

Supporting Information

Thiamine hydrochloride (VB₁): an efficient promoter for the one-pot synthesis of benzo[4,5]imidazo[1,2-*a*]pyrimidine and [1,2,4]triazolo[1,5-*a*]pyrimidine derivatives in water medium

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S1.	LCMS	spectrum	of	ethyl	
2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimidine-3-carboxylate (5a).					8
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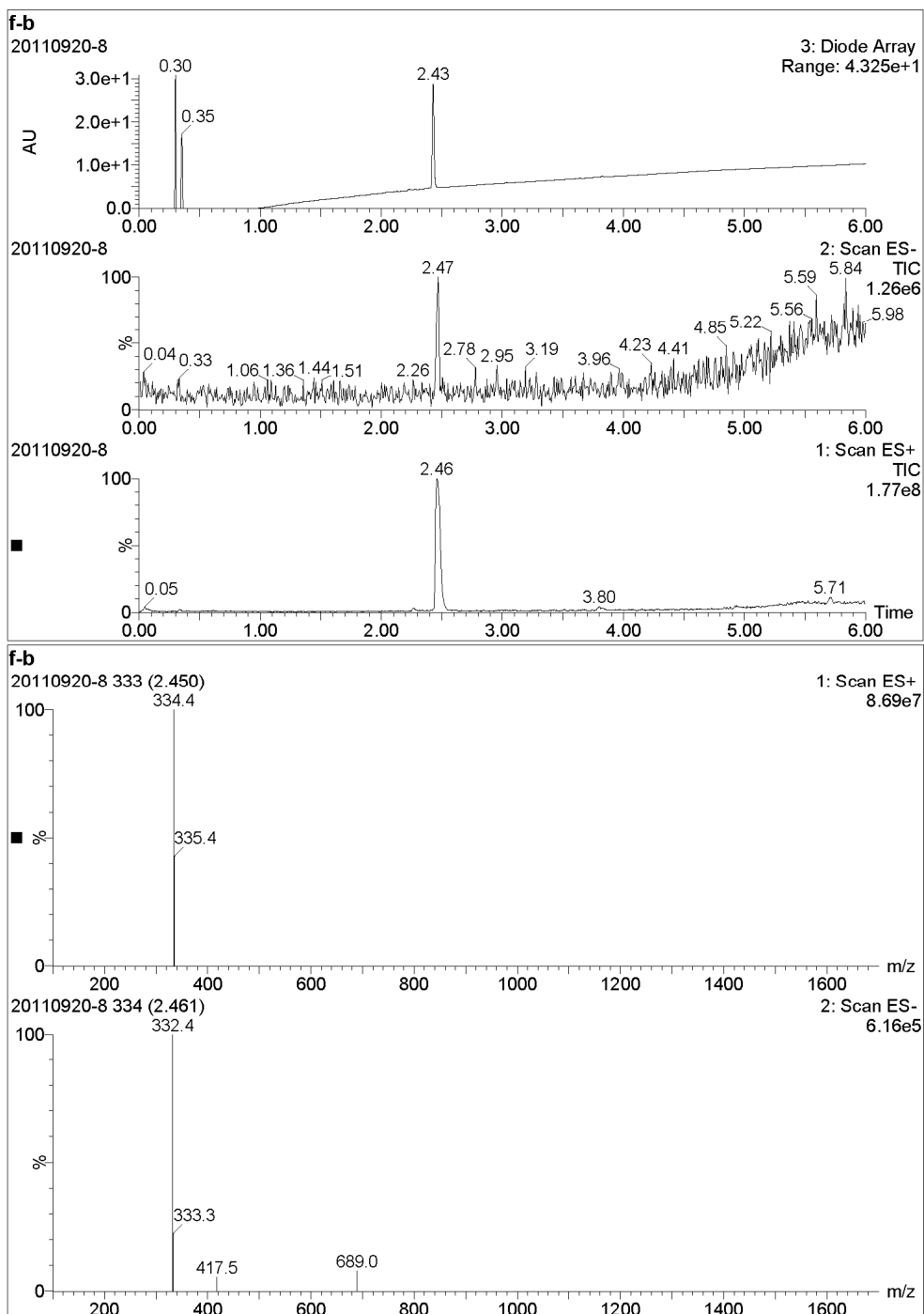
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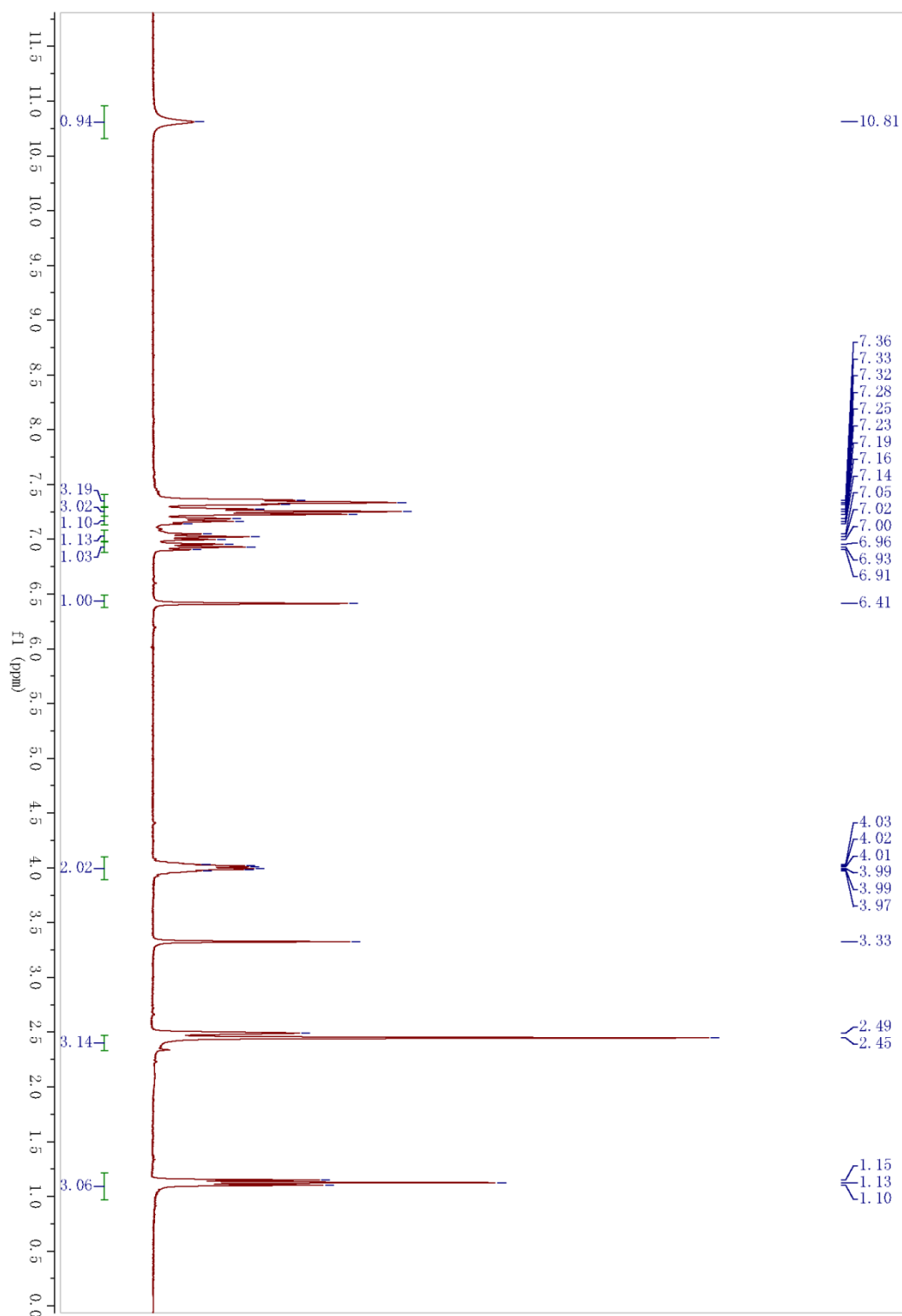
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7-(3,4-dimethoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5- <i>a</i>]pyrimidine-6-carboxylate (6d) in DMSO- <i>d</i> ₆ .						76

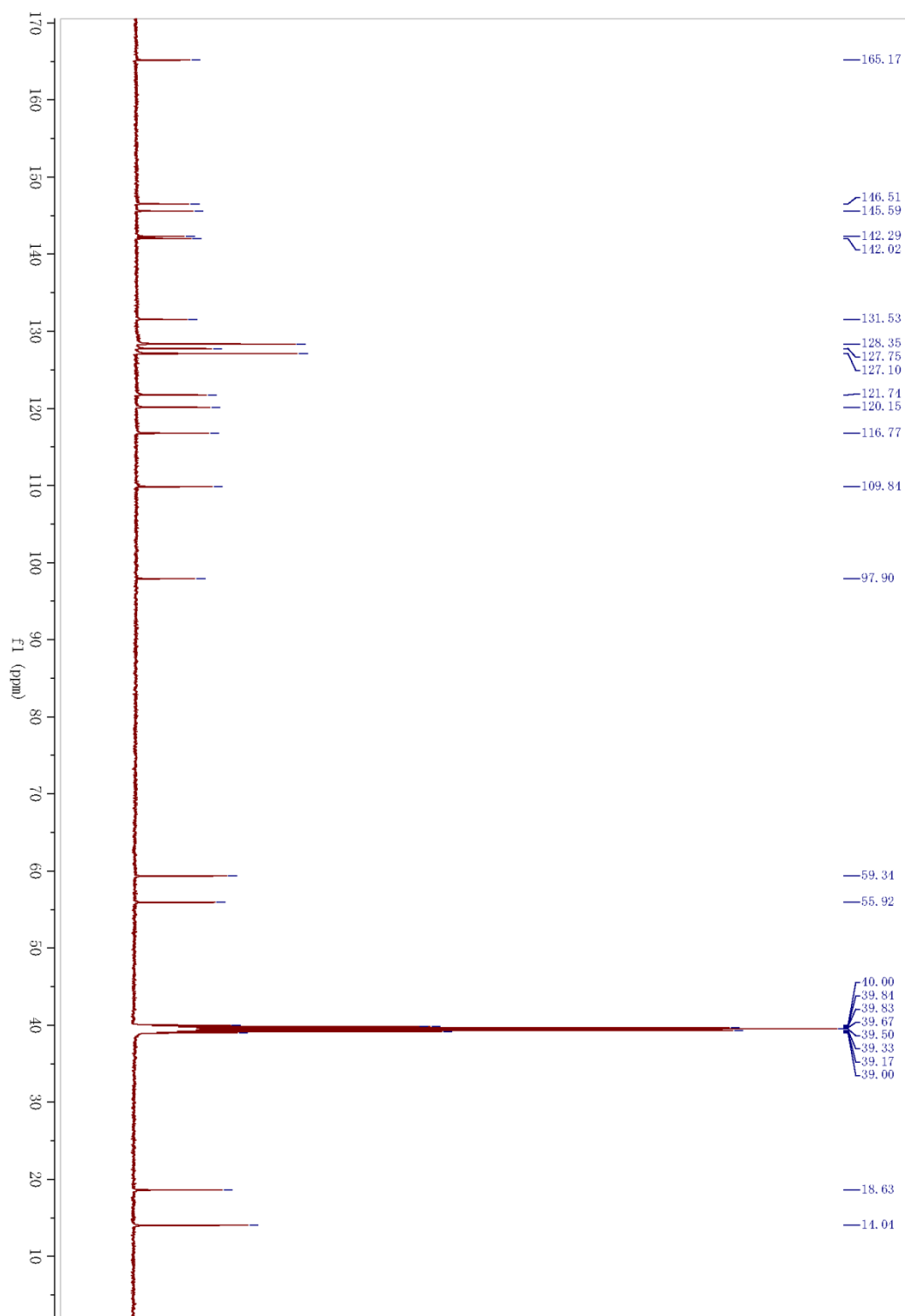
S1. LCMS spectrum of ethyl
2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5a**).



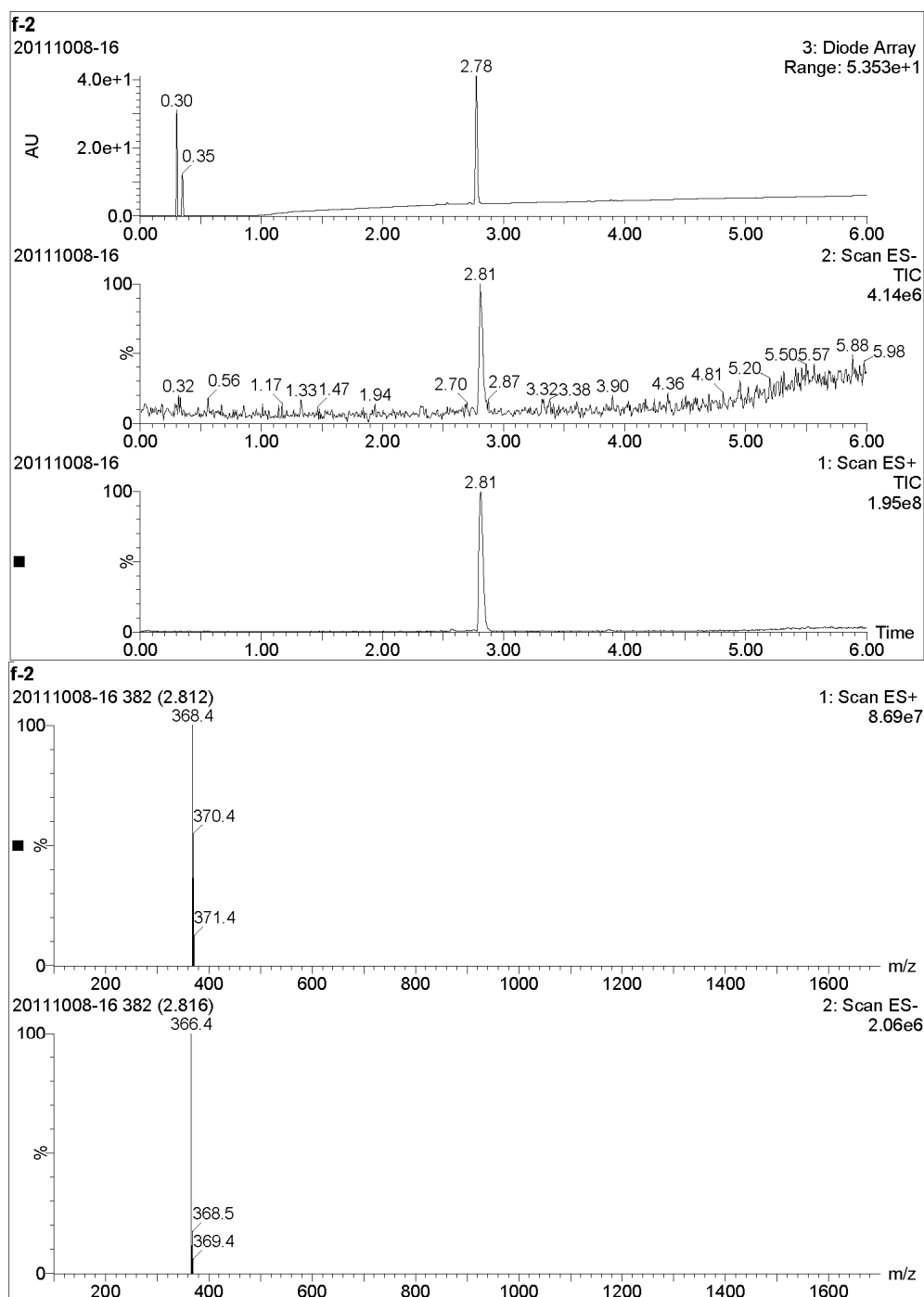
S2. ^1H NMR spectrum of ethyl 2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5a**) in $\text{DMSO-}d_6$.



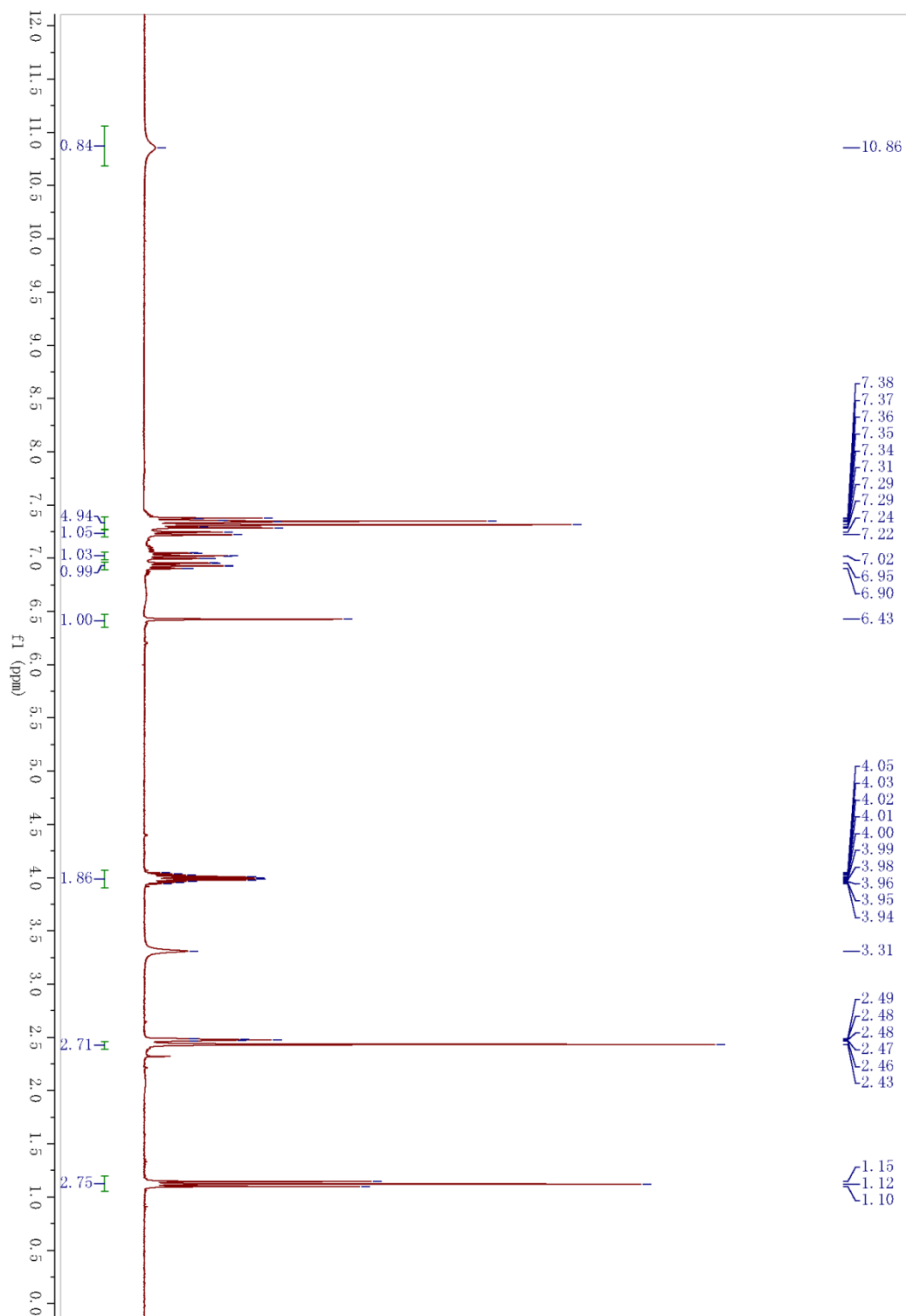
S3. ^{13}C NMR spectrum of ethyl 2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5a**) in DMSO- d_6 .



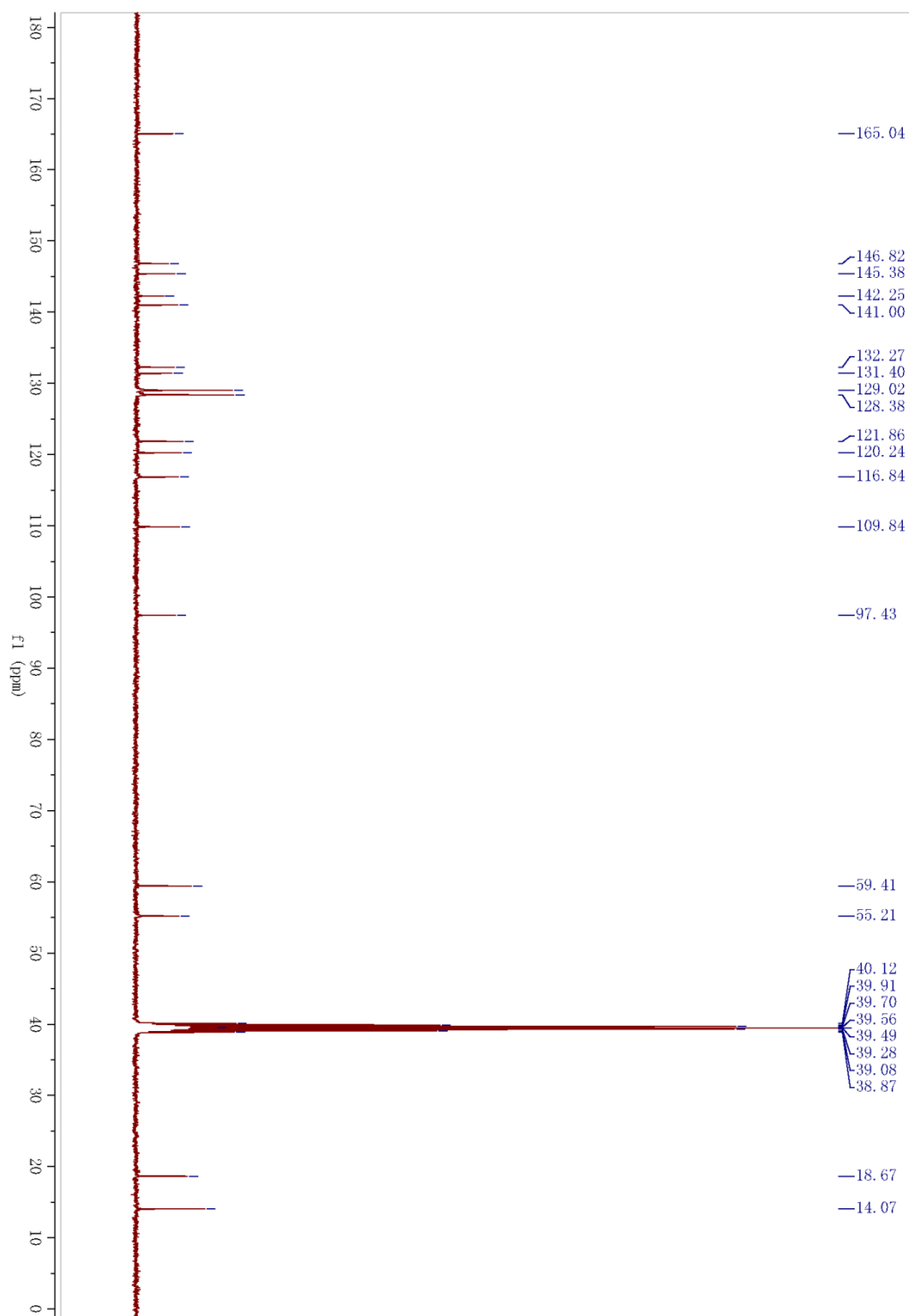
S4. LCMS spectrum of ethyl 4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5b**).



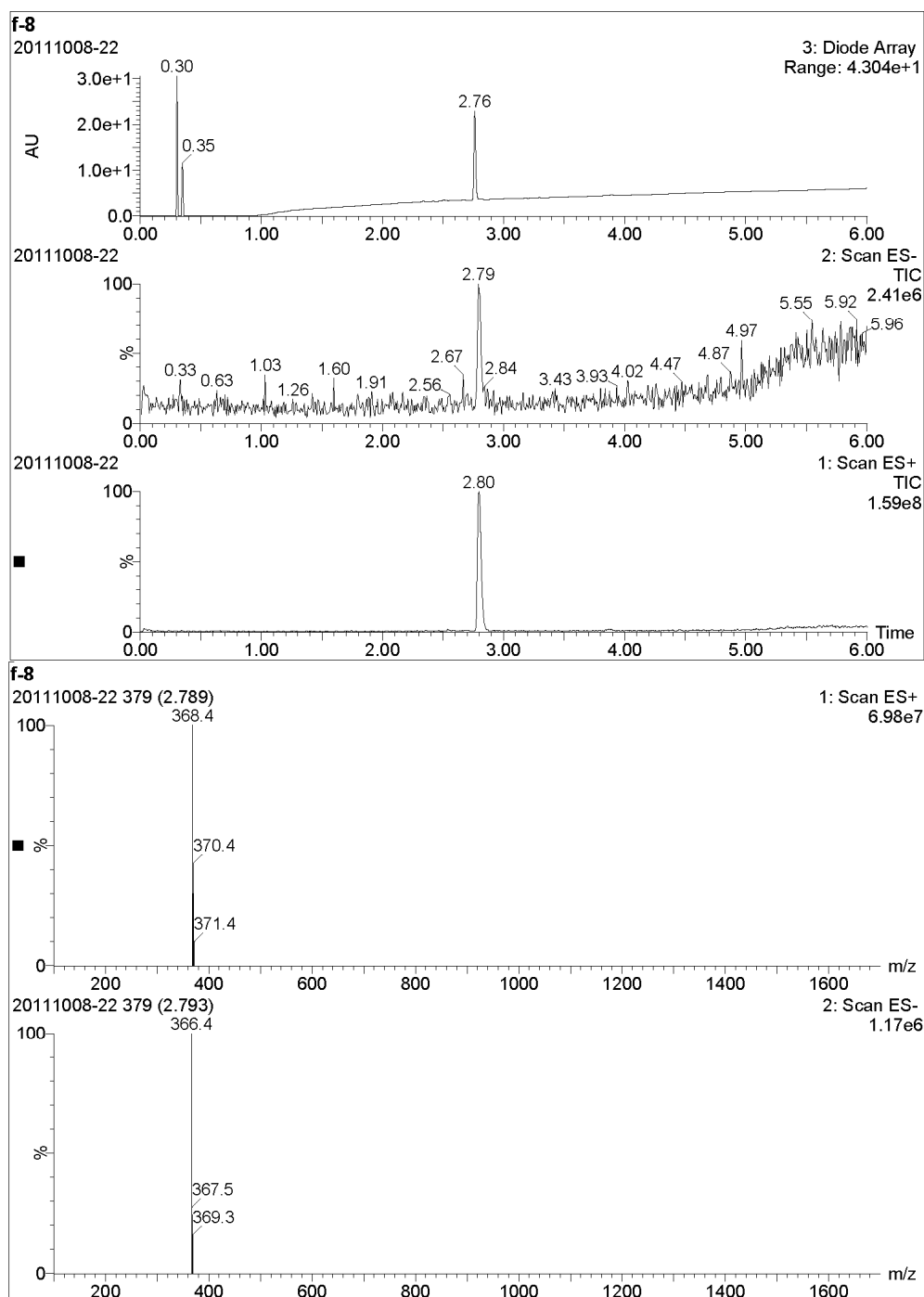
S5. ^1H NMR spectrum of ethyl 4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5b**) in $\text{DMSO-}d_6$.



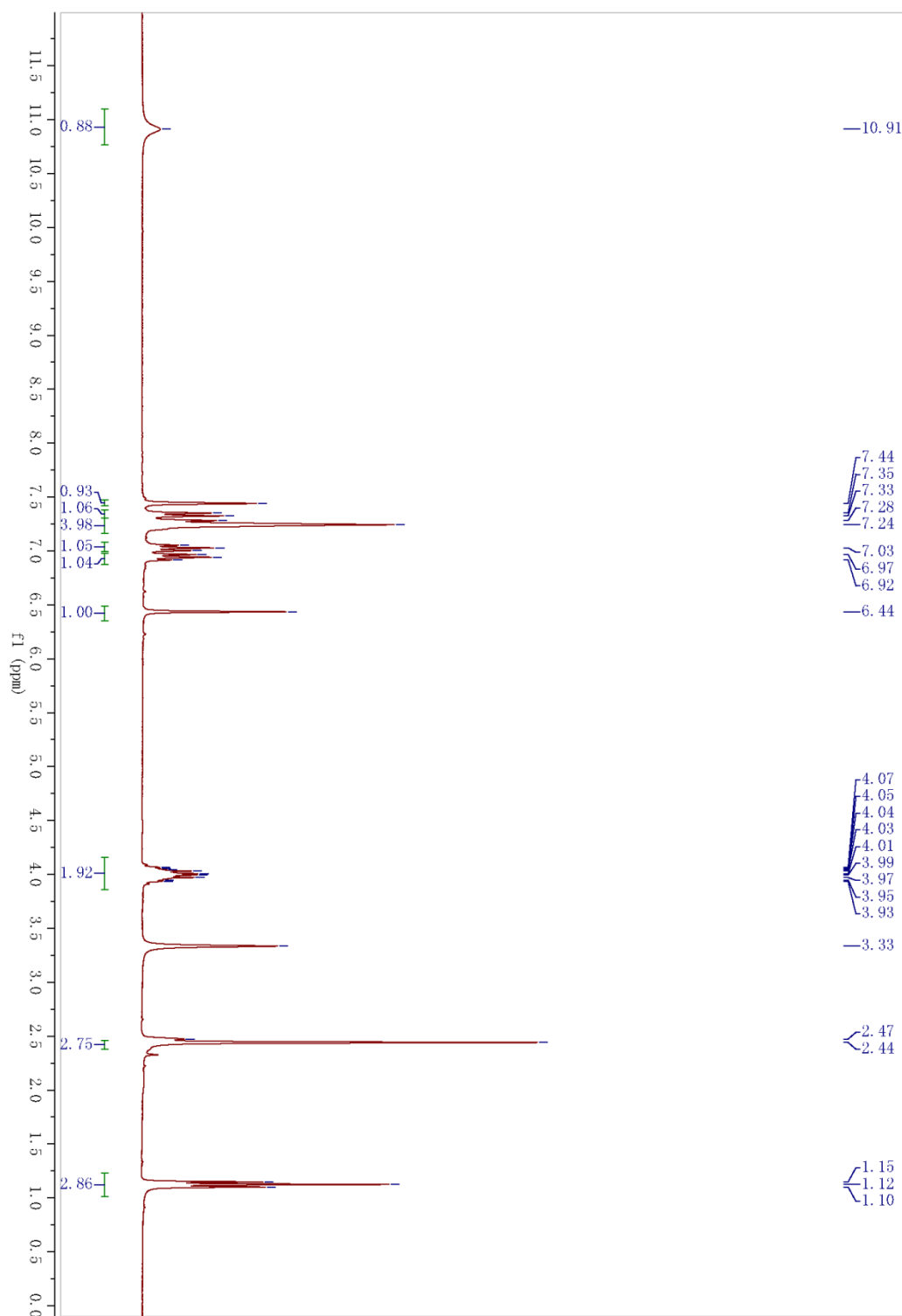
S6. ^{13}C NMR spectrum of ethyl 4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5b**) in $\text{DMSO-}d_6$.



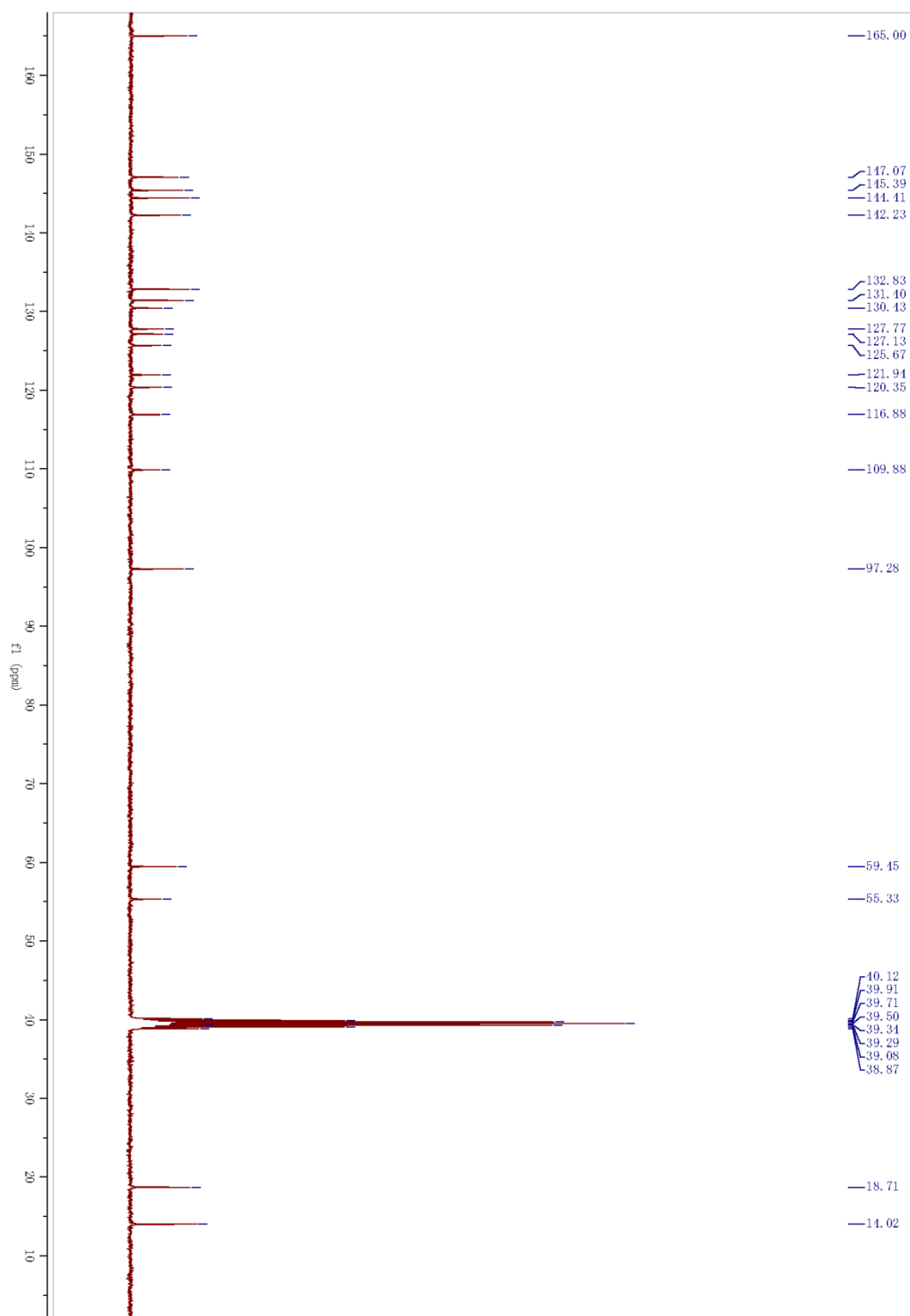
S7. LCMS spectrum of ethyl 4-(3-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5c**).



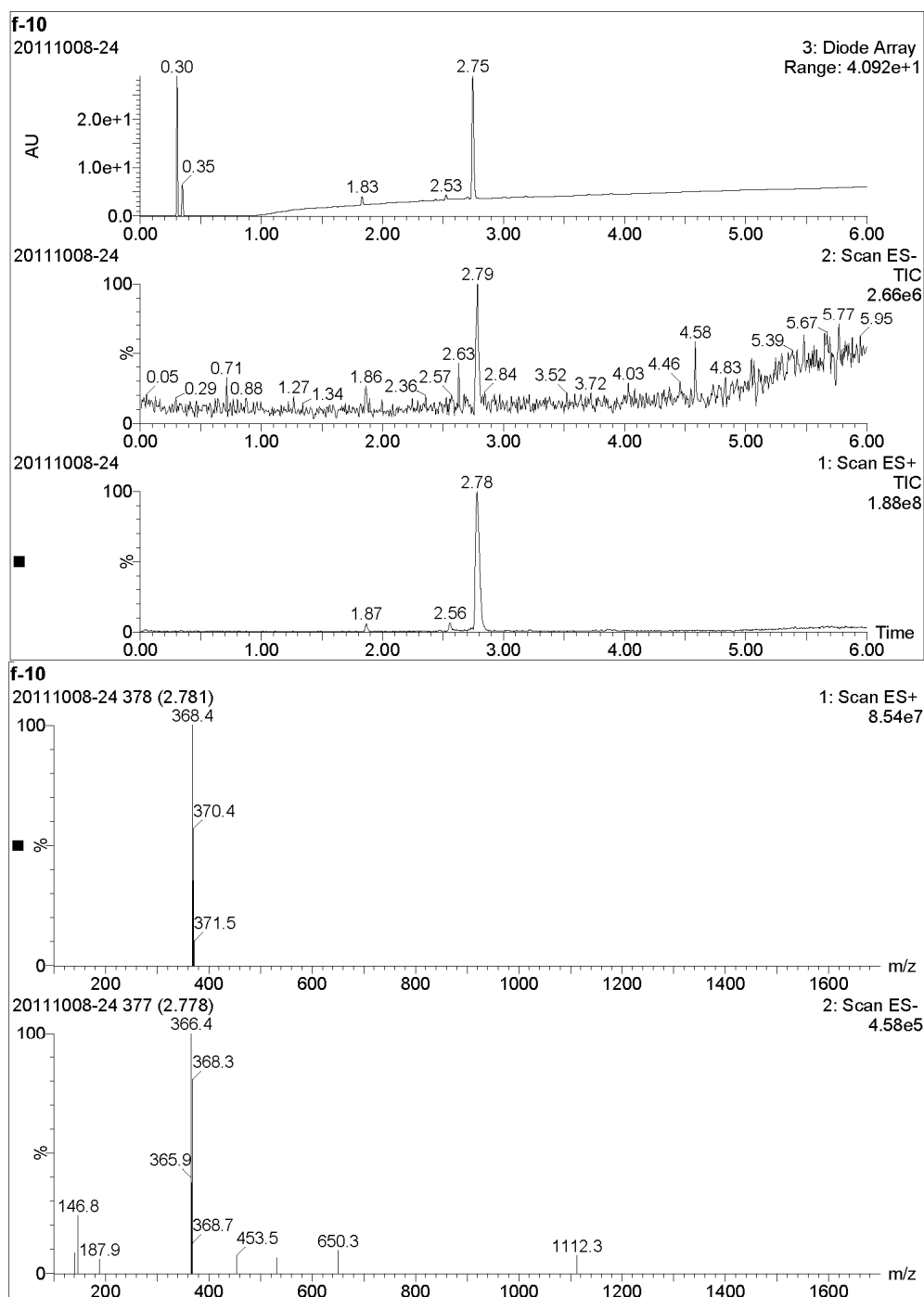
S8. ^1H NMR spectrum of ethyl 4-(3-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5c**) in $\text{DMSO-}d_6$.



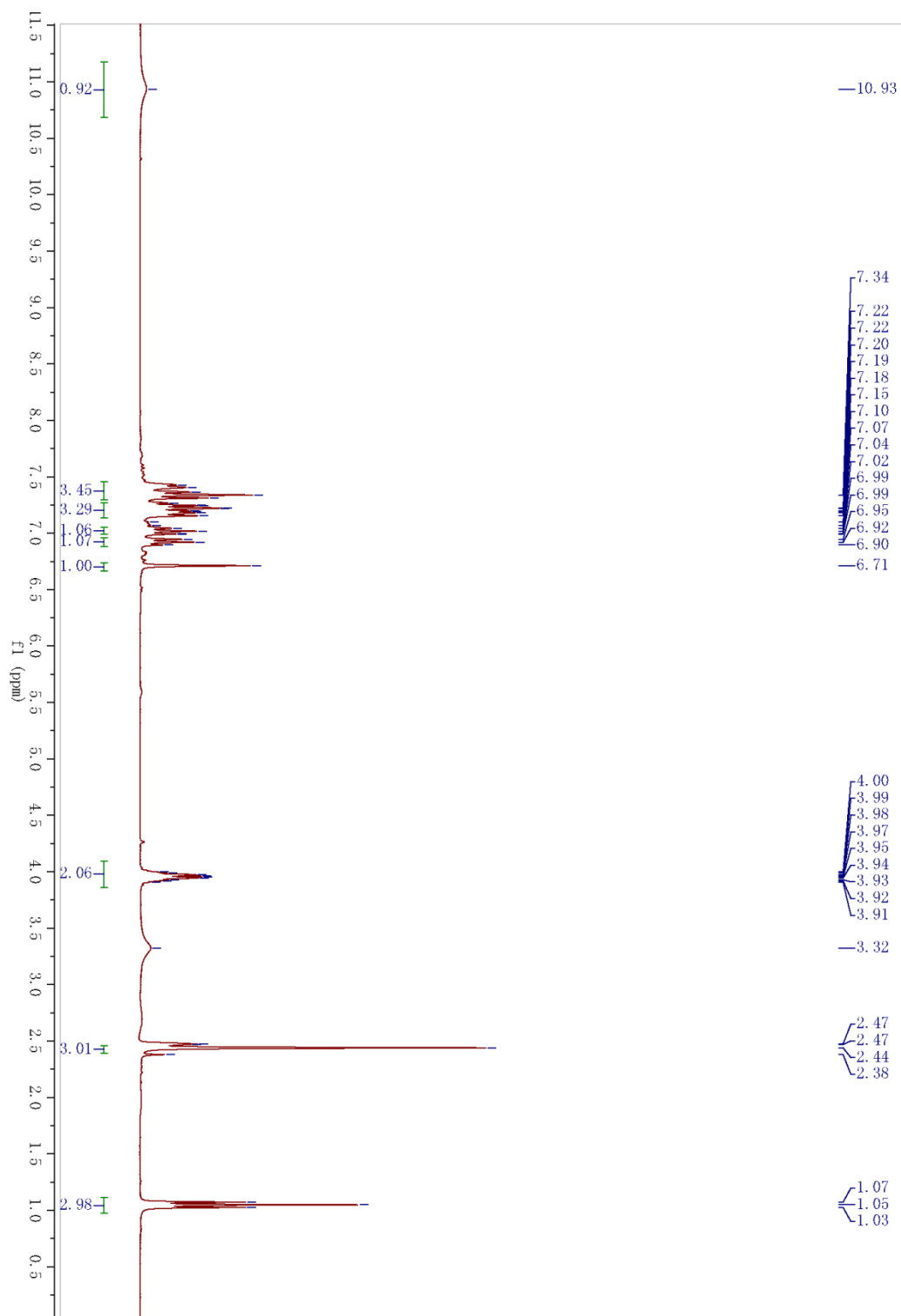
S9. ^{13}C NMR spectrum of ethyl 4-(3-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5c**) in $\text{DMSO-}d_6$.



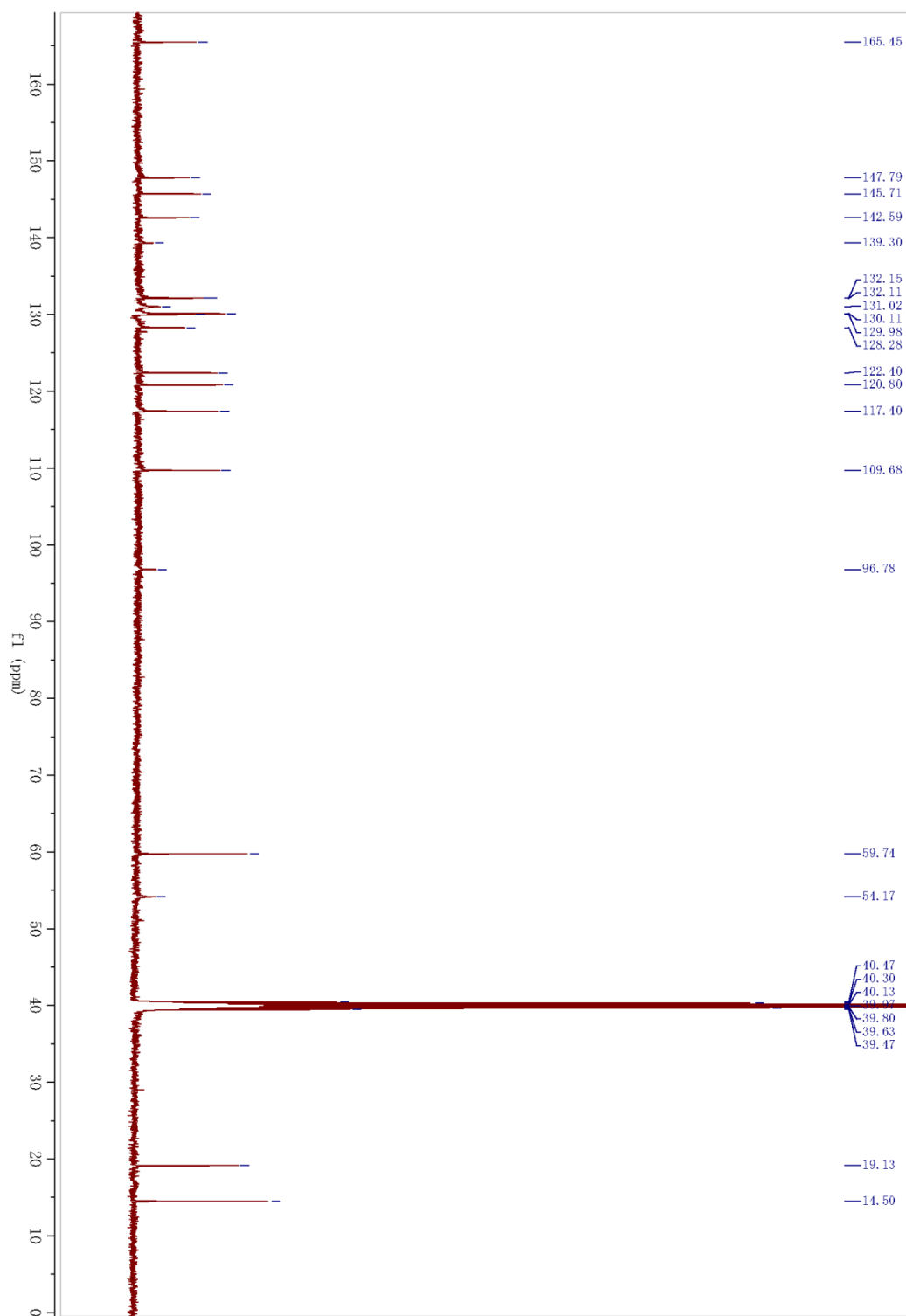
S10. LCMS spectrum of ethyl 4-(2-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5d**).



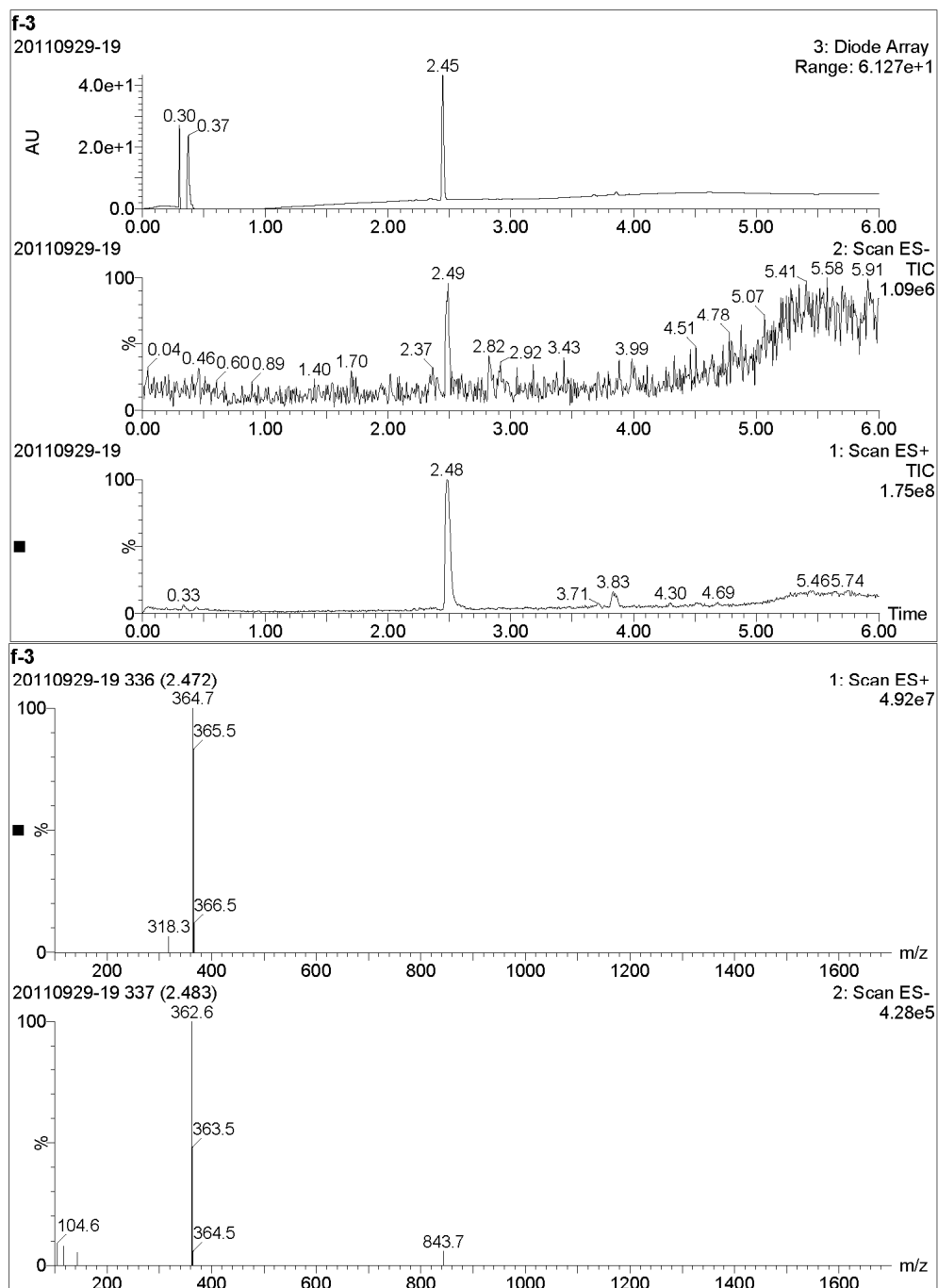
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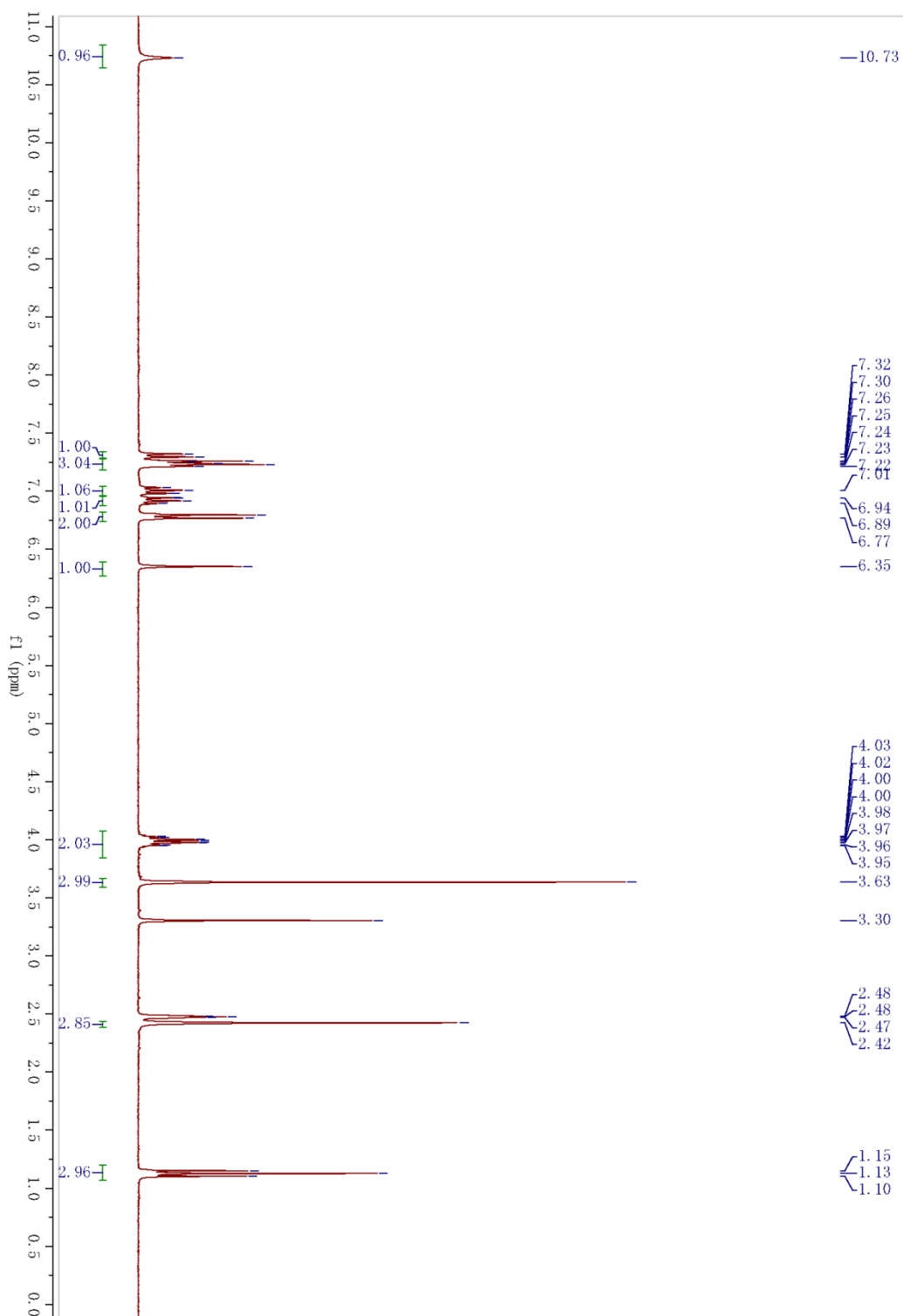
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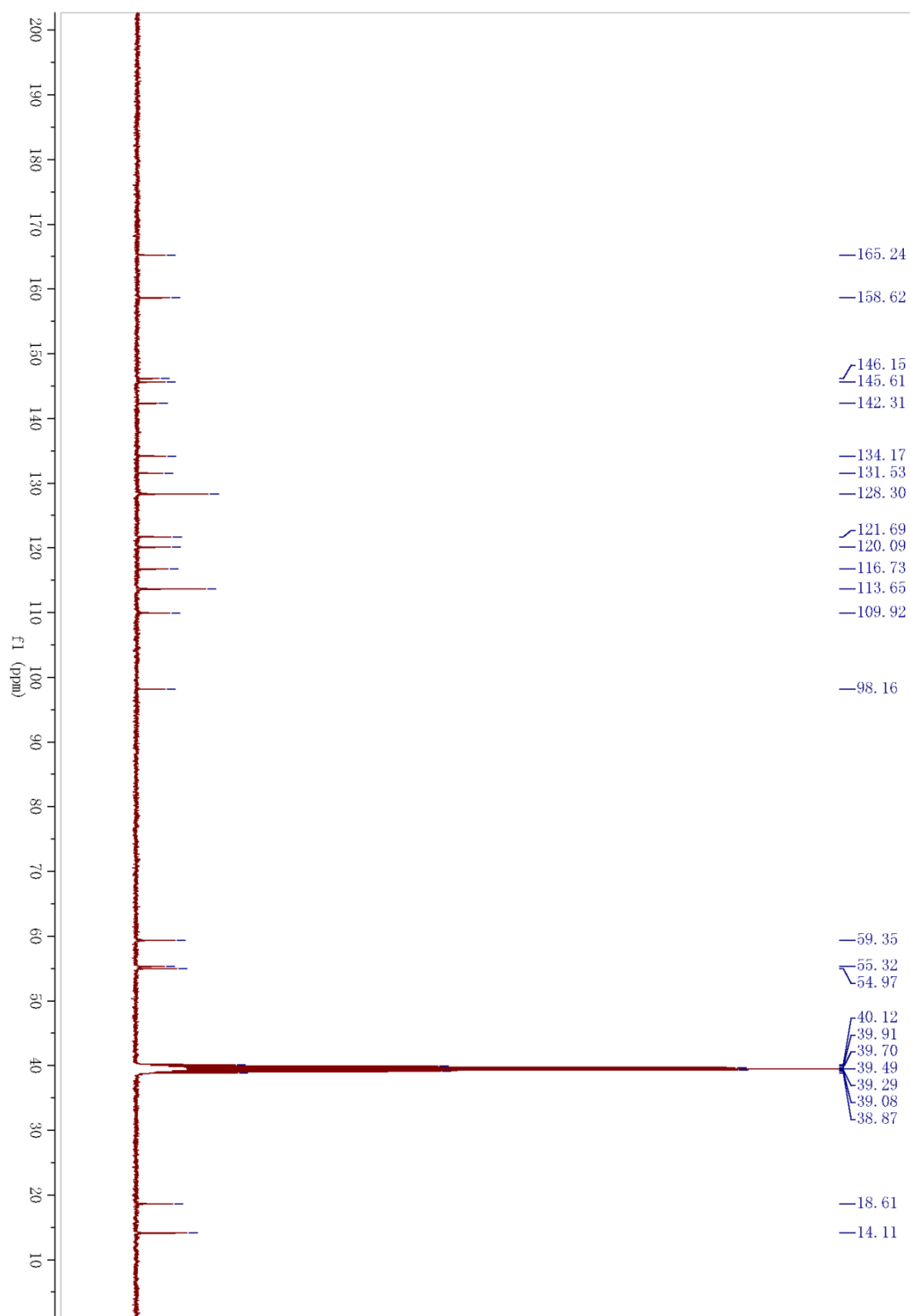
S13. LCMS spectrum of ethyl 4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5e**).



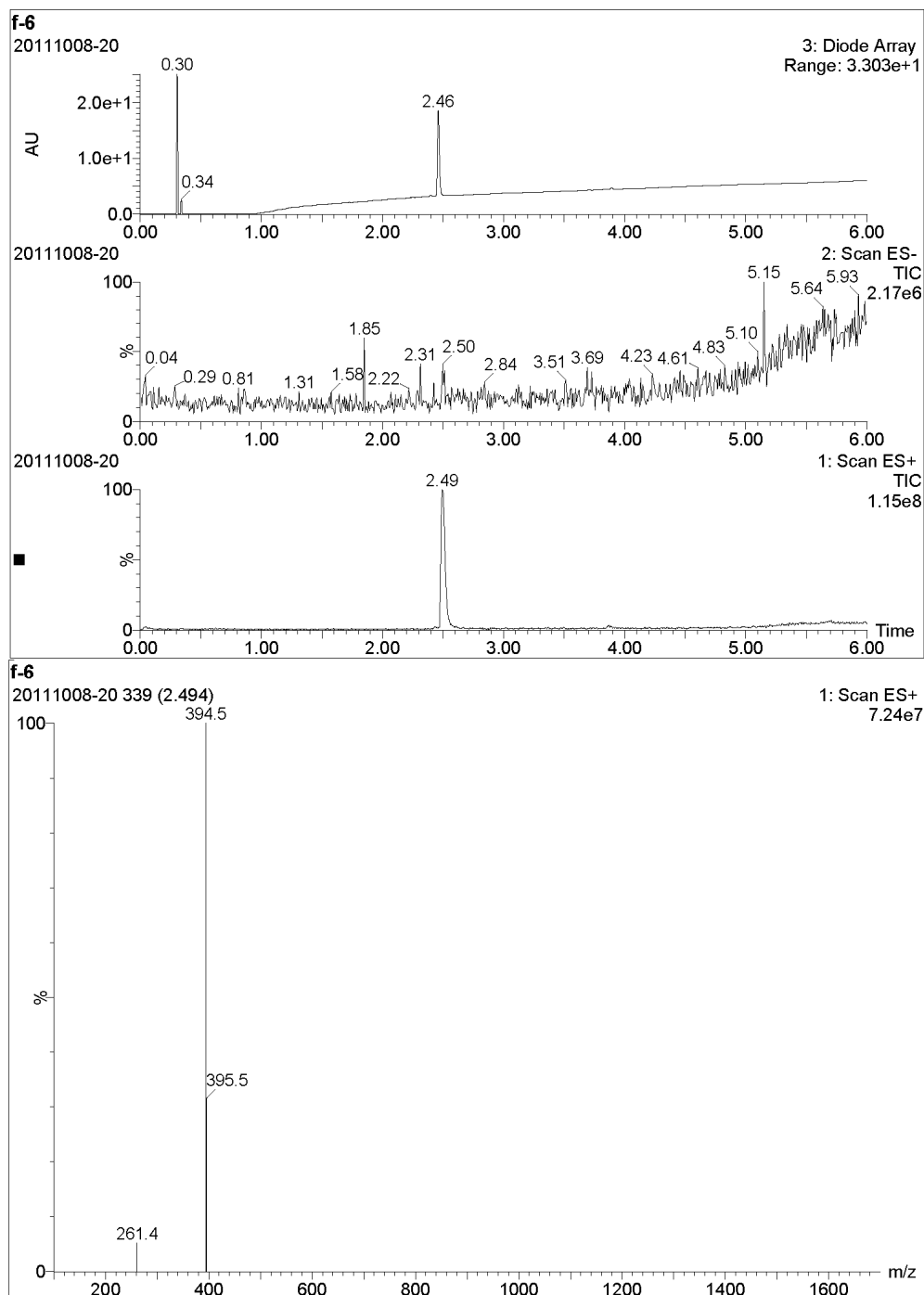
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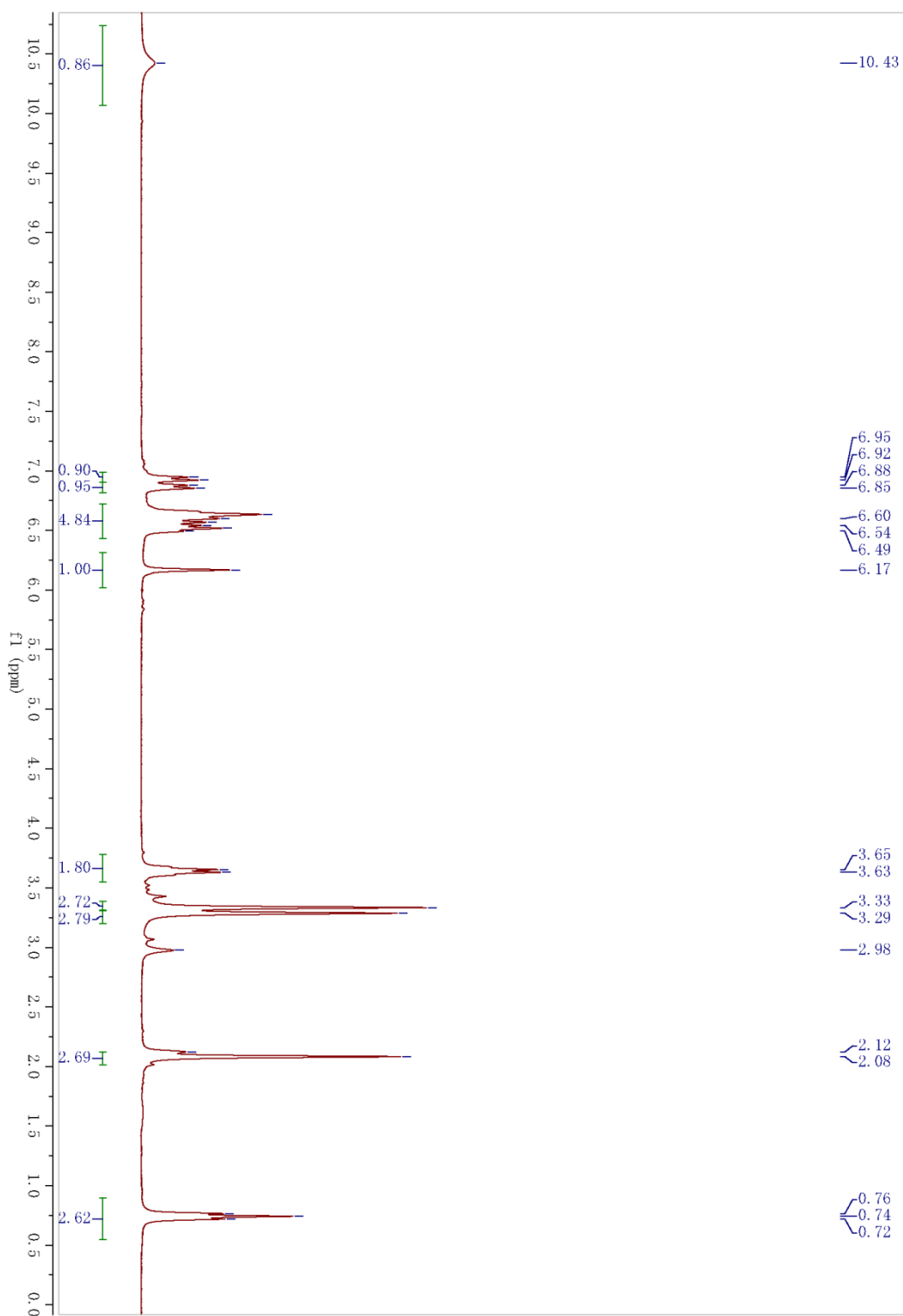
S15. ^{13}C NMR spectrum of ethyl 4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5e**) in $\text{DMSO-}d_6$.



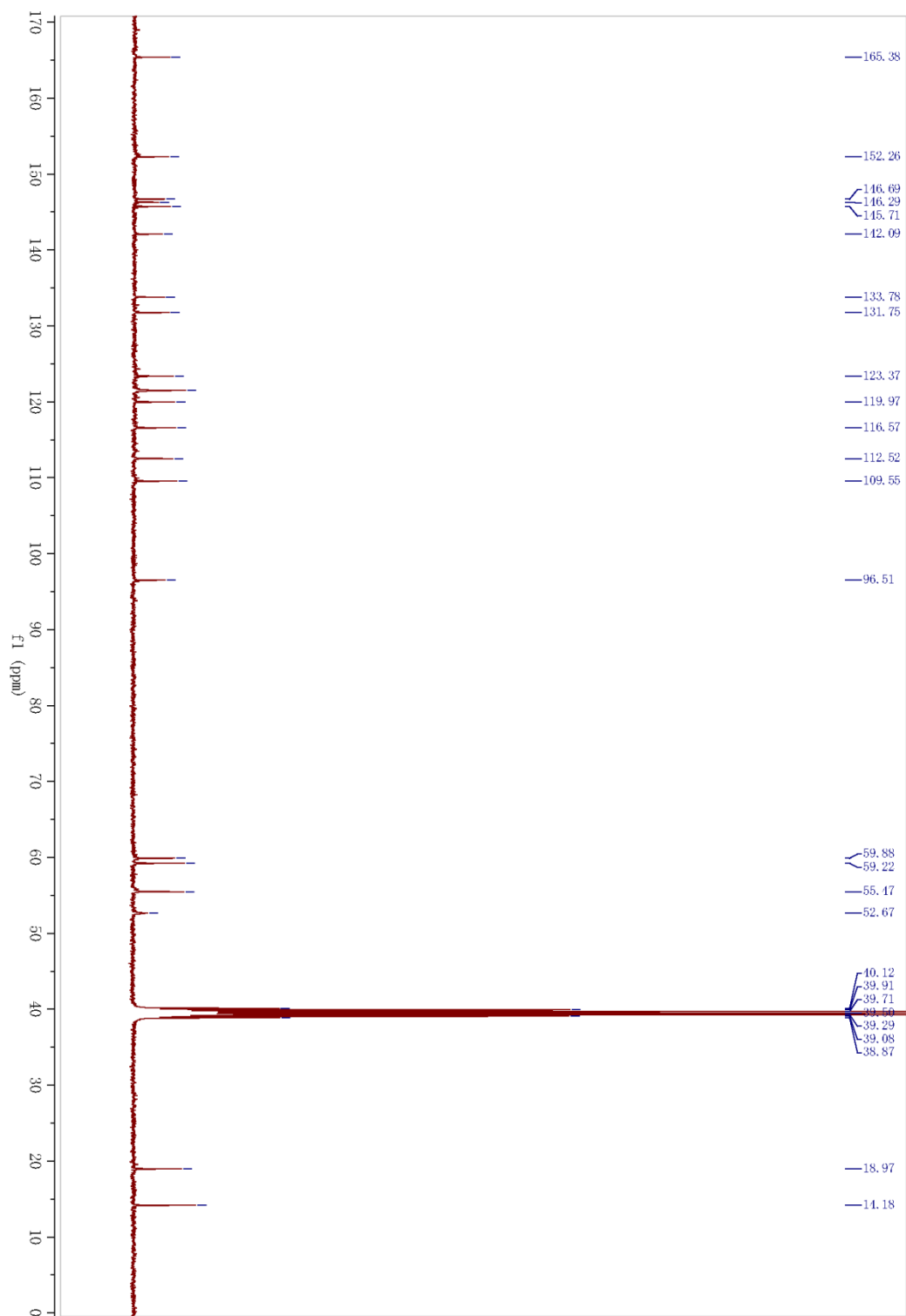
S16. LCMS spectrum of ethyl 4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5f**).



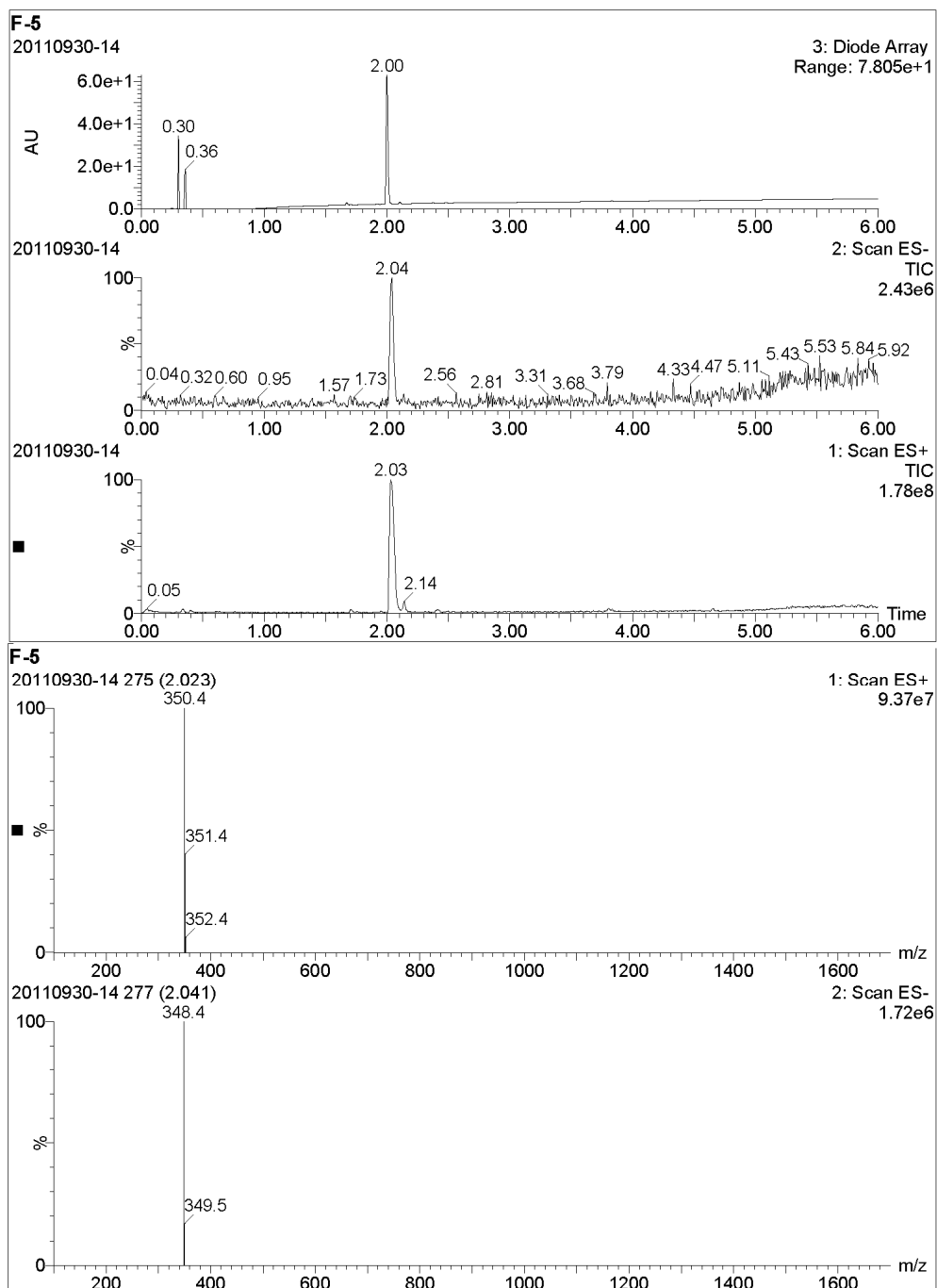
S17. ^1H NMR spectrum of ethyl 4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5f**) in $\text{DMSO-}d_6$.



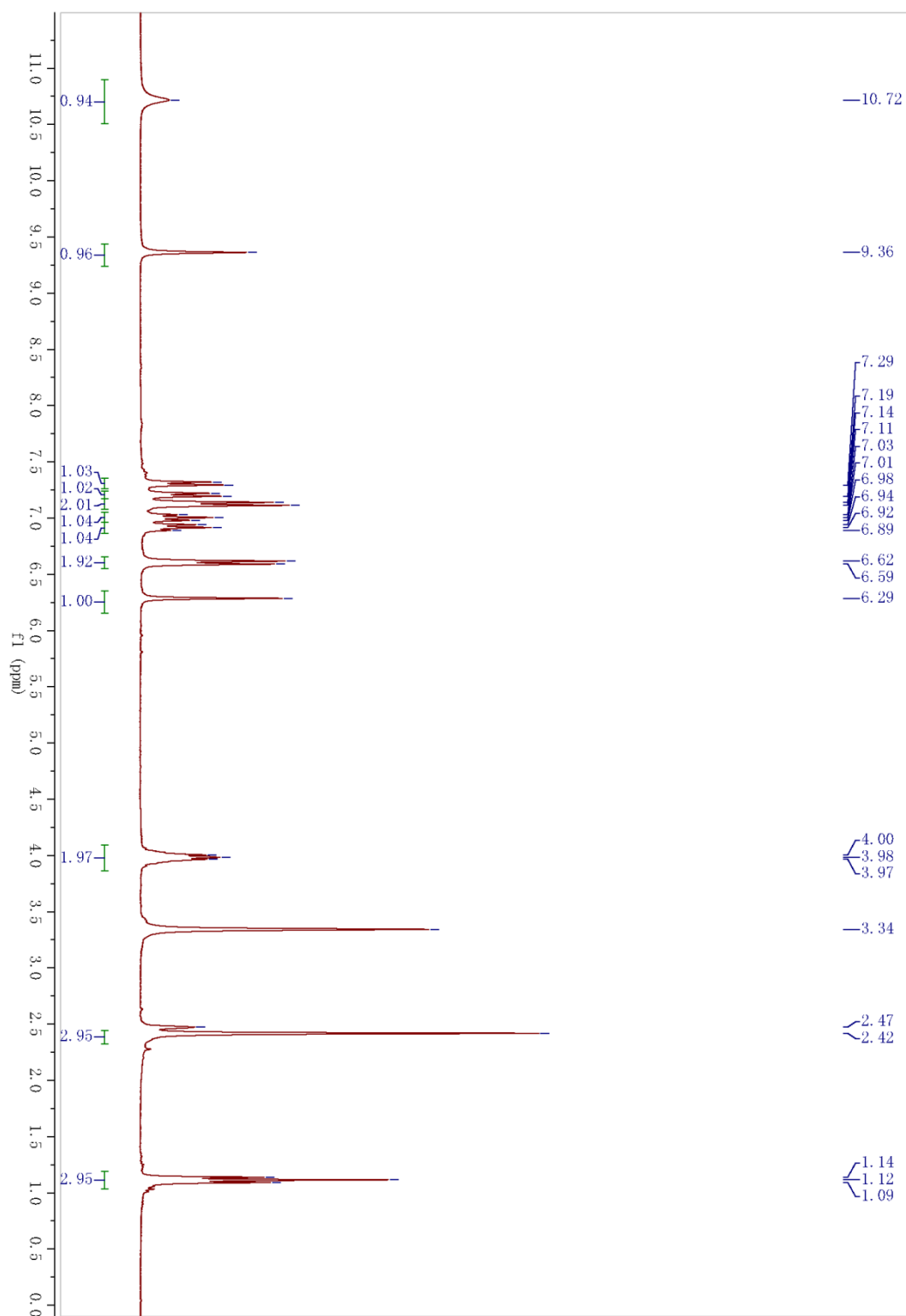
S18. ^{13}C NMR spectrum of ethyl 4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5f**) in $\text{DMSO-}d_6$.



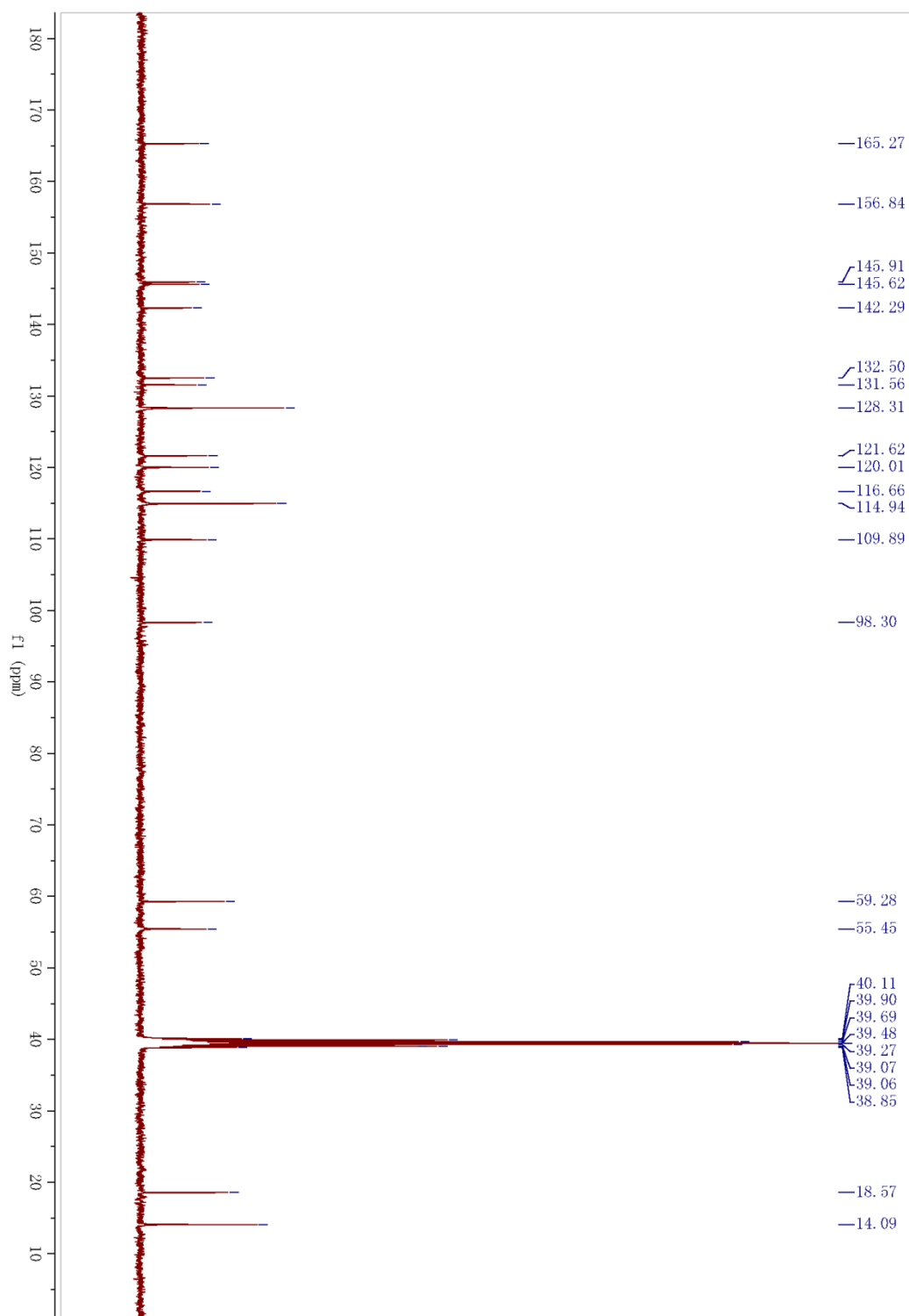
S19. LCMS spectrum of ethyl 4-(4-hydroxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5g**).



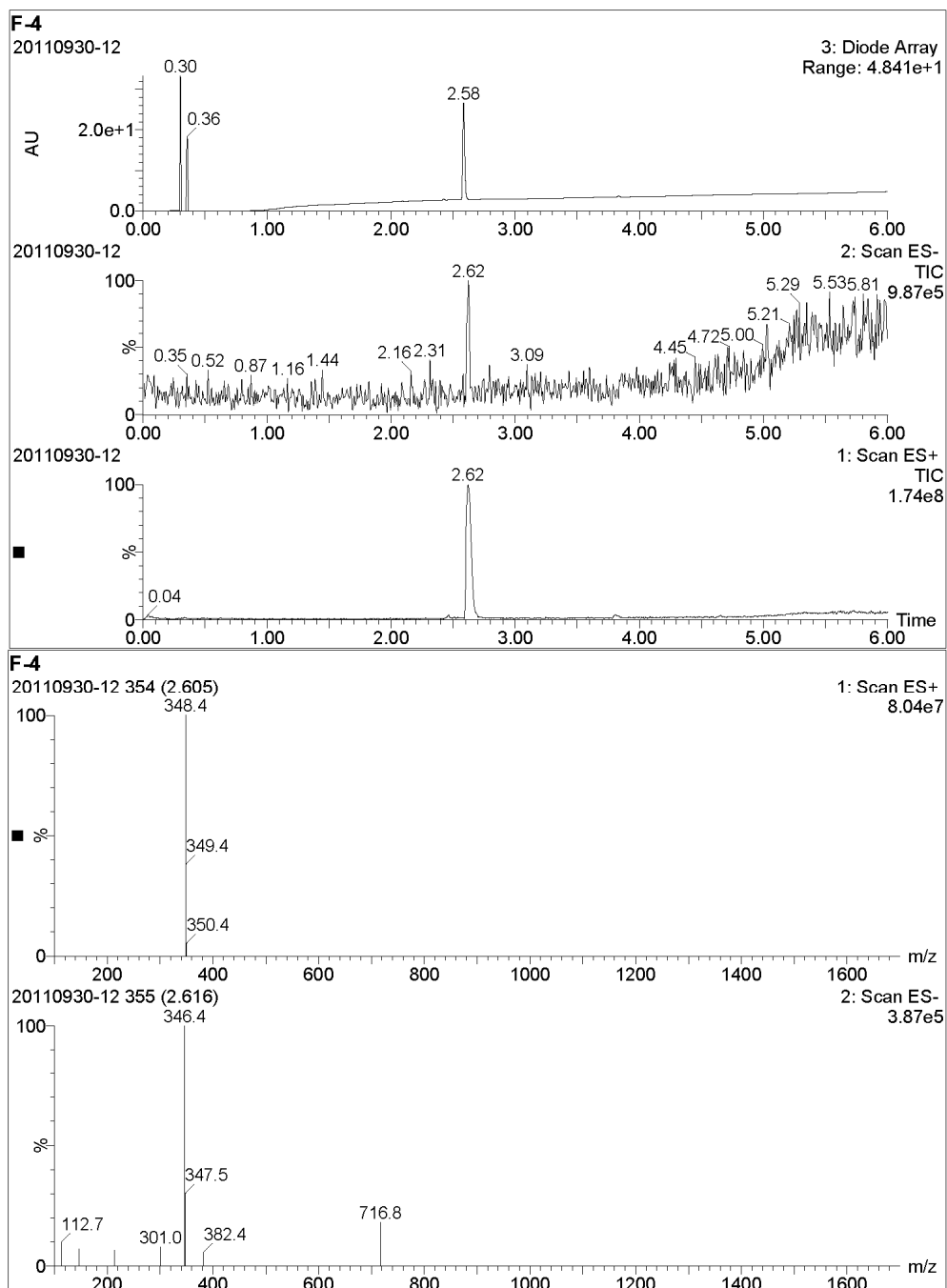
S20. ^1H NMR spectrum of ethyl 4-(4-hydroxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5g**) in $\text{DMSO-}d_6$.



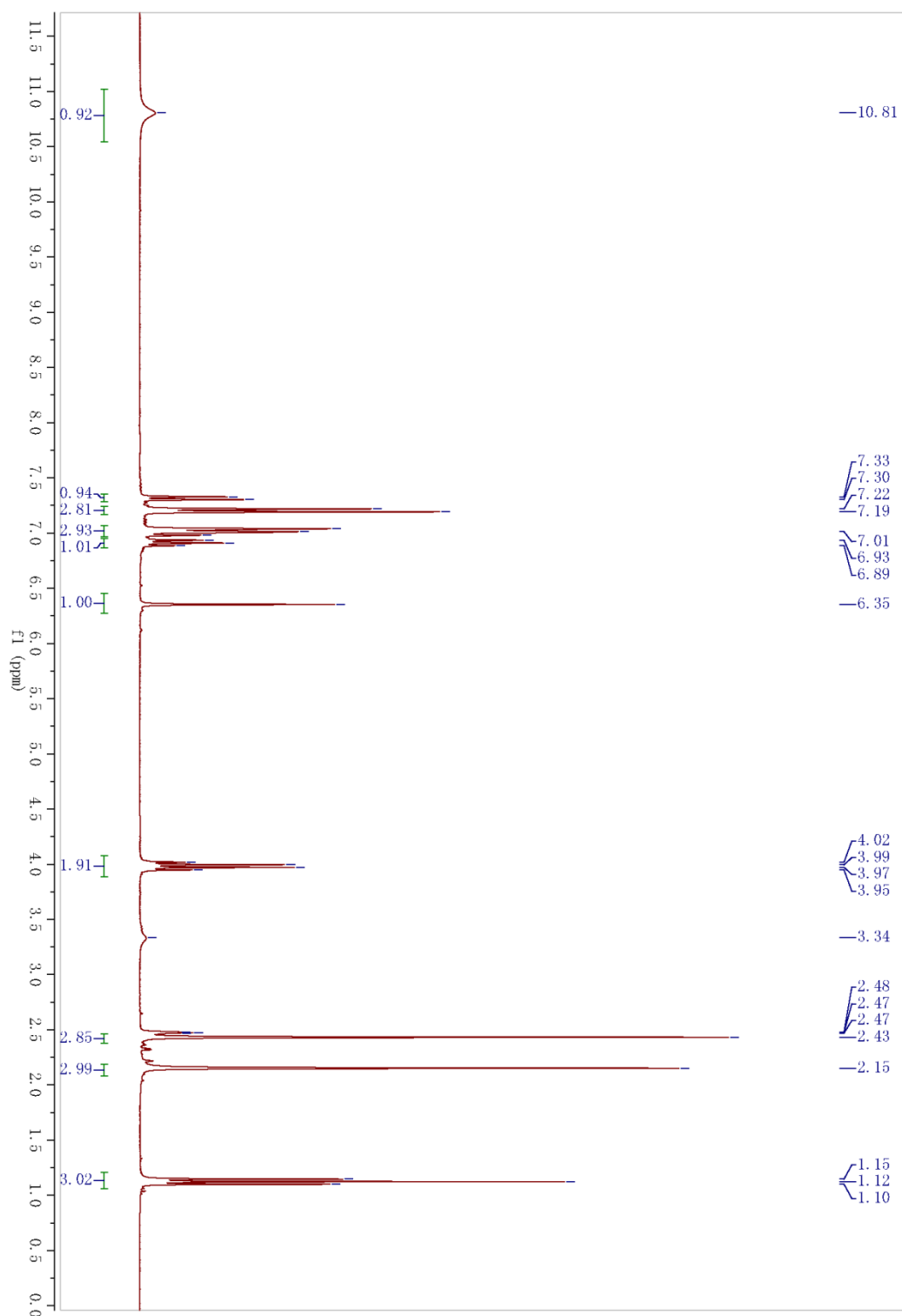
S21. ^{13}C NMR spectrum of ethyl 4-(4-hydroxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5g**) in $\text{DMSO-}d_6$.



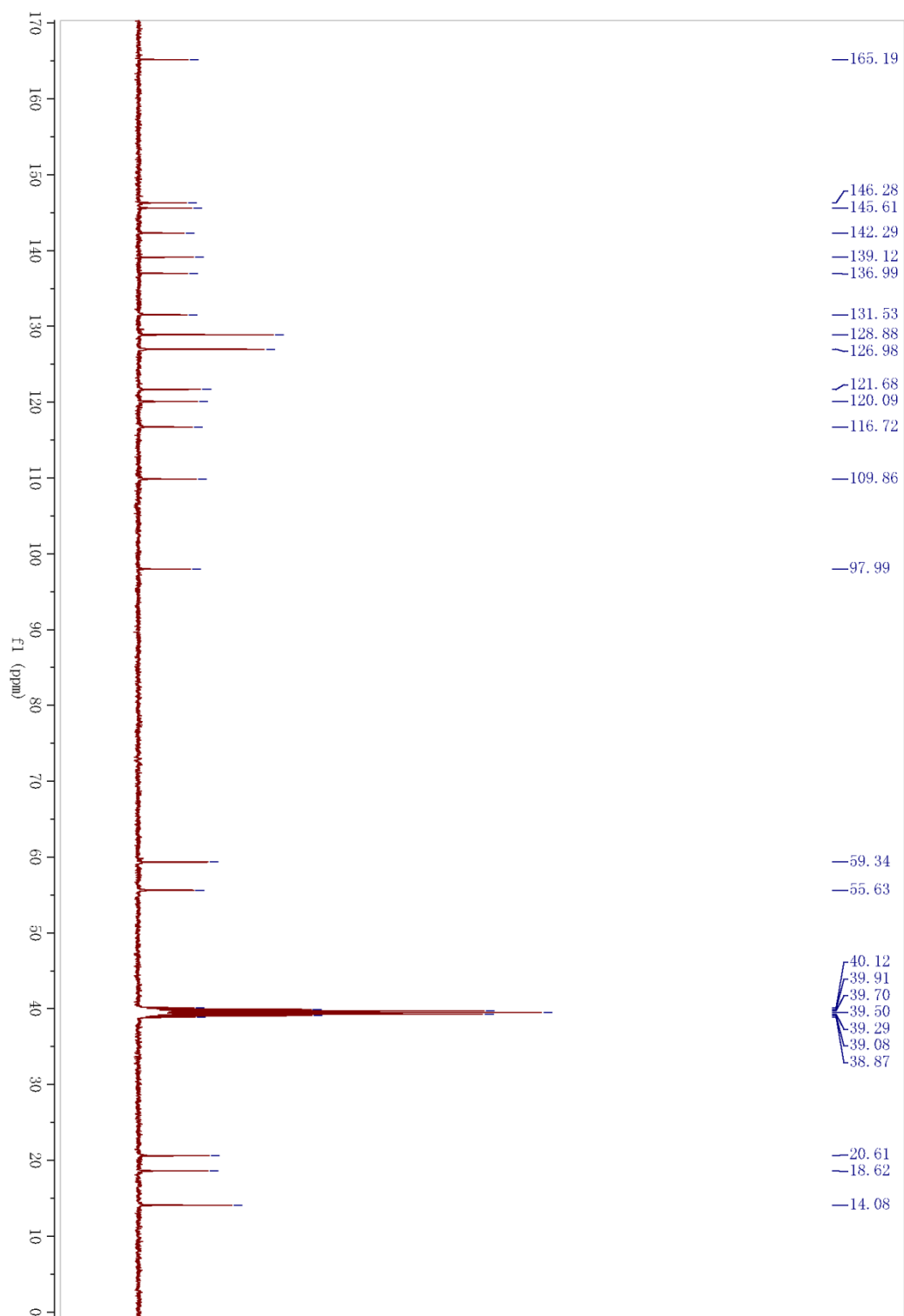
S22. LCMS spectrum of ethyl
2-methyl-4-(p-tolyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5h**).



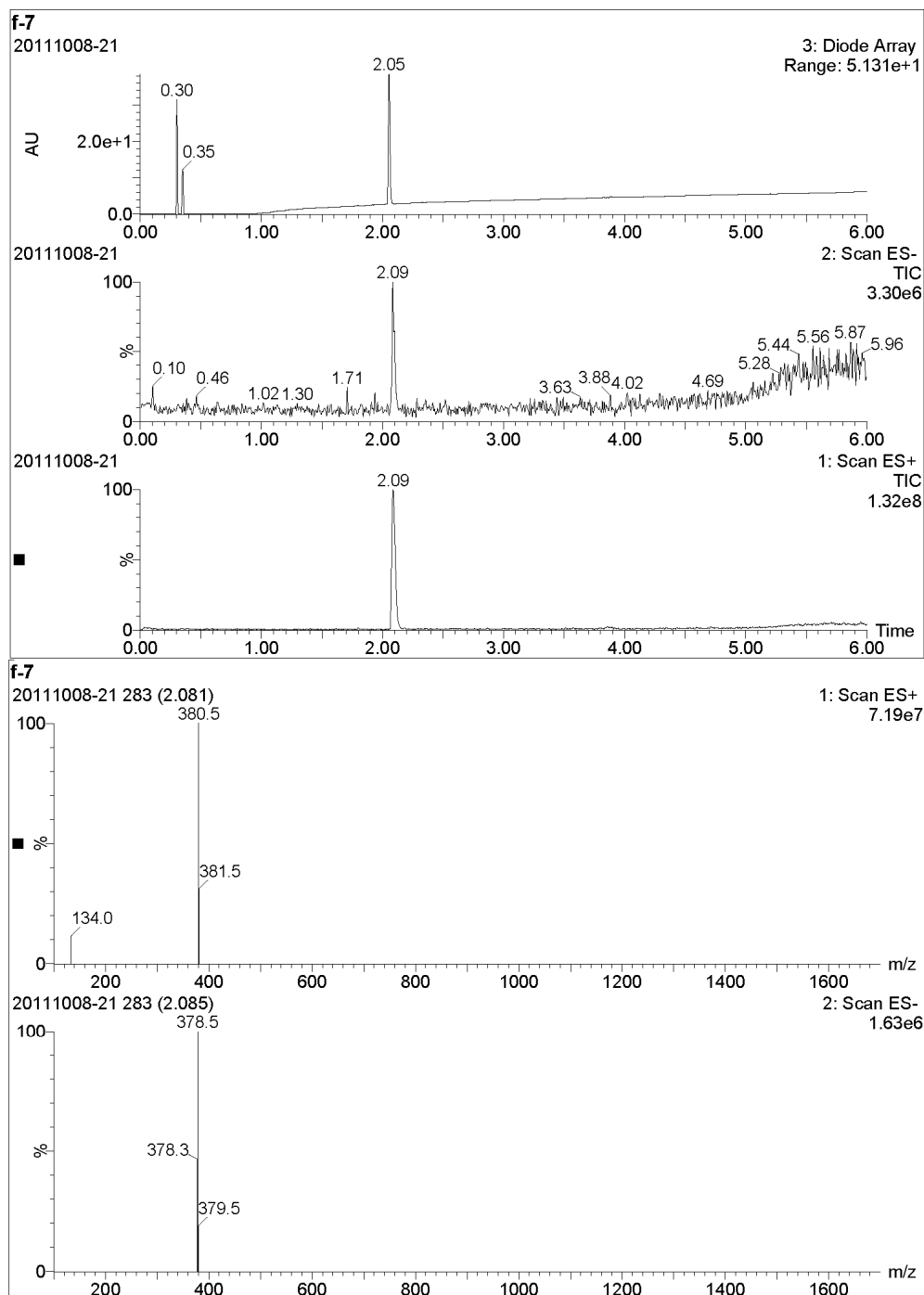
S23. ^1H NMR spectrum of ethyl
2-methyl-4-(p-tolyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5h**) in $\text{DMSO-}d_6$.



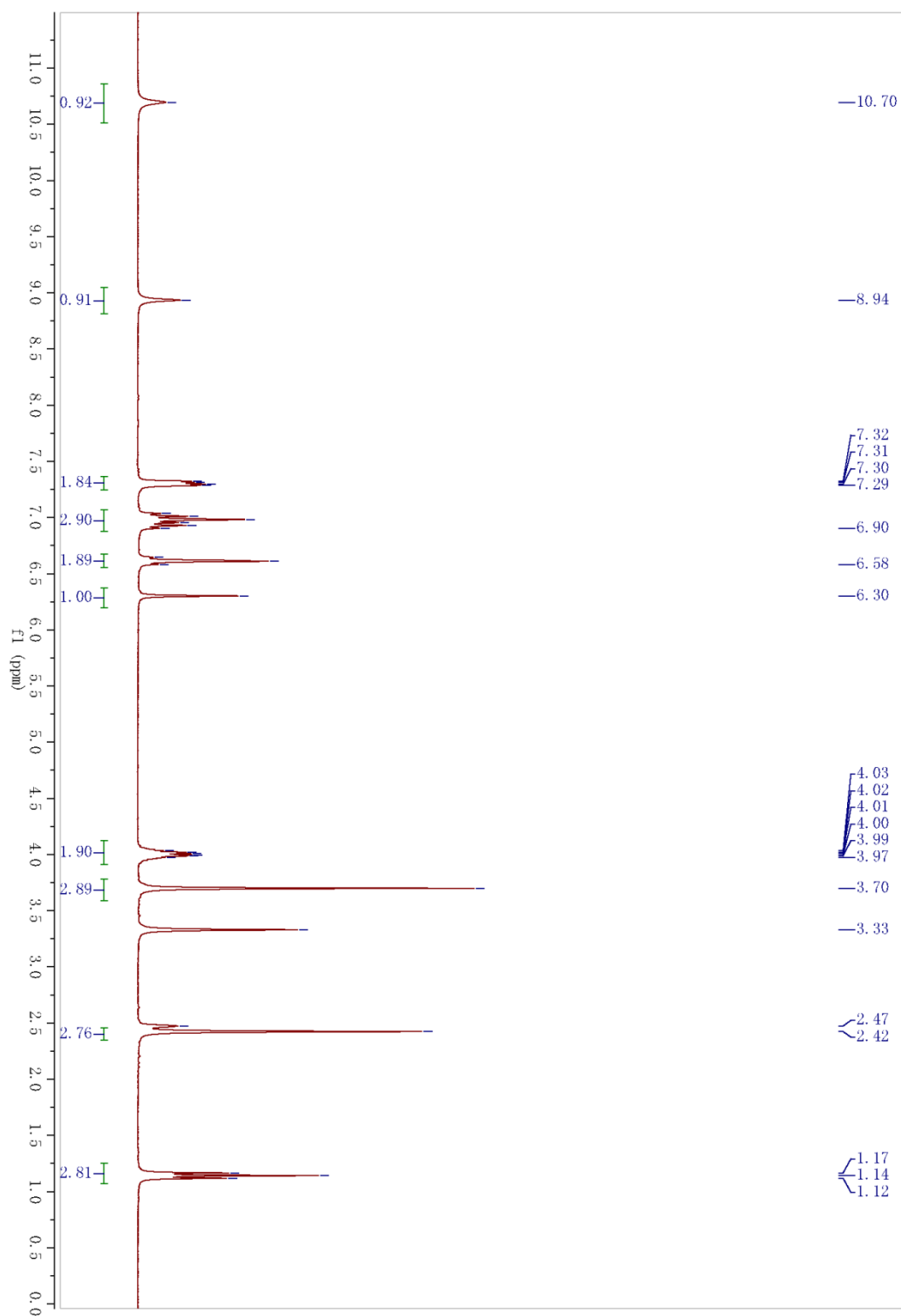
S24. ^{13}C NMR spectrum of ethyl
2-methyl-4-(p-tolyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5h**) in $\text{DMSO-}d_6$.



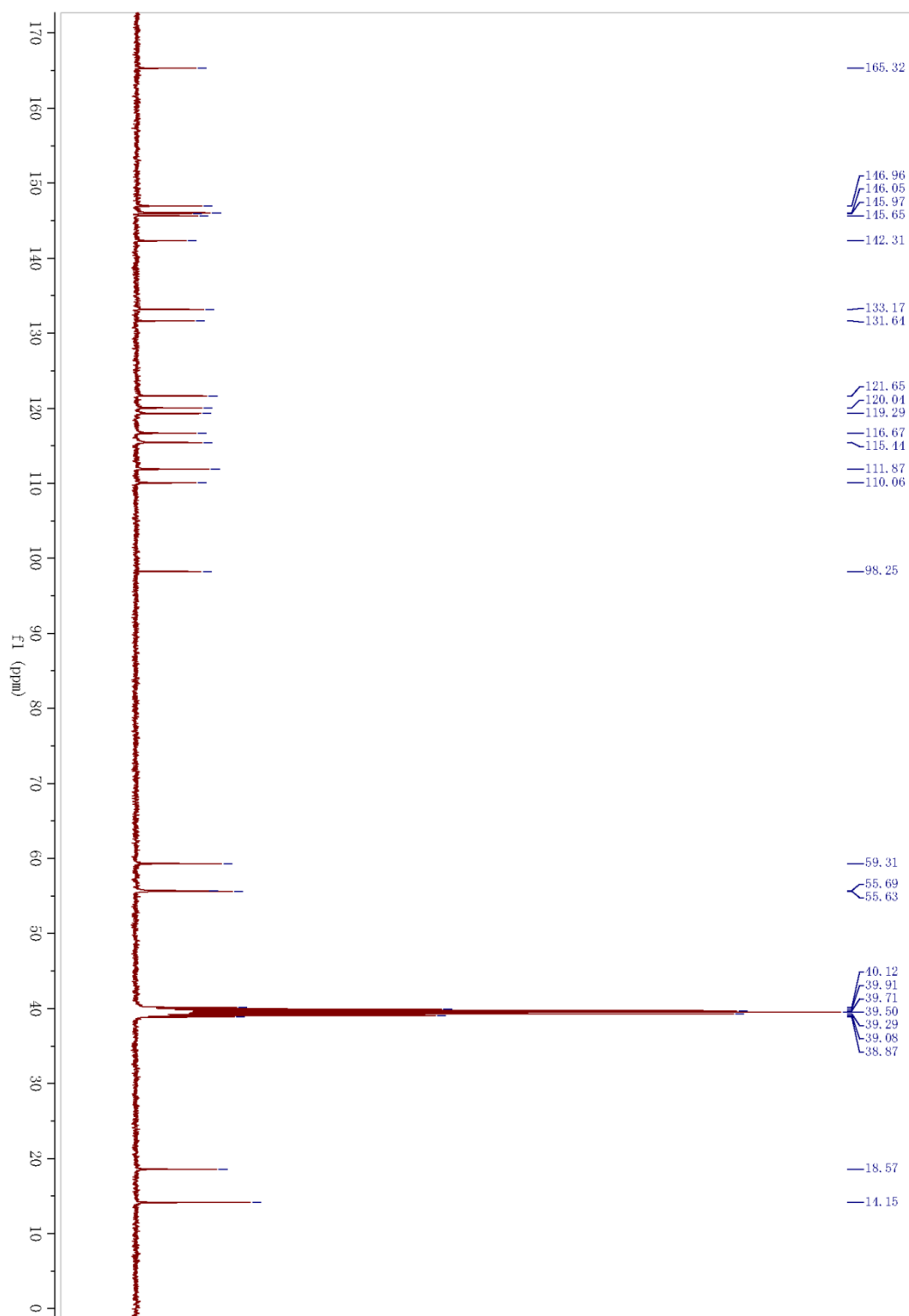
S25. LCMS spectrum of ethyl 4-(4-hydroxy-3-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5i**).



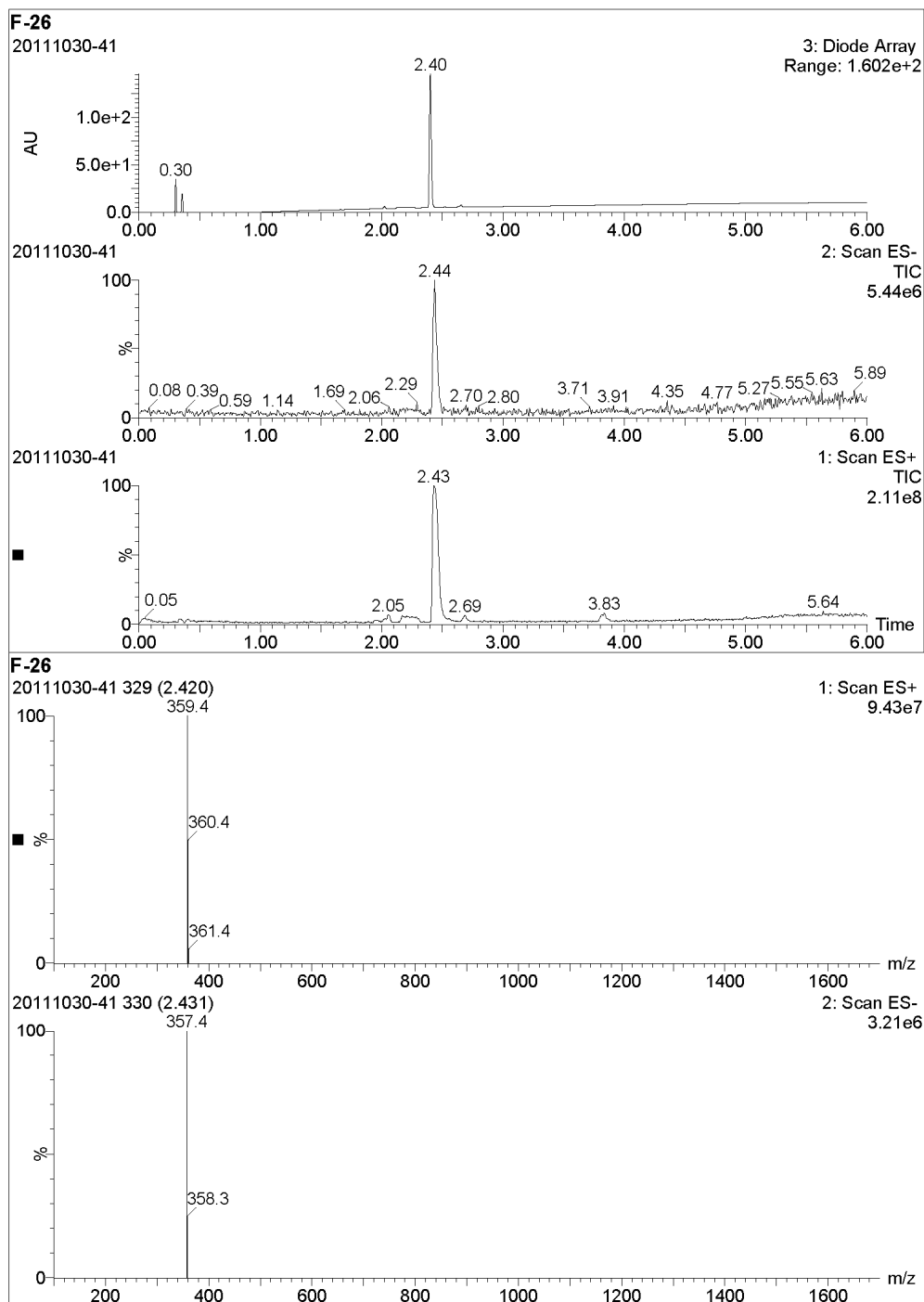
S26. ^1H NMR spectrum of ethyl 4-(4-hydroxy-3-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5i**) in $\text{DMSO}-d_6$.



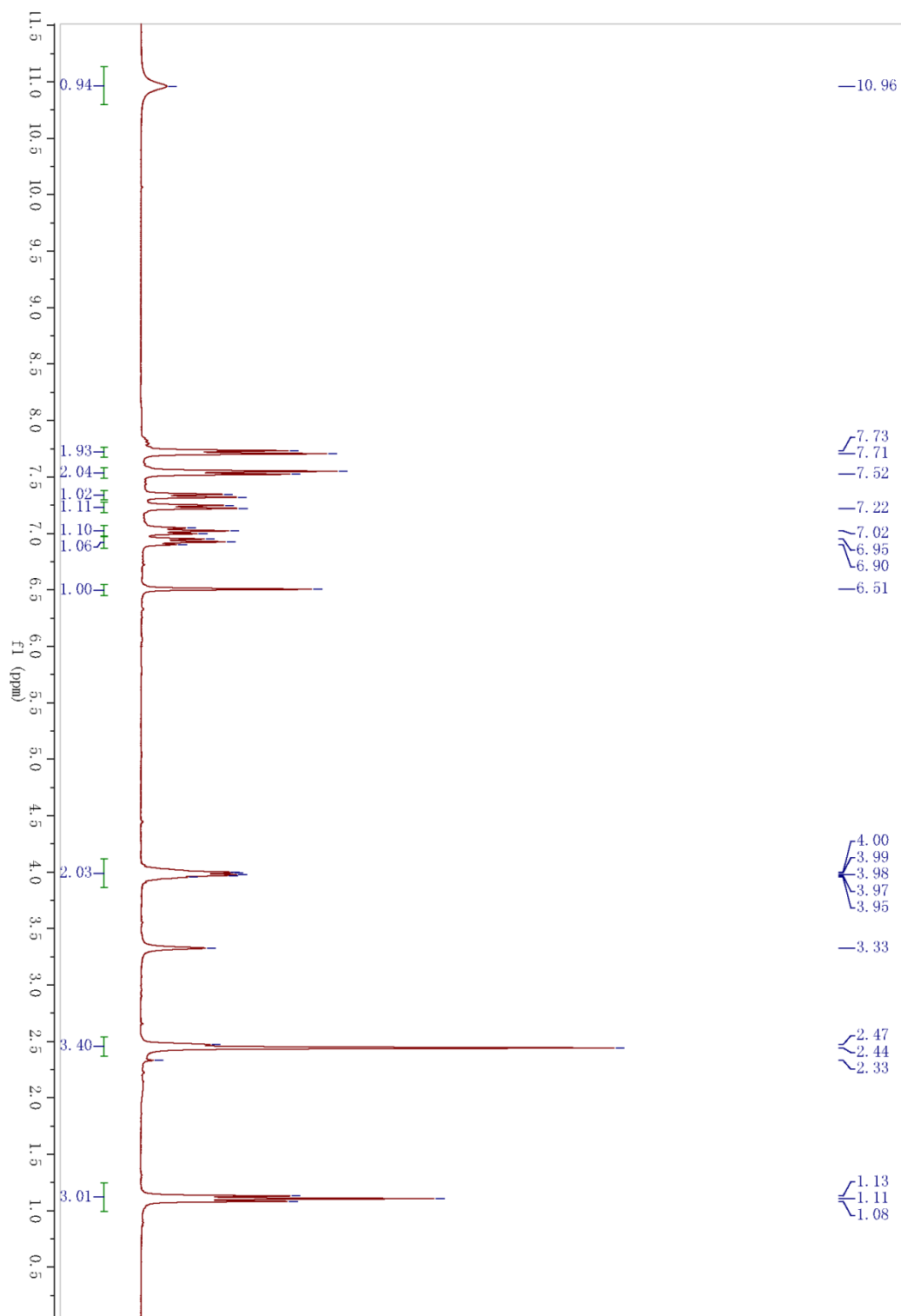
S27. ^{13}C NMR spectrum of ethyl 4-(4-hydroxy-3-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5i**) in $\text{DMSO-}d_6$.



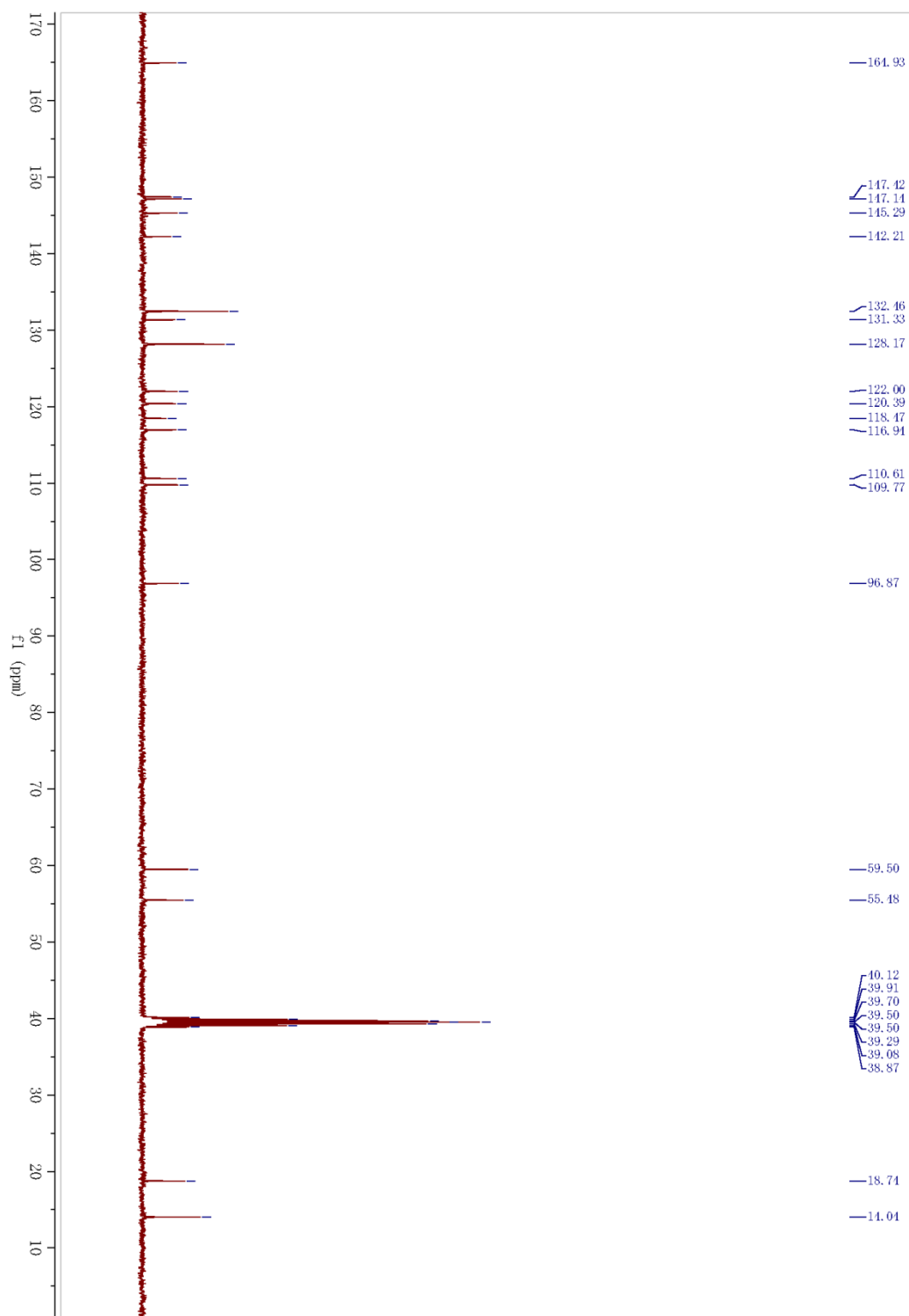
S28. LCMS spectrum of ethyl 4-(4-cyanophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5j**).



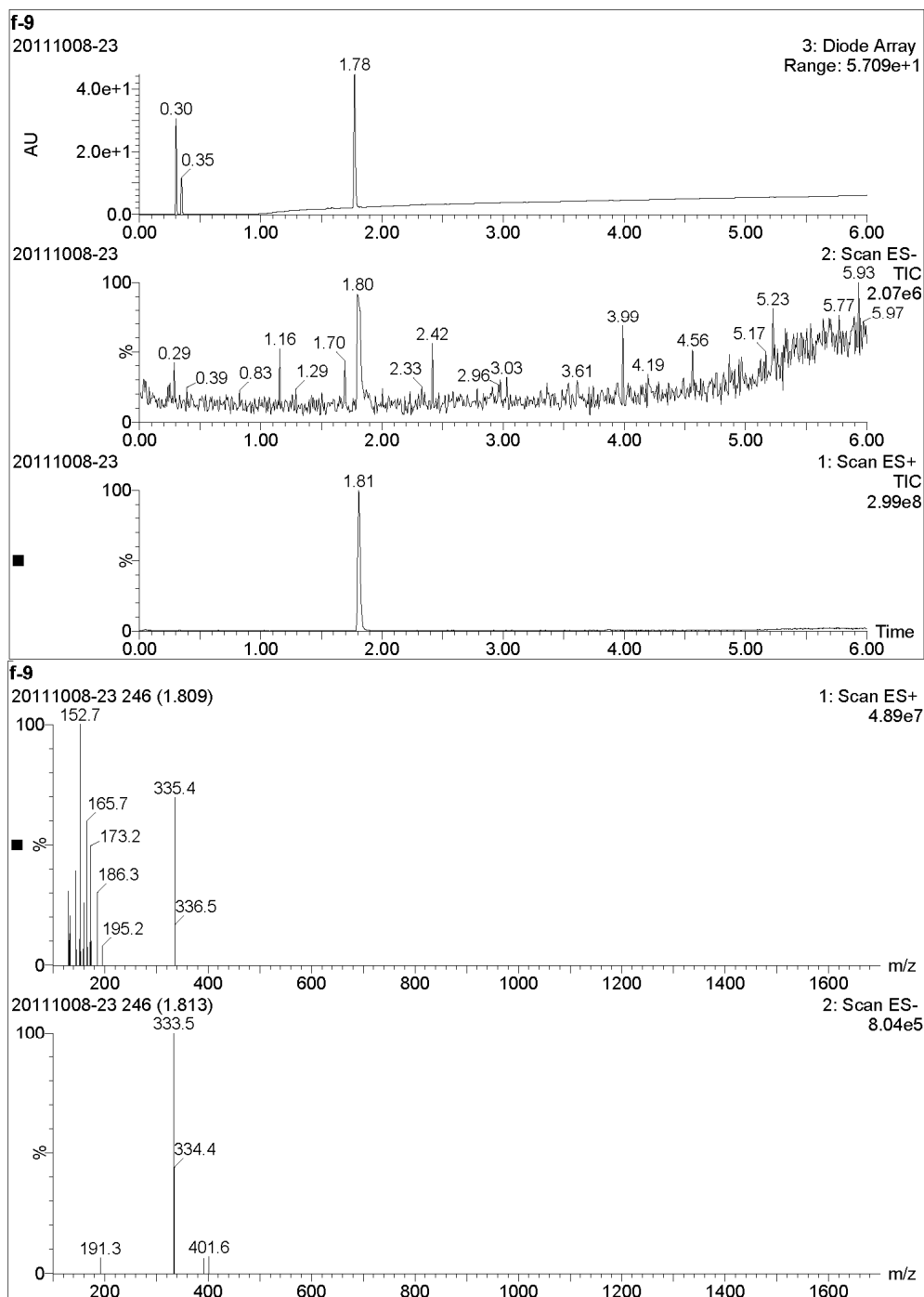
S29. ^1H NMR spectrum of ethyl 4-(4-cyanophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5j**) in $\text{DMSO-}d_6$.



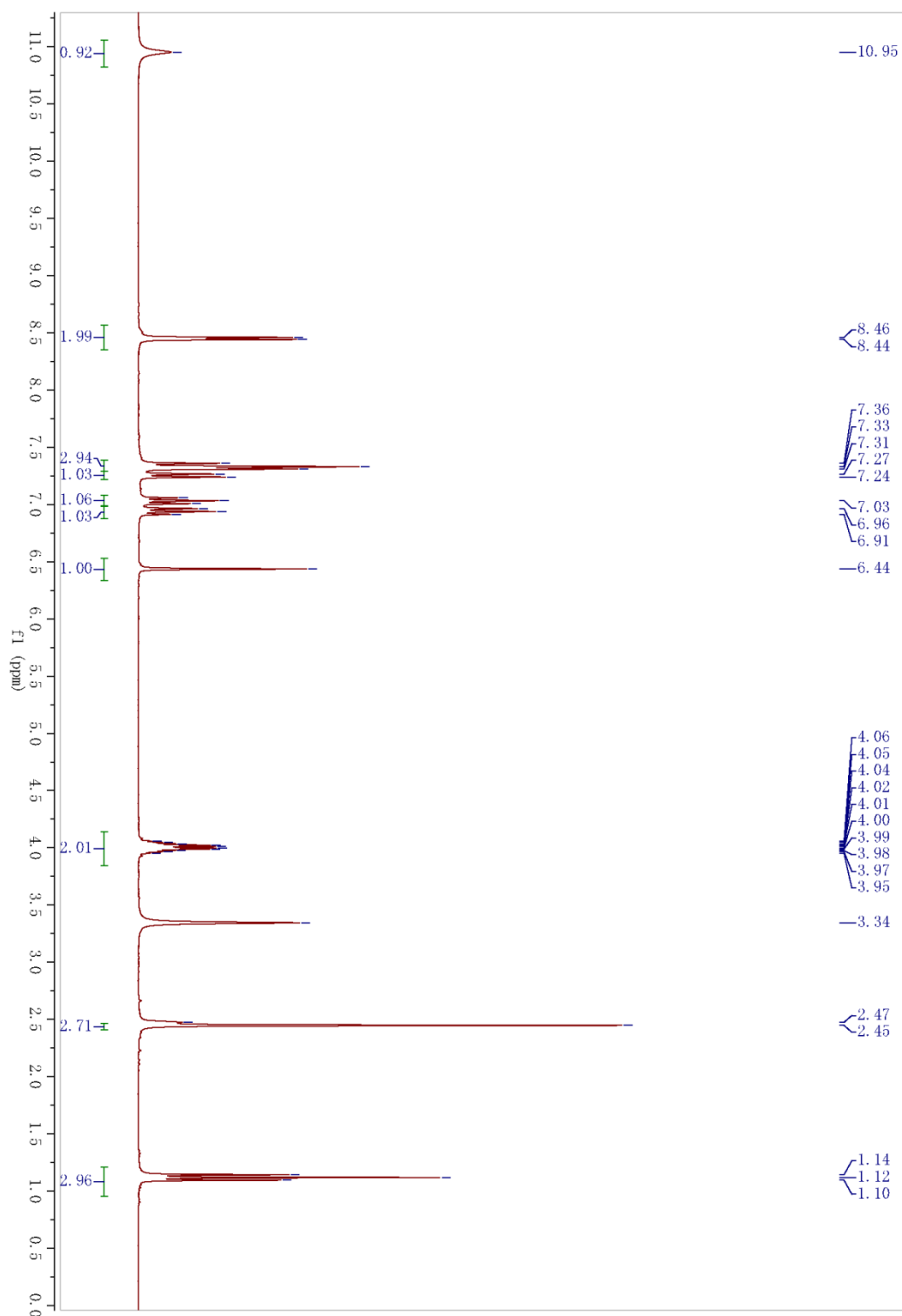
S30. ^{13}C NMR spectrum of ethyl 4-(4-cyanophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5j**) in $\text{DMSO-}d_6$.



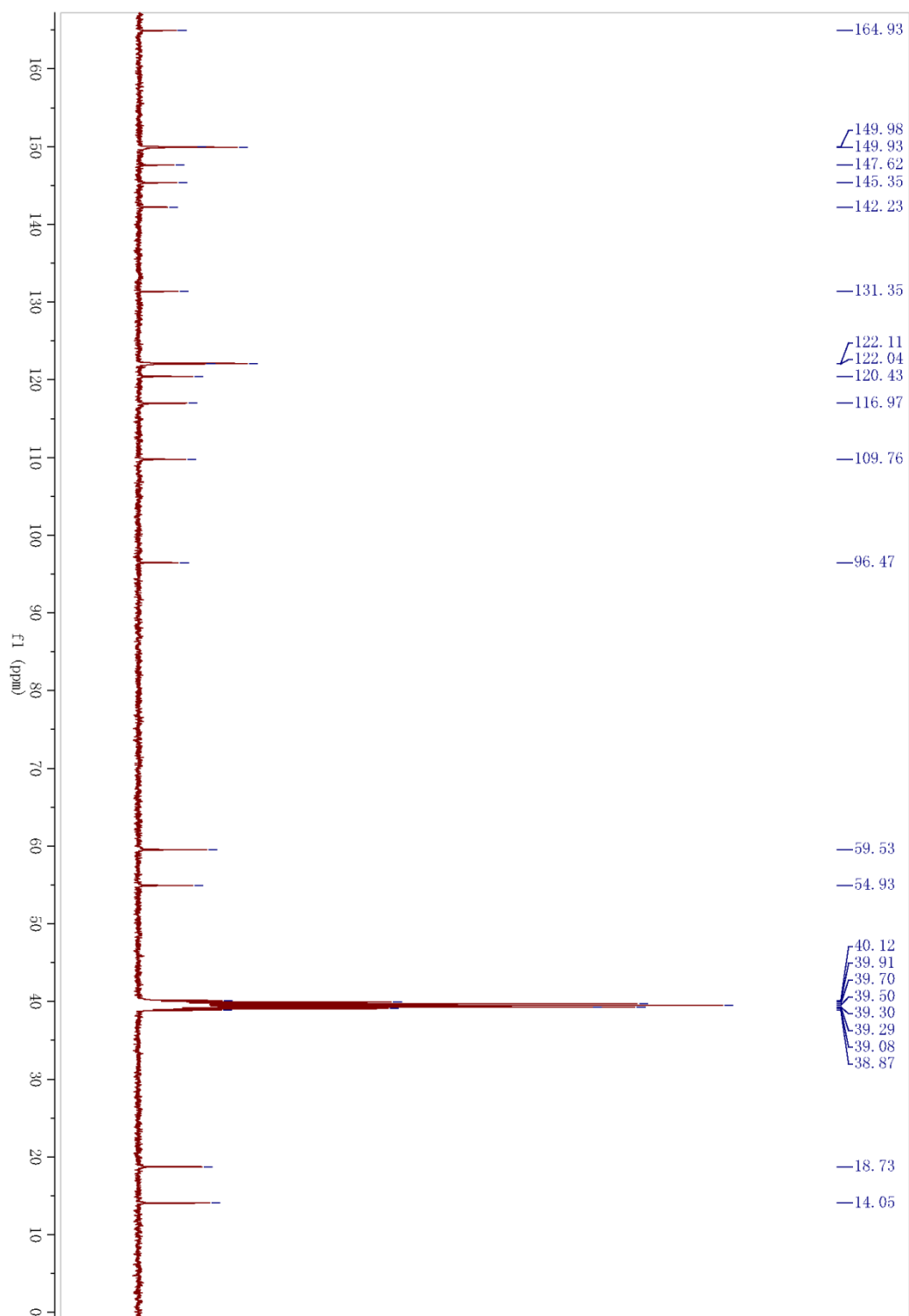
S31. LCMS spectrum of ethyl 2-methyl-4-(pyridin-4-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5k**).



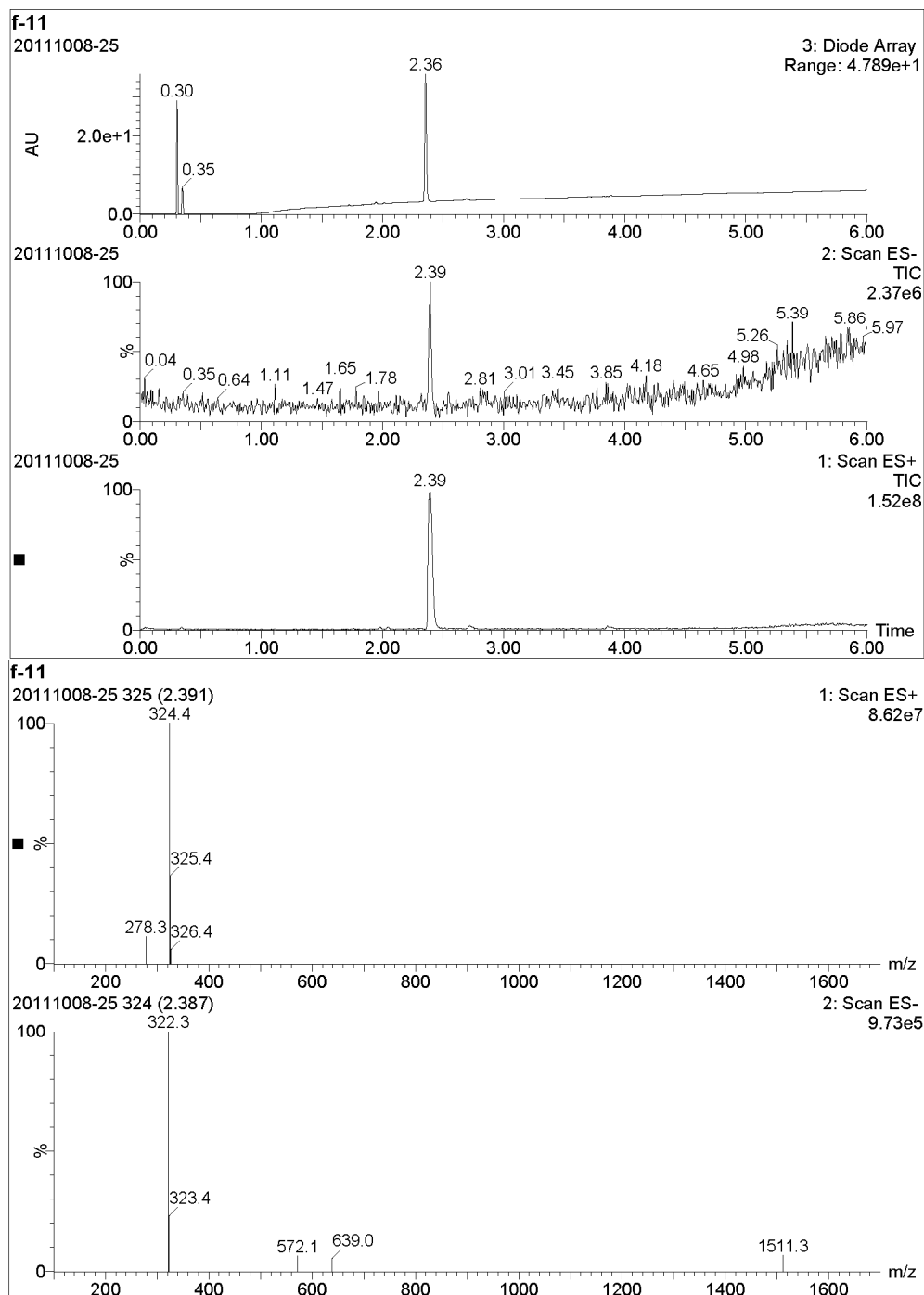
S32. ^1H NMR spectrum of ethyl 2-methyl-4-(pyridin-4-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5k**) in $\text{DMSO-}d_6$.



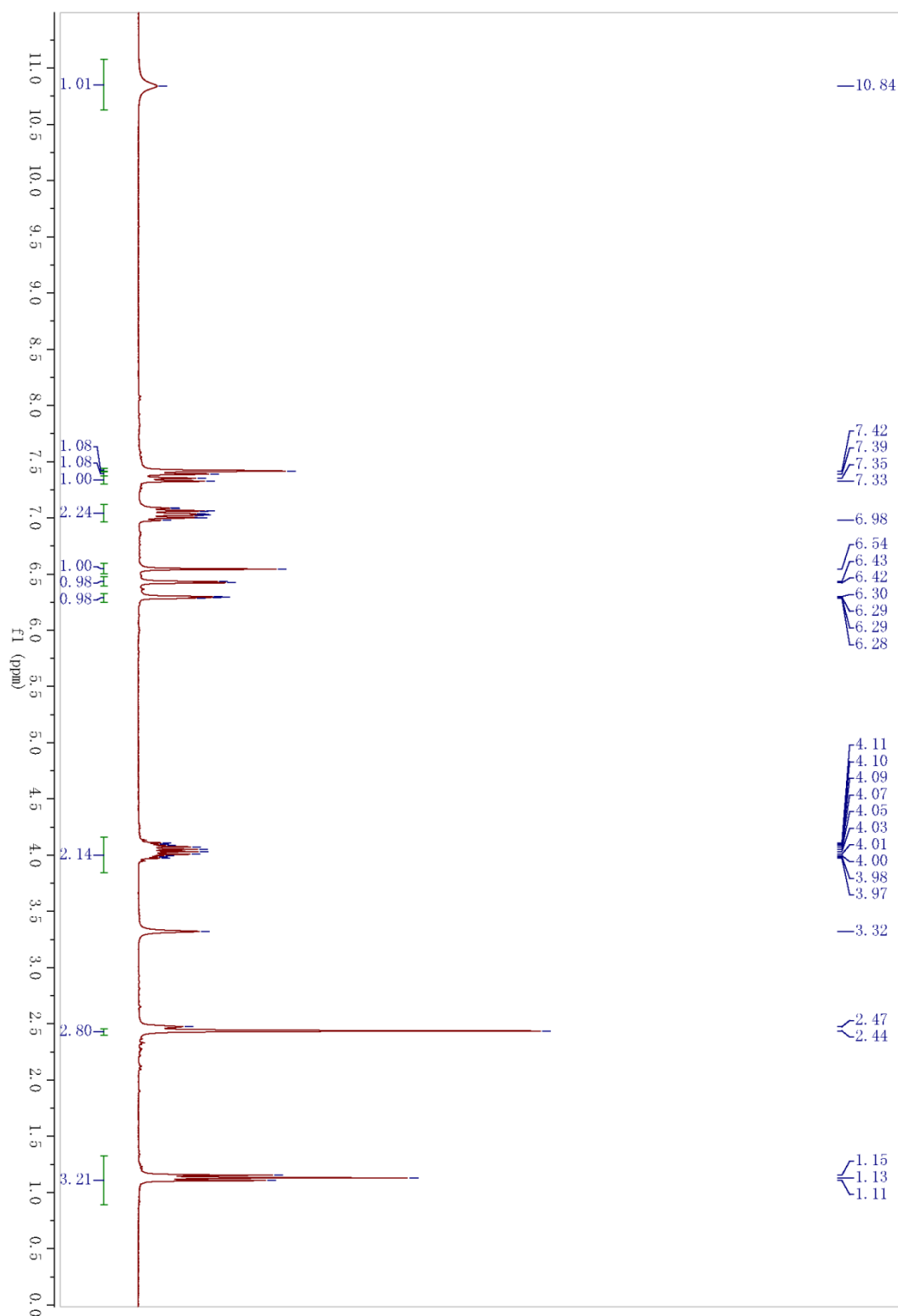
S33. ^{13}C NMR spectrum of ethyl 2-methyl-4-(pyridin-4-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5k**) in $\text{DMSO-}d_6$.



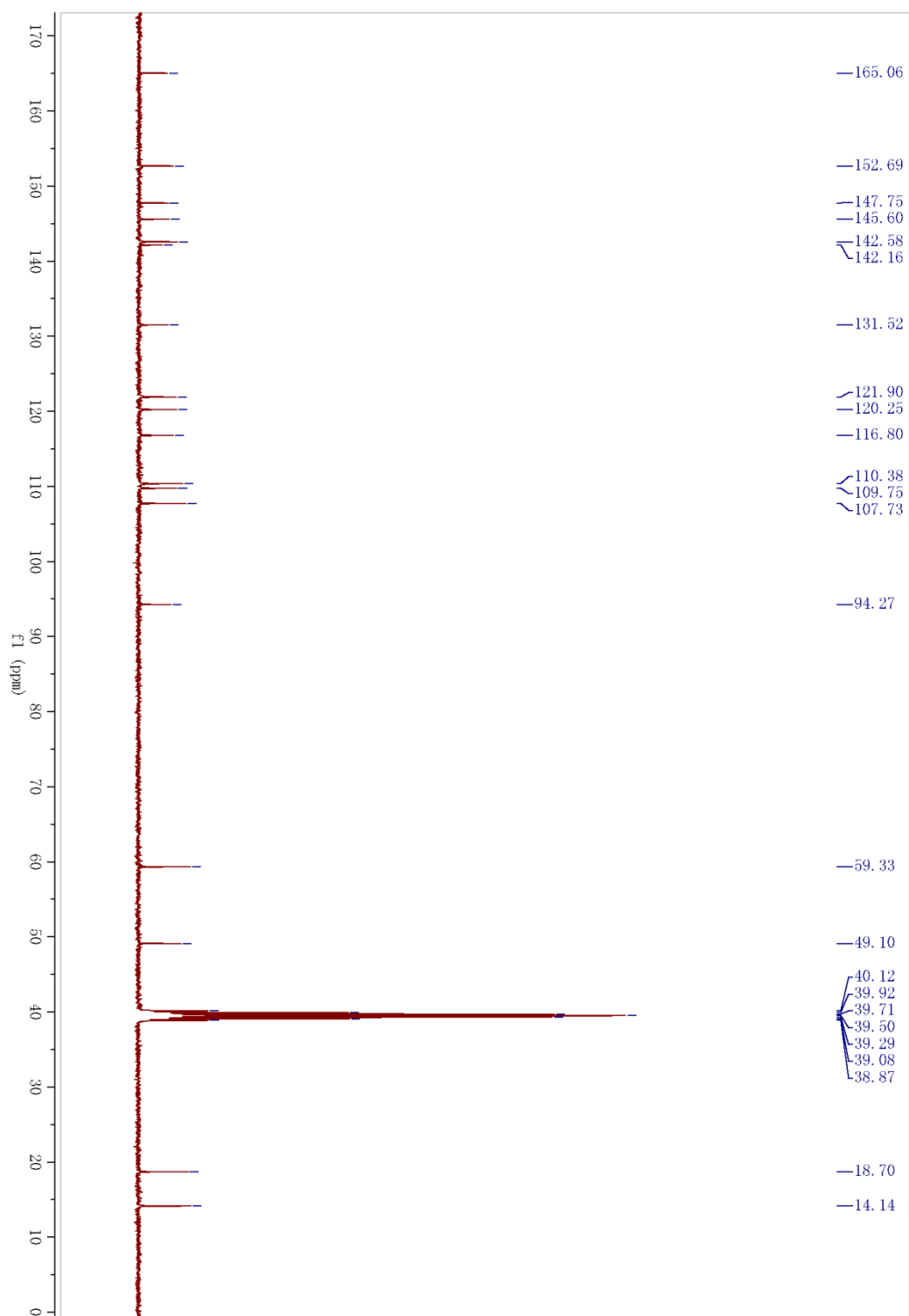
S34. LCMS spectrum of ethyl 4-(furan-2-yl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5I**).



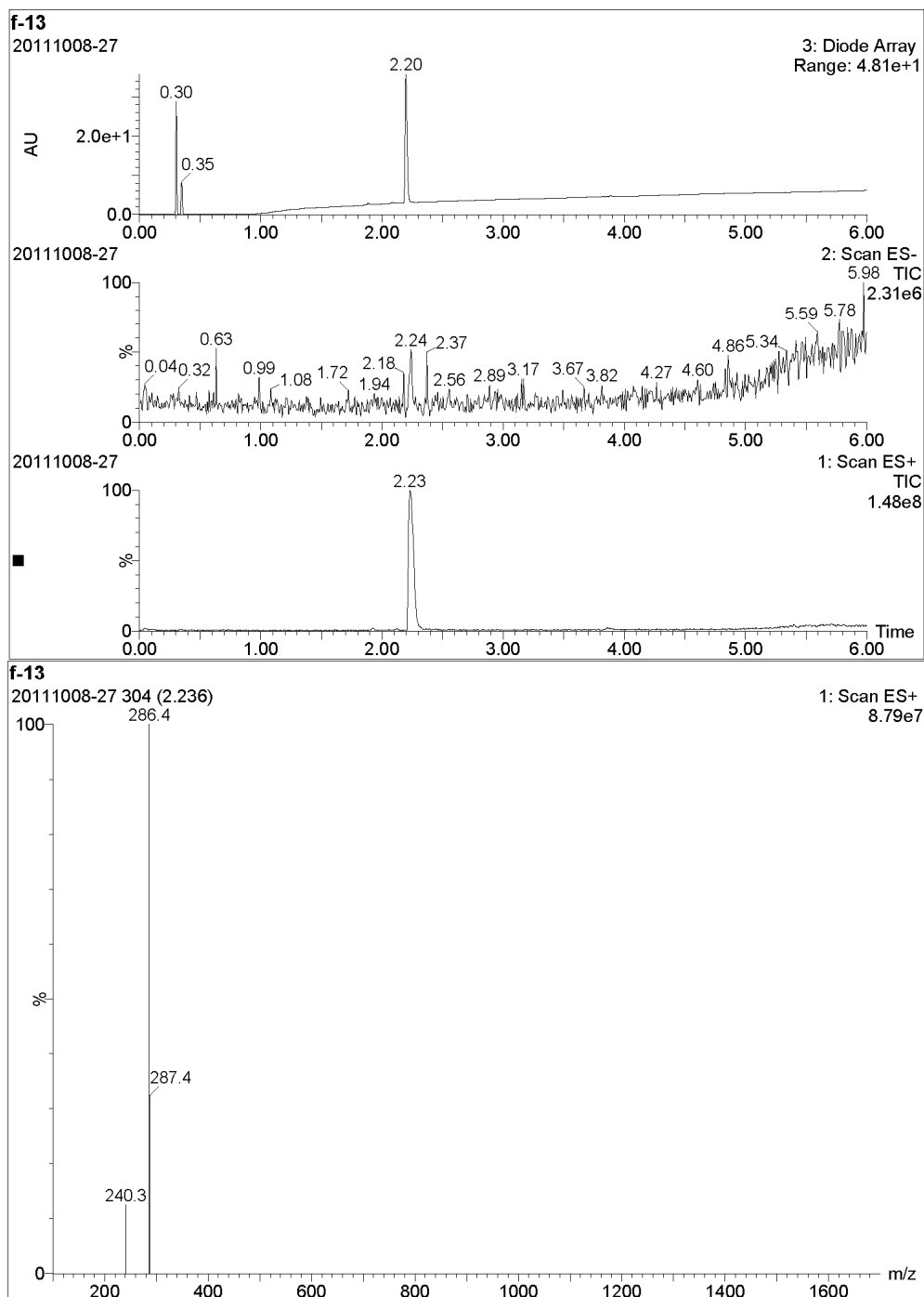
S35. ^1H NMR spectrum of ethyl 4-(furan-2-yl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5I**) in $\text{DMSO-}d_6$.



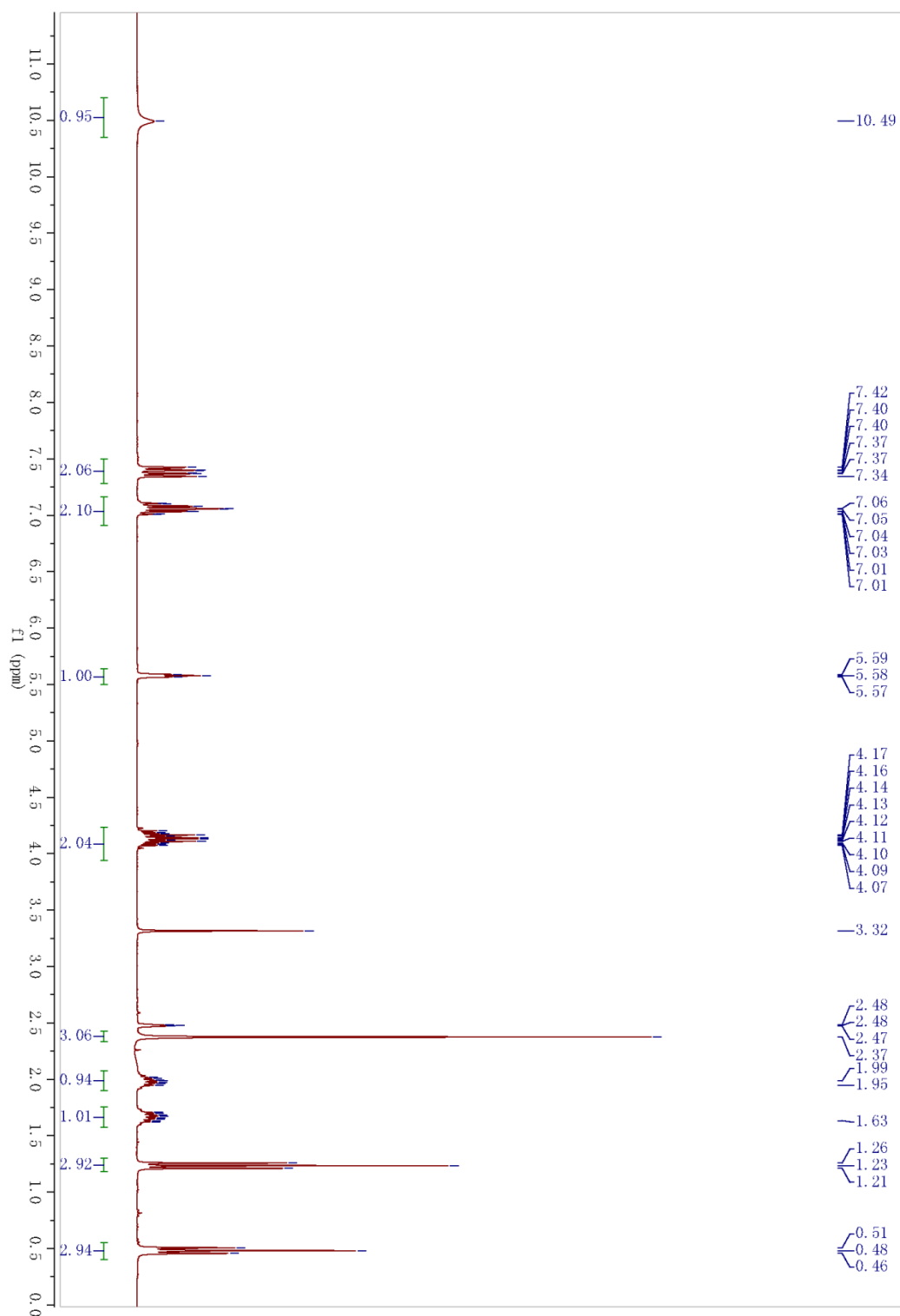
S36. ^{13}C NMR spectrum of ethyl 4-(furan-2-yl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5I**) in $\text{DMSO-}d_6$.



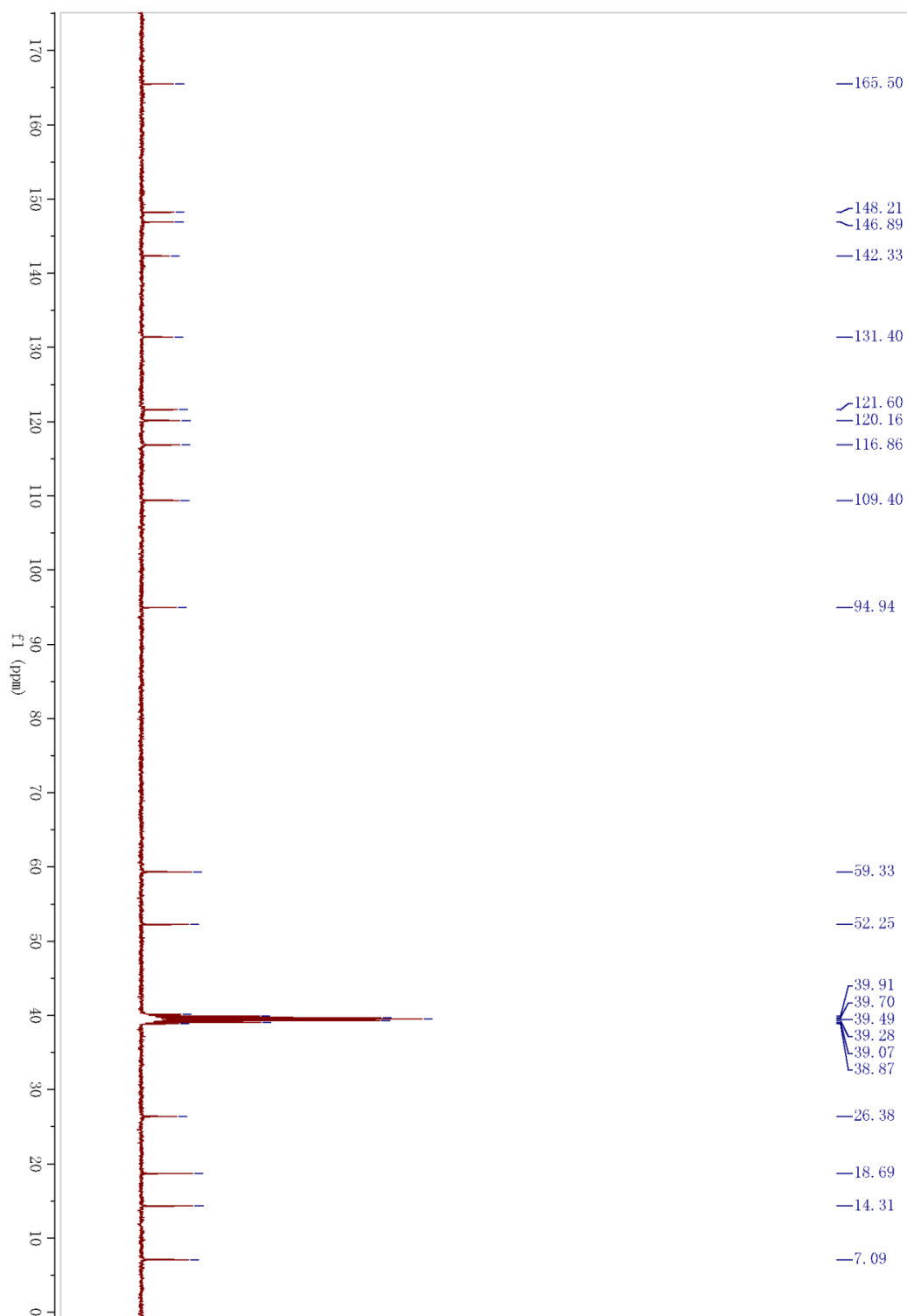
S37. LCMS spectrum of ethyl
4-ethyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(5m).



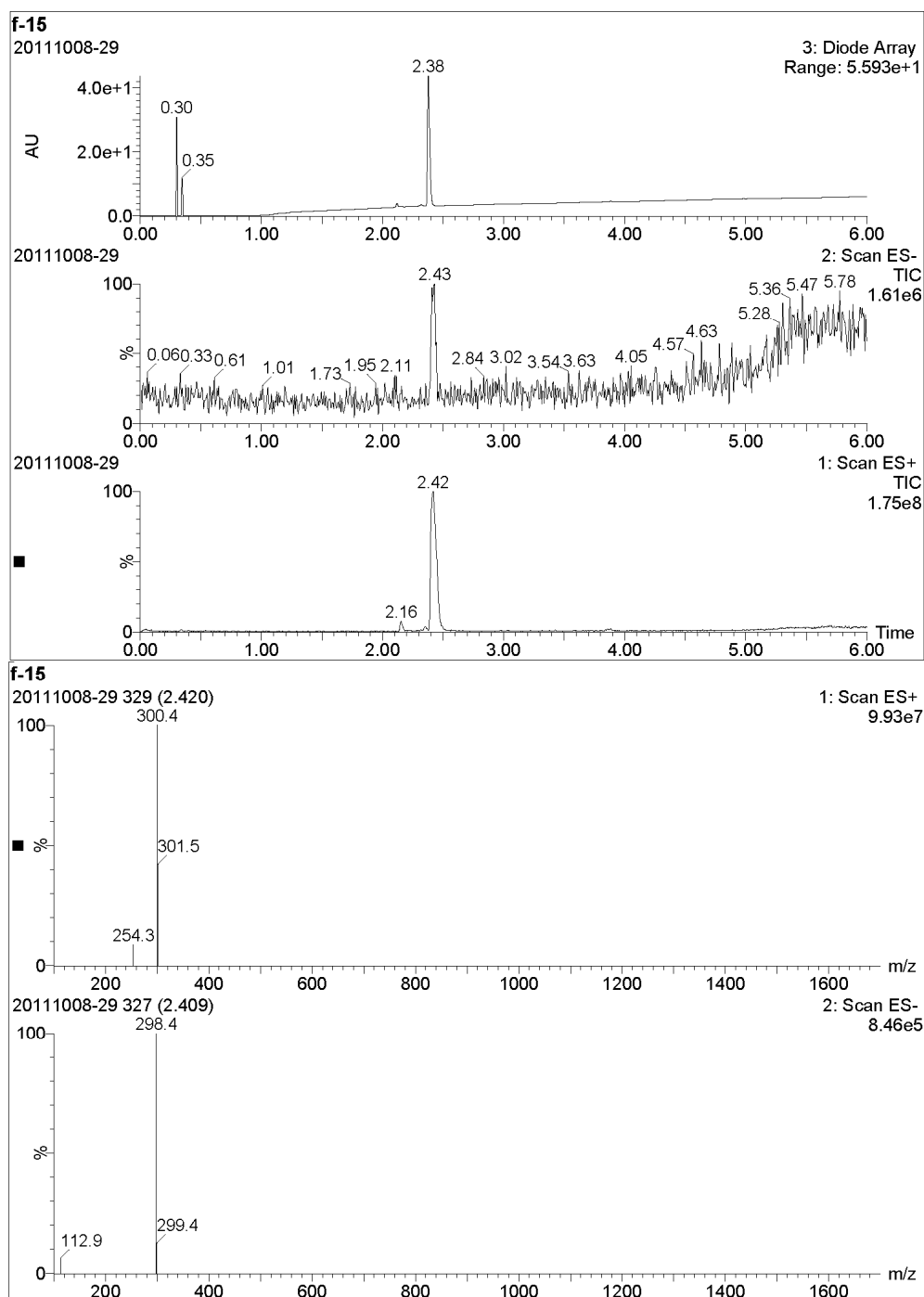
S38. ^1H NMR spectrum of ethyl 4-ethyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5m**) in $\text{DMSO-}d_6$.



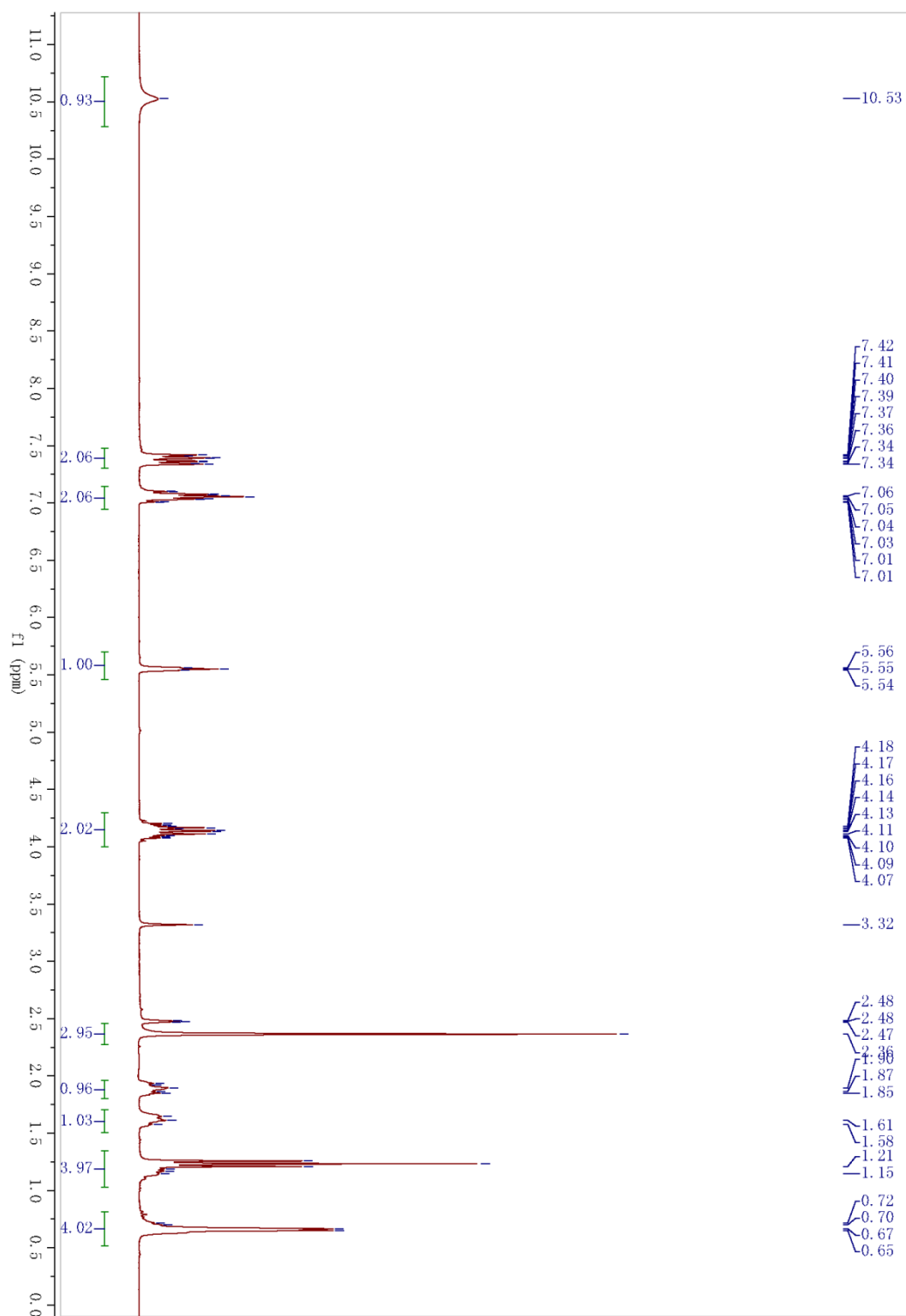
S39. ^{13}C NMR spectrum of ethyl 4-ethyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5m**) in DMSO- d_6 .



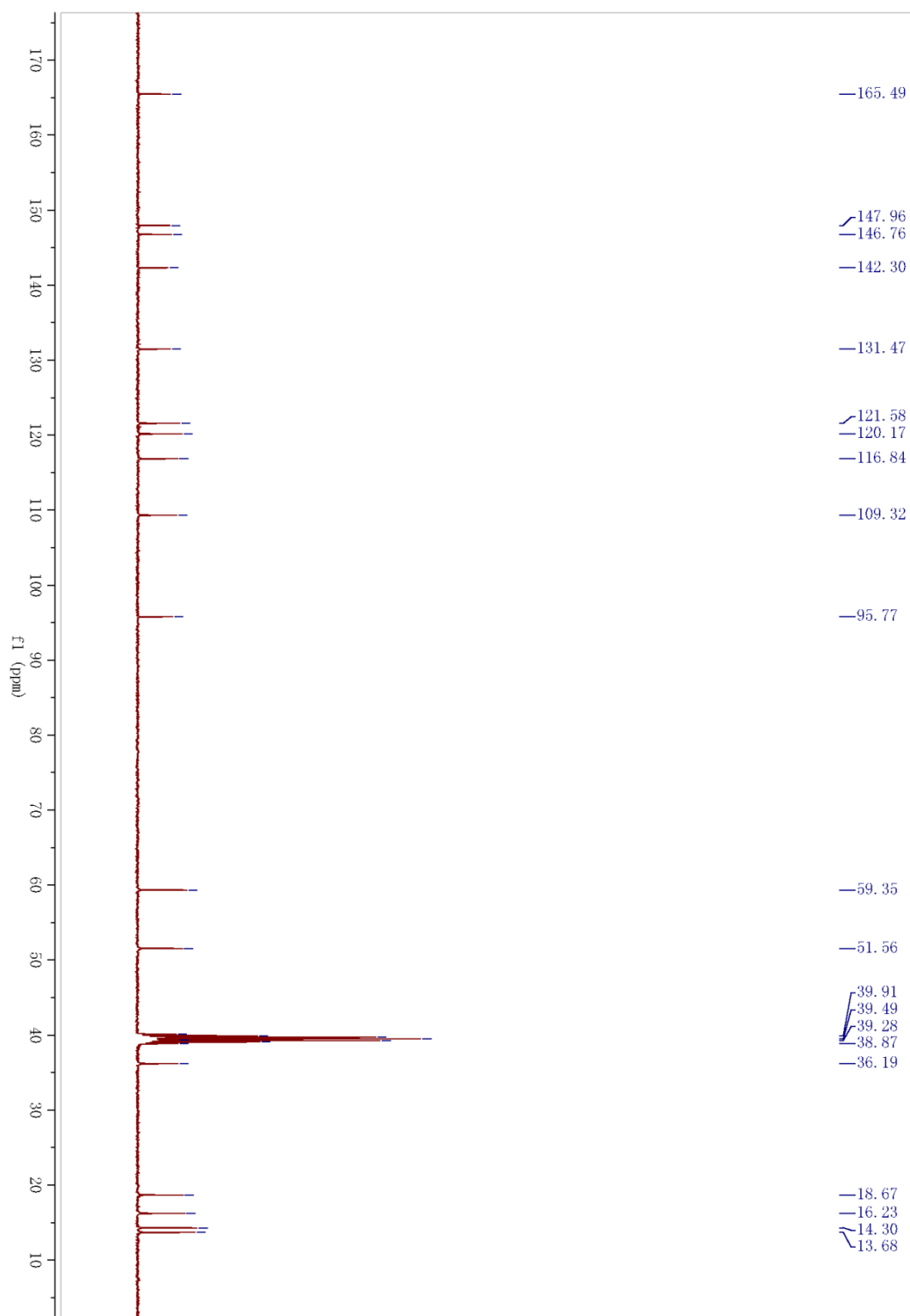
S40. LCMS spectrum of ethyl
2-methyl-4-propyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5n**).



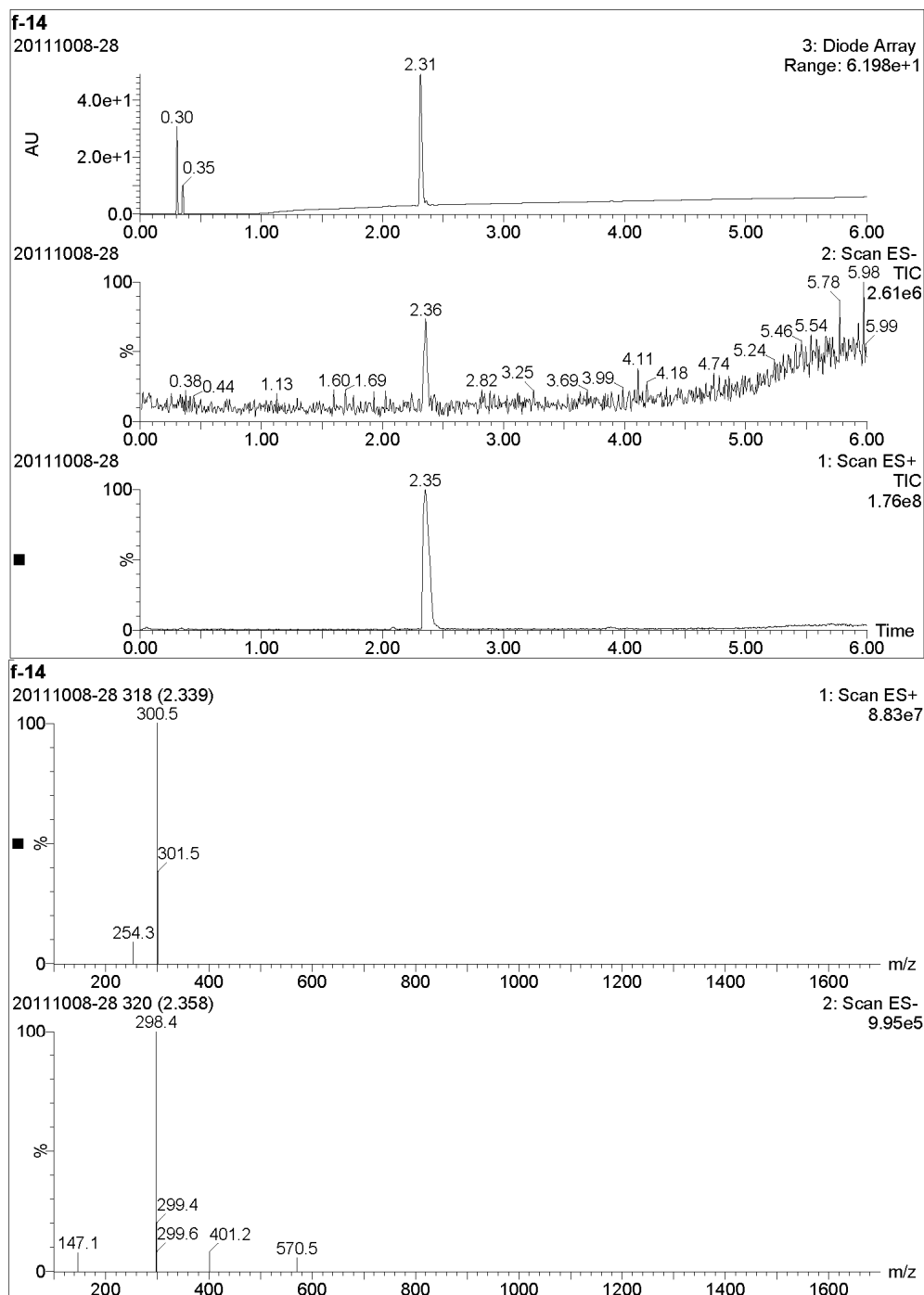
S41. ^1H NMR spectrum of ethyl 2-methyl-4-propyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5n**) in DMSO- d_6 .



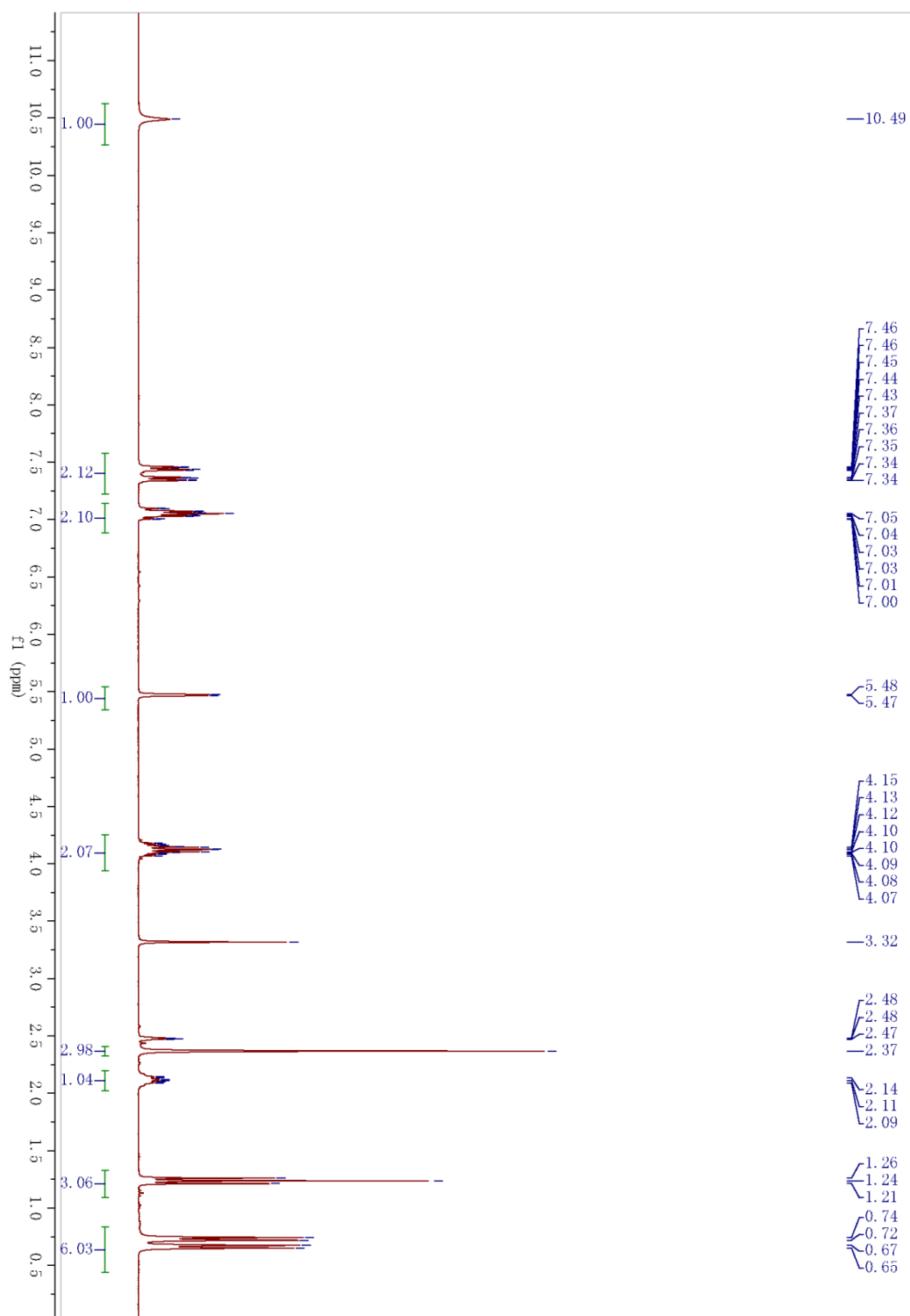
S42. ^{13}C NMR spectrum of ethyl 2-methyl-4-propyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5n**) in DMSO- d_6 .



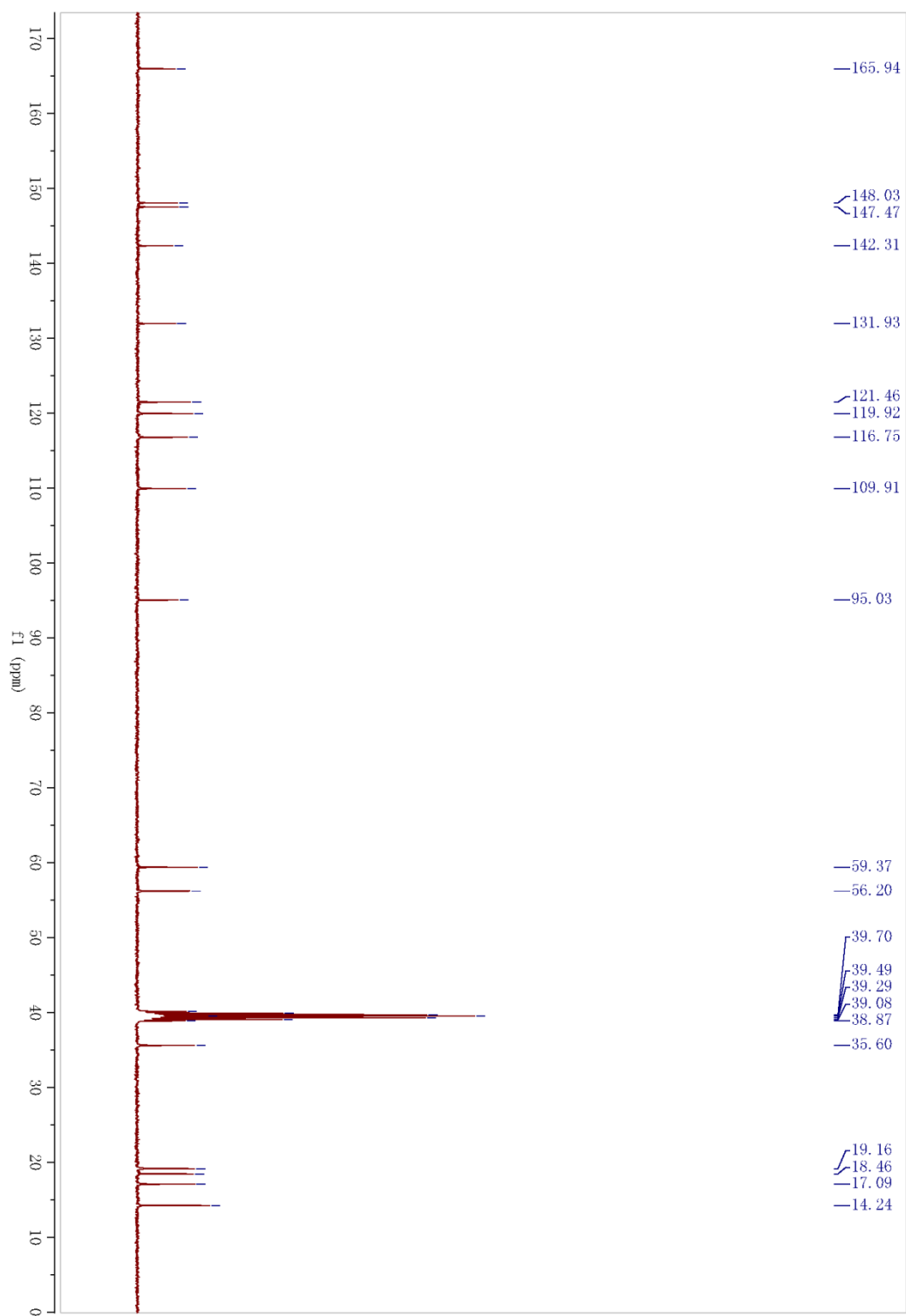
S43. LCMS spectrum of ethyl
4-isopropyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5o**).



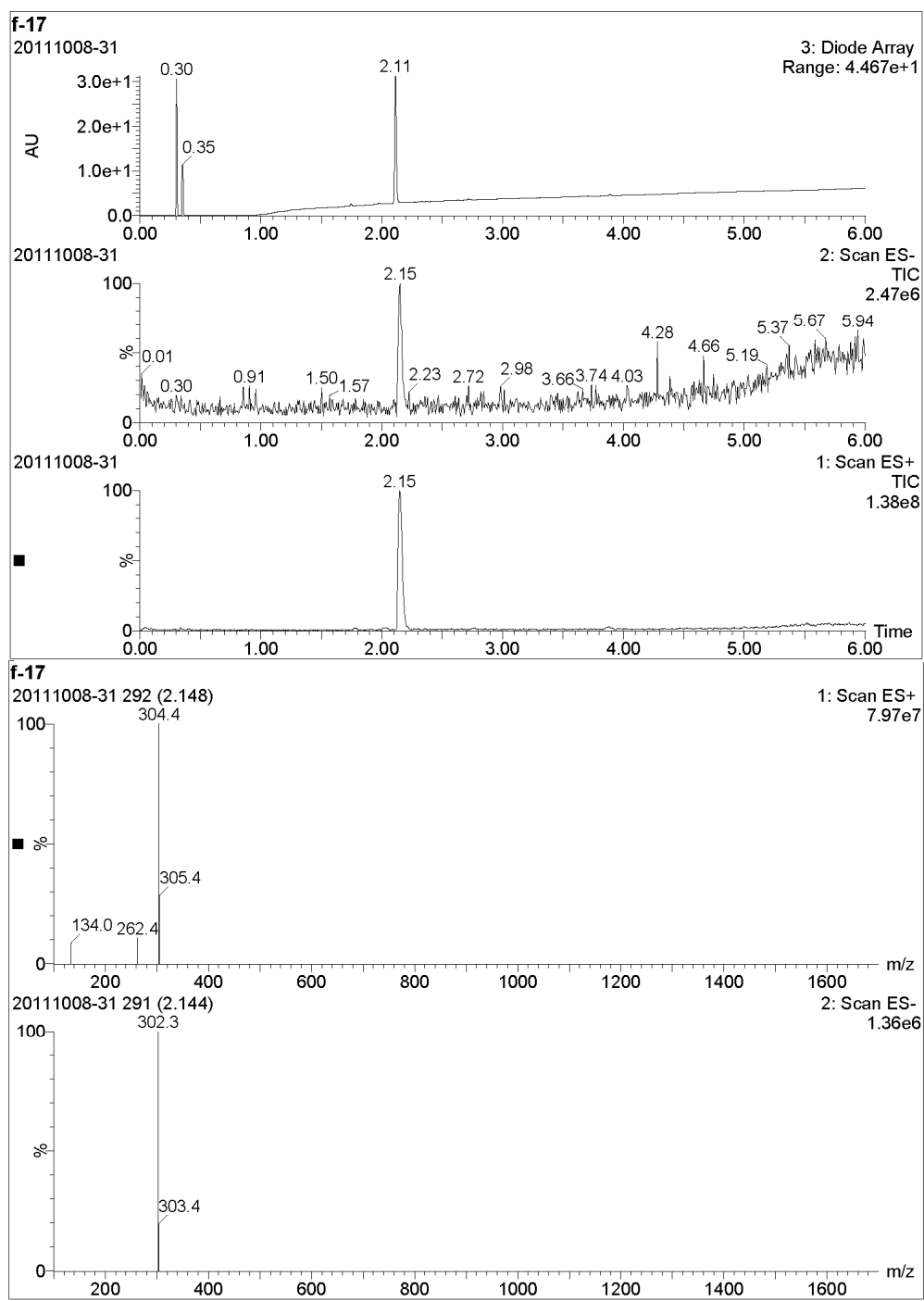
S44. ^1H NMR spectrum of ethyl 4-isopropyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5o**) in $\text{DMSO-}d_6$.



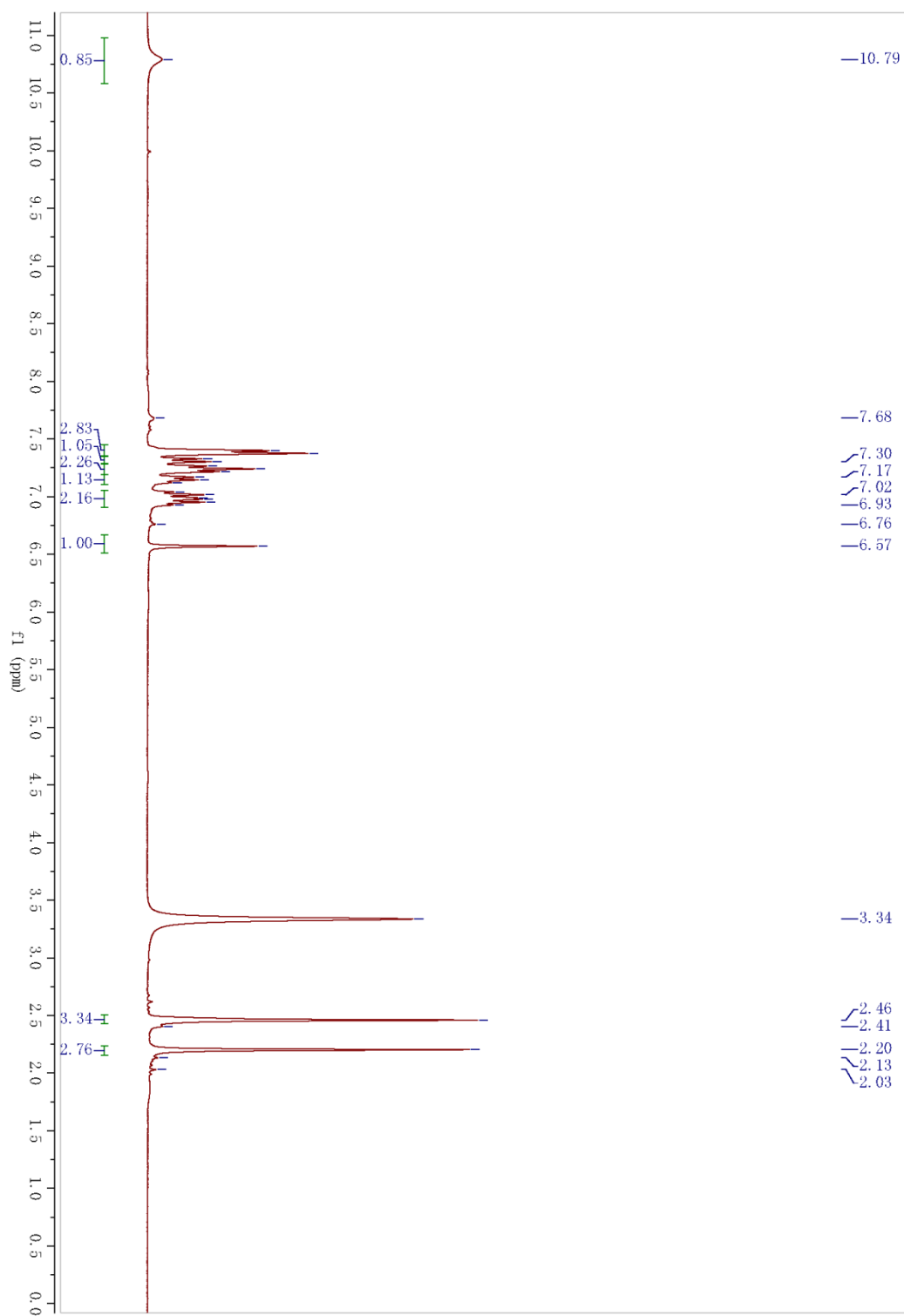
S45. ^{13}C NMR spectrum of ethyl
4-isopropyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate
(**5o**) in $\text{DMSO-}d_6$.



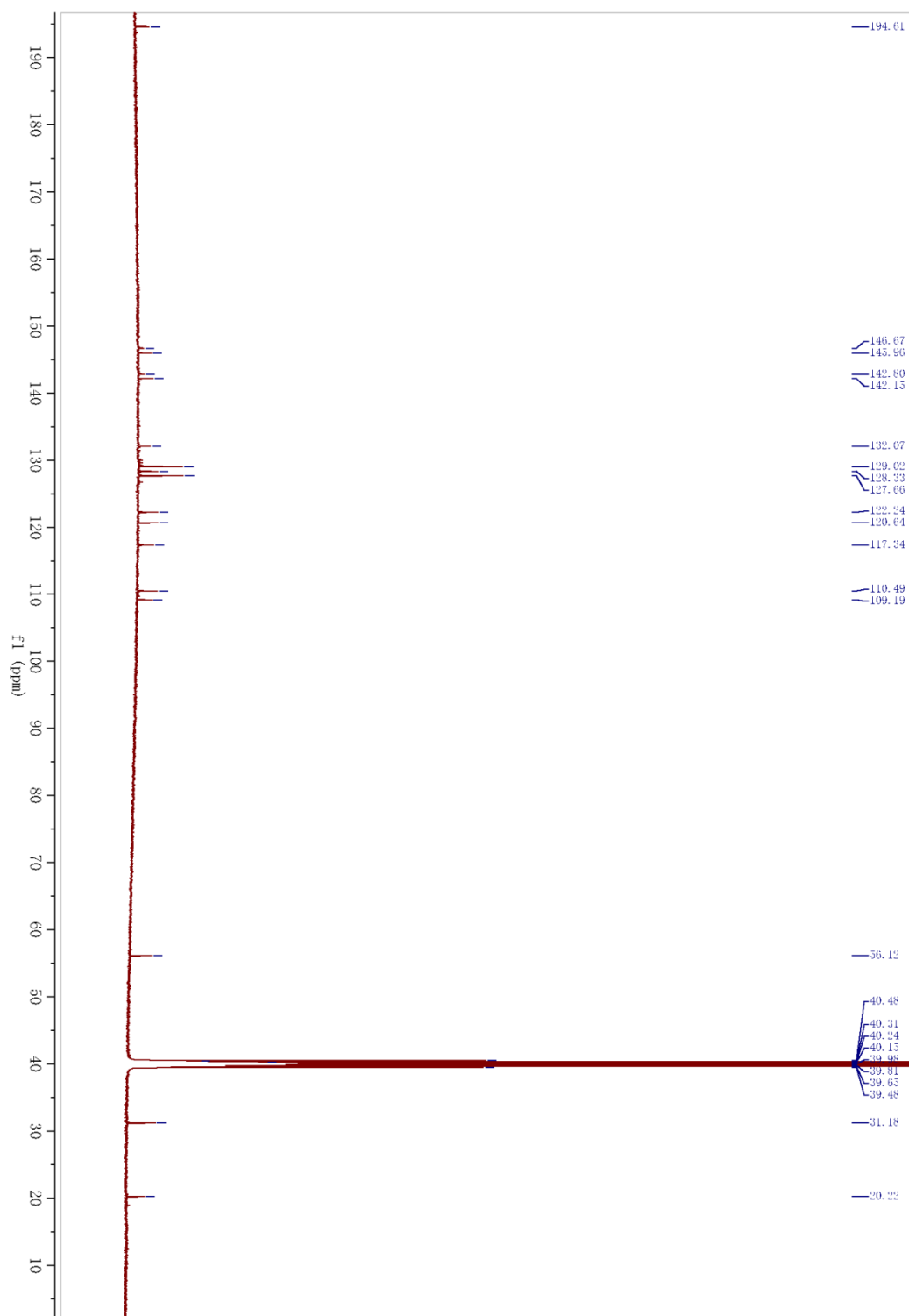
S46. LCMS spectrum of
1-(2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone
(5p).



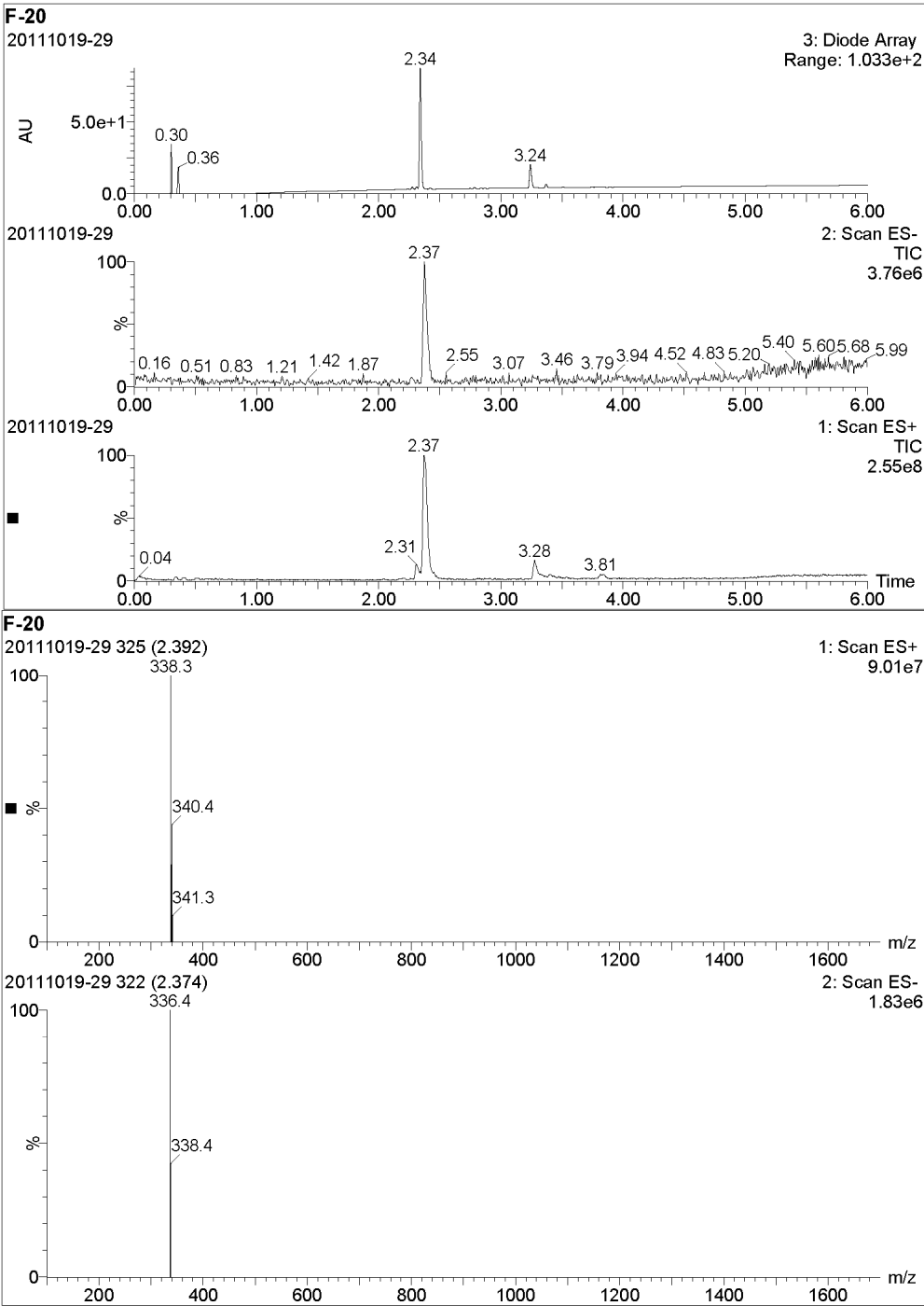
S47. ^1H NMR spectrum of
1-(2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone
(**5p**) in $\text{DMSO-}d_6$.



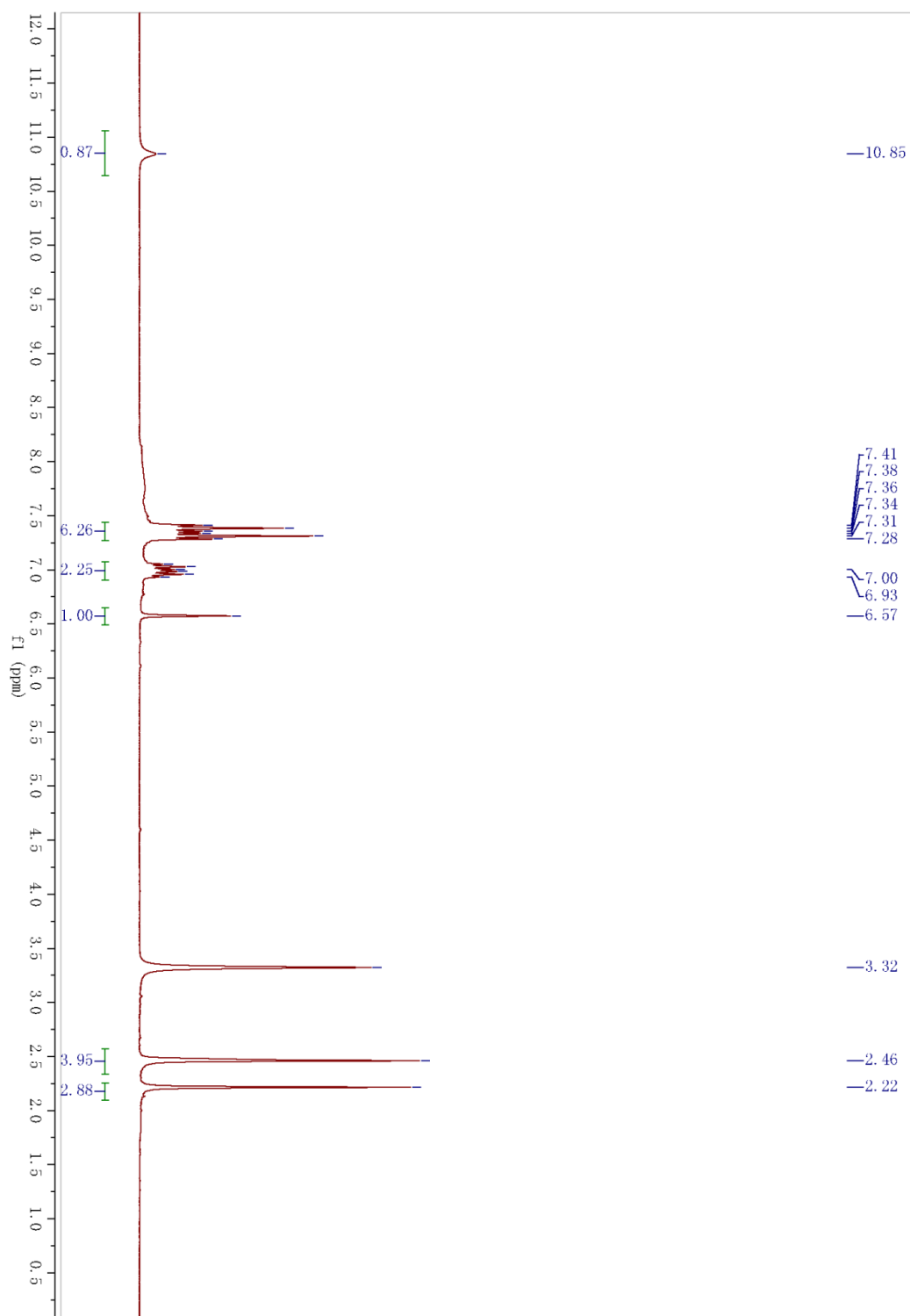
S48. ^{13}C NMR spectrum of
1-(2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone
(**5p**) in $\text{DMSO-}d_6$.



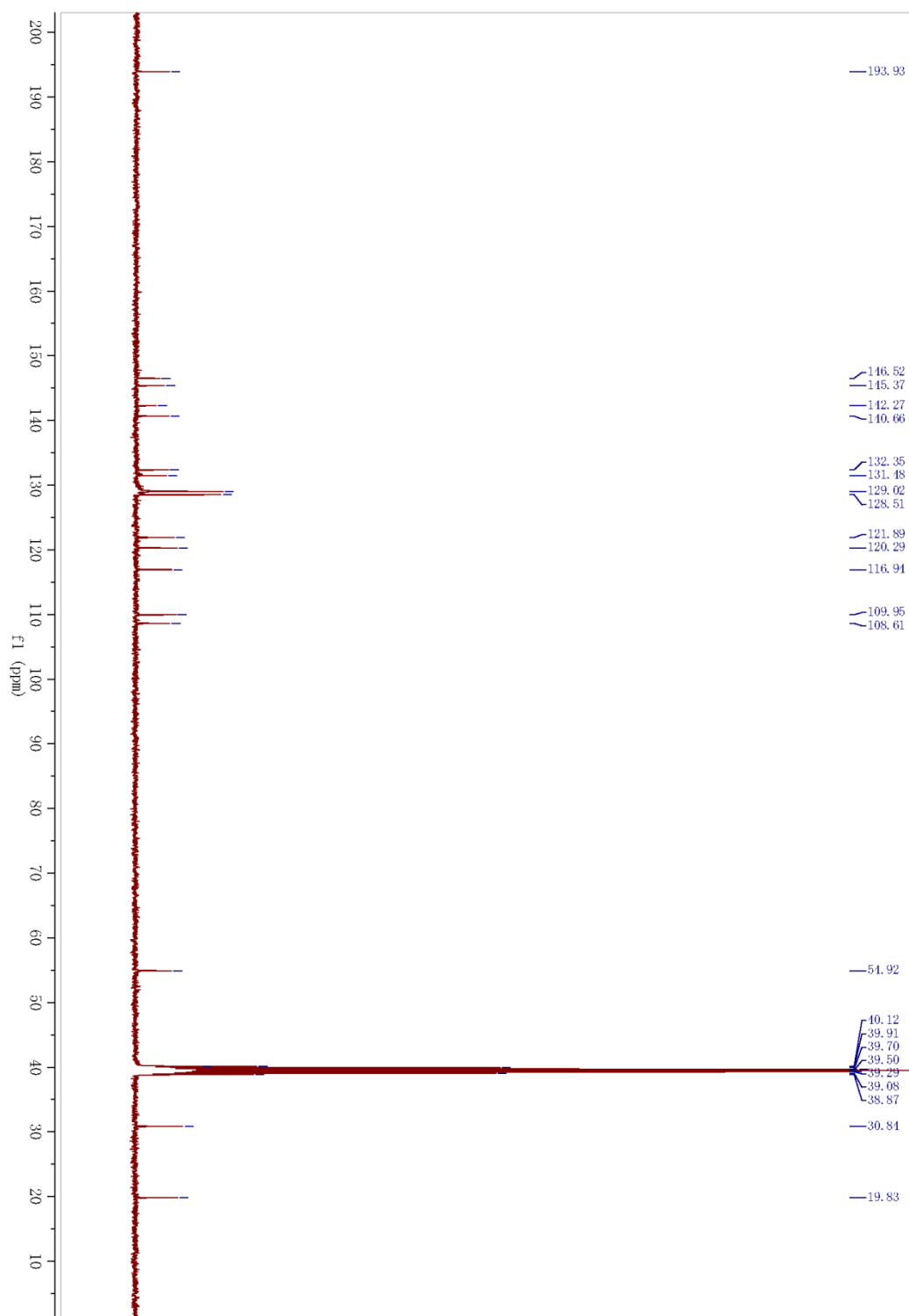
S49. LCMS spectrum of
1-(4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)
ethanone (**5q**).



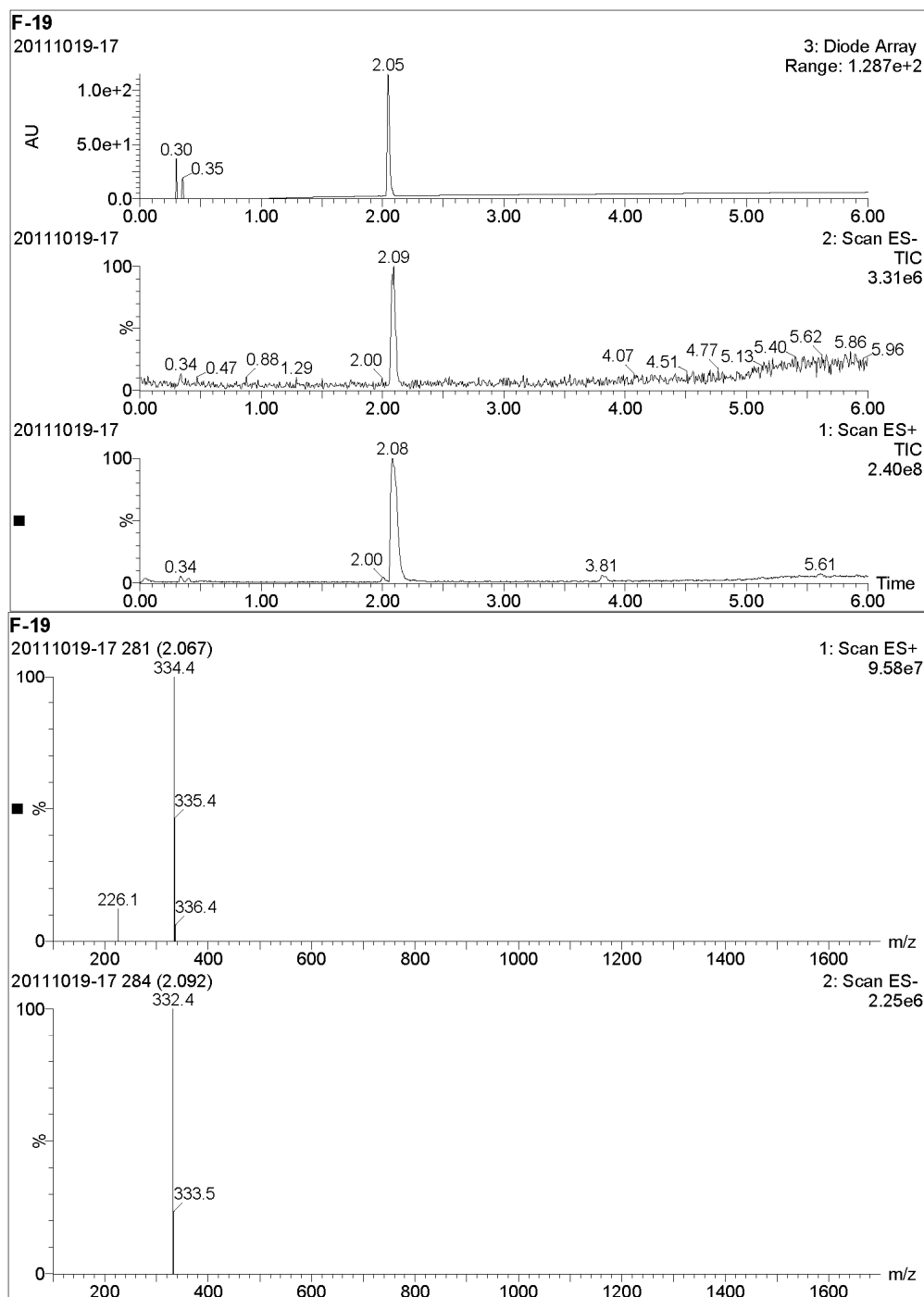
S50. ^1H NMR spectrum of
1-(4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)
ethanone (**5q**) in $\text{DMSO-}d_6$.



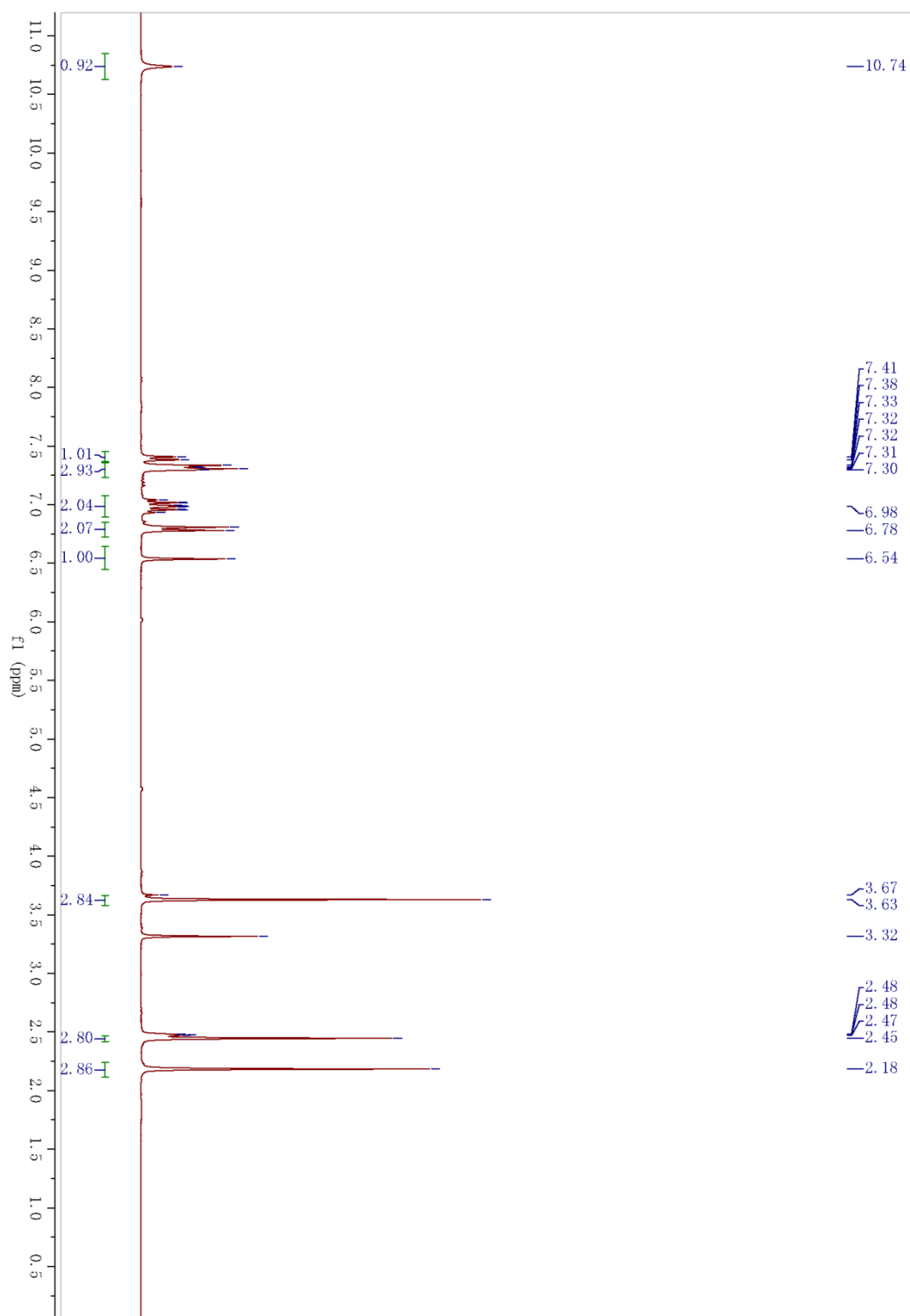
S51. ^{13}C NMR spectrum of
1-(4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)
ethanone (**5q**) in $\text{DMSO-}d_6$.



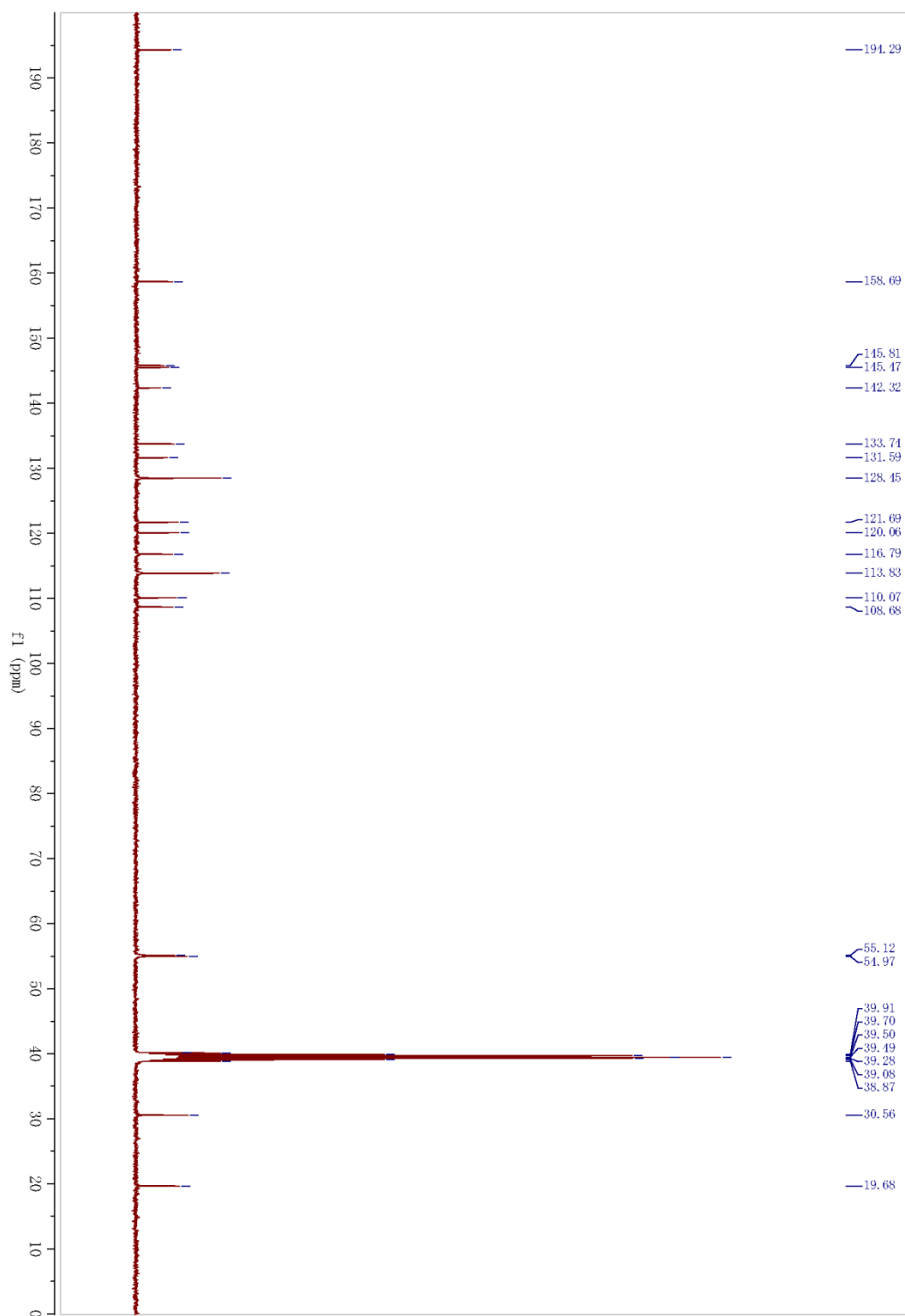
S52. LCMS spectrum of
1-(4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone (**5r**).



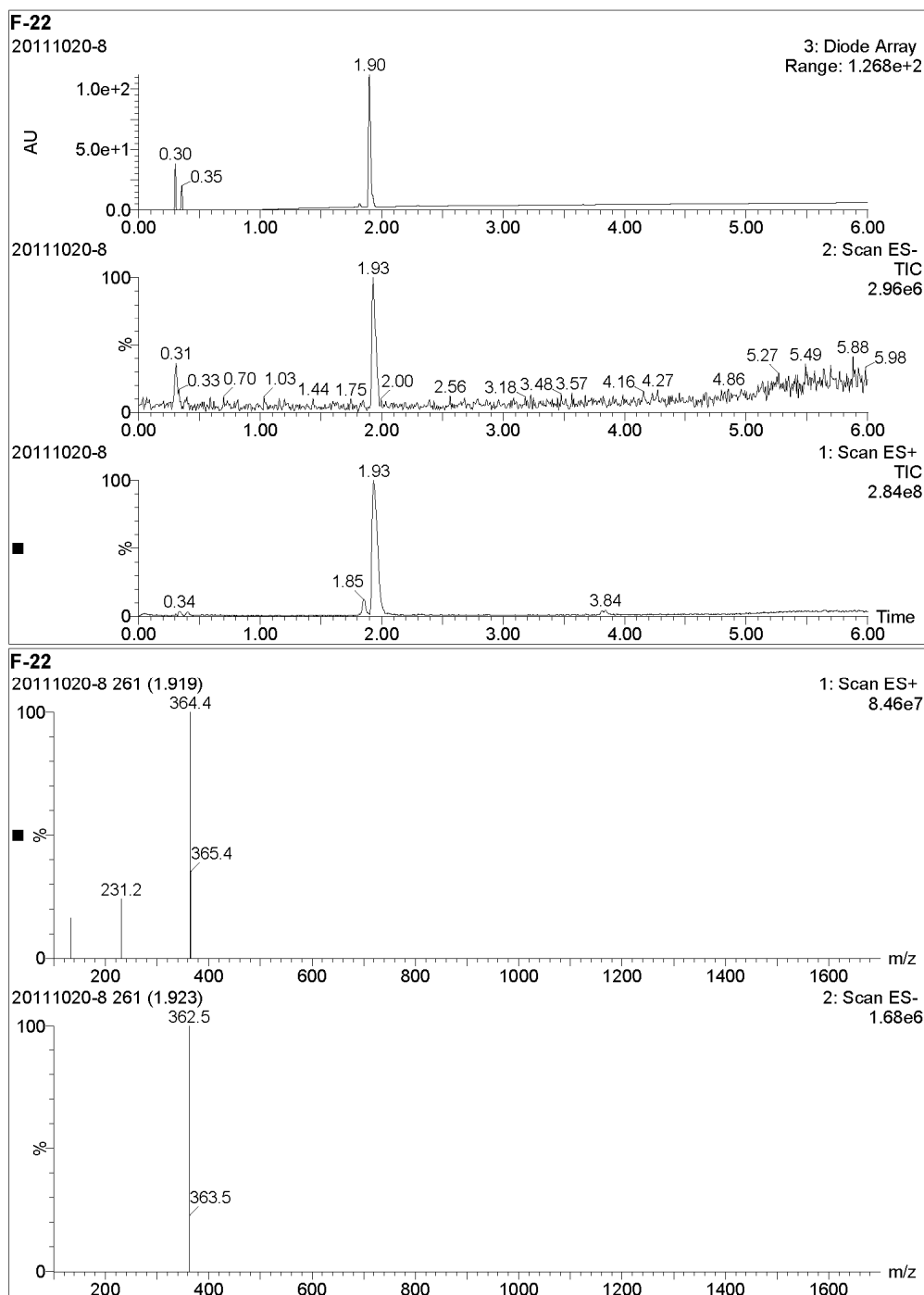
S53. ^1H NMR spectrum of
1-(4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone (**5r**) in $\text{DMSO-}d_6$.



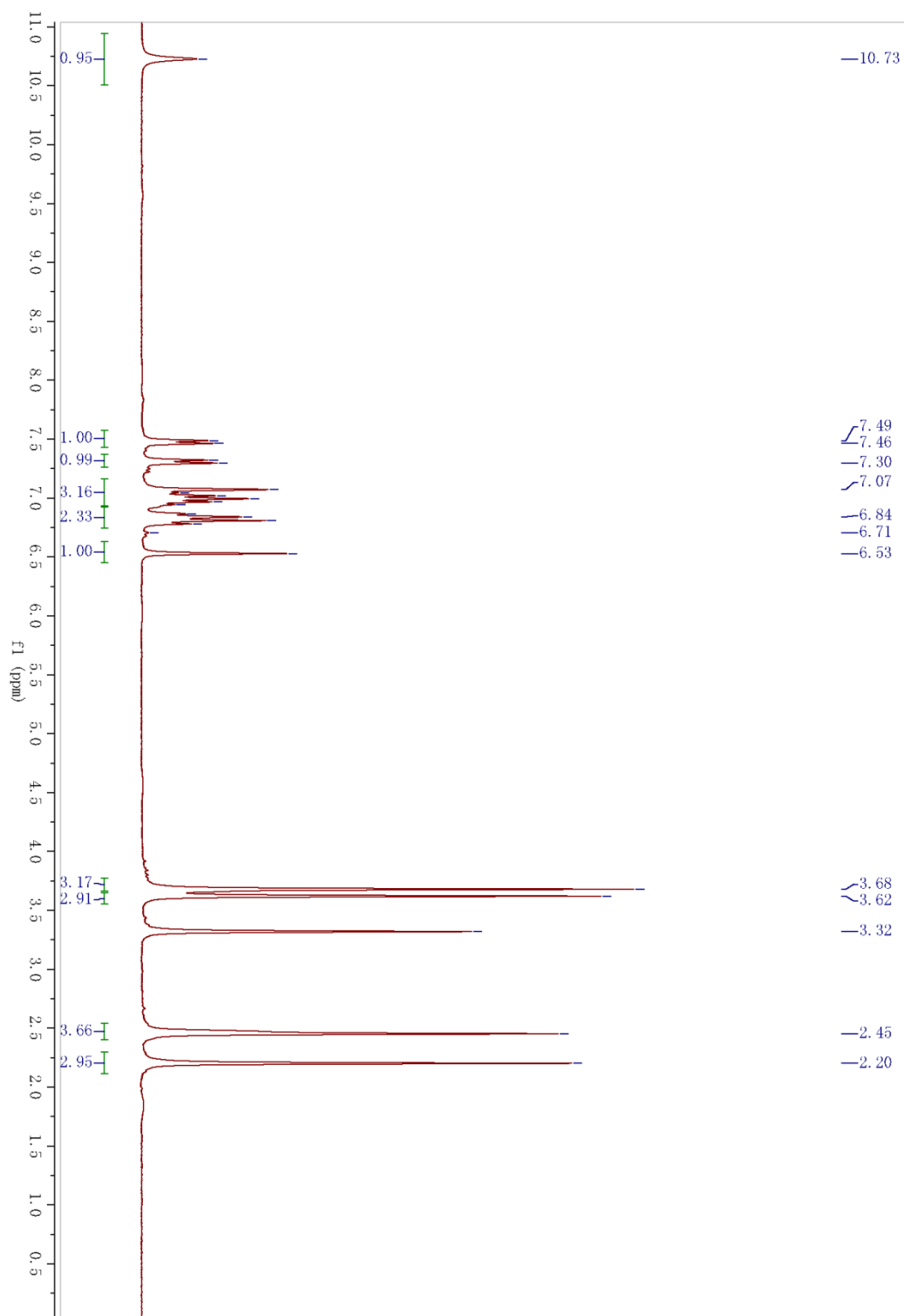
S54. ^{13}C NMR spectrum of
1-(4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin-3-yl)ethanone (**5r**) in $\text{DMSO-}d_6$.



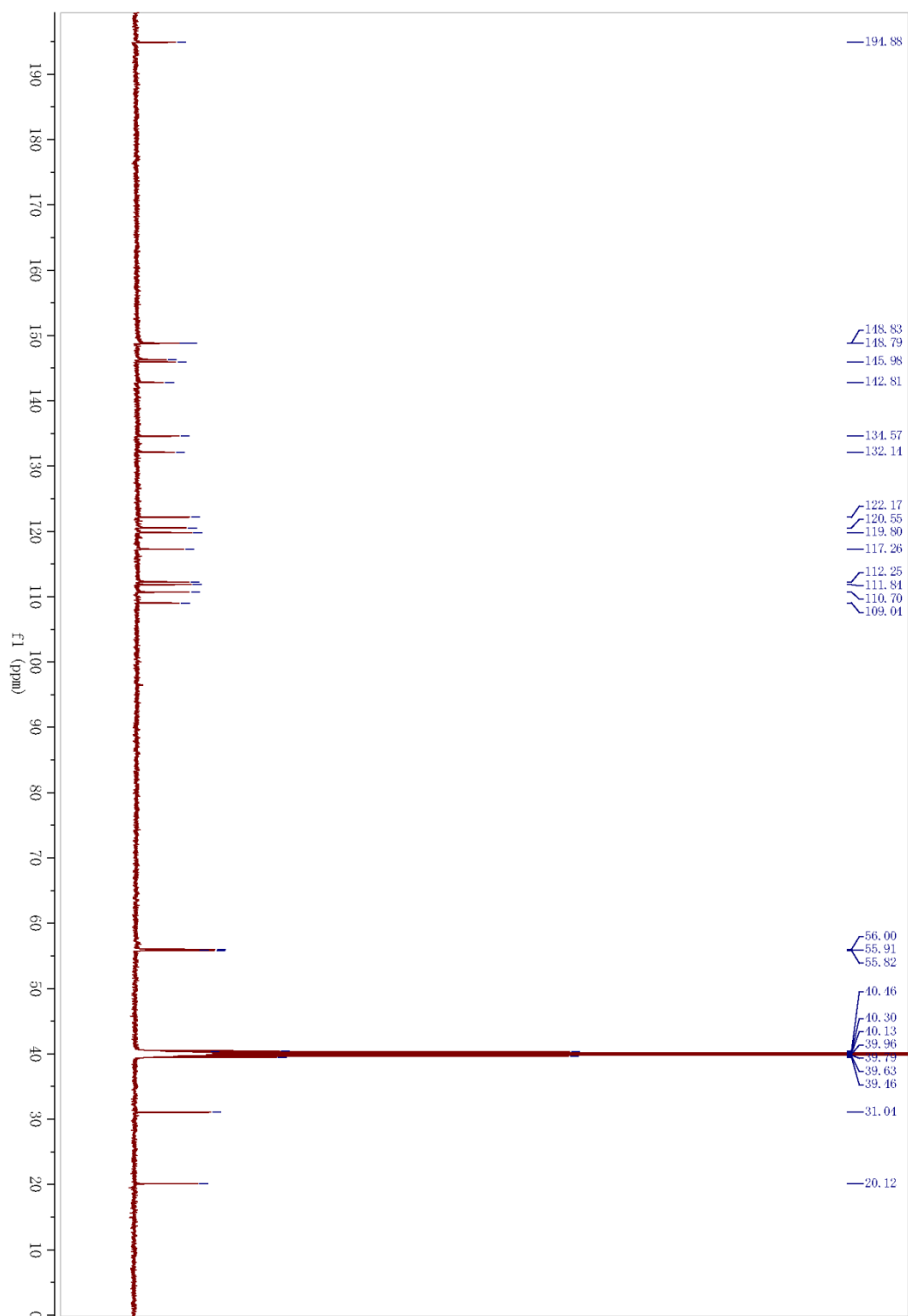
S55. LCMS spectrum of
1-(4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin
-3-yl)ethanone (**5s**).



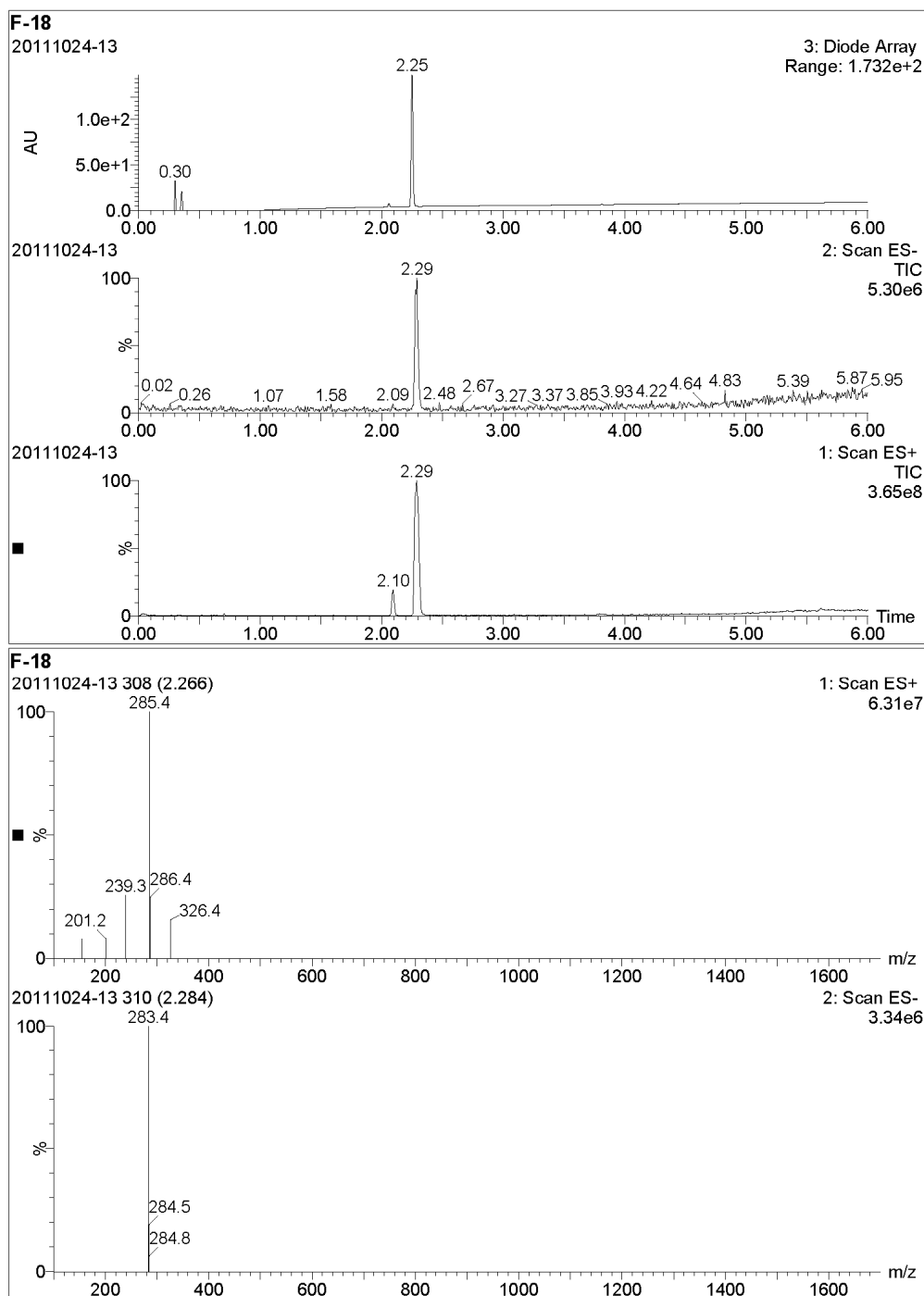
S56. ^1H NMR spectrum of
1-(4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin
-3-yl)ethanone (**5s**) in $\text{DMSO}-d_6$.



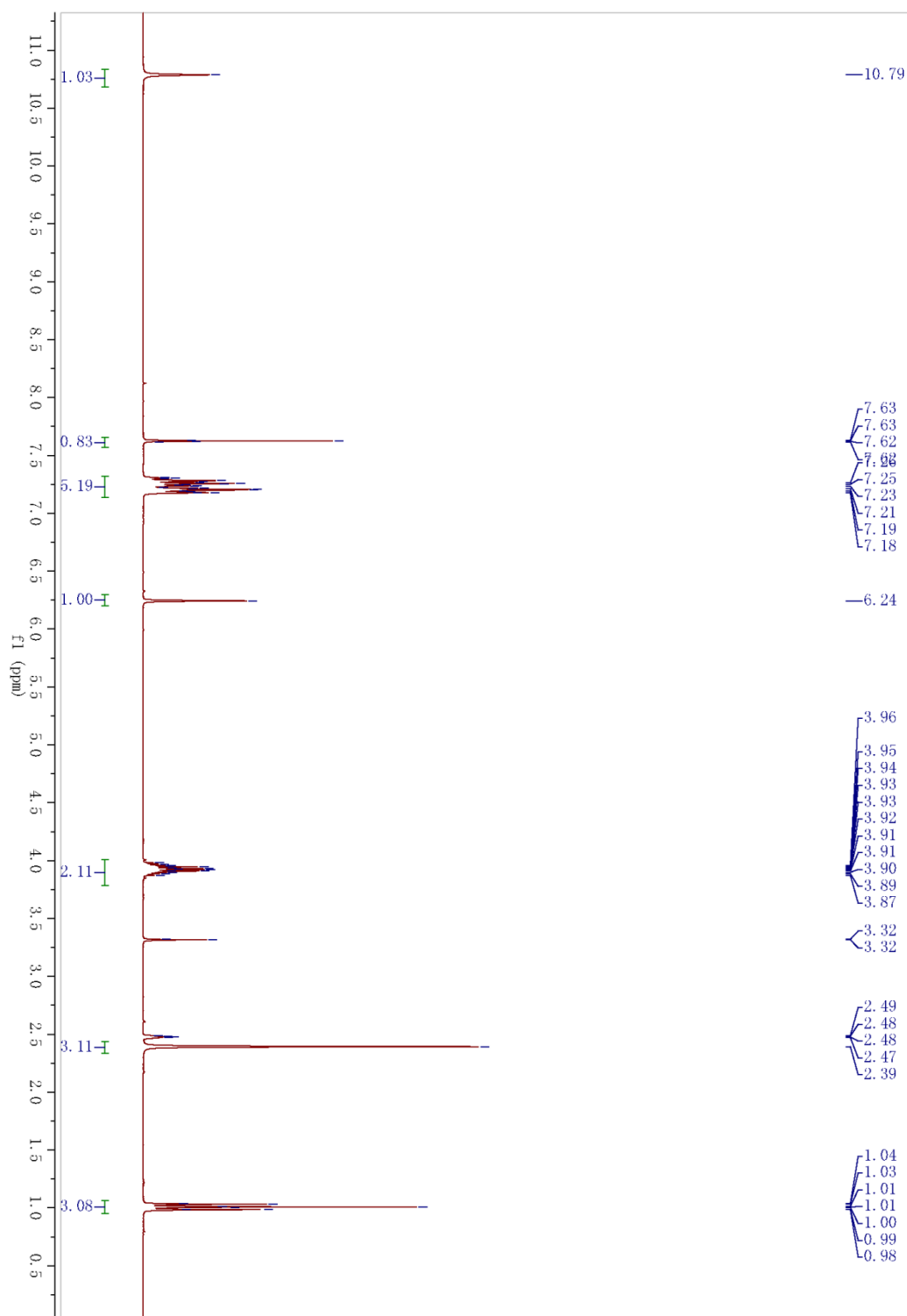
S57. ^{13}C NMR spectrum of
1-(4-(3,4-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidin
-3-yl)ethanone (**5s**) in $\text{DMSO-}d_6$.



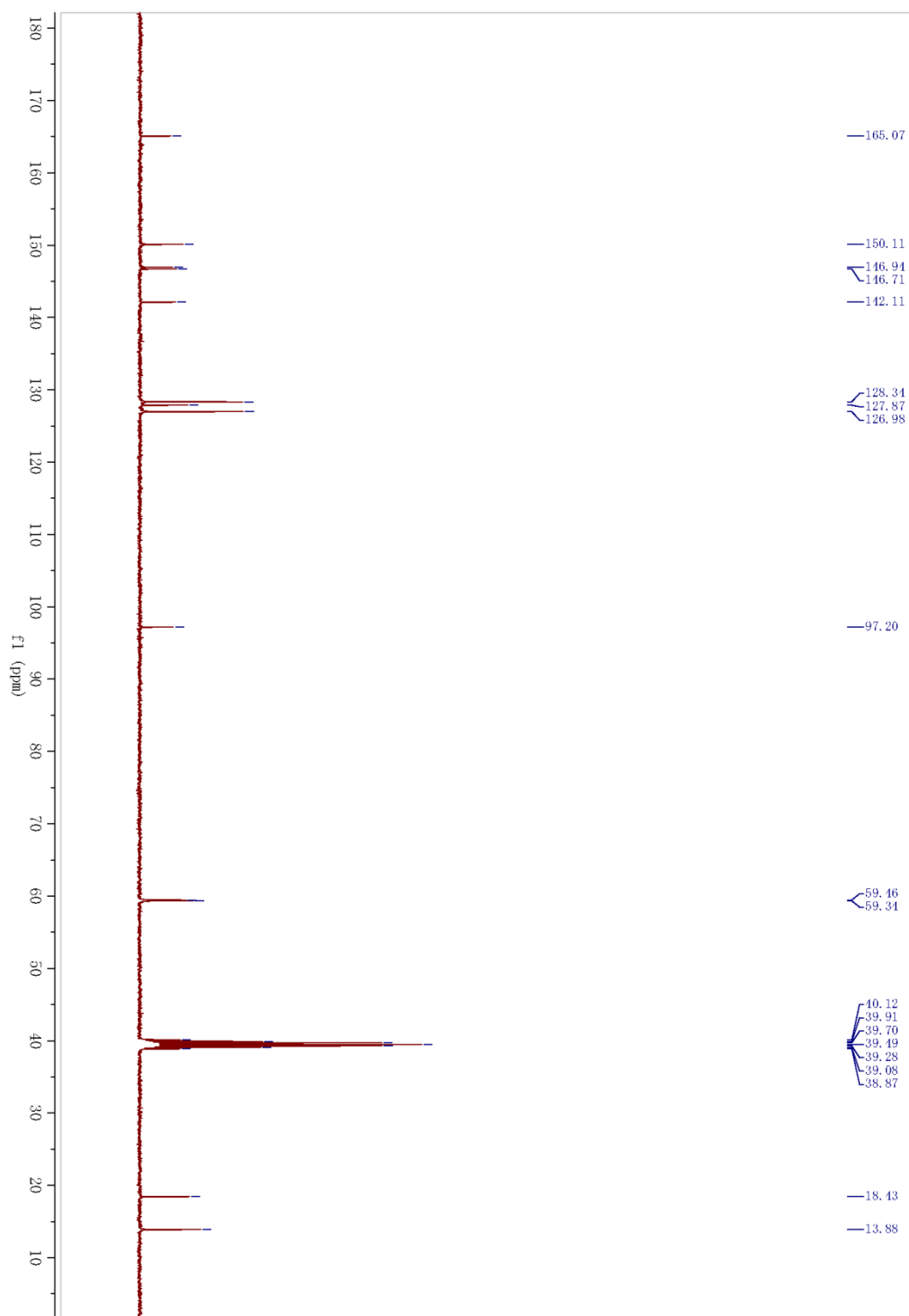
S58. LCMS spectrum of ethyl
5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6a**).



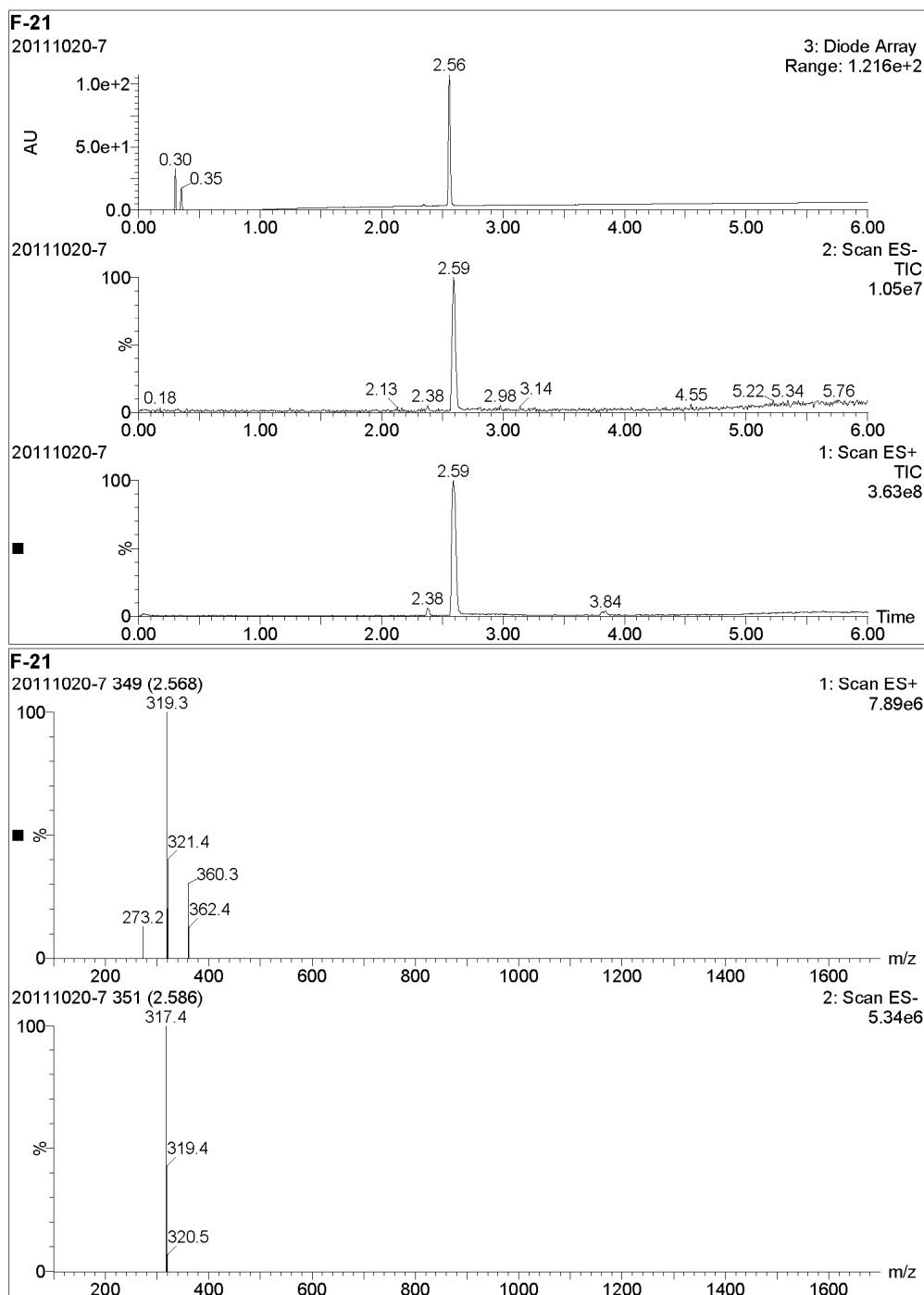
S59. ^1H NMR spectrum of ethyl 5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6a**) in $\text{DMSO-}d_6$.



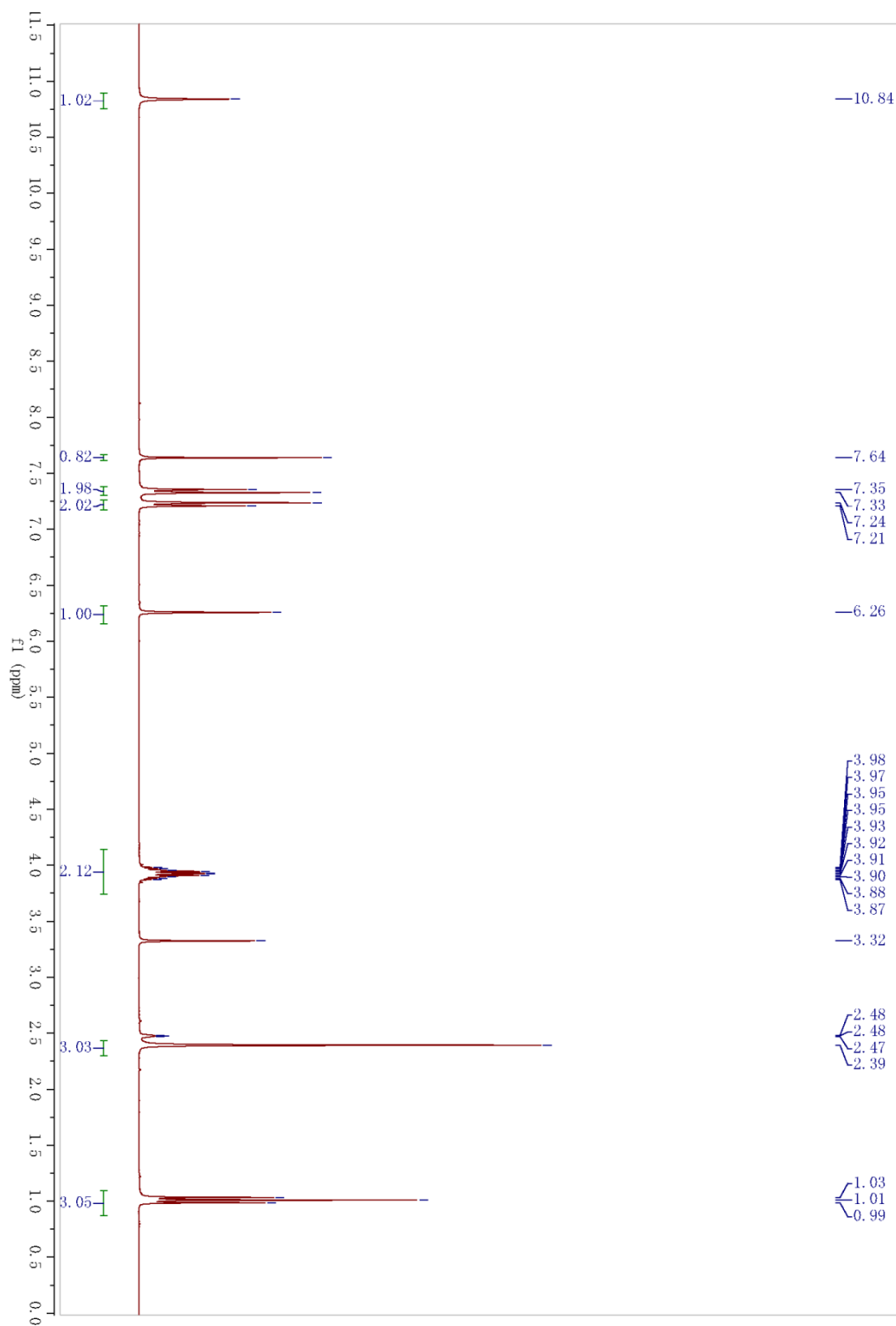
S60. ^{13}C NMR spectrum of ethyl 5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6a**) in DMSO- d_6 .



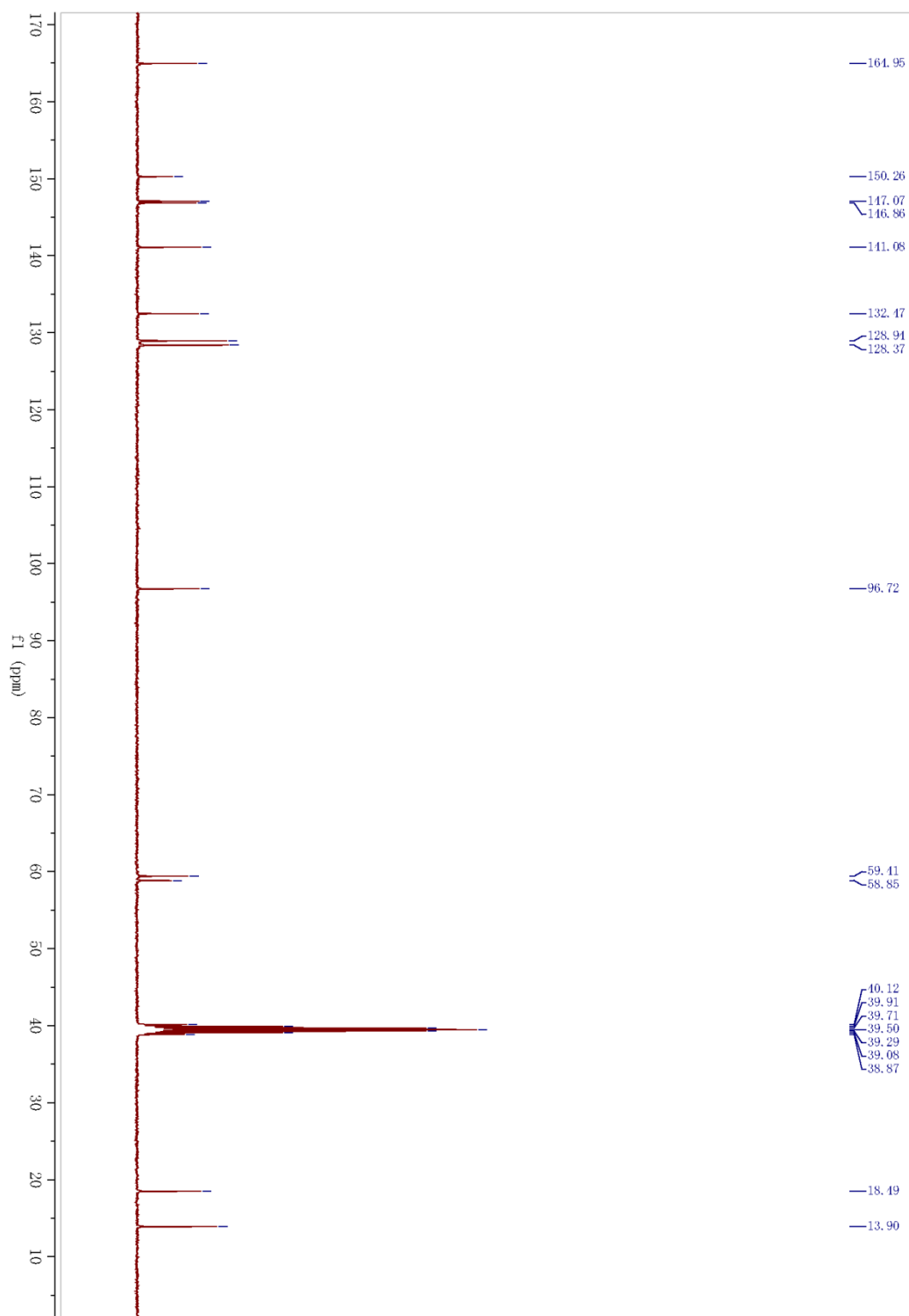
S61. LCMS spectrum of ethyl 7-(4-chlorophenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6b**).



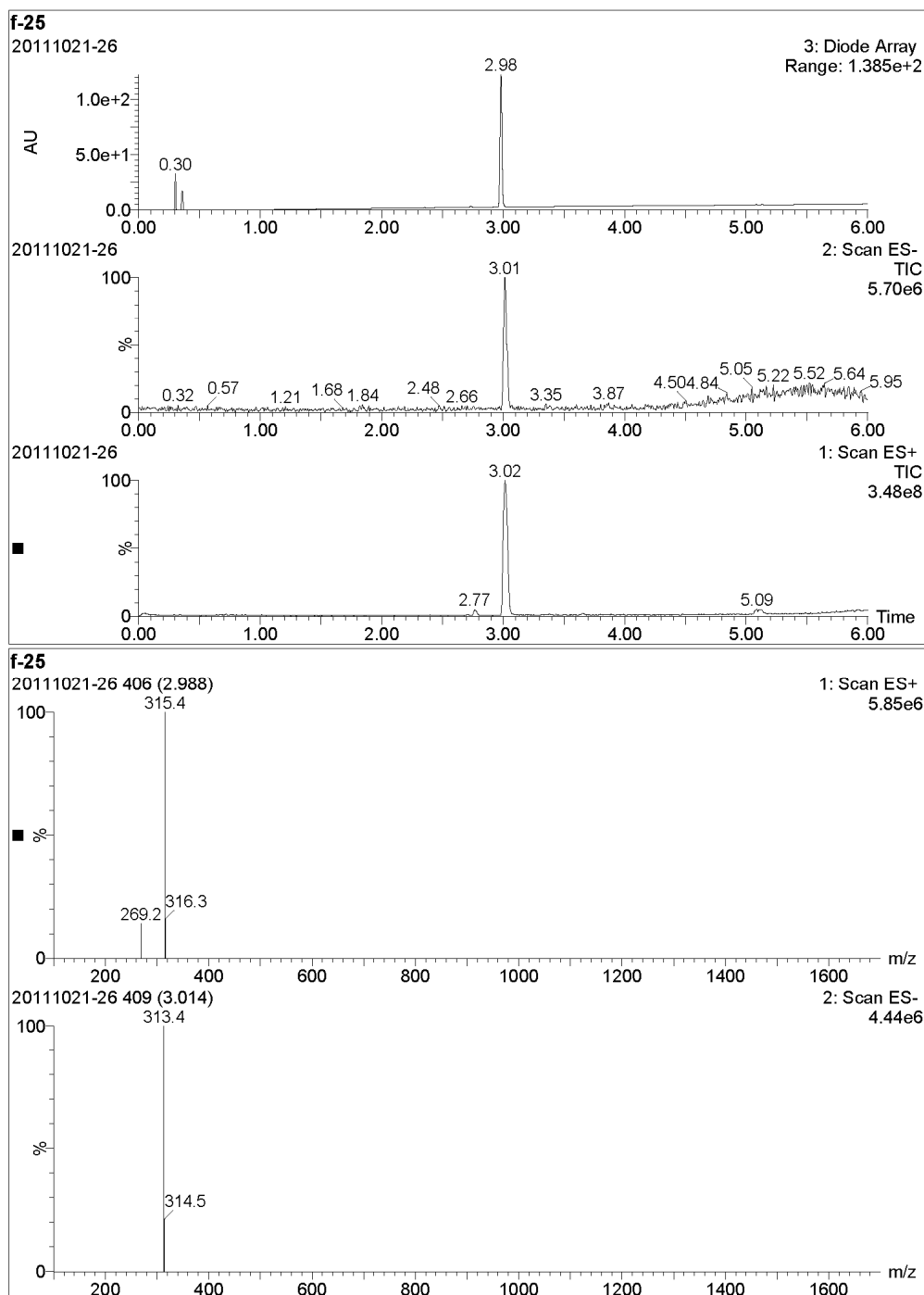
S62. ^1H NMR spectrum of ethyl 7-(4-chlorophenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6b**) in $\text{DMSO-}d_6$.



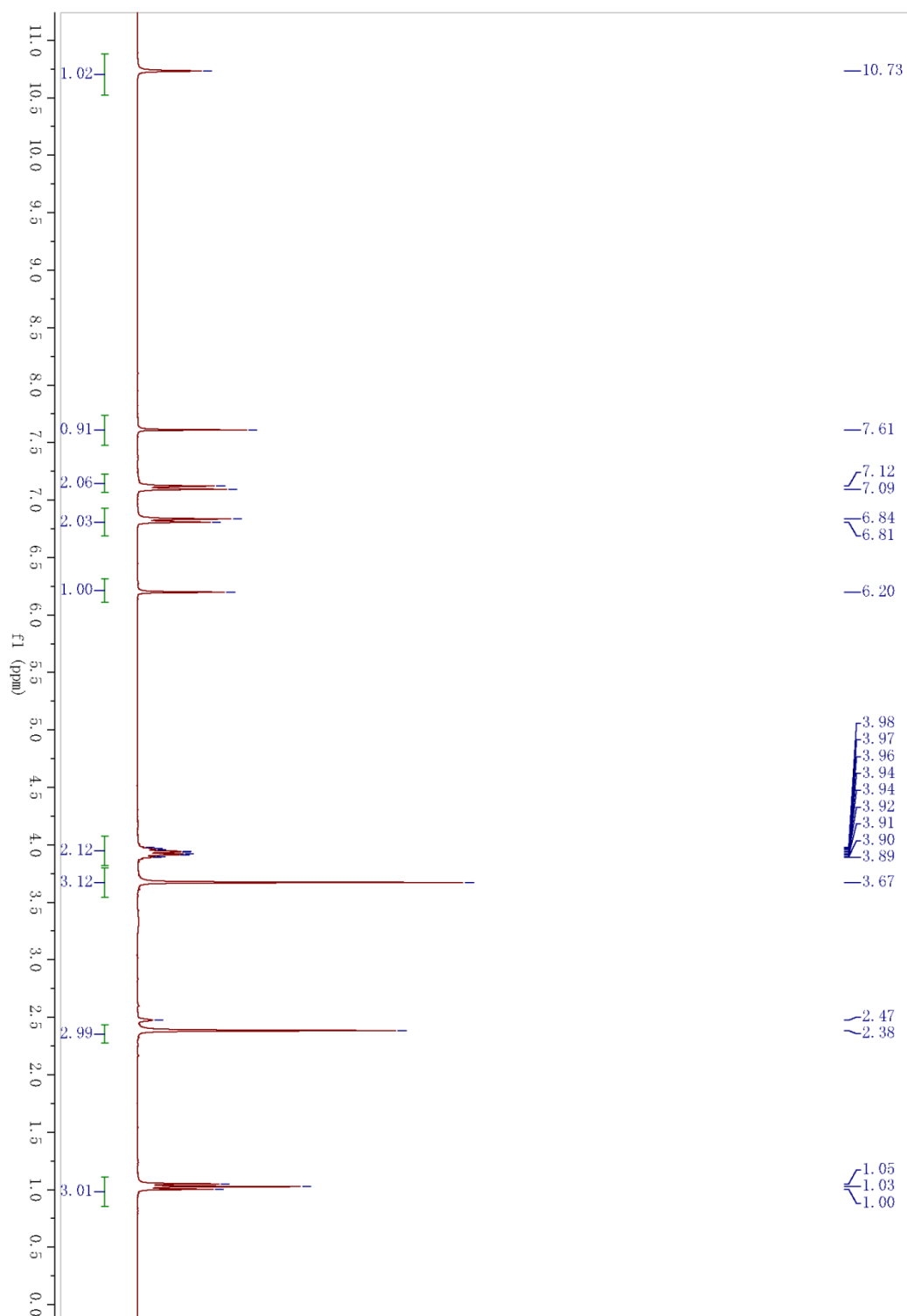
S63. ^{13}C NMR spectrum of ethyl 7-(4-chlorophenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6b**) in $\text{DMSO-}d_6$.



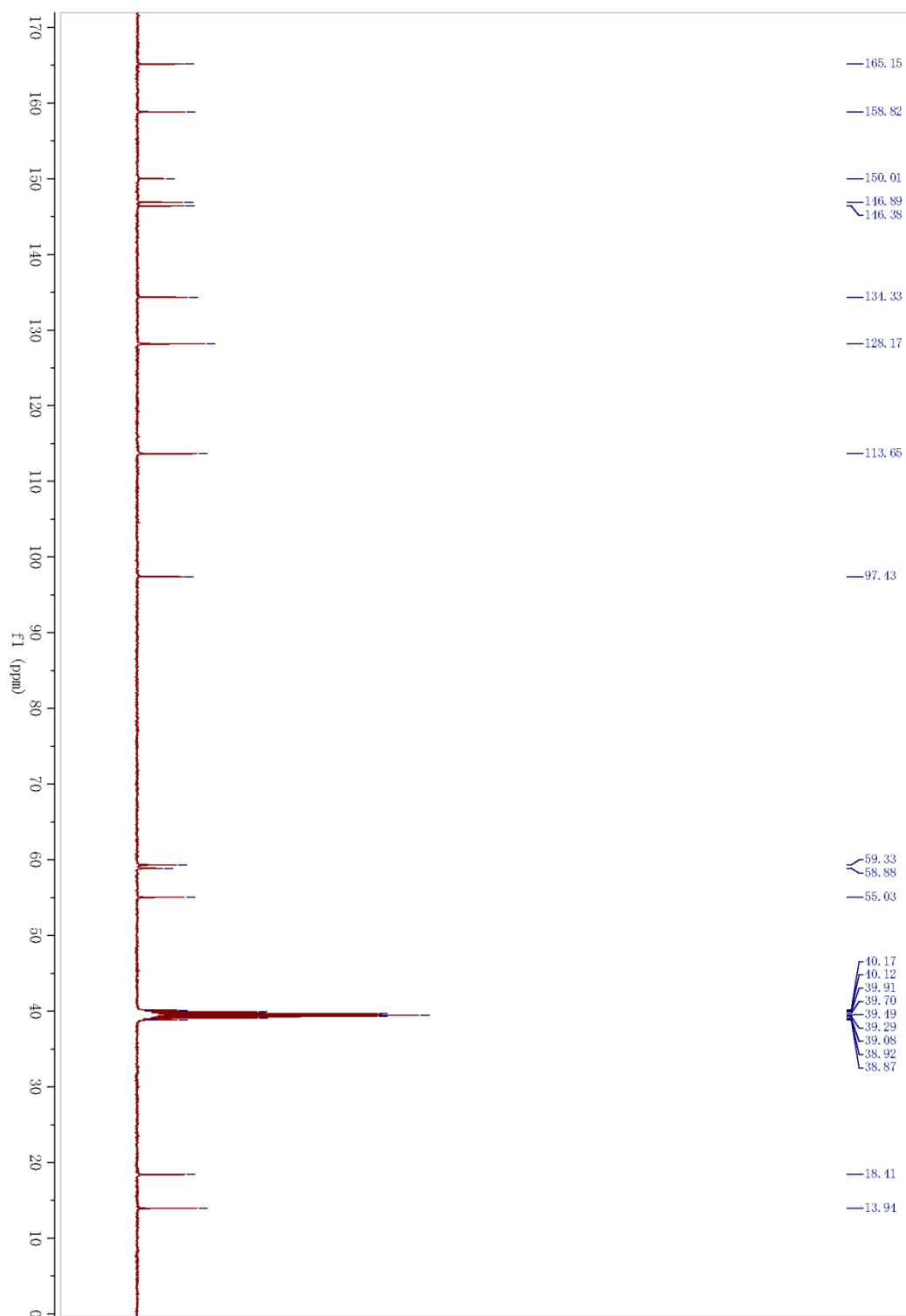
S64. LCMS spectrum of ethyl 7-(4-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6c**).



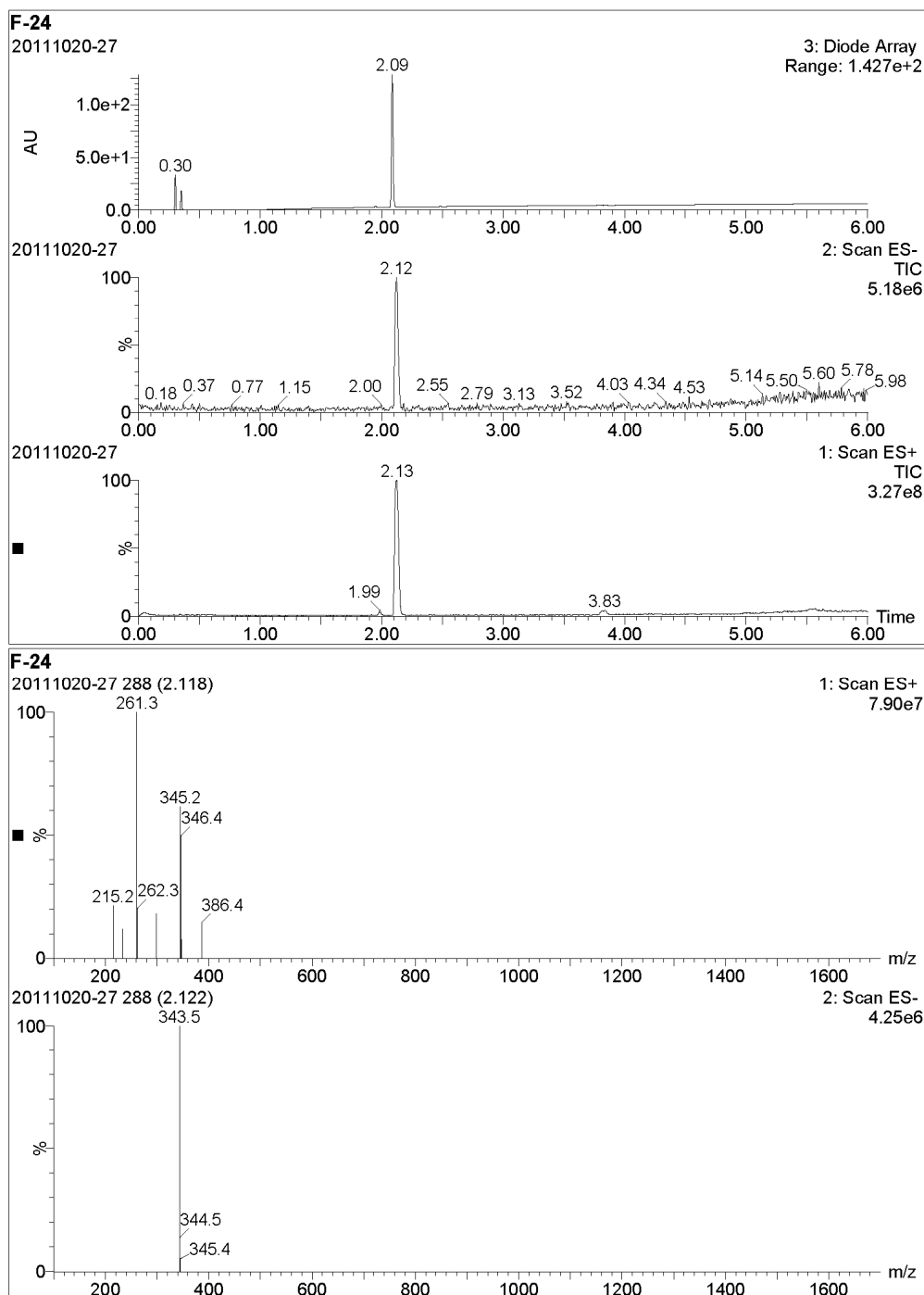
S65. ^1H NMR spectrum of ethyl 7-(4-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6c**) in $\text{DMSO-}d_6$.



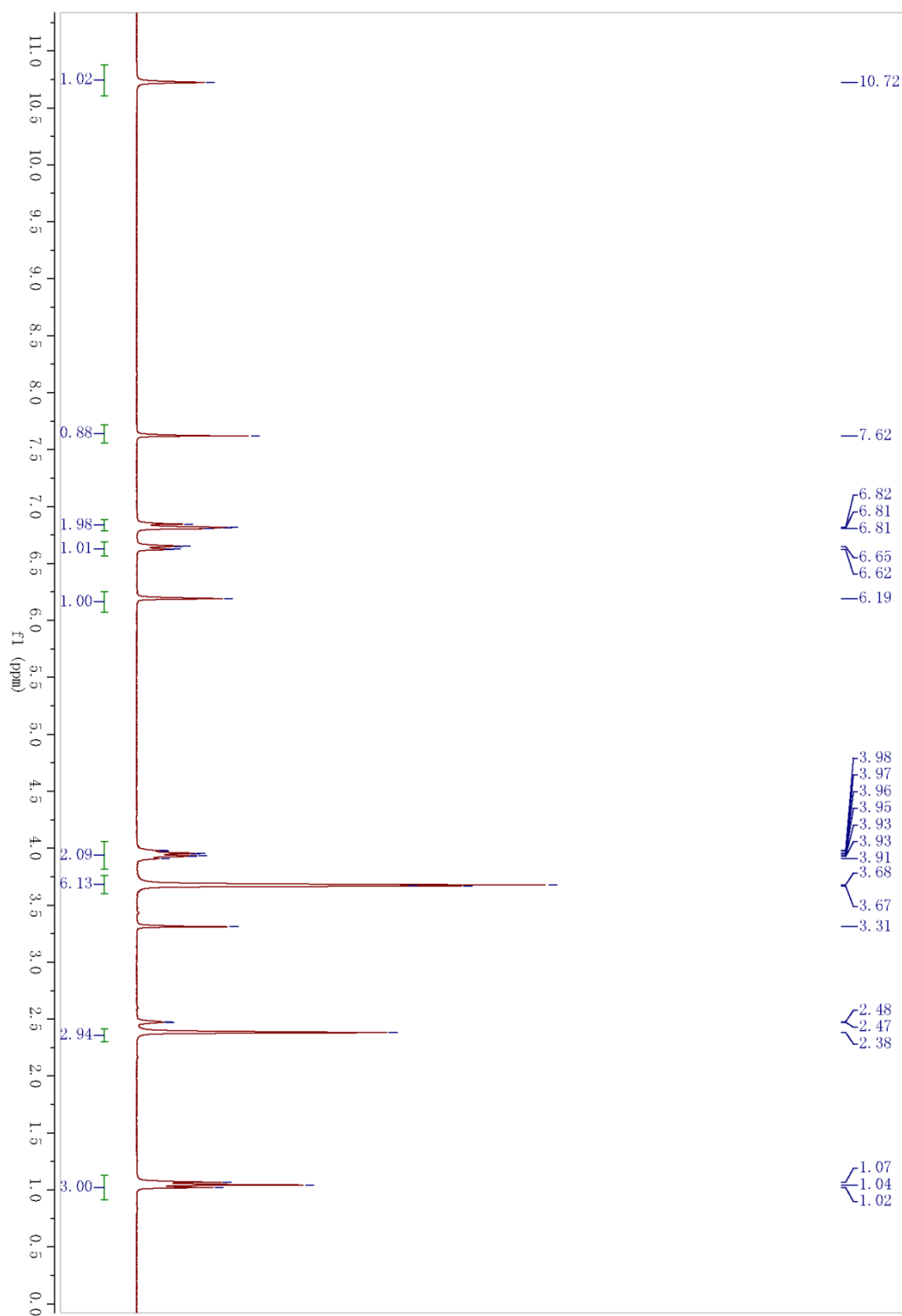
S66. ^{13}C NMR spectrum of ethyl 7-(4-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6c**) in $\text{DMSO-}d_6$.



S67. LCMS spectrum of ethyl 7-(3,4-dimethoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6d**).



S68. ^1H NMR spectrum of ethyl 7-(3,4-dimethoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6d**) in $\text{DMSO}-d_6$.



S69. ^{13}C NMR spectrum of ethyl 7-(3,4-dimethoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carboxylate (**6d**) in $\text{DMSO-}d_6$.

