Synthesis, Antimicrobial and Cytotoxicity Studies of Some Novel Modified Strobilurin Derivatives

Ajjanna M. Sridhara,^{a,b} Kallam R. Venugopala Reddy,^{*,b} Jathi Keshavayya,^c Dasannana Malige S. Ambika,^e Vadiraj S. Gopinath,^a Prosenjit Bose,^a Sanath Kumar Goud^a and Sanenahalli K. Peethambar^d

^aAdvinus Therapeutics Pvt. Ltd, 21 & 22, Peenya II phase, Bangalore-560 058, India

^bDepartment of Studies in Industrial Chemistry, ^cDepartment of Studies in Chemistry and ^dDepartment of Biochemistry, Kuvempu University, Jnana Sahyadri, Shankaragatta-577 451, Karnataka, India

^eDepartment of Plant Pathology, G.K.V.K, UAS, Bangalore-65 India



Figure S1. Mass spectrum of methyl 2-(3-allyl-4-oxo-3,4-dihydrophthalazin-1-yl)acetate (5).

^{*}e-mail: venurashmi30@rediffmail.com



Figure S2. ¹H NMR spectrum of methyl 2-(3-allyl-4-oxo-3,4-dihydrophthalazin-1-yl)acetate (5).



Figure S3. Mass spectrum of methyl 2-(3-allyl-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxy acrylate (6).



Figure S4. ¹H NMR spectrum of methyl 2-(3-allyl-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxy acrylate (6).



Figure S5. Mass spectrum of methyl 3-methoxy-2-(3-((3-methyl-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)acrylate (7a).



Figure S6. ¹H NMR spectrum of methyl 3-methoxy-2-(3-((3-methyl-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)acrylate (7a).



Figure S7. Mass spectrum of methyl 3-methoxy-2-(4-oxo-3-((3-phenyl-4,5-dihydroisoxazol-5-yl)methyl)-3,4-dihydrophthalazin-1-yl)acrylate (7b).



Figure S8. ¹H NMR spectrum of methyl 3-methoxy-2-(4-oxo-3-((3-phenyl-4,5-dihydroisoxazol-5-yl)methyl)-3,4-dihydrophthalazin-1-yl)acrylate (7b).



Figure S9. Mass spectrum of methyl 2-(3-((3-((3-((3-((A-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7c).



 $Figure S10. \ \ 'HNMR \ spectrum of methyl 2-(3-((3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7c).$



Figure S11. Mass spectrum of methyl 2-(3-((3-(4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7d).



 $Figure S12. \ \ 'HNMR \ spectrum of methyl 2-(3-((3-(4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3, 4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7d).$



 $Figure S13. {}^{13}CNMR spectrum of methyl 2-(3-((3-(4-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3, 4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7d).$



Figure S14. Mass spectrum of methyl 2-(3-((3-(3,4-dimethoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7e).



Figure S15. ¹H NMR spectrum of methyl 2-(3-((3-(3,4-dimethoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7e).



Figure S16. Mass spectrum of methyl 2-(3-((3-(3,4-dimethoxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7f).



Figure S17. ¹H NMR spectrum of methyl 3-methoxy-2-(4-oxo-3-((3-(thiophen-2-yl)-4,5-dihydroisoxazol-5-yl) methyl)-3,4-dihydrophthalazin-1-yl) acrylate (7h).



Figure S18. Mass spectrum of methyl 2-(3-((3-(4-bromo-3-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7i).



Figure S19. ¹H NMR spectrum of methyl 2-(3-((3-((4-bromo-3-fluorophenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7i).



 $\label{eq:Figure S20. ^{1}H NMR spectrum of methyl 3-methoxy-2-(4-oxo-3-((3-(1-pivaloylpiperidin-4-yl)-4,5-dihydroisoxazol-5-yl)methyl)-3, 4-dihydrophthalazin-1-yl)acrylate (7j).$



 $\label{eq:Figure S21.} Figure S21. {}^{13}C NMR spectrum of methyl 3-methoxy-2-(4-oxo-3-((3-(1-pivaloylpiperidin-4-yl)-4,5-dihydroisoxazol-5-yl)methyl)-3,4-dihydrophthalazin-1-yl)acrylate (7j).$



Figure S22. Mass spectrum of methyl 2-(3-((3-(1-benzylpiperidin-4-yl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (7k).



Figure S23. Mass spectrum of methyl 2-(3-((3-(2-hydroxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (71).



Figure S24. ¹H NMR spectrum of methyl 2-(3-((3-((2-hydroxyphenyl)-4,5-dihydroisoxazol-5-yl)methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)-3-methoxyacrylate (71).