

Supporting information

RSK1 vs RSK2 inhibitory activity of the marine β -carboline alkaloid Manzamine A: a biochemical, cervical cancer protein expression and computational docking study

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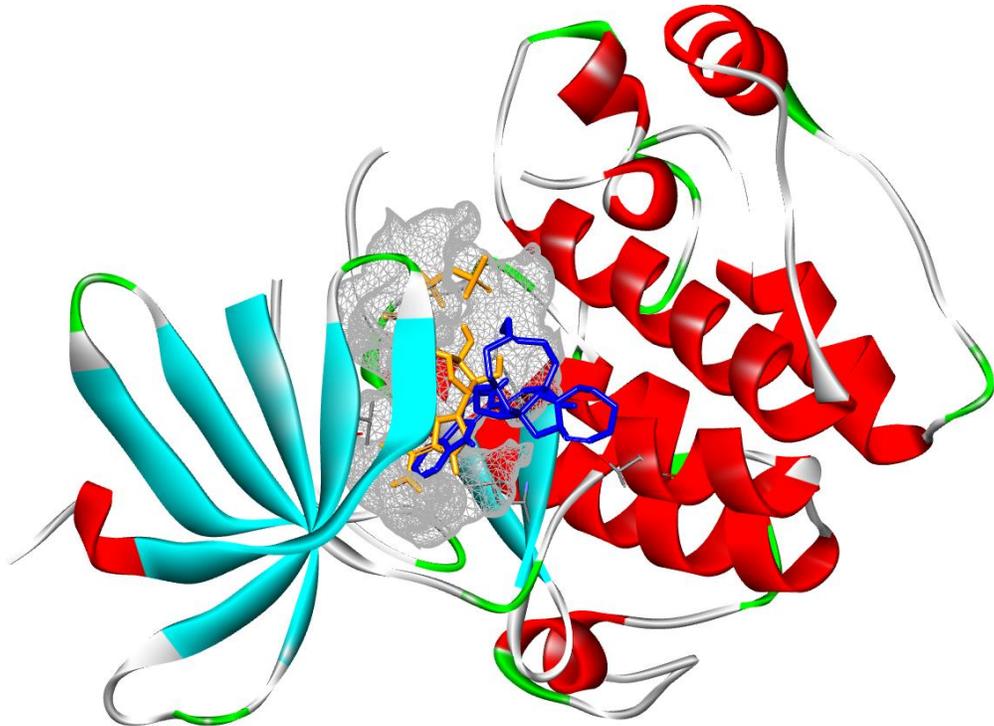


Figure S1: MZA (blue) and ATP (orange) is shown docked to MAPK-activated protein kinase-1 α (binding pocket is shown as gray mesh) (MAPKAP-K1 α) (PDB ID: 2Z7Q)

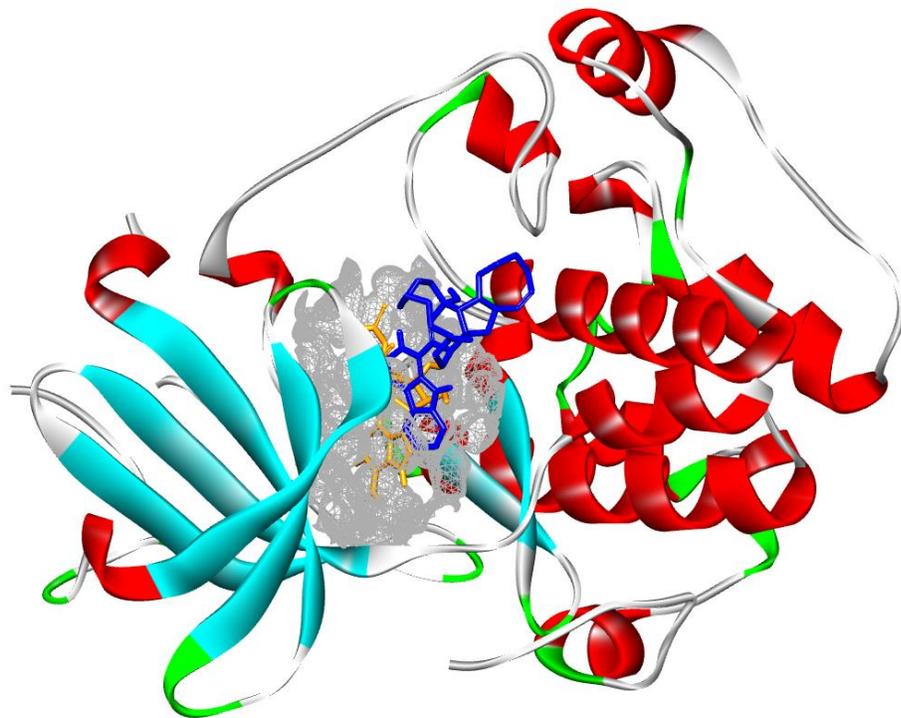


Figure S2: MZA (blue) and ATP (orange) is shown docked to serum and glucocorticoid-induced kinase (binding pocket is shown as gray mesh) (SGK) (PDB ID: 2R5T)

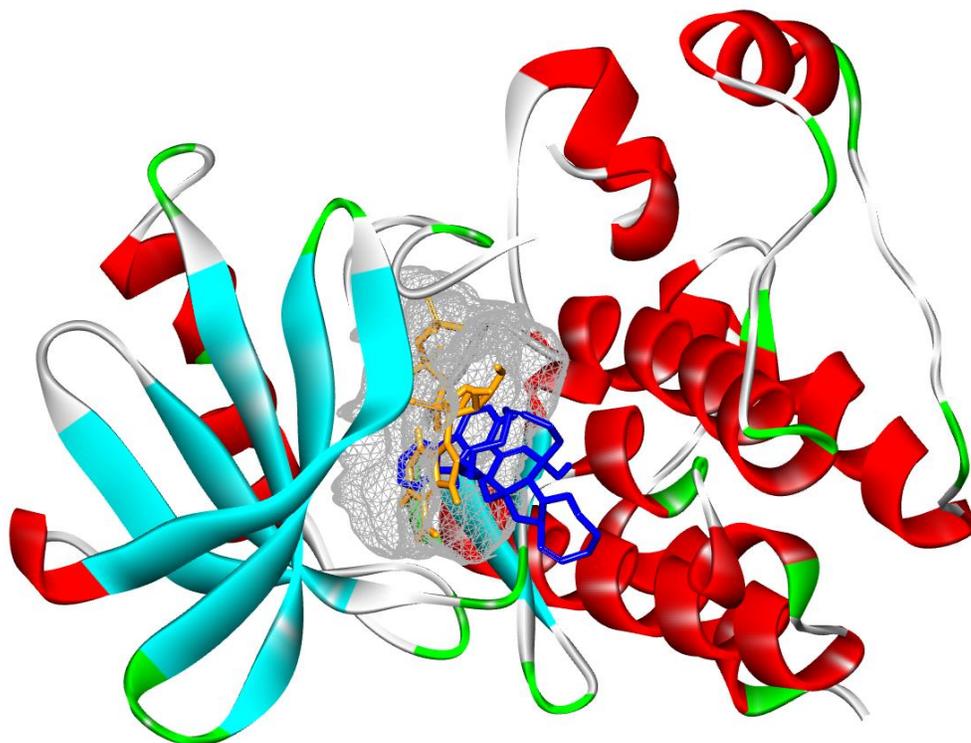


Figure S3: MZA (blue) and ATP (orange) is shown docked to lymphocyte kinase (binding pocket is shown as gray mesh) (LCK) (PDB ID: 3MPM)

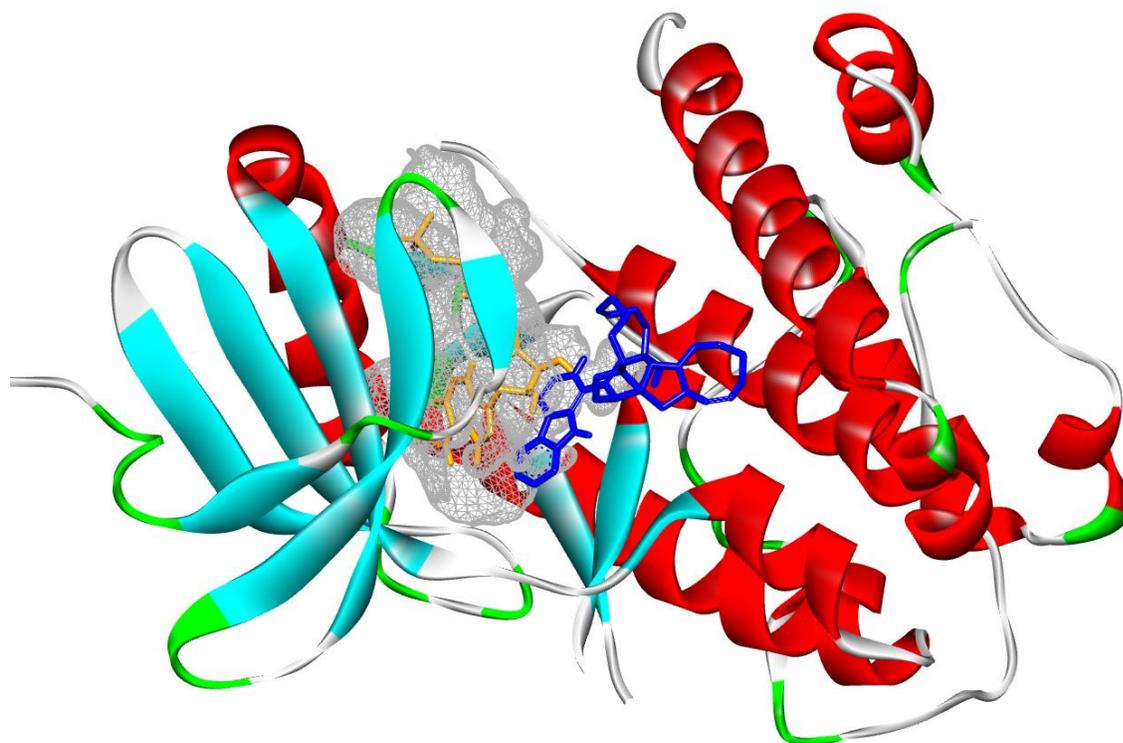


Figure S4: MZA (blue) and ATP (orange) is shown docked to mitogen and stress-activated protein kinase-1 (binding pocket is shown as gray mesh) (MSK1) (PDB ID: 3KN5)

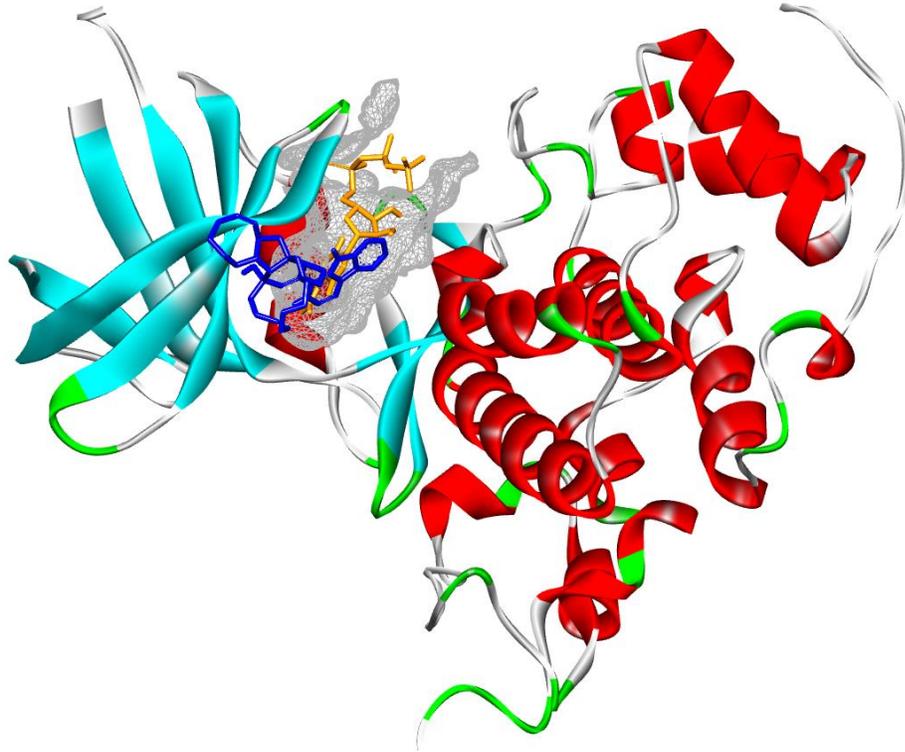


Figure S5: MZA (blue) and ATP (orange) is shown docked to glycogen synthase kinase-3 β (binding pocket is shown as gray mesh) (GSK3 β) (PDB ID: 1Q5K)

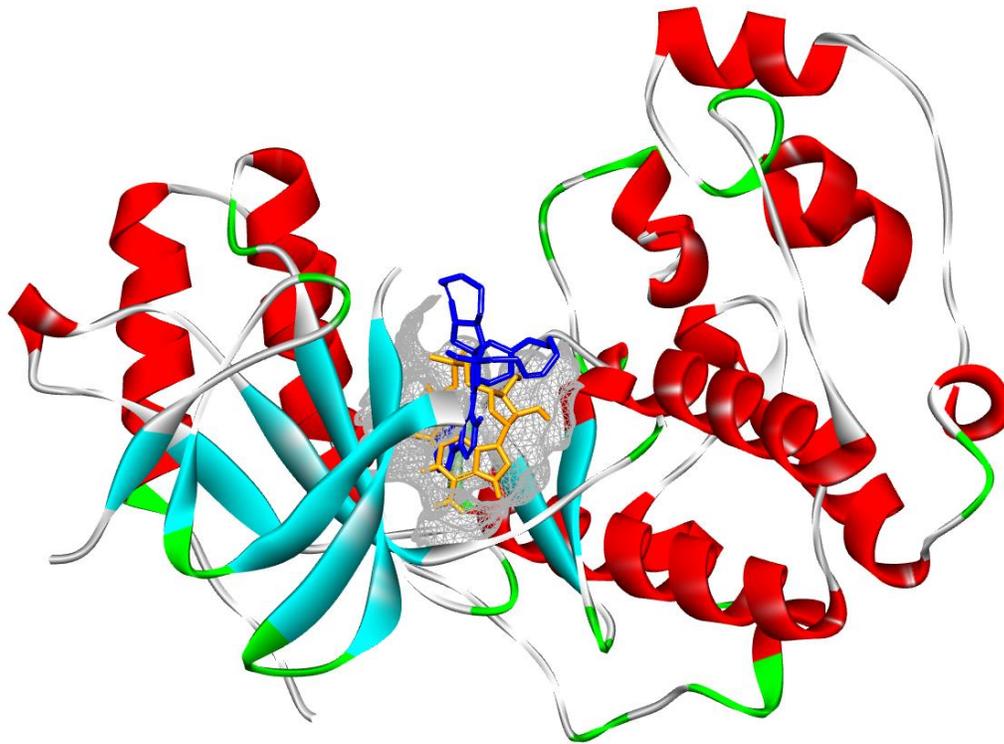


Figure S6: MZA (blue) and ATP (orange) is shown docked to stress-activated protein kinase-2 α (binding pocket is shown as gray mesh) (SAPK2 α /P38) (PDB ID: 5OMH)

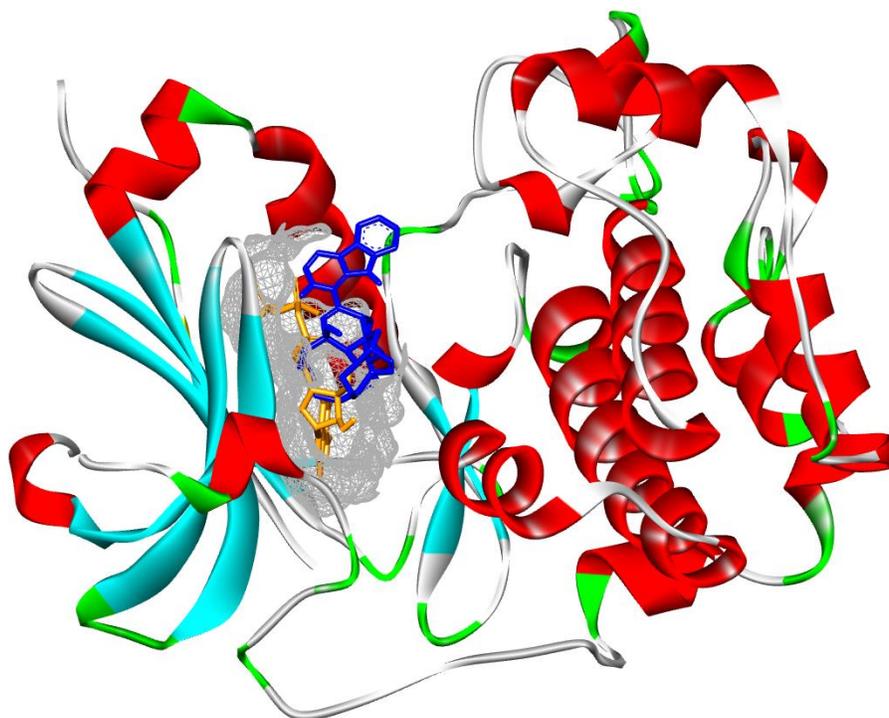


Figure S7: MZA (blue) and ATP (orange) is shown docked to protein kinase B (binding pocket is shown as gray mesh) (PKB α) (PDB ID: 3CQW)

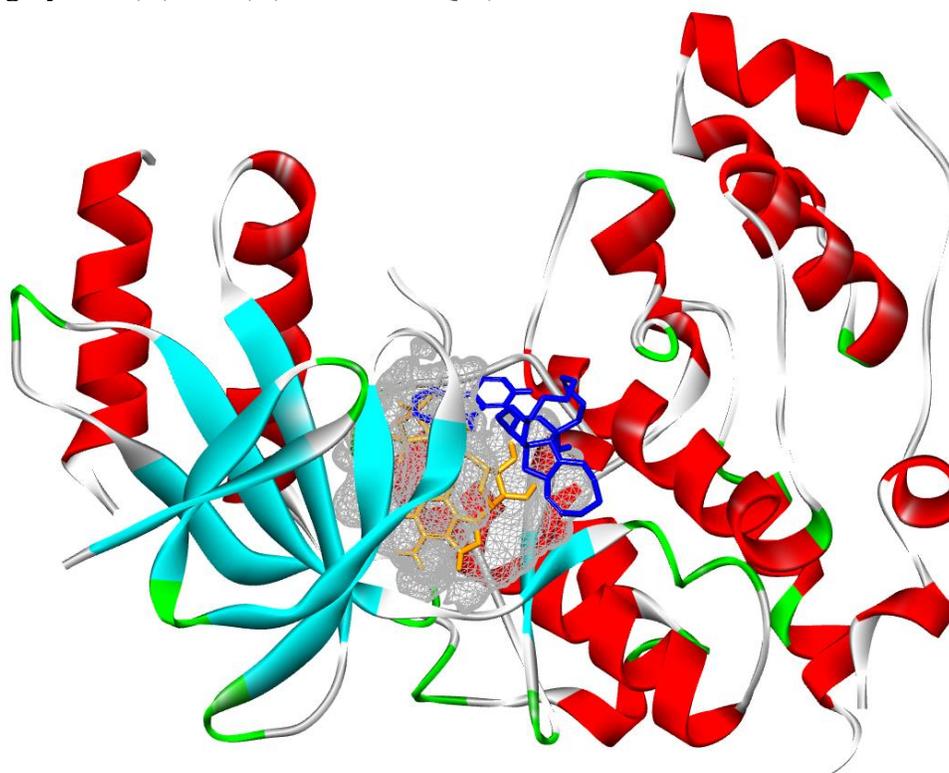


Figure S8: MZA (blue) and ATP (orange) is shown docked to c-Jun N-terminal kinase (binding pocket is shown as gray mesh) (JNK1 α 1) (PDB ID: 1UKI)

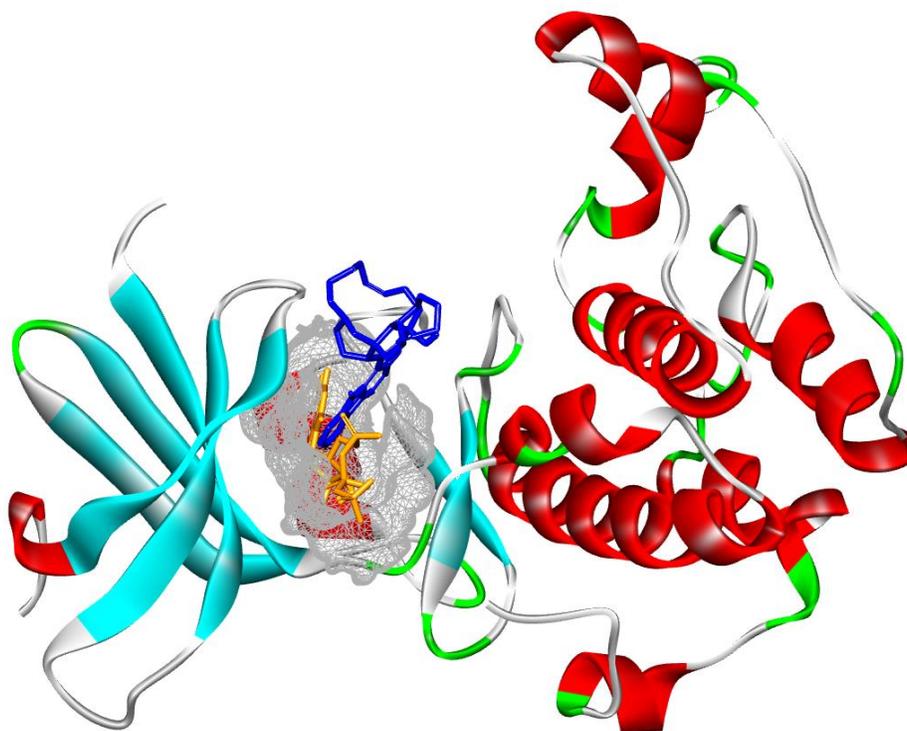


Figure S9: MZA (blue) and ATP (orange) is shown docked to p70 ribosomal protein S6 kinase (binding pocket is shown as gray mesh) (S6K1) (PDB ID: 3A60)

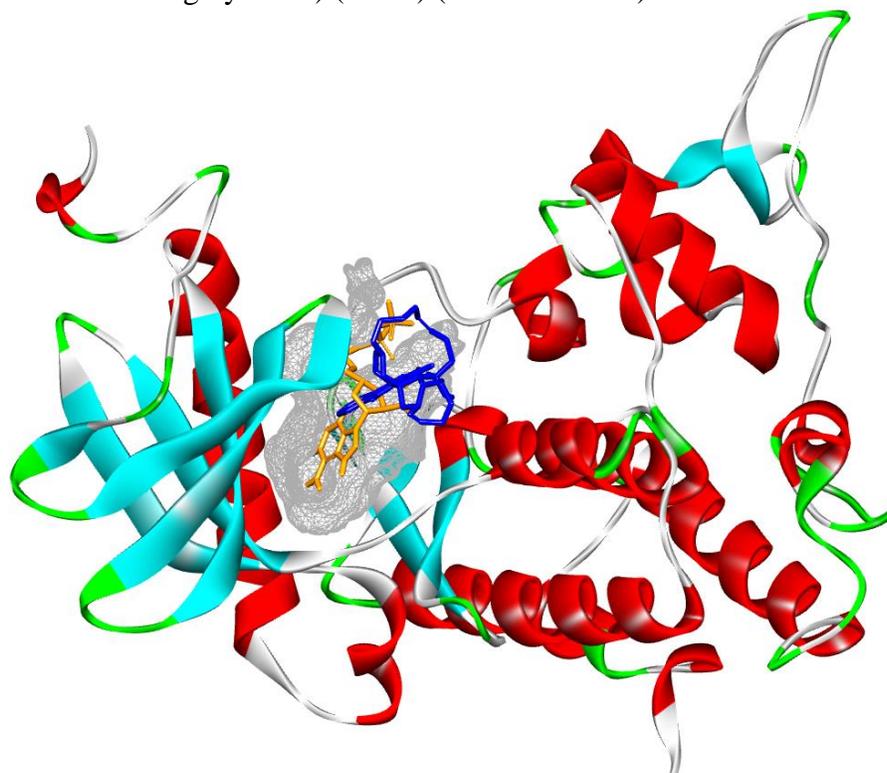


Figure S10: MZA (blue) and ATP (orange) is shown docked to dual tyrosine phosphorylated and regulated kinase 1A (binding pocket is shown as gray mesh) (DYRK1A) (PDB ID: 2VX3)

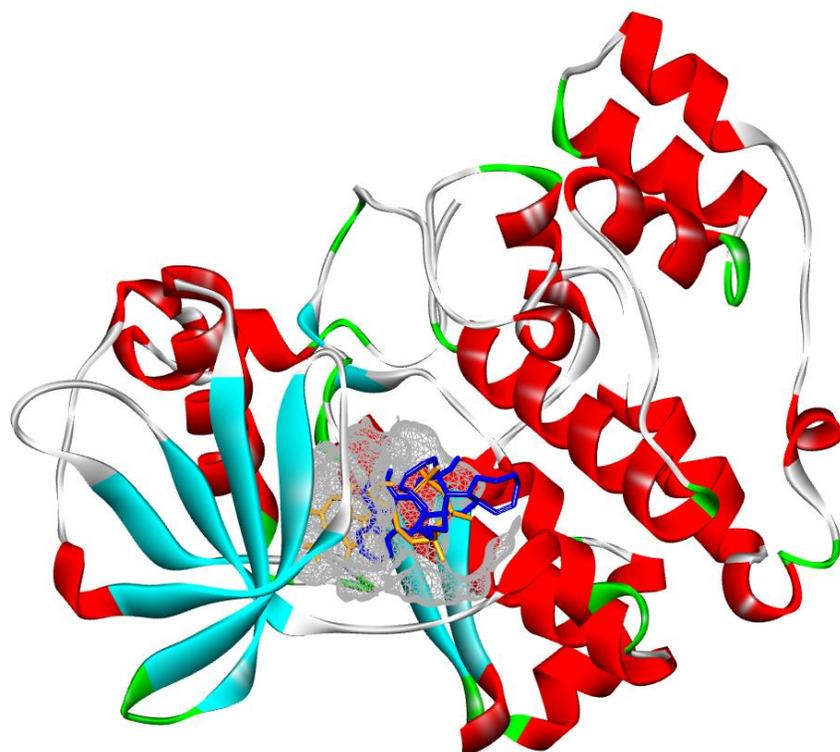


Figure S11: MZA (blue) and ATP (orange) is shown docked to casein kinase-2 (binding pocket is shown as gray mesh) (CK2) (PDB ID: 1J91)

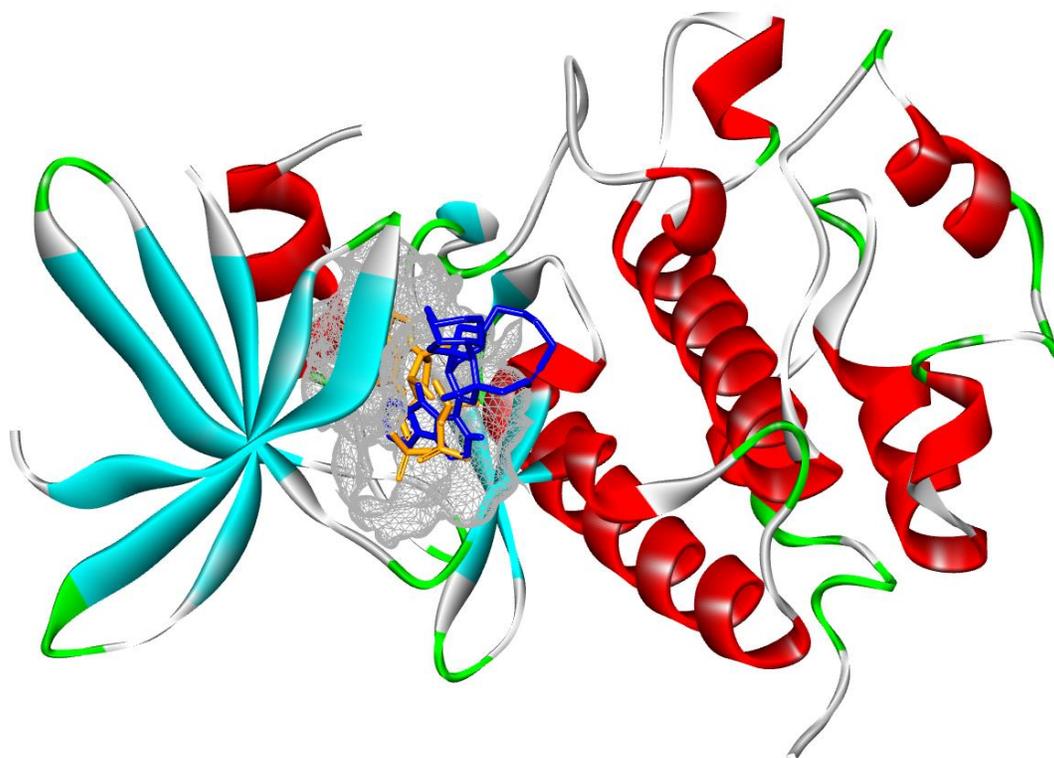


Figure S12: MZA (blue) and ATP (orange) is shown docked to checkpoint kinase-1 (binding pocket is shown as gray mesh) (CHK1) (PDB ID: 3U9N)

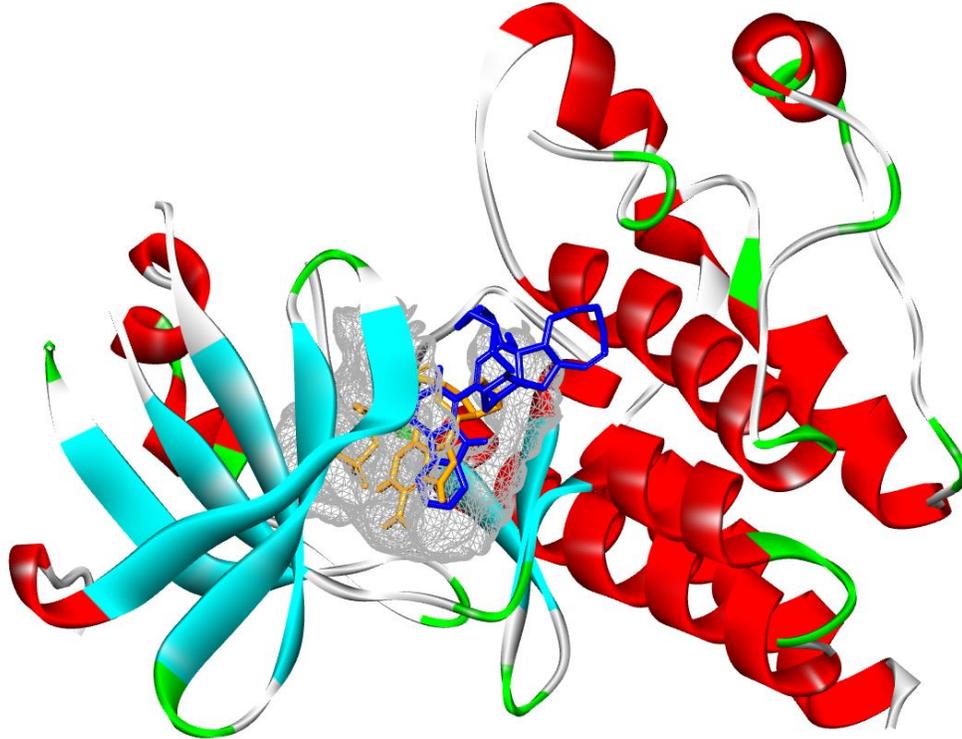


Figure S13: MZA (blue) and ATP (orange) is shown docked to C-terminal Src kinase (binding pocket is shown as gray mesh) (CSK) (PDB ID: 1BYG)

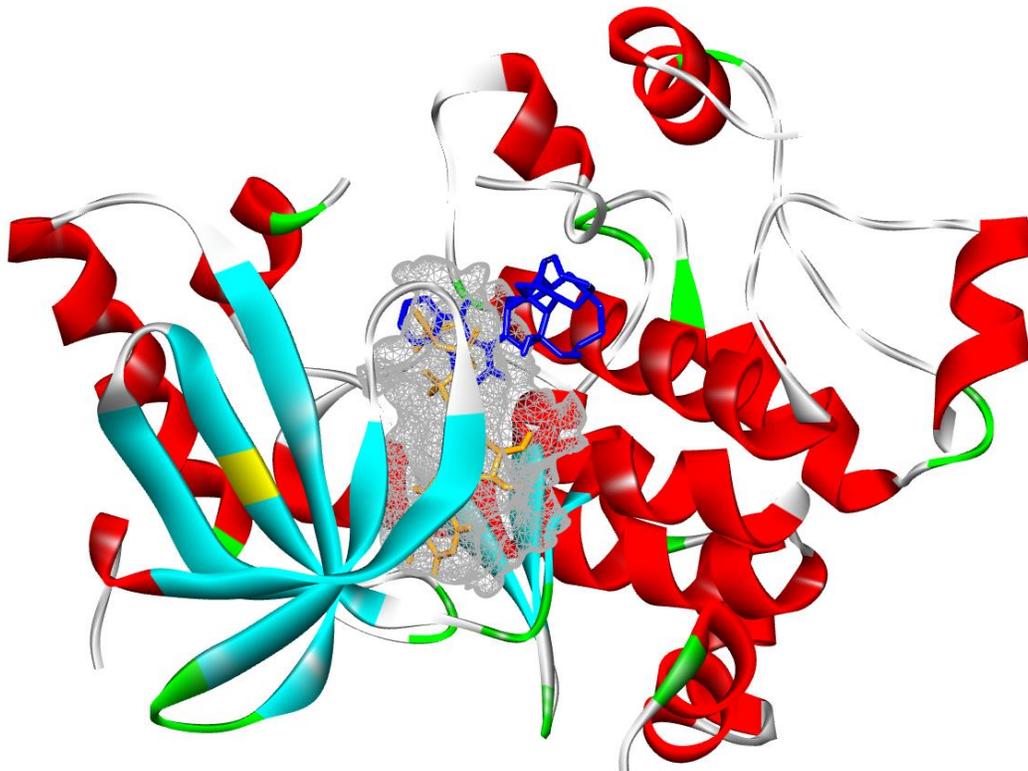


Figure S14: MZA (blue) and ATP (orange) is shown docked to MAPK kinase (mitogen-activated protein kinase) (binding pocket is shown as gray mesh) (MKK1) (PDB ID: 1S9J)

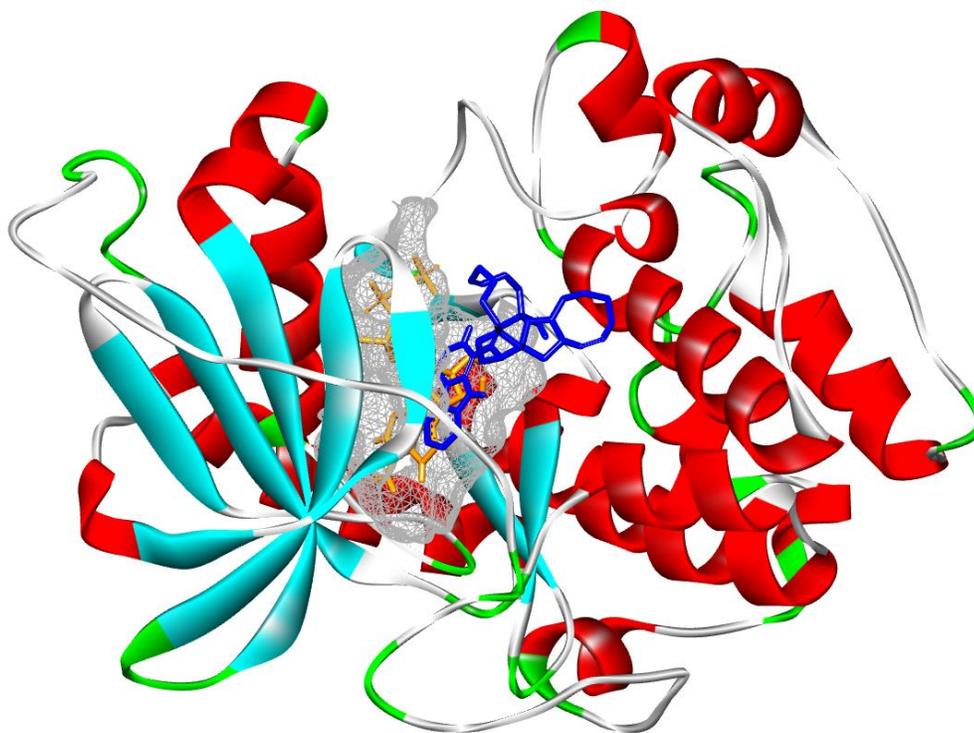


Figure S15: MZA (blue) and ATP (orange) is shown docked to cyclic AMP-dependent protein kinase (binding pocket is shown as gray mesh) (PKA) (PDB ID: 2JDS)

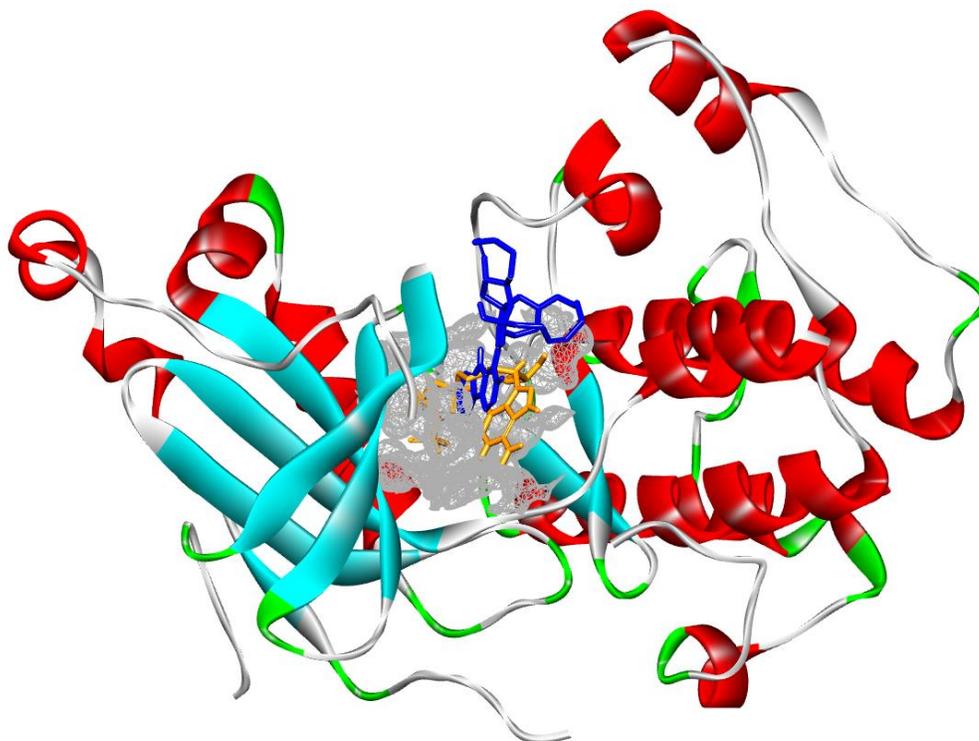


Figure S16: MZA (blue) and ATP (orange) is shown docked to protein kinase C (binding pocket is shown as gray mesh) (PKC α) (PDB ID: 3IW4)

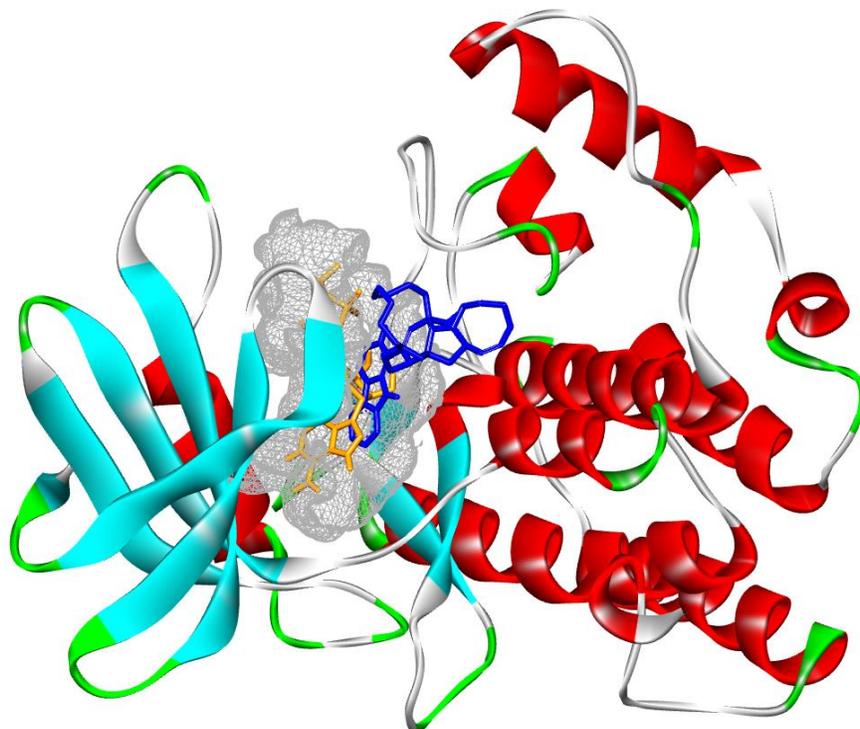


Figure S17: MZA (blue) and ATP (orange) is shown docked to casein kinase-1 (binding pocket is shown as gray mesh) (CK1) (PDB ID: 1CSN)

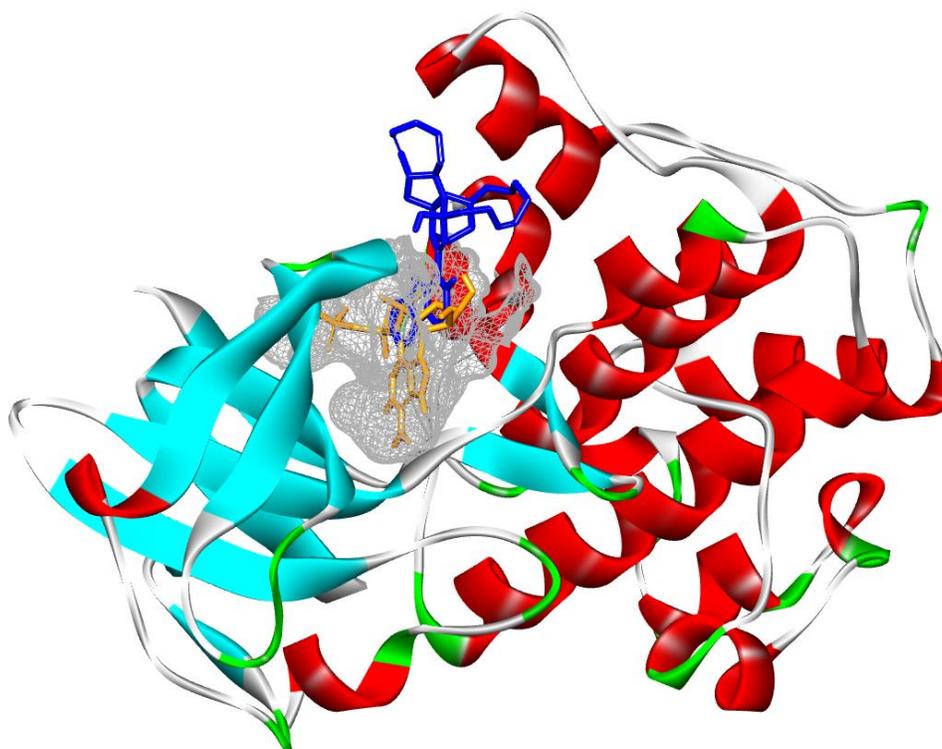


Figure S18: MZA (blue) and ATP (orange) is shown docked to MAPK-activated protein kinase-2 (binding pocket is shown as gray mesh) (MAPKAP-K2 (RSK-2)) (PDB ID: 3G51)

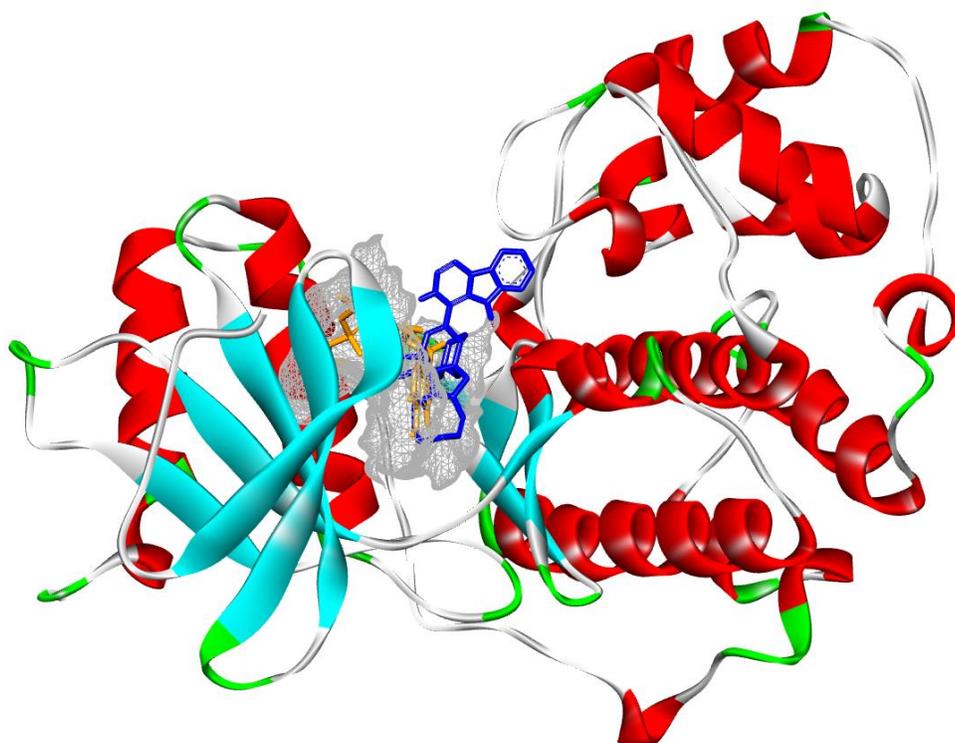


Figure S19: MZA (blue) and ATP (orange) is shown docked to mitogen-activated protein kinase (binding pocket is shown as gray mesh) (MAPK2/ERK2) (PDB ID: 2OJJ)

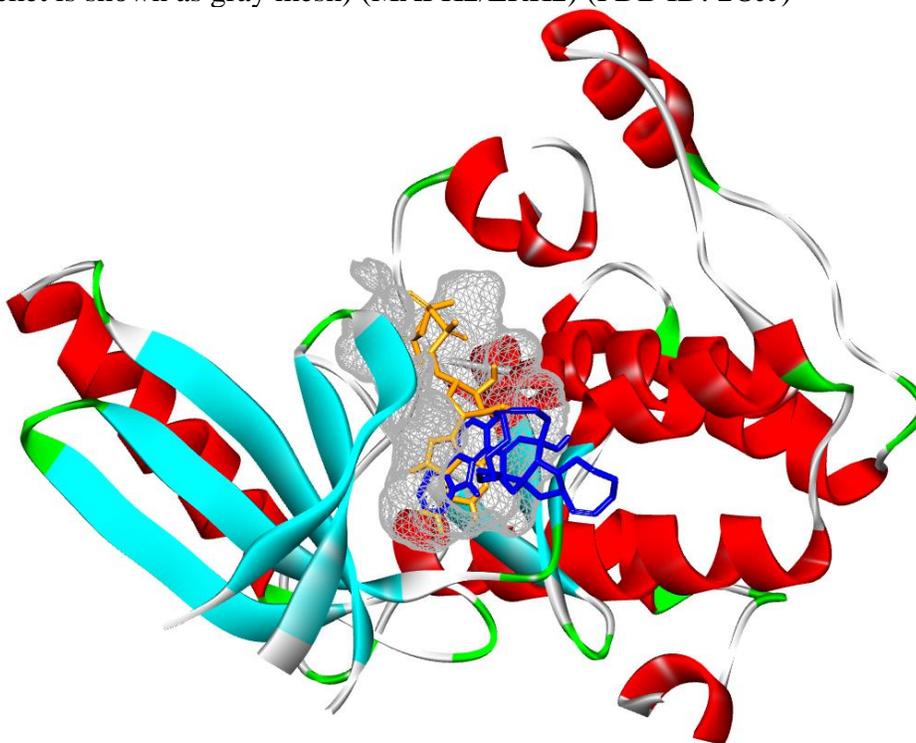


Figure S20: MZA (blue) and ATP (orange) is shown docked to NIMA-related protein kinase 2α (binding pocket is shown as gray mesh) (NEK2α) (PDB ID: 5M53)

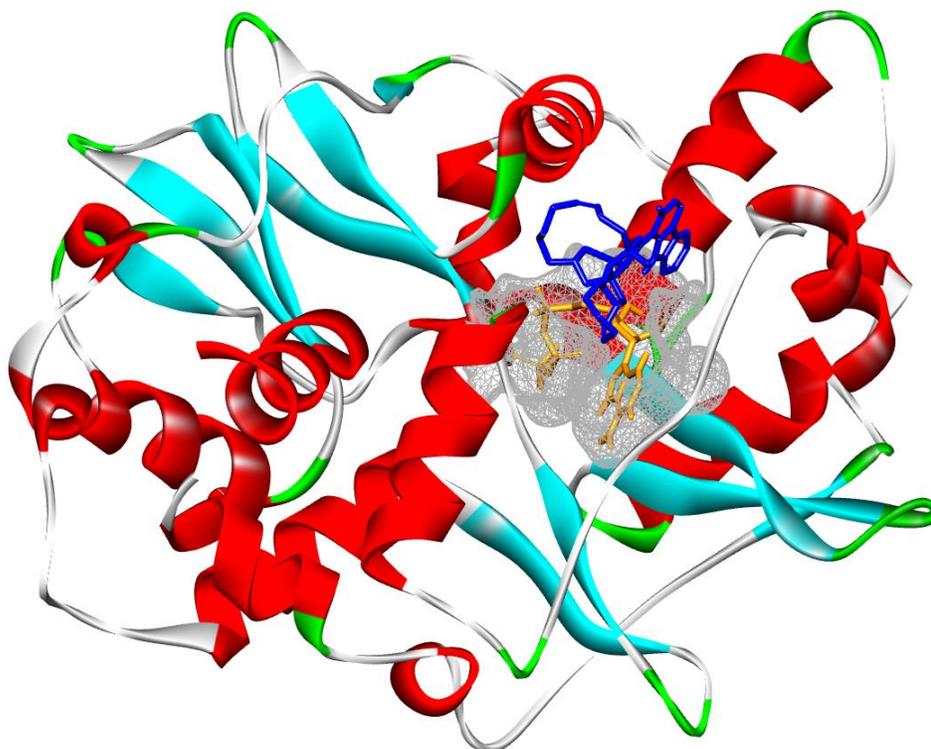


Figure S21: MZA (blue) and ATP (orange) is shown docked to AMP-activated protein kinase (binding pocket is shown as gray mesh) (AMPK) (PDB ID: 2YA3)

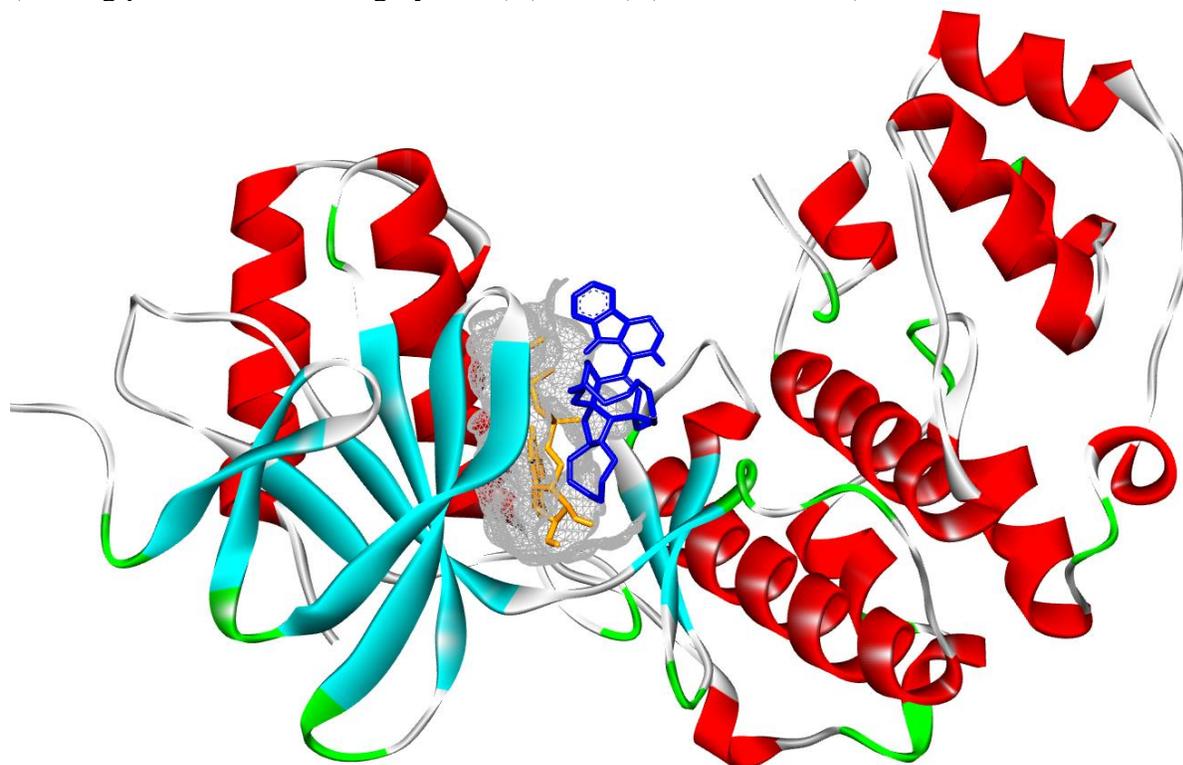


Figure S22: MZA (blue) and ATP (orange) is shown docked to stress-activated protein kinase-4 (binding pocket is shown as gray mesh) (SAPK4/P38δ) (PDB ID: 5ekn)

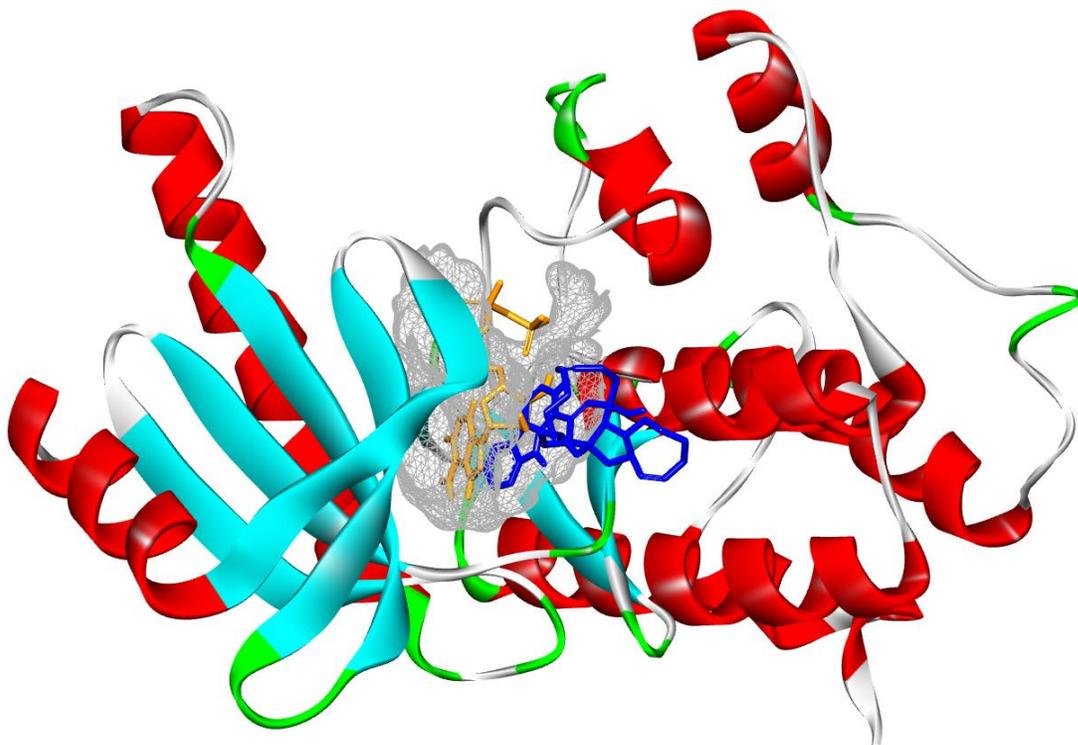


Figure S23: MZA (blue) and ATP (orange) is shown docked to phosphorylase kinase (binding pocket is shown as gray mesh) (PHK) (PDB ID: 2Y7J)



Figure S24: MZA (blue) and ATP (orange) is shown docked to stress-activated protein kinase-3 (binding pocket is shown as gray mesh) (SAPK3/P38 γ) (PDB ID: 1CM8)

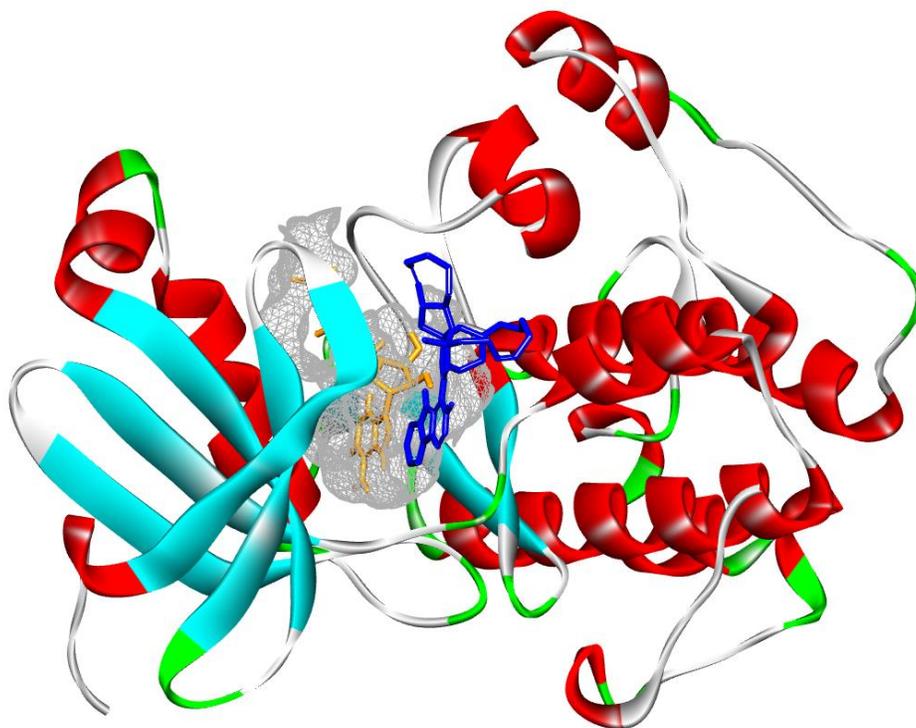


Figure S25: MZA (blue) and ATP (orange) is shown docked to 3-phosphoinositide-dependent protein kinase-1 (binding pocket is shown as gray mesh) (PDK1) (PDB ID: 5LVL)

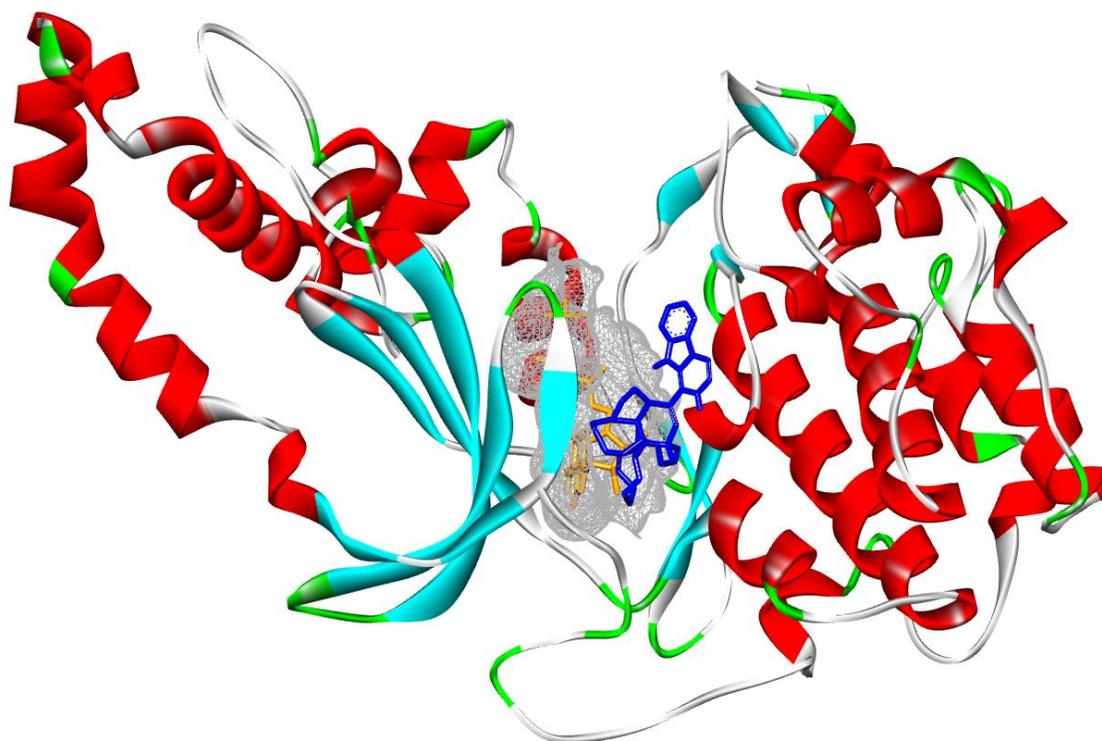


Figure S26: MZA (blue) and ATP (orange) is shown docked to Rho-dependent protein kinase (binding pocket is shown as gray mesh) (ROCK-II) (PDB ID: 6ED6)

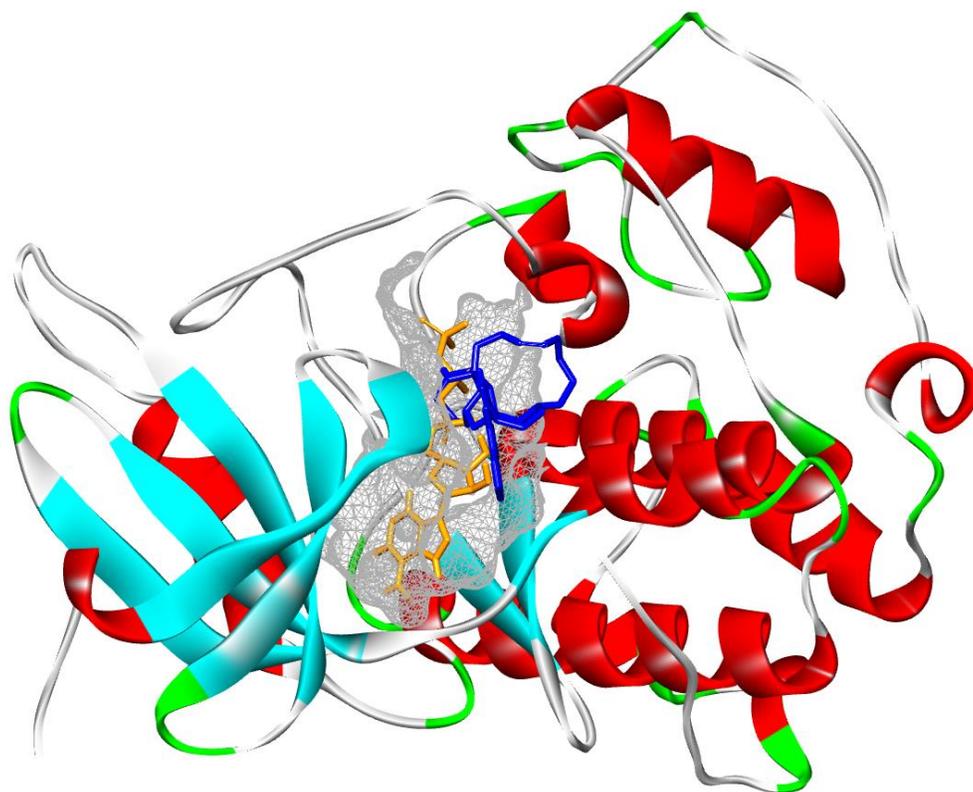


Figure S27: MZA (blue) and ATP (orange) is shown docked to cyclin-dependent kinase 2-cyclin A complex (binding pocket is shown as gray mesh) (CDK2/cyclin A) (PDB ID: 4EZ7)

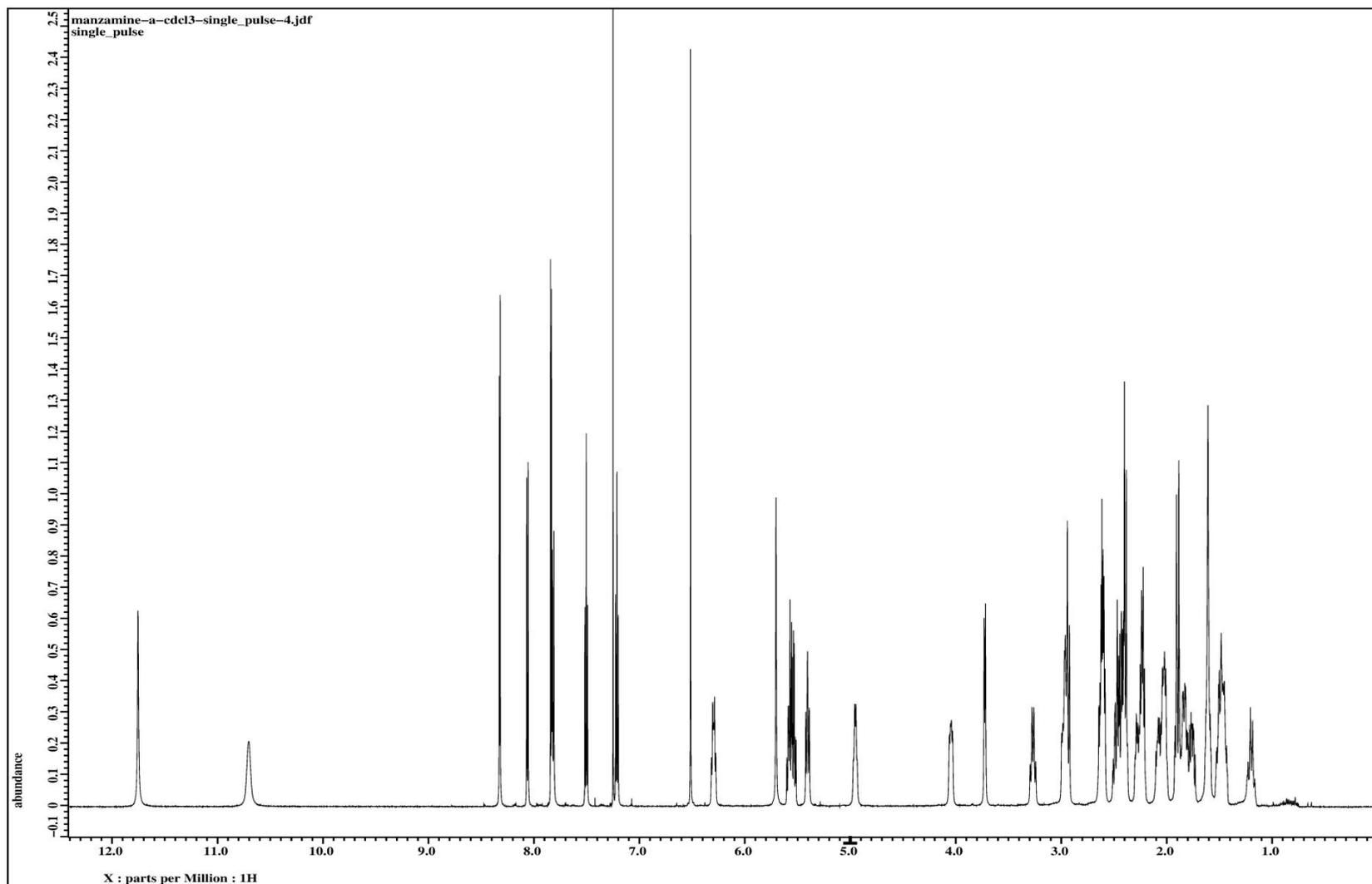


Figure S28. ^1H NMR of Manzamine A (CDCl_3 , 600 MHz)

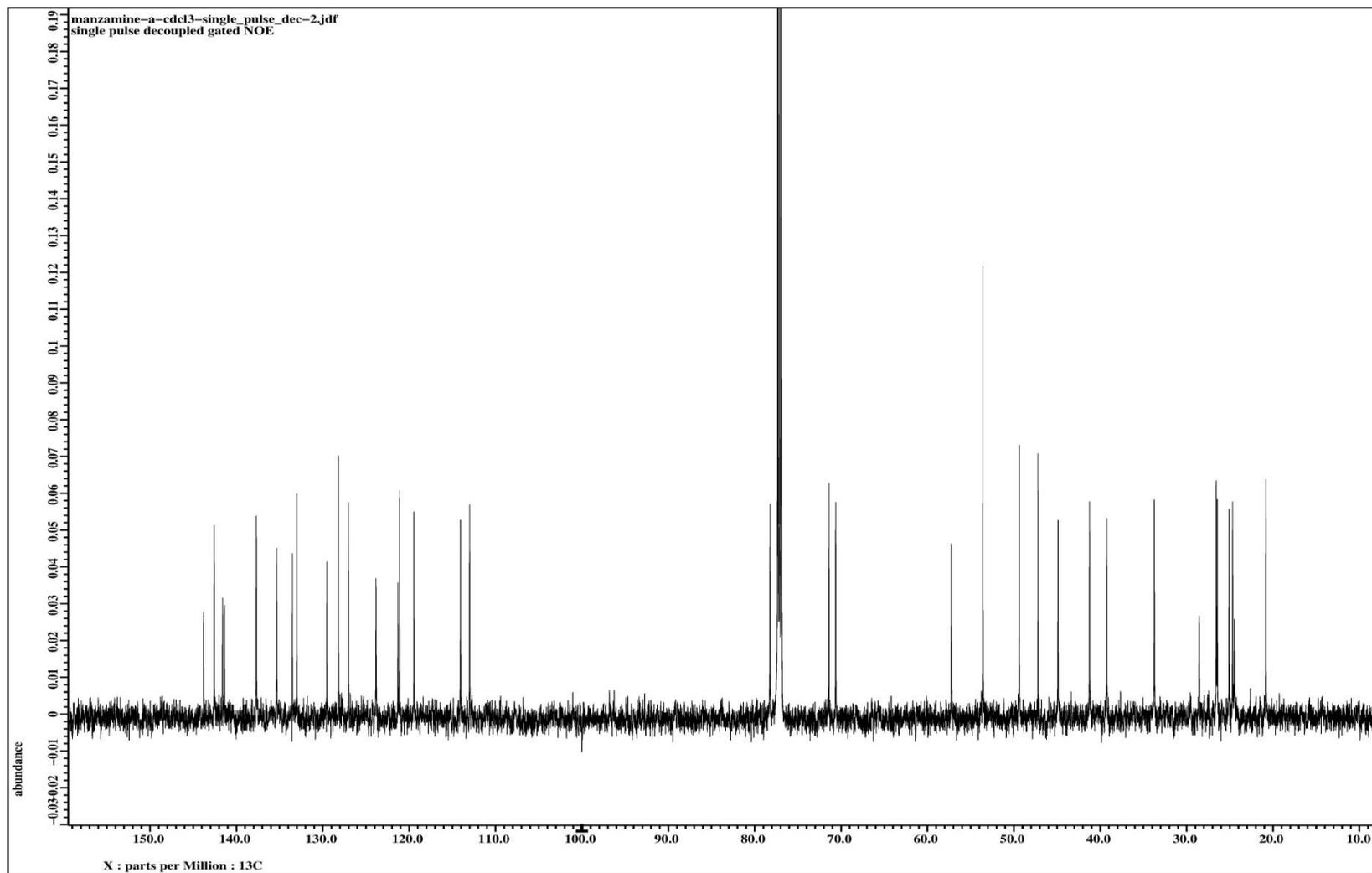


Figure S29. ^{13}C NMR of Manzamine A (CDCl_3 , 150 MHz)

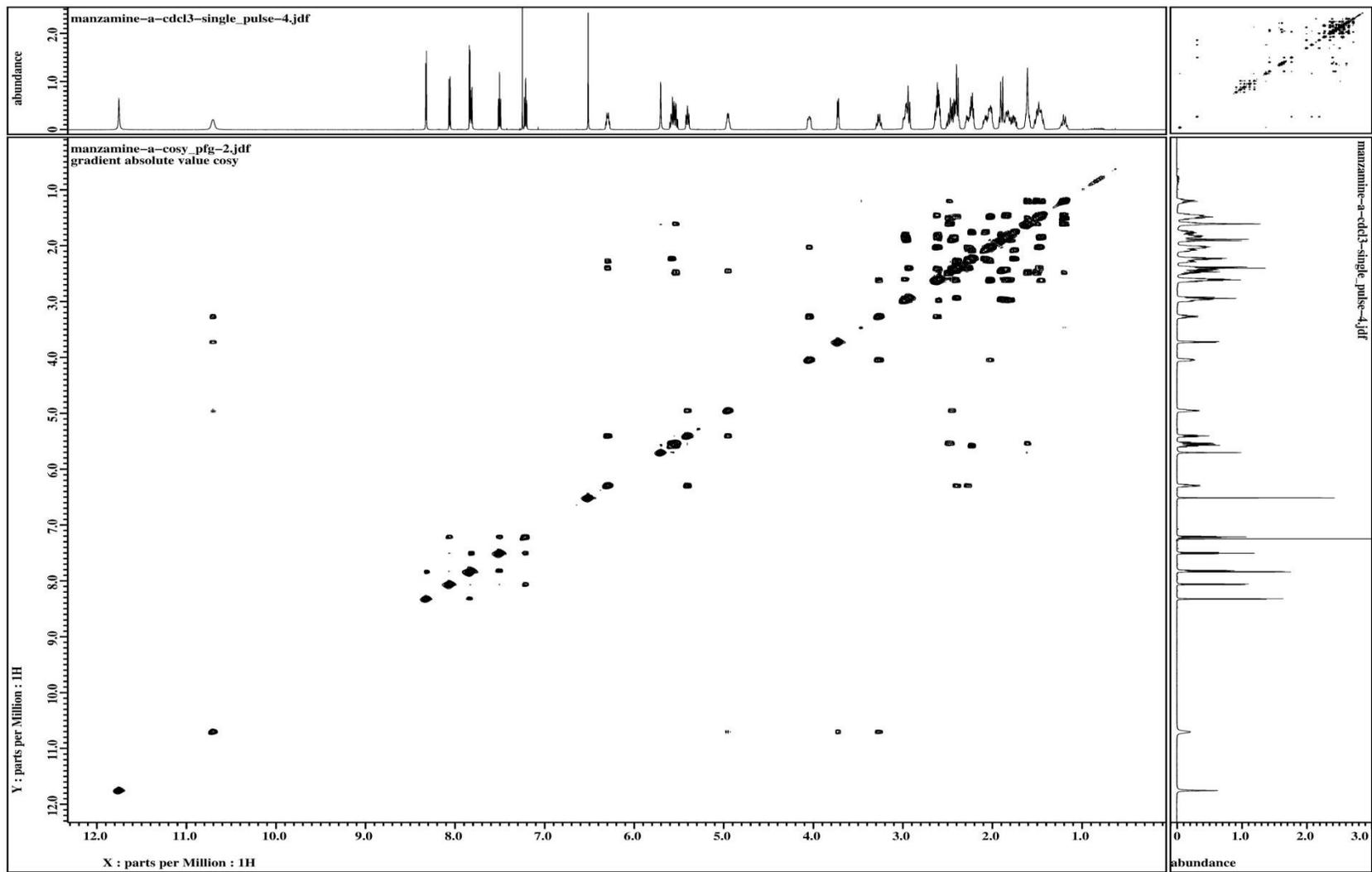


Figure S30. 2D-COSY Spectrum Manzamine A (CDCL₃, 600 MHz)

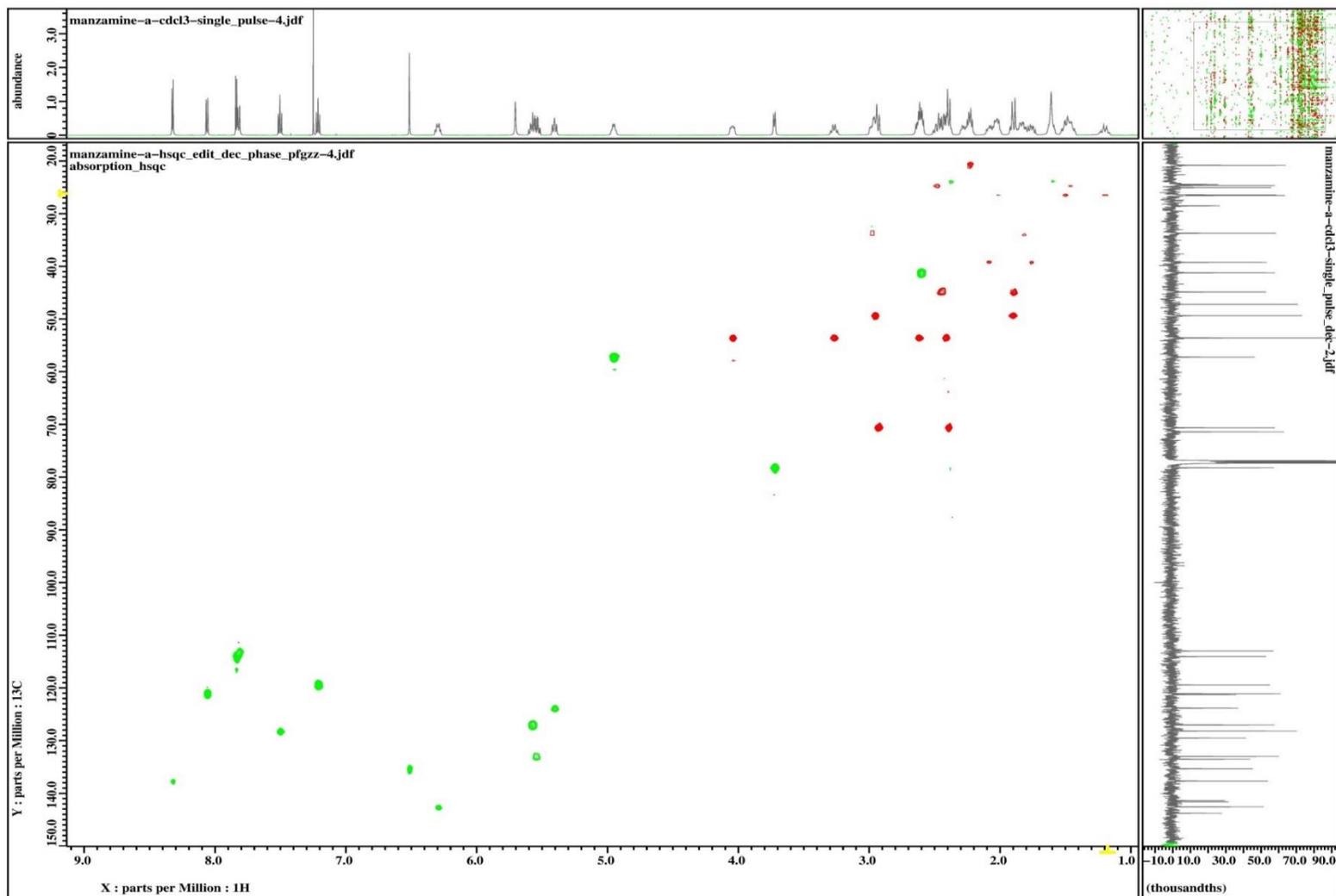


Figure S31. 2D edited g-HSQC Spectrum of Manzamine A (CDCL₃, 600 MHz)