

Supporting Information

Synthesis of 2-substituted-3-(1*H*-indol-3-yl)isoindolin-1-one derivatives in water under catalyst-free conditions

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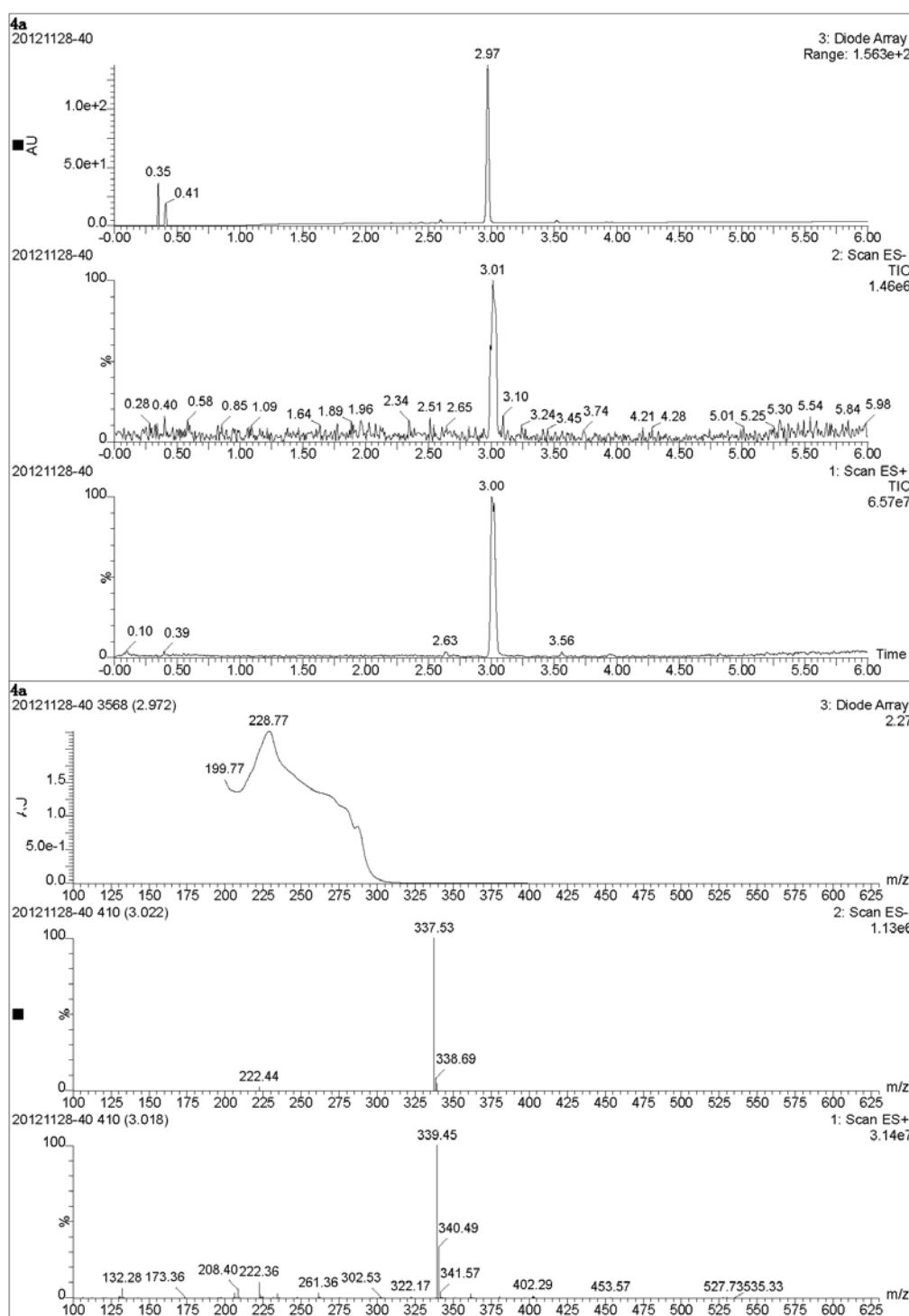
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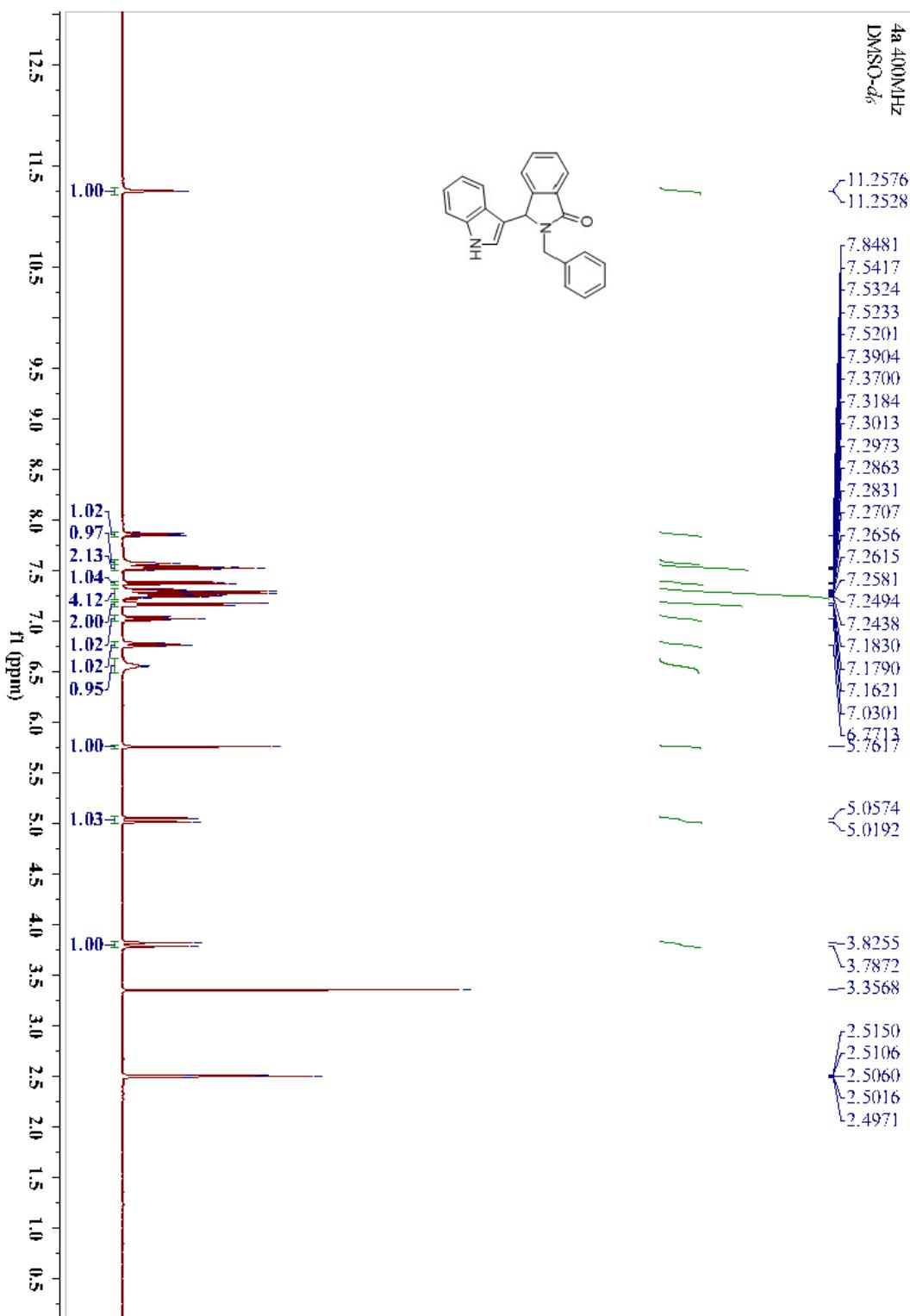
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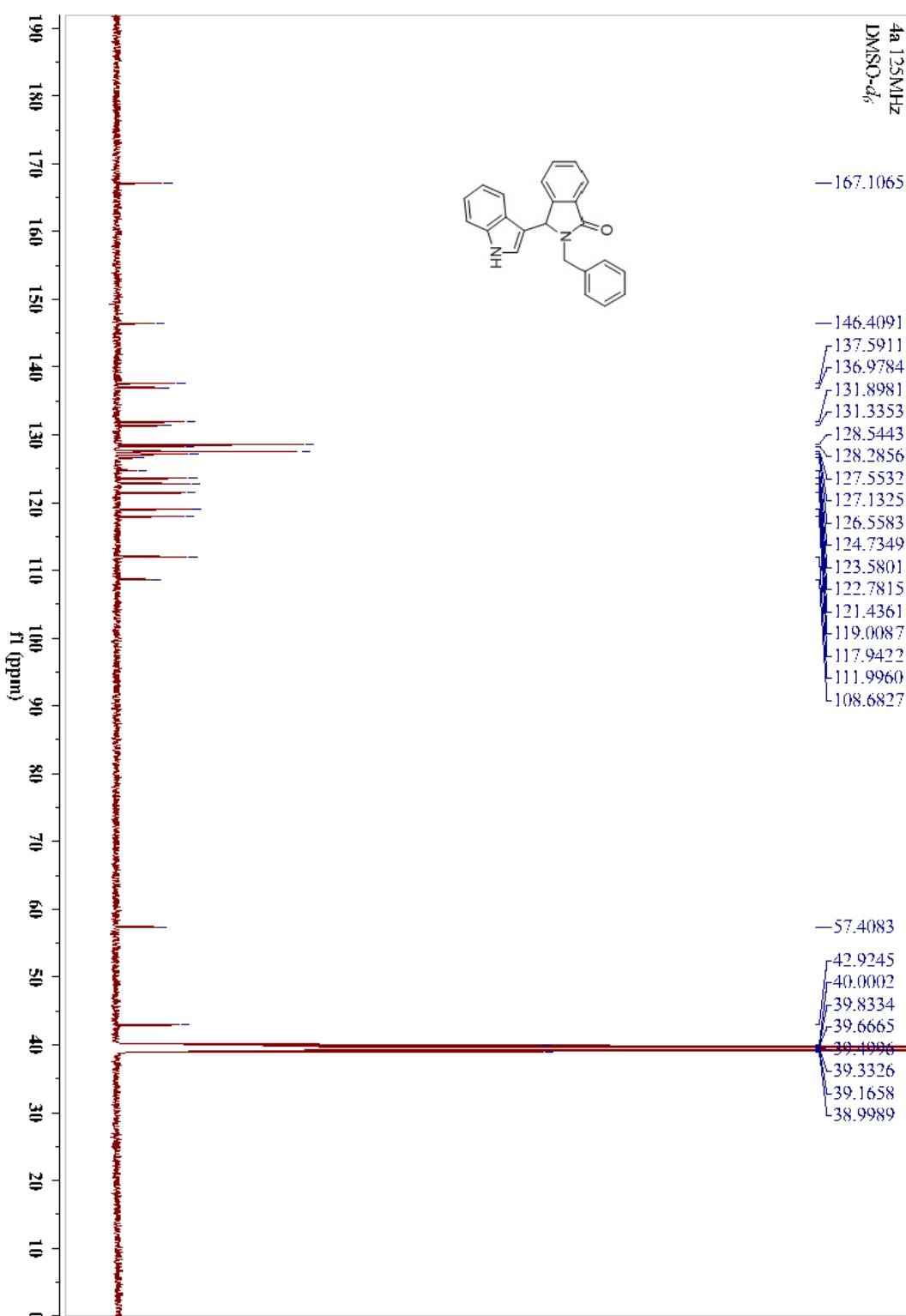
S1. LCMS spectrum of 2-benzyl-3-(1*H*-indol-3-yl)isoindolin-1-one (4a**).**



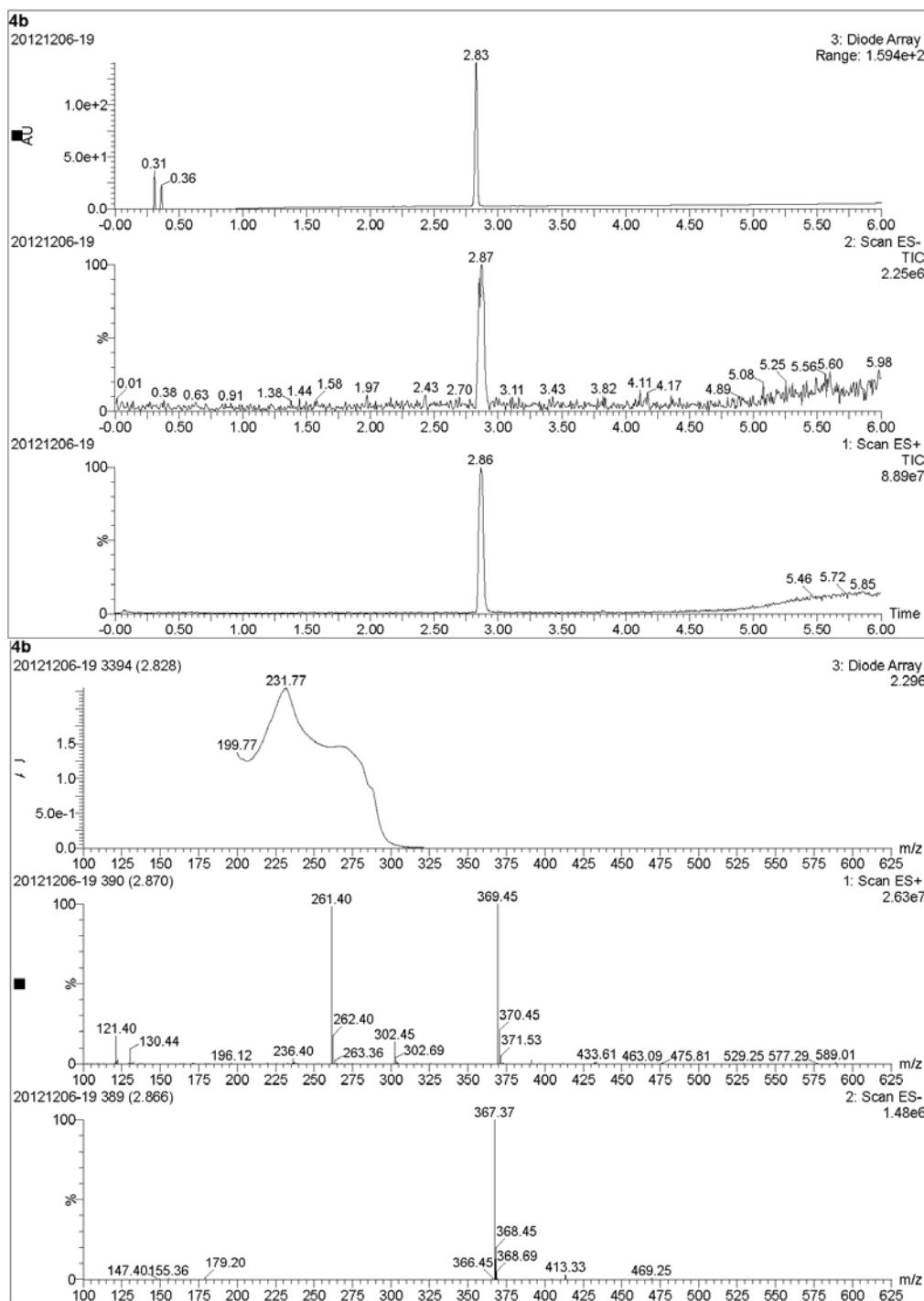
S2. ^1H NMR spectrum of 2-benzyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4a**) in $\text{DMSO}-d_6$.



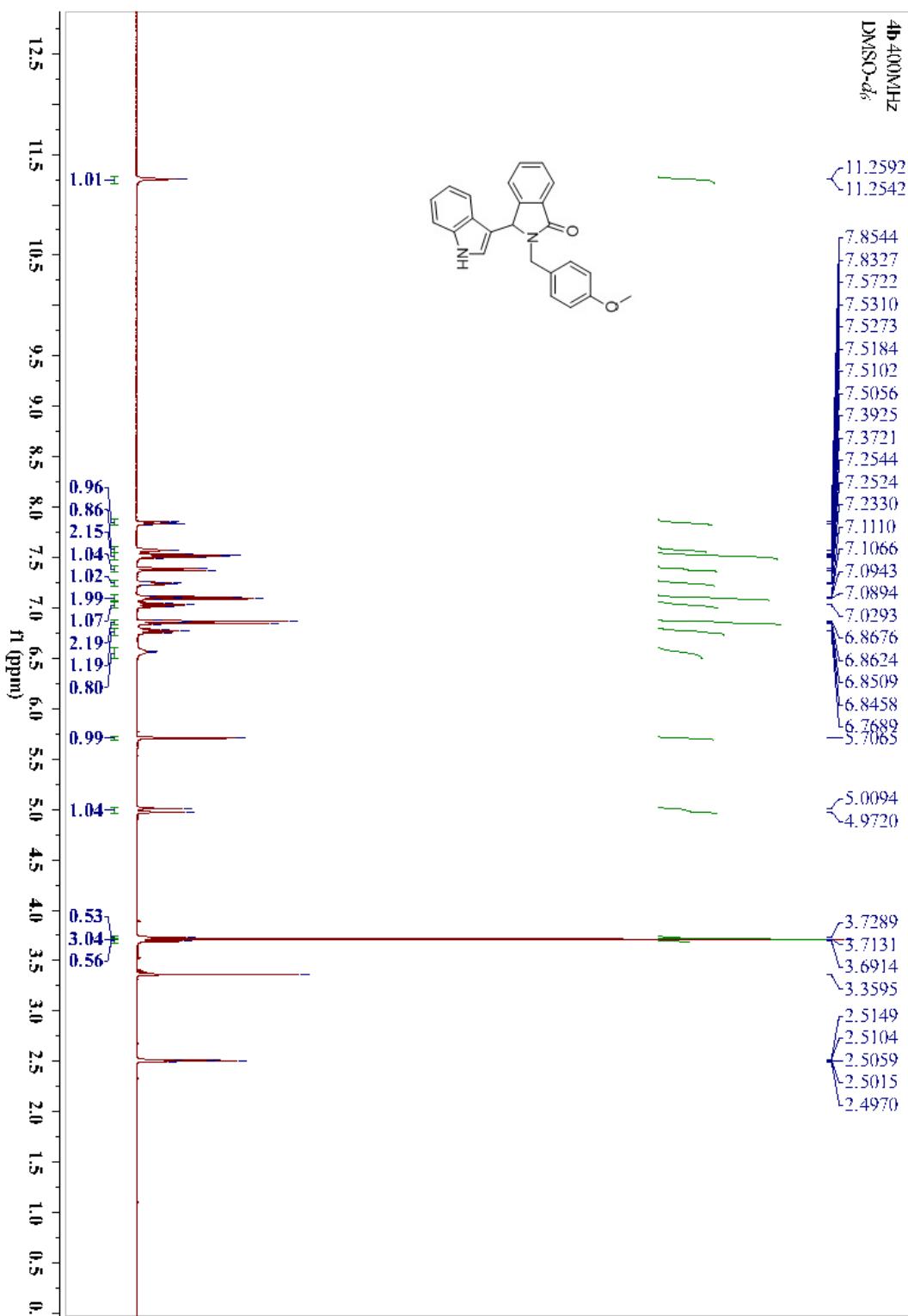
S3. ^{13}C NMR spectrum of 2-benzyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4a**) in $\text{DMSO}-d_6$.



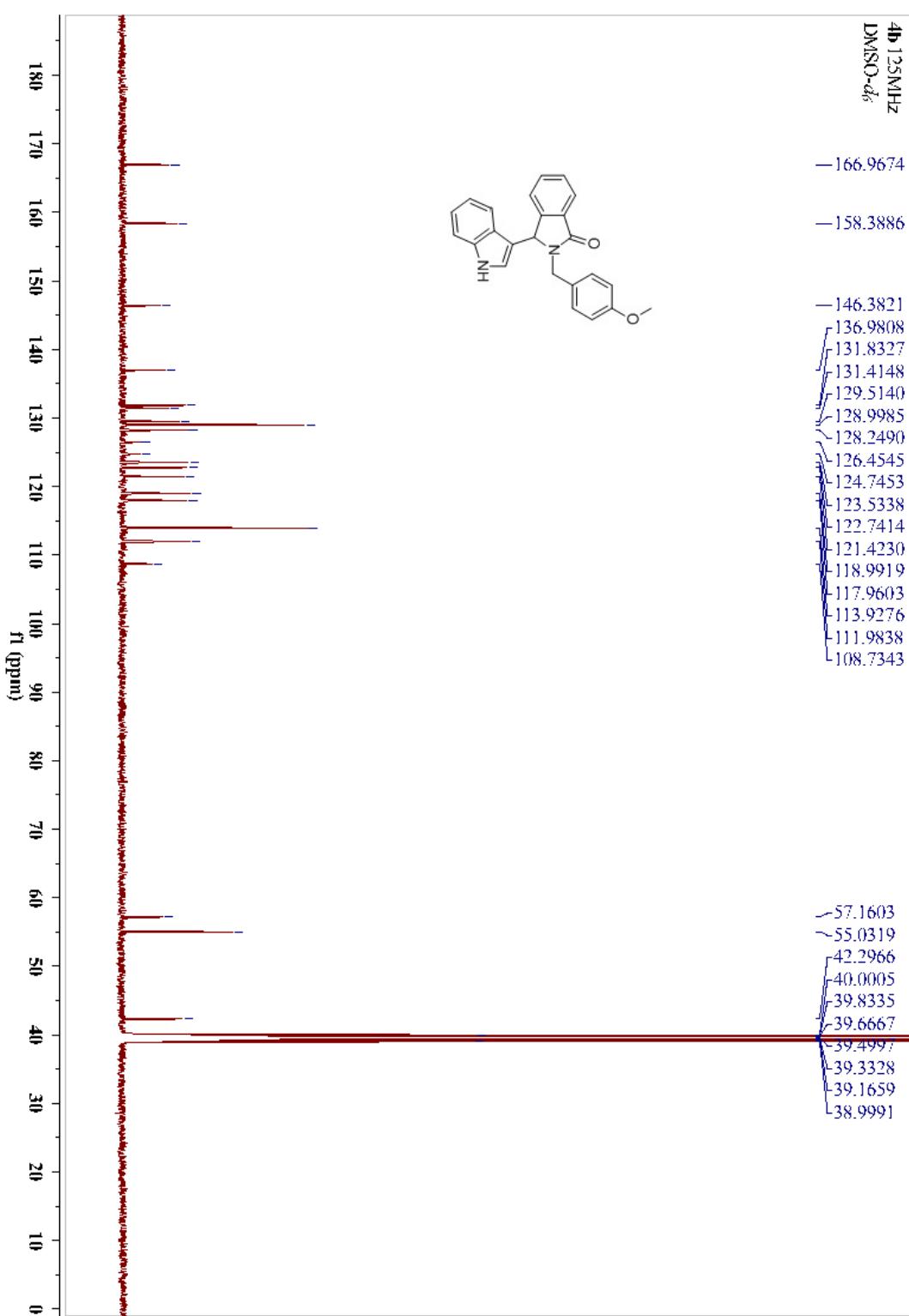
S4. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one (4b**).**



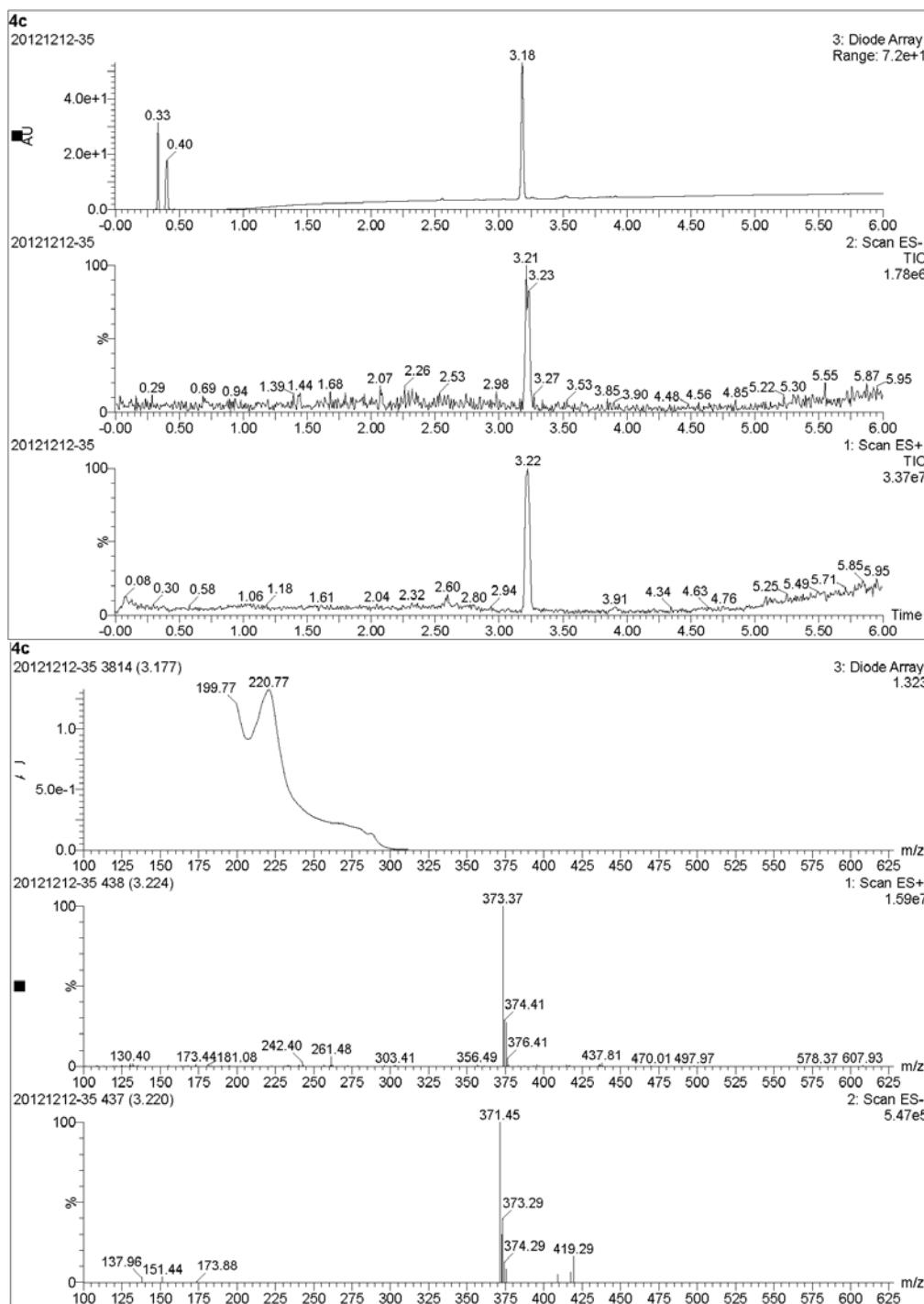
S5. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one (**4b**) in DMSO-*d*₆.



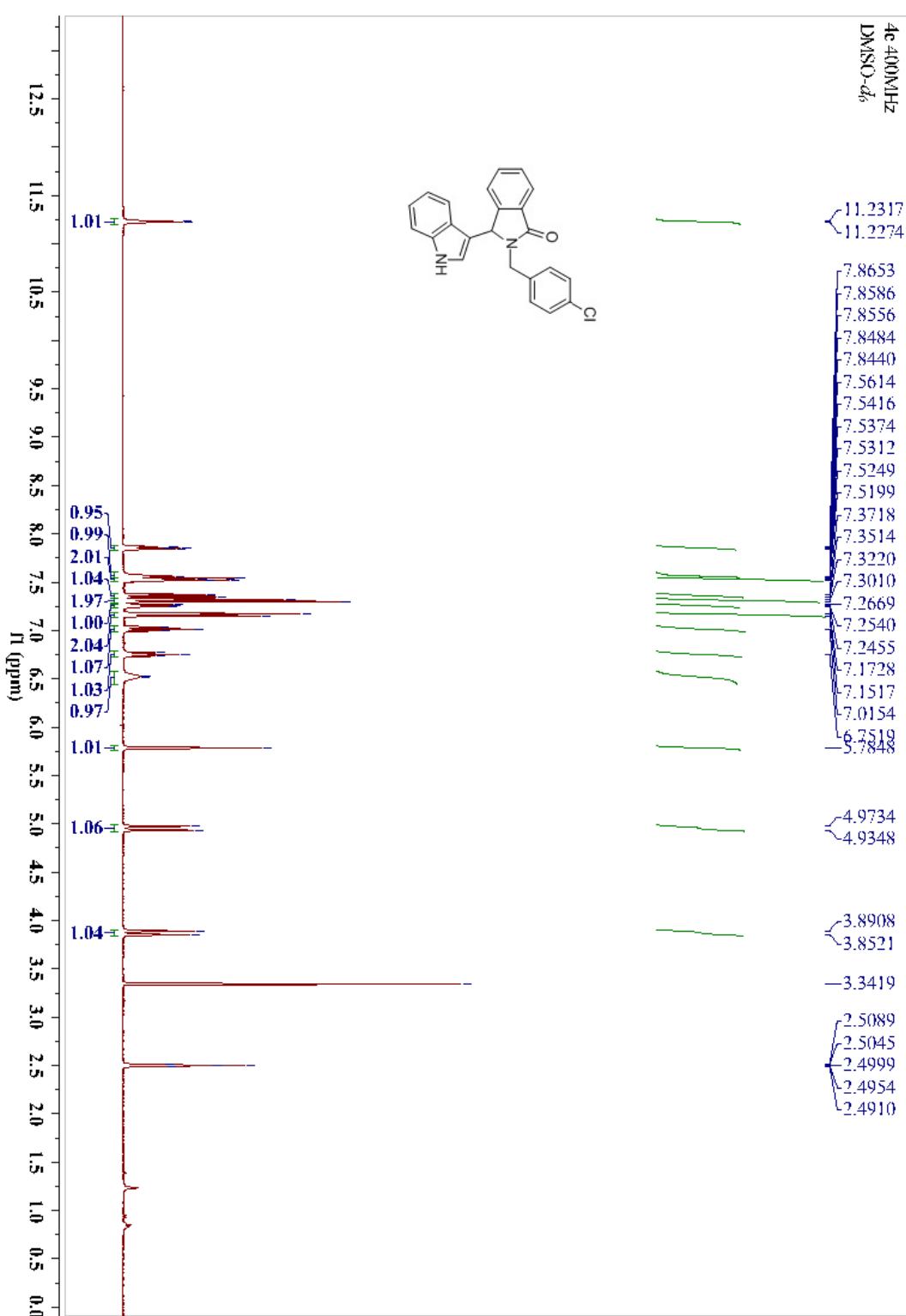
S6. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one (**4b**) in DMSO-*d*₆.



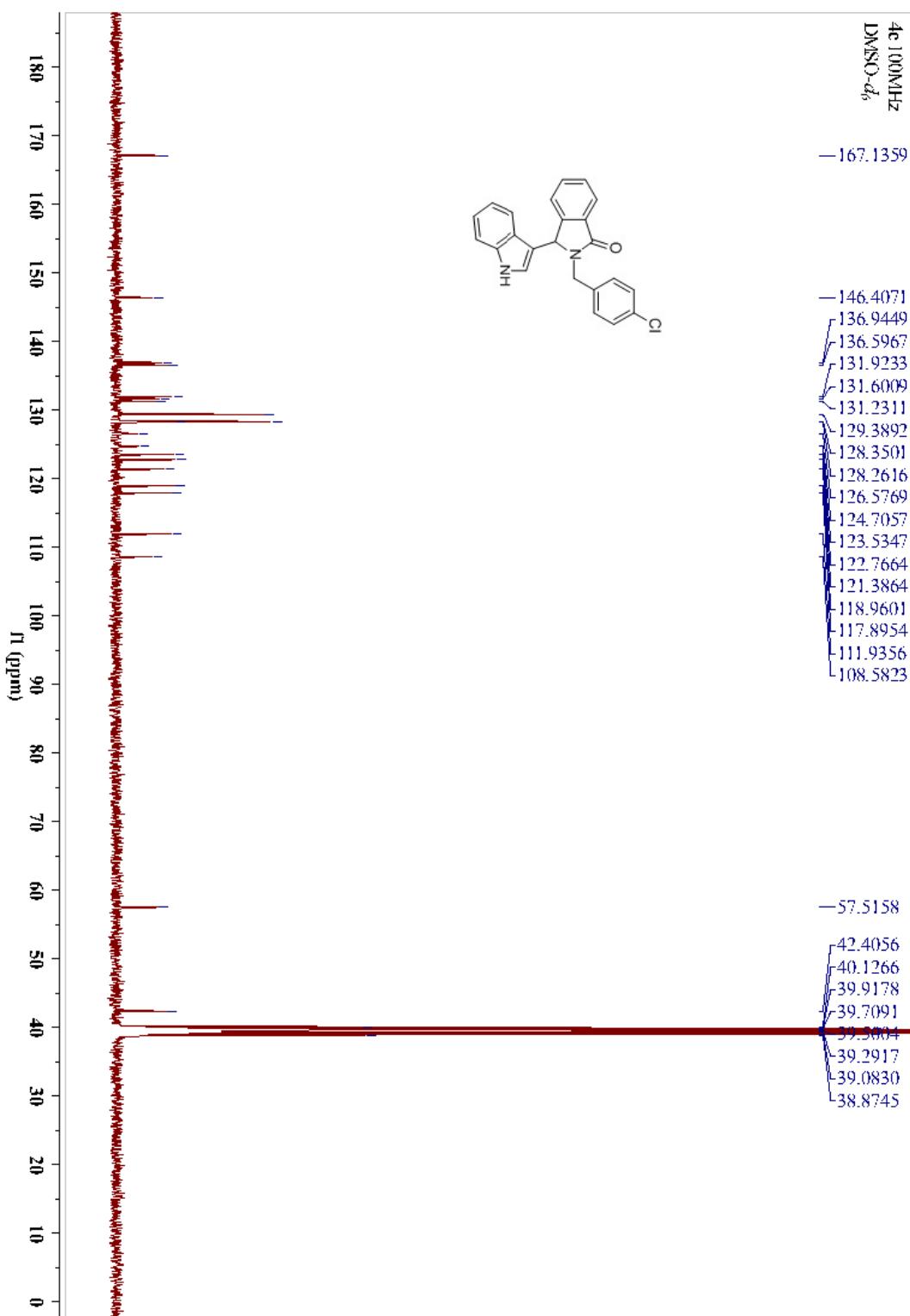
S7. LCMS spectrum of 2-(4-chlorobenzyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (4c**).**



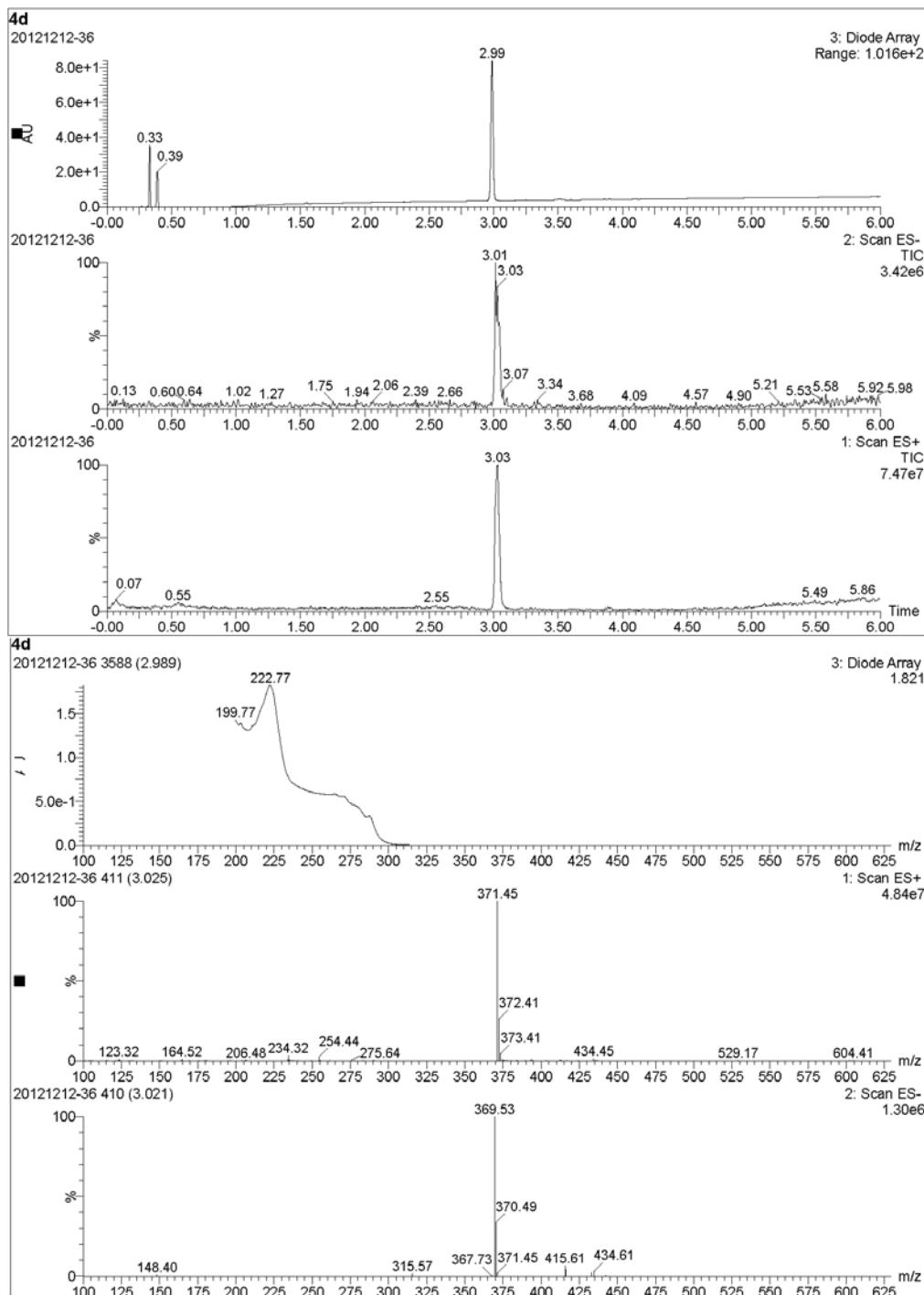
S8. ^1H NMR spectrum of 2-(4-chlorobenzyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4c**) in $\text{DMSO}-d_6$.



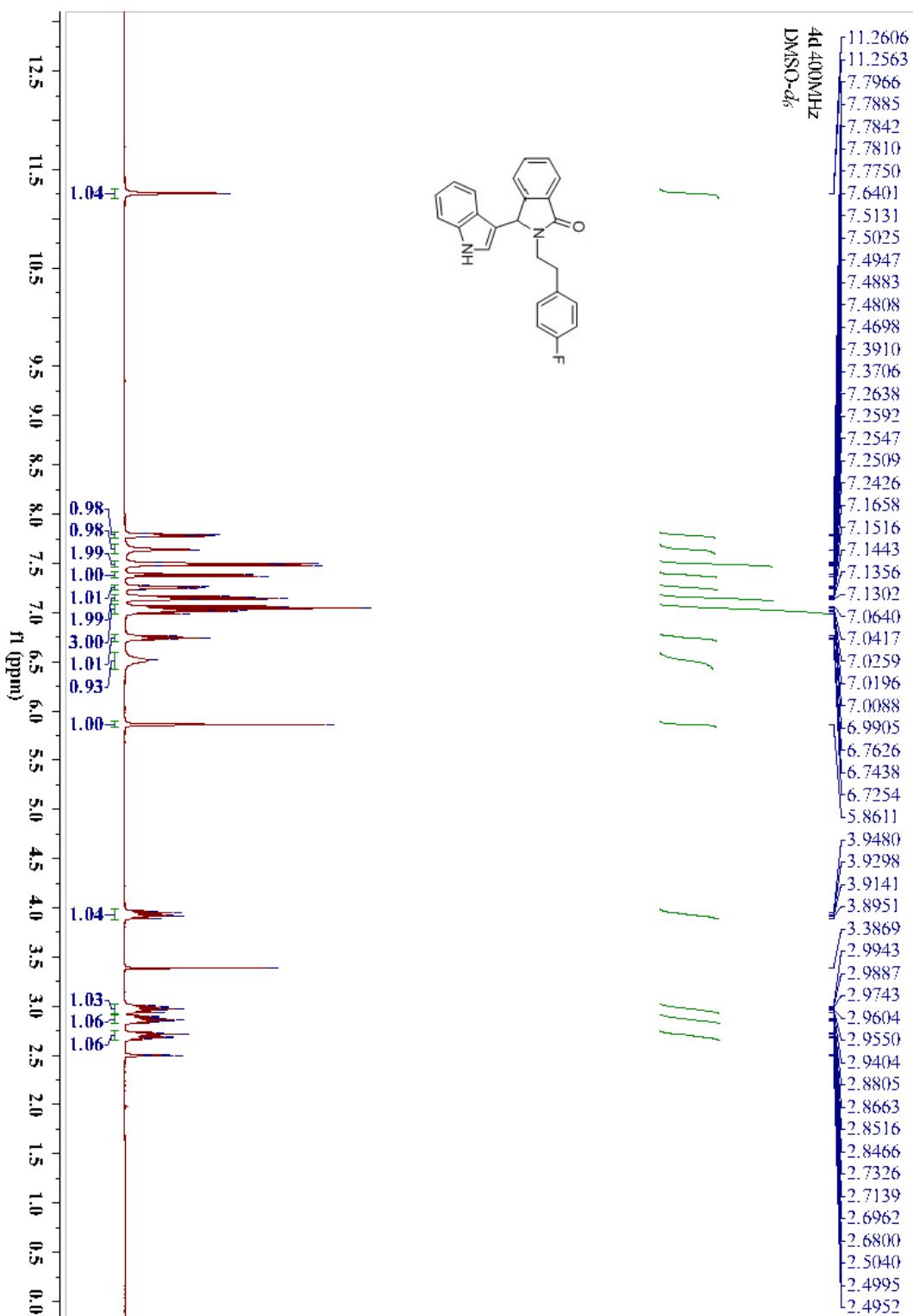
S9. ^{13}C NMR spectrum of 2-(4-chlorobenzyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4c**) in $\text{DMSO}-d_6$.



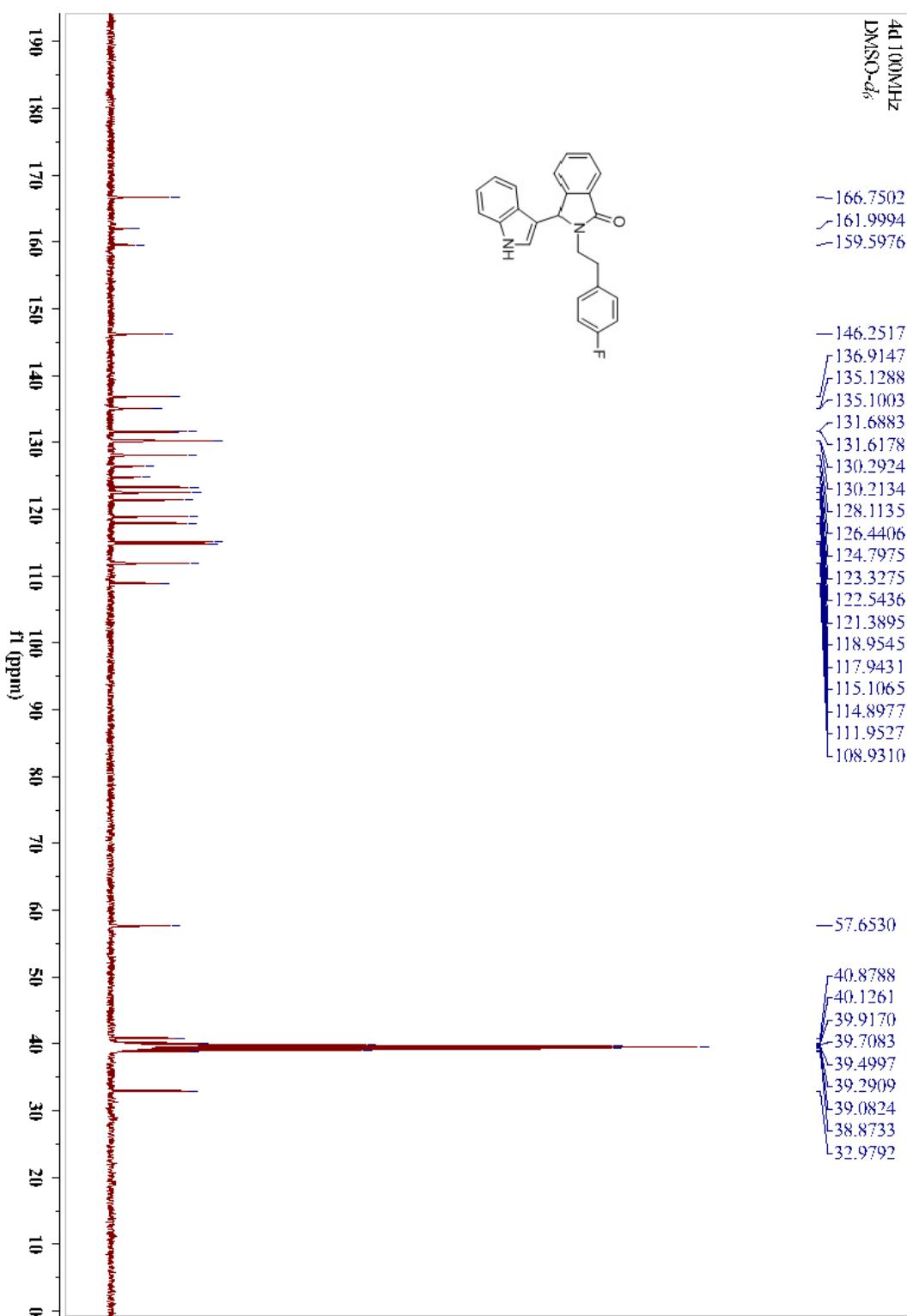
S10. LCMS spectrum of 2-(4-fluorophenethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (4d).



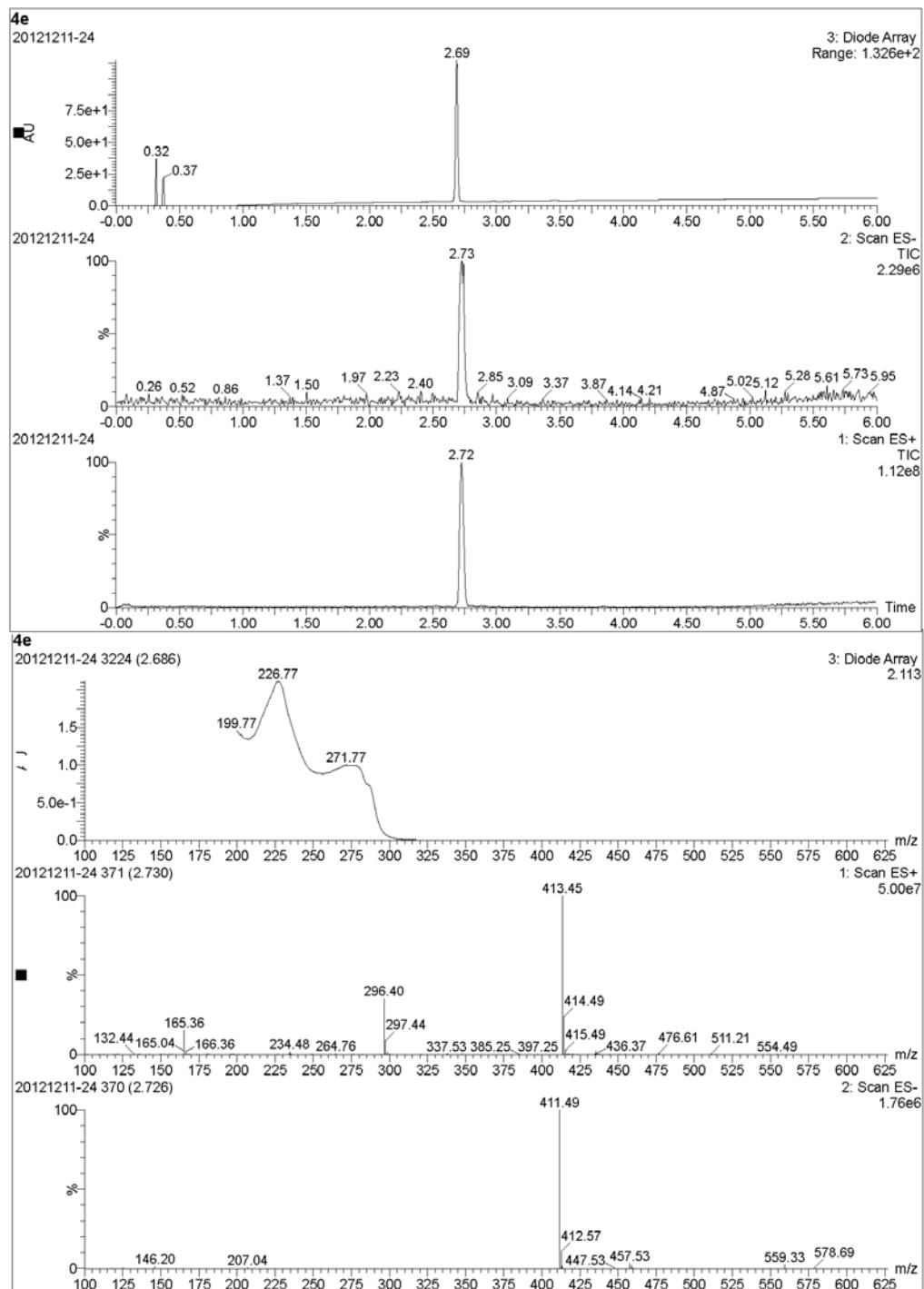
S11. ^1H NMR spectrum of 2-(4-fluorophenethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4d**) in $\text{DMSO}-d_6$.



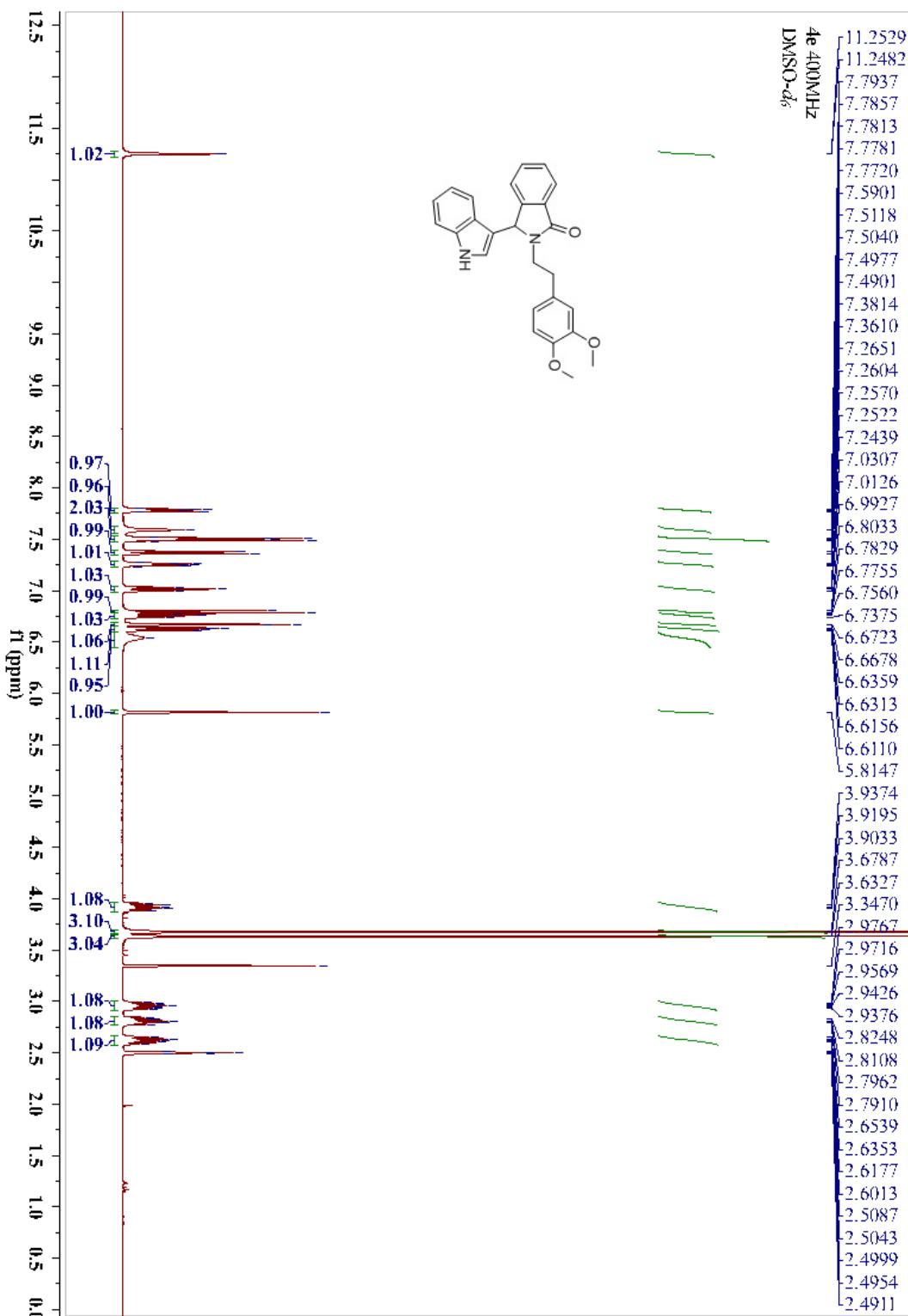
S12. ^{13}C NMR spectrum of 2-(4-fluorophenethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4d**) in $\text{DMSO}-d_6$.



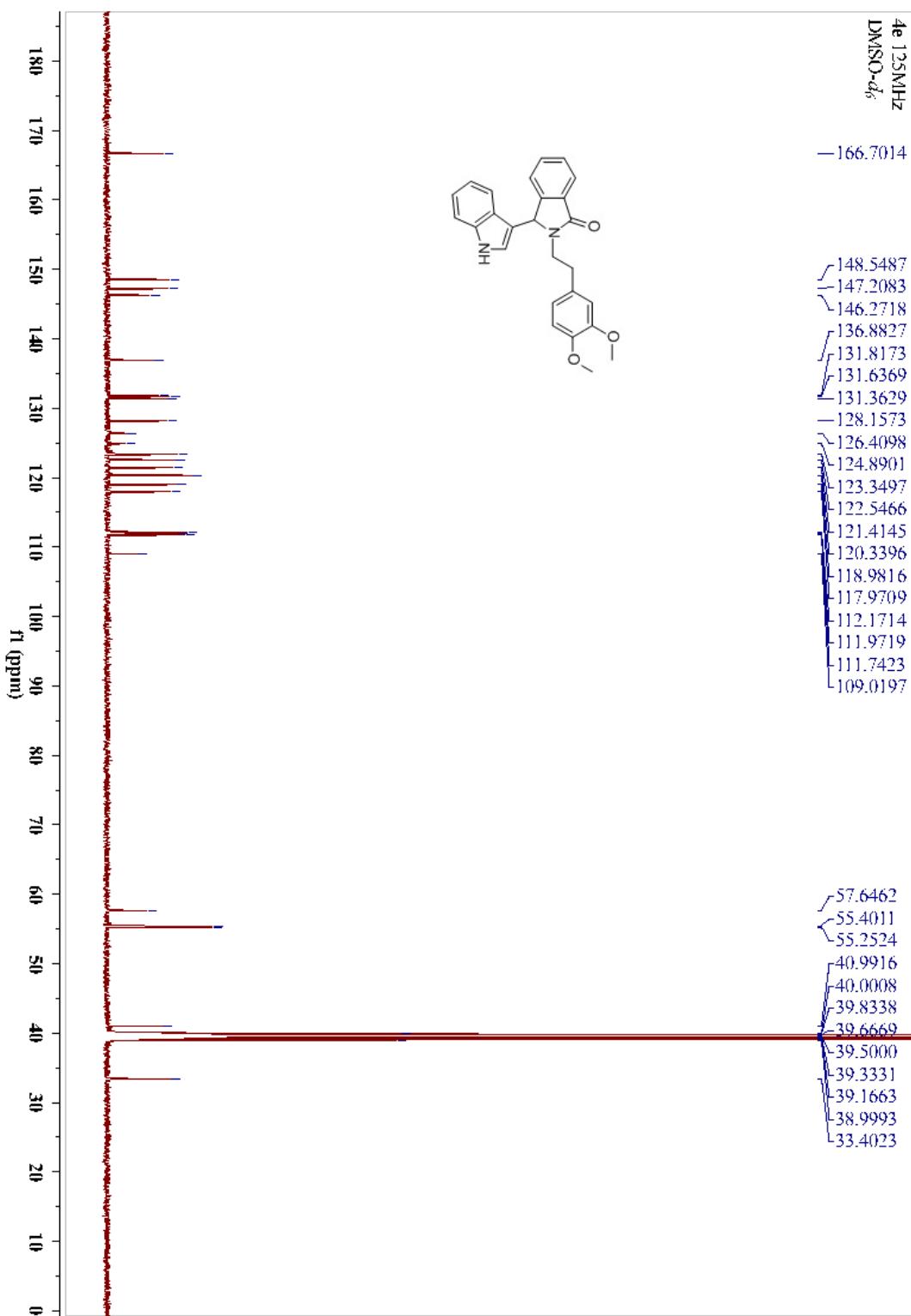
S13. LCMS spectrum of 2-(3,4-dimethoxyphenethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4e**).



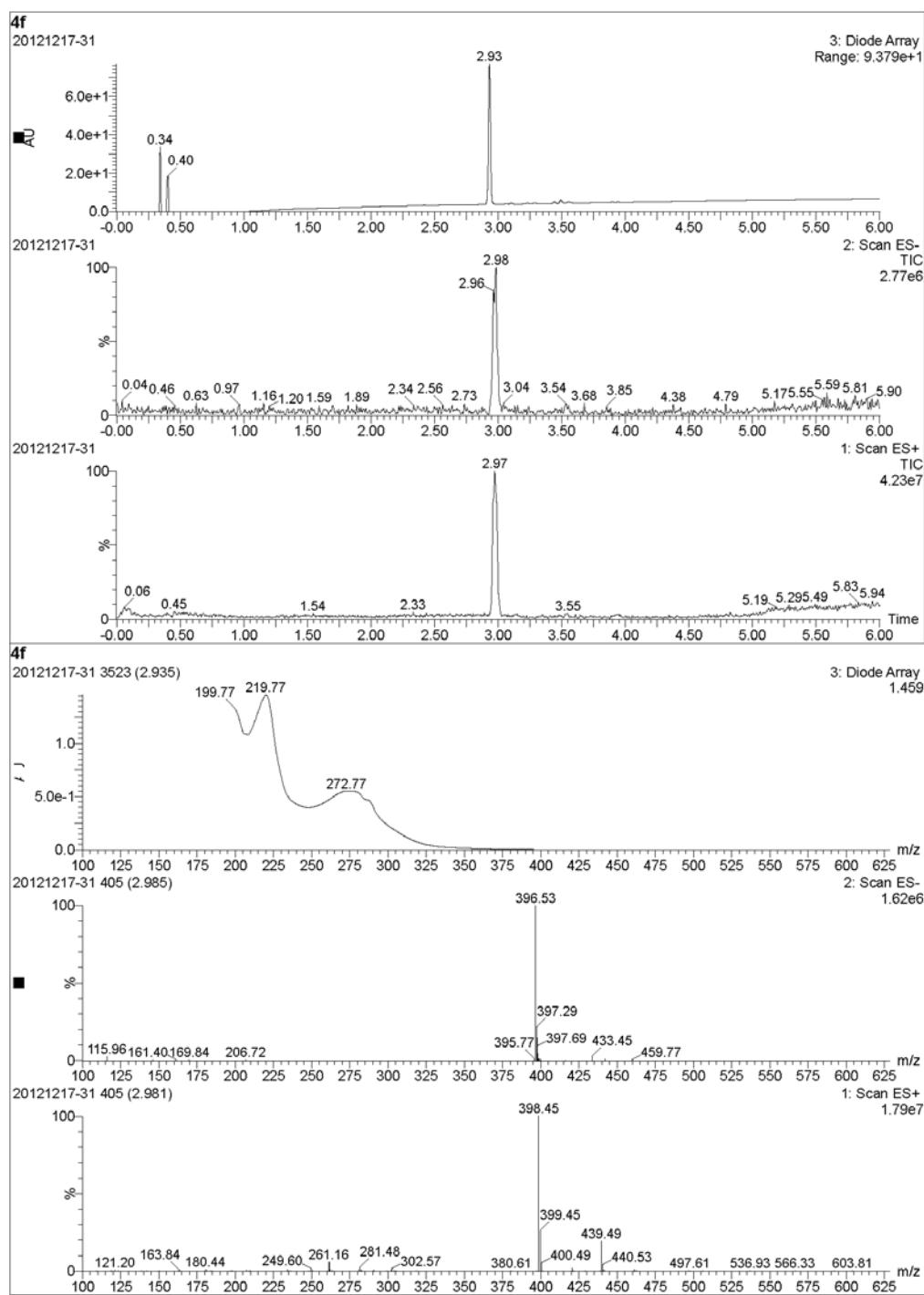
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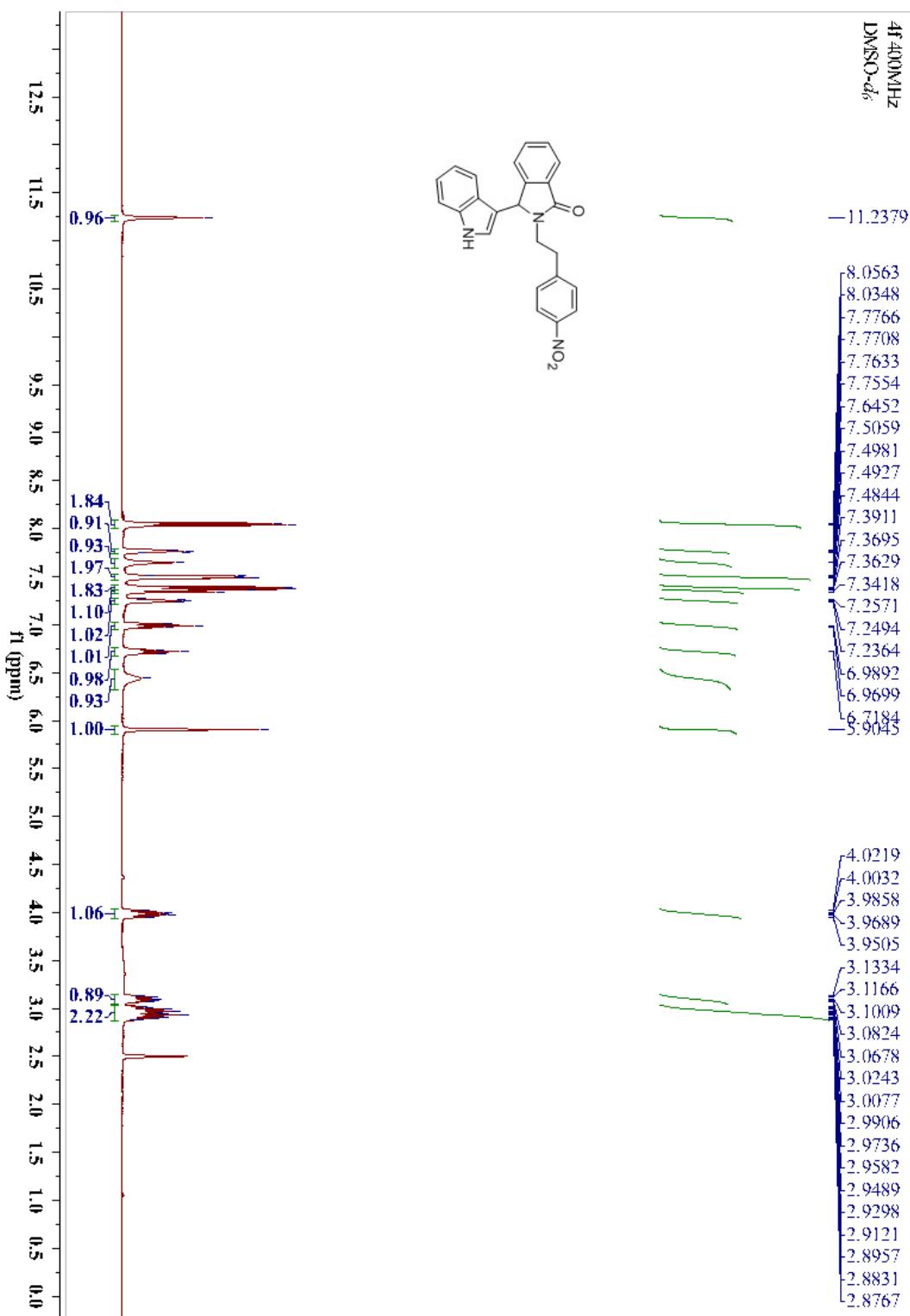
S15. ^{13}C NMR spectrum of 2-(3,4-dimethoxyphenethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4e**) in $\text{DMSO}-d_6$.



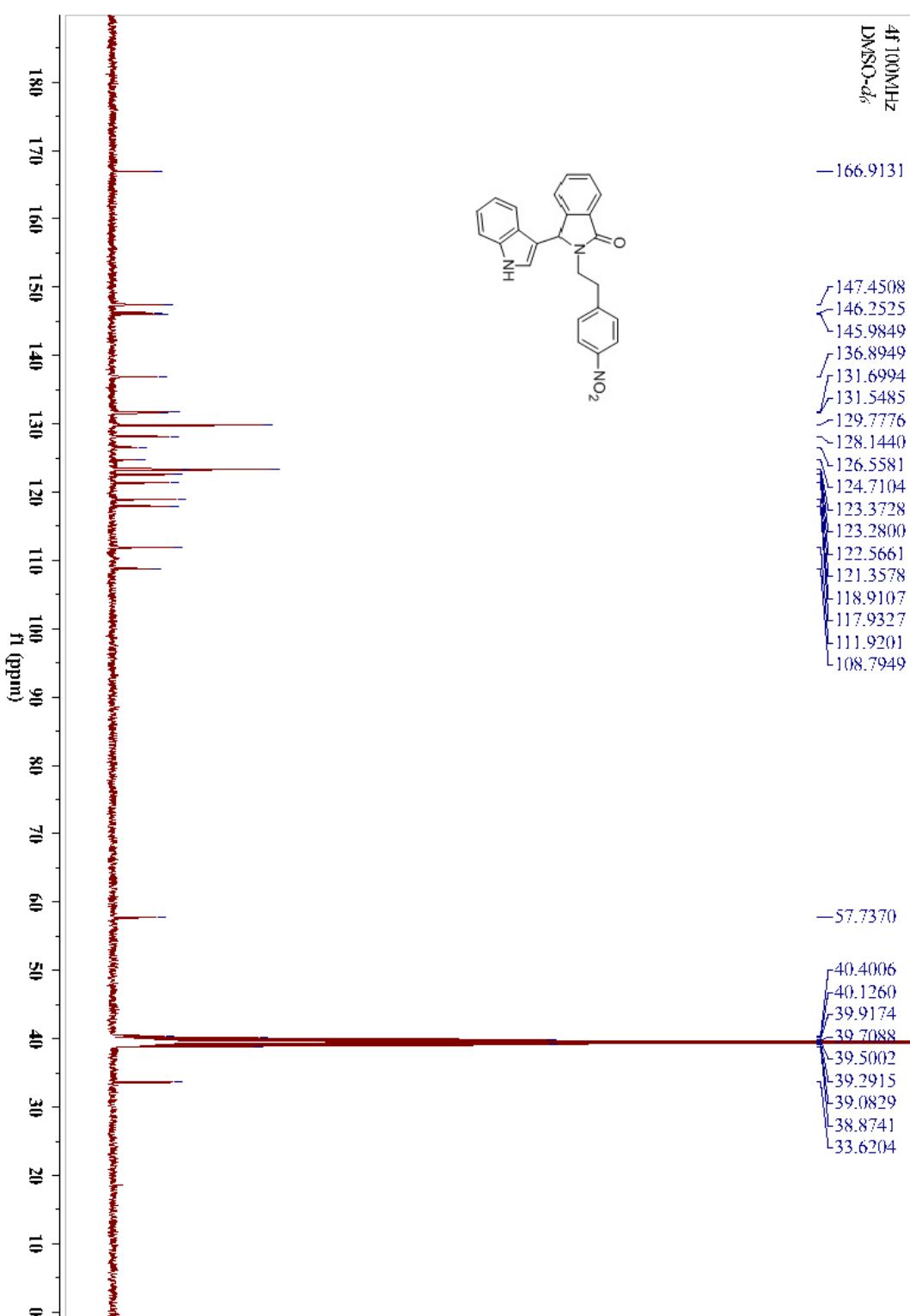
S16. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-(4-nitrophenethyl)isoindolin-1-one (**4f**).



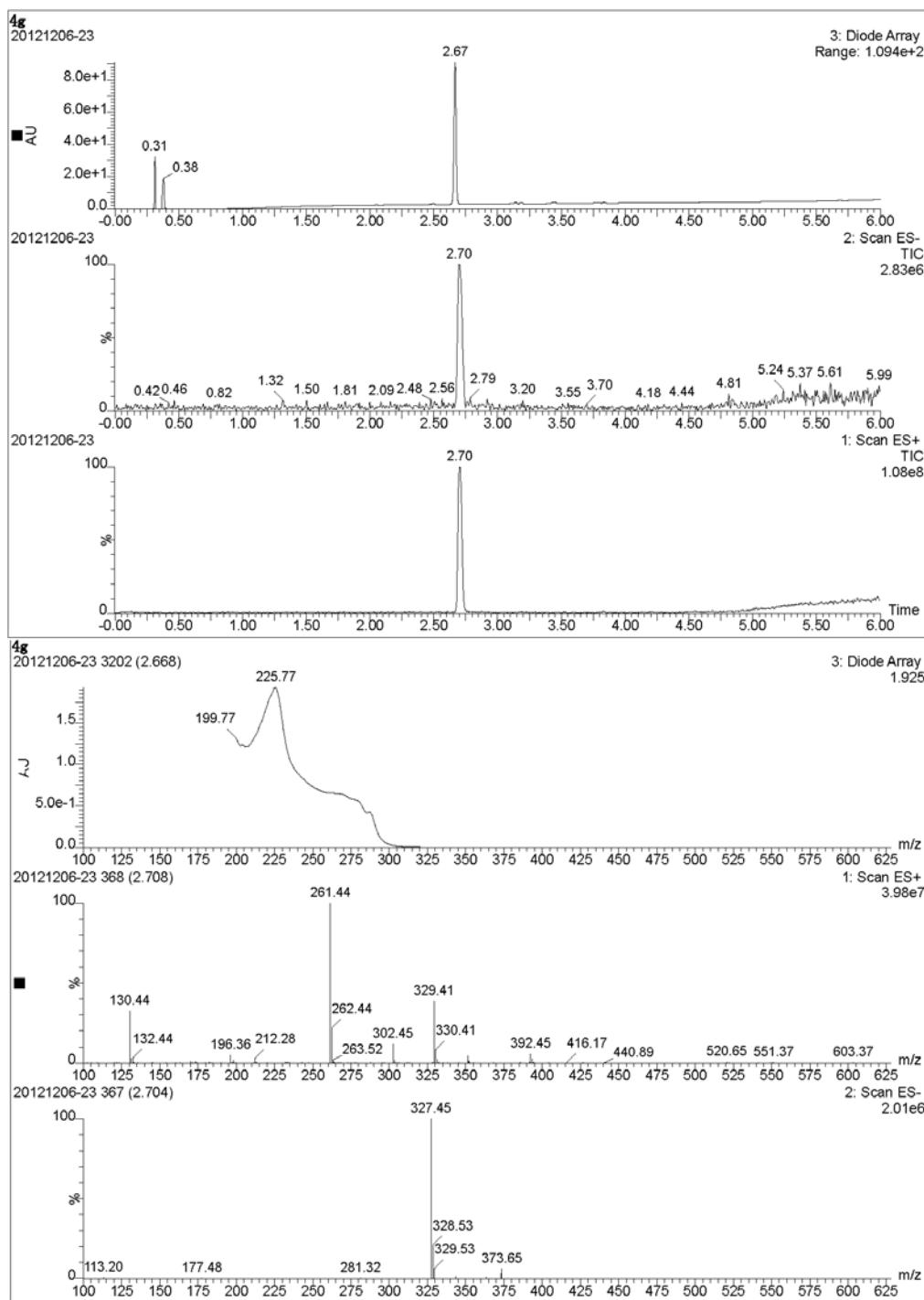
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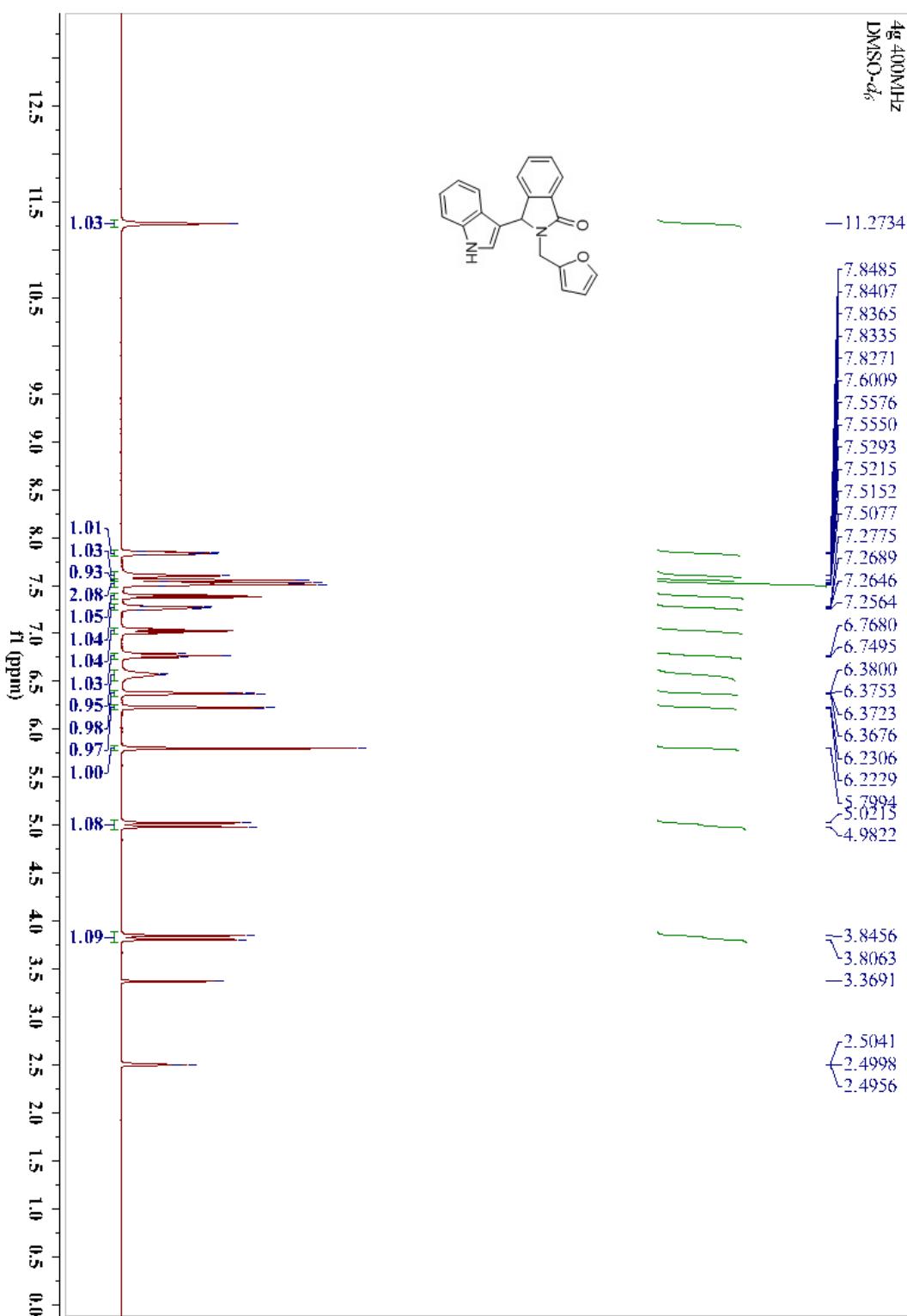
S18. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-(4-nitrophenethyl)isoindolin-1-one (**4f**) in $\text{DMSO}-d_6$.



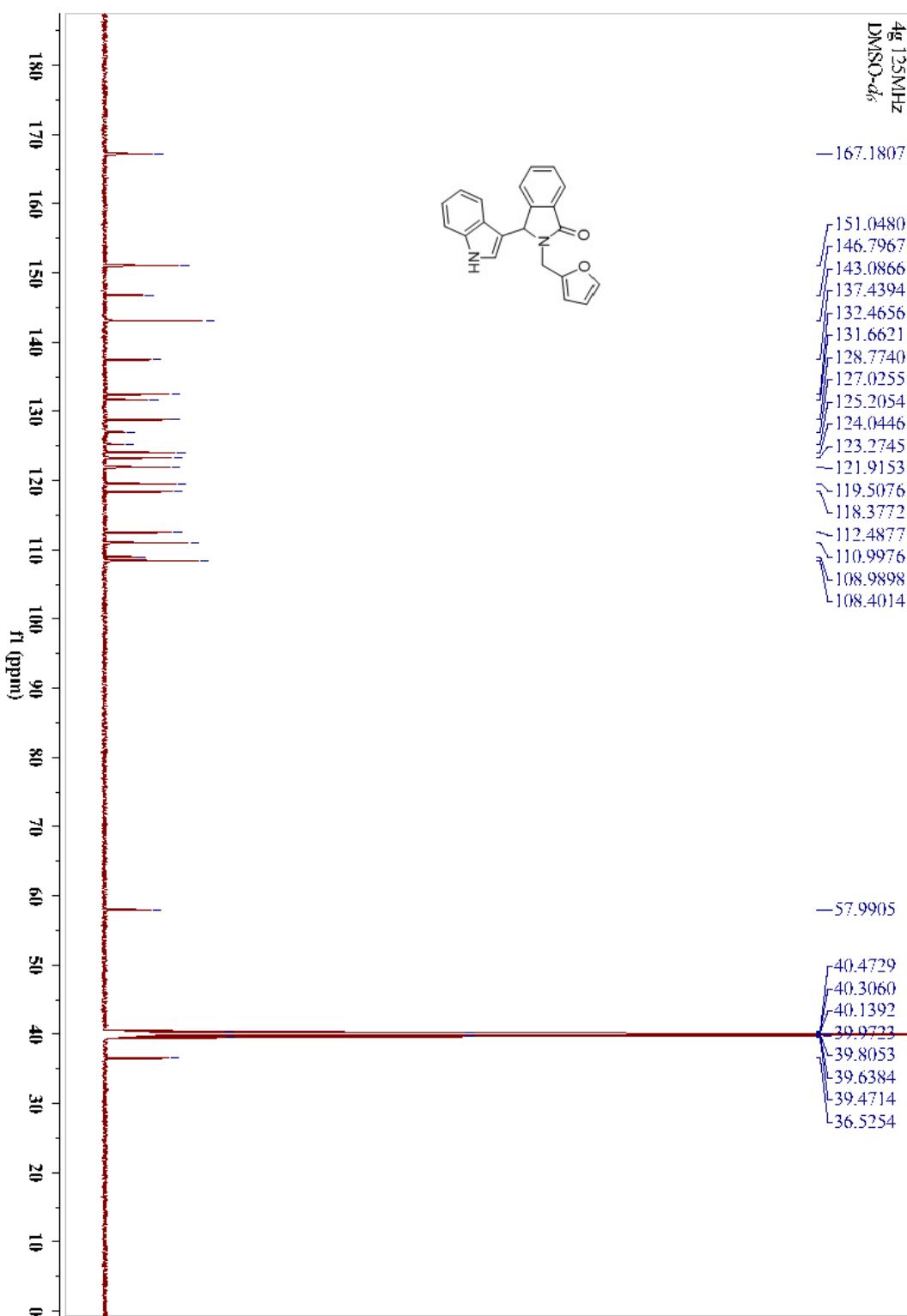
S19. LCMS spectrum of 2-(furan-2-ylmethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4g**).



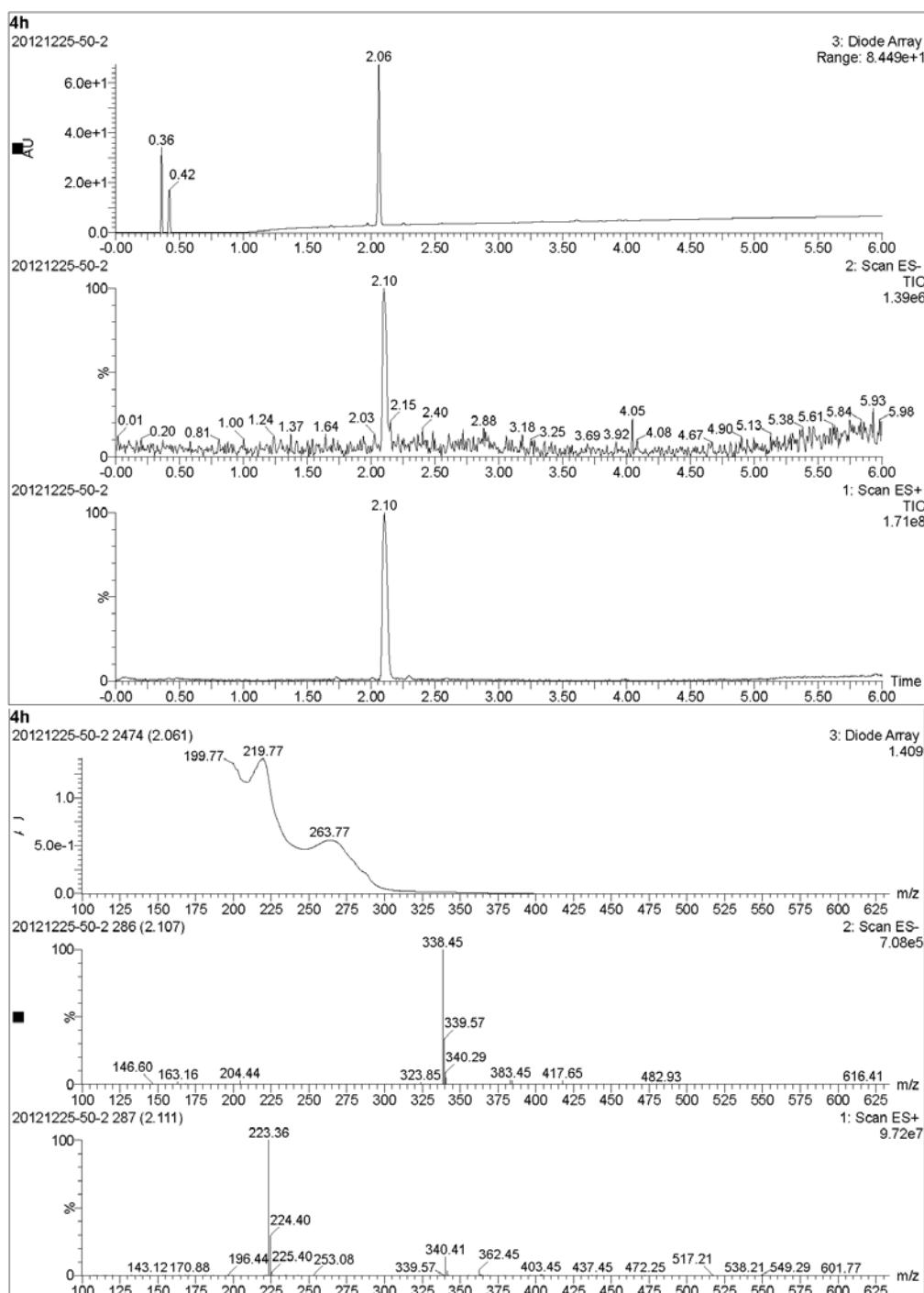
S20. ^1H NMR spectrum of 2-(furan-2-ylmethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4g**) in $\text{DMSO}-d_6$.



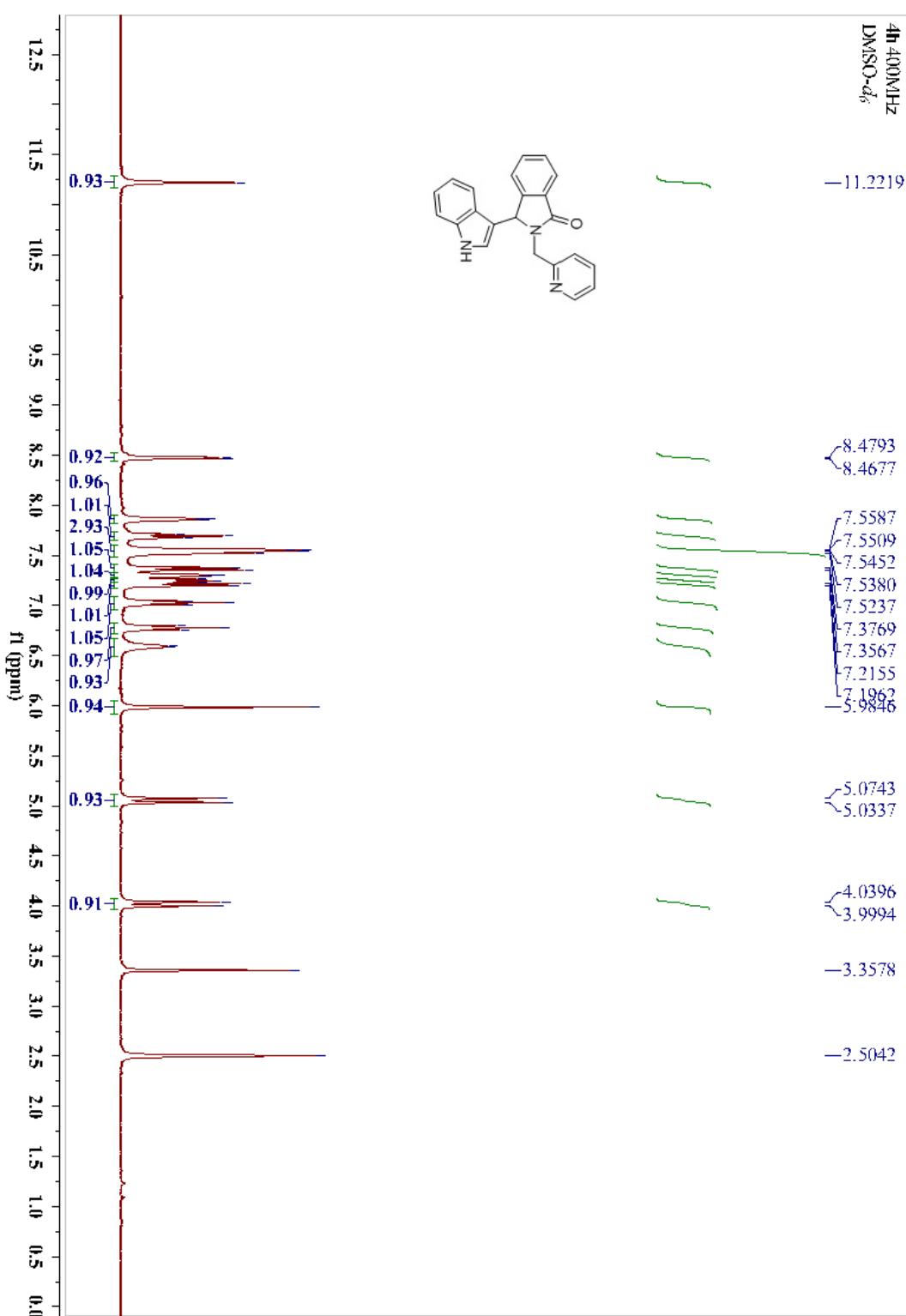
S21. ^{13}C NMR spectrum of 2-(furan-2-ylmethyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4g**) in $\text{DMSO}-d_6$.



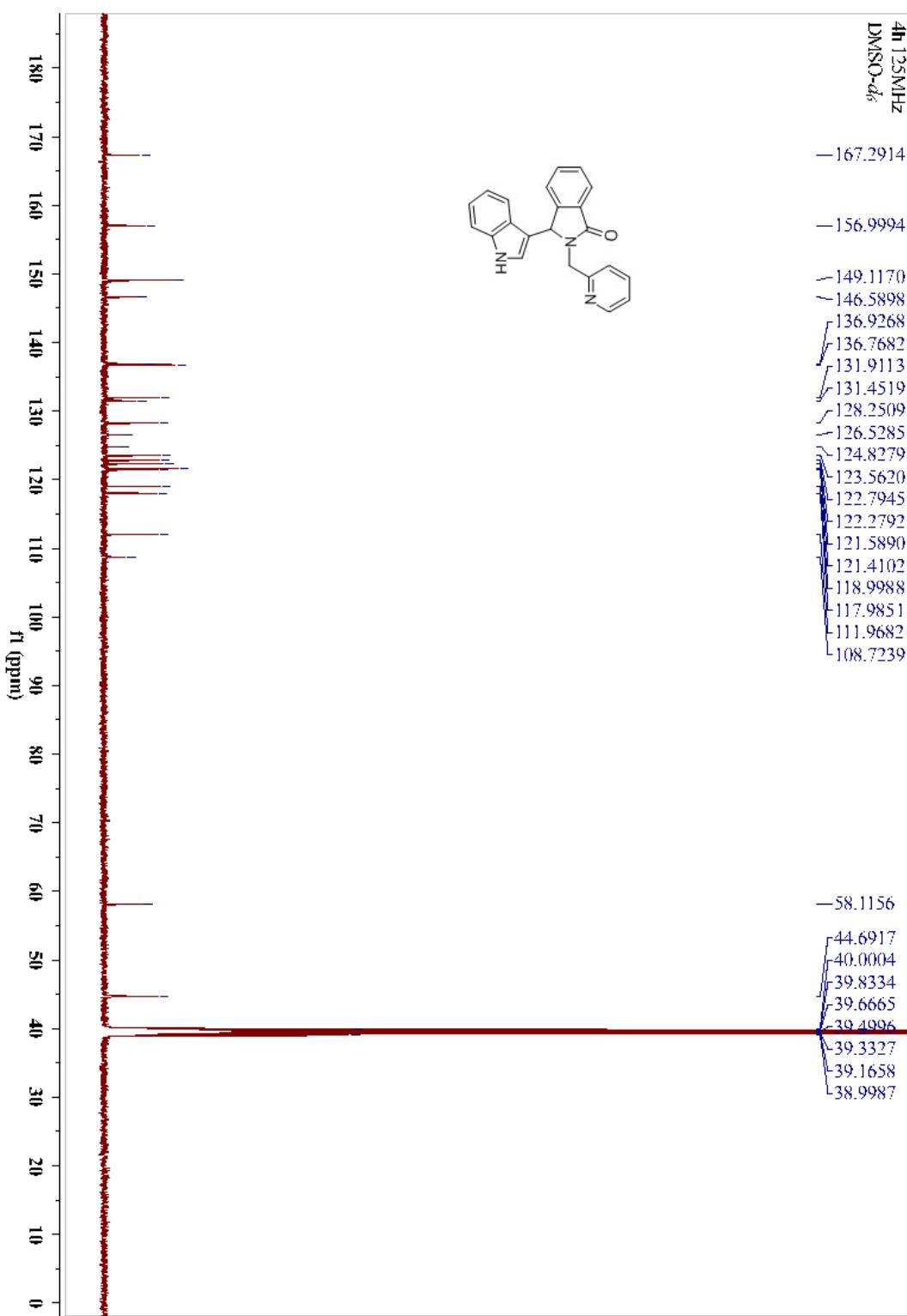
S22. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-(pyridin-2-ylmethyl)isoindolin-1-one (**4h**).



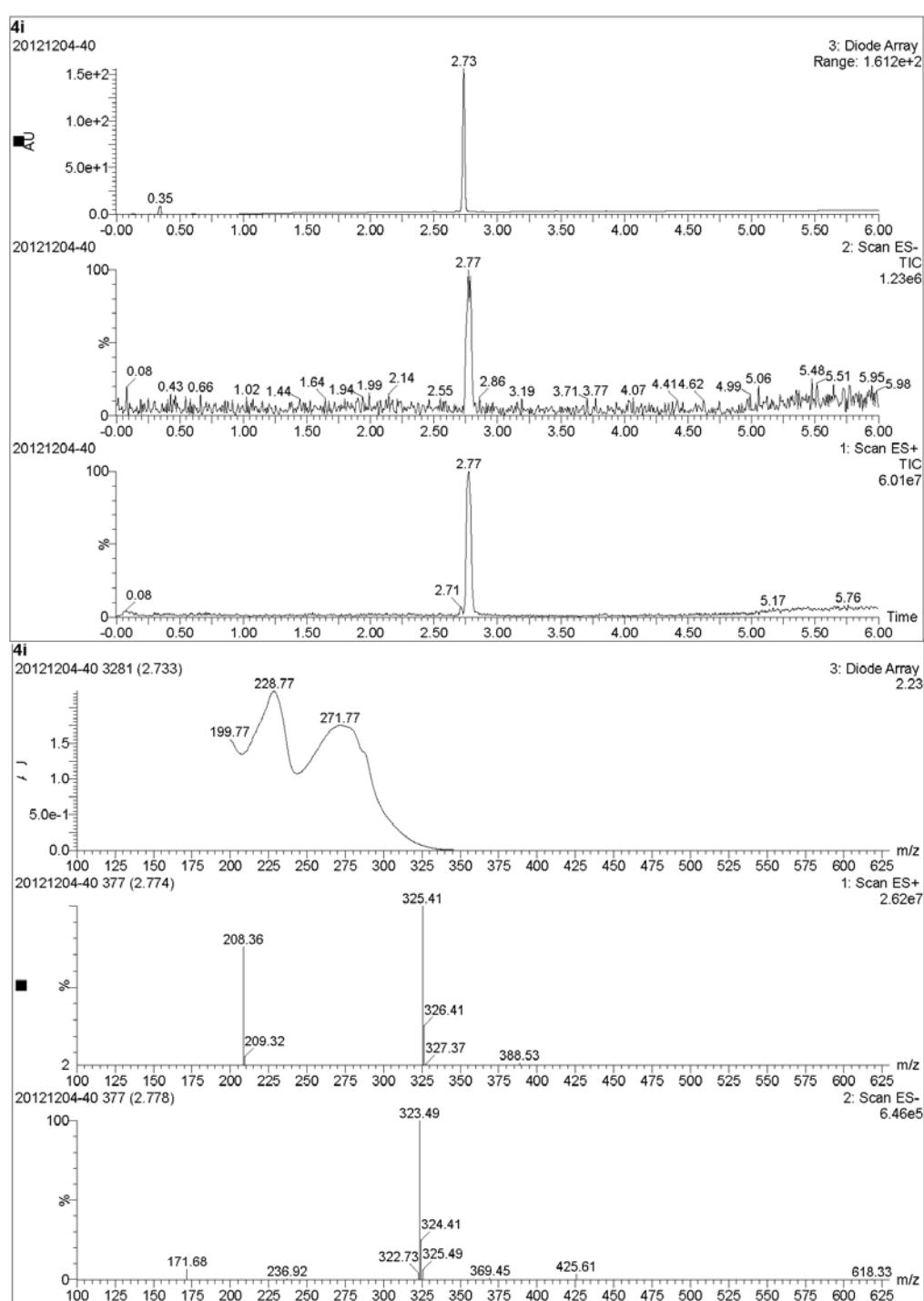
S23. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)-2-(pyridin-2-ylmethyl)isoindolin-1-one (**4h**) in $\text{DMSO}-d_6$.



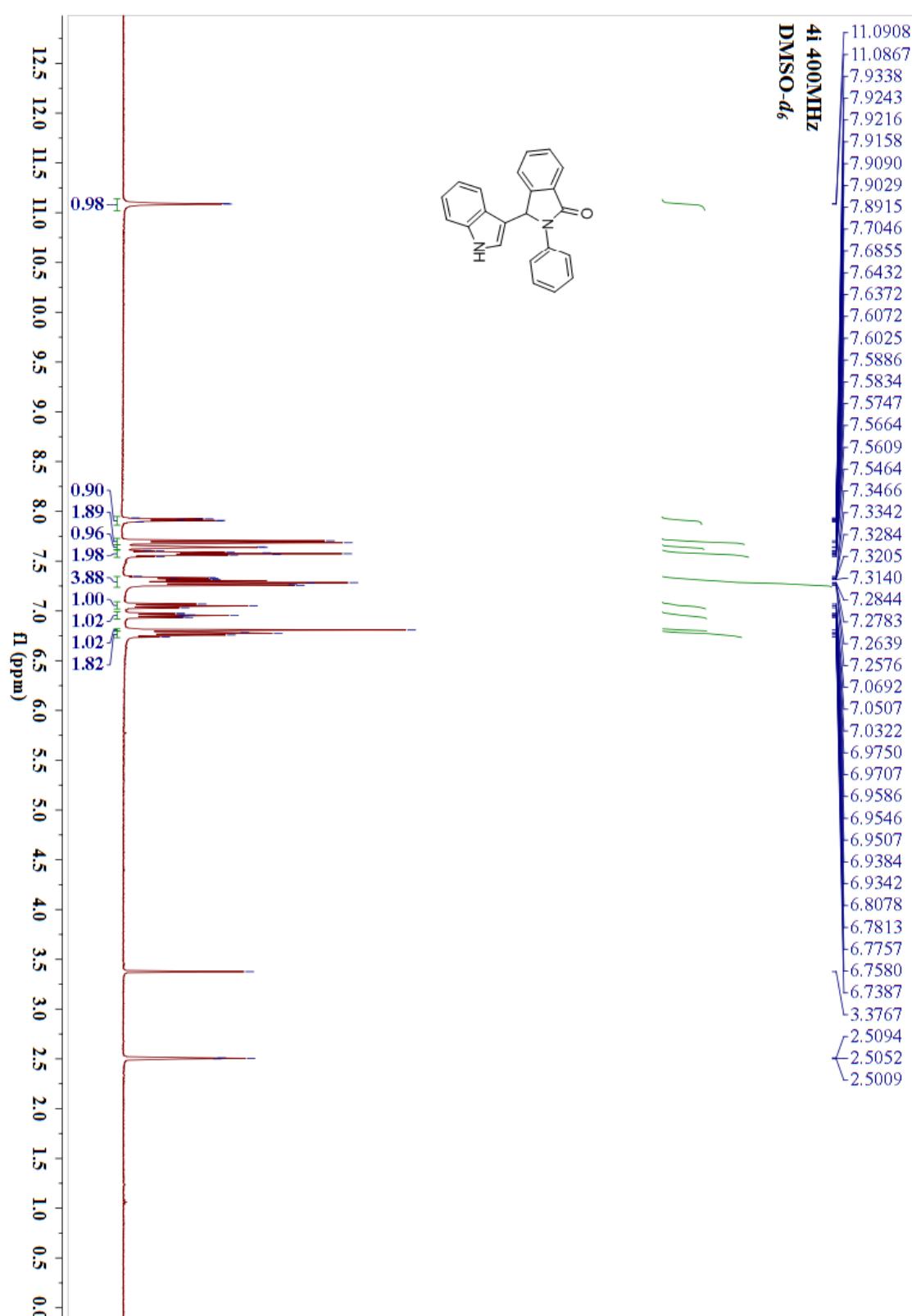
S24. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-(pyridin-2-ylmethyl)isoindolin-1-one (**4h**) in $\text{DMSO}-d_6$.



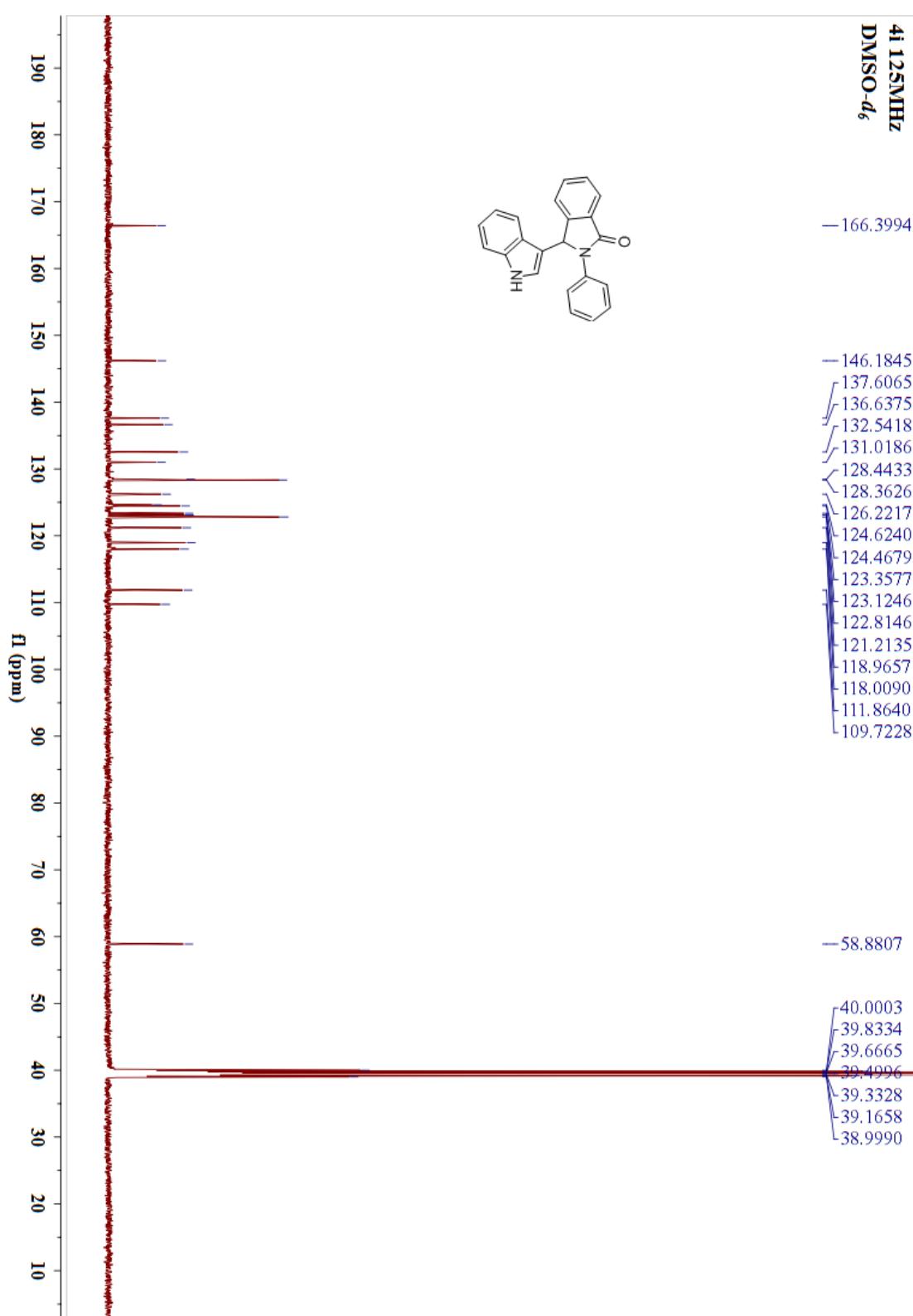
S25. LCMS spectrum of 3-(1*H*-Indol-3-yl)-2-phenylisoindolin-1-one (**4i**).



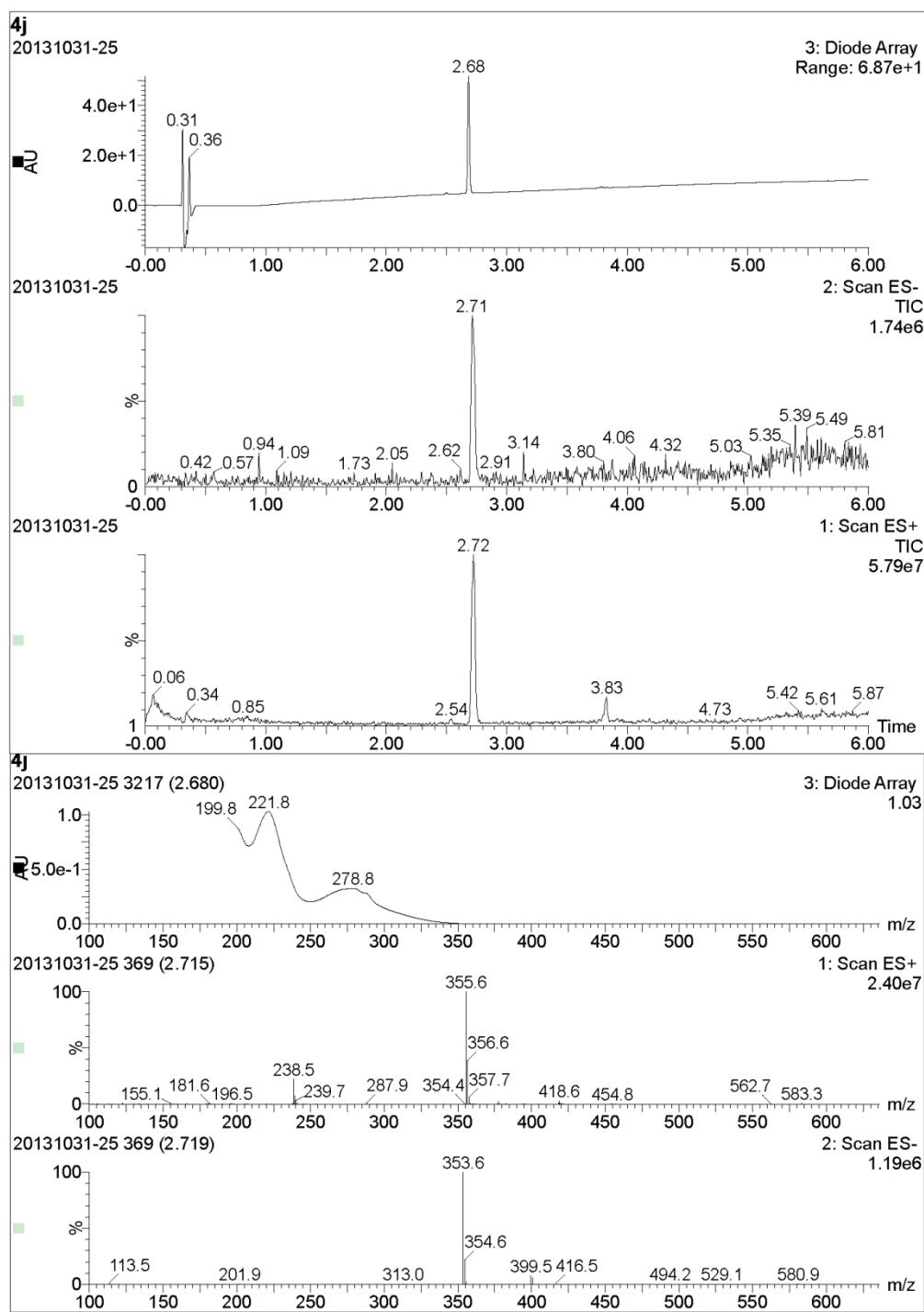
S26. ^1H NMR spectrum of 3-(1*H*-Indol-3-yl)-2-phenylisoindolin-1-one (**4i**) in $\text{DMSO}-d_6$.



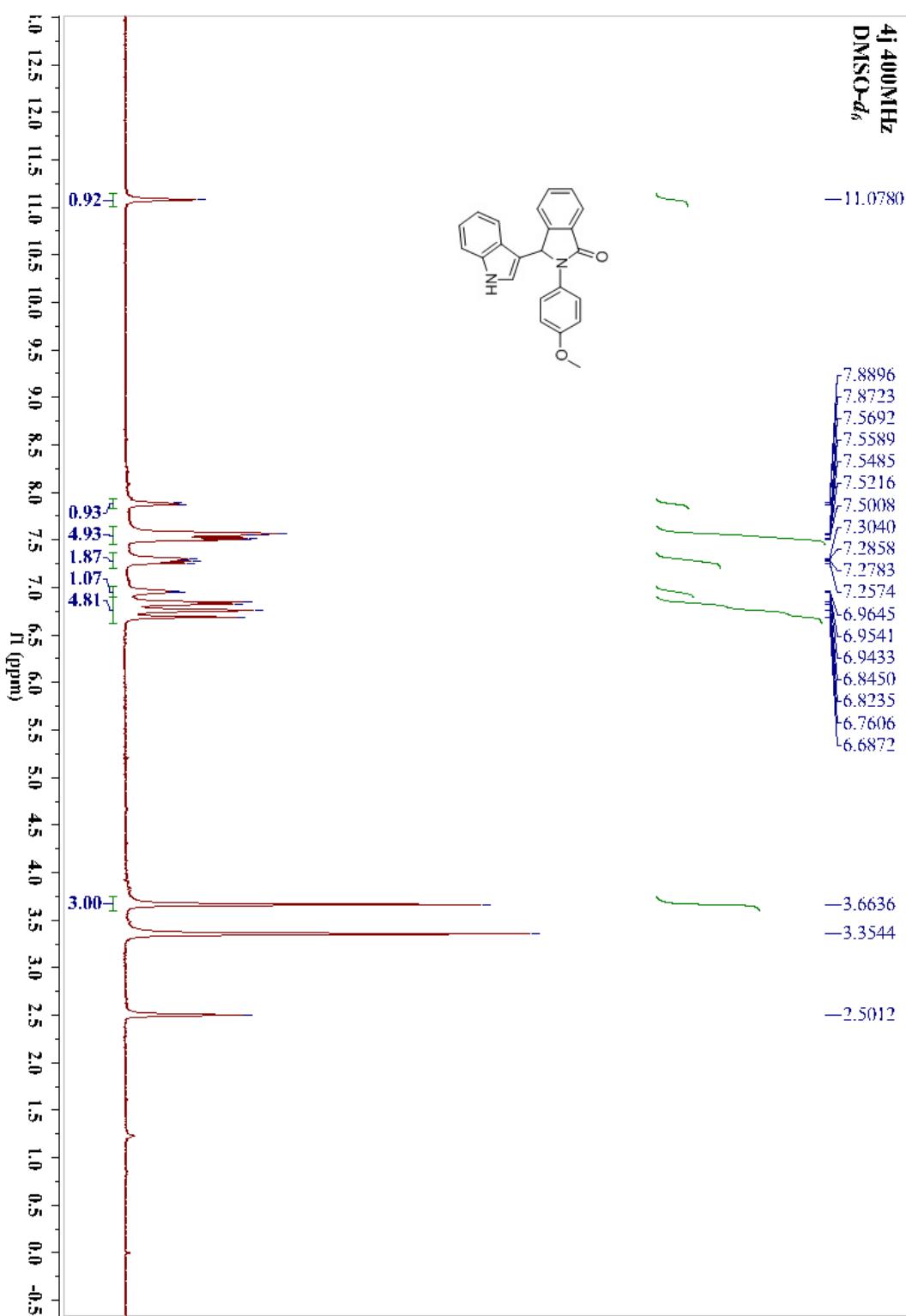
S27. ^{13}C NMR spectrum of 3-(1*H*-Indol-3-yl)-2-phenylisoindolin-1-one (**4i**) in $\text{DMSO}-d_6$.



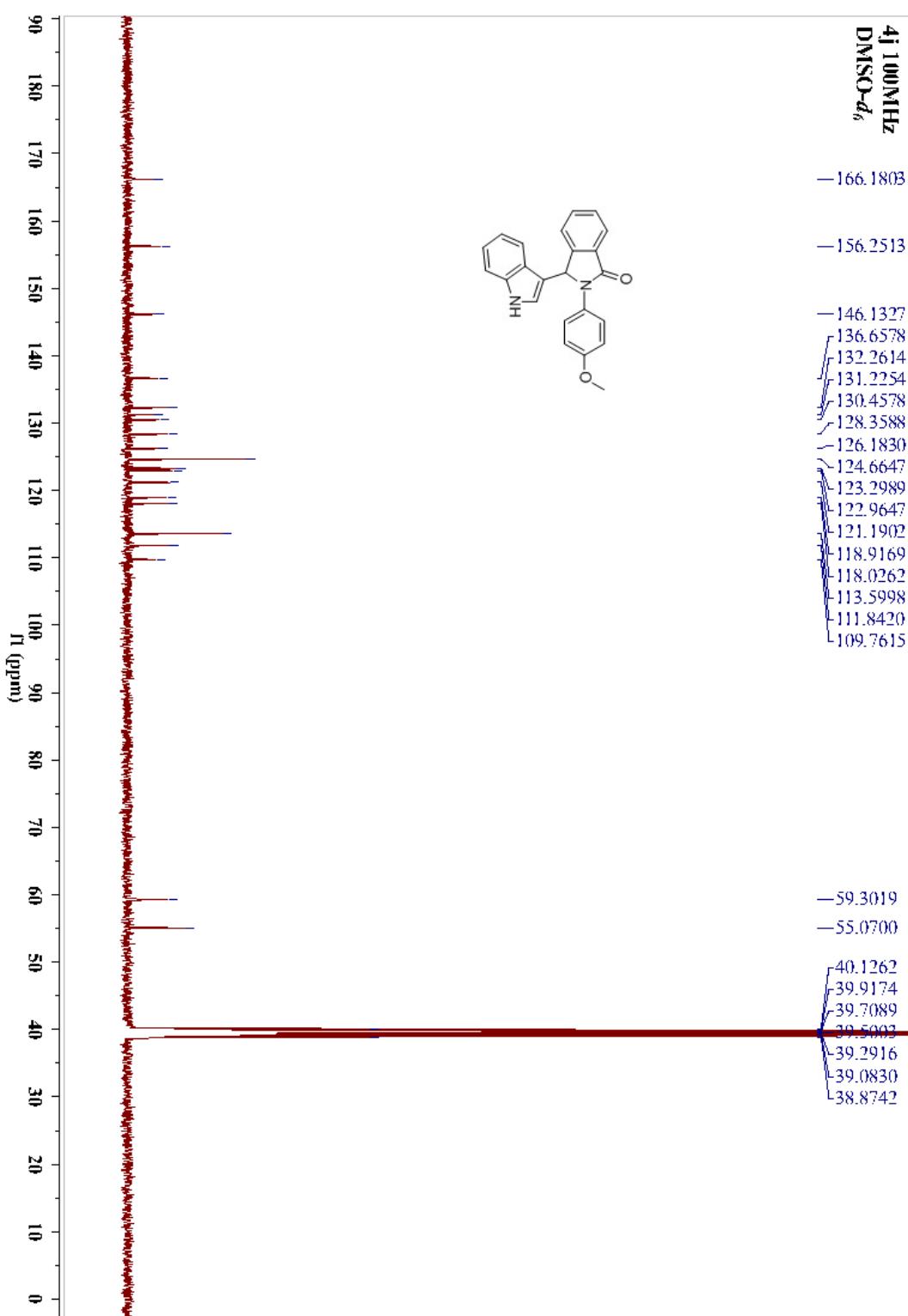
S28. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)isoindolin-1-one (**4j**).



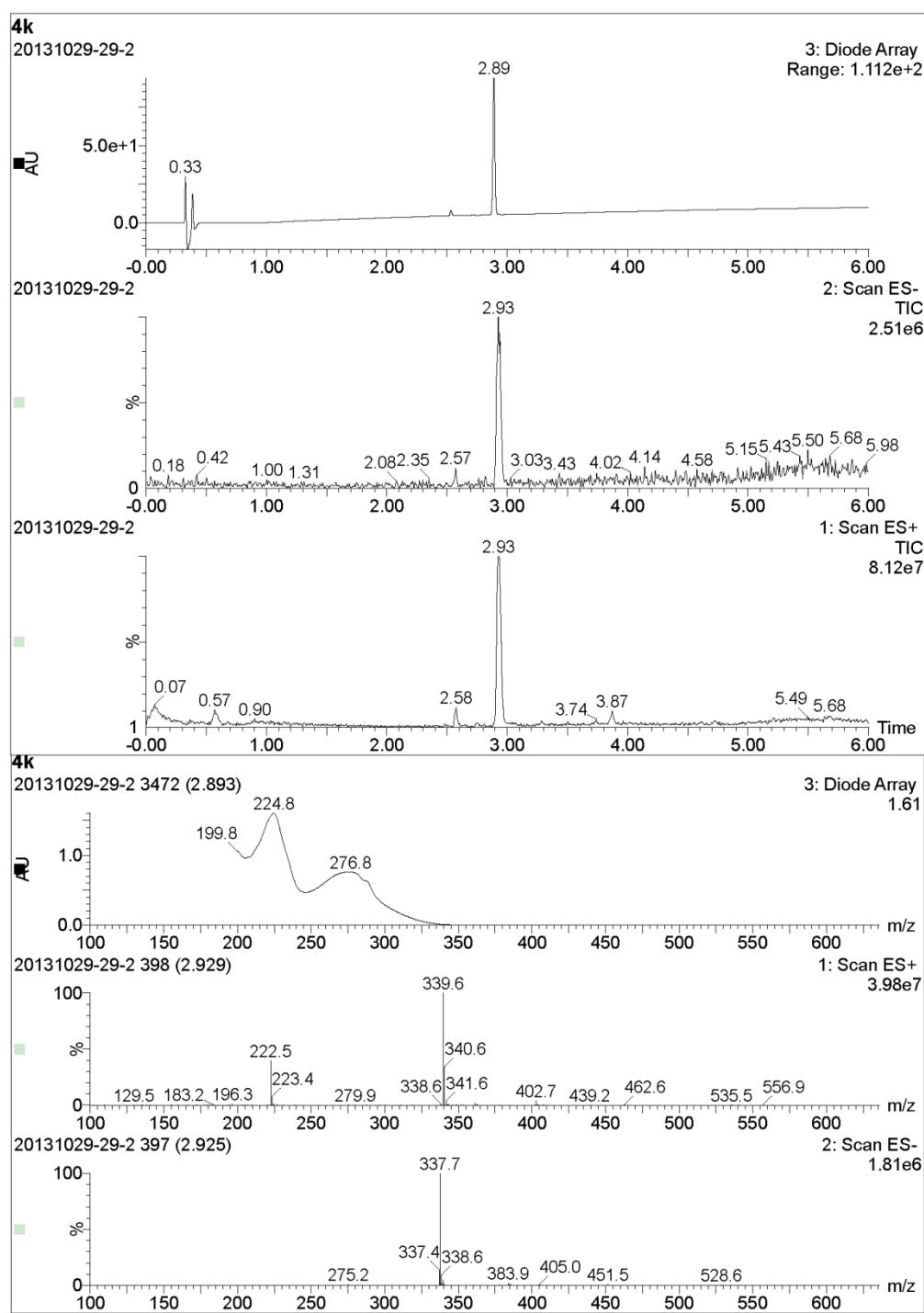
S29. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)isoindolin-1-one (**4j**) in $\text{DMSO}-d_6$.



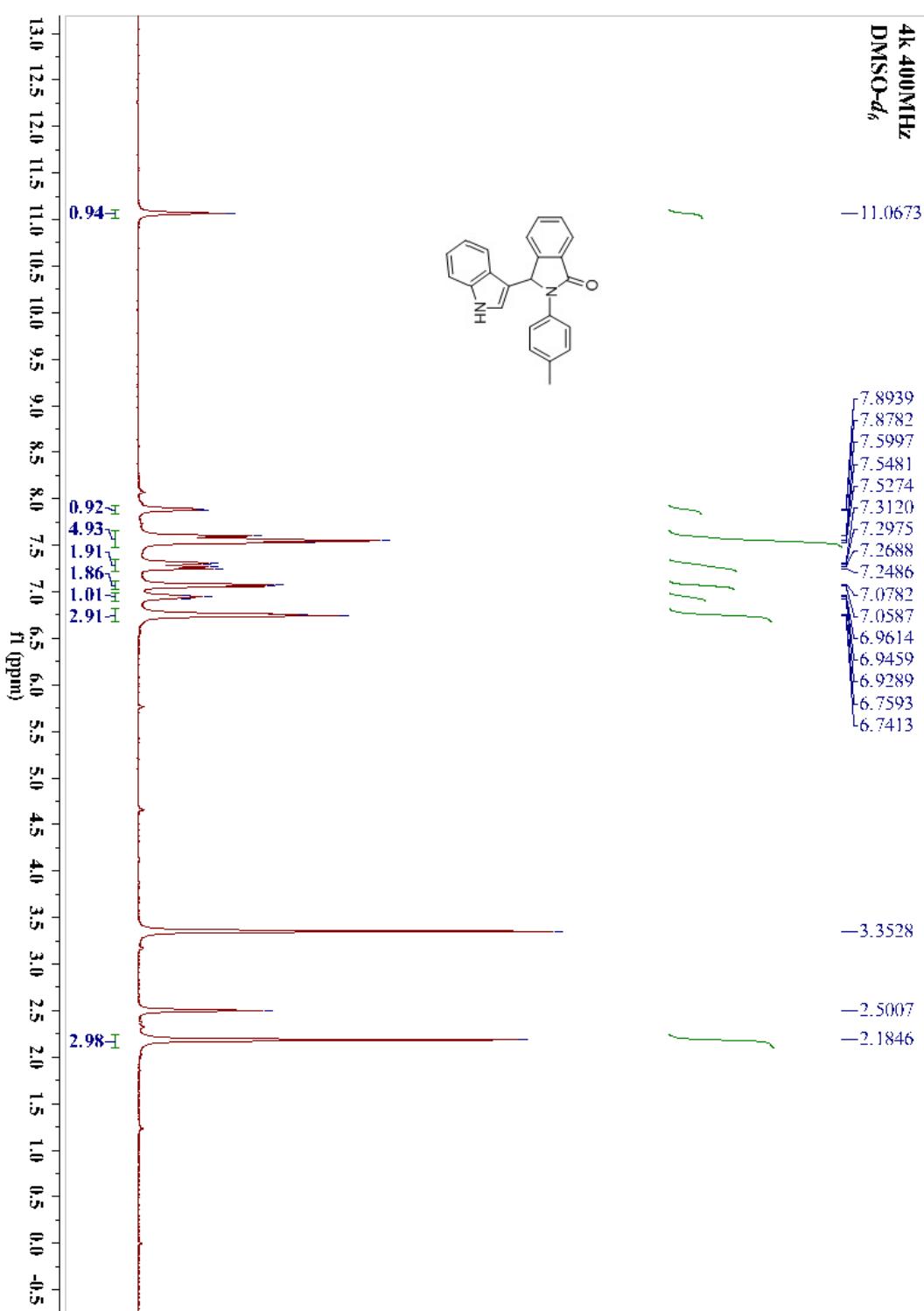
S30. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)isoindolin-1-one (**4j**) in $\text{DMSO}-d_6$.



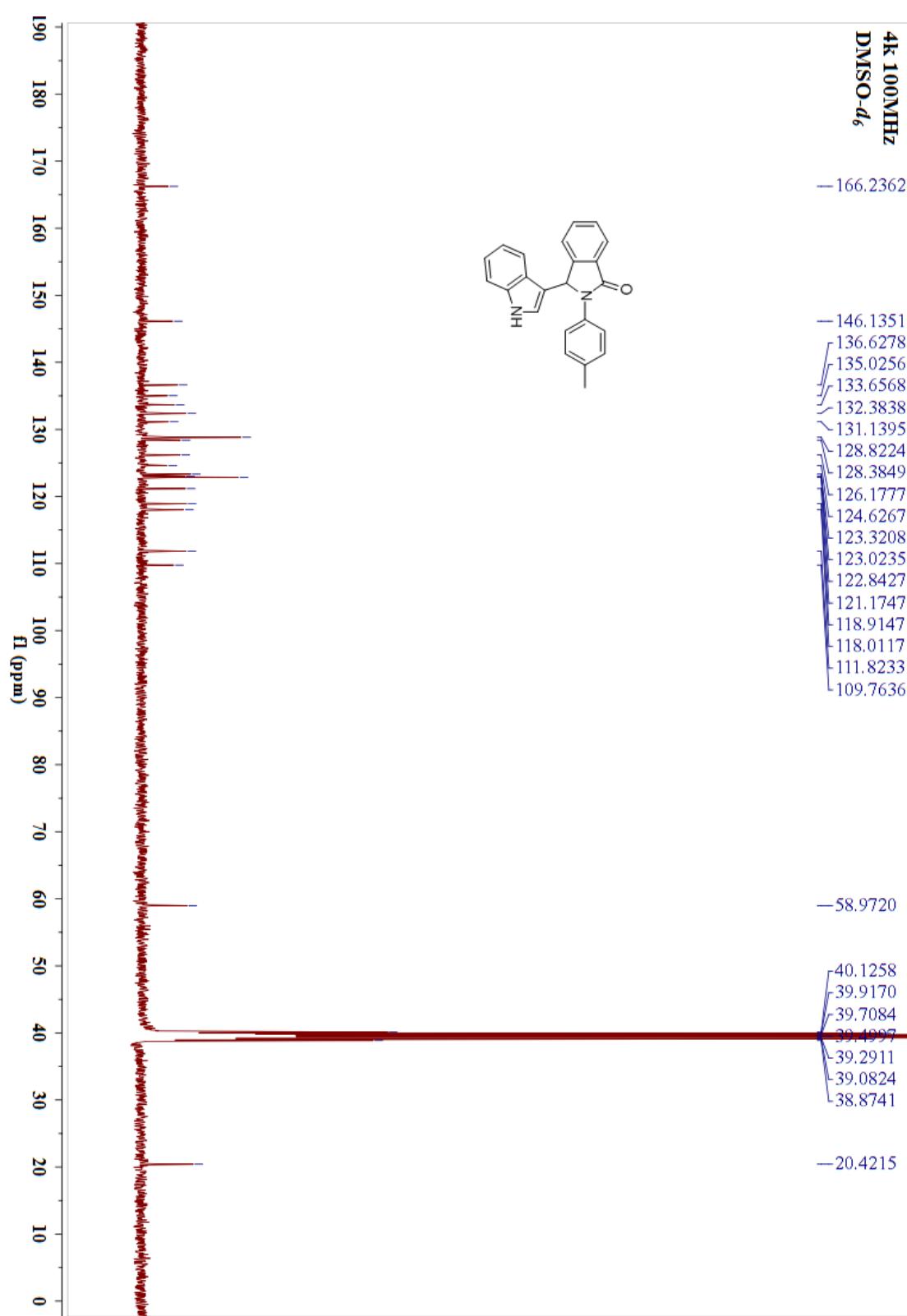
S31. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-(*p*-tolyl)isoindolin-1-one (**4k**).



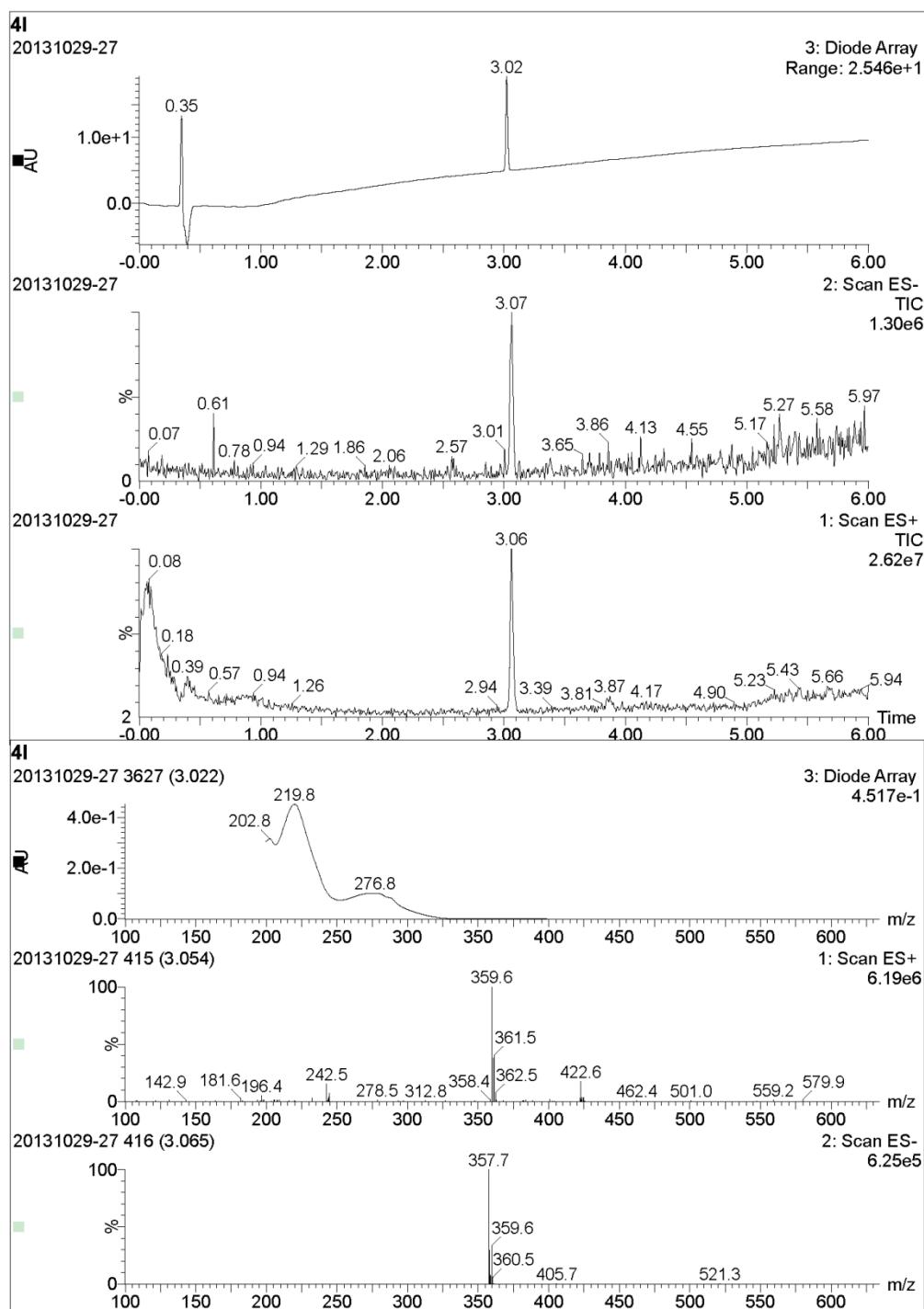
S32. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)-2-(*p*-tolyl)isoindolin-1-one (**4k**) in DMSO-*d*₆.



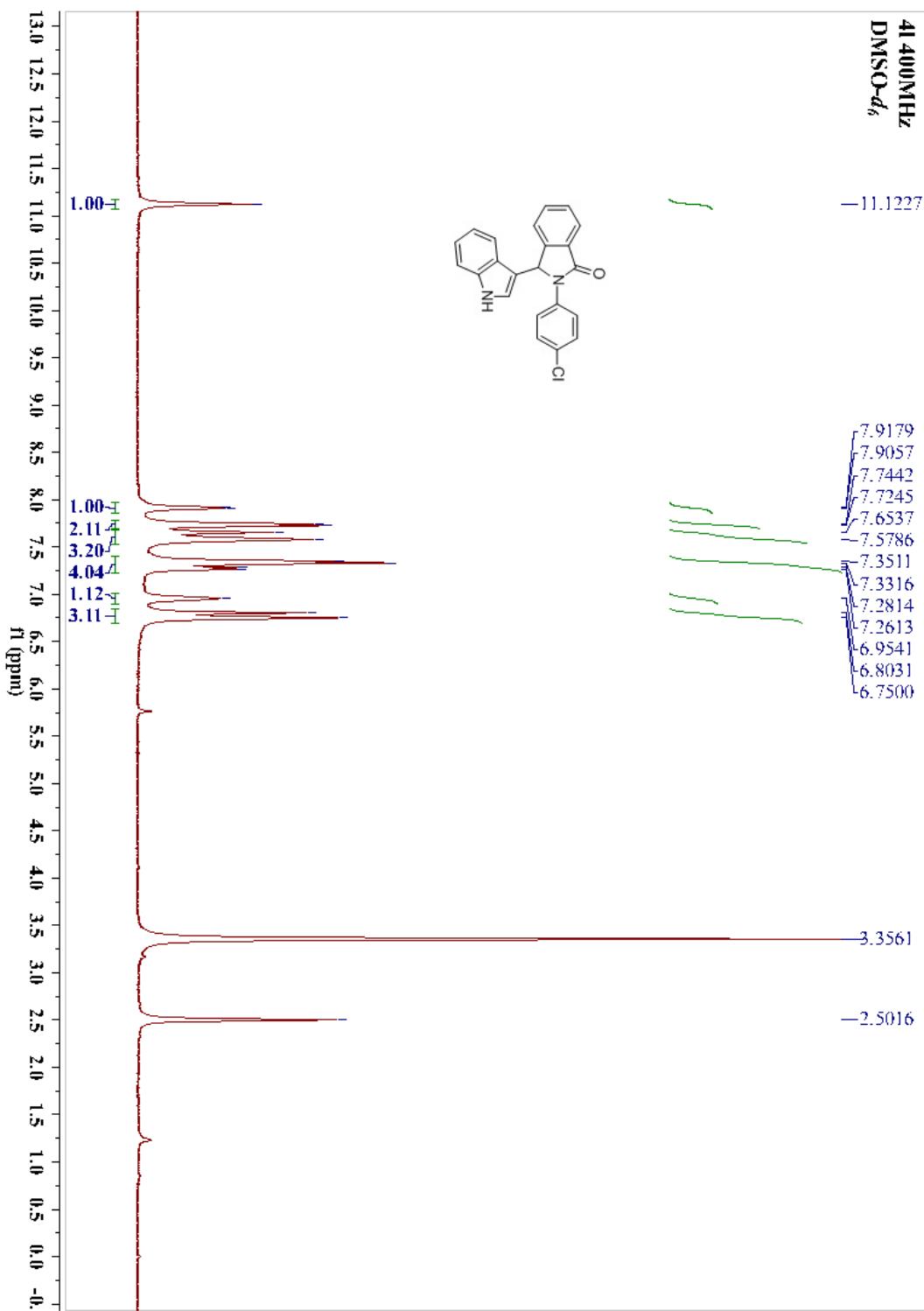
S33. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-(*p*-tolyl)isoindolin-1-one (**4k**) in DMSO-*d*₆.



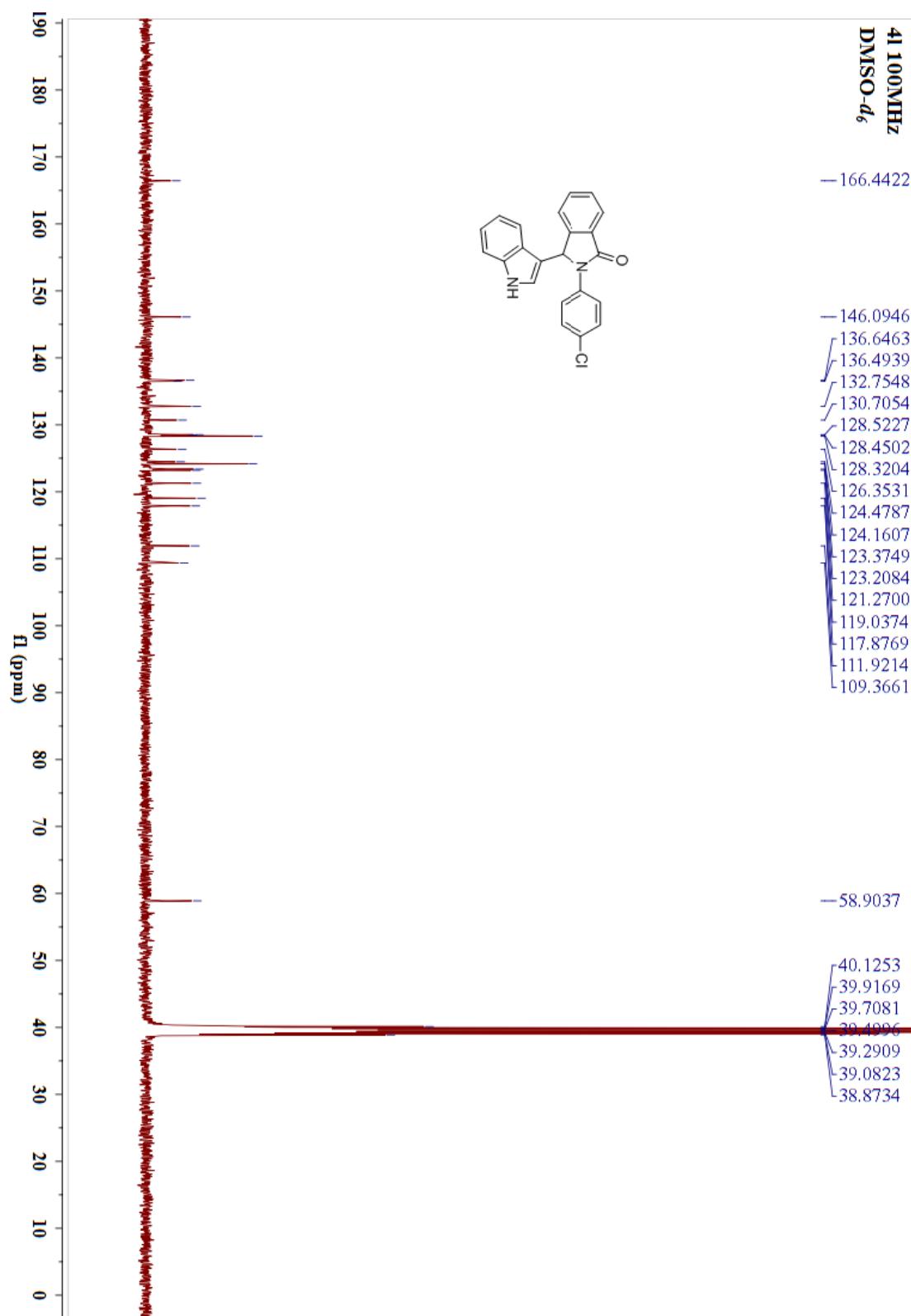
S34. LCMS spectrum of 2-(4-chlorophenyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4l**).



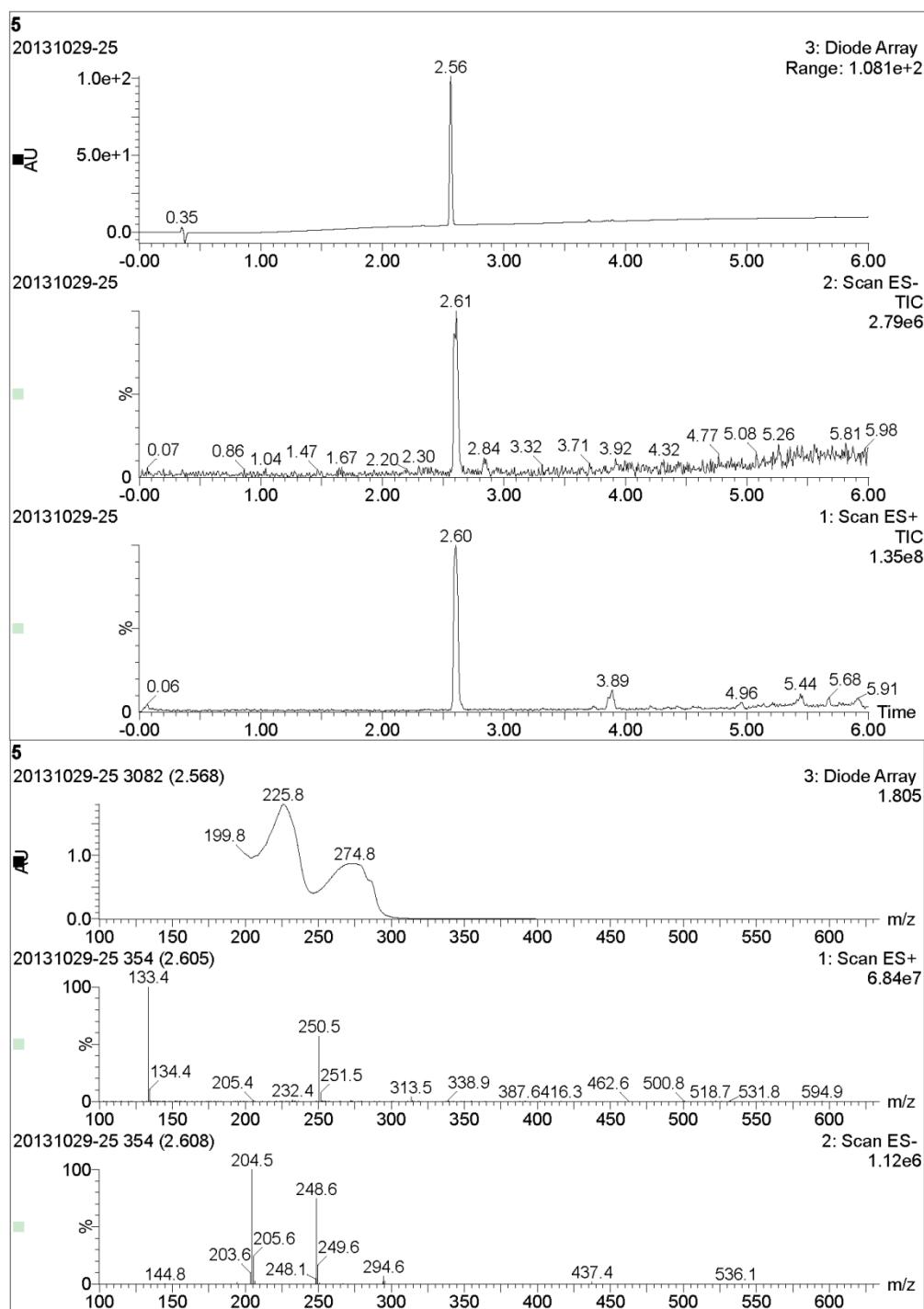
S35. ^1H NMR spectrum of 2-(4-chlorophenyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4I**).
in $\text{DMSO}-d_6$.



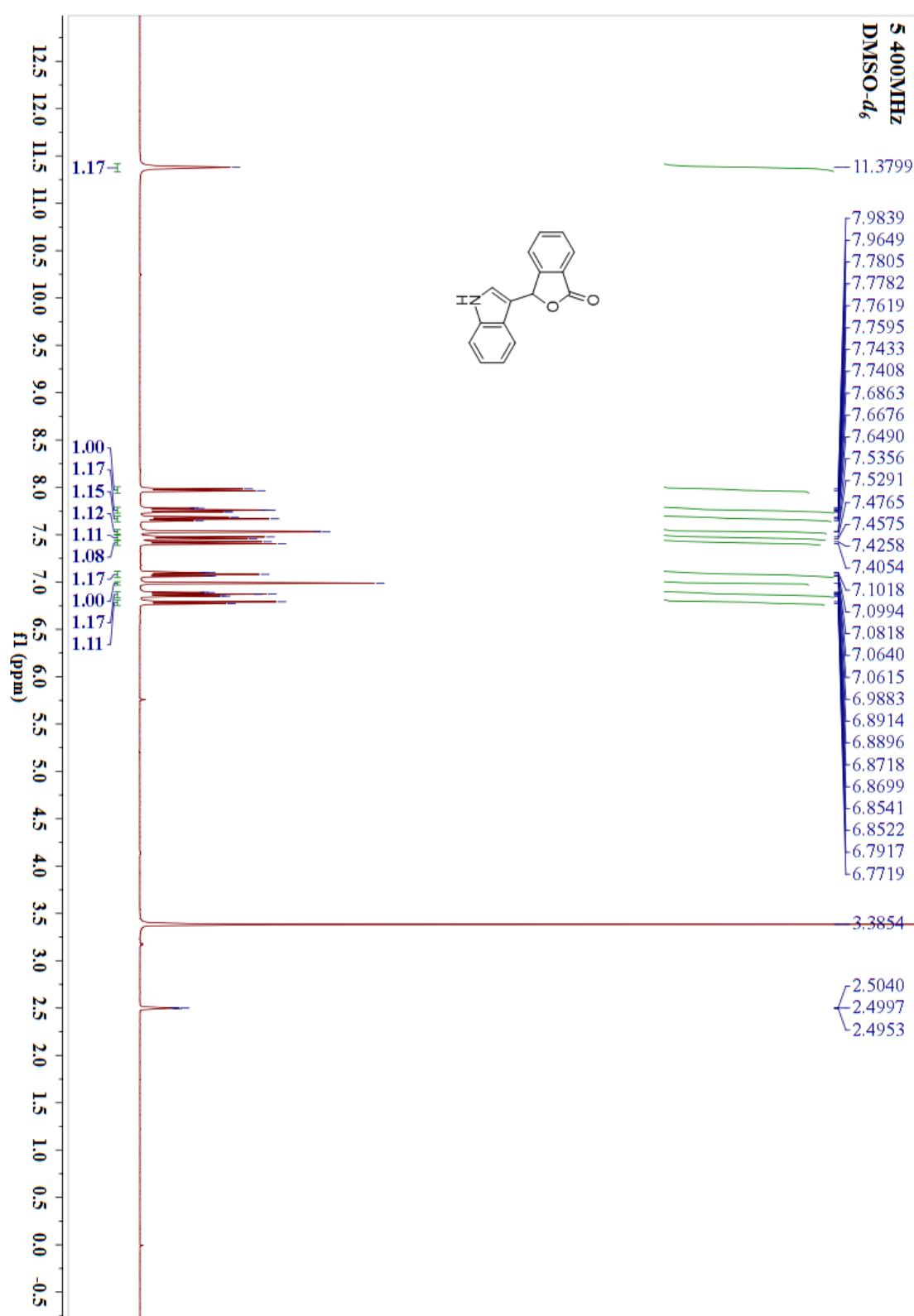
S36. ^{13}C NMR spectrum of 2-(4-chlorophenyl)-3-(1*H*-indol-3-yl)isoindolin-1-one (**4I**).
in $\text{DMSO}-d_6$.



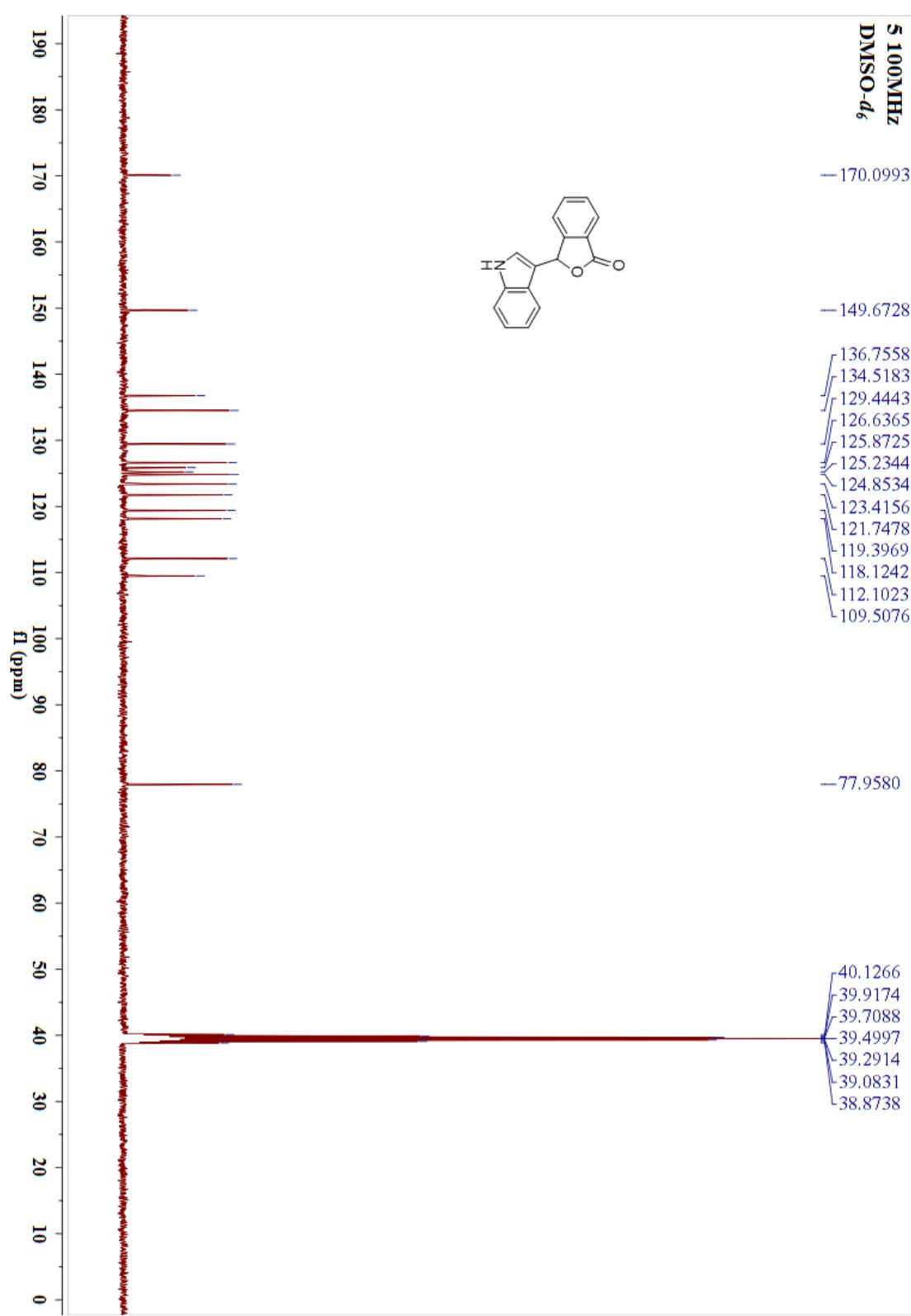
S37. LCMS spectrum of 3-(1*H*-indol-3-yl)isobenzofuran-1(*3H*)-one (**5**).



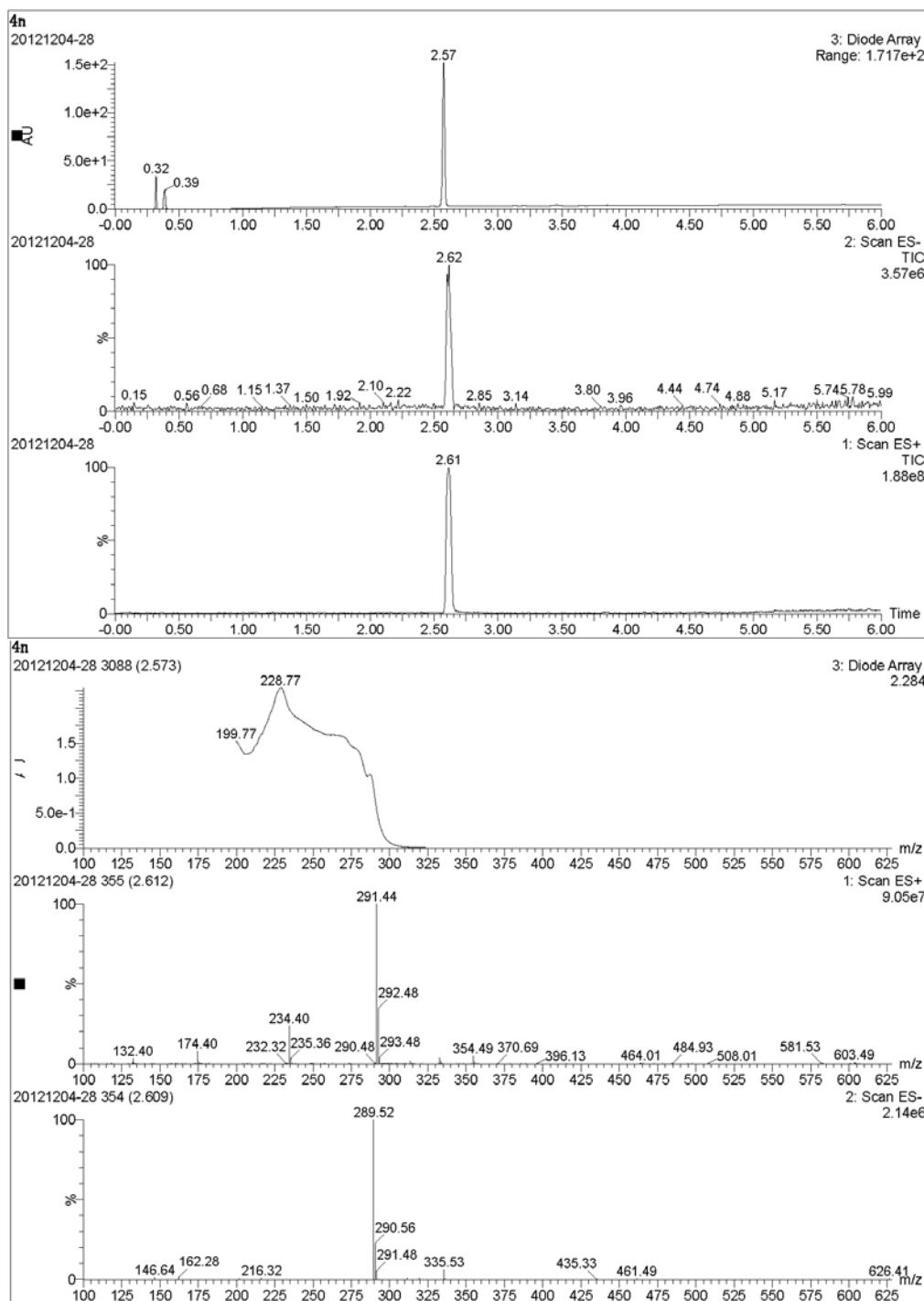
S38. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)isobenzofuran-1(*3H*)-one (**5**) in $\text{DMSO}-d_6$.



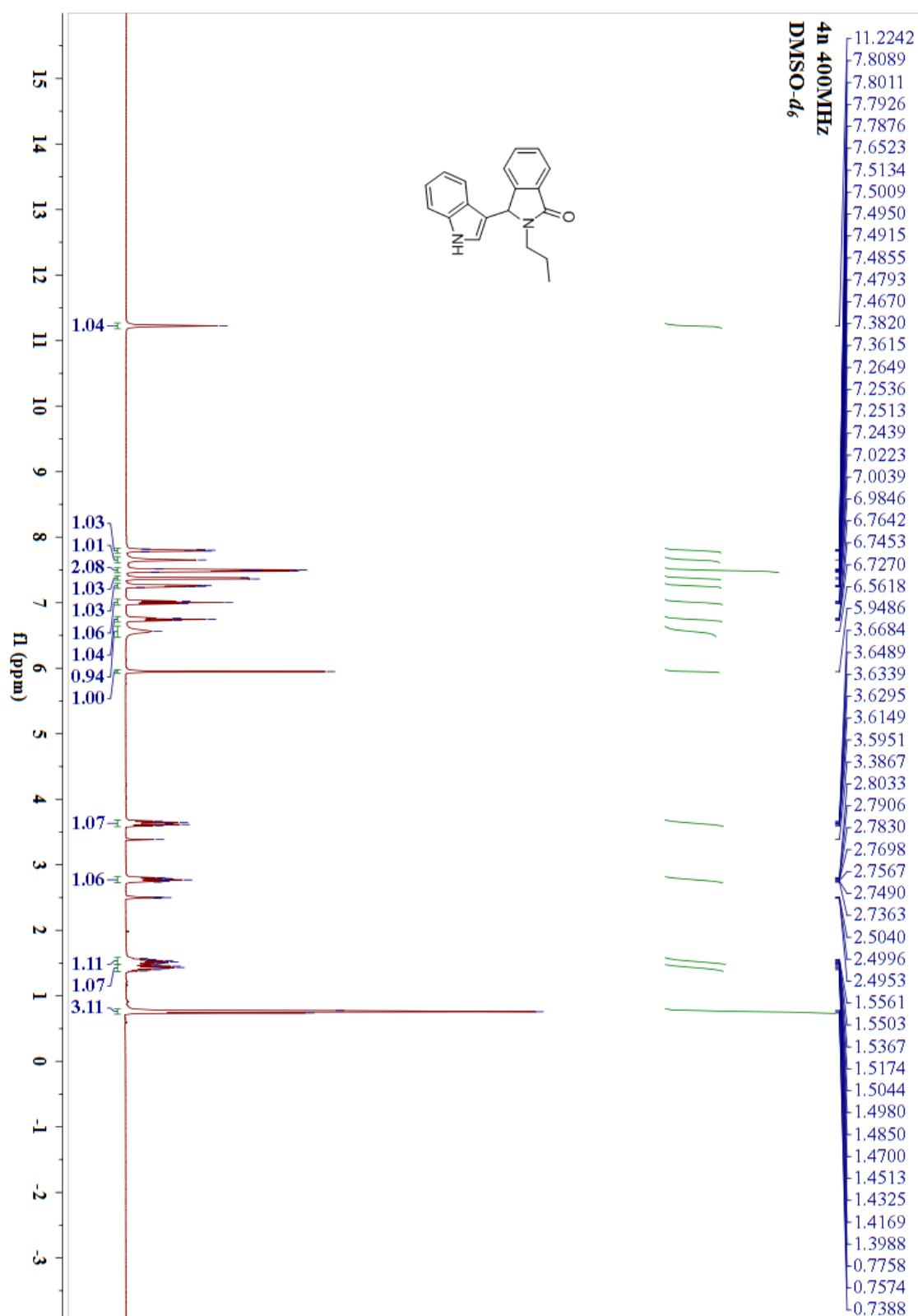
S39. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)isobenzofuran-1(*3H*)-one (**5**) in $\text{DMSO}-d_6$.



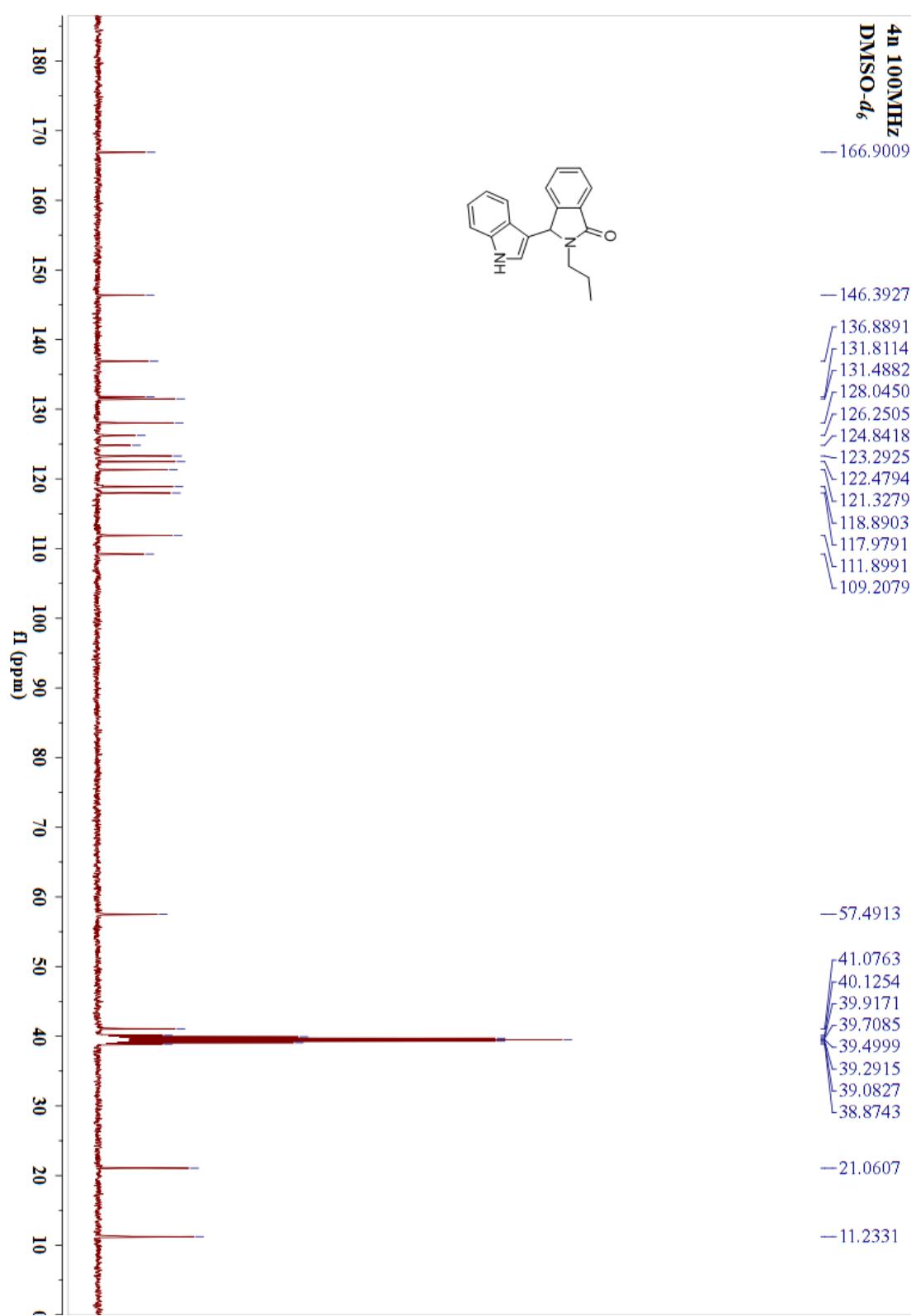
S40. LCMS spectrum of 3-(1*H*-Indol-3-yl)-2-propylisoindolin-1-one (**4n**).



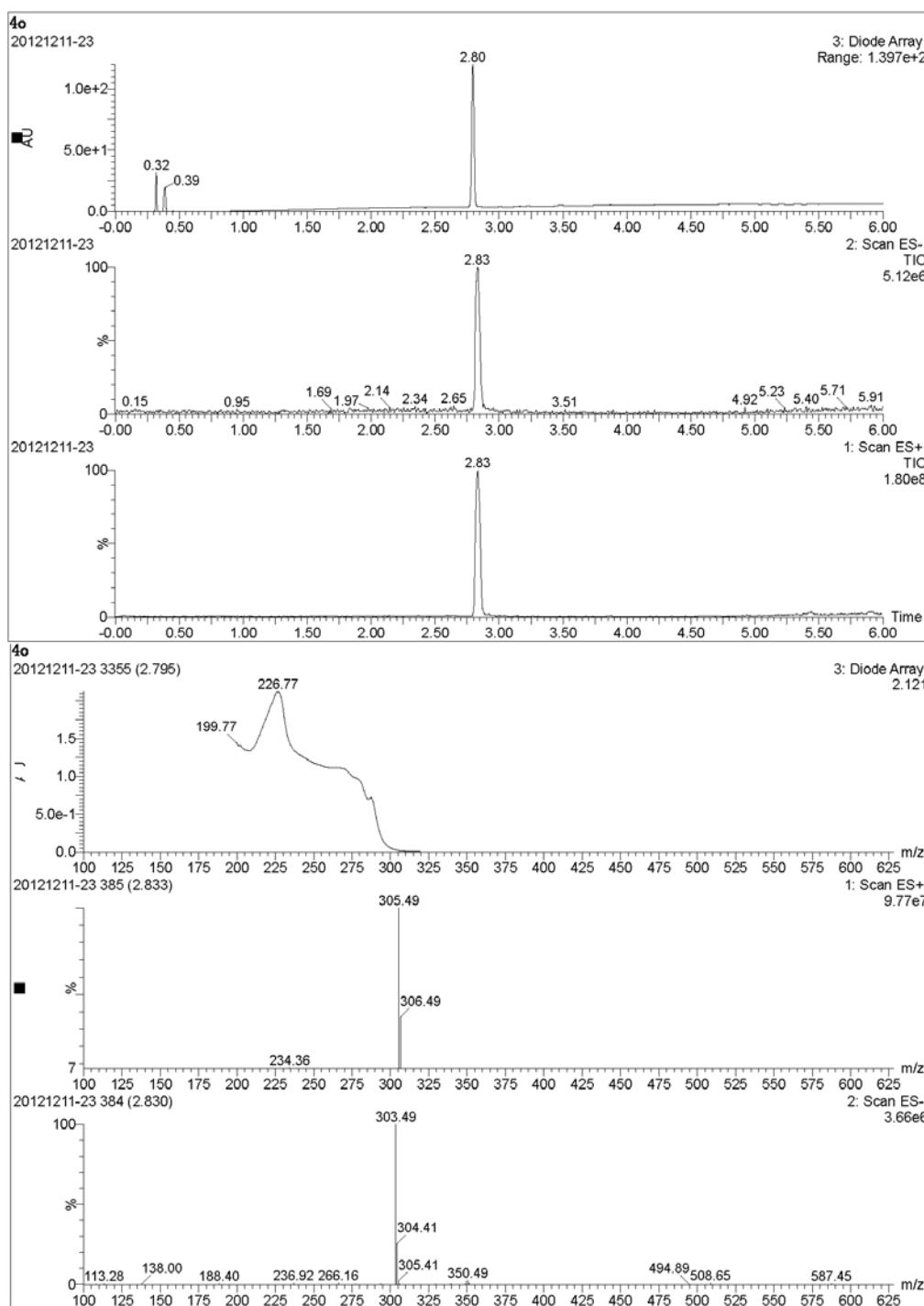
S41. ^1H NMR spectrum of 3-(1*H*-Indol-3-yl)-2-propylisoindolin-1-one (**4n**) in $\text{DMSO}-d_6$.



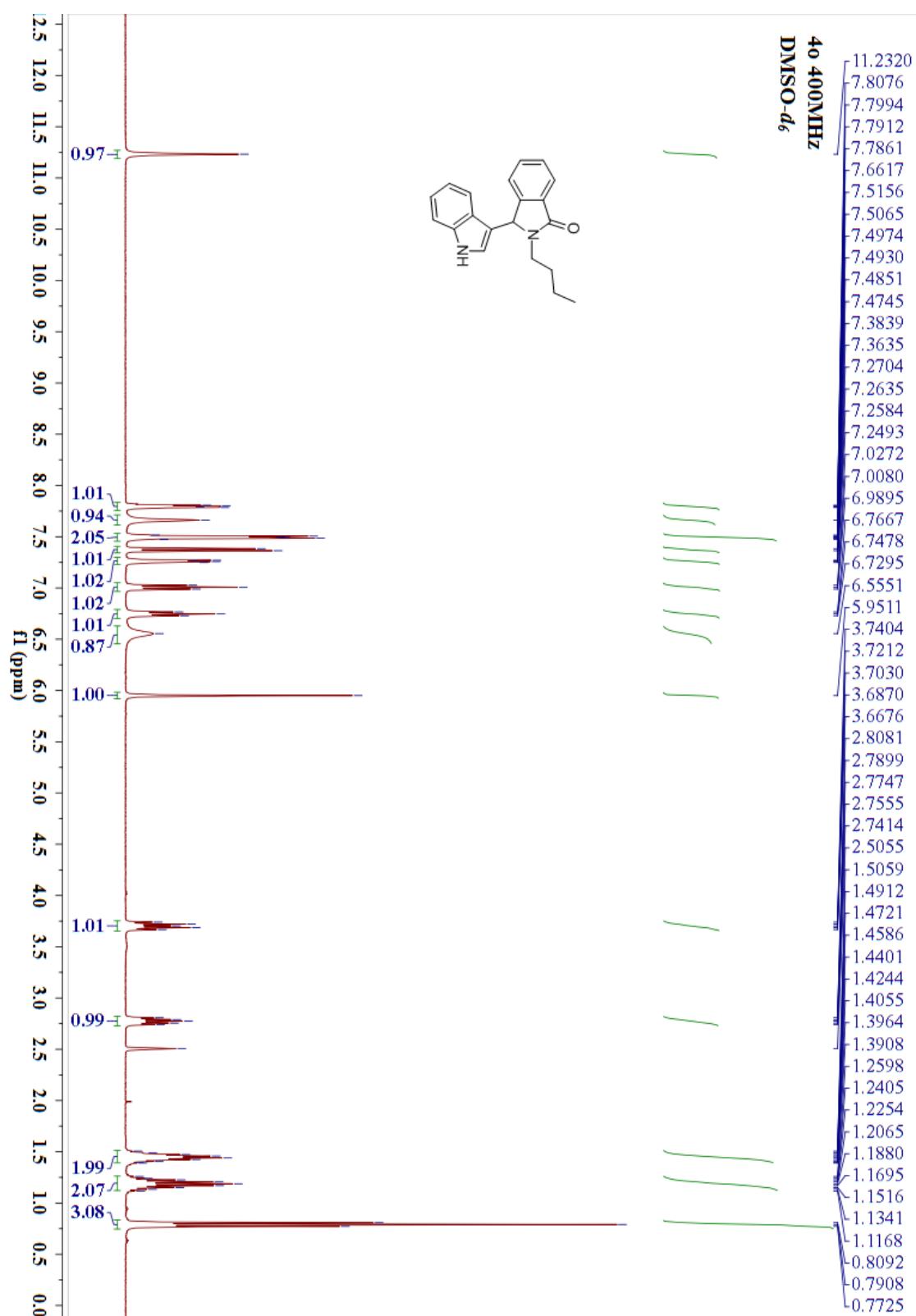
S42. ^{13}C NMR spectrum of 3-(1*H*-Indol-3-yl)-2-propylisoindolin-1-one (**4n**) in $\text{DMSO}-d_6$.



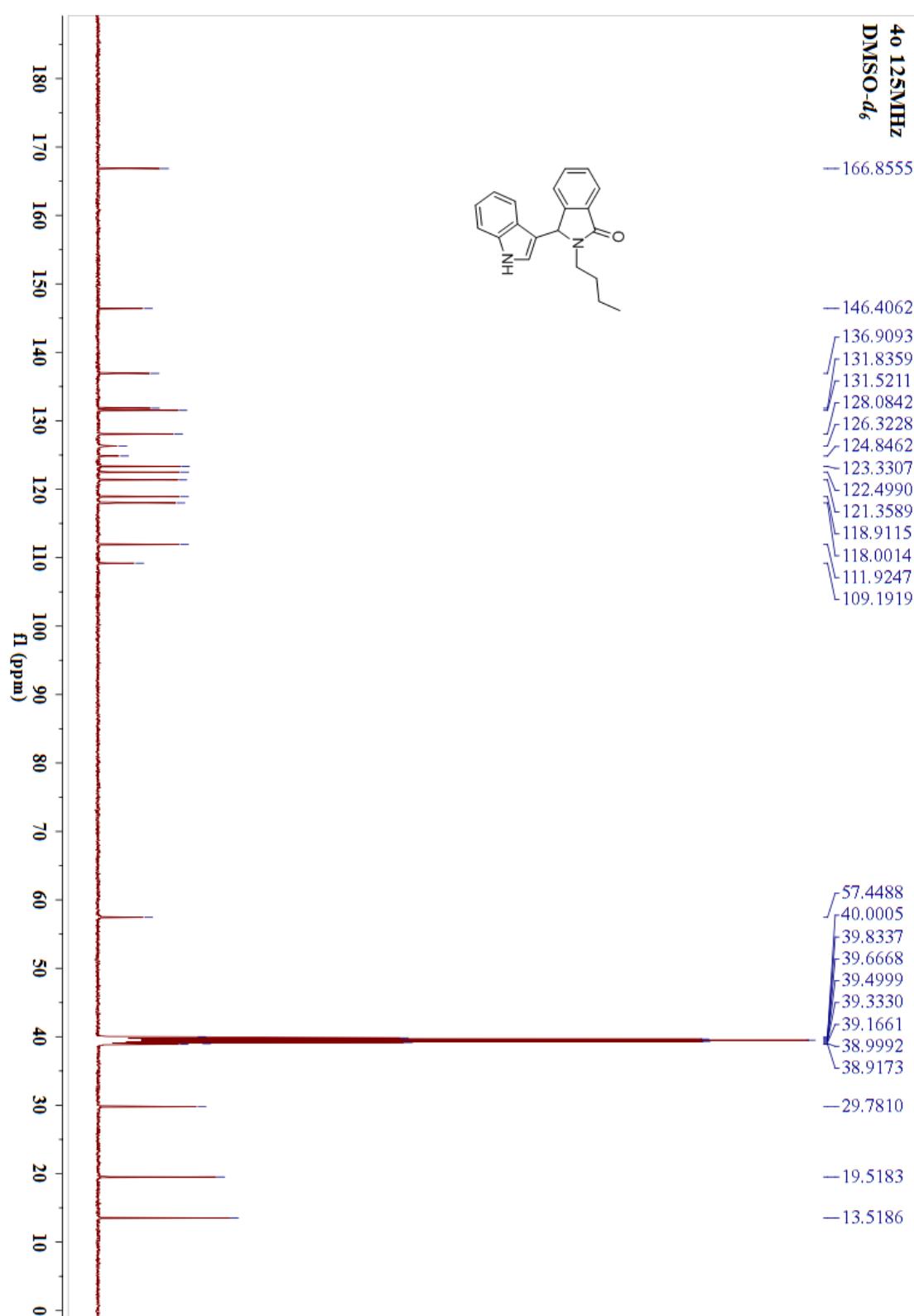
S43. LCMS spectrum of 2-butyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4o**).



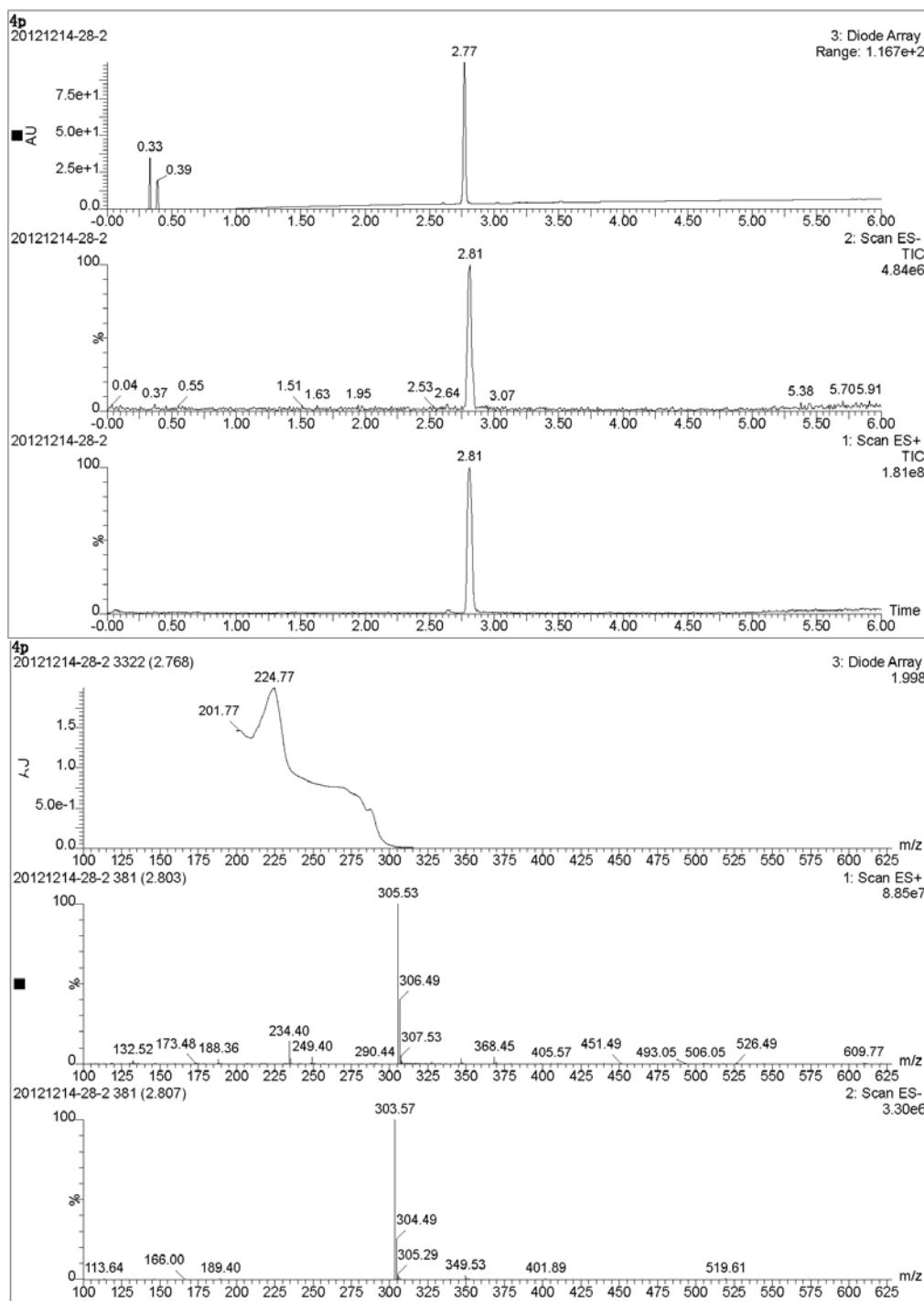
S44. ^1H NMR spectrum of 2-butyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4o**) in $\text{DMSO}-d_6$.



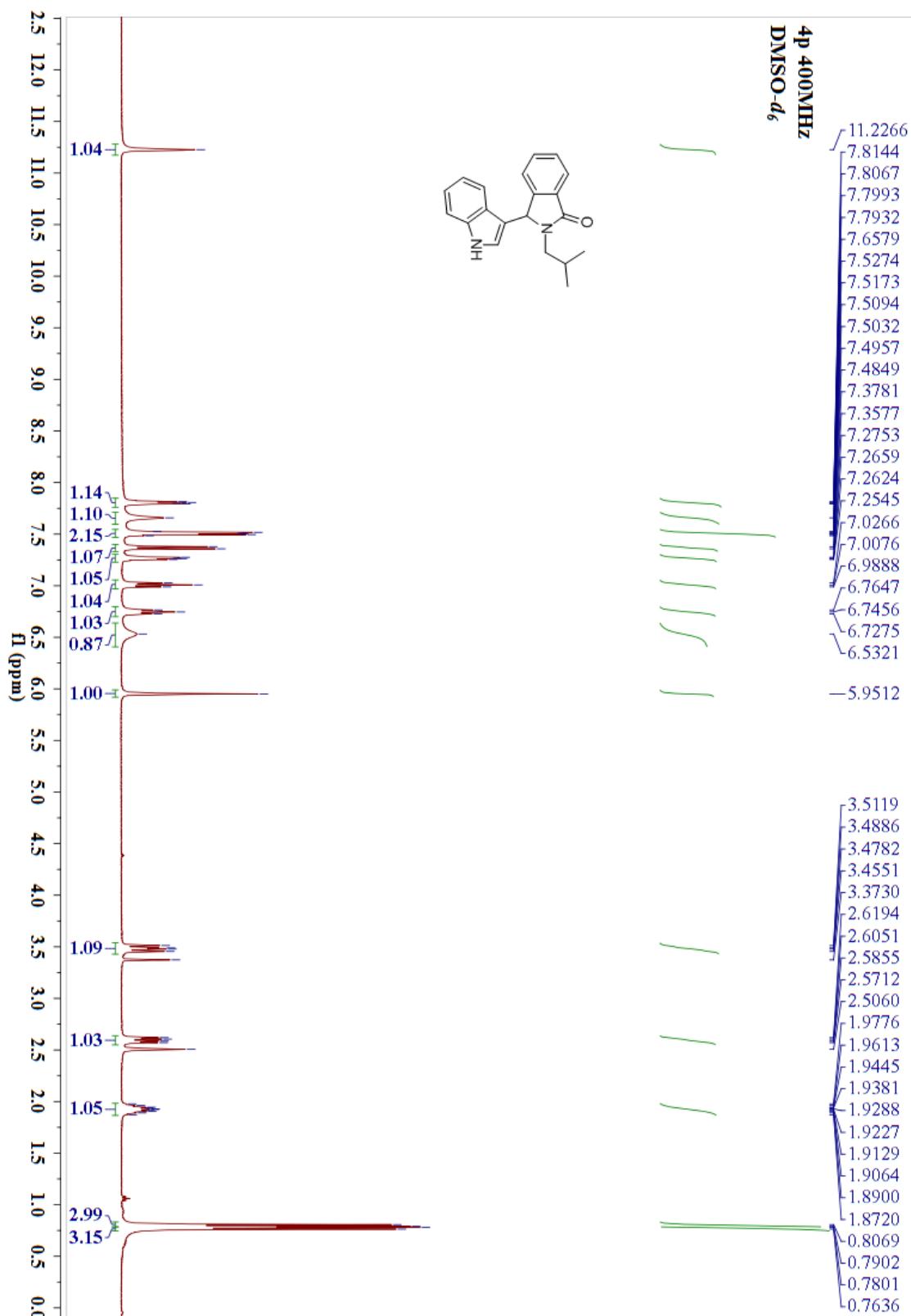
S45. ^{13}C NMR spectrum of 2-butyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4o**) in $\text{DMSO}-d_6$.



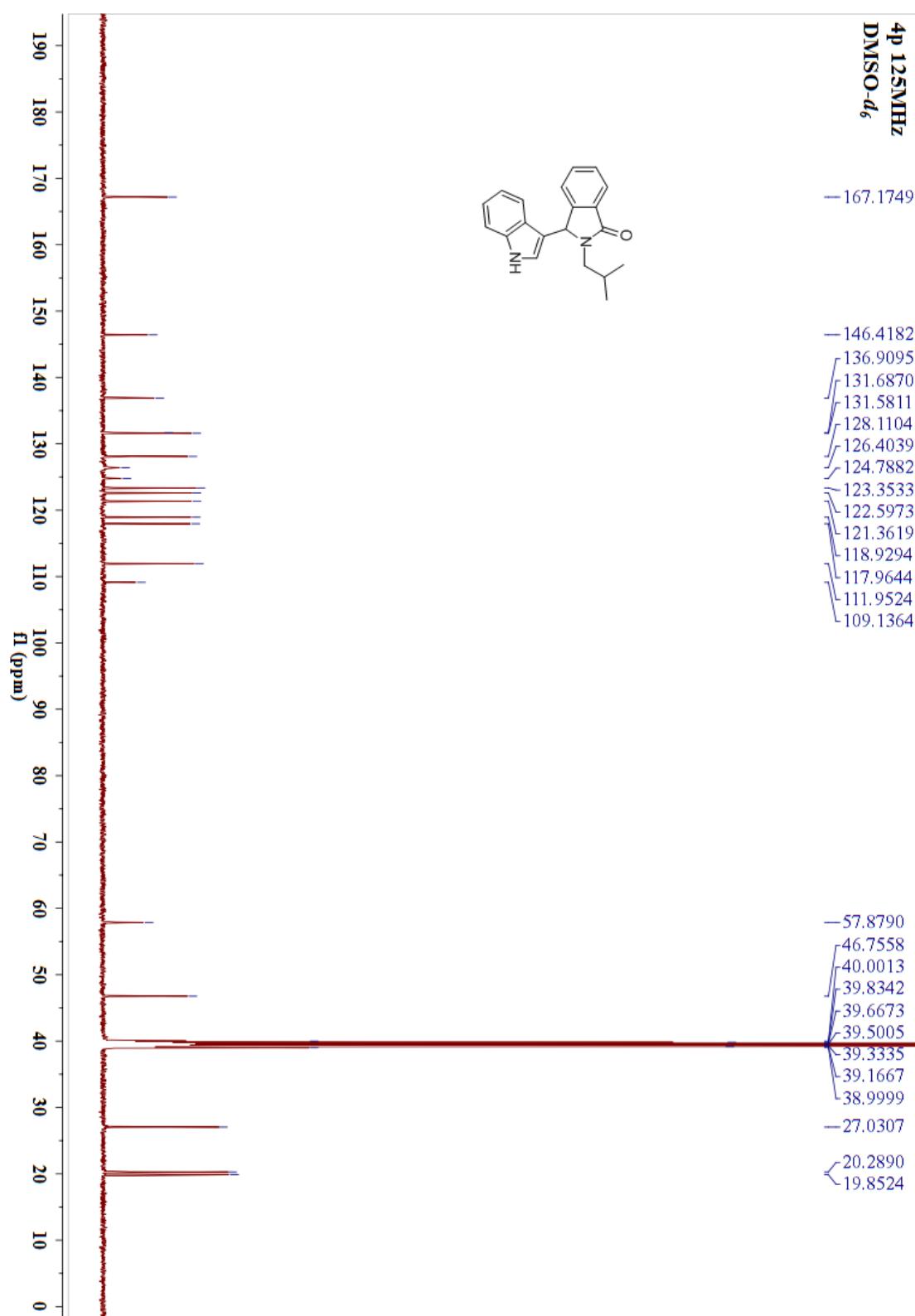
S46. LCMS spectrum of 3-(1*H*-Indol-3-yl)-2-isobutylisoindolin-1-one (**4p**).



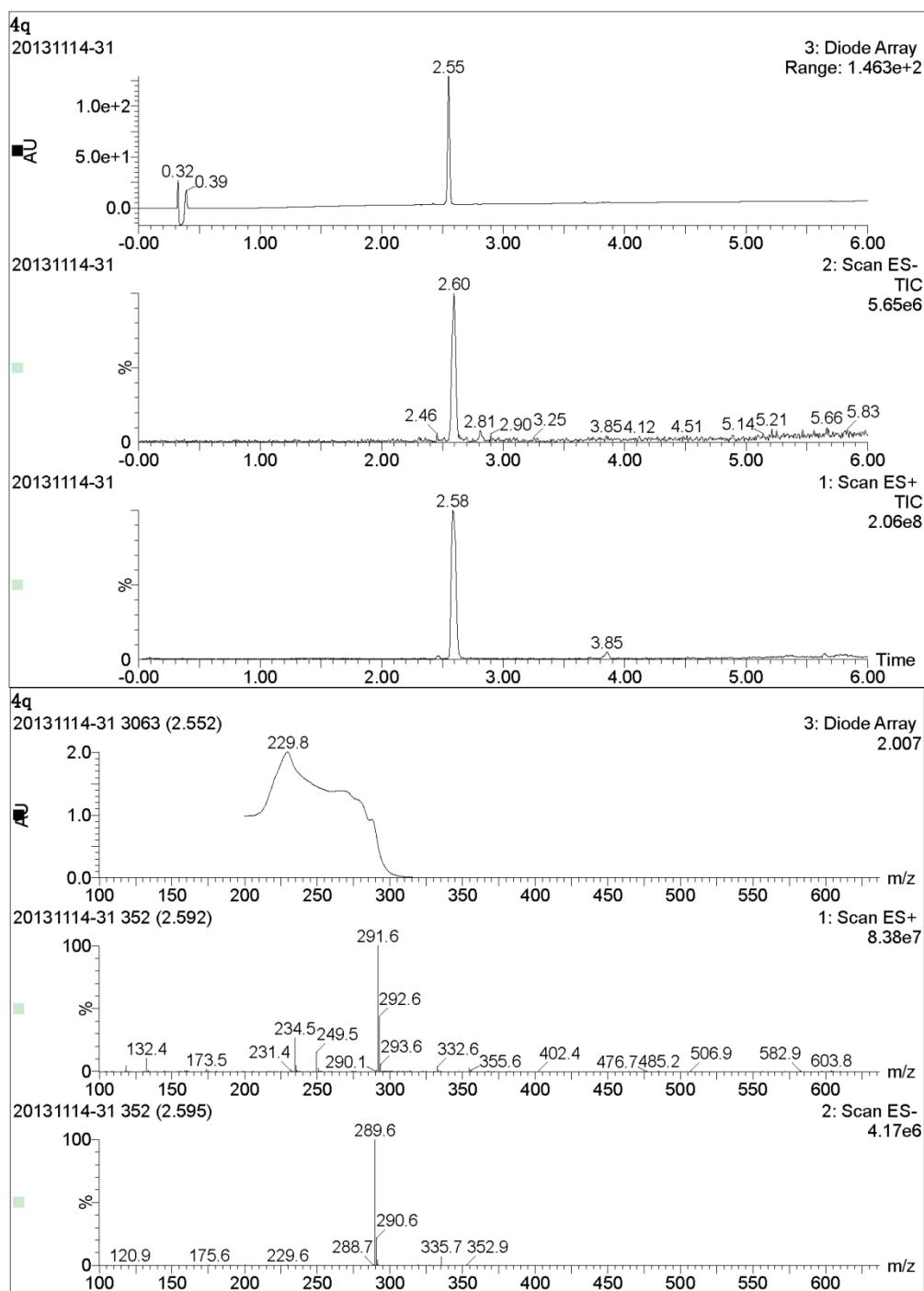
S47. ^1H NMR spectrum of 3-(1*H*-Indol-3-yl)-2-isobutylisoindolin-1-one (**4p**) in $\text{DMSO}-d_6$.



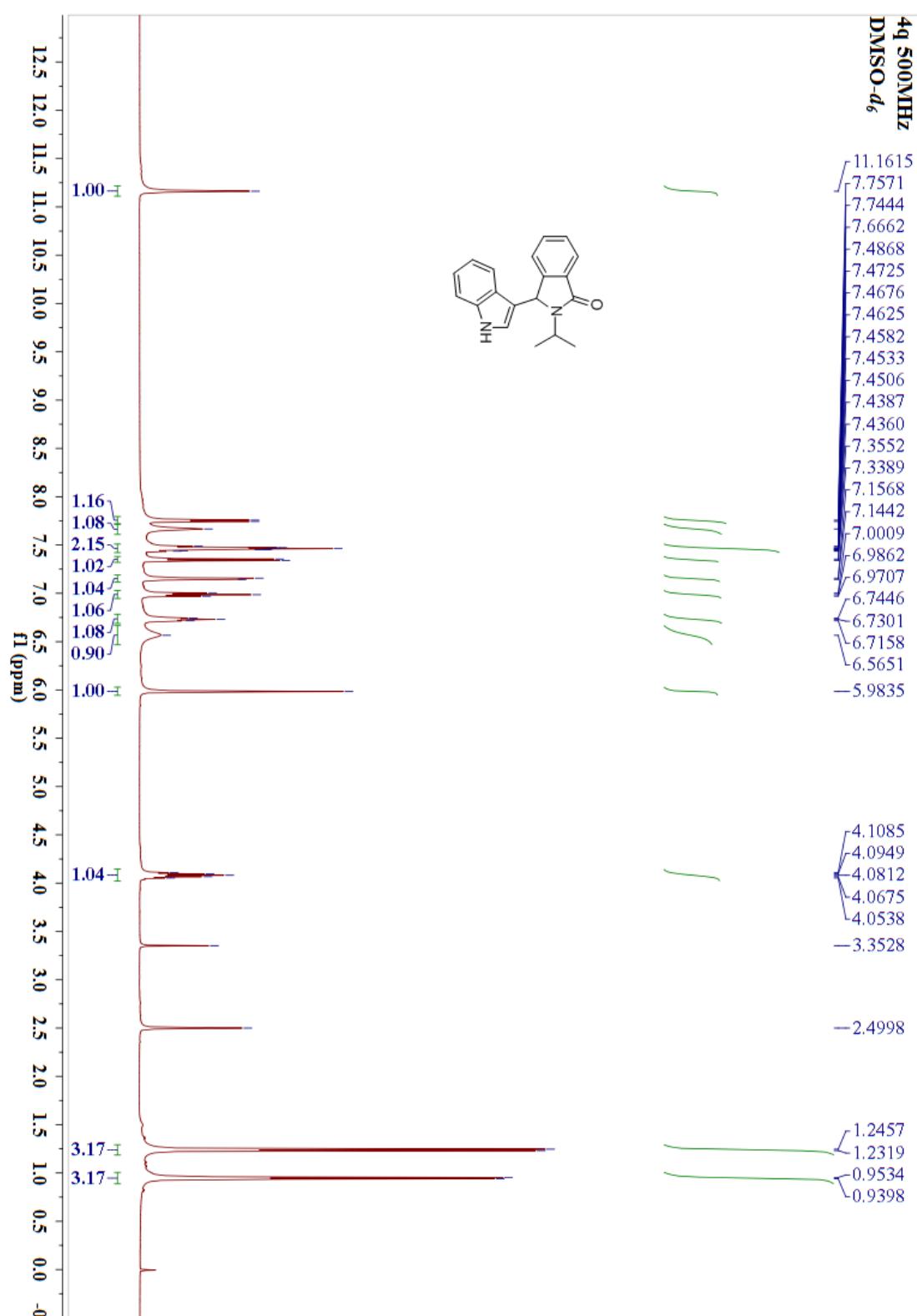
S48. ^{13}C NMR spectrum of 3-(1*H*-Indol-3-yl)-2-isobutylisoindolin-1-one (**4p**) in $\text{DMSO}-d_6$.



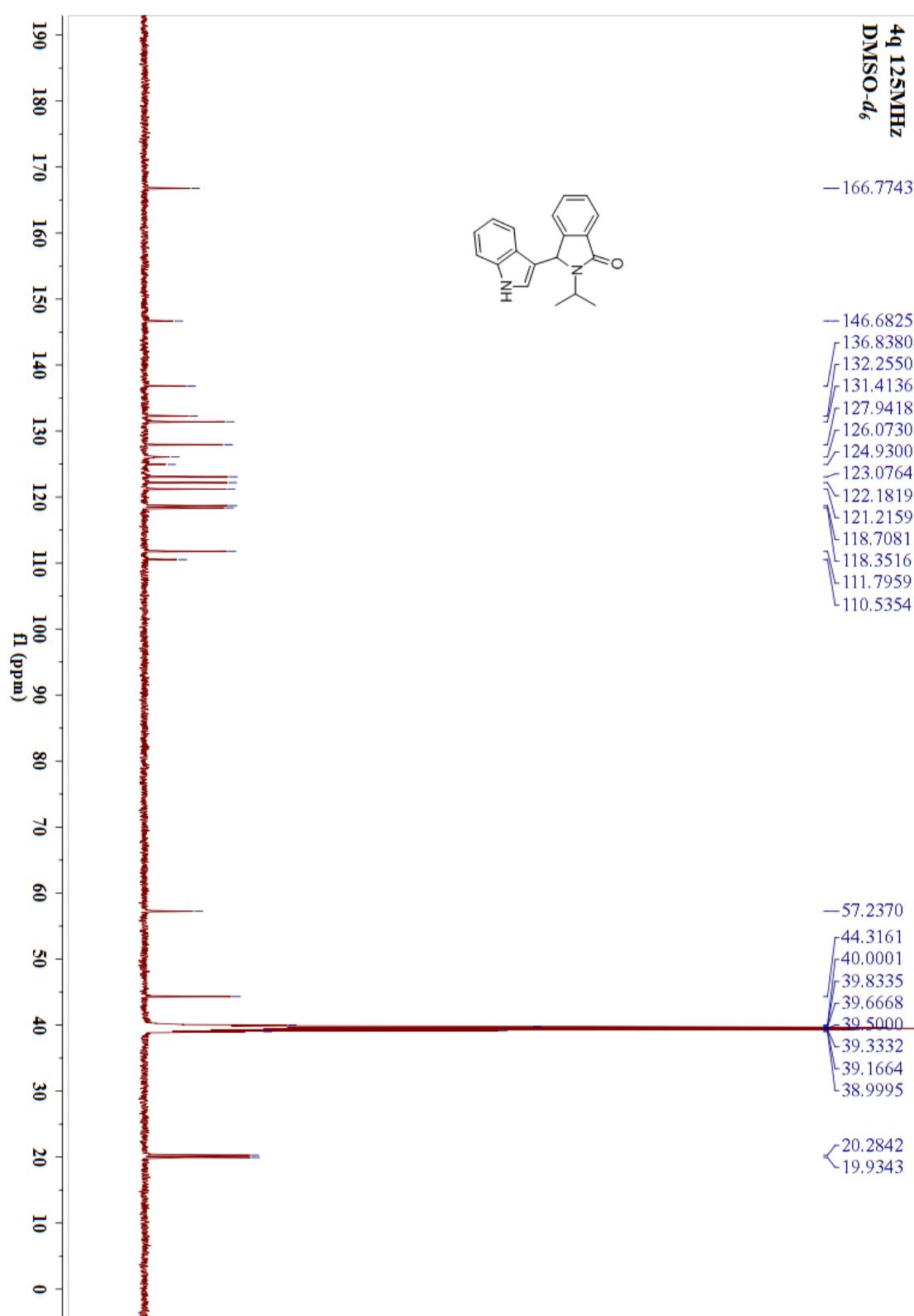
S49. LCMS spectrum of 3-(1*H*-indol-3-yl)-2-isopropylisoindolin-1-one (**4q**).



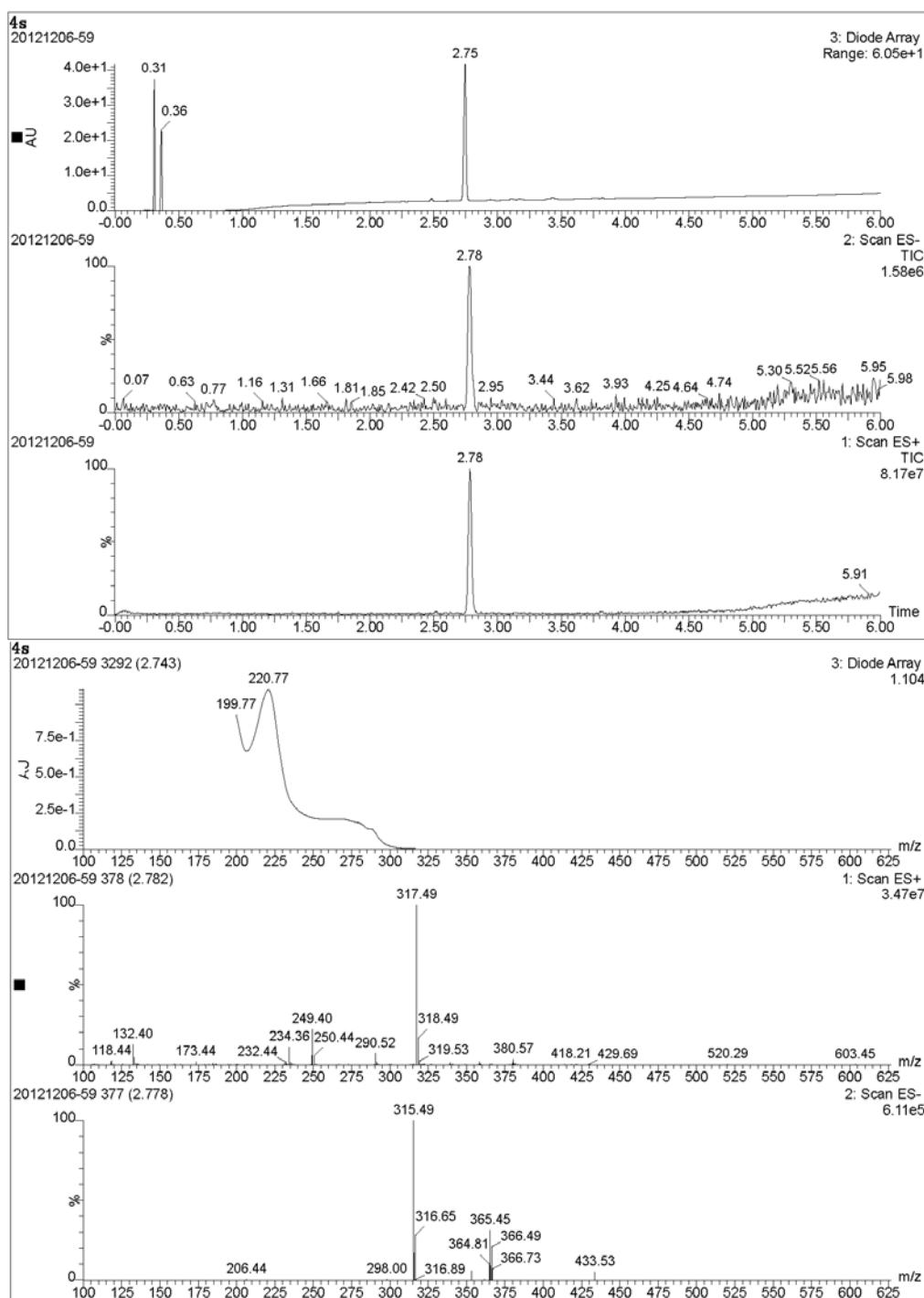
S50. ^1H NMR spectrum of 3-(1*H*-indol-3-yl)-2-isopropylisoindolin-1-one (**4q**) in DMSO-*d*₆.



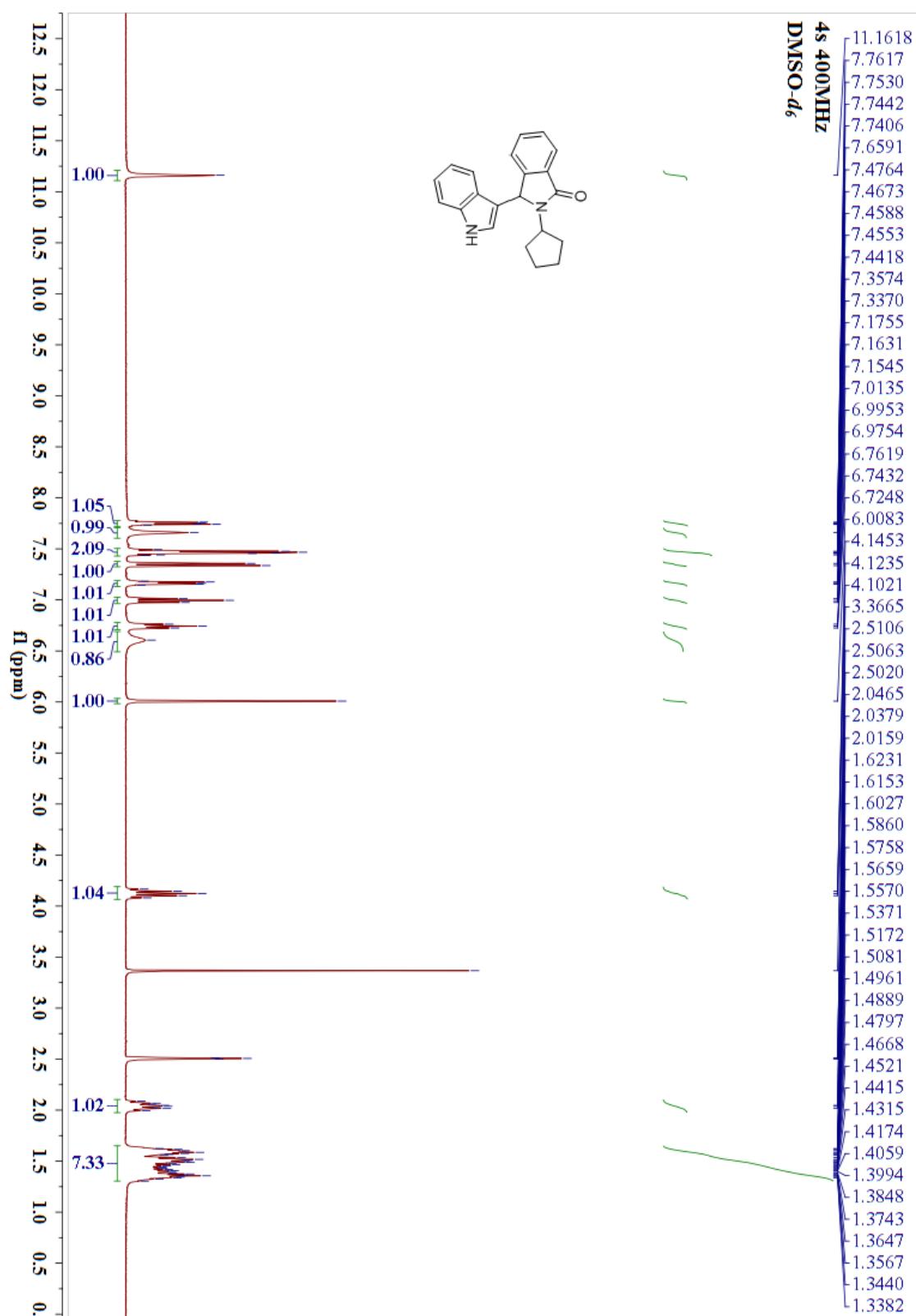
S51. ^{13}C NMR spectrum of 3-(1*H*-indol-3-yl)-2-isopropylisoindolin-1-one (**4q**) in $\text{DMSO}-d_6$.



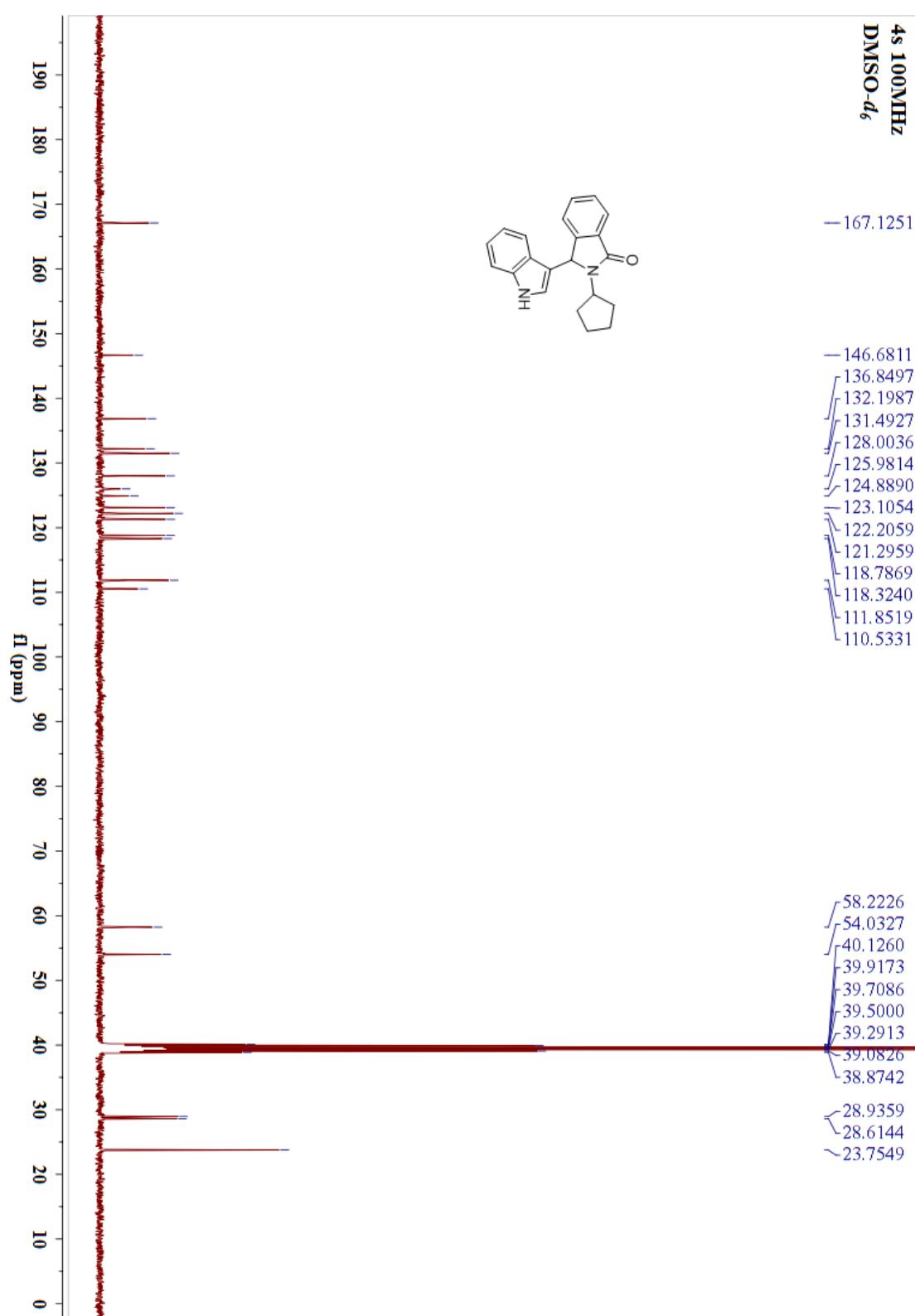
S52. LCMS spectrum of 2-cyclopentyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4s**).



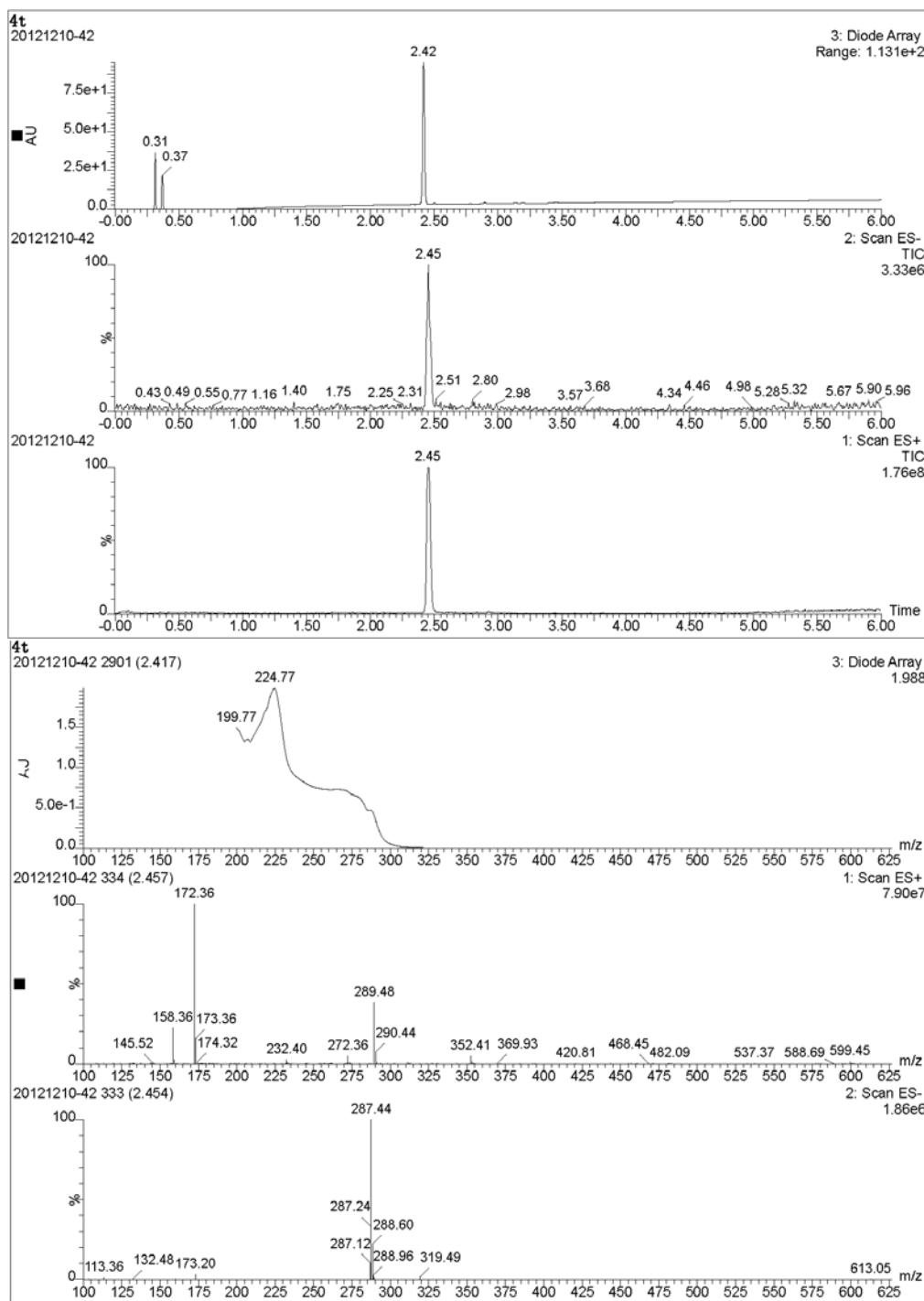
S53. ^1H NMR spectrum of 2-cyclopentyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4s**) in $\text{DMSO}-d_6$.



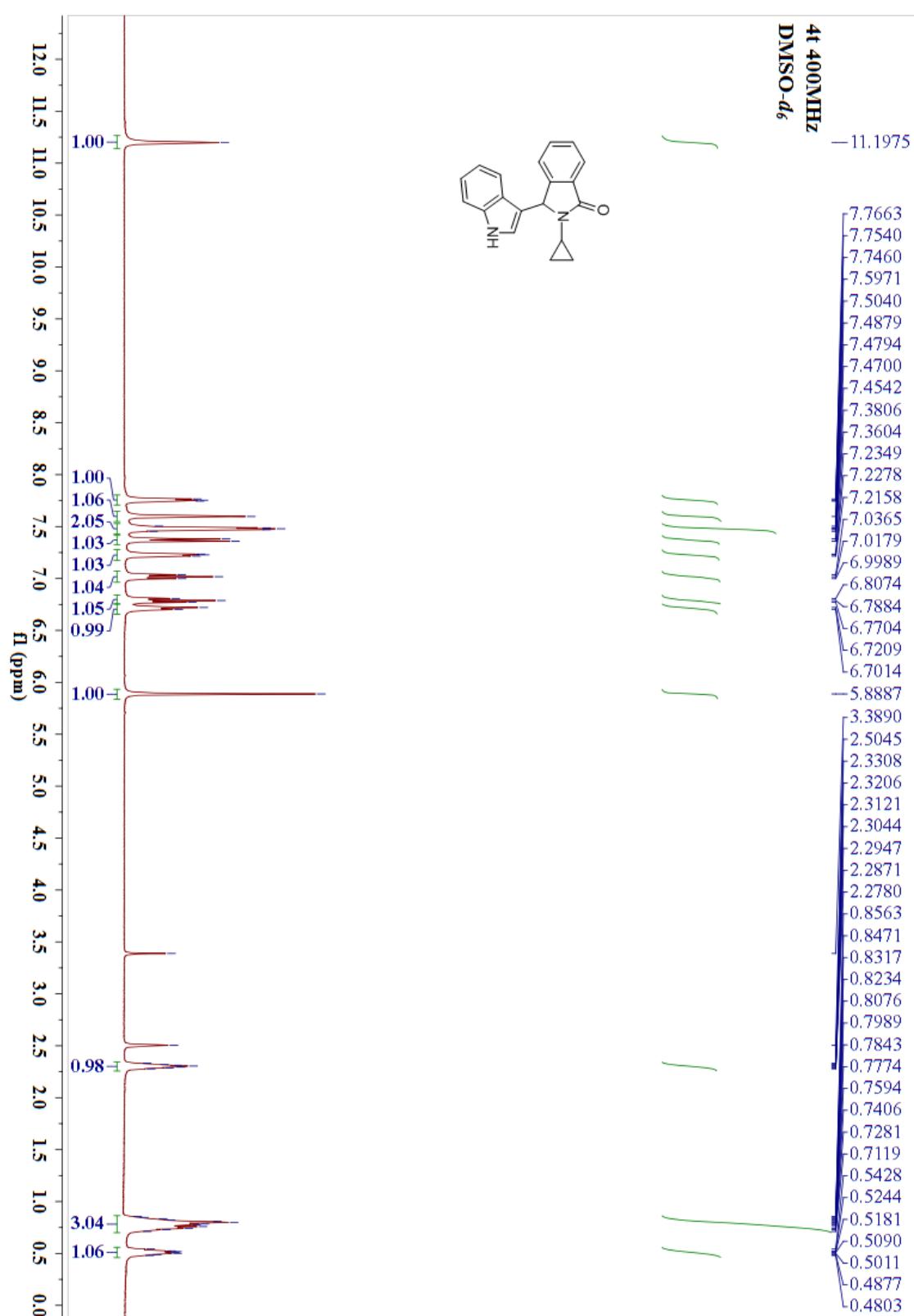
S54. ^{13}C NMR spectrum of 2-cyclopentyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4s**) in $\text{DMSO}-d_6$.



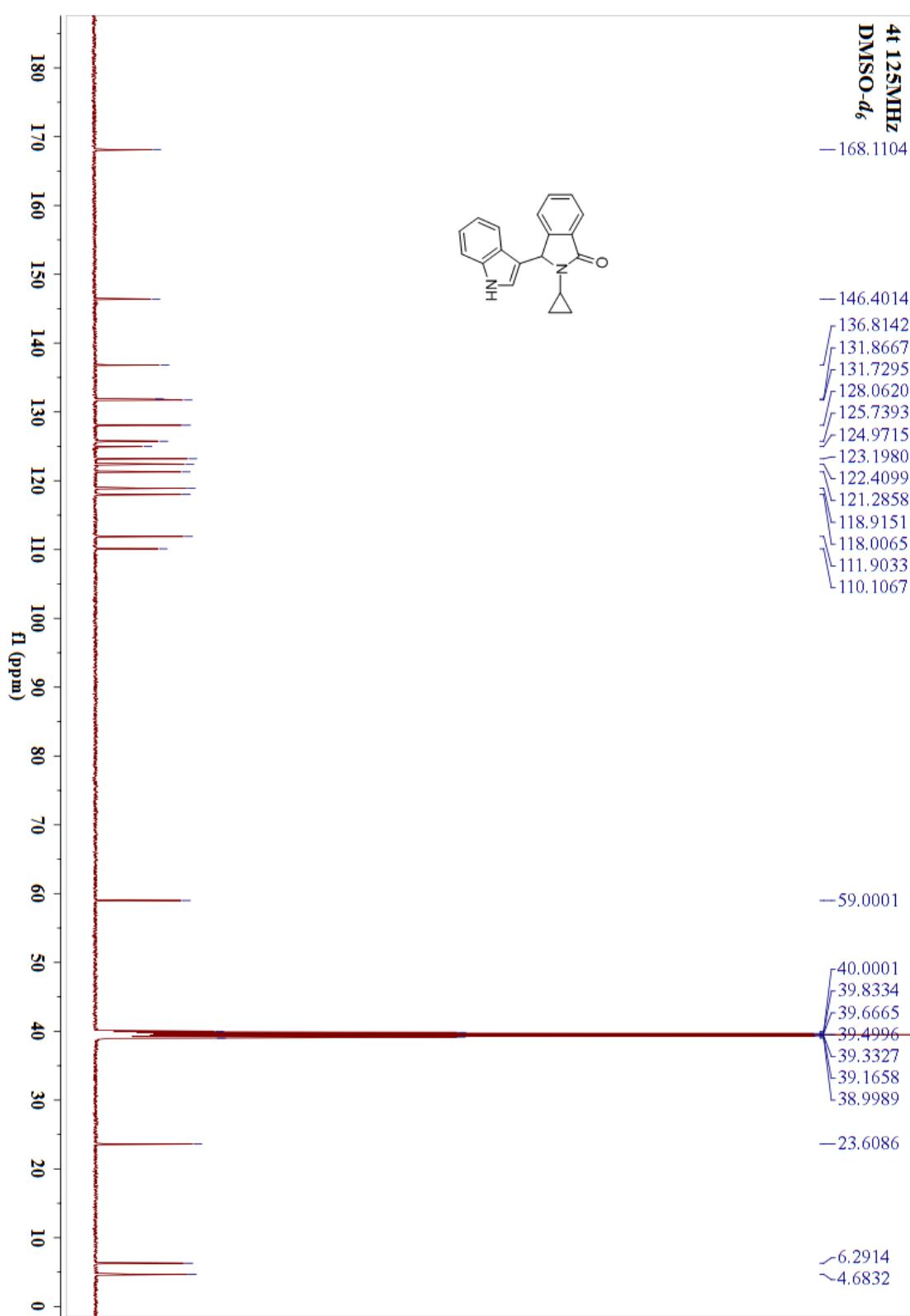
S55. LCMS spectrum of 2-cyclopropyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4t**).



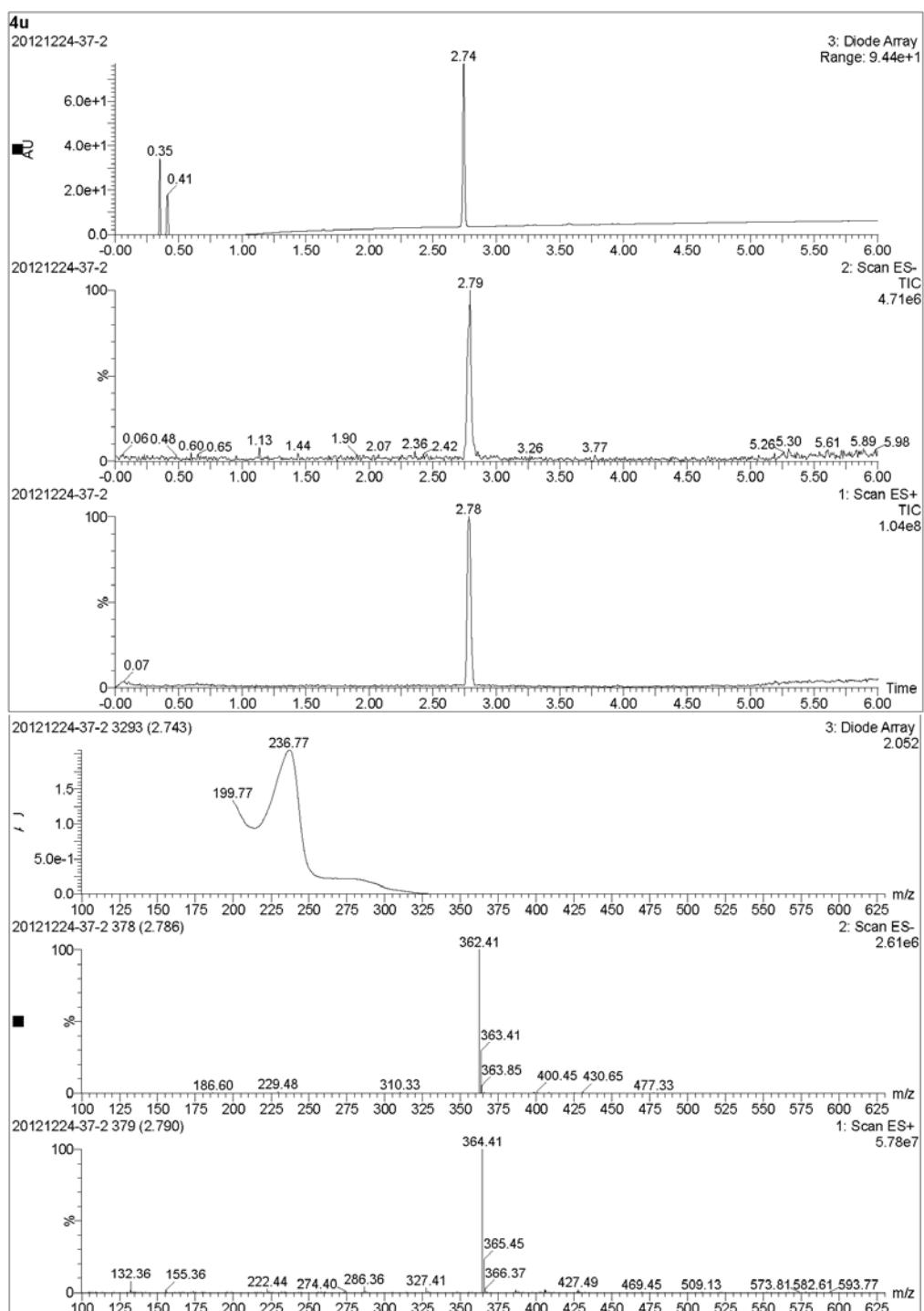
S56. ^1H NMR spectrum of 2-cyclopropyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4t**) in $\text{DMSO}-d_6$.



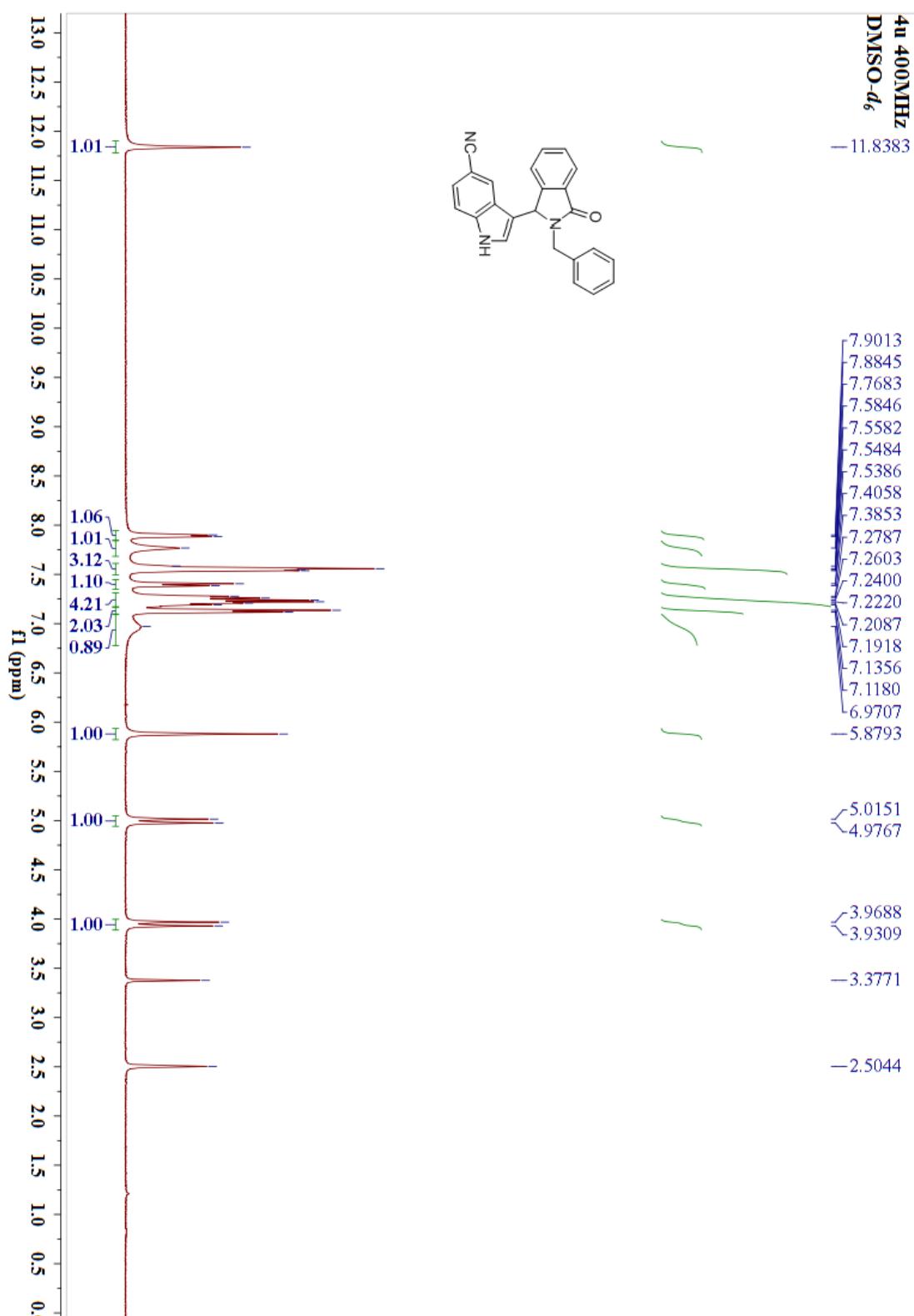
S57. ^{13}C NMR spectrum of 2-cyclopropyl-3-(1*H*-indol-3-yl)isoindolin-1-one (**4t**) in $\text{DMSO}-d_6$.



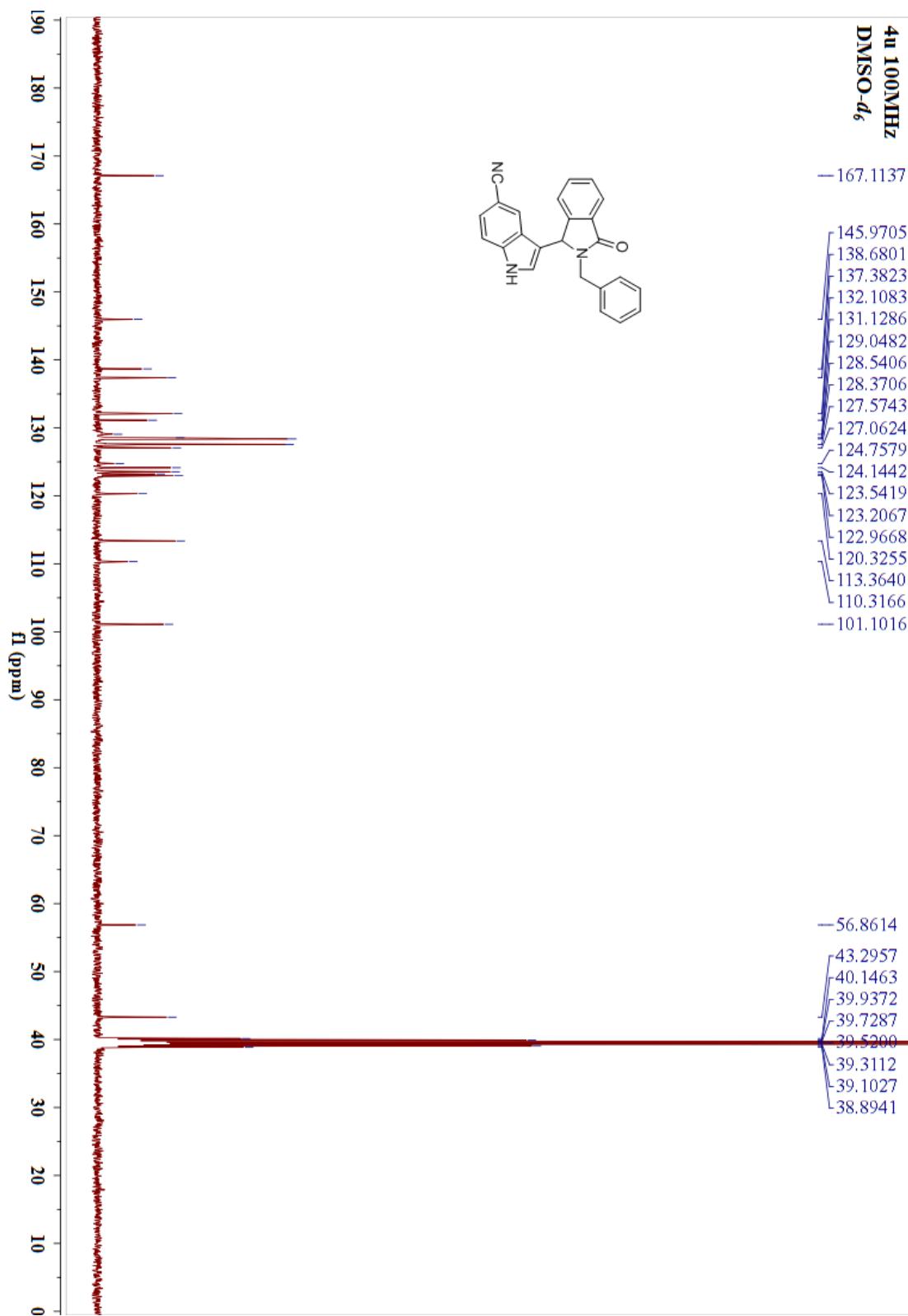
S58. LCMS spectrum of 3-(2-benzyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4u**).



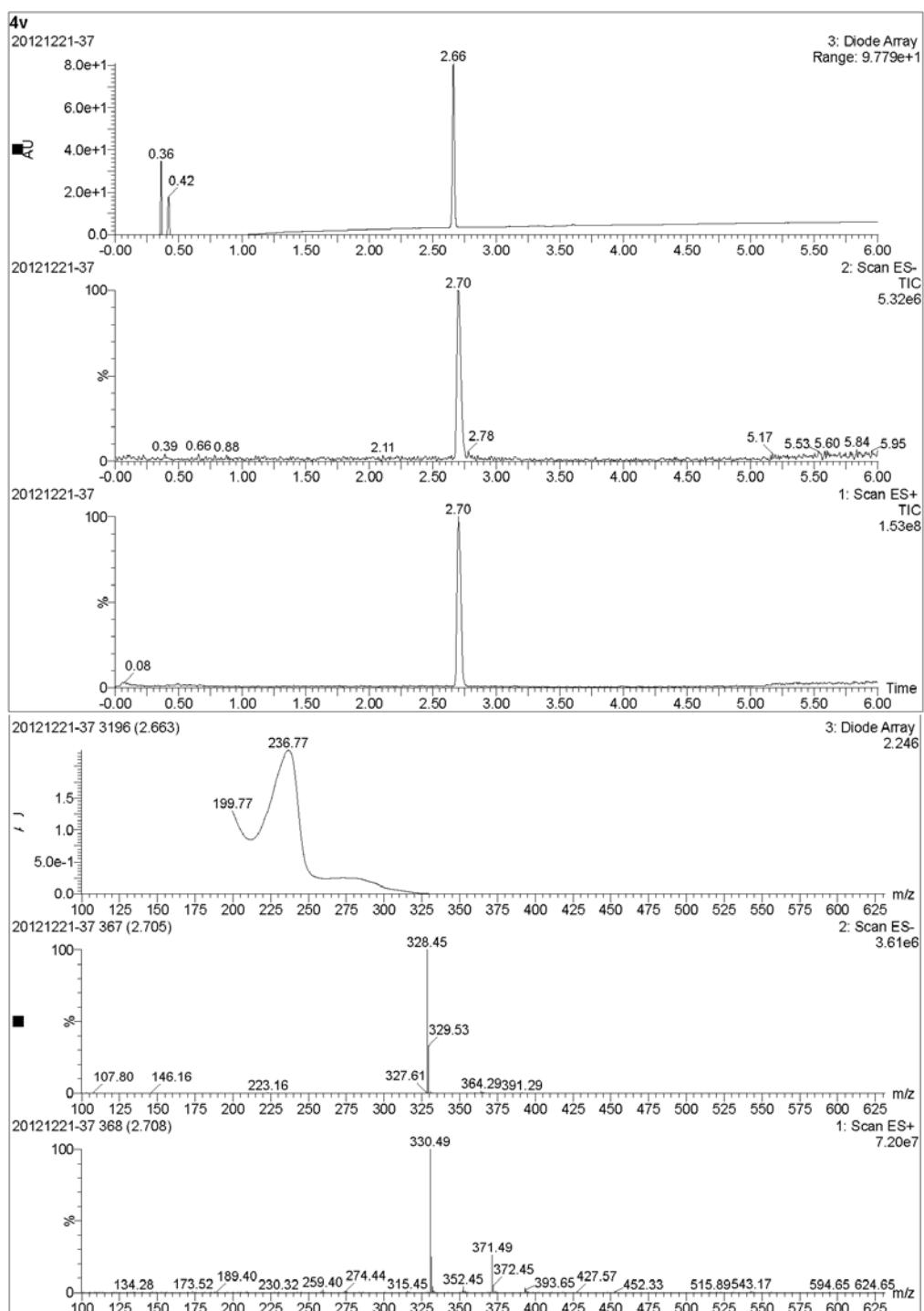
S59. ^1H NMR spectrum of 3-(2-benzyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4u**) in $\text{DMSO}-d_6$.



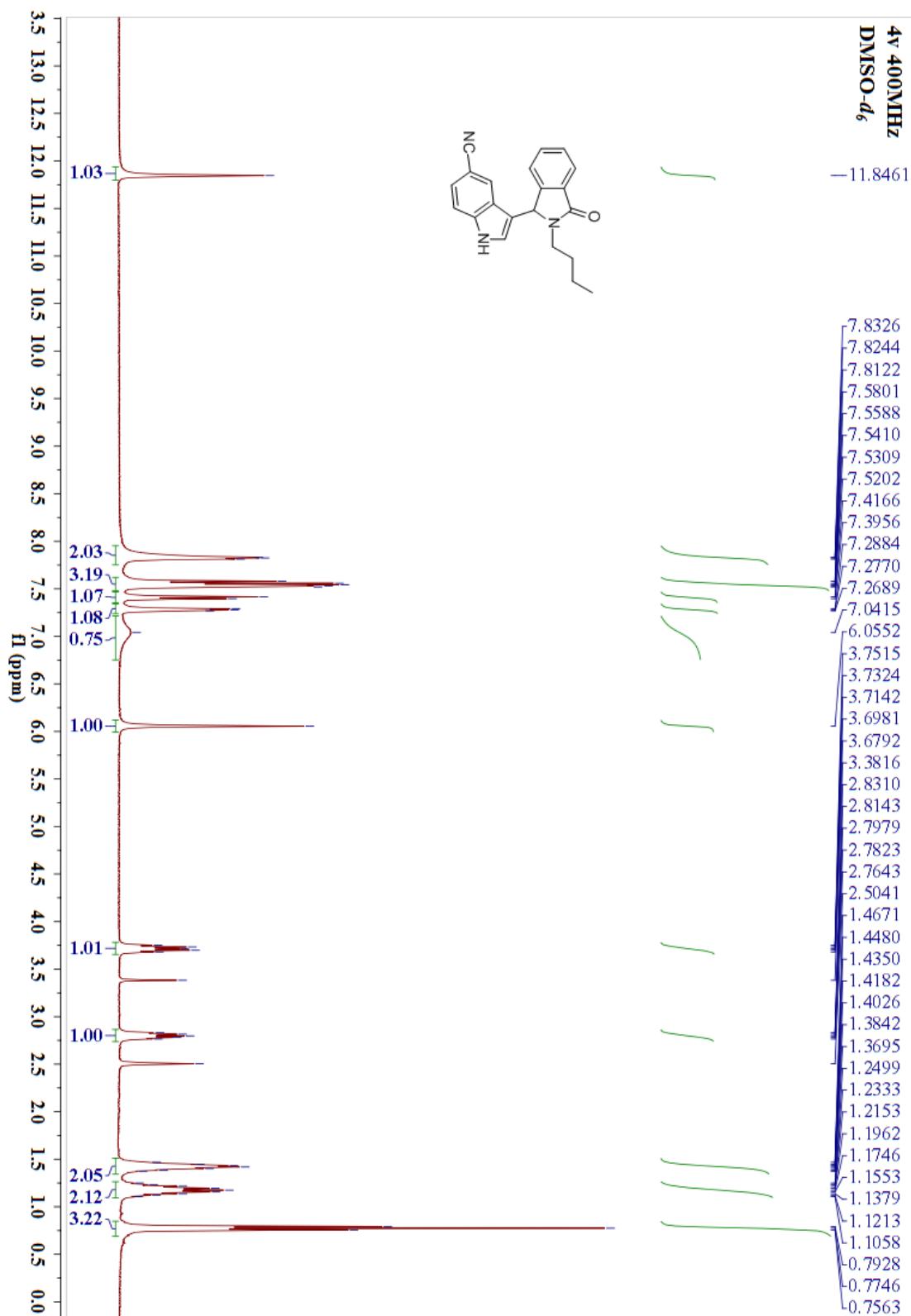
S60. ^{13}C NMR spectrum of 3-(2-benzyl-3-oxoisoindolin-1-yl)-1*H*-indole-5-carbonitrile (**4u**) in $\text{DMSO}-d_6$.



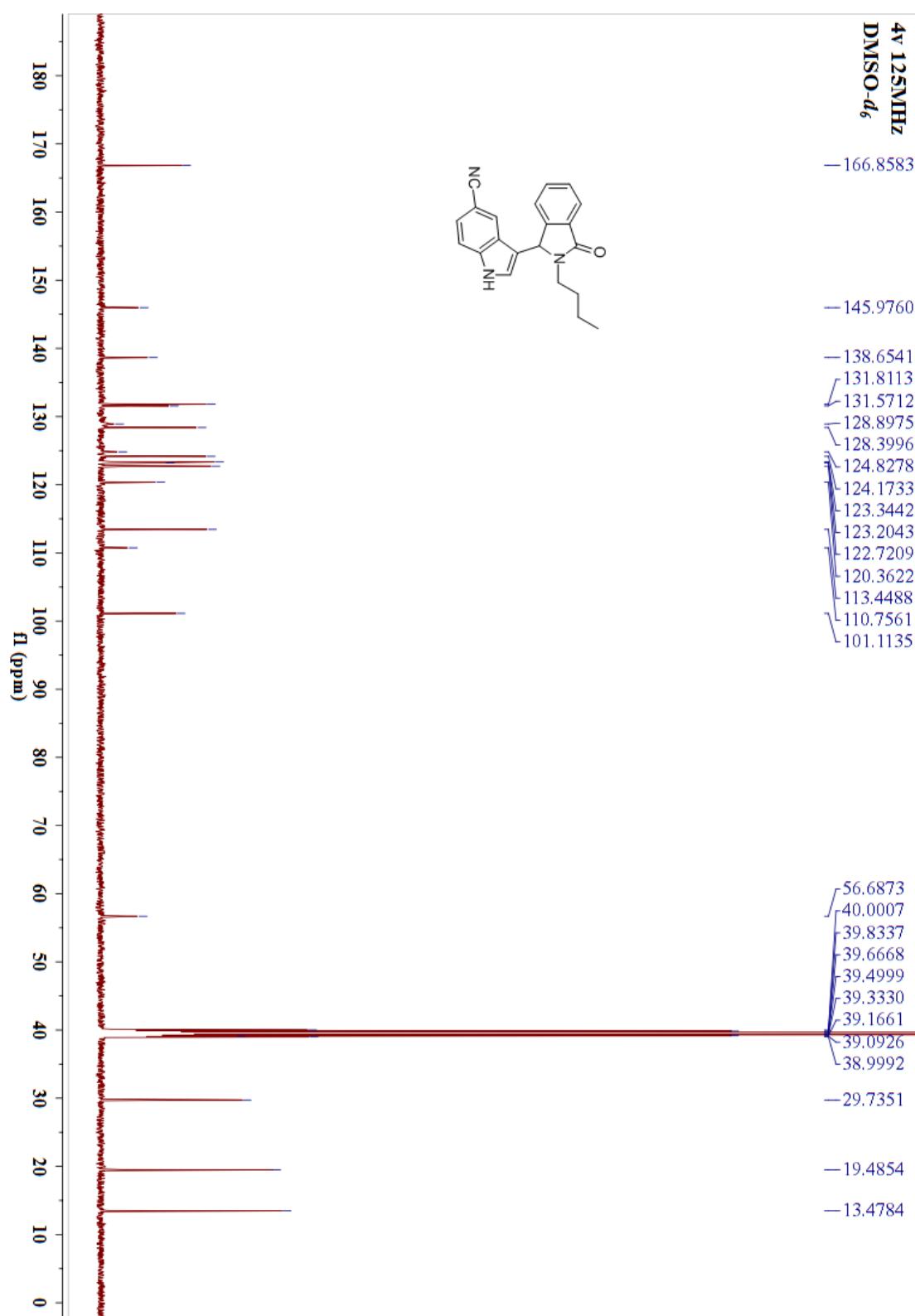
S61. LCMS spectrum of 3-(2-butyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4v**).



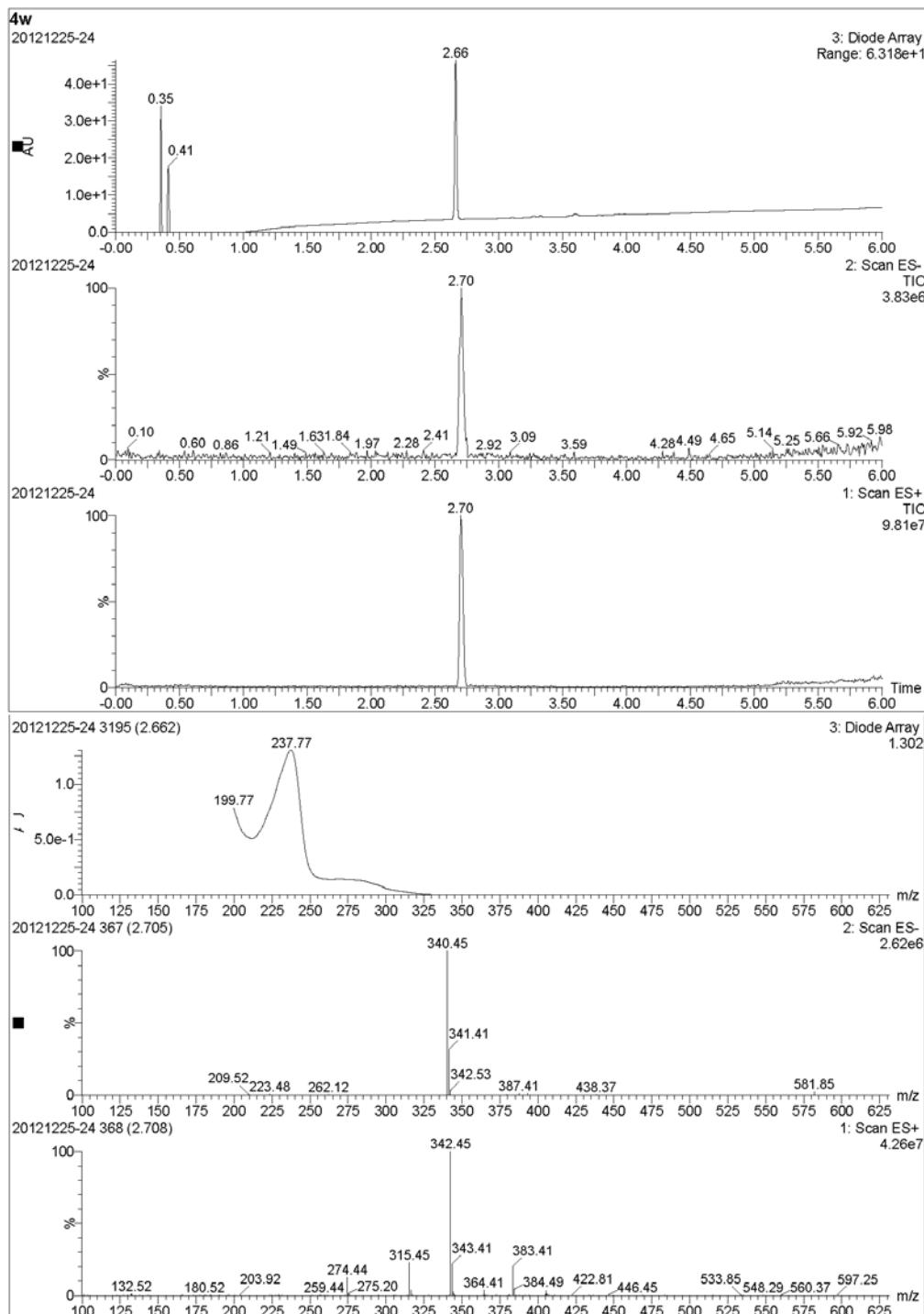
S62. ^1H NMR spectrum of 3-(2-butyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4v**) in $\text{DMSO}-d_6$.



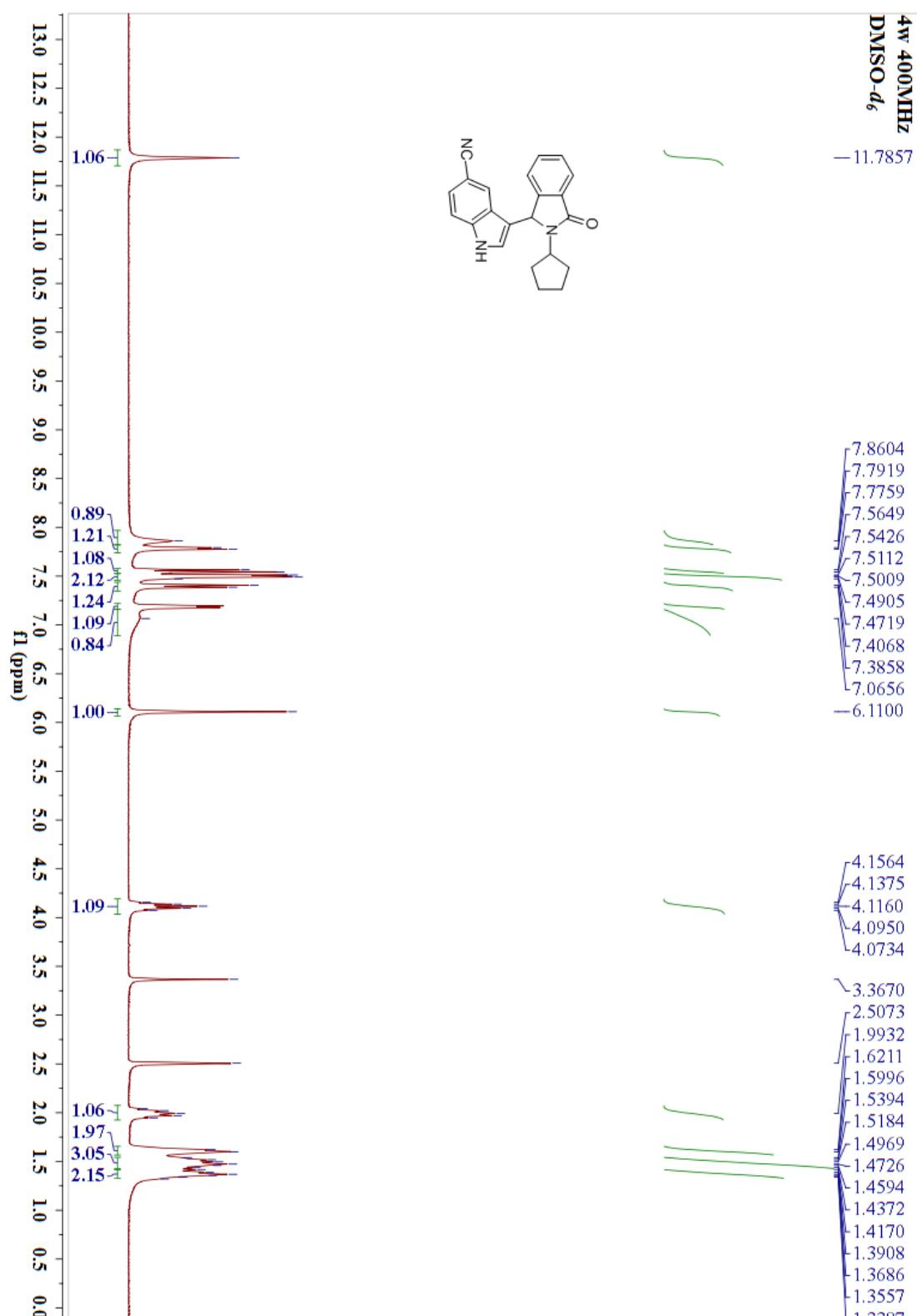
S63. ^{13}C NMR spectrum of 3-(2-butyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4v**) in $\text{DMSO}-d_6$.



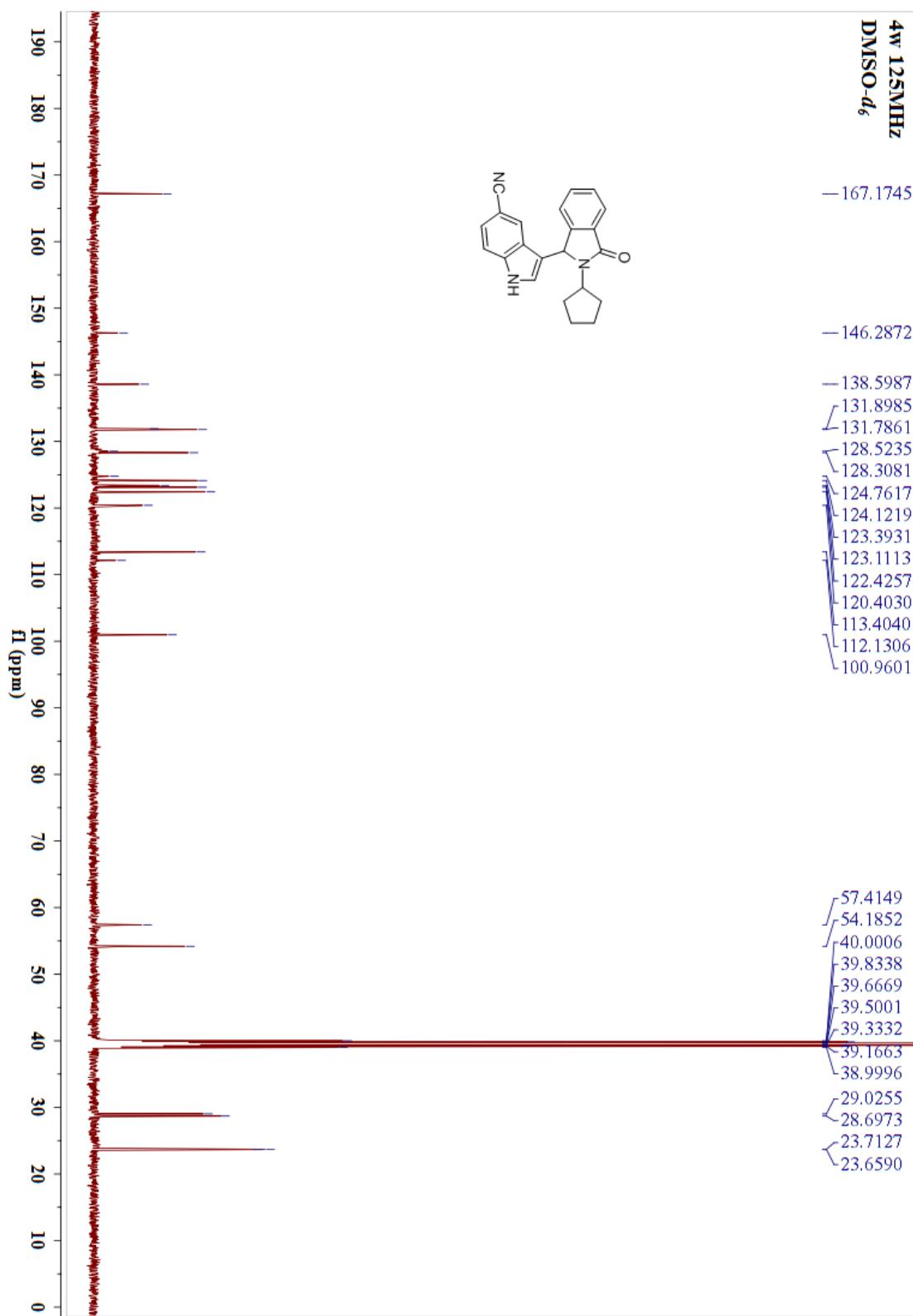
S64. LCMS spectrum of
3-(2-cyclopentyl-3-oxoisindolin-1-yl)-1*H*-indole-5-carbonitrile (**4w**).



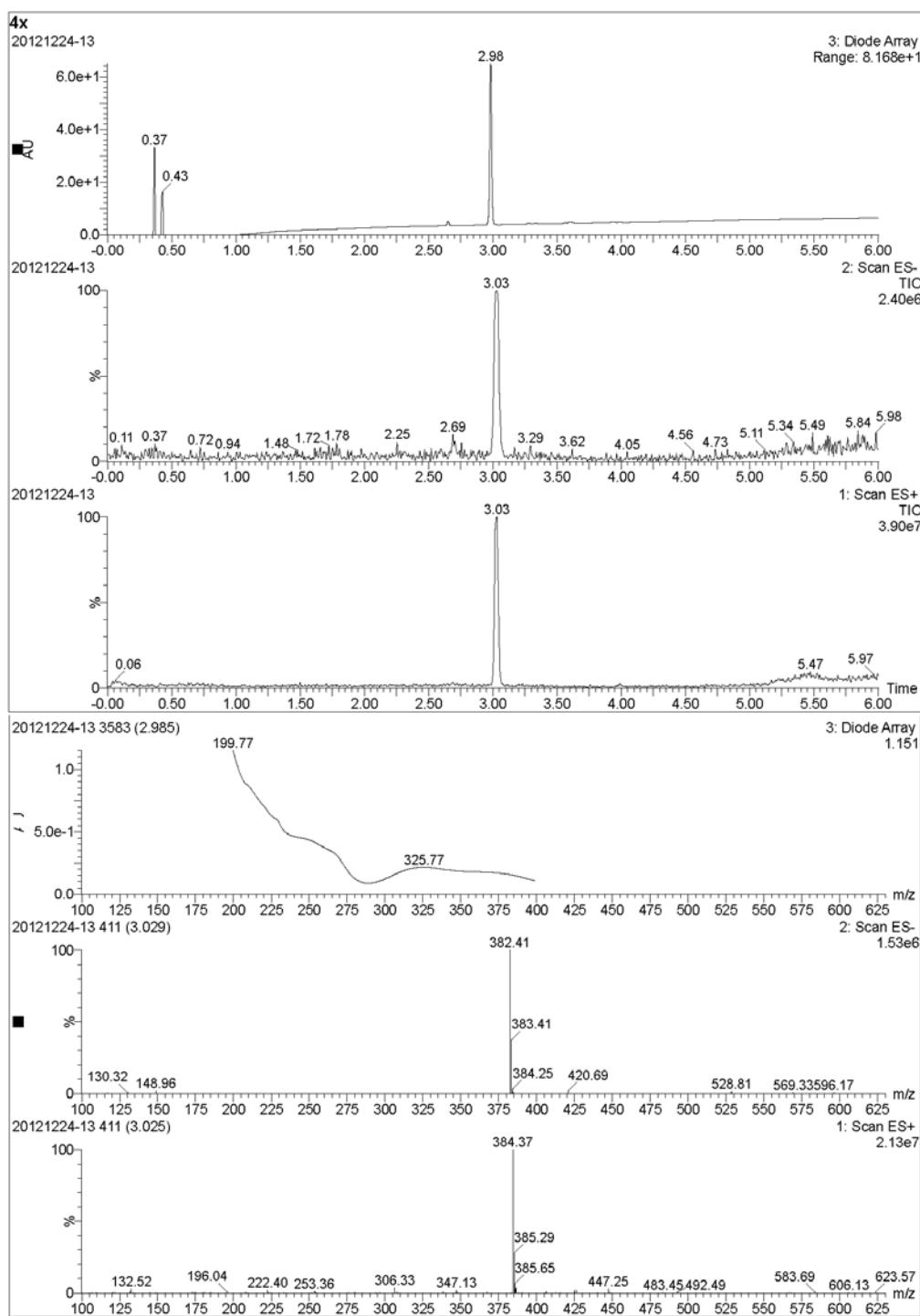
S65. ^1H NMR spectrum of 3-(2-cyclopentyl-3-oxoisoindolin-1-yl)-1*H*-indole-5-carbonitrile (**4w**) in $\text{DMSO}-d_6$.



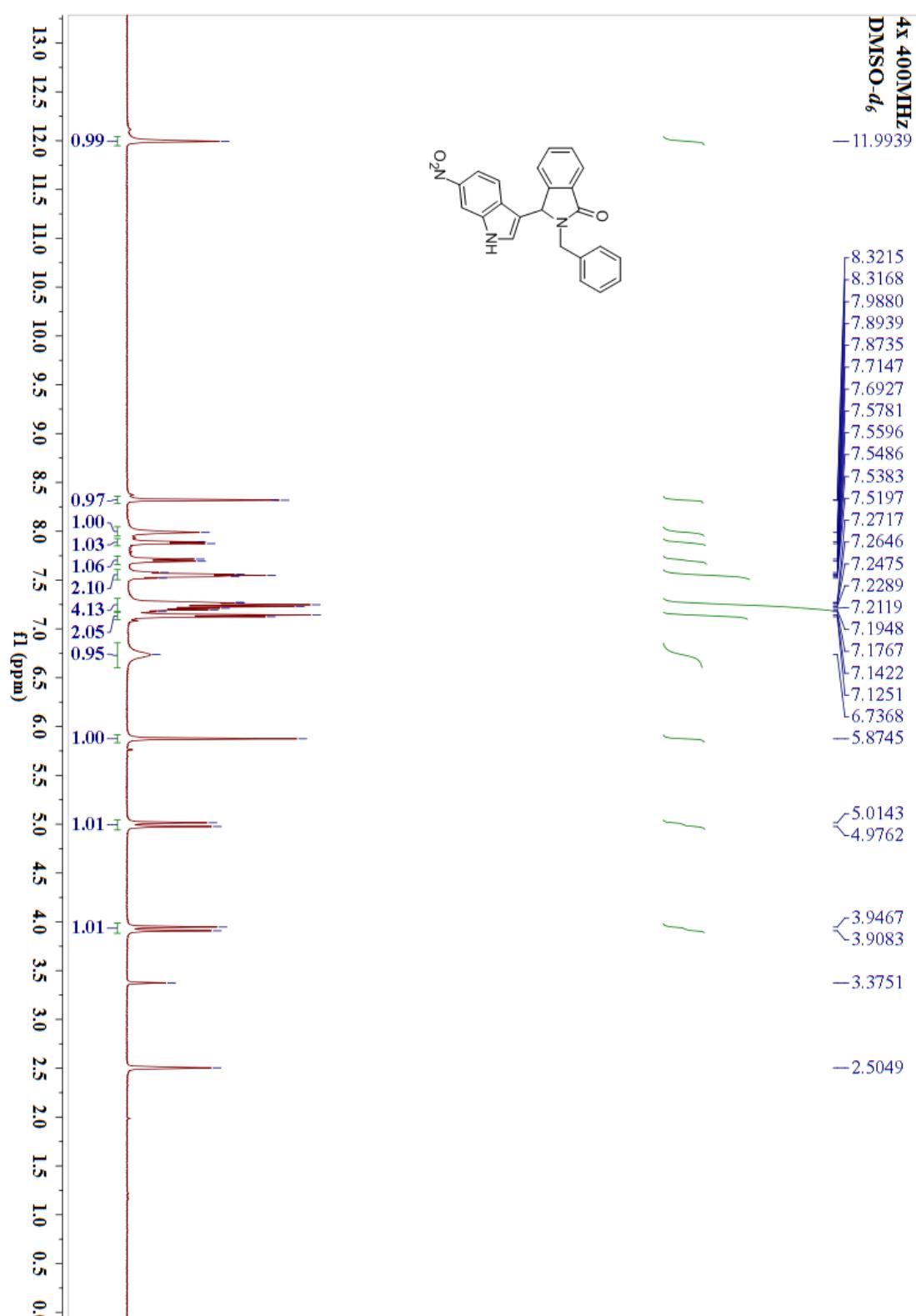
S66. ^{13}C NMR spectrum of
3-(2-cyclopentyl-3-oxoindolin-1-yl)-1*H*-indole-5-carbonitrile (**4w**) in $\text{DMSO}-d_6$.



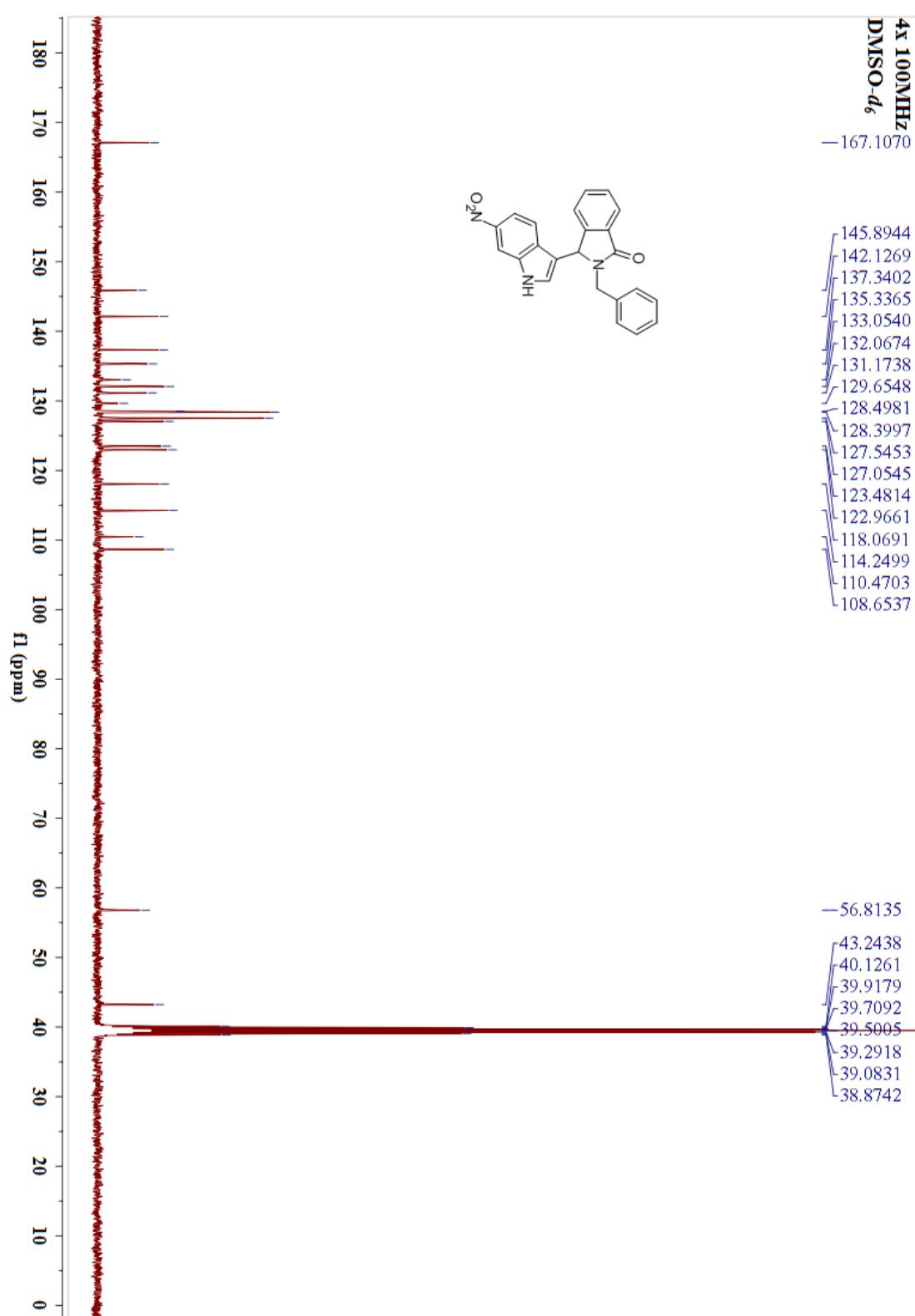
S67. LCMS spectrum of 2-benzyl-3-(6-nitro-1*H*-indol-3-yl)isoindolin-1-one (**4x**).



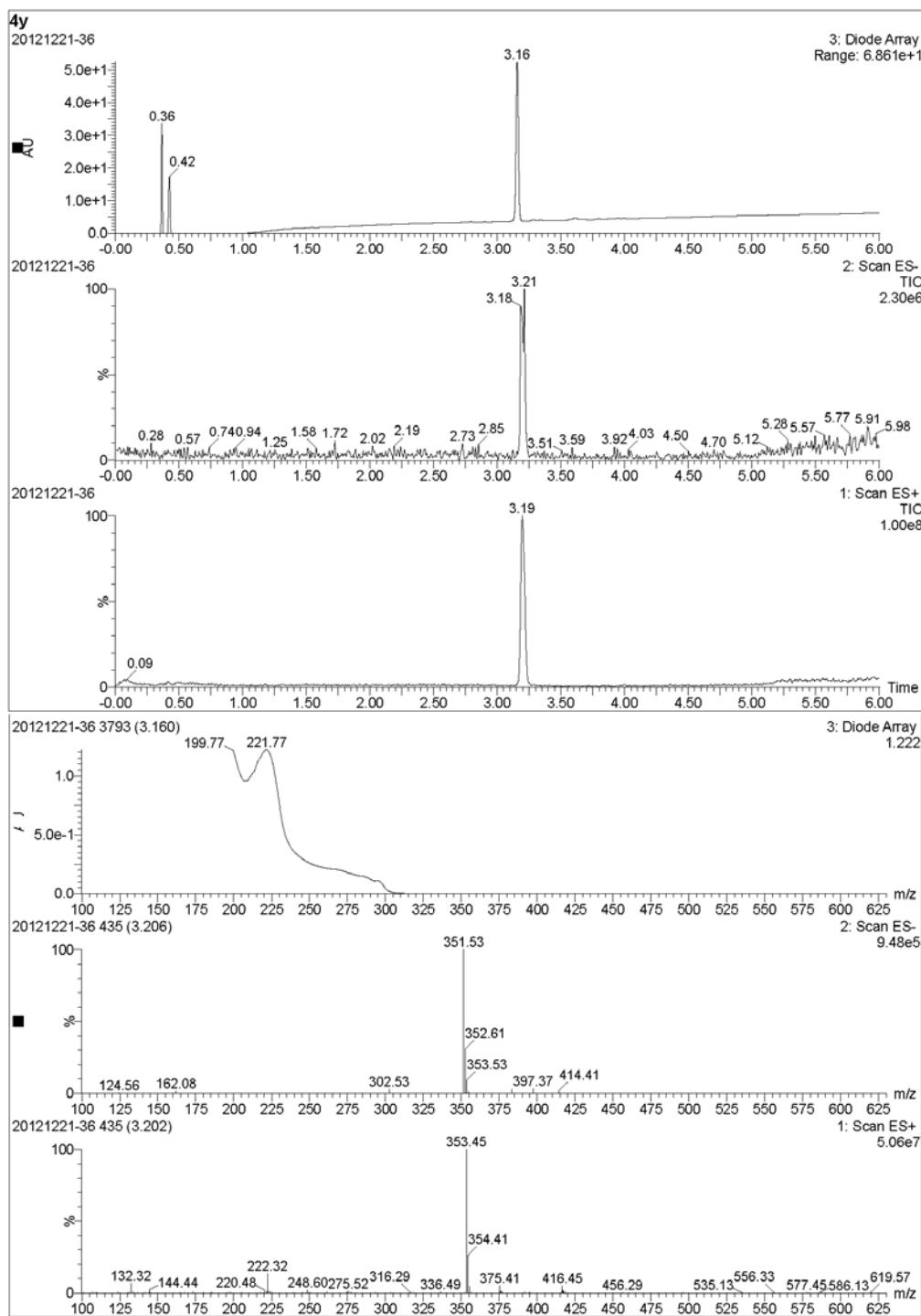
S68. ^1H NMR spectrum of 2-benzyl-3-(6-nitro-1*H*-indol-3-yl)isoindolin-1-one (**4x**) in $\text{DMSO}-d_6$.



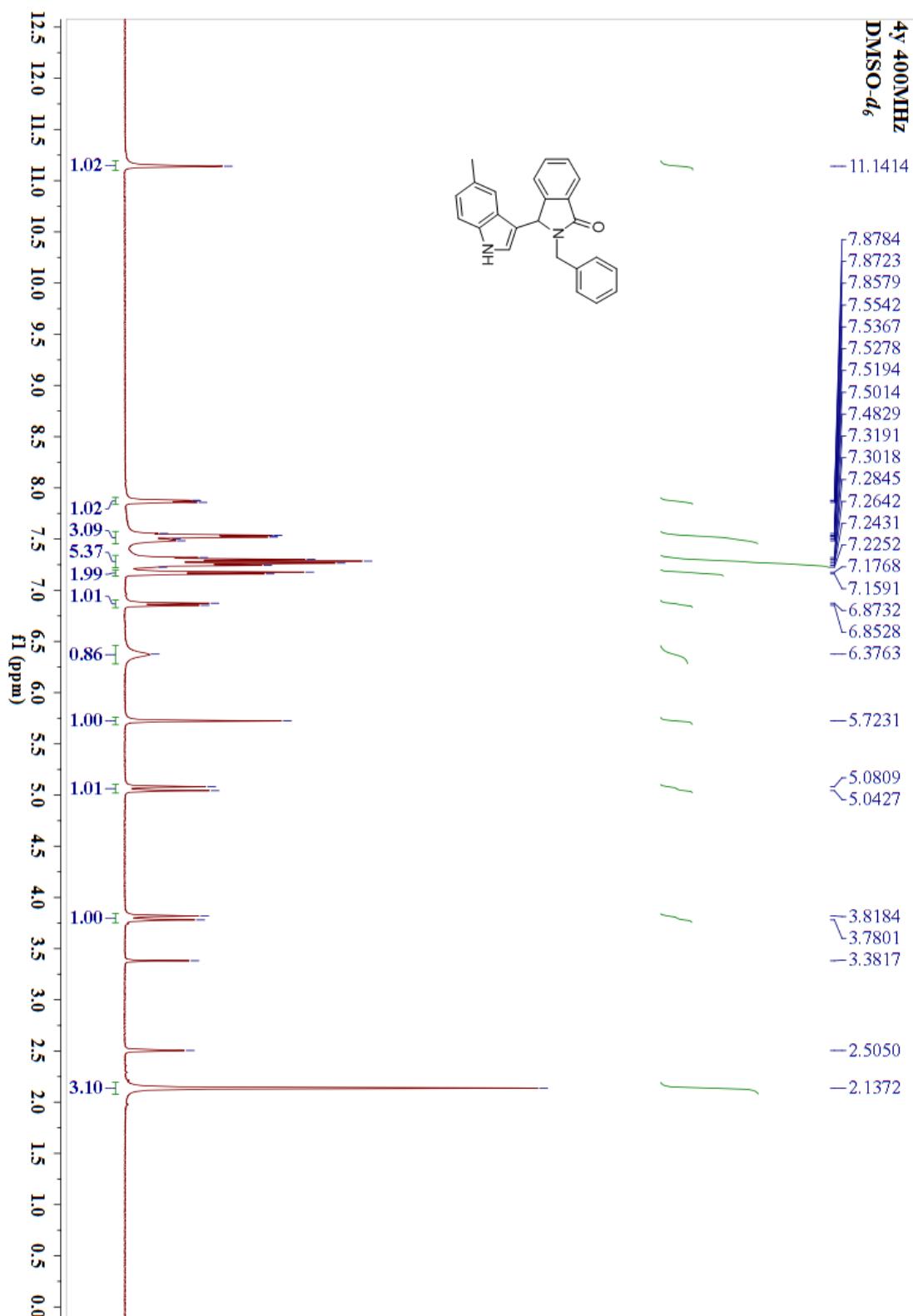
S69. ^{13}C NMR spectrum of 2-benzyl-3-(6-nitro-1*H*-indol-3-yl)isoindolin-1-one (**4x**) in $\text{DMSO}-d_6$.



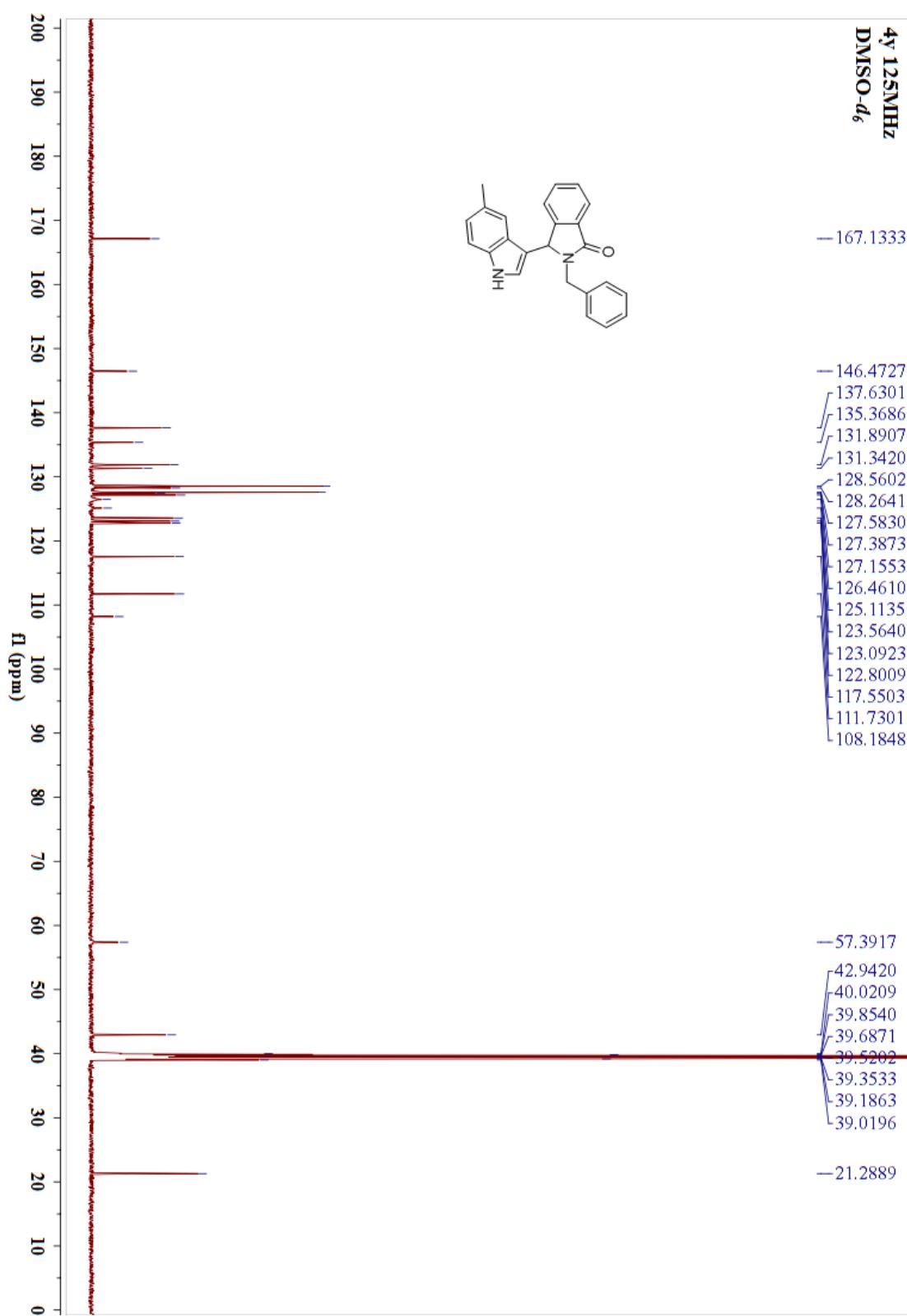
S70. LCMS spectrum of 2-benzyl-3-(5-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4y**).



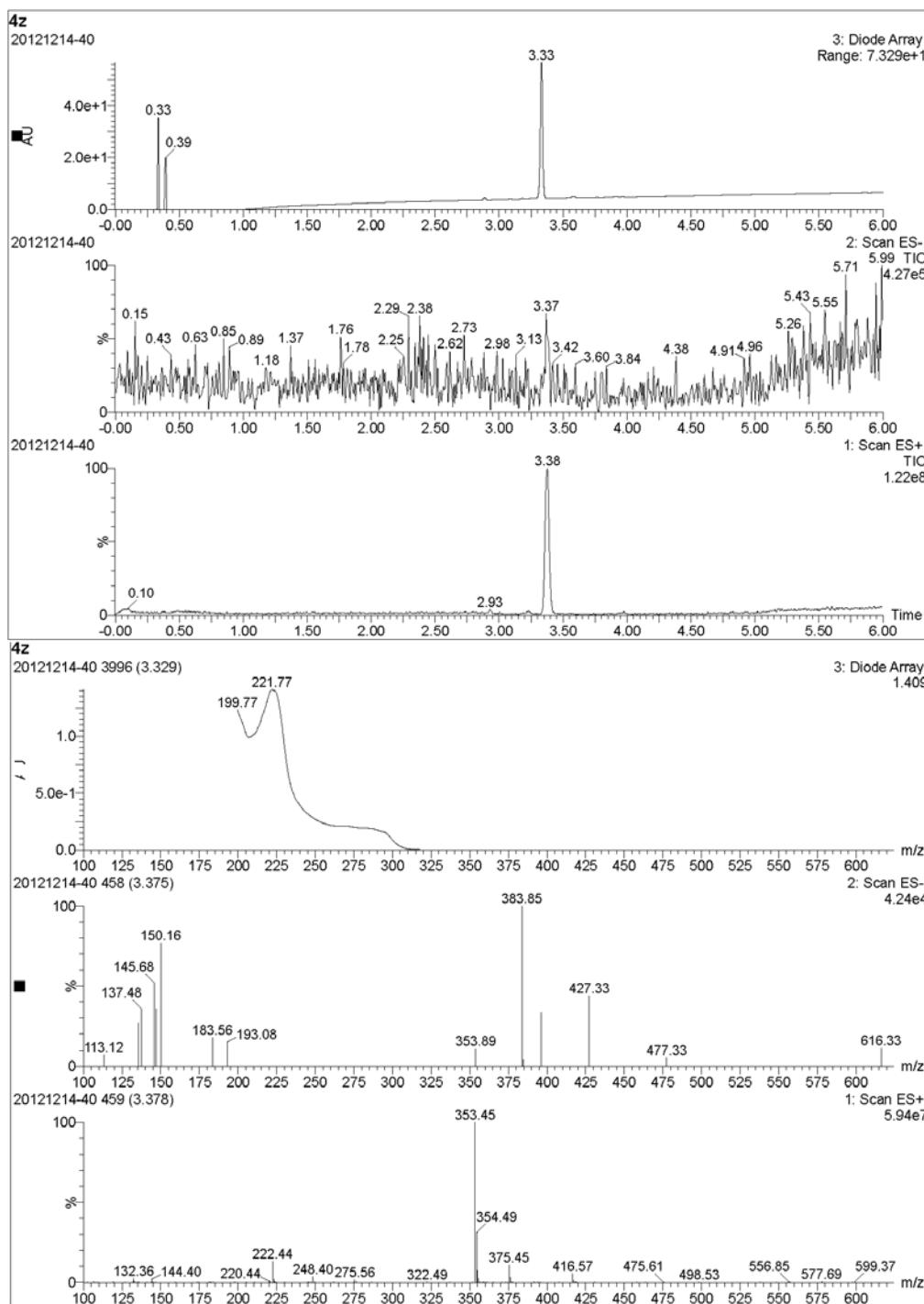
S71. ^1H NMR spectrum of 2-benzyl-3-(5-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4y**) in DMSO-*d*₆.



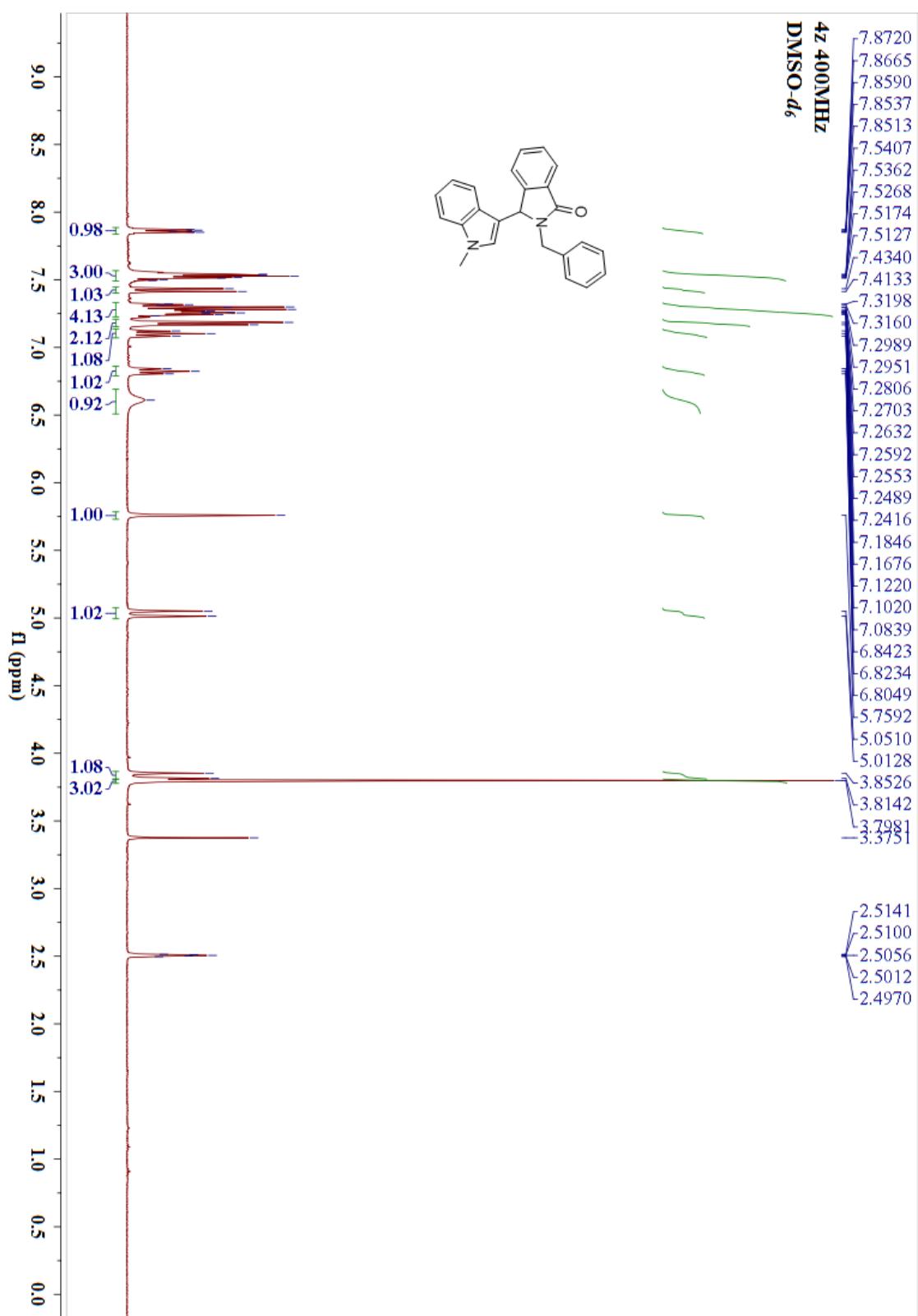
S72. ^{13}C NMR spectrum of 2-benzyl-3-(5-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4y**) in $\text{DMSO}-d_6$.



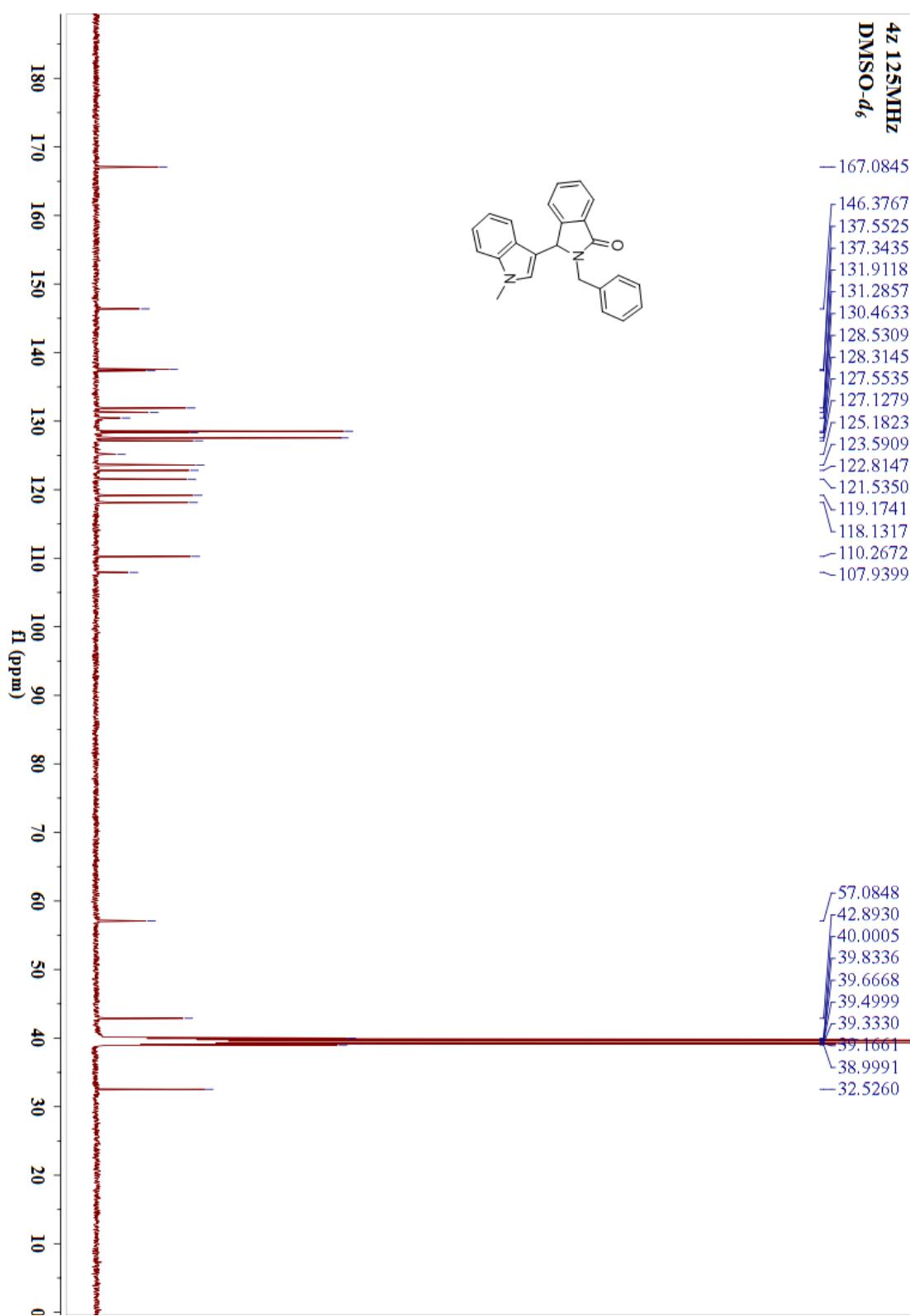
S73. LCMS spectrum of 2-benzyl-3-(1-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4z**).



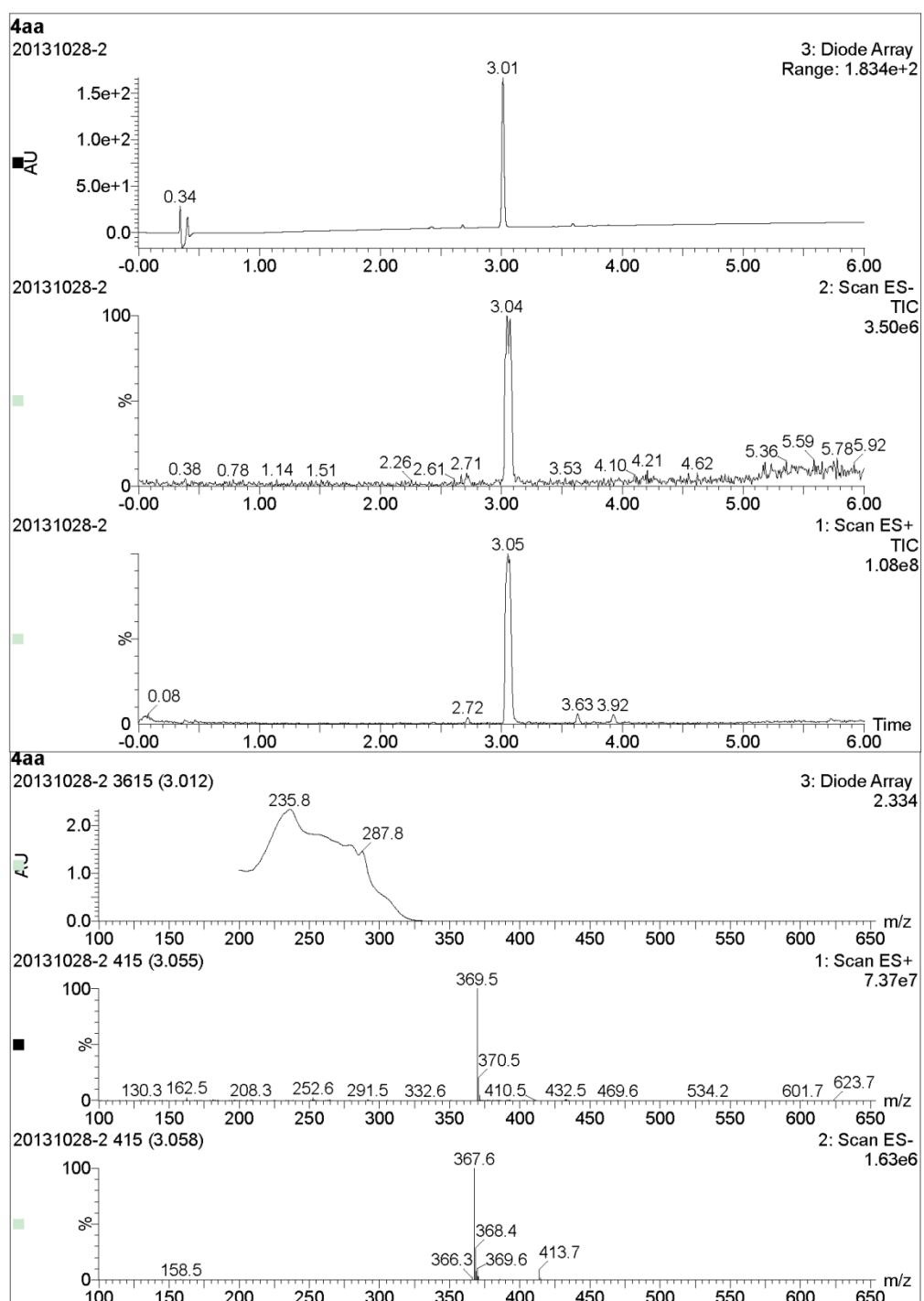
S74. ^1H NMR spectrum of 2-benzyl-3-(1-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4z**) in $\text{DMSO}-d_6$.



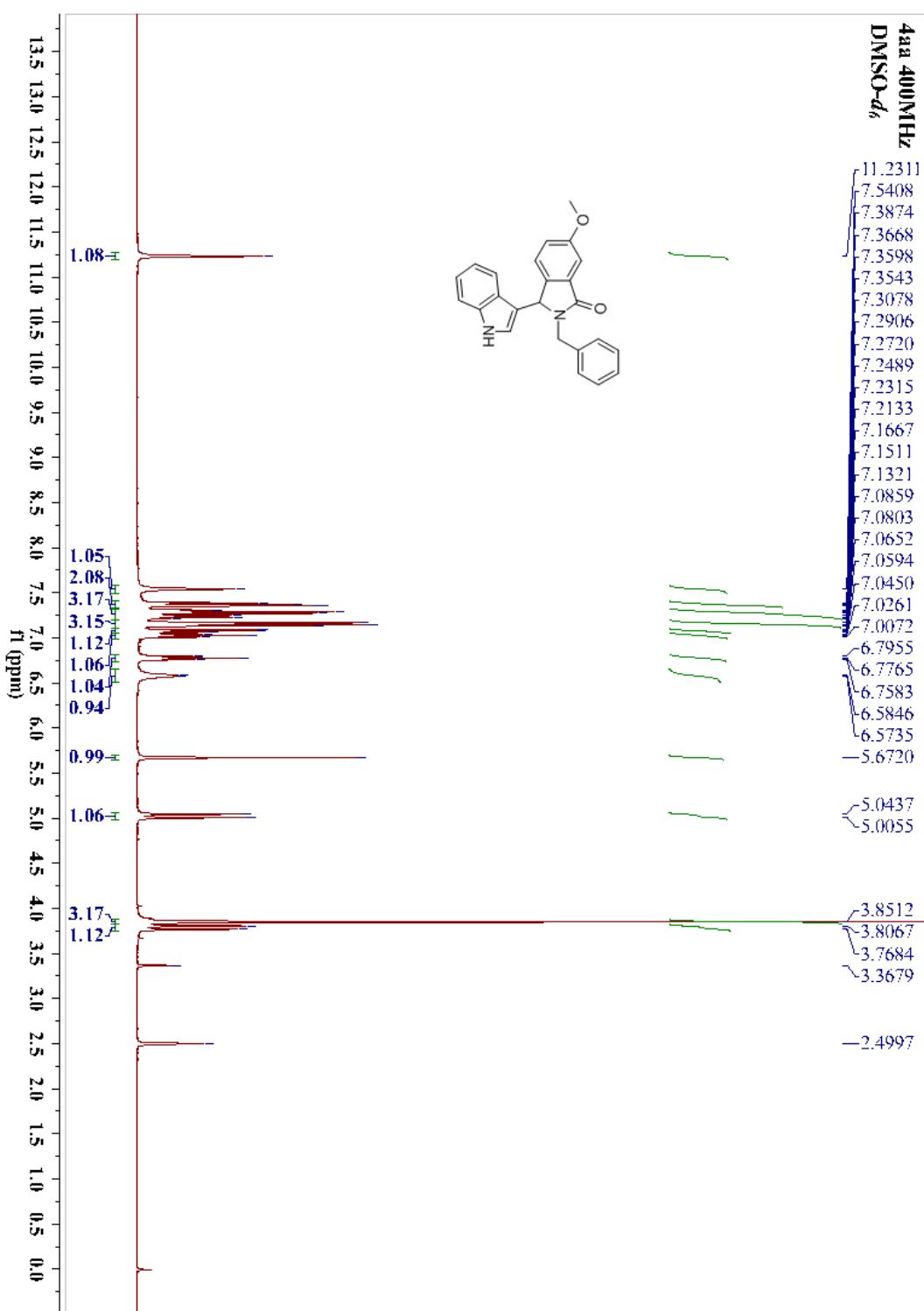
S75. ^{13}C NMR spectrum of 2-benzyl-3-(1-methyl-1*H*-indol-3-yl)isoindolin-1-one (**4z**) in $\text{DMSO}-d_6$.



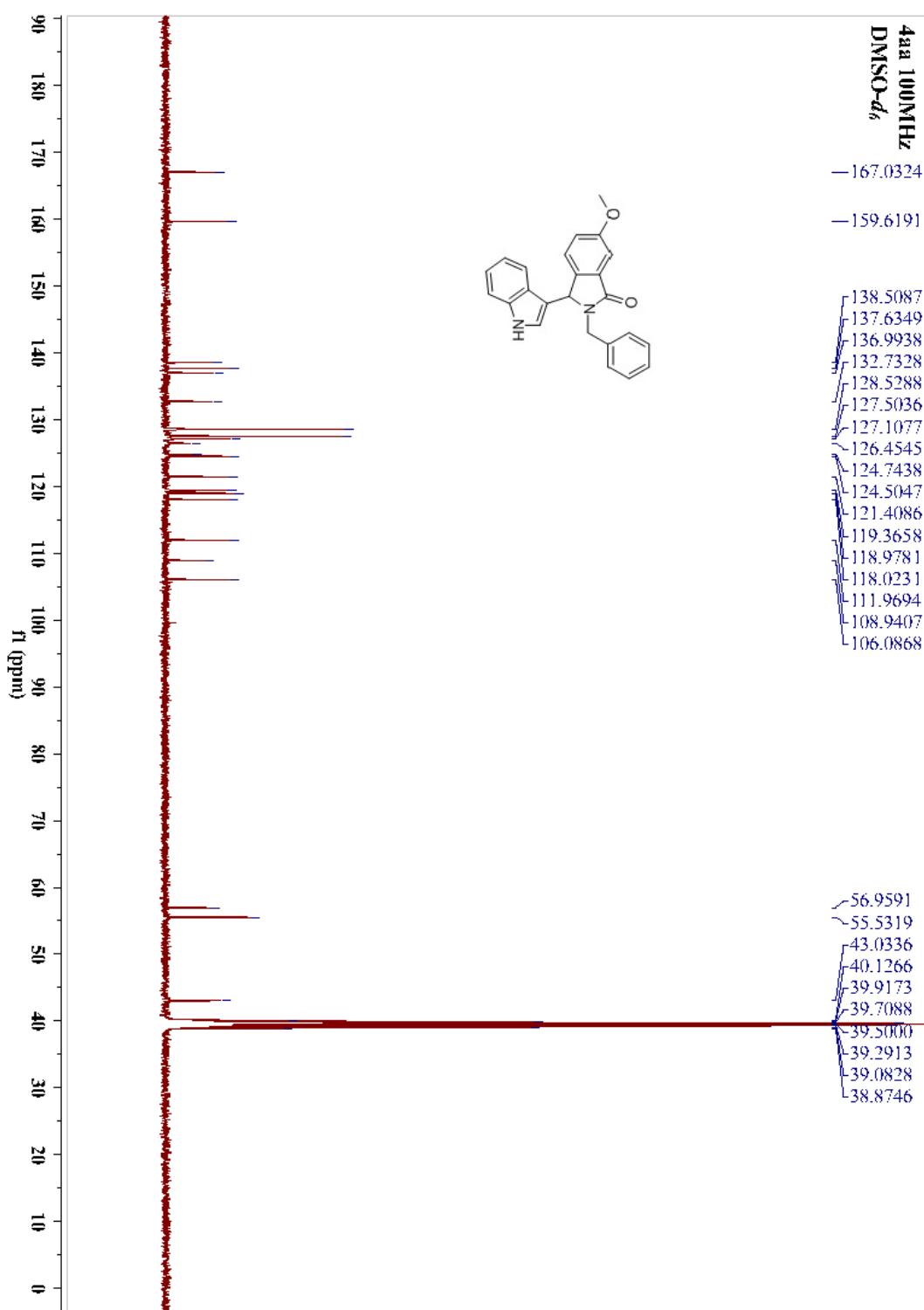
S76. LCMS spectrum of 2-benzyl-3-(1*H*-indol-3-yl)-6-methoxyisoindolin-1-one (4aa).



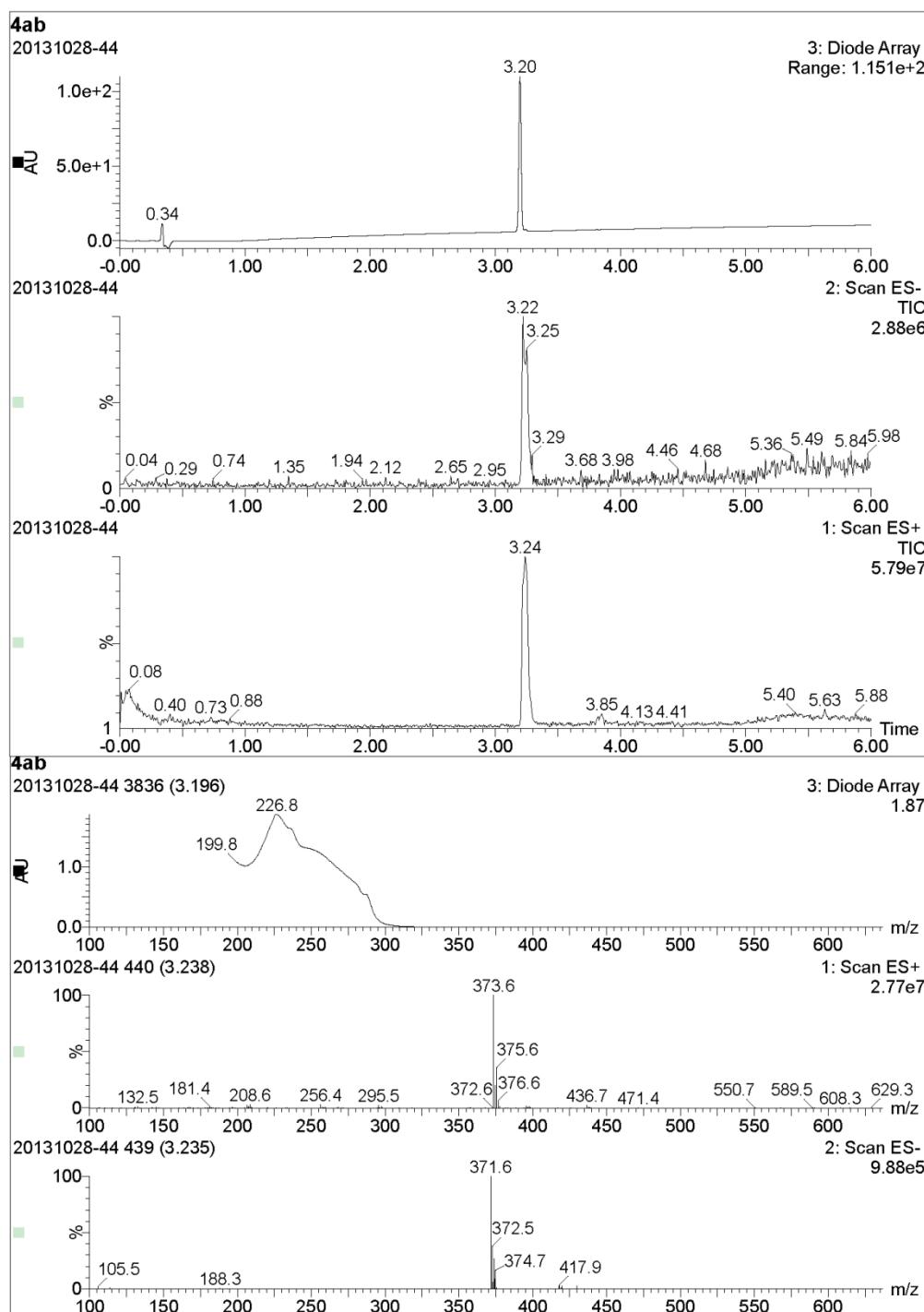
S77. ^1H NMR spectrum of 2-benzyl-3-(1*H*-indol-3-yl)-6-methoxyisoindolin-1-one (**4aa**) in $\text{DMSO}-d_6$.



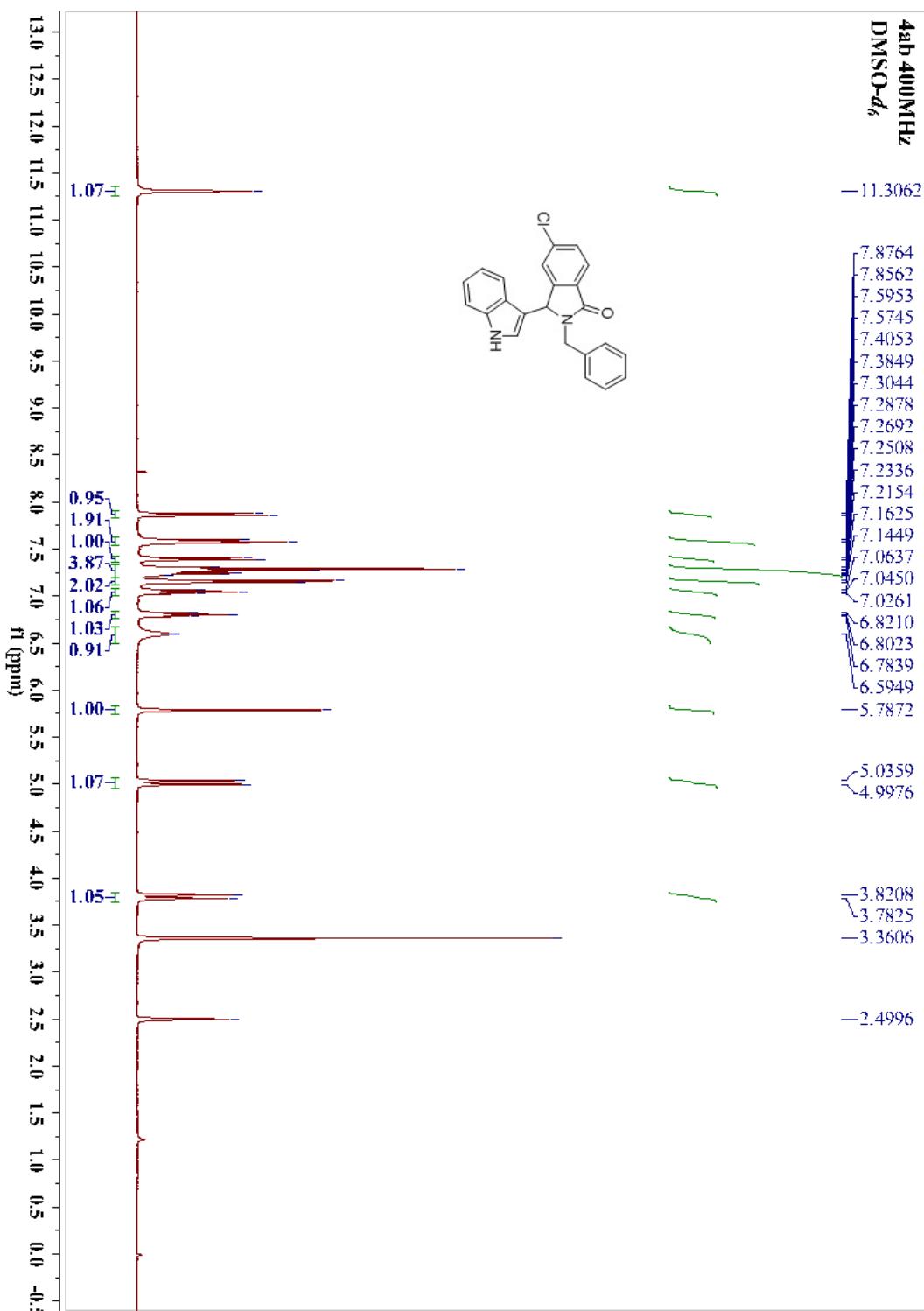
S78. ^{13}C NMR spectrum of 2-benzyl-3-(1*H*-indol-3-yl)-6-methoxyisoindolin-1-one (**4aa**) in $\text{DMSO}-d_6$.



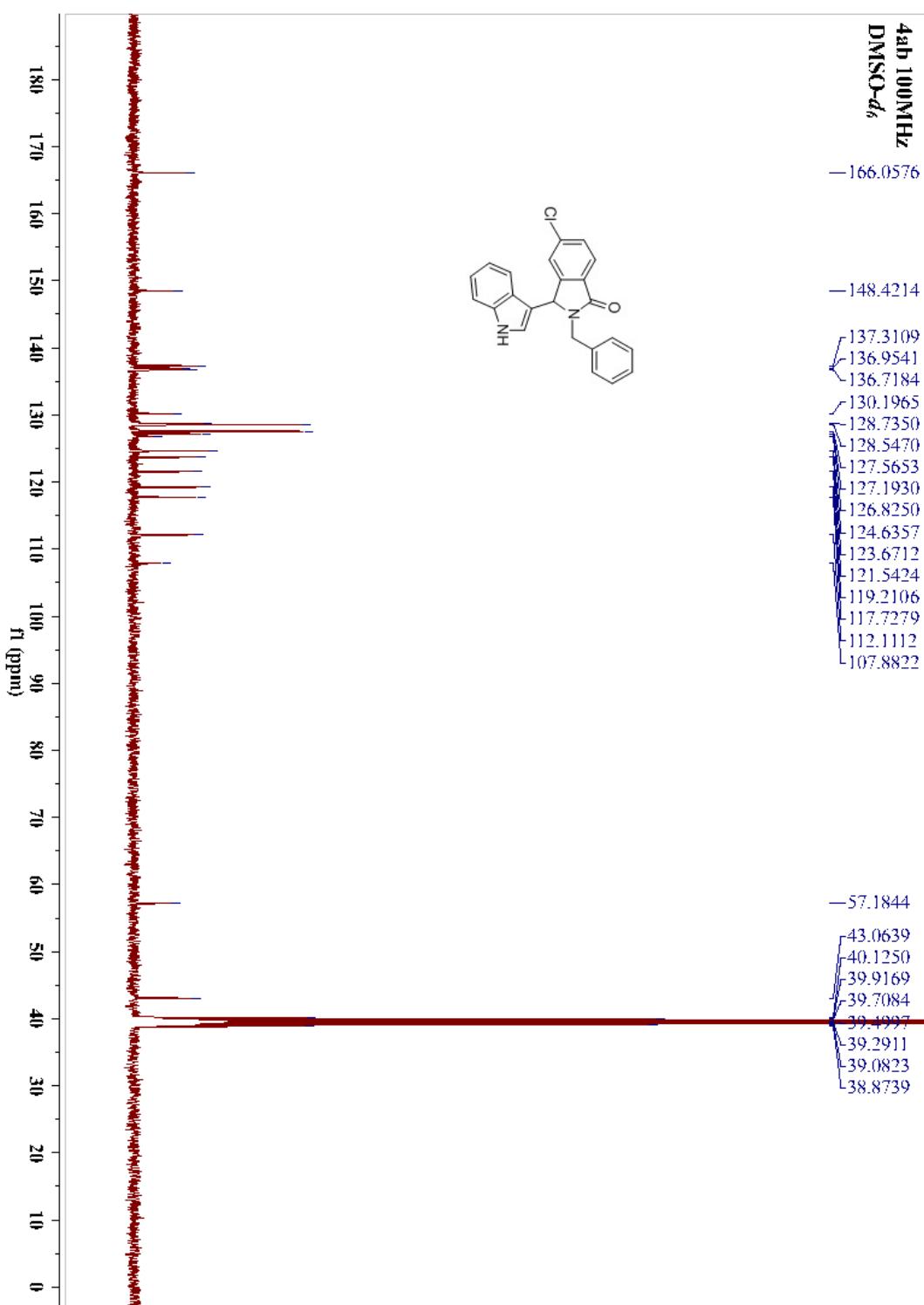
S79. LCMS spectrum of 2-benzyl-5-chloro-3-(1*H*-indol-3-yl)isoindolin-1-one (**4ab**).



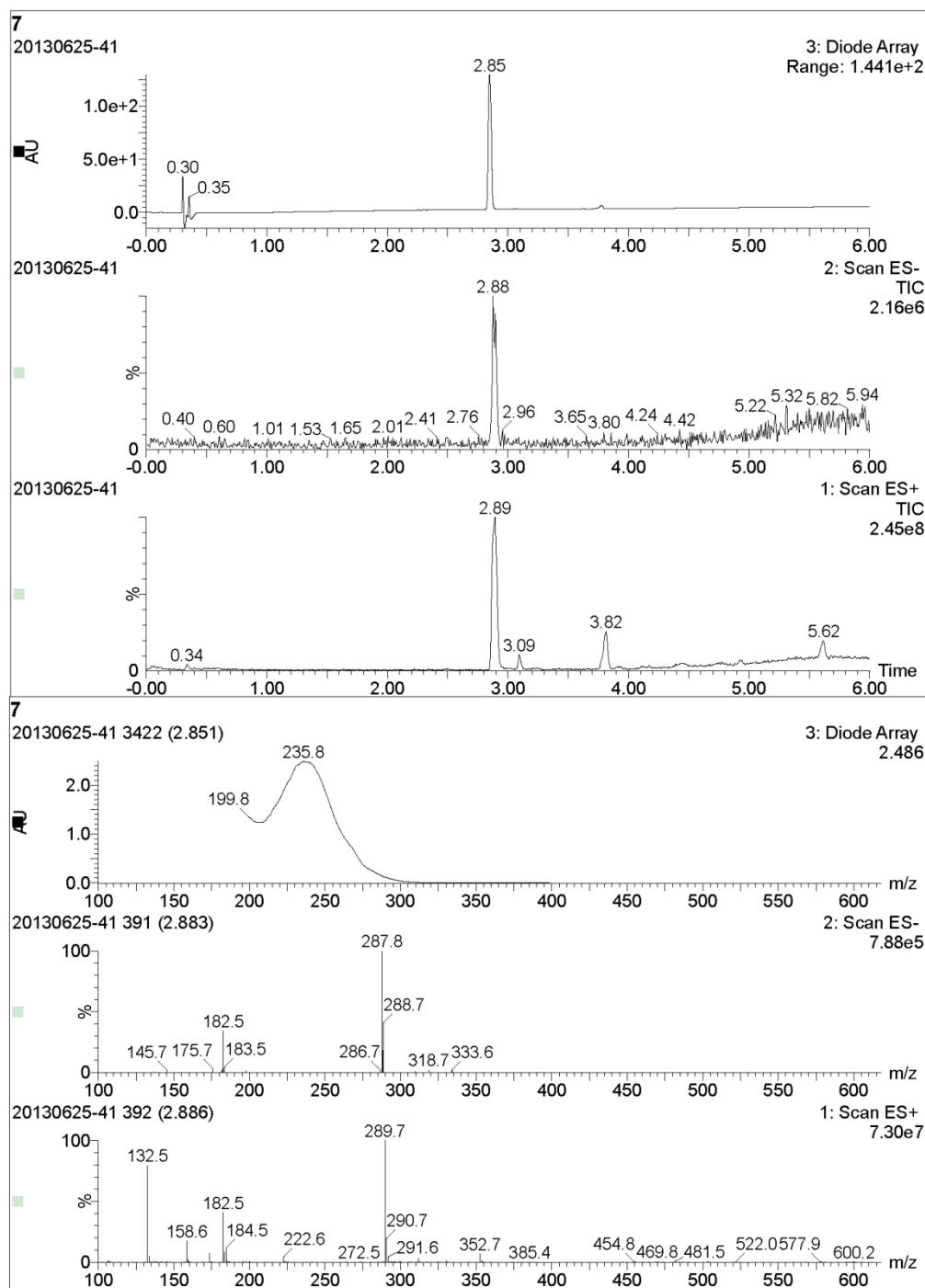
S80. ^1H NMR spectrum of 2-benzyl-5-chloro-3-(1*H*-indol-3-yl)isoindolin-1-one (**4ab**) in $\text{DMSO}-d_6$.



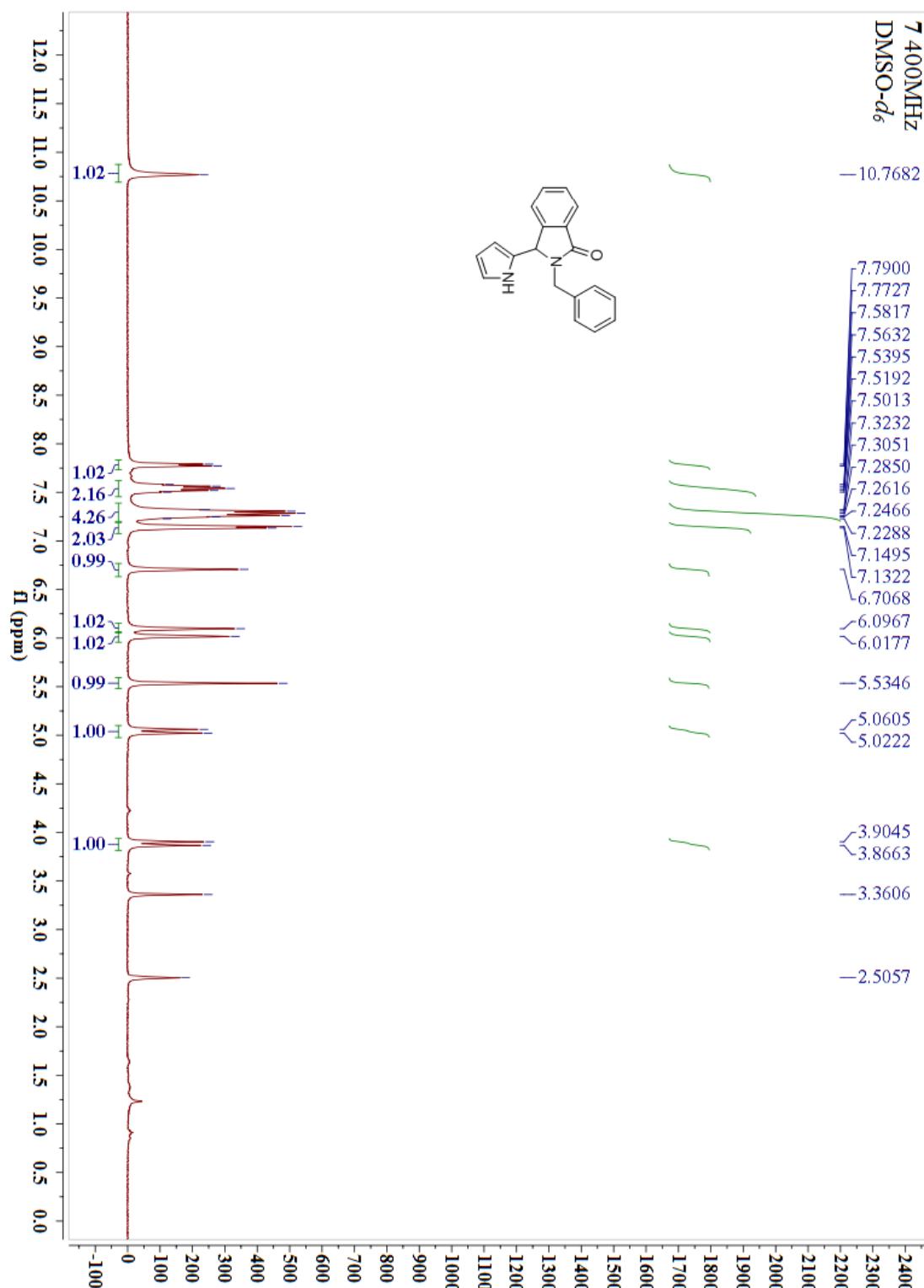
S81. ^{13}C NMR spectrum of 2-benzyl-5-chloro-3-(1*H*-indol-3-yl)isoindolin-1-one (**4ab**) in $\text{DMSO}-d_6$.



S82. LCMS spectrum of 2-benzyl-3-(1*H*-pyrrol-2-yl)isoindolin-1-one (**7**).



S83. ^1H NMR spectrum of 2-benzyl-3-(1*H*-pyrrol-2-yl)isoindolin-1-one (**7**) in DMSO-*d*₆.



S84. ^{13}C NMR spectrum of 2-benzyl-3-(1*H*-pyrrol-2-yl)isoindolin-1-one (**7**) in $\text{DMSO}-d_6$.

