SYNTHESIS OF NITROMETHYL AND (OR) N-METHYLINDOLYL SUBSTITUTED 1,4-BENZOTHIAZINE(DIAZINE)ONES AND 3-METHYL-1,4-BENZOXAZINONES BASED ON ALKYL-3-NITROACRYLATES

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SUPPLEMENTARY INFORMATION

Figure 1. IR spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CHCl₃.
Figure 2. IR spectrum of 2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4a in KBr.

Figure 3. IR spectrum of 2-(1-methyl-1H-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4b in KBr.
**Figure 4.** IR spectrum of ethyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6a in CHCl₃.

**Figure 5.** IR spectrum of methyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6b in CHCl₃.
**Figure 6.** IR spectrum of ethyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6c in CHCl₃.

**Figure 7.** IR spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CHCl₃.
Figure 8. IR spectrum of 3-methyl-2H-1,4-benzoxazin-2-one 7a in KBr.

Figure 9. IR spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in KBr.
**Figure 10.** IR spectrum of 3-(1-methyl-1\textit{H}-indol-3-yl)quinoxalin-2(1\textit{H})-one 10a in KBr.

**Figure 11.** IR spectrum of 6,7-dichloro-3-(1-methyl-1\textit{H}-indol-3-yl)quinoxalin-2(1\textit{H})-one 10b in KBr.
Figure 12. $^1$H NMR spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CDCl$_3$.

Figure 13. $^{13}$C{$^1$H} NMR spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CDCl$_3$.
Figure 14. $^1$H-$^1$H COSY spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CDCl$_3$.

Figure 15. $^1$H-$^{13}$C HMQC spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CDCl$_3$. 
Figure 16. $^1$H-$^{13}$C HMBC spectrum of ethyl 2-[(2-aminophenyl)sulfanyl]-3-nitropropanoate 3a in CDCl$_3$.

Figure 17. $^1$H NMR spectrum of 2-(nitromethyl)-2$H$-1,4-benzothiazin-3(4H)-one 4a in DMSO-$d_6$. 
Figure 18. $^{13}$C\text{(}^{1}H\text{)} NMR spectrum of 2-(nitromethyl)-2$H$-1,4-benzothiazin-3(4$H$)-one 4a in DMSO-$d_{6}$.

Figure 19. $^1$H-$^{13}$C HMQC spectrum of 2-(nitromethyl)-2$H$-1,4-benzothiazin-3(4$H$)-one 4a in DMSO-$d_{6}$. 
Figure 20. $^1$H-$^{13}$C HMBC spectrum of 2-(nitromethyl)-2H-1,4-benzothiazin-3(4$H$)-one 4a in DMSO-$d_6$.

Figure 21. $^1$H NMR spectrum of 2-(1-methyl-1$H$-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4$H$)-one 4b in DMSO-$d_6$. 
Figure 22. $^{13}$C-$^1$H NMR spectrum of 2-(1-methyl-1H-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4b in DMSO-$d_6$.

Figure 23. $^1$H-$^1$H COSY spectrum of 2-(1-methyl-1H-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4b in DMSO-$d_6$. 

12
Figure 24. $^1$H-$^{13}$C HMQC spectrum of 2-(1-methyl-1H-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4b in DMSO-$d_6$.

Figure 25. $^1$H-$^{13}$C HMBC spectrum of 2-(1-methyl-1H-indol-3-yl)-2-(nitromethyl)-2H-1,4-benzothiazin-3(4H)-one 4b in DMSO-$d_6$. 
**Figure 26.** $^1$H NMR spectrum of ethyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6a in CDCl$_3$.

**Figure 27.** $^{13}$C($^1$H) NMR spectrum of ethyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6a in CDCl$_3$.
Figure 28. $^1$H NMR spectrum of methyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6b in CDCl$_3$.

Figure 29. $^{13}$C $^1$H NMR spectrum of methyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6b in CDCl$_3$. 
Figure 30. $^1$H-$^1$C HMQC spectrum of methyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6b in CDCl$_3$.

Figure 31. $^1$H-$^1$C HMBC spectrum of methyl 2-[(2-hydroxyphenyl)amino]-3-nitropropanoate 6b in CDCl$_3$. 
Figure 32. $^1$H NMR spectrum of ethyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6c in CDCl$_3$.

Figure 33. $^{13}$C-$^1$H NMR spectrum of ethyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6c in CDCl$_3$. 
Figure 34. $^1$H-$^{13}$C HMQC spectrum of ethyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6c in CDCl$_3$.

Figure 35. $^1$H-$^{13}$C HMBC spectrum of ethyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6c in CDCl$_3$. 
**Figure 36.** $^1$H NMR spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl₃.

**Figure 37.** $^{13}$C{$^{1}$H} NMR spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl₃.
Figure 38. $^1$H-$^1$H COSY spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl$_3$.

Figure 39. $^1$H-$^{13}$C HMQC spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl$_3$. 
Figure 40. $^1$H-$^{13}$C HMBC spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl$_3$.

Figure 41. $^1$H-$^{15}$N HMBC spectrum of methyl 2-[(5-bromo-2-hydroxyphenyl)amino]-3-nitropropanoate 6d in CDCl$_3$. 
Figure 42. $^1$H NMR spectrum of 3-methyl-2$H$-1,4-benoxazin-2-one 7a in DMSO-$d_6$.

Figure 43. $^{13}$C{$^1$H} NMR spectrum of 3-methyl-2$H$-1,4-benoxazin-2-one 7a in DMSO-$d_6$. 
Figure 44. $^1$H-$^{13}$C HMQC spectrum of 3-methyl-$2H$-1,4-benzoxazin-2-one 7a in DMSO-$d_6$.

Figure 45. $^1$H-$^{13}$C HMBC spectrum of 3-methyl-$2H$-1,4-benzoxazin-2-one 7a in DMSO-$d_6$. 
Figure 46. $^1$H NMR spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in DMSO-$d_6$.

Figure 47. $^{13}$C-€€$^1$H} NMR spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in DMSO-$d_6$. 

24
Figure 48. $^1$H-$^{13}$C HMQC spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in DMSO-$d_6$.

Figure 49. $^1$H-$^{13}$C HMBC spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in DMSO-$d_6$. 

25
Figure 50. $^1$H-$^{15}$N HMBC spectrum of 6-bromo-3-methyl-2H-1,4-benzoxazin-2-one 7b in DMSO-$d_6$.

Figure 51. $^1$H NMR spectrum of 3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10a in DMSO-$d_6$. 

26
Figure 52. $^{13}$C-$^{1}$H NMR spectrum of 3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10a in DMSO-$d_6$.

Figure 53. $^1$H-$^1$H COSY spectrum of 3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10a in DMSO-$d_6$. 
Figure 54. $^1$H-$^{13}$C HMQC spectrum of 3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10a in DMSO-$d_6$.

Figure 55. $^1$H-$^{13}$C HMBC spectrum of 3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10a in DMSO-$d_6$. 
Figure 56. $^1$H NMR spectrum of 6,7-dichloro-3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10b in DMSO-$d_6$.

Figure 57. $^{13}$C{$^1$H} NMR spectrum of 6,7-dichloro-3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10b in DMSO-$d_6$. 
Figure 58. $^1$H-$^1$H COSY spectrum of 6,7-dichloro-3-(1-methyl-$^1$H-indol-3-yl)quinoxalin-2($^1$H)-one 10b in DMSO-$d_6$.

Figure 59. $^1$H-$^{13}$C HMQC spectrum of 6,7-dichloro-3-(1-methyl-$^1$H-indol-3-yl)quinoxalin-2($^1$H)-one 10b in DMSO-$d_6$. 
Figure 60. $^1$H-$^{13}$C HMBC spectrum of 6,7-dichloro-3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one 10b in DMSO-$d_6$. 