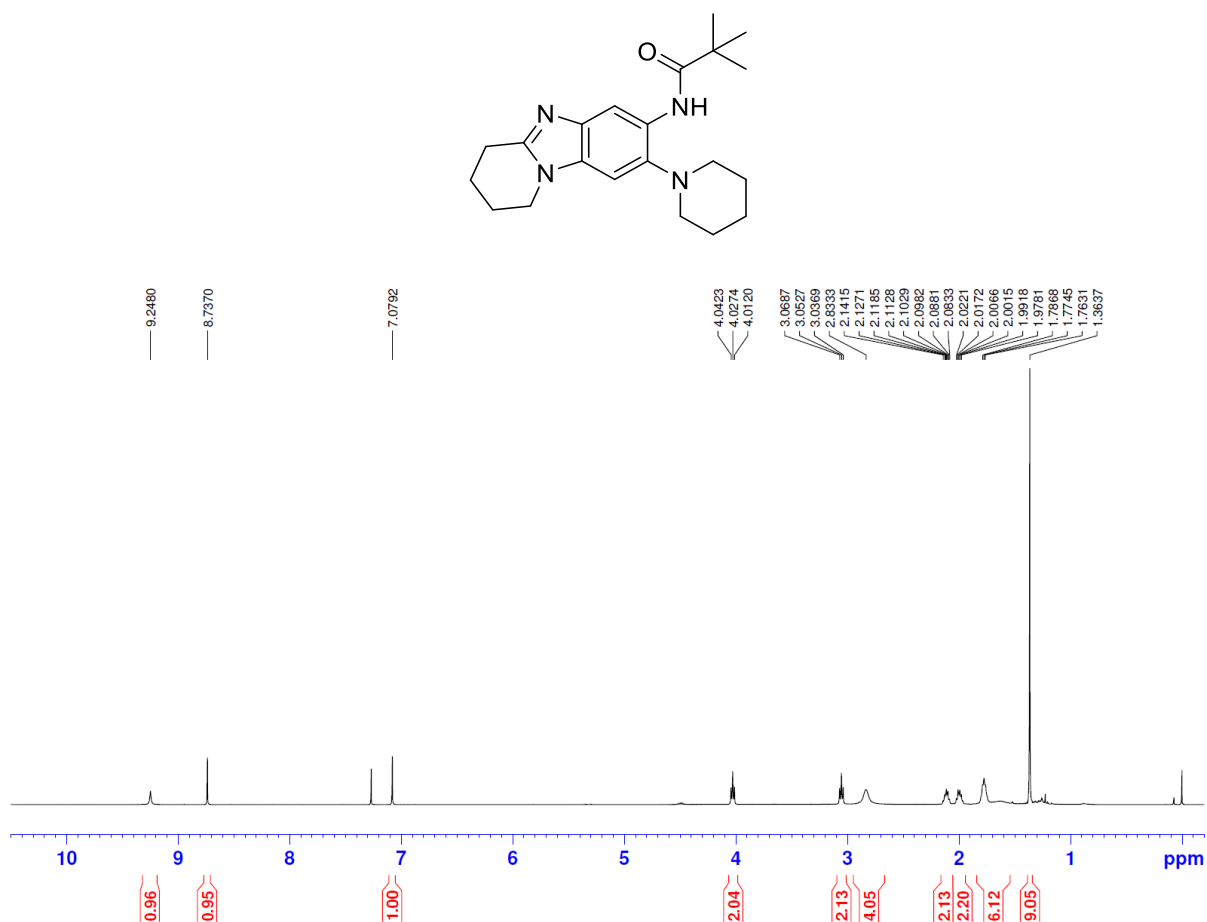
^1H NMR (400 MHz) of *N,N'*-[4,6-di(piperidin-1-yl)-1,3-phenylene]bis(2,2-dimethylpropanamide) (11) in CDCl_3 

^{13}C NMR (100 MHz) of *N,N'*-[4,6-di(piperidin-1-yl)-1,3-phenylene]bis(2,2-dimethylpropanamide) (11) in CDCl_3 

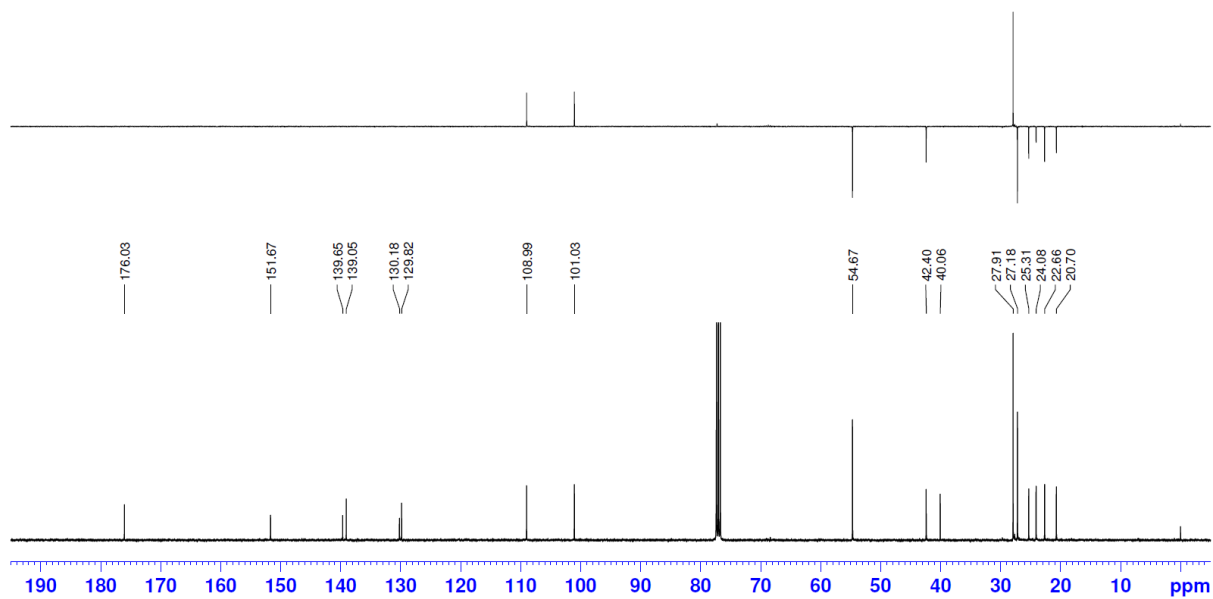
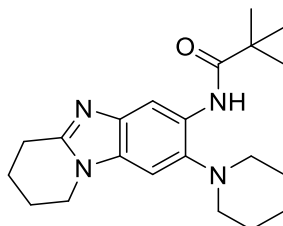
¹H NMR (400 MHz) of 2,2-dimethyl-N-[8-(1-oxidopiperidin-1-yl)-1,2,3,4-tetrahydropyrido[1,2- α]benzimidazol-7-yl]propanamide (12) in CDCl₃

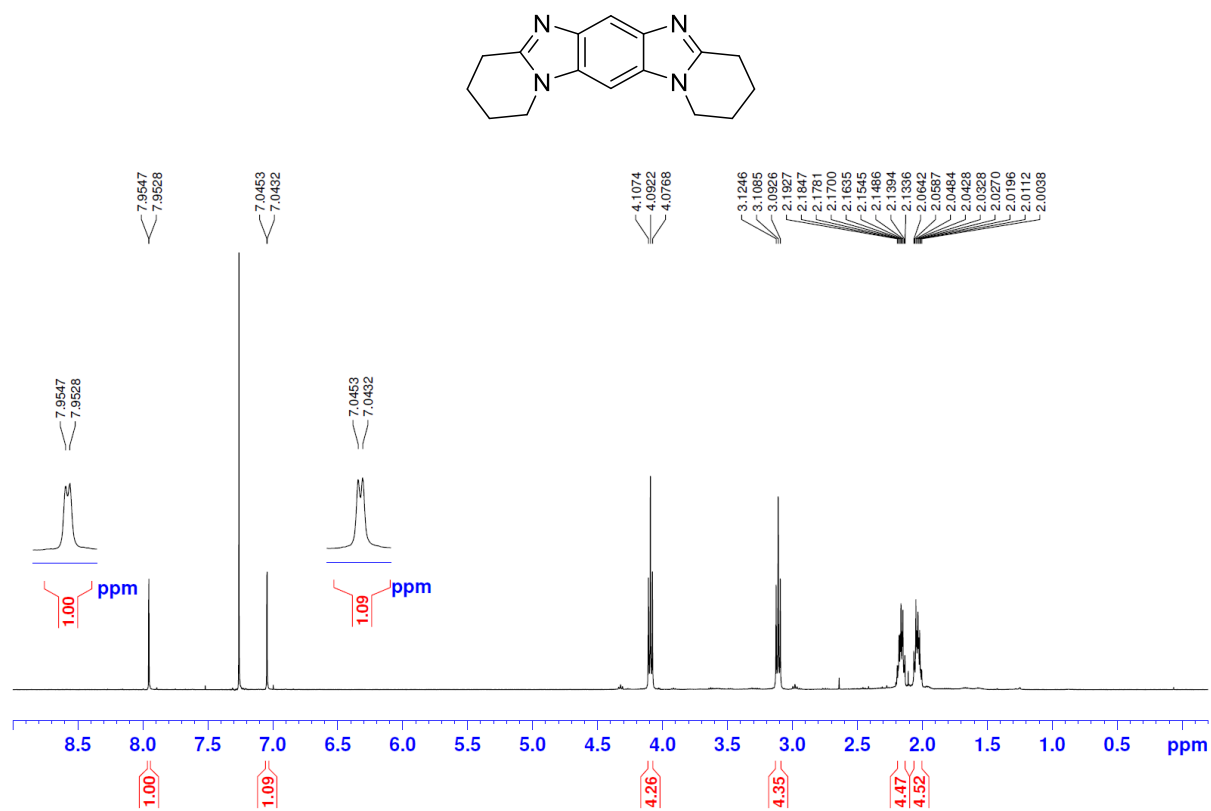
^{13}C NMR (100 MHz) of 2,2-dimethyl-*N*-[8-(1-oxidopiperidin-1-yl)-1,2,3,4-tetrahydropyrido[1,2-*a*]benzimidazol-7-yl]propanamide (12) in CDCl_3



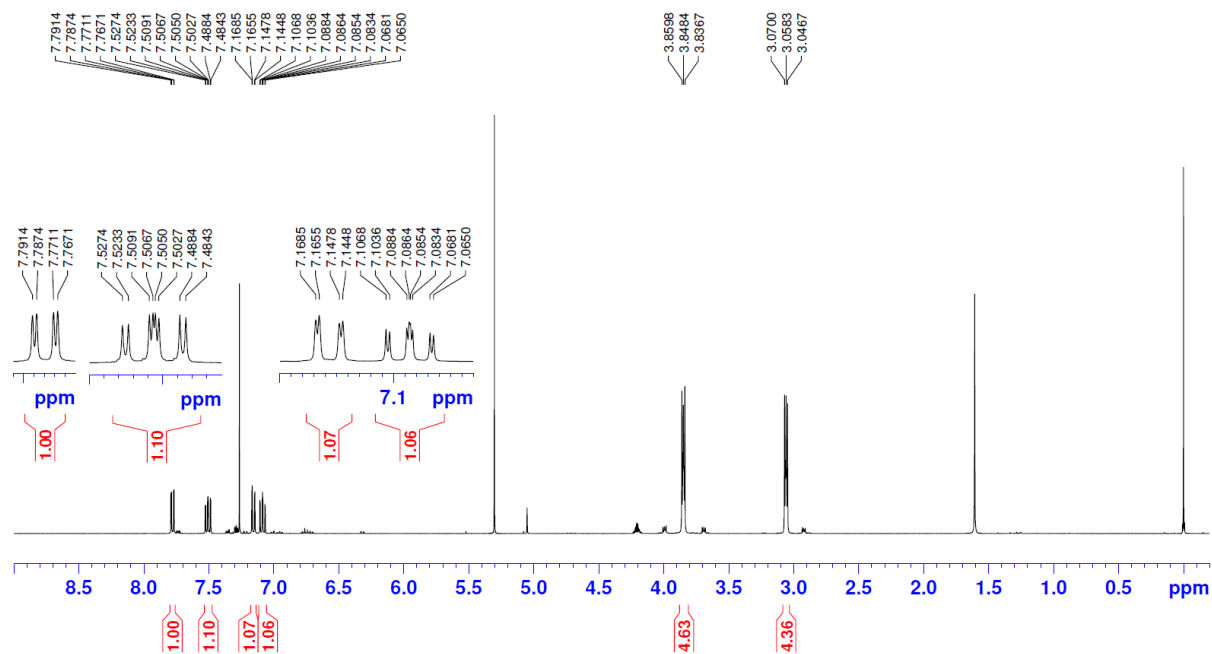
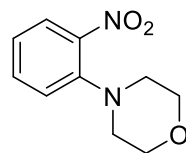
^1H NMR (400 MHz) of 2,2-dimethyl-*N*-[8-(piperidin-1-yl)-1,2,3,4-tetrahydropyrido[1,2-*a*]benzimidazol-7-yl]propanamide (13) in CDCl_3 

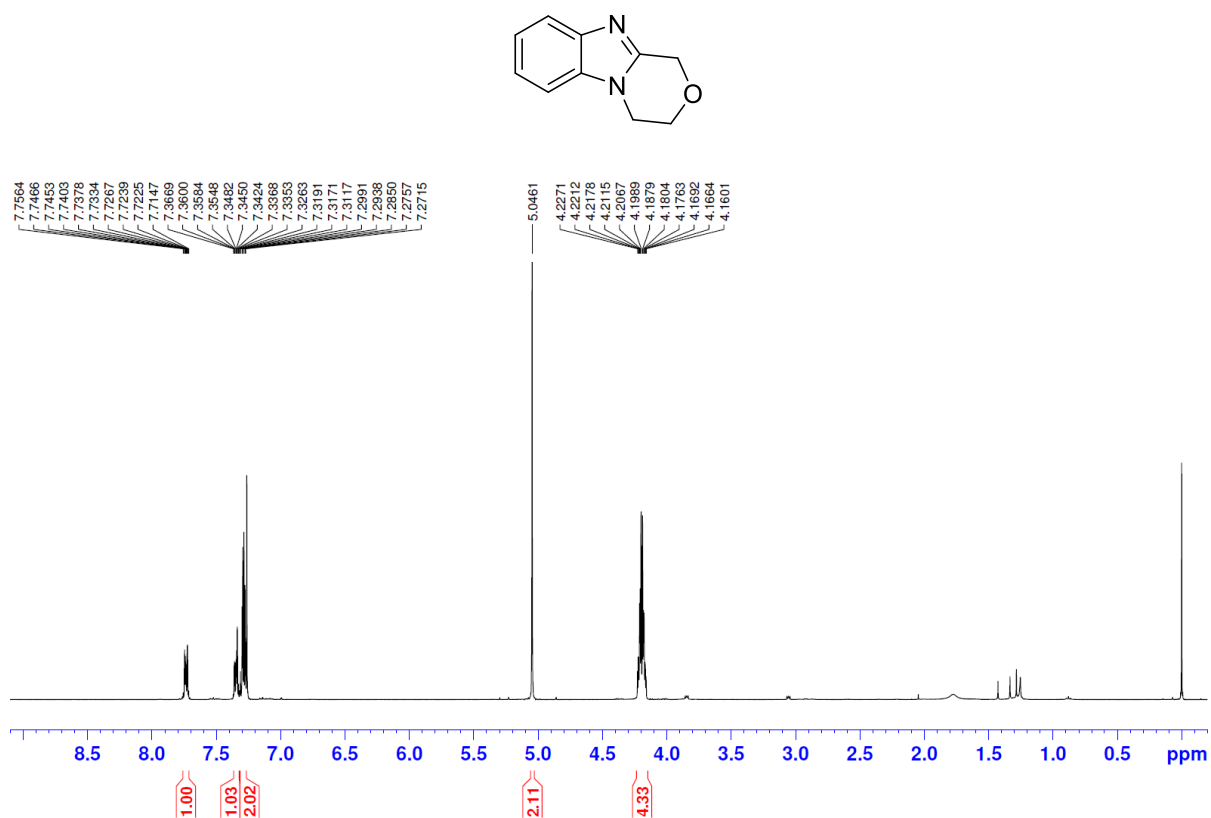
^{13}C NMR (100 MHz) of 2,2-dimethyl-*N*-[8-(piperidin-1-yl)-1,2,3,4-tetrahydropyrido[1,2-*a*]benzimidazol-7-yl]propanamide (13) in CDCl_3

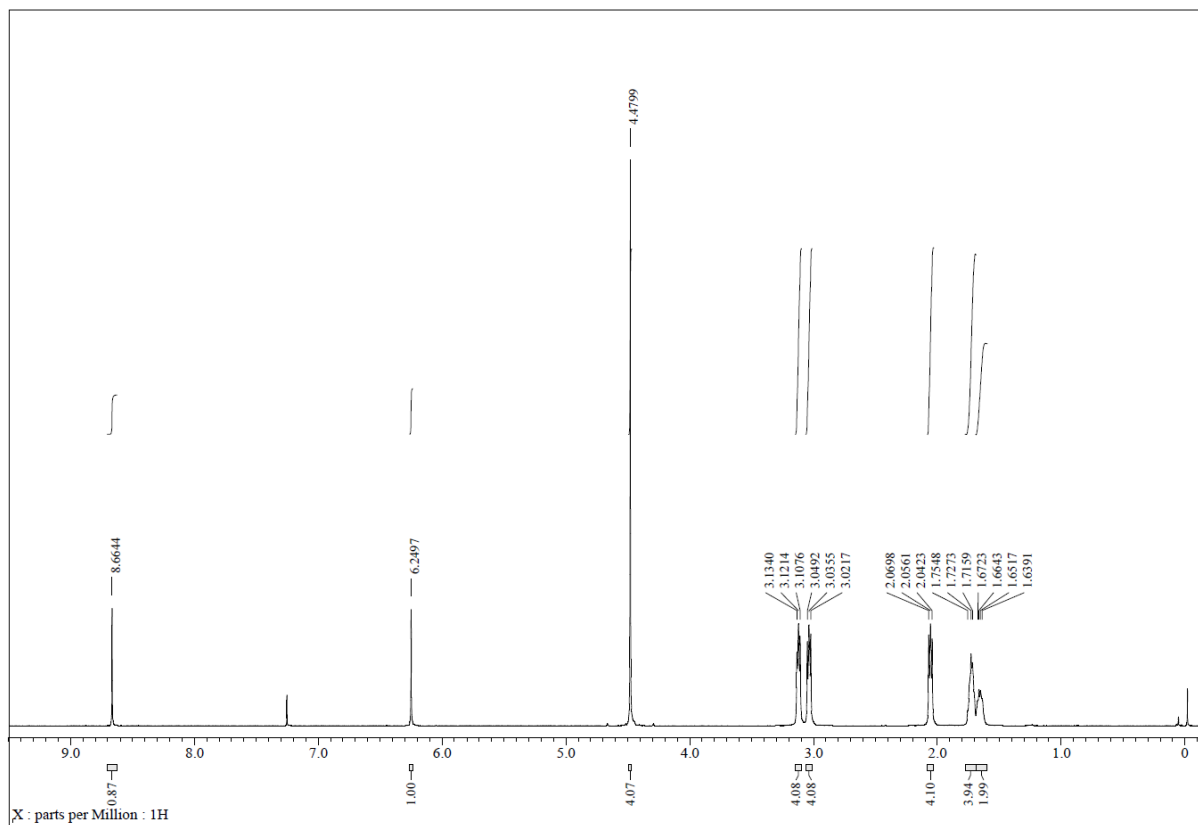
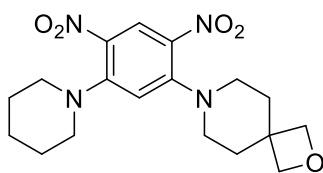


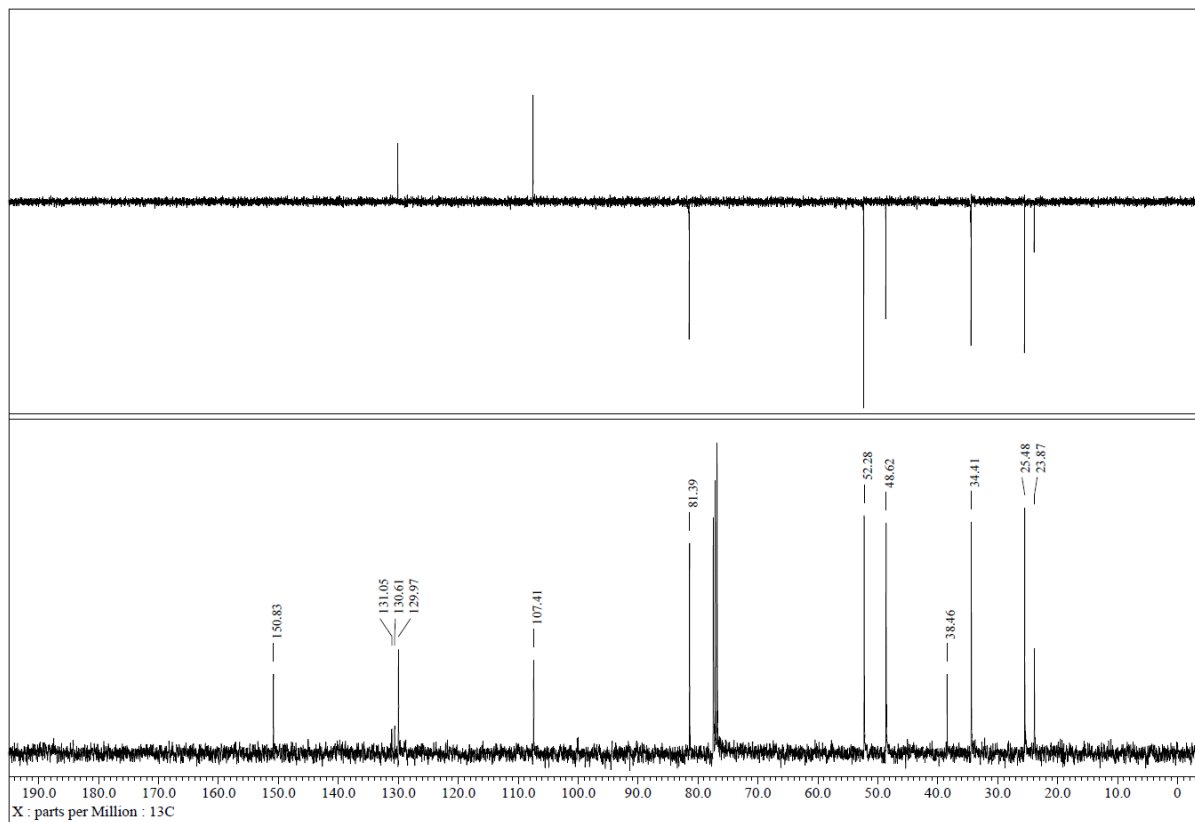
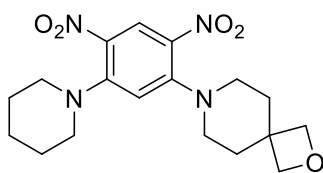
^1H NMR (400 MHz) of 1,2,3,4,8,9,10,11-octahydropyrido[1,2-*a*]pyrido[1',2':1,2]imidazo[4,5-*f*]benzimidazole (14) in CDCl_3 

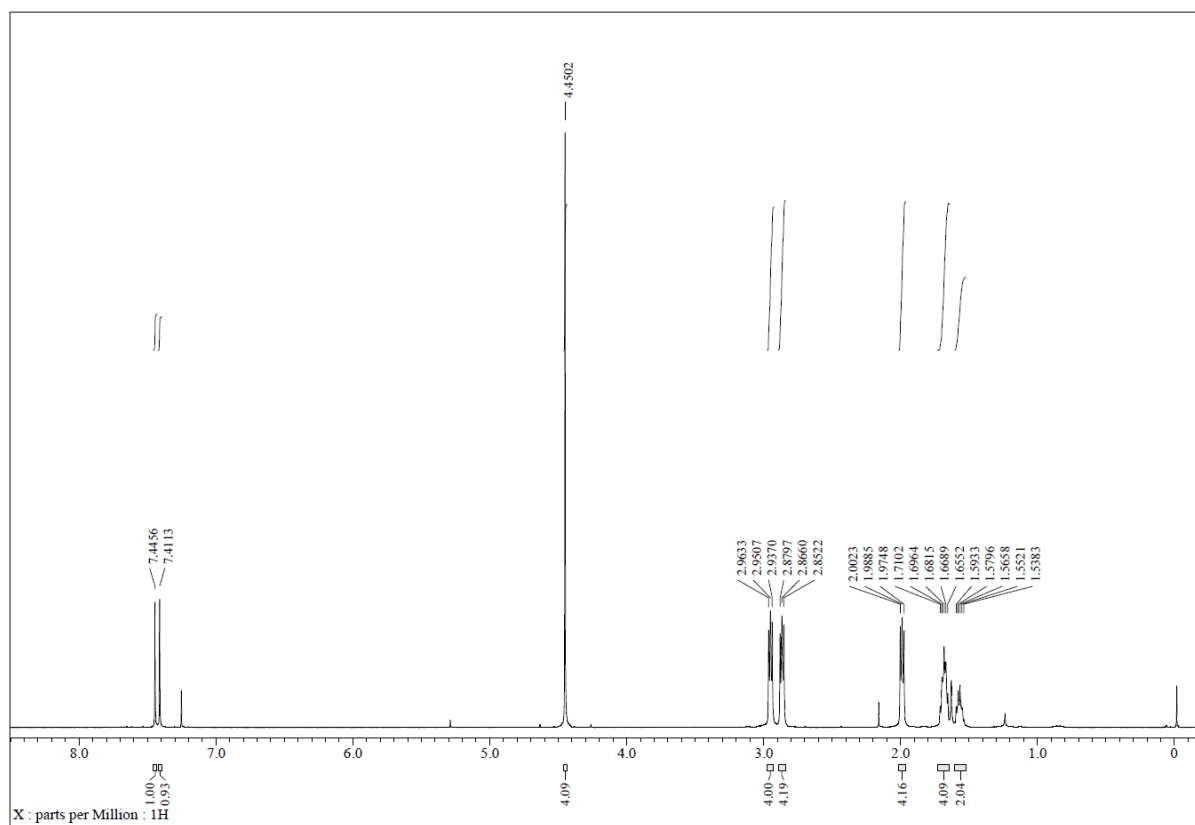
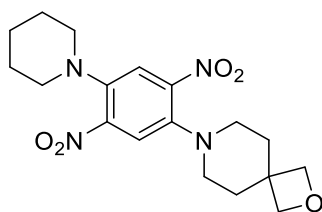
^1H NMR (400 MHz) of 4-(2-nitrophenyl)morpholine (18) in CDCl_3 (CH_2Cl_2 peak at 5.3 ppm, H_2O peak at 1.6 ppm)

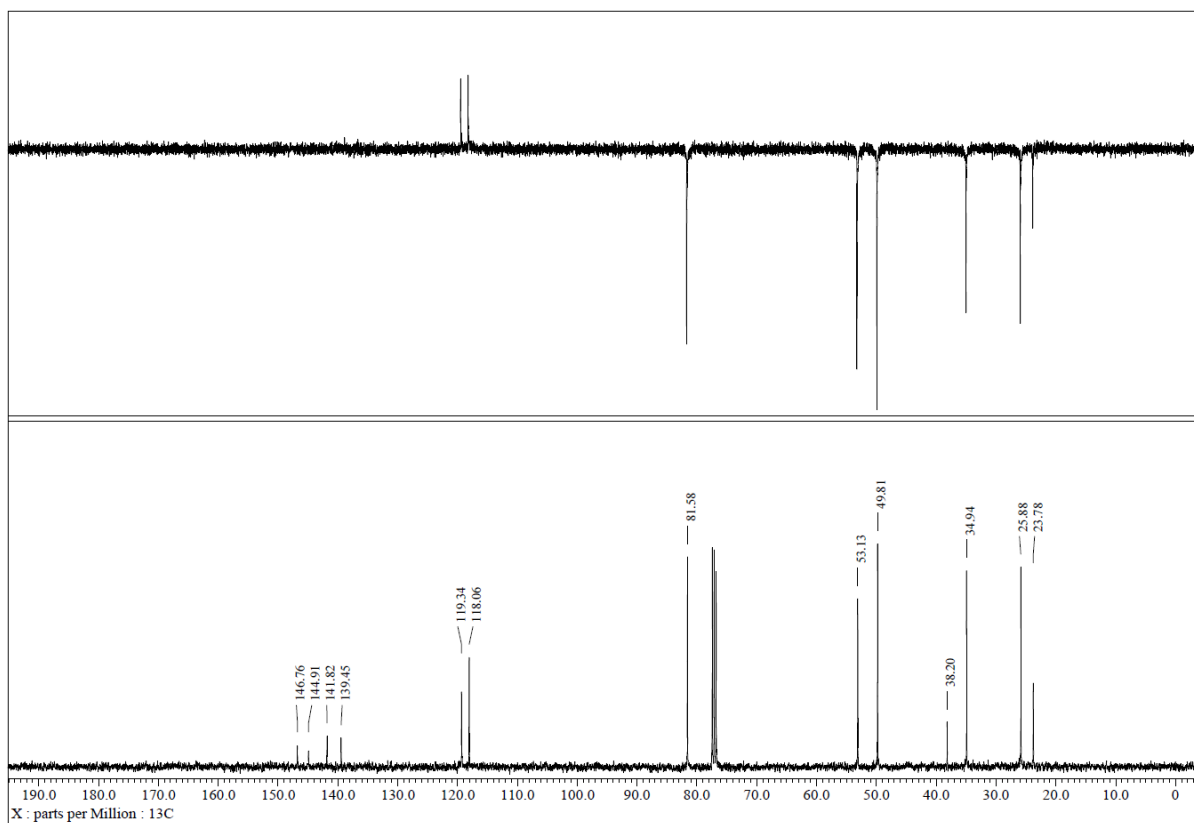
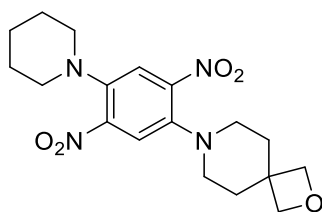


^1H NMR (400 MHz) of 3,4-dihydro-1*H*-[1,4]oxazino[4,3-*a*]benzimidazole (17) in CDCl_3 

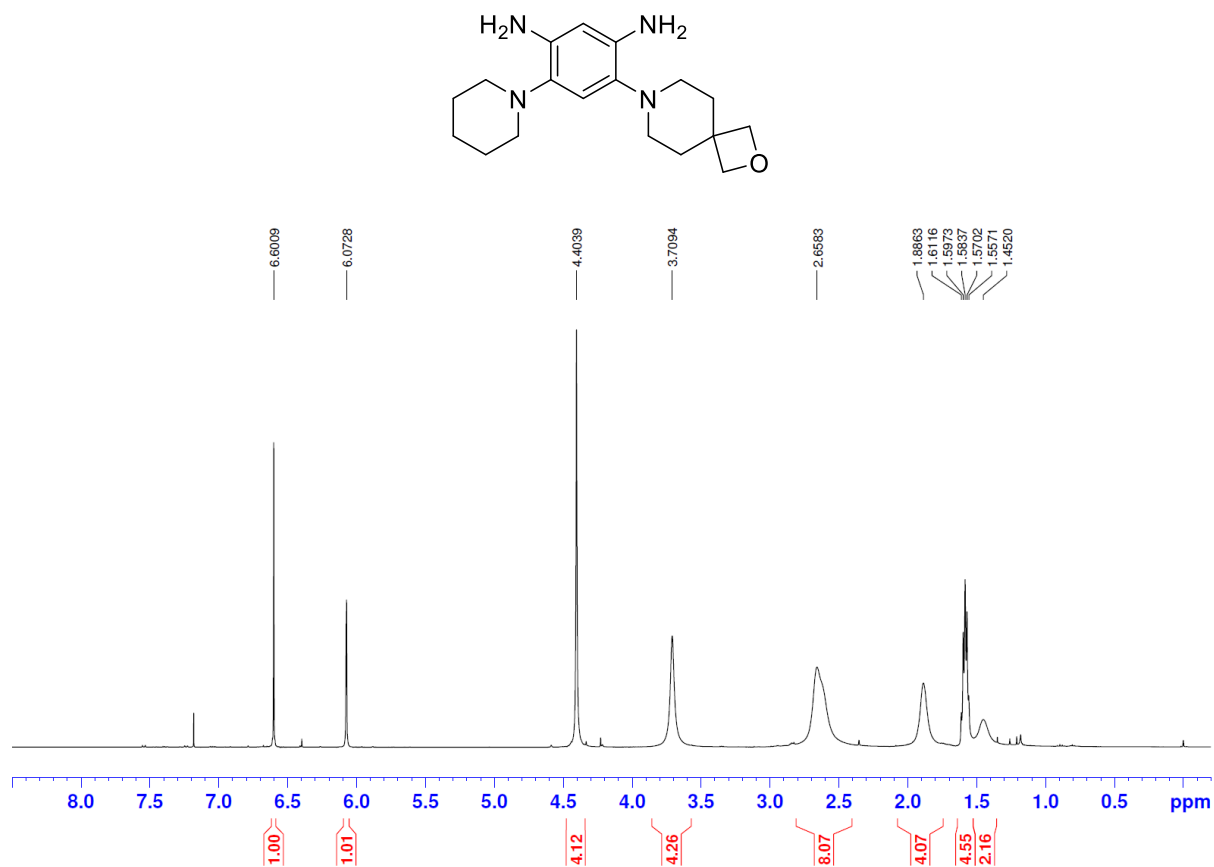
^1H NMR (400 MHz) of 7-(2,4-dinitro-5-piperidin-1-ylphenyl)-2-oxa-7-azaspiro[3.5]nonane (19) in CDCl_3 

^{13}C NMR (100 MHz) of 7-(2,4-dinitro-5-piperidin-1-ylphenyl)-2-oxa-7-azaspiro[3.5]nonane (19) in CDCl_3 

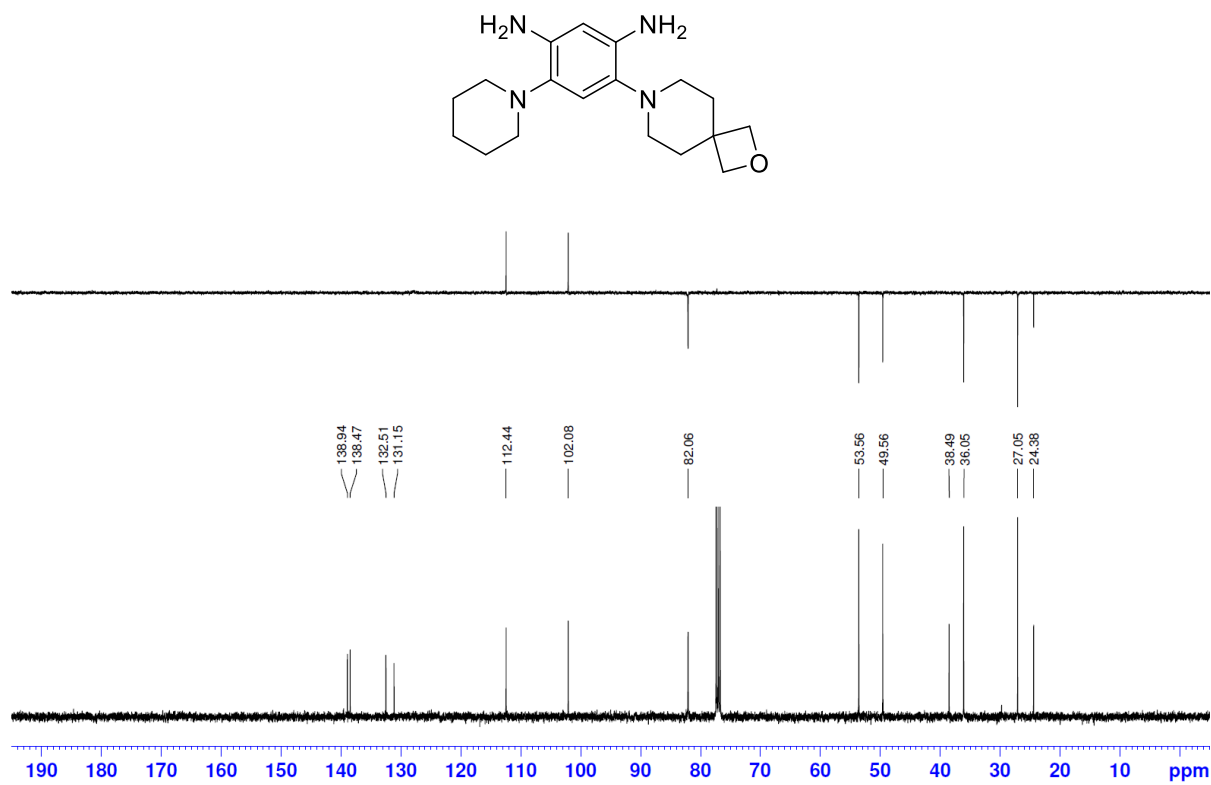
^1H NMR (400 MHz) of 7-(2,5-dinitro-4-piperidin-1-ylphenyl)-2-oxa-7-azaspiro[3.5]nonane (22) in CDCl_3 

^{13}C NMR (100 MHz) of 7-(2,5-dinitro-4-piperidin-1-ylphenyl)-2-oxa-7-azaspiro[3.5]nonane (22) in CDCl_3 

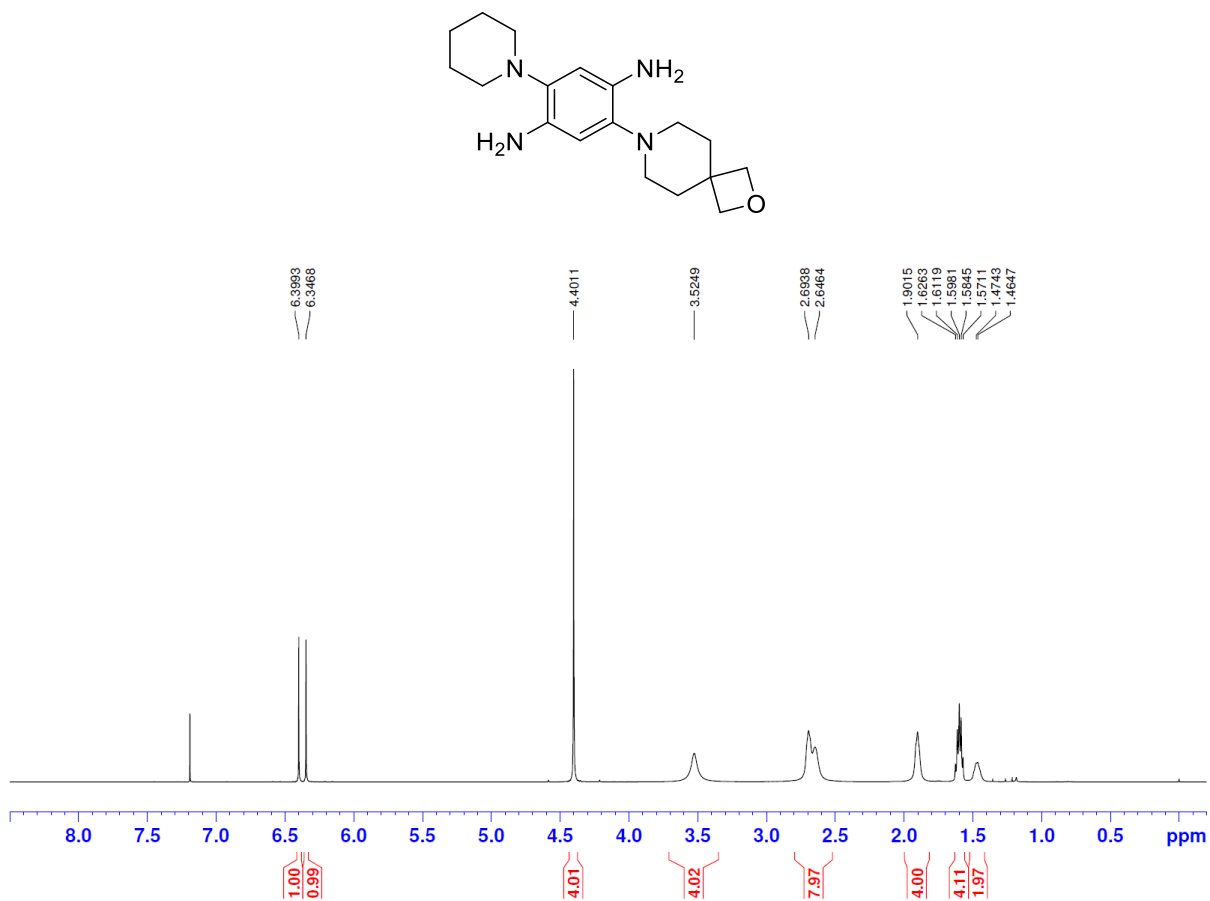
^1H NMR (400 MHz) of 4-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-6-(piperidin-1-yl)benzene-1,3-diamine (20) in CDCl_3



^{13}C NMR (100 MHz) of 4-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-6-(piperidin-1-yl)benzene-1,3-diamine (20) in CDCl_3

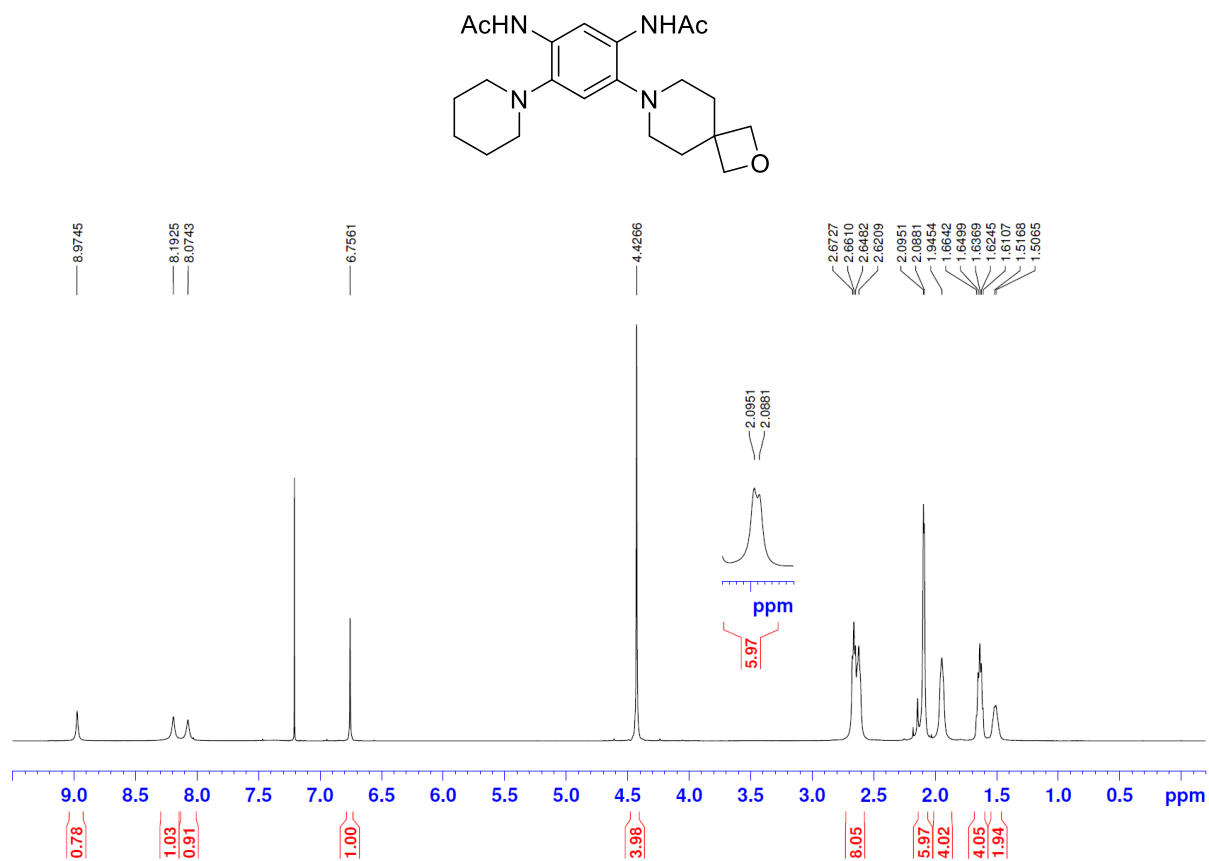


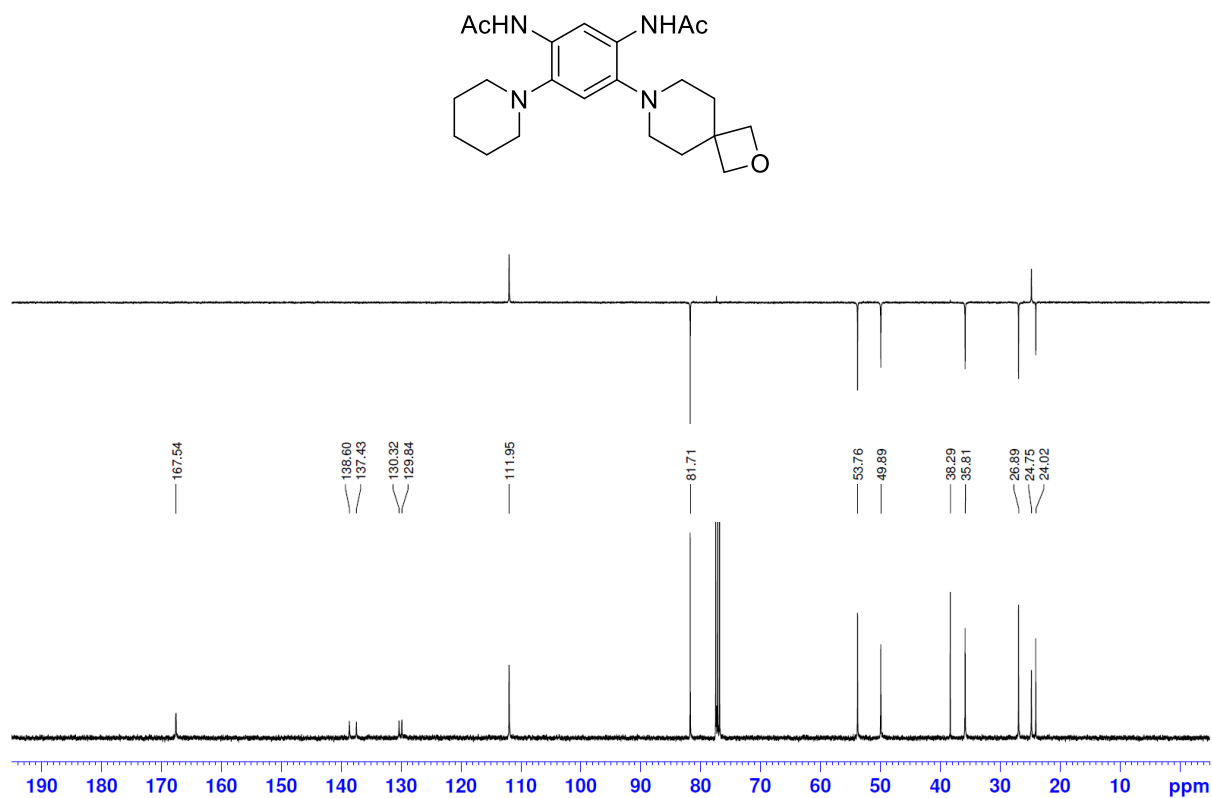
^1H NMR (400 MHz) of 2-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-5-(piperidin-1-yl)benzene-1,4-diamine (23) in CDCl_3

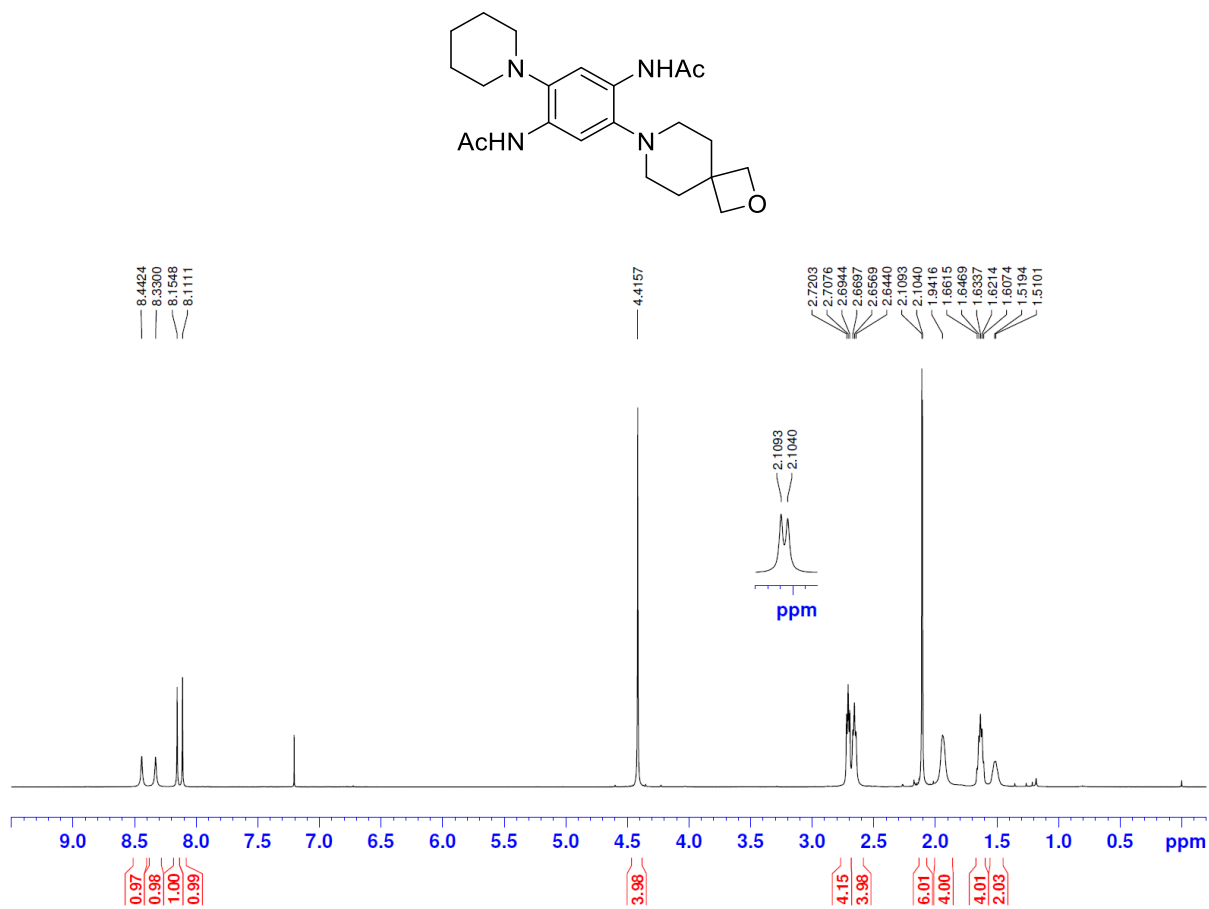


^{13}C NMR (100 MHz) of 2-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-5-(piperidin-1-yl)benzene-1,4-diamine (23) in CDCl_3



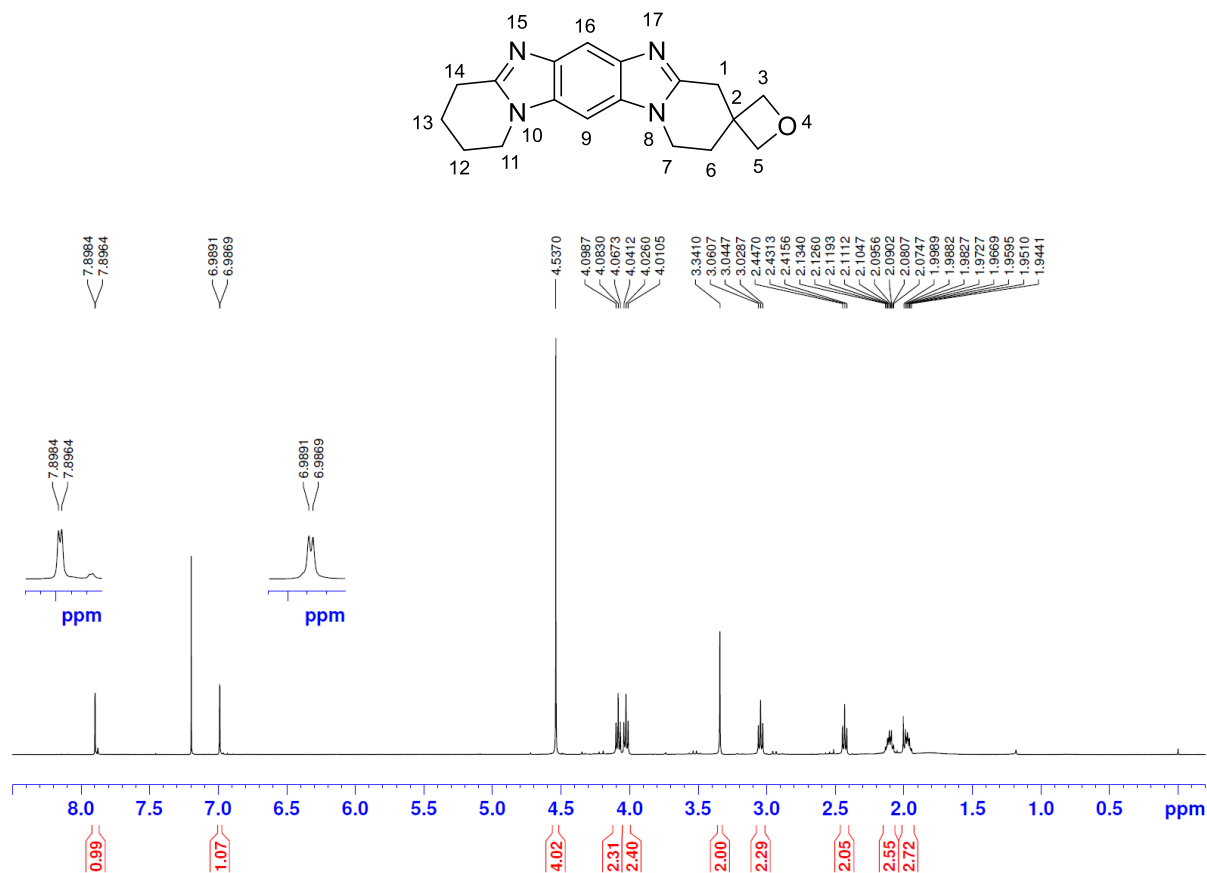
^1H NMR (400 MHz) of *N,N'*-[4-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-6-piperidin-1-yl]-1,3-phenylene]diacetamide (21) in CDCl_3 

^{13}C NMR (100 MHz) of *N,N'*-[4-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-6-piperidin-1-yl-1,3-phenylene]diacetamide (21) in CDCl_3 

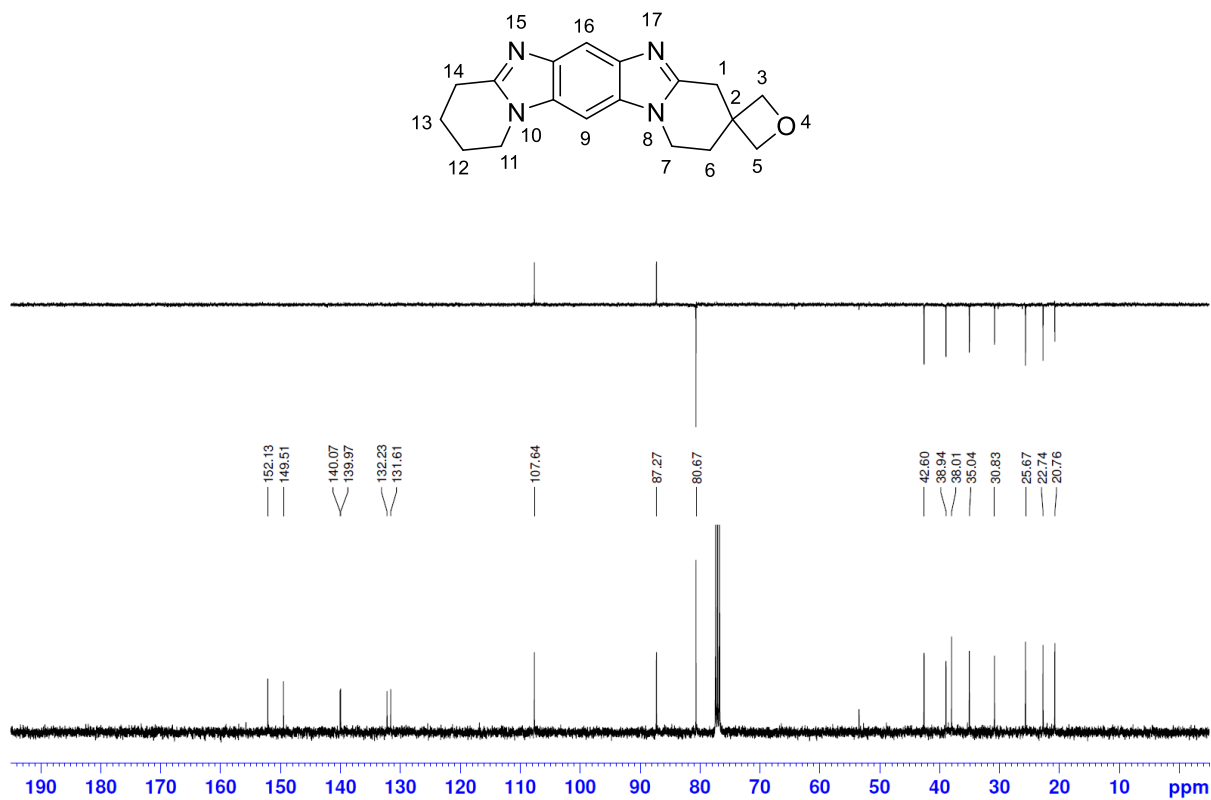
^1H NMR (400 MHz) of *N,N'*-[2-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-5-(piperidin-1-yl)-1,4-phenylene]diacetamide (24) in CDCl_3 

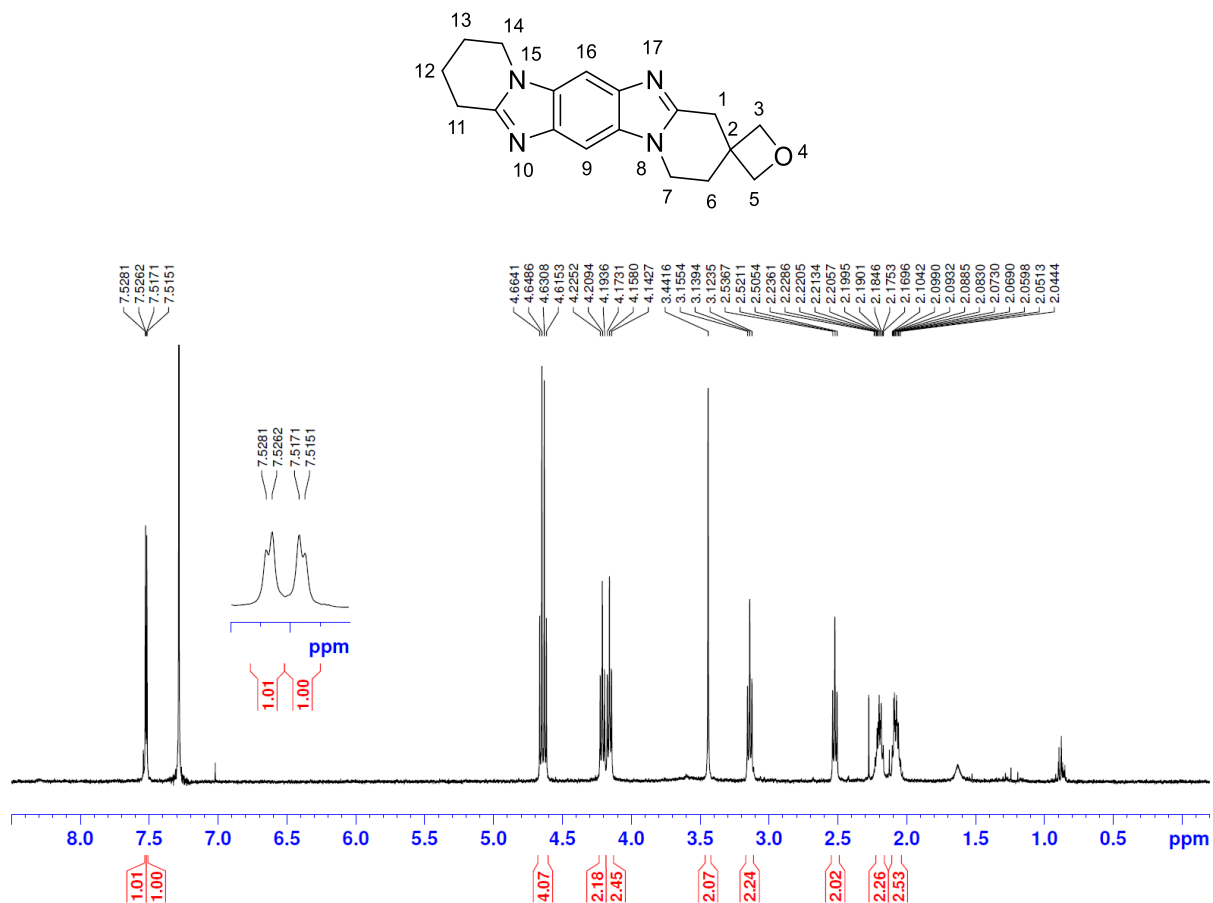
^{13}C NMR (100 MHz) of *N,N'*-[2-(2-oxa-7-azaspiro[3.5]nonan-7-yl)-5-(piperidin-1-yl)-1,4-phenylene]diacetamide (24) in CDCl_3



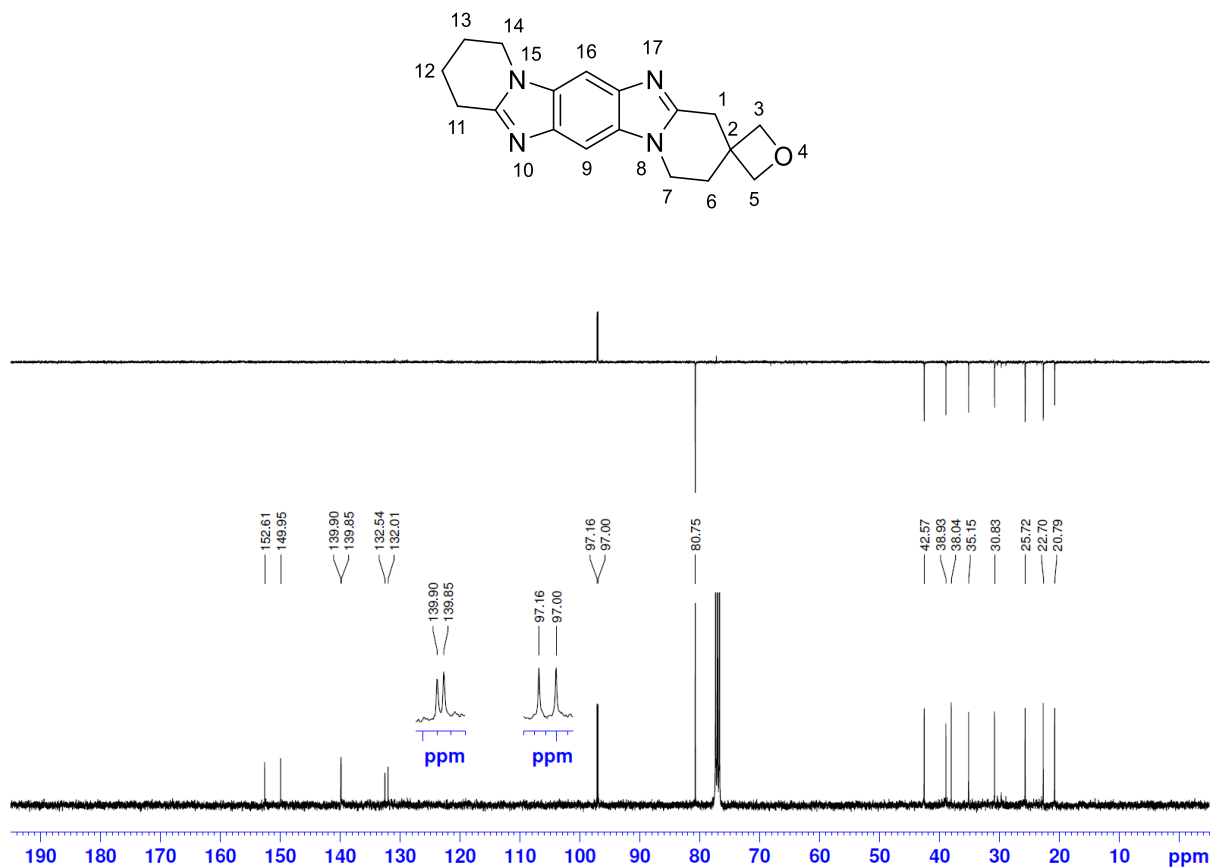
¹H NMR (400 MHz) of 6,7,11,12,13,14-hexahydro-1H-2-oxa-7-azaspiro[3.5]nonan[1,2-*α*]pyrido[1',2':1,2]imidazo[4,5-*f*]benzimidazole (4) in CDCl₃

^{13}C NMR (100 MHz) of 6,7,11,12,13,14-hexahydro-1*H*-2-oxa-7-azaspiro[3.5]nonan[1,2-*a*]pyrido[1',2':1,2]imidazo[4,5-*f*]benzimidazole (4) in CDCl_3



^1H NMR (400 MHz) of 6,7,11,12,13,14-hexahydro-1*H*-2-oxa-7-azaspiro[3.5]nonan[1,2- α]pyrido[1',2':1,2]imidazo[5,4-*f*]benzimidazole (5) in CDCl_3 

^{13}C NMR (100 MHz) of 6,7,11,12,13,14-hexahydro-1*H*-2-oxa-7-azaspiro[3.5]nonan[1,2-*a*]pyrido[1',2':1,2]imidazo[5,4-*f*]benzimidazole (5) in CDCl_3



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