Supporting Information
Anti-inflammatory Chalcone–Isoflavone Dimers and Chalcone Dimers from
*Caragana jubata*

Lina Wang,† Xuedong Yang,* ‡ Yi Zhang,† Ruixue Chen,† Yuanyuan Cui, † and Qiulin Wang†

† School of Pharmaceutical Science and Technology, Health Sciences Platform, Tianjin University, 92 Weijin Road, Nankai District, Tianjin 300072, People’s Republic of China

*Corresponding author:* Xuedong Yang
Tel.: 86 22 87401152
E-mail: yangxd@tju.edu.cn
## Contents

Figure S1. UV Spectrum of Compound 1 ................................................................. 4
Figure S2. IR Spectrum of Compound 1 ................................................................. 4
Figure S3. HRESIMS of Compound 1 ................................................................. 4
Figure S4. 1H-NMR Spectrum of Compound 1 (DMSO-d$_6$) ................................. 5
Figure S5. 13C-NMR Spectrum of Compound 1 (DMSO-d$_6$) ................................. 5
Figure S6. DEPT-135 NMR Spectrum of Compound 1 (DMSO-d$_6$) ......................... 6
Figure S7. COSY Spectrum of Compound 1 (DMSO-d$_6$) ........................................ 7
Figure S8. HSQC Spectrum of Compound 1 (DMSO-d$_6$) ........................................ 7
Figure S9. HMBC Spectrum of Compound 1 (DMSO-d$_6$) ....................................... 8
Figure S10. HMBC Correlations of H-6'/H-6''/H-8'/H-7' and C-9' for Compound 1 .... 8
Figure S11. HMBC Correlations of H-7' and C-2'' for Compound 1 ............................ 9
Figure S12. UV Spectrum of Compound 2 .............................................................. 10
Figure S13. IR Spectrum of Compound 2 .............................................................. 10
Figure S14. HRESIMS of Compound 2 ............................................................... 11
Figure S15. 1H-NMR Spectrum of Compound 2 (DMSO-d$_6$) ................................. 11
Figure S16. 13C-NMR Spectrum of Compound 2 (DMSO-d$_6$) ............................... 12
Figure S17. DEPT-135 NMR Spectrum of Compound 2 (DMSO-d$_6$) ...................... 12
Figure S18. COSY Spectrum of Compound 2 (DMSO-d$_6$) ..................................... 13
Figure S19. HSQC Spectrum of Compound 2 (DMSO-d$_6$) .................................... 13
Figure S20. HMBC Spectrum of Compound 2 (DMSO-d$_6$) .................................. 14
Figure S21. HMBC Correlation of H-6'' and C-7' for Compound 2 ......................... 14
Figure S22. HMBC Correlation of H-6'/H-7'/H-8'/H-6'' and C-9' for Compound 2 ... 15
Figure S23. UV Spectrum of Compound 3 ............................................................ 16
Figure S24. IR Spectrum of Compound 3 ............................................................ 16
Figure S25. HRESIMS of Compound 3 ............................................................... 17
Figure S26. 1H-NMR Spectrum of Compound 3 (DMSO-d$_6$) ............................... 17
Figure S27. 13C-NMR Spectrum of Compound 3 (DMSO-d$_6$) ............................. 18
Figure S28. DEPT-135 NMR Spectrum of Compound 3 (DMSO-d$_6$) .................... 18
Figure S29. COSY Spectrum of Compound 3 (DMSO-d$_6$) .................................. 19
Figure S30. HSQC Spectrum of Compound 3 (DMSO-d$_6$) .................................. 19
Figure S31. HMBC Spectrum of Compound 3 (DMSO-d$_6$) ................................. 20
Figure S32. HMBC Correlations of H-5 and C-4 for Compound 3 ............................ 20
Figure S33. HMBC Correlations of H-2 and C-9 for Compound 3 ............................ 21
Figure S34. HMBC Correlations of H-6'' and C-11 for Compound 3 ......................... 21
Figure S35. HMBC Correlations of H-13 and C-2'' for Compound 3 ......................... 22
Figure S36. HMBC Correlations of H-4 and C-11 for Compound 3 ........................... 22
Figure S37. HMBC Correlations of H-12/H-13 and C-4 for Compound 3 .................. 23
Figure S38. NOESY Spectrum of Compound 3 (DMSO-d$_6$) ................................. 23
Figure S39. UV Spectrum of Compound 4 ............................................................ 24
Figure S40. IR Spectrum of Compound 4 ............................................................ 24
Figure S41. HRESIMS of Compound 4 ............................................................... 25
Figure S42. $^1$H-NMR Spectrum of Compound 4 (DMSO-$d_6$) ........................................25
Figure S43. $^{13}$C-NMR Spectrum of Compound 4 (DMSO-$d_6$) ....................................26
Figure S44. DEPT-135 NMR Spectrum of Compound 4 (DMSO-$d_6$) .........................26
Figure S45. COSY Spectrum of Compound 4 (DMSO-$d_6$) ........................................27
Figure S46. HSQC Spectrum of Compound 4 (DMSO-$d_6$) ........................................27
Figure S47. HMBC Spectrum of Compound 4 (DMSO-$d_6$) ........................................28
Figure S48. HMBC Correlations of H-2 and C-3/C-4 for Compound 4 ..........................28
Figure S49. HMBC Correlations of H-2 and C-9 for Compound 4 ..................................29
Figure S50. HMBC Correlation of H-5 and C-4 for Compound 4 ..................................29
Figure S51. HMBC Correlation of H-12/H-13 and C-4 for Compound 4 .......................30
Figure S52. HMBC Correlation of H-13 and C-2"" for Compound 4 ...............................30
Figure S53. HMBC Correlation of H-2"" and C-11 for Compound 4 ...............................31
Figure S54. HMBC Correlation of H-6' and C-2 for Compound 4 .................................31
Figure S55. NOESY Spectrum of Compound 4 (DMSO-$d_6$) .....................................32
Figure S56. HRESIMS of Compound 5 .................................................................33
Figure S57. $^1$H-NMR Spectrum of Compound 5 (DMSO-$d_6$) ..................................33
Figure S58. $^{13}$C-NMR Spectrum of Compound 5 (DMSO-$d_6$) .................................34
Figure S59. HRESIMS of Compound 6 ........................................................................35
Figure S60. $^1$H-NMR Spectrum of Compound 6 (DMSO-$d_6$) ..................................35
Figure S61. $^{13}$C-NMR Spectrum of Compound 6 (DMSO-$d_6$) ..................................36
Figure S62. HRESIMS of Compound 7 ........................................................................37
Figure S63. $^1$H-NMR Spectrum of Compound 7 (DMSO-$d_6$) ..................................37
Figure S64. $^{13}$C-NMR Spectrum of Compound 7 (DMSO-$d_6$) ..................................38
Figure S65. HRESIMS of Compound 8 ........................................................................39
Figure S66. $^1$H-NMR spectrum of Compound 8 (CDCl$_3$) ........................................39
Figure S67. $^{13}$C-NMR Spectrum of Compound 8 (CDCl$_3$) ........................................40
Figure S68. HRESIMS of Compound 9 ........................................................................41
Figure S69. $^1$H-NMR Spectrum of Compound 9 (DMSO-$d_6$) ..................................41
Figure S70. $^{13}$C-NMR Spectrum of Compound 9 (DMSO-$d_6$) ..................................42
Figure S71. HRESIMS of Compound 10 .......................................................................43
Figure S72. $^1$H-NMR Spectrum of Compound 10 (DMSO-$d_6$) ..............................43
Figure S73. $^{13}$C-NMR Spectrum of Compound 10 (DMSO-$d_6$) ..............................44
Figure S74. HRESIMS of Compound 11 .......................................................................45
Figure S75. $^1$H-NMR Spectrum of Compound 11 (DMSO-$d_6$) ..............................45
Figure S76. $^{13}$C-NMR Spectrum of Compound 11 (DMSO-$d_6$) ..............................46
Figure S77. HRESIMS of Compound 12 .......................................................................47
Figure S78. $^1$H-NMR Spectrum of Compound 12 (CDCl$_3$) ....................................47
Figure S79. $^{13}$C-NMR Spectrum of Compound 12 (CDCl$_3$) ....................................48
Figure S80. Scheme of Plausible Biosynthetic Pathways for Compounds 1 and 2 .......49
Figure S81. Scheme of Plausible Biosynthetic Pathways for Compounds 3 and 4 .......50
Figure S1. UV Spectrum of Compound 1

Figure S2. IR Spectrum of Compound 1
Figure S3. HRESIMS of Compound 1

Figure S4. $^1$H-NMR Spectrum of Compound 1 (DMSO-$d_6$)
Figure S5. $^{13}$C-NMR Spectrum of Compound 1 (DMSO-$d_6$)

Figure S6. DEPT-135 NMR Spectrum of Compound 1 (DMSO-$d_6$)
Figure S7. COSY Spectrum of Compound 1 (DMSO-$d_6$)

Figure S8. HSQC Spectrum of Compound 1 (DMSO-$d_6$)
Figure S9. HMBC Spectrum of Compound 1 (DMSO-\textit{d}_6)

Figure S10. HMBC Correlations of H-6'/H-6''/H-8'/H-7' and C-9' for Compound 1
Figure S11. HMBC Correlations of H-7' and C-2''' for Compound 1
Figure S12. UV Spectrum of Compound 2

Figure S13. IR Spectrum of Compound 2
Figure S14. HRESIMS of Compound 2

Figure S15. $^1$H-NMR Spectrum of Compound 2 (DMSO-$d_6$)
Figure S16. $^{13}$C-NMR Spectrum of Compound 2 (DMSO-$d_6$)

Figure S17. DEPT-135 NMR Spectrum of Compound 2 (DMSO-$d_6$)
**Figure S18.** COSY Spectrum of Compound 2 (DMSO-$d_6$)

**Figure S19.** HSQC Spectrum of Compound 2 (DMSO-$d_6$)
**Figure S20.** HMBC Spectrum of Compound 2 (DMSO-\textit{d}_6)

**Figure S21.** HMBC Correlation of H-6" and C-7' for Compound 2
Figure S22. HMBC Correlation of H-6'/H-7'/H-8'/H-6''' and C-9' for Compound 2
Figure S23. UV Spectrum of Compound 3

Figure S24. IR Spectrum of Compound 3
Figure S25. HRESIMS of Compound 3

Figure S26. $^1$H-NMR Spectrum of Compound 3 (DMSO-$d_6$)
**Figure S27.** $^{13}$C-NMR Spectrum of Compound 3 (DMSO-$d_6$)

**Figure S28.** DEPT-135 NMR Spectrum of Compound 3 (DMSO-$d_6$)
**Figure S29.** COSY Spectrum of Compound 3 (DMSO-$d_6$)

**Figure S30.** HSQC Spectrum of Compound 3 (DMSO-$d_6$)
Figure S31. HMBC Spectrum of Compound 3 (DMSO-d<sub>6</sub>)

Figure S32. HMBC Correlations of H-5 and C-4 for Compound 3
Figure S33. HMBC Correlations of H-2 and C-9 for Compound 3

Figure S34. HMBC Correlations of H-6" and C-11 for Compound 3
Figure S35. HMBC Correlations of H-13 and C-2'' for Compound 3

Figure S36. HMBC Correlations of H-4 and C-11 for Compound 3
Figure S37. HMBC Correlations of H-12/H-13 and C-4 for Compound 3

Figure S38. NOESY Spectrum of Compound 3 (DMSO-\textit{d}_6)
Figure S39. UV Spectrum of Compound 4

Figure S40. IR Spectrum of Compound 4
Figure S41. HRESIMS of Compound 4

Figure S42. $^1$H-NMR Spectrum of Compound 4 (DMSO-$d_6$)
Figure S43. $^{13}$C-NMR Spectrum of Compound 4 (DMSO-$d_6$)

Figure S44. DEPT-135 Spectrum of Compound 4 (DMSO-$d_6$)
Figure S45. COSY Spectrum of Compound 4 (DMSO-$d_6$)

Figure S46. HSQC Spectrum of Compound 4 (DMSO-$d_6$)
Figure S47. HMBC Spectrum of Compound 4 (DMSO-$d_6$)

Figure S48. HMBC Correlations of H-2 and C-3/C-4 for Compound 4
Figure S49. HMBC Correlations of H-2 and C-9 for Compound 4

Figure S50. HMBC Correlation of H-5 and C-4 for Compound 4
Figure S51. HMBC Correlation of H-12/H-13 and C-4 for Compound 4

Figure S52. HMBC Correlation of H-13 and C-2"" for Compound 4
Figure S53. HMBC Correlation of H-2” and C-11 for Compound 4

Figure S54. HMBC Correlation of H-6’ and C-2 for Compound 4
Figure S55. NOESY Spectrum of Compound 4 (DMSO-$d_6$)
Figure S56. HRESIMS of Compound 5

Figure S57. $^1$H-NMR Spectrum of Compound 5 (DMSO-$d_6$)
Figure S58. $^{13}$C-NMR Spectrum of Compound 5 (DMSO-$d_6$)
Figure S59. HRESIMS of Compound 6

Figure S60. $^1$H-NMR Spectrum of Compound 6 (DMSO-$d_6$)
Figure S61. $^{13}$C-NMR Spectrum of Compound 6 (DMSO-$d_6$)
Figure S62. HRESIMS of Compound 7

Figure S63. $^1$H-NMR Spectrum of Compound 7 (DMSO-$d_6$)
**Figure S64.** $^{13}$C-NMR Spectrum of Compound 7 (DMSO-$d_6$)
Figure S65. HRESIMS of Compound 8

Figure S66. $^1$H-NMR Spectrum of Compound 8 (CDCl$_3$)
Figure S67. $^{13}$C-NMR Spectrum of Compound 8 (CDCl$_3$)
Figure S68. HRESIMS of Compound 9

Figure S69. $^1$H-NMR Spectrum of Compound 9 (DMSO-$d_6$)
Figure S70. $^{13}$C-NMR Spectrum of Compound 9 (DMSO-$d_6$)
**Figure S71.** HRESIMS of Compound 10

**Figure S72.** $^1$H-NMR Spectrum of Compound 10 (DMSO-$d_6$)
Figure S73. $^{13}$C-NMR Spectrum ofCompound 10 (DMSO-$d_6$)
Figure S74. HRESIMS of Compound 11

Figure S75. $^1$H-NMR Spectrum of Compound 11 (DMSO-$d_6$)
Figure S76. $^{13}$C-NMR Spectrum of Compound 11 (DMSO-$d_6$)
Figure S77. HRESIMS of Compound 12

Figure S78. $^1$H-NMR Spectrum of Compound 12 (CDCl$_3$)
**Figure S79.** $^{13}$C-NMR Spectrum of Compound 12 (CDCl$_3$)
Figure S80. Scheme of Plausible Biosynthetic Pathways for Compounds 1 and 2
Figure S81. Scheme of Plausible Biosynthetic Pathways for Compounds 3 and 4