Supplementary Materials

Palladium-Catalyzed Synthesis of 6-aryl Dopamine Derivatives

Andrea Calcaterra [1], Santiago Fernández García [1], Federico Marrone [1], Roberta Bernini [2,*], Giancarlo Fabrizi [1,*], Antonella Goggiamani [1] and Antonia Iazzetti [3,4]

[1] Department of Chemistry and Technology of Drugs, Sapienza—University of Rome, P.le Aldo Moro 5, 00185 Rome, Italy; andrea.calcaterra@uniroma1.it (A.C.); federico.marrone@uniroma1.it (F.M.); antonella.goggiamani@uniroma1.it (A.G.)
[2] Department of Agriculture and Forest Sciences (DAFNE), University of Tuscia, Via San Camillo de Lellis, 01100 Viterbo, Italy
[3] Dipartimento di Scienze Biotecnologiche di base, Cliniche Intensivologiche e Perioperatorie, Università Cattolica del Sacro Cuore, L.go Francesco Vito 1, 00168 Rome, Italy; antonia.iazzetti@unicatt.it
[4] Policlinico Universitario 'A. Gemelli' Foundation-IRCCS, 00168 Rome, Italy
* Correspondence: roberta.bernini@unitus.it (R.B.); giancarlo.fabrizi@uniroma1.it (G.F.)

Index: Pag.

Figure S1. ^{1}H NMR of Methyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1a**) 4

Figure S2. ^{13}C NMR of Methyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1a**) 4

Figure S3. ^{1}H NMR of Methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**) 5

Figure S4. ^{13}C NMR of Methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**) 5

Figure S5. DEPT 135 NMR of methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**) 6

Figure S6. ^{1}H NMR of *tert*-butyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**13**) 7

Figure S7. ^{13}C NMR of *tert*-butyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**13**) 7

Figure S8. ^{1}H NMR of (*tert*-butoxycarbonyl)(2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b**) 8

Figure S9. ^{13}C NMR of (*tert*-butoxycarbonyl)(2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b**) 7

Figure S10. ^{1}H NMR of *tert*-butyl (2-(2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b'**) 9

Figure S11. ^{13}C NMR of *tert*-butyl (2-(2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b'**) 9

Figure S12. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3ba**) 10

Figure S13. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3ba**) 10

Figure S14. ^{1} H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-acetylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bb**) 11

Figure S15. ^{13} C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-acetylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bb**) 11

Figure S16. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methoxyphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bc**) 12

Figure S17. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methoxyphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bc**) 12

Figure S18. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-methylphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bd**) 13

Figure S19. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-methylphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bd**) 13

Figure S20. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-fluoro-3-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3be**) 14

Figure S21. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-fluoro-3-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3be**) 14

Figure S22. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)ethyl)carbamate (**3bf**) 15

Figure S23. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)ethyl)carbamate (**3bf**) 15

Figure S24. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-formylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol -5-yl)ethyl)carbamate (**3bh**) 16

Figure S25. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-hydroxymethylphenyl)-2,2-dimethylbenzo[d] [1,3]dioxol-5-yl)ethyl)carbamate (**3bh'**) 17

Figure S26. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-hydroxymethylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol-5-yl)ethyl)carbamate (**3bh'**) 17

Figure S27. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(3-formylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol -5-yl)ethyl)carbamate (**3bi**) 18

Figure S28. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(3-formylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol -5-yl)ethyl)carbamate (**3bi**) 18

Figure S29. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-formylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol -5-yl)ethyl)carbamate (**3bj**) 19

Figure S30. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-formylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol -5-yl)ethyl)carbamate (**3bj**) 19

Figure S31. ^{1}H NMR of methyl 3-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)benzoate (**3bl**) 20

Figure S32. ^{13}C NMR of methyl 3-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)benzoate (**3bl**) 20

Figure S33. ^{1}H NMR of methyl 4-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)benzoate (**3bm**) 21

Figure S34. ^{13}C NMR of methyl 4-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)benzoate (**3bm**) 21

Figure S35. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-([1,1'-biphenyl]-4-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bn**) 22

Figure S36. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-([1,1'-biphenyl]-4-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bn**) 22

Figure S37. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(naphtalen-1-yl)-2,2-dimethylbenzo[d][1,3]dioxol -5-yl)ethyl)carbamate (**3bo**) 23

Figure S38. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(naphtalen-1-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bo**) 23

Figure S39. ^{1}H NMR of *tert*-butyl (2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**4a**) 24

Figure S40. ^{13}C NMR of *tert*-butyl (2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**4a**) 24

Figure S41. ^{1}H NMR of 2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethanamine (**5a**) 25

Figure S42. ^{13}C NMR of 2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethanamine (**5a**) 25

Figure S43. ^{1}H NMR of 6-(2-aminoethyl)-[1,1'-biphenyl]-3,4-diol (**6a**) 26

Figure S44. ^{13}C NMR of 6-(2-aminoethyl)-[1,1'-biphenyl]-3,4-diol (**6a**) 26

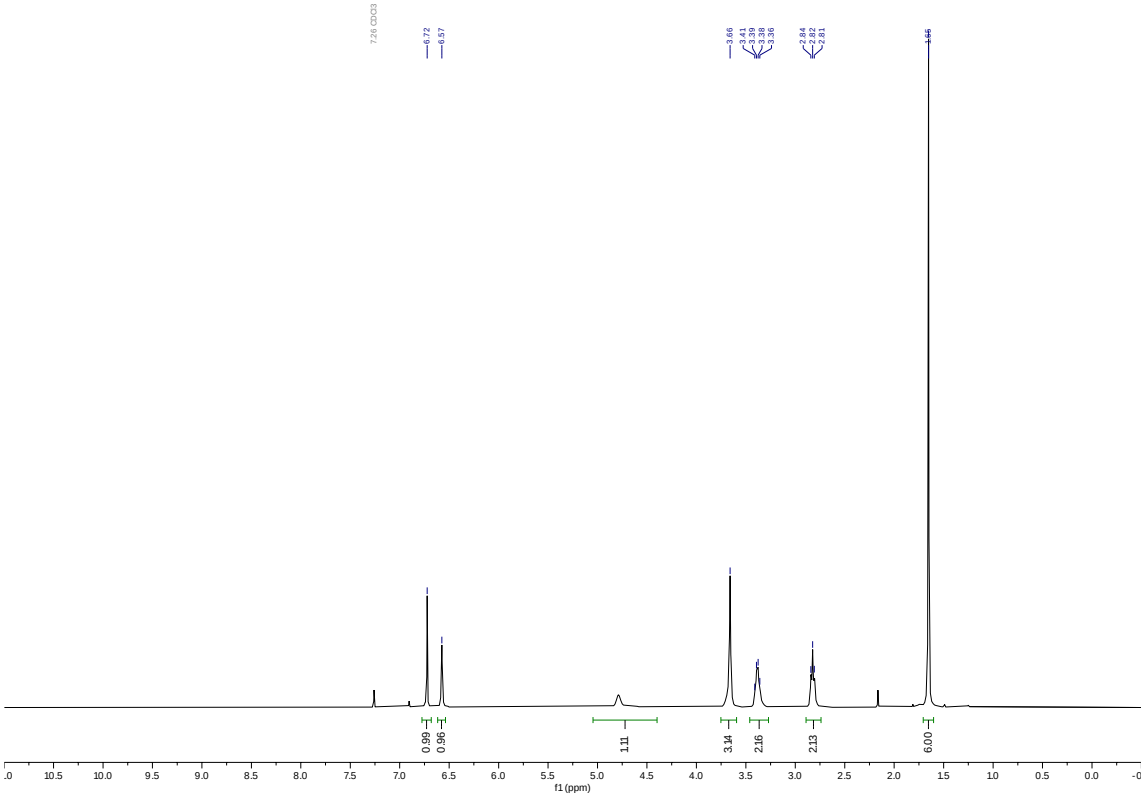


Figure S1. ^{1}H NMR of Methyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1a**).

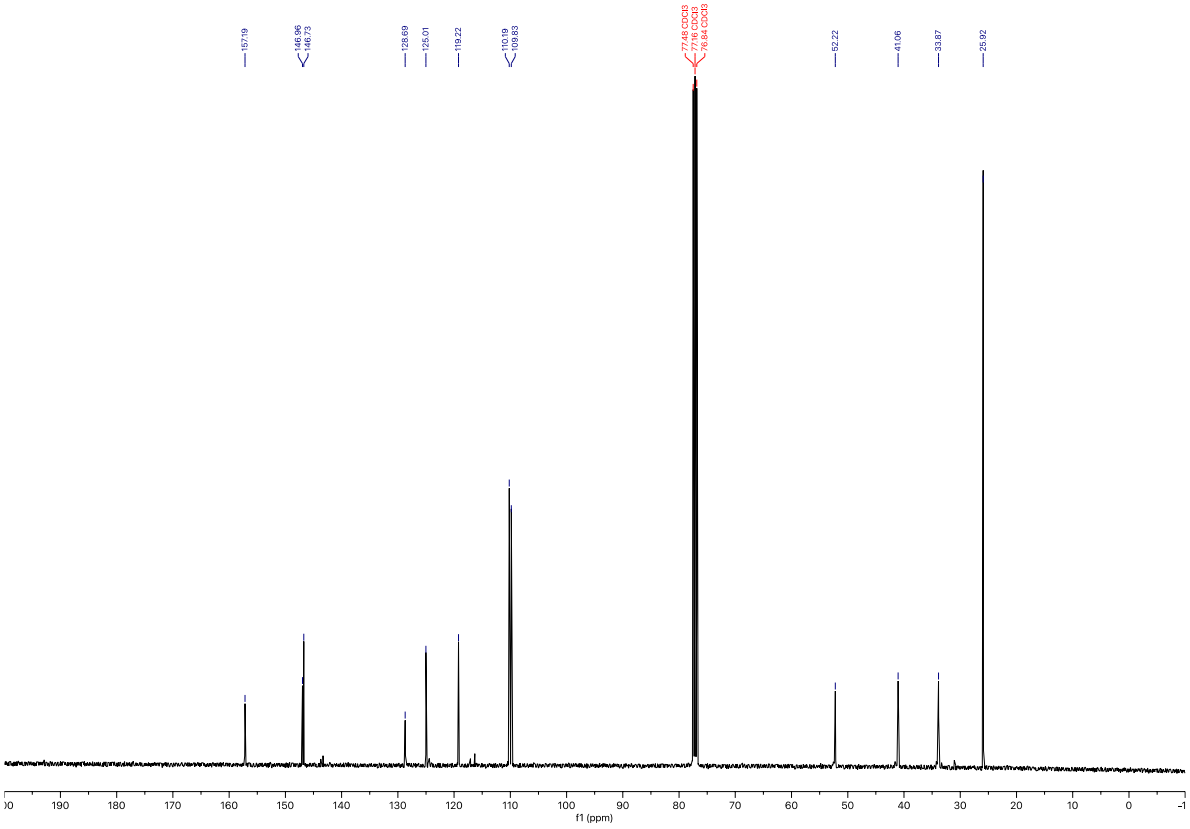


Figure S2. ^{13}C NMR of methyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1a**).

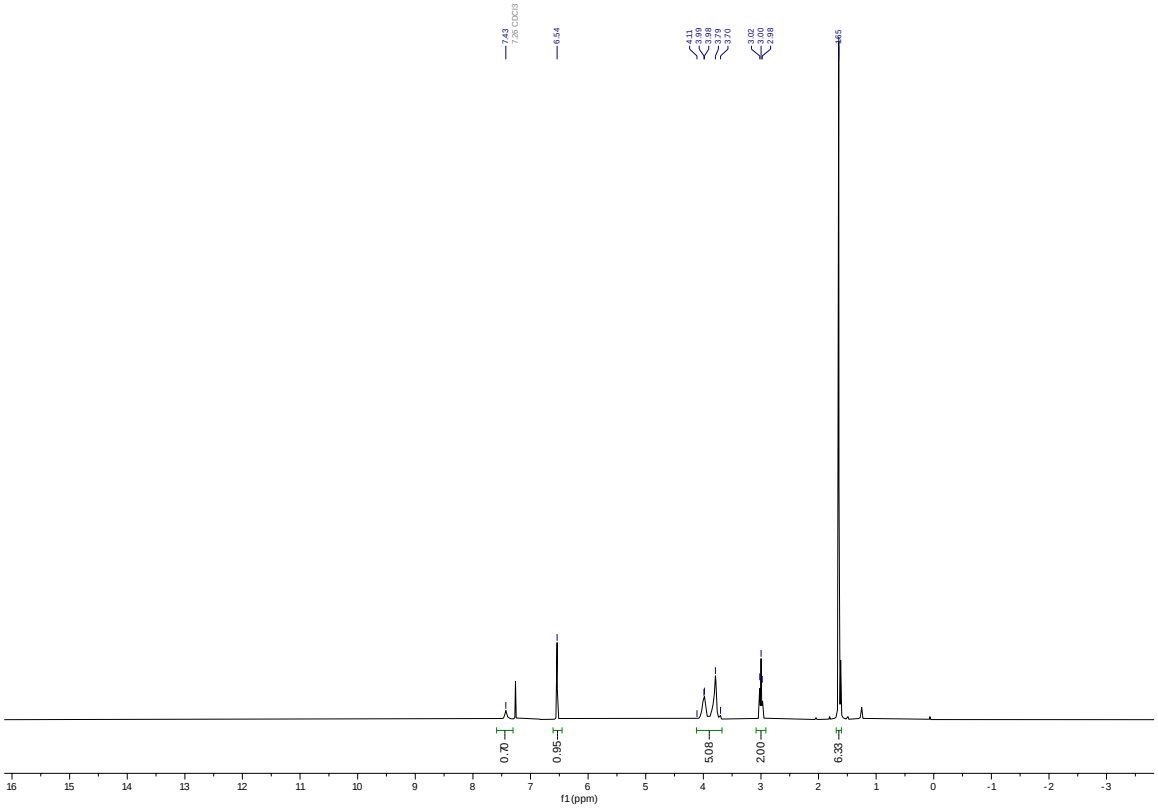


Figure S3. ^{1}H NMR of methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**).

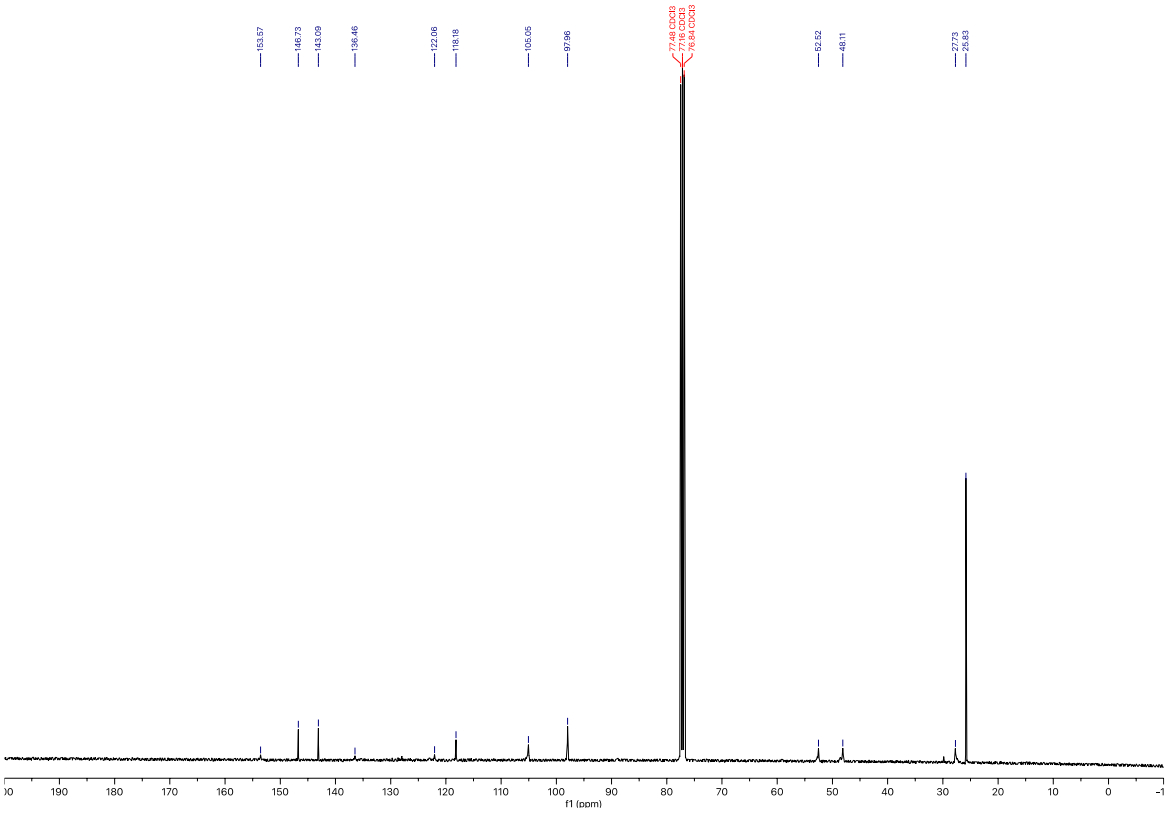


Figure S4. ^{13}C NMR of methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**).

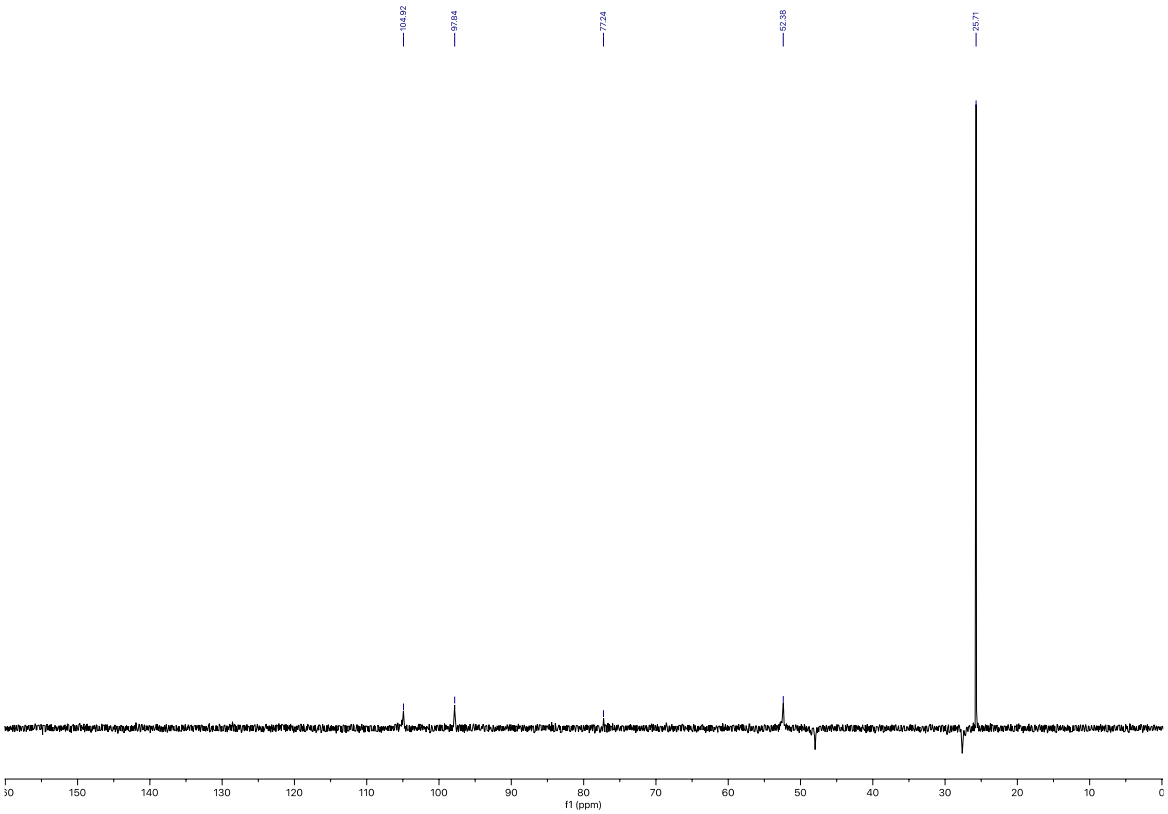


Figure S5. DEPT 135 NMR experiment of methyl 2,2-dimethyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]indole-5-carboxylate (**9**).

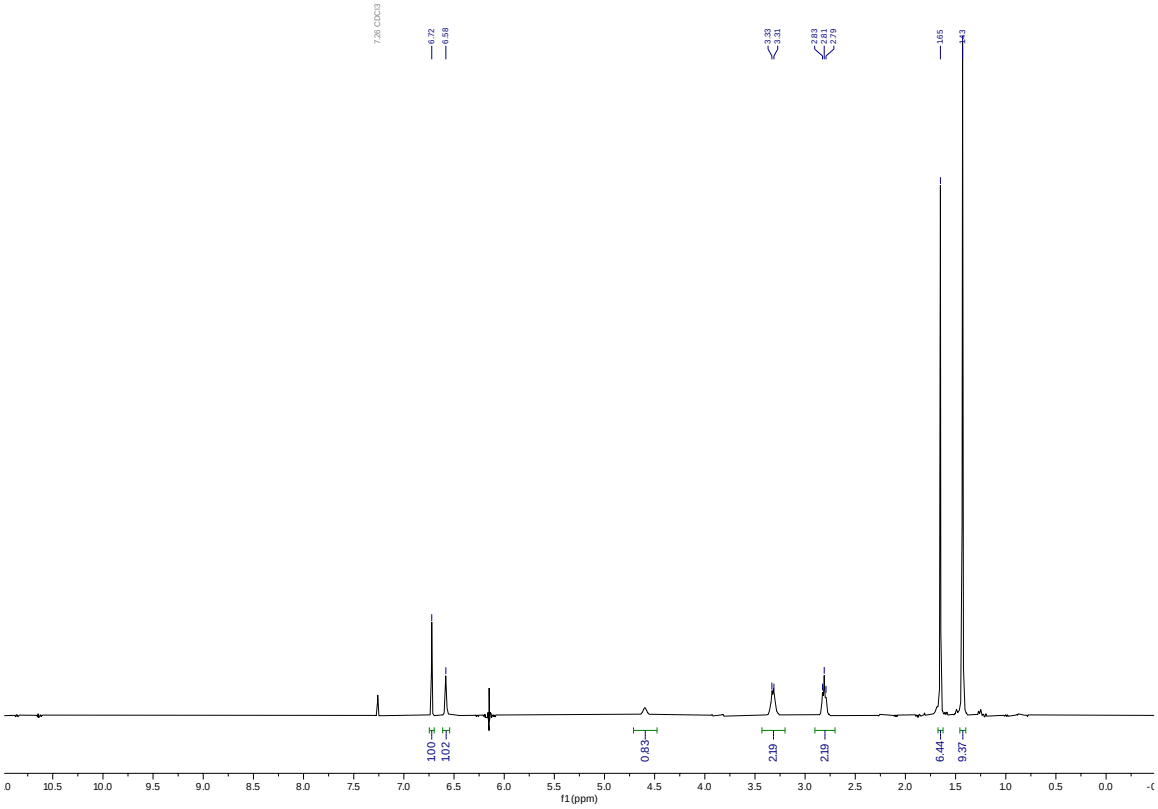


Figure S6. [1]H NMR of *tert*-butyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**13**).

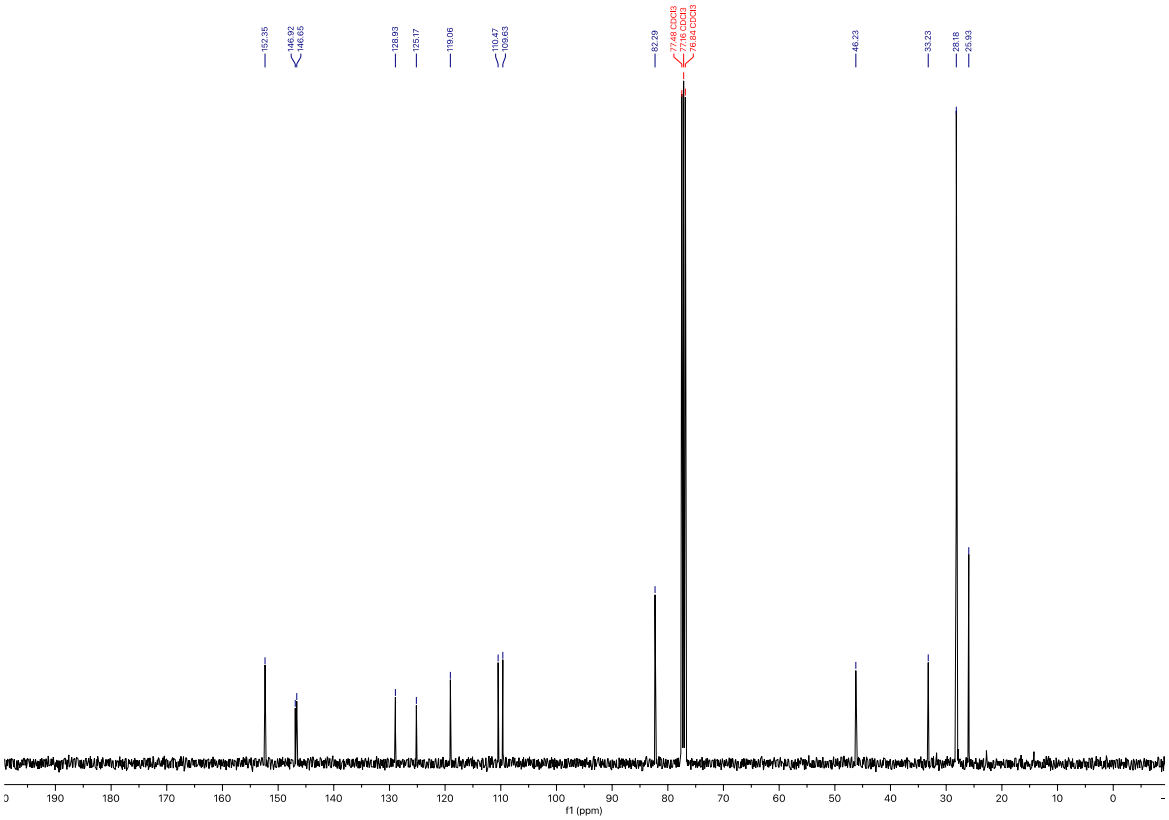


Figure S7. [13]C NMR of *tert*-butyl (2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**13**).

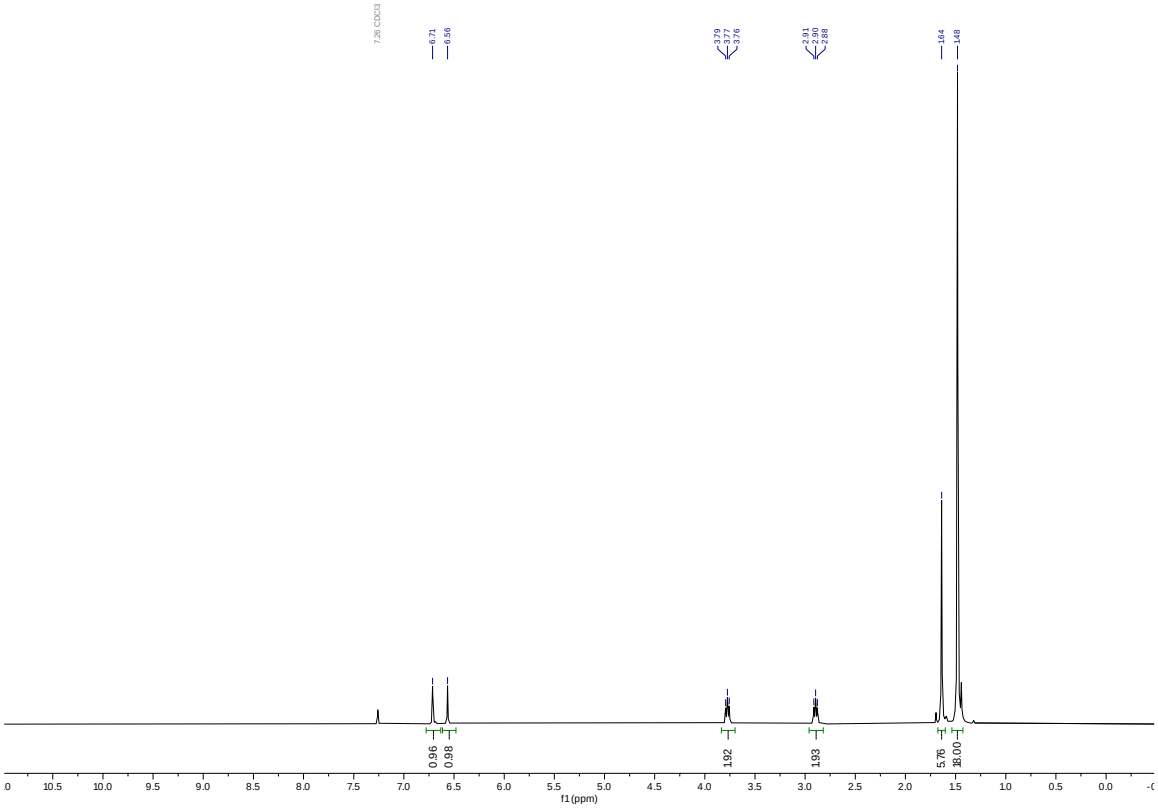


Figure S8. [1]H NMR of (*tert*-butoxycarbonyl)(2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b**).

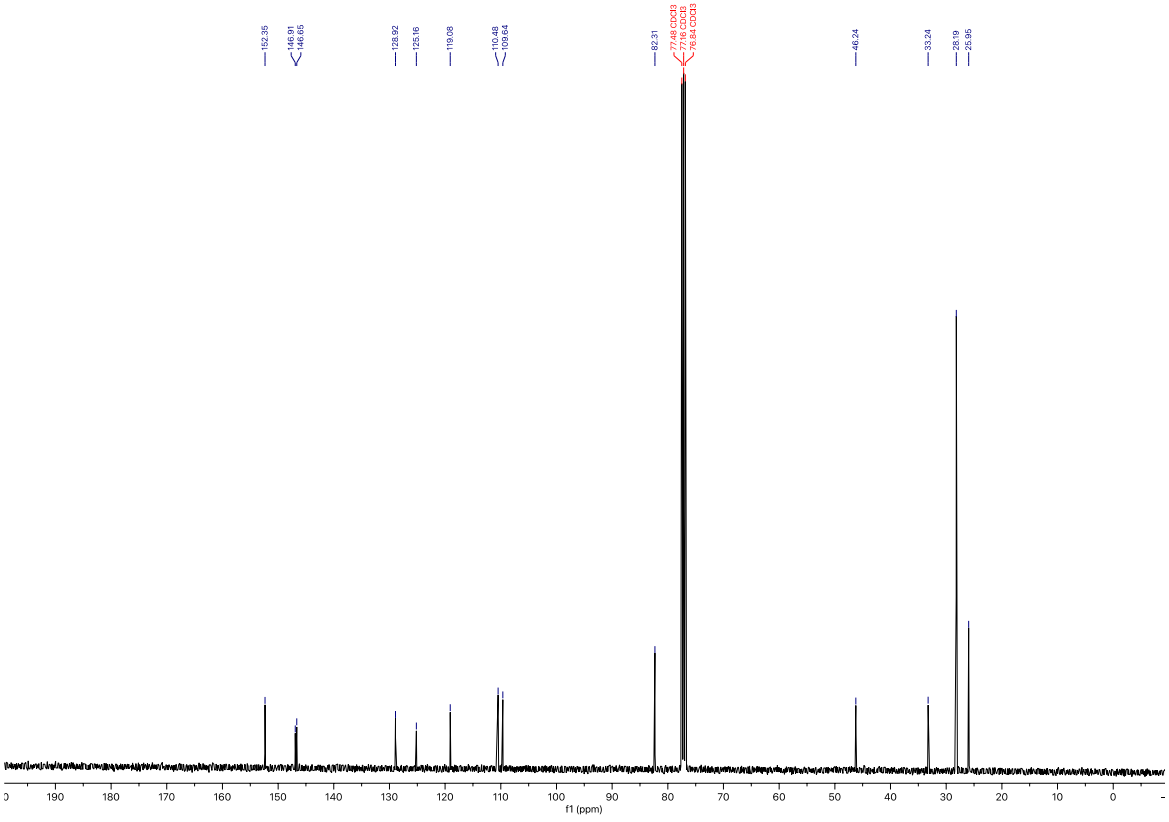


Figure S9. [13]C NMR of (*tert*-butoxycarbonyl)(2-(6-chloro-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b**).

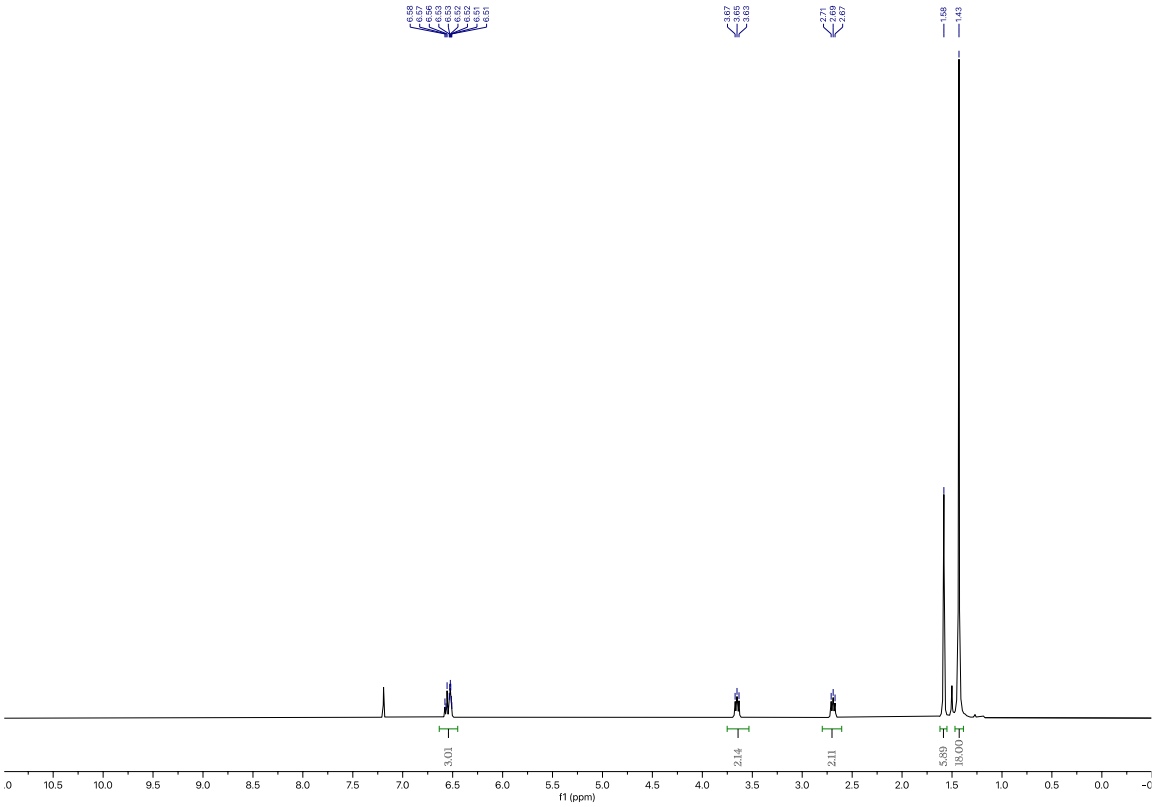


Figure S10. [1]H NMR of *tert*-butyl (2-(2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b'**)

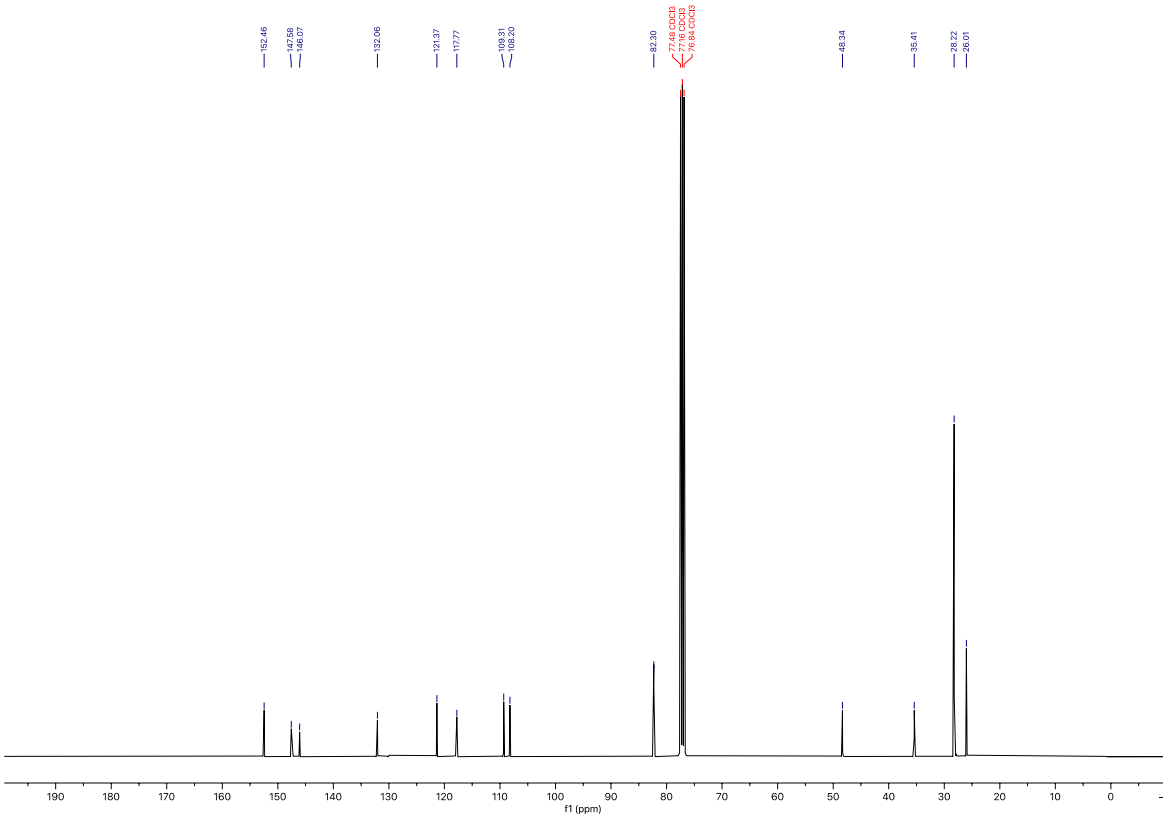


Figure S11. [13]C NMR of *tert*-butyl (2-(2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**1b'**).

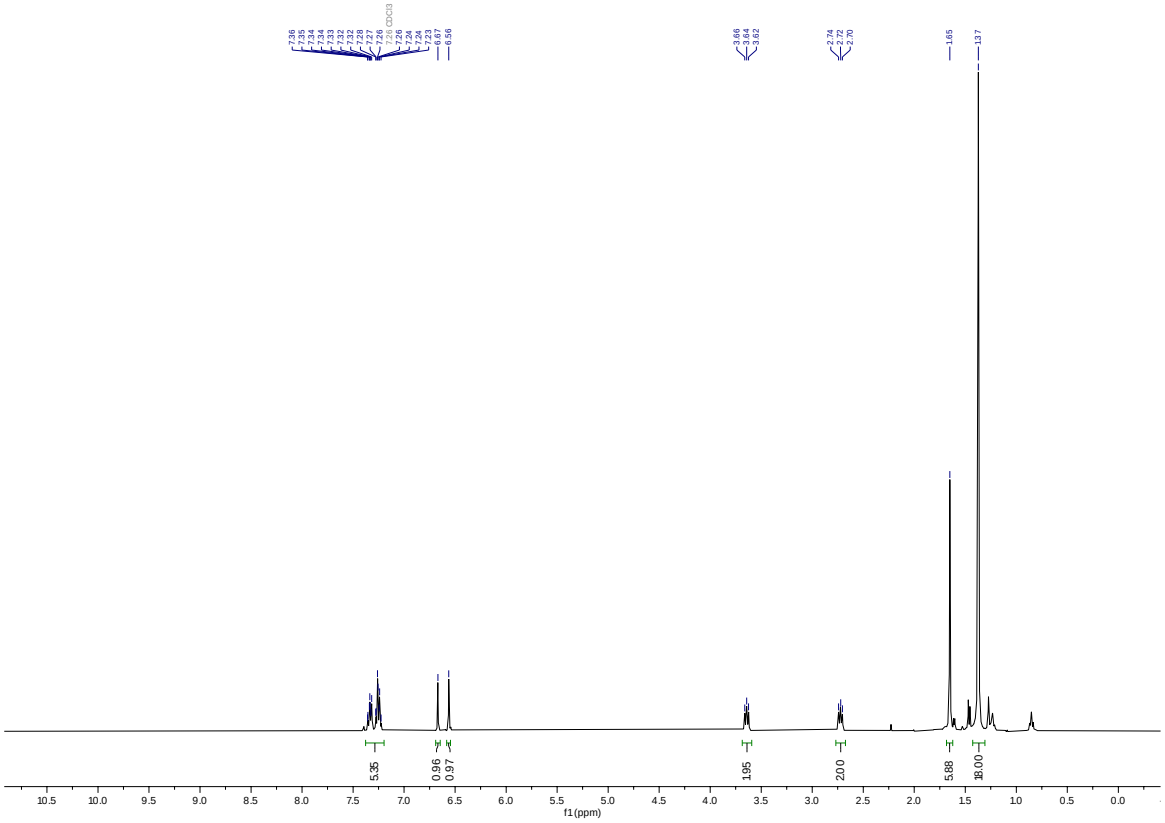


Figure S12. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3ba**).

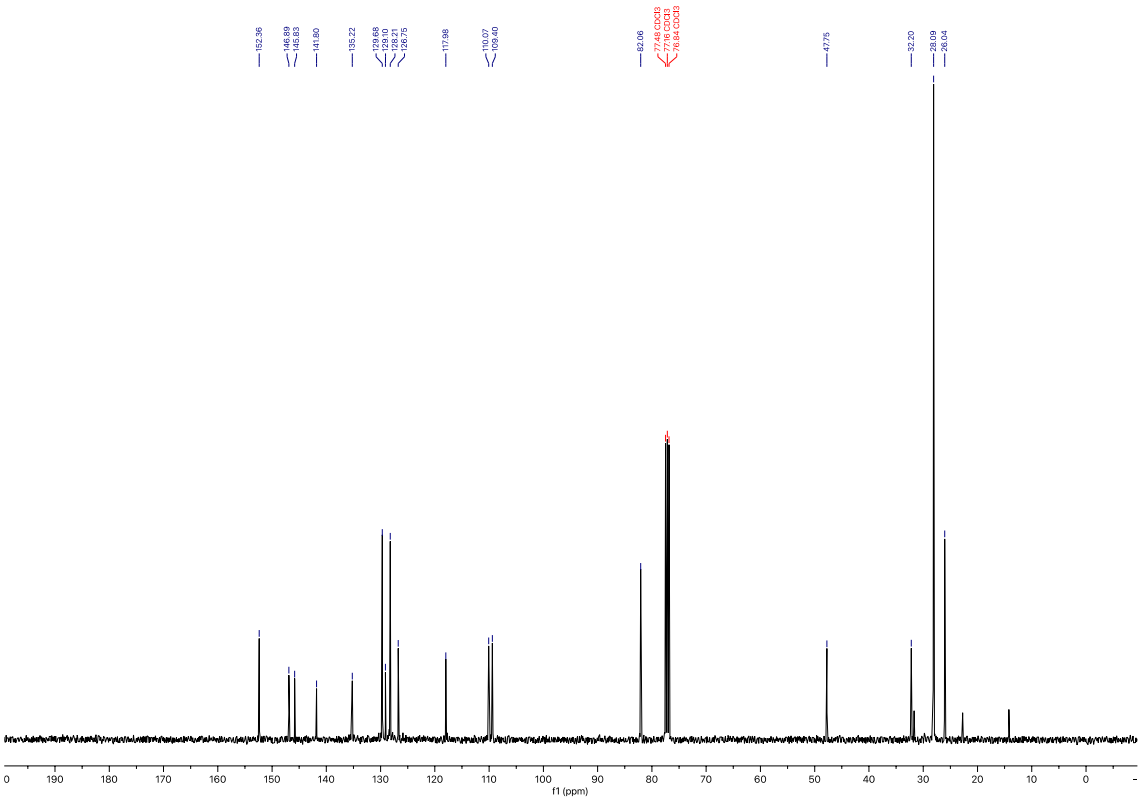


Figure S13. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3ba**).

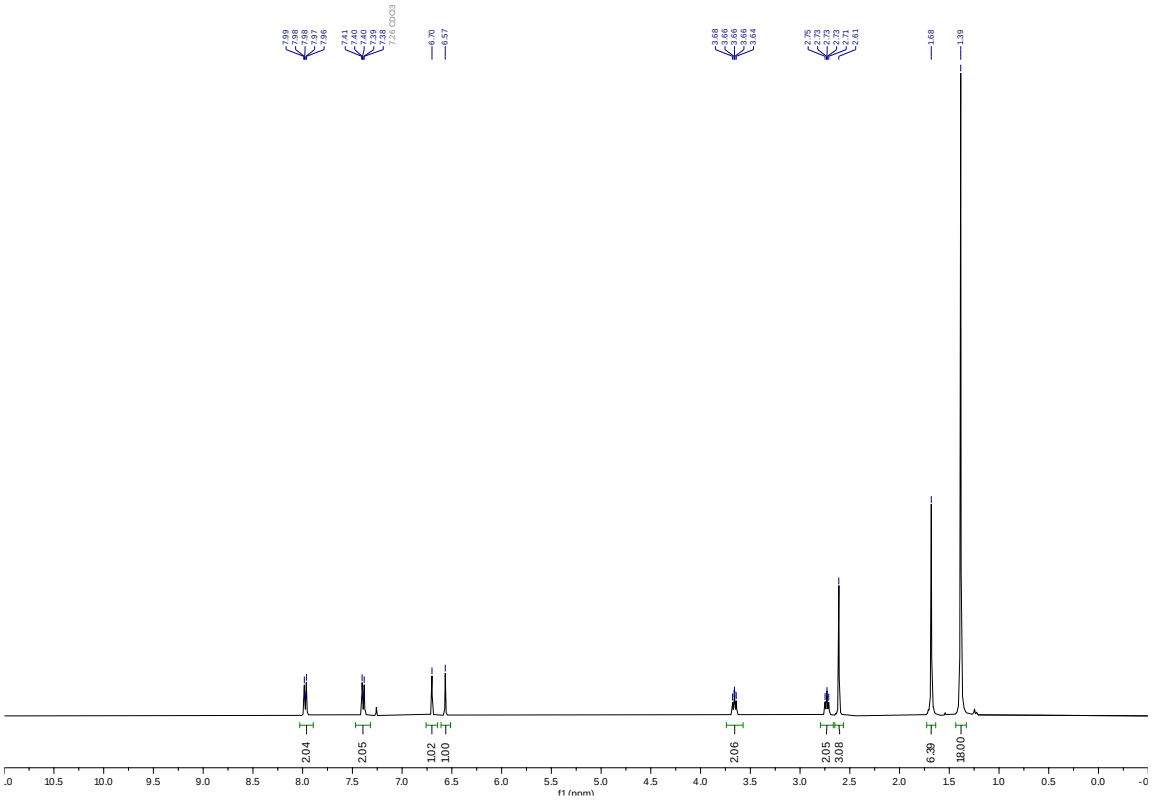


Figure S14. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-acetylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bb**).

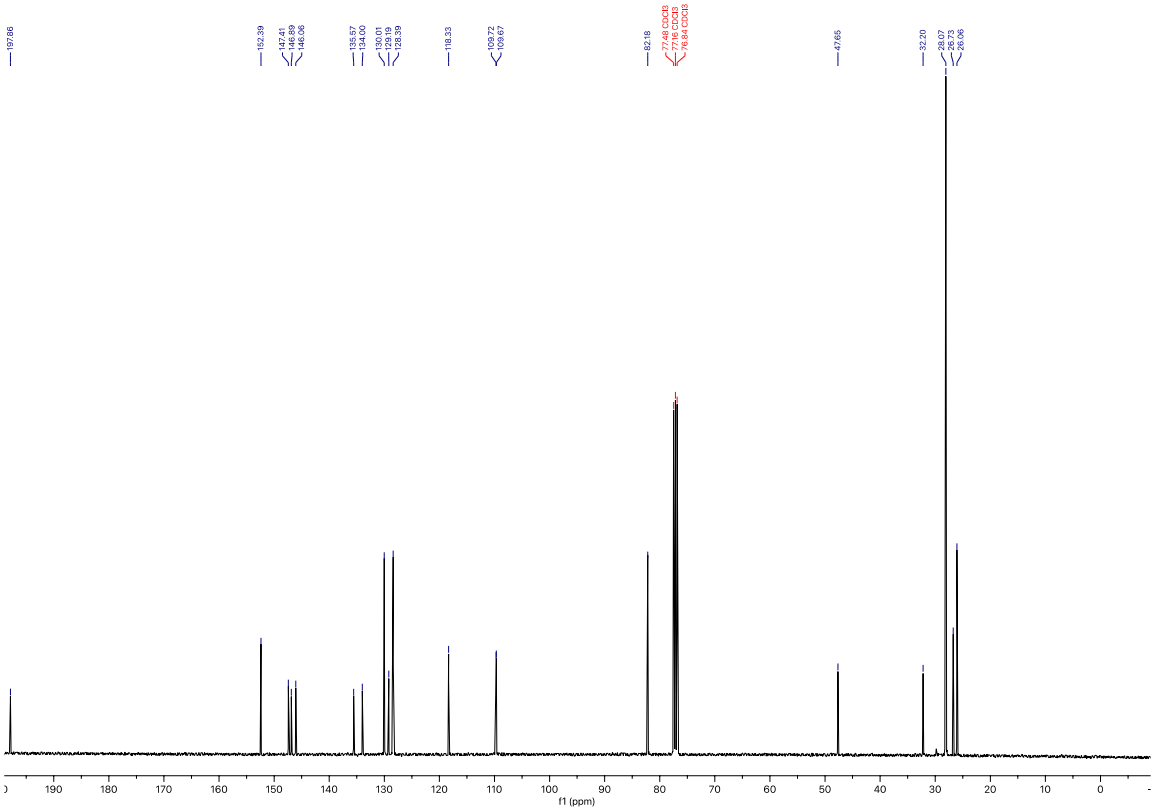


Figure S15. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-acetylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bb**).

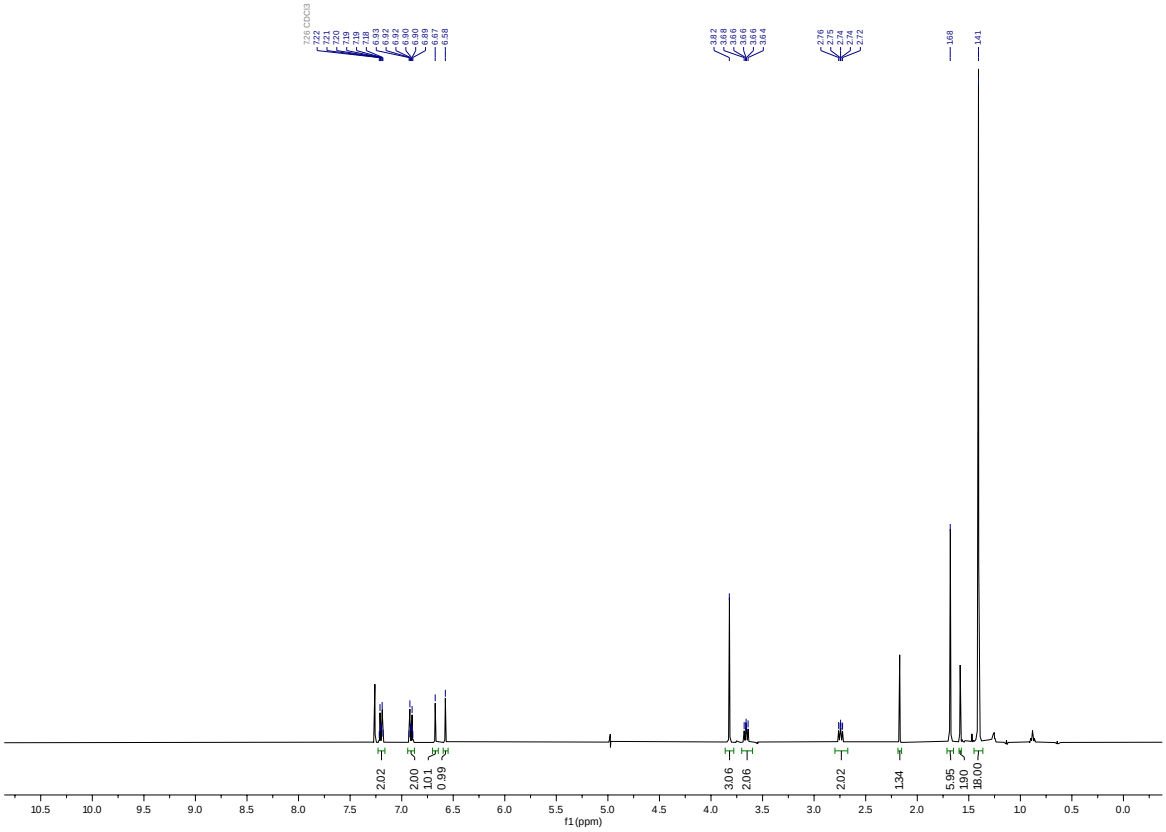


Figure S16. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methoxyphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bc**).

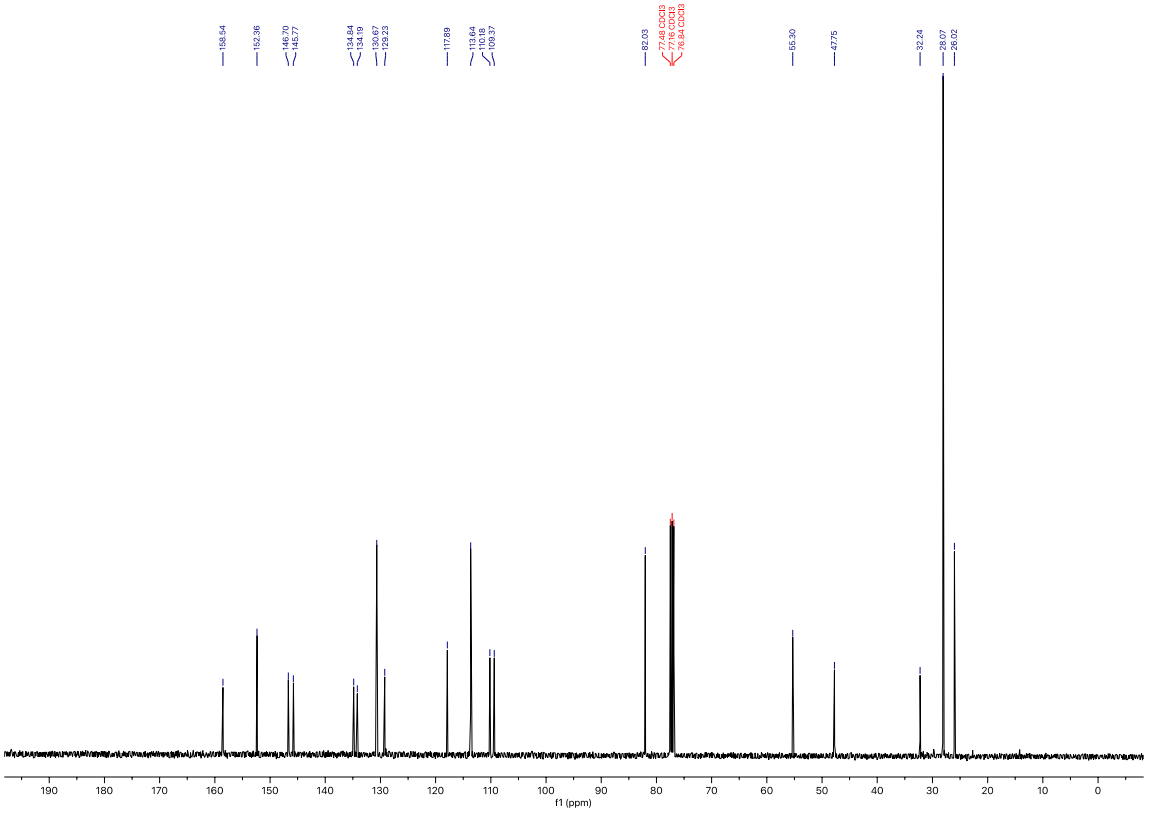


Figure S17. [13] C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methoxyphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bc**).

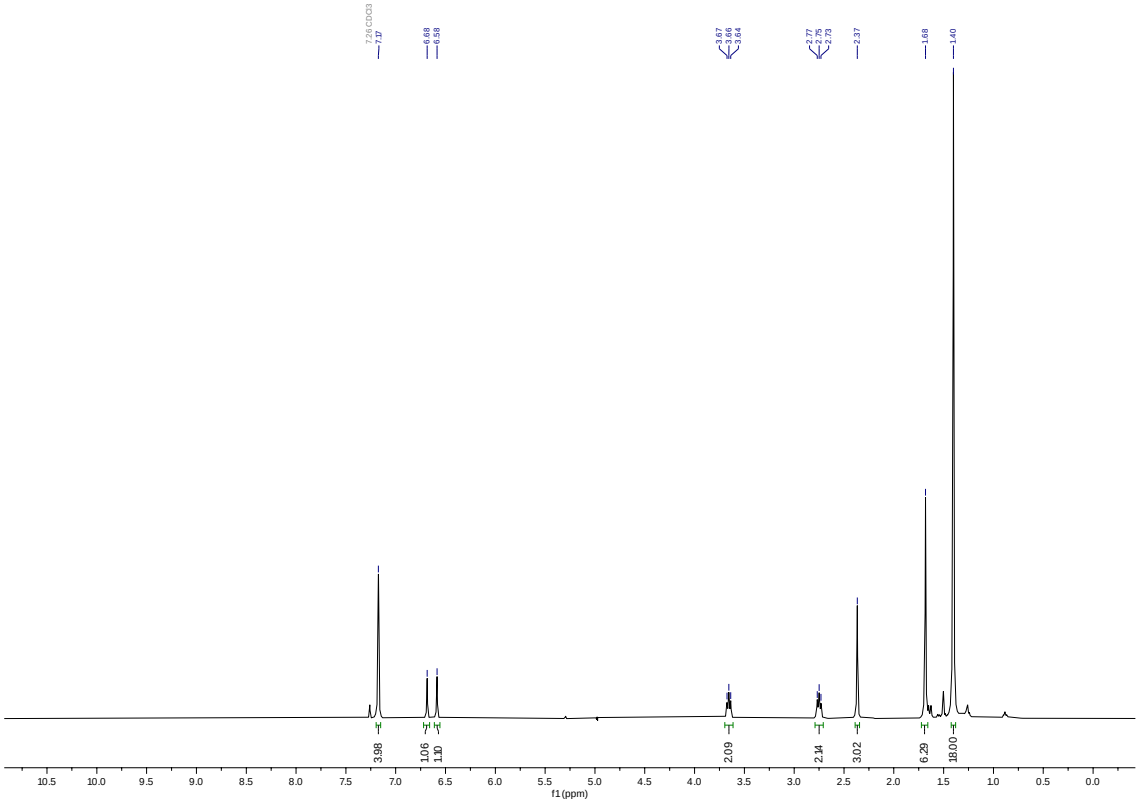


Figure S18. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-methylphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bd**).

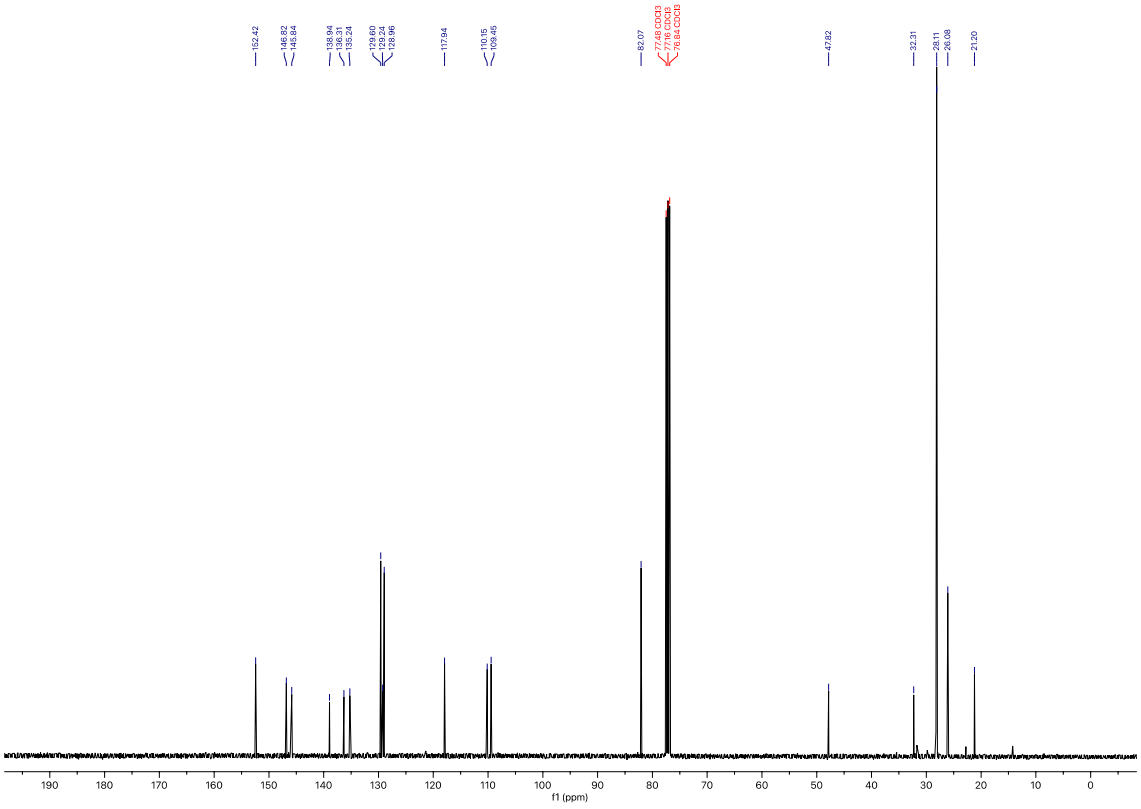


Figure S19. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-methylphenyl)-2,2-dimethylbenzo[d][1,3] dioxol-5-yl)ethyl)carbamate (**3bd**).

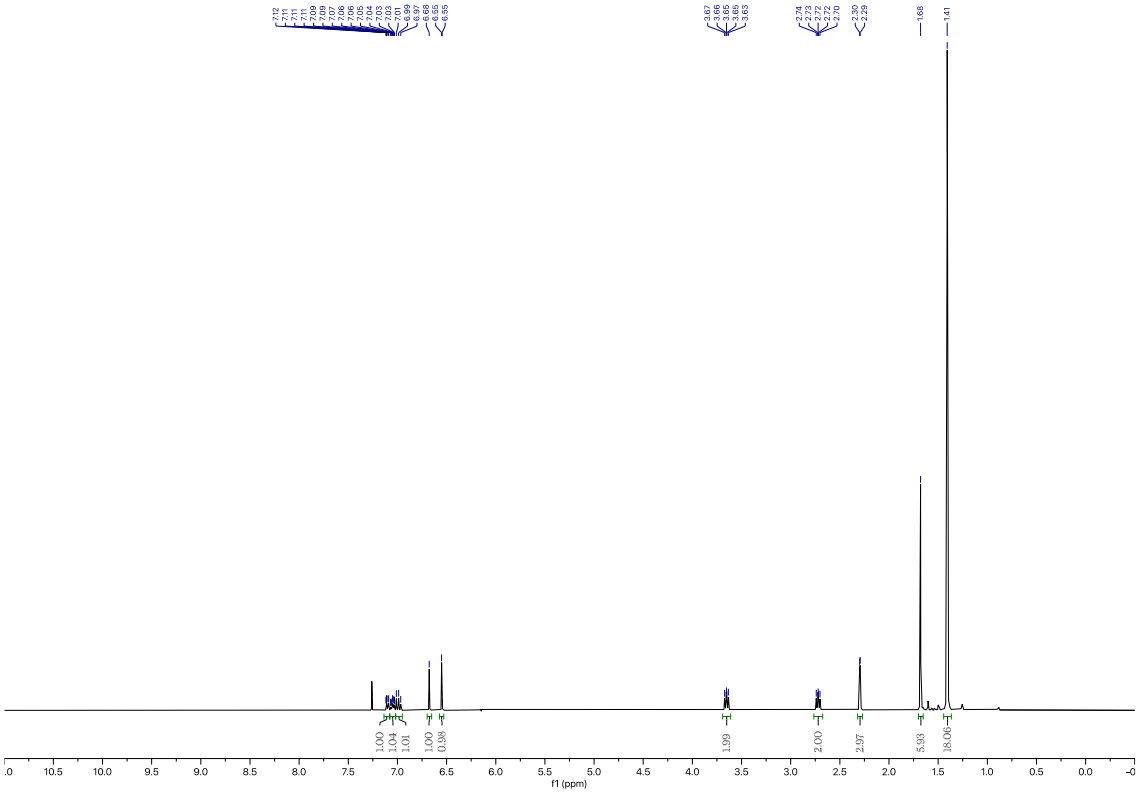


Figure S20. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-fluoro-3-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3be**).

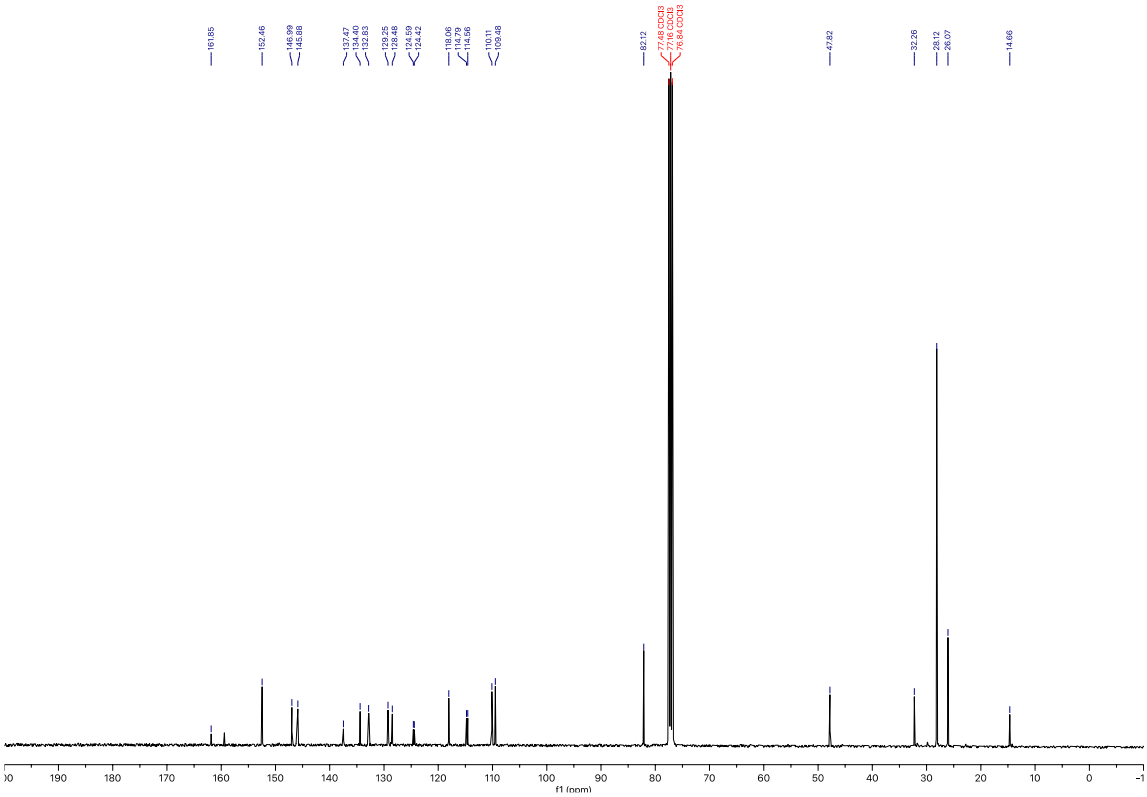


Figure S21. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-fluoro-3-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3be**).

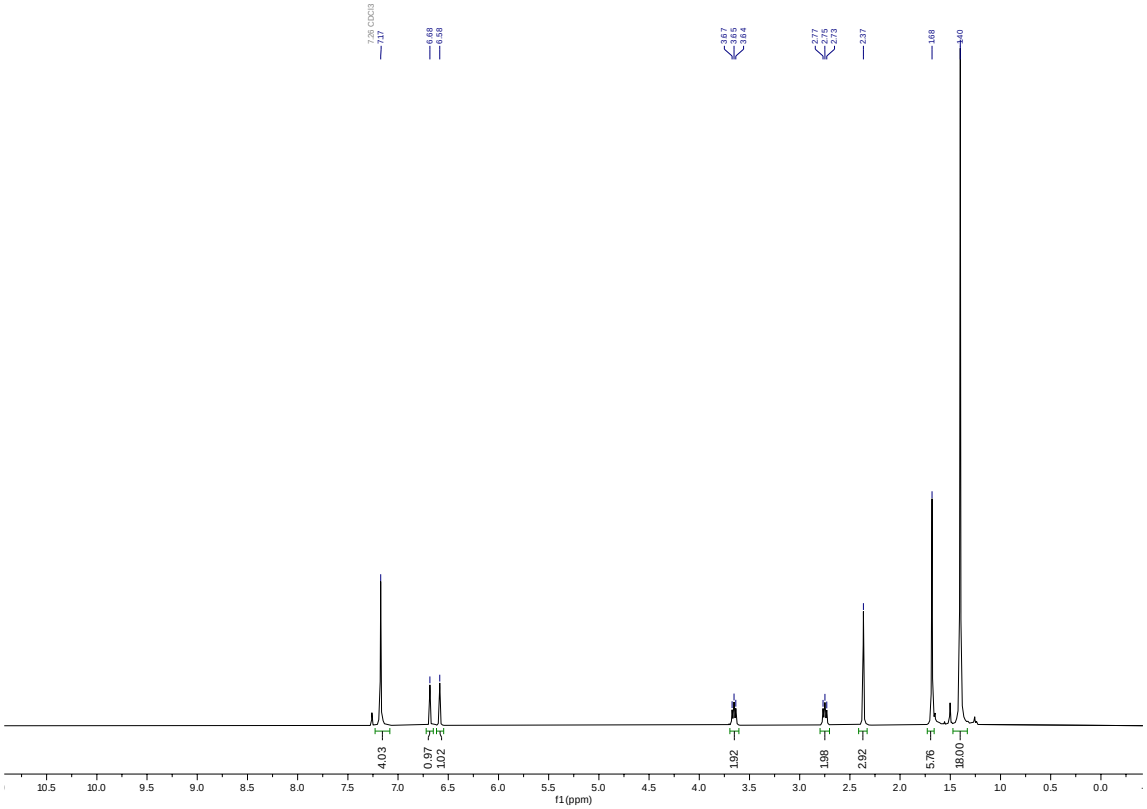


Figure S22. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bf**).

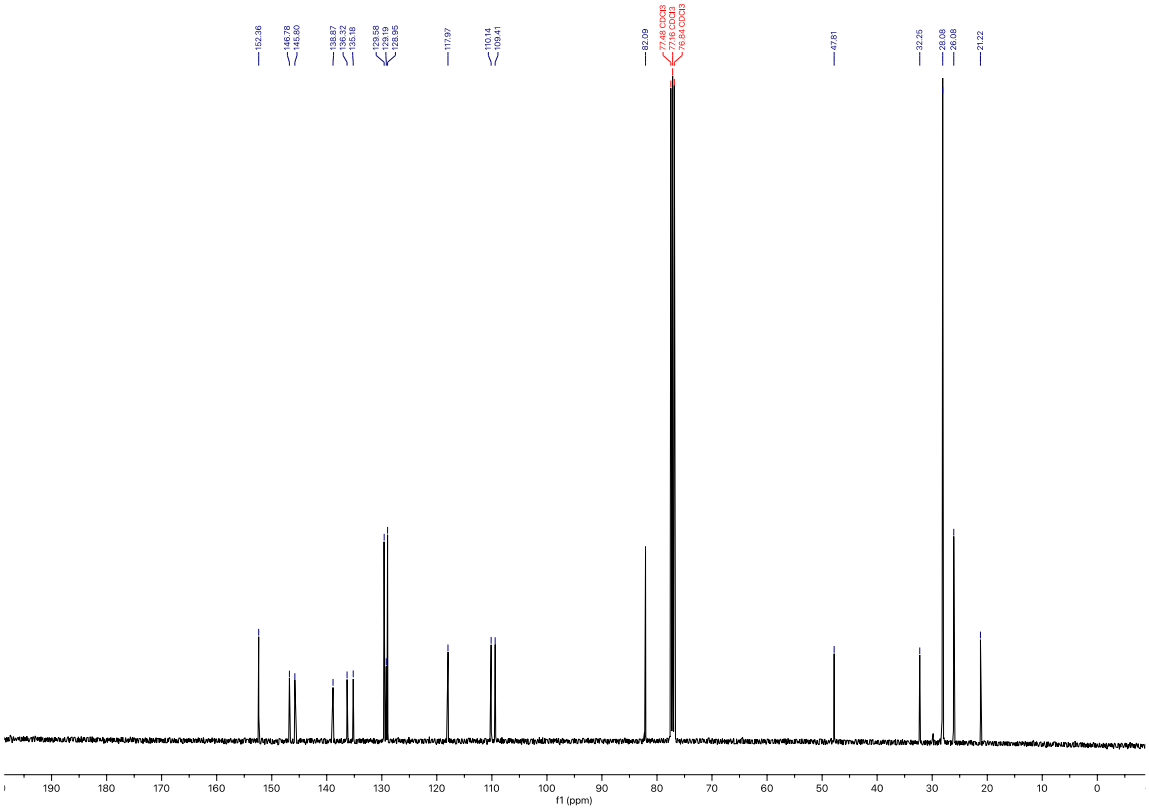


Figure S23. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-methylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bf**).

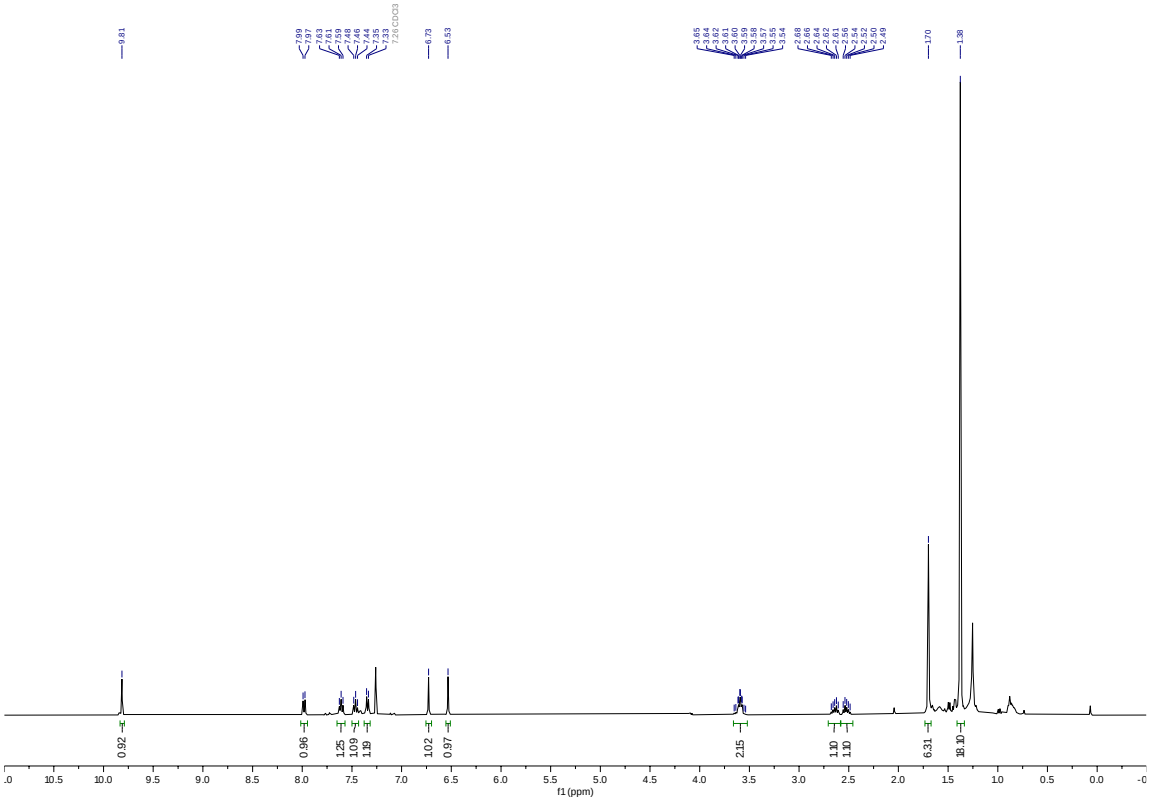


Figure S24. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-formylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bh**).

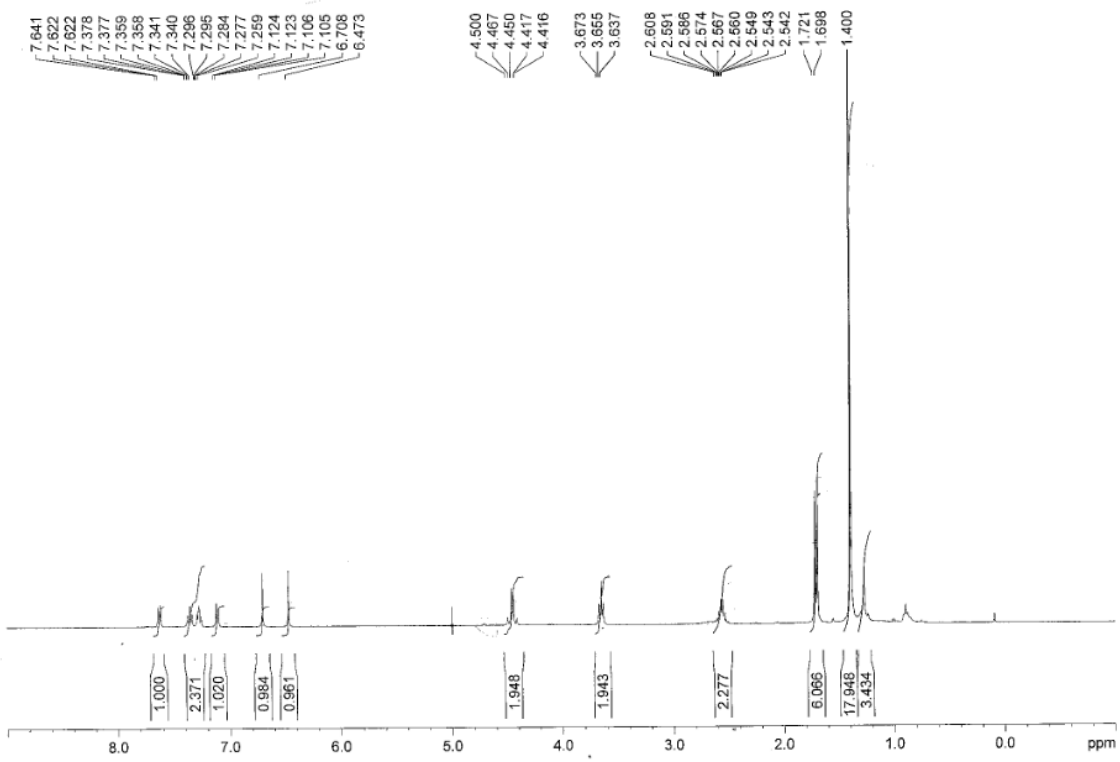


Figure S25. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-hydroxymethylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol-5-yl)ethyl)carbamate (**3bh'**).

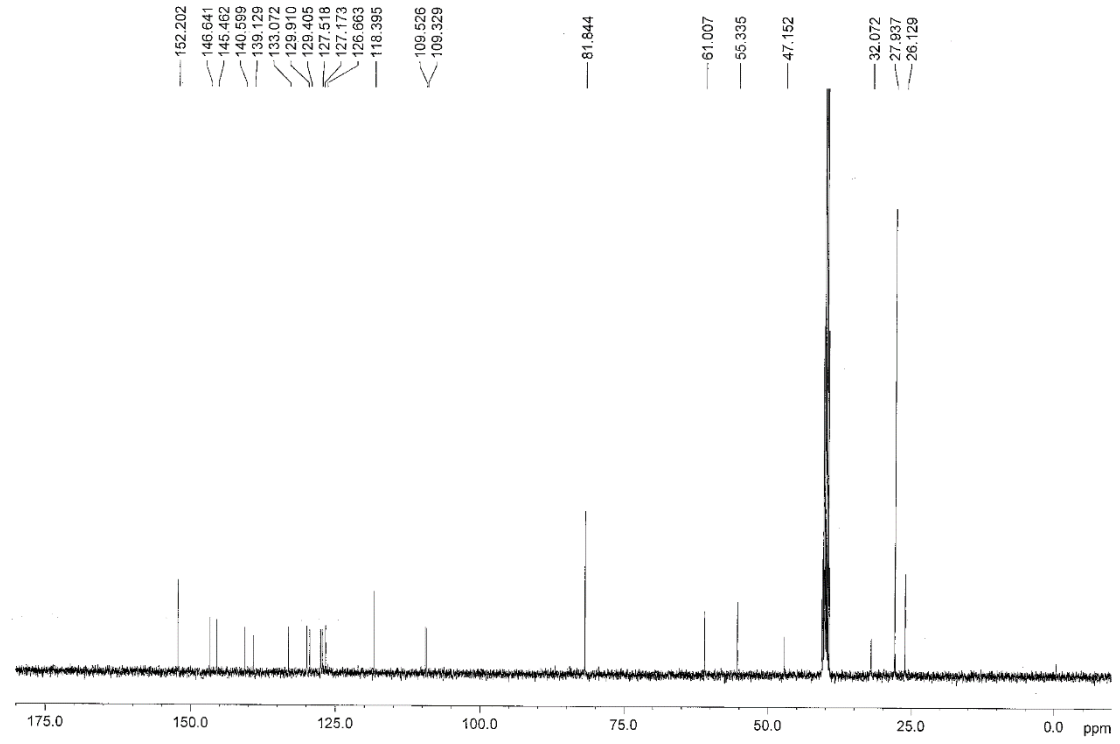


Figure S26. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(2-hydroxymethylphenyl)-2,2-dimethylbenzo[d][1,3]d ioxol-5-yl)ethyl)carbamate (**3bh'**).

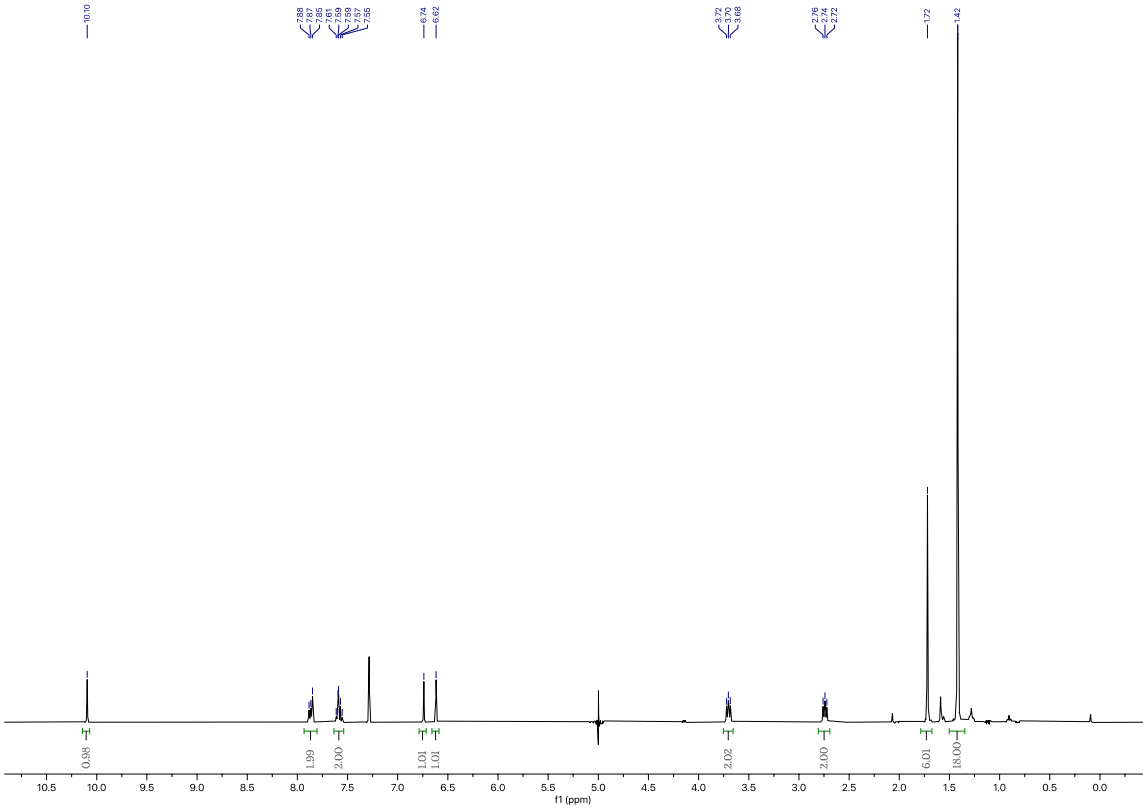


Figure S27. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(3-formylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bi**).

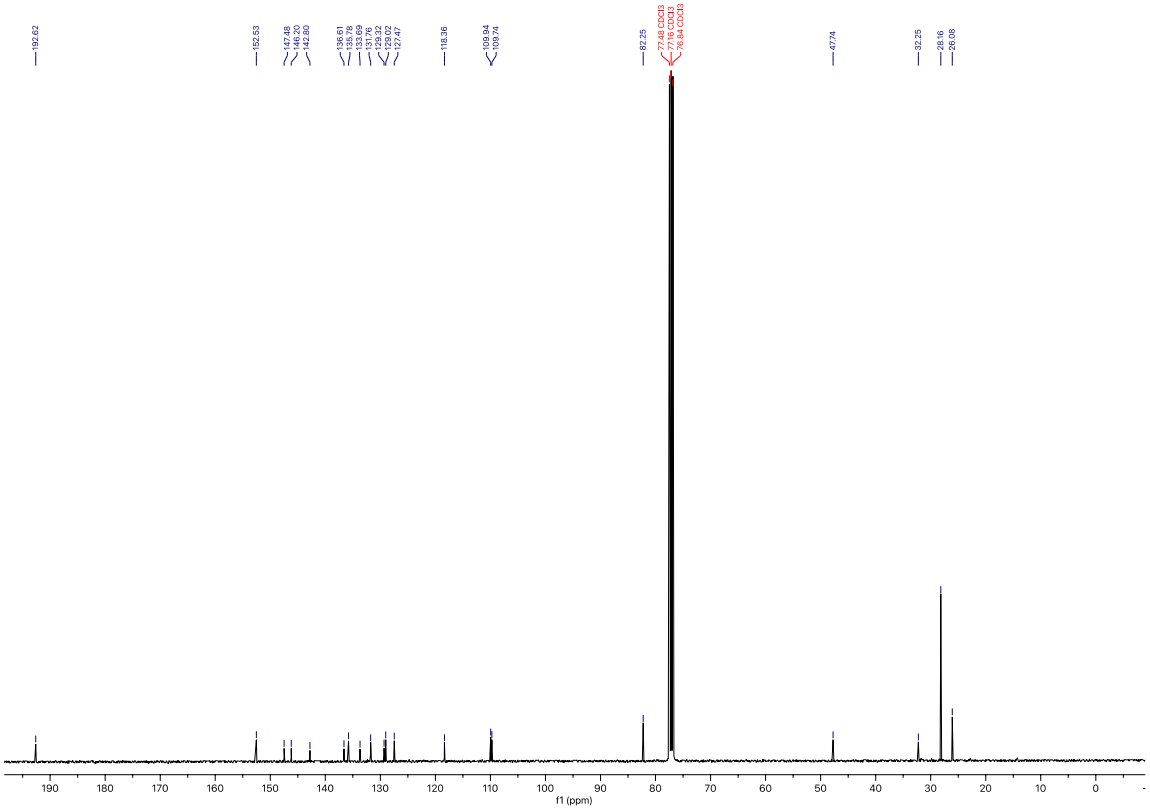


Figure S28. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(3-formylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bi**).

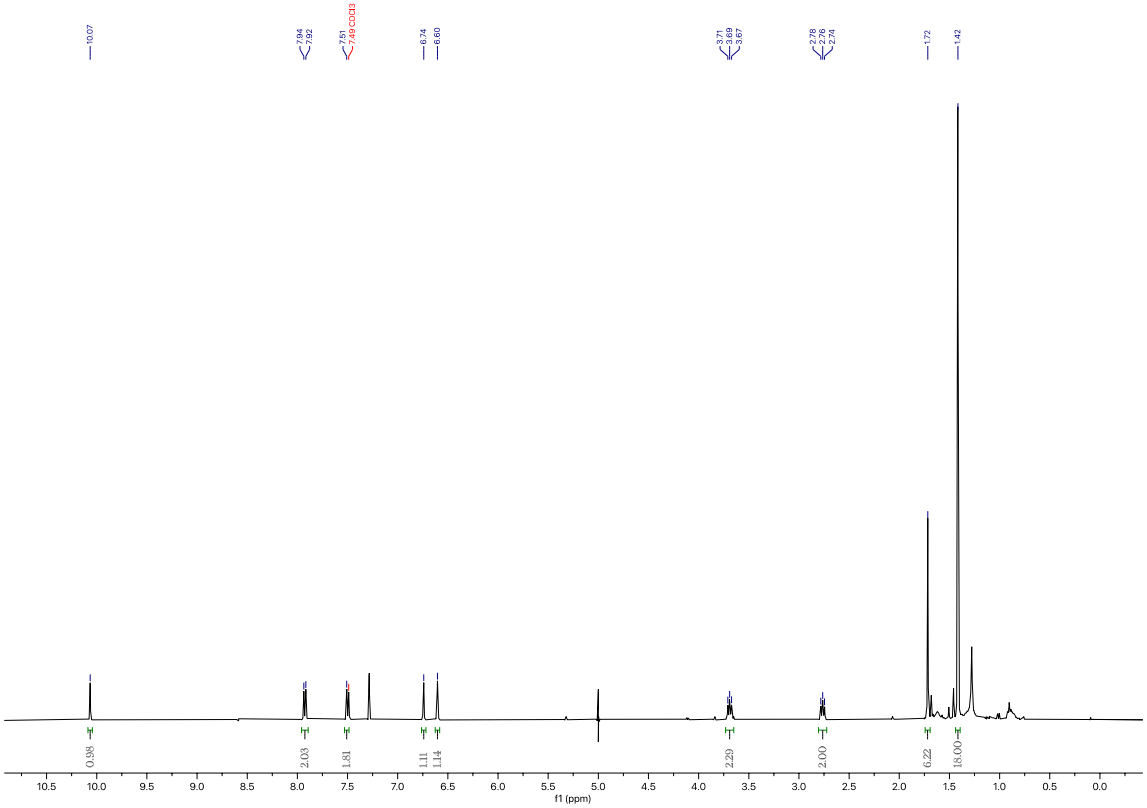


Figure S29. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-formylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bj**).

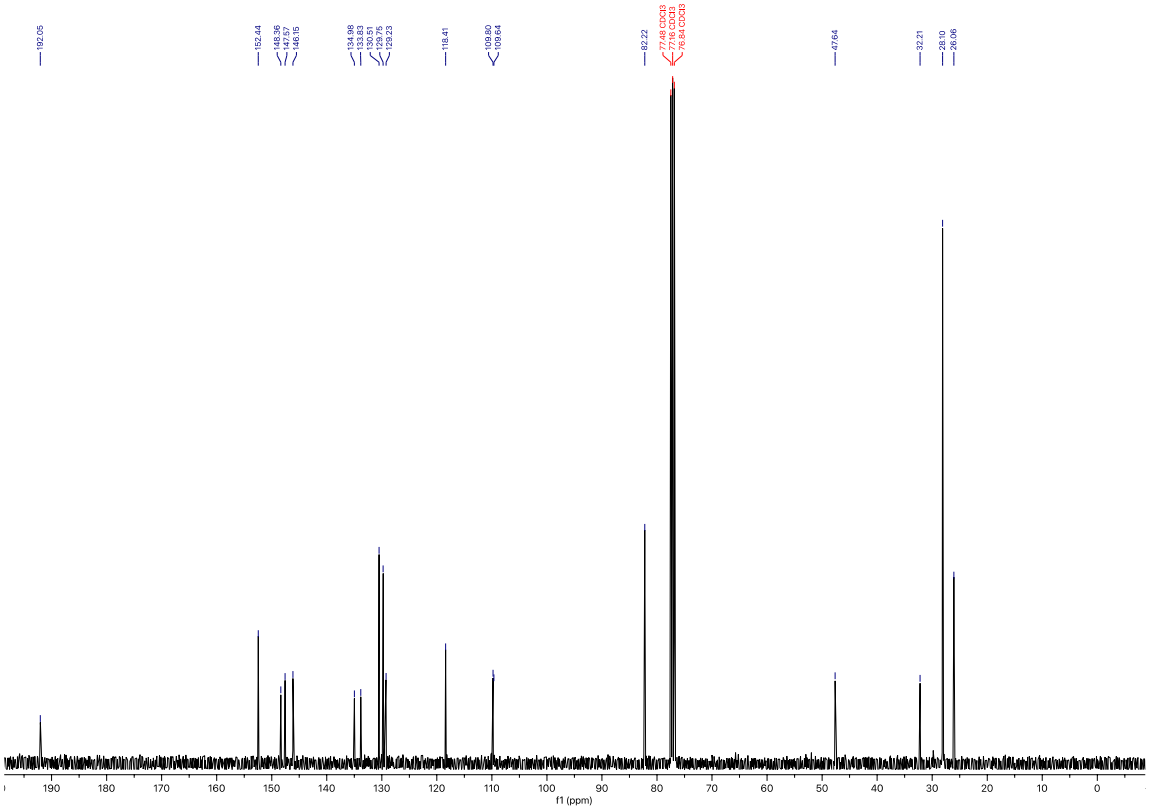


Figure S30. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(4-formylphenyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bj**).

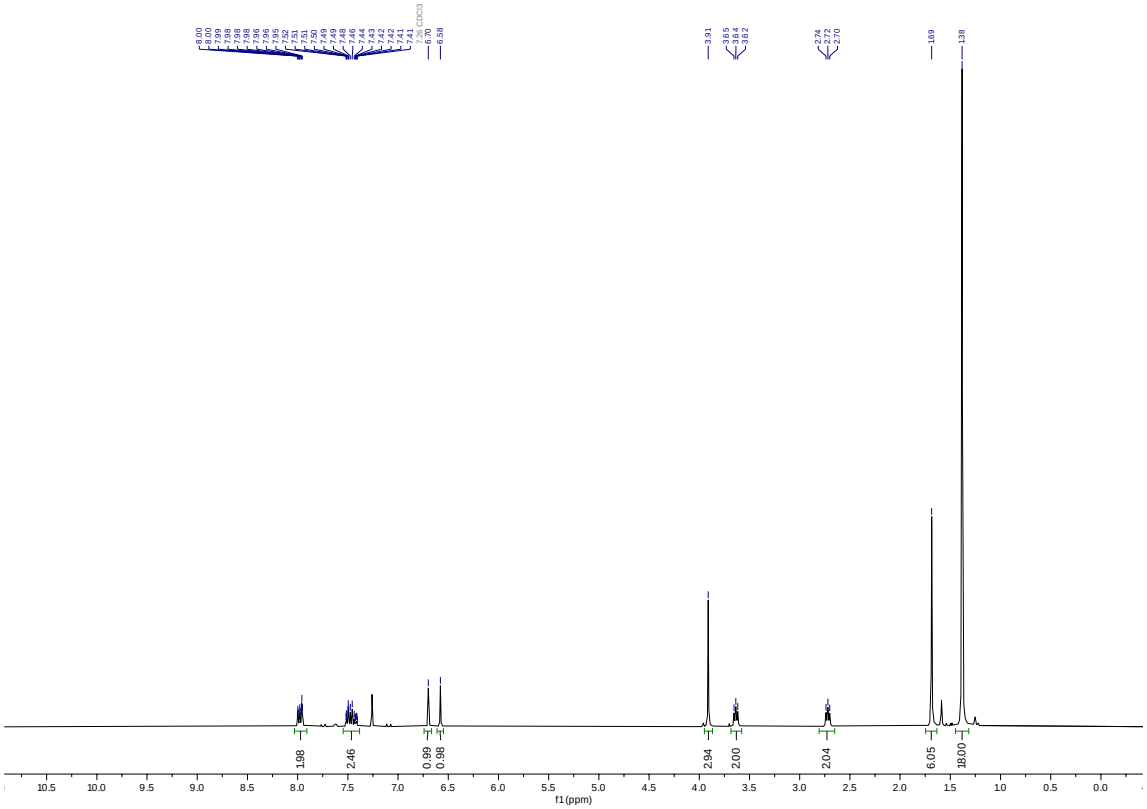


Figure S31. ^{1}H NMR of methyl 3-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)benzoate (**3bl**).

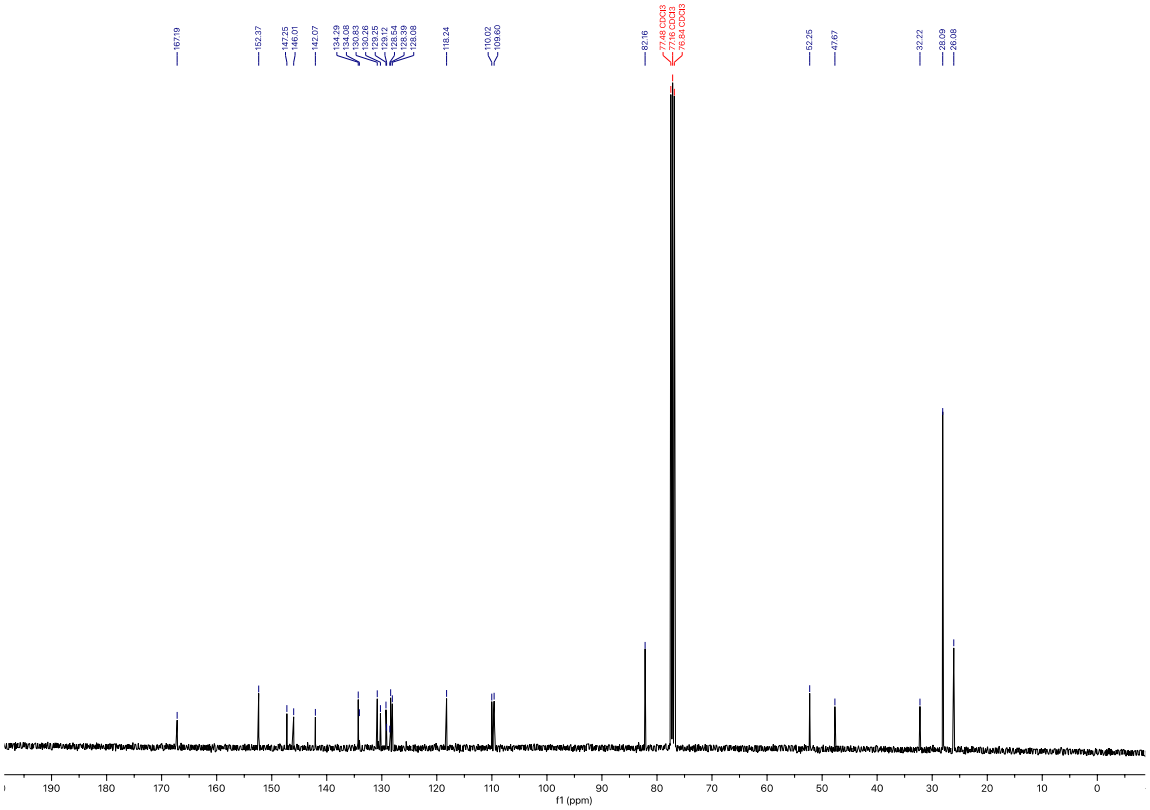


Figure S32. ^{13}C NMR of methyl 3-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)benzoate (**3bl**).

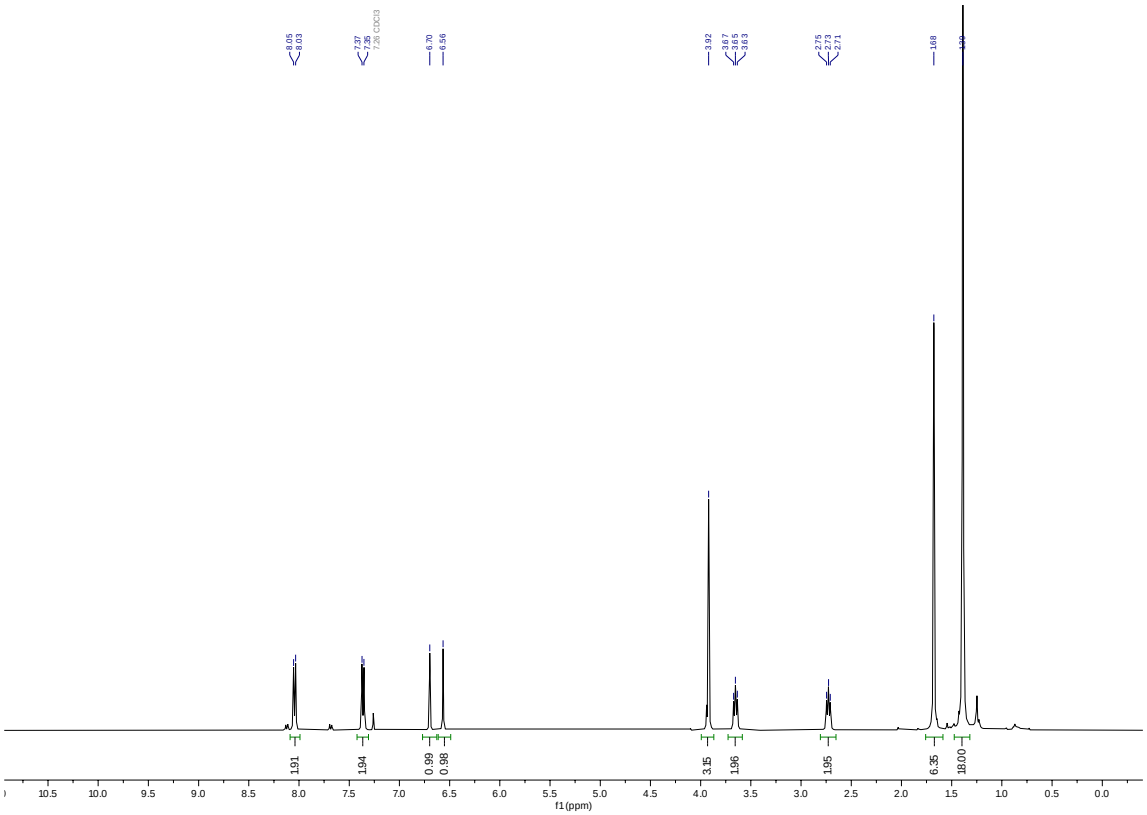


Figure S33. ^{1}H NMR of methyl 4-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)benzoate (**3bm**).

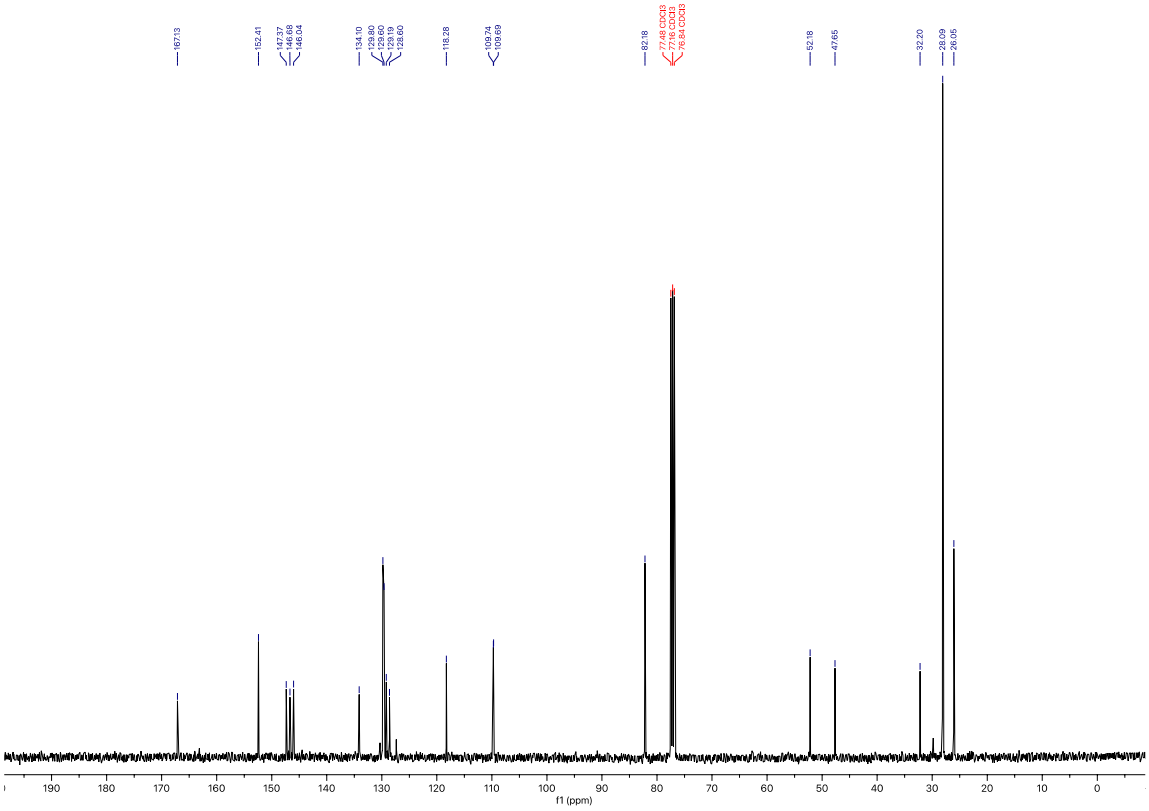


Figure S34. ^{13}C NMR of methyl 4-(6-(2-(bis(*tert*-butoxycarbonyl)amino)ethyl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)benzoate (**3bm**).

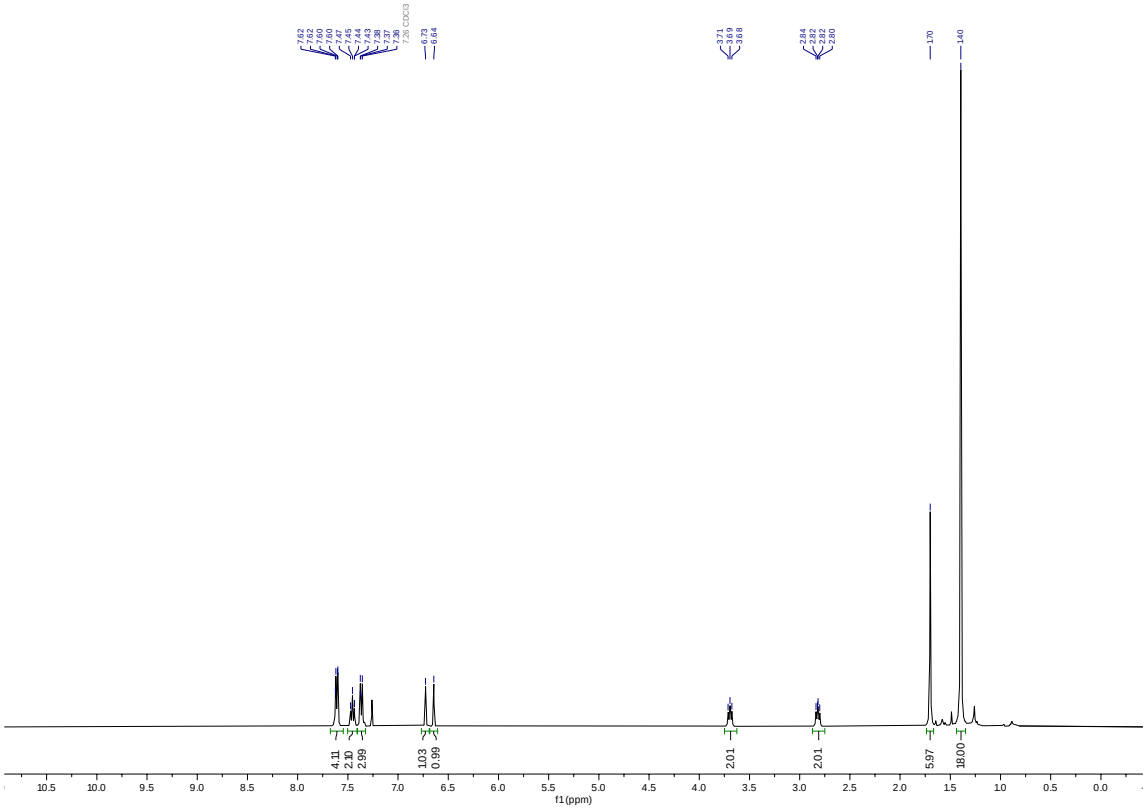


Figure S35. [1]H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-([1,1'-biphenyl]-4-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bn**).

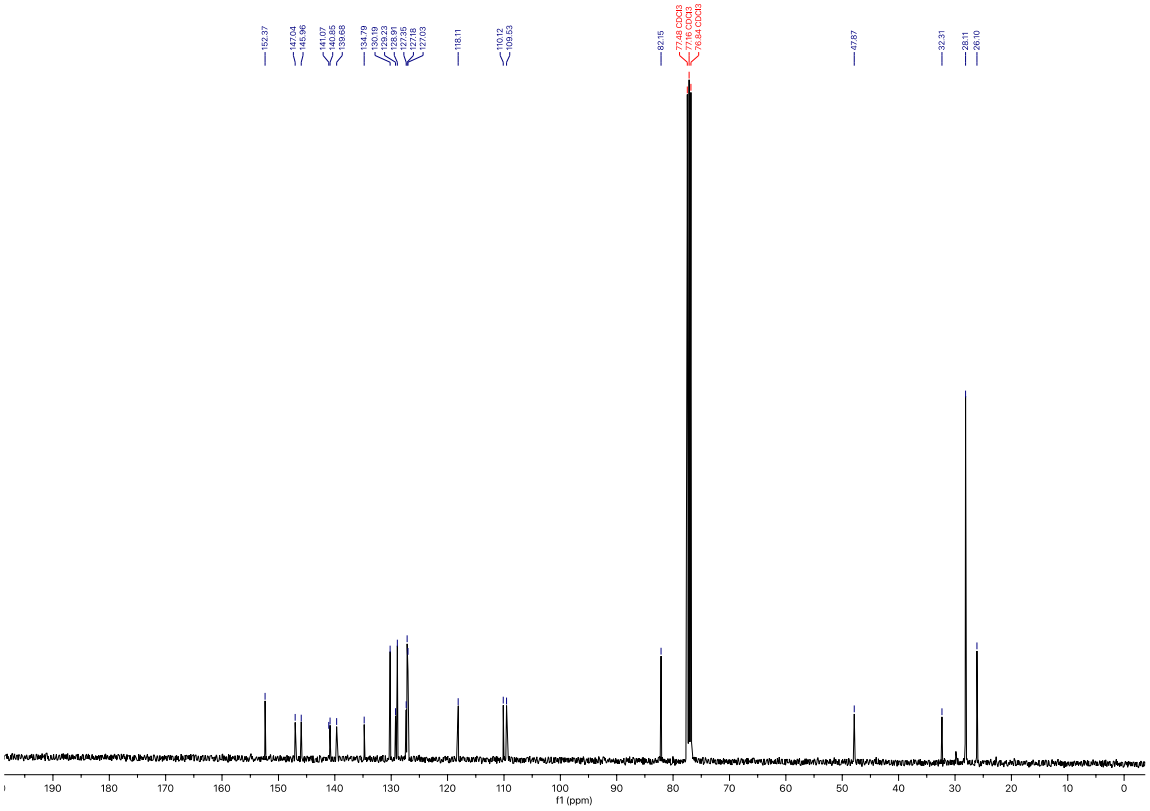


Figure S36. [13]C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-([1,1'-biphenyl]-4-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bn**).

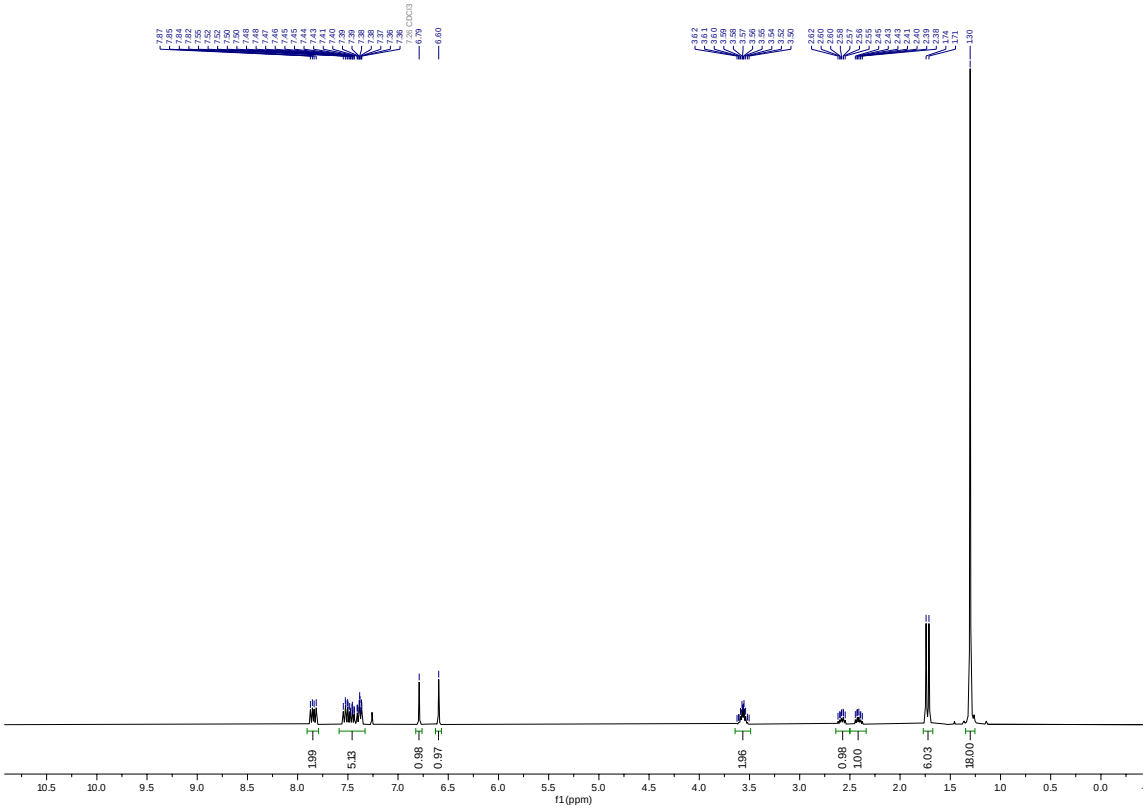


Figure S37. ^{1}H NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(naphtalen-1-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bo**).

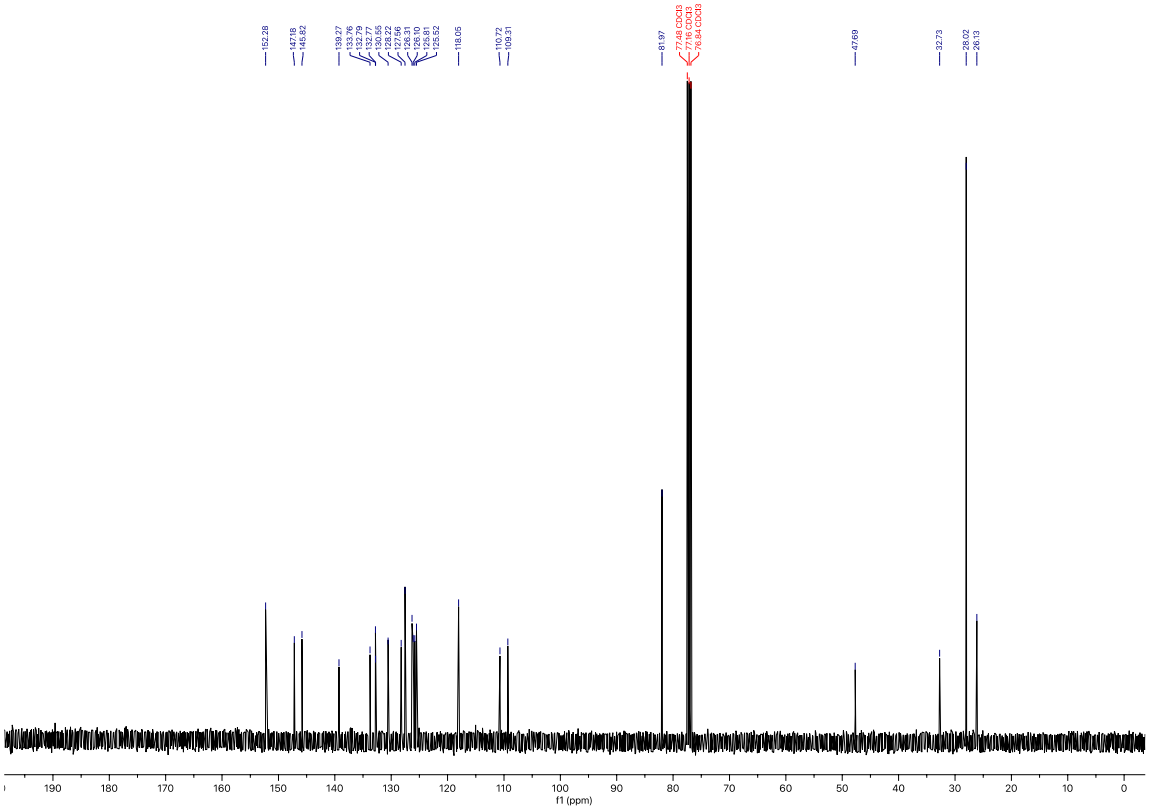


Figure S38. ^{13}C NMR of *tert*-butyl (*tert*-butoxycarbonyl)(2-(6-(naphtalen-1-yl)-2,2-dimethylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**3bo**).

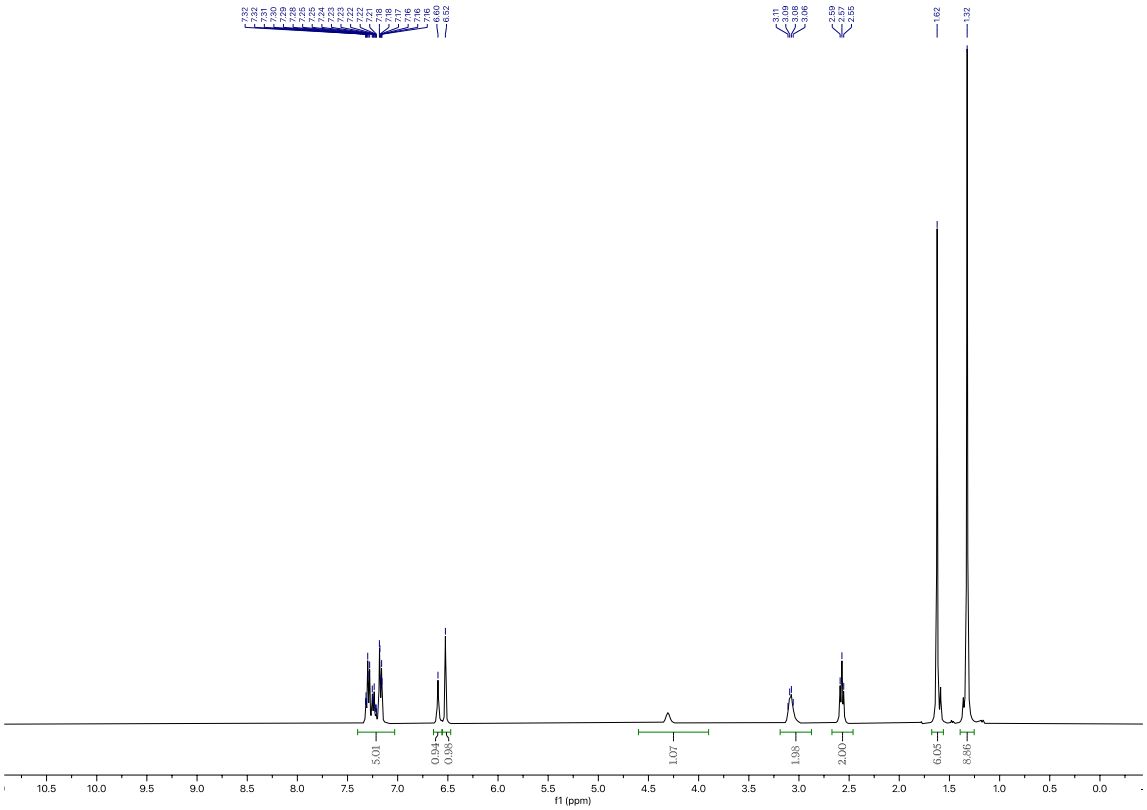


Figure S39. [1]H NMR of *tert*-butyl (2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**4a**).

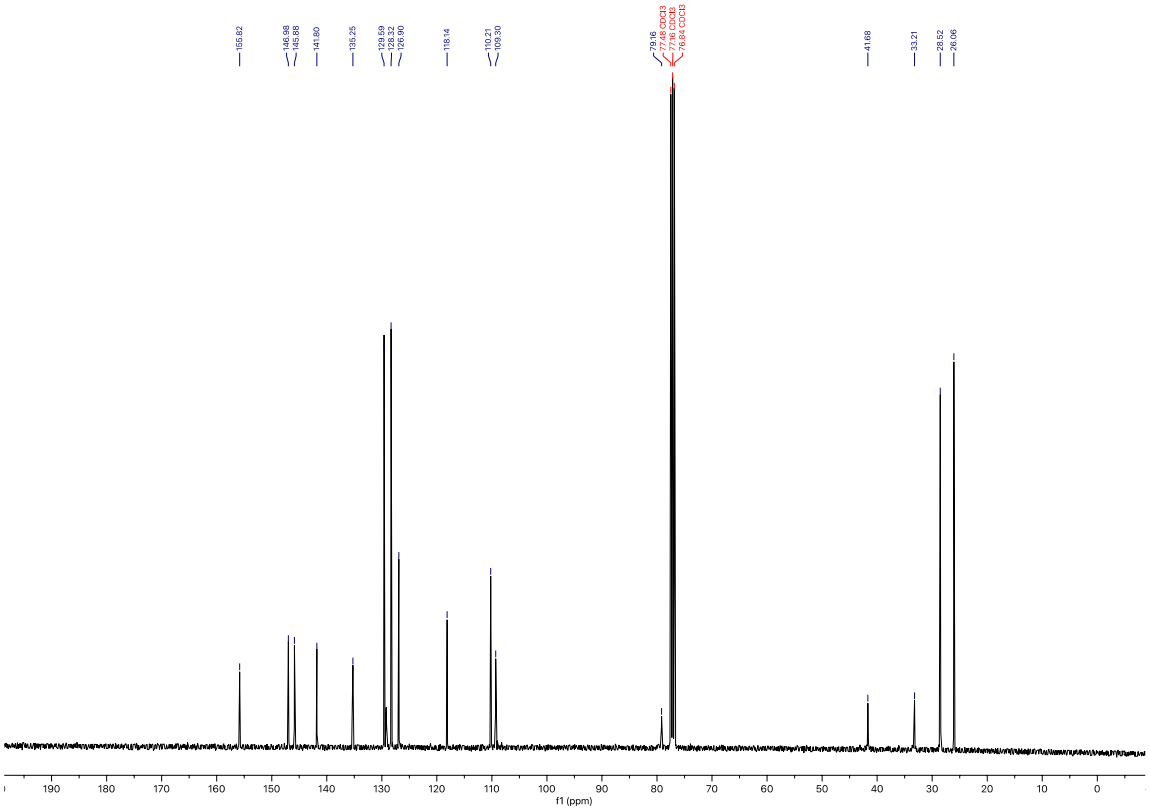


Figure S40. [13]C NMR of *tert*-butyl (2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethyl)carbamate (**4a**).

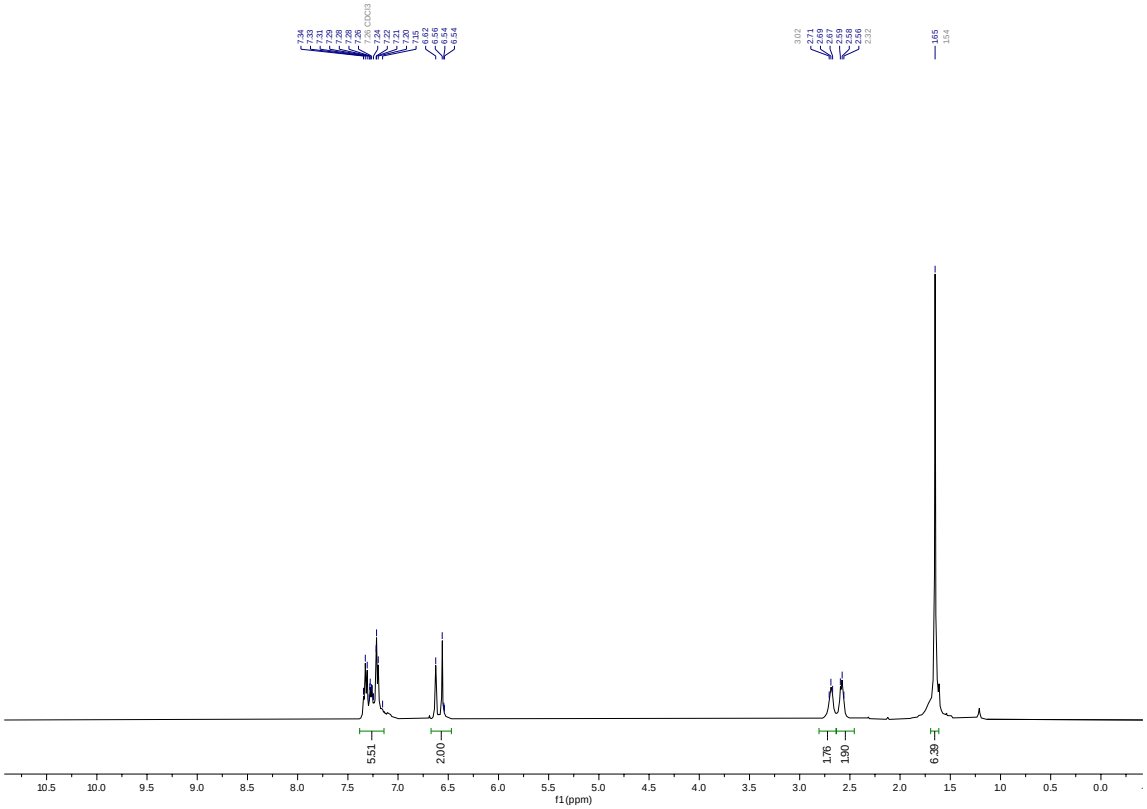


Figure S41. [1]H NMR of 2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethanamine (**5a**).

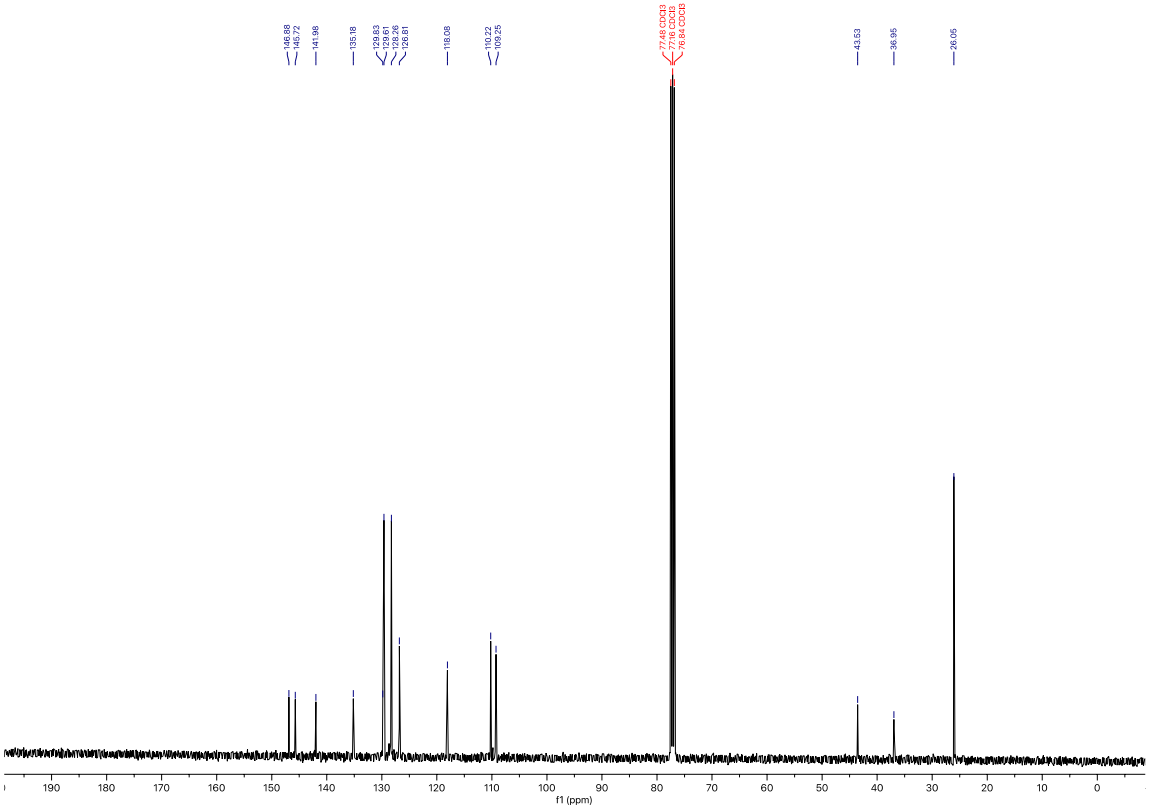


Figure S42. [13]C NMR of 2-(2,2-dimethyl-6-phenylbenzo[d][1,3]dioxol-5-yl)ethanamine (**5a**).

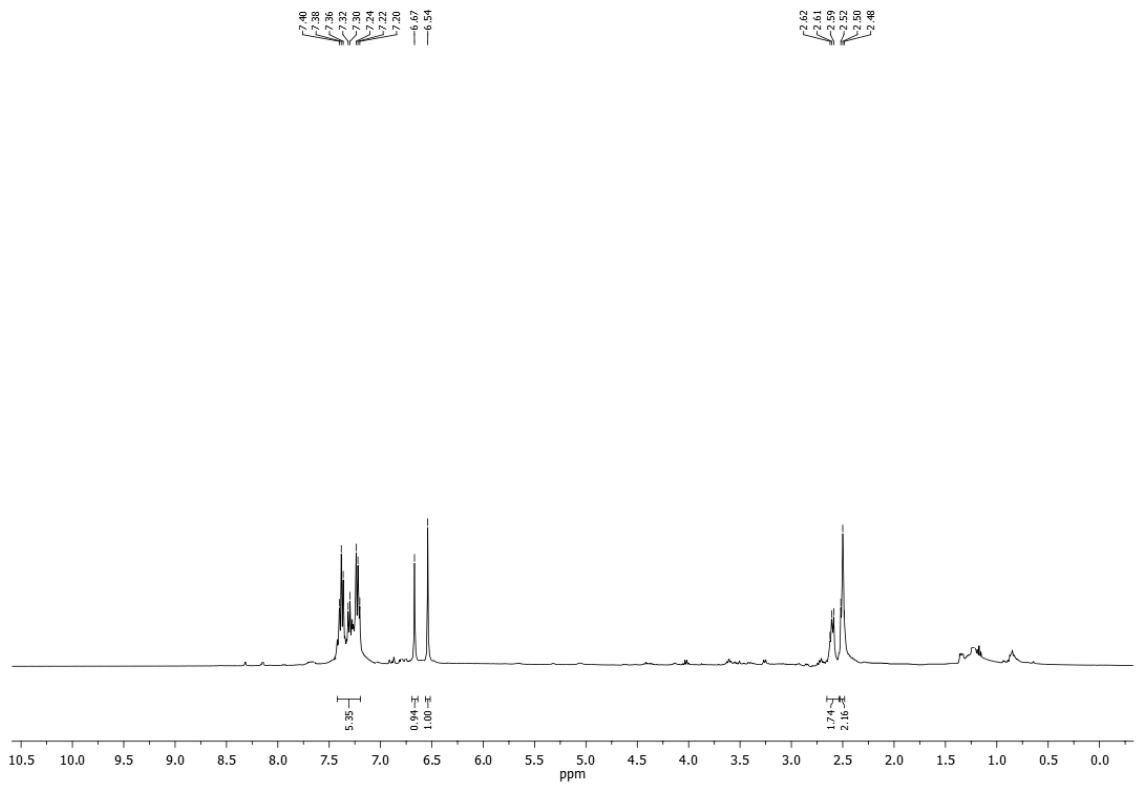


Figure S43. [1]H NMR of 6-(2-aminoethyl)-[1,1'-biphenyl]-3,4-diol (**6a**).

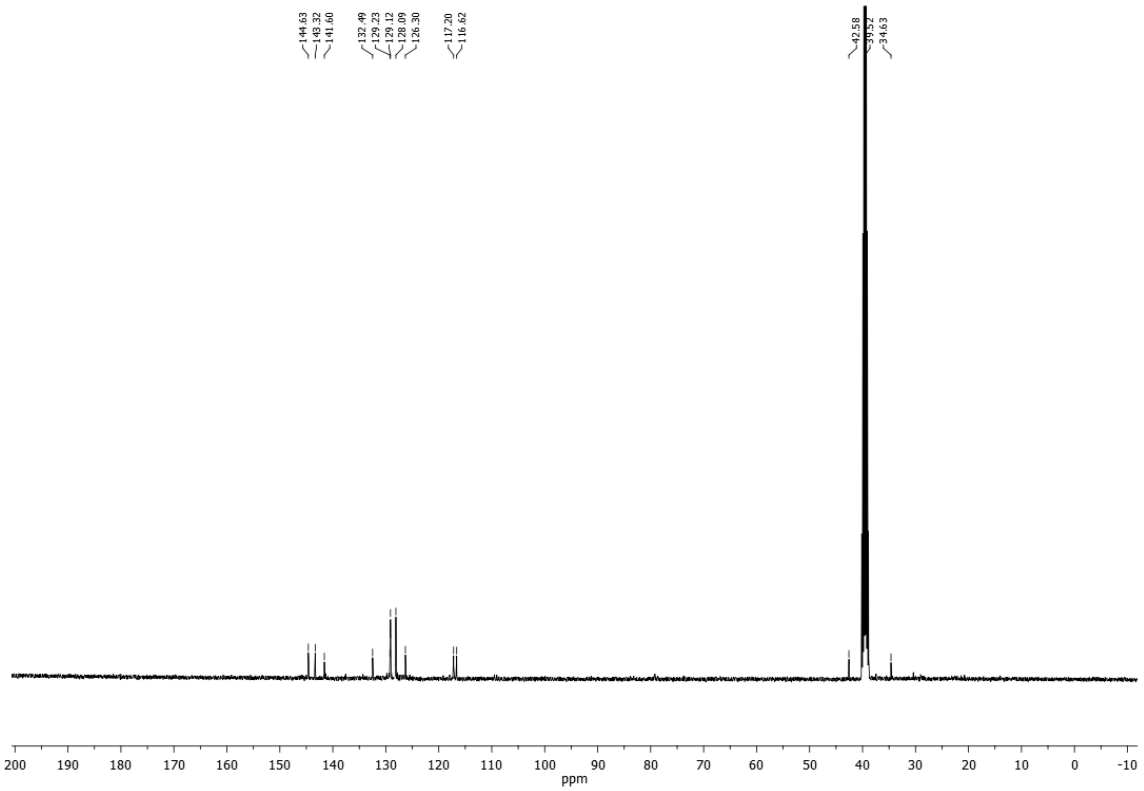


Figure S44. [13]C NMR of 6-(2-aminoethyl)-[1,1'-biphenyl]-3,4-diol (**6a**).