

Position-Selective Synthesis and Biological Evaluation of Four Isomeric A-Ring Amino Derivatives of the Alkaloid Luotonin A

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Supplementary Material

IL1; 2-Nitrophenyl-Amid / DMSO 1H

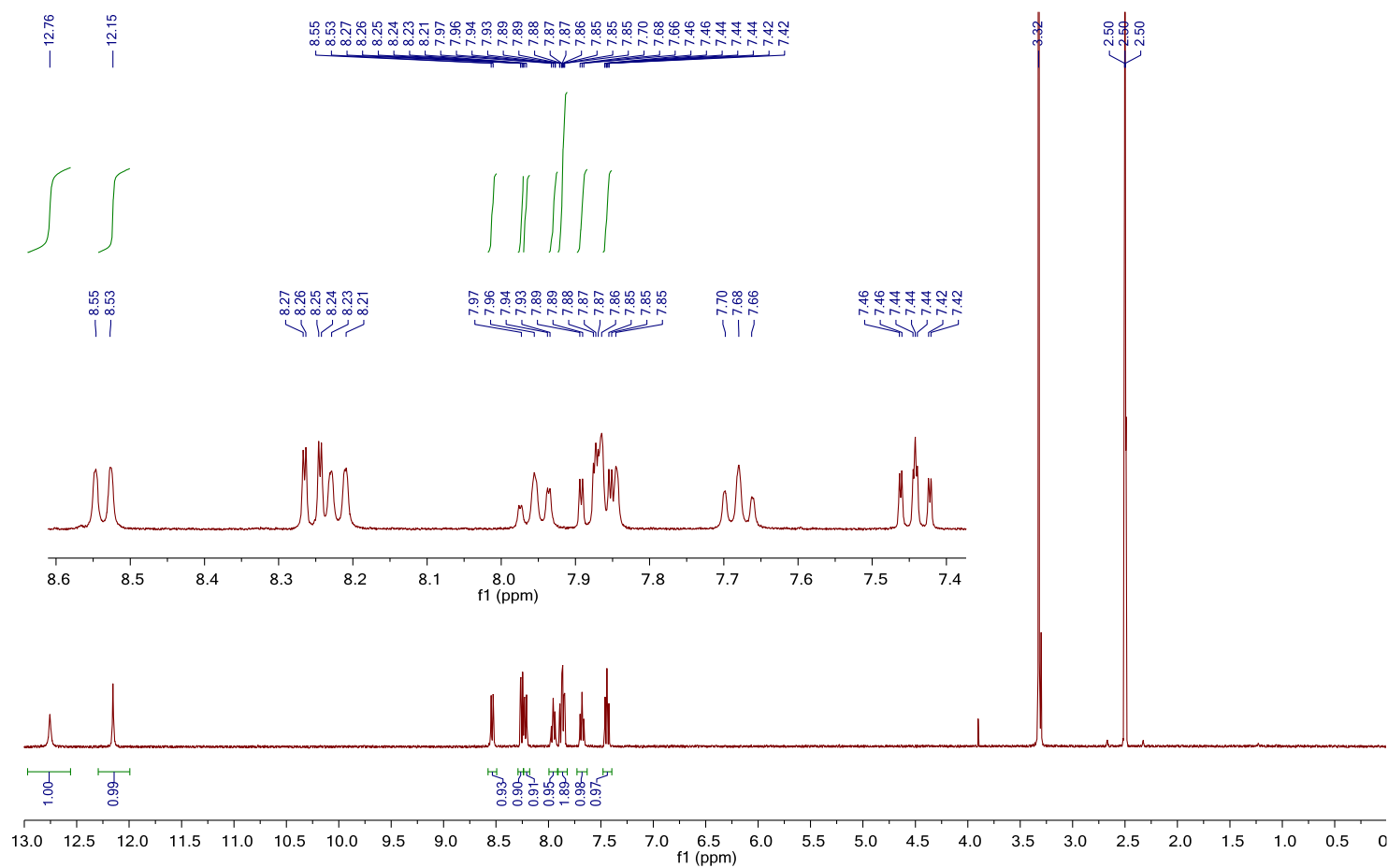


Figure S1. ¹H NMR spectrum of *N*-(2-nitrophenyl)-4-oxo-3,4-dihydroquinazoline-2-carboxamide (**2b**).

IL1; 2-Nitrophenyl-Amid / DMSO 13C CPD

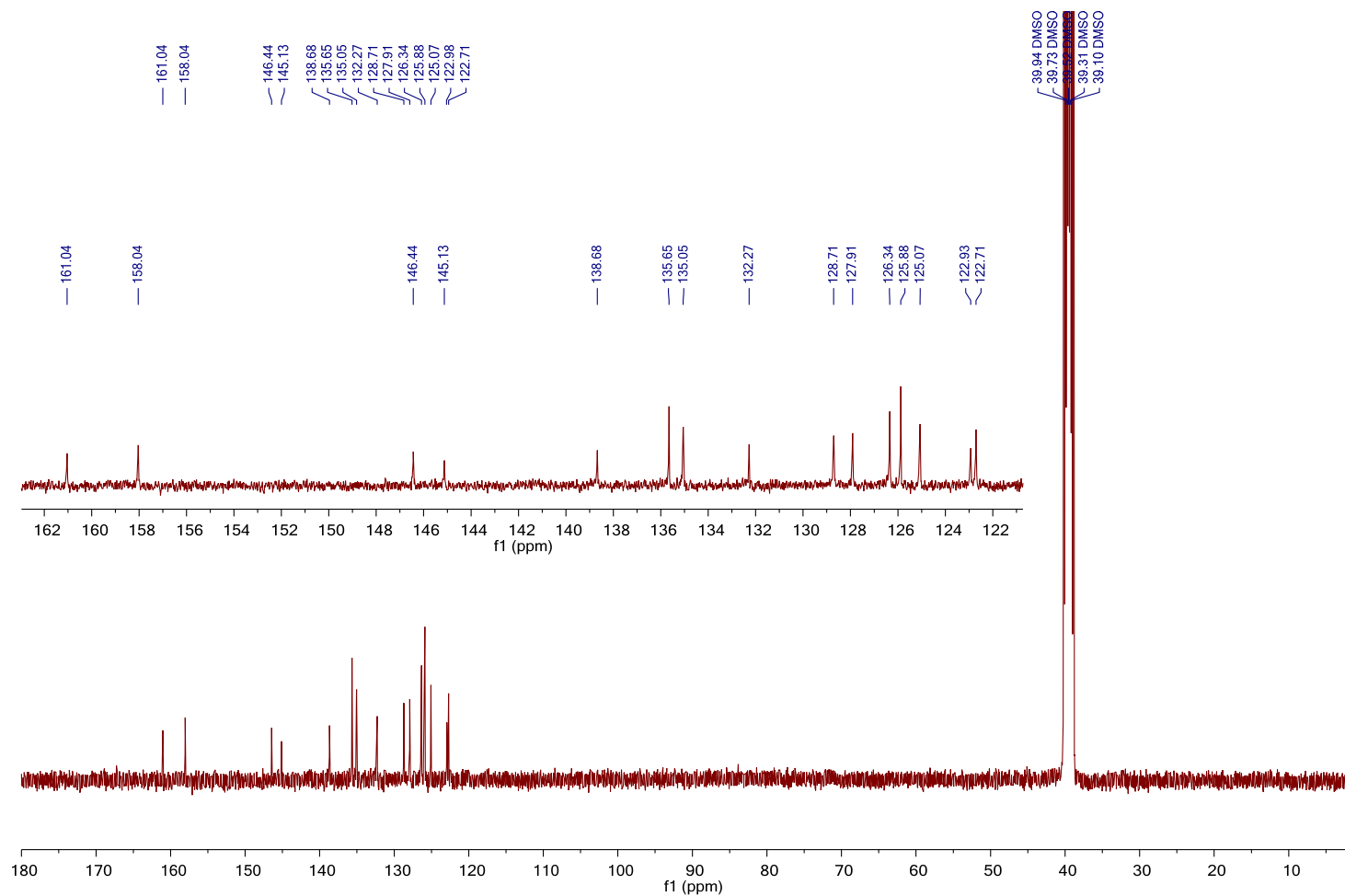


Figure S2. ^{13}C NMR spectrum of *N*-(2-nitrophenyl)-4-oxo-3,4-dihydroquinazoline-2-carboxamide (2b).

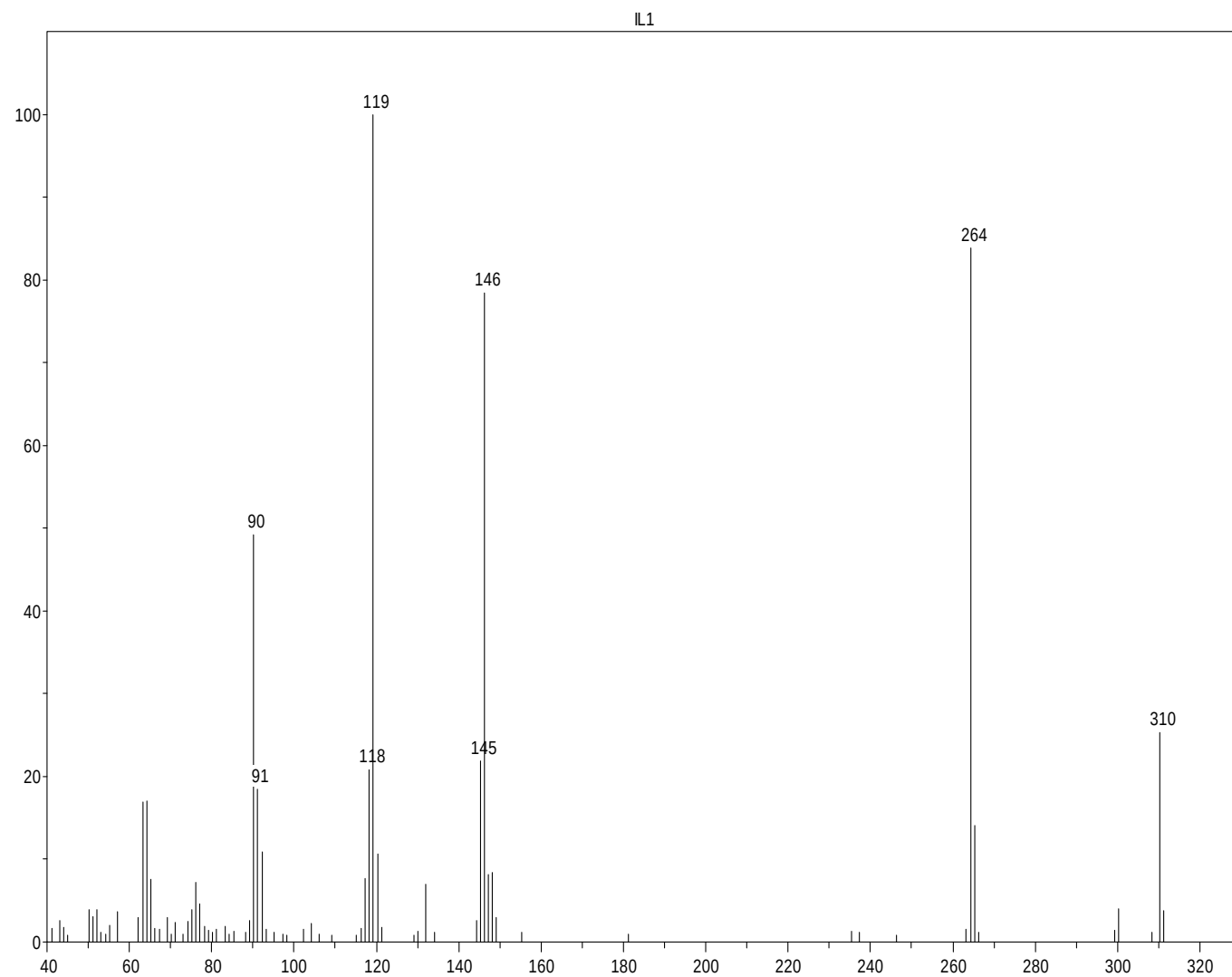


Figure S3. EI-MS of *N*-(2-nitrophenyl)-4-oxo-3,4-dihydroquinazoline-2-carboxamide (**2b**).

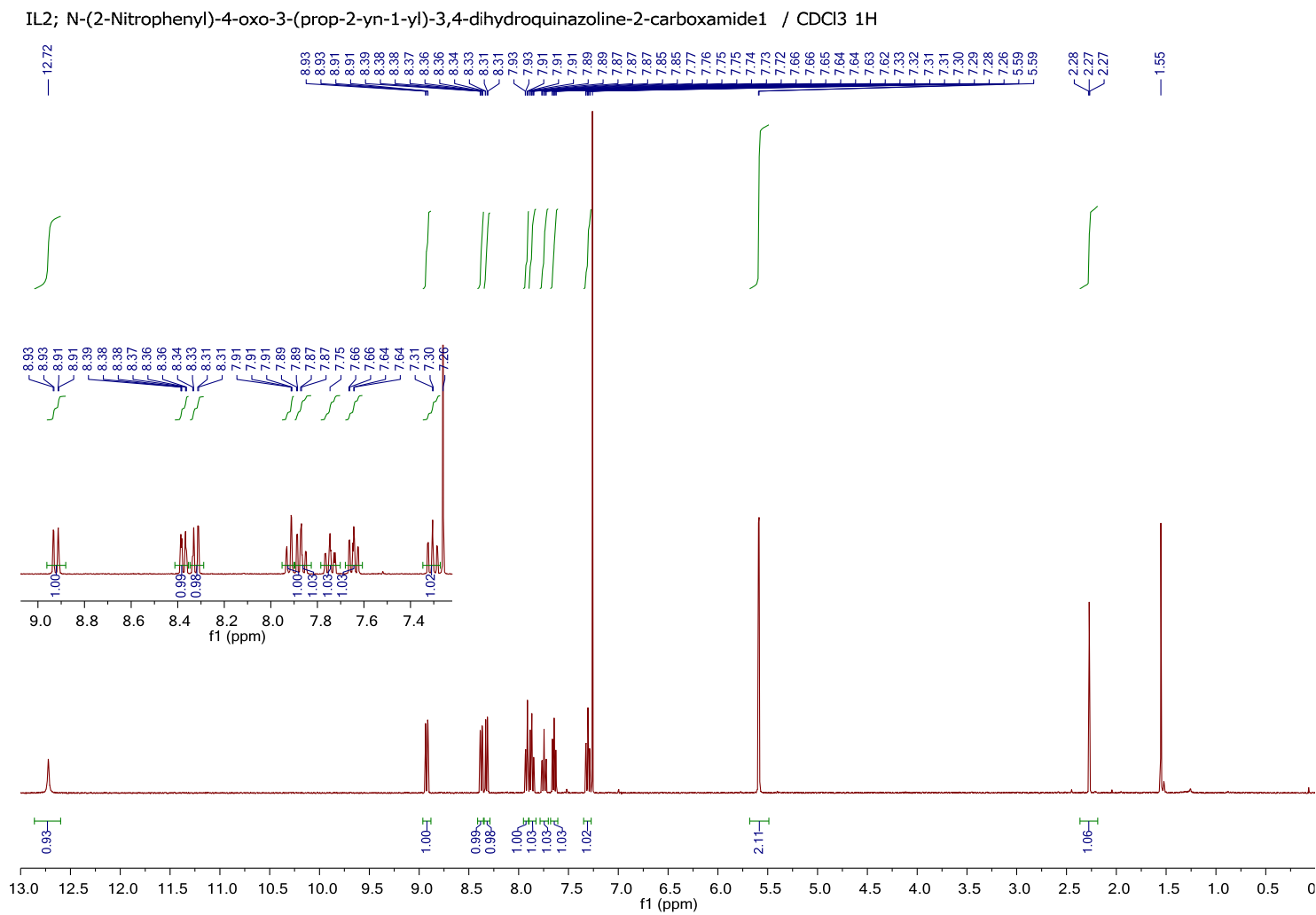


Figure S4. ¹H NMR spectrum of *N*-(2-nitrophenyl)-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide (**3b**).

IL2; N-(2-Nitrophenyl)-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide1 / CDCl₃ C13APT

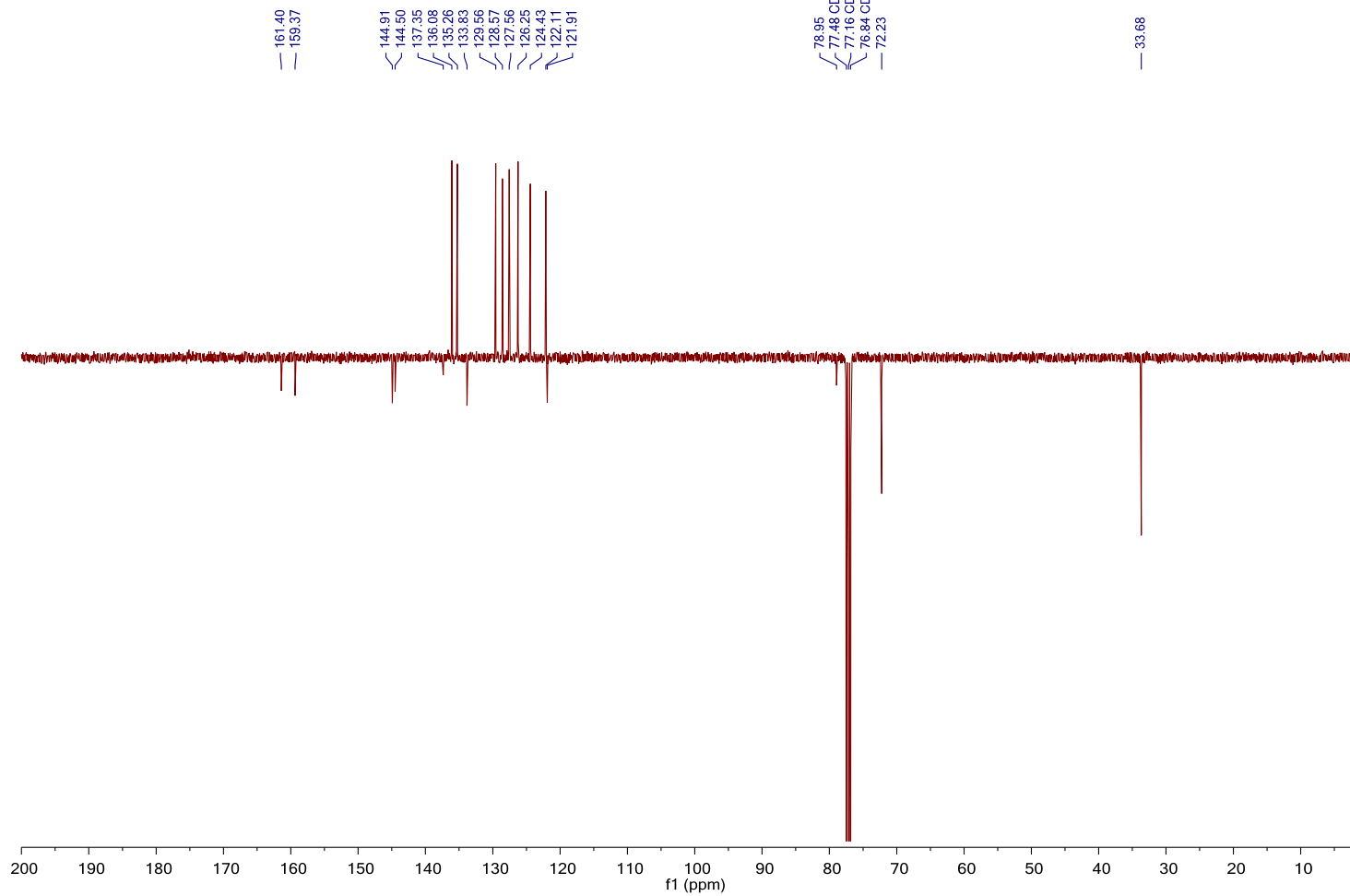


Figure S5. ¹³C NMR spectrum of N-(2-nitrophenyl)-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide (**3b**).

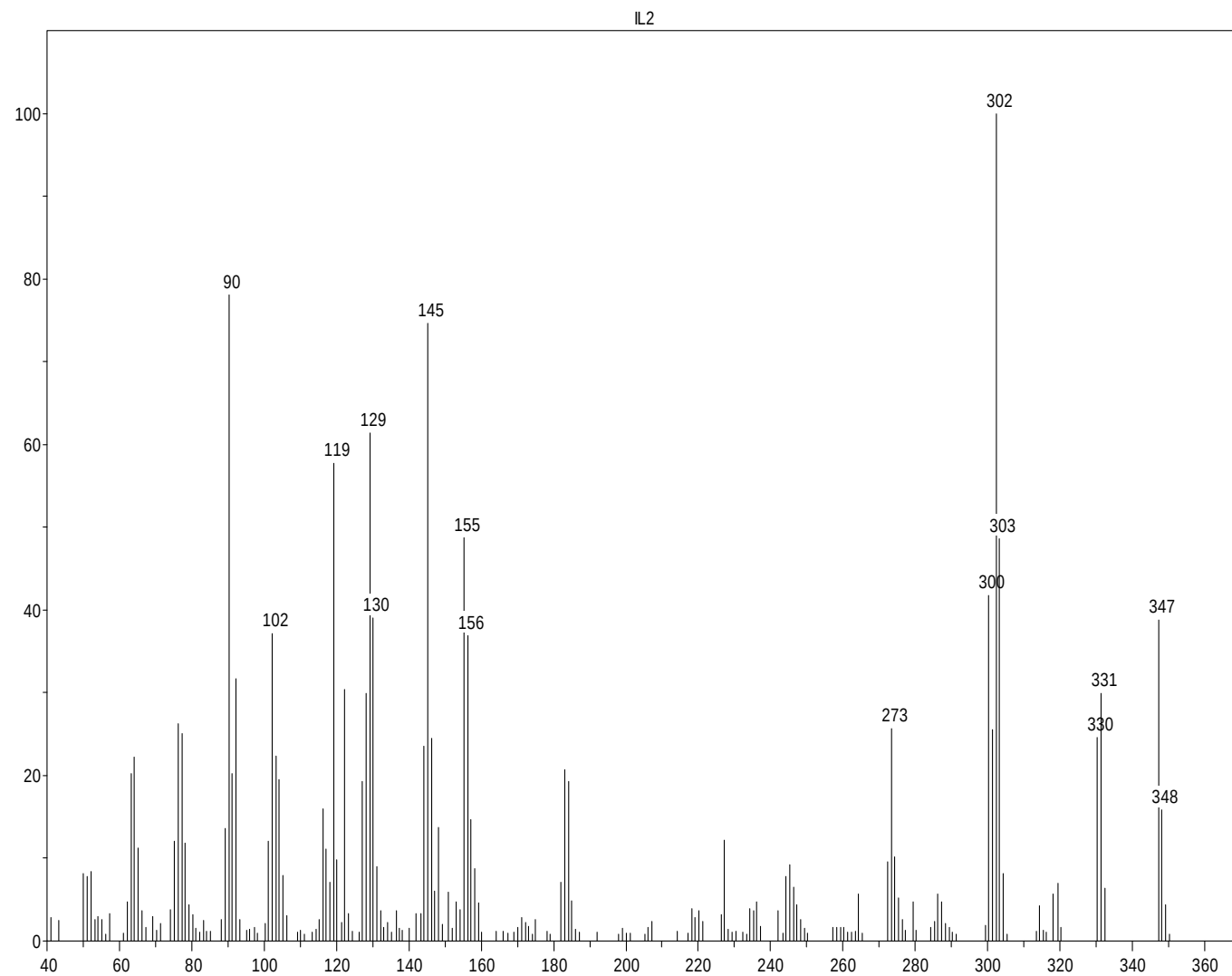


Figure S6. EI-MS of *N*-(2-nitrophenyl)-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide (**3b**).

IL4; 4-Nitroquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO 1H

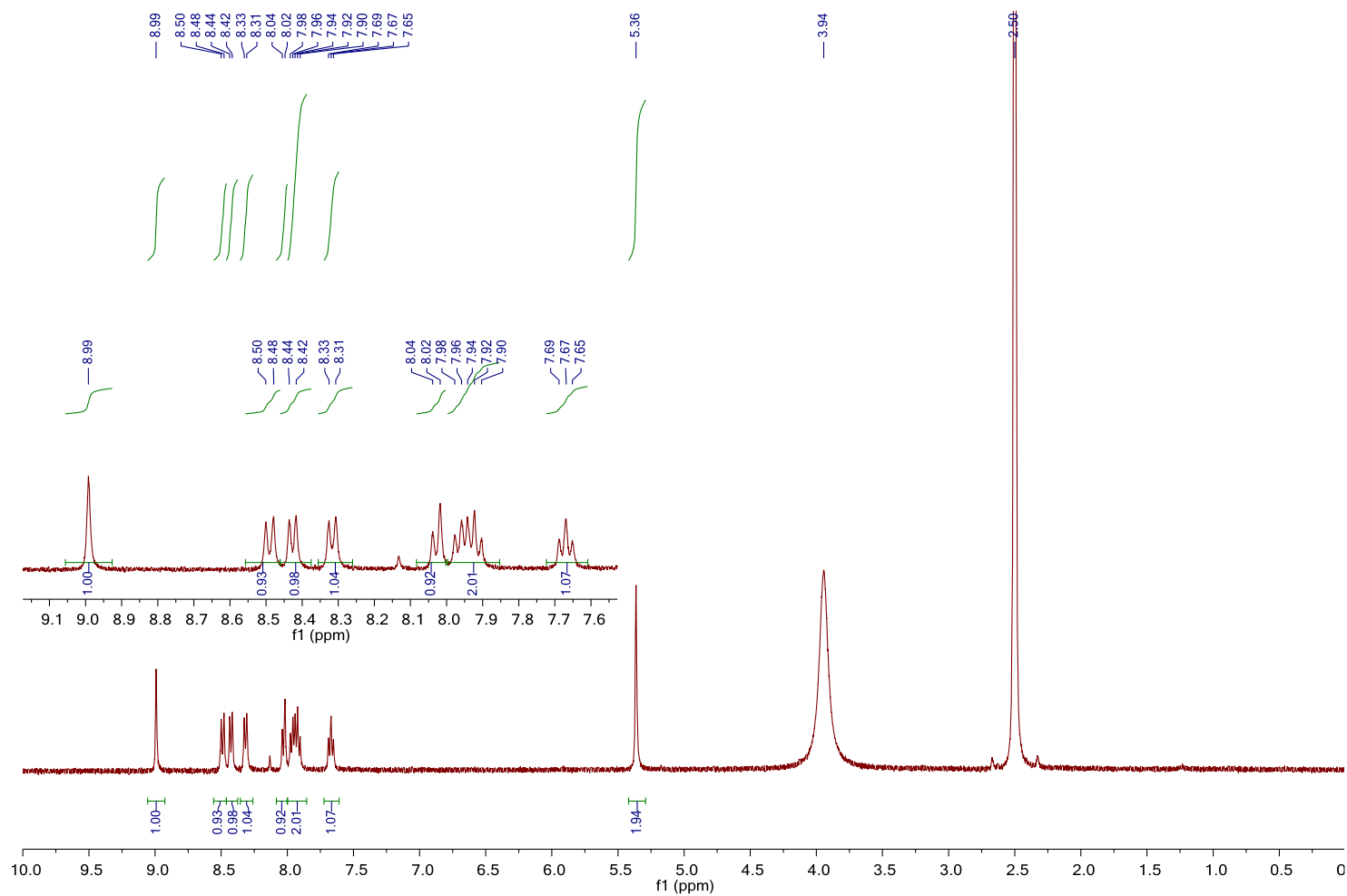


Figure S7. ^1H NMR spectrum of 4-Nitroquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one (**4b**).

IL4; 4-Nitroquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO C13CPD

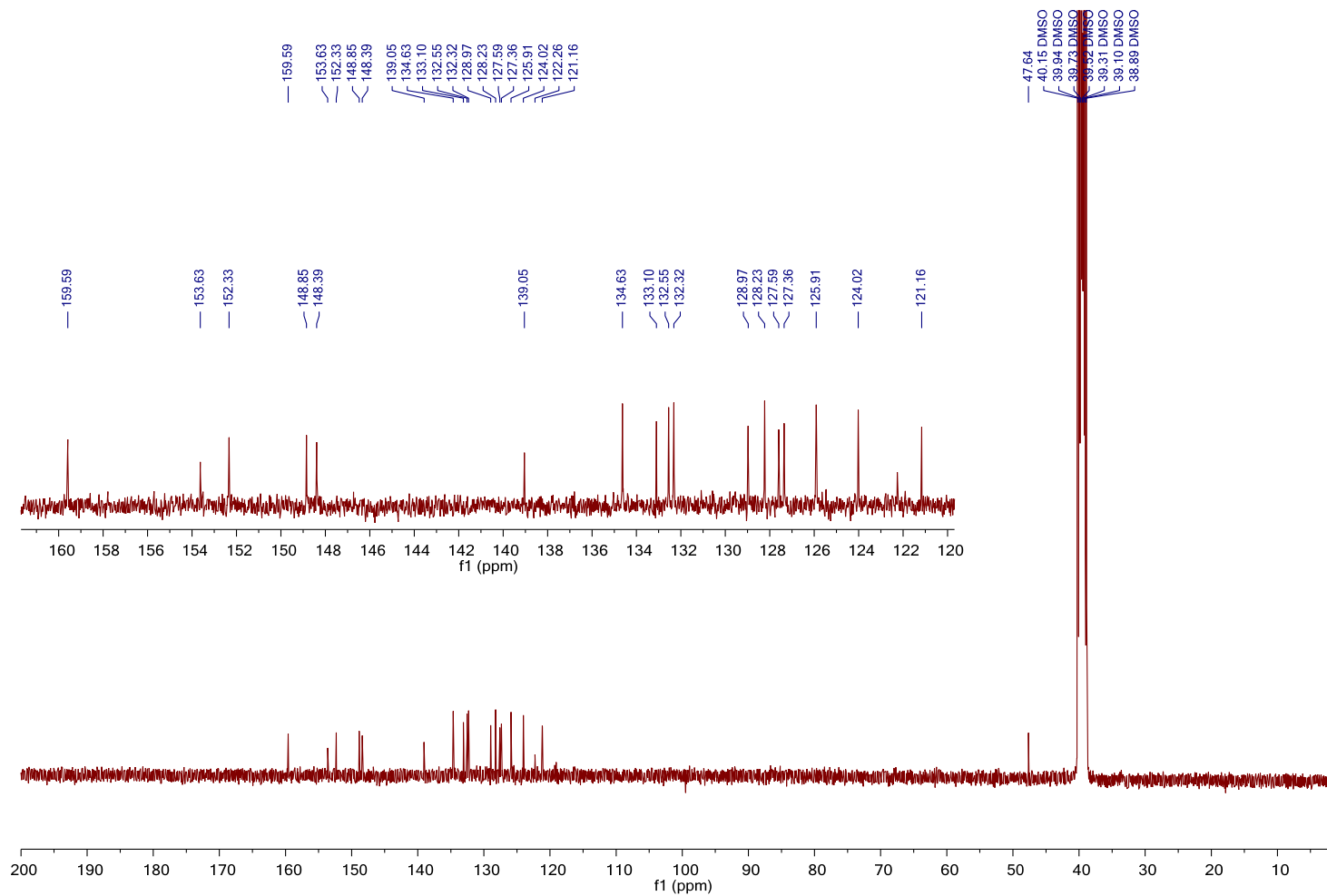


Figure S8. ^{13}C NMR spectrum of 4-Nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**4b**).

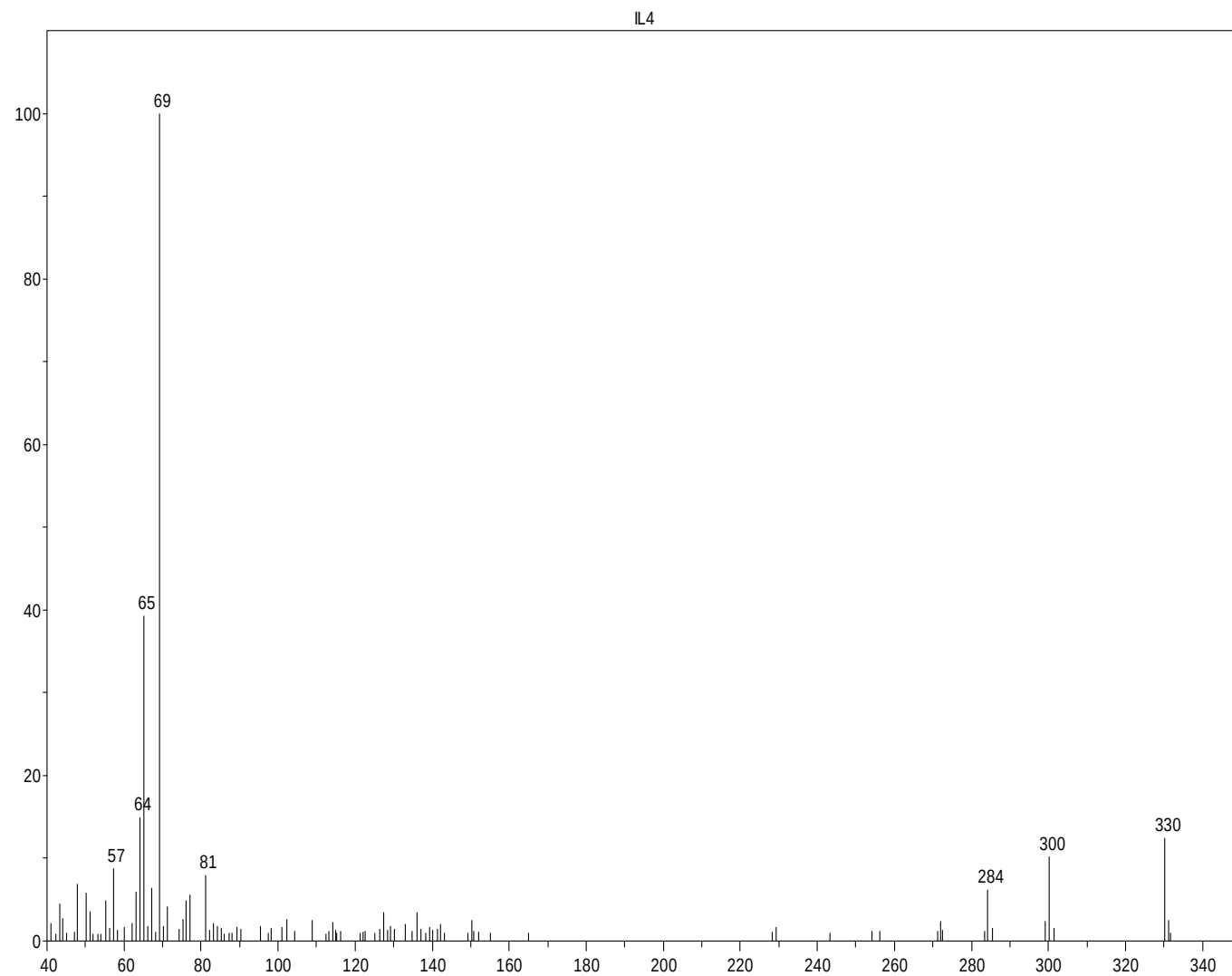


Figure S9. EI-MS of 4-Nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**4b**).

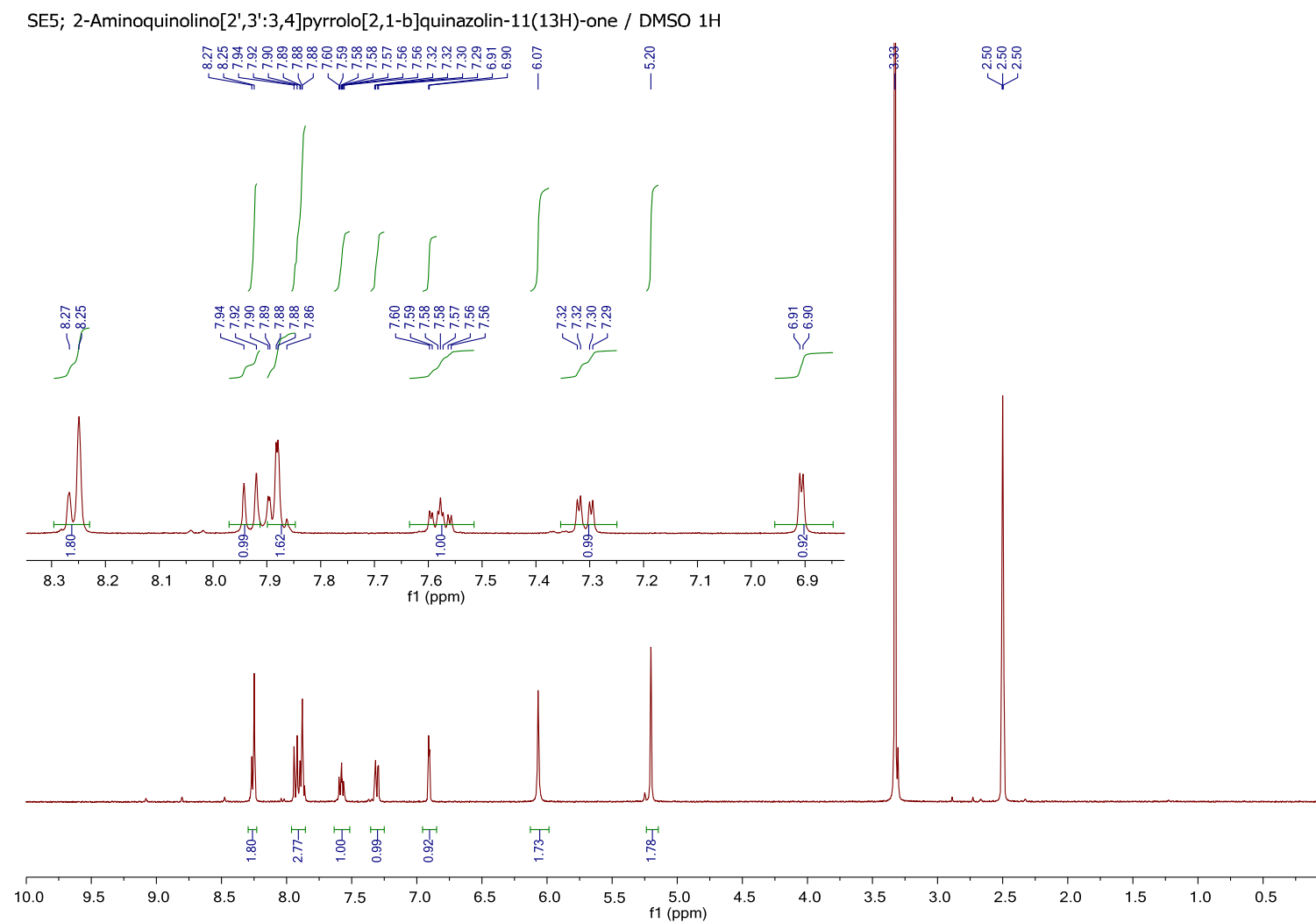


Figure S10. ^1H NMR spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one (5a).

SE5; 2-Aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one / DMSO COSY

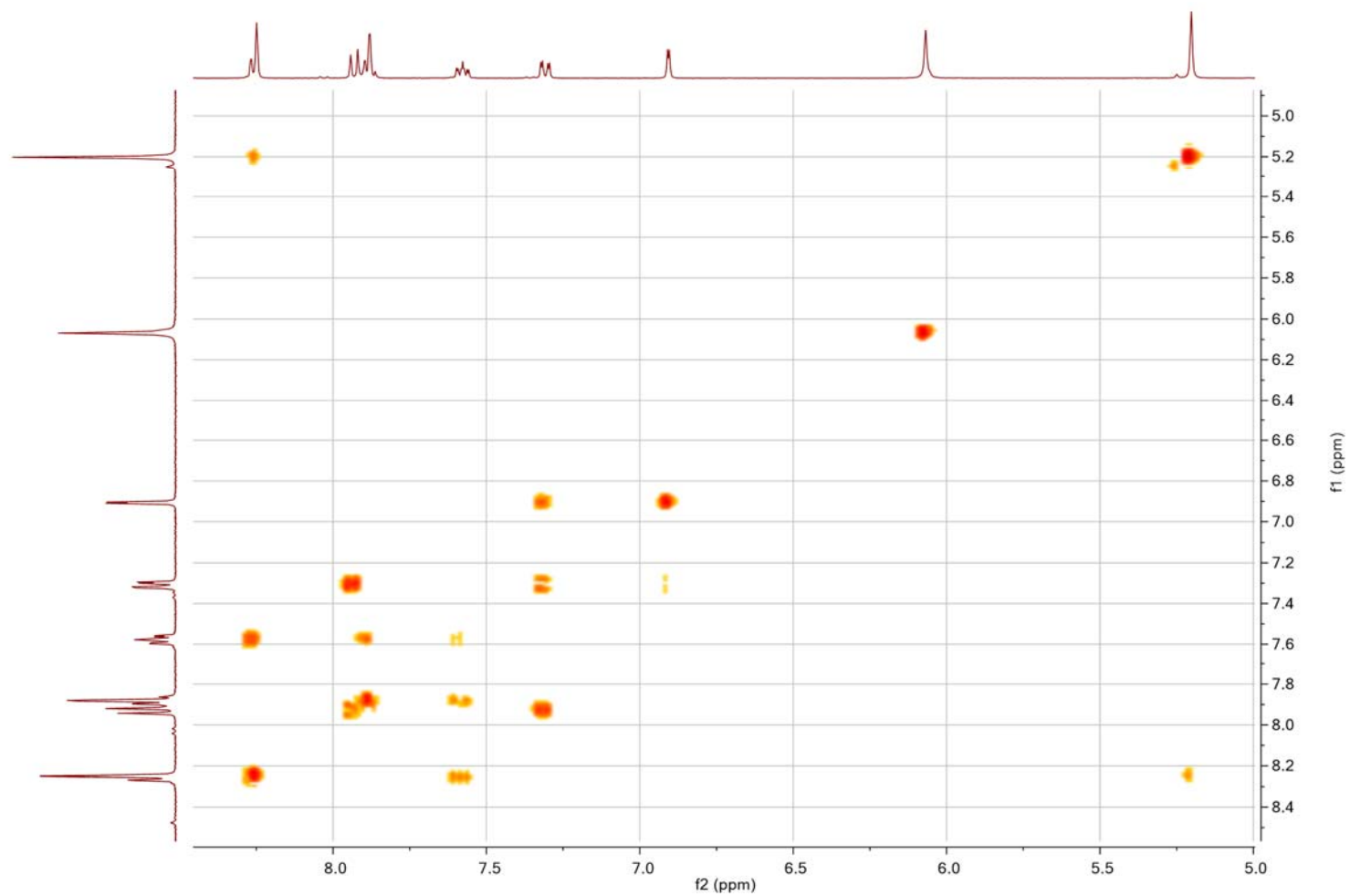


Figure S11. COSY spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5a**).

SE5; 2-Aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one / DMSO NOESY

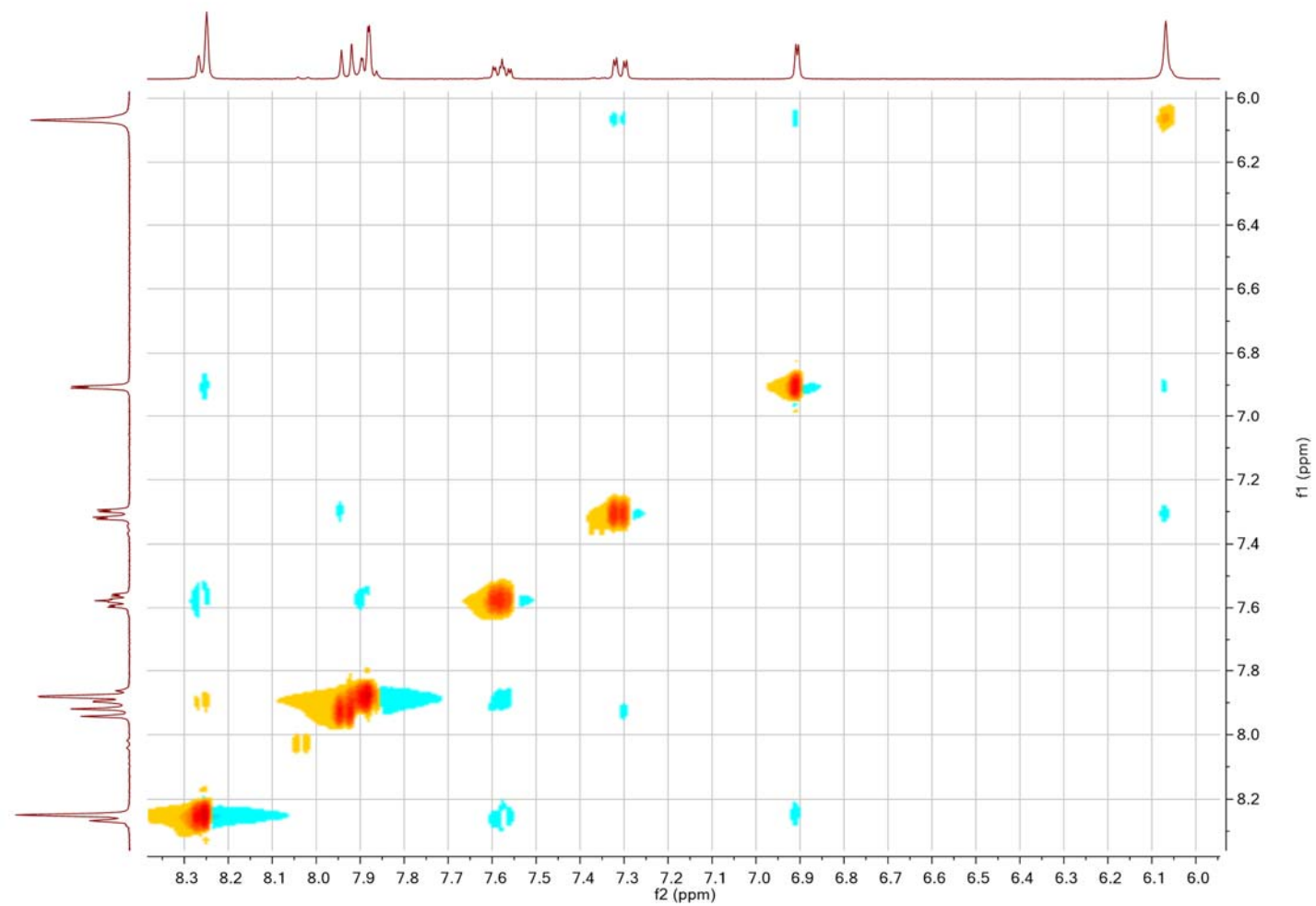


Figure S12. NOESY spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (5a).

SE5; 2-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO C13APT

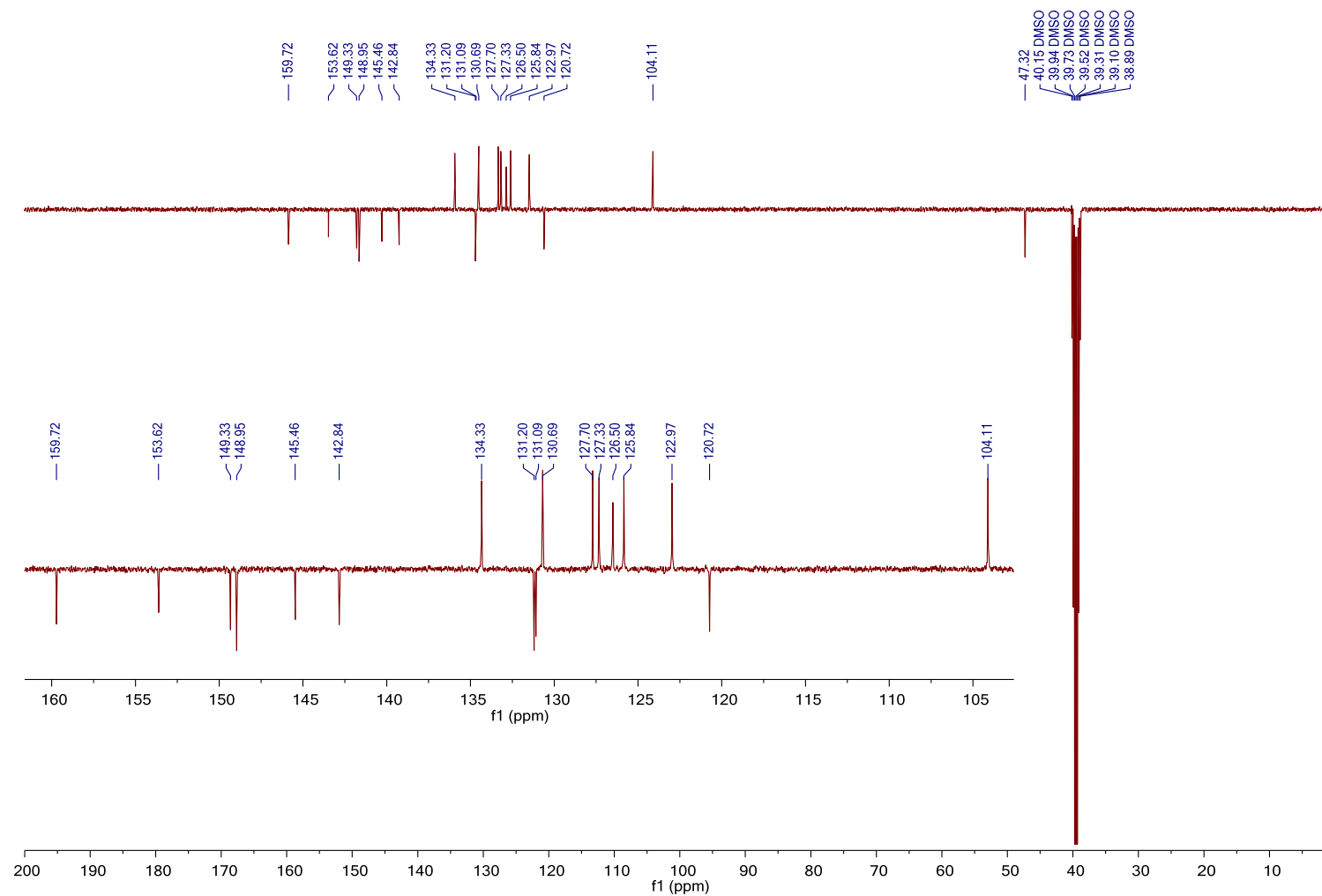


Figure S13. ^{13}C NMR spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one (**5a**).

SE5; 2-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO HSQC

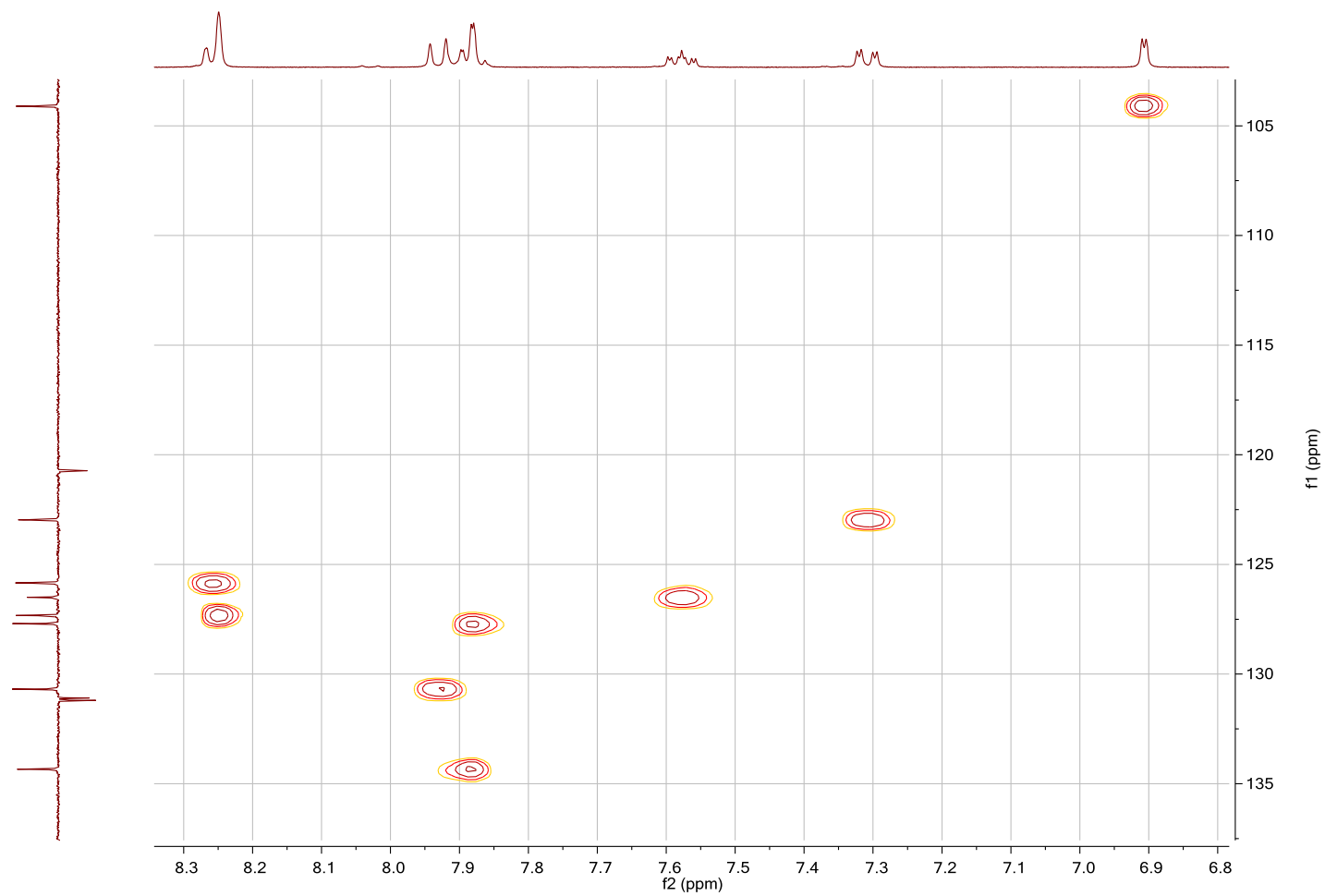


Figure S14. HSQC spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one (**5a**).

SE5; 2-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO HMBC

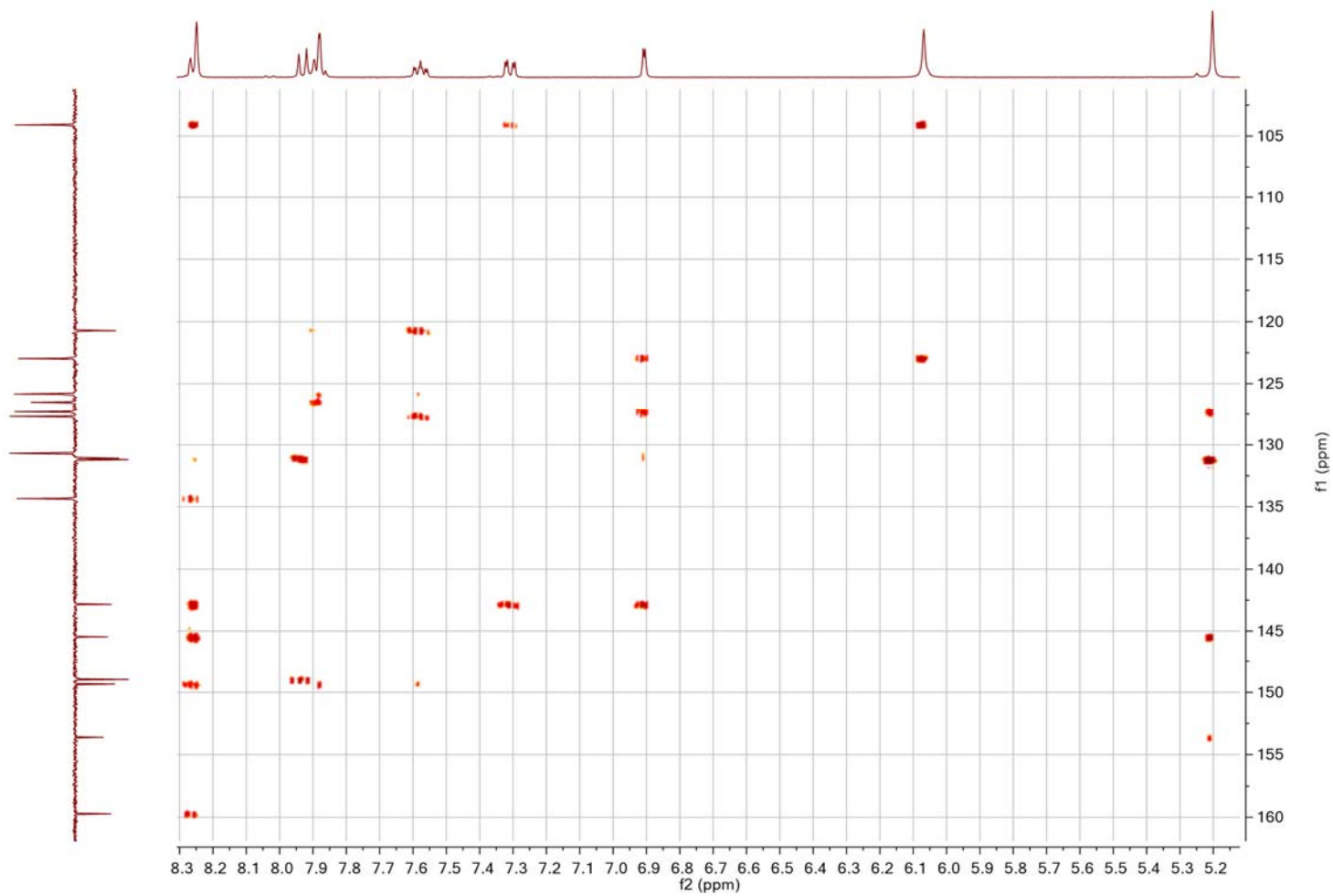


Figure S15. HMBC spectrum of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5a**).

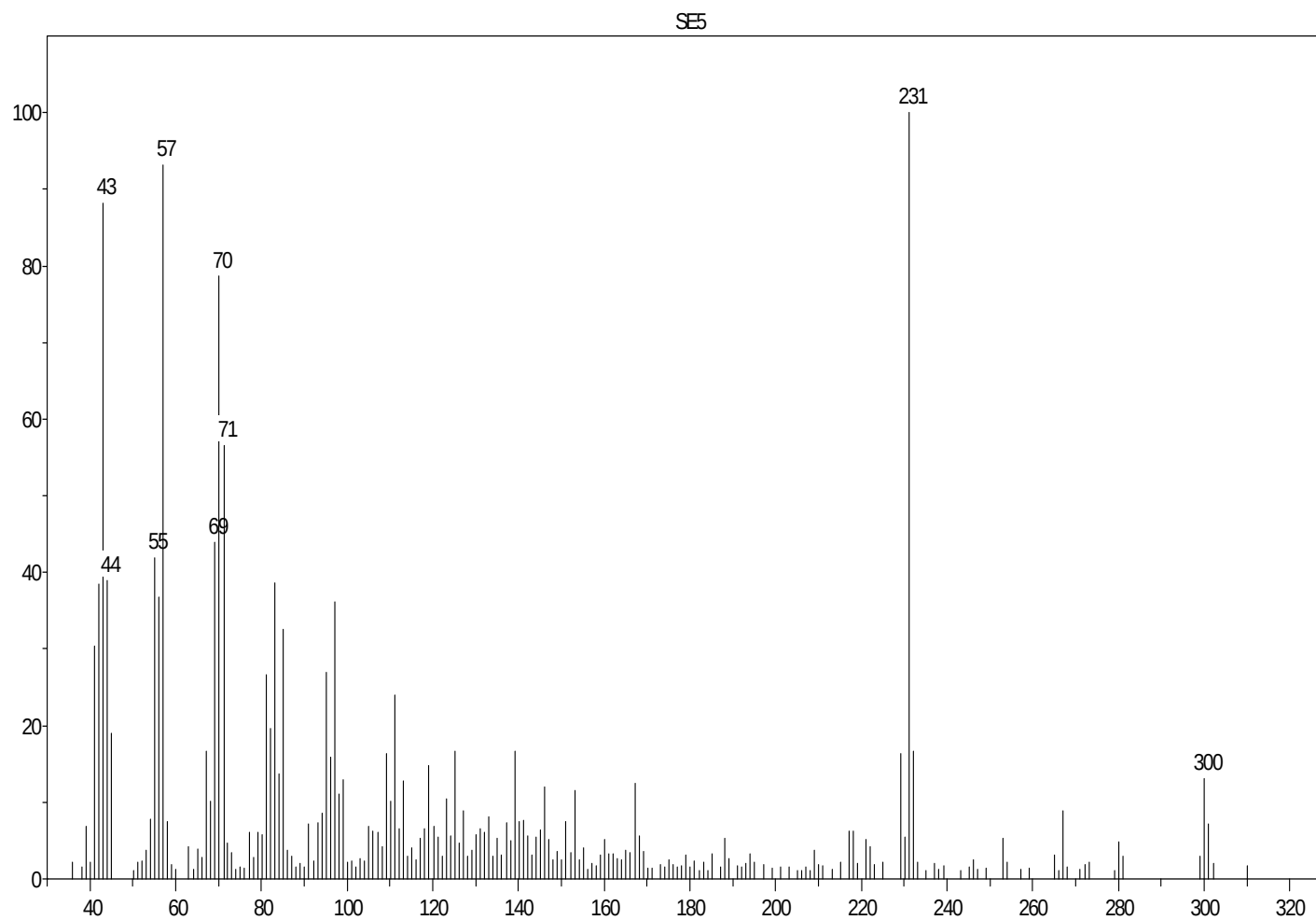


Figure S16. EI-MS of 2-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5a**).

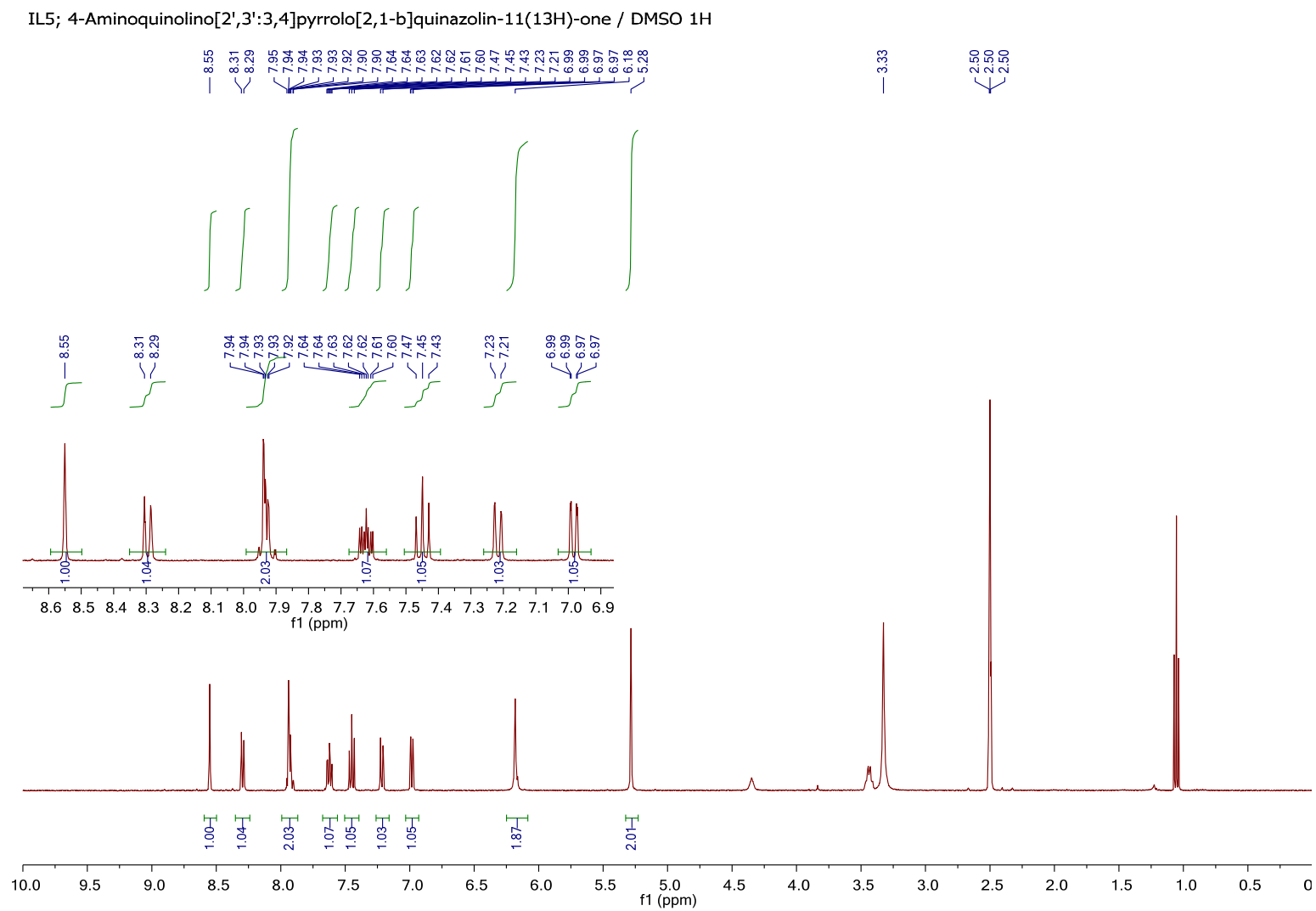


Figure S17. ^1H NMR spectrum of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13H)-one (**5b**).

IL5; 4-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO COSY

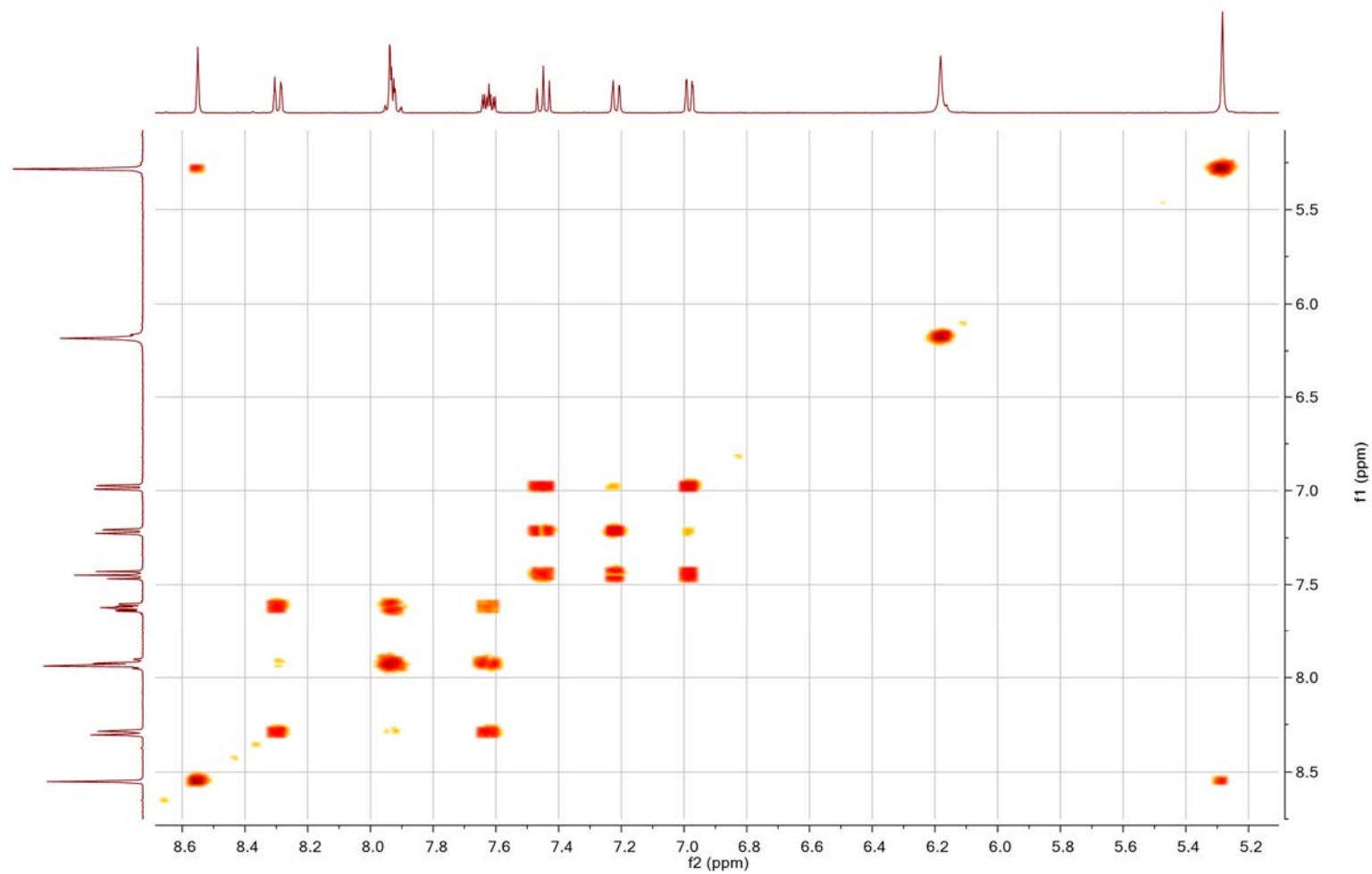


Figure S18. COSY spoection of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5b**).

IL5; 4-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO NOESY

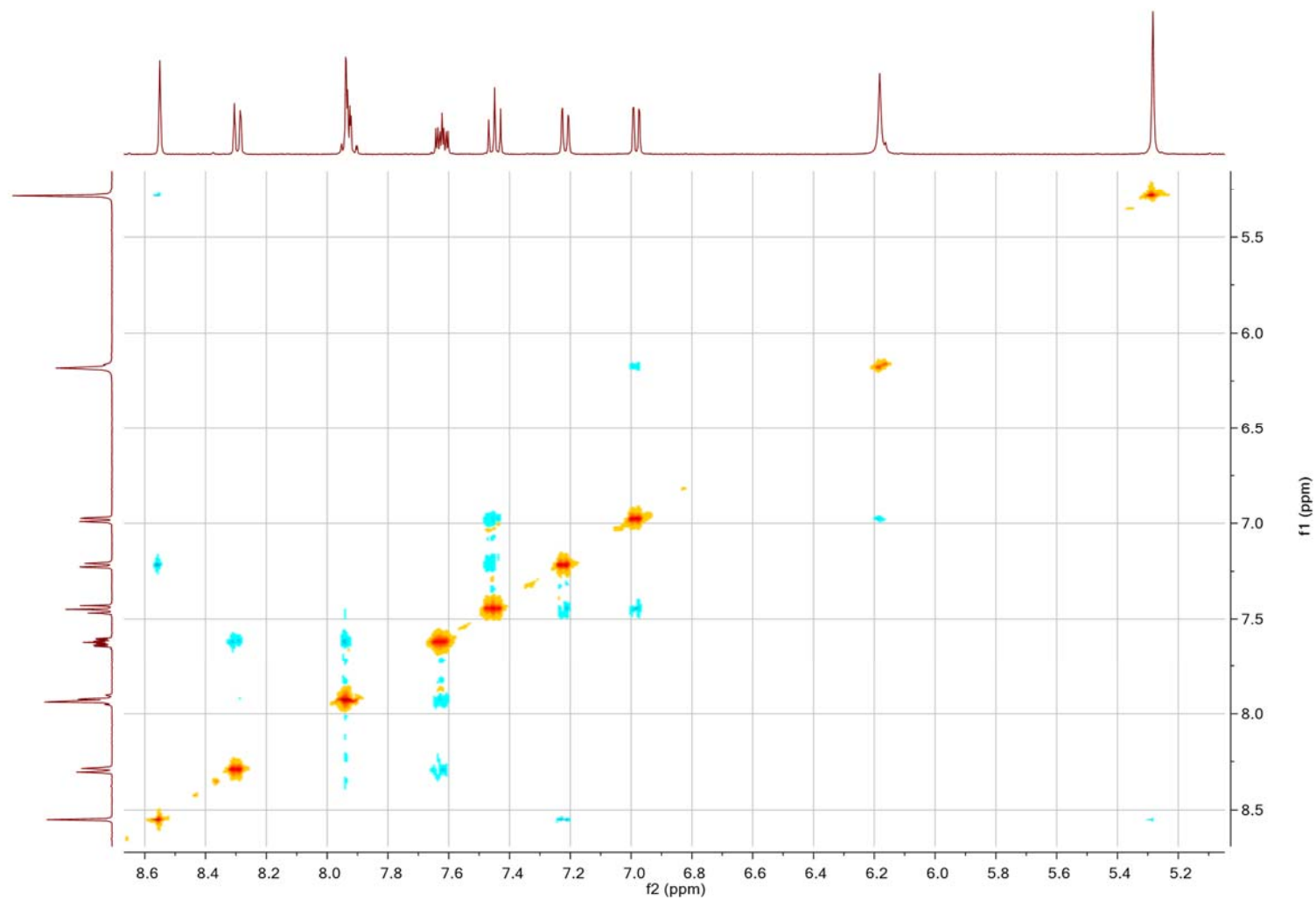


Figure S19. NOESY spectrum of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5b**).

IL5; 4-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO C13APT

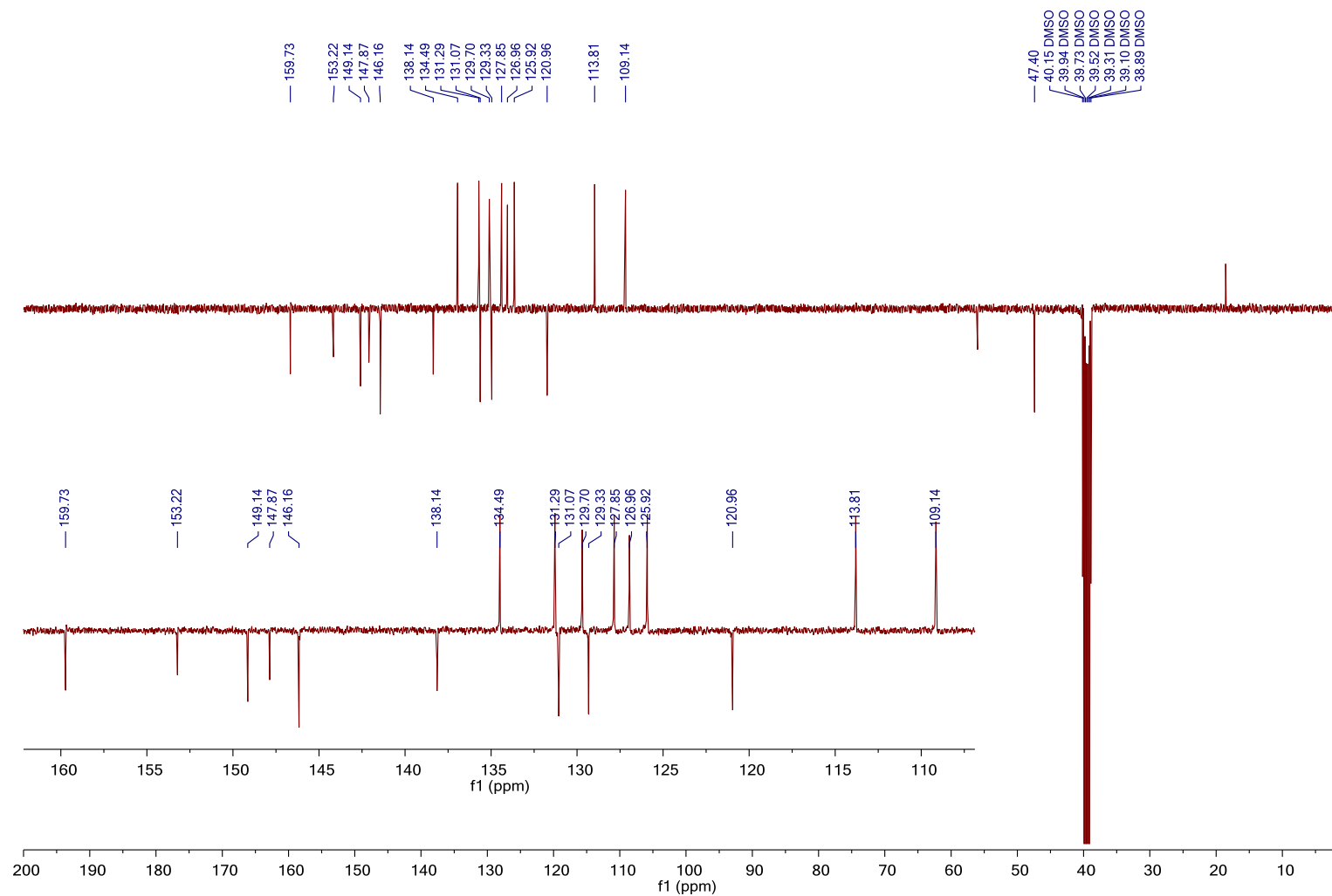


Figure S20. ^{13}C NMR spectrum of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one (**5b**).

IL5; 4-Aminoquinolino[2',3':3,4]pyrrolo[2,1-b]quinazolin-11(13H)-one / DMSO HSQC

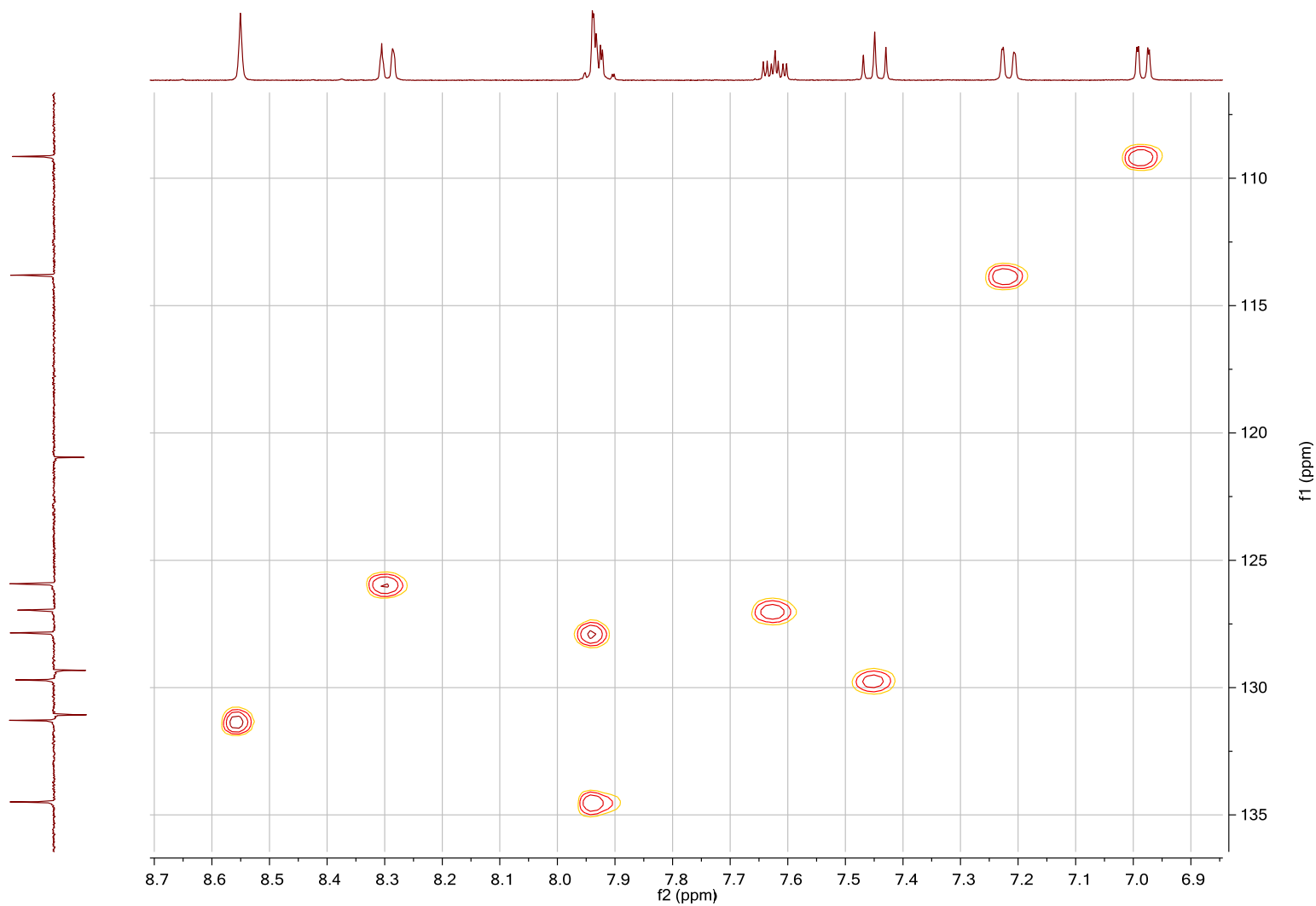


Figure S21. HSQC spoection of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5b**).

IL5; 4-Aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one / DMSO HMBC

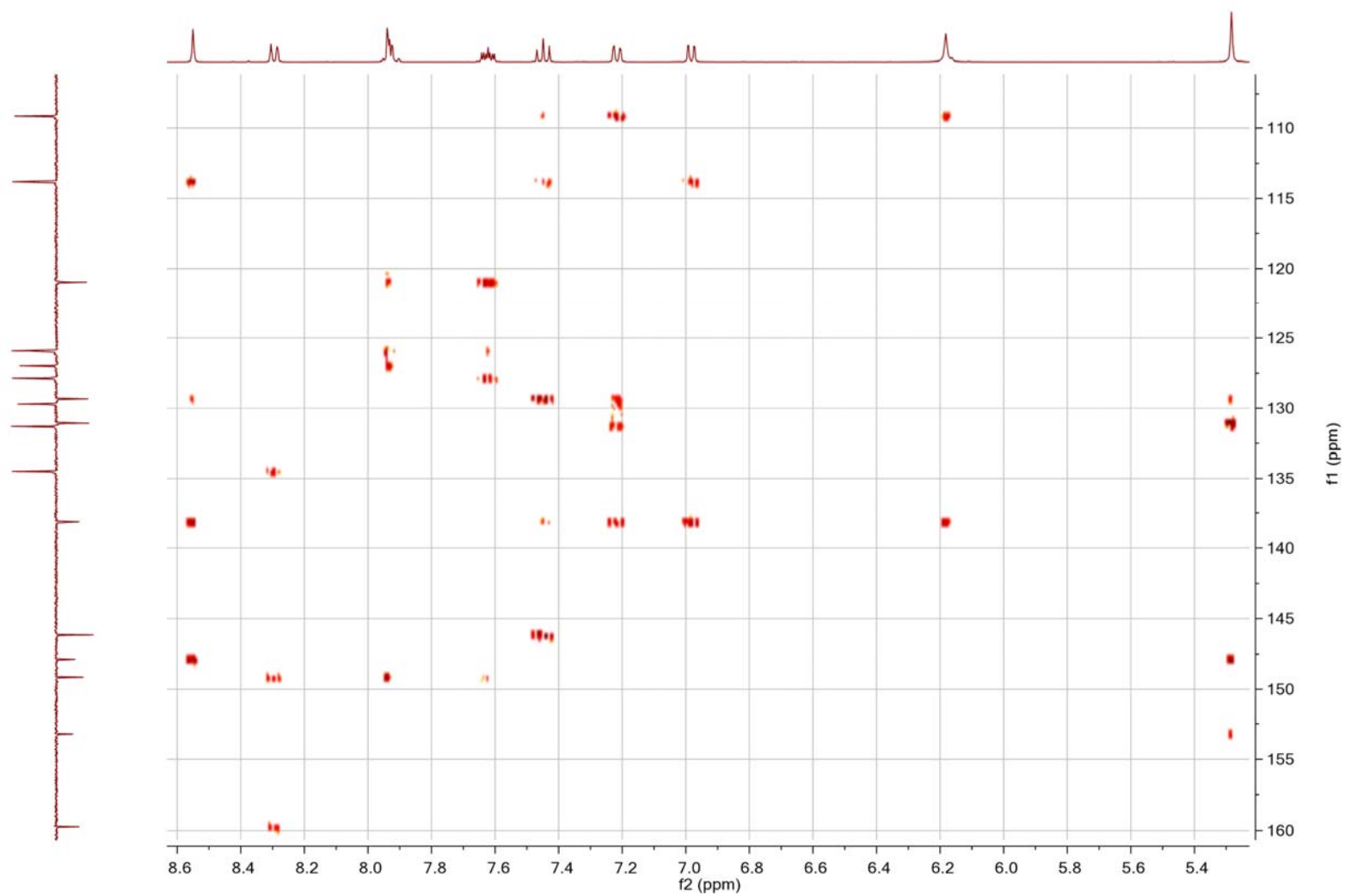


Figure S22. HMBC spectrum of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5b**).

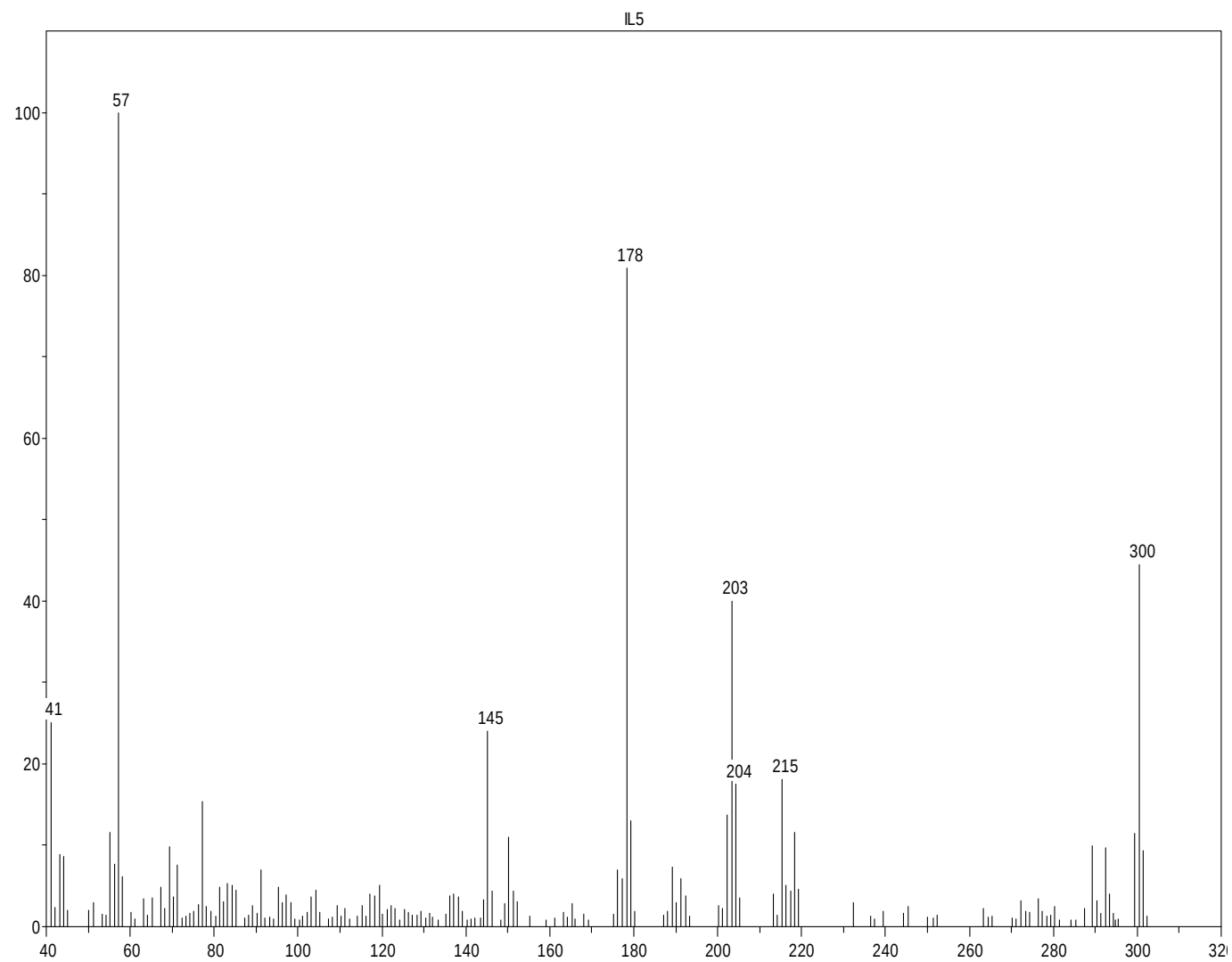


Figure S23. EI-MS of 4-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**5b**).

med1/1

MED1; 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide / DMSO 1H

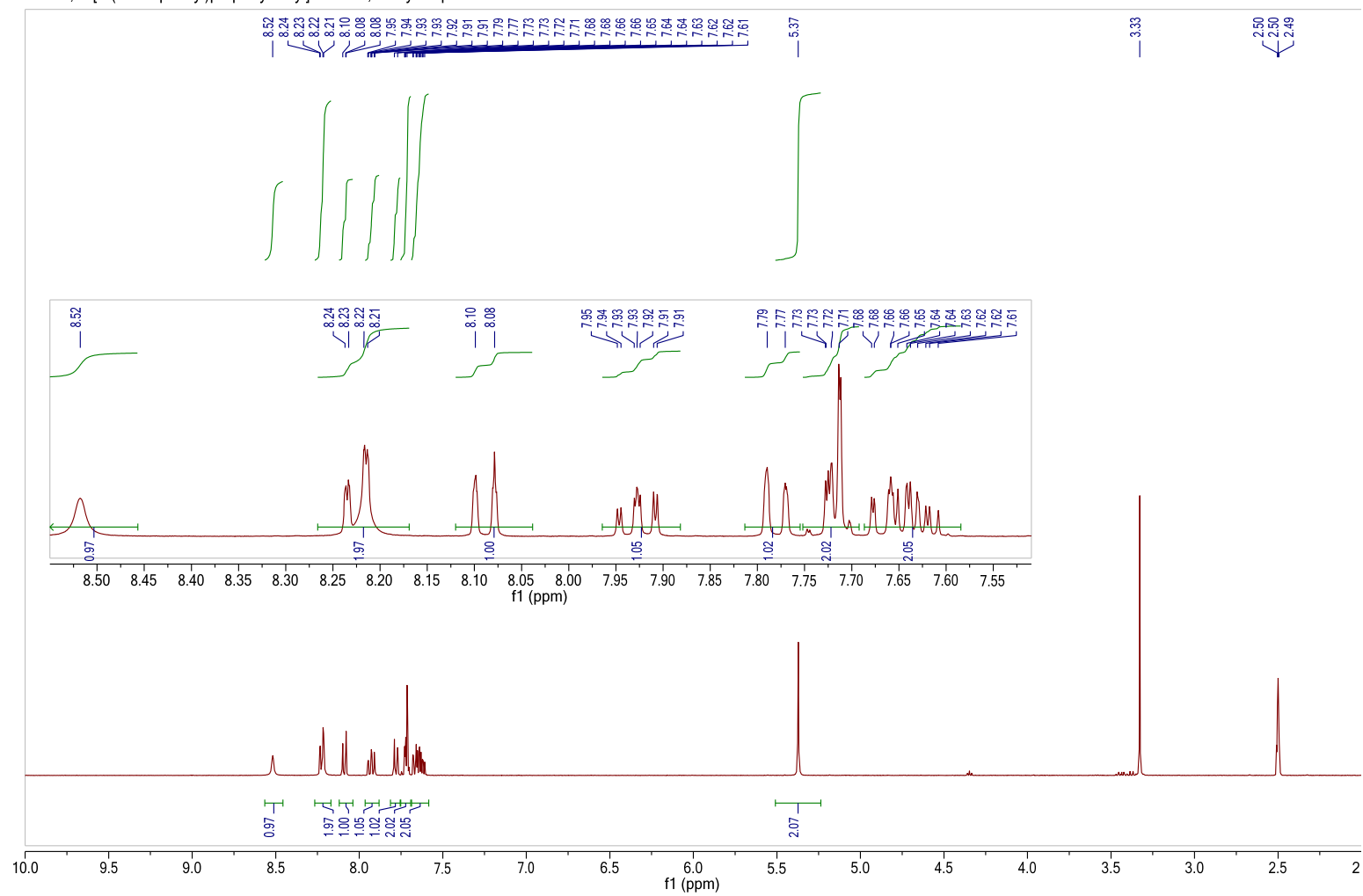


Figure S24. ^1H NMR spectrum of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (7a).

med1/1

MED1; 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide / DMSO C13APT

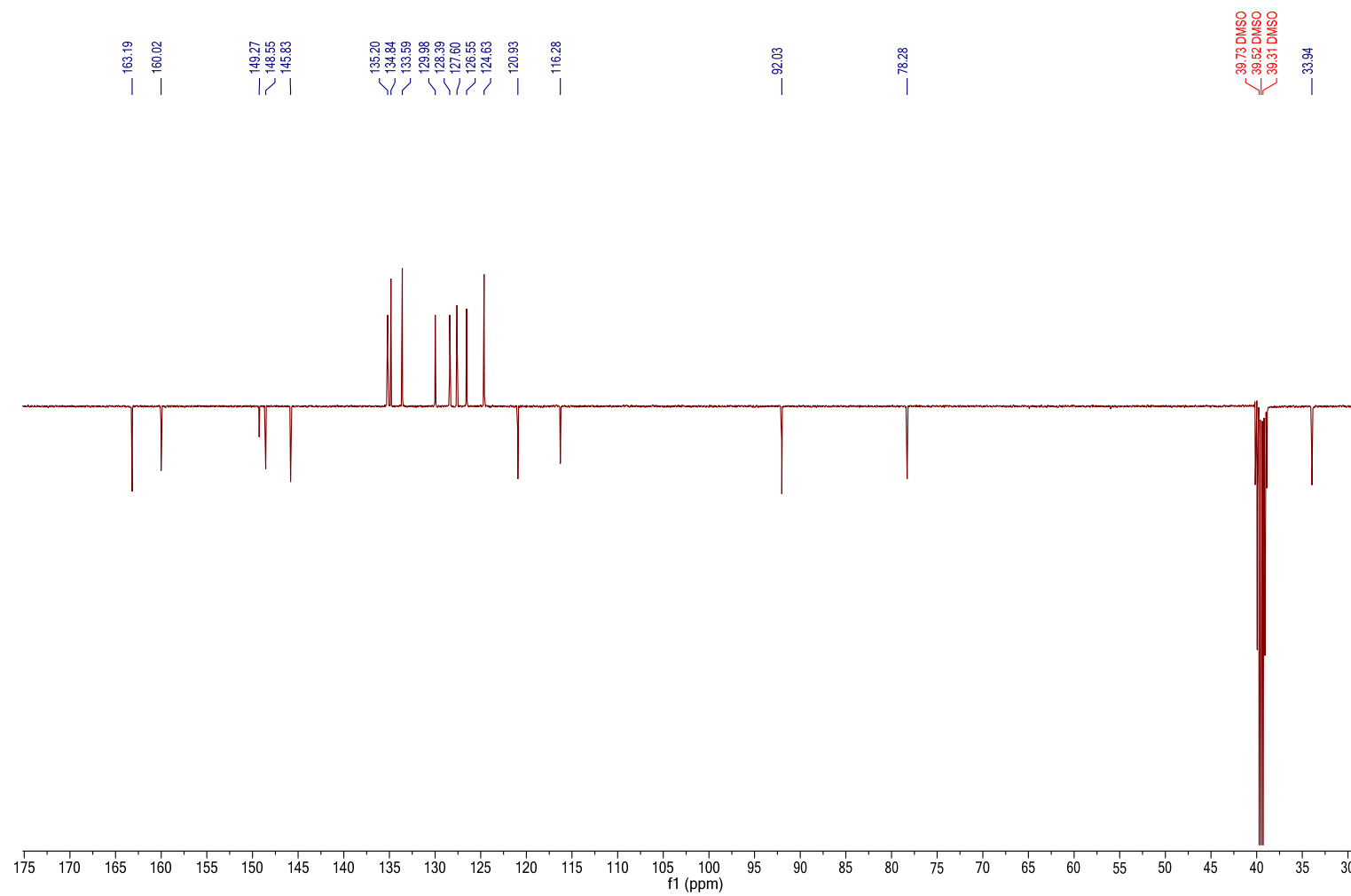


Figure S25. ¹³C NMR spectrum of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (7a).

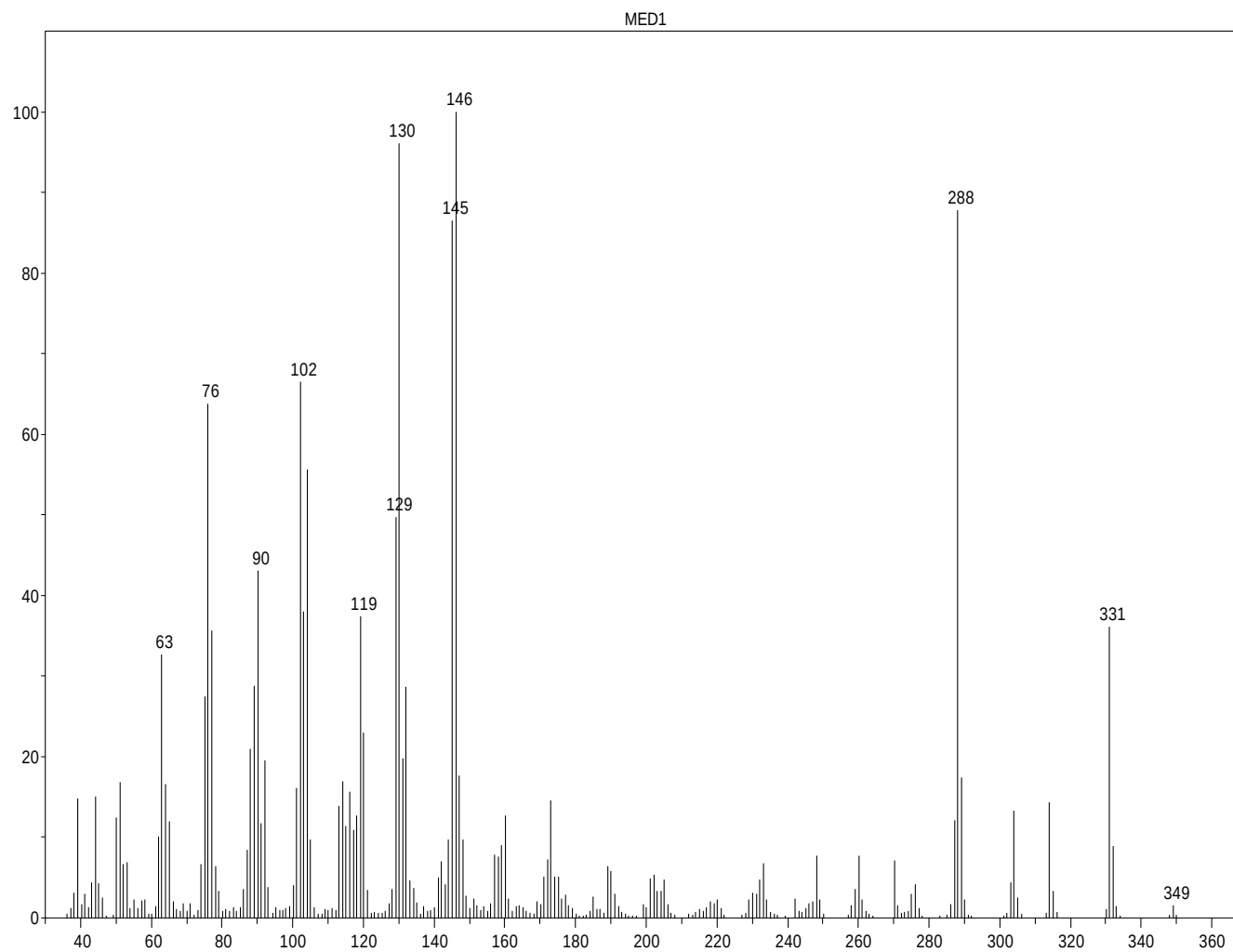


Figure S26. EI-MS of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (**7a**).

LT1; 4-Nitrophenylpropargyl-Amid / DMSO

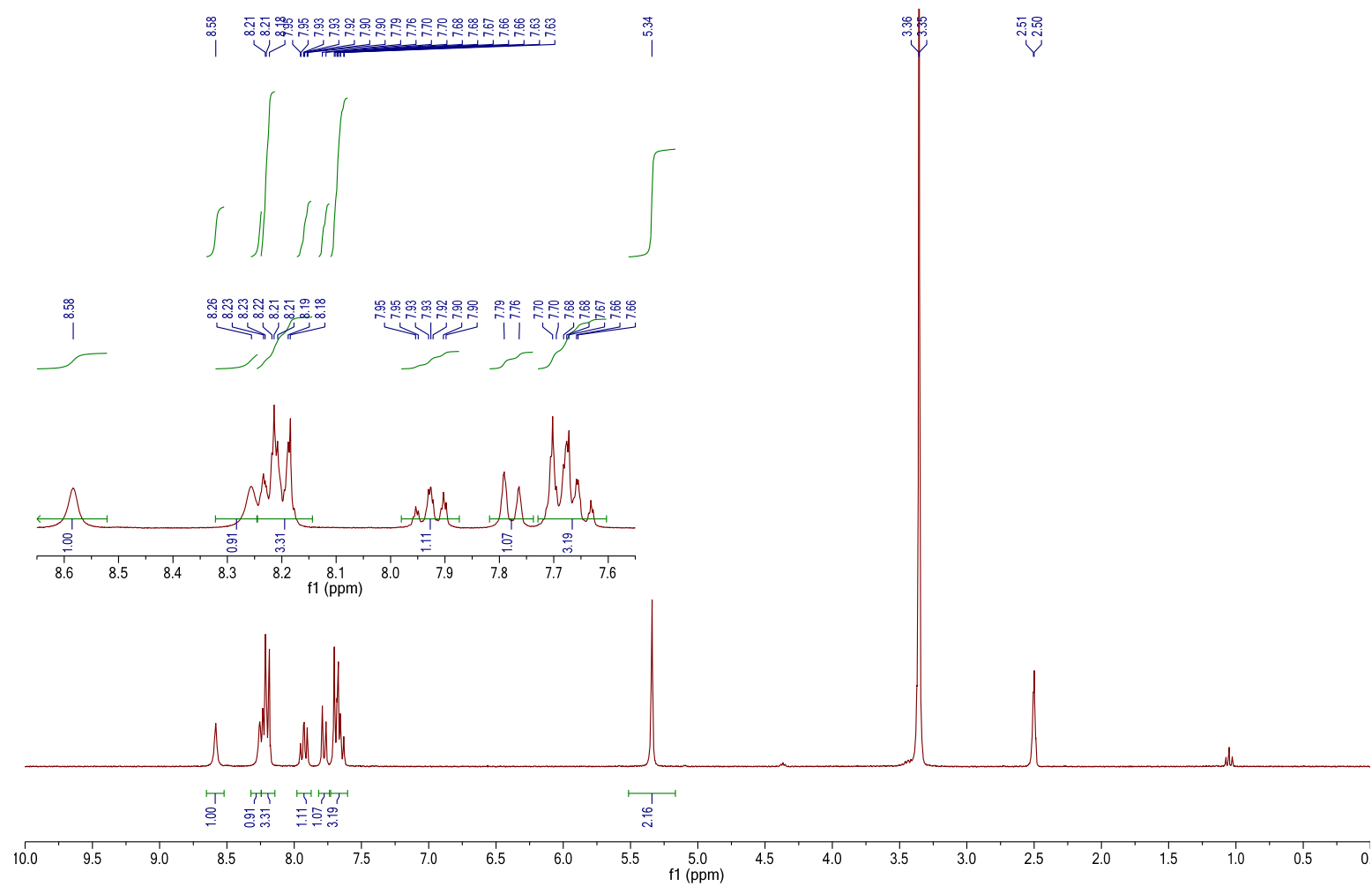


Figure S27. ^1H NMR spectrum of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (7b).

LT1; 4-Nitrophenylpropargyl-Amid / DMSO

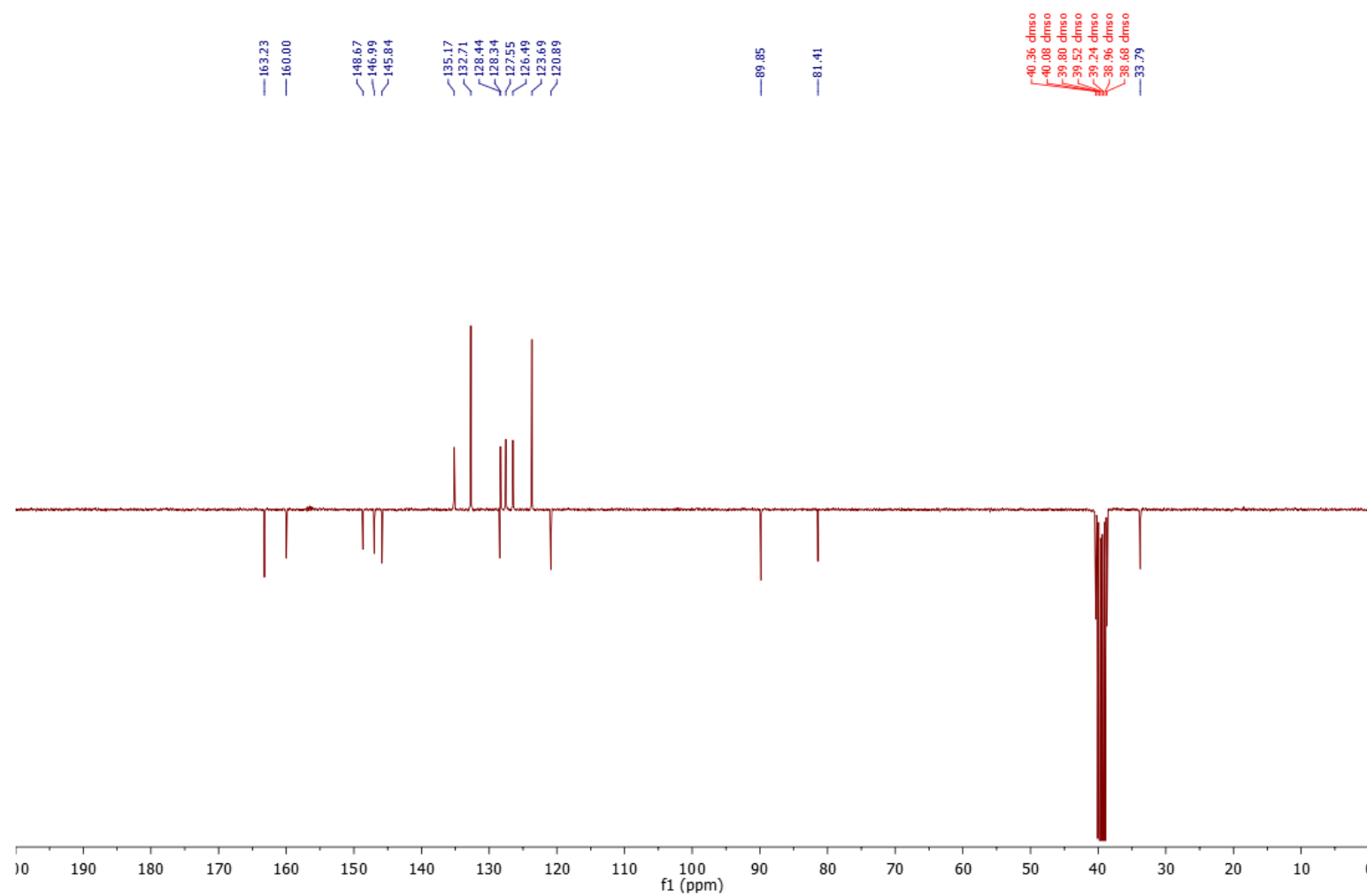


Figure S28. ^{13}C NMR spectrum of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (**7b**).

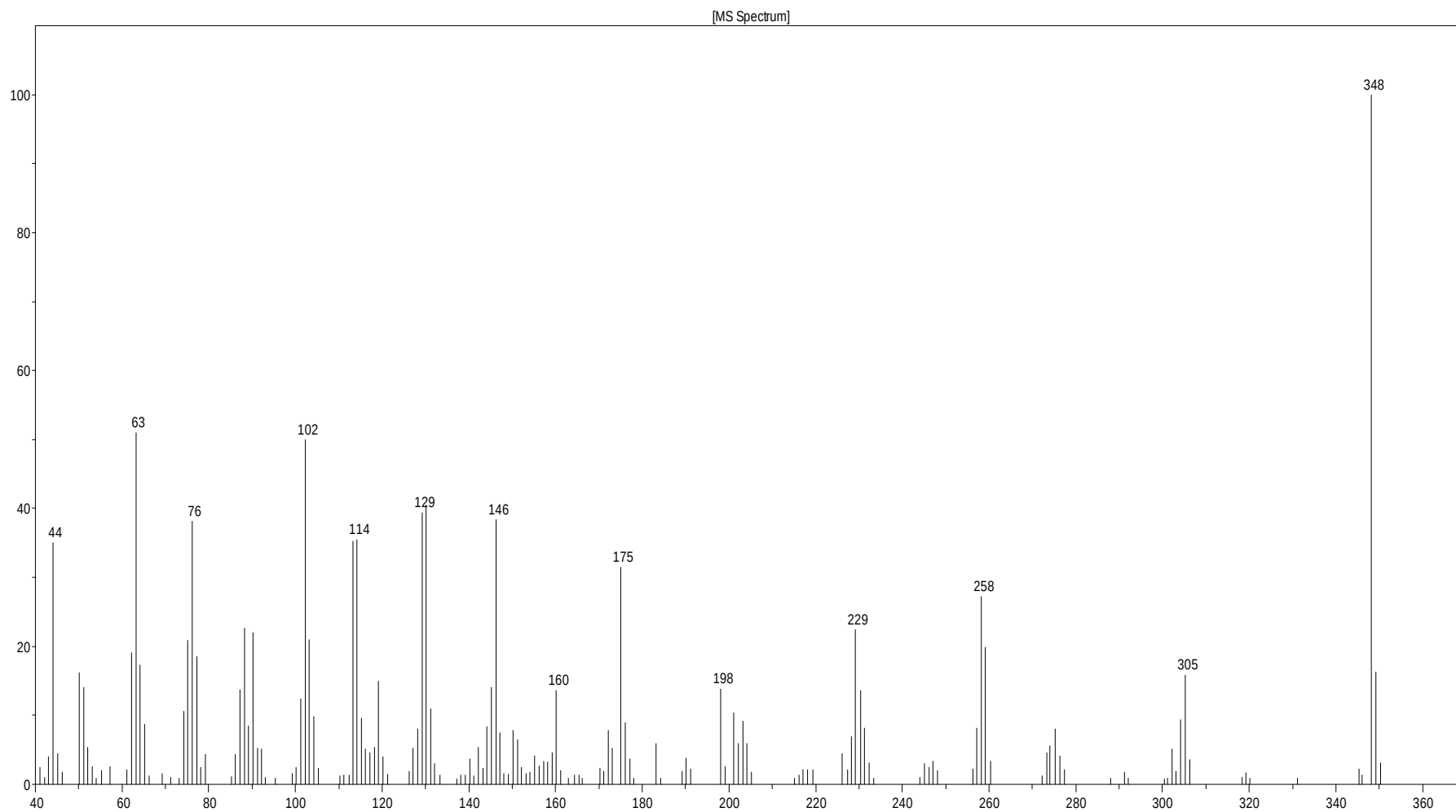


Figure S29. EI-MS of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (**7b**).

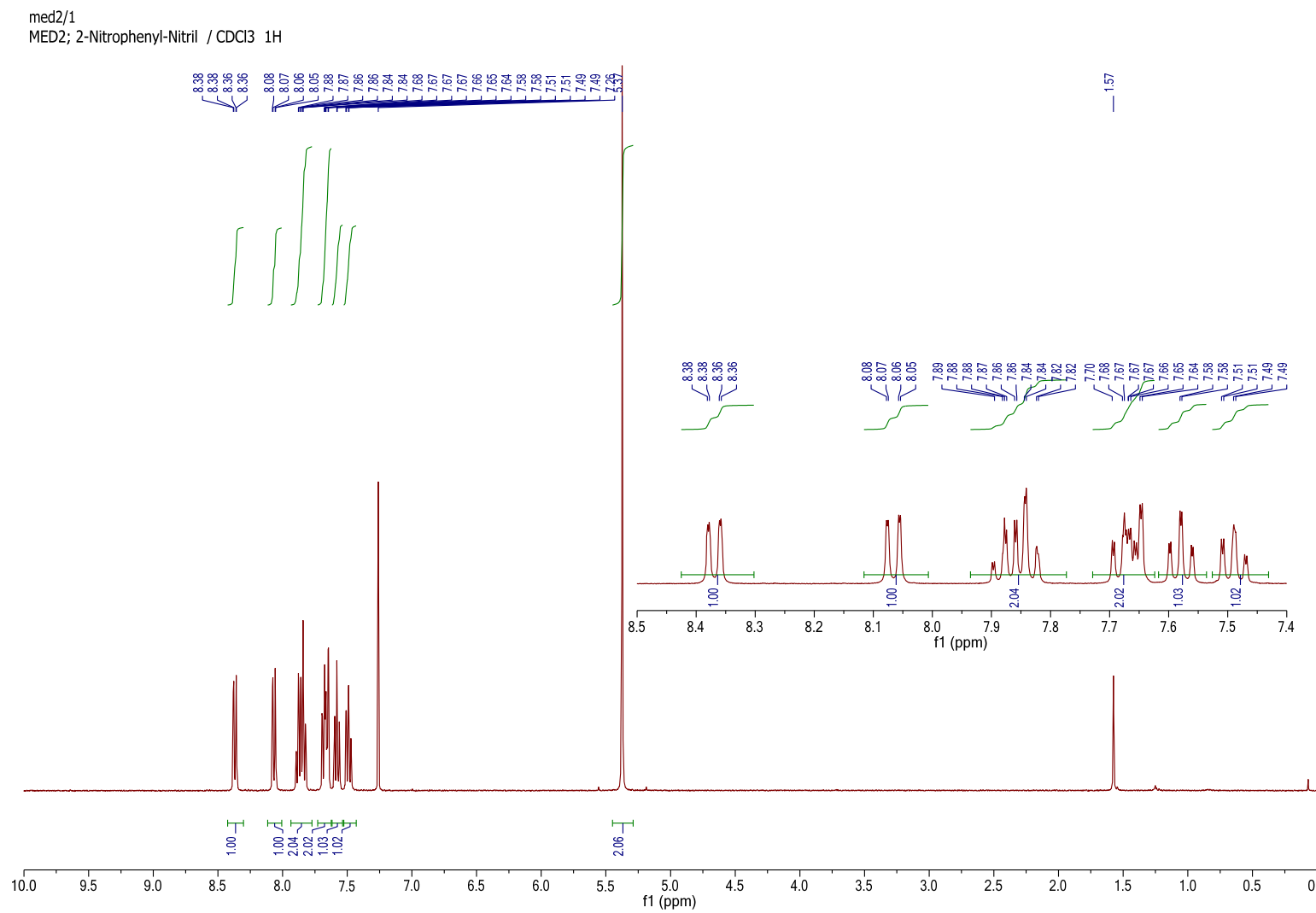


Figure S30. ¹H NMR spectrum of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8a**).

med2/1
MED2; 2-Nitrophenyl-Nitril / CDCl₃ 13C APT

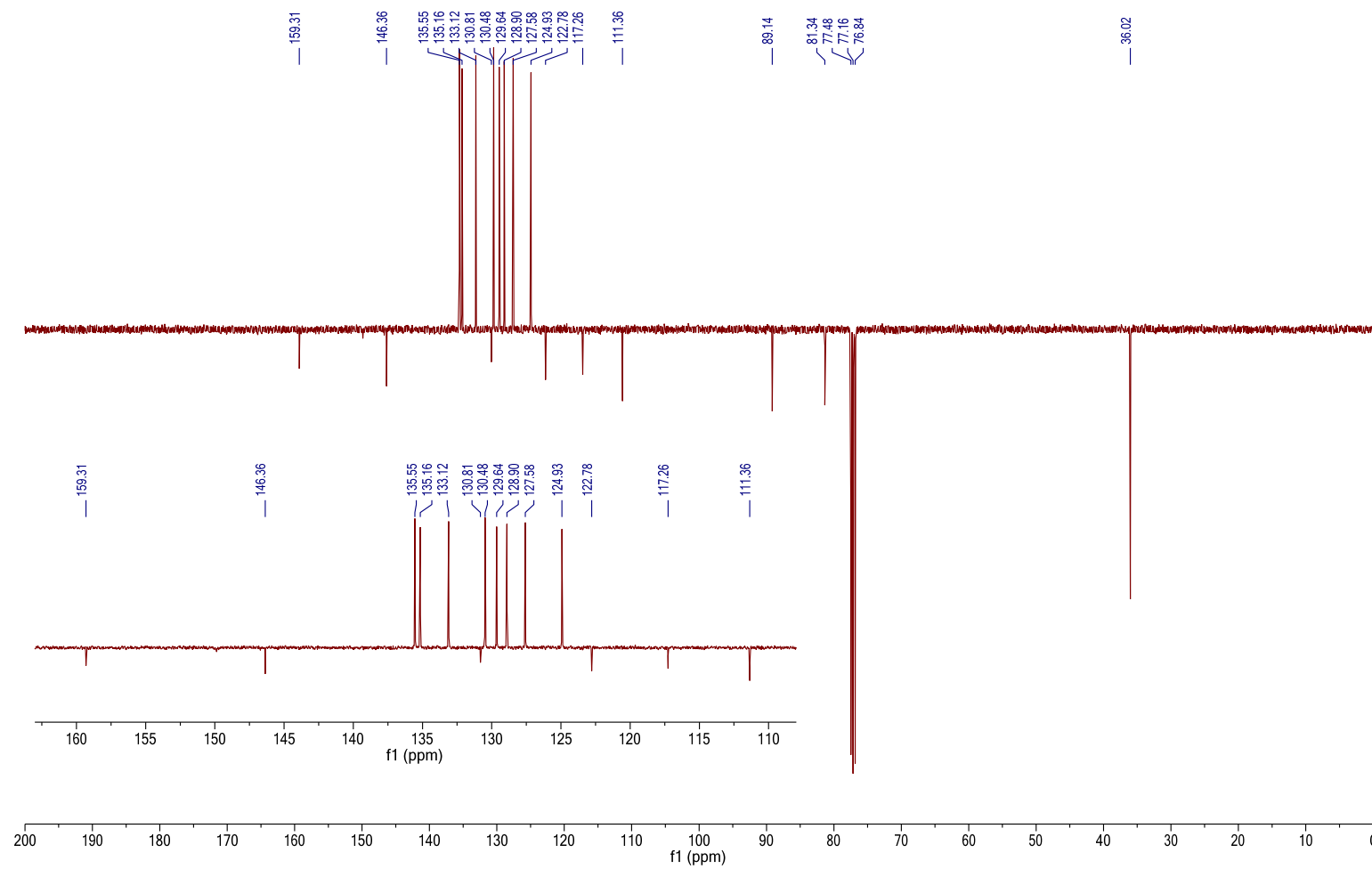


Figure S31. ¹H NMR spectrum of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8a**).

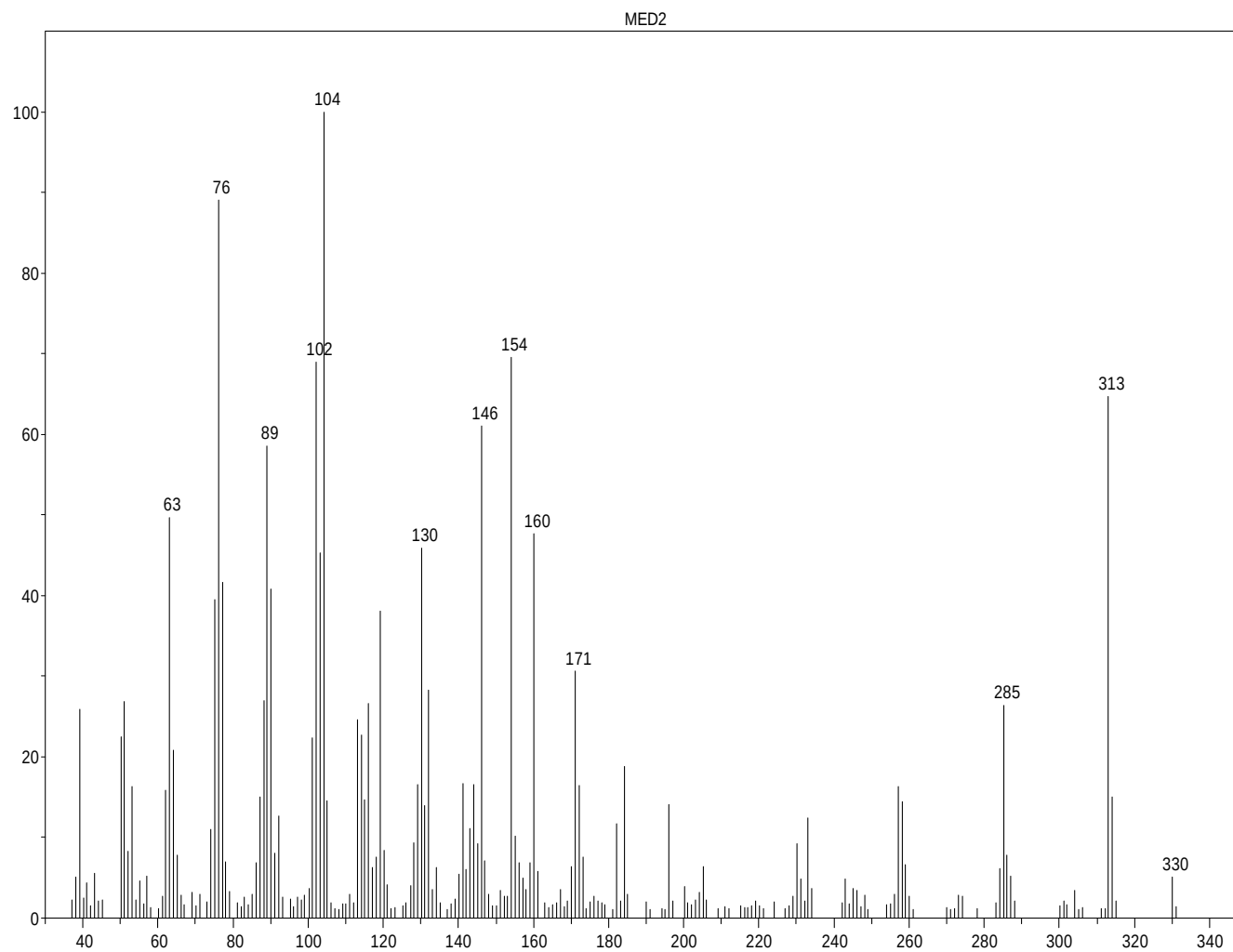


Figure S32. EI-MS of 3-[3-(2-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8a**).

LT2; 4-Nitrophenylpropargyl-Nitril / CDCl₃

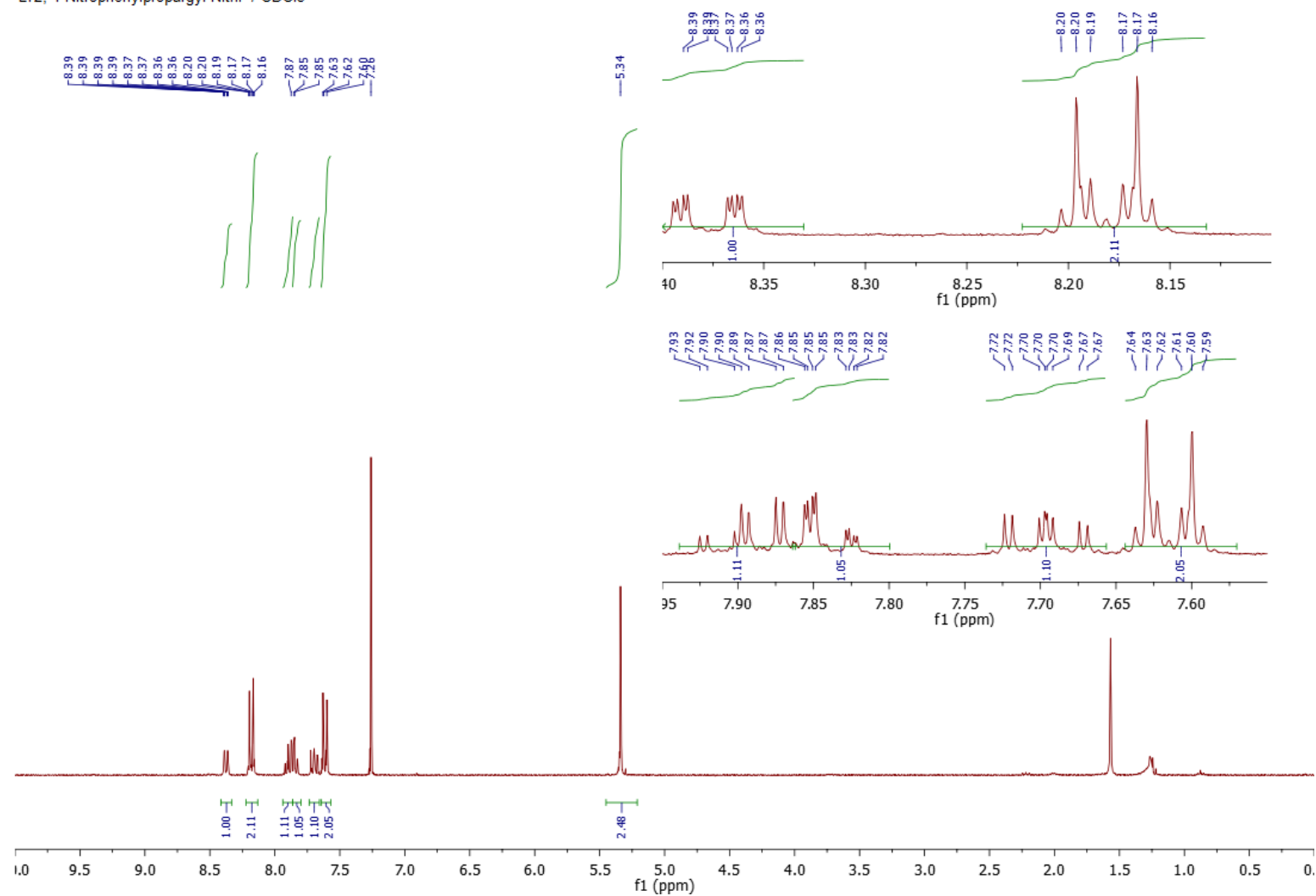


Figure S33. ¹H NMR spectrum of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8b**).

LT2; 4-Nitrophenylpropargyl-Nitril / CDCl₃

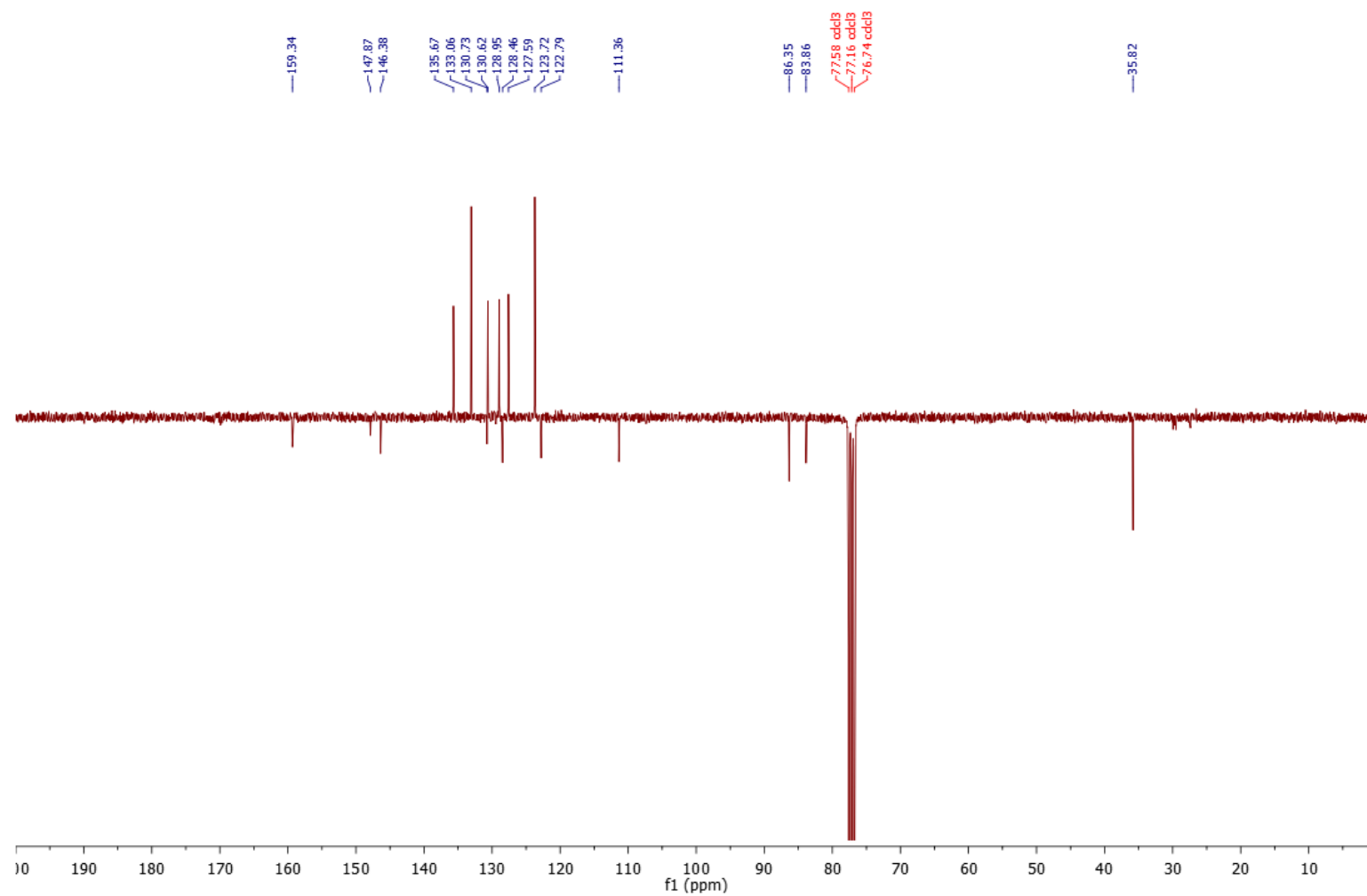


Figure S34. ¹³C NMR spectrum of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8b**).

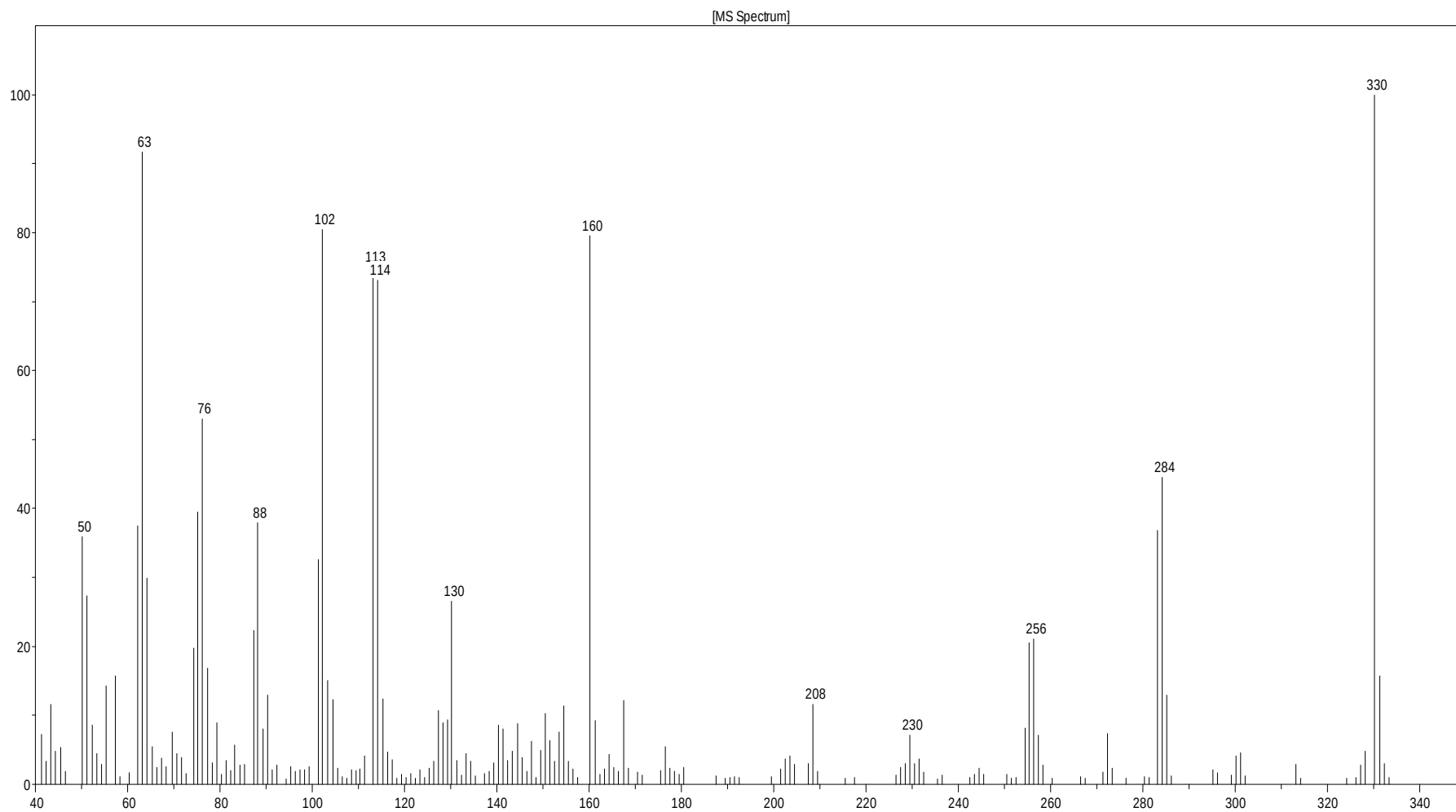


Figure S35. EI-MS of 3-[3-(4-nitrophenyl)prop-2-yn-1-yl]-4-oxo-3,4-dihydroquinazoline-2-carbonitrile (**8b**).

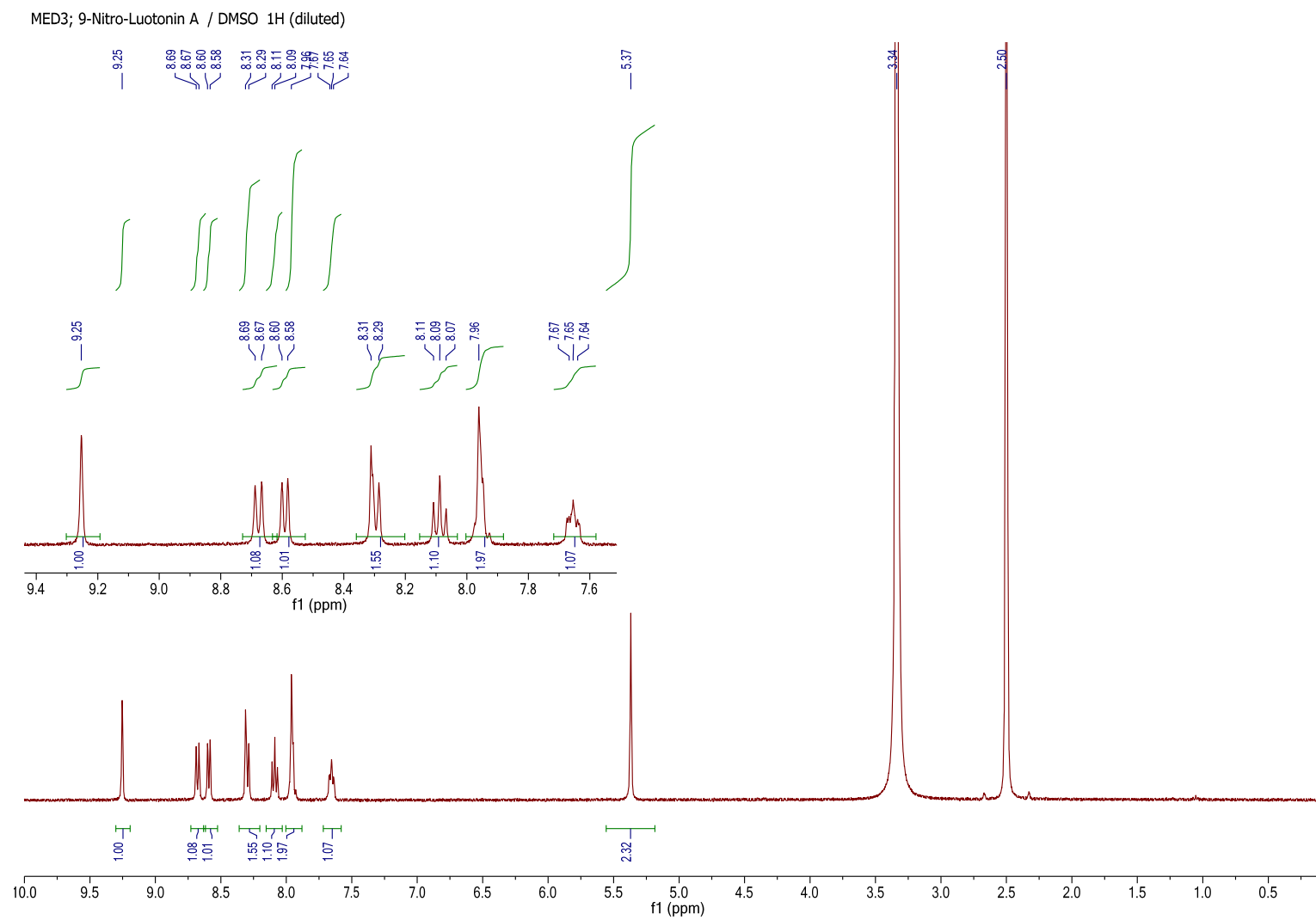
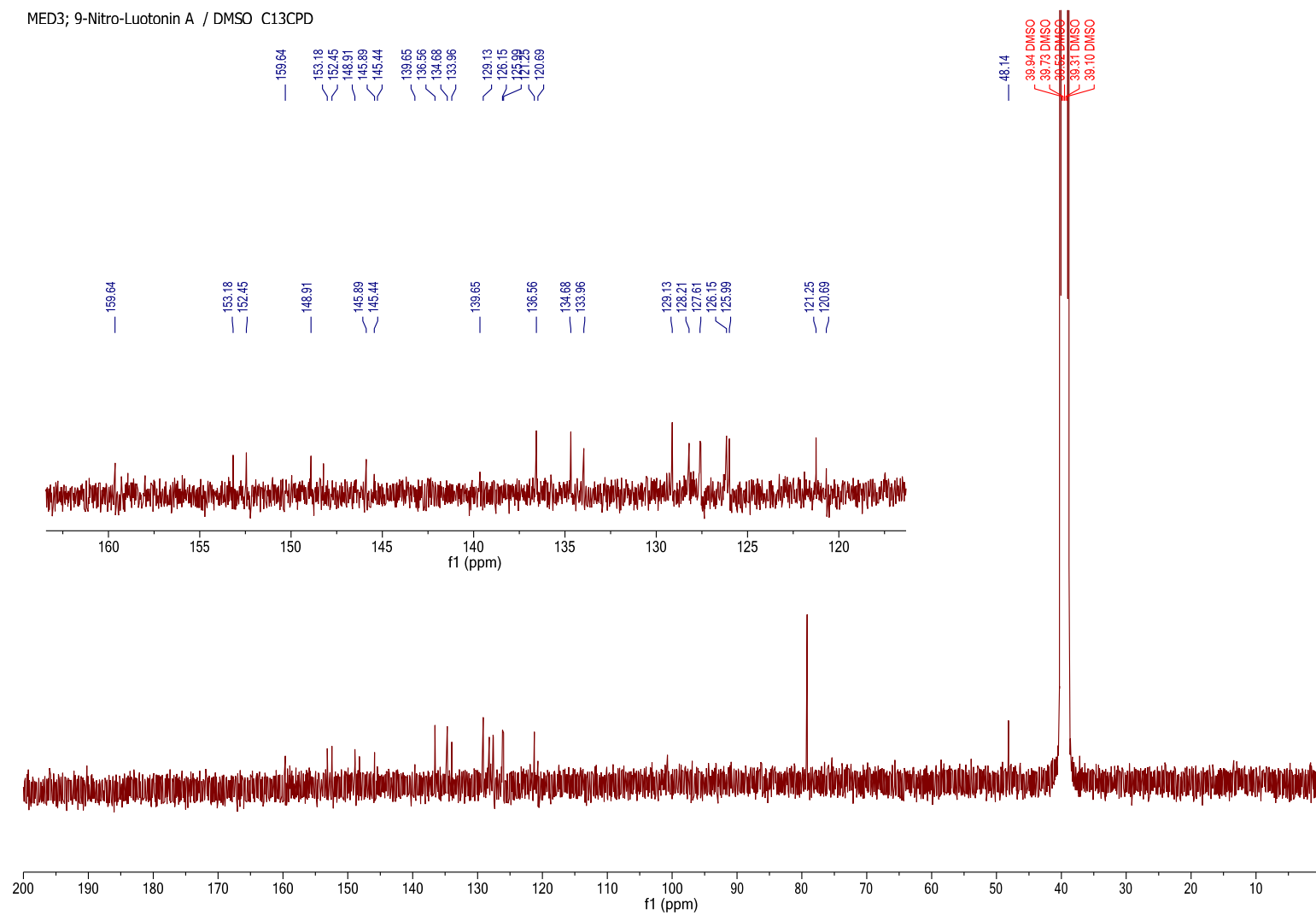


Figure S36. ^1H NMR spectrum of 1-nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**9a**).



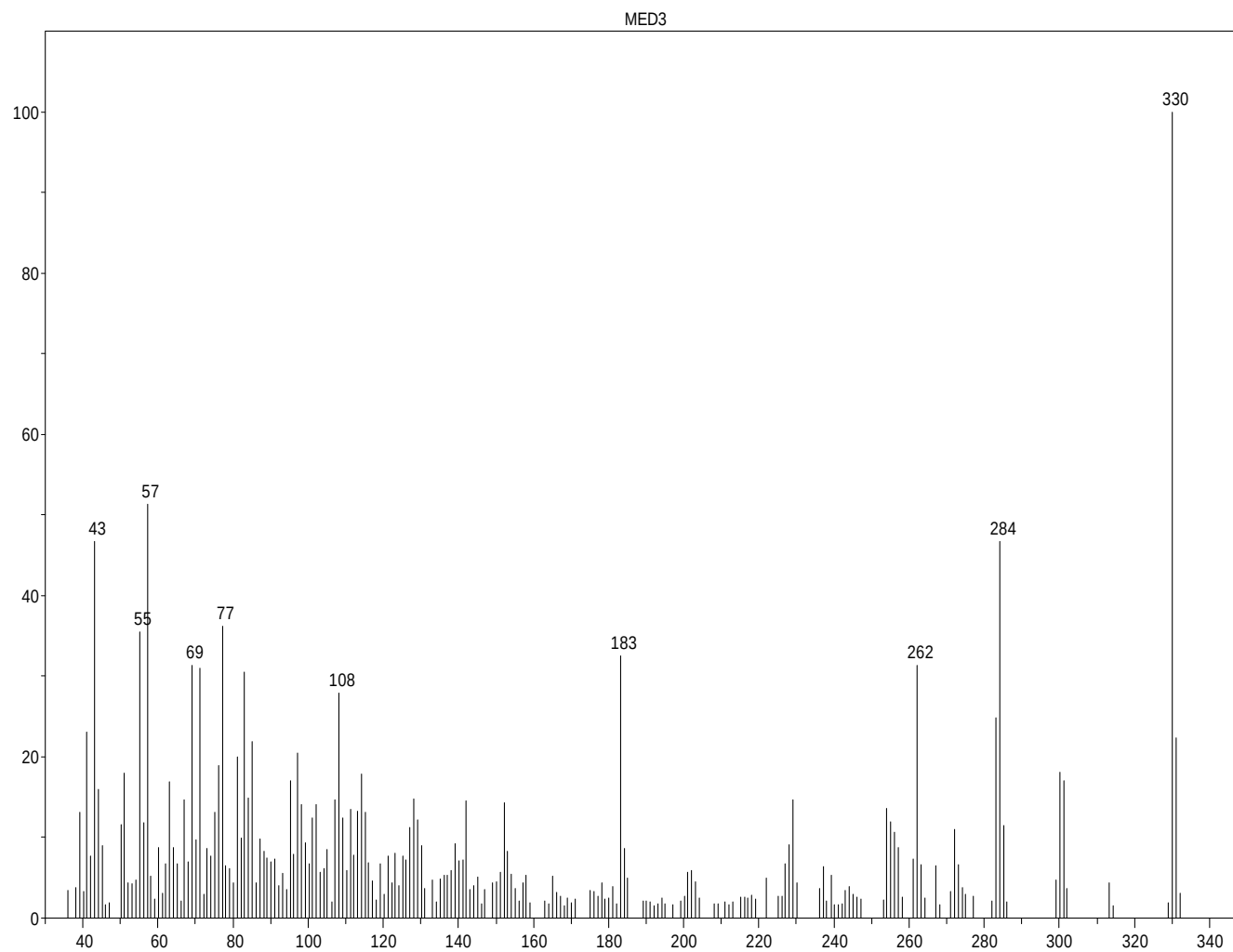


Figure S38. EI-MS of 1-nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**9a**).

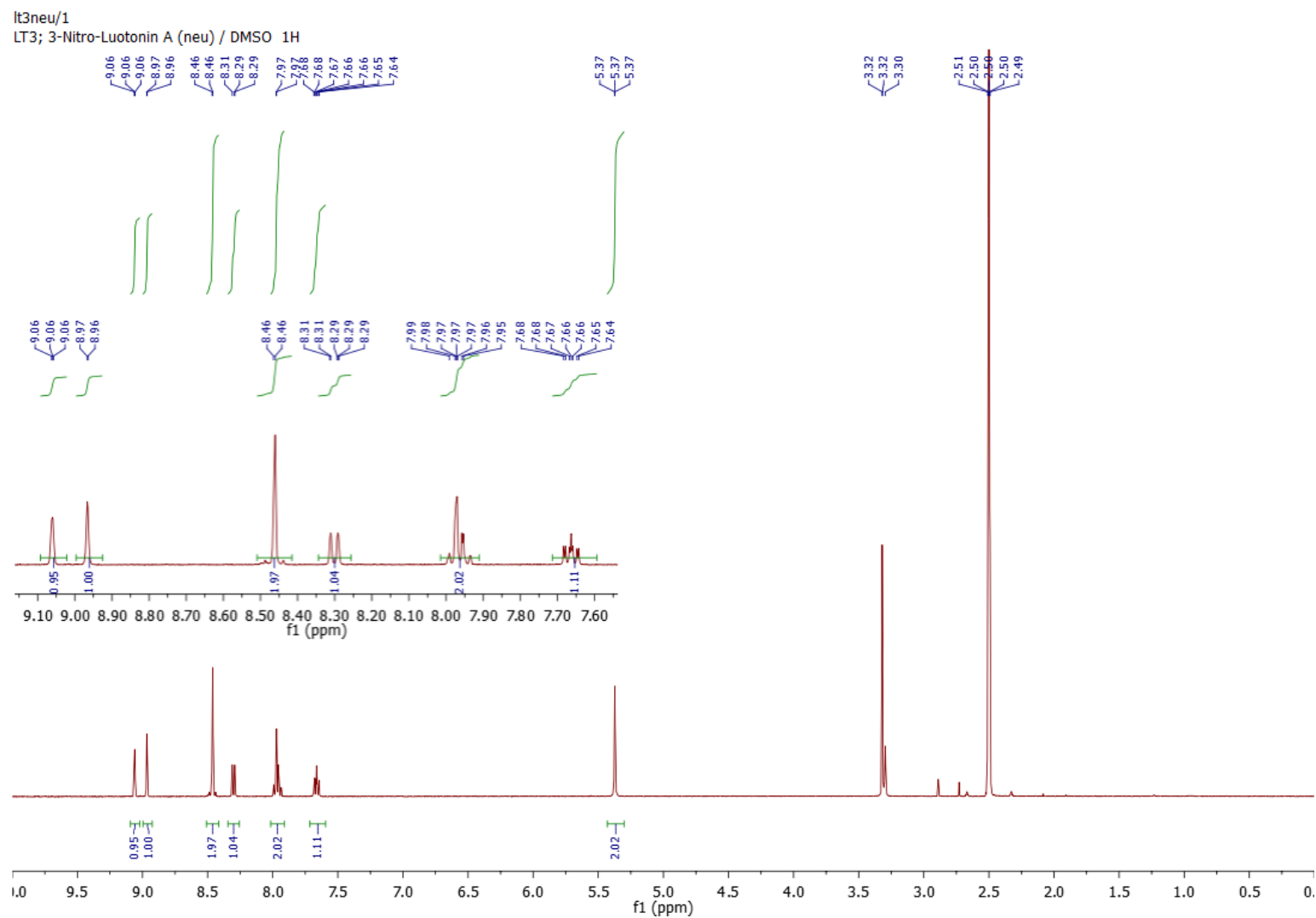


Figure S39. ^1H NMR spectrum of 3-nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**9b**).

lt3neu/1
LT3; 3-Nitro-Luotonin A (neu) / DMSO 1H

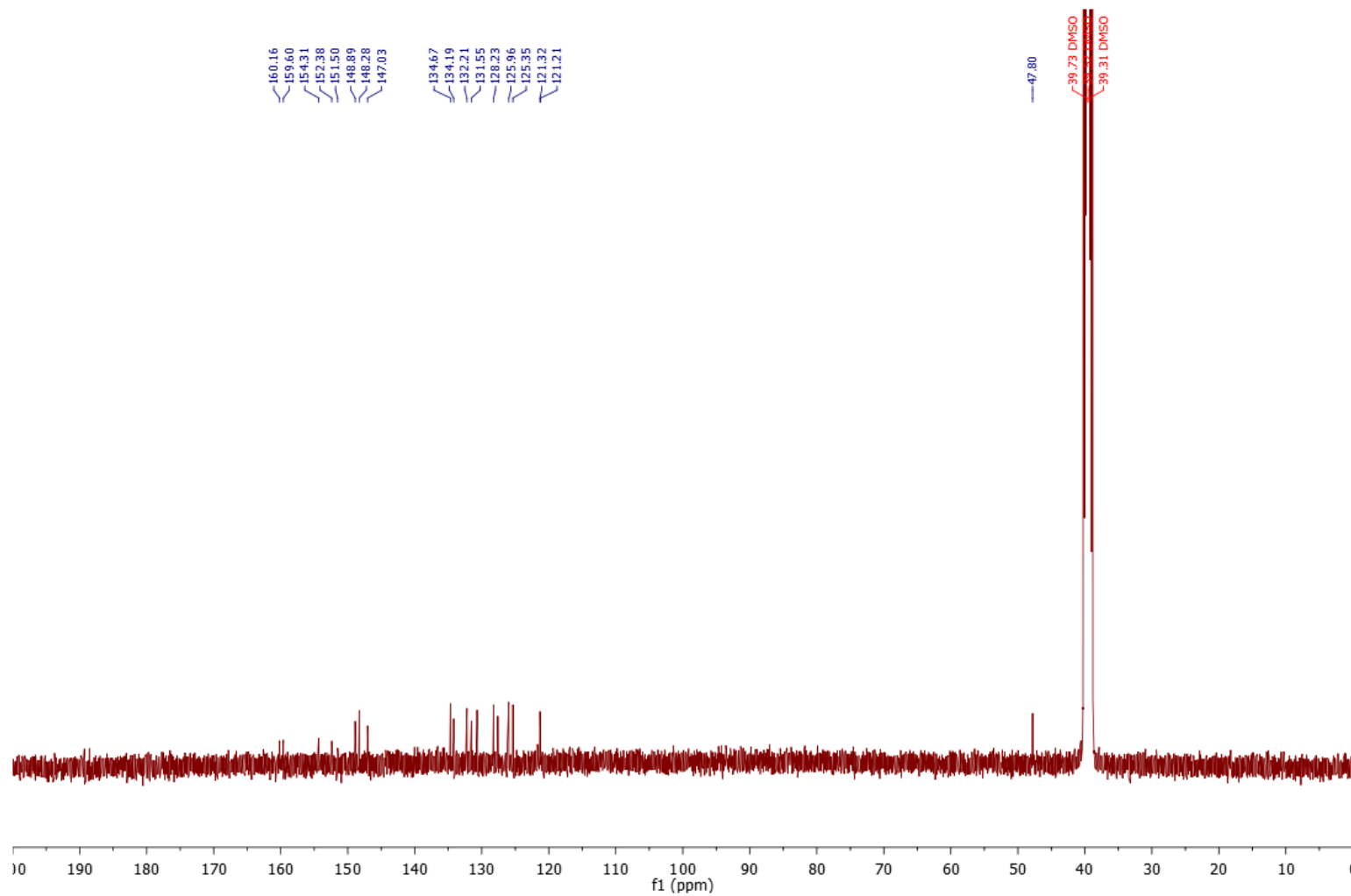


Figure S40. ¹³C NMR spectrum of 3-nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (9b).

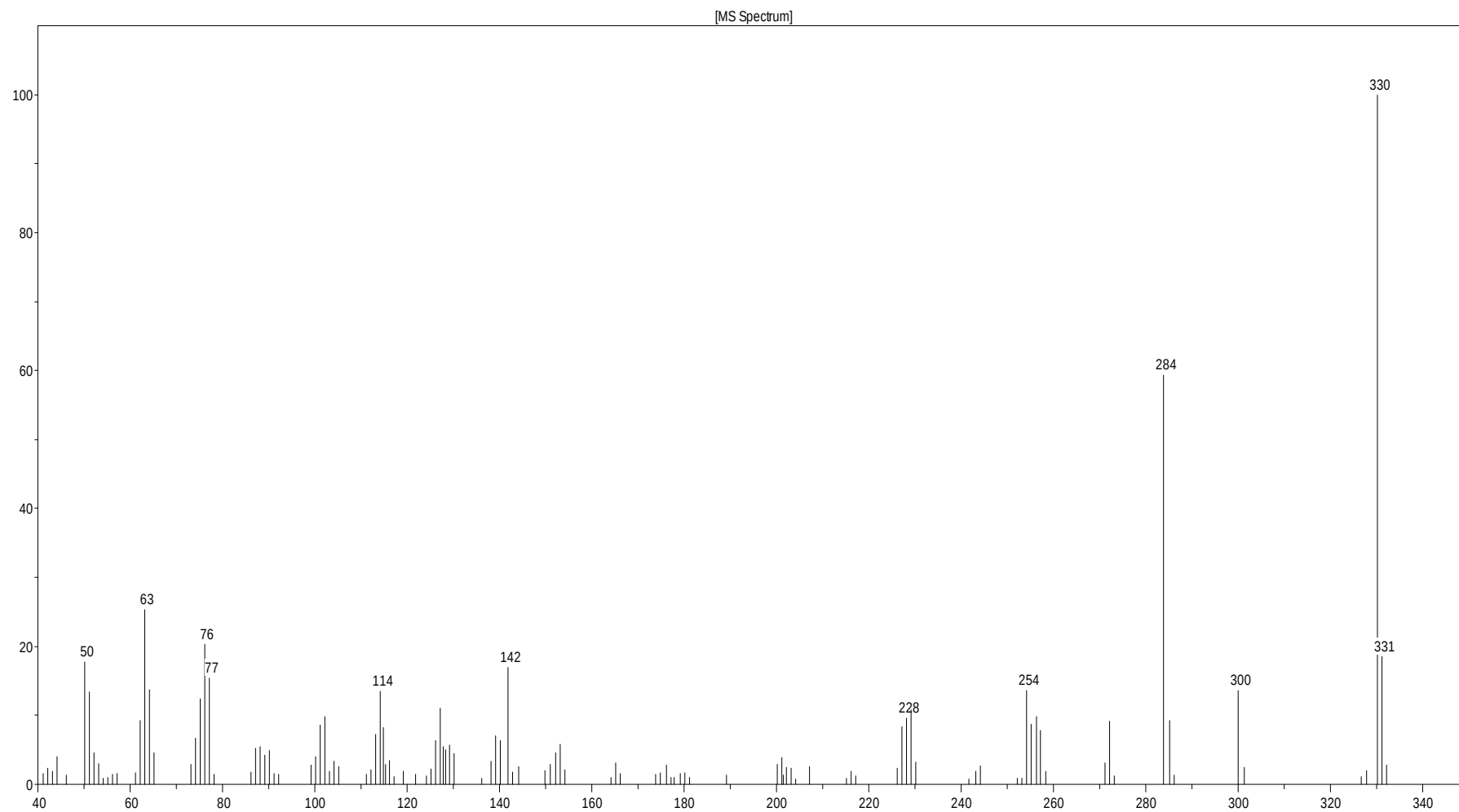


Figure S41. EI-MS of 3-nitroquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**9b**).

MED4; 9-Amino-Luotonin A / DMSO 1H

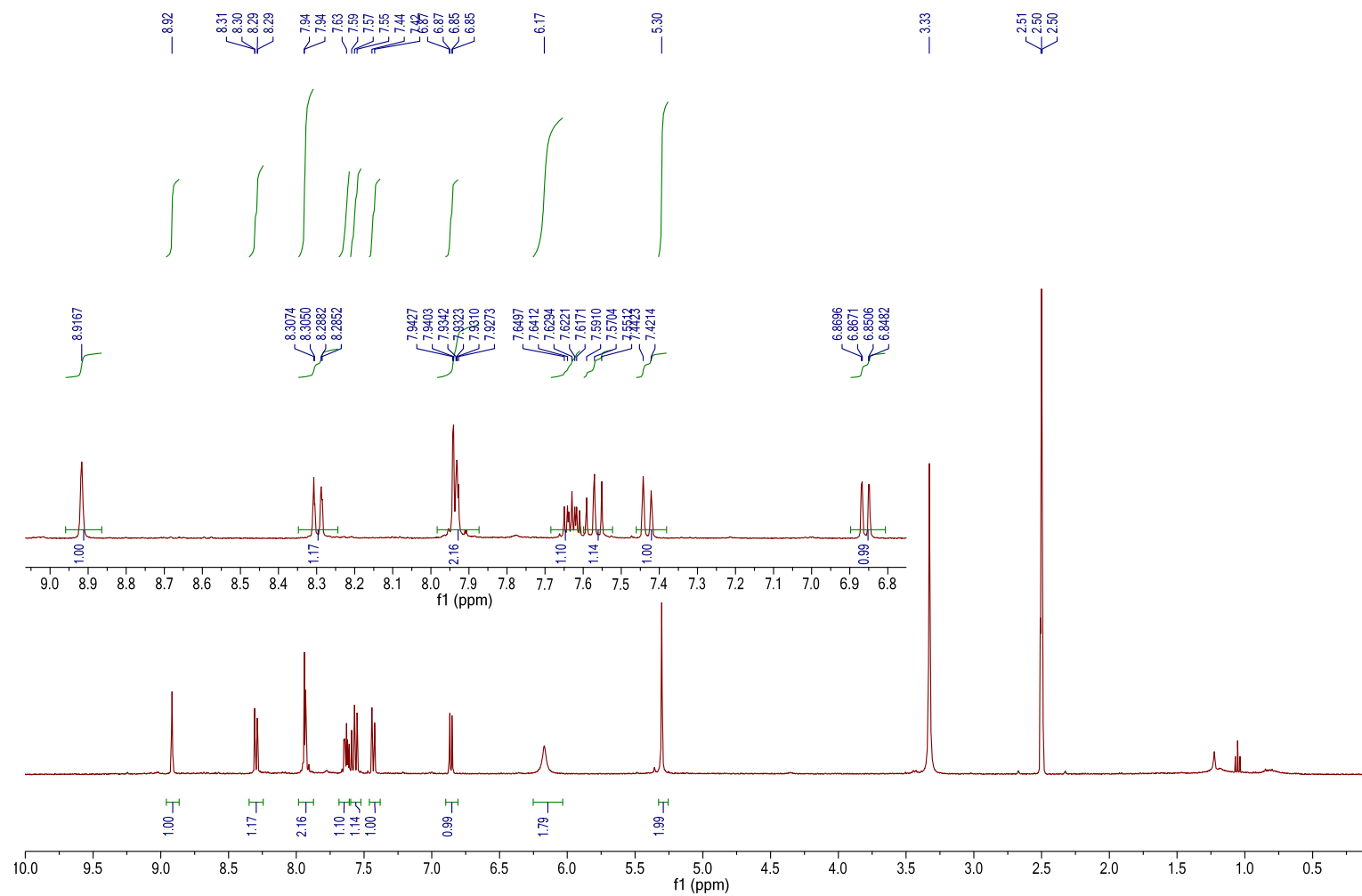


Figure S42. ^1H NMR spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

MED4; 9-Amino-Luotonin A / DMSO COSY

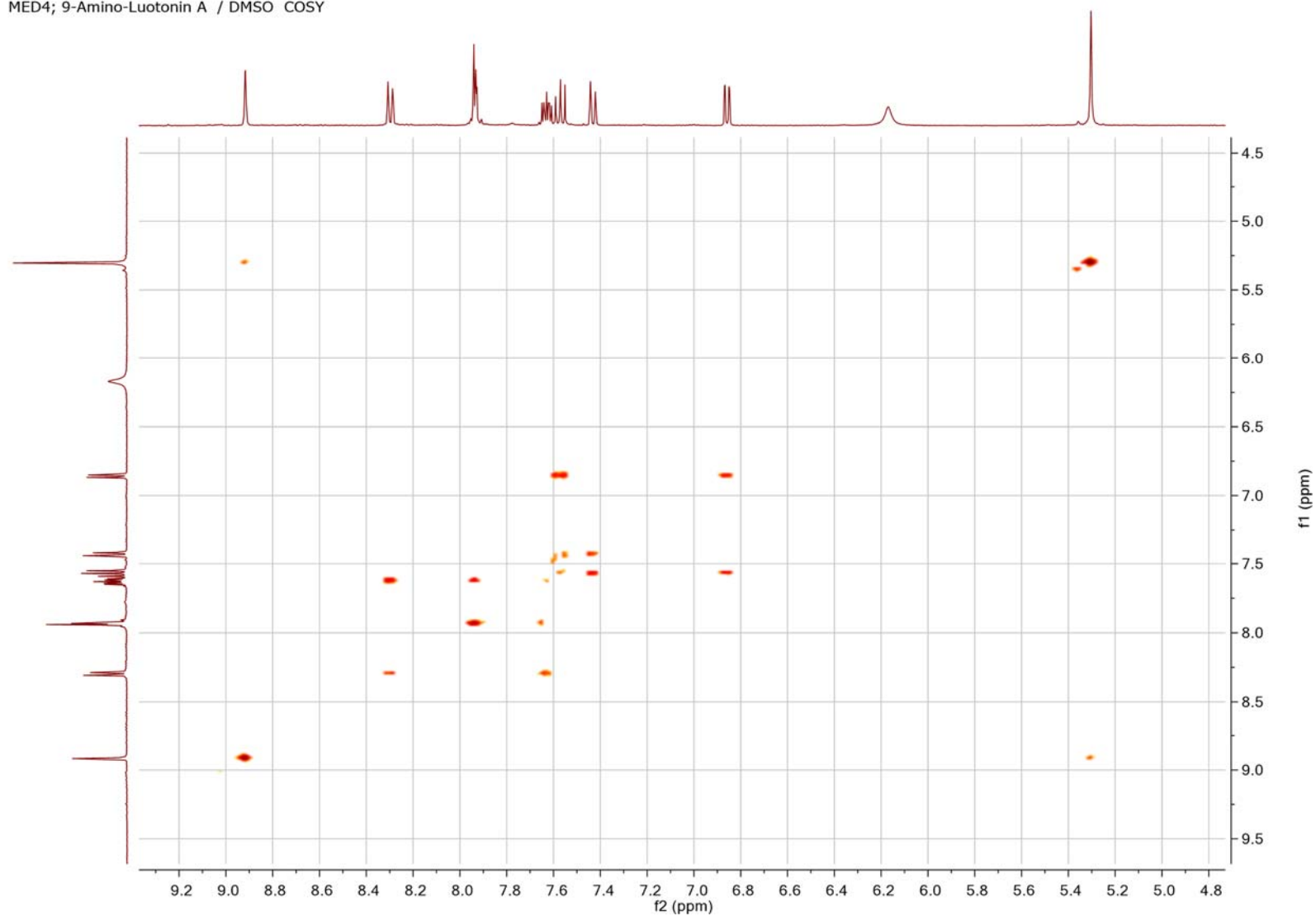


Figure S43. COSY spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

MED4; 9-Amino-Luotonin A / DMSO NOESY

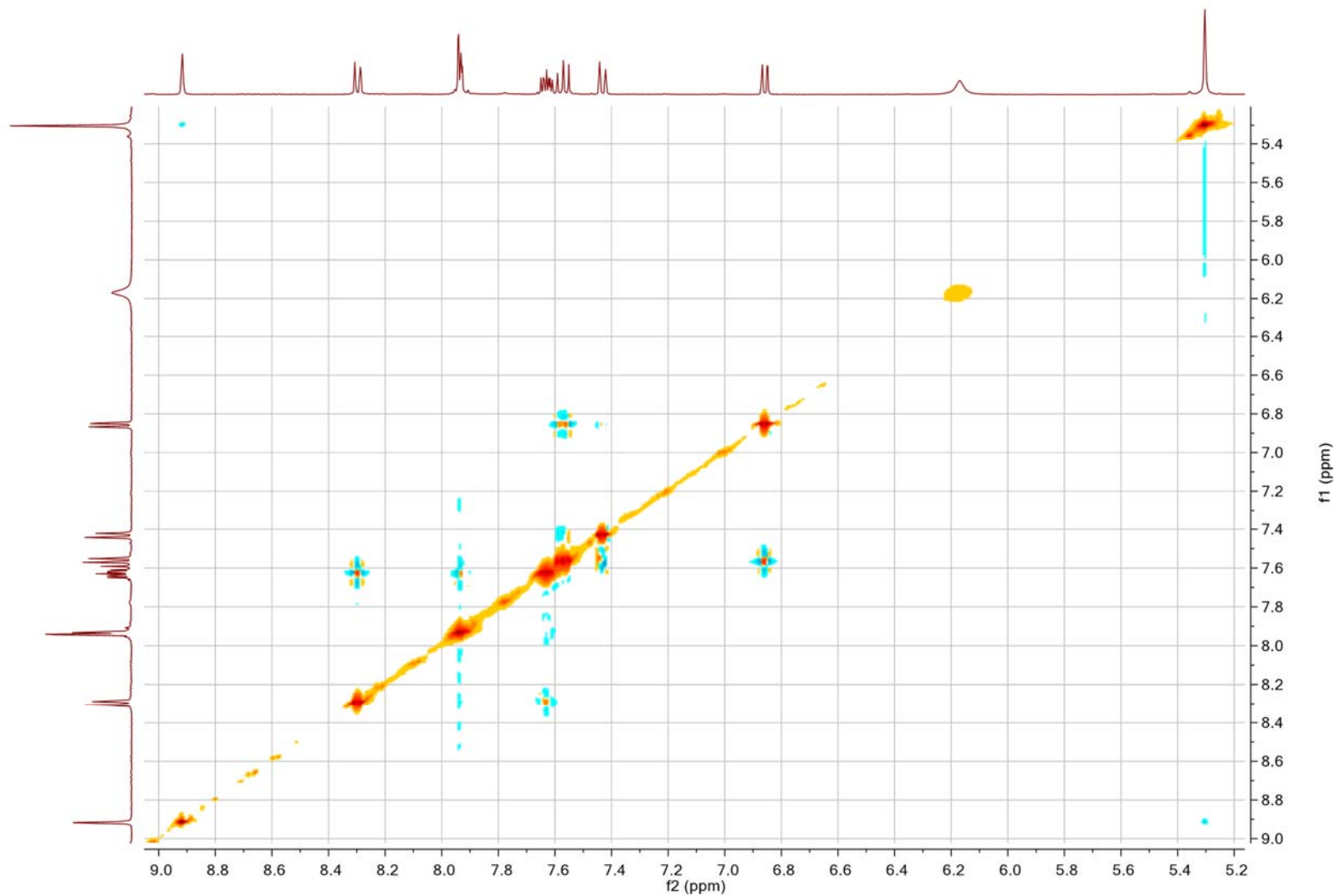


Figure S44. NOESY spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

MED4; 9-Amino-Luotonin A / DMSO C13APT

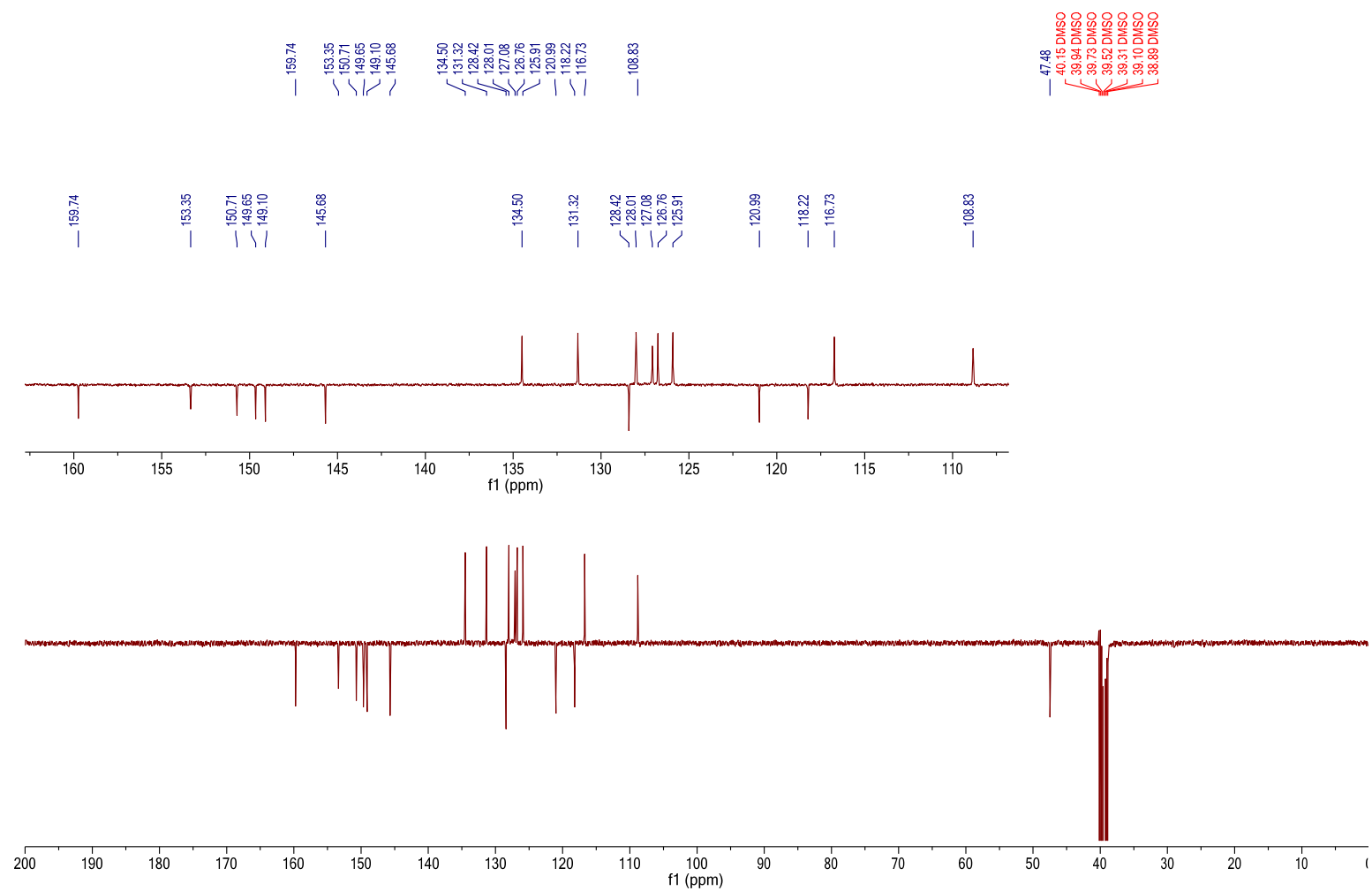


Figure S45. ^{13}C NMR spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

MED4; 9-Amino-Luotonin A / DMSO HSQC

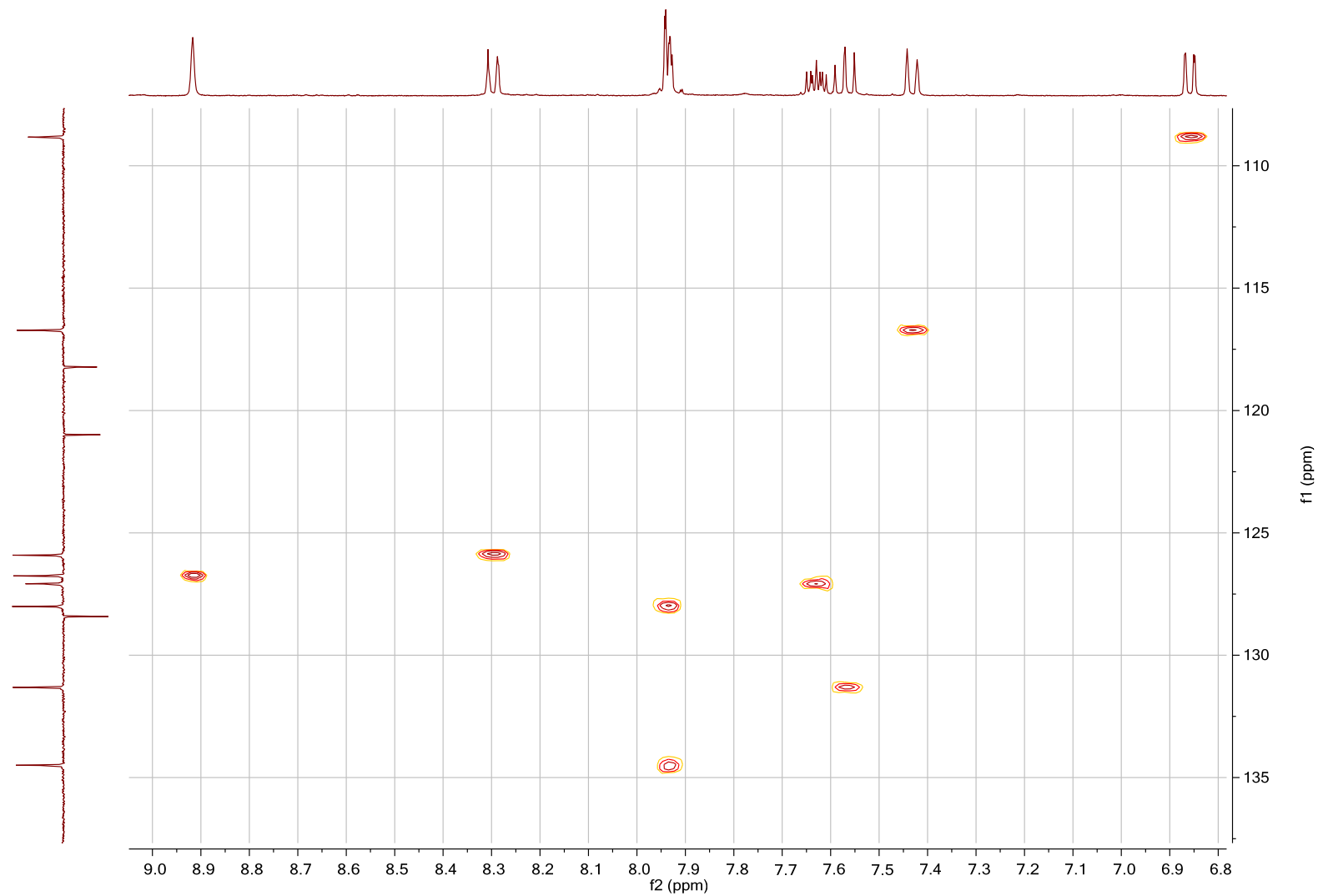


Figure S46. HSQC spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

MED4; 9-Amino-Luotonin A / DMSO HMBC

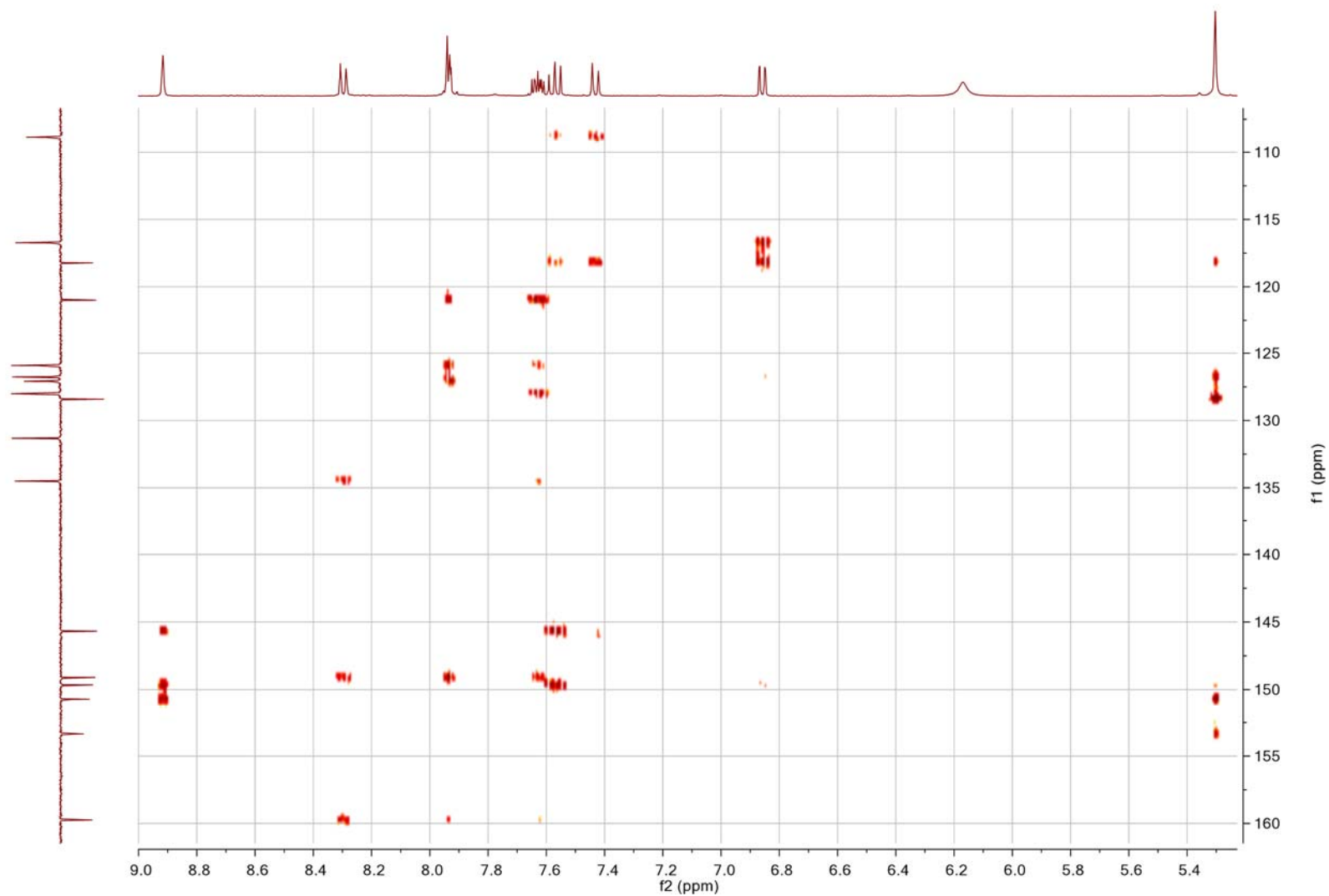


Figure S47. HMBC spectrum of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

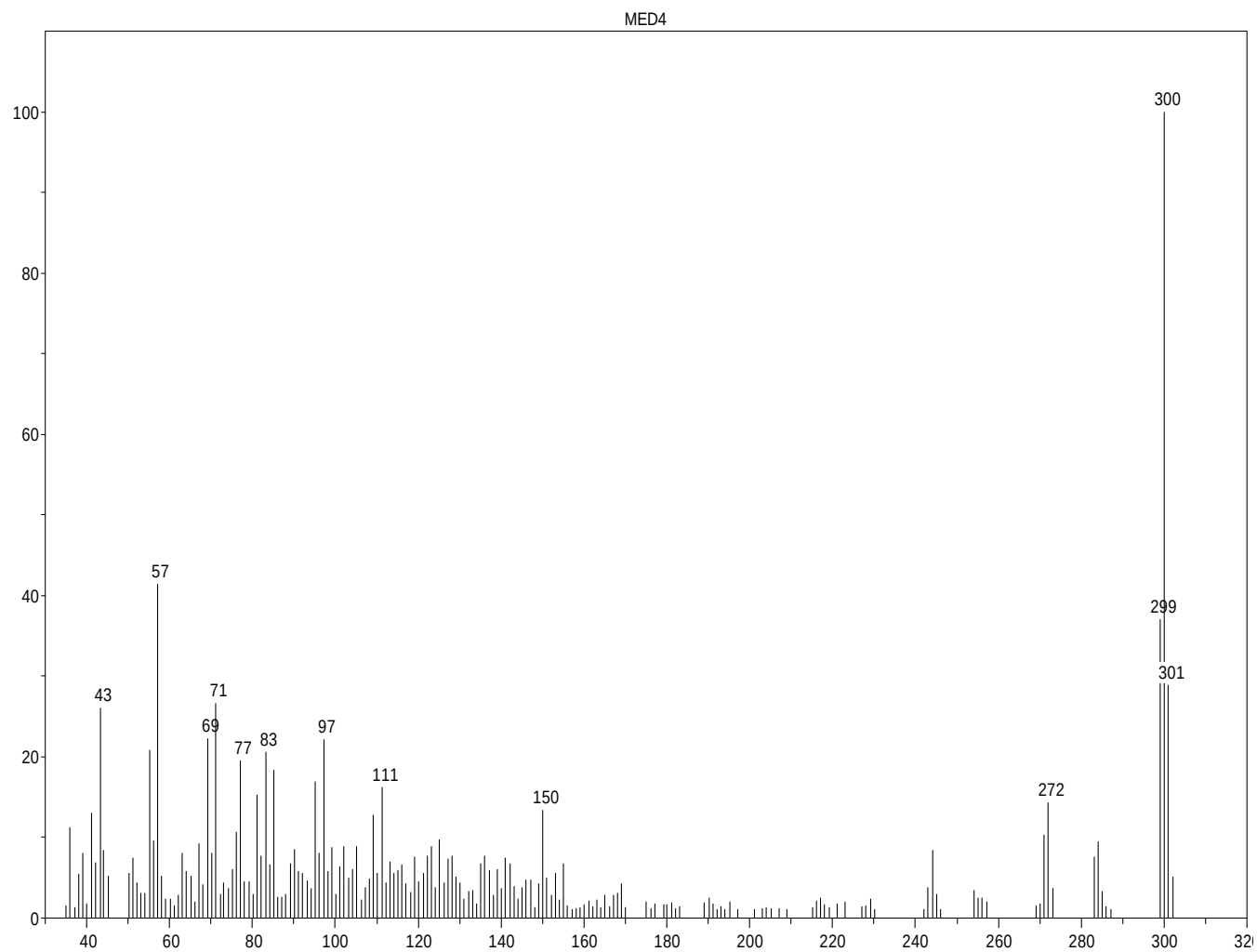


Figure S48. EI-MS of 1-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10a**).

LT4; 11-Amino-Luotonin A (roh) / DMSO 1H
lt4_1/1

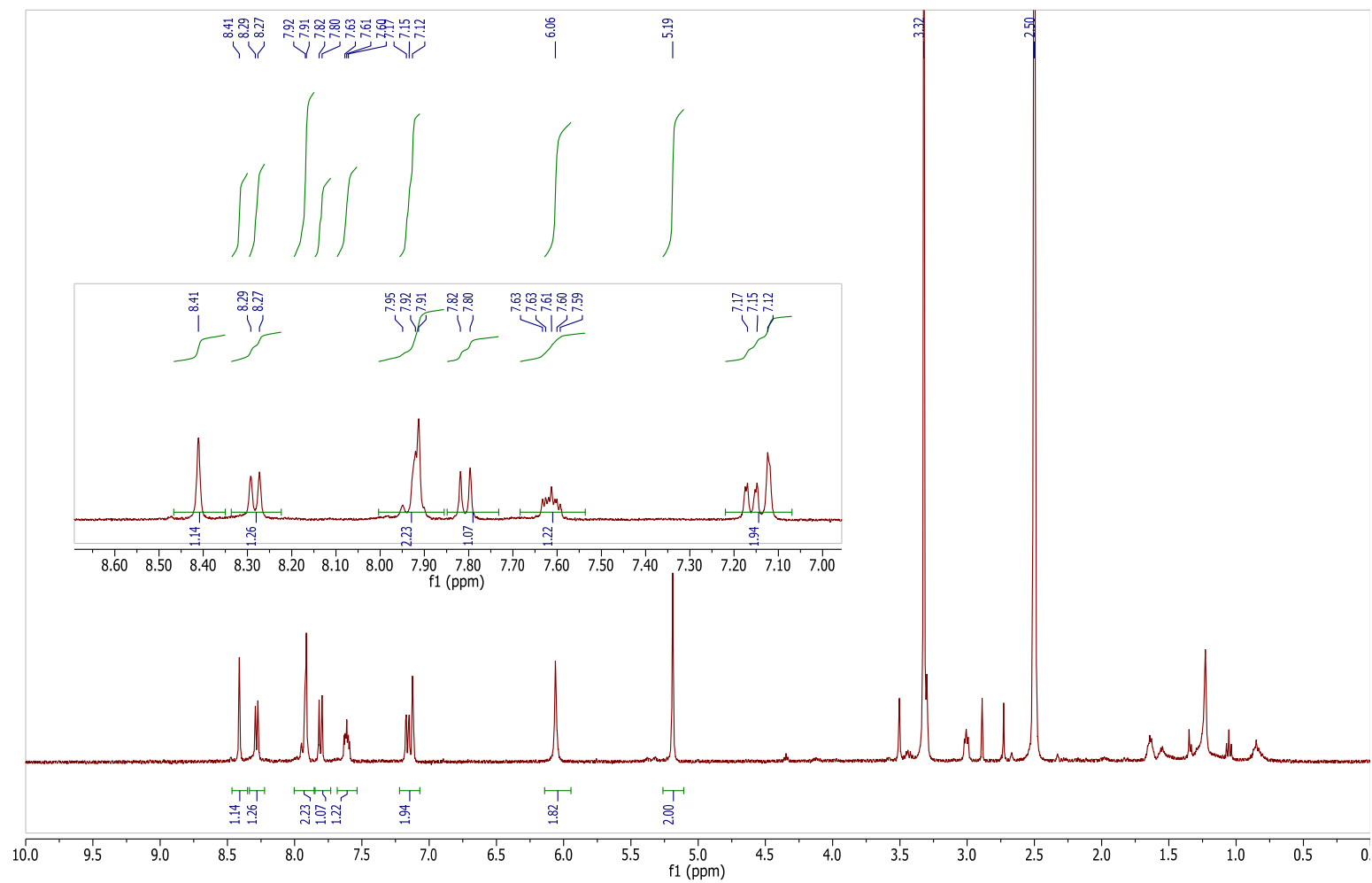


Figure S49. ^1H NMR spectrum of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

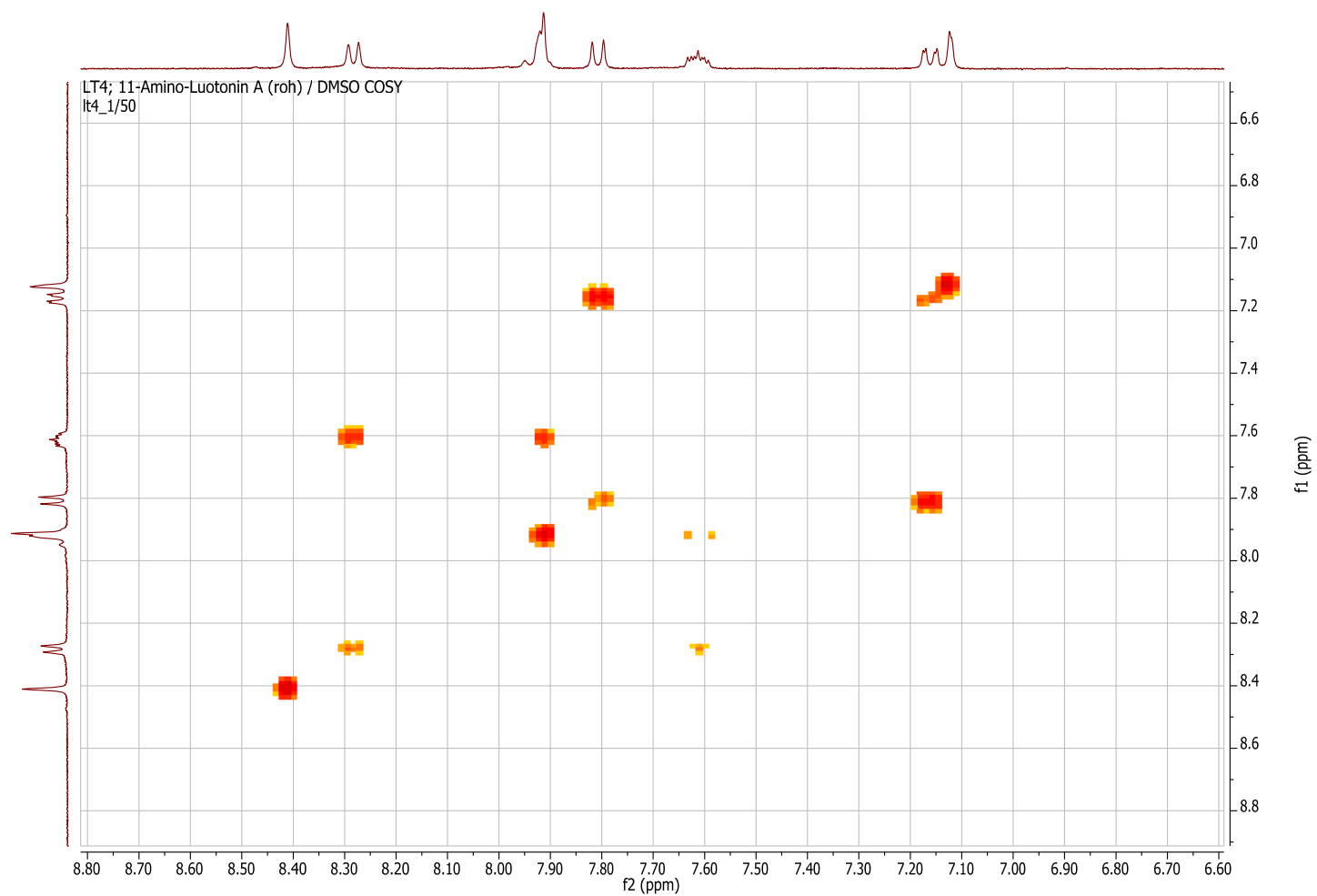


Figure S50. COSY spectrum of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

LT4; 11-Amino-Luotonin A (roh) / DMSO 1H
lt4_1/1

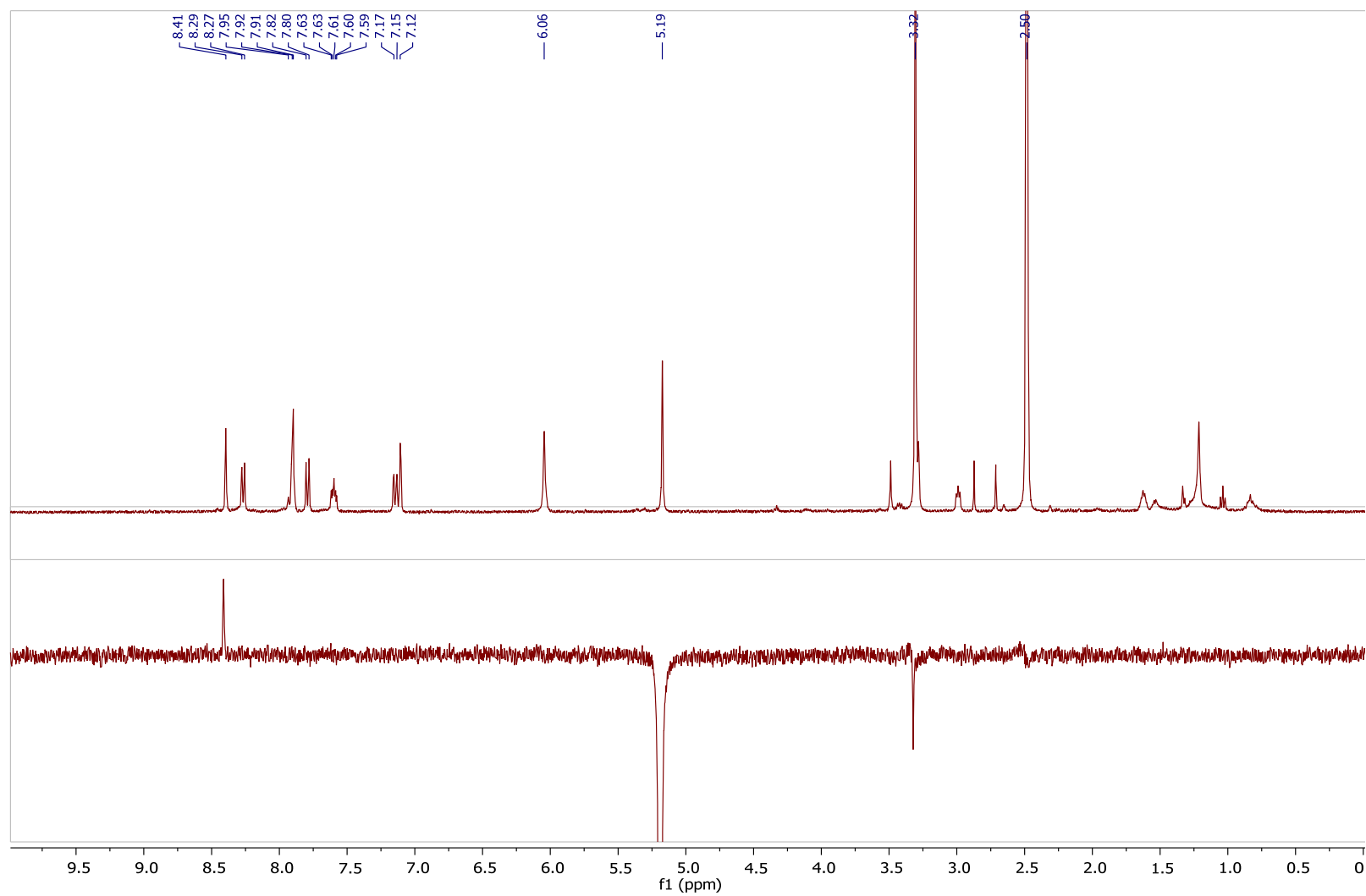


Figure S51. NOE difference spoectrum #1 of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

LT4; 11-Amino-Luotonin A (roh) / DMSO 1H
lt4_1/1

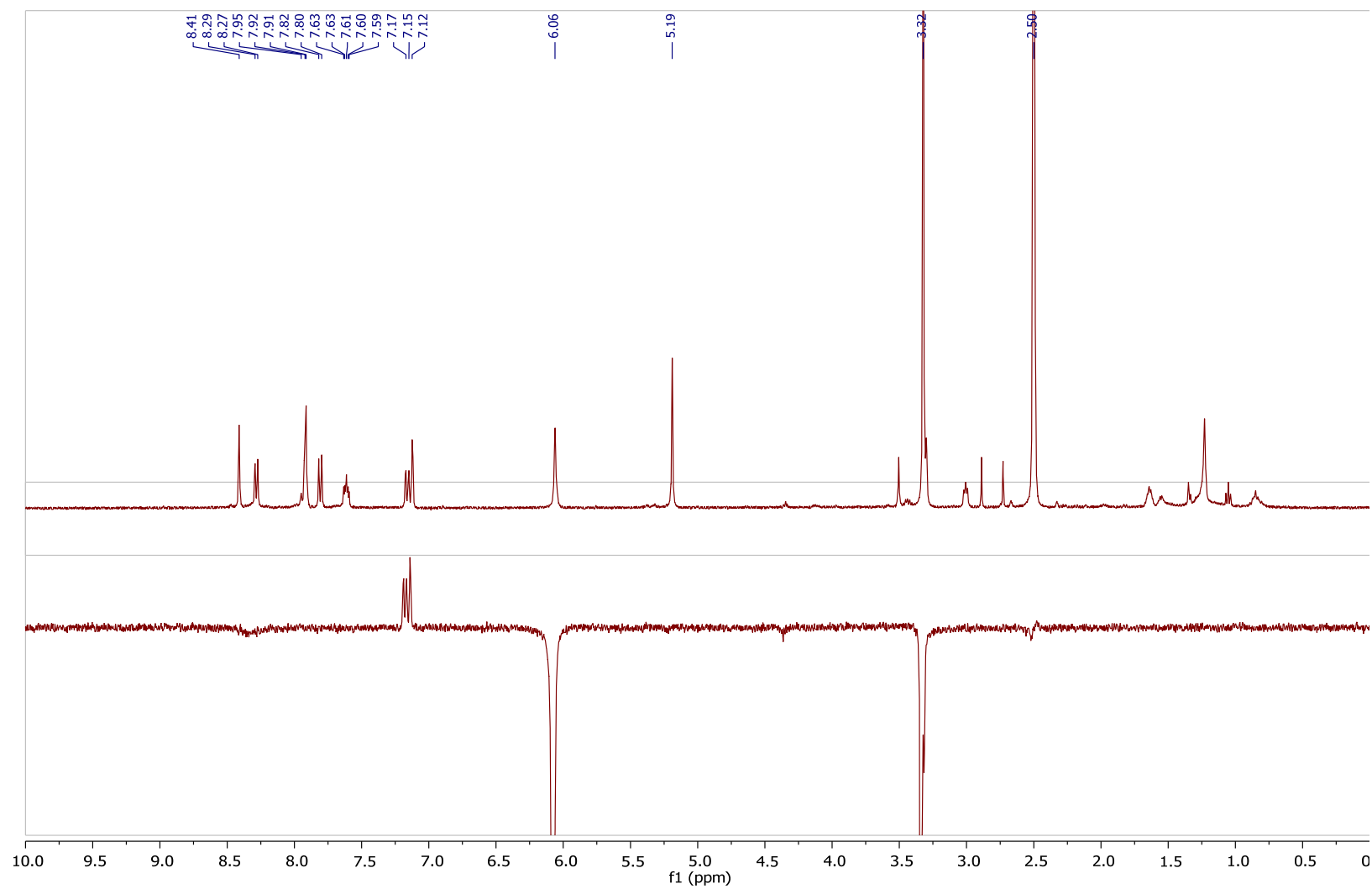


Figure S52. NOE difference spoectrum #2 of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

LT4; 11-Amino-Luotonin A (roh) / DMSO 1H
lt4_1/1

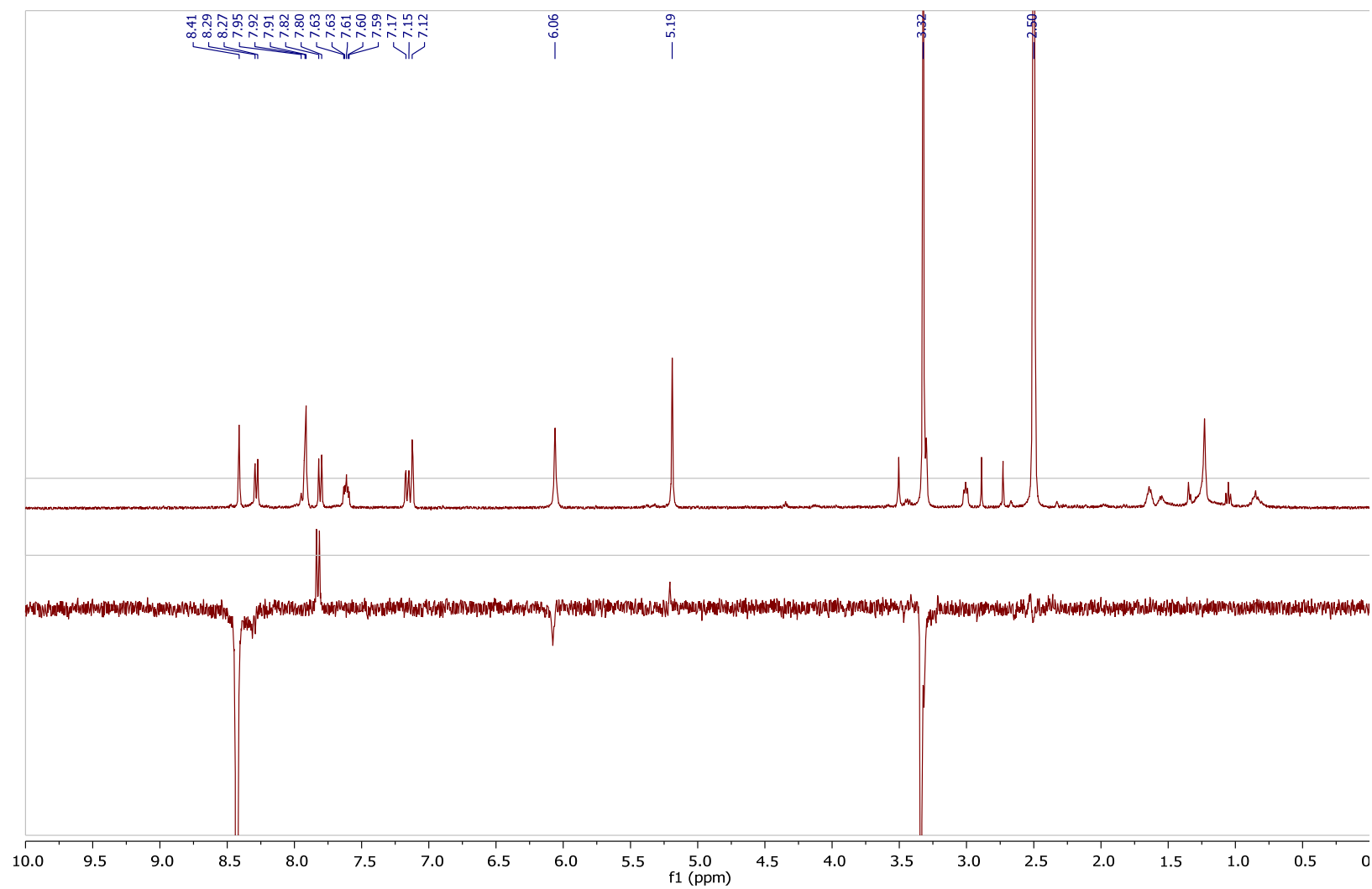


Figure S53. NOE difference spoectrum #3 of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

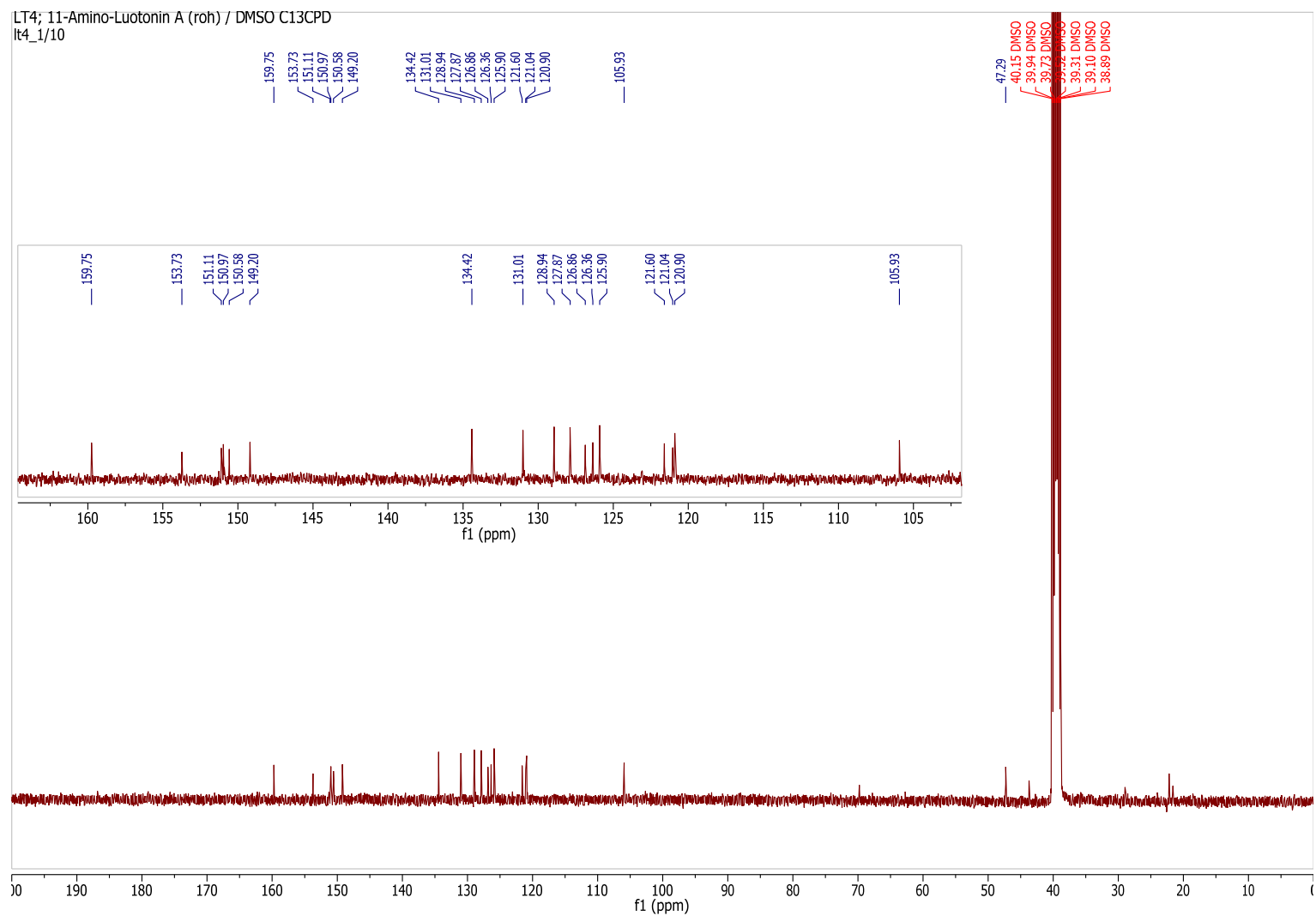


Figure S54. ^{13}C NMR spectrum of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

LT4; 11-Amino-Luotonin A (roh) / DMSO HSQC

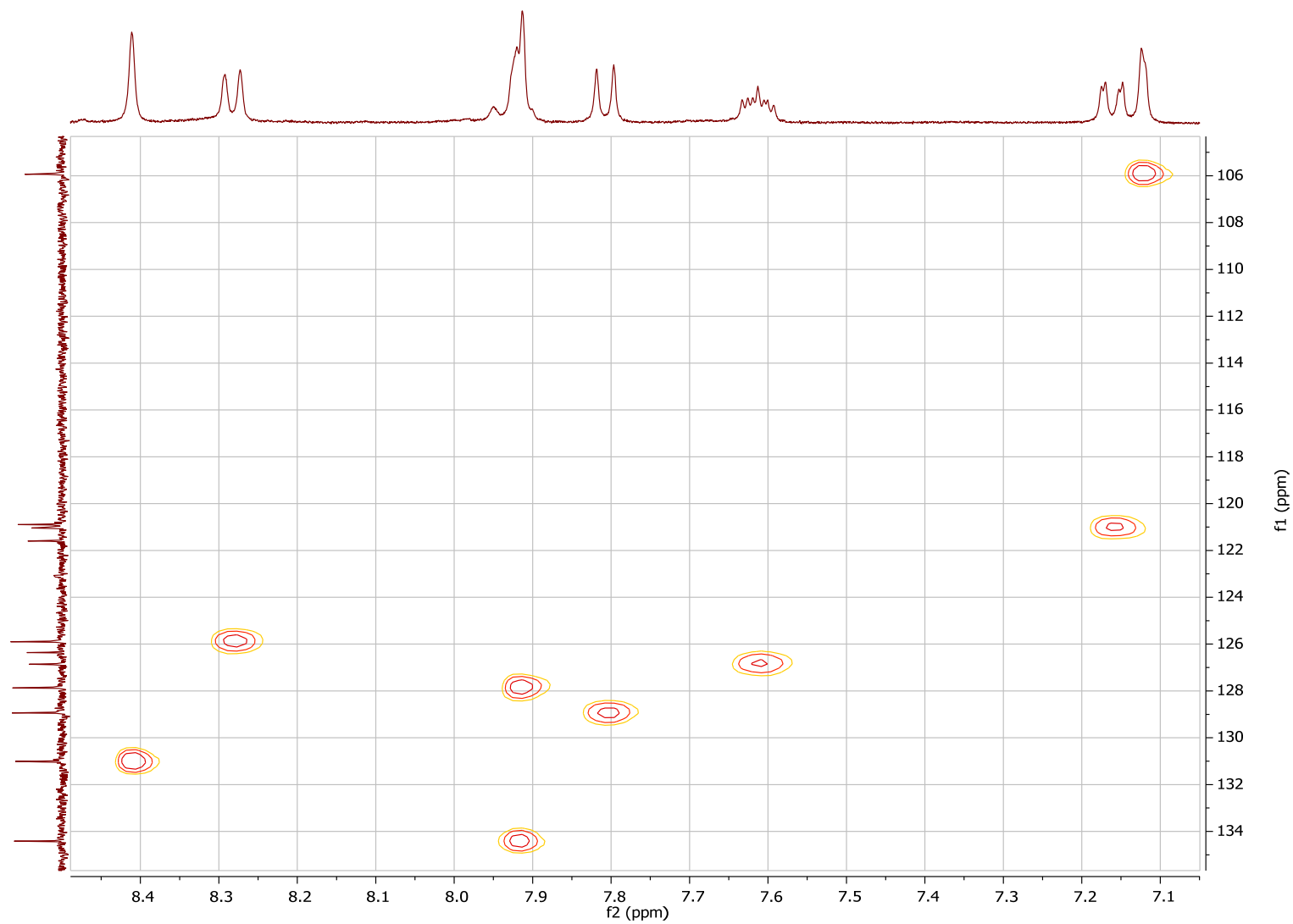


Figure S55. HSQC spectrum of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

LT4; 11-Amino-Luotonin A (roh) / DMSO HMBC

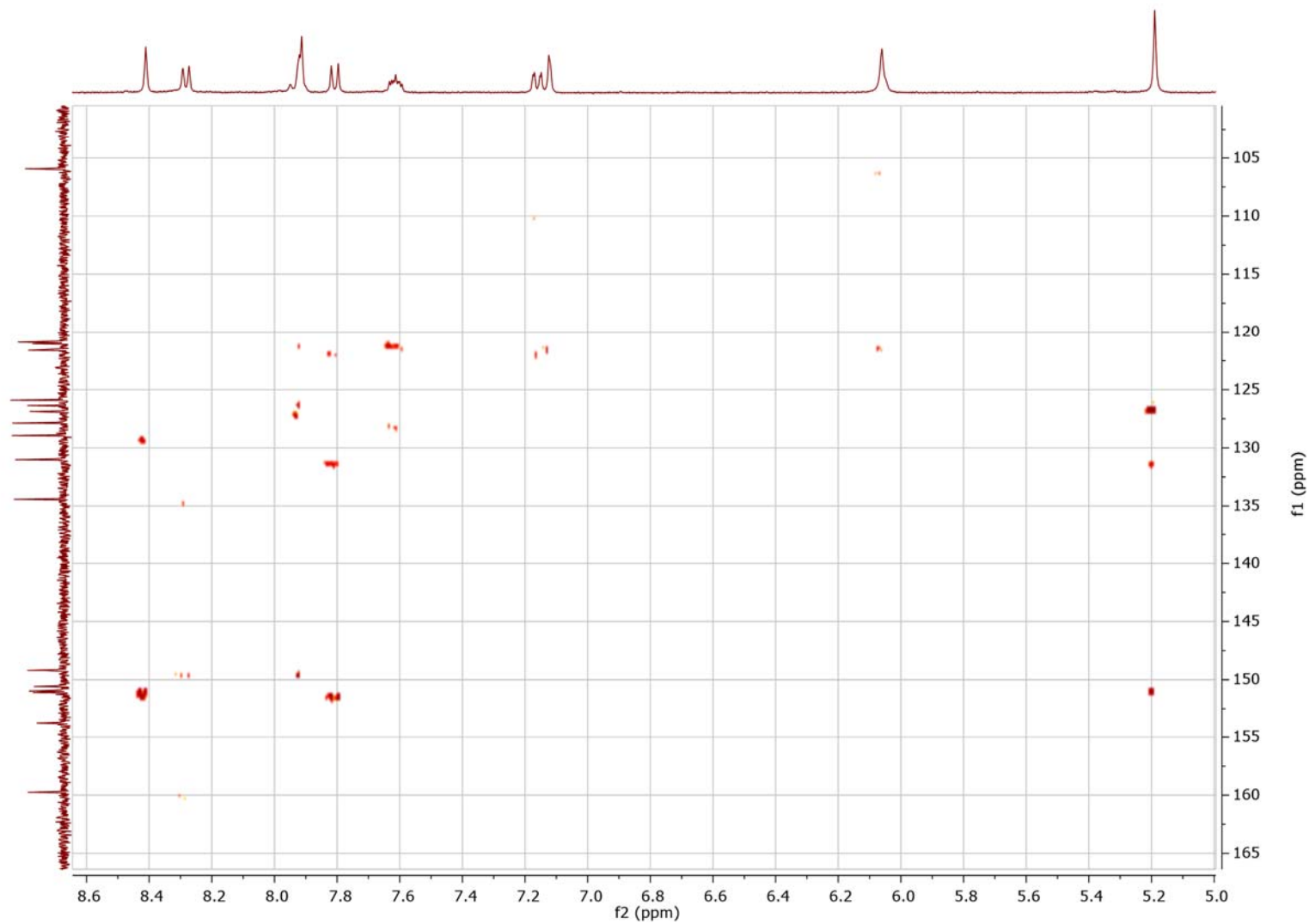


Figure S56. HMBC spoepectrum of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).

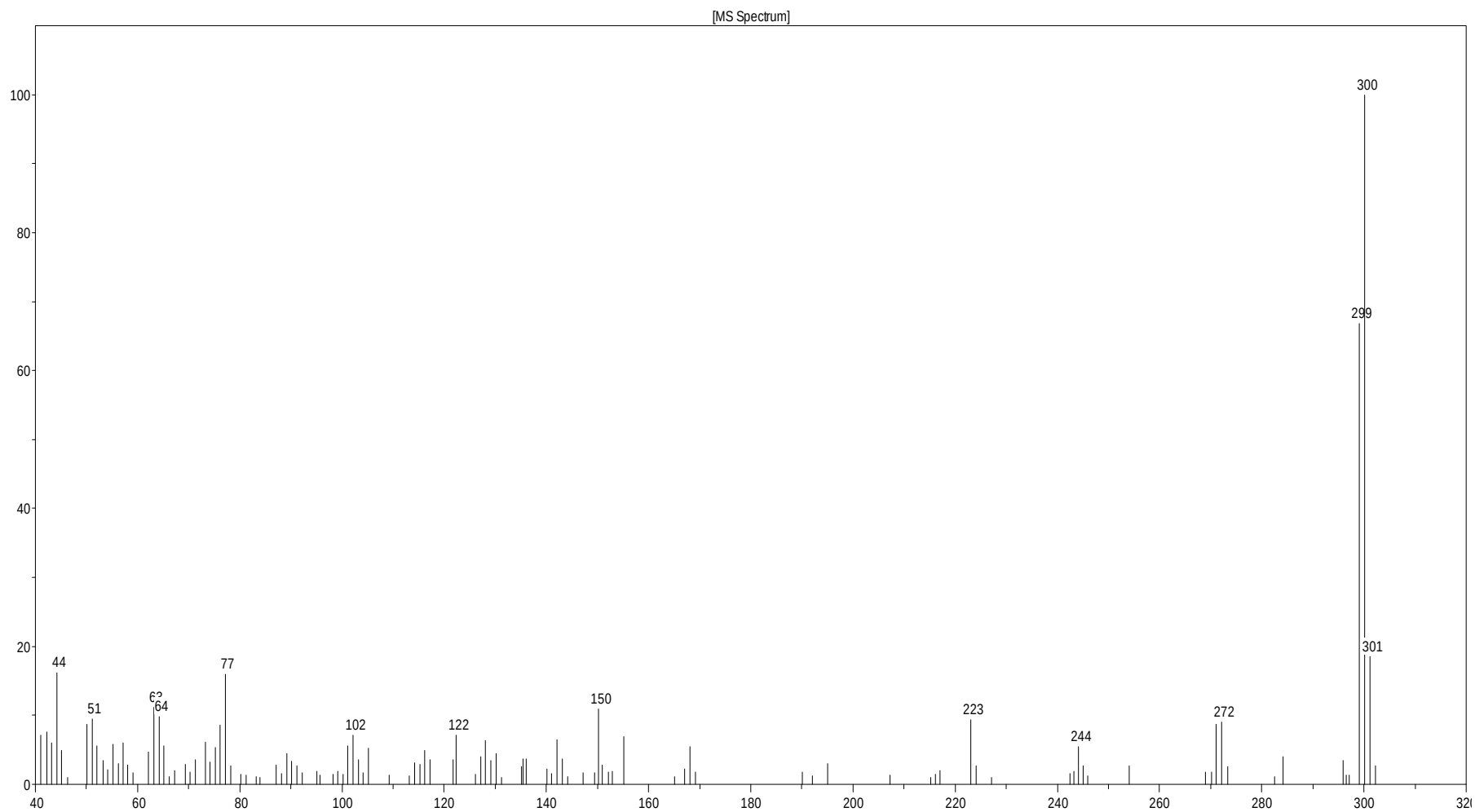


Figure S57. EI-MS of 3-aminoquinolino[2',3':3,4]pyrrolo[2,1-*b*]quinazolin-11(13*H*)-one (**10b**).