

**Design, synthesis and biological activity of novel methoxy and hydroxy substituted
N- benzimidazole derived carboxamides**

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2. Figures S63: Reaction scheme for the preparation of compounds **1–6**

Figure S1. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-phenylacrylonitrile 17

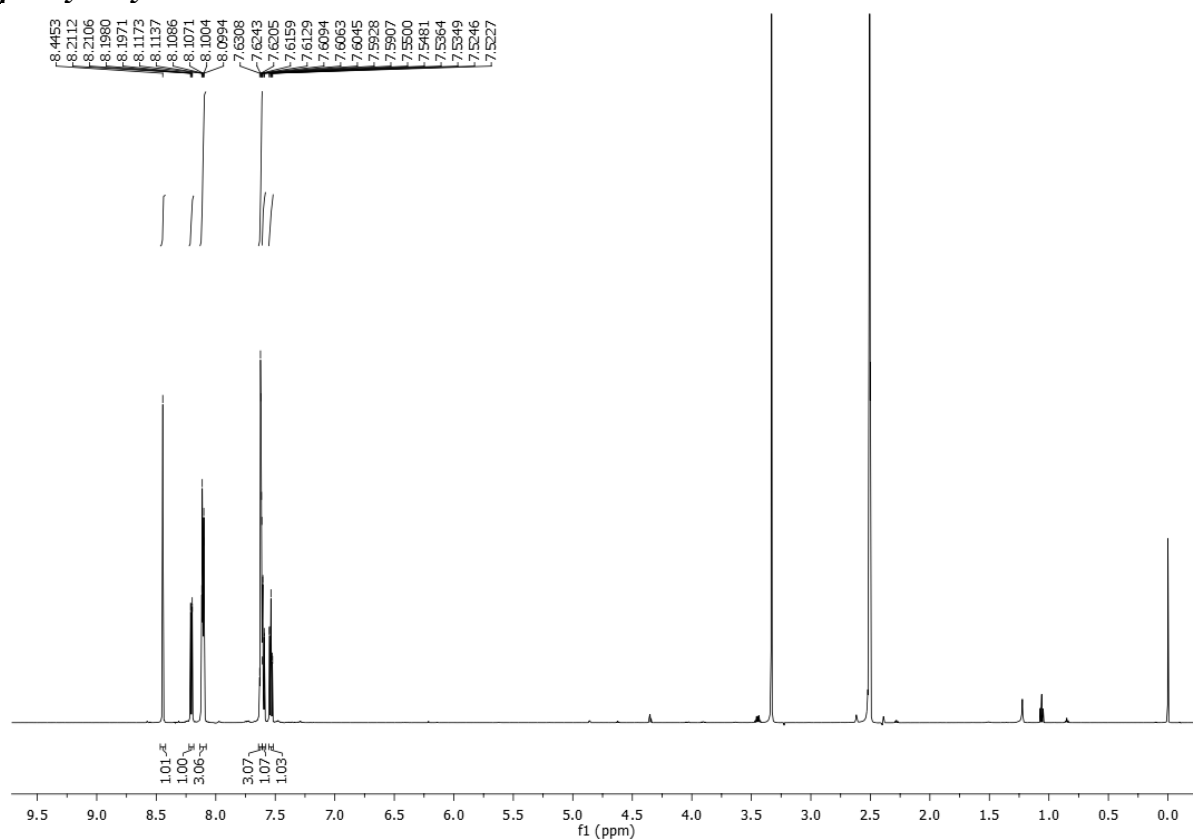


Figure S2. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-phenylacrylonitrile 17

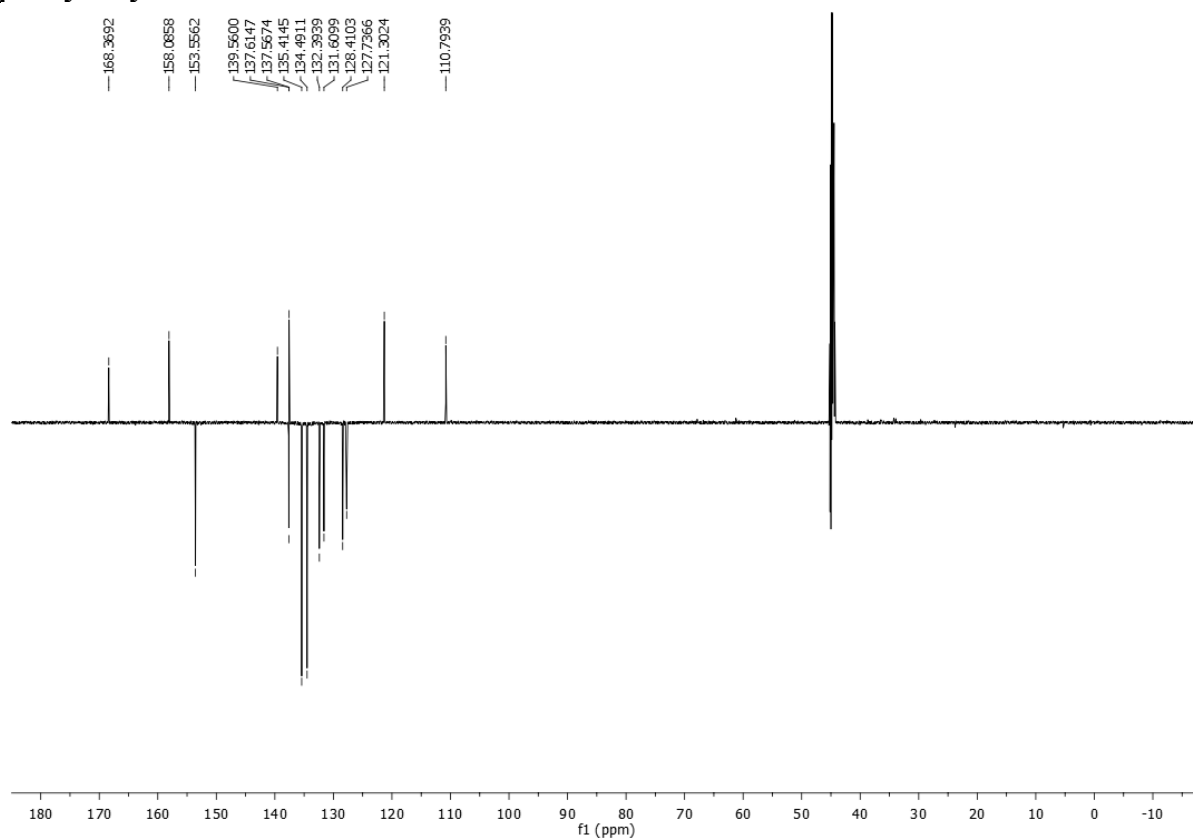


Figure S3. ^1H NMR spectrum (DMSO- d_6 , 300 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(2-methoxyphenyl)acrylonitrile 18

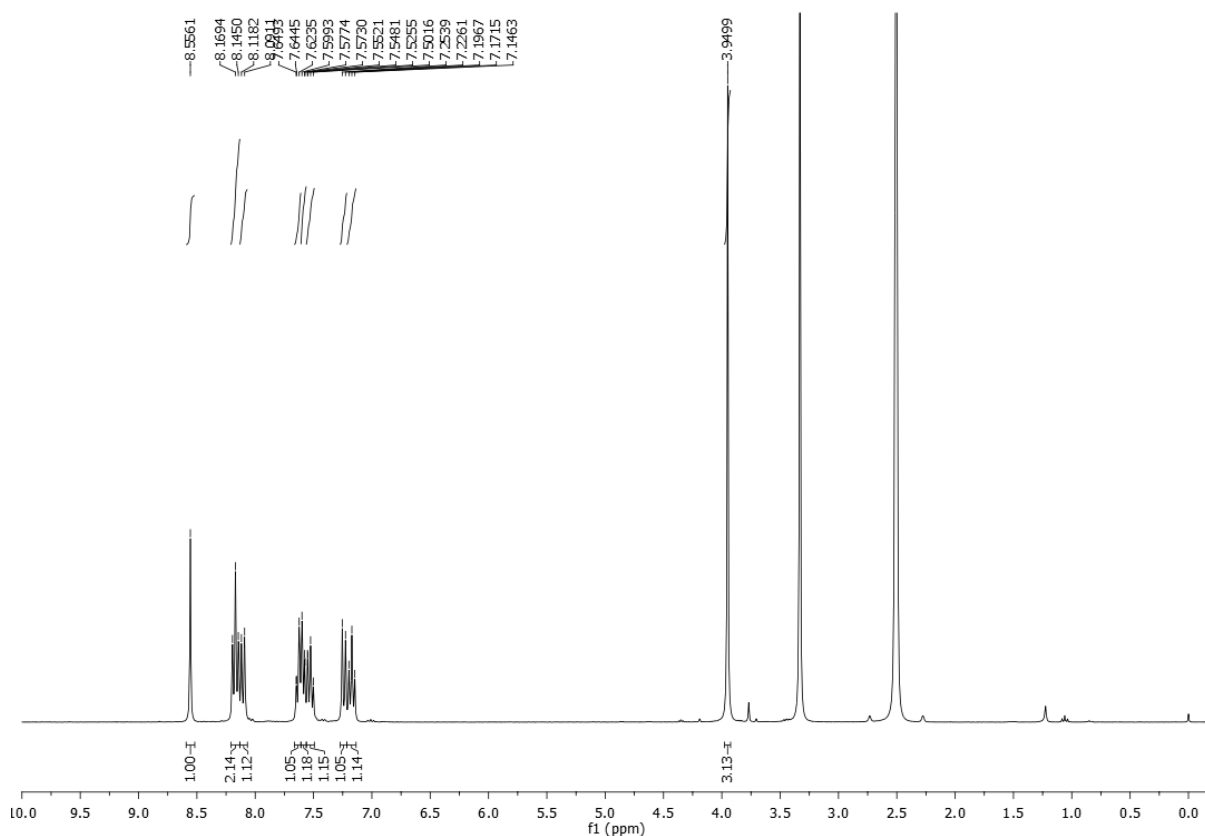


Figure S4. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(2-methoxyphenyl)acrylonitrile 18

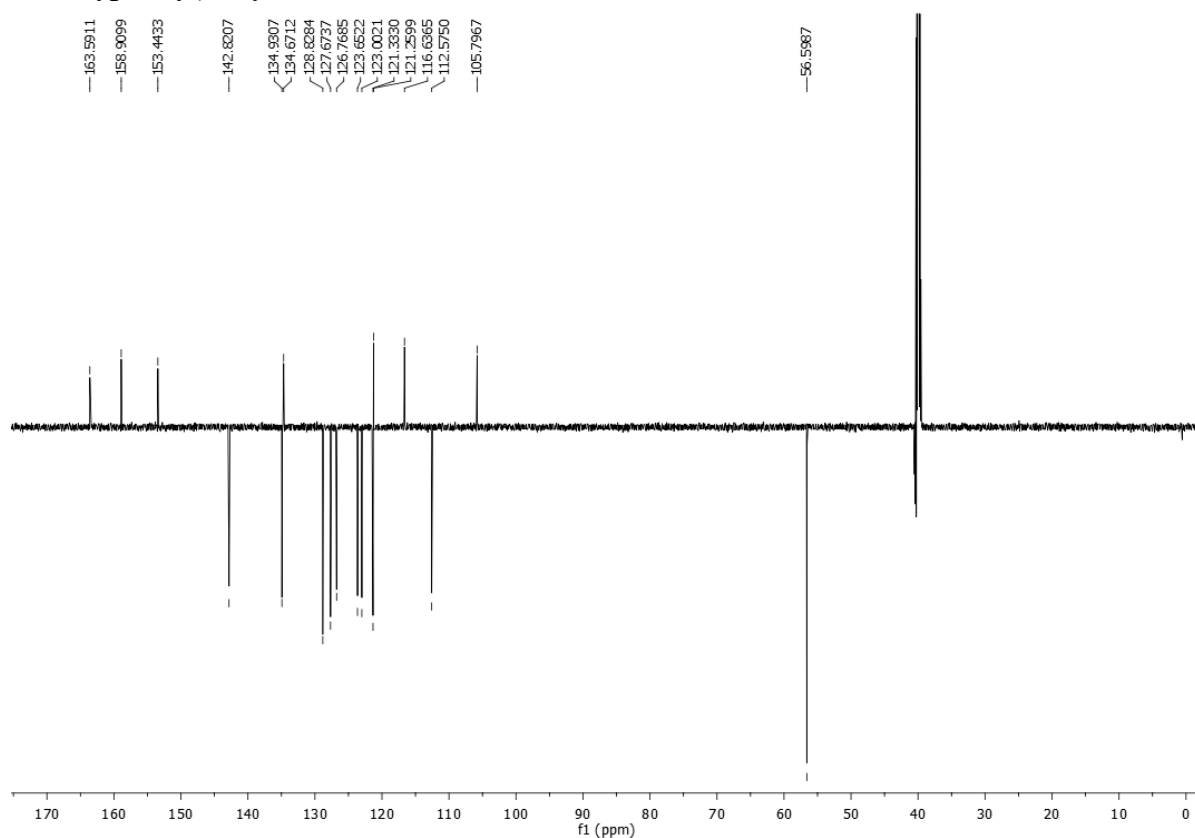


Figure S5. ^1H NMR spectrum (DMSO- d_6 , 300 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(2,4-dimethoxyphenyl)acrylonitrile 19

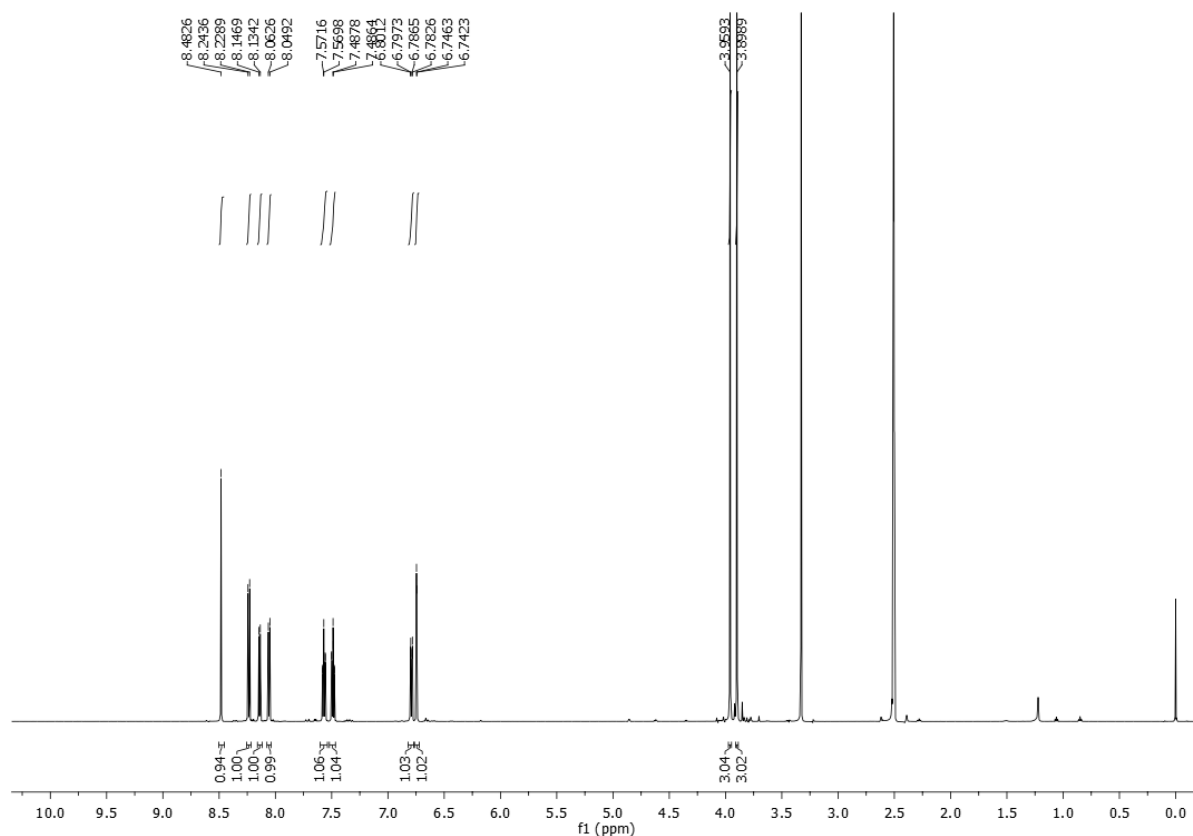


Figure S6. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(2,4-dimethoxyphenyl)acrylonitrile 19

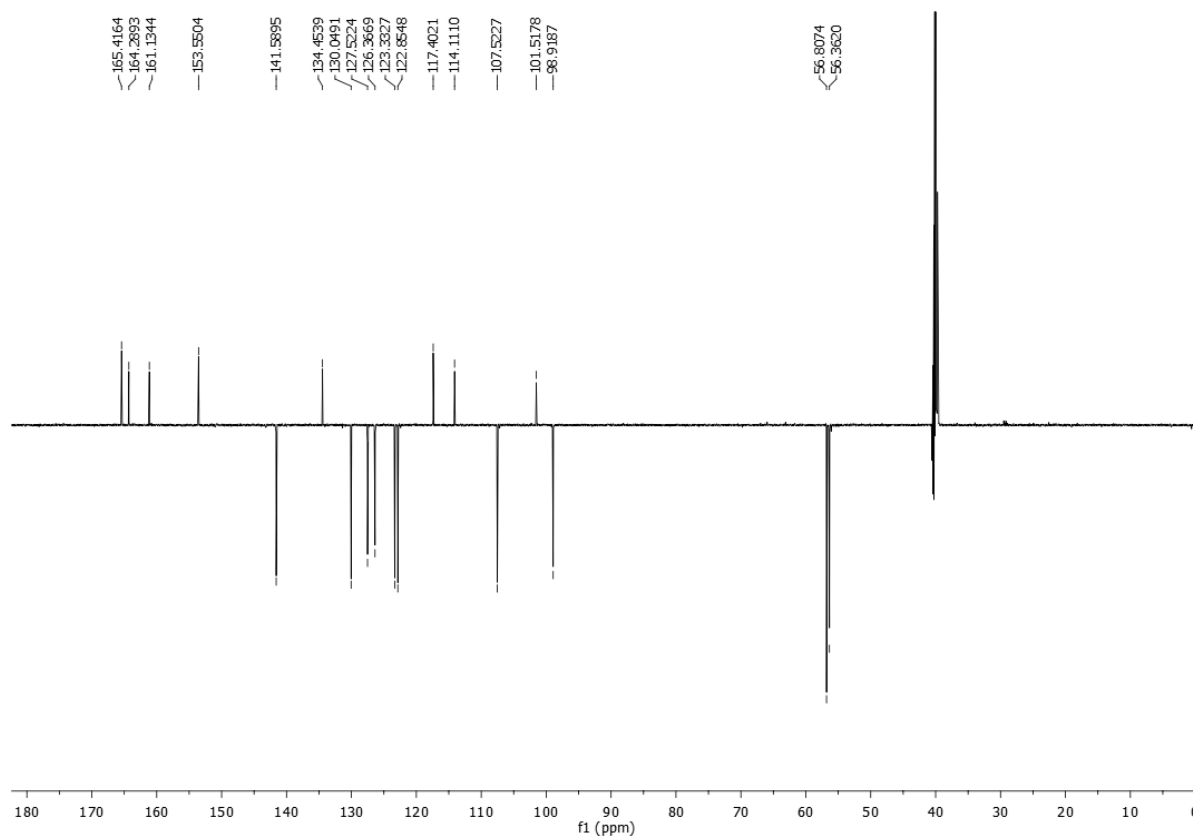


Figure S7. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4,5-trimethoxyphenyl)acrylonitrile 20

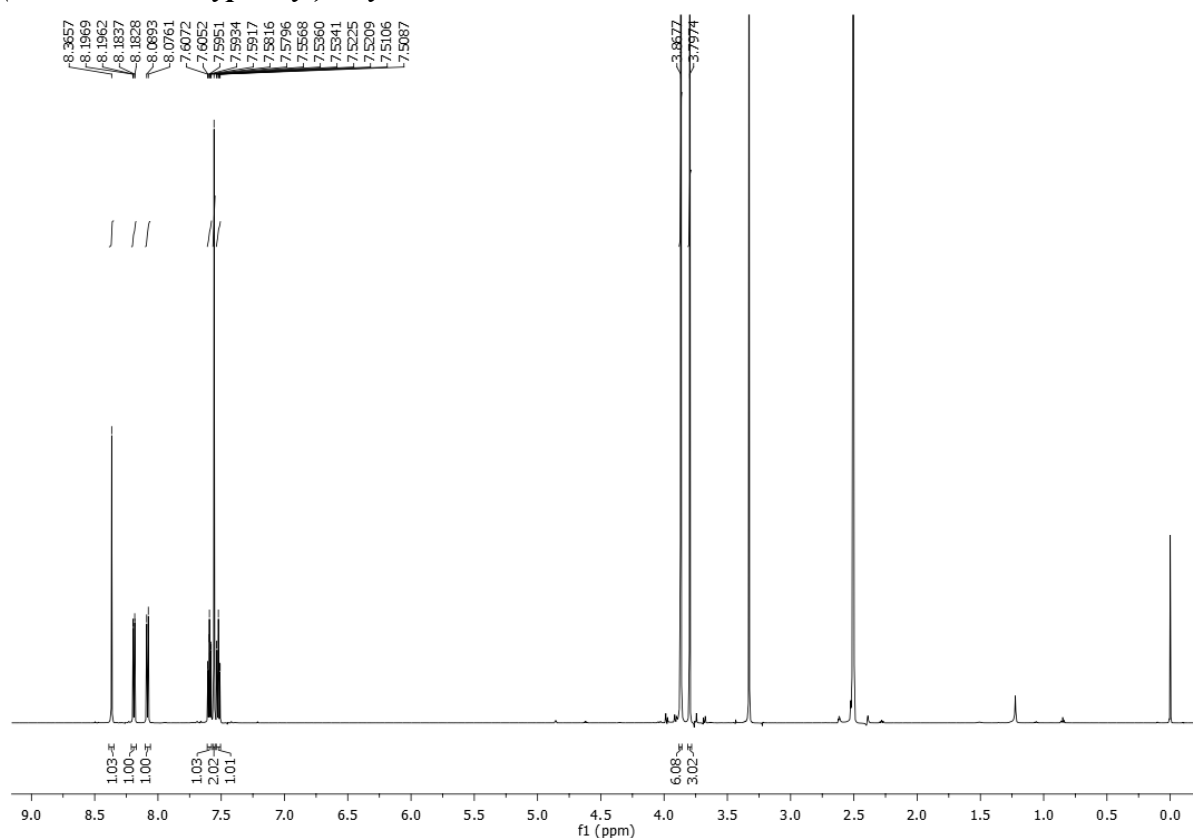


Figure S8. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4,5-trimethoxyphenyl)acrylonitrile 20

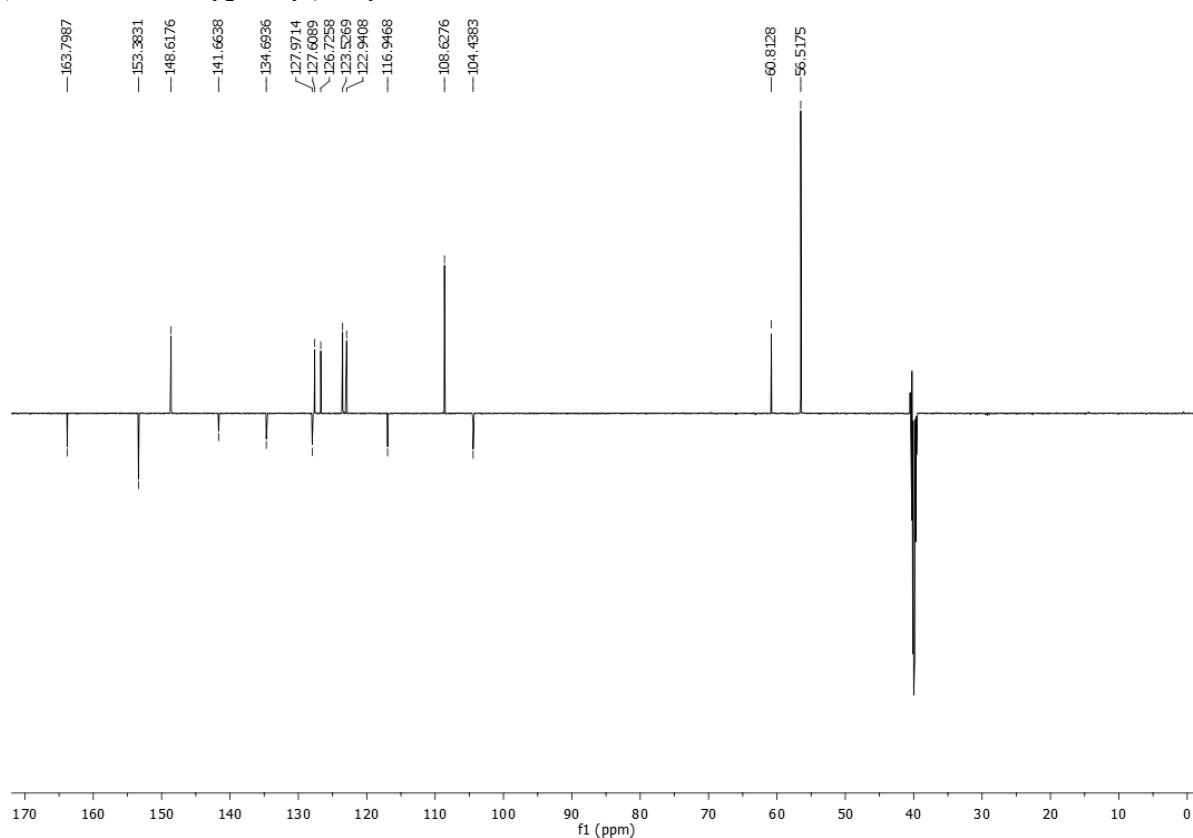


Figure S9. ^1H NMR spectrum (DMSO- d_6 , 300 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(4-hydroxyphenyl)acrylonitrile 21

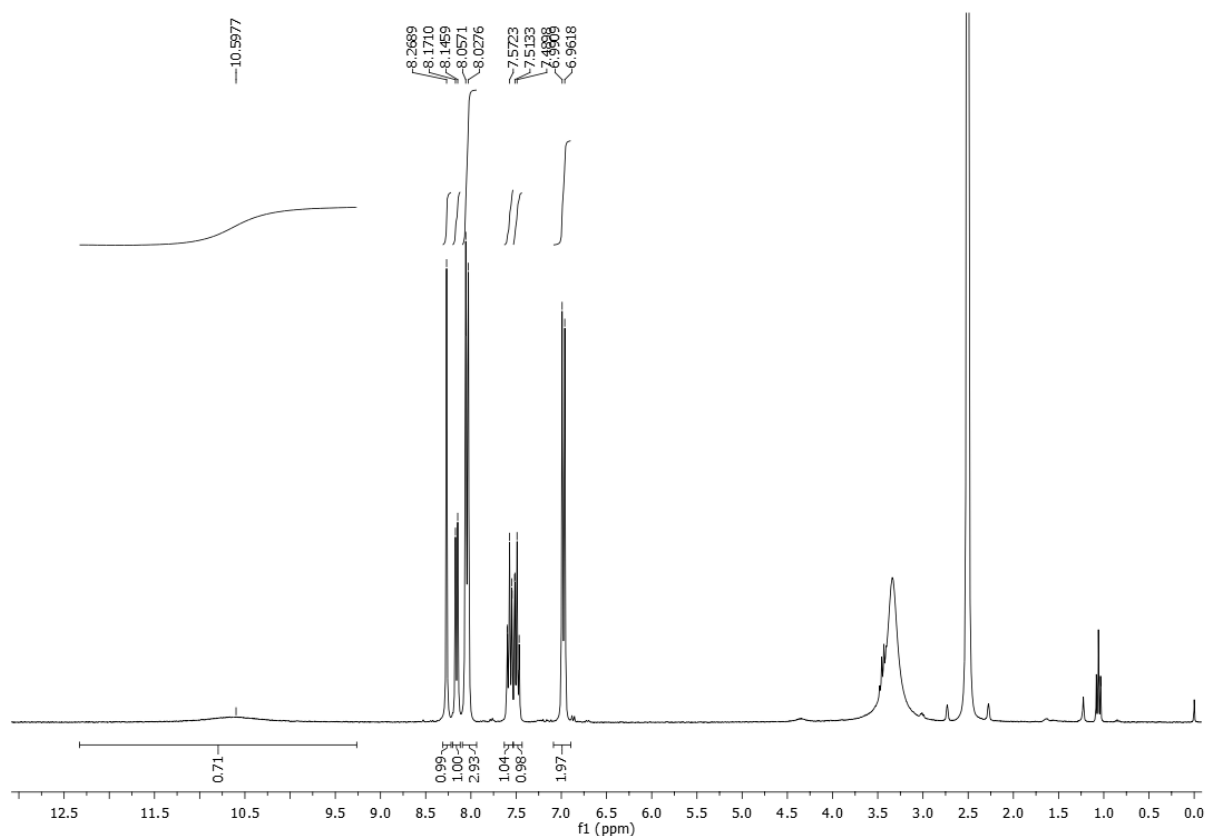


Figure S10. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(4-hydroxyphenyl)acrylonitrile 21

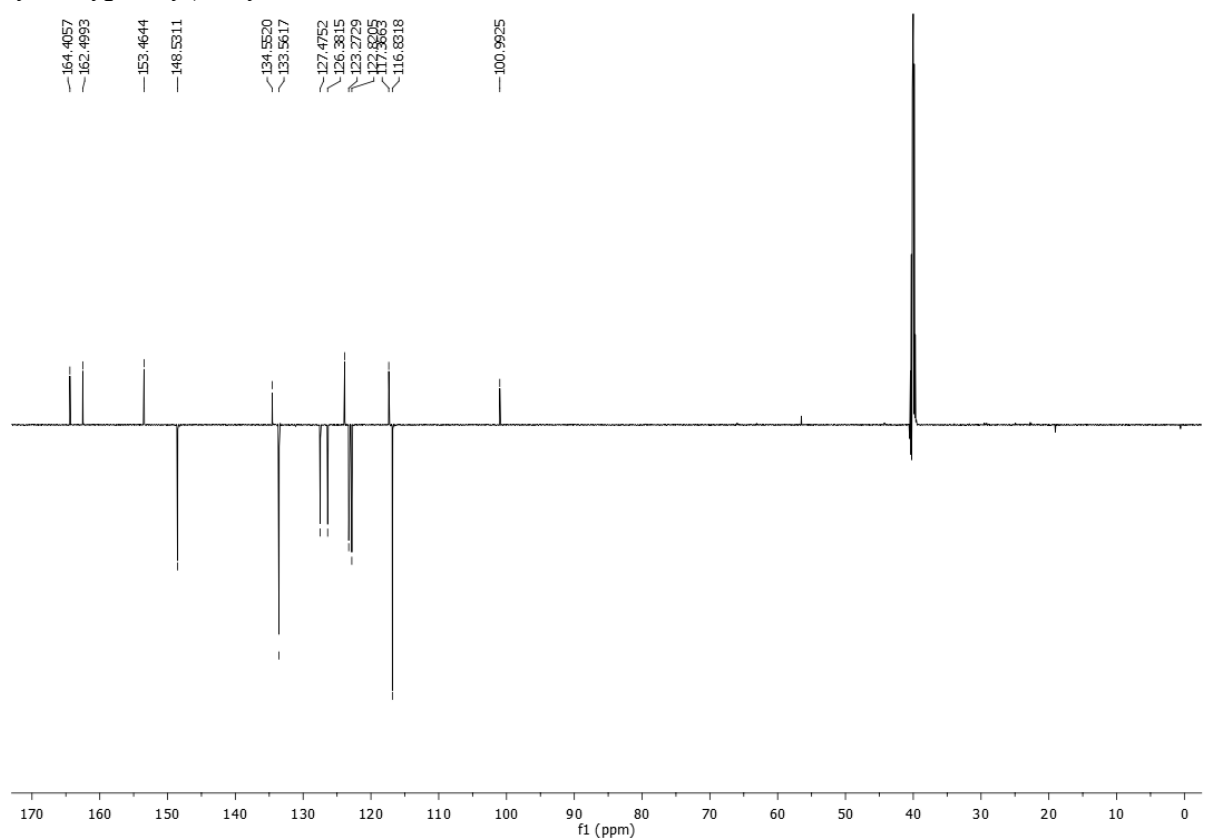


Figure S11. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4-dihydroxyphenyl)acrylonitrile 22

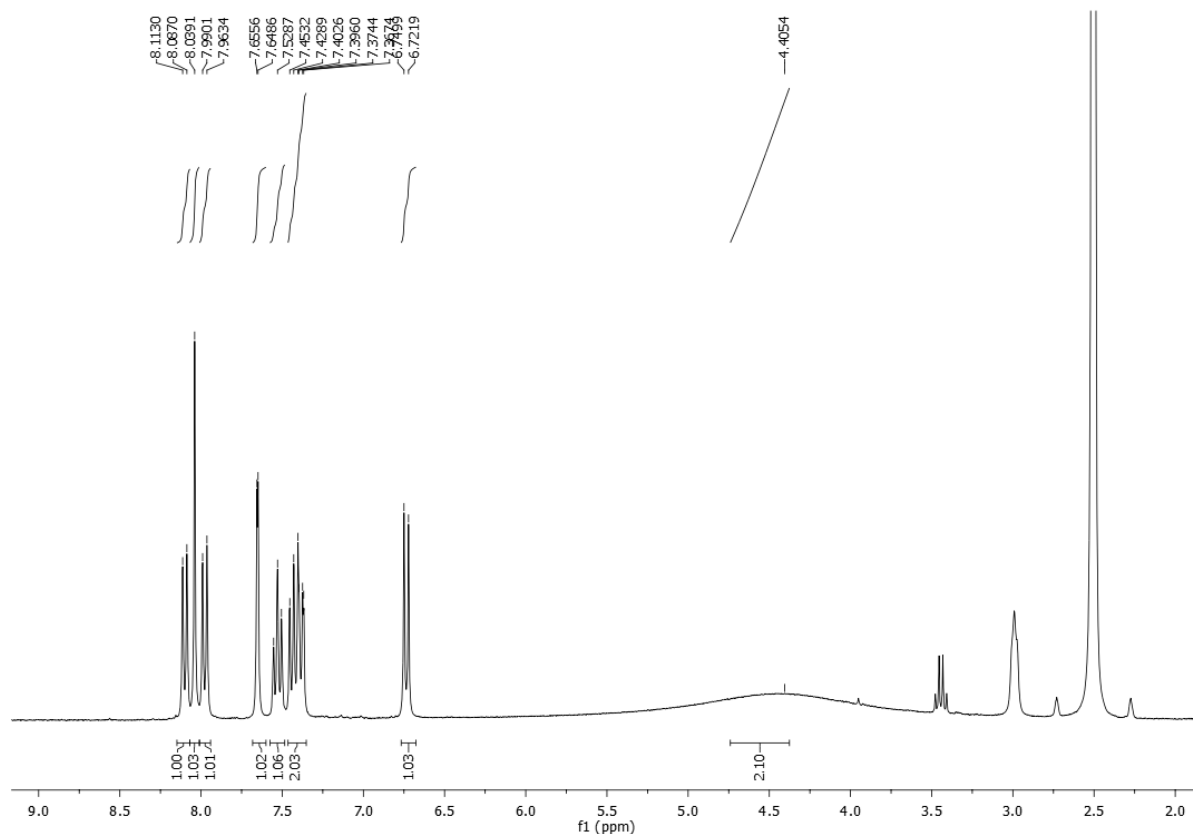


Figure S12. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4-dihydroxyphenyl)acrylonitrile 22

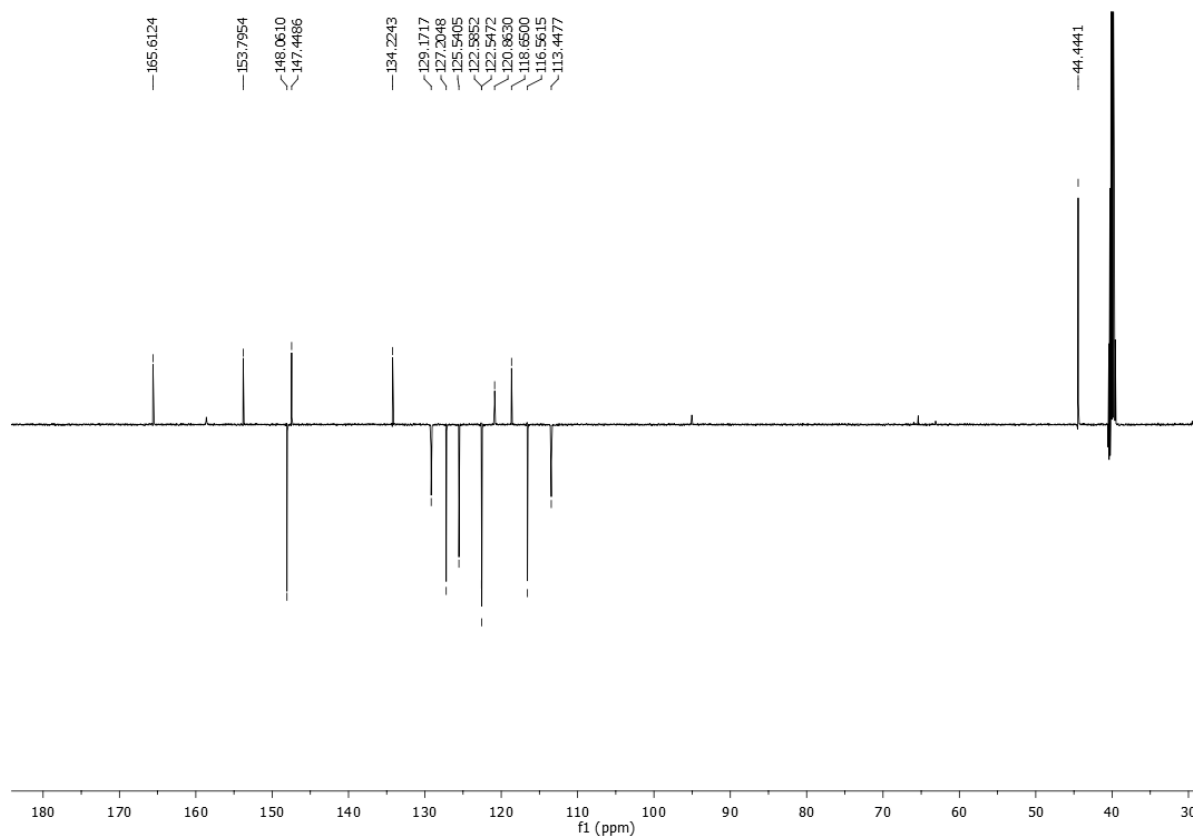


Figure S13. ^1H NMR spectrum (DMSO- d_6 , 300 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 23

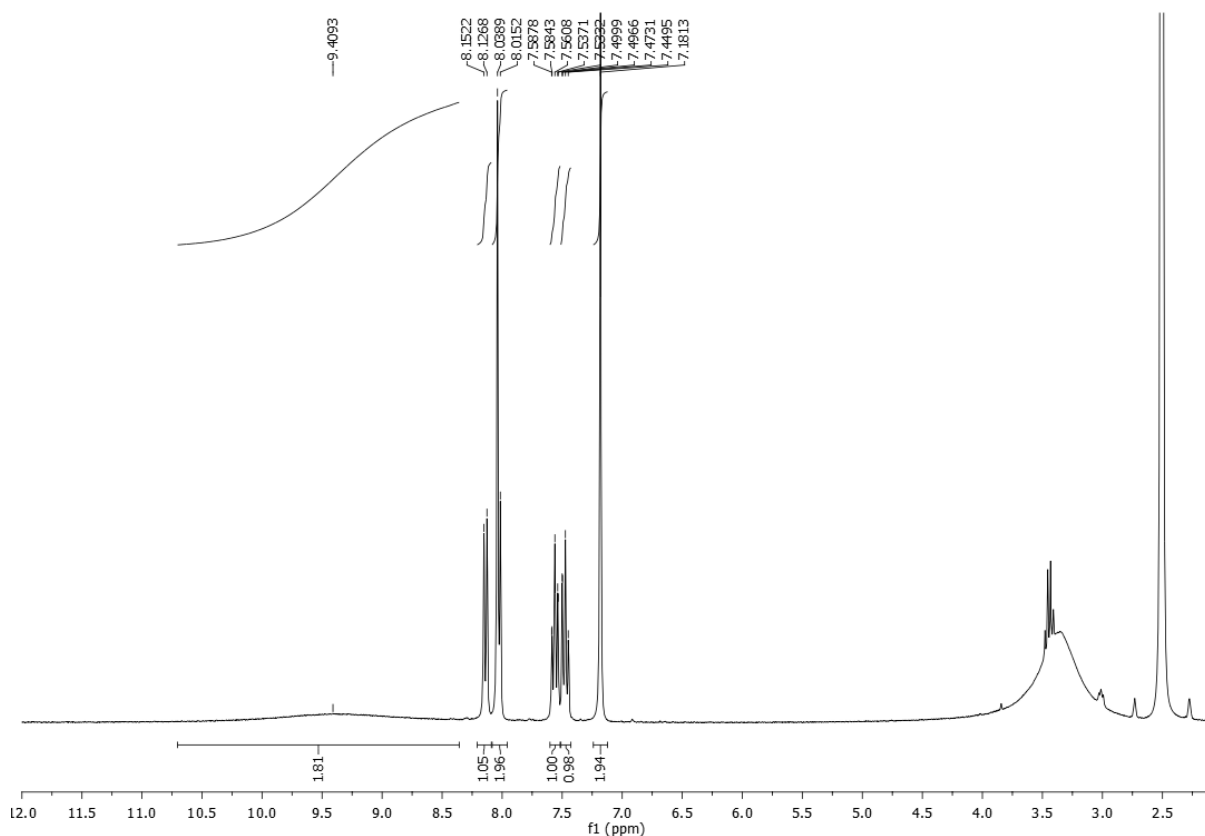


Figure S14. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(benzo[d]thiazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 23

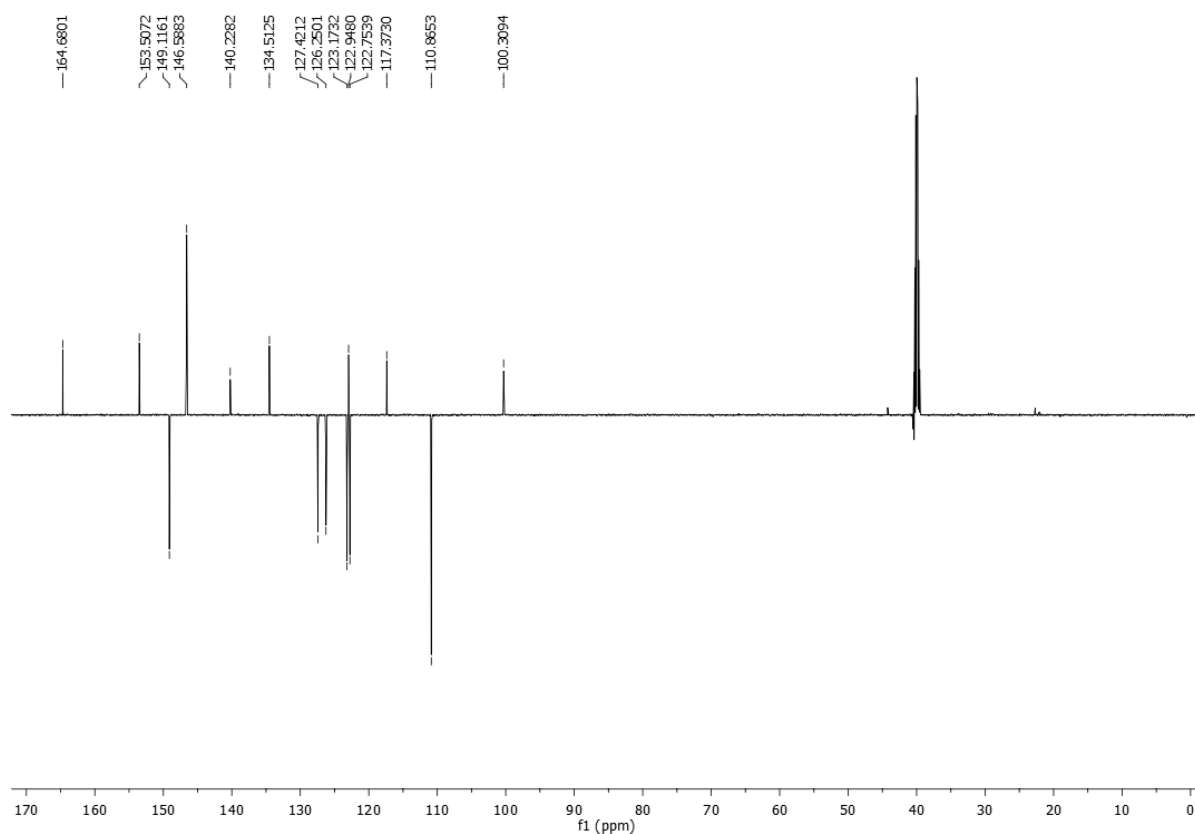


Figure S15. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(4-hydroxyphenyl)acrylonitrile 24

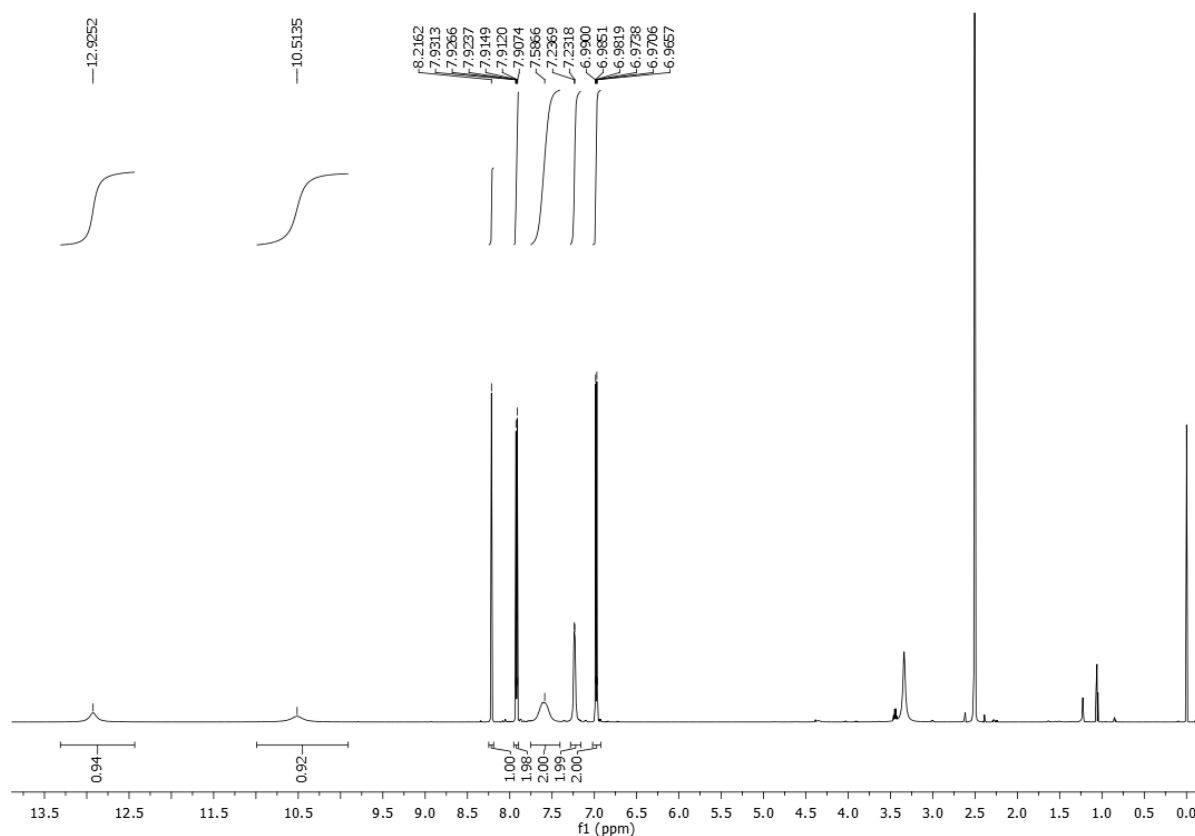


Figure S16. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(4-hydroxyphenyl)acrylonitrile 24

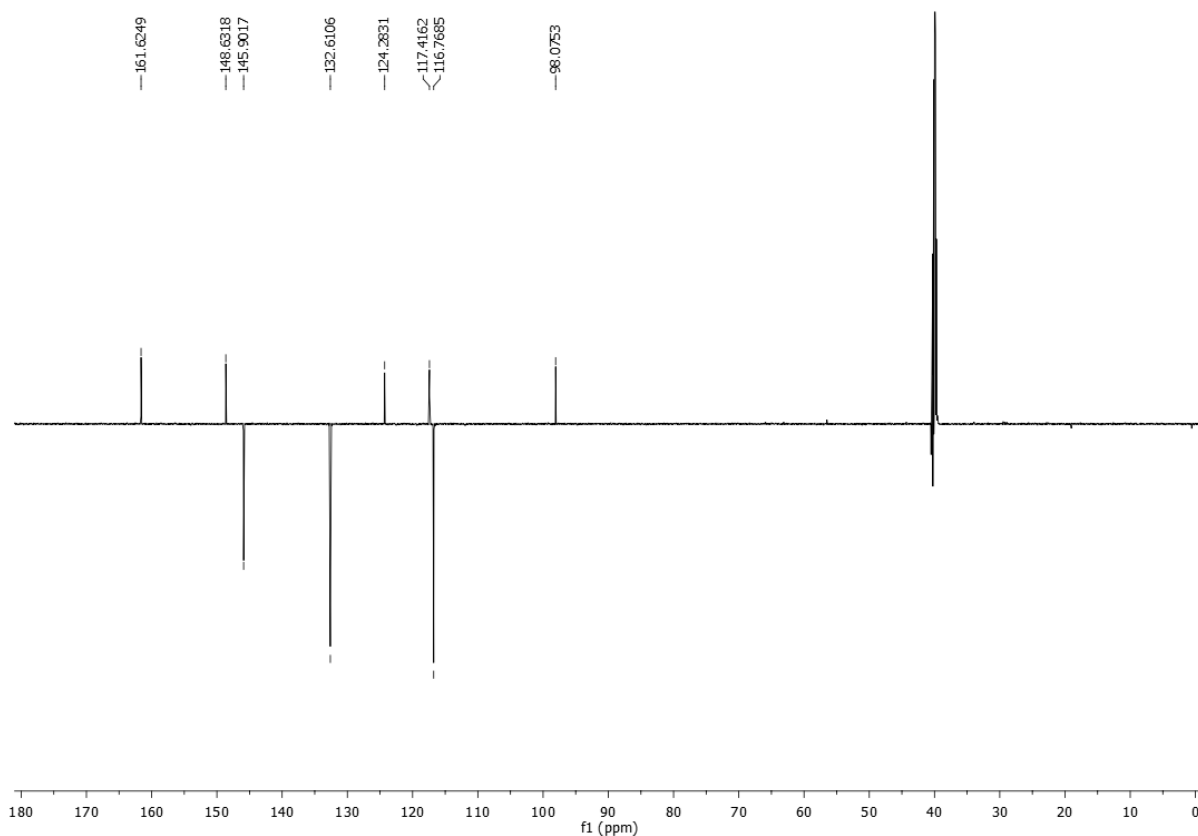


Figure S17. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(3,4-dihydroxyphenyl)acrylonitrile 25

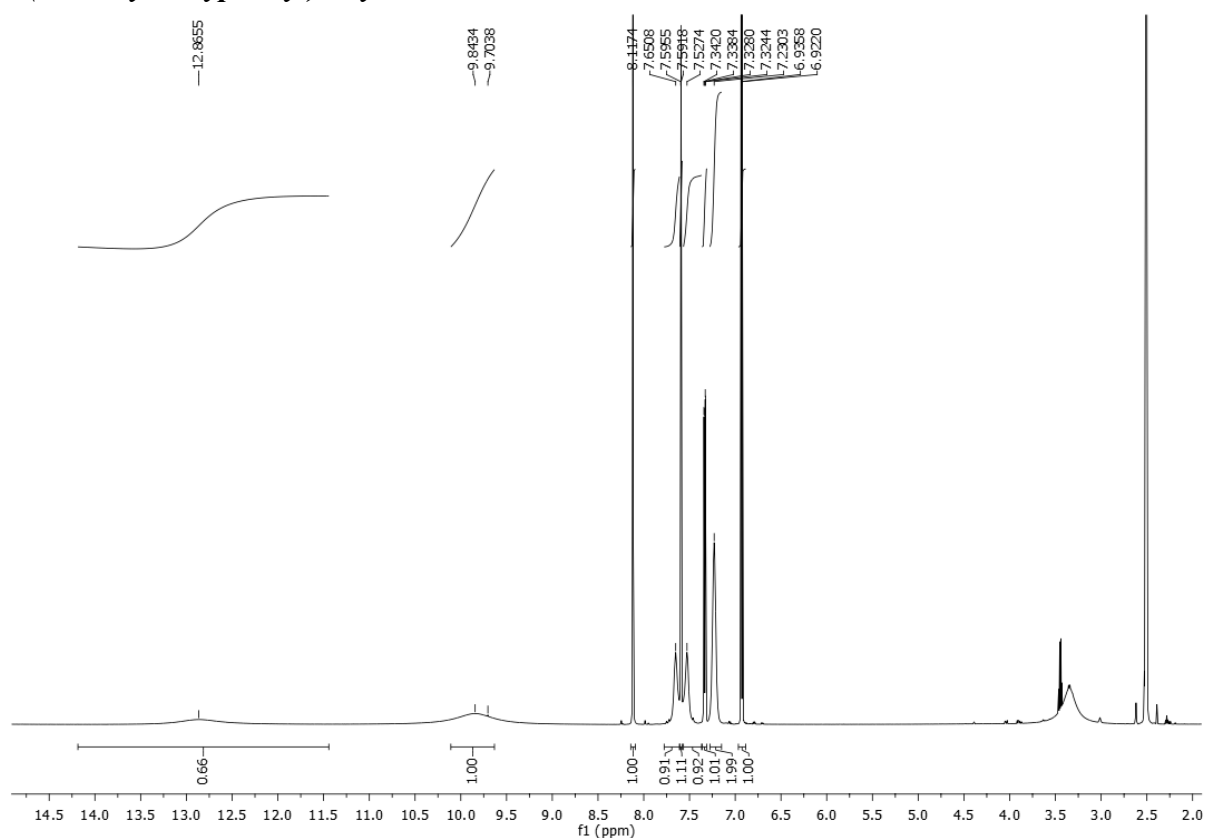


Figure S18. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(3,4-dihydroxyphenyl)acrylonitrile 25

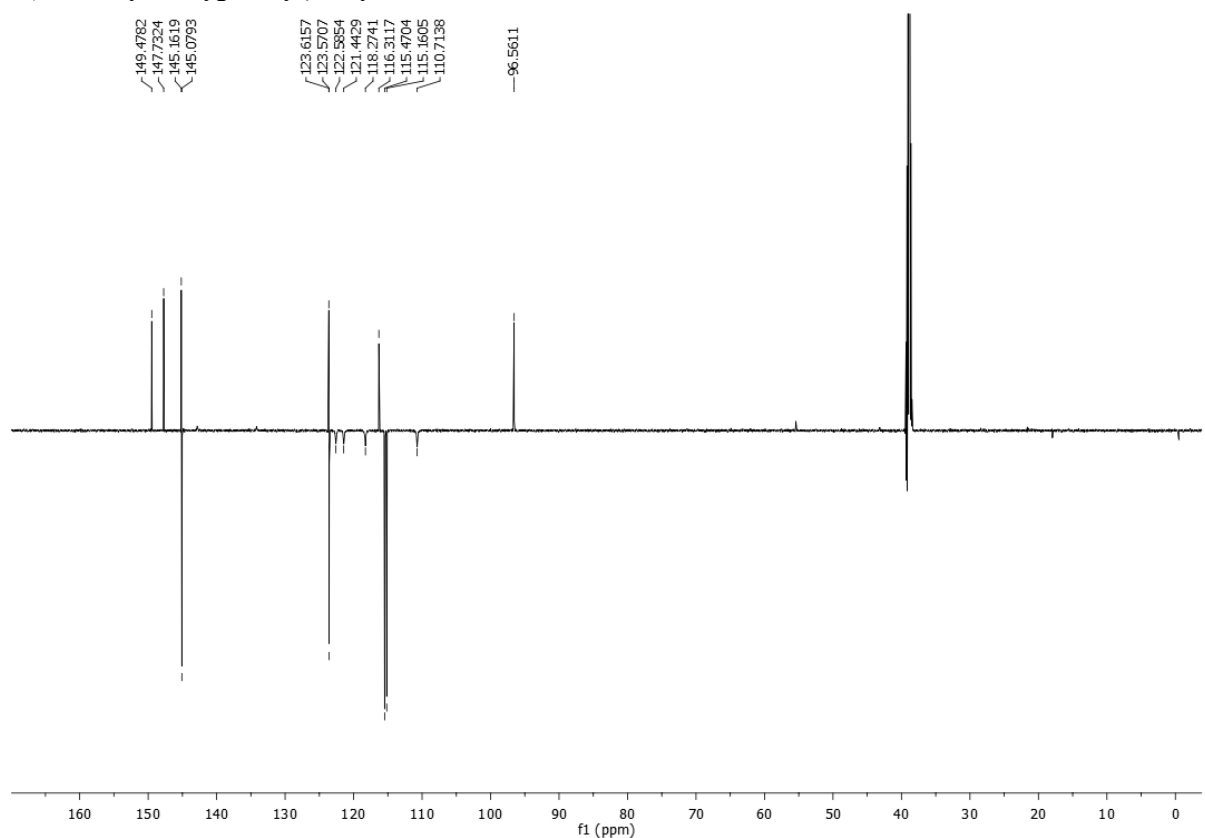


Figure S19. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile **26**

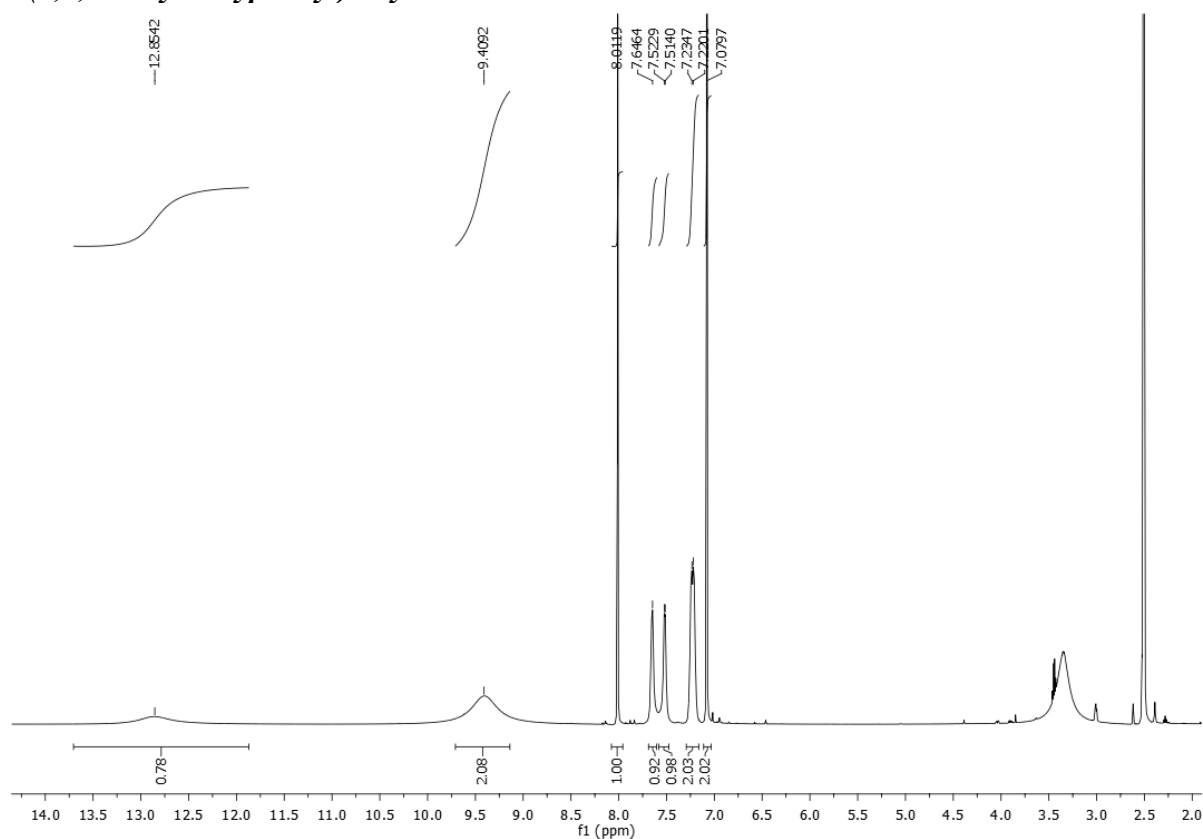


Figure S20. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1*H*-benzo[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile **26**

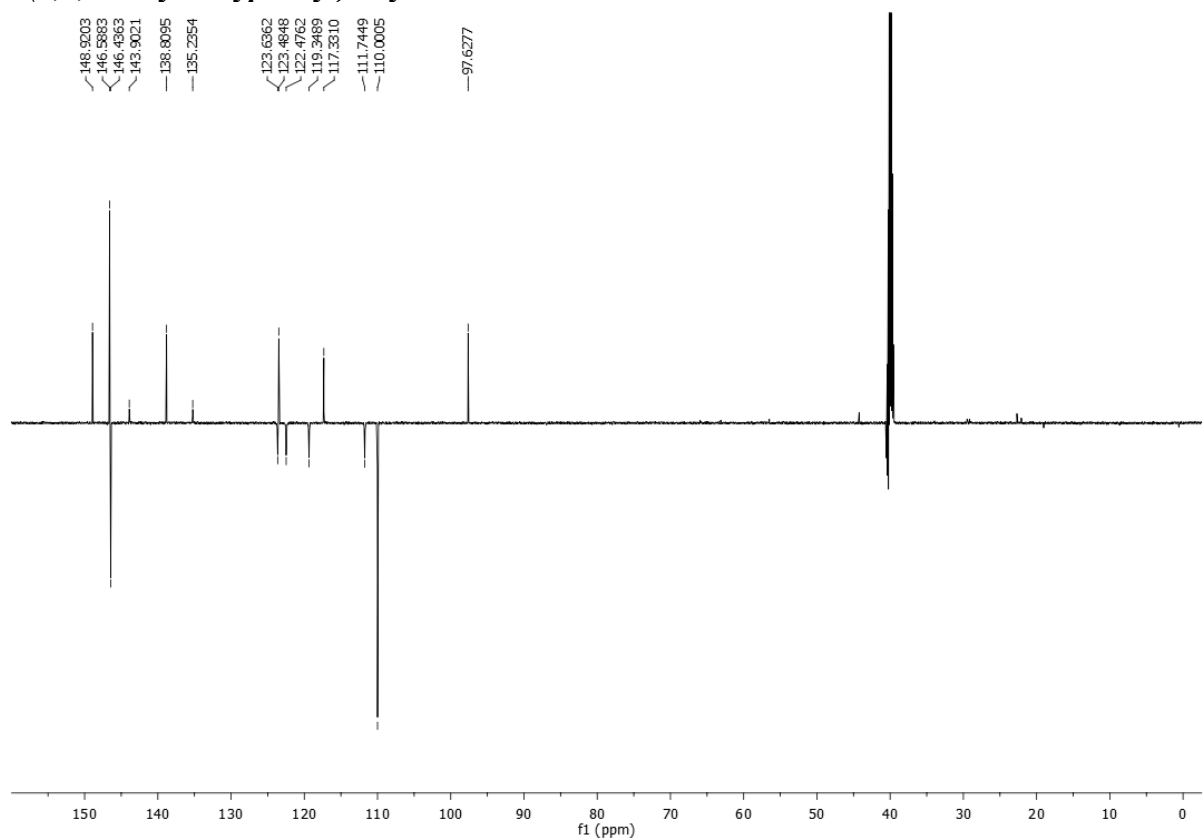


Figure S21. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1*H*-benzo[d]imidazole-5(6)-carbonitrile 27

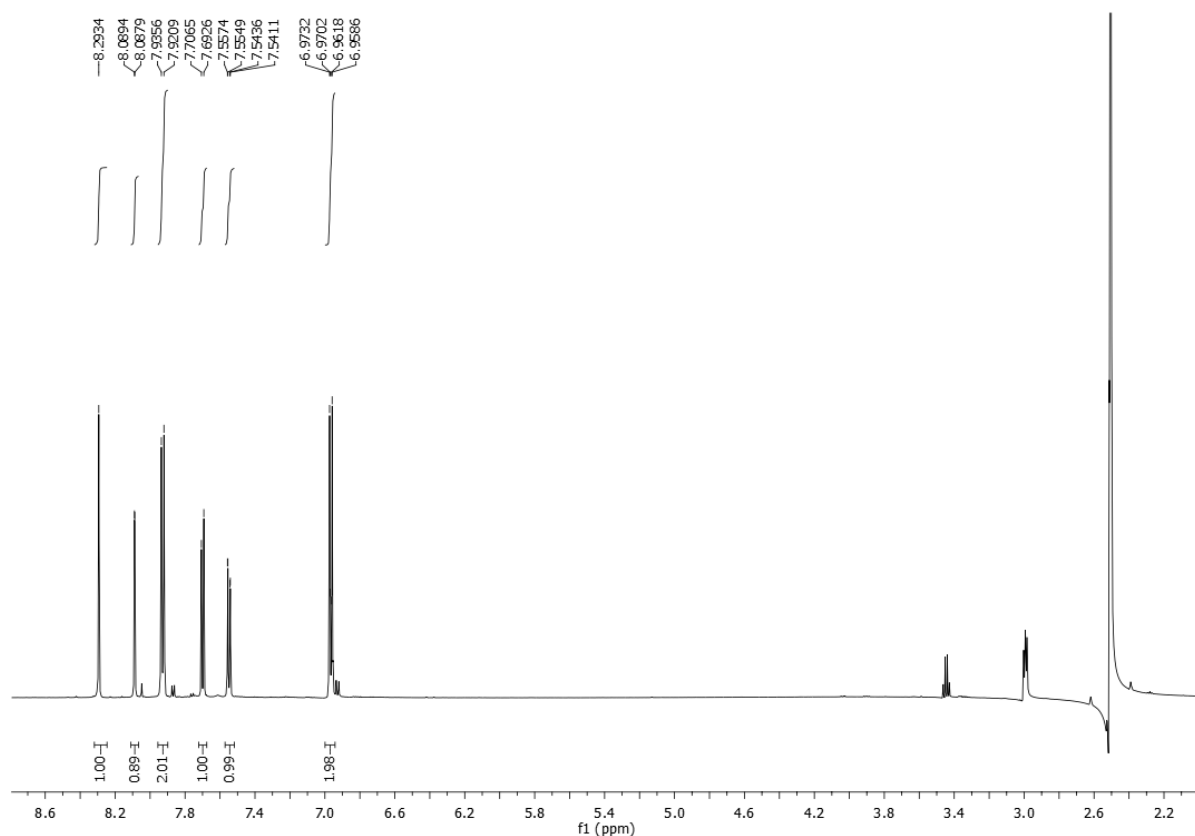


Figure S22. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1*H*-benzo[d]imidazole-5(6)-carbonitrile 27

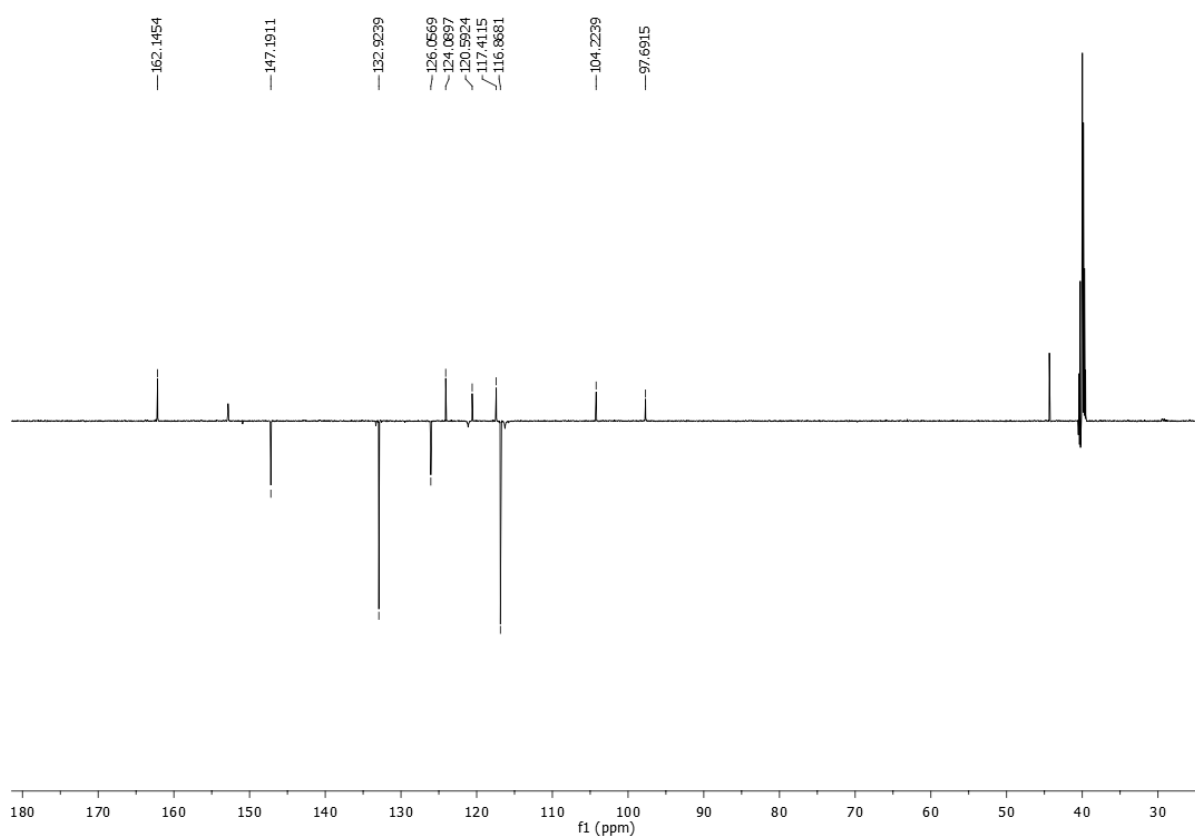


Figure S23. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1H-benzo[d]imidazole-5(6)-carbonitrile 28

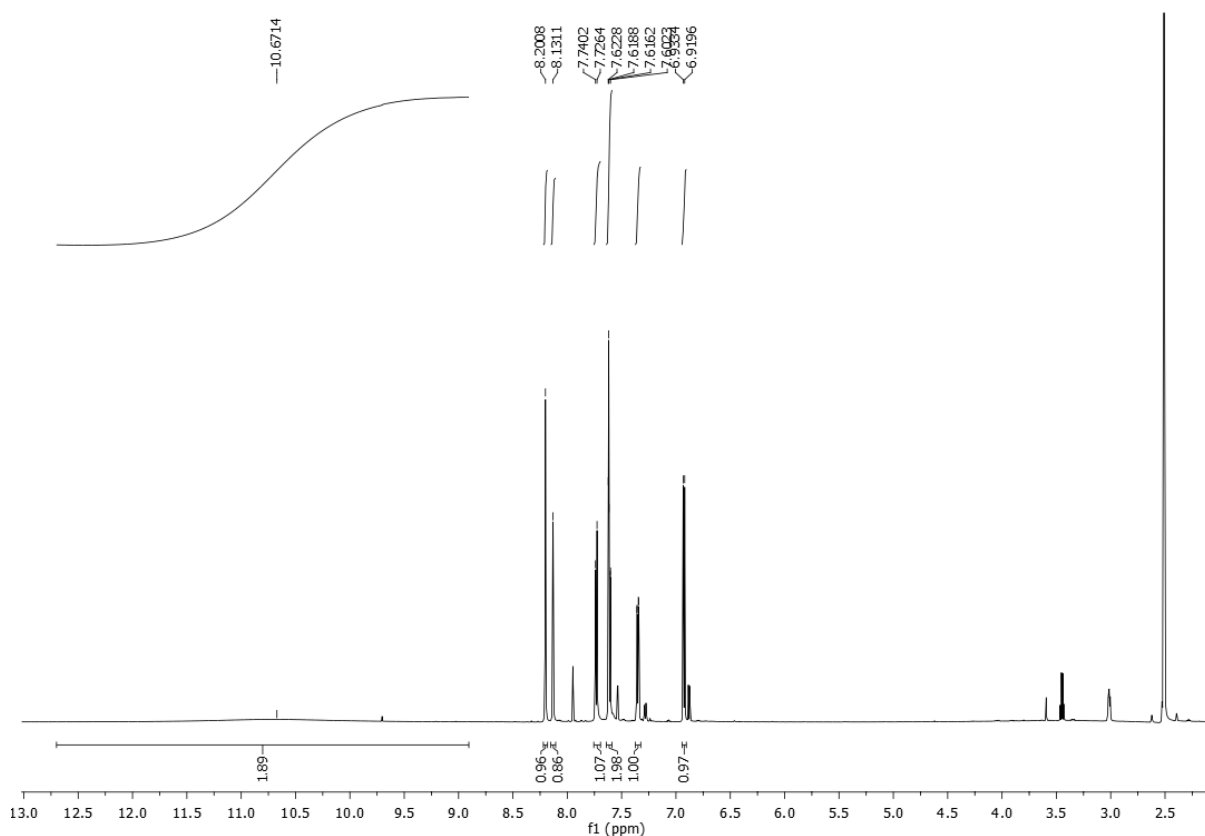


Figure S24. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1H-benzo[d]imidazole-5(6)-carbonitrile 28

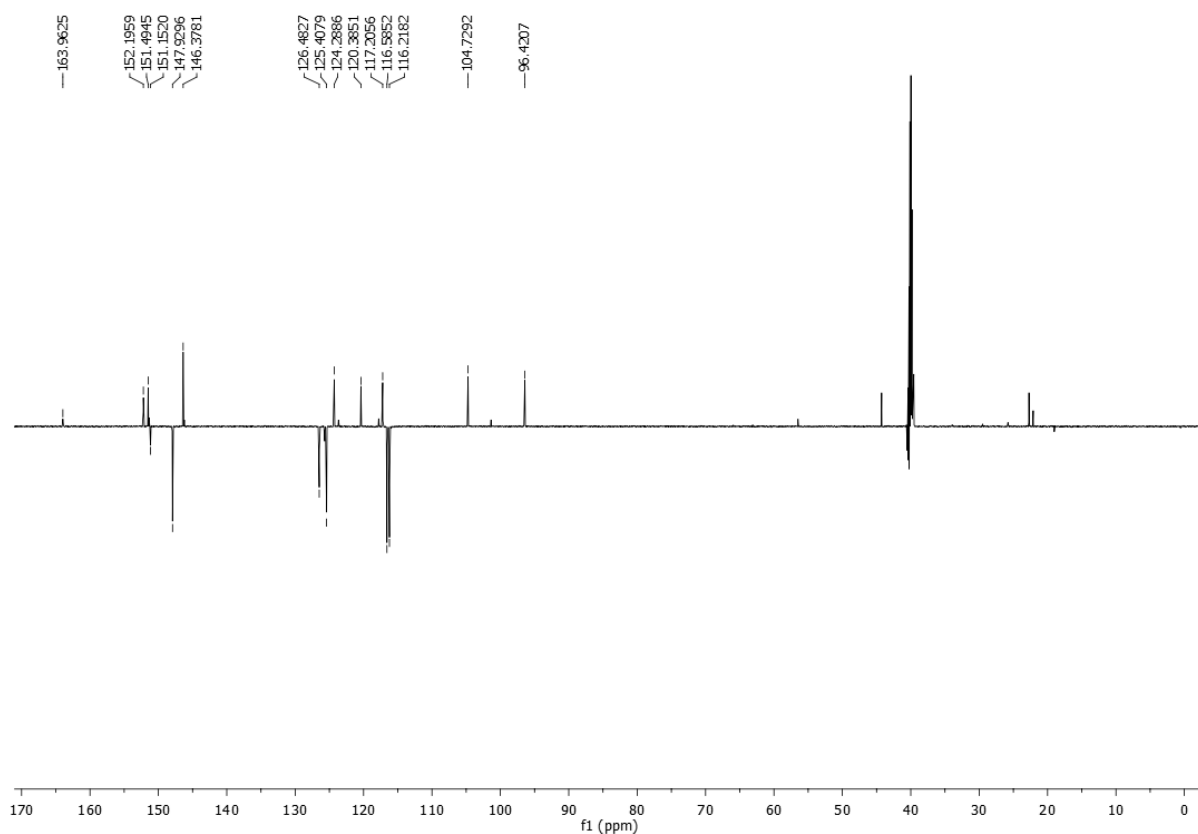


Figure S25. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1H-benzo[d]imidazole-5(6)-carbonitrile 29

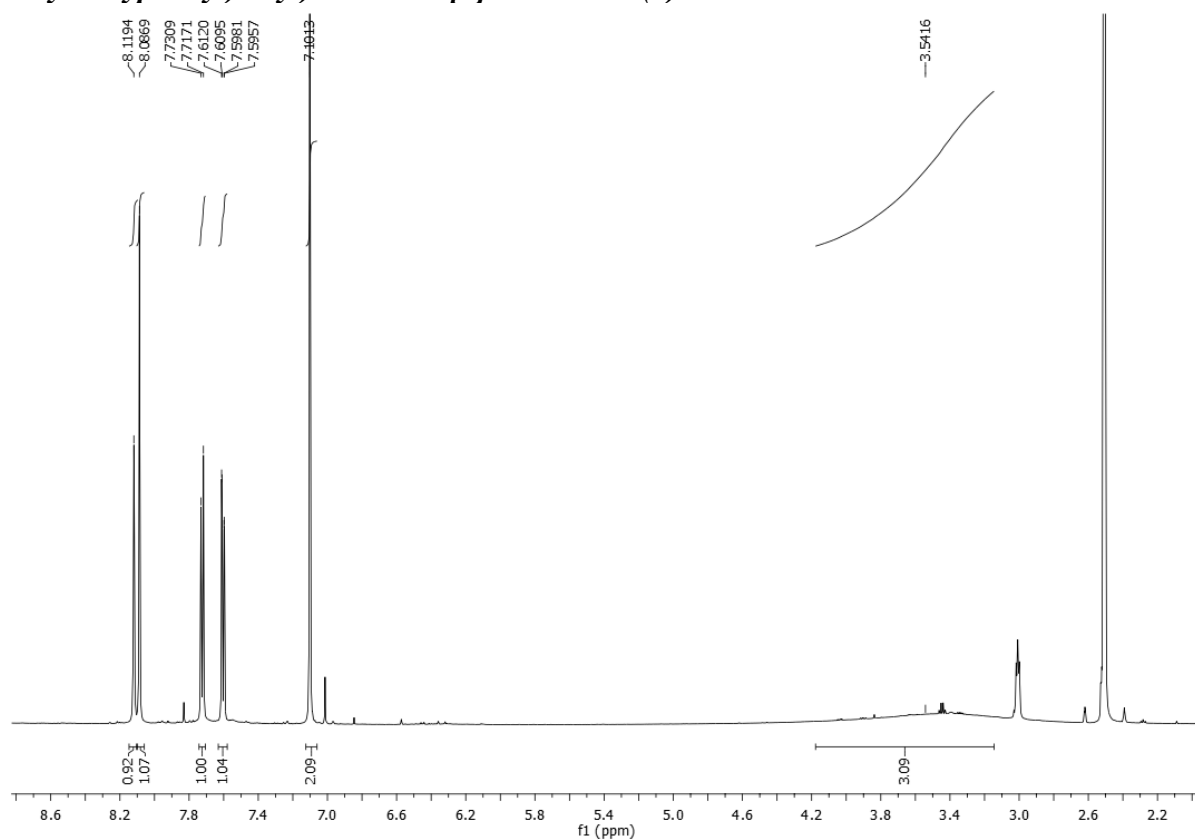


Figure S26. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1H-benzo[d]imidazole-5(6)-carbonitrile 29

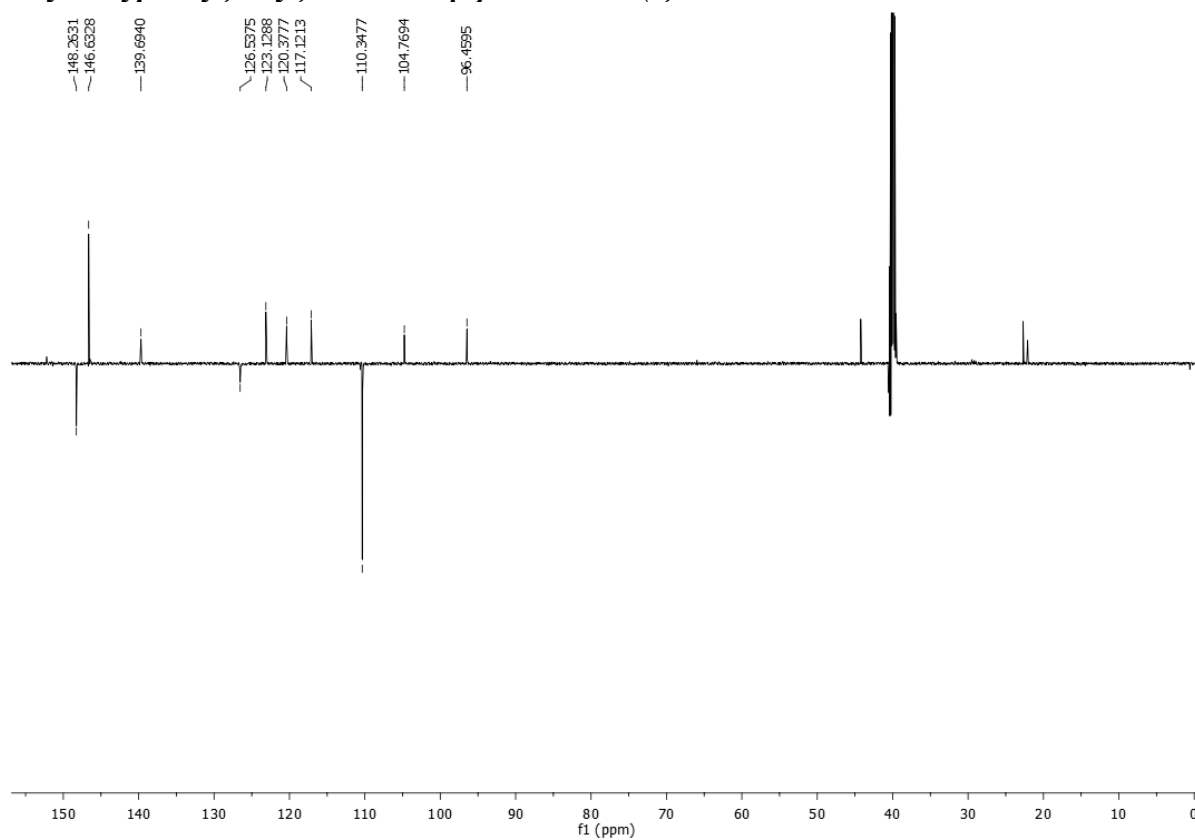


Figure S27. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 30

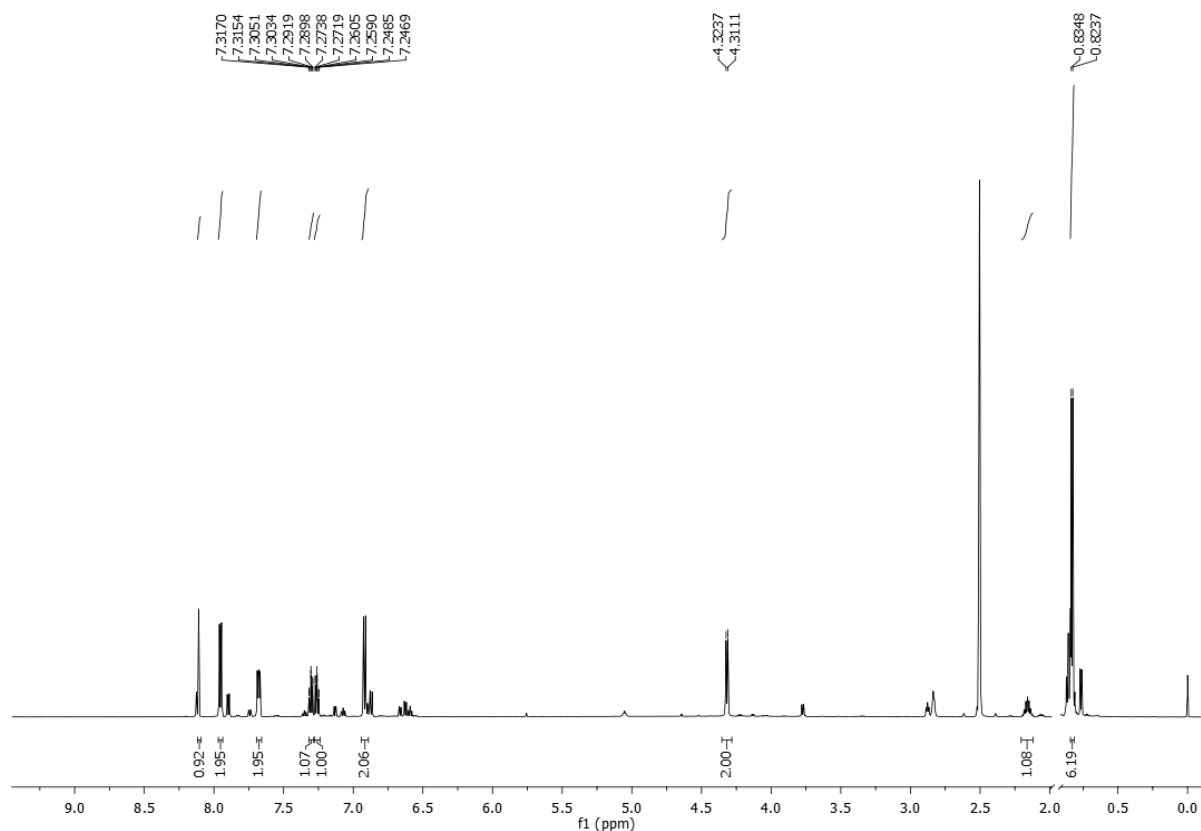


Figure S28. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 30

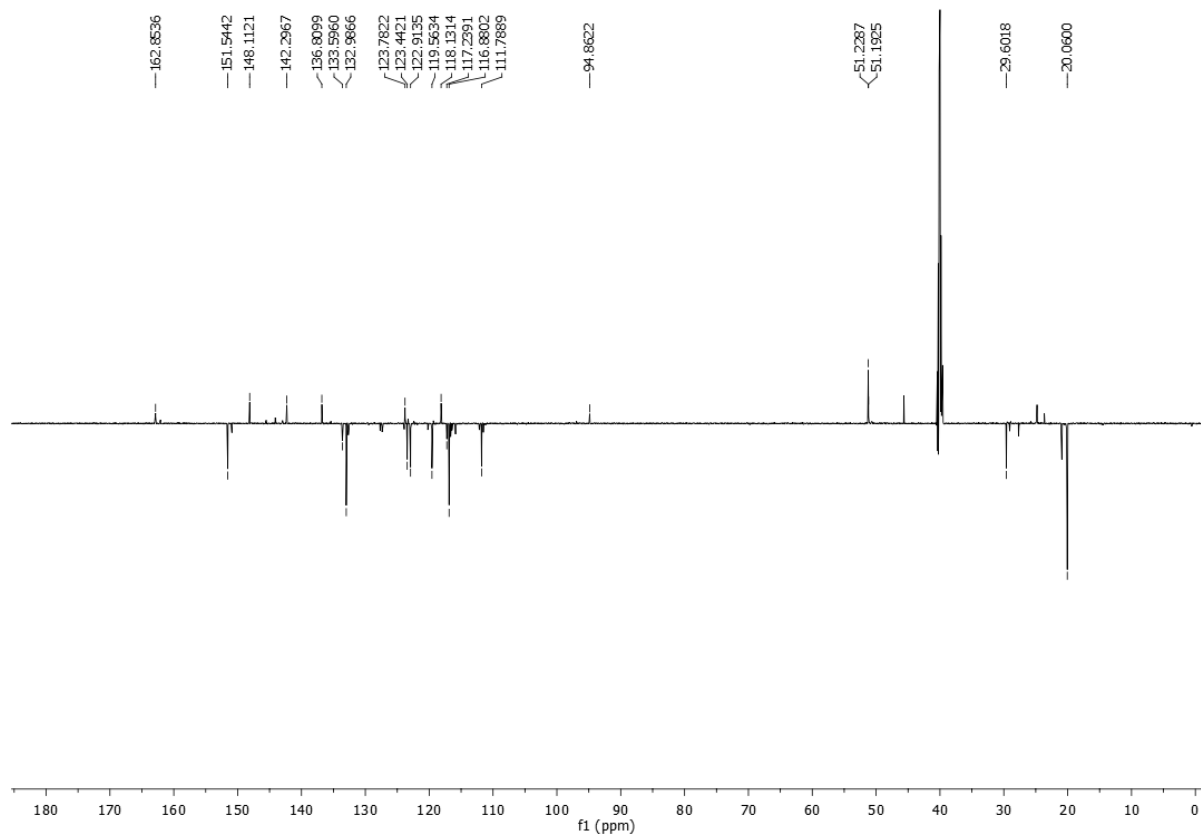


Figure S29. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 31

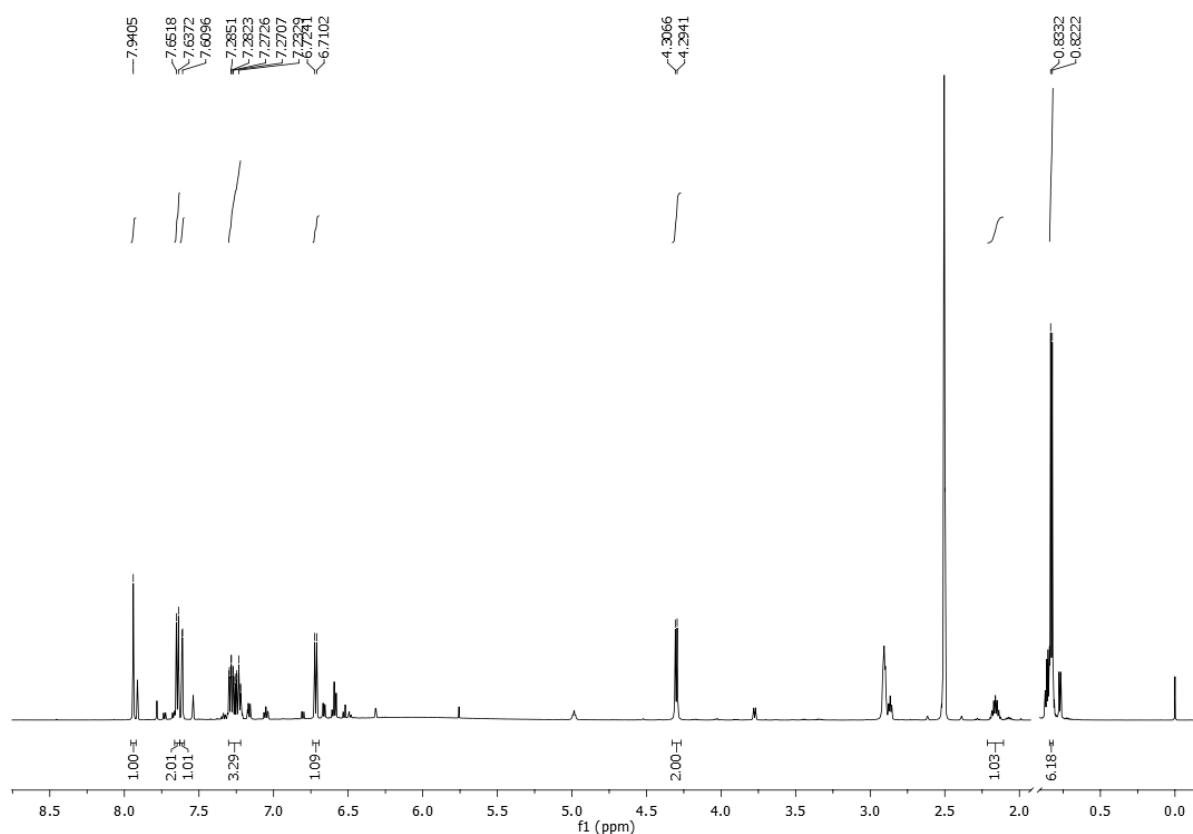


Figure S30. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 31

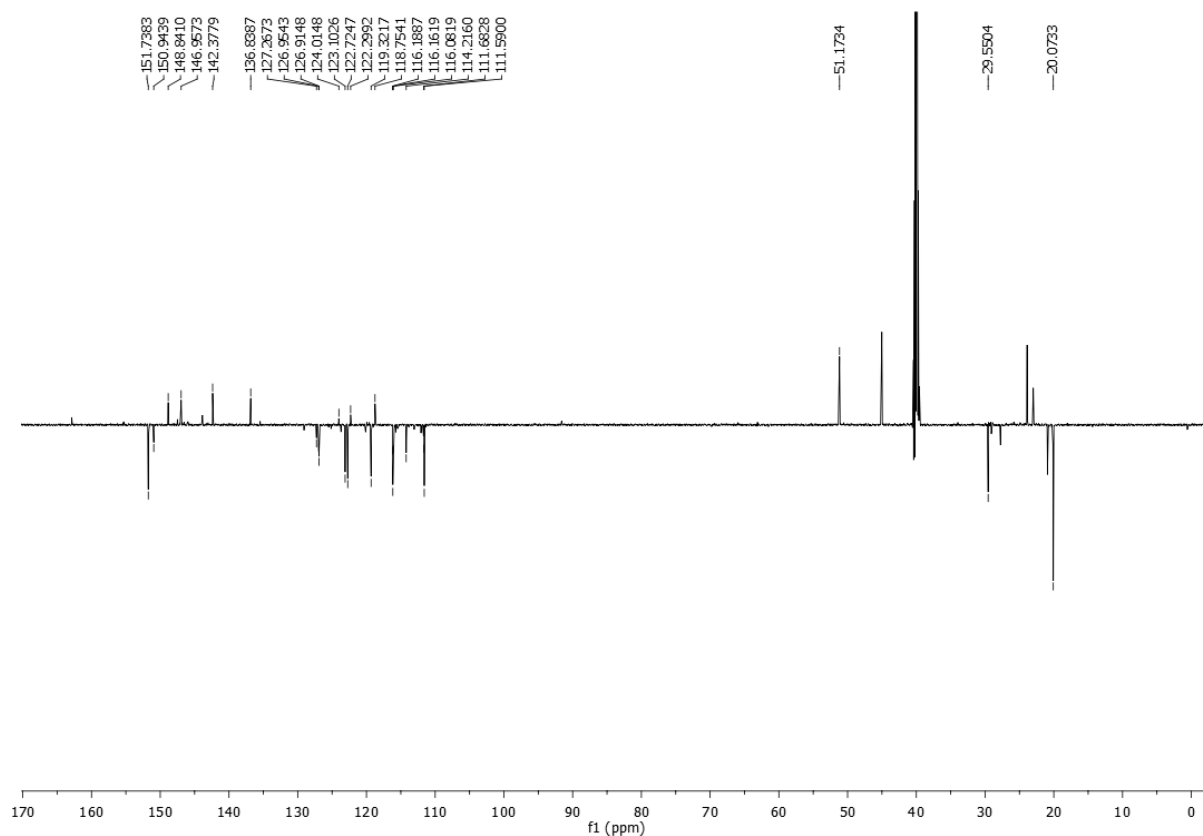


Figure S31. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 32

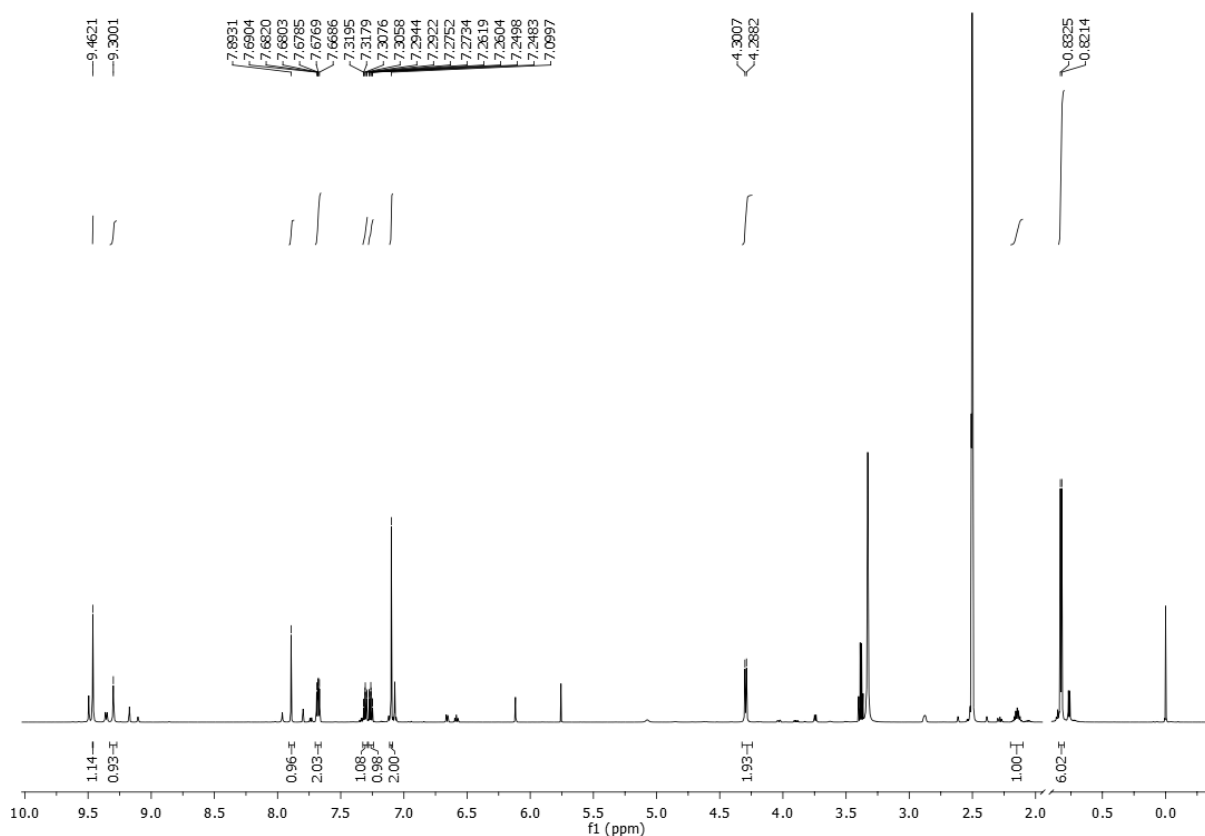


Figure S32. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-isobutyl-1H-benzo[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 32

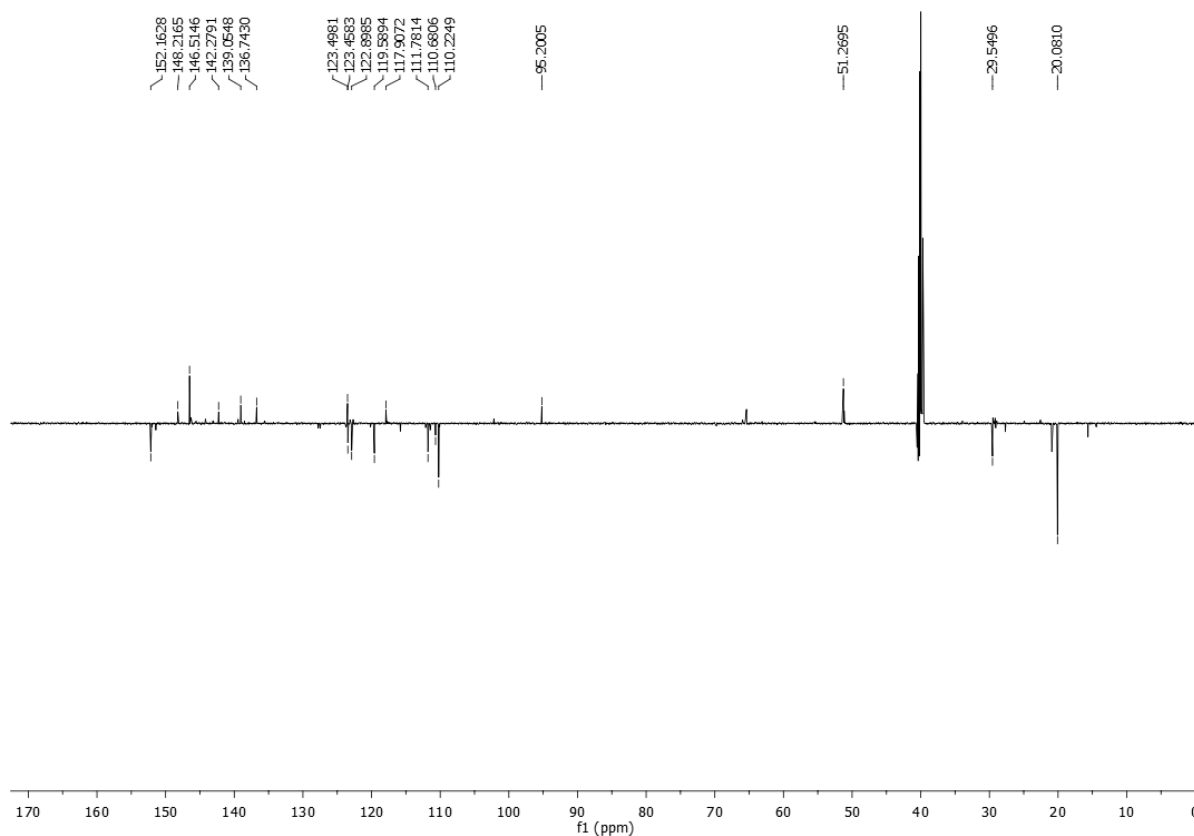


Figure S33. ^1H NMR spectrum ($\text{DMSO-}d_6$, 600 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-isobutyl-1H-benzo[d]imidazole-6-carbonitrile **33**

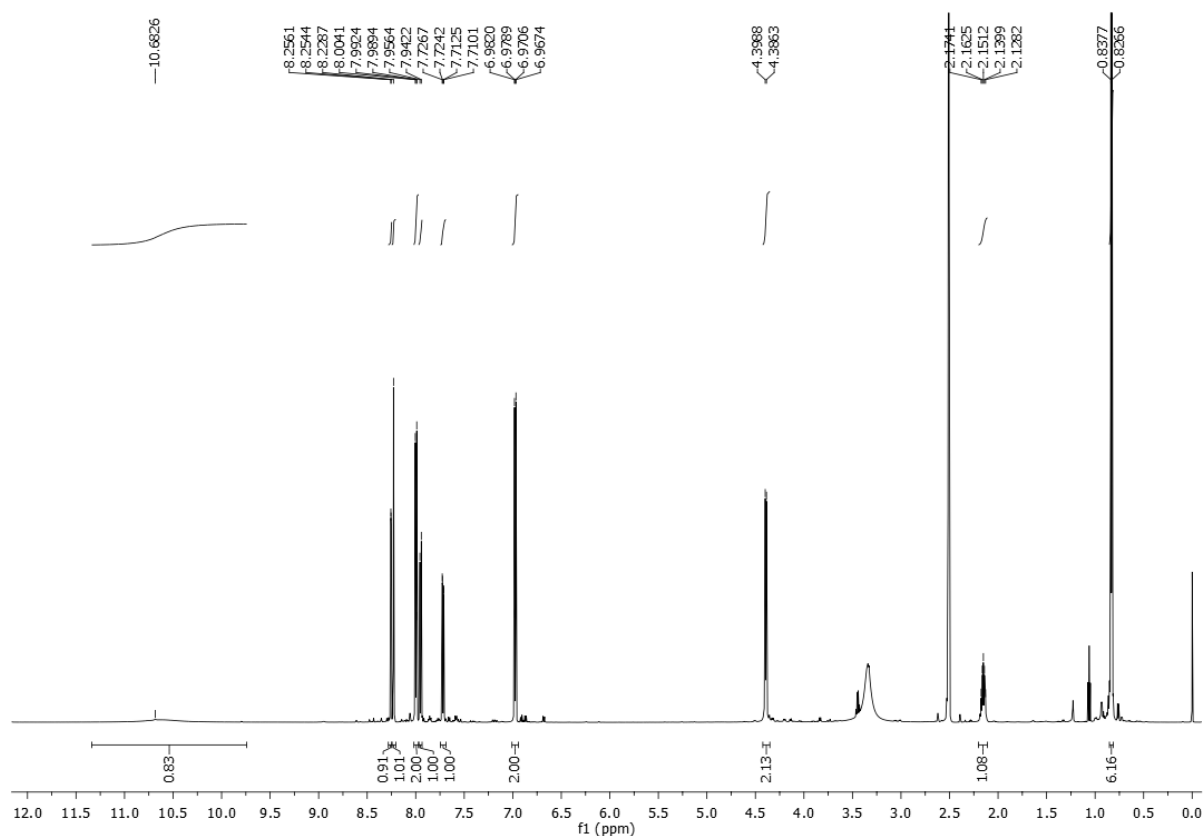


Figure S34. ^{13}C NMR spectrum ($\text{DMSO-}d_6$, 151 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-isobutyl-1H-benzo[d]imidazole-6-carbonitrile **33**

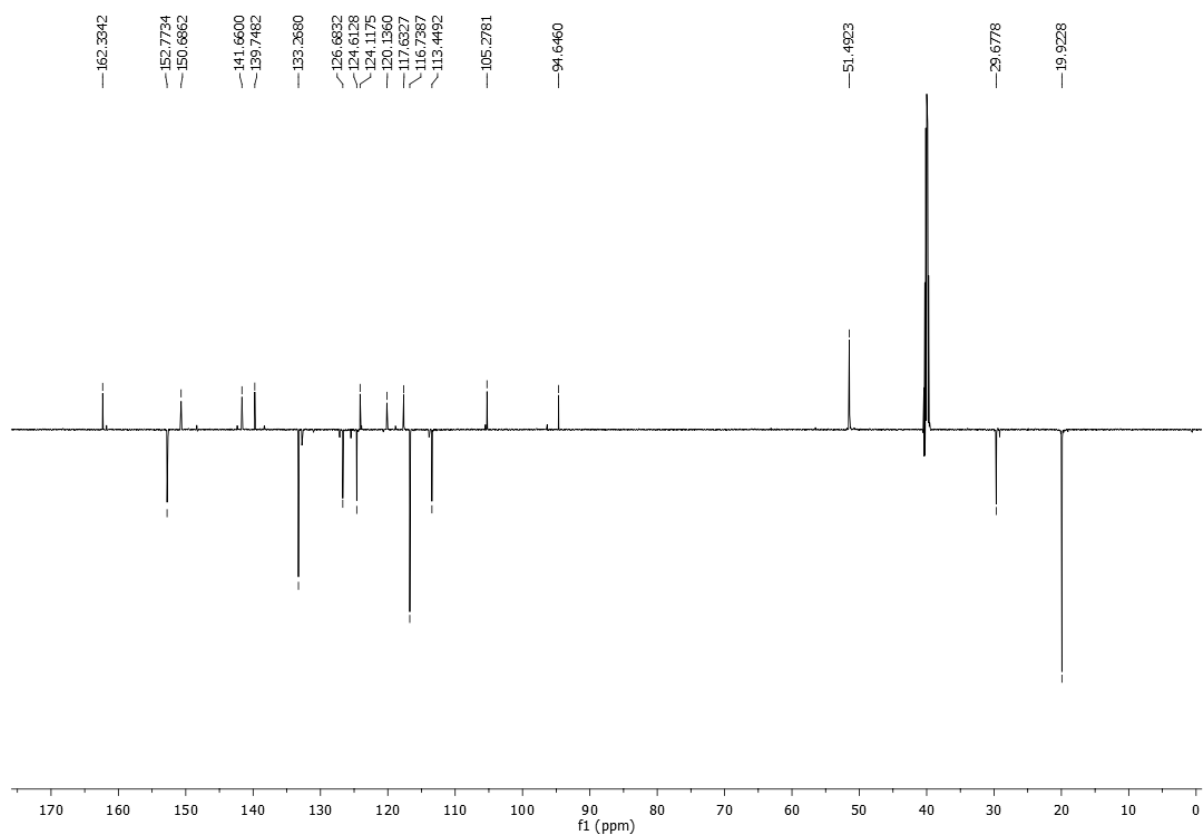


Figure S35. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-isobutyl-1H-benzod[*d*]imidazole-6-carbonitrile 34

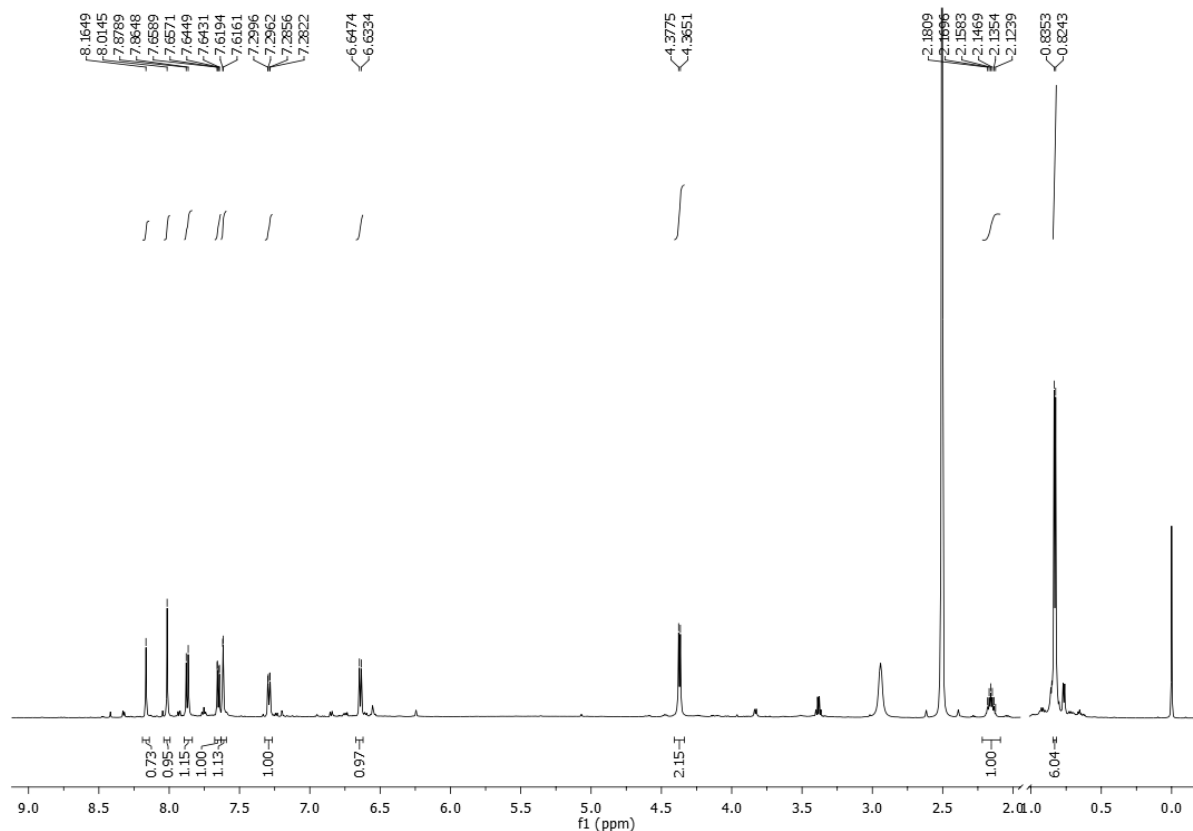


Figure S36. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-isobutyl-1H-benzod[*d*]imidazole-6-carbonitrile 34

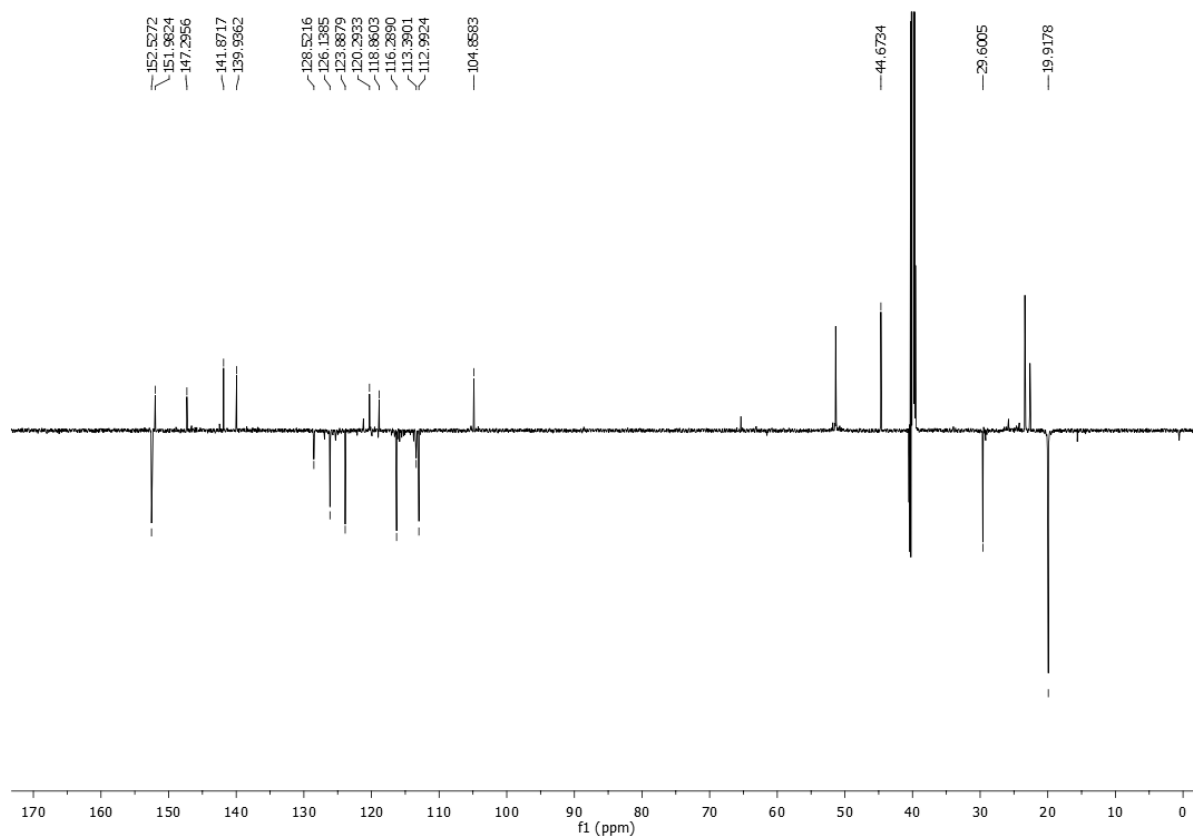


Figure S37. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-isobutyl-1H-benzo[d]imidazole-6-carbonitrile 35

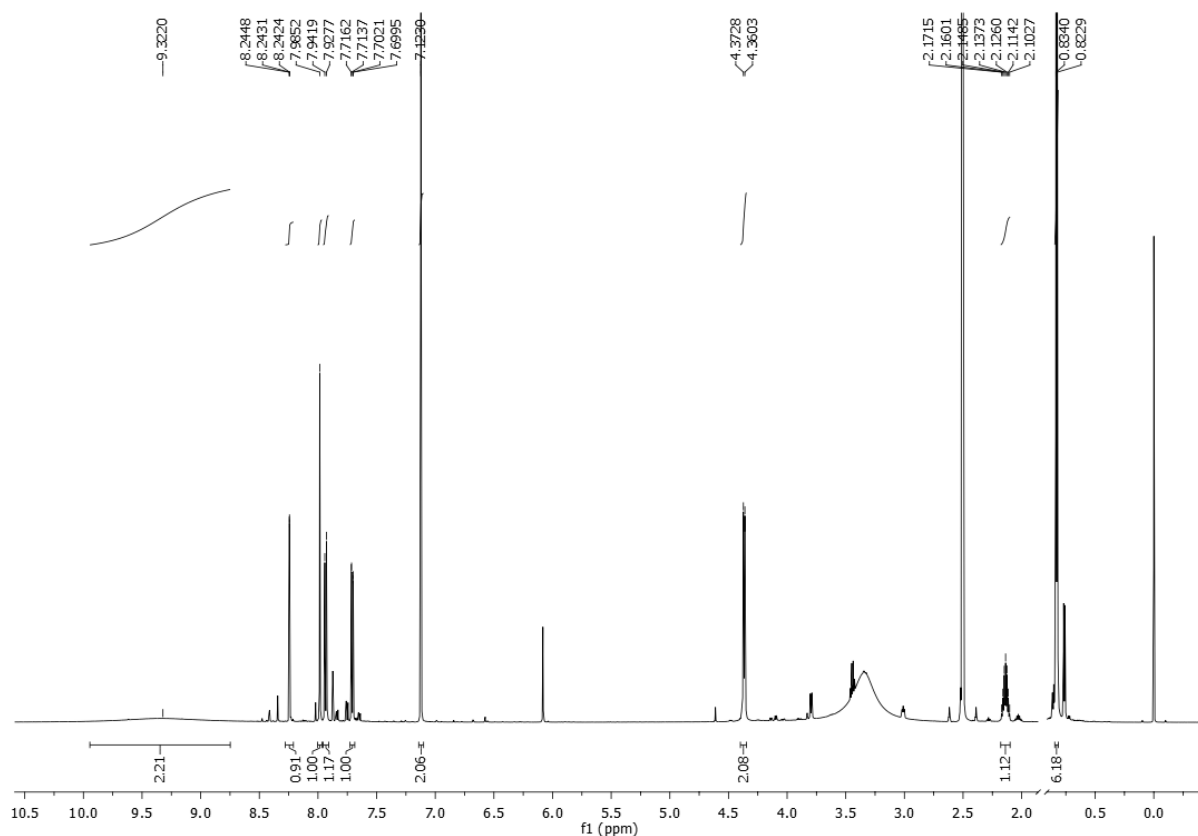


Figure S38. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-isobutyl-1H-benzo[d]imidazole-6-carbonitrile 35

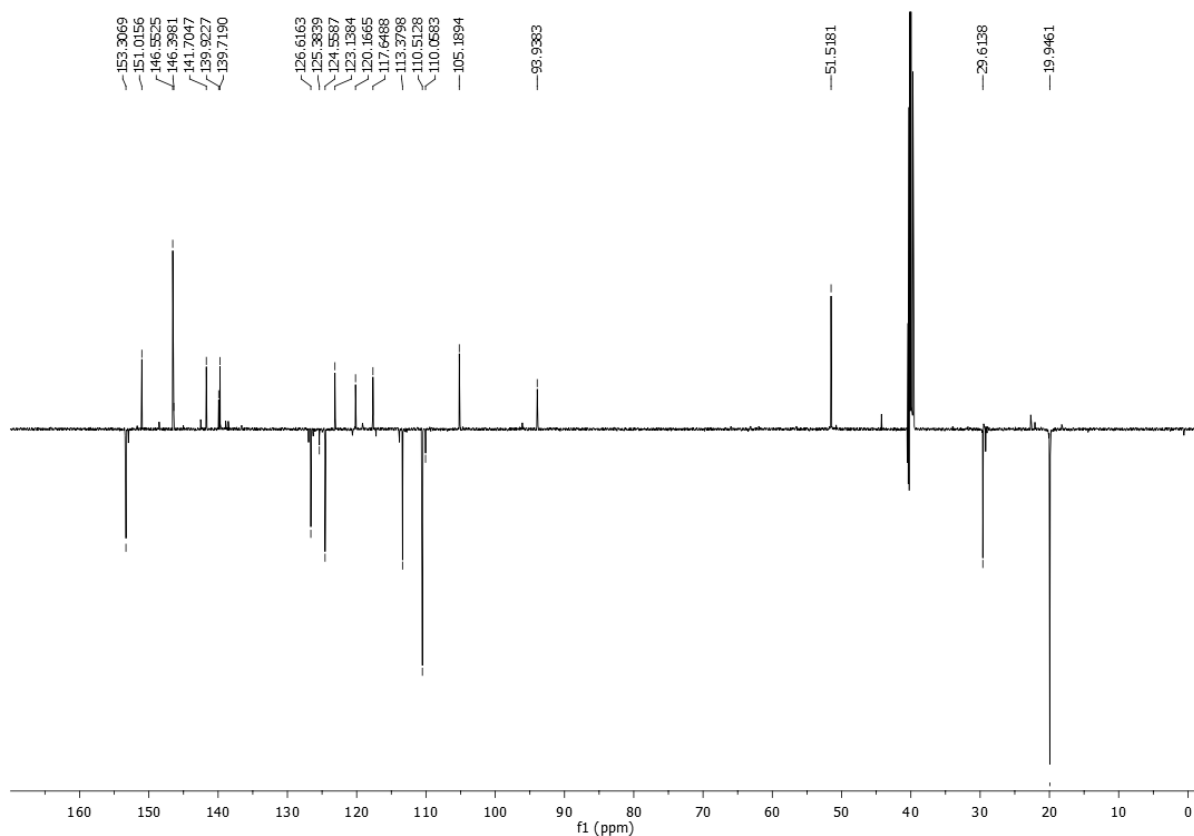


Figure S39. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-methyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 36

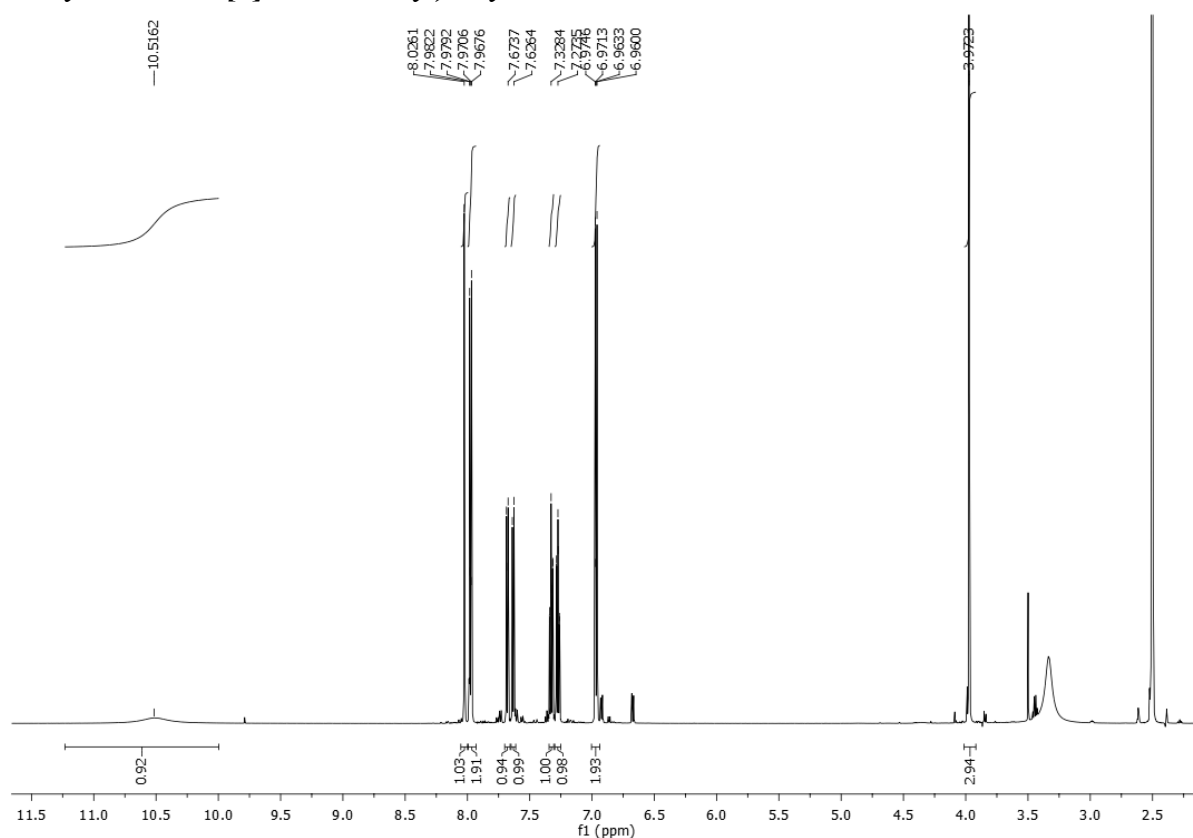


Figure S40. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-methyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 36

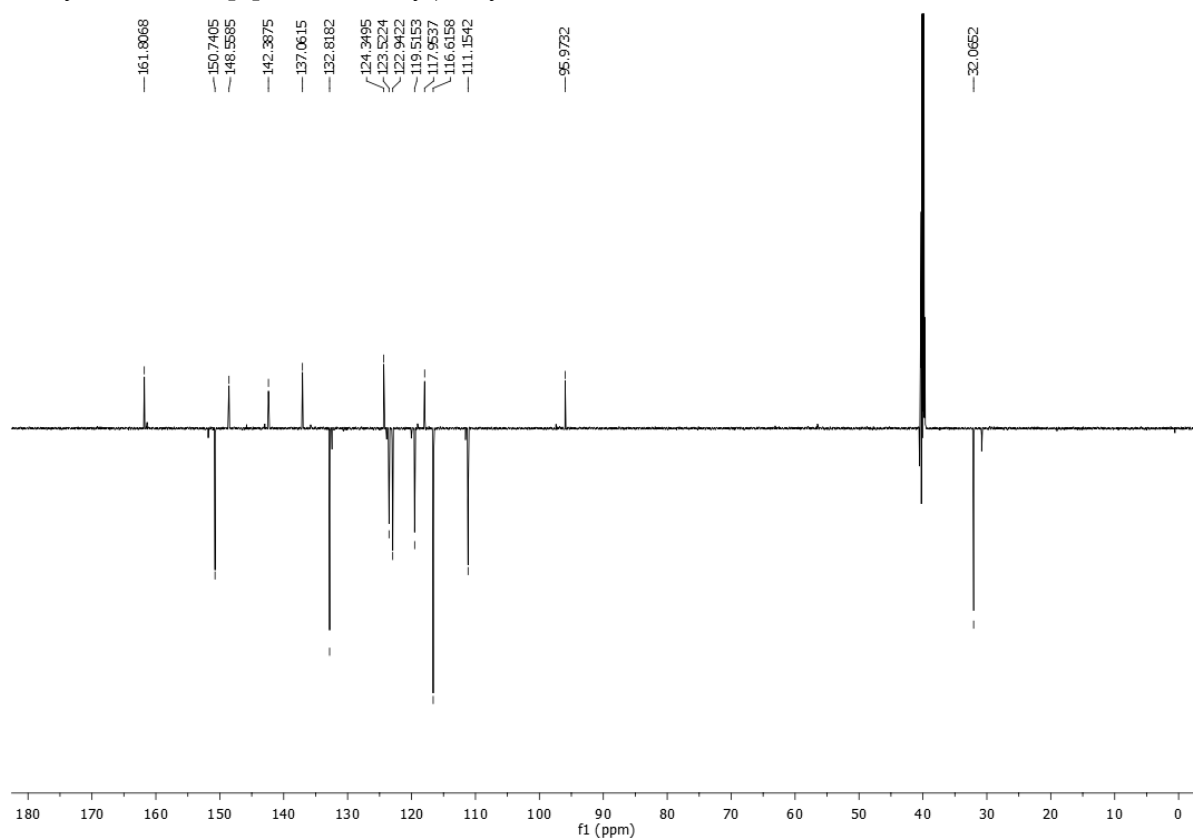


Figure S41. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-methyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 37

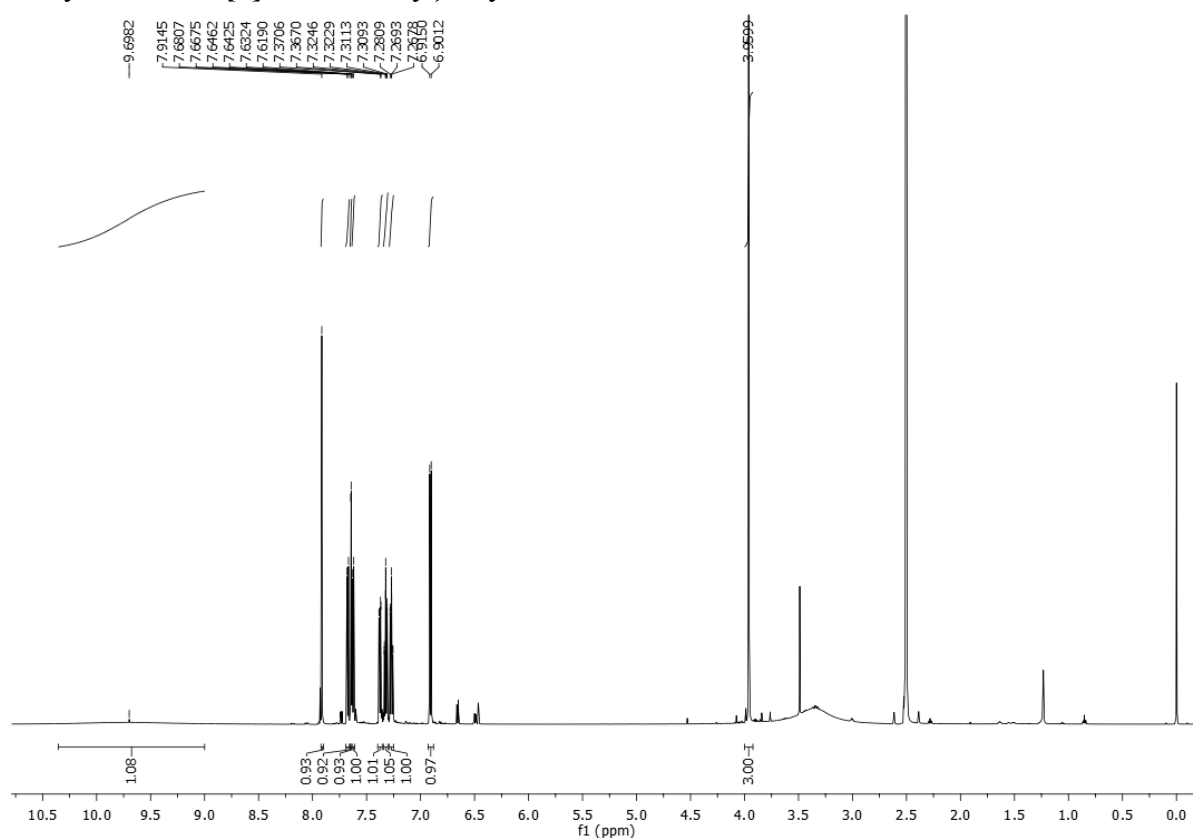


Figure S42. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-methyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 37

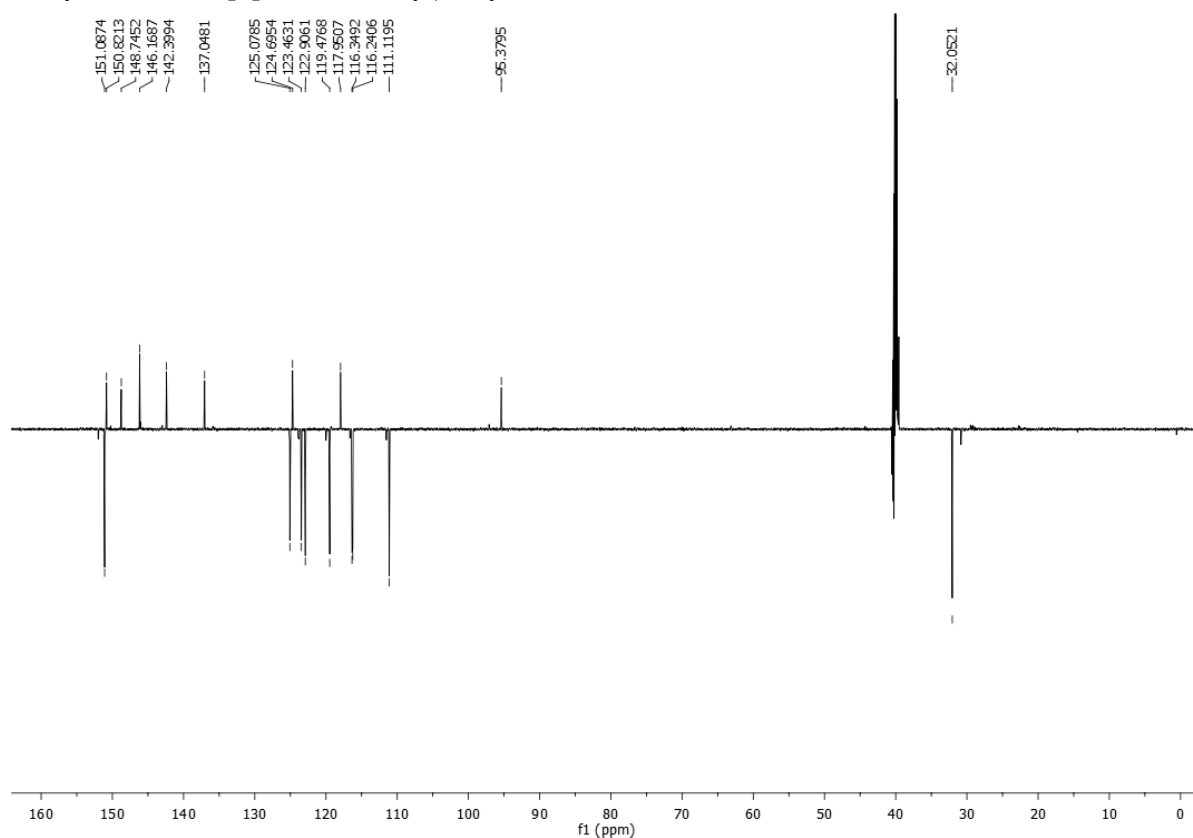


Figure S43. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-methyl-1H-benzof[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile **38**

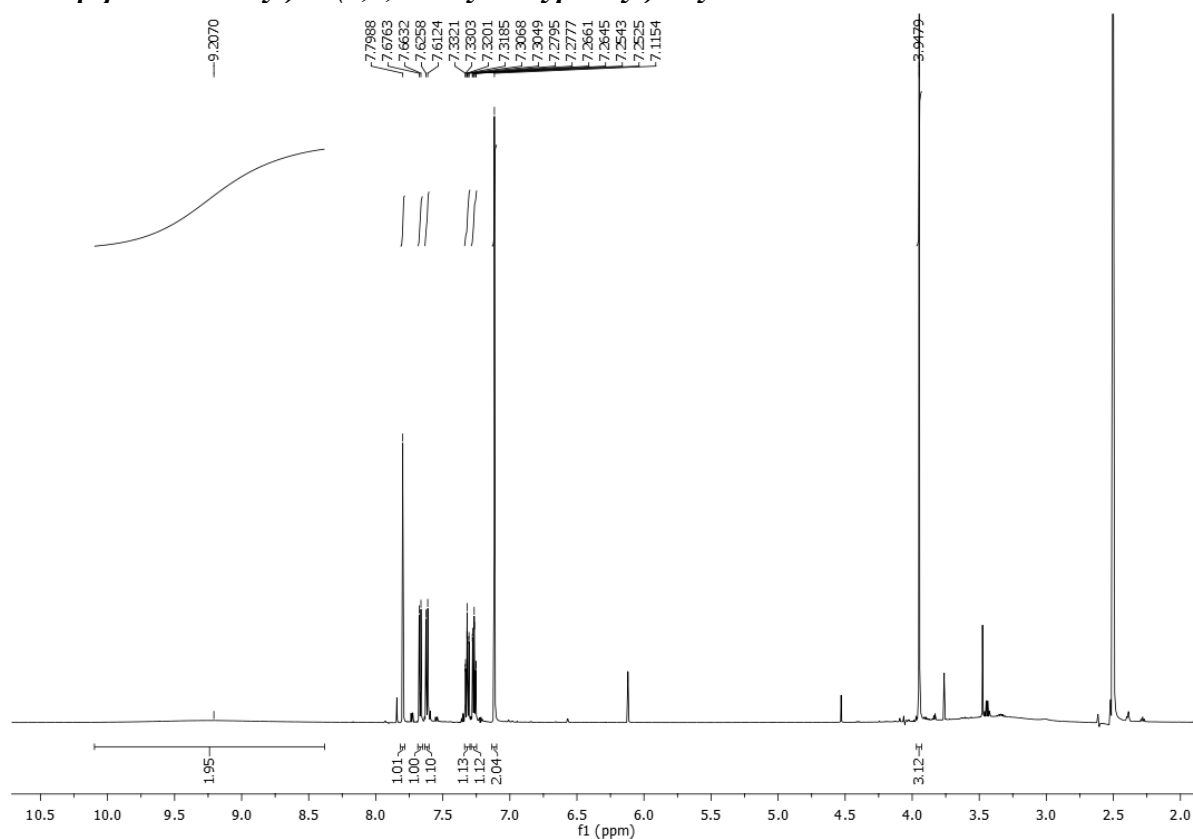


Figure S44. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-methyl-1H-benzof[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile **38**

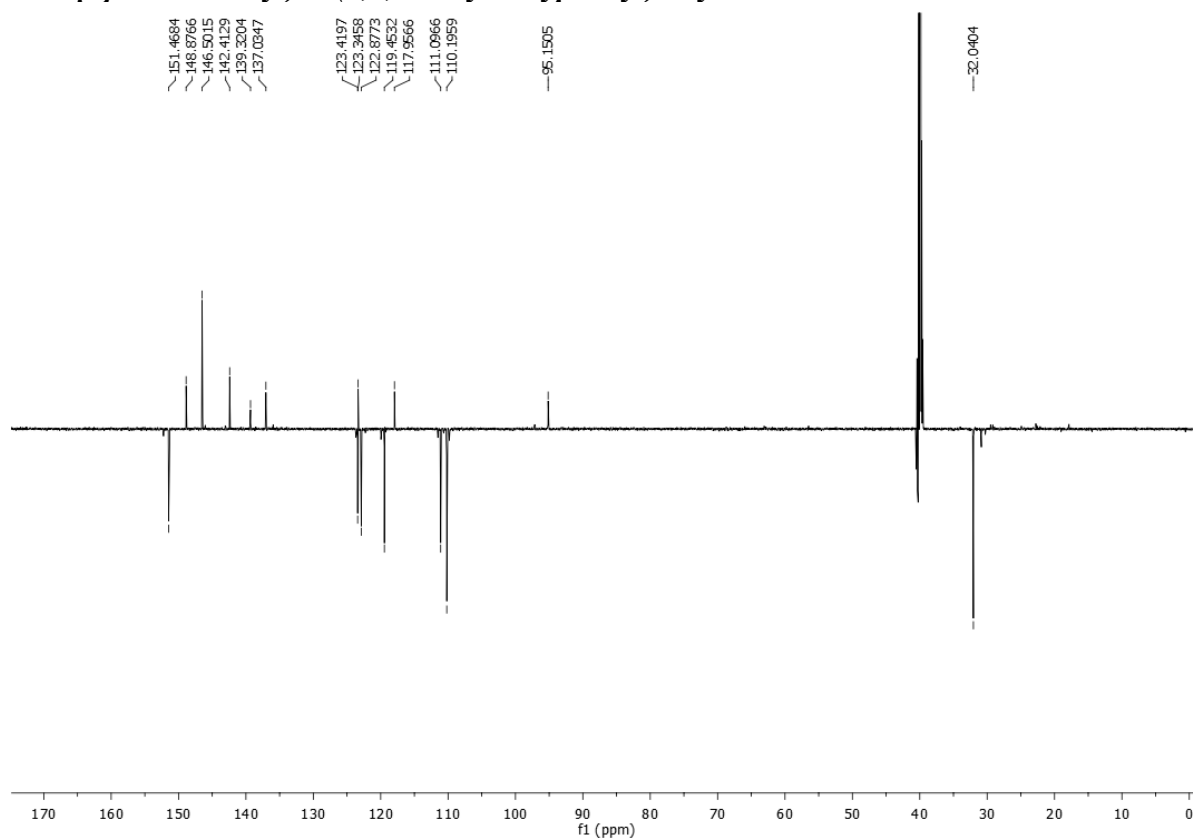


Figure S45. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile **39**

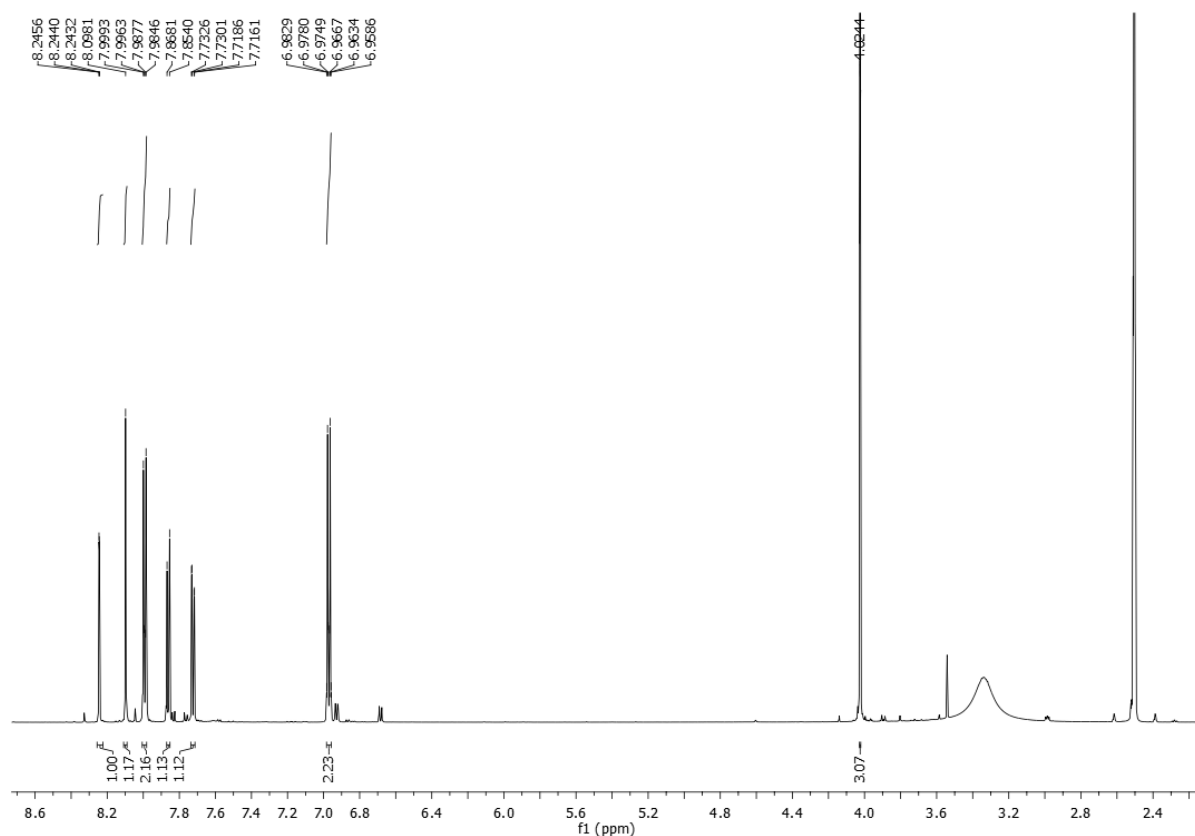


Figure S46. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile **39**

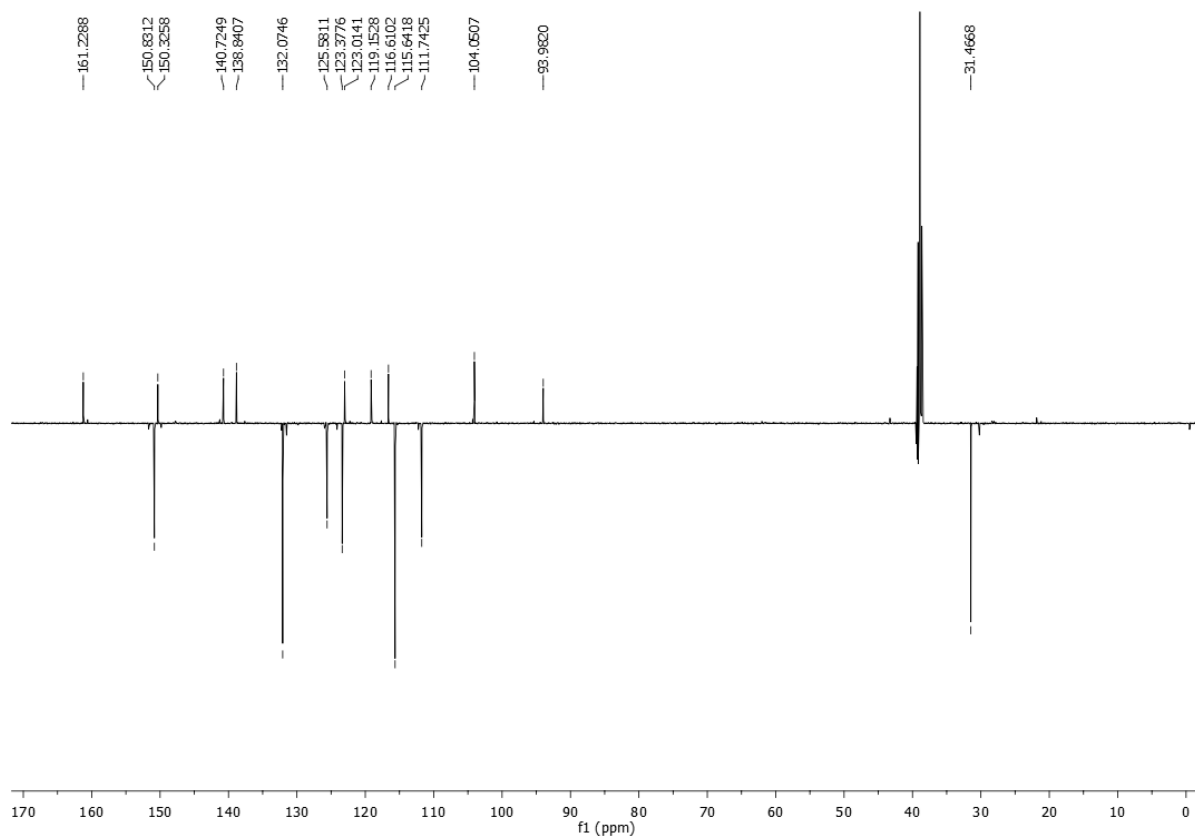


Figure S47. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile 40

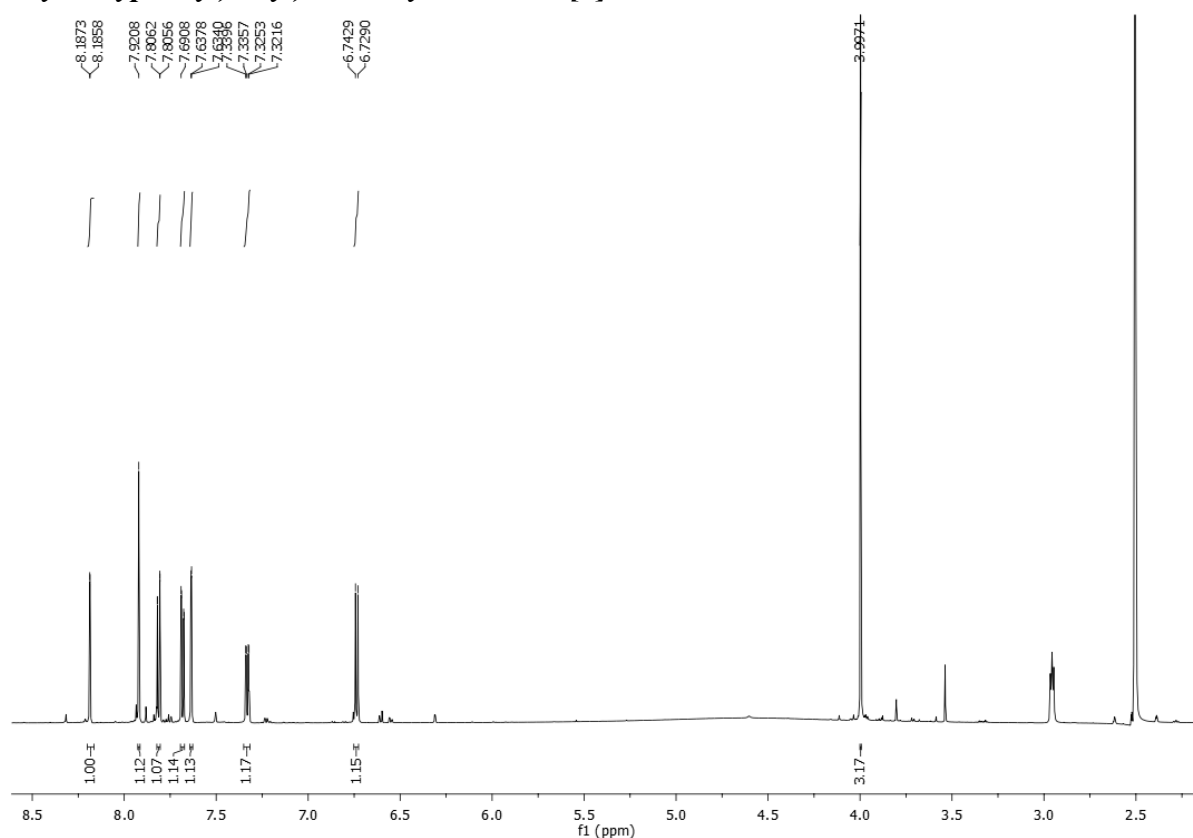


Figure S48. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile 40

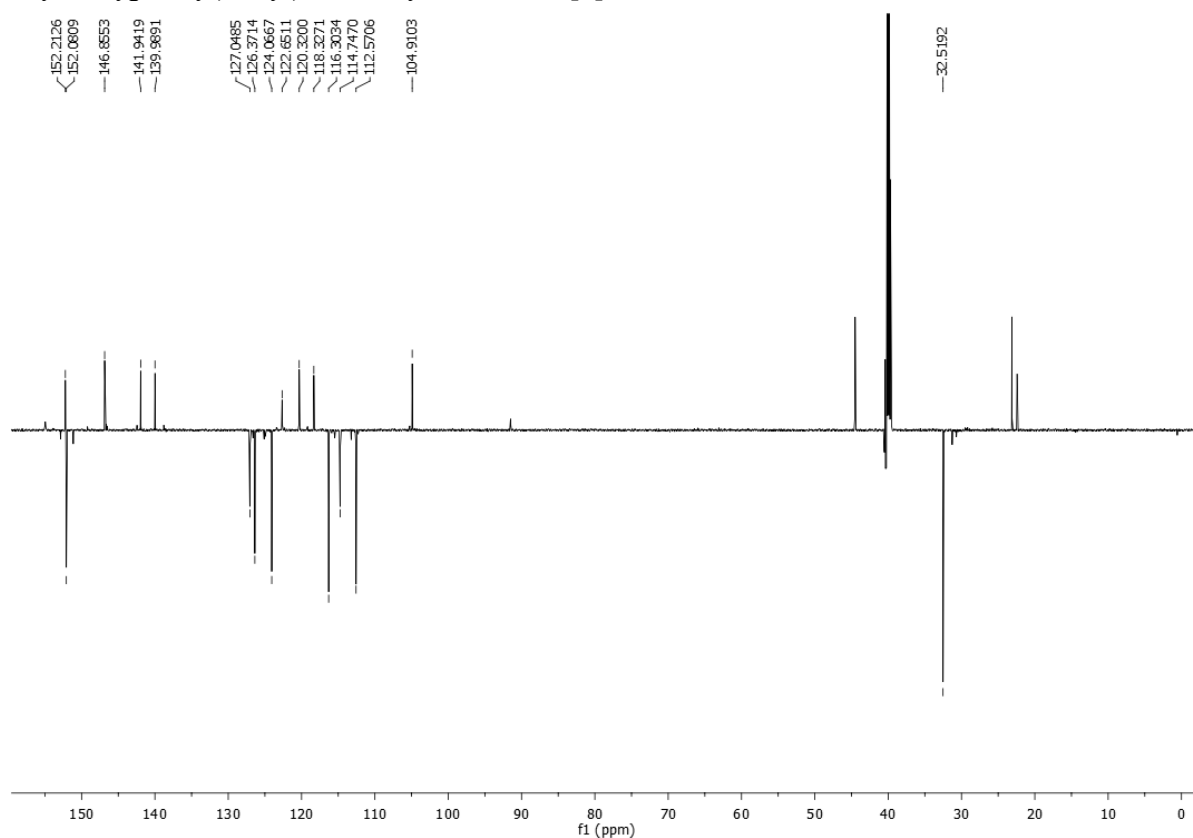


Figure S49. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile 41

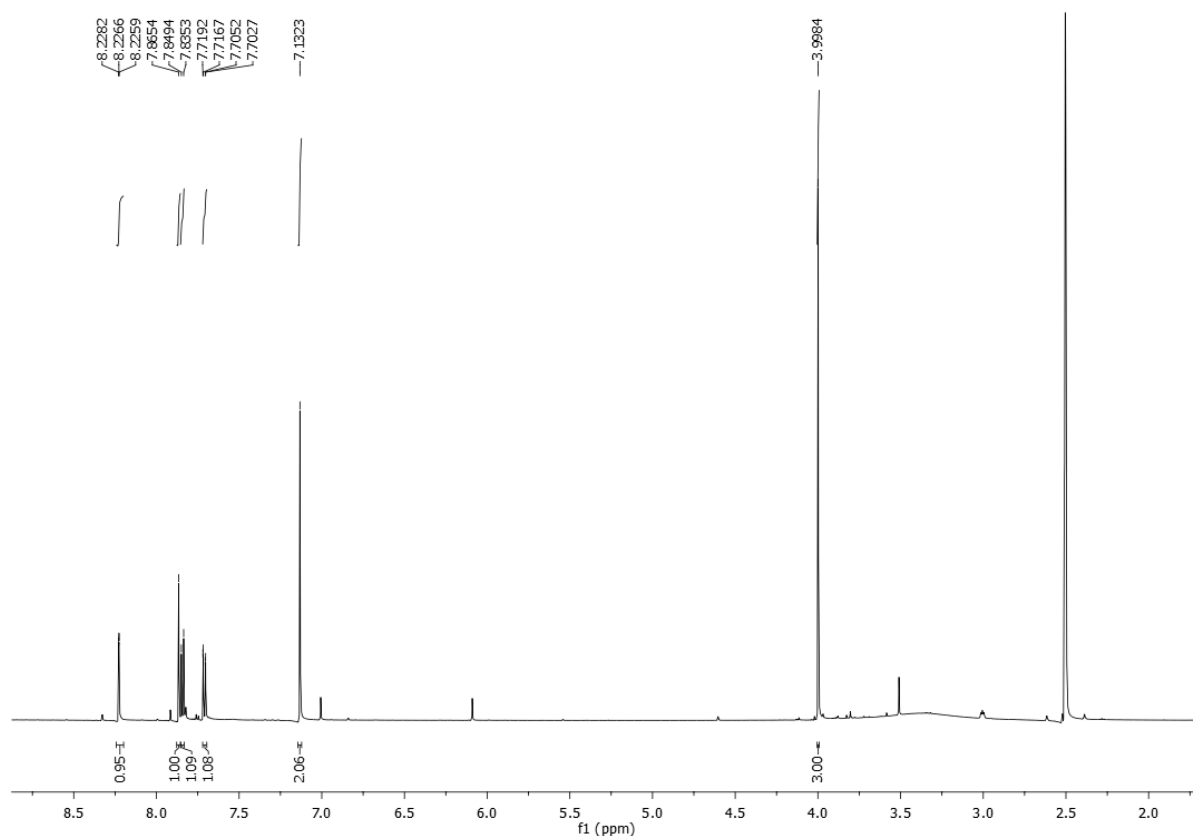


Figure S50. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-methyl-1H-benzo[d]imidazole-6-carbonitrile 41

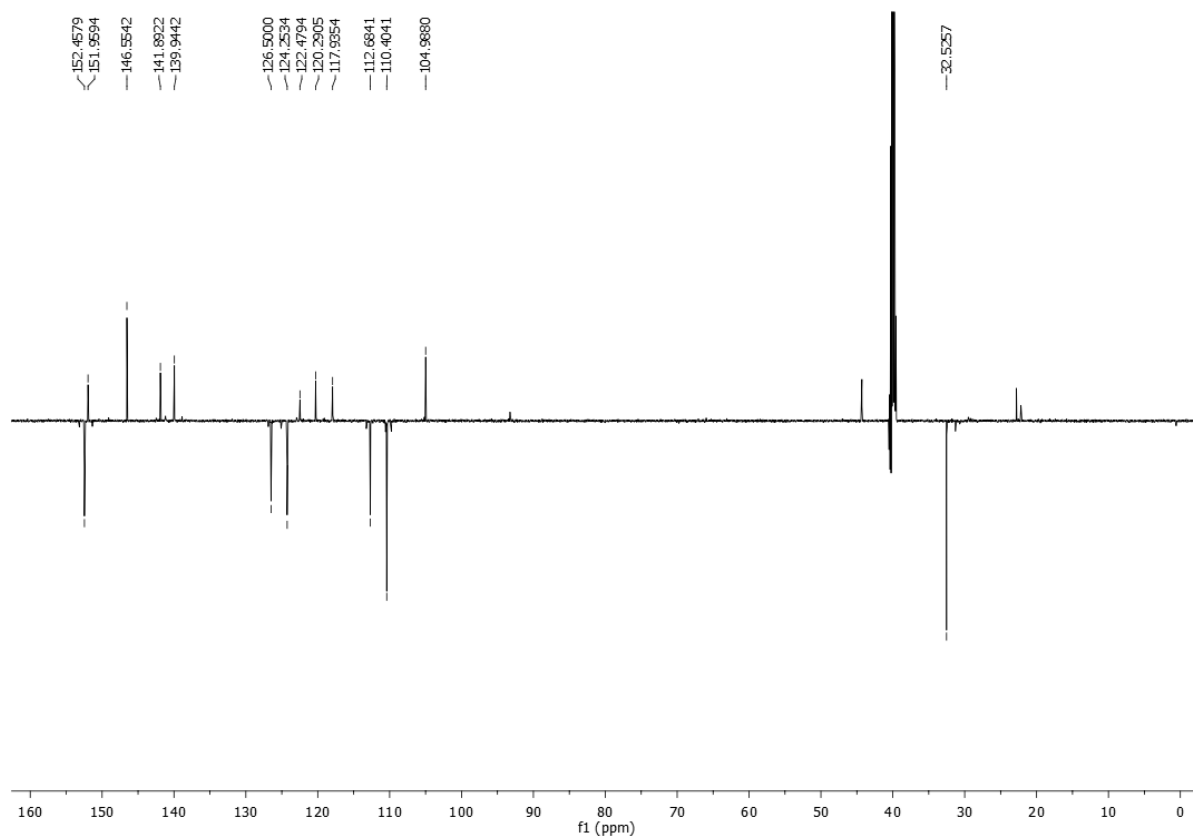


Figure S51. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-phenyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 42

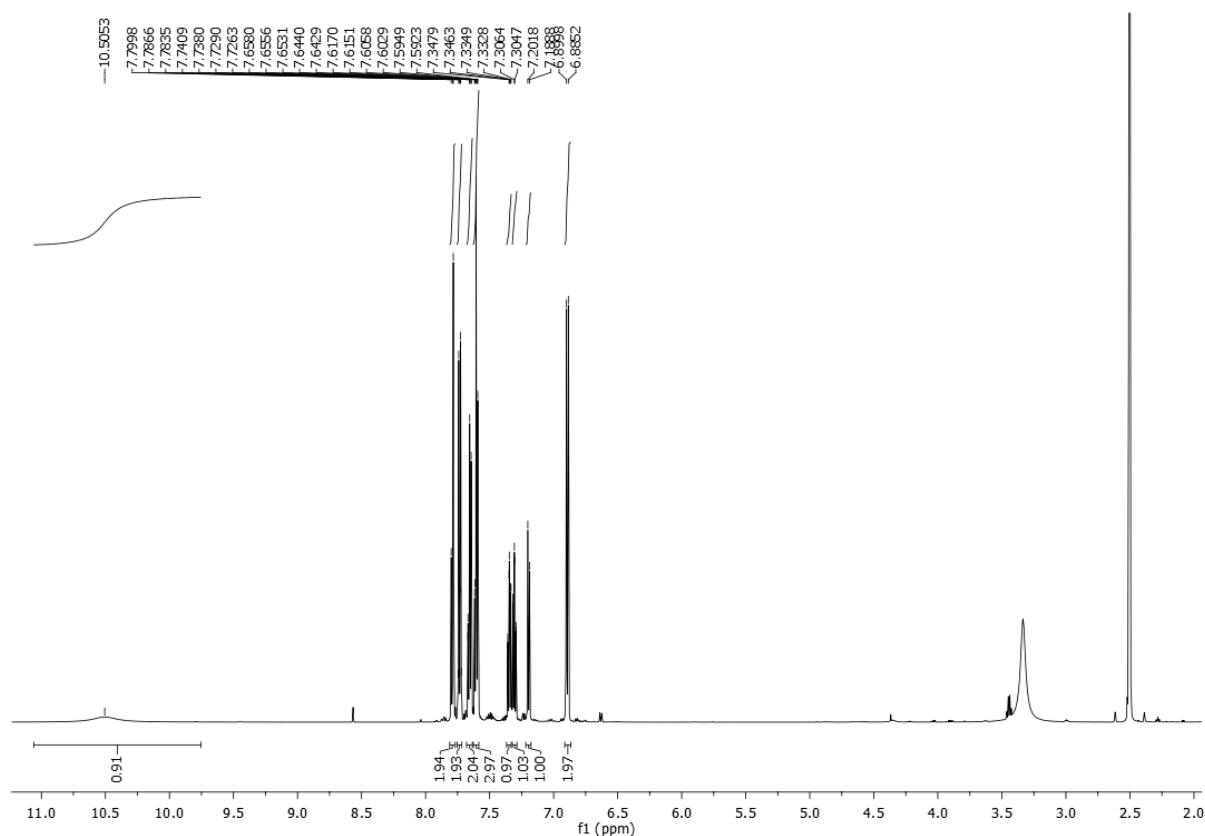


Figure S52. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(4-hydroxyphenyl)-2-(1-phenyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 42

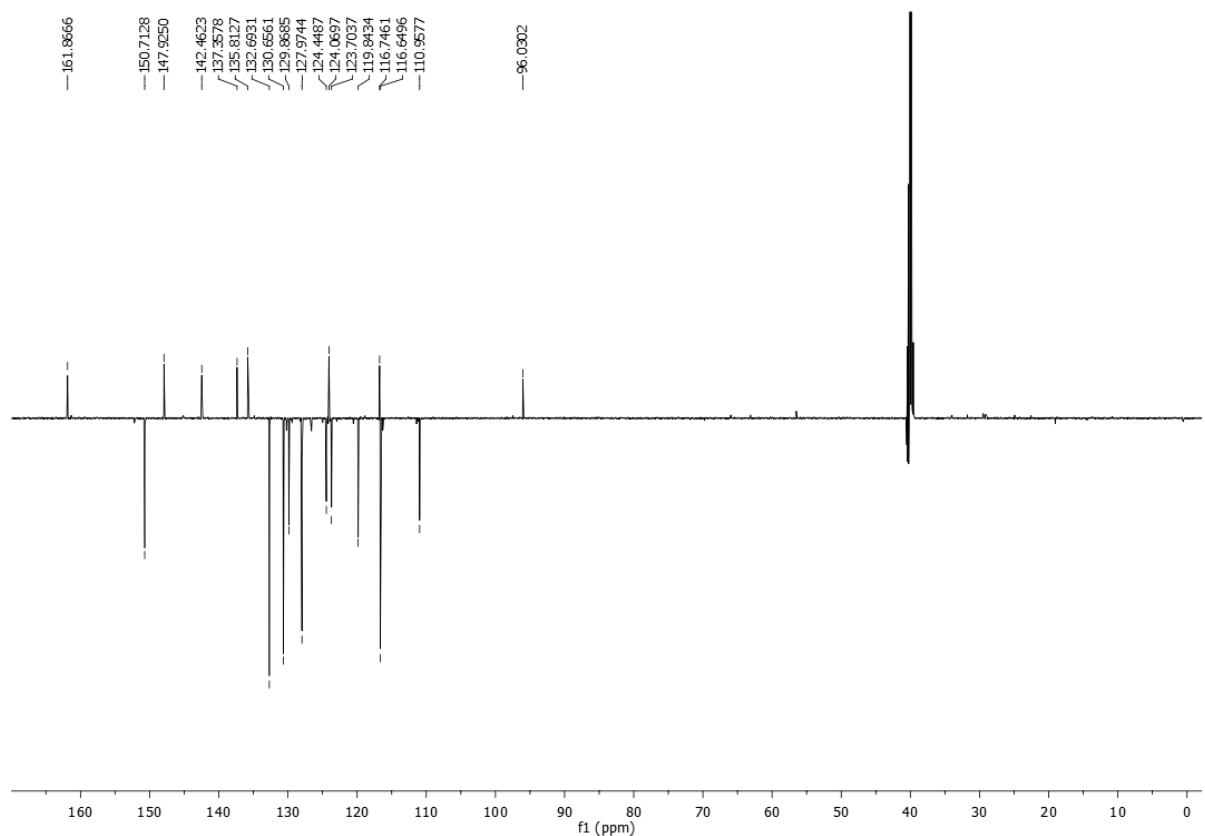


Figure S53. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-phenyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 43

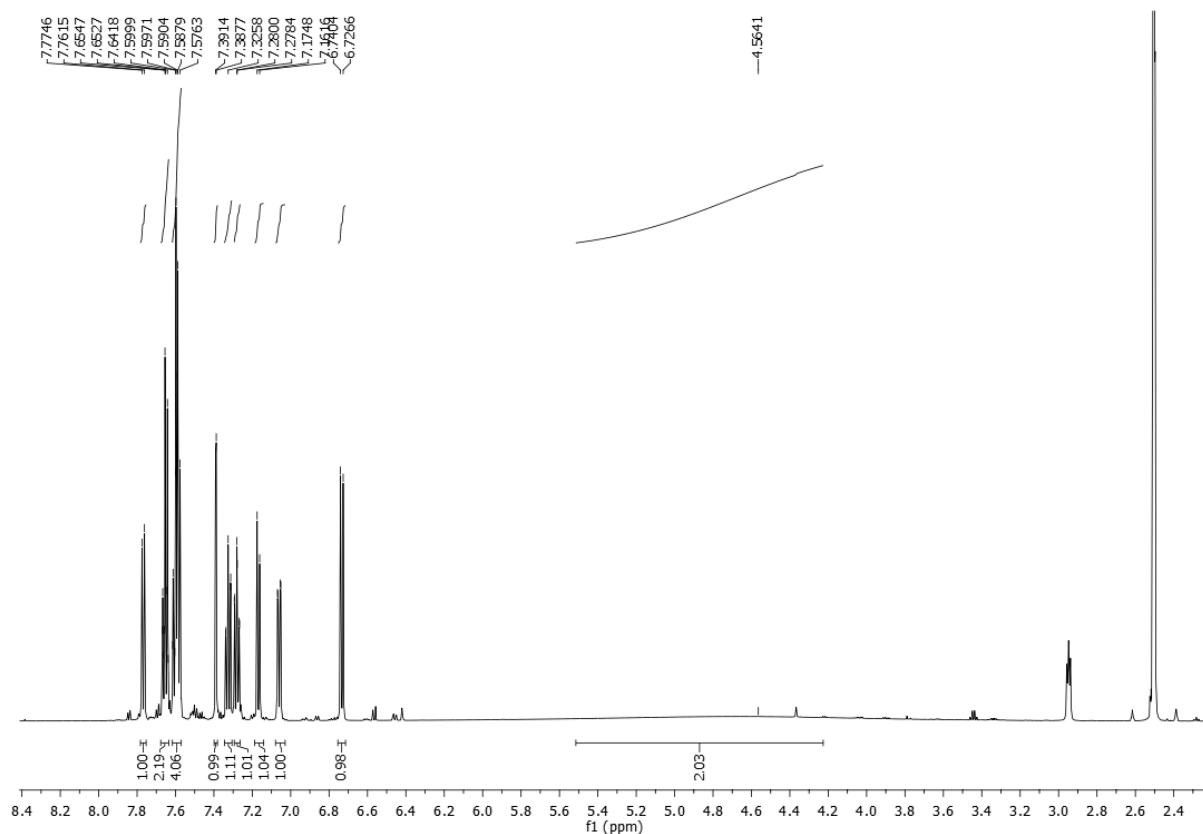


Figure S54. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-3-(3,4-dihydroxyphenyl)-2-(1-phenyl-1H-benzo[d]imidazol-2-yl)acrylonitrile 43

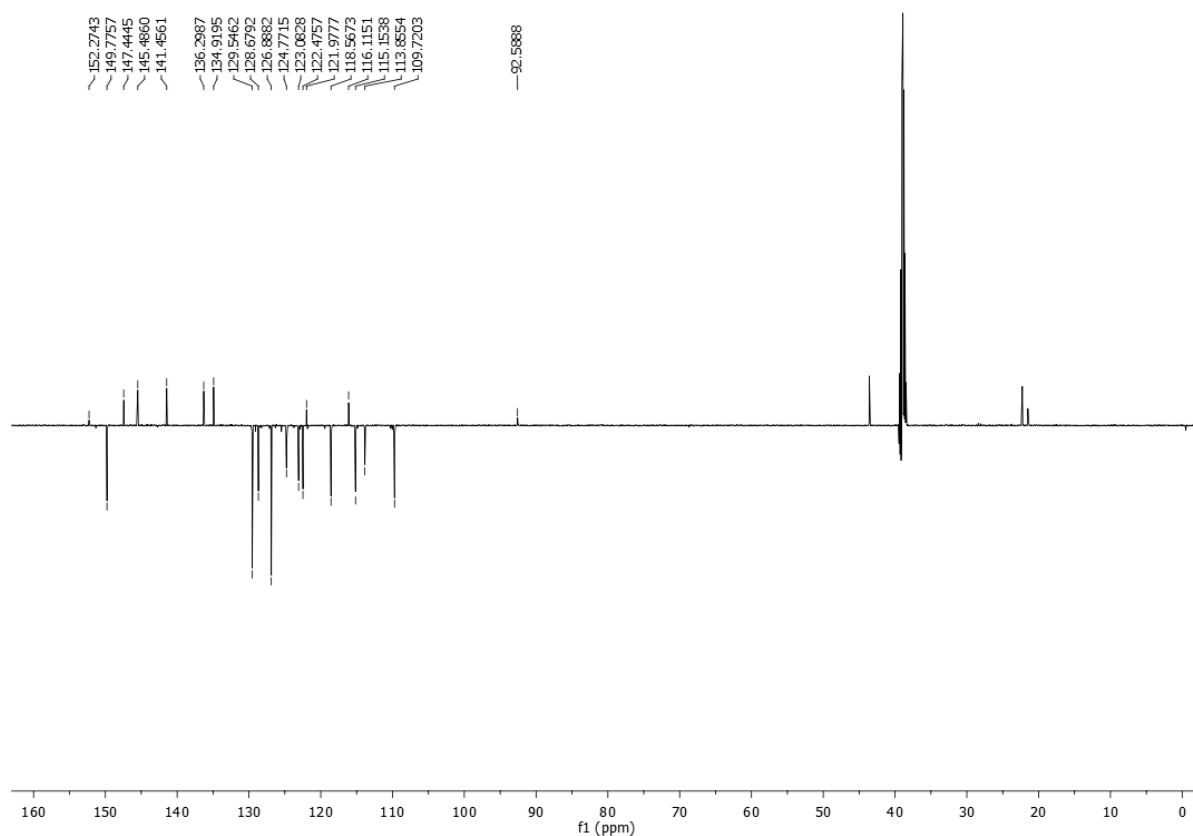


Figure S55. ^1H NMR spectrum ($\text{DMSO-}d_6$, 600 MHz) of *(E)*-2-(1-phenyl-1H-benzof[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 44

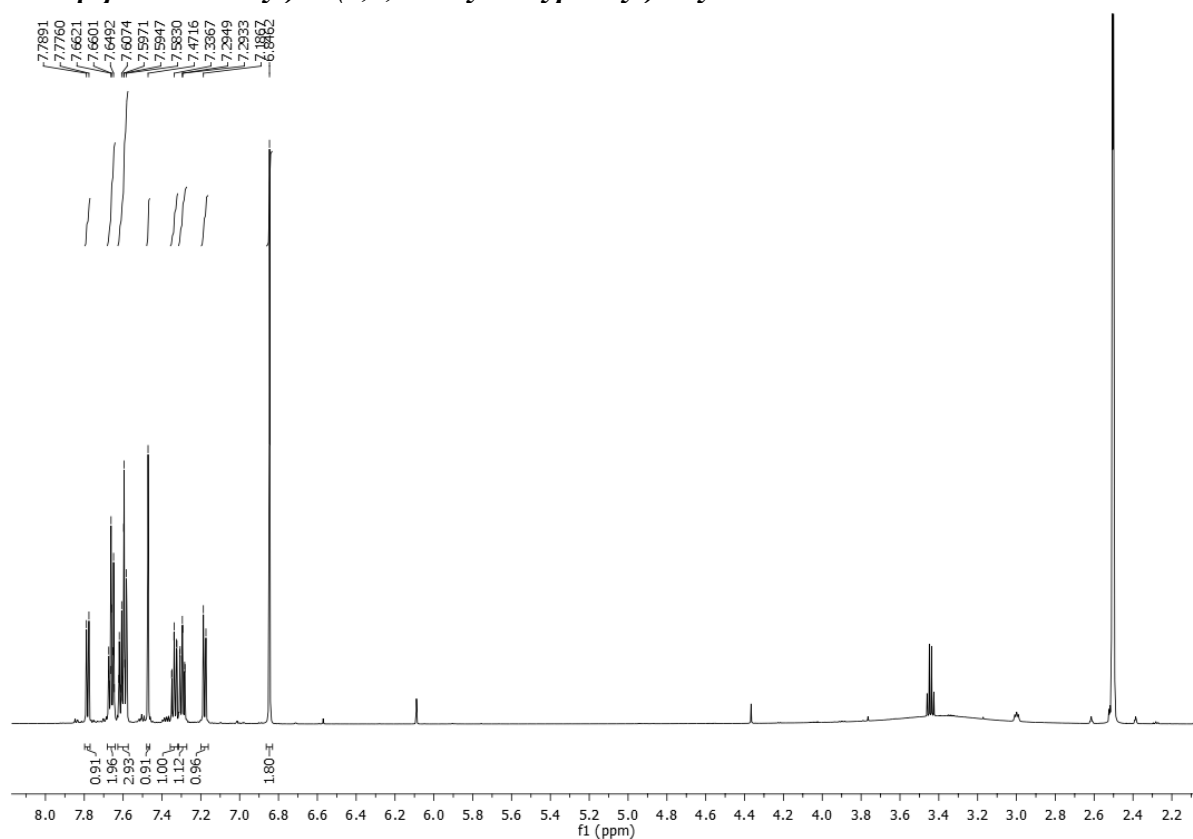


Figure S56. ^{13}C NMR spectrum ($\text{DMSO-}d_6$, 151 MHz) of *(E)*-2-(1-phenyl-1H-benzof[d]imidazol-2-yl)-3-(3,4,5-trihydroxyphenyl)acrylonitrile 44

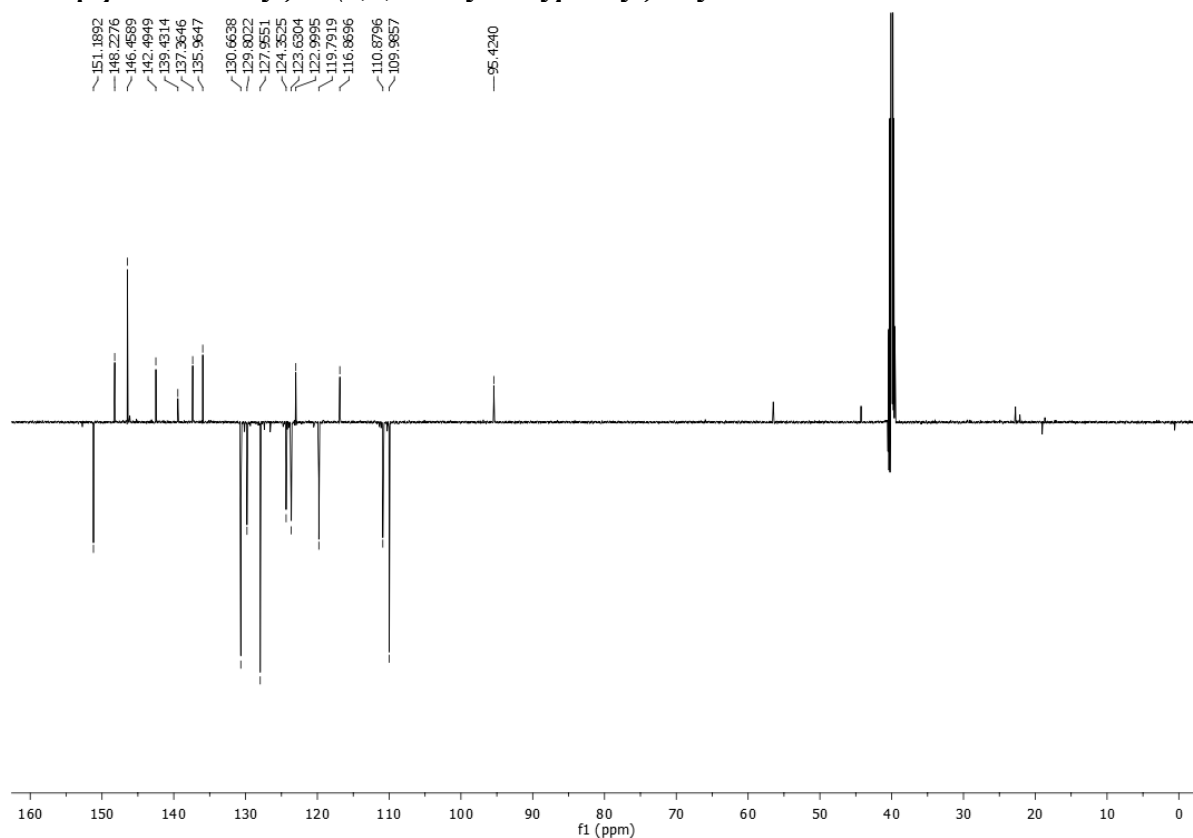


Figure S57. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 45

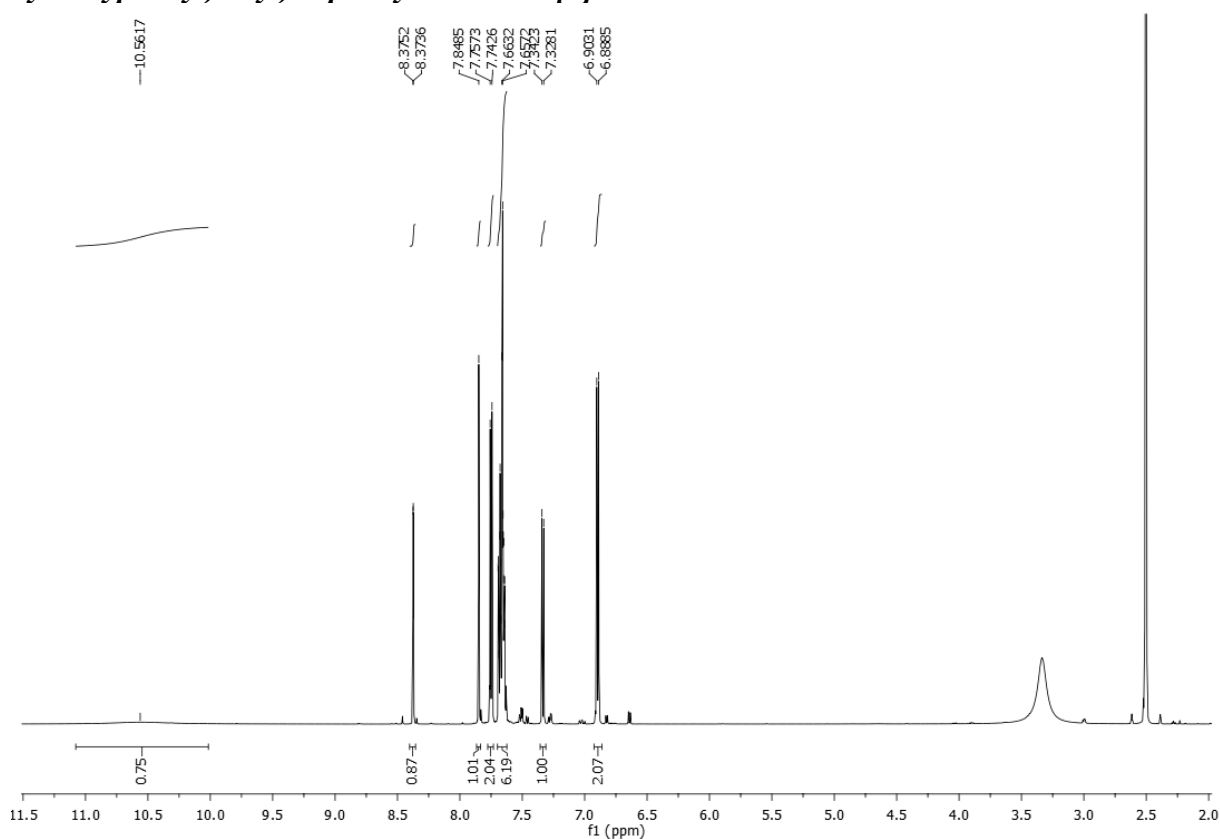


Figure S58. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(4-hydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 45

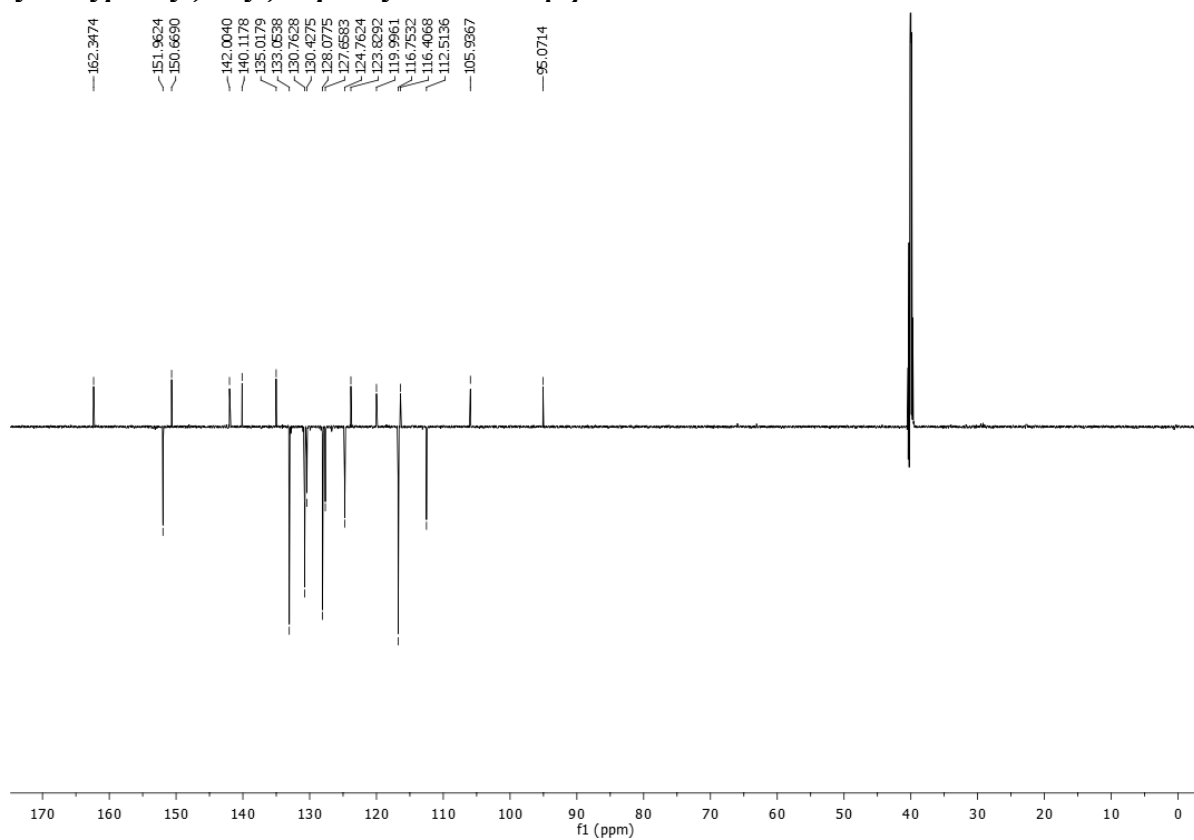


Figure S59. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 46

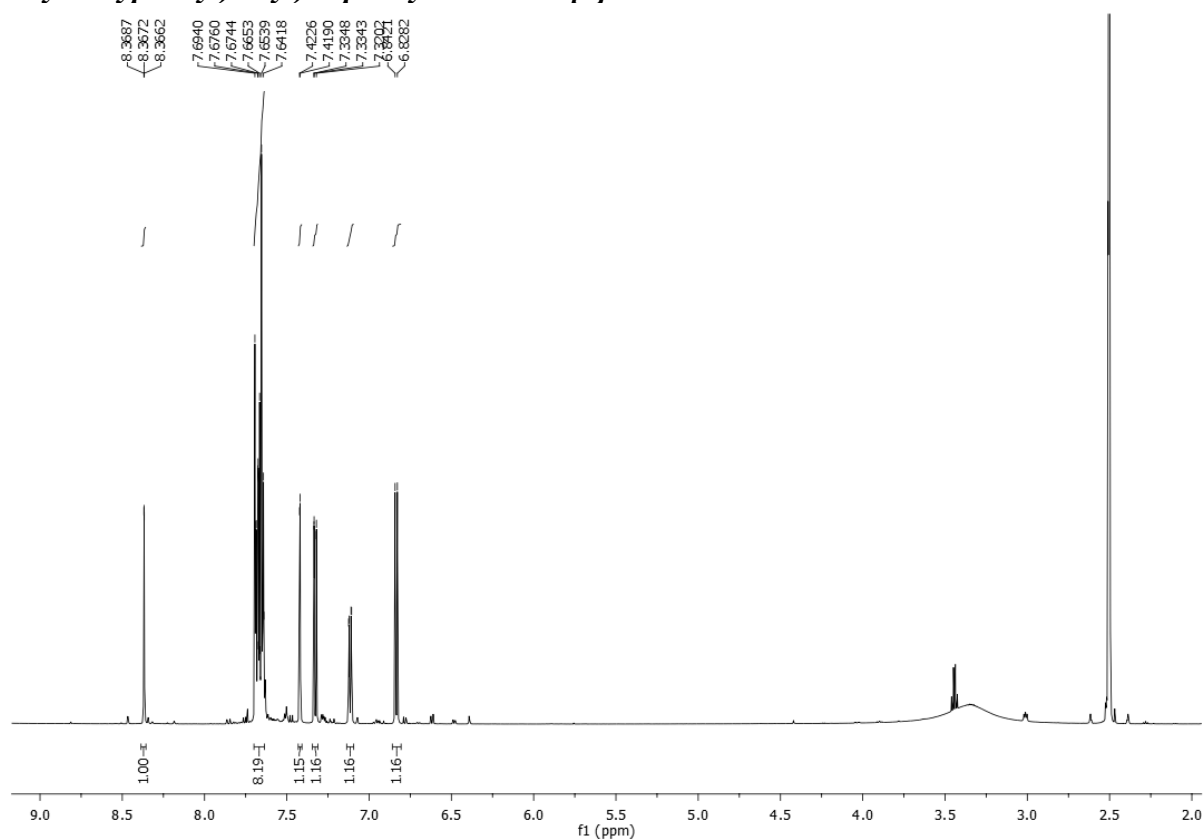


Figure S60. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4-dihydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 46

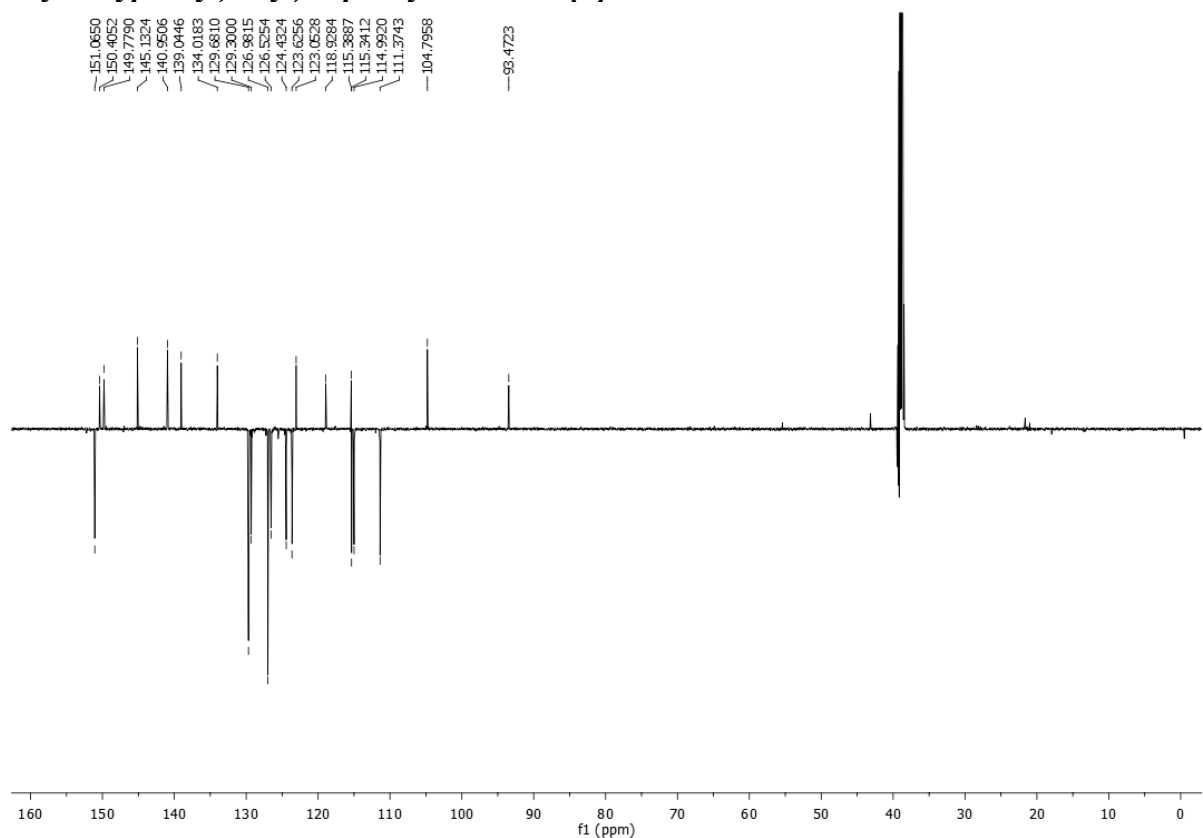


Figure S61. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 47

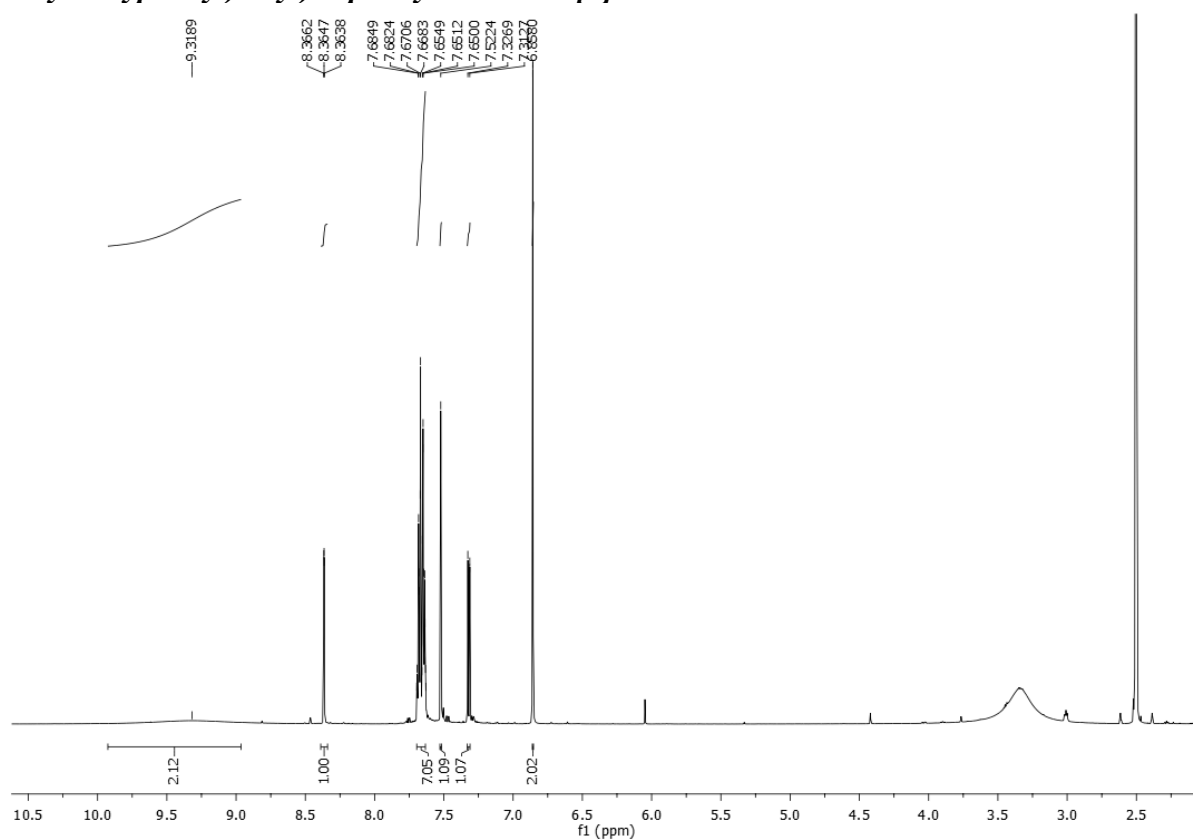


Figure S62. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of *(E)*-2-(1-cyano-2-(3,4,5-trihydroxyphenyl)vinyl)-1-phenyl-1H-benzo[d]imidazole-6-carbonitrile 47

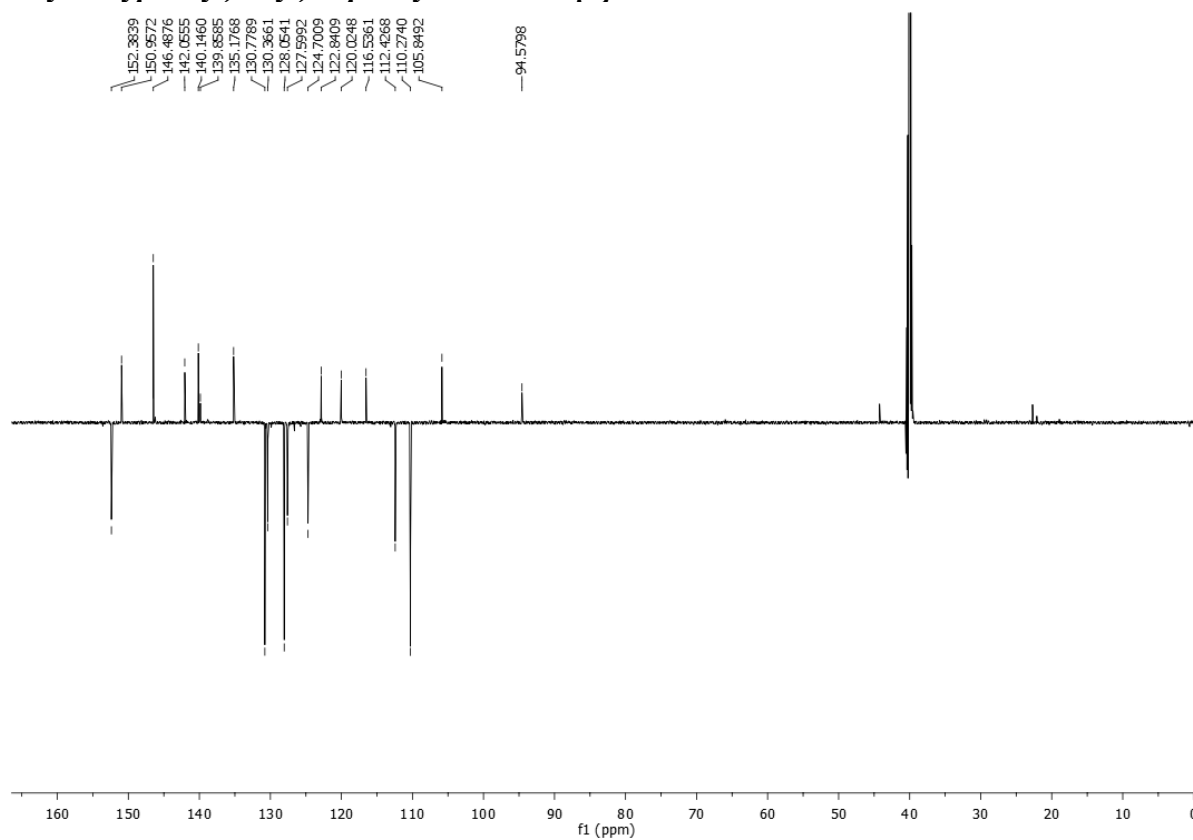


Figure S63. Reaction scheme for preparing the compounds **1-6** which synthesis has been already published.

