Table of contents

S1-S19. ¹H NMR and ¹³C NMR of MGF and intermediates A1-A18

S20-S37. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G1-G18

S38-S55. HPLC of G1-G18

S56. Stability of MGF derivative G1 in mice plasma

S1. ¹H NMR and ¹³C NMR of MGF



¹³C NMR spectrum of compound MGF



S2. ¹H NMR and ¹³C NMR of intermediates A1





S3. ¹H NMR and ¹³C NMR of intermediates A2



S4. ¹H NMR and ¹³C NMR of intermediates A3





S5. ¹H NMR and ¹³C NMR of intermediates A4





S6. ¹H NMR and ¹³C NMR of intermediates A5





S7. ¹H NMR and ¹³C NMR of intermediates A6



S8. ¹H NMR and ¹³C NMR of intermediates A7

¹³C NMR spectrum of compound A7



S9. ¹H NMR and ¹³C NMR of intermediates A8





S10. ¹H NMR and ¹³C NMR of intermediates A9

¹³C NMR spectrum of compound A9









S12. ¹H NMR and ¹³C NMR of intermediates A11





S13. ¹H NMR and ¹³C NMR of intermediates A12

¹³C NMR spectrum of compound A12



S14. ¹H NMR and ¹³C NMR of intermediates A13





S15. ¹H NMR and ¹³C NMR of intermediates A14

¹³C NMR spectrum of compound A14



S16. ¹H NMR and ¹³C NMR of intermediates A15





S17. ¹H NMR and ¹³C NMR of intermediates A16



¹³C NMR spectrum of compound A16



S18. ¹H NMR and ¹³C NMR of intermediates A17





S19. ¹H NMR and ¹³C NMR of intermediates A18

¹³C NMR spectrum of compound A18



S20. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G1

¹³C NMR spectrum of compound G1



HRESIMS of compound G1





¹H NMR spectrum of compound G2





m/z



S22. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G3



BW #272 RT: 1.18 AV: 1 NL: 2.94E6 T: FTMS + p ESI Full ms [850.0000-1500.0000]



HRESIMS of compound G3









HRESIMS of compound G4



S24. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G5





HRESIMS of compound G5















S26. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G7



HRESIMS of compound G7











1141.6520 1185.6777 1229.7040 1287.7084

1<u>053</u>,5997

1323,5304

1361,4854

1403,4705

1430.4894

14<u>46</u>,4622

lh h

hù.

Relative Abundance

0^Ξ

877.4962 921.5222 965.5479 1009.5741

S28. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G9



¹³C NMR spectrum of compound G9



HRESIMS of compound G9













¹³C NMR spectrum of compound G11











¹³C NMR spectrum of compound G13



S33. ¹H NMR, ¹³C NMR and HRESIMS of MGF derivatives G14







HRESIMS of compound G14



¹³C NMR spectrum of compound G15



HRESIMS of compound G15





















HRESIMS of compound G18



Purity analysis of the G1: 96.01%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%



Purity analysis of the G2: 99.06%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 68%: 32%





Purity analysis of the G3: 99.31%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%



Purity analysis of the G4: 99.76%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%





Purity analysis of the G5: 95.35%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 75%: 25%

S43. HPLC of G6



Purity analysis of the G6: 95.37%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%



Purity analysis of the G7: 98.04%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 68%: 32%



Purity analysis of the G8: 96.32%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 72%: 28%

S46. HPLC of G9



Purity analysis of the G9: 98.76%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 55%: 45%



Purity analysis of the G10: 97.32%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%





Purity analysis of the G11: 98.59%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 68%: 32%

S49. HPLC of G12



Purity analysis of the G12: 99.76%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 57%: 43%

S50. HPLC of G13



Purity analysis of the G13: 99.56%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 65%: 35%



Purity analysis of the G14: 97.50%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 75%: 25%

S52. HPLC of G15



Purity analysis of the G15: 95.40%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%



Purity analysis of the G16: 99.17%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 68%: 32%





Purity analysis of the G17: 99.78%. The mobile phase was methanol (A)-0.1% formic acid in

water (B), and the mobile phase ratio was A: B = 75%: 25%

S55. HPLC of G18



Purity analysis of the G18: 95.14%. The mobile phase was methanol (A)-0.1% formic acid in water (B), and the mobile phase ratio was A: B = 75%: 25%

S56. Stability of MGF derivative G1 in mice plasma









HPLC of the product of the complete hydrolysis of methyl ester



The curve of incubation time and residual substrate concentration