

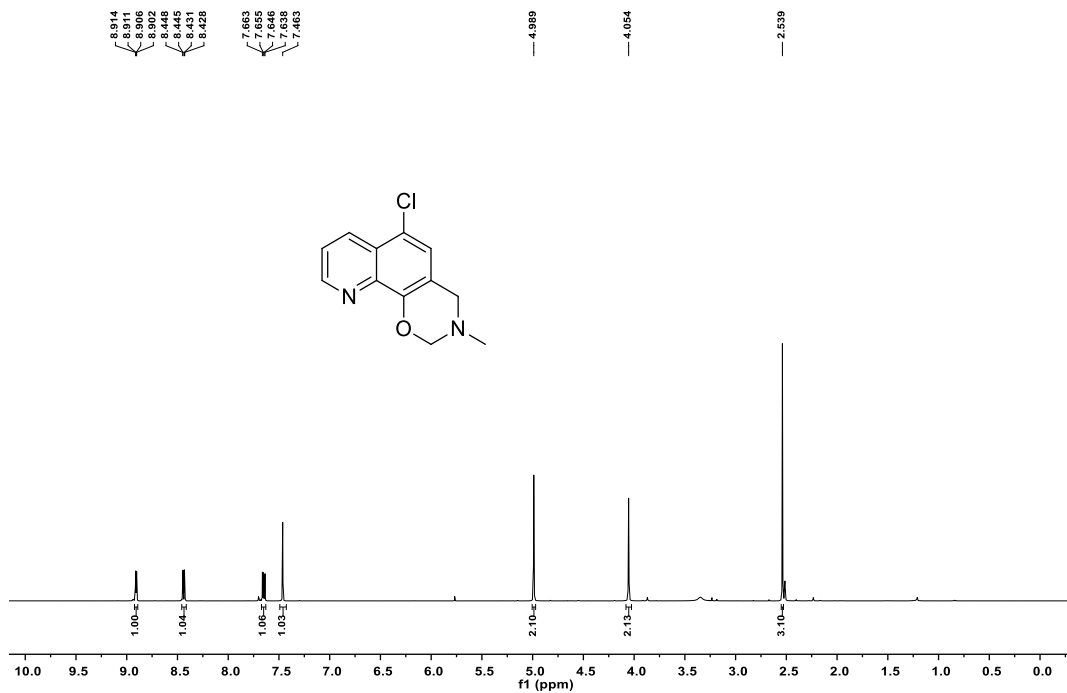
Supporting Information

Synthesis and Biological evaluation of quinoline derivatives as a novel class of broad-spectrum antibacterial agents

Hai-Gen Fu, Zhi-Wen Li, Xin-Xin Hu, Xue-Lian Zhang, Shu-Yi Si, Xue-Fu You,
Sheng Tang, Yan-Xiang Wang, Dan-Qing Song

Figure S1. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-13-methyl-3, 4-dihydro-2H-[1, 3]oxazino-[5, 6-h]quinoline (**4a**)

20140630-D-20
 BRUKER AV-III-500 1H-NMR D-20a IN DMSO 2014.06.30
 PROTON DMSO E:\\ kangjunsu 9



20140704-D-20
 BRUKER AV-III-500 13C-NMR D-20 IN CDCL3 2014.07.04
 C13CPD CDCL3 E:\\ kangjunsu 4

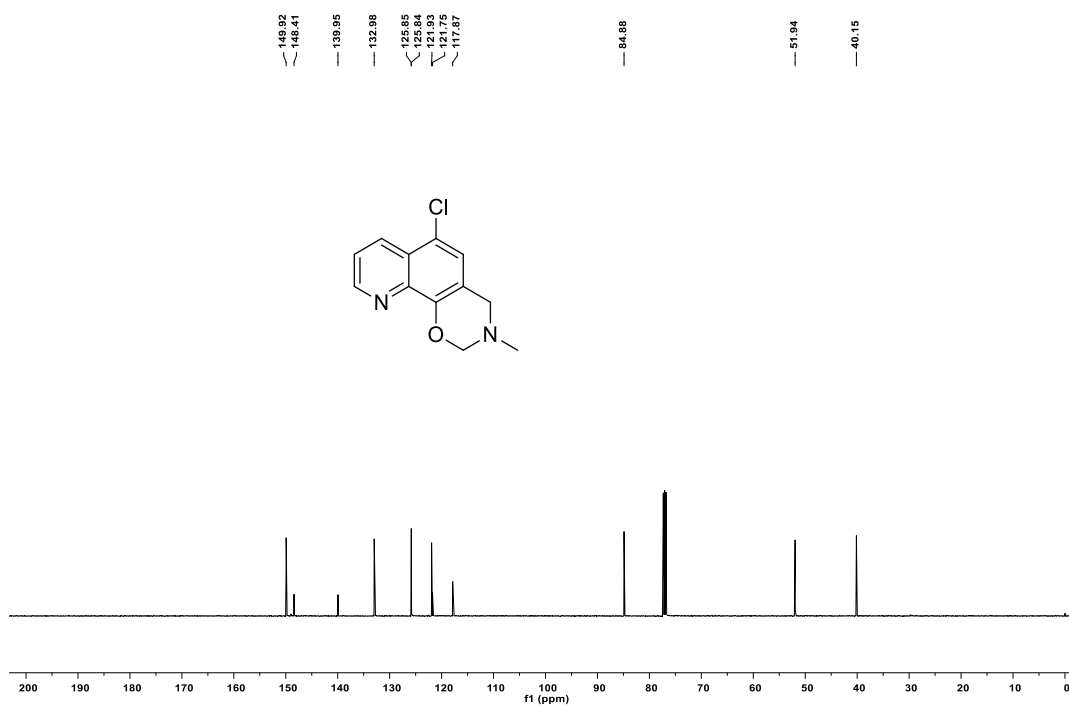
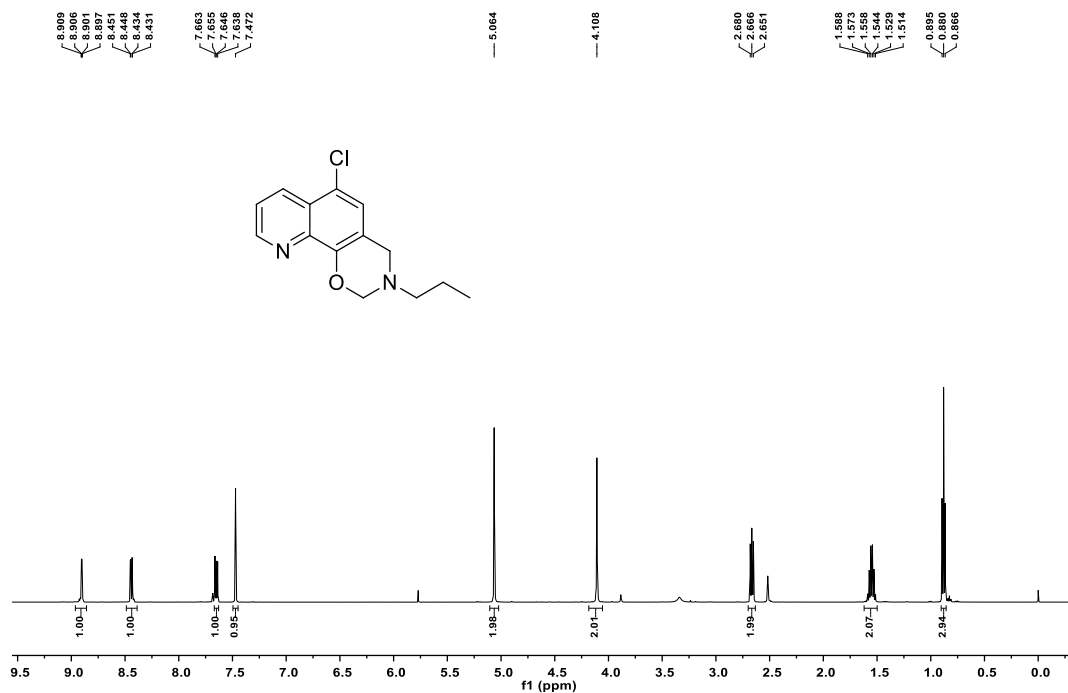


Figure S2. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-propyl-3, 4-dihydro-2H-[1,3]oxazino-[5, 6-h]quinoline (**4b**)

20140704-D-21a
 BRUKER AV-111-500 ^1H -NMR D-21a IN DMSO 2014.07.04
 PROTON DMSO E:\ kangjunsu 6



20140708-D-21a
 BRUKER AV-111-500 ^{13}C -NMR D-21a IN DMSO 2014.07.08
 C13CPD DMSO E:\ songdanqing 38

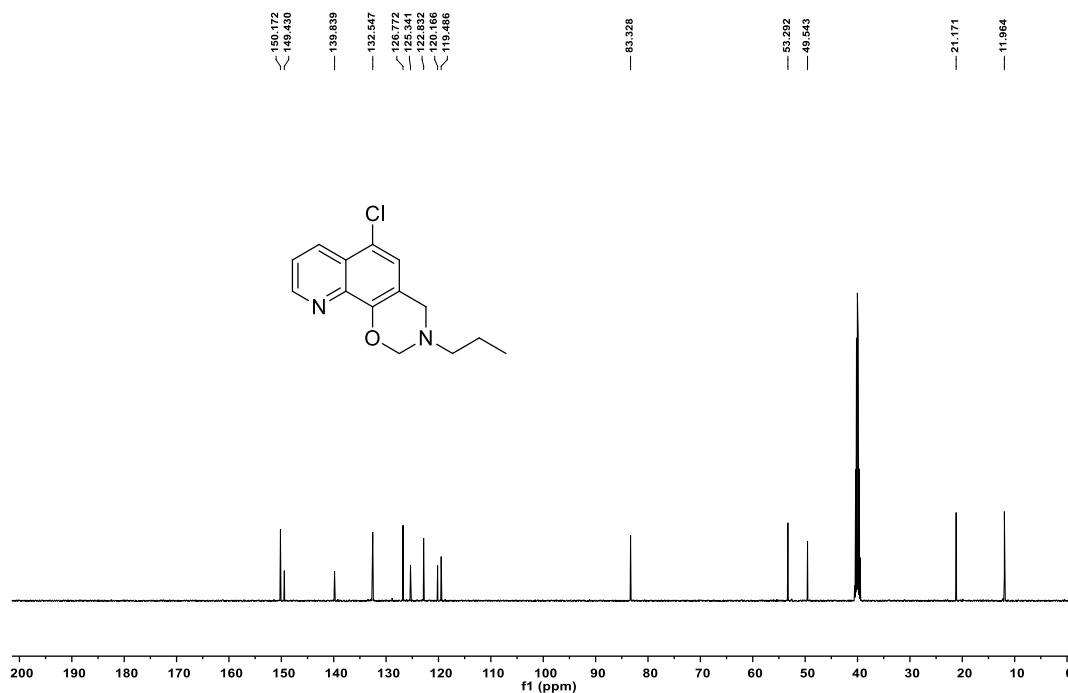
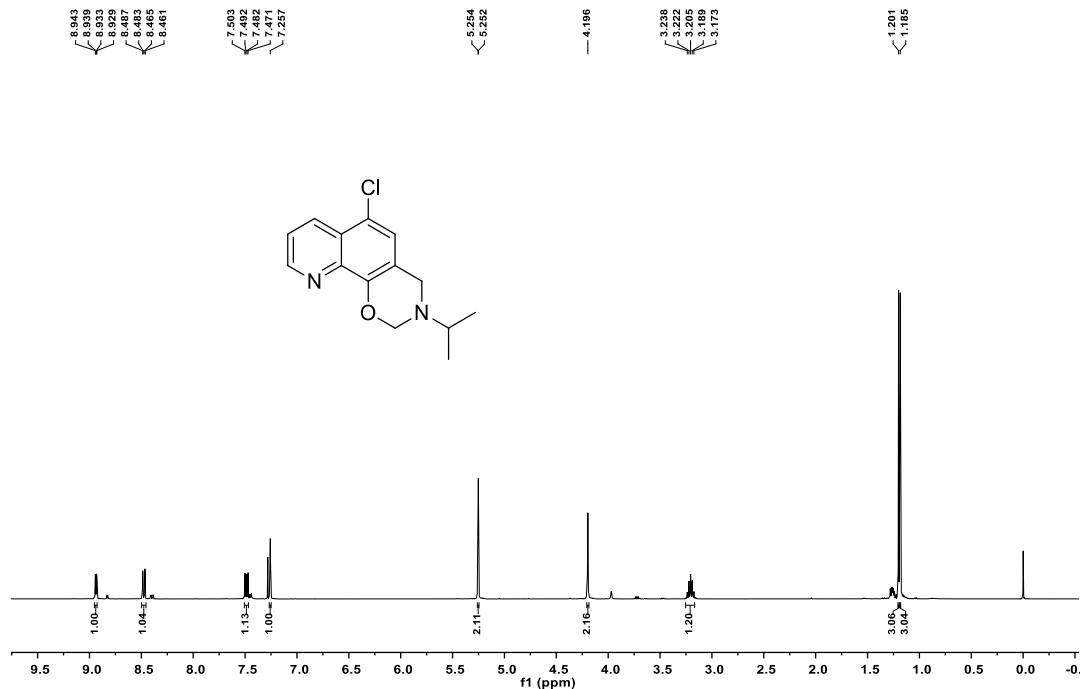


Figure S3. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-13-isopropyl-3,4-dihydro-2H-[1,3]oxazino-[5,6-h]quinoline (**4c**)

D-33

single_pulse



20140901 D-33
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 C13 CDCl3 D:\DATA-2014 44

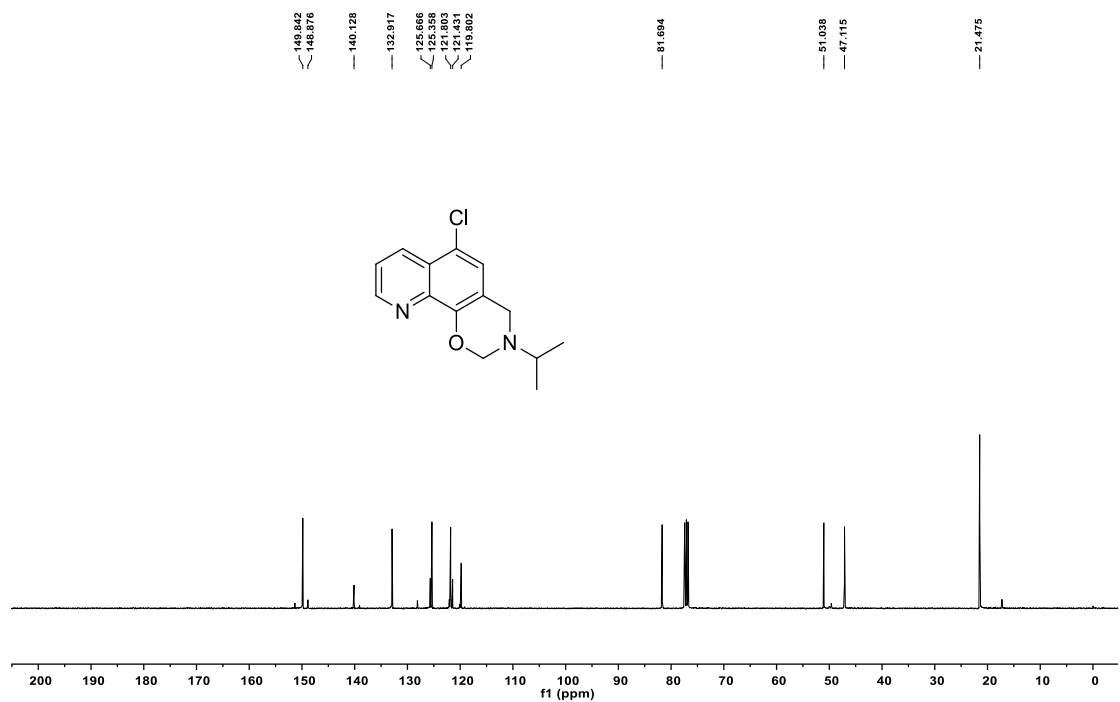
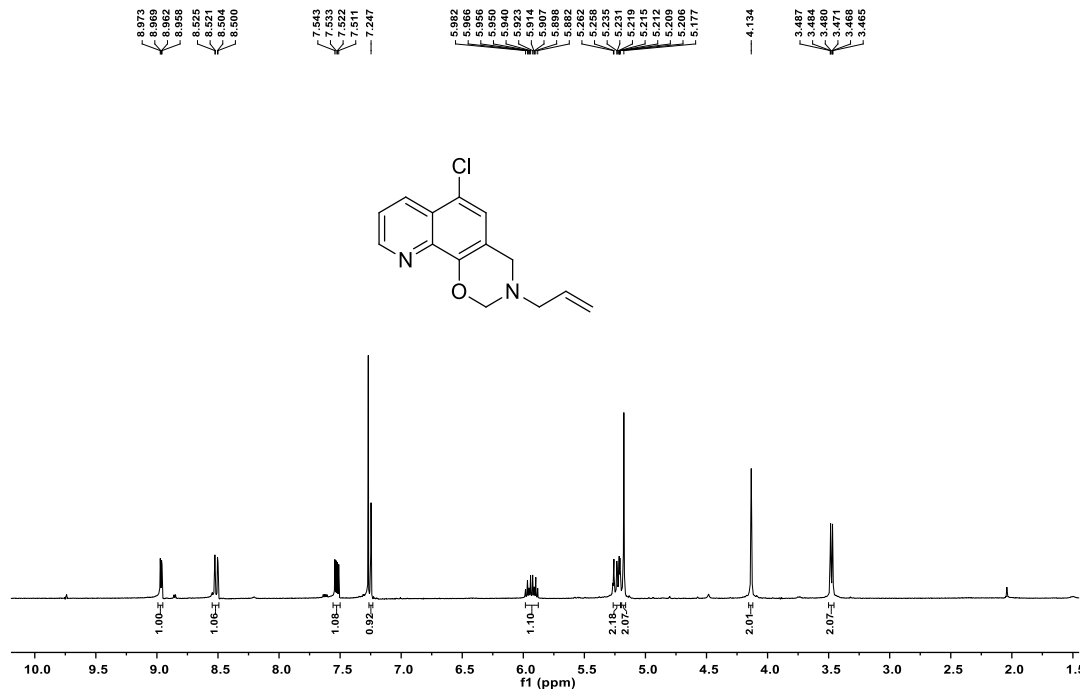


Figure S4. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-13-allyl-3, 4-dihydro-2H-[1, 3]oxazino-[5, 6-h]quinoline (**4d**)

D-28

single_pulse



D-28

single pulse decoupled gated NOE

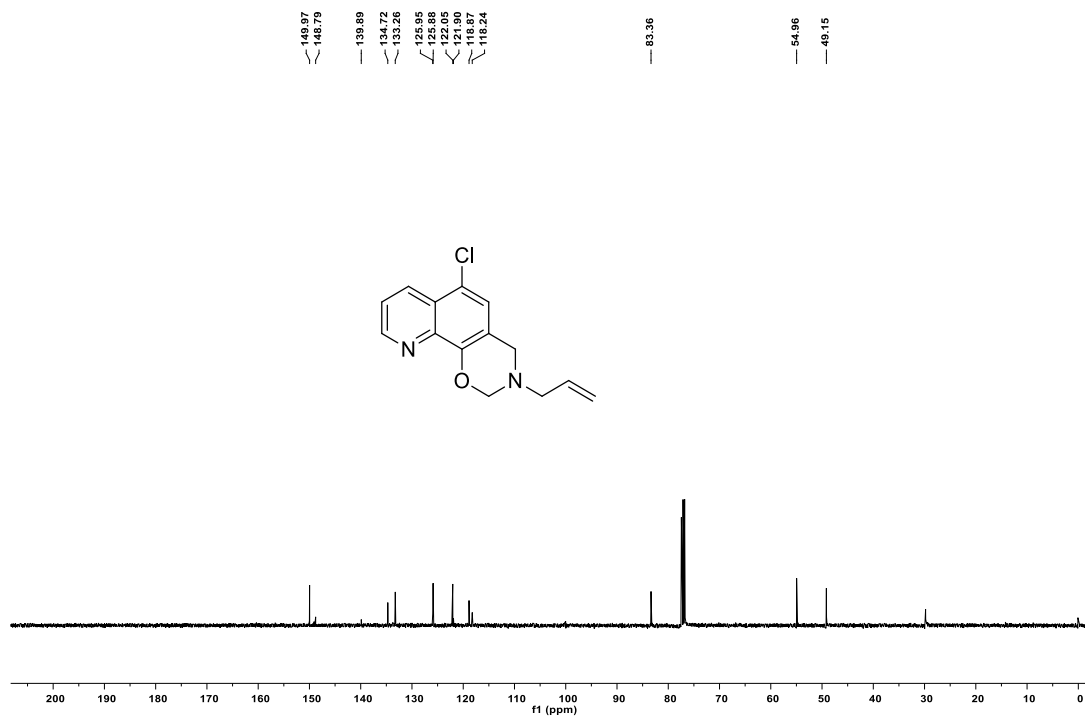
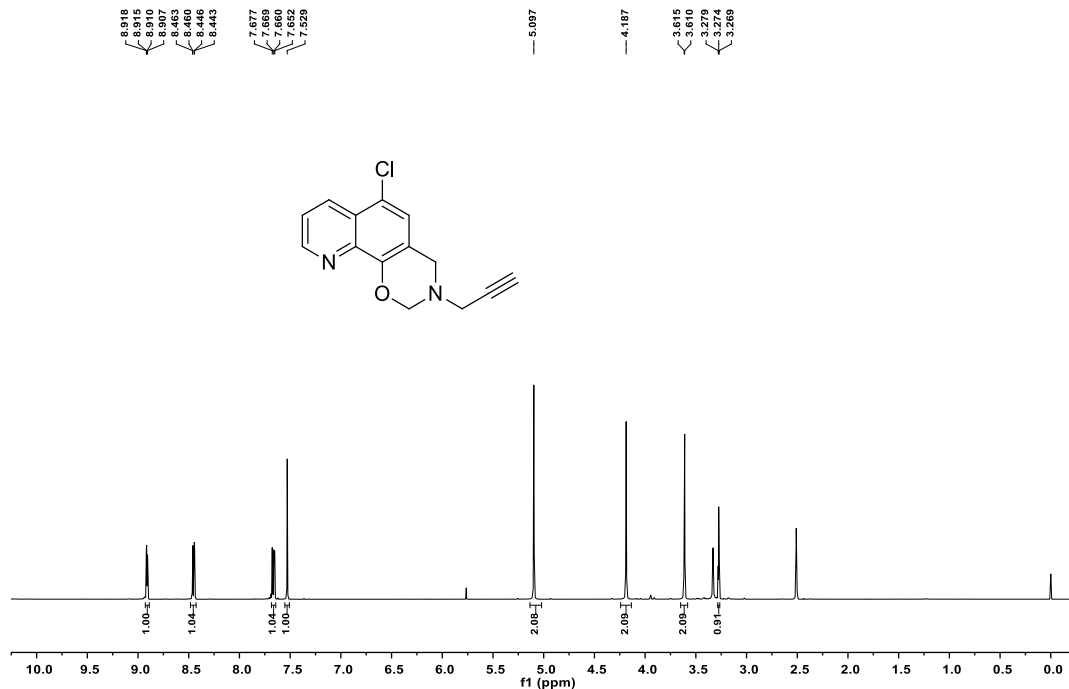


Figure S5. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-(prop-2-yn-1-yl)-3,4-dihydro-2H-[1,3]oxazino-[5,6-h]quinoline (**4e**)

20140702-D-22
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 PROTON DMSO E:\ kangjunsu 13



20140704-D-22
 BRUKER AV-111-500 13C-NMR D-22 IN DMSO 2014.07.04
 C13CPD DMSO E:\ kangjunsu 5

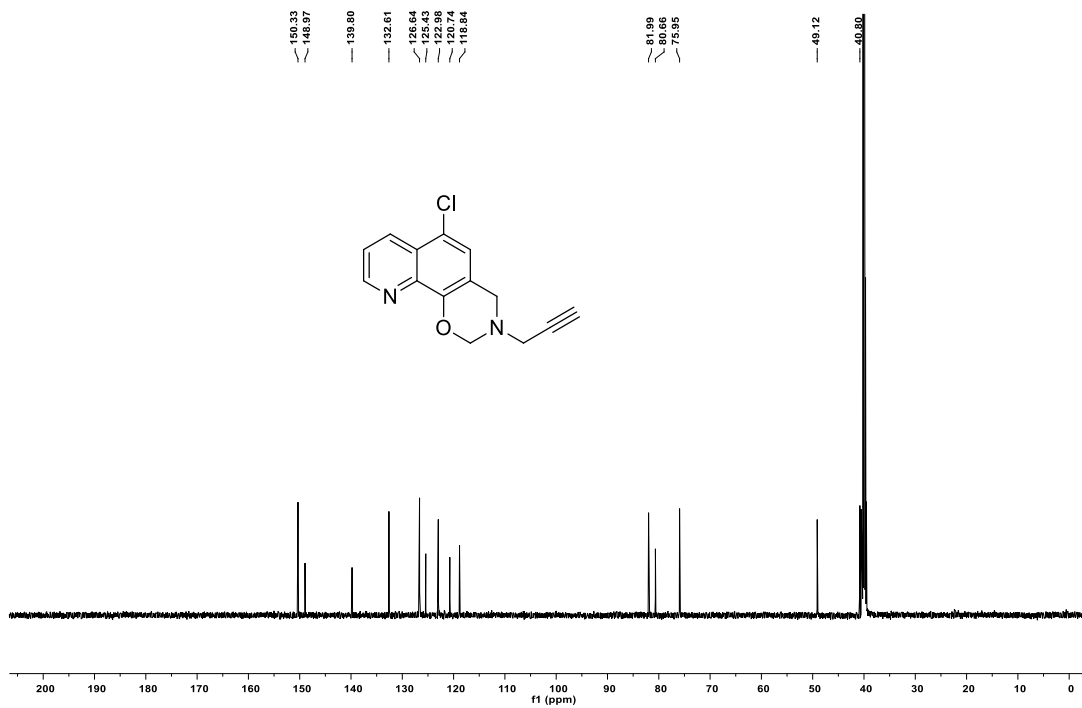
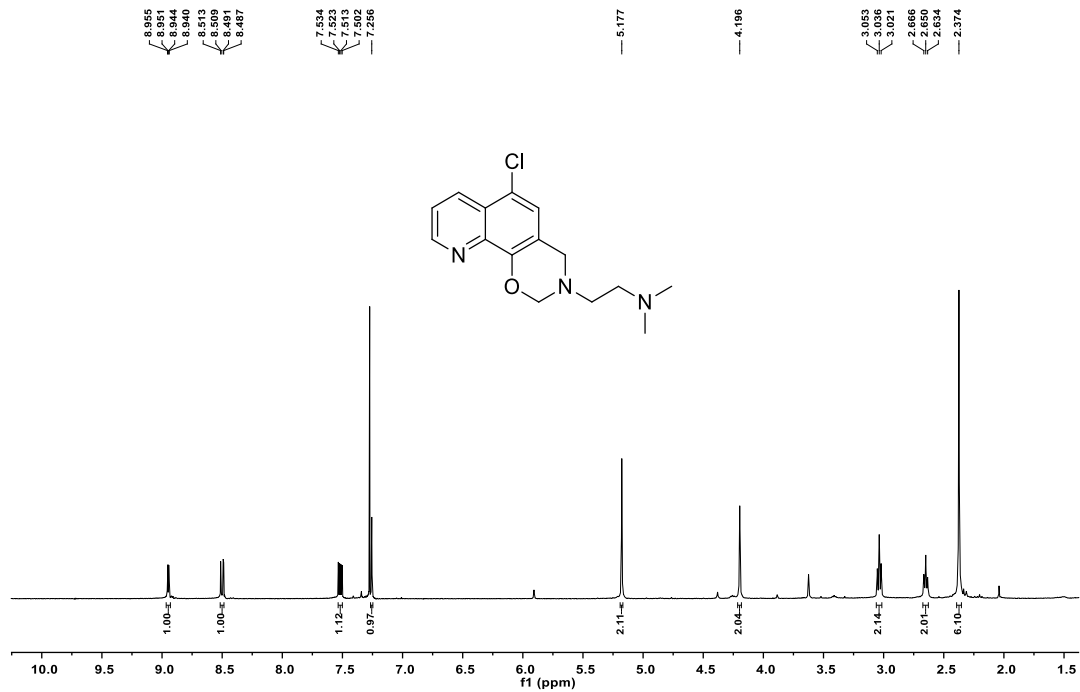


Figure S6. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-(2-dimethylaminoethyl)-3,4-dihydro-2H-[1,3]oxazino-[5,6-h]quinoline (**4f**)

D-31
single_pulse



D-31
single_pulse decoupled gated NOE

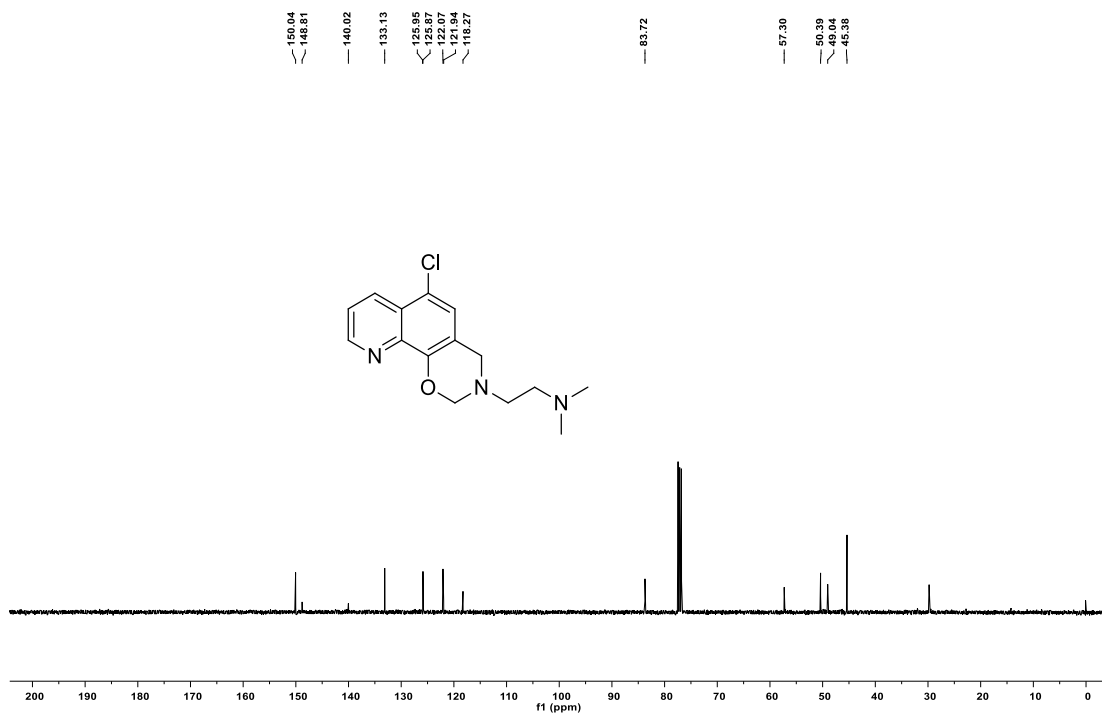
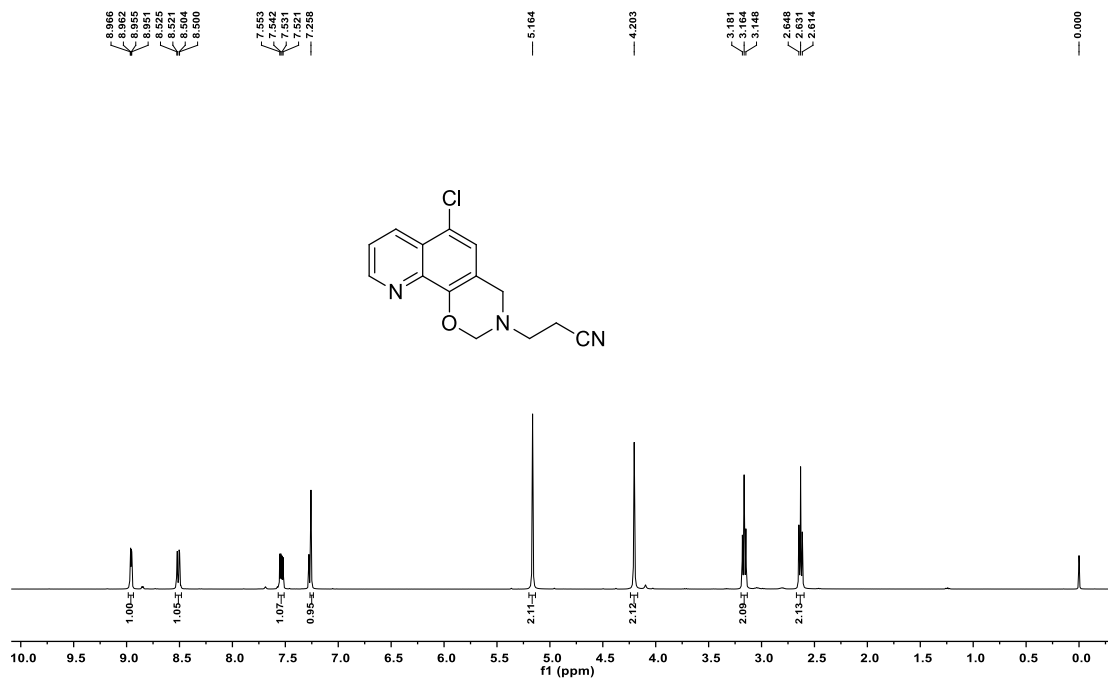


Figure S7. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-13-cyanoethyl-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (4g)

20140825 D-40
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20140828 D-40
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 C13 CDC13 D:\ \ DATA-2014 30

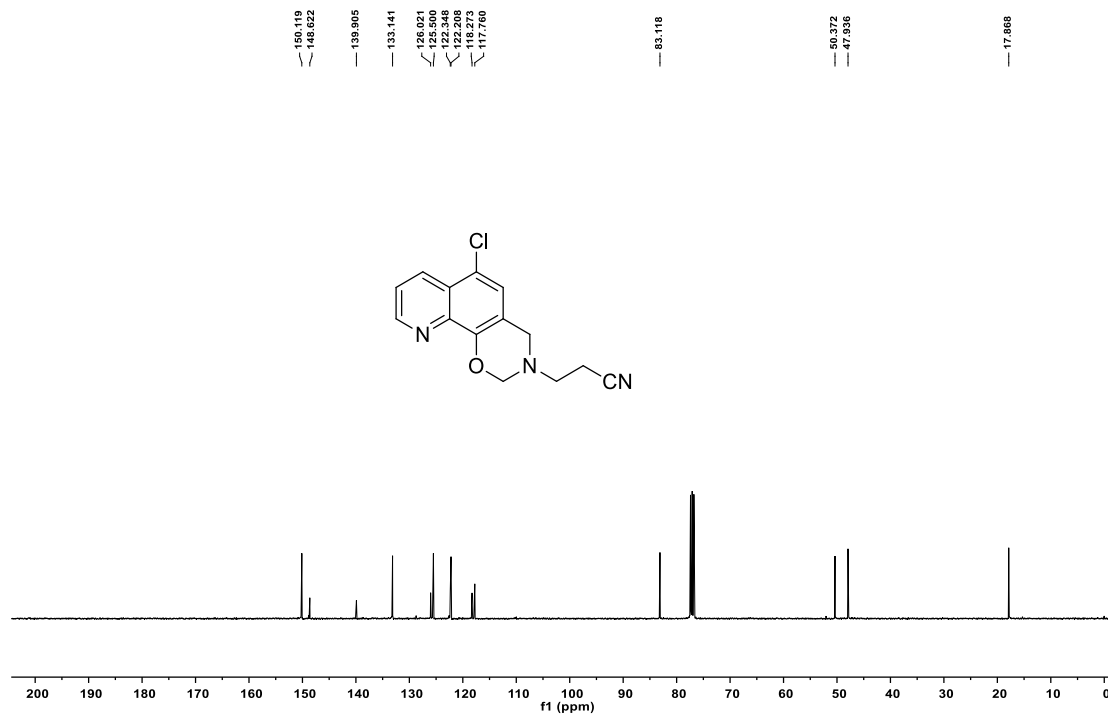
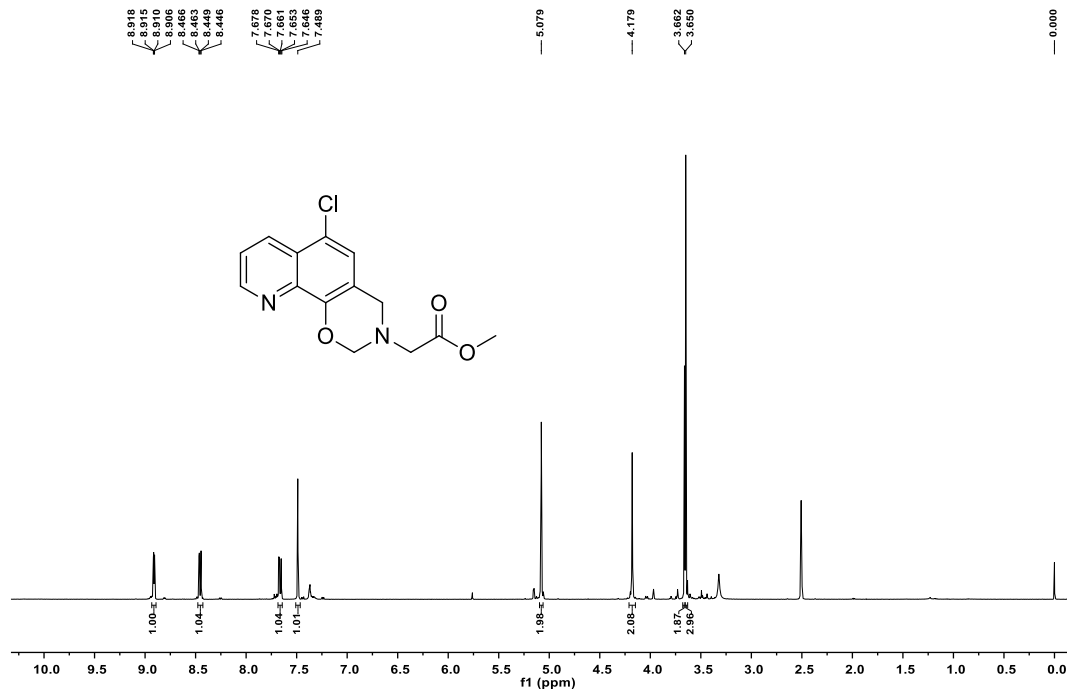


Figure S8. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-methoxycarbonylmethyl-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4h**)

20140708-D-24
 BRUKER AV-111-500 1H-NMR D-24 IN DMSO 2014.07.08
 PROTON DMSO E:\\ songdanqing 39



20140709-D-24
 BRUKER AV-111-500 13C-NMR D-24 IN DMSO 2014.07.09
 C13CPD DMSO E:\\ songdanqing 58

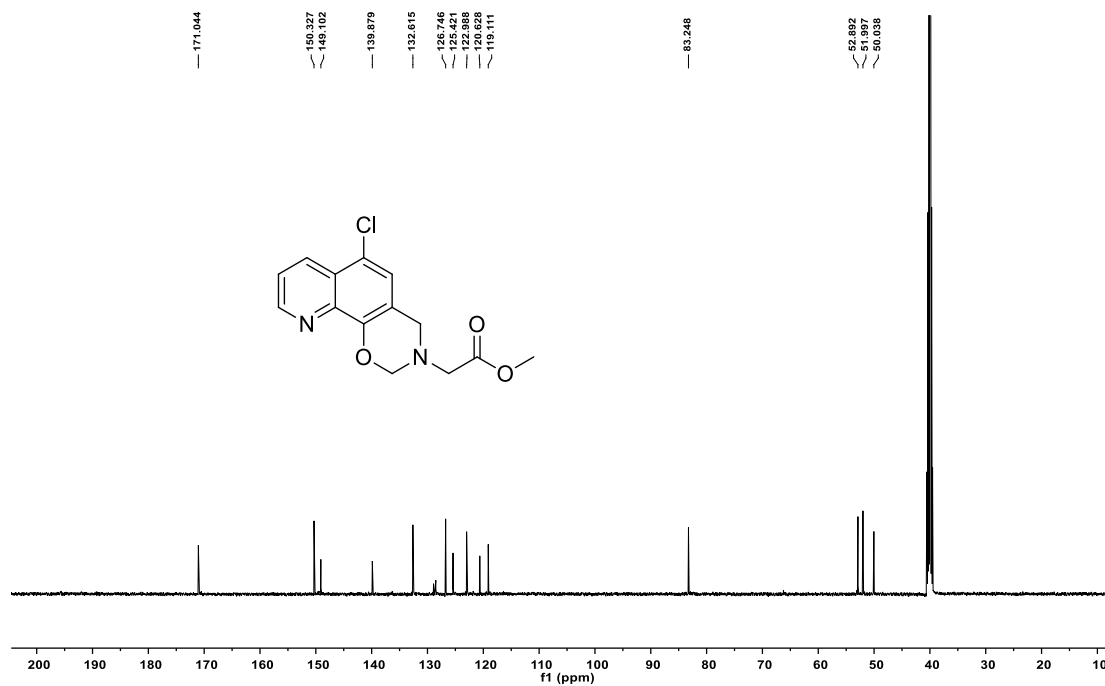
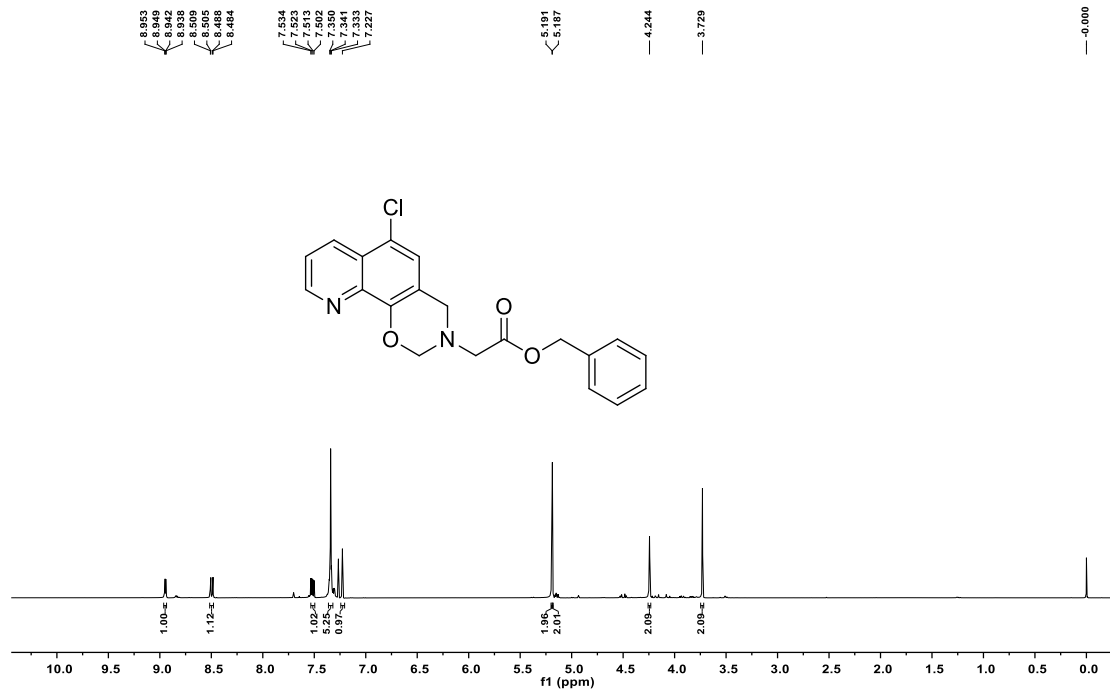


Figure S9. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-13-benzoxycarbonylmethyl-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4i**)

20140825 D-27
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20140828 D-27
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 C13 CDC13 D:\ DATA-2014 27

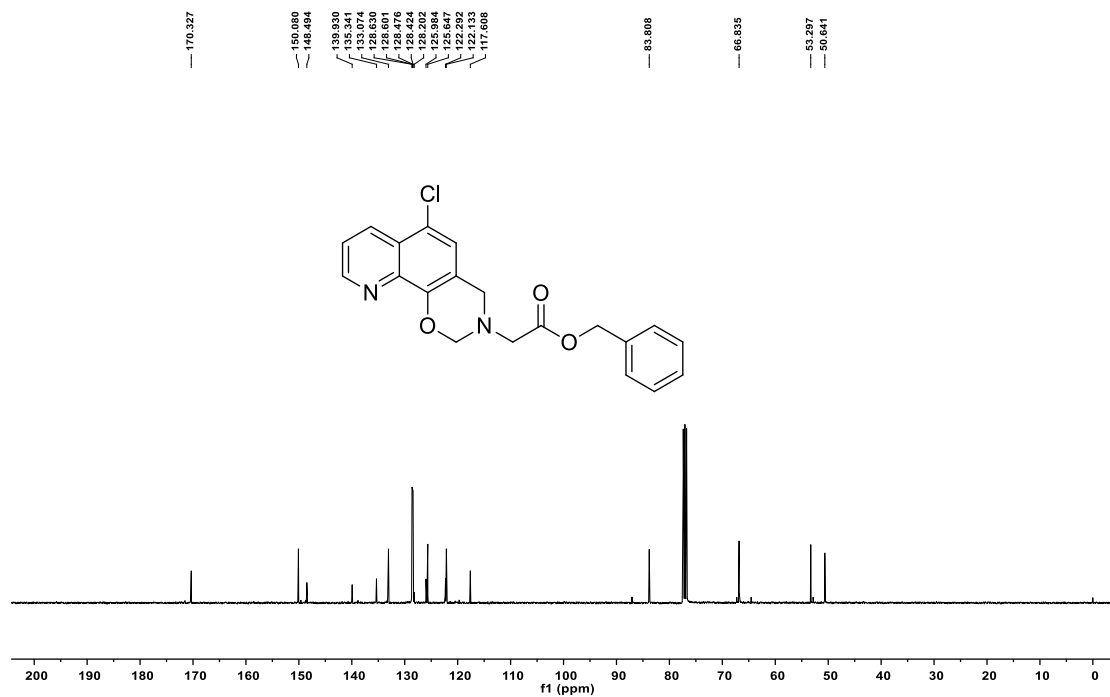
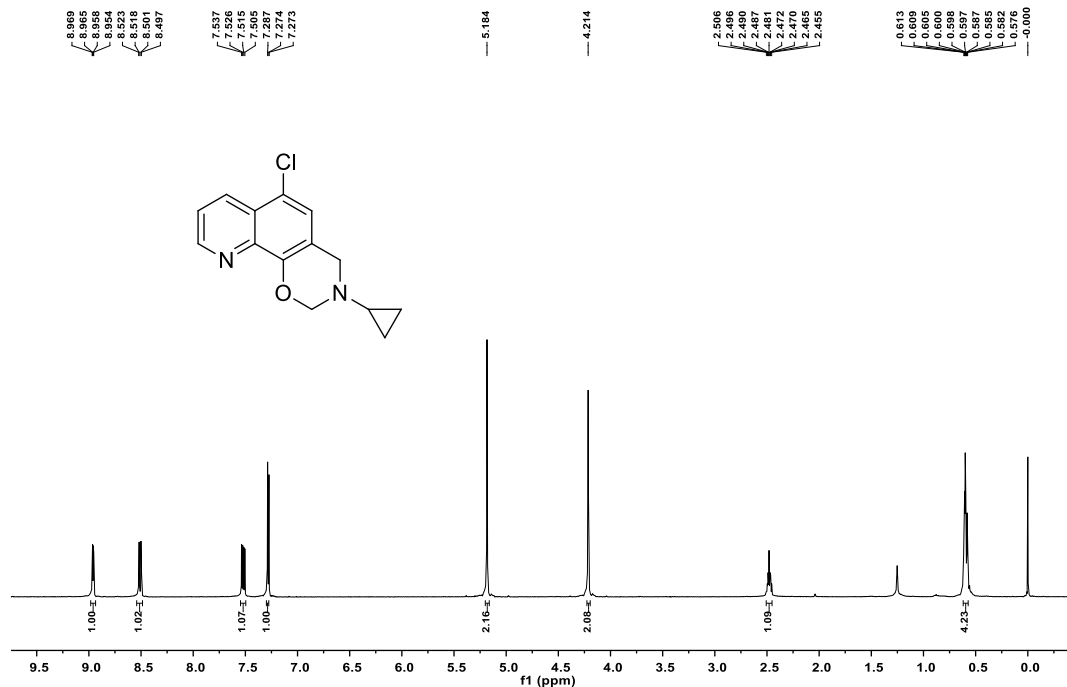


Figure S10. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-cyclopropyl-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4j**)

D-34
single_pulse



D-34
single_pulse decoupled gated NOE

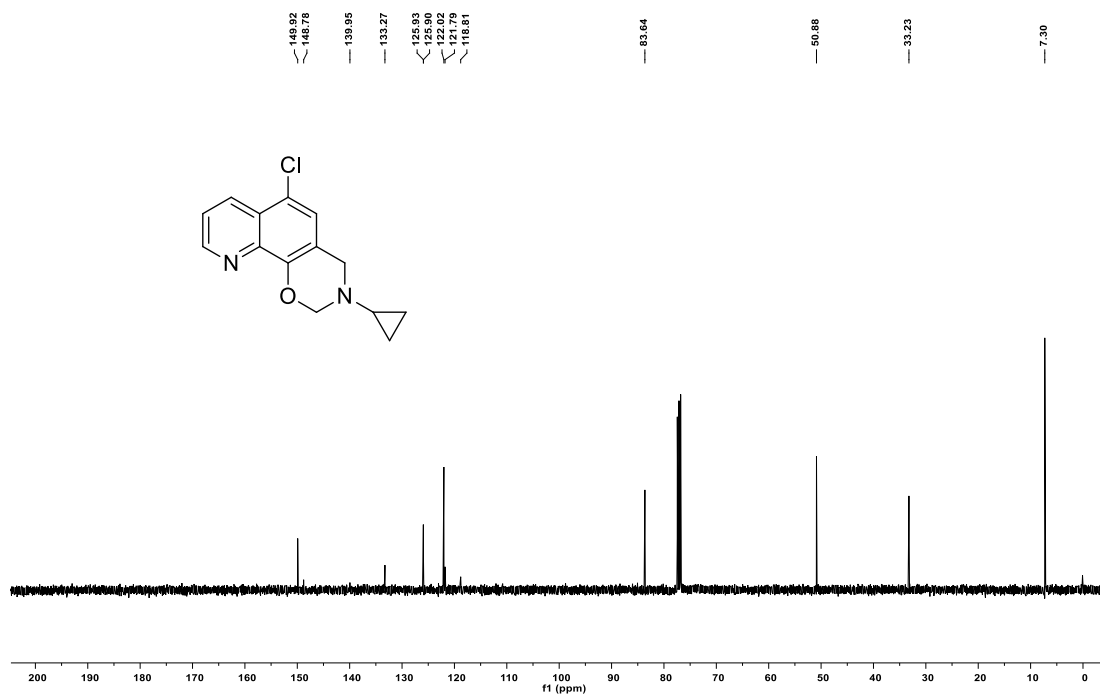
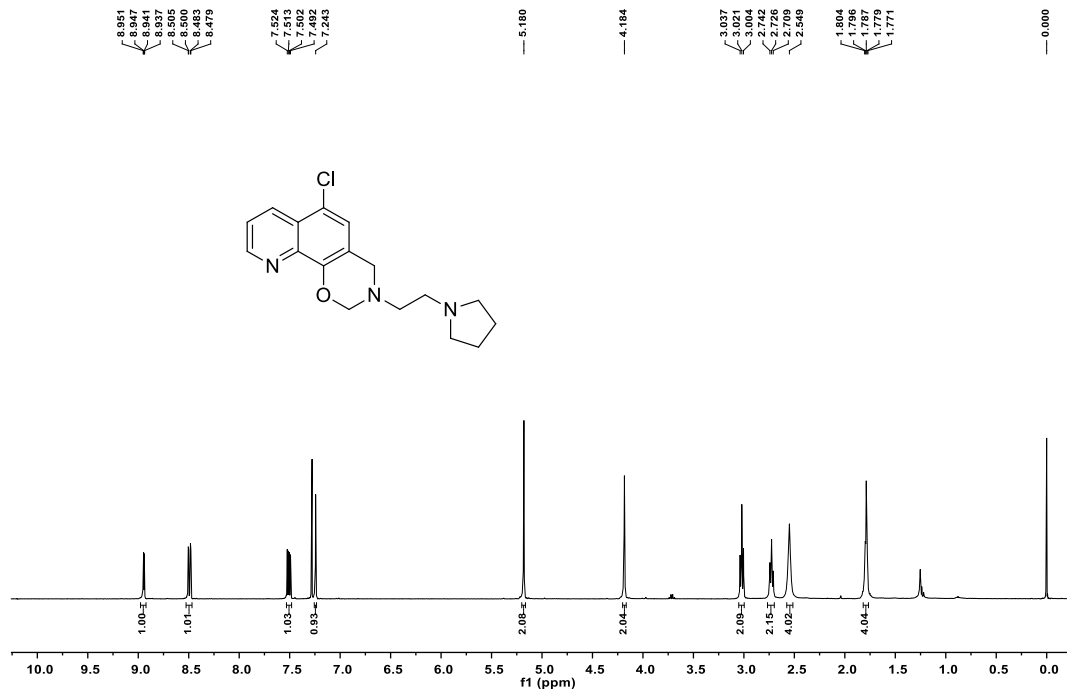


Figure S11. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-[2-(pyrrolidin-1-yl)ethyl]-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4k**)

D-36

single_pulse



D-36

single_pulse decoupled gated NOE

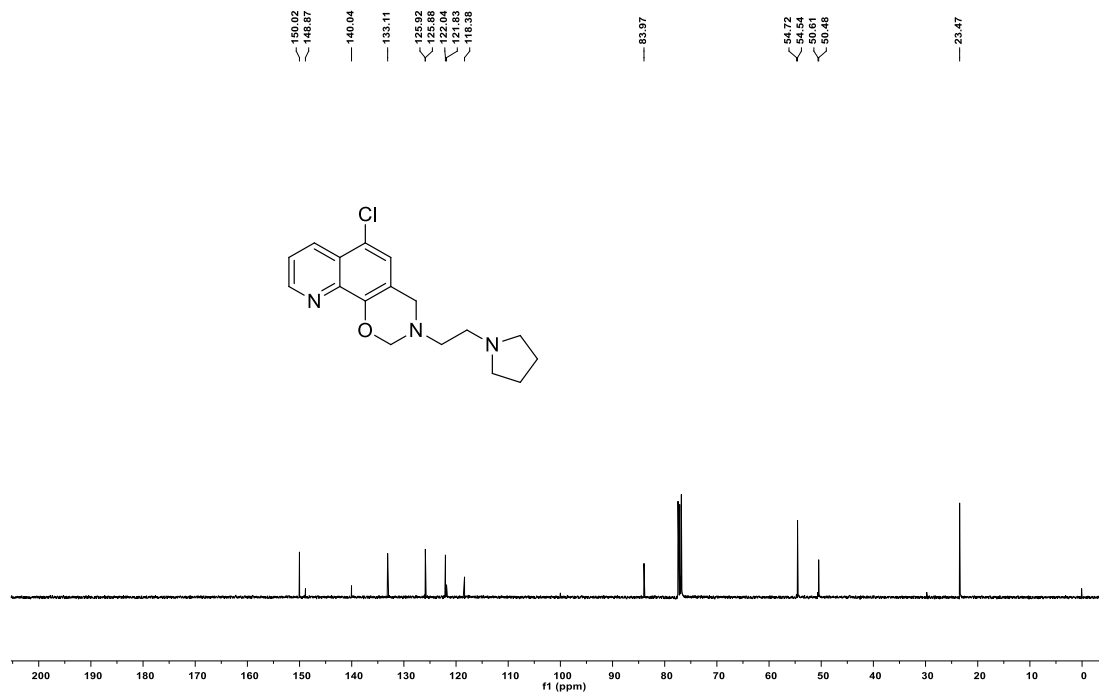
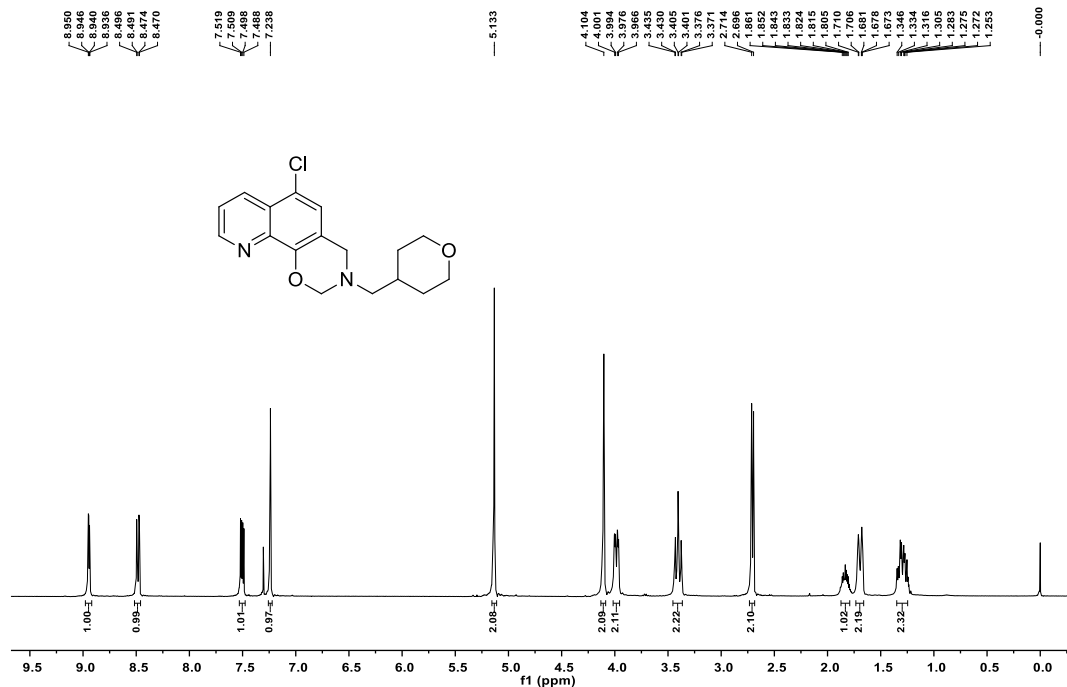


Figure S12. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-[(tetrahydro-2H-pyran-4-yl)methyl]-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4I**)

D-29

single_pulse



D-29

single_pulse decoupled gated NOE

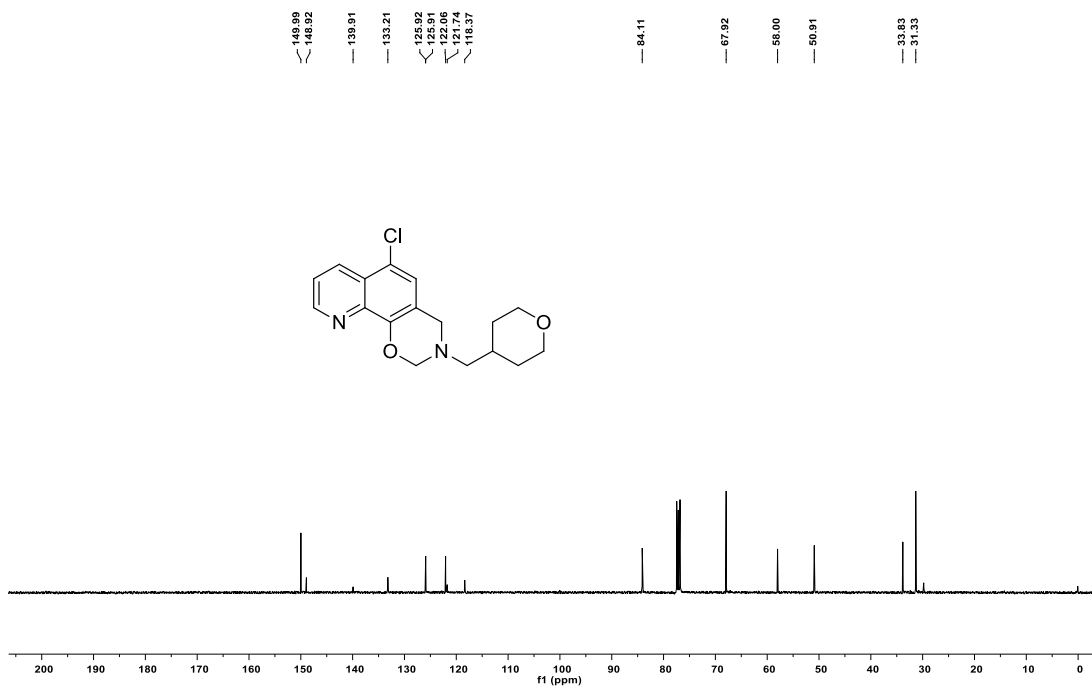
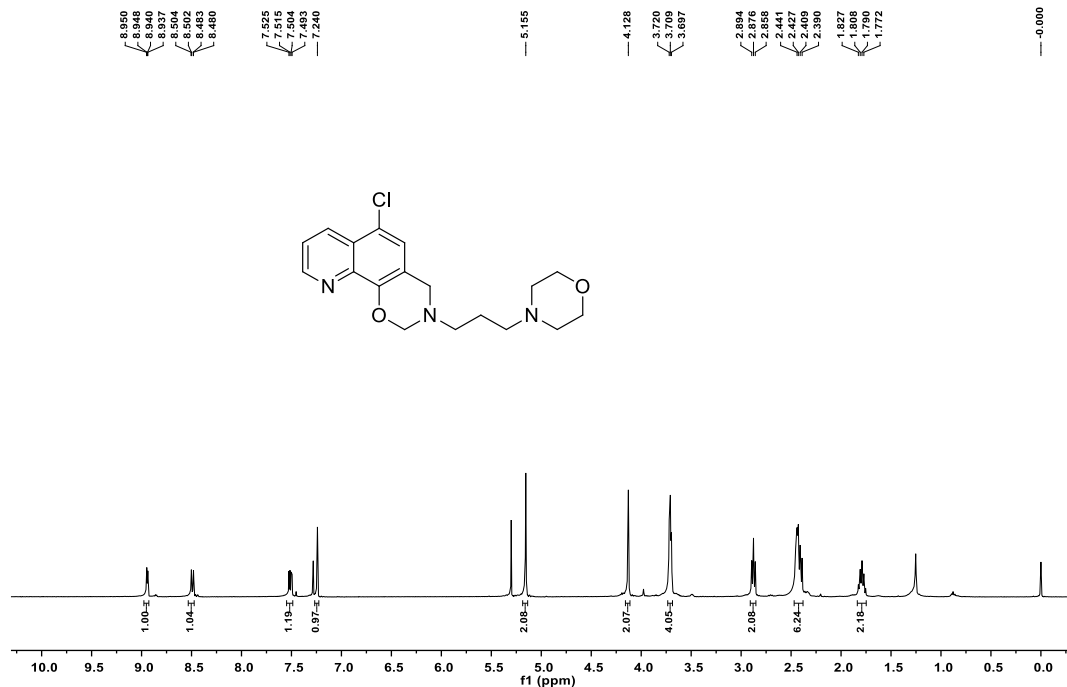


Figure S13. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-13-morpholinopropyl-3,4-dihydro-2H-[1,3]oxazino[5,6-h]quinoline (**4m**)

D-35

single_pulse



D-35

single pulse decoupled gated NOE

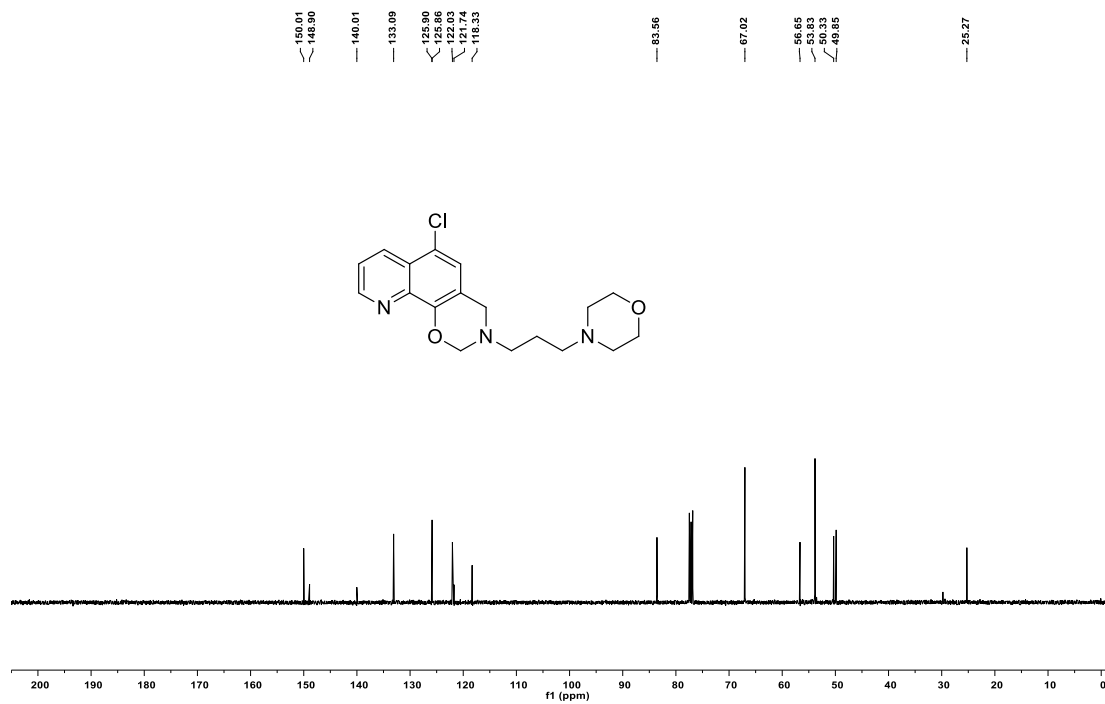
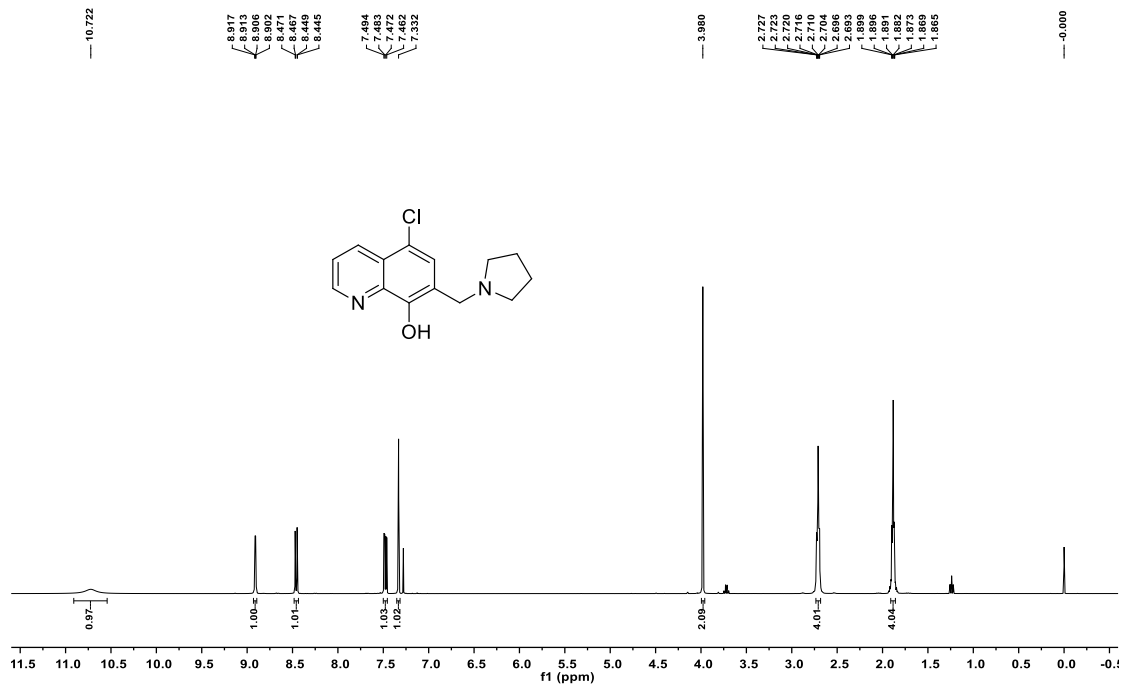


Figure S14. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-7-(pyrrolidin-1-yl-methyl)quinolin-8-ol

(5a)

20140828 D-52
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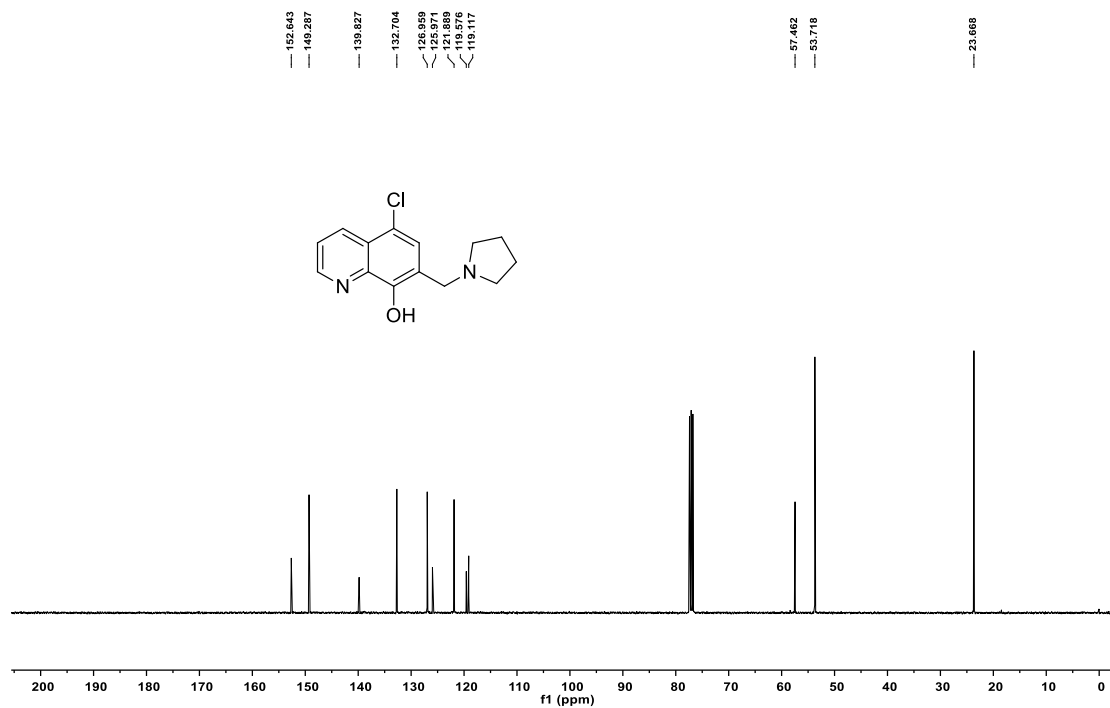
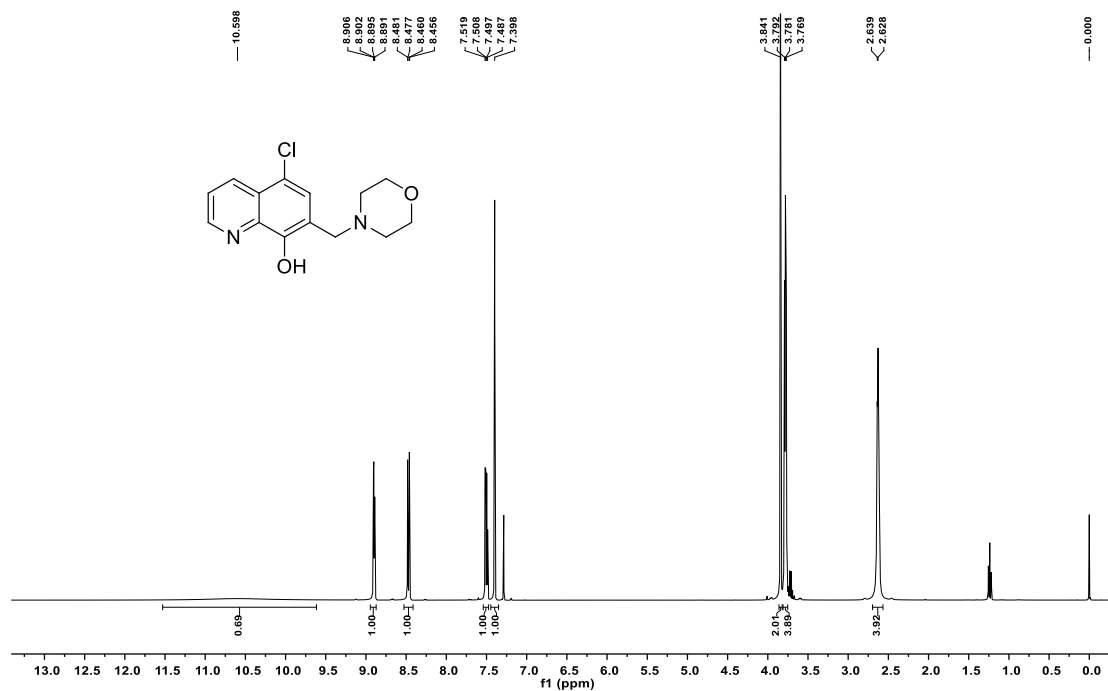


Figure S15. ^1H NMR (top) and ^{13}C NMR (bottom) of 5-Chloro-7-(morpholinomethyl)quinolin-8-ol (**5b**)

20140826 D-51
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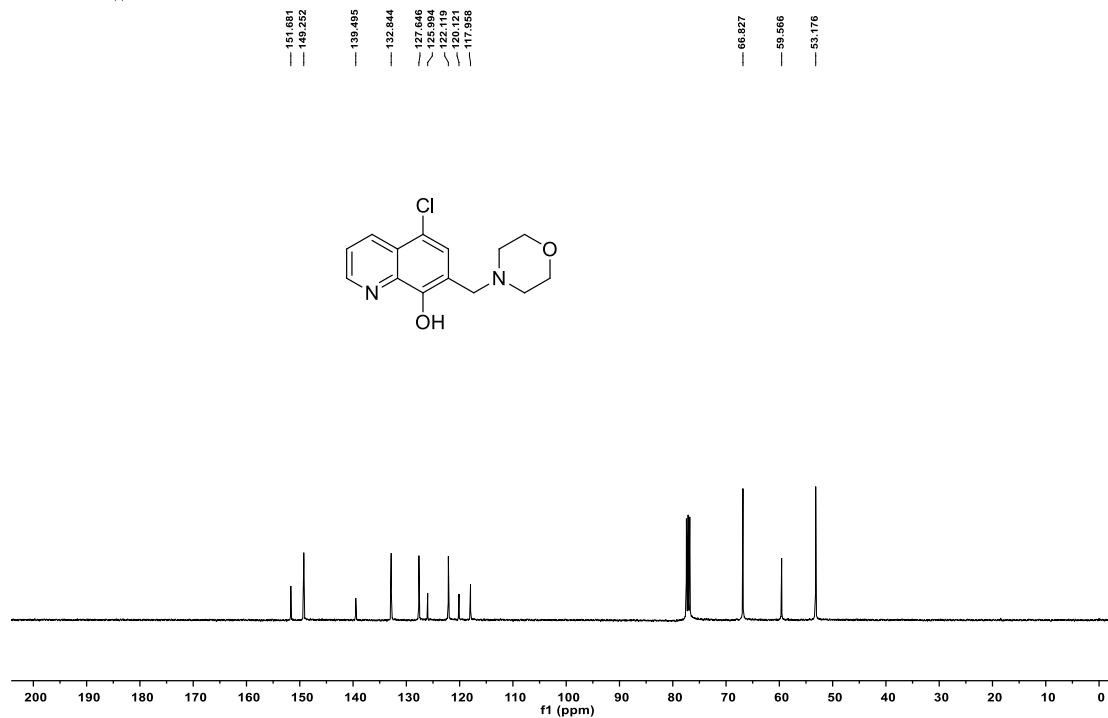


Figure S16. ¹H NMR (top) and ¹³C NMR (bottom) of 5-Chloro-7-[(4-methylpiperazin-1-yl)methyl]quinolin-8-ol (5c)

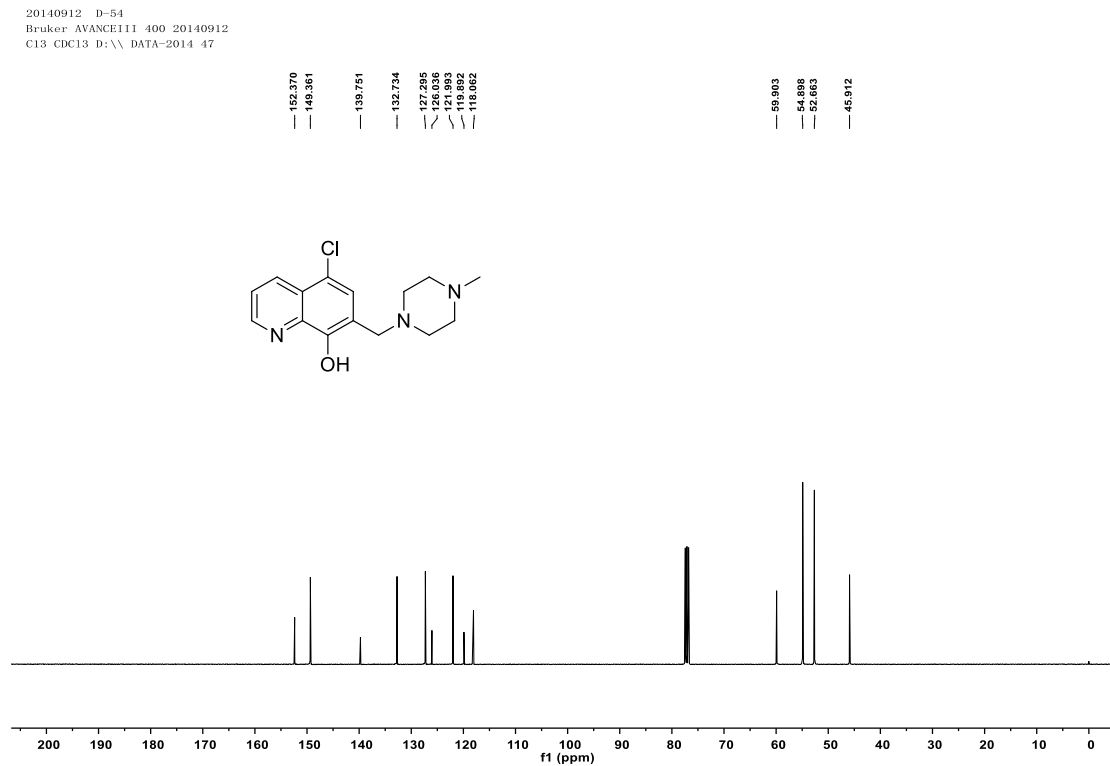
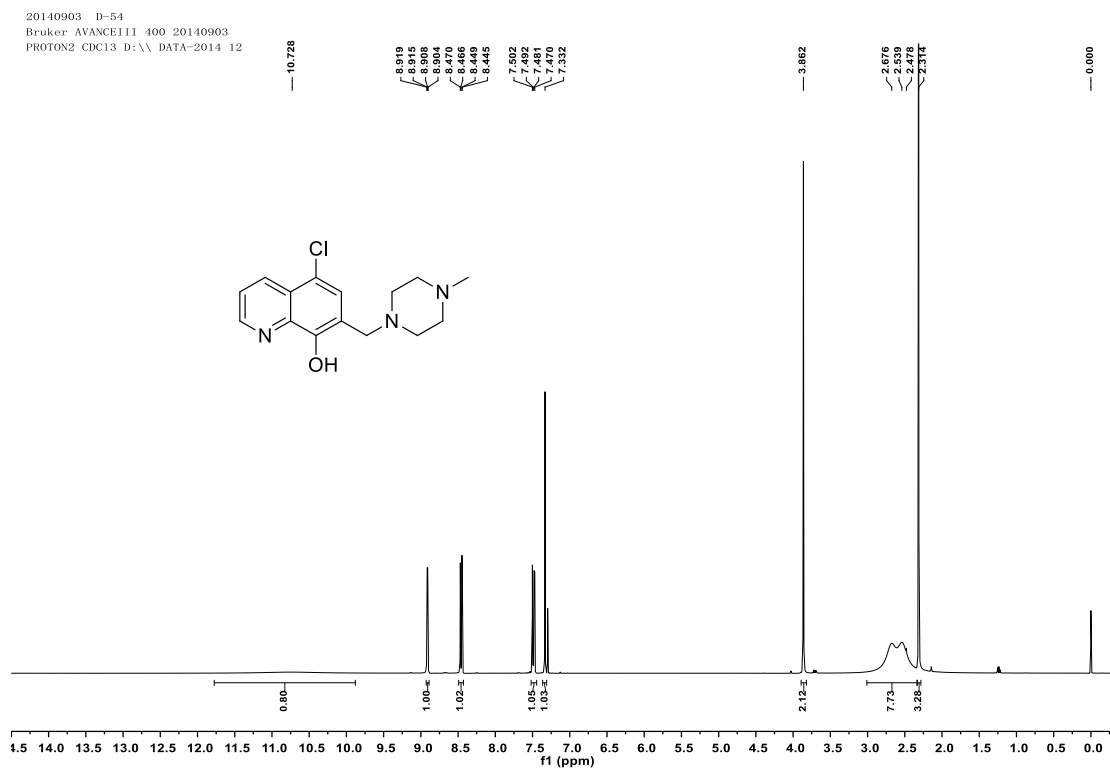


Figure S17. ^1H NMR (top) and ^{13}C NMR (bottom) of 7-[4-[(5-chloro-8-hydroxyquinolin-7-yl)methyl]piperazin-1-yl]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid (**5d**)

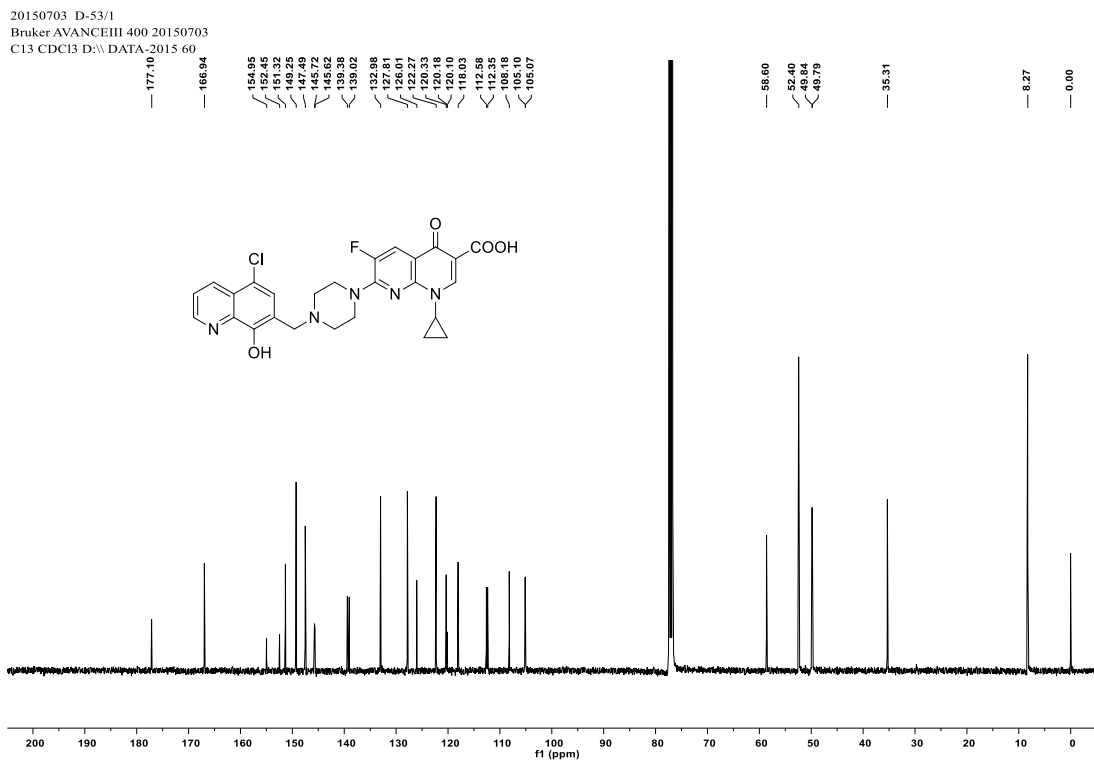
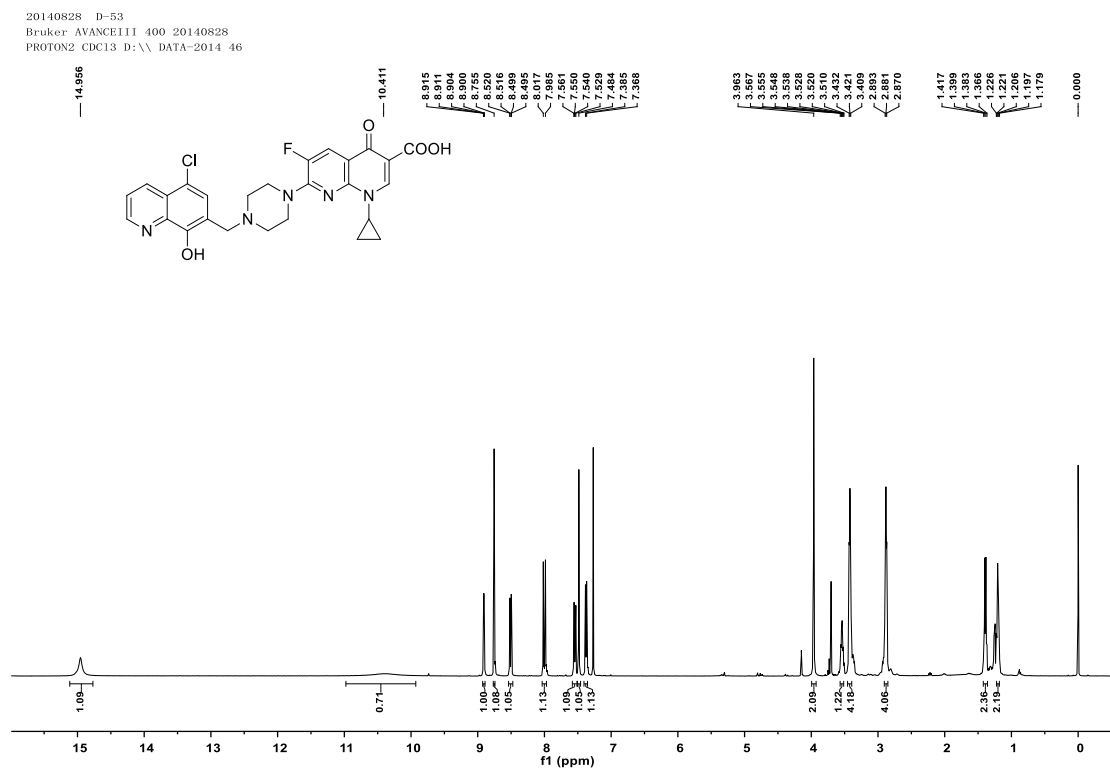
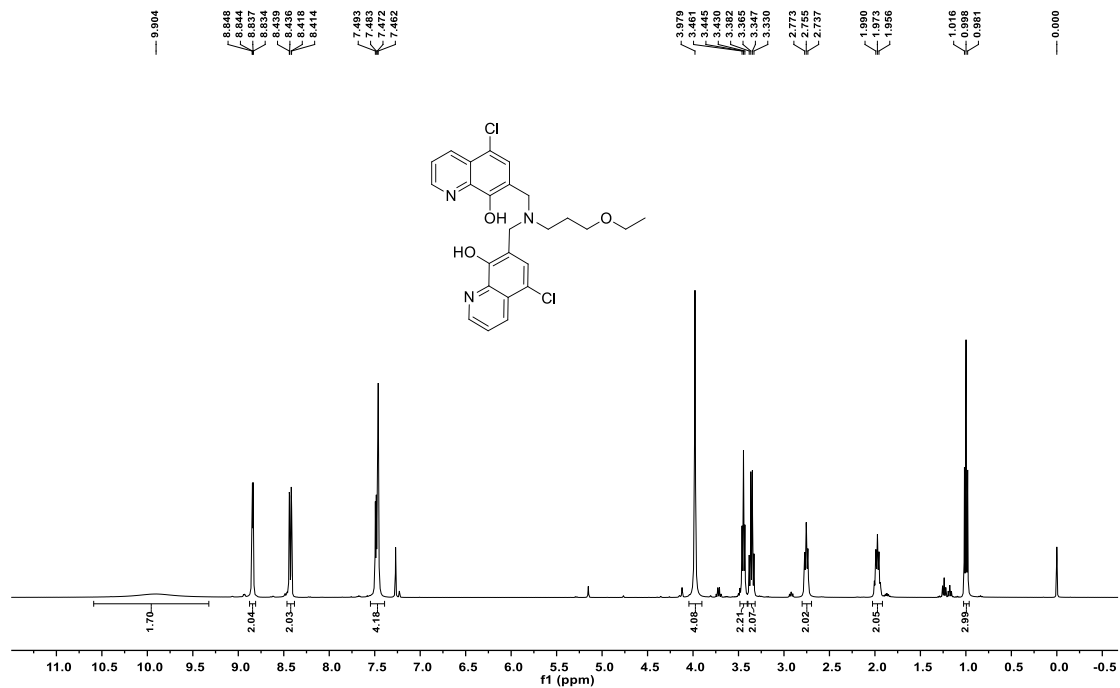


Figure S18. ¹H NMR (top) and ¹³C NMR (bottom) of 7,7'-[[3-ethoxypropyl)azanediy]bis(methylene)]bis(5-chloroquinolin-8-ol) (**6a**)

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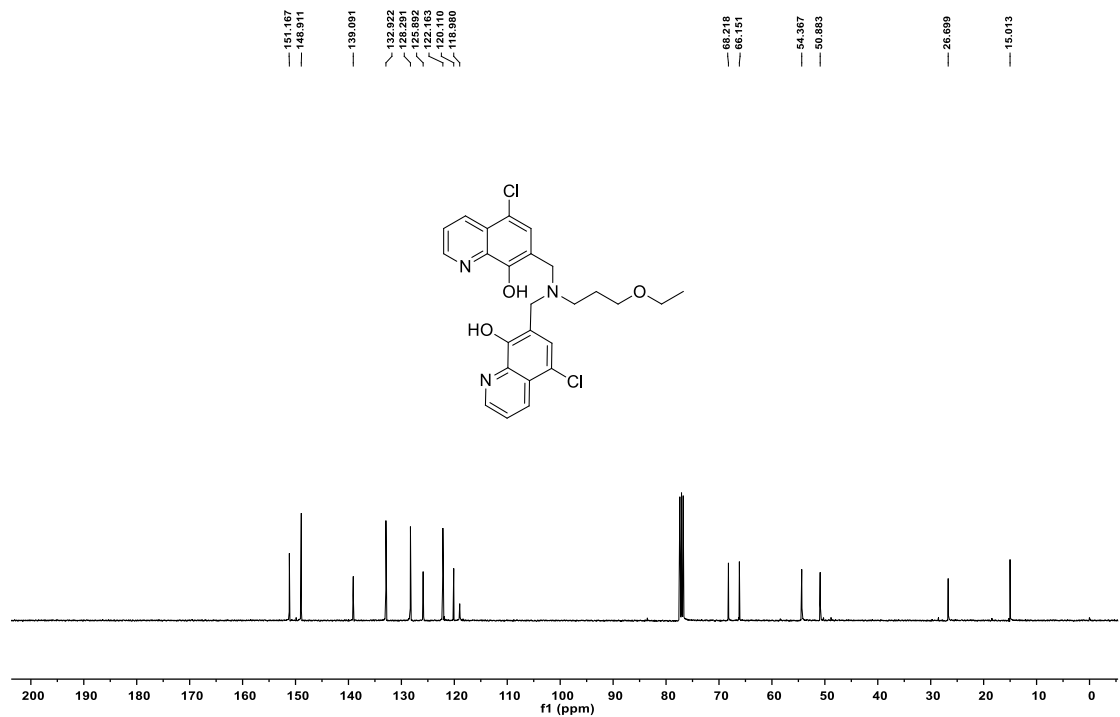


Figure S19. ^1H NMR (top) and ^{13}C NMR (bottom) of (*S*)-ethyl-2-[bis[(5-chloro-8-hydroxyquinolin-7-yl)methyl]amino]-3-phenylpropanoate (**6b**)

