

Supplementary Material:

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1. The copies of ^1H NMR and ^{13}C NMR spectra for compounds 2a-c

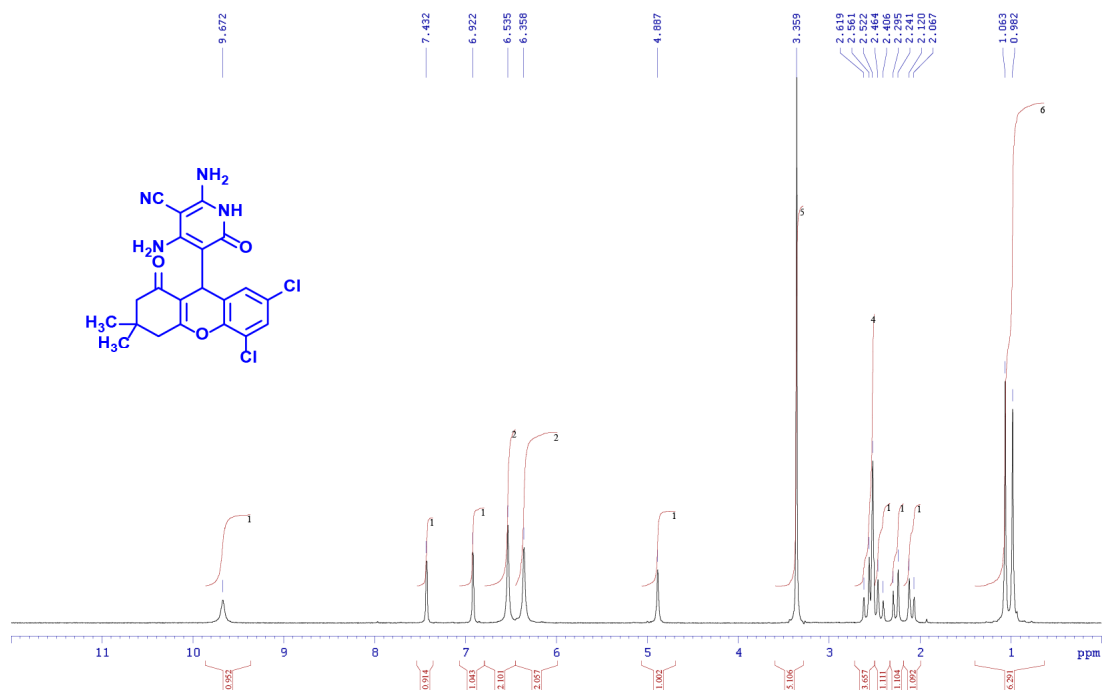


Figure S1. ^1H NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in DMSO- d_6 .

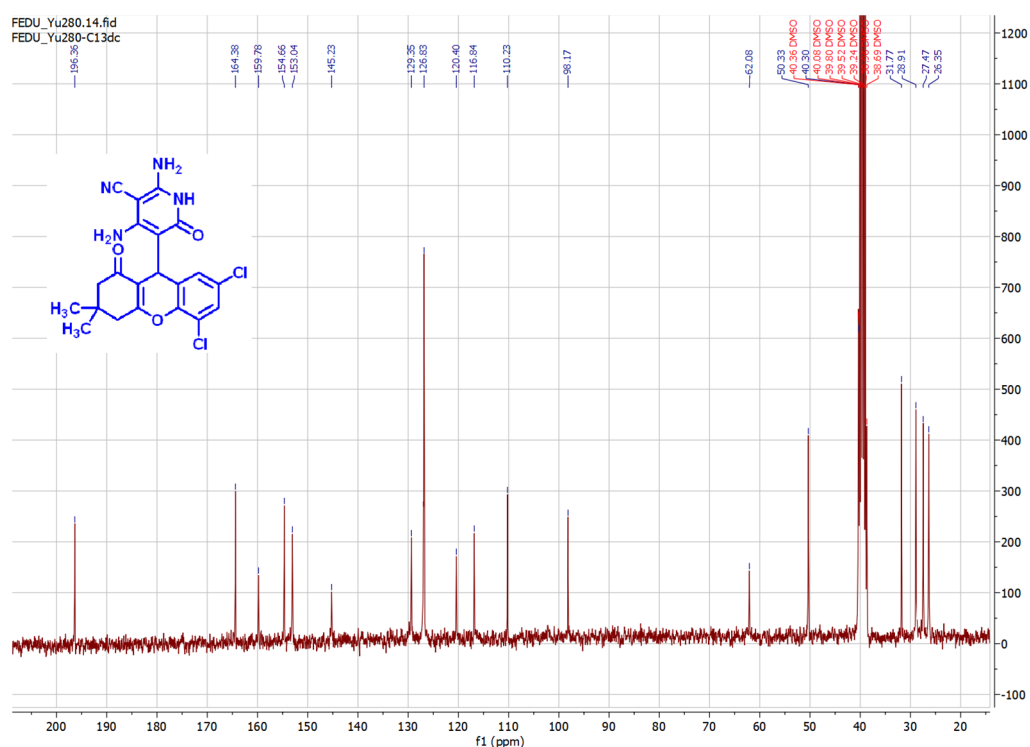


Figure S2. ^{13}C NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in DMSO- d_6 .

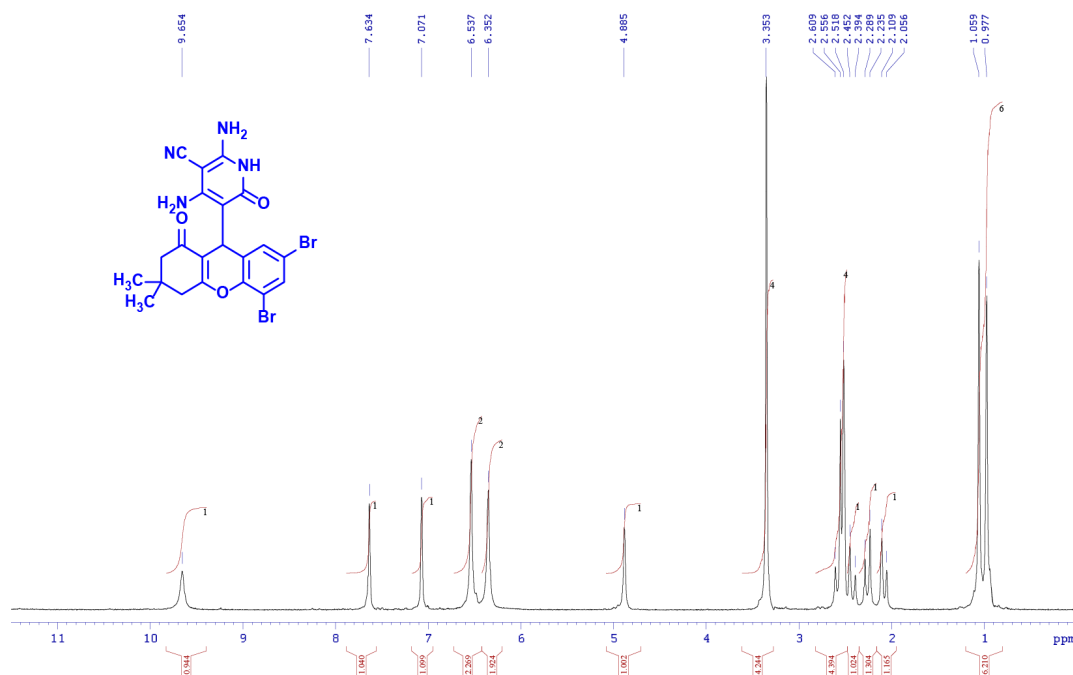


Figure S3. ¹H NMR spectrum of 2,4-diamino-5-(5,7-dibromo-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2b** in DMSO-*d*₆.

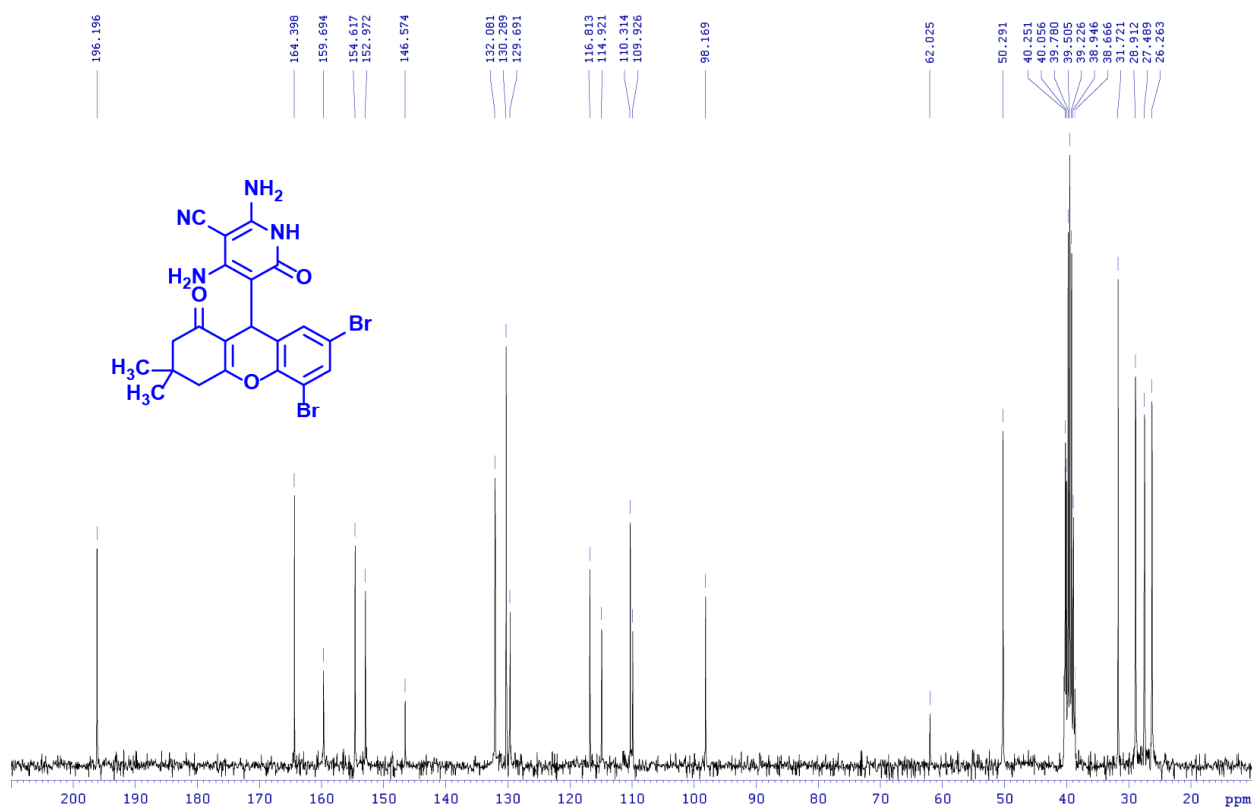


Figure S4. ¹³C NMR spectrum of 2,4-diamino-5-(5,7-dibromo-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2b** in DMSO-*d*₆.

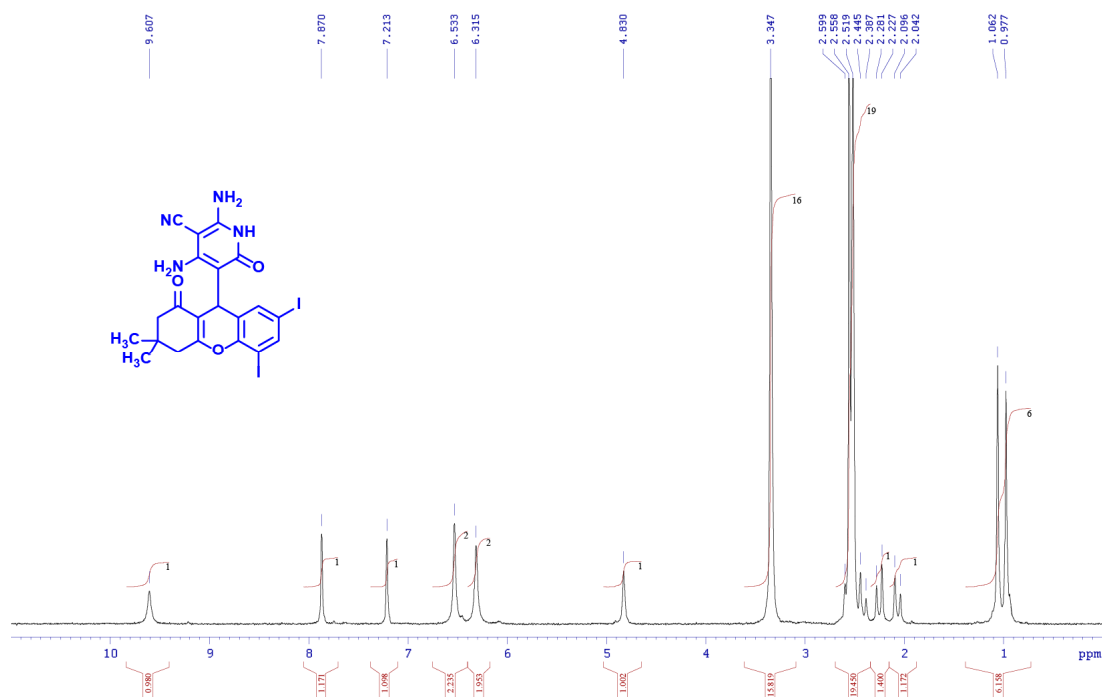


Figure S5. ^1H NMR spectrum of 2,4-diamino-5-(5,7-diiodo-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1H-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2c** in $\text{DMSO}-d_6$.

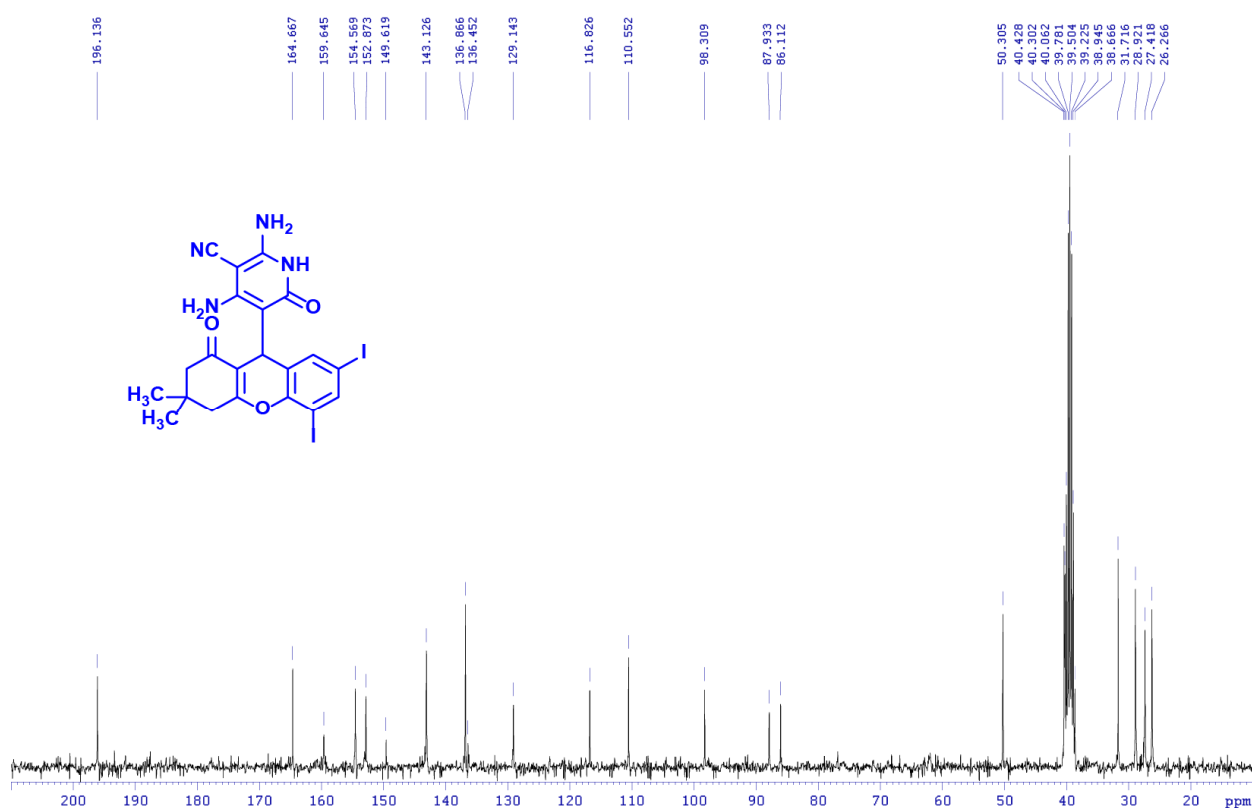


Figure S6. ^{13}C NMR spectrum of 2,4-diamino-5-(5,7-diiodo-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1H-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2c** in $\text{DMSO}-d_6$.

2. The copies of ^1H NMR and ^{13}C NMR spectra for compounds 3a-c

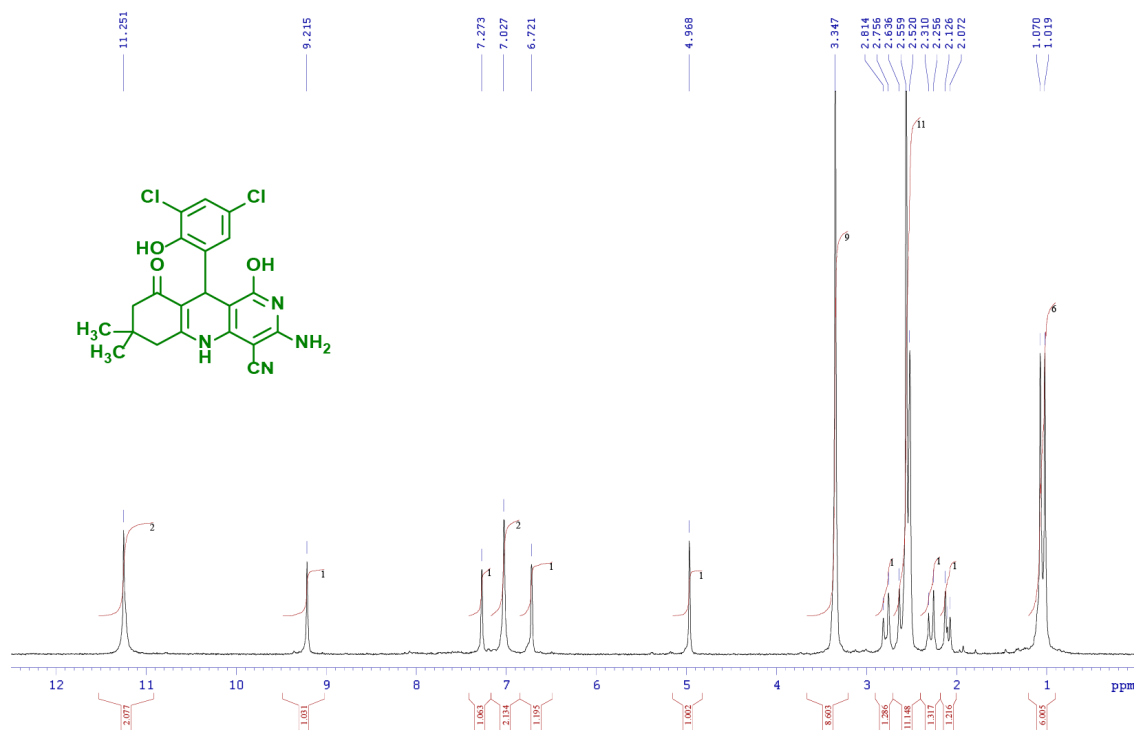


Figure S7. ^1H NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in DMSO- d_6 .

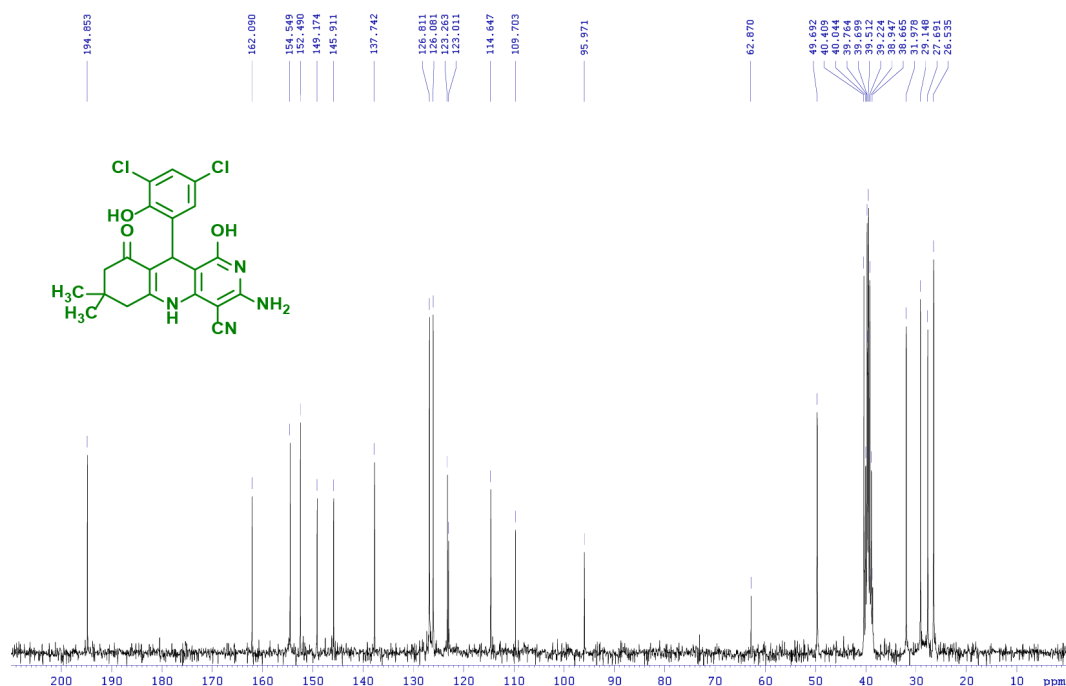


Figure S8. ^{13}C NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in DMSO- d_6 .

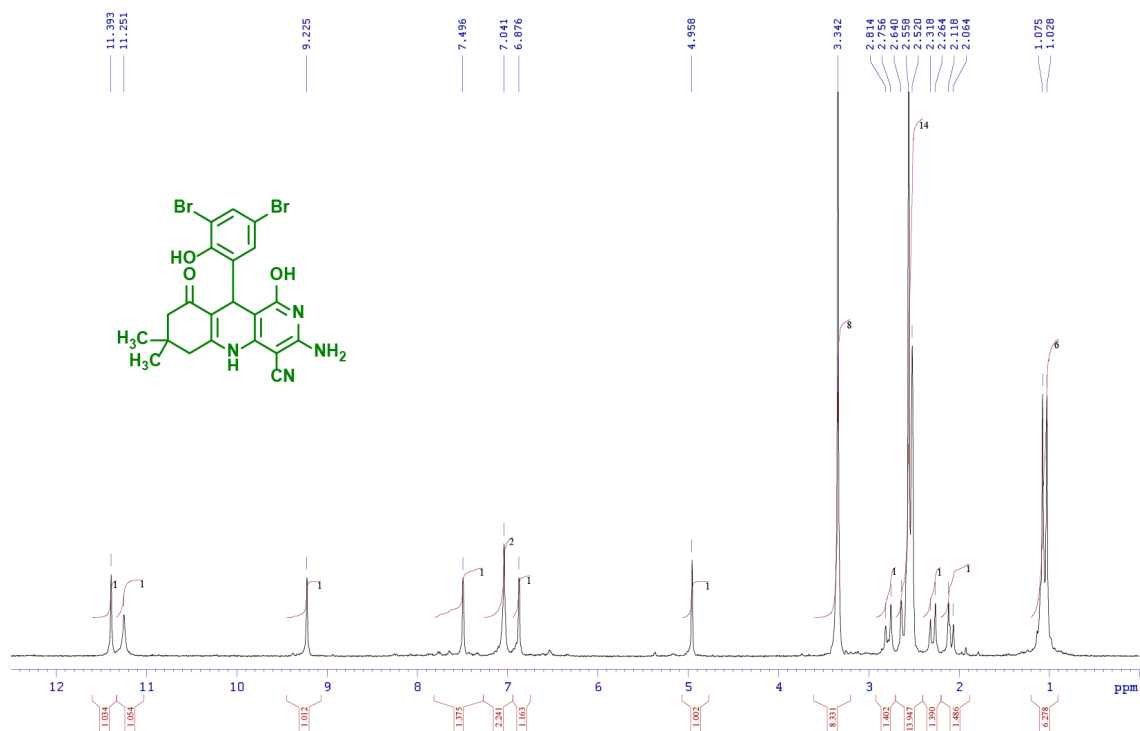


Figure S9. ^1H NMR spectrum of 3-amino-10-(3,5-dibromo-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3b** in $\text{DMSO-}d_6$.

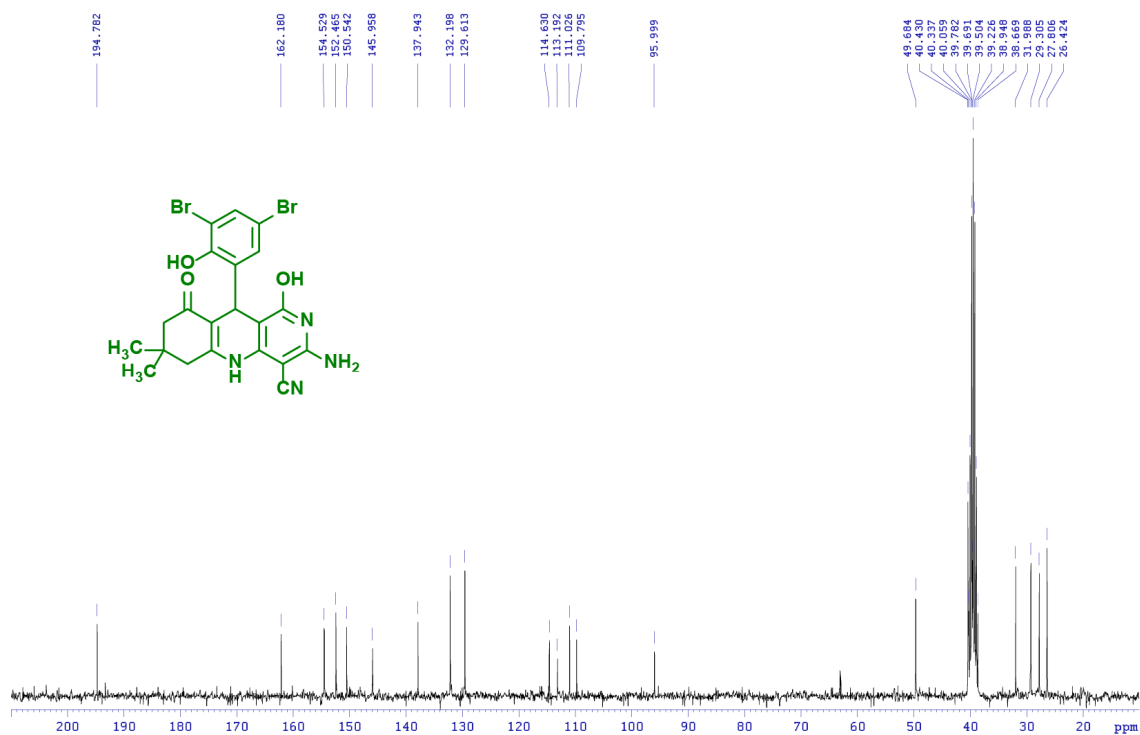


Figure S10. ^{13}C NMR spectrum of 3-amino-10-(3,5-dibromo-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3b** in $\text{DMSO-}d_6$.

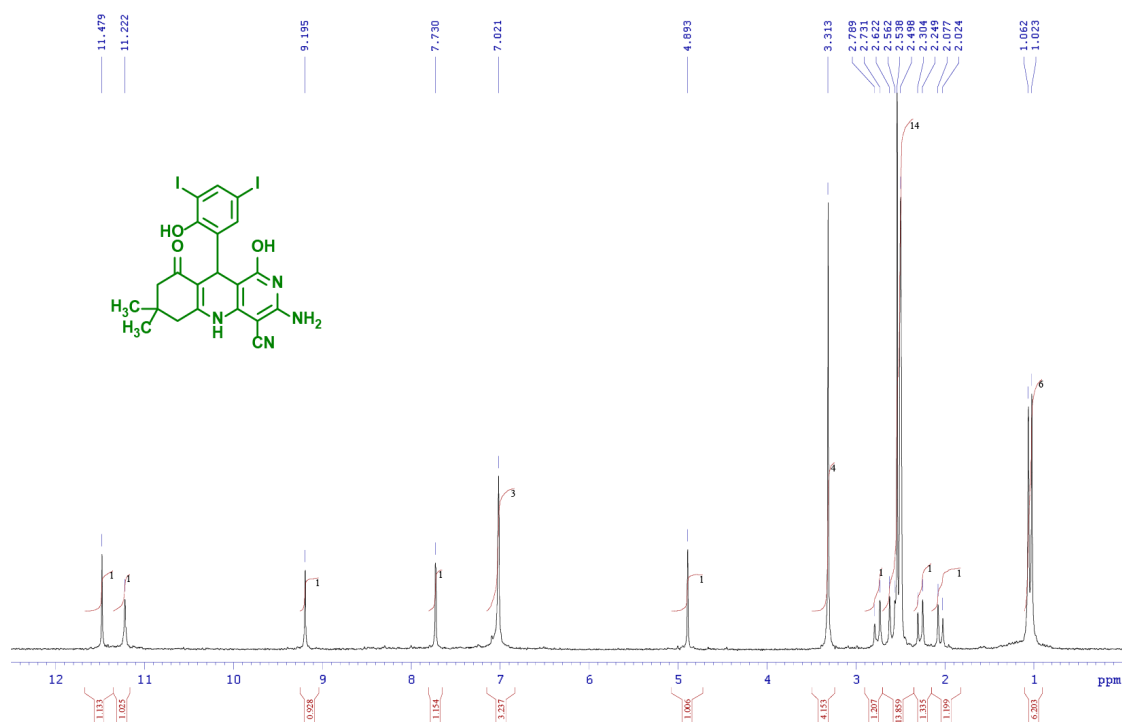


Figure S11. ¹H NMR spectrum of 3-amino-1-hydroxy-10-(2-hydroxy-3,5-diiodophenyl)-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3c** in DMSO-*d*₆.

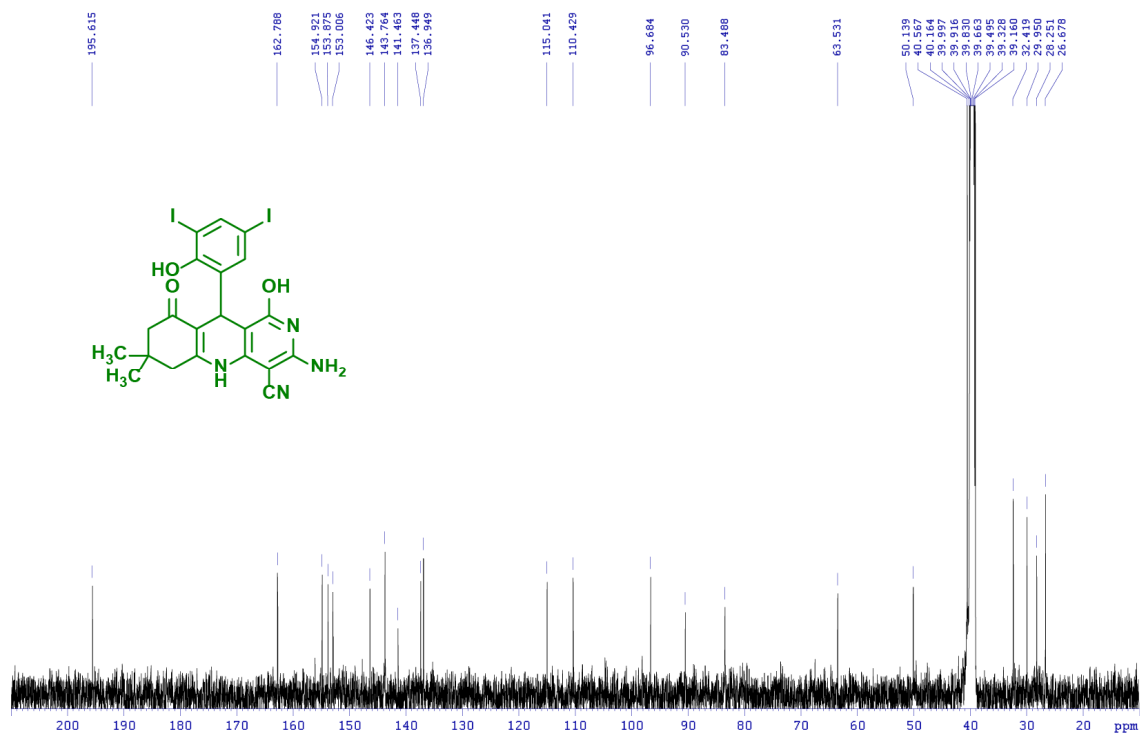


Figure S12. ¹³C NMR spectrum of 3-amino-1-hydroxy-10-(2-hydroxy-3,5-diiodophenyl)-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3c** in DMSO-*d*₆.

3. ^{15}N and 2D NMR spectra for compound **2a**

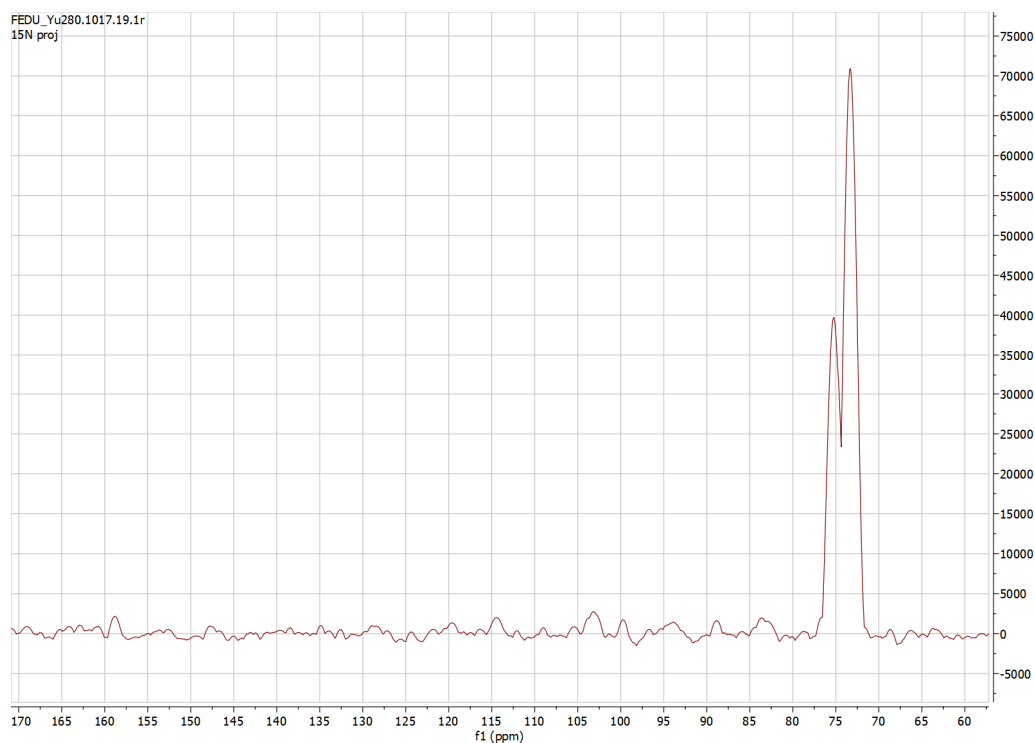


Figure S13. ^{15}N NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in $\text{DMSO-}d_6$.

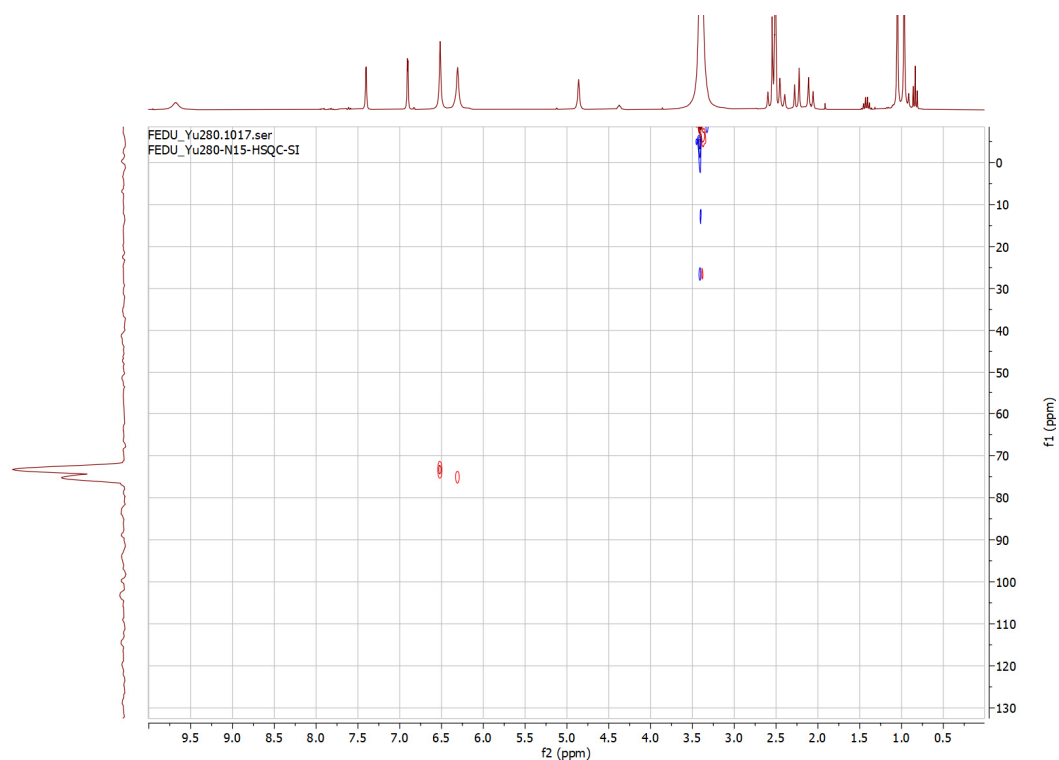


Figure S14. ^1H - ^{15}N HSQC NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in $\text{DMSO-}d_6$.

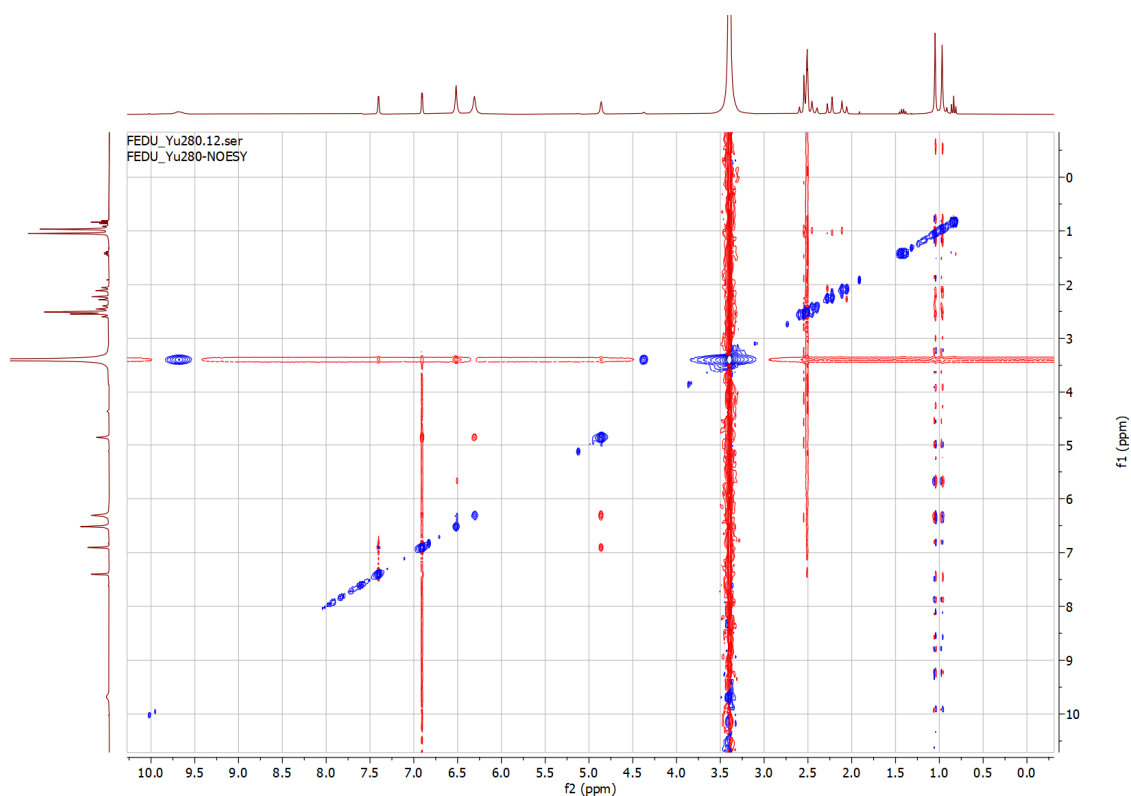


Figure S15. ^1H - ^1H NOESY NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in $\text{DMSO-}d_6$.

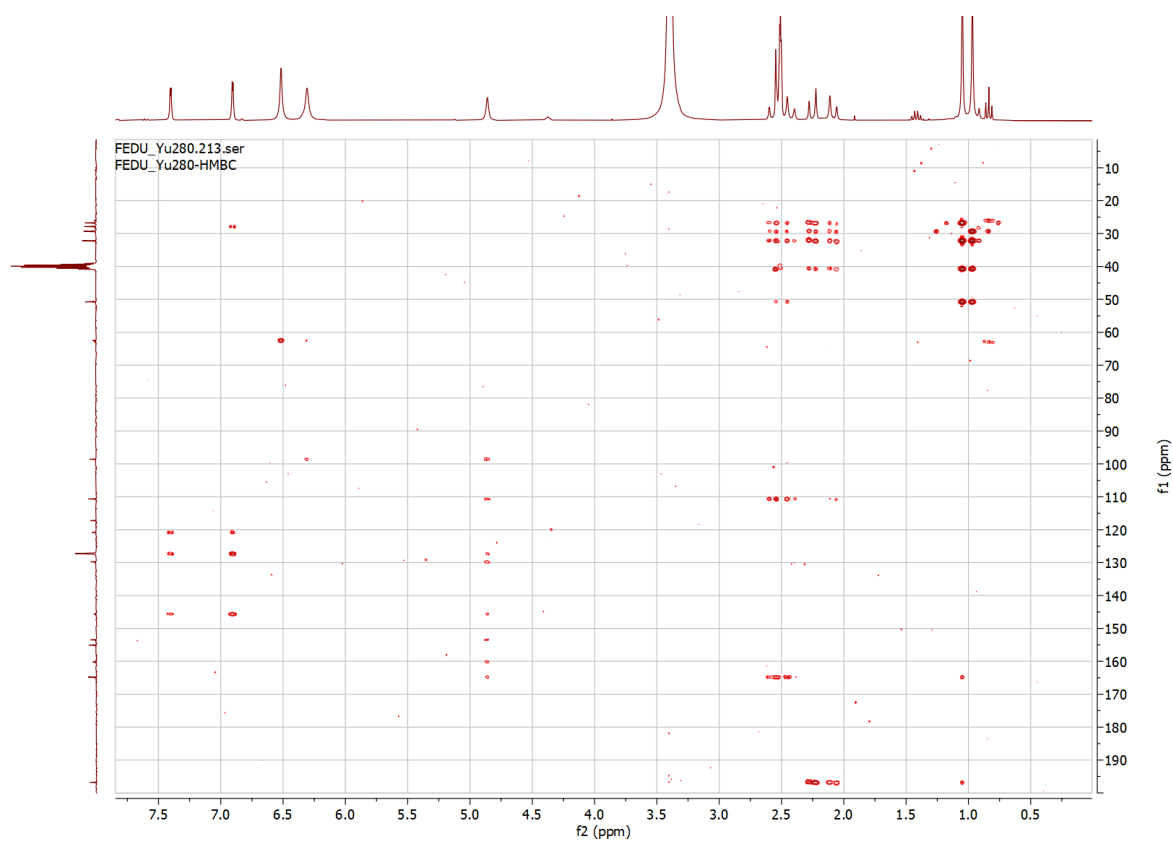


Figure S16. ^1H - ^{13}C HMBC NMR spectrum of 2,4-diamino-5-(5,7-dichloro-3,3-dimethyl-1-oxo-2,3,4,9-tetrahydro-1*H*-xanthen-9-yl)-6-oxo-1,6-dihydropyridine-3-carbonitrile **2a** in $\text{DMSO-}d_6$.

4. ^{15}N and 2D NMR spectra for compound **3a**

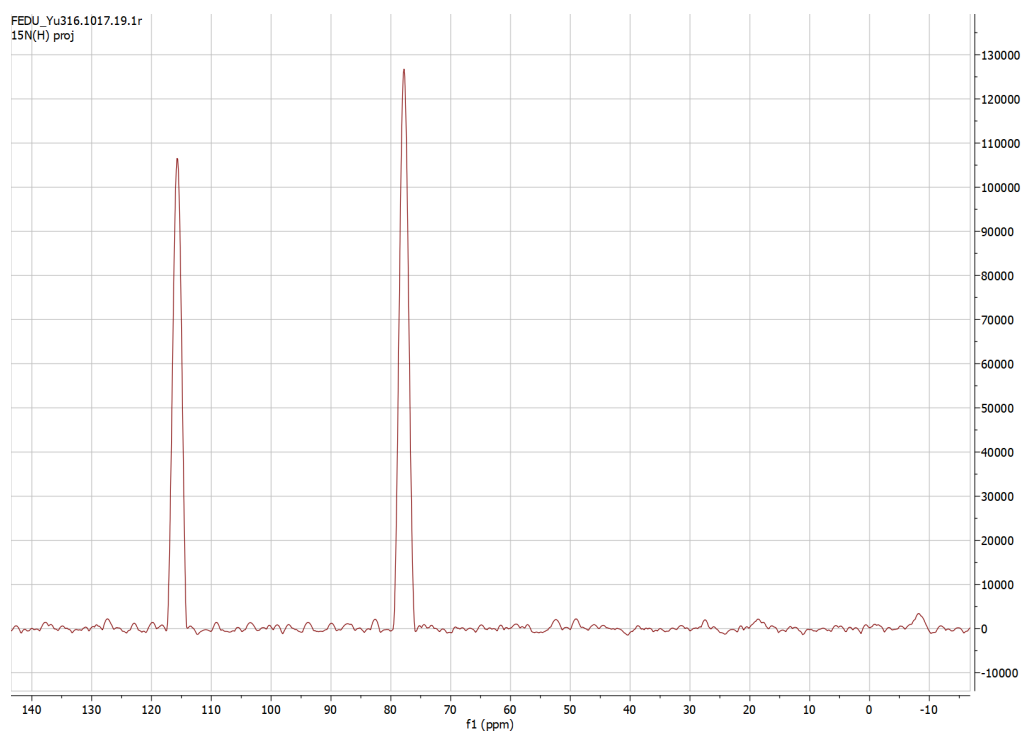


Figure S17. ^{15}N NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in $\text{DMSO-}d_6$.

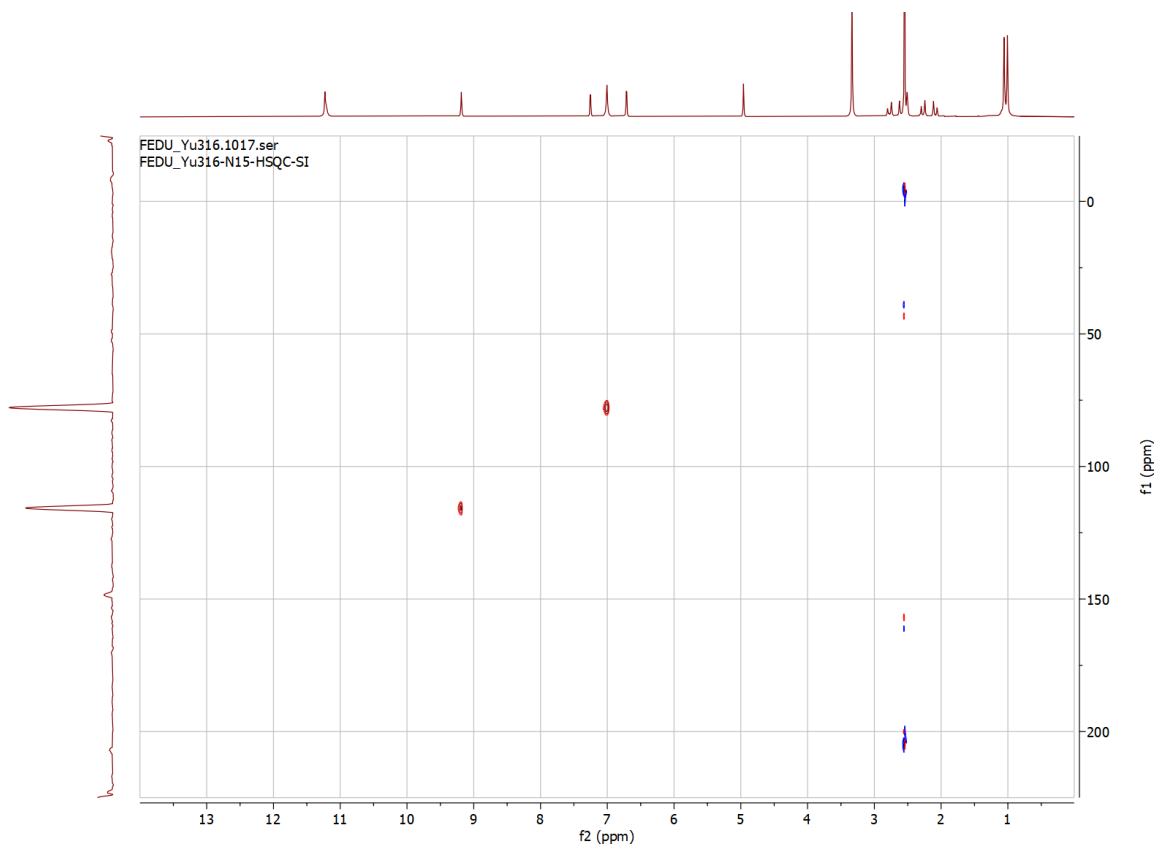


Figure S18. ^1H - ^{15}N HSQC NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in $\text{DMSO-}d_6$.

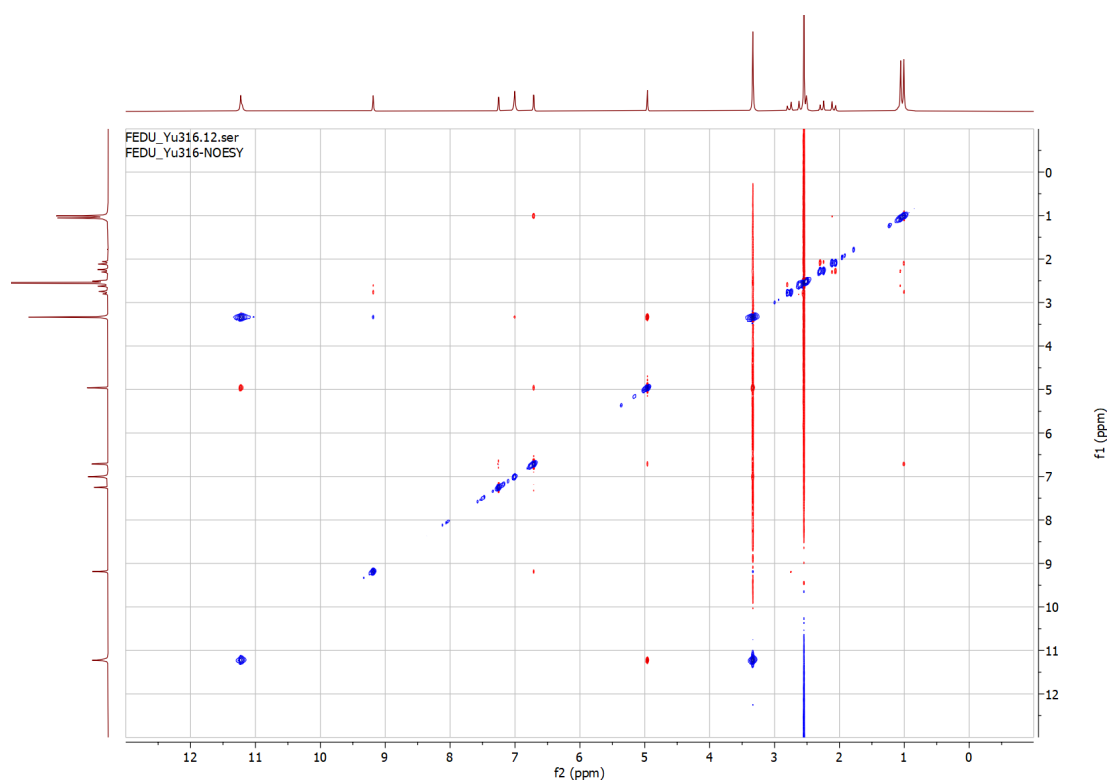


Figure S19. ^1H - ^1H NOESY NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in $\text{DMSO-}d_6$.

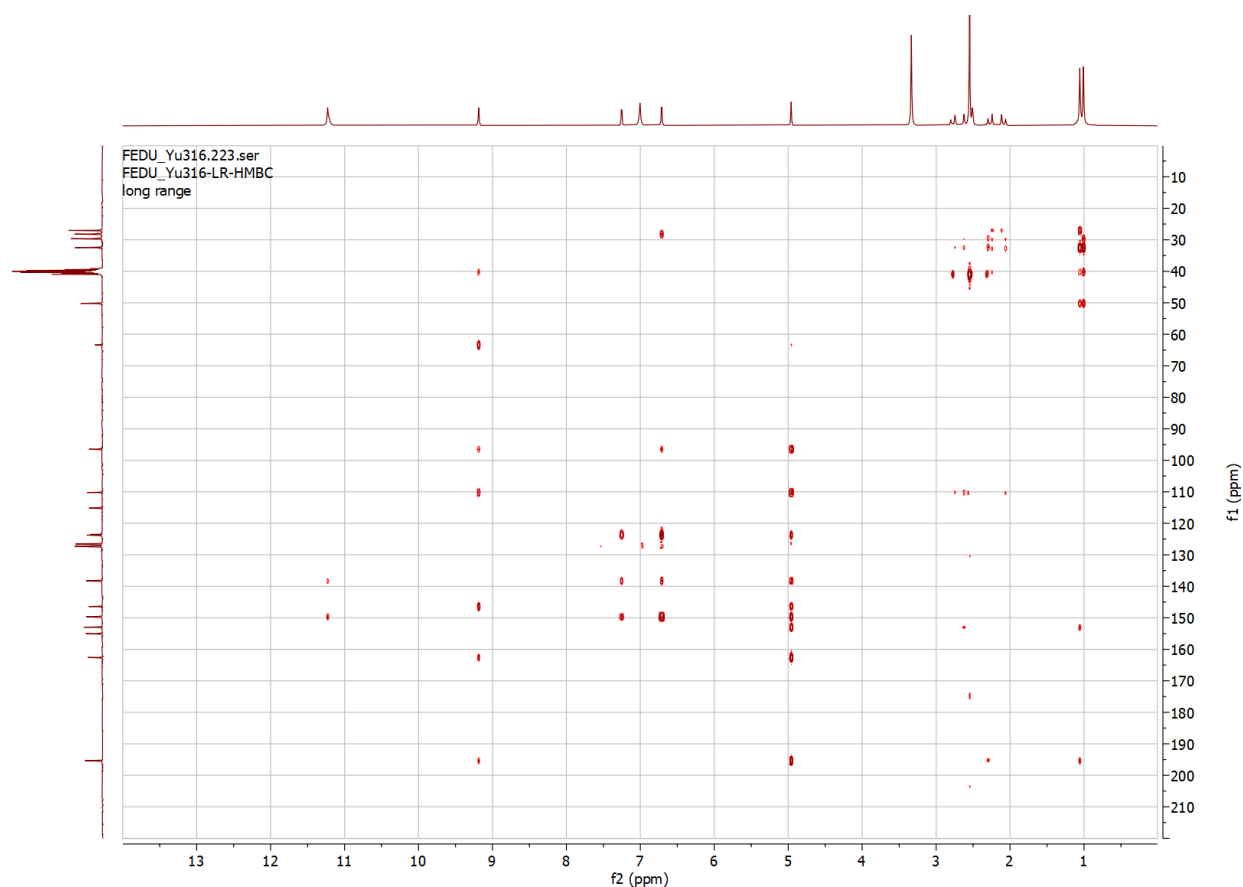


Figure S20. ^1H - ^{13}C HMBC NMR spectrum of 3-amino-10-(3,5-dichloro-2-hydroxyphenyl)-1-hydroxy-7,7-dimethyl-9-oxo-5,6,7,8,9,10-hexahydrobenzo[*b*][1,6]naphthyridine-4-carbonitrile **3a** in $\text{DMSO-}d_6$.