## **Supporting Information for**

## (+)-Meyeniins A–C, Novel Hexahydroimidazo[1,5-*c*]thiazole Derivatives from the Tubers of *Lepidium meyenii*: Complete Structural Elucidation by Biomimetic Synthesis and Racemic Crystallization

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Figure S1. <sup>1</sup>H NMR spectrum of natural (+)-meyeniin A (1)

Figure S2. <sup>13</sup>C NMR spectrum of natural (+)-meyeniin A (1)



Figure S3. HSQC spectrum of natural (+)-meyeniin A (1)



Figure S4. HMBC spectrum of natural (+)-meyeniin A (1)



Figure S5. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of natural (+)-meyeniin A (1)



Figure S6. ROESY spectrum of natural (+)-meyeniin A (1)



Figure S7. CD of natural (+)-meyeniin A (1)





Figure S8. <sup>1</sup>H NMR spectrum of natural (+)-meyeniin B (2)

Figure S9. <sup>13</sup>C NMR spectrum of natural (+)-meyeniin B (2)





Figure S10. HSQC spectrum of natural (+)-meyeniin B (2)

Figure S11. HMBC spectrum of natural (+)-meyeniin B (2)





Figure S12. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of natural (+)-meyeniin B (2)

Figure S13. ROESY spectrum of natural (+)-meyeniin B (2)









Figure S15. <sup>1</sup>H NMR spectrum of natural (+)-meyeniin C (3)

Figure S16. <sup>13</sup>C NMR spctrum of natural (+)-meyeniin C (3)



Figure S17. HSQC spectrum of natural (+)-meyeniin C (3)



Figure S18. HMBC spectrum of natural (+)-meyeniin C (3)



(mpg) 11  $\cap$ (+)-meyeniin C (3) 8.0 2.5 2.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 f2 (ppm) 3.5 3.0 1.5 1.0 0.5

Figure S19. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of natural (+)-meyeniin C (**3**)

Figure S20. ROESY spectrum of natural (+)-meyeniin C (3)



Figure S21. CD of natural (+)-meyeniin C (3)





Figure S22. <sup>1</sup>H NMR spectrum of synthetic (+)-meyeniin A (1)

Figure S23. <sup>13</sup>C NMR spectrum of synthetic (+)-meyeniin A (1)



Figure S24. CD of synthetic (+)-meyeniin A (1)





Figure S25. <sup>1</sup>H NMR spectrum of synthetic (-)-meyeniin A (1)

Figure S26. <sup>13</sup>C NMR spectrum of synthetic (-)-meyeniin A (1)





Figure S28. X-ray structure of synthetic racemic meyeniin A (1)





Figure S29. <sup>1</sup>H NMR spectrum of synthetic (+)-meyeniin B (2)

Figure S30. <sup>13</sup>C NMR spectrum of synthetic (+)-meyeniin B (2)



Figure S31. CD of synthetic (+)-meyeniin B (2)





Figure S32. <sup>1</sup>H NMR spectrum of synthetic (-)-meyeniin B (2)

Figure S33. <sup>13</sup>C NMR spectrum of synthetic (-)-meyeniin B (2)









Figure S35. <sup>1</sup>H NMR spectrum of synthetic (+)-meyeniin C (**3**)

Figure S36. <sup>13</sup>C NMR spectrum of synthetic (+)-meyeniin C (3)

![](_page_23_Figure_3.jpeg)

Figure S37. CD of synthetic (+)-meyeniin C (3)

![](_page_24_Figure_1.jpeg)

![](_page_25_Figure_0.jpeg)

Figure S38. <sup>1</sup>H NMR spectrum of synthetic (-)-meyeniin C (3)

Figure S25. <sup>13</sup>C NMR spectrum of synthetic (-)-meyeniin C (**3**)

![](_page_25_Figure_3.jpeg)

![](_page_26_Figure_1.jpeg)