Synthesis of fluorescent boron difluoride complexes of 3-acyl-4-hydroxycoumarins

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Supporting Information

Nomenclature of synthesized compounds

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Absorption spectra of 3-acyl-4-hydroxycoumarins 15-20 and corresponding boron difluoride complexes 22-27
Nomenclature of synthesized compounds

9-hydroxy-10-(undec-10'-ynoyl)-2,3,6,7-tetrahydro-1H,5H,11H-pyranof2,3-fpyrido3,2-ijquinolin-11-one

3-(hept-6-ynoyl)-4-hydroxy-5,6,7-trimethoxy-2H-chromen-2-one

3-methyl-2,3,8,9,12,13-hexahydro-4H,5H,7H,11H-pyranof2',3':4,5]pyranof2,3-fpyrido3,2-ijquinoline-4,5-dione

Figure S1. Atom labels of 3-acyl-4-hydroxycoumarins according to IUPAC nomenclature.
$^1$H and $^{13}$C NMR spectra of products

Figure S2. $^1$H NMR spectrum of compound 6

Figure S3. $^{13}$C NMR spectrum of compound 6
Figure S4. $^1$H NMR spectrum of compound 7

Figure S5. $^{13}$C NMR spectrum of compound 7
Figure S6. $^1$H NMR spectrum of compound 8

Figure S7. $^{13}$C NMR spectrum of compound 8
Figure S8. $^1$H NMR spectrum of compound 9

Figure S9. $^{13}$C NMR spectrum of compound 9
Figure S10. $^1$H NMR spectrum of compound 10

Figure S11. $^{13}$C NMR spectrum of compound 10
Figure S12. $^1$H NMR spectrum of compound 11

Figure S13. $^{13}$C NMR spectrum of compound 11
Figure S14. $^1$H NMR spectrum of compound 12

Figure S15. $^{13}$C NMR spectrum of compound 12
Figure S16. $^1$H NMR spectrum of compound 14

Figure S17. $^{13}$C NMR spectrum of compound 14
Figure S18. $^1$H NMR spectrum of compound 15

Figure S19. $^{13}$C NMR spectrum of compound 15
Figure S20. $^1$H NMR spectrum of compound 16 (7.6-1.2 ppm region).

Figure S21. $^1$H NMR spectrum of compound 16
Figure S22. $^{13}$C NMR spectrum of compound 16

Figure S23. $^1$H NMR spectrum of compound 17
Figure S24. $^1$H NMR spectrum of compound 17 (7.6-1.3 ppm region)

Figure S25. $^{13}$C NMR spectrum of compound 17
Figure S26. $^1$H NMR spectrum of compound 18

Figure S27. $^1$H NMR spectrum of compound 18 (7.4-1.2 ppm region)
Figure S28. $^{13}$C NMR spectrum of compound 18

Figure S29. $^1$H NMR spectrum of compound 19
Figure S30. $^{13}$C NMR spectrum of compound 19

Figure S31. $^1$H NMR spectrum of compound 20
Figure S32. $^{13}$C NMR spectrum of compound 20

Figure S33. $^1$H NMR spectrum of compound 21
Figure S34. $^{13}$C NMR spectrum of compound 21

Figure S35. $^1$H NMR spectrum of compound 22
Figure S36. $^{13}$C NMR spectrum of compound 22

Figure S37. $^1$H NMR spectrum of compound 23
Figure S38. $^{13}$C NMR spectrum of compound 23

Figure S39. $^1$H NMR spectrum of compound 24
Figure S40. $^{13}$C NMR spectrum of compound 24

Figure S41. $^1$H NMR spectrum of compound 25
Figure S42. $^{13}$C NMR spectrum of compound 25

Figure S43. $^1$H NMR spectrum of compound 26
Figure S44. $^{13}$C NMR spectrum of compound 26

Figure S45. $^1$H NMR spectrum of compound 27
Figure S46. $^{13}$C NMR spectrum of compound 27
Emission spectra of 3-acyl-4-hydroxycoumarins 15-20 and corresponding boron difluoride complexes 22-27

Emission spectra were measured in acetonitrile at $5 \cdot 10^{-6}$ M for compounds 15-20 and $1 \cdot 10^{-6}$ M for compounds 22-27 concentrations.

Figure S47. Normalized emission spectra of 3-acyl-4-hydroxycoumarin 15 (black) and corresponding boron difluoride complex 22 (red)
Figure S48. Normalized emission spectra of 3-acyl-4-hydroxycoumarin 16 (black) and corresponding boron difluoride complex 23 (red)

Figure S49. Normalized emission spectra of 3-acyl-4-hydroxycoumarin 17 (black) and corresponding boron difluoride complex 24 (red)
Figure S50. Normalized emission spectra of 3-acyl-4-hydroxycoumarin **18** (black) and corresponding boron difluoride complex **25** (red).

Figure S51. Normalized emission spectra of 3-acyl-4-hydroxycoumarin **19** (black) and corresponding boron difluoride complex **26** (red).
Figure S52. Normalized emission spectra of 3-acyl-4-hydroxycoumarin 20 (black) and corresponding boron difluoride complex 27 (red)
Absorption spectra of 3-acyl-4-hydroxycoumarins 15-20 and corresponding boron difluoride complexes 22-27

Absorption spectra were measured in acetonitrile at $5 \cdot 10^{-6} \text{ M}$ for compounds 15-20 and $1 \cdot 10^{-6} \text{ M}$ for compounds 22-27.

Figure S53. Absorption spectrum of compound 15
Figure S54. Absorption spectrum of compound 16

Figure S55. Absorption spectrum of compound 17
Figure S56. Absorption spectrum of compound 18

Figure S57. Absorption spectrum of compound 19
Figure S58. Absorption spectrum of compound 20

Figure S59. Absorption spectrum of compound 22
Figure S60. Absorption spectrum of compound 23

Figure S61. Absorption spectrum of compound 24
Figure S62. Absorption spectrum of compound 25

Figure S63. Absorption spectrum of compound 26
Figure S64. Absorption spectrum of compound 27