### Supporting Information

# Design and Synthesis of Novel Insecticidal 3-Isothiazolols as Potential Antagonists of Insect GABA Receptors

Zihang Ye<sup>a</sup>, Congwei Zhou<sup>a</sup>, Minghong Jiang<sup>a</sup>, Xiaogang Luo<sup>a, b</sup>, Fengshou Wu<sup>a</sup>, ZhiQiang Xu<sup>a</sup>, Qi Sun<sup>a, \*</sup>, Genyan Liu<sup>a, \*</sup>

<sup>a</sup> Key Laboratory for Green Chemical Process of Ministry of Education, Hubei Key Laboratory of Novel Reactor and Green Chemical Technology, School of Chemical Engineering and Pharmacy, Wuhan Institute of Technology, Wuhan 430205, P. R. China <sup>b</sup> School of Materials Science and Engineering, Zhengzhou University, No.100 Science Avenue, Zhengzhou 450001, Henan Province, P. R. China

\*Corresponding authors: Genyan Liu, PhD & Professor; Qi Sun, PhD & Professor *E-mail addresses*: liugenyan@wit.edu.cn (G. Liu); qisun@wit.edu.cn (Q. Sun)

## Contents

1. <sup>1</sup> H NMR spectra of compounds <b>2-5</b> and <b>7</b>	3
2. <sup>1</sup> H NMR spectra of compounds <b>8a-8k</b>	5
3. <sup>1</sup> H NMR spectra of compounds <b>10</b> , <b>11</b> and <b>13</b>	11
4. <sup>1</sup> H NMR spectra of compounds <b>14a-14k</b>	12
5. <sup>1</sup> H NMR spectra and <sup>13</sup> C NMR spectra of compounds 6, 9a-9k	18
6. <sup>1</sup> H NMR spectra and <sup>13</sup> C NMR spectra of compounds <b>12</b> , <b>15a-15k</b>	
7. HRMS of compounds 6, 9a-9k, 12, and 15a-15k	42









Figure S3. <sup>1</sup>H NMR spectra of compound 4



Figure S4. <sup>1</sup>H NMR spectra of compound 5



Figure S5. <sup>1</sup>H NMR spectra of compound 7

## 2. <sup>1</sup>H NMR spectra of compounds 8a-8k



Figure S6. <sup>1</sup>H NMR spectra of compound 8a



Figure S7. <sup>1</sup>H NMR spectra of compound 8b



Figure S8. <sup>1</sup>H NMR spectra of compound 8c



Figure S9. <sup>1</sup>H NMR spectra of compound 8d



Figure S10. <sup>1</sup>H NMR spectra of compound 8e



Figure S11. <sup>1</sup>H NMR spectra of compound 8f



Figure S12. <sup>1</sup>H NMR spectra of compound 8g



Figure S13. <sup>1</sup>H NMR spectra of compound 8h



Figure S14. <sup>1</sup>H NMR spectra of compound 8i



Figure S15. <sup>1</sup>H NMR spectra of compound 8j



Figure S16. <sup>1</sup>H NMR spectra of compound 8k



### 3. <sup>1</sup>H NMR spectra of compounds 10, 11 and 13

Figure S18. <sup>1</sup>H NMR spectra of compound 11



Figure S19. <sup>1</sup>H NMR spectra of compound 13

### 4. <sup>1</sup>H NMR spectra of compounds 14a-14k







Figure S21. <sup>1</sup>H NMR spectra of compound 14b



Figure S22. <sup>1</sup>H NMR spectra of compound 14c



Figure S23. <sup>1</sup>H NMR spectra of compound 14d



Figure S24. <sup>1</sup>H NMR spectra of compound 14e



Figure S25. <sup>1</sup>H NMR spectra of compound 14f



Figure S26. <sup>1</sup>H NMR spectra of compound 14g



Figure S27. <sup>1</sup>H NMR spectra of compound 14h



Figure S28. <sup>1</sup>H NMR spectra of compound 14i







Figure S30. <sup>1</sup>H NMR spectra of compound 14k

5. <sup>1</sup>H NMR spectra and <sup>13</sup>C NMR spectra of compounds 6, 9a-9k



Figure S32. <sup>1</sup>H NMR spectra of compound 9a











Figure S35. <sup>1</sup>H NMR spectra of compound 9d



Figure S36. <sup>1</sup>H NMR spectra of compound 9e



Figure S37. <sup>1</sup>H NMR spectra of compound 9f



Figure S38. <sup>1</sup>H NMR spectra of compound 9g



Figure S39. <sup>1</sup>H NMR spectra of compound 9h



Figure S40. <sup>1</sup>H NMR spectra of compound 9i







Figure S42. <sup>1</sup>H NMR spectra of compound 9k



Figure S44. <sup>13</sup>C NMR spectra of compound 9a



Figure S46. <sup>13</sup>C NMR spectra of compound 9c



Figure S48. <sup>13</sup>C NMR spectra of compound 9e











Figure S52. <sup>13</sup>C NMR spectra of compound 9i



Figure S54. <sup>13</sup>C NMR spectra of compound 9k



6. <sup>1</sup>H NMR spectra and <sup>13</sup>C NMR spectra of compounds 12, 15a-15k

Figure S56. <sup>1</sup>H NMR spectra of compound 15a



Figure S57. <sup>1</sup>H NMR spectra of compound 15b







Figure S59. <sup>1</sup>H NMR spectra of compound 15d



Figure S60. <sup>1</sup>H NMR spectra of compound 15e



Figure S61. <sup>1</sup>H NMR spectra of compound 15f



Figure S62. <sup>1</sup>H NMR spectra of compound 15g



Figure S63. <sup>1</sup>H NMR spectra of compound 15h



Figure S64. <sup>1</sup>H NMR spectra of compound 15i



Figure S65. <sup>1</sup>H NMR spectra of compound 15j



Figure S66. <sup>1</sup>H NMR spectra of compound 15k



Figure S68. <sup>13</sup>C NMR spectra of compound 15a



Figure S70. <sup>13</sup>C NMR spectra of compound 15c



Figure S72. <sup>13</sup>C NMR spectra of compound 15e



Figure S73. <sup>13</sup>C NMR spectra of compound 15f



Figure S74. <sup>13</sup>C NMR spectra of compound 15g



Figure S76. <sup>13</sup>C NMR spectra of compound 15i



Figure S78. <sup>13</sup>C NMR spectra of compound 15k

#### 7. HRMS of compounds 6, 9a-9k, 12, and 15a-15k





























Figure S88. HRMS of compound 9i



Figure S90. HRMS of compound 9k



















315.0948 ([C15H18N2O2S]+Na)

308 310 312 314 Counts vs. Mass-to-Charge (m/z)

Figure S96. HRMS of compound 15e

 \_\_\_\_\_329.0747 ([C15H18N2O2S]+K)+

331.0669 ([C15H18N2O2S]+K)+





Figure S98. HRMS of compound 15g



Figure S99. HRMS of compound 15h



Figure S100. HRMS of compound 15i



Figure S101. HRMS of compound 15j



Figure S102. HRMS of compound 15k