

**Design, synthesis of 2-phenyl-1H-benzo[d]imidazole derivatives as 17 β -HSD10
inhibitor for the treatment of Alzheimer's Disease**

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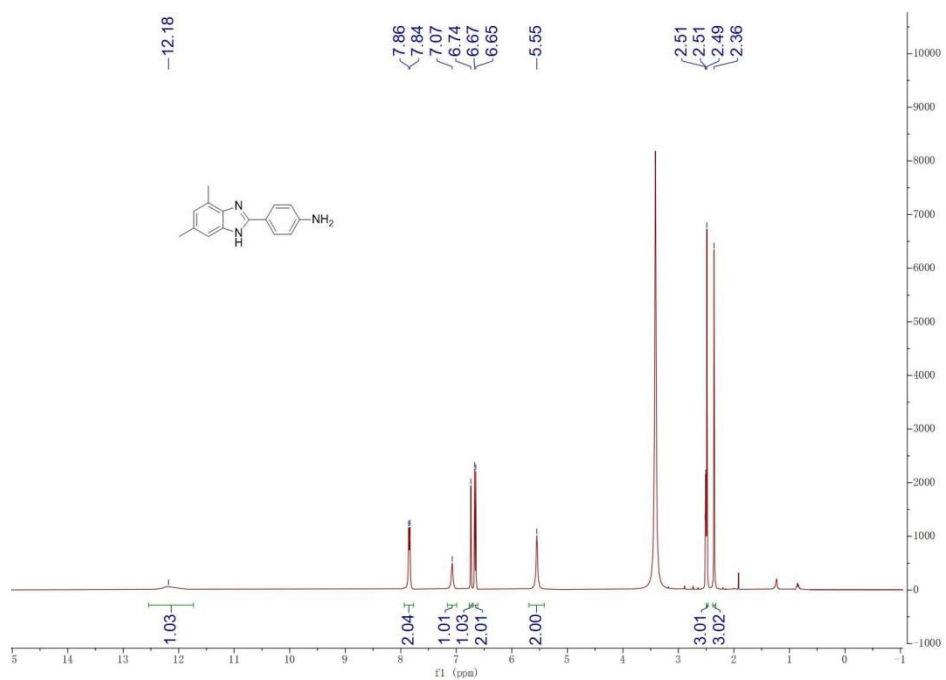
Nanjing 210023, P. R. China;

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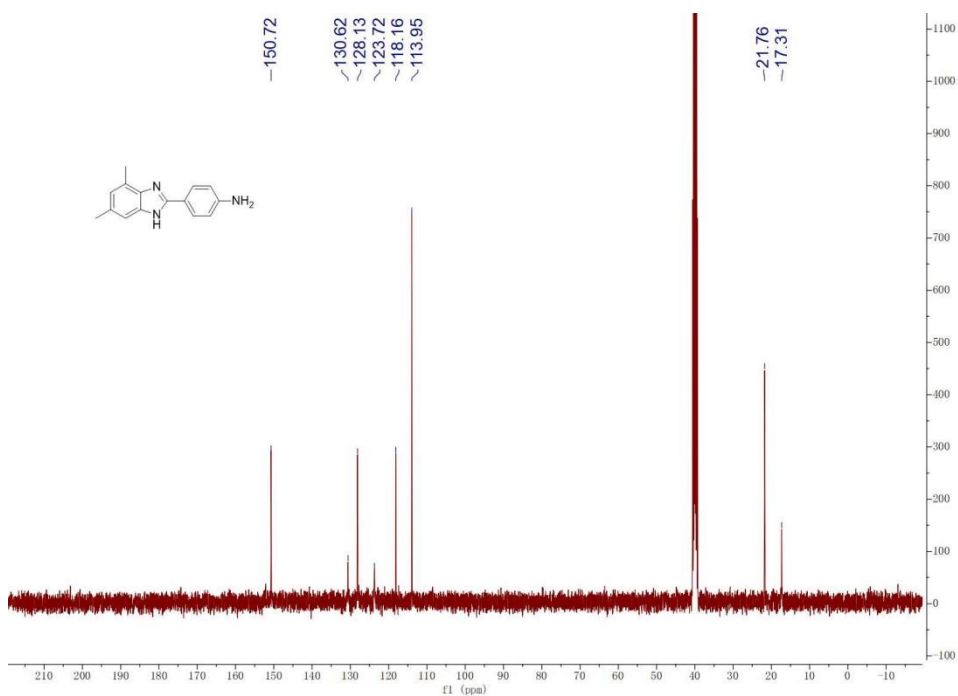
Contents

1. ¹H NMR, ¹³C NMR, HRMS.....S2

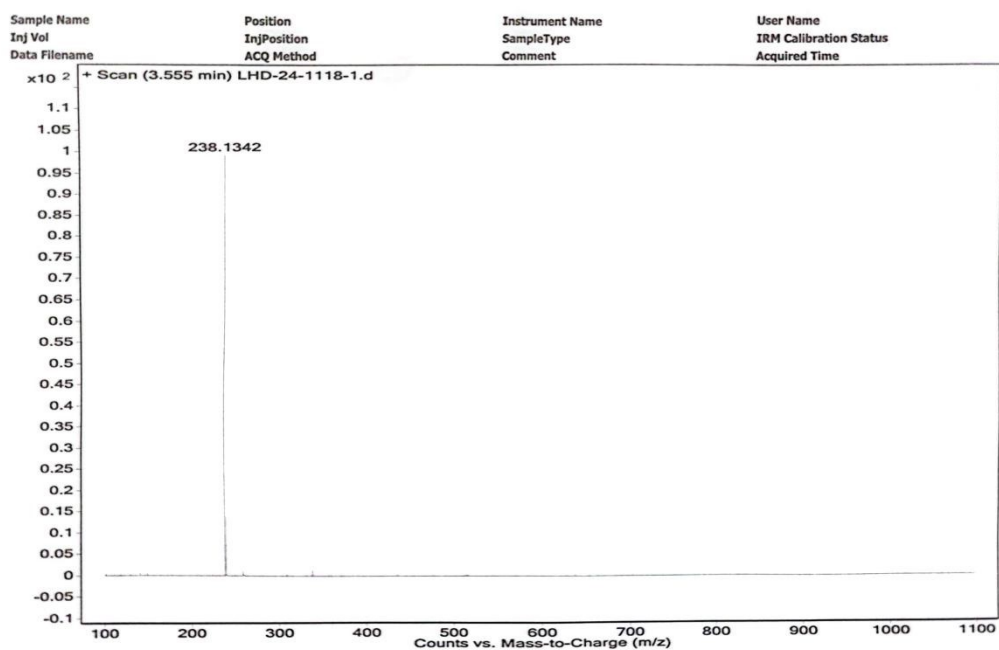
4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)aniline (H1)



¹H NMR of compound H1

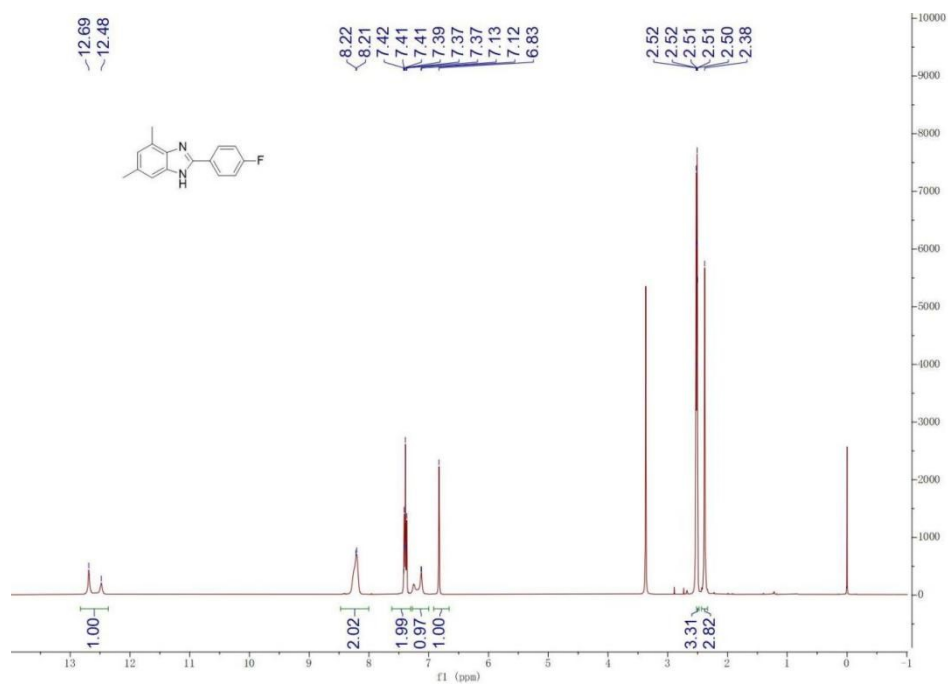


¹³C NMR of compound H1

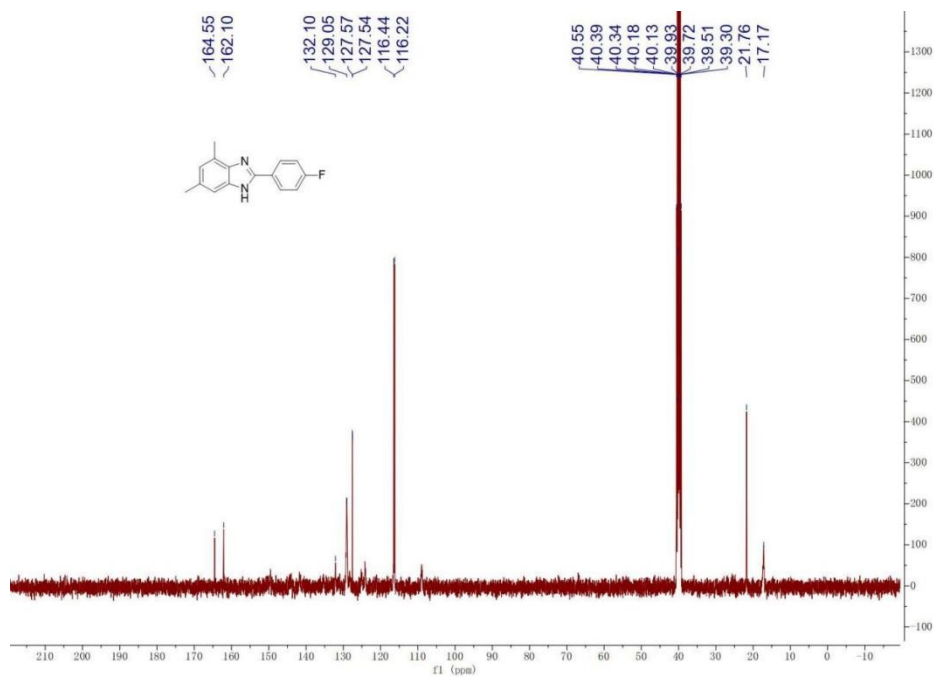


HR-MS of compound H1

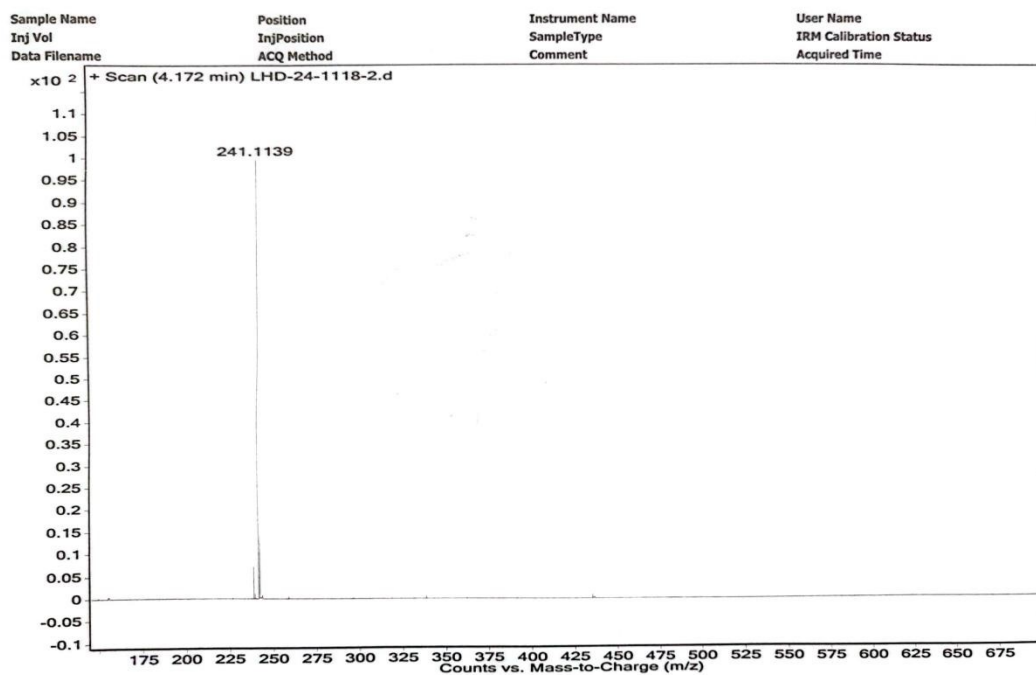
2-(4-fluorophenyl)-4,6-dimethyl-1H-benzo[d]imidazole (1)



¹H NMR of compound 1

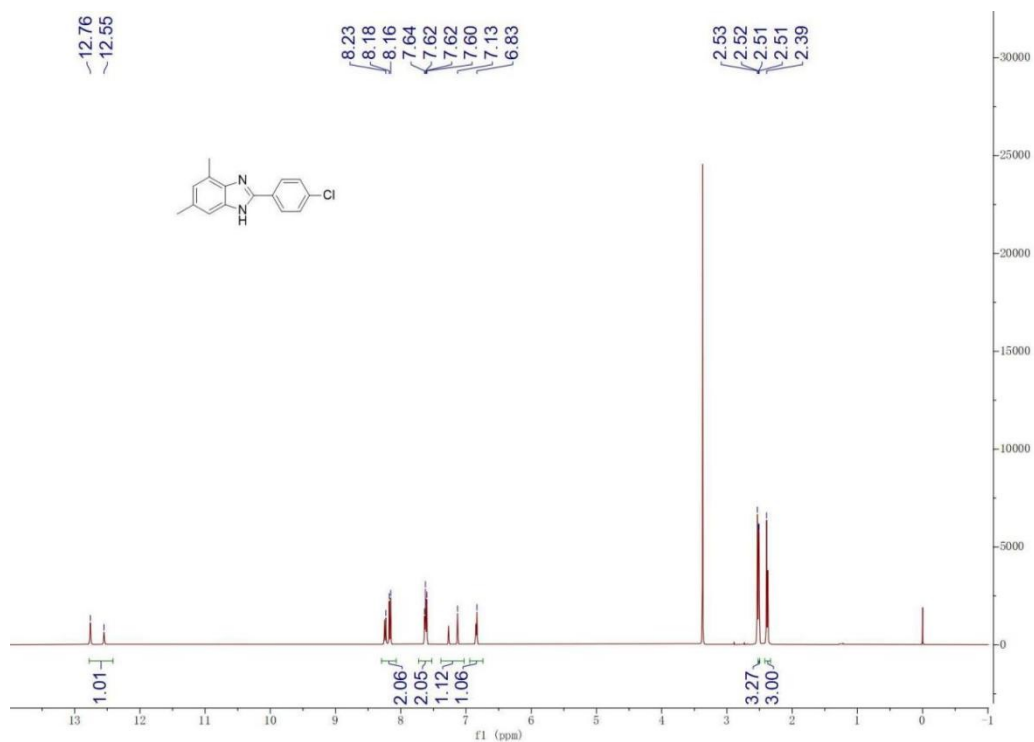


¹³C NMR of compound 1

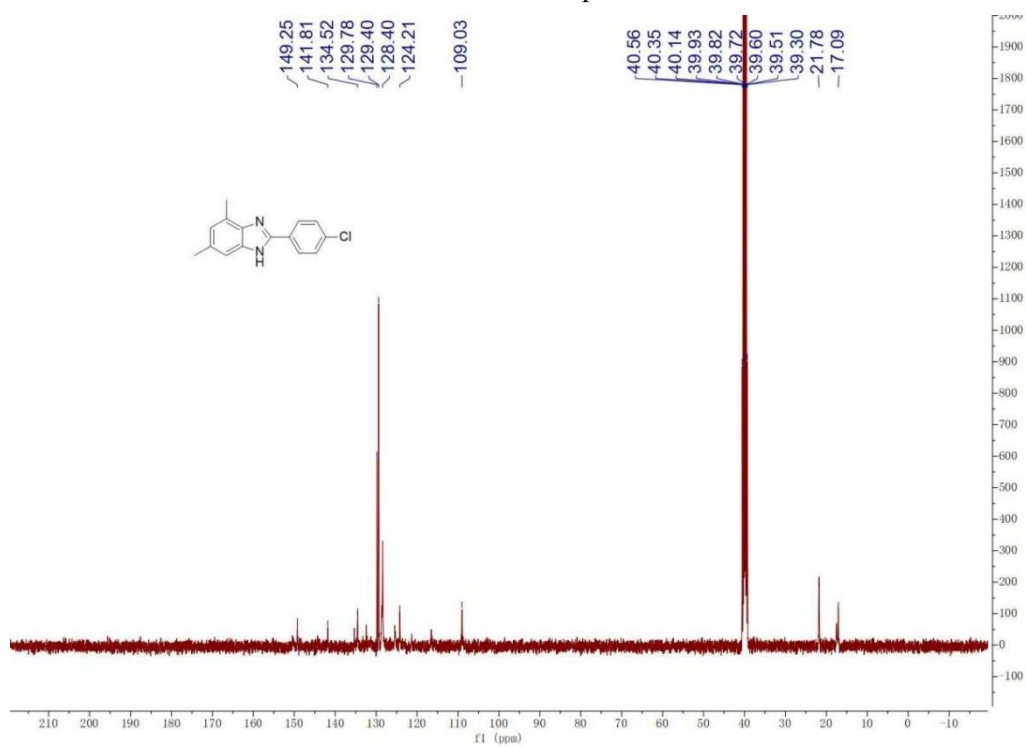


HR-MS of compound 1

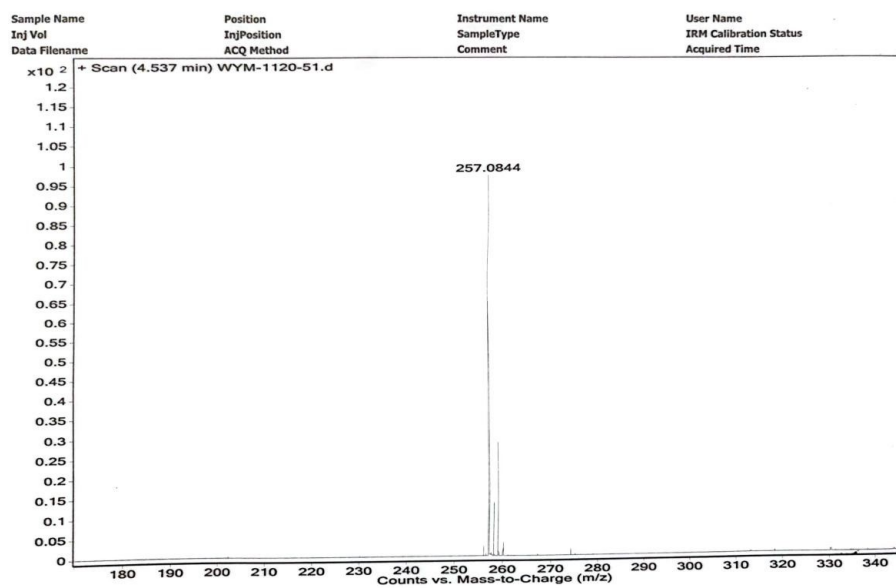
2-(4-chlorophenyl)-4,6-dimethyl-1H-benzo[d]imidazole (2)



¹H NMR of compound 2

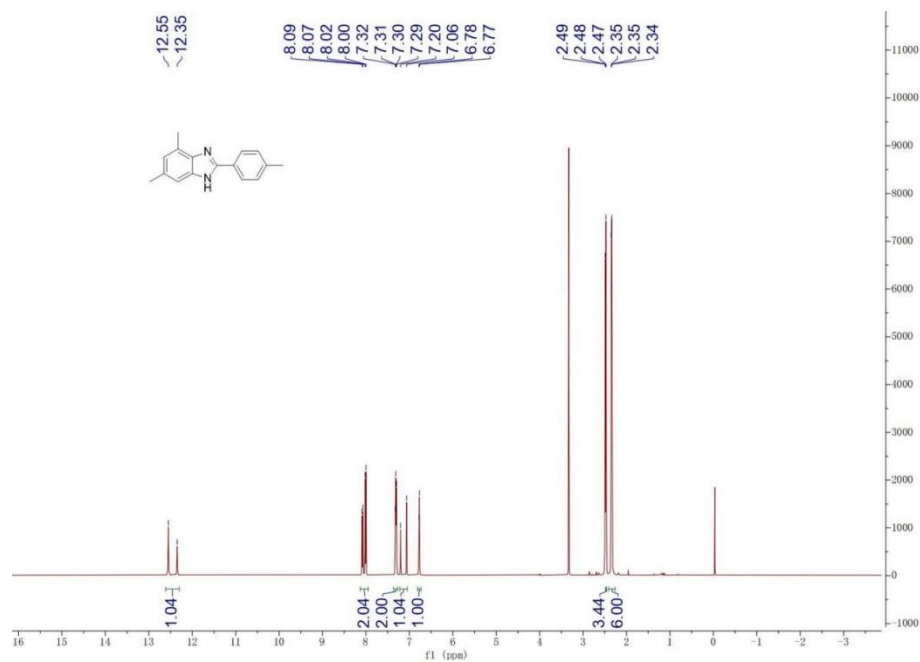


¹³C NMR of compound 2

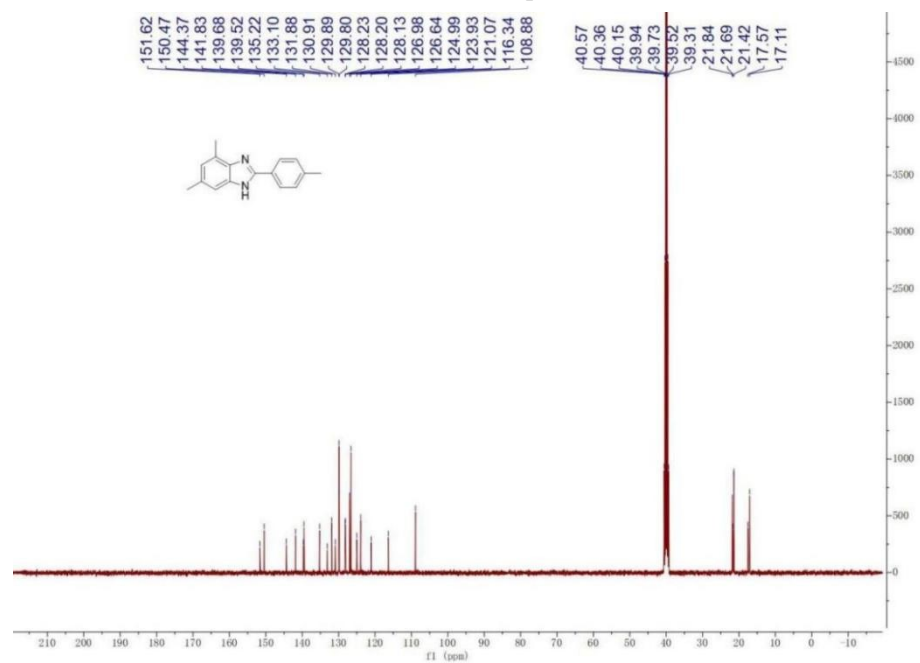


HR-MS of compound 2

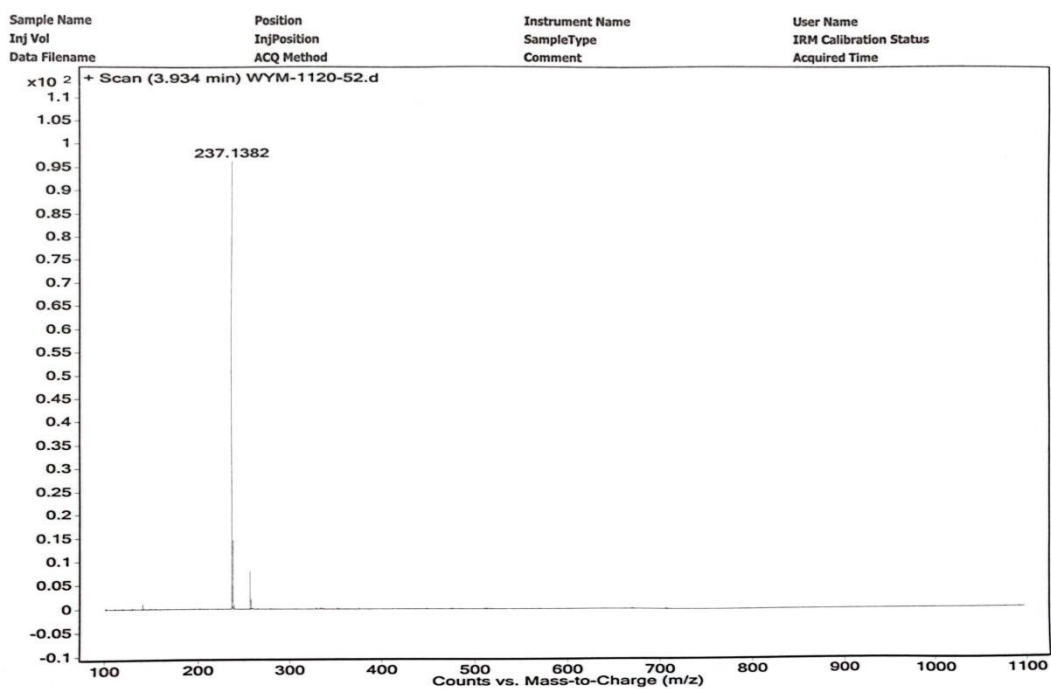
4,6-dimethyl-2-(p-tolyl)-1H-benzo[d]imidazole (3)



¹H NMR of compound 3

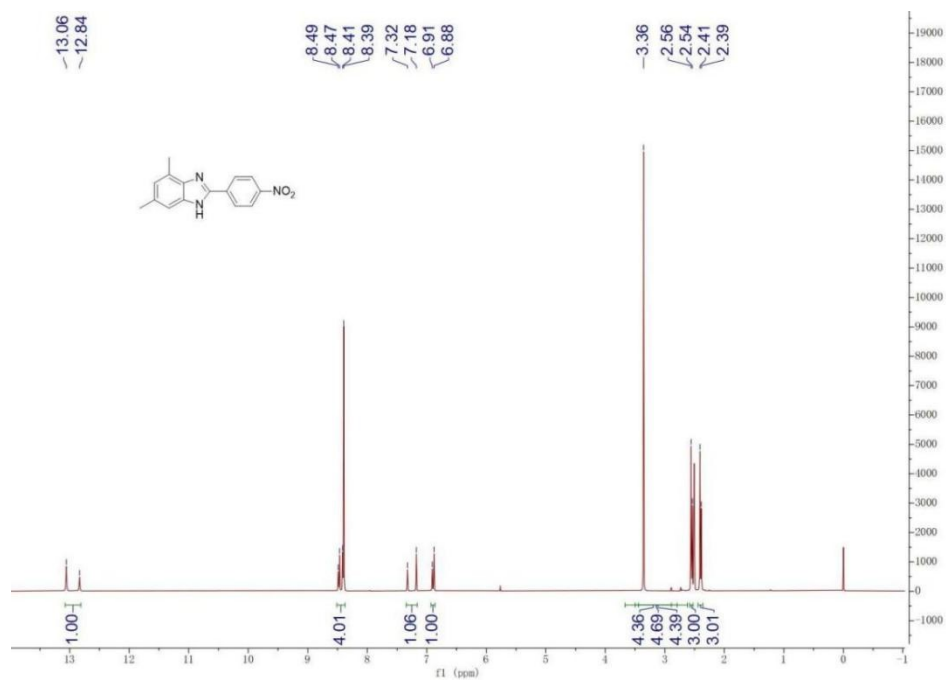


¹³C NMR of compound 3

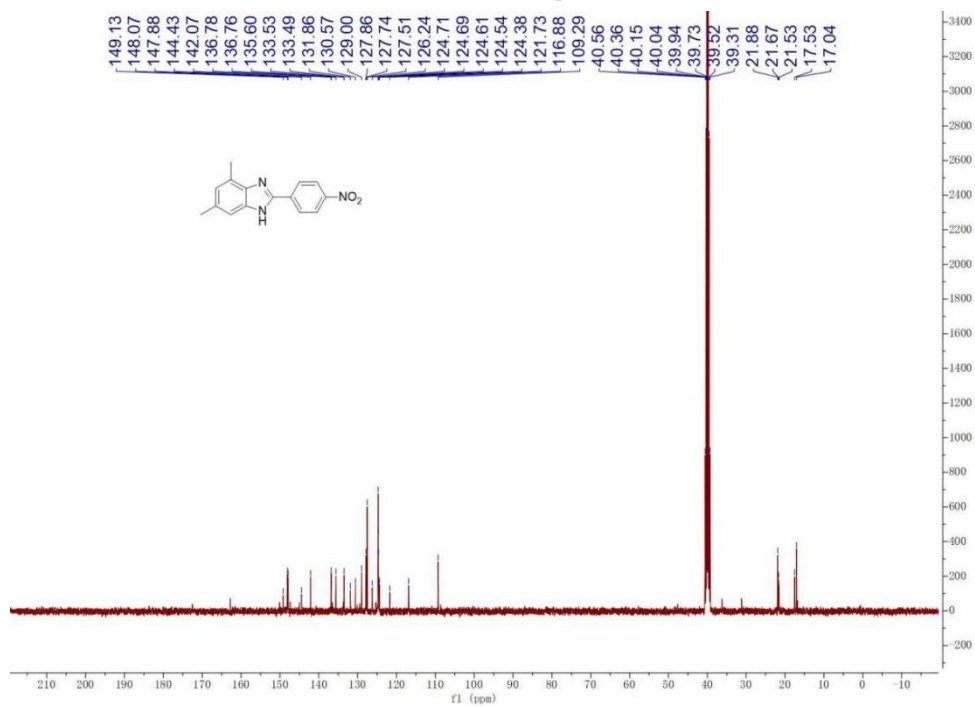


HR-MS of compound 3

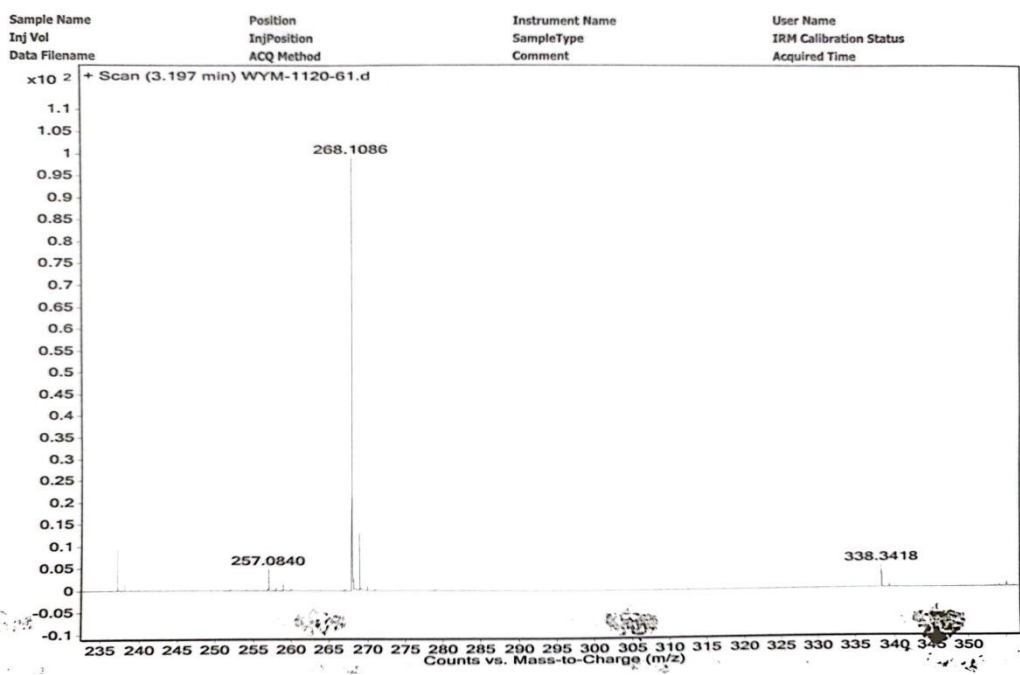
4,6-dimethyl-2-(4-nitrophenyl)-1H-benzo[d]imidazole (4)



¹H NMR of compound 4

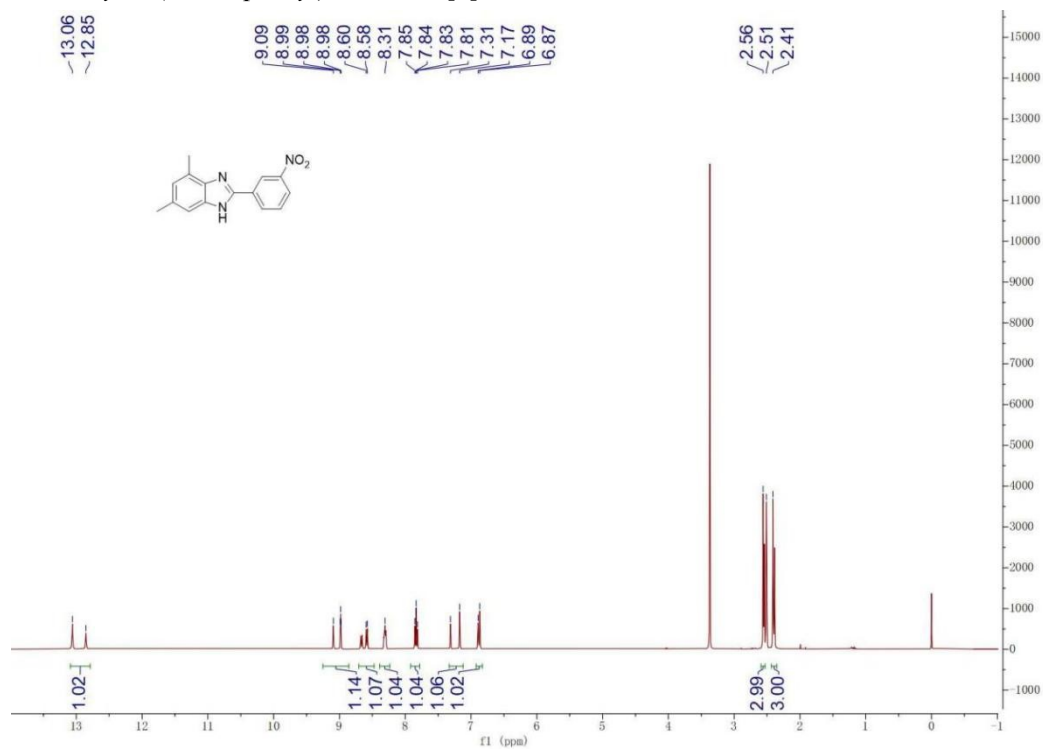


¹³C NMR of compound 4

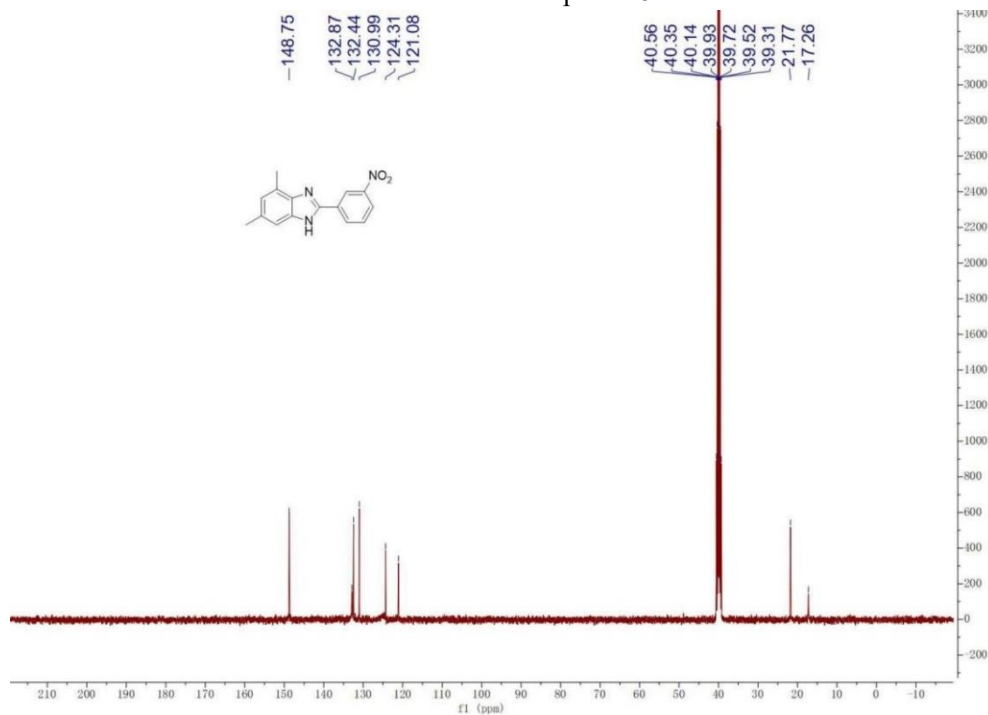


HR-MS of compound 4

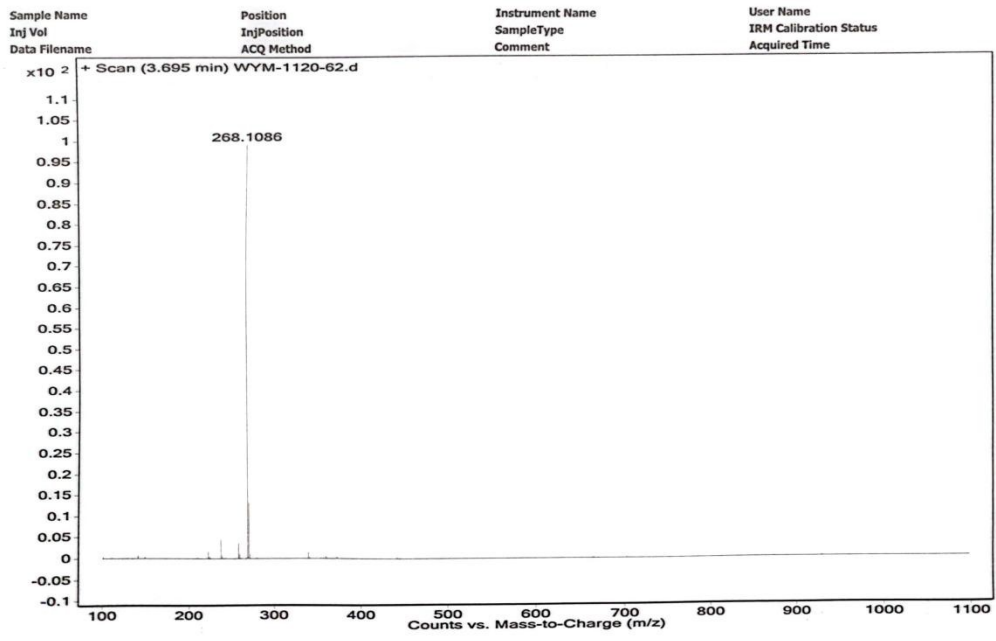
4,6-dimethyl-2-(3-nitrophenyl)-1H-benzo[d]imidazole (5)



¹H NMR of compound 5

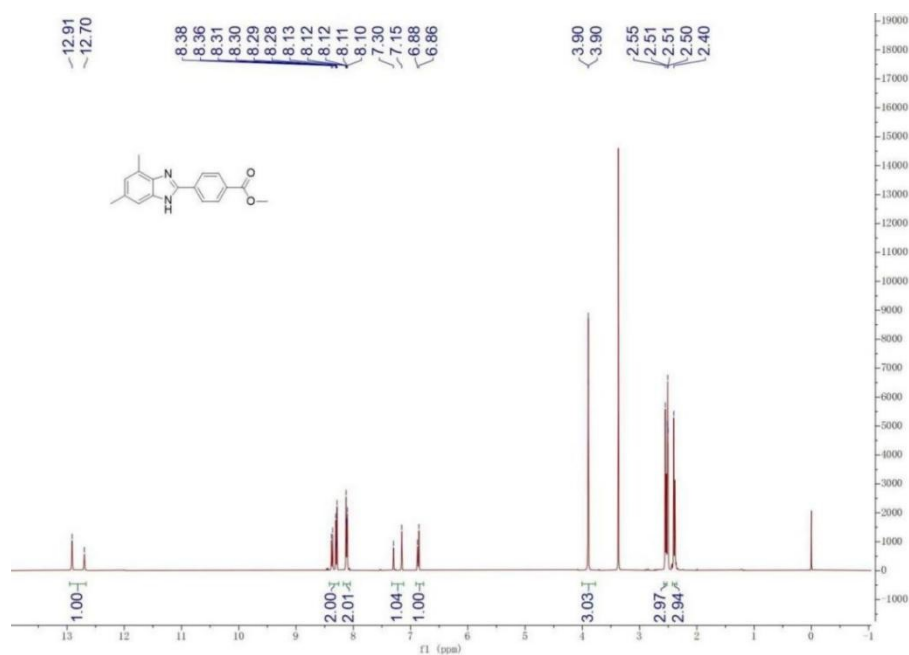


¹³C NMR of compound 5

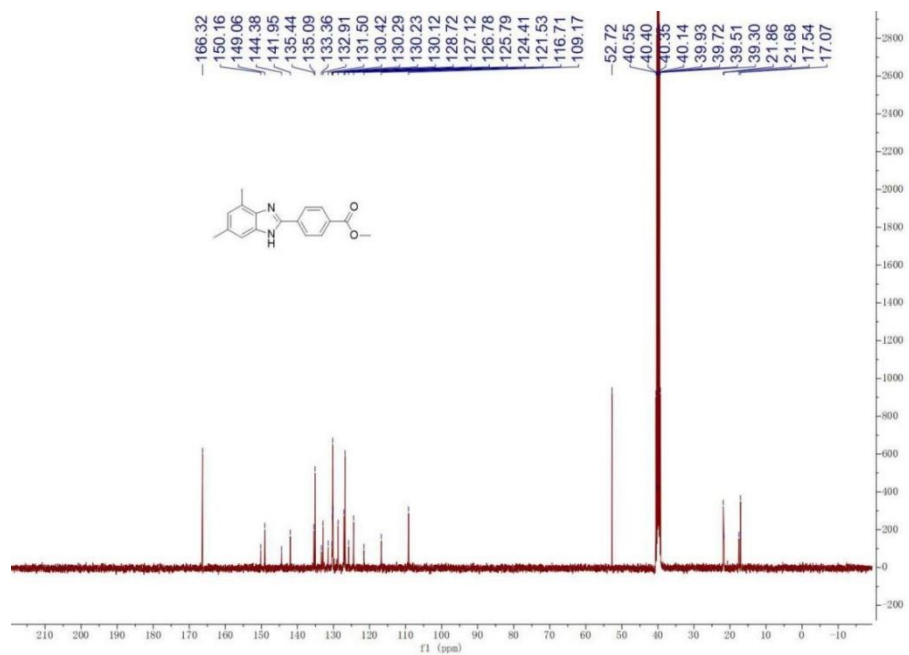


HR-MS of compound 5

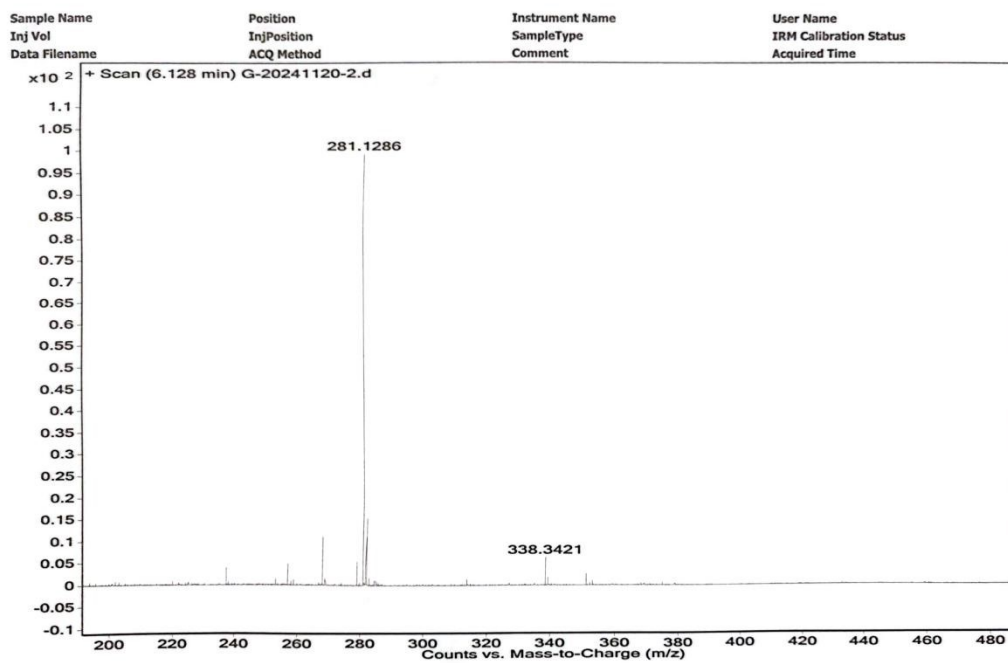
methyl 4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)benzoate (6)



¹H NMR of compound 6

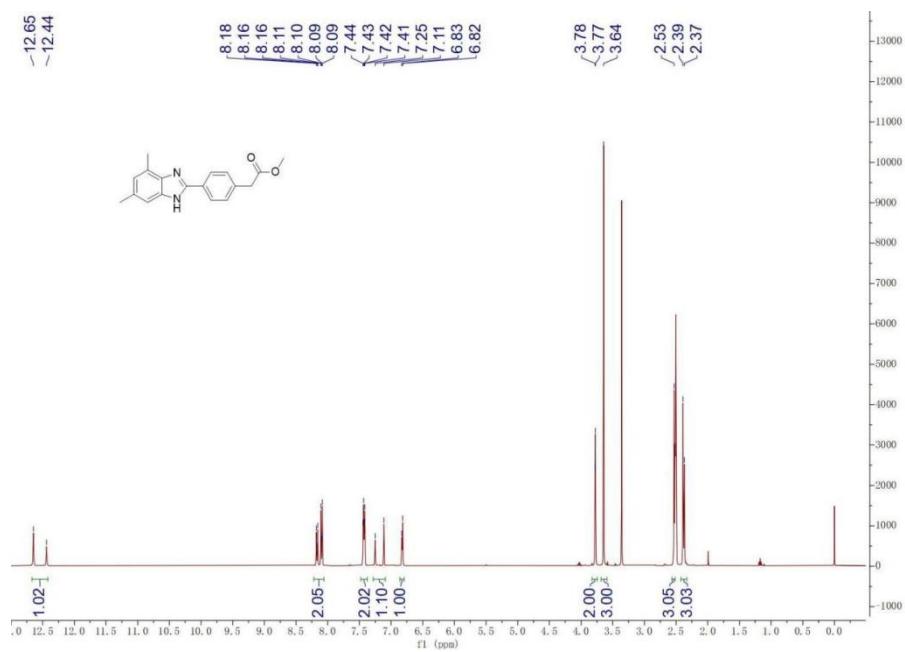


¹³C NMR of compound 6

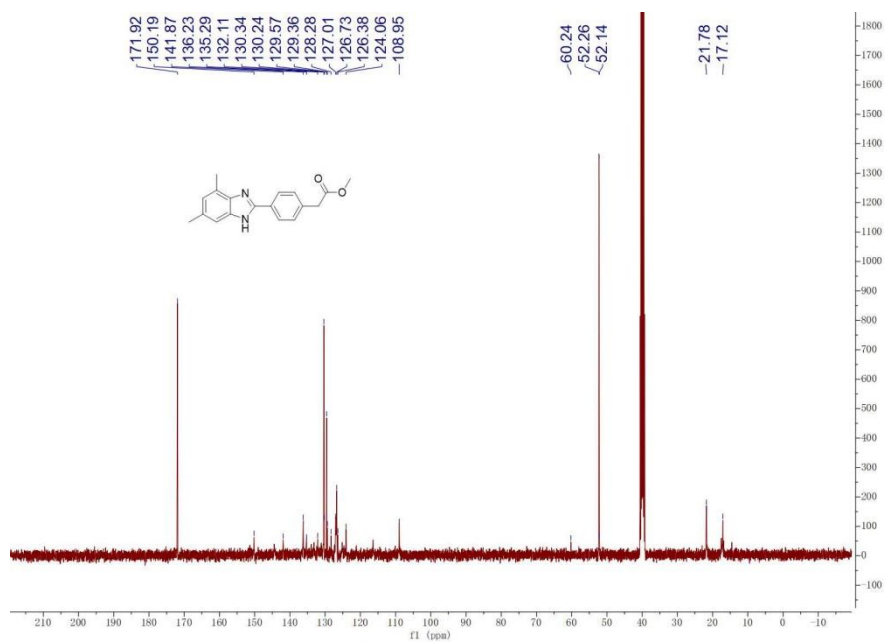


HR-MS of compound 6

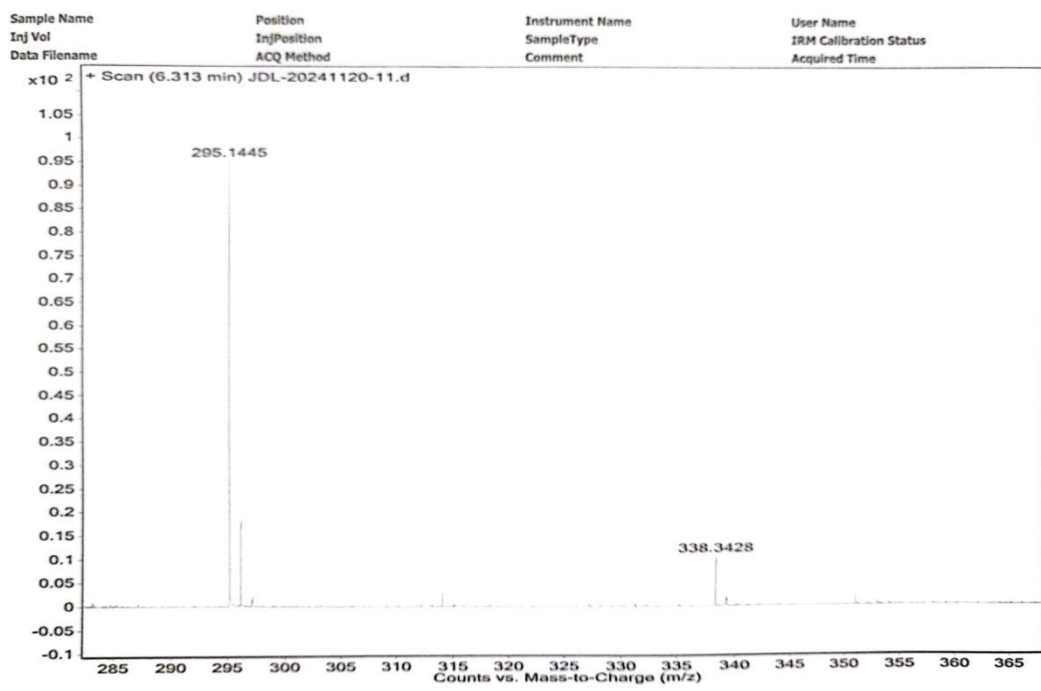
methyl 2-(4-(4,6-dimethyl-1H-benzodimidazol-2-yl)phenyl)acetate (7)



¹H NMR of compound 7

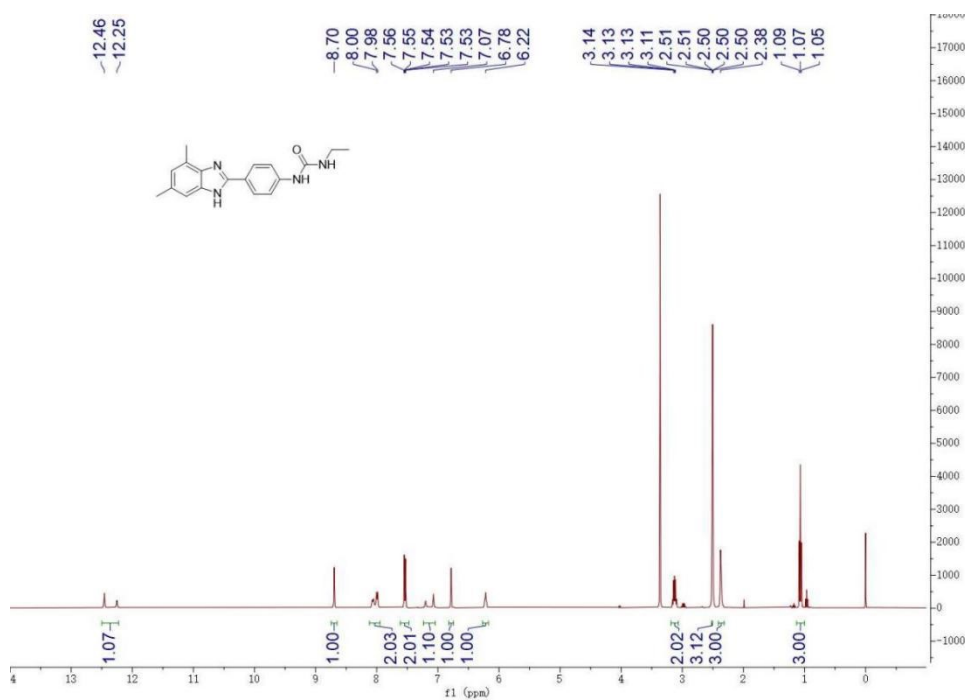


¹³C NMR of compound 7

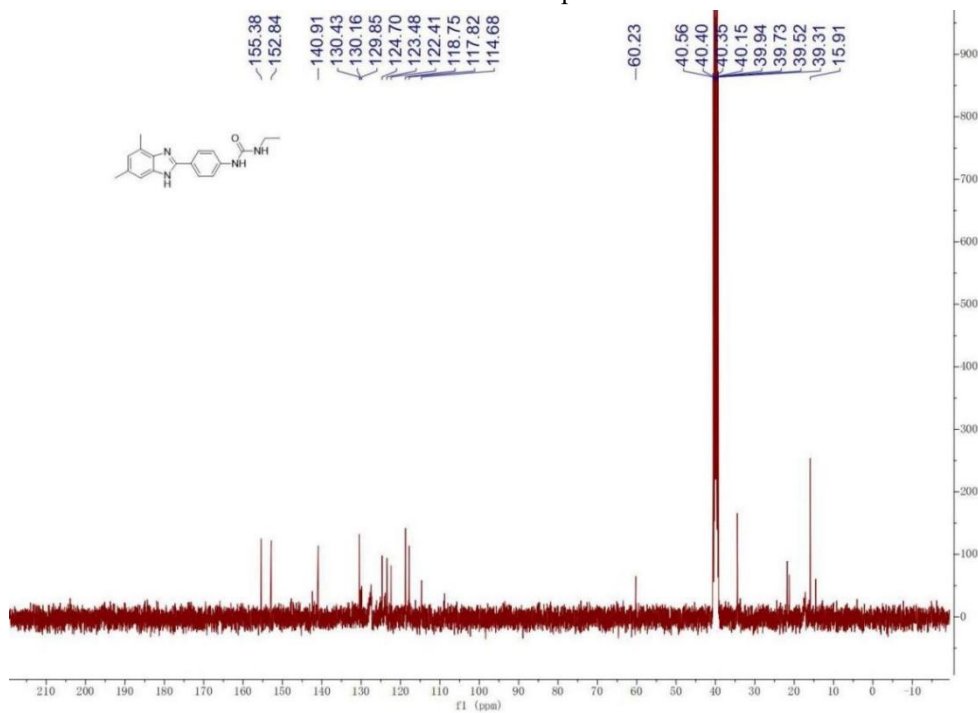


HR-MS of compound 7

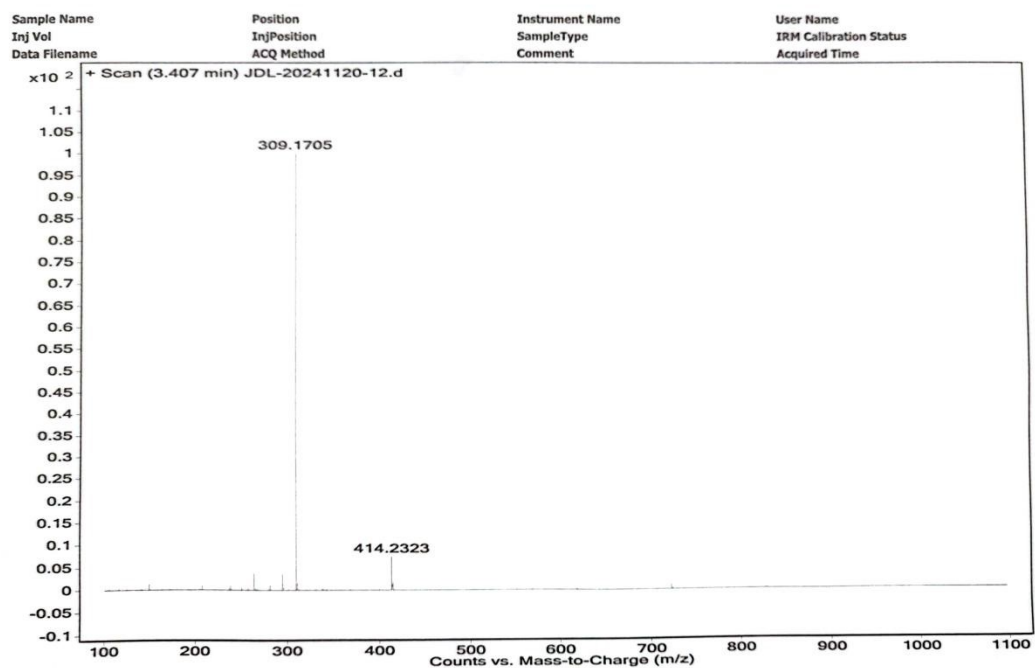
1-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)-3-ethylurea (8)



¹H NMR of compound 8

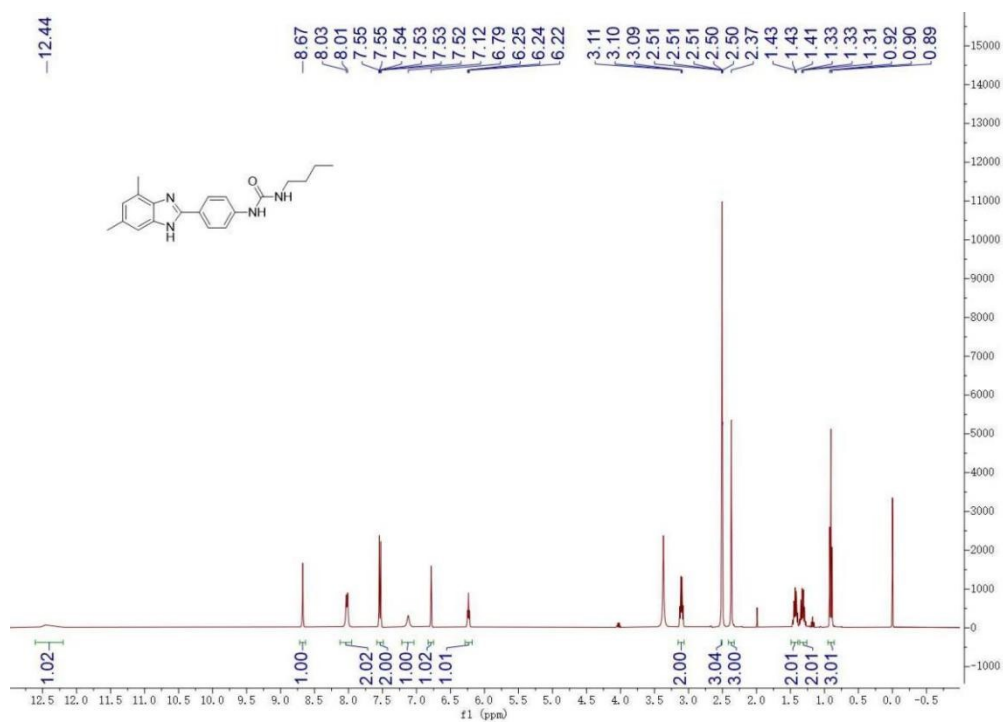


¹³C NMR of compound 8

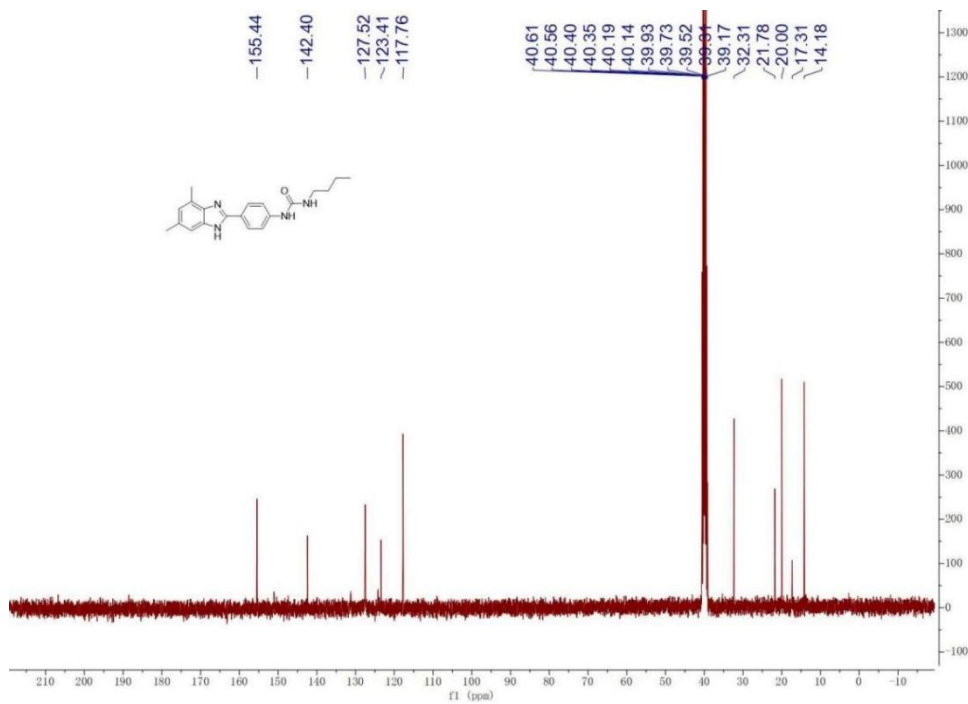


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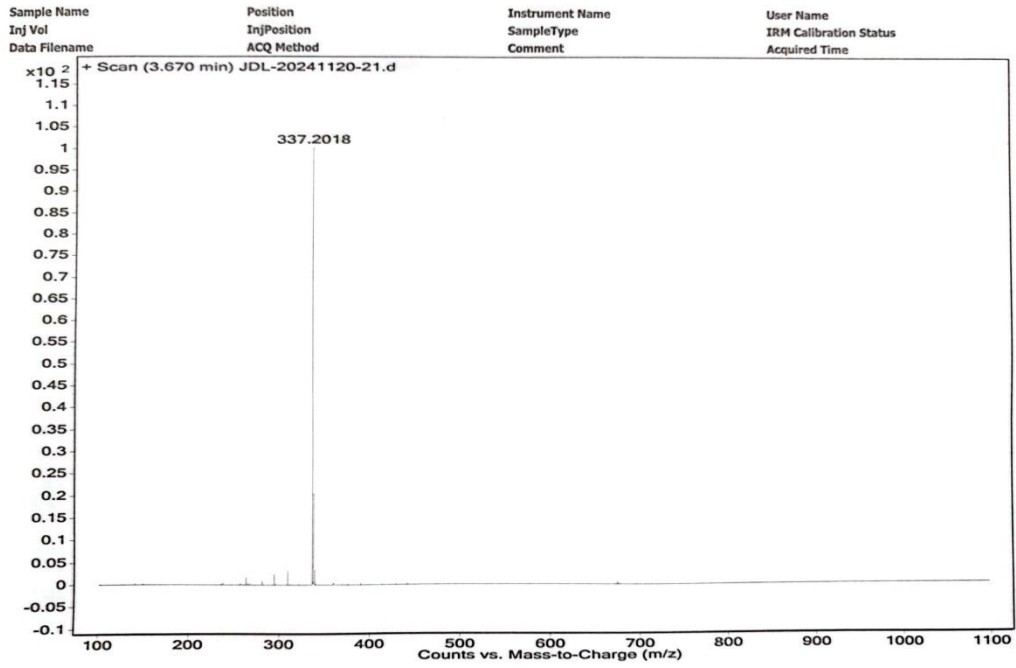
1-butyl-3-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)urea (9)



¹H NMR of compound 9

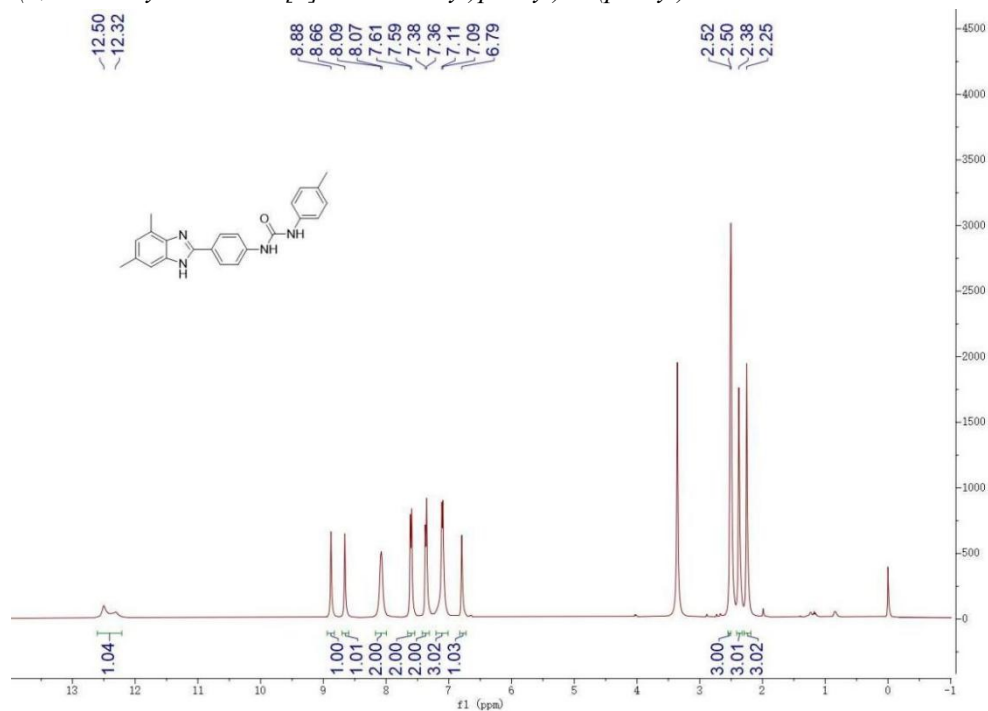


¹³C NMR of compound 9

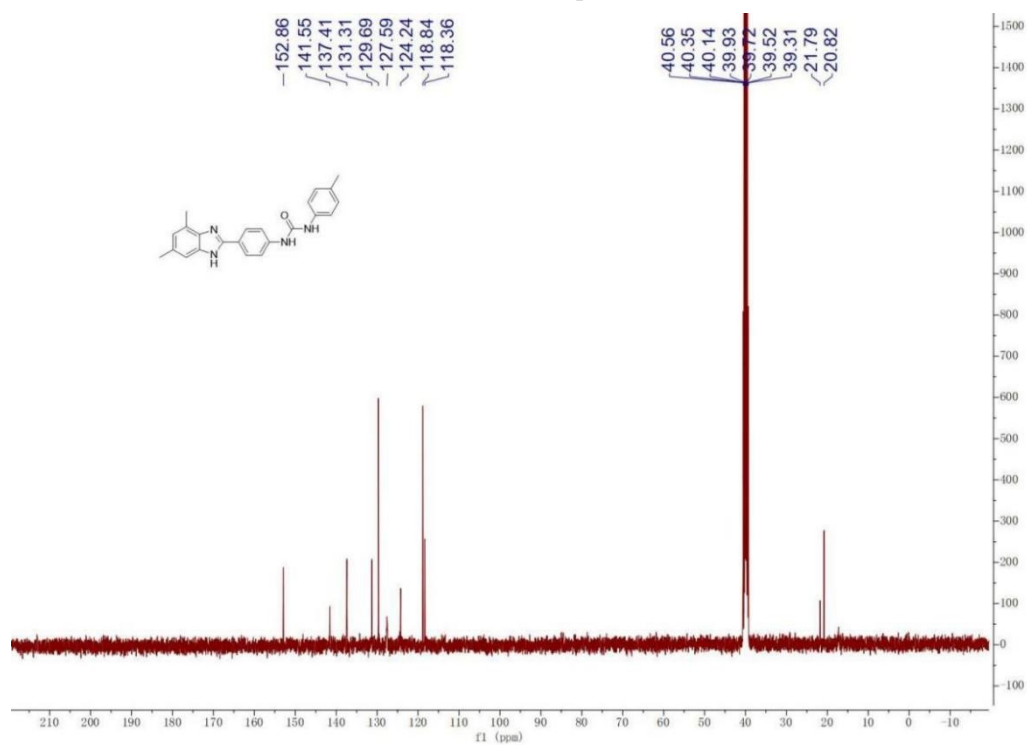


HR-MS of compound 9

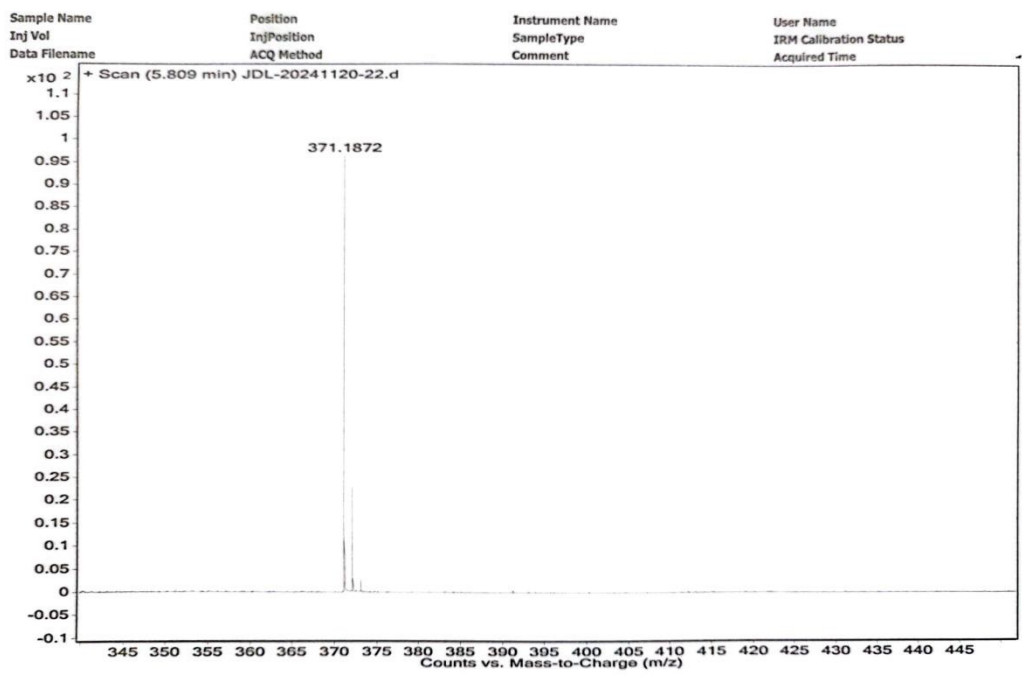
1-(4-(4,6-dimethyl-1H-benzof[d]imidazol-2-yl)phenyl)-3-(p-tolyl)urea (10)



¹H NMR of compound 10

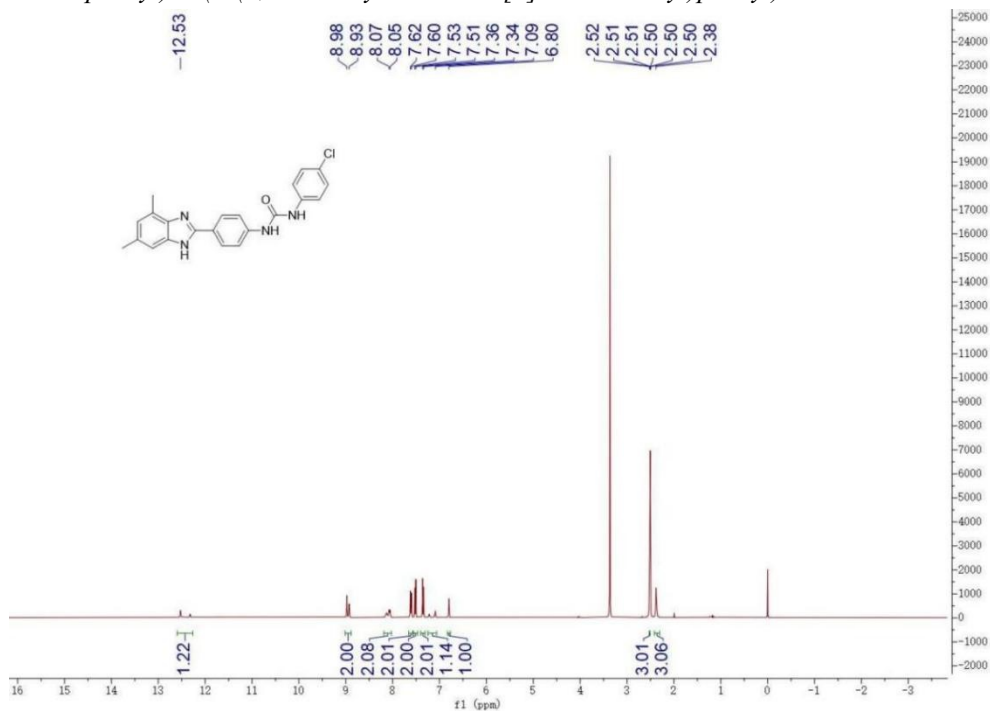


¹³C NMR of compound 10

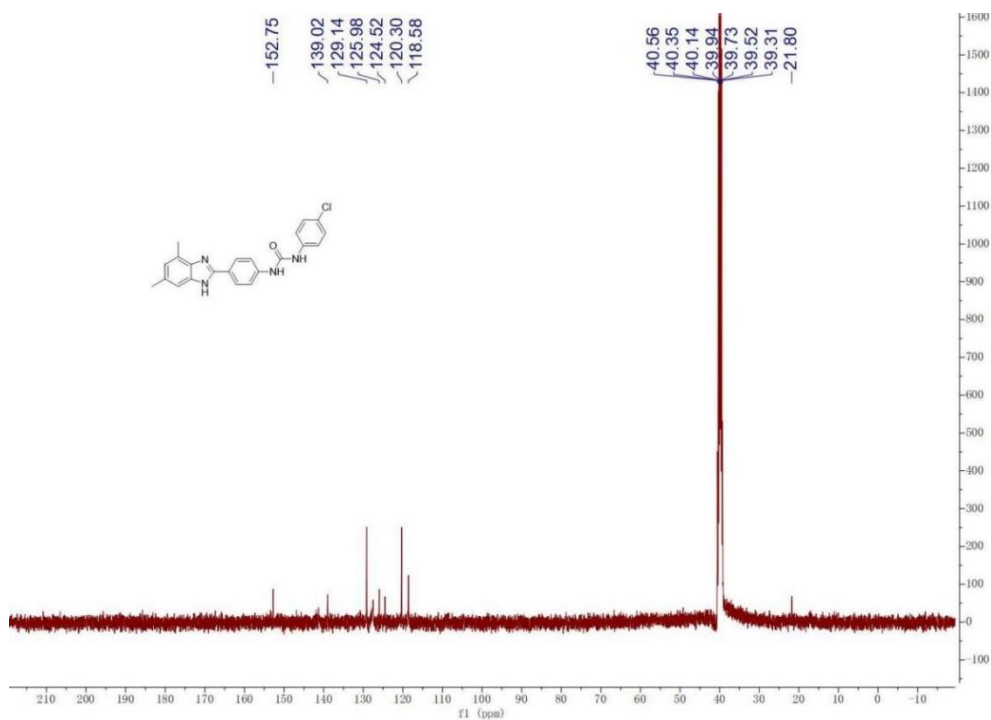


HR-MS of compound 10

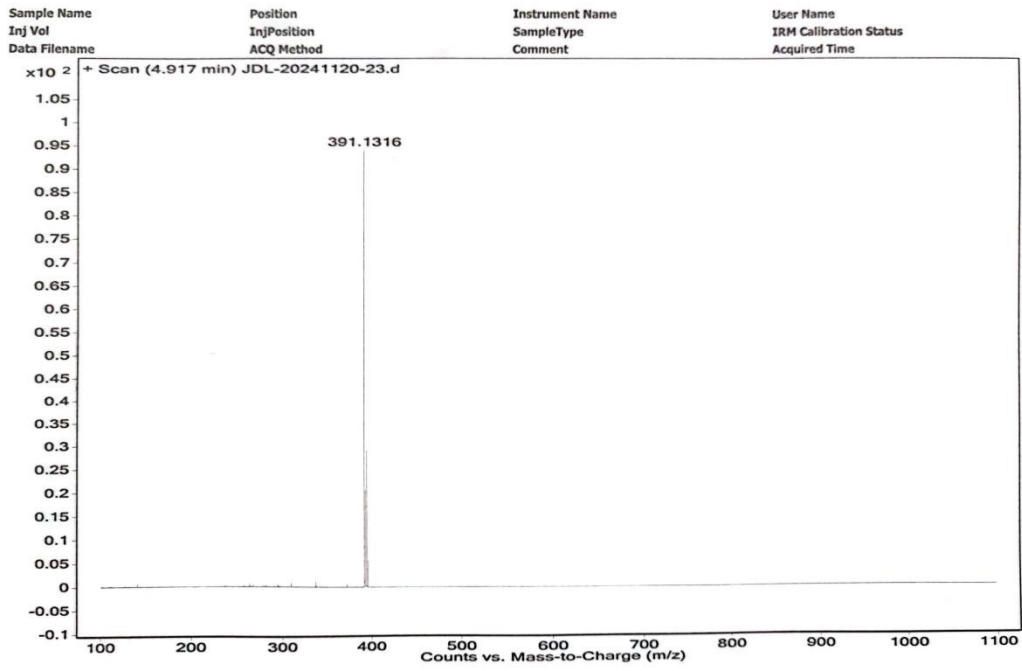
1-(4-chlorophenyl)-3-(4-(4,6-dimethyl-1H-benzof[d]imidazol-2-yl)phenyl)urea (**11**)



¹H NMR of compound **11**

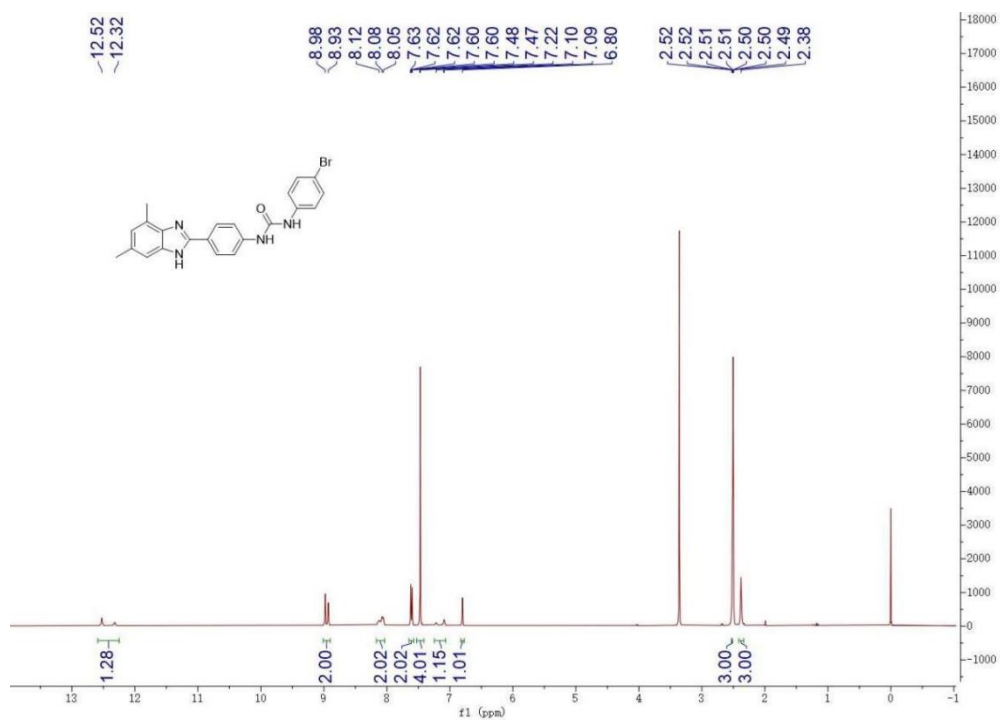


¹³C NMR of compound **11**

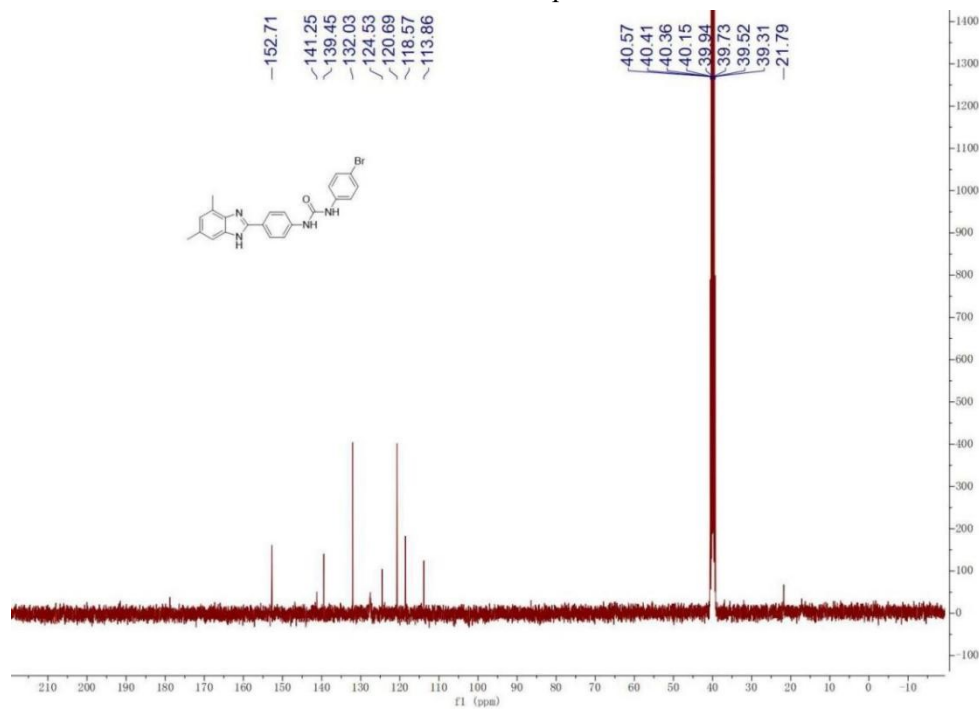


HR-MS of compound 11

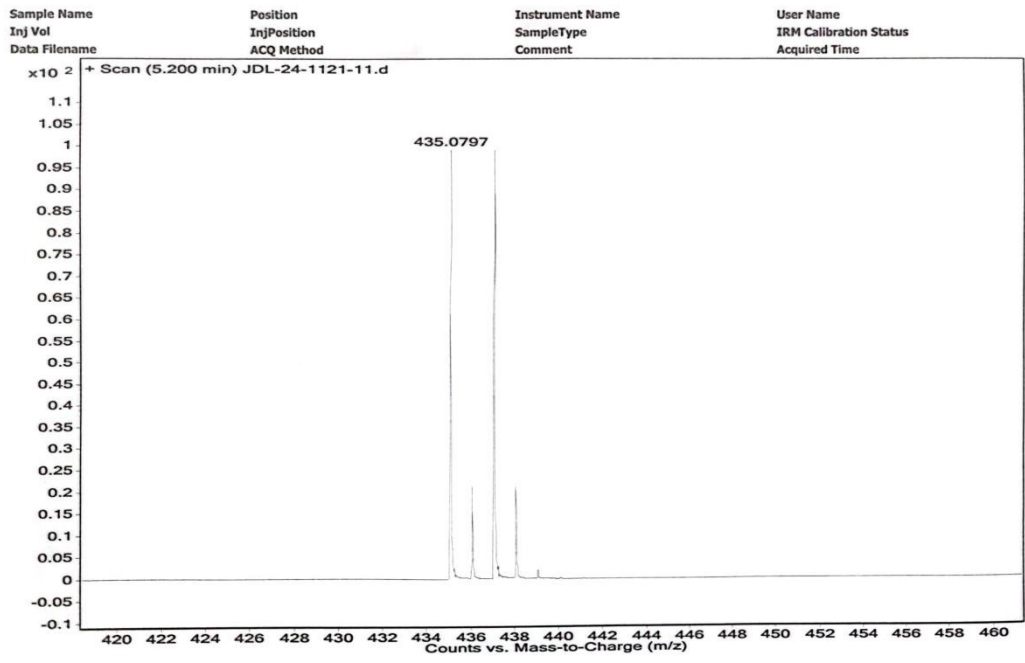
1-(4-bromophenyl)-3-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)urea (12)



¹H NMR of compound 12

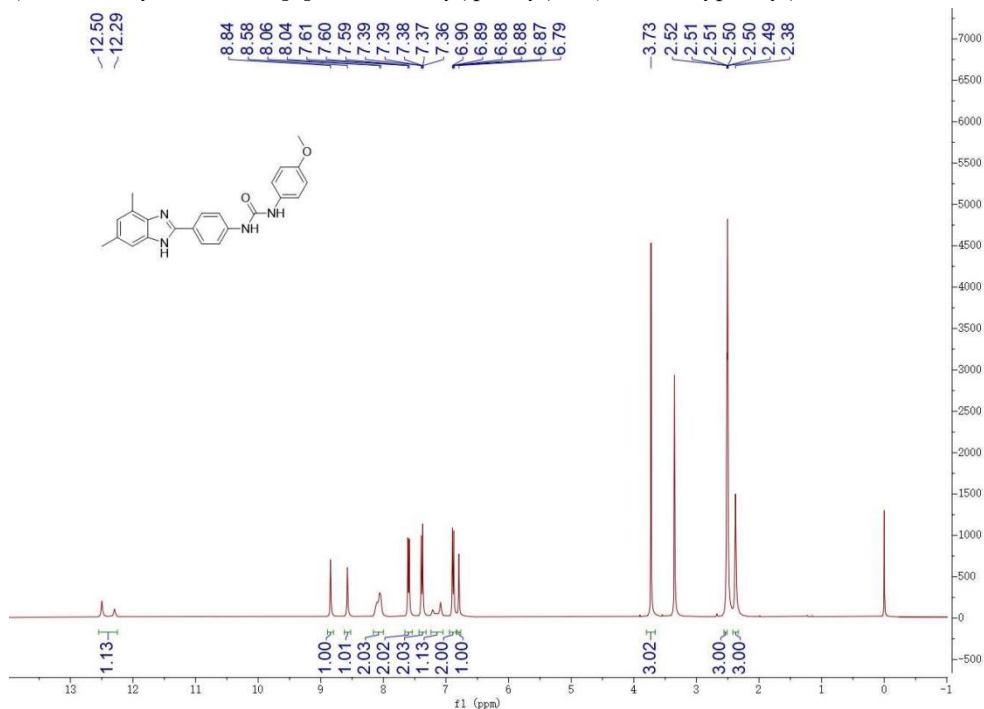


¹³C NMR of compound 12

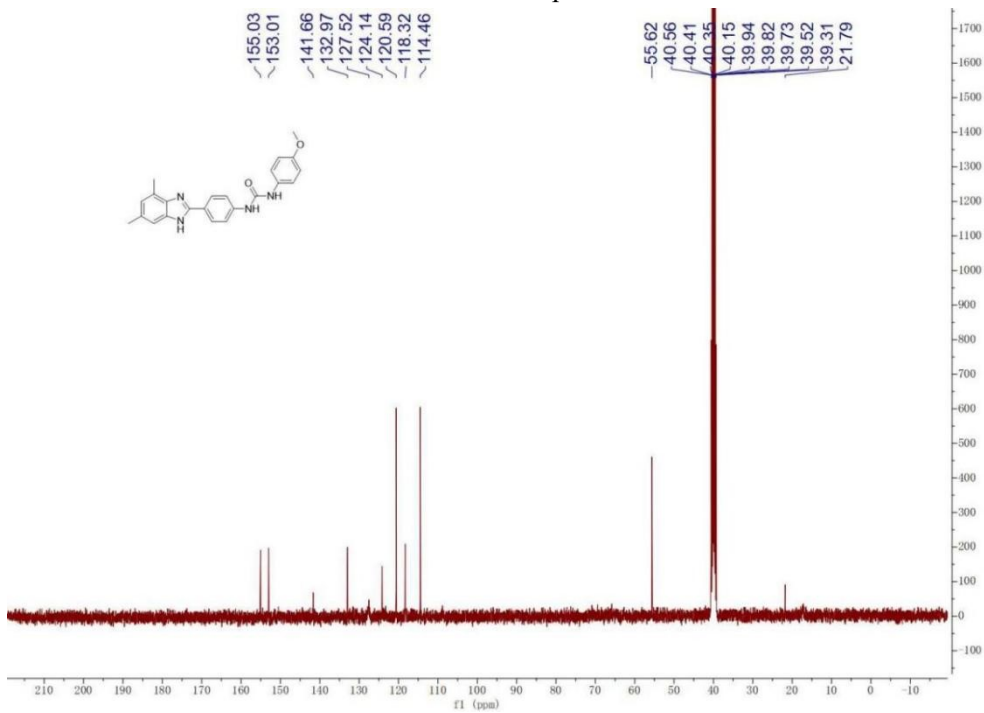


HR-MS of compound 12

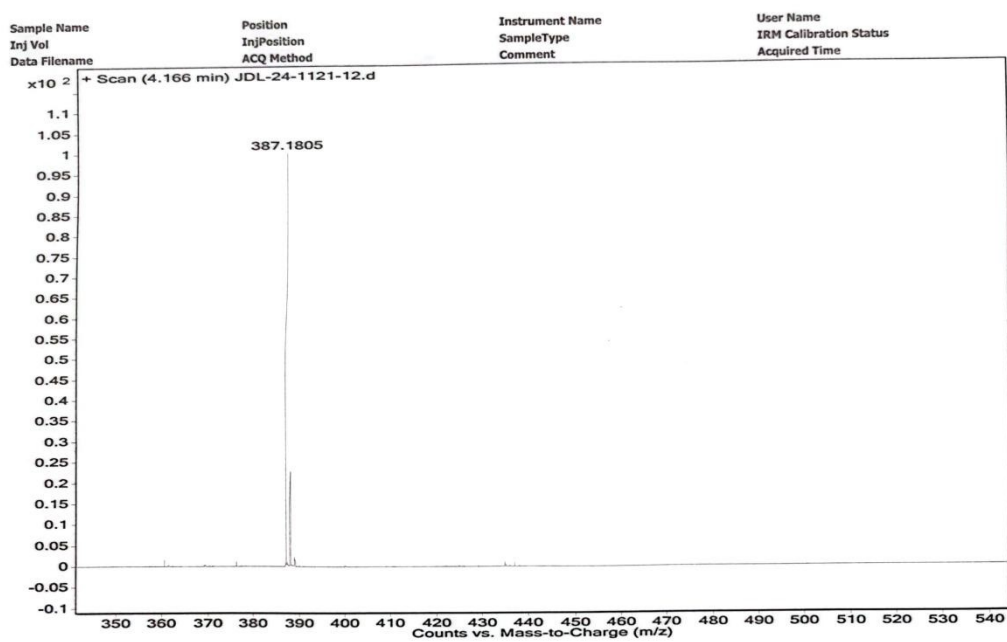
1-(4-(4,6-dimethyl-1H-benzof[d]imidazol-2-yl)phenyl)-3-(4-methoxyphenyl)urea (13)



¹H NMR of compound 13

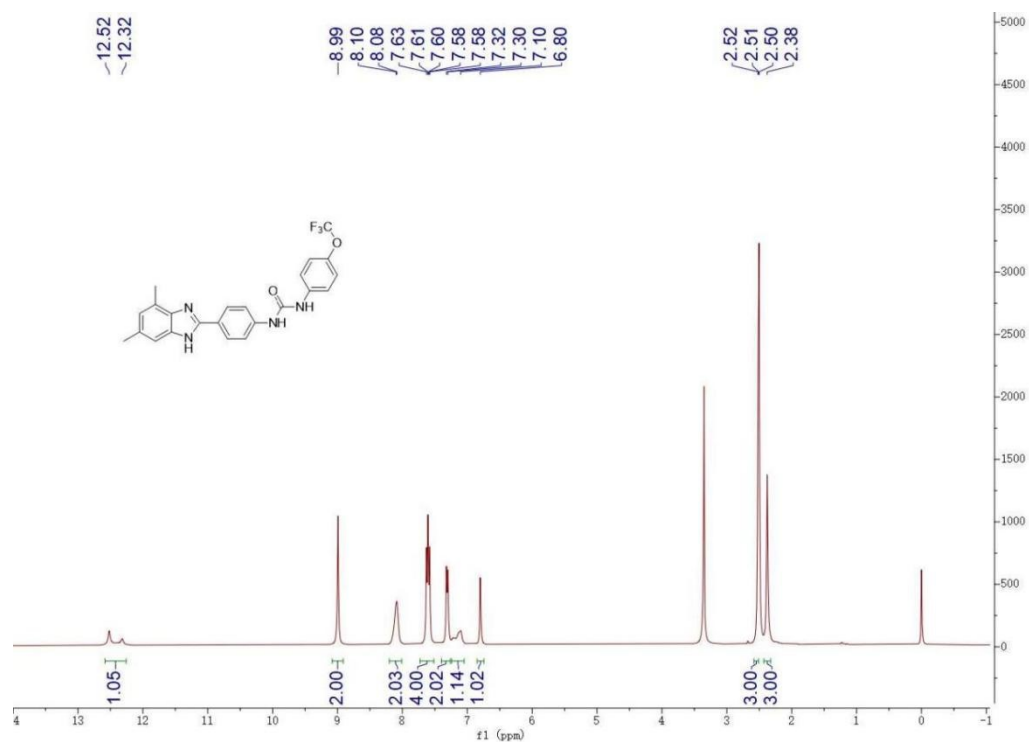


¹³C NMR of compound 13

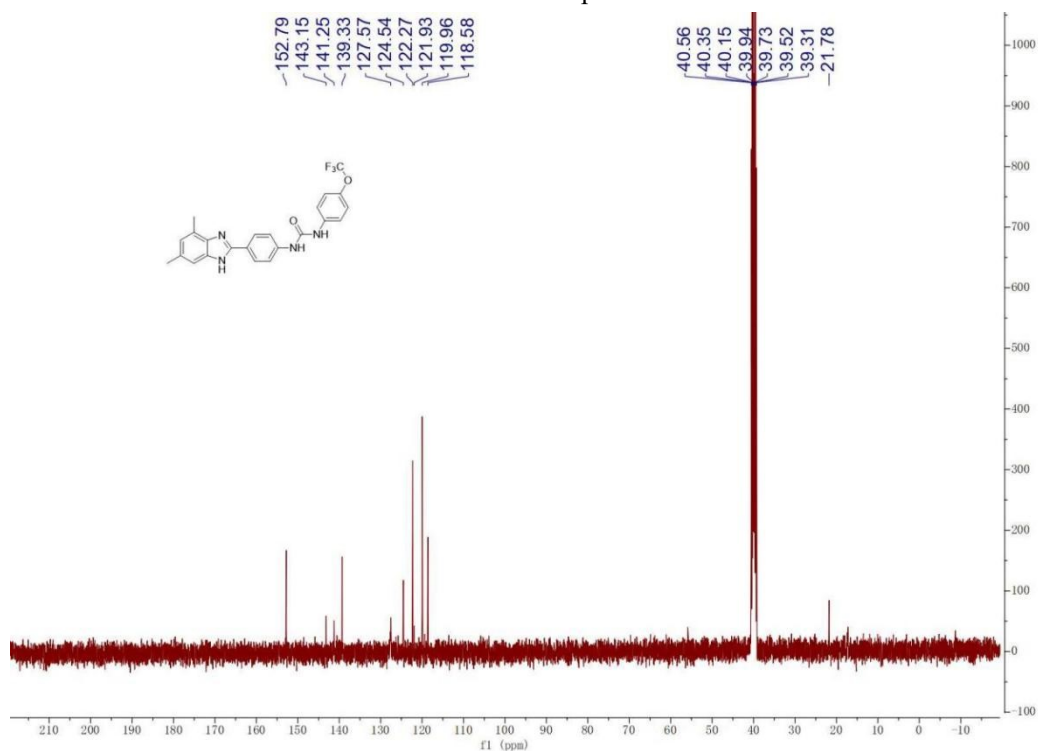


HR-MS of compound 13

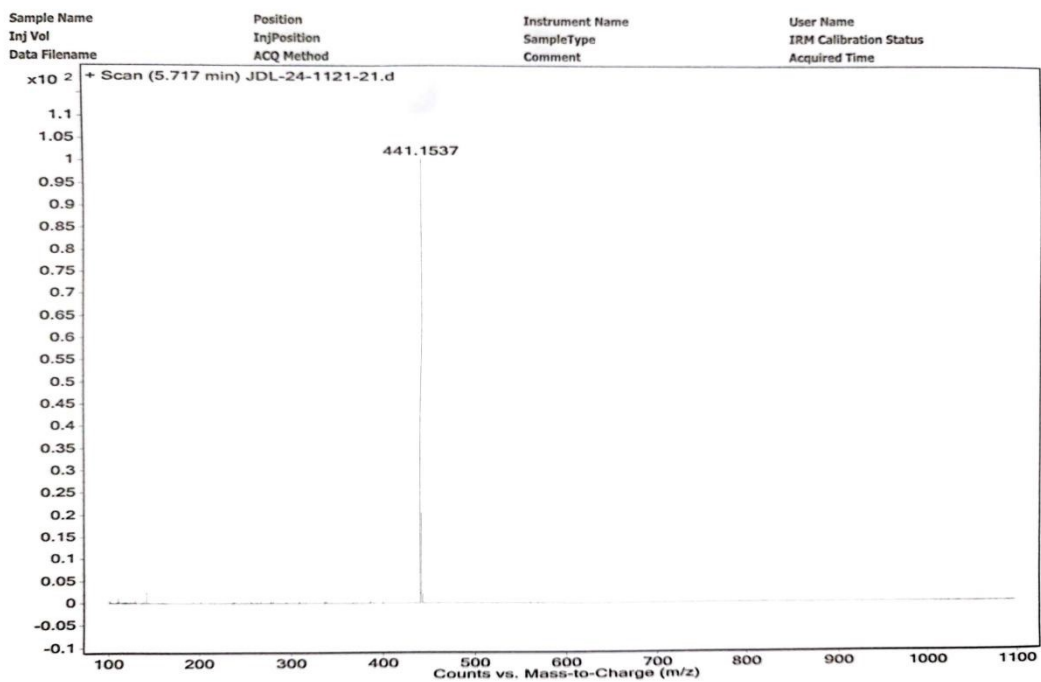
1-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)-3-(4-(trifluoromethoxy)phenyl)urea (**14**)



¹H NMR of compound 14

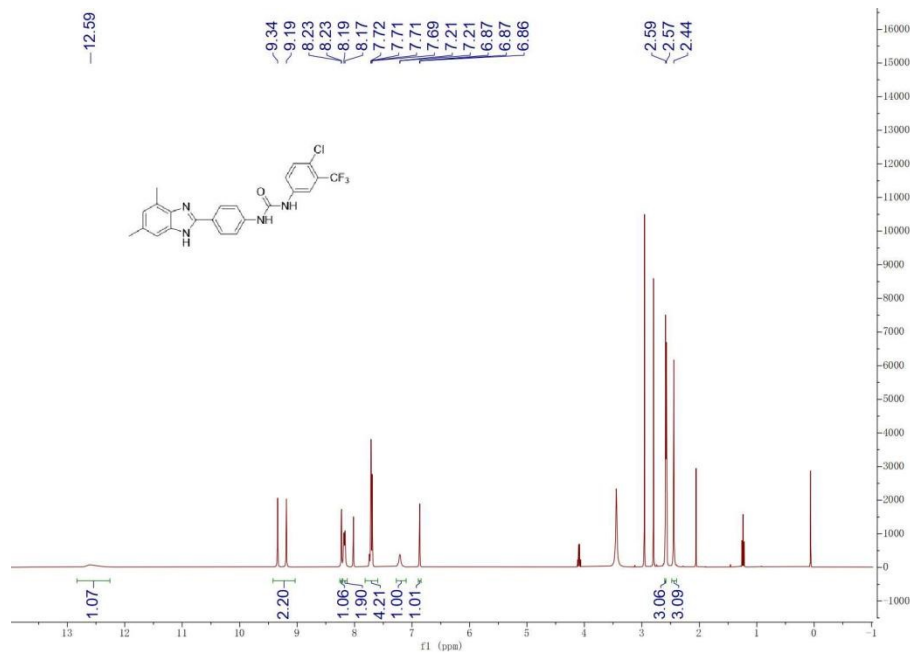


¹³C NMR of compound 14

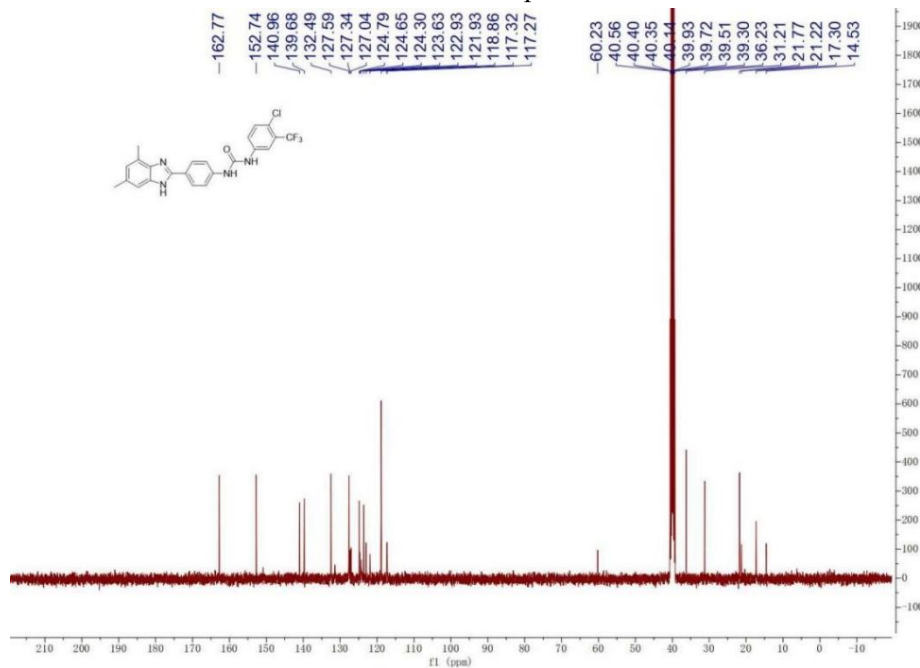


HR-MS of compound 14

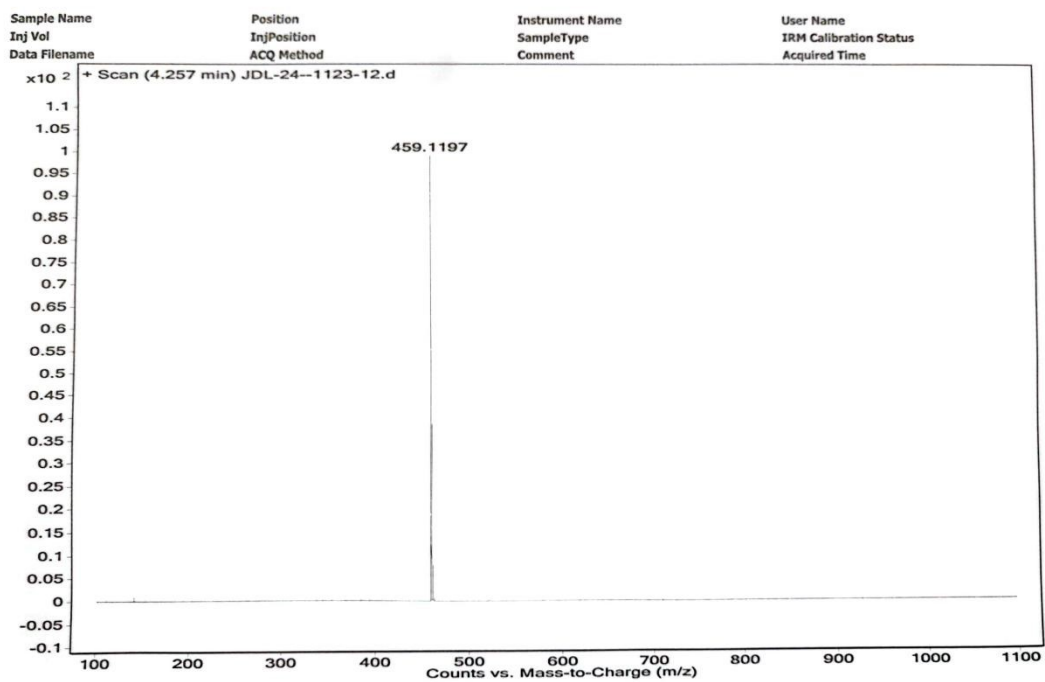
1-(4-chloro-3-(trifluoromethyl)phenyl)-3-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)urea (15)



¹H NMR of compound 15

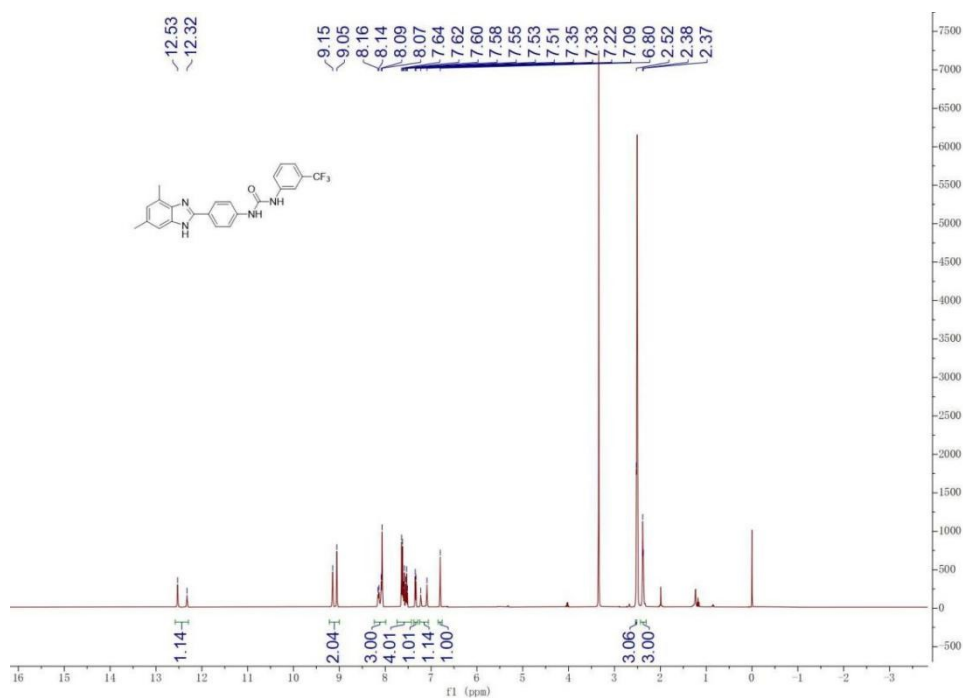


¹³C NMR of compound 15

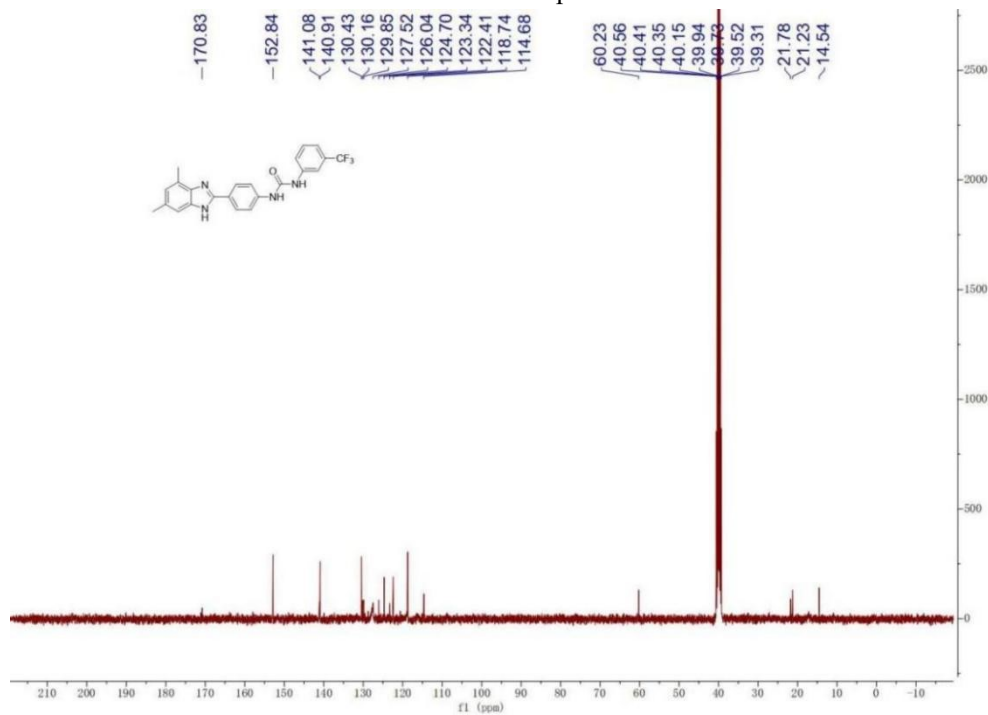


HR-MS of compound 15

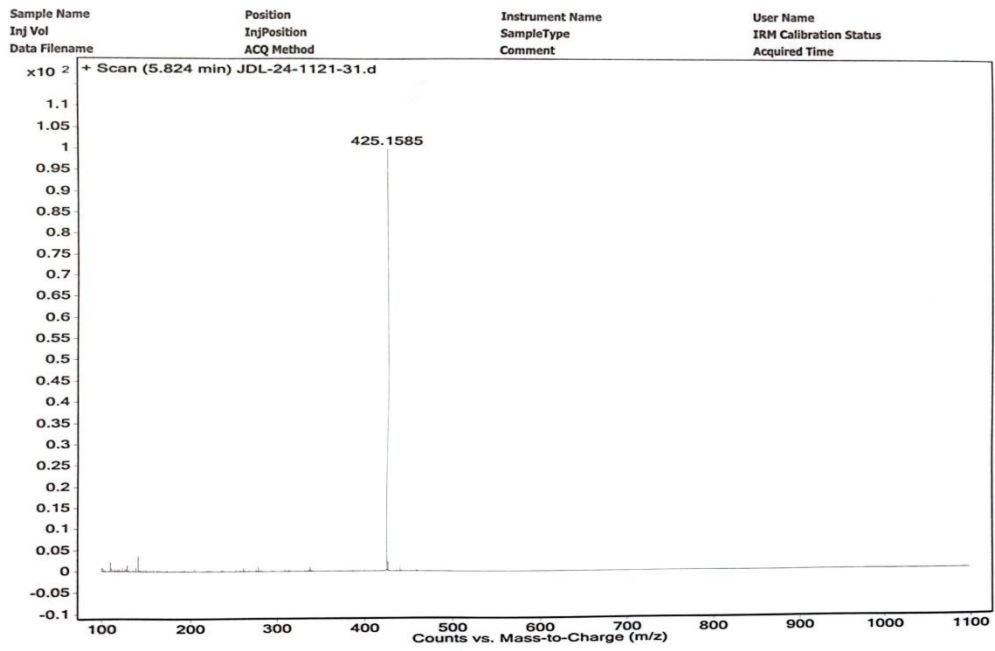
1-(4-(4,6-dimethyl-1H-benzodimidazol-2-yl)phenyl)-3-(3-(trifluoromethyl)phenyl)urea (16)



¹H NMR of compound 16

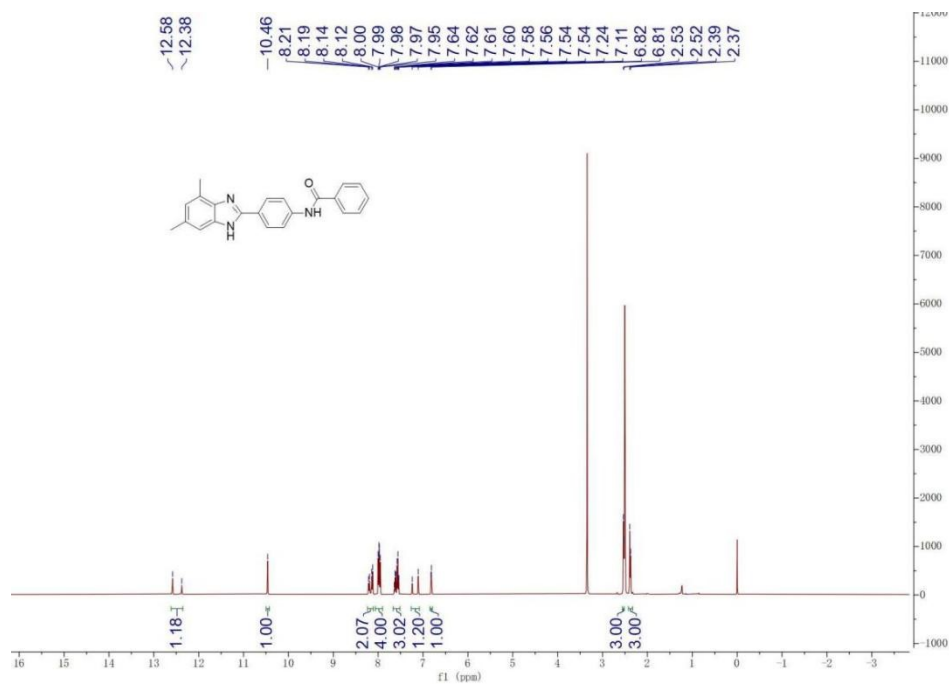


¹³C NMR of compound 16

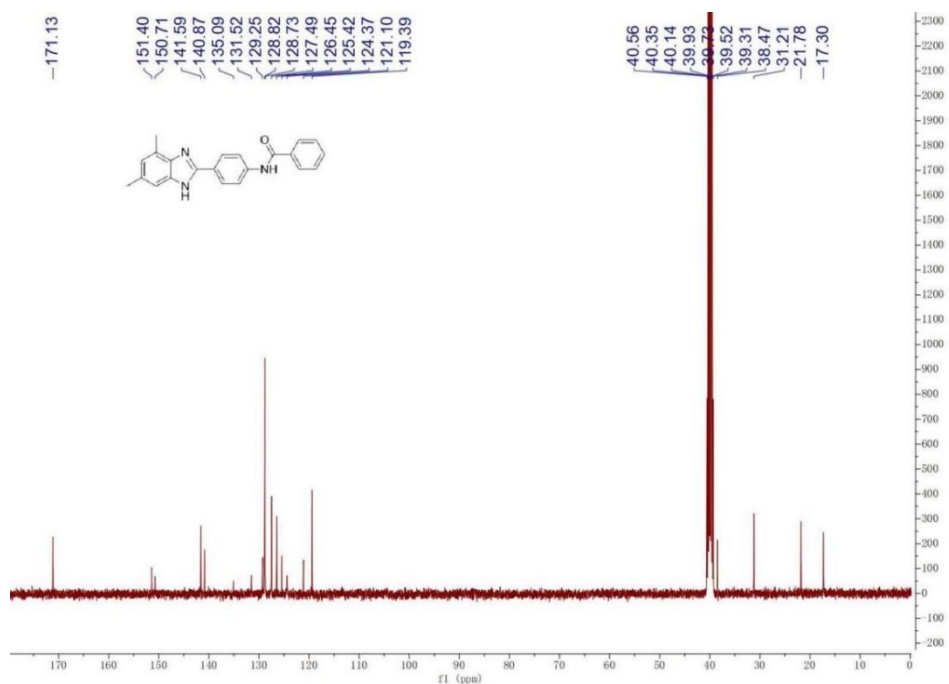


HR-MS of compound 16

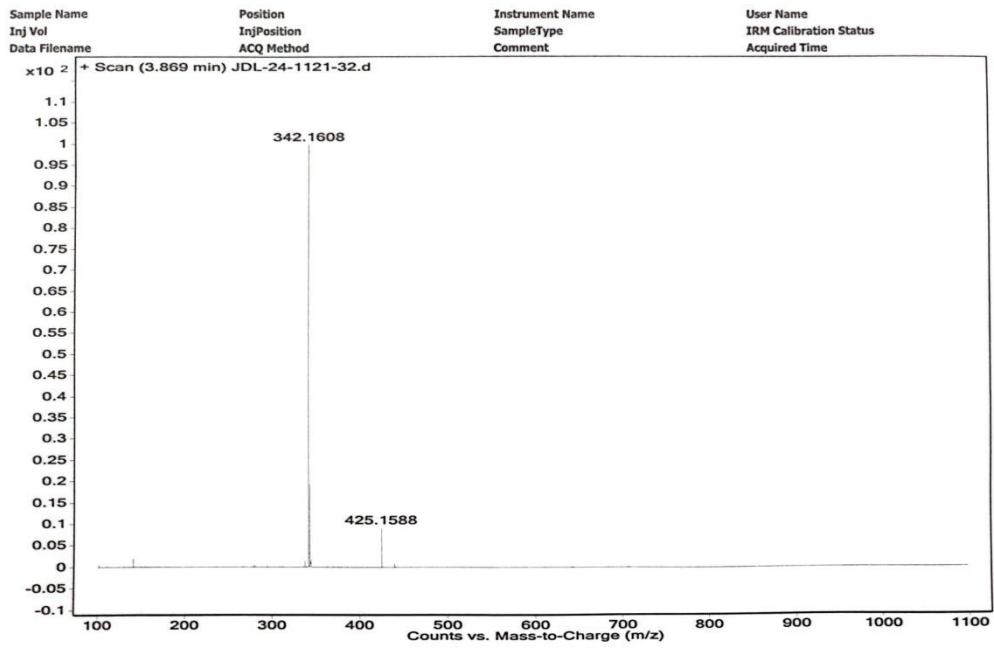
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)benzamide (**17**)



¹H NMR of compound **17**

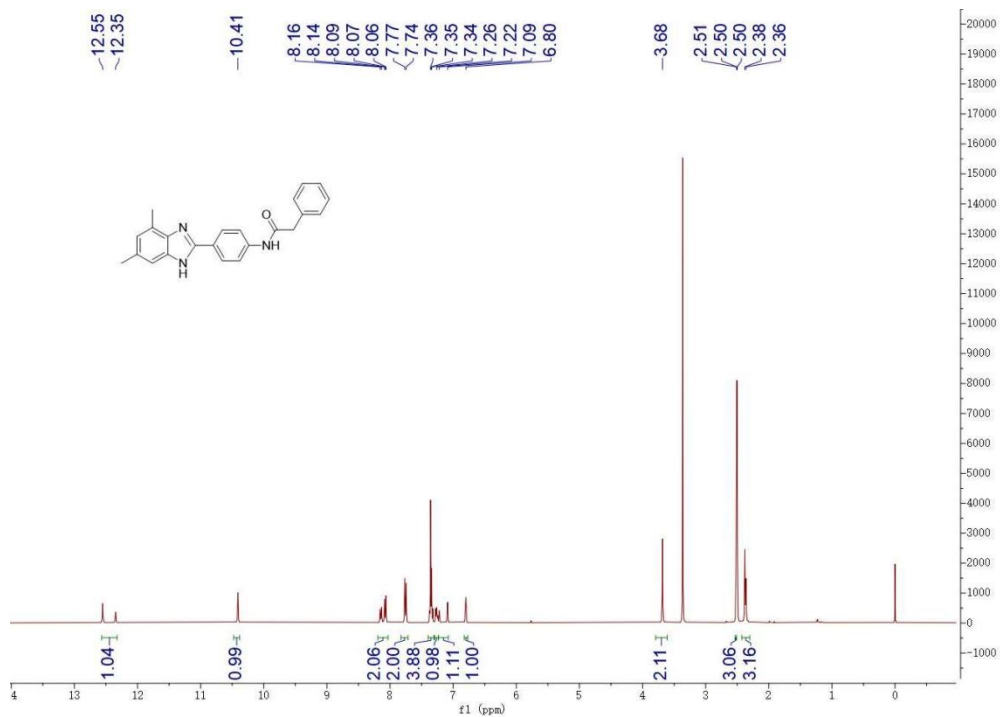


¹³C NMR of compound **17**

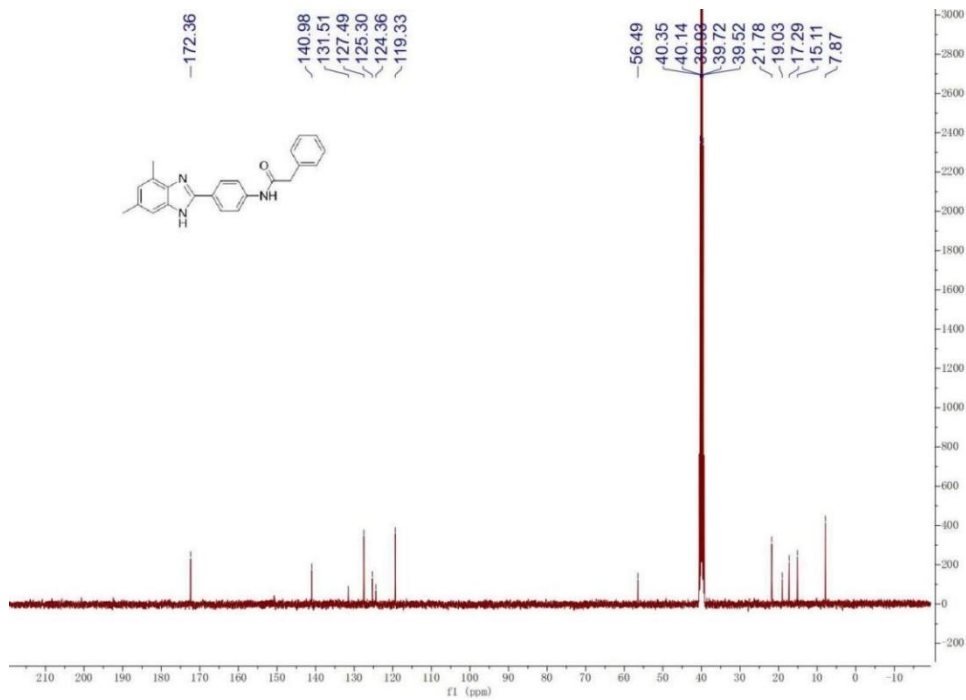


HR-MS of compound 17

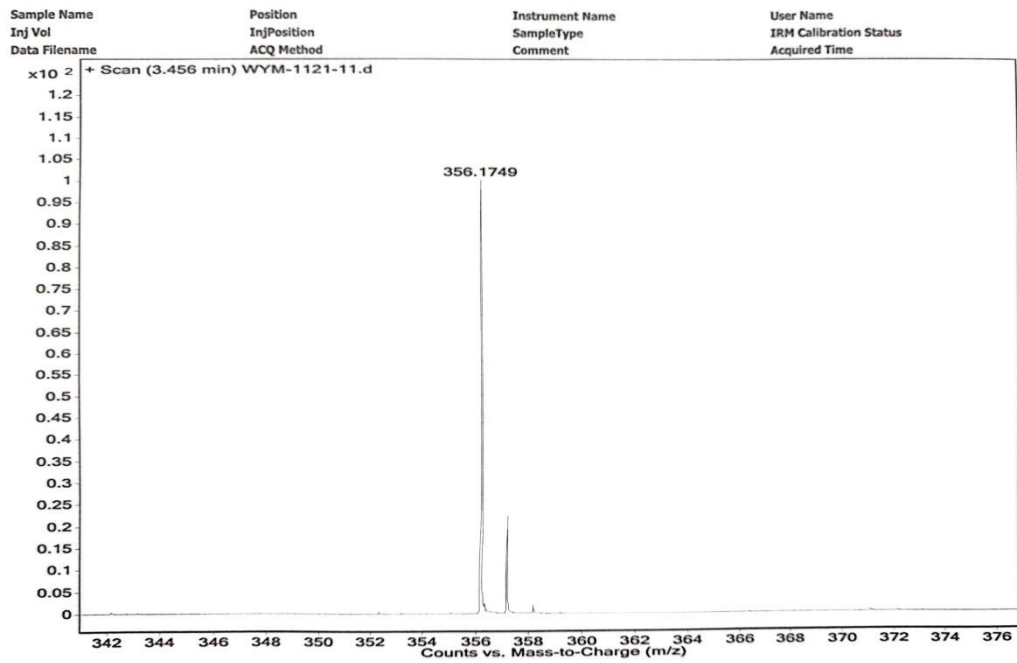
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)-2-phenylacetamide (**18**)



¹H NMR of compound 18

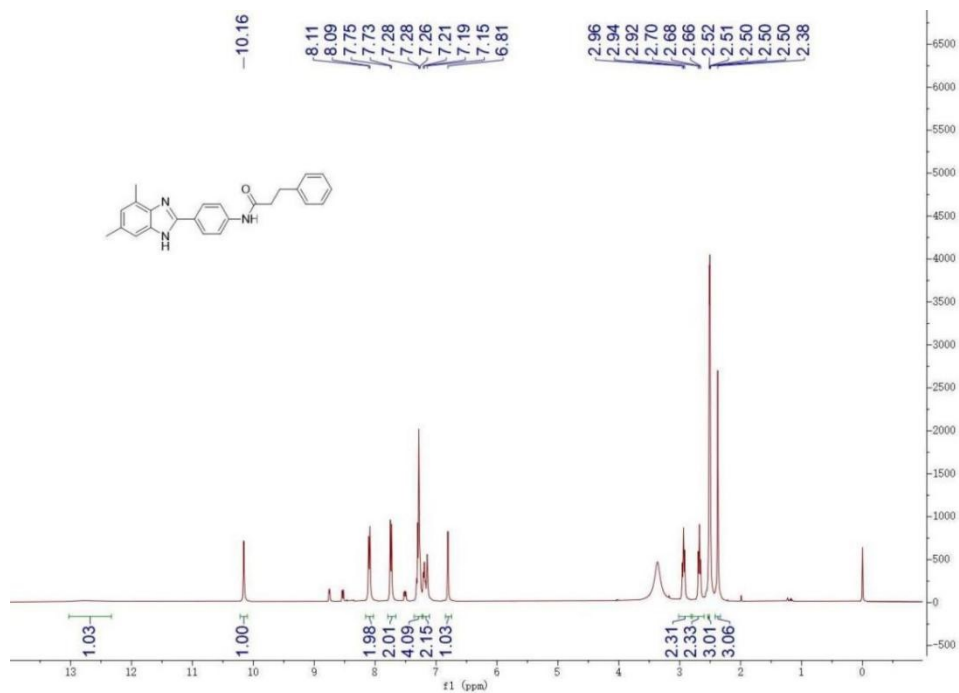


¹³C NMR of compound 18

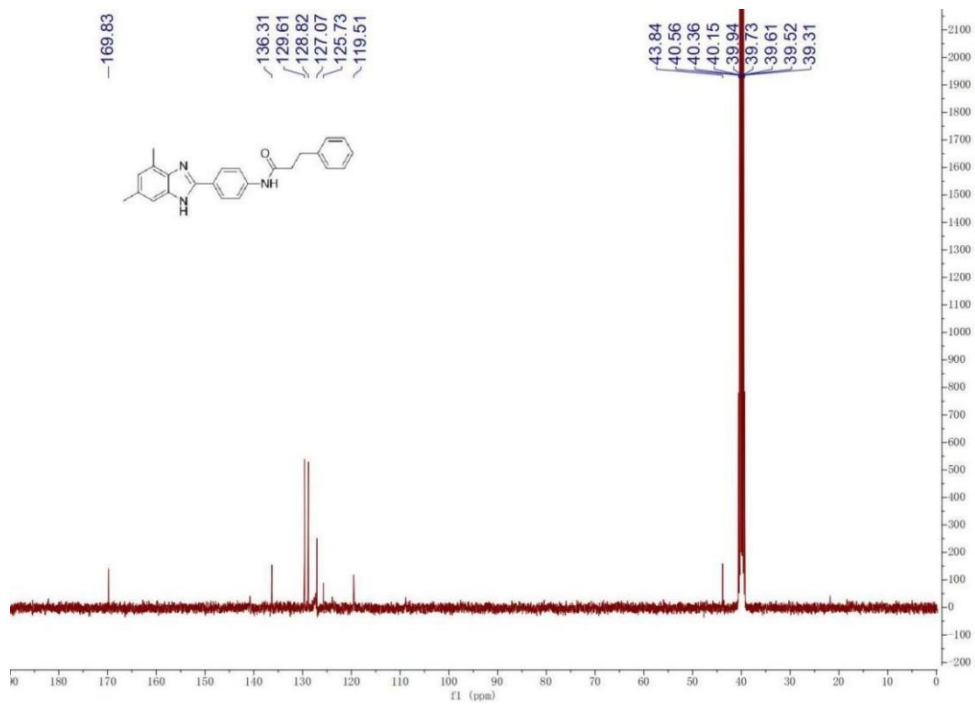


HR-MS of compound 18

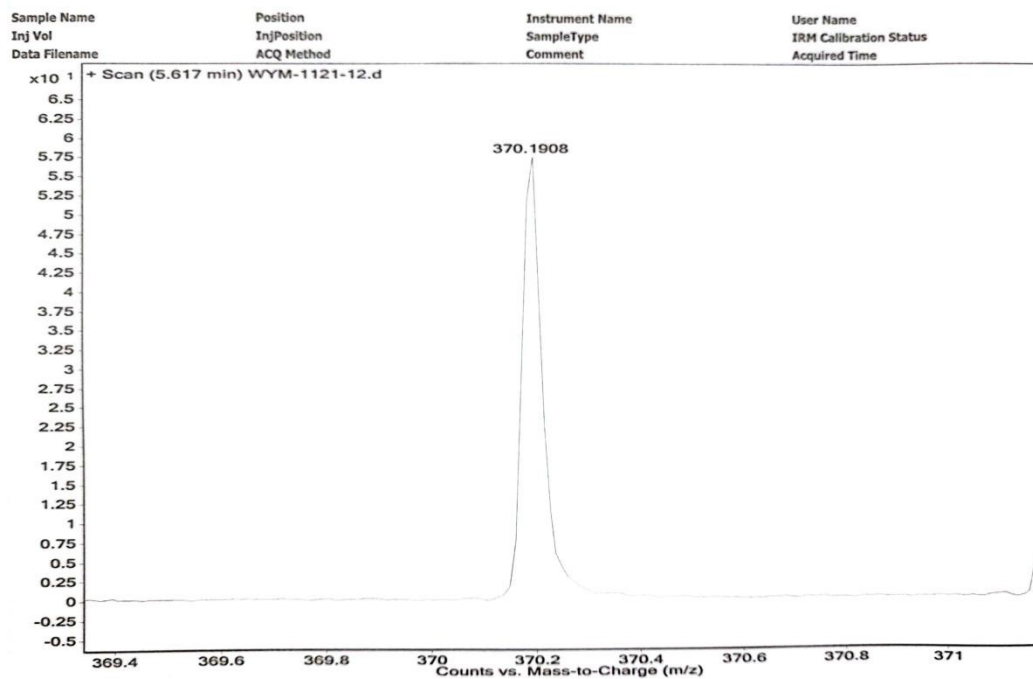
N-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)-3-phenylpropanamide (**19**)



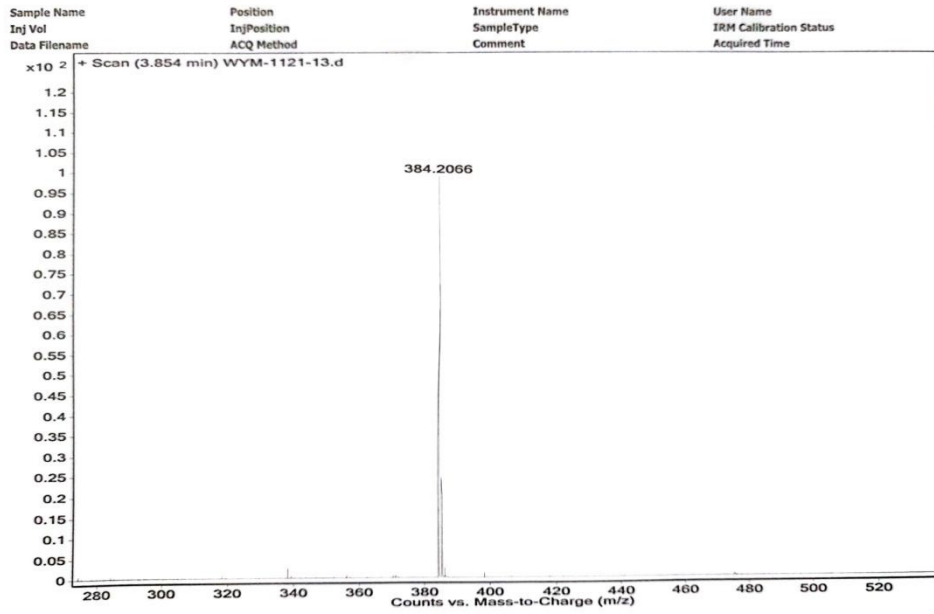
¹H NMR of compound 19



¹³C NMR of compound 19

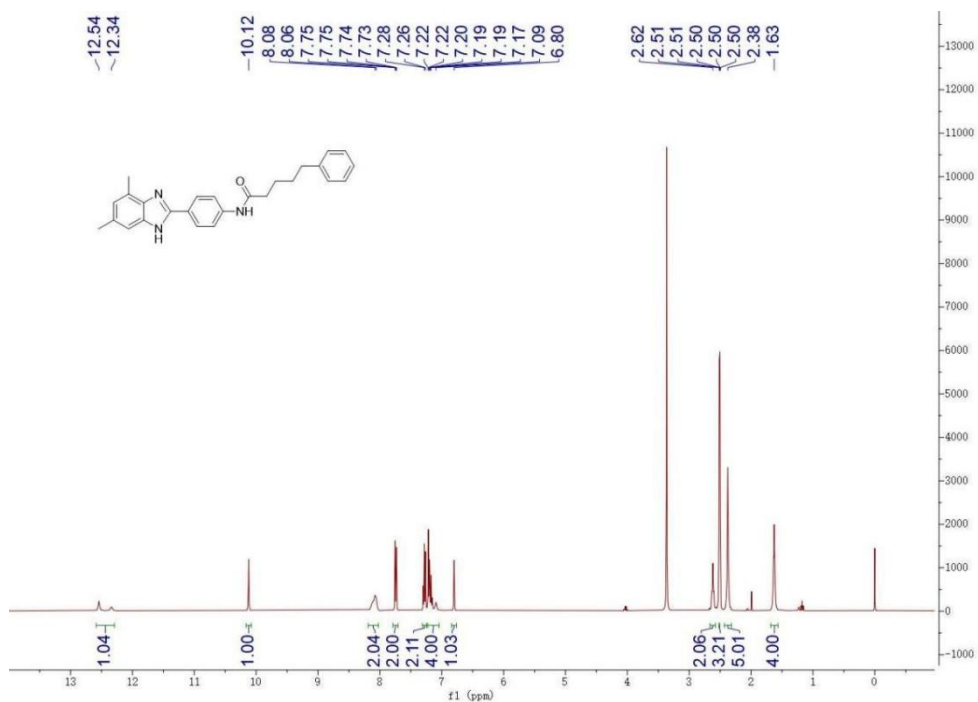


HR-MS of compound 19

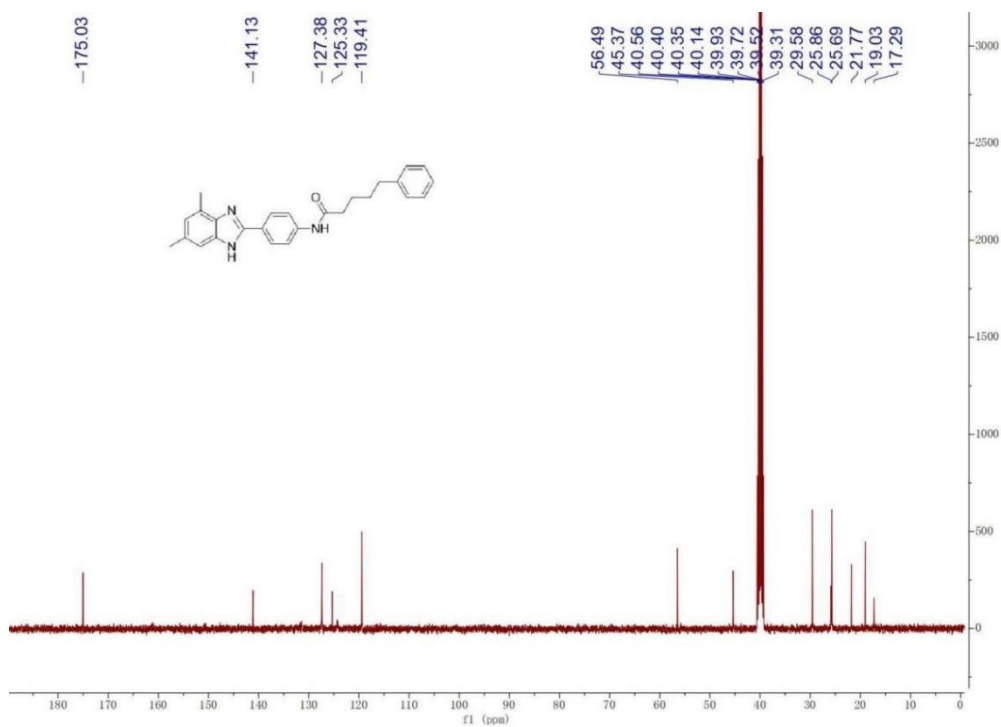


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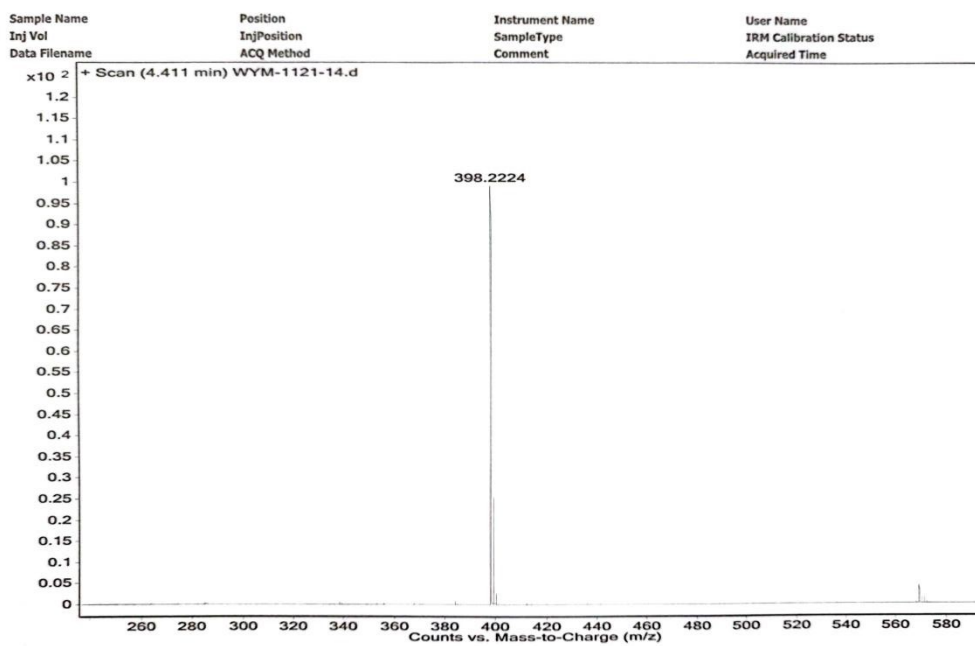
N-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)-5-phenylpentanamide (21)



¹H NMR of compound 21

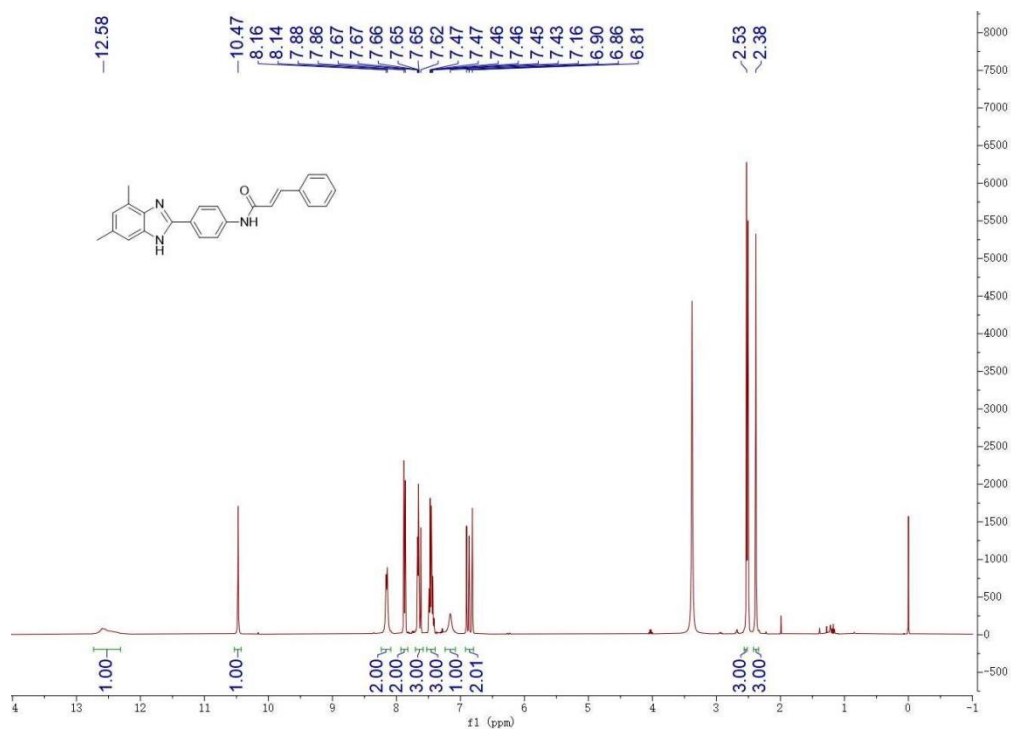


¹³C NMR of compound 21

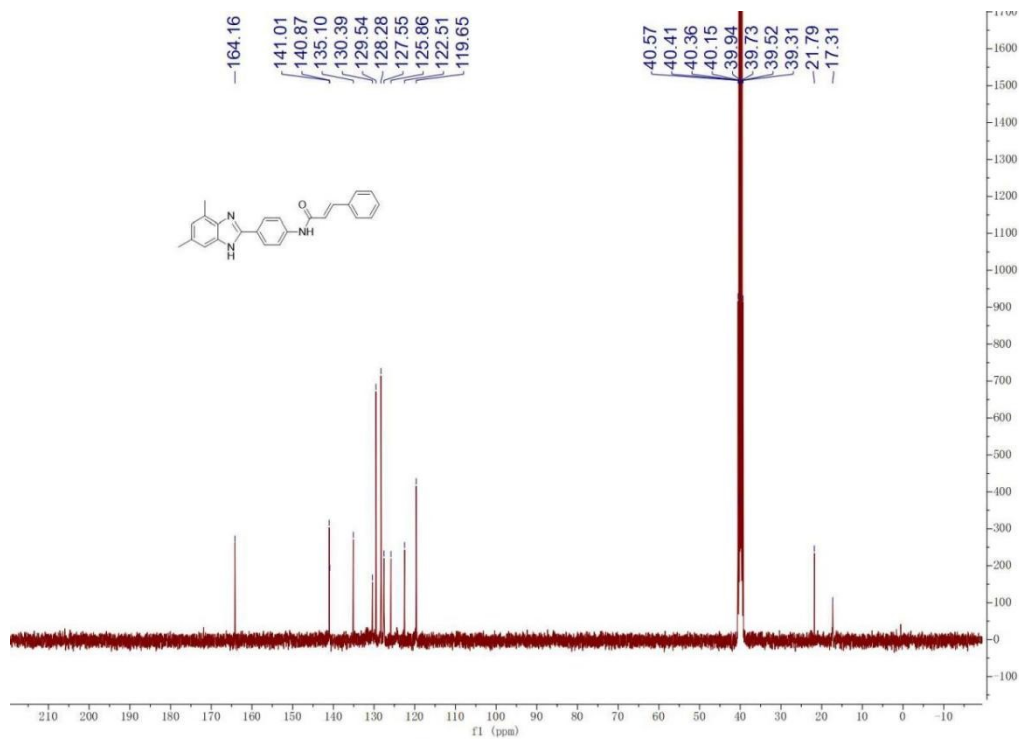


HR-MS of compound 21

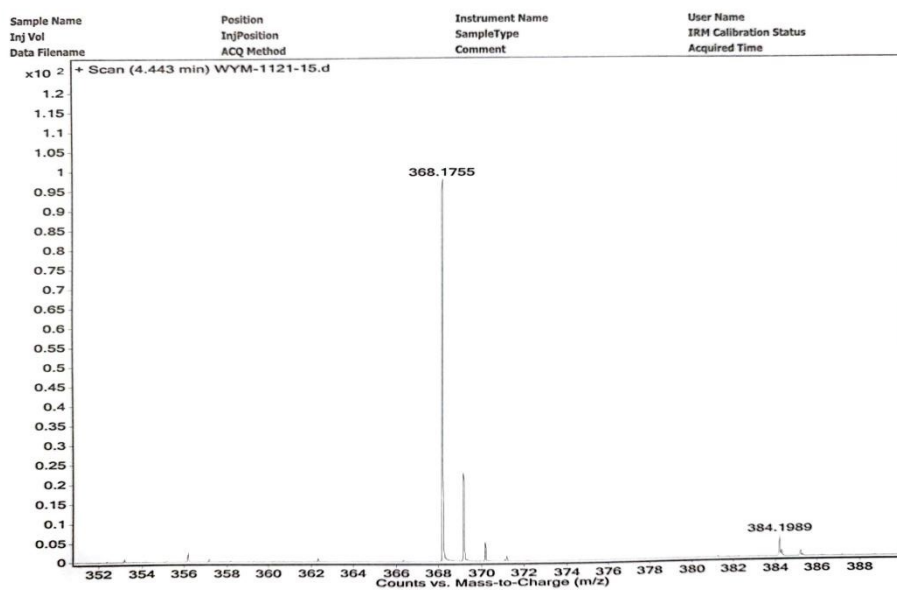
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)cinnamamide (**22**)



¹H NMR of compound **22**

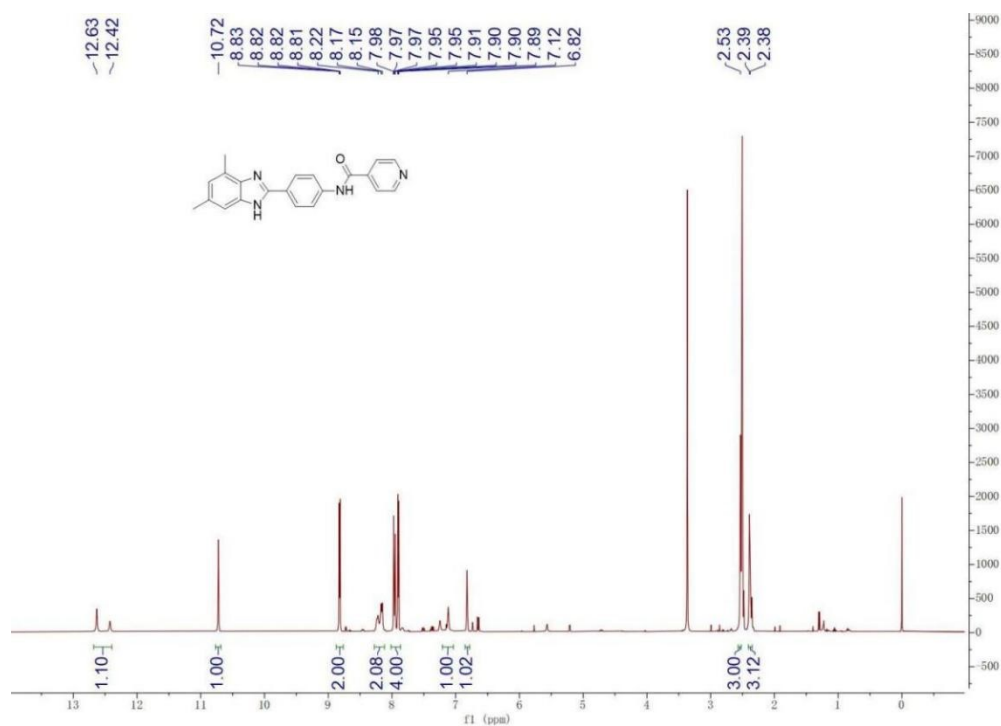


¹³C NMR of compound **22**

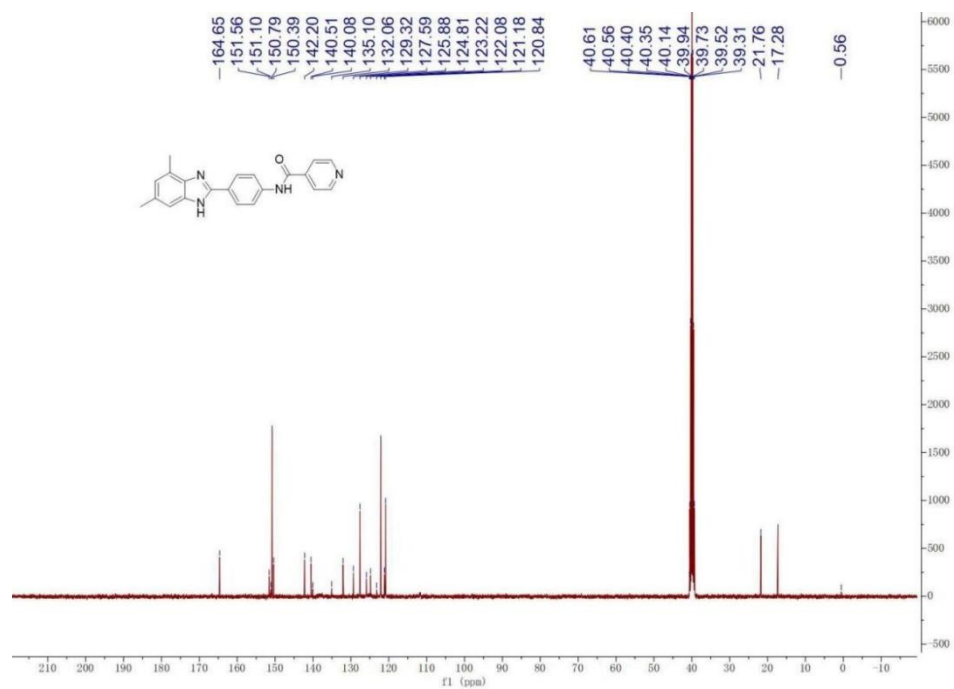


HR-MS of compound 22

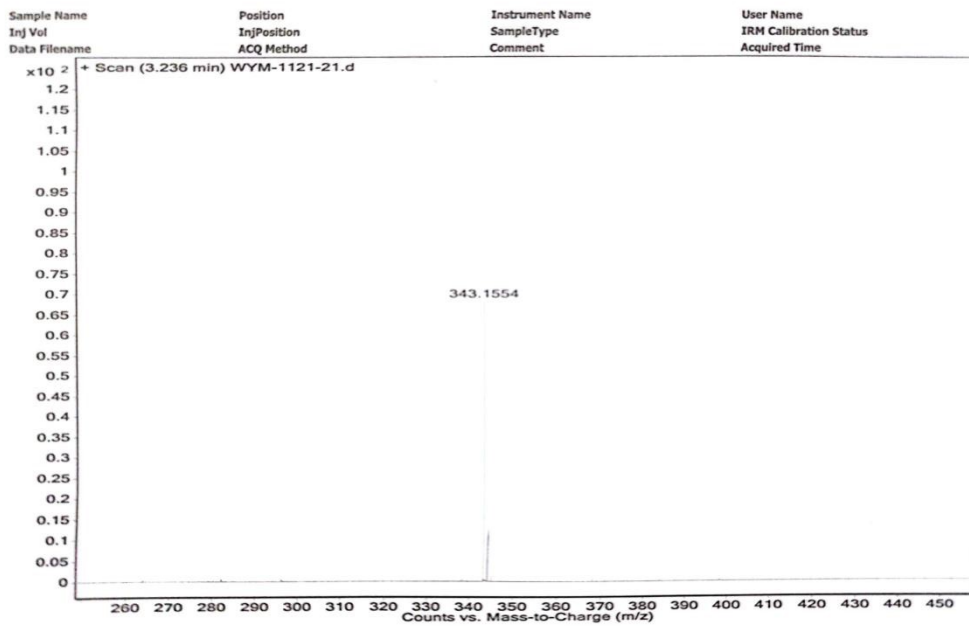
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)isonicotinamide (**23**)



¹H NMR of compound **23**

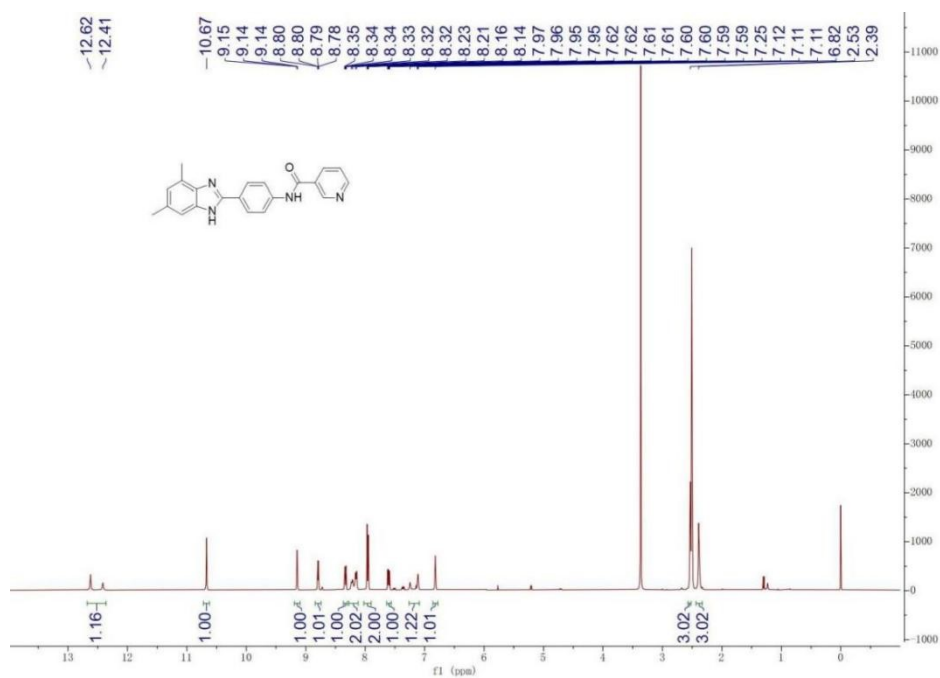


¹³C NMR of compound **23**

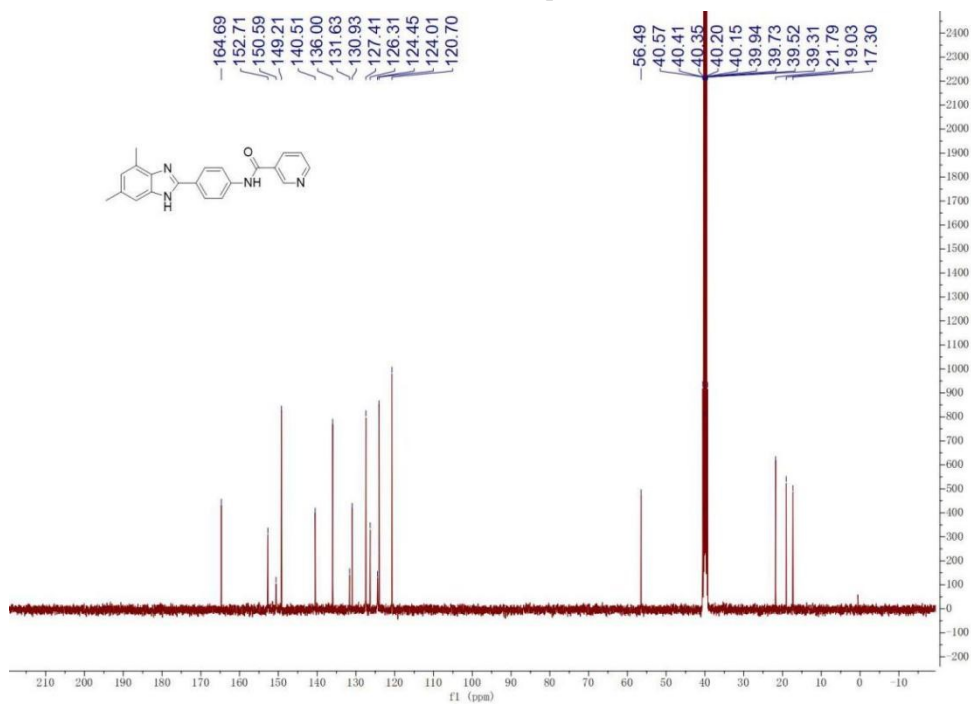


HR-MS of compound 23

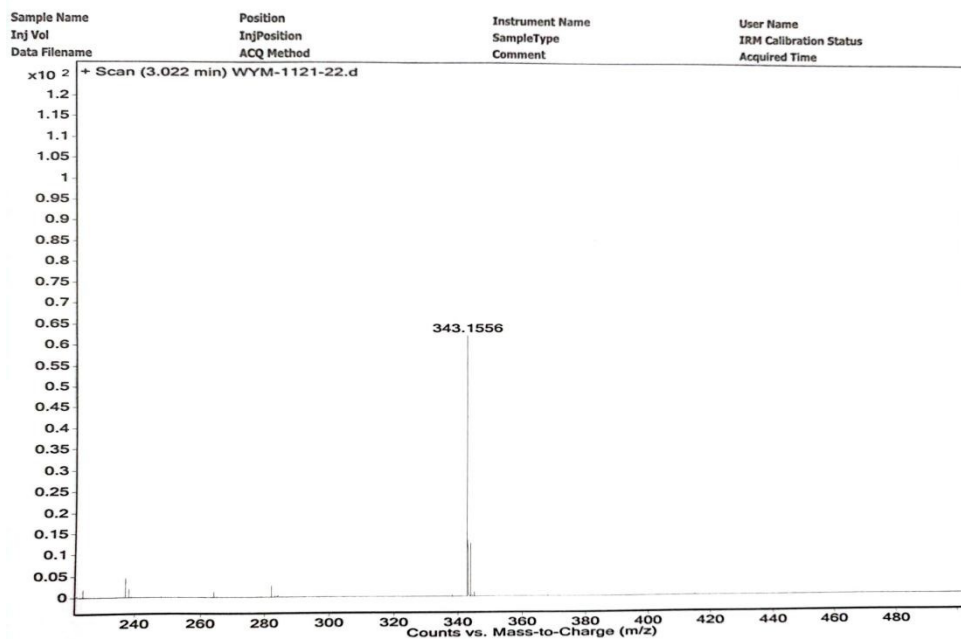
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)nicotinamide (**24**)



¹H NMR of compound **24**

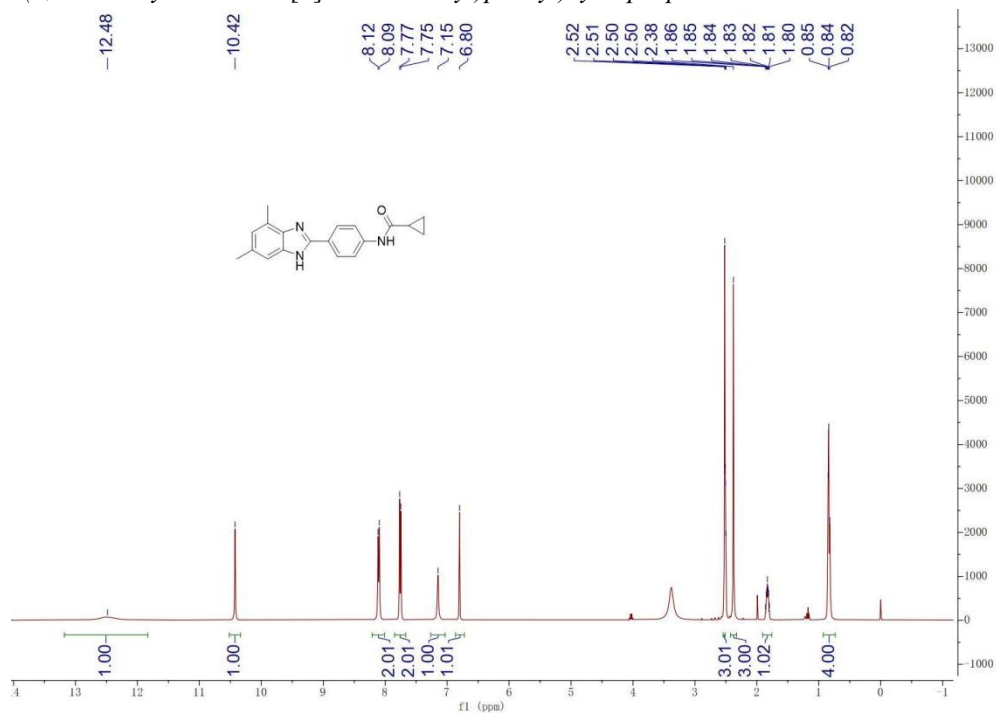


¹³C NMR of compound **24**

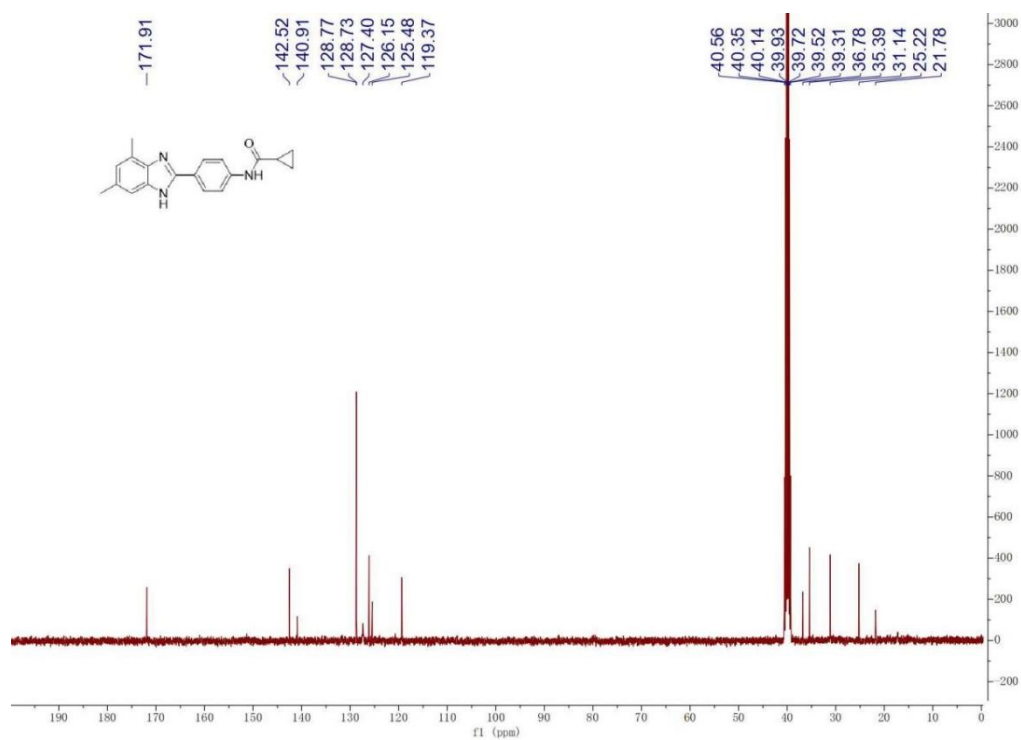


HR-MS of compound 24

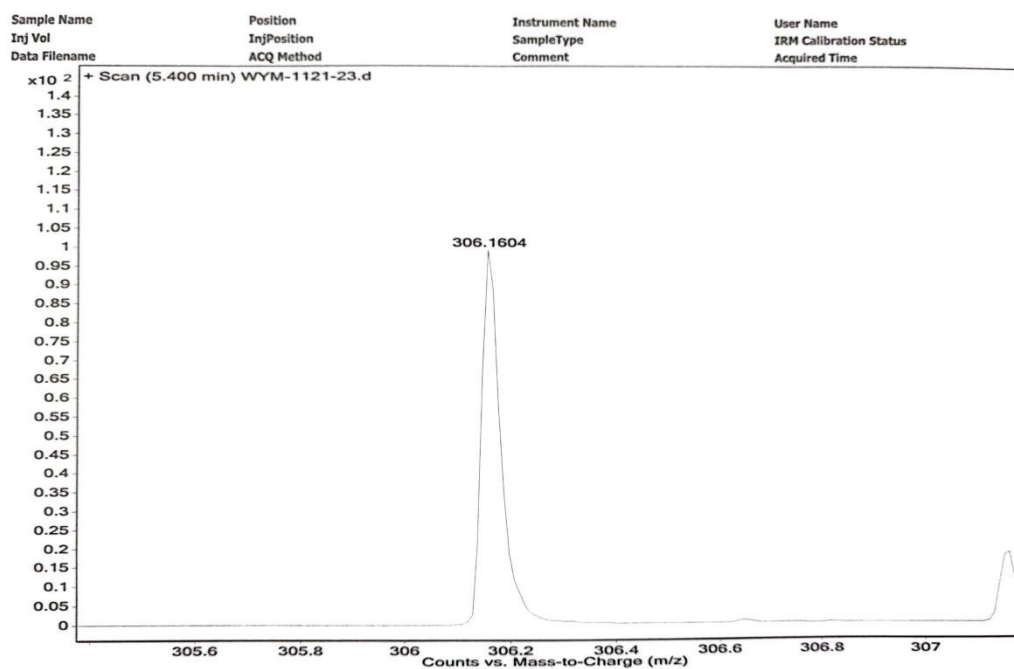
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)cyclopropanecarboxamide (**25**)



¹H NMR of compound **25**

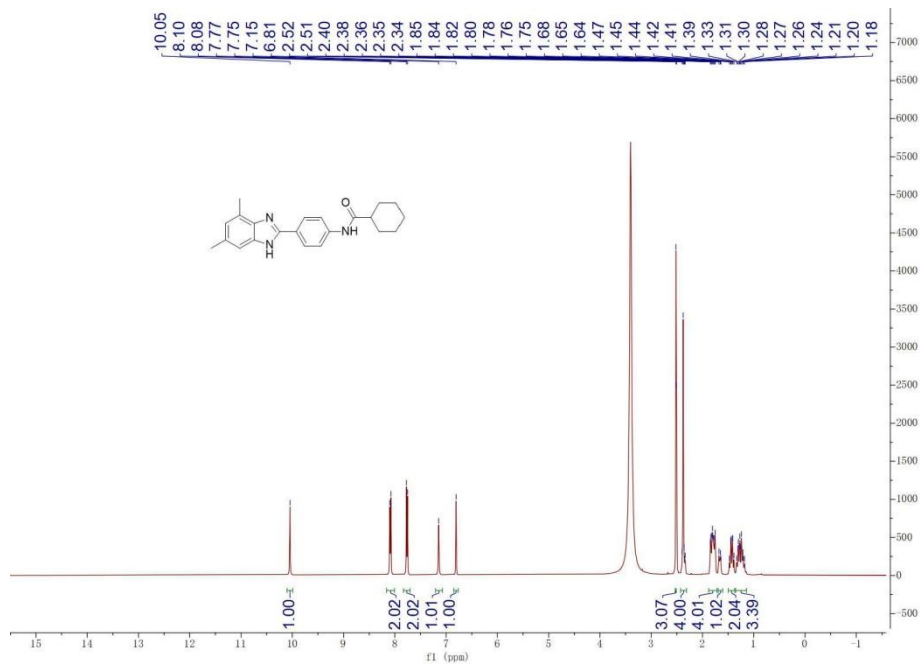


¹³C NMR of compound **25**

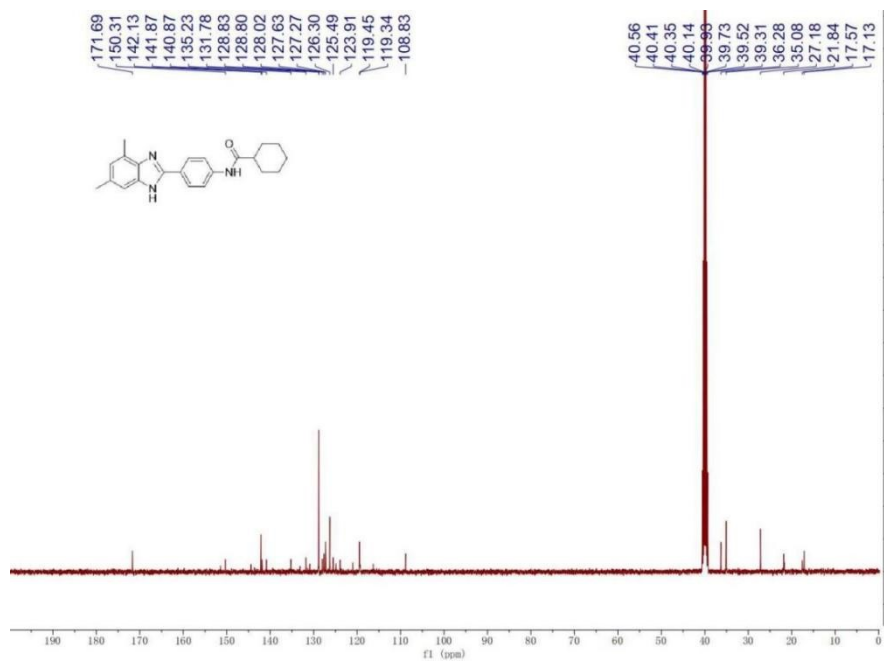


HR-MS of compound 25

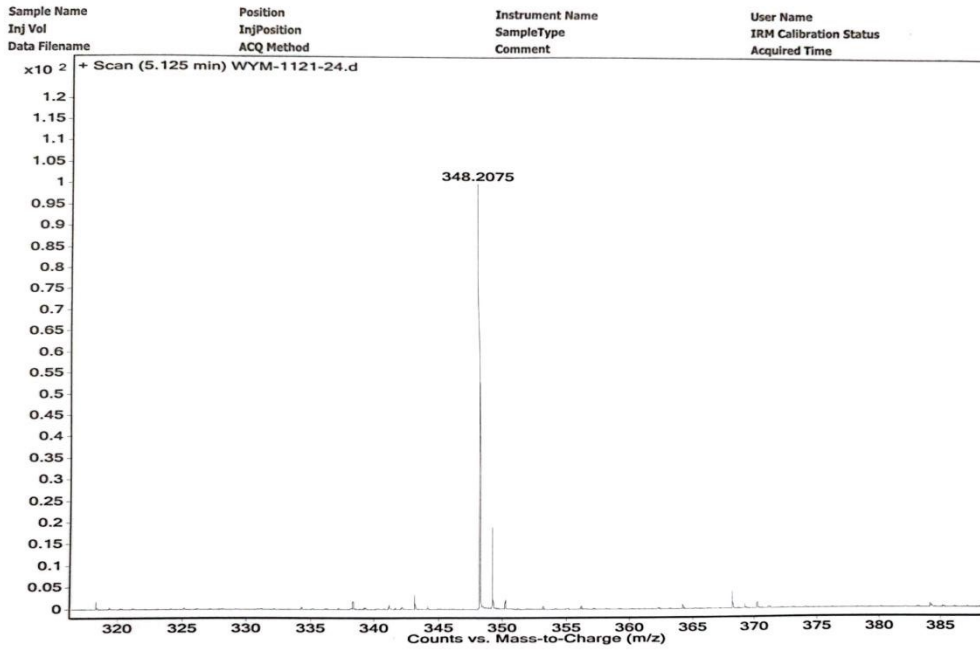
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)cyclohexanecarboxamide (**26**)



¹H NMR of compound **26**

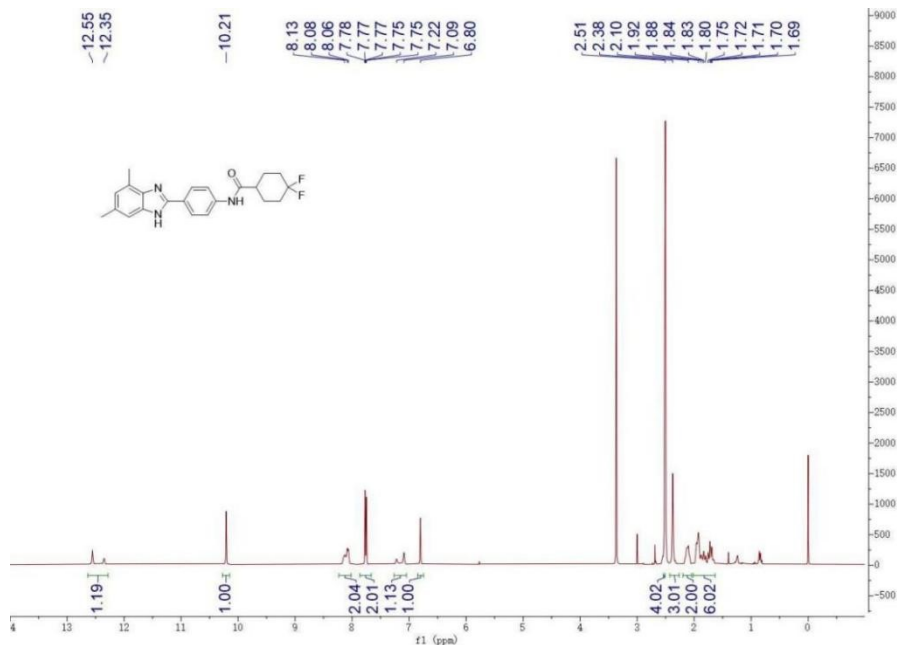


¹³C NMR of compound **26**

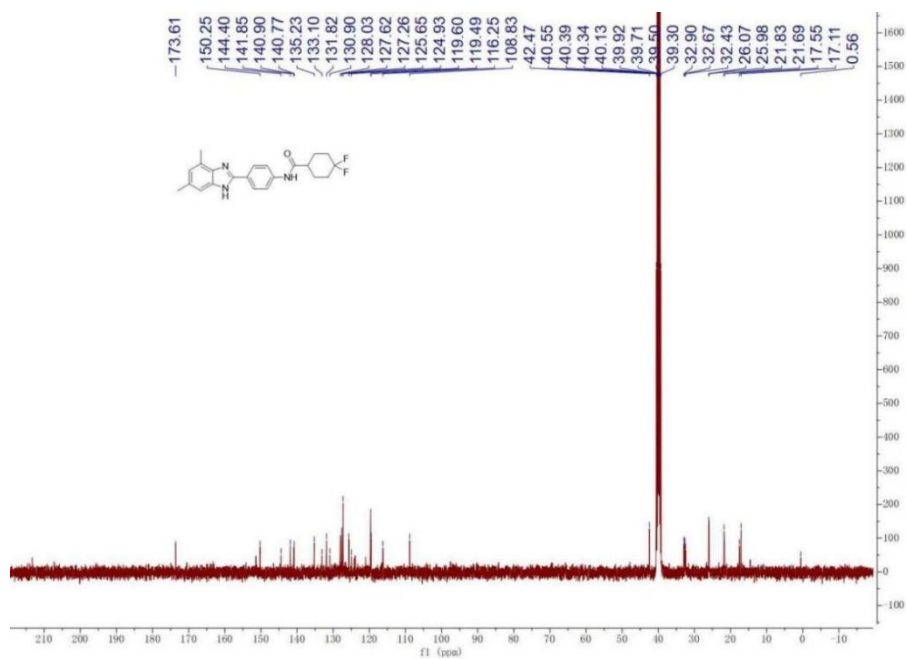


HR-MS of compound 26

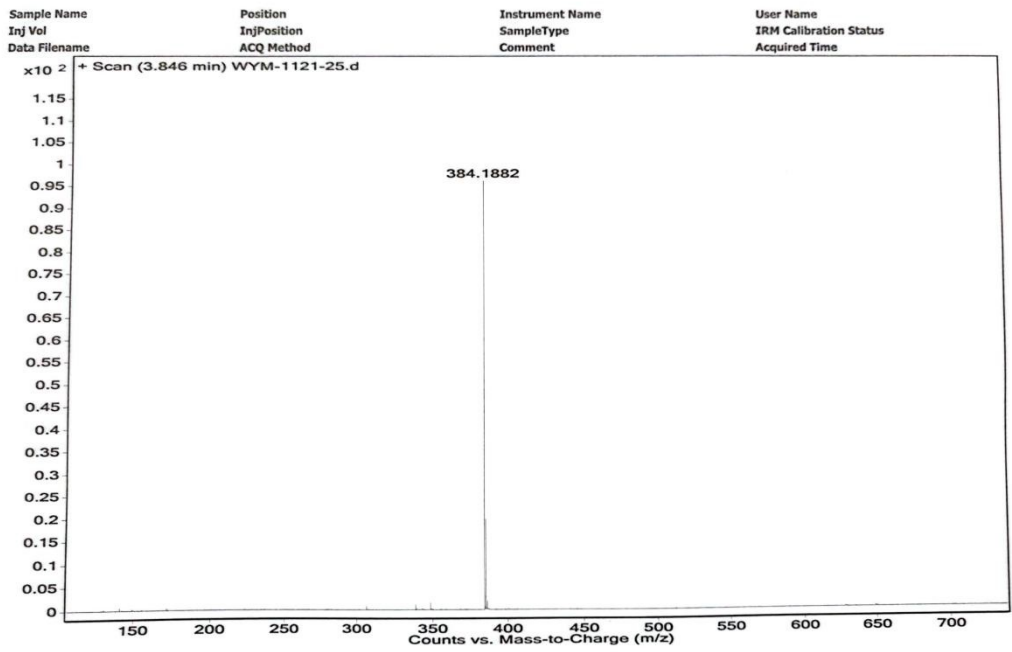
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)-4,4-difluorocyclohexane-1-carboxamide (27)



¹H NMR of compound 27

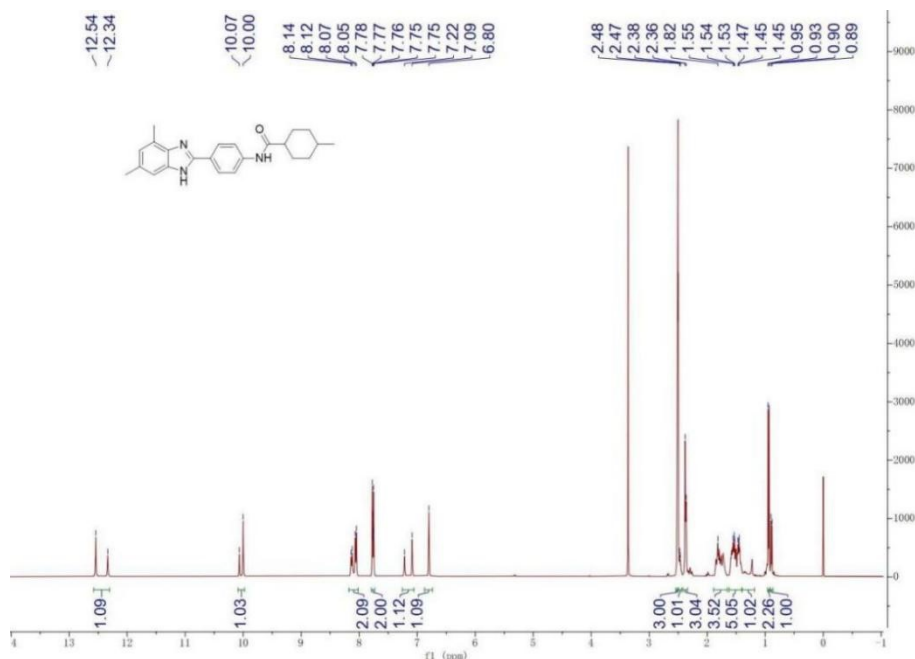


¹³C NMR of compound 27

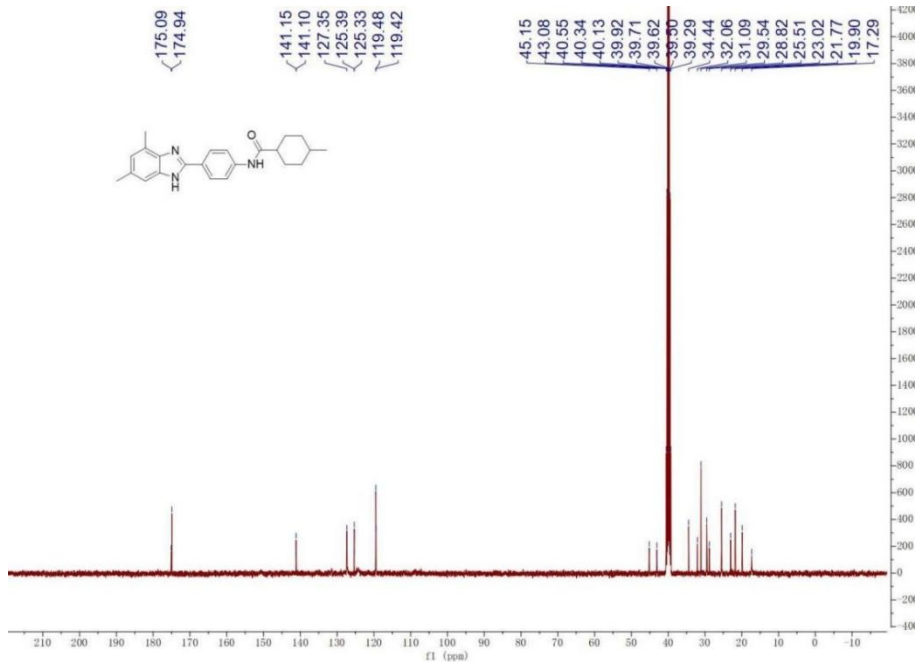


HR-MS of compound 27

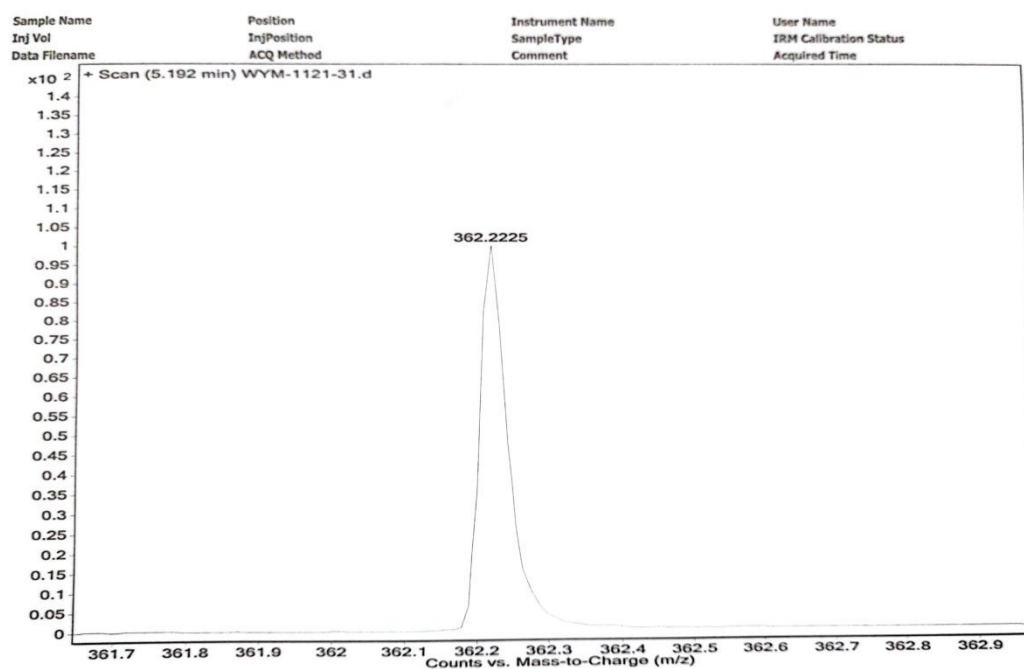
N-(4-(4,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)-4-methylcyclohexane-1-carboxamide (**28**)



¹H NMR of compound **28**

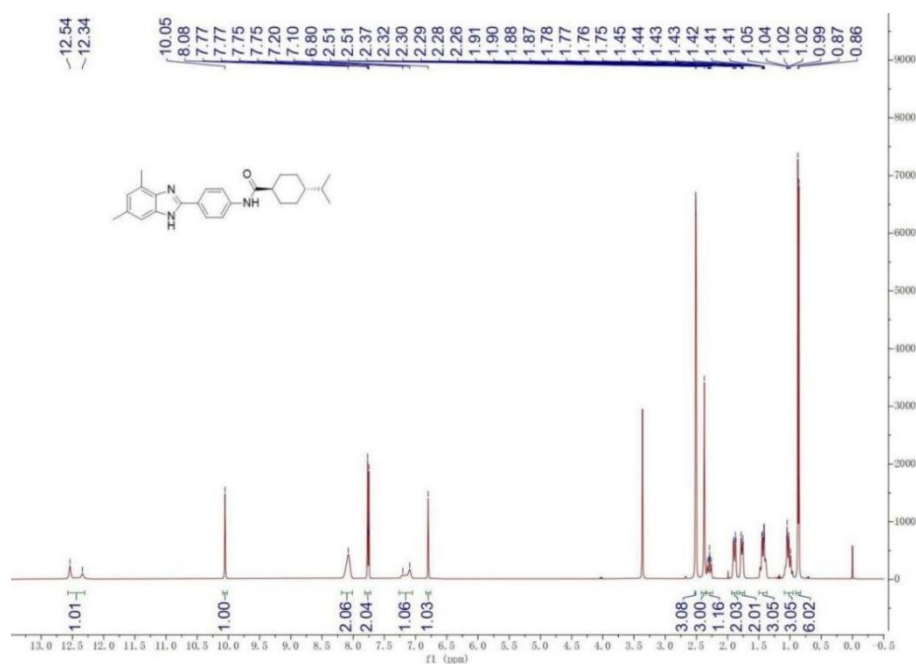


¹³C NMR of compound **28**

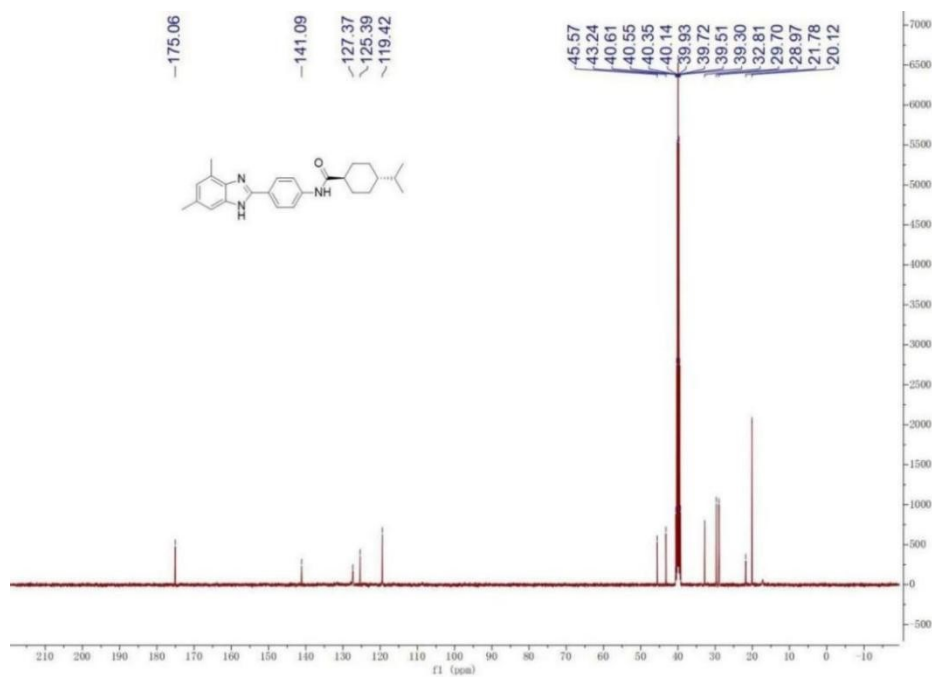


HR-MS of compound 28

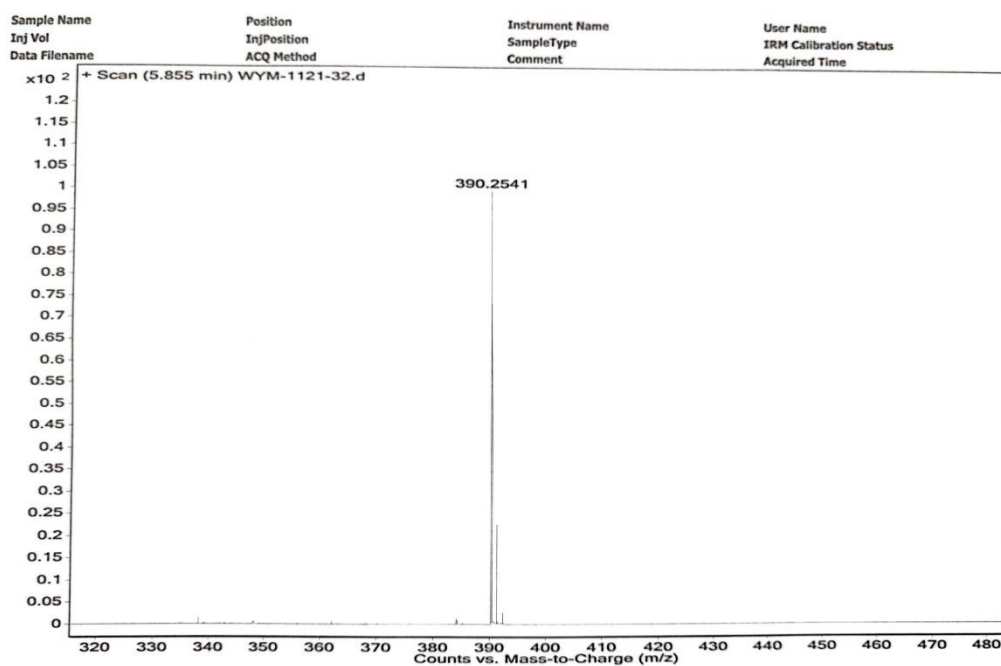
(1r,4r)-N-(4-(4,6-dimethyl-1H-benzo[d]imidazol-2-yl)phenyl)-4-isopropylcyclohexane-1-carboxamide (**29**)



^1H NMR of compound **29**

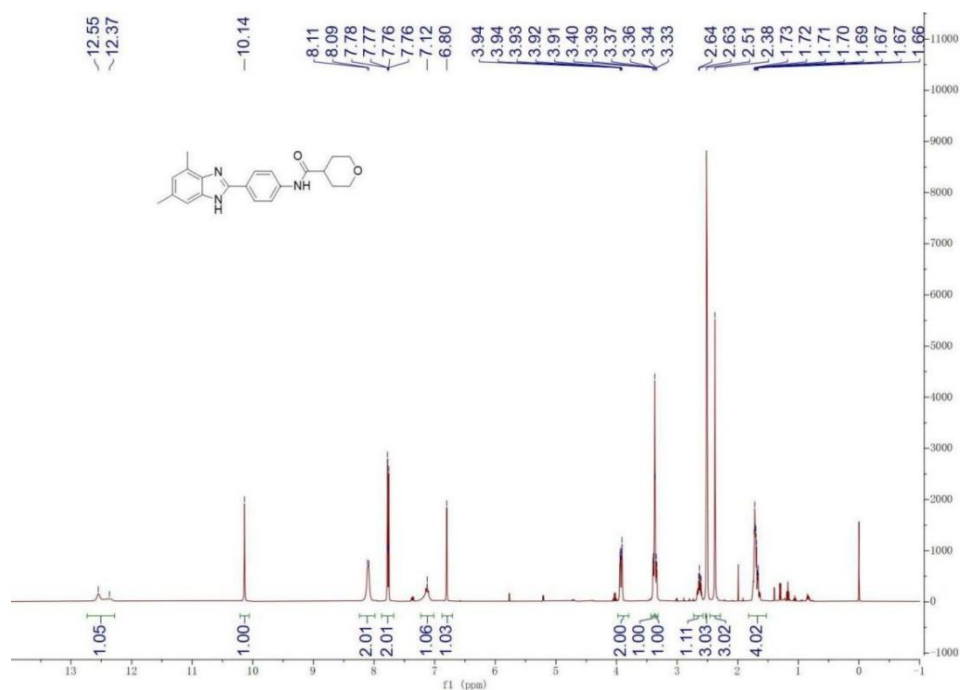


^{13}C NMR of compound **29**

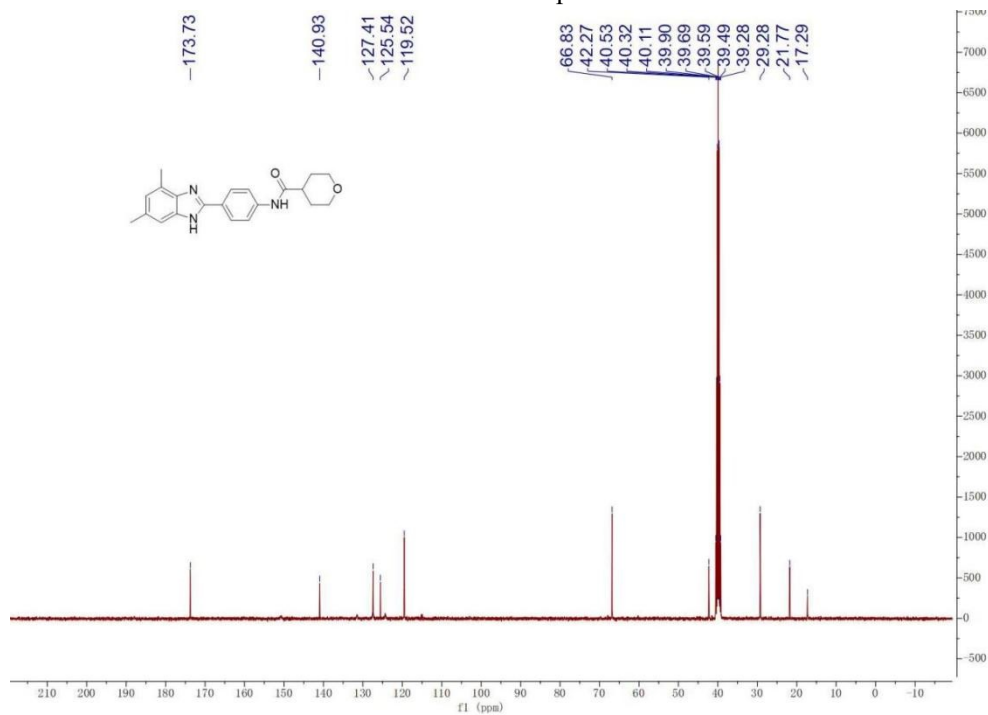


HR-MS of compound 29

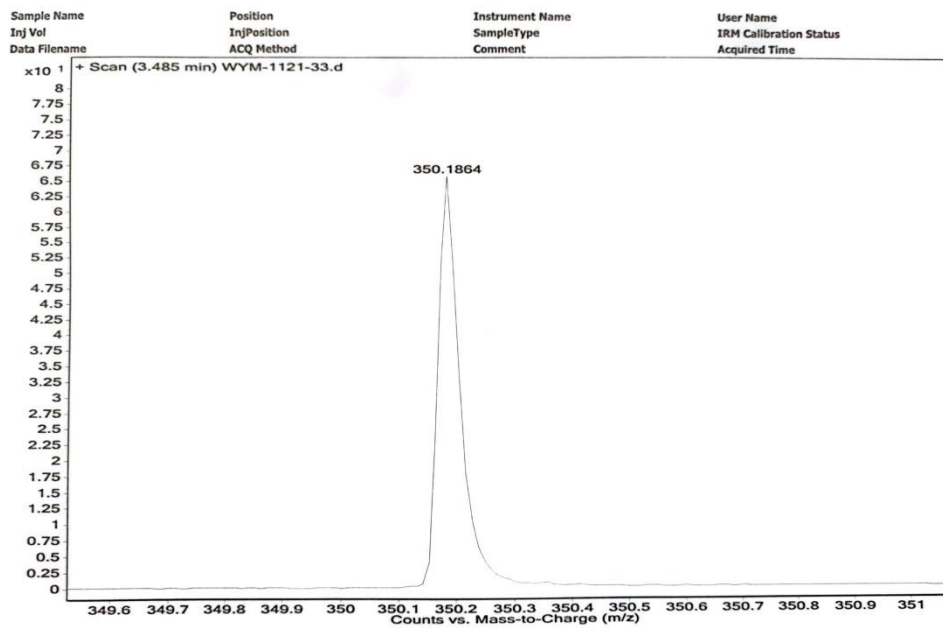
N-(4-(4,6-dimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)tetrahydro-2*H*-pyran-4-carboxamide (**30**)



¹H NMR of compound **30**

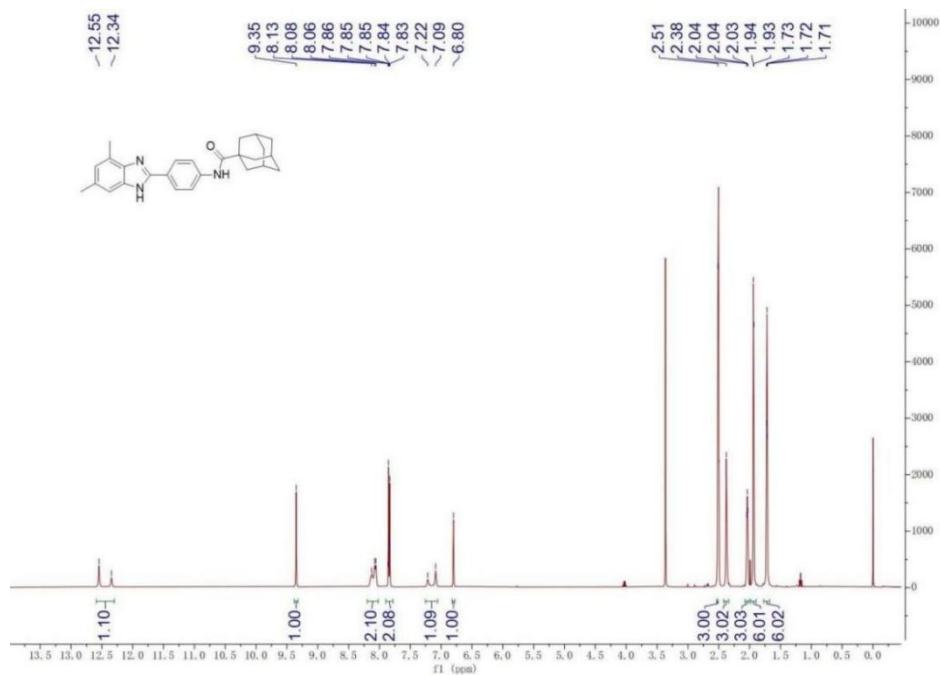


¹³C NMR of compound **30**

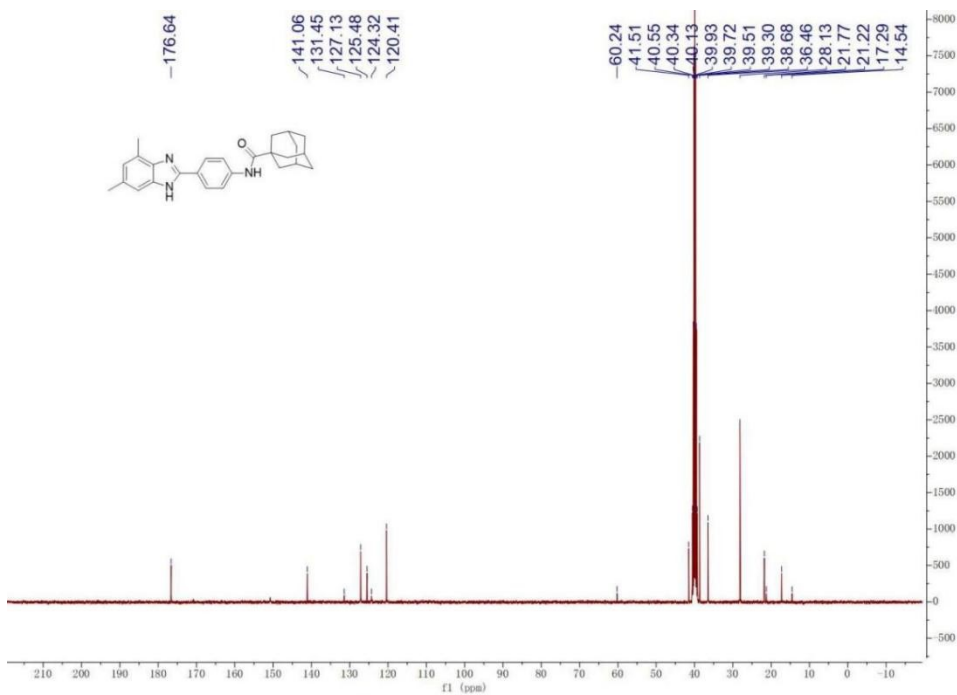


HR-MS of compound 30

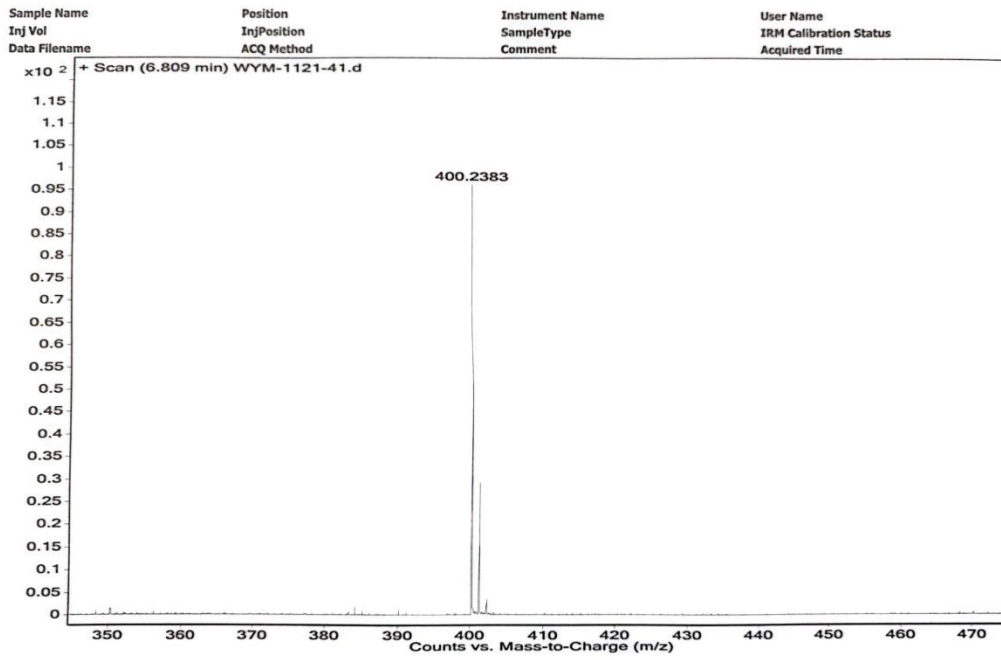
(3*r*,5*r*,7*r*)-*N*-(4-(4,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)adamantane-1-carboxamide (**31**)



¹H NMR of compound 31

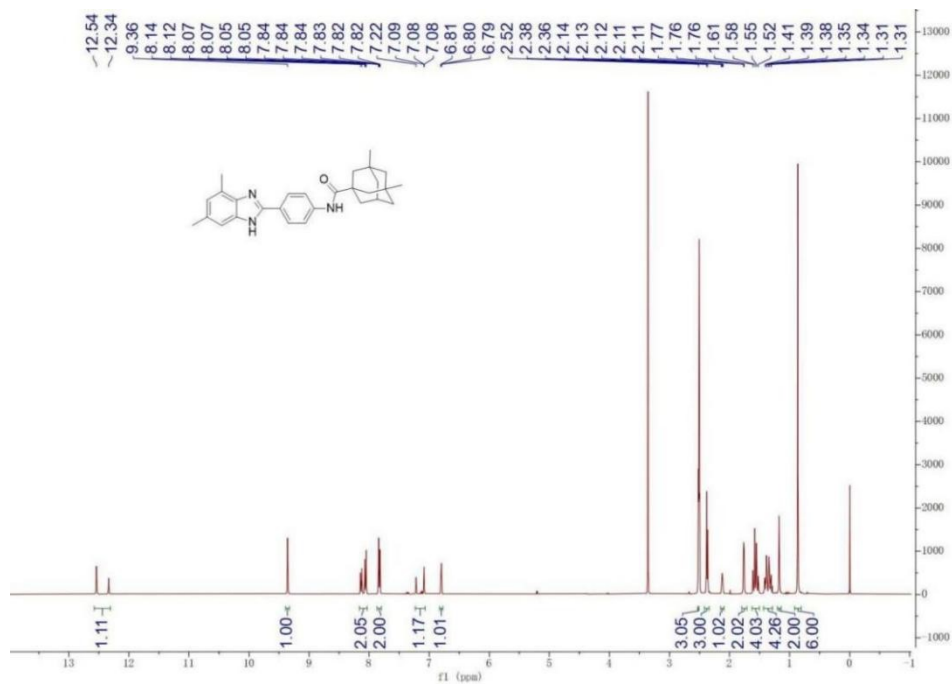


¹³C NMR of compound 31

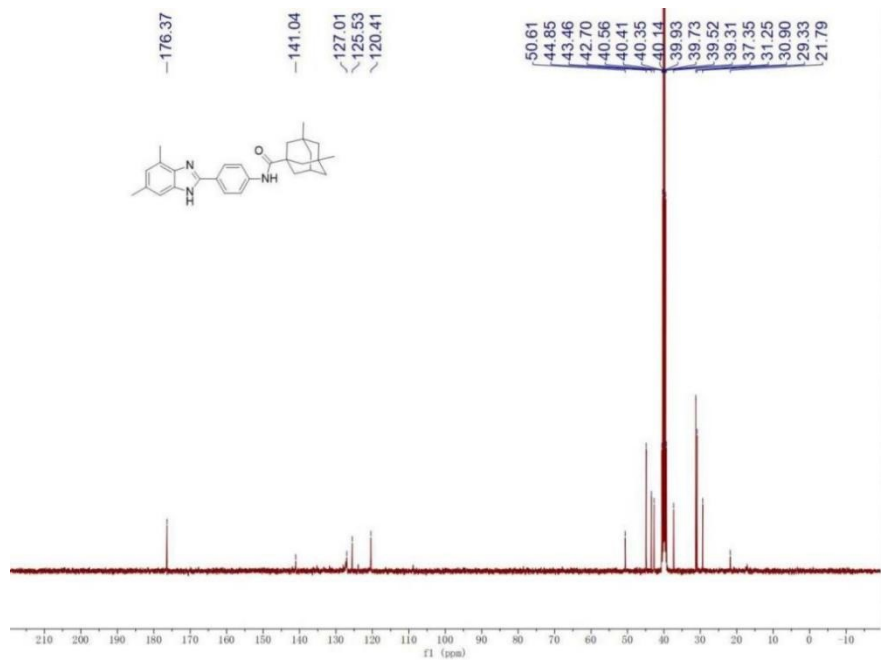


HR-MS of compound 31

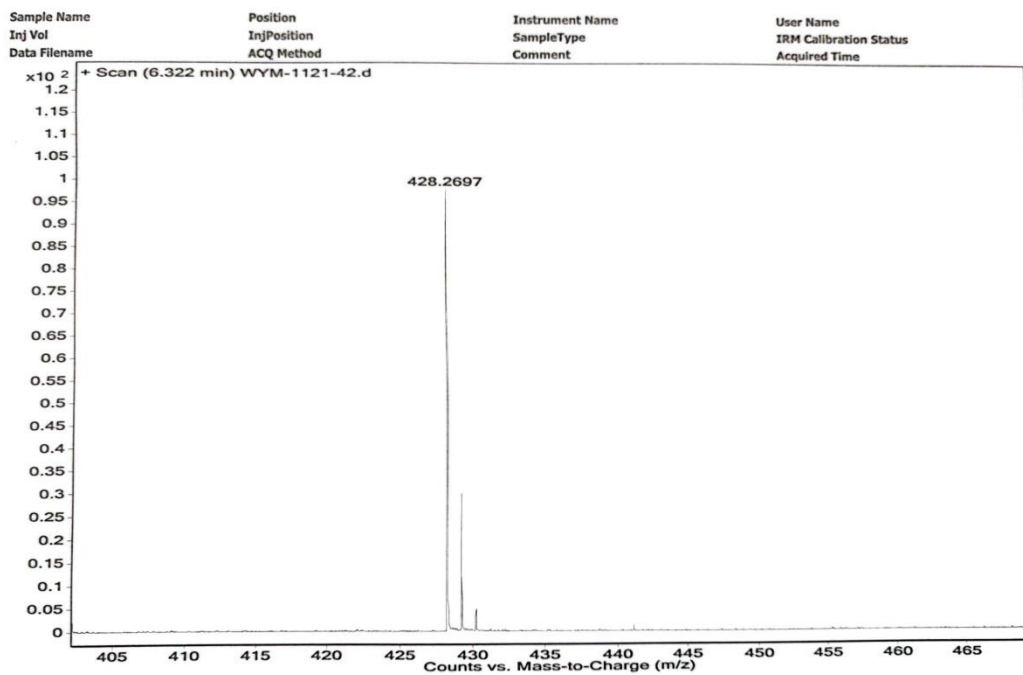
(1r,3R,5S,7r)-N-(4-(4,6-dimethyl-1H-benzodimidazol-2-yl)phenyl)-3,5-dimethyladamantane-1-carboxamide (**32**)



¹H NMR of compound 32

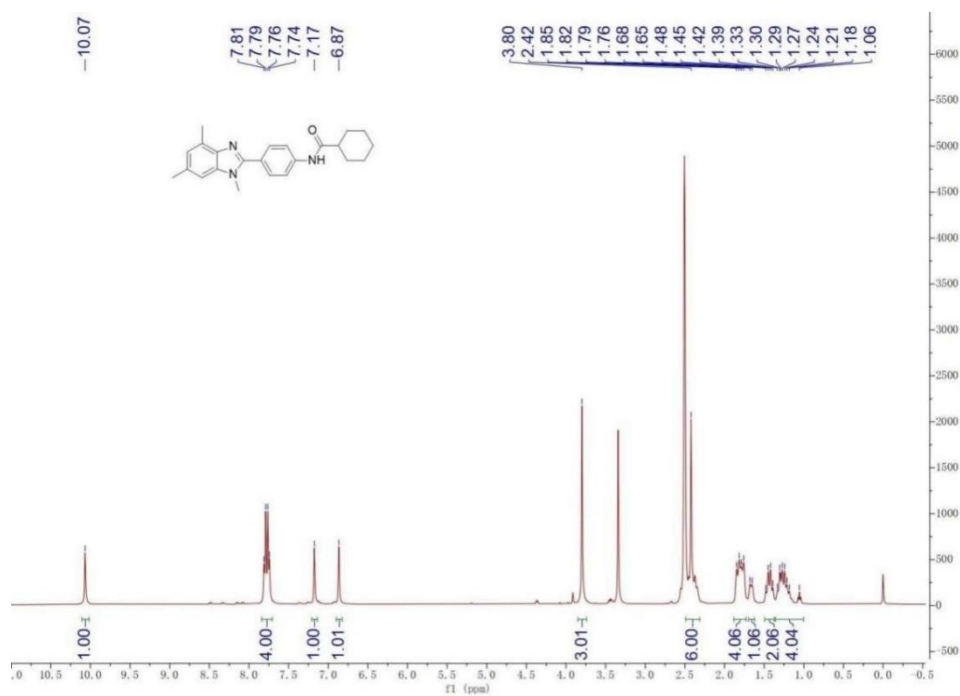


¹³C NMR of compound 32

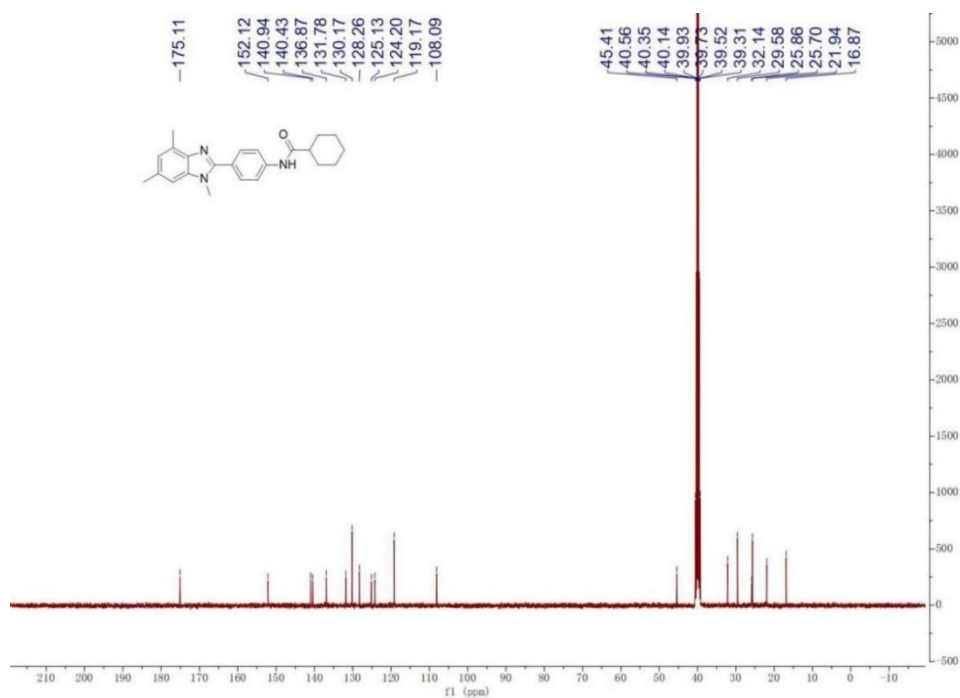


HR-MS of compound 32

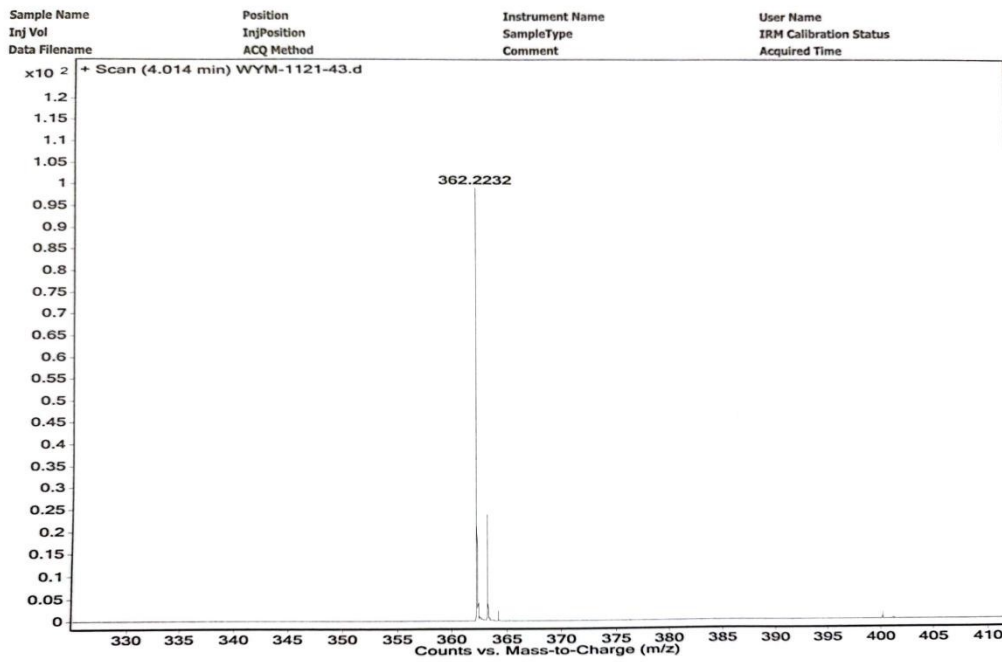
N-(4-(1,4,6-trimethyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)cyclohexanecarboxamide (**33**)



¹H NMR of compound 33

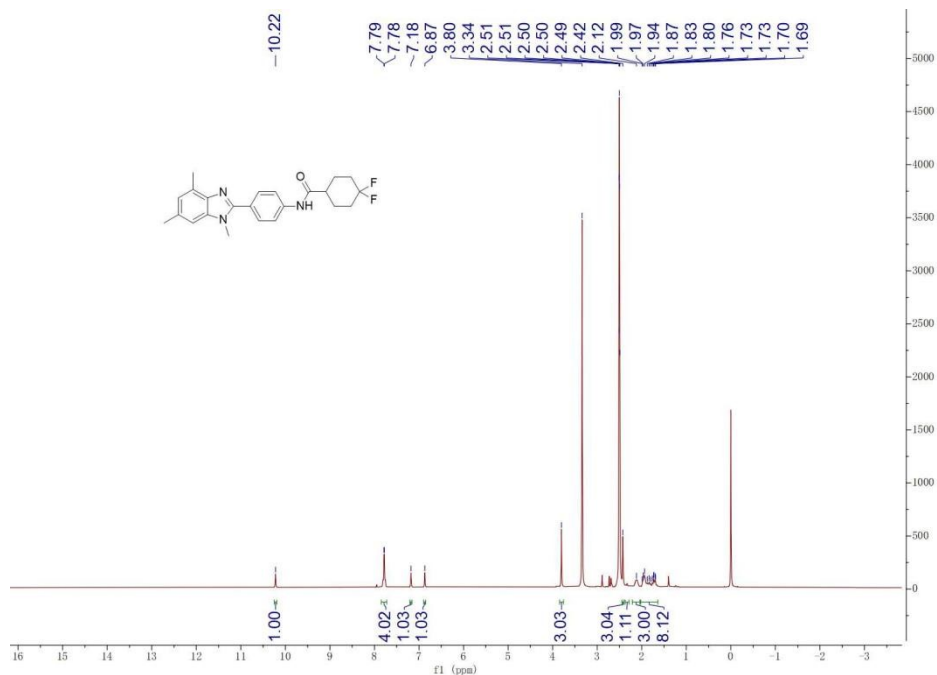


¹³C NMR of compound 33

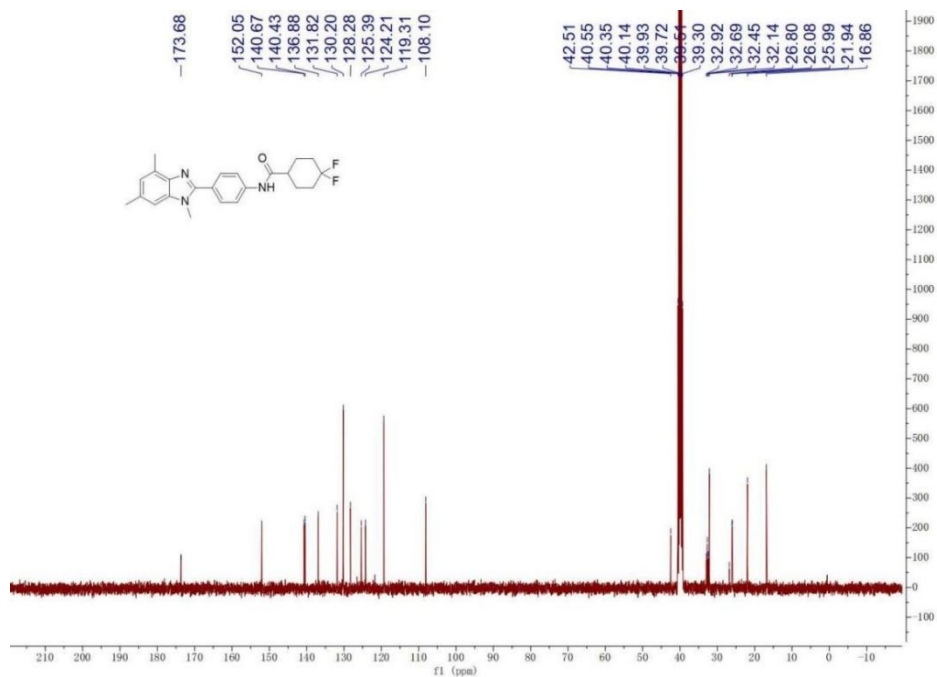


HR-MS of compound 33

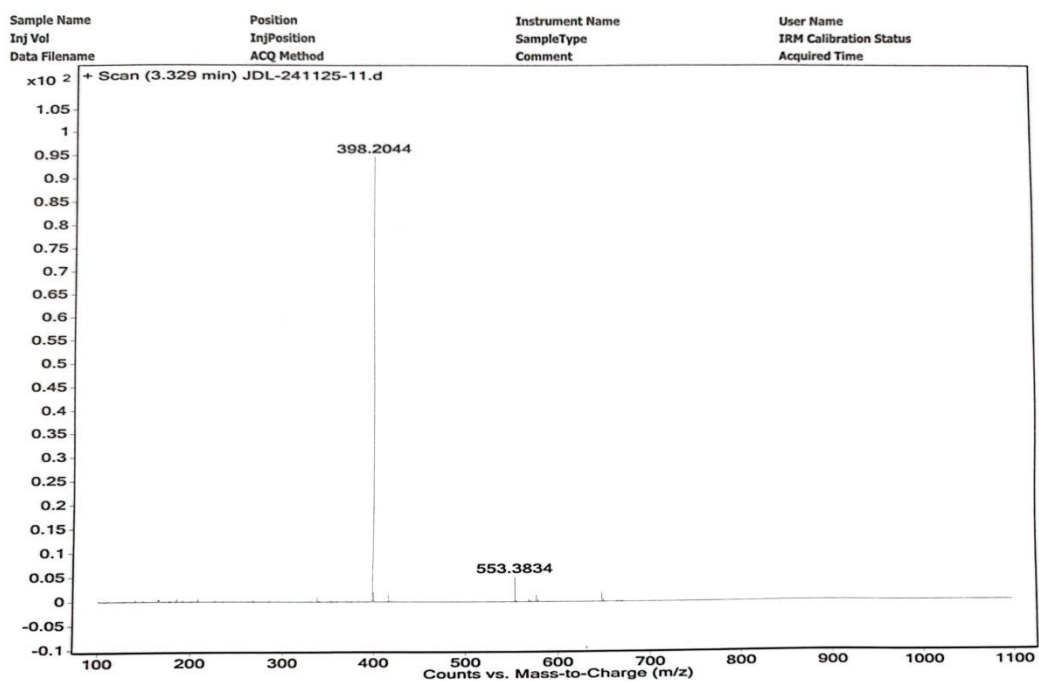
4,4-difluoro-N-(4-(1,4,6-trimethyl-1H-benzo[d]imidazol-2-yl)phenyl)cyclohexane-1-carboxamide (34)



¹H NMR of compound 34

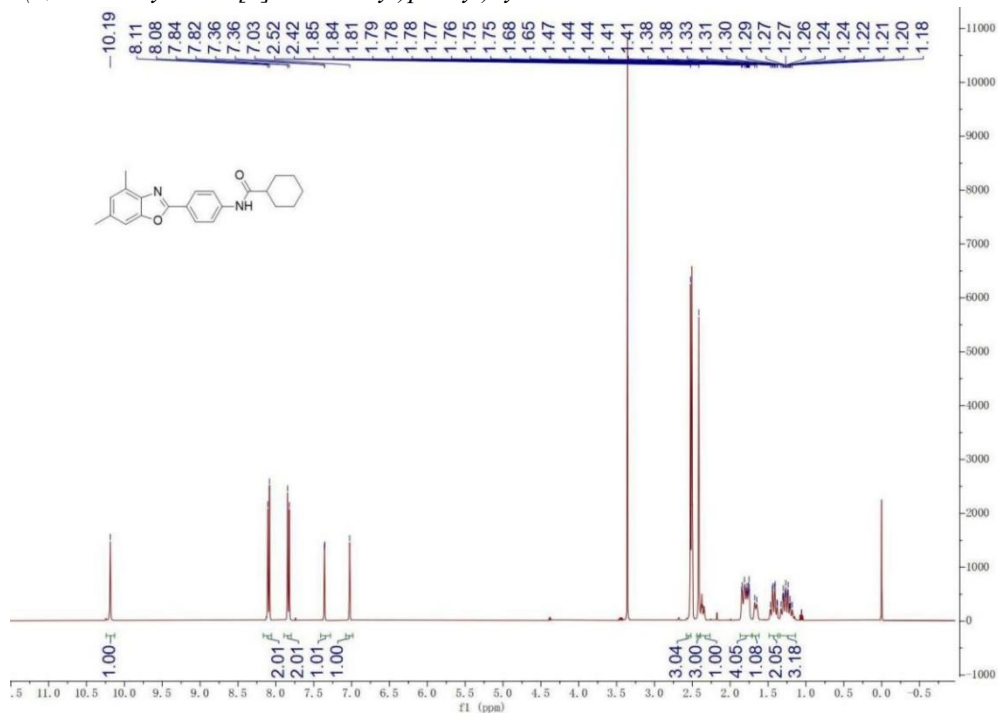


¹³C NMR of compound 34

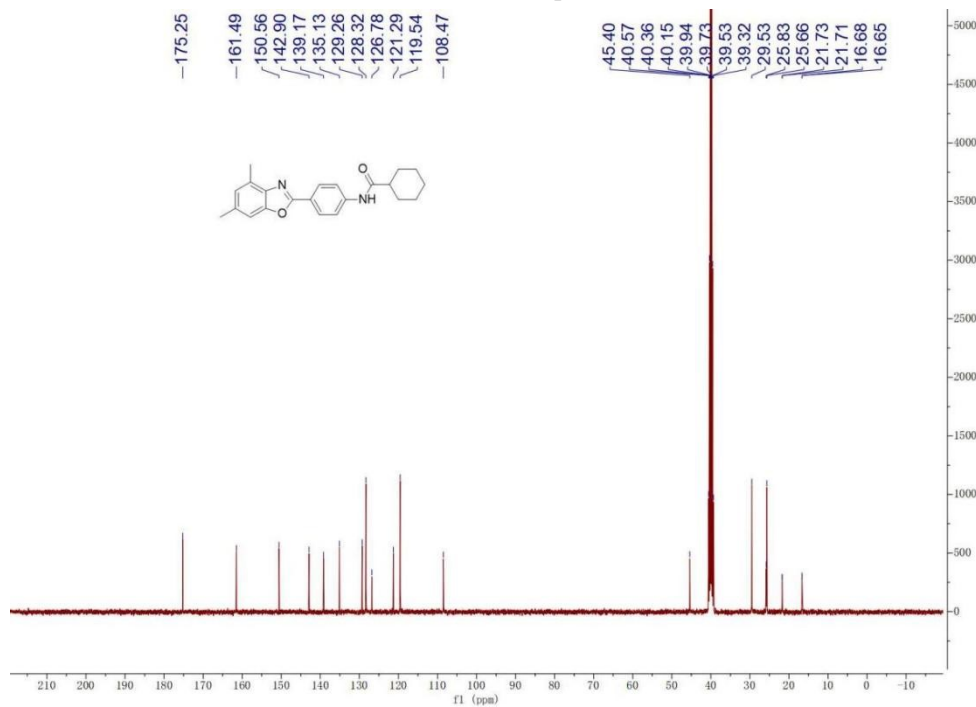


HR-MS of compound 34

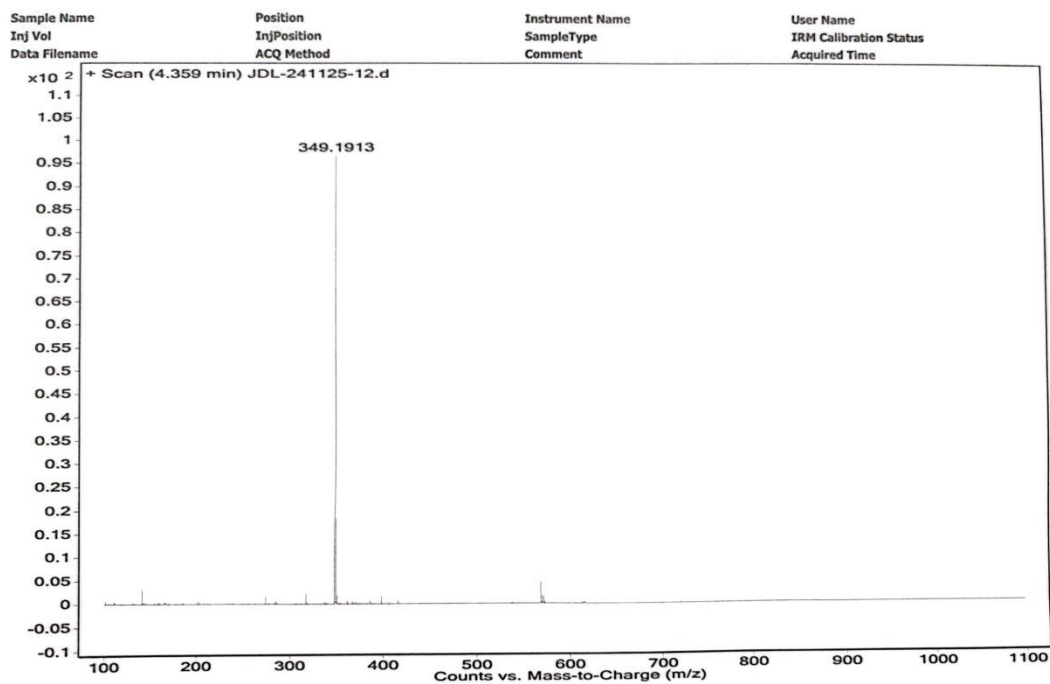
N-(4-(4,6-dimethylbenzo[d]oxazol-2-yl)phenyl)cyclohexanecarboxamide (**35**)



¹H NMR of compound 35

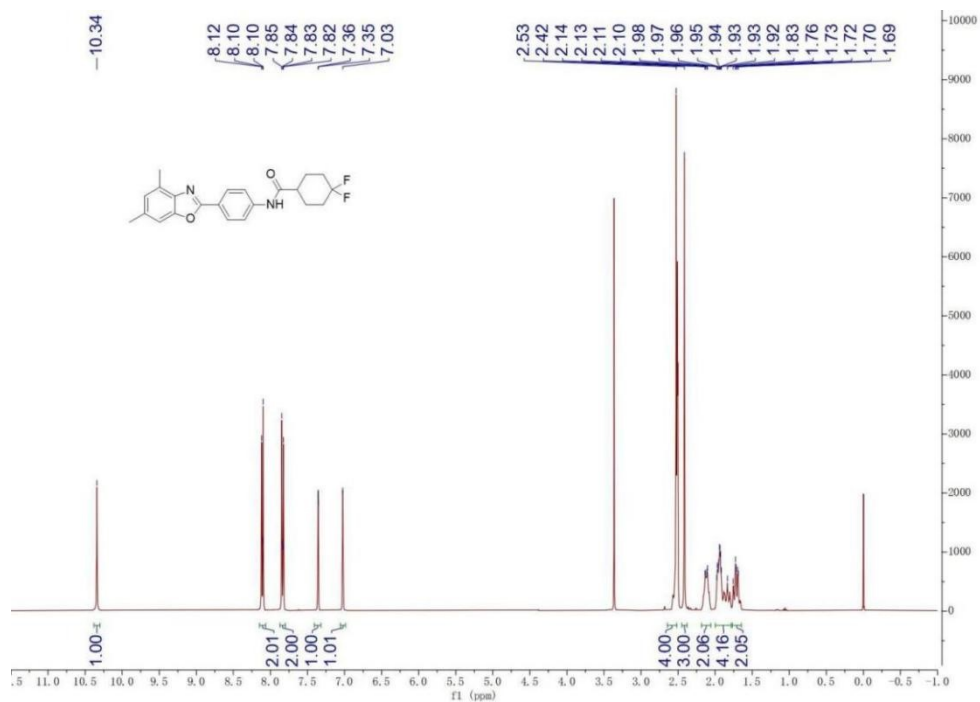


¹³C NMR of compound 35

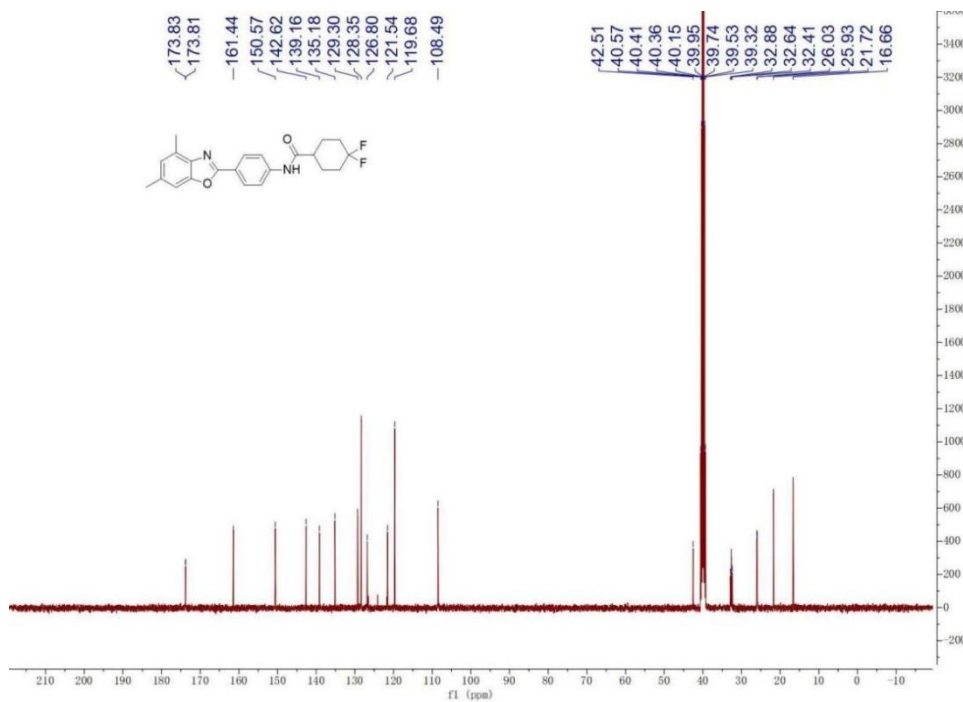


HR-MS of compound 35

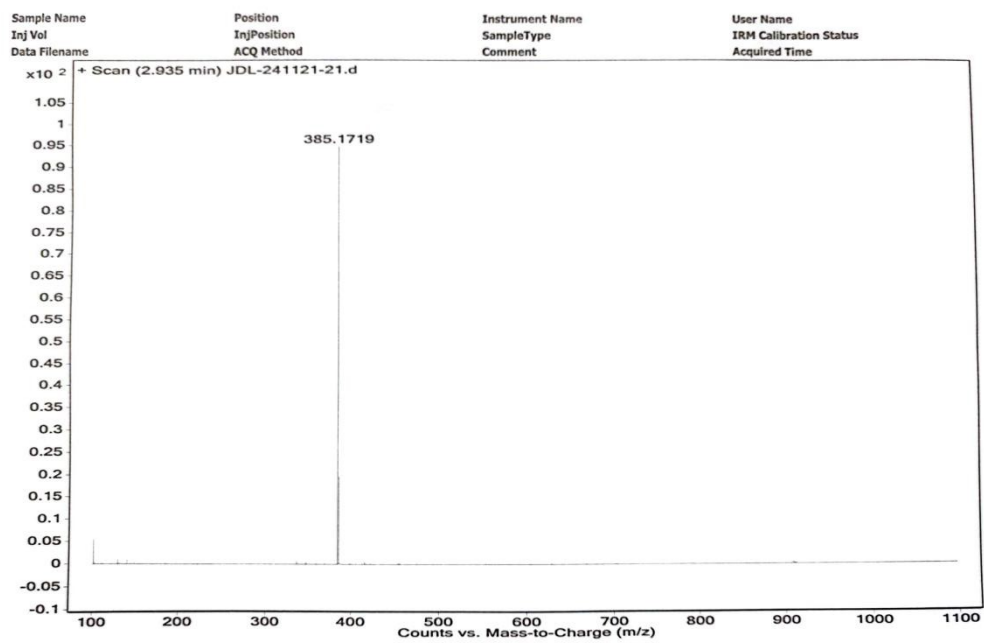
N-(4-(4,6-dimethylbenzo[d]oxazol-2-yl)phenyl)-4,4-difluorocyclohexane-1-carboxamide (36)



¹H NMR of compound 36

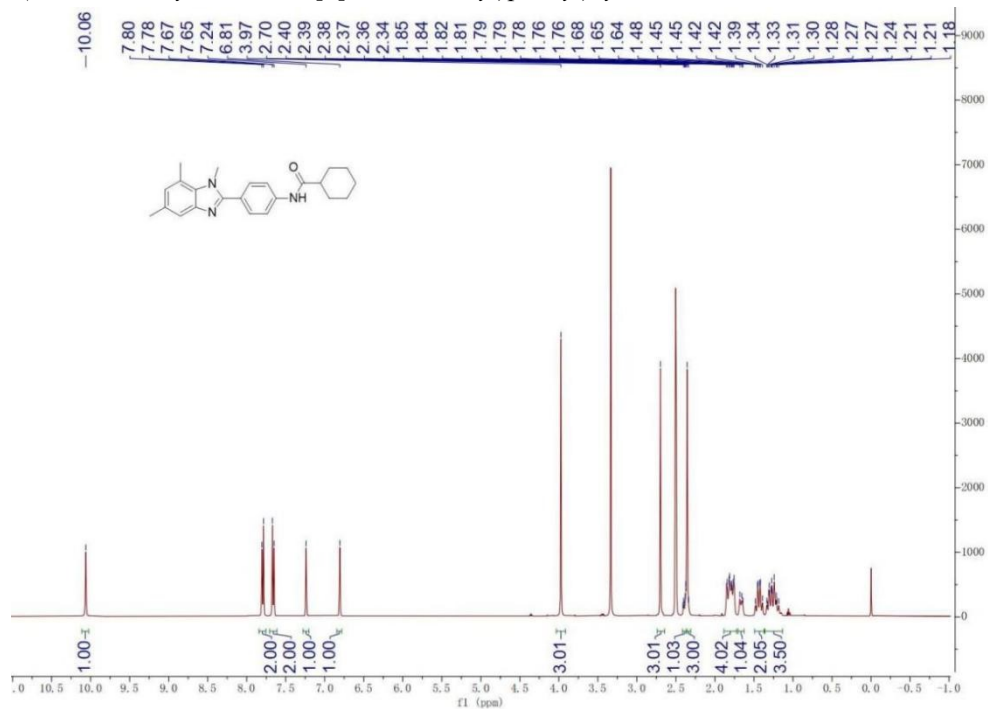


¹³C NMR of compound 36

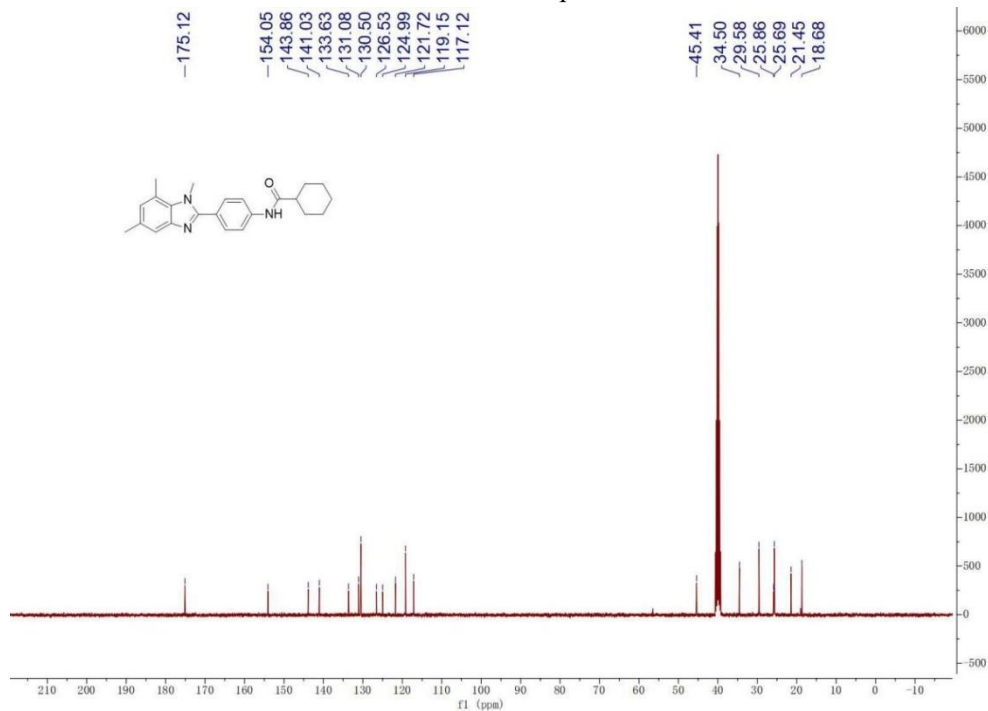


HR-MS of compound 36

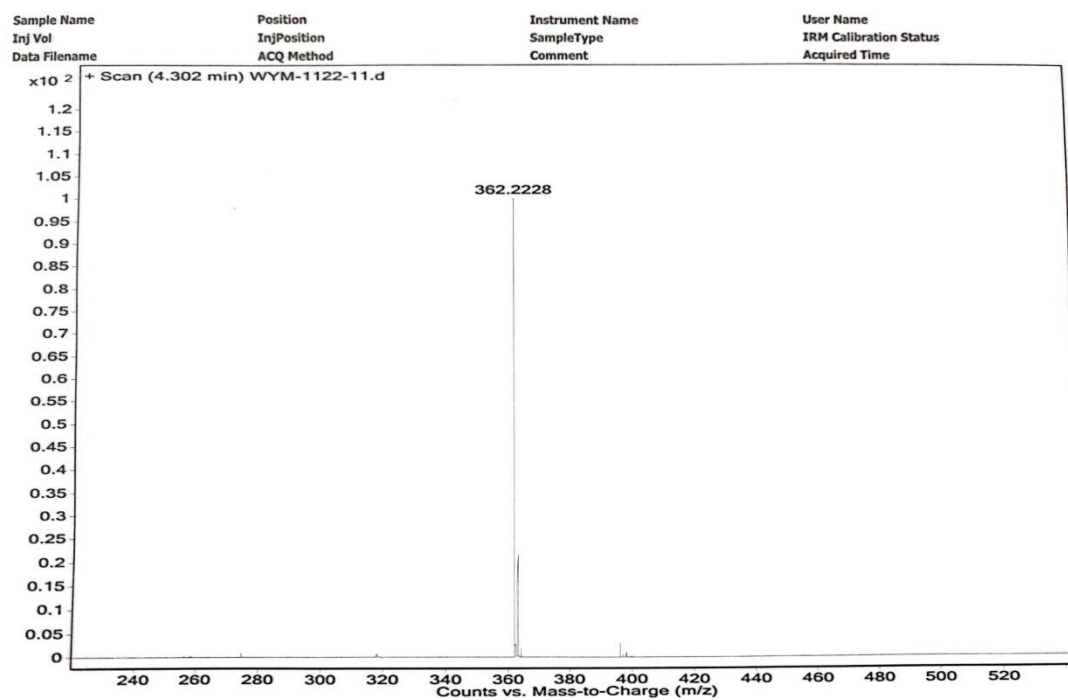
N-(4-(1,5,7-trimethyl-1*H*-benzo[d]imidazol-2-yl)phenyl)cyclohexanecarboxamide (**37**)



¹H NMR of compound **37**

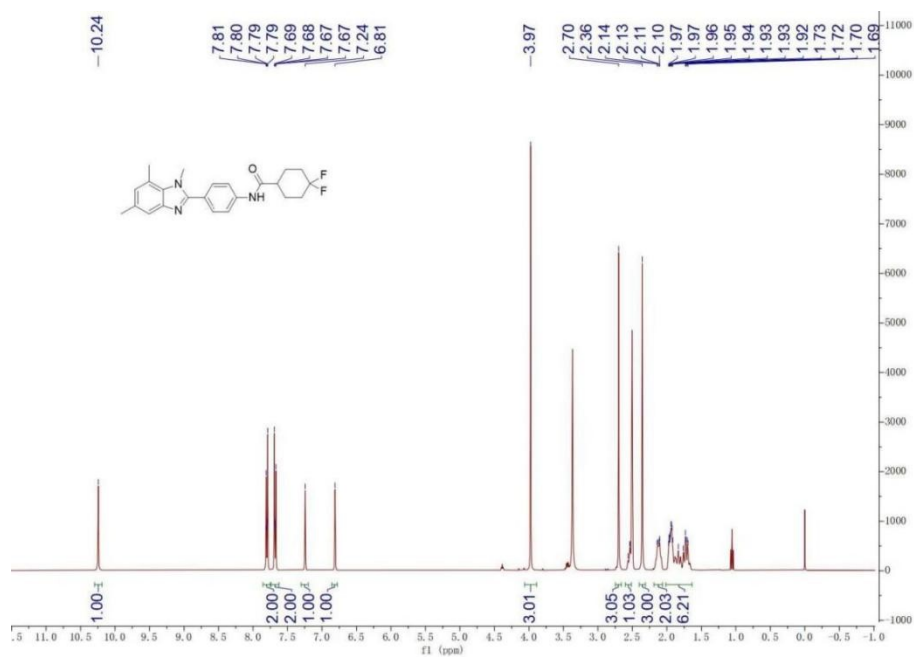


¹³C NMR of compound **37**

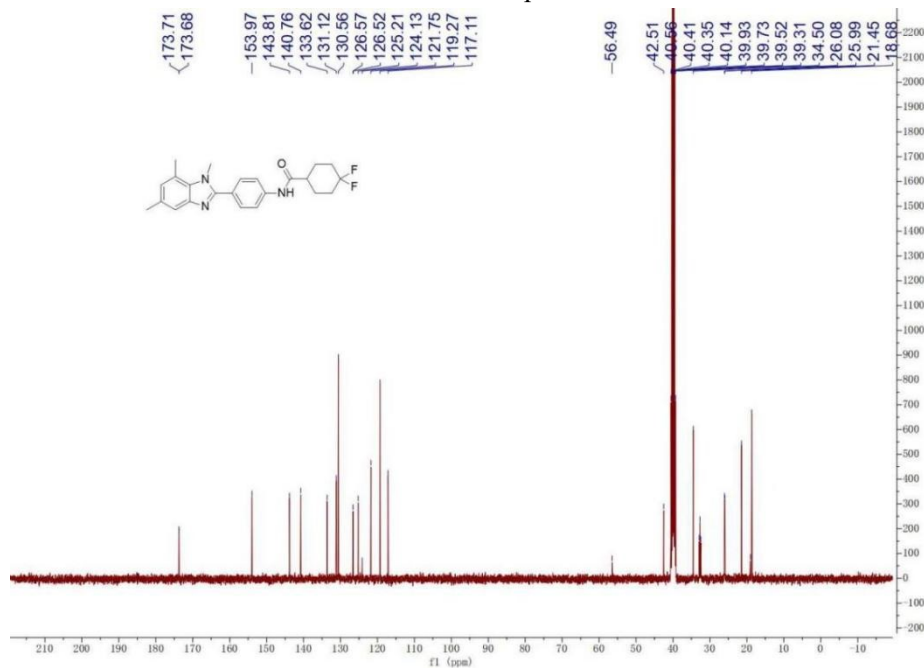


HR-MS of compound 37

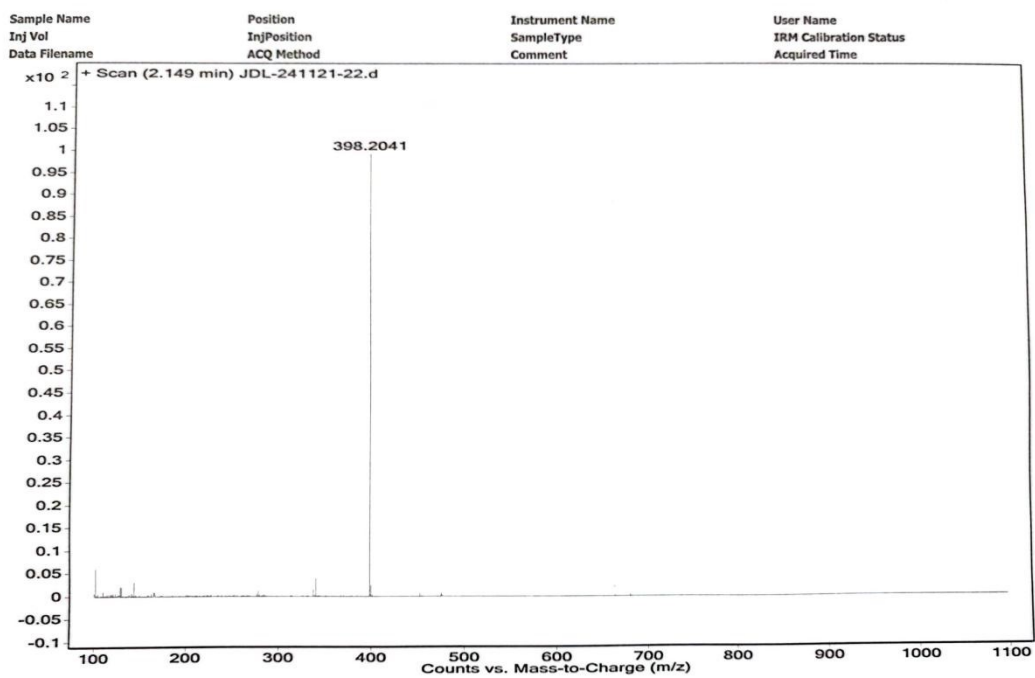
4,4-difluoro-N-(4-(1,5,7-trimethyl-1H-benzo[d]imidazol-2-yl)phenyl)cyclohexane-1-carboxamide (38)



¹H NMR of compound 38

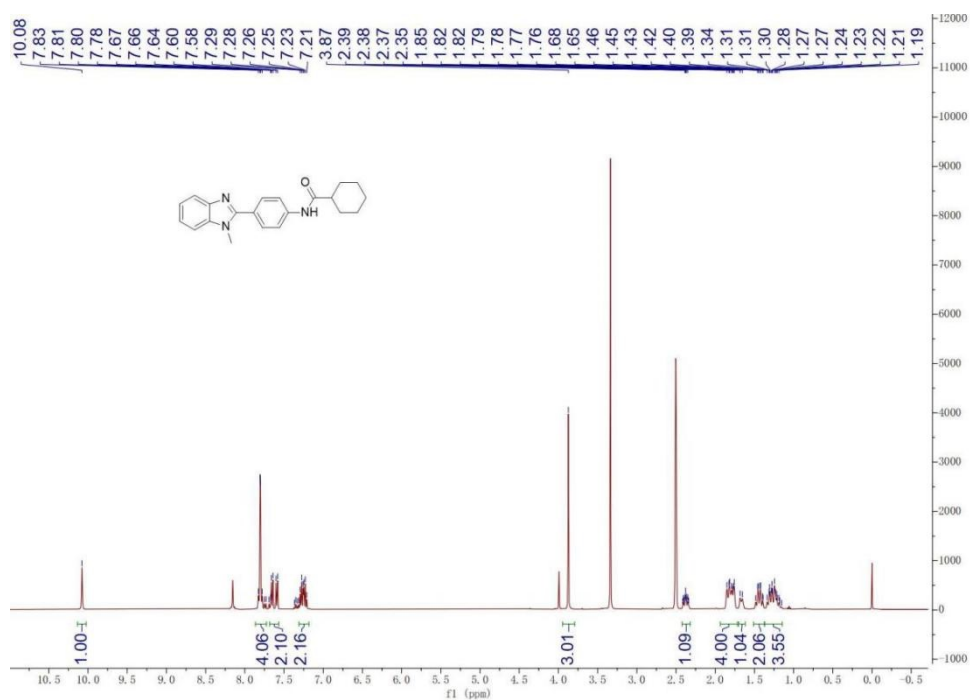


¹³C NMR of compound 38

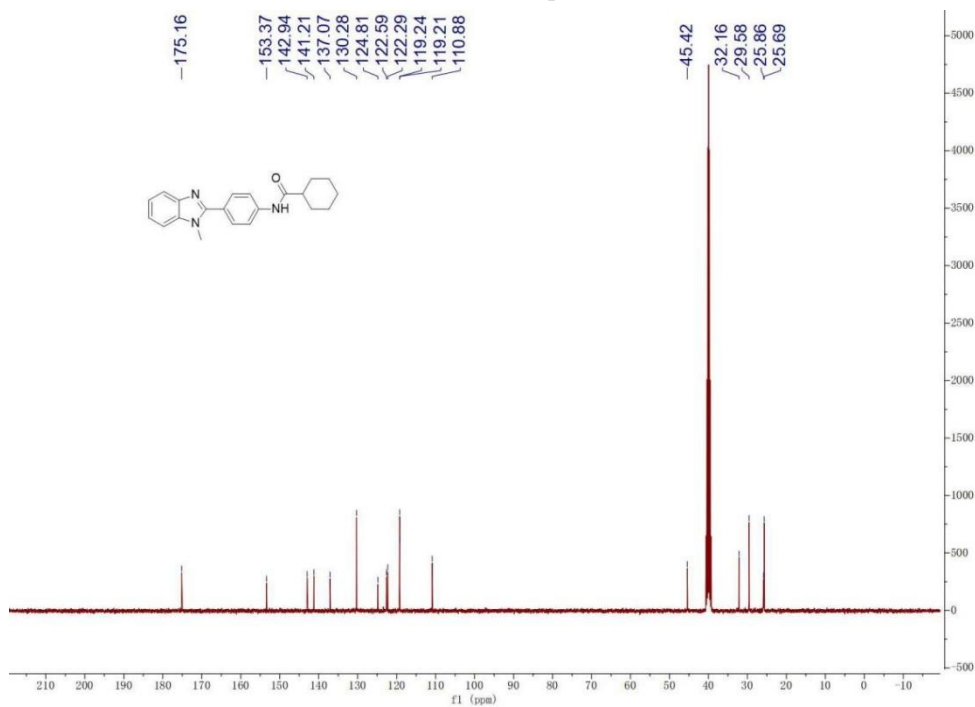


HR-MS of compound 38

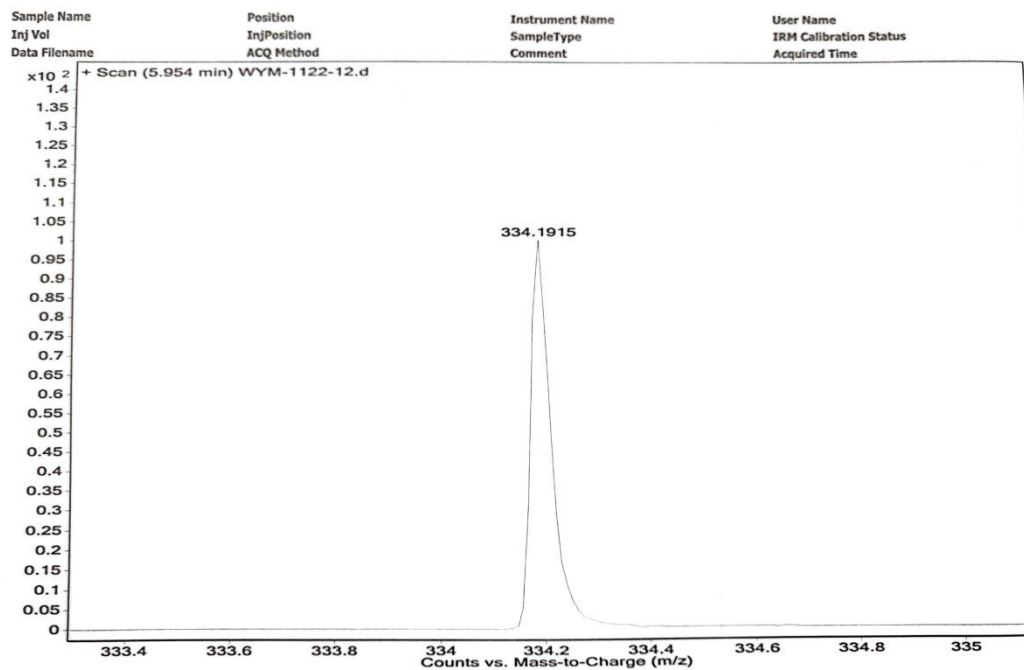
N-(4-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)cyclohexanecarboxamide (**39**)



¹H NMR of compound 39

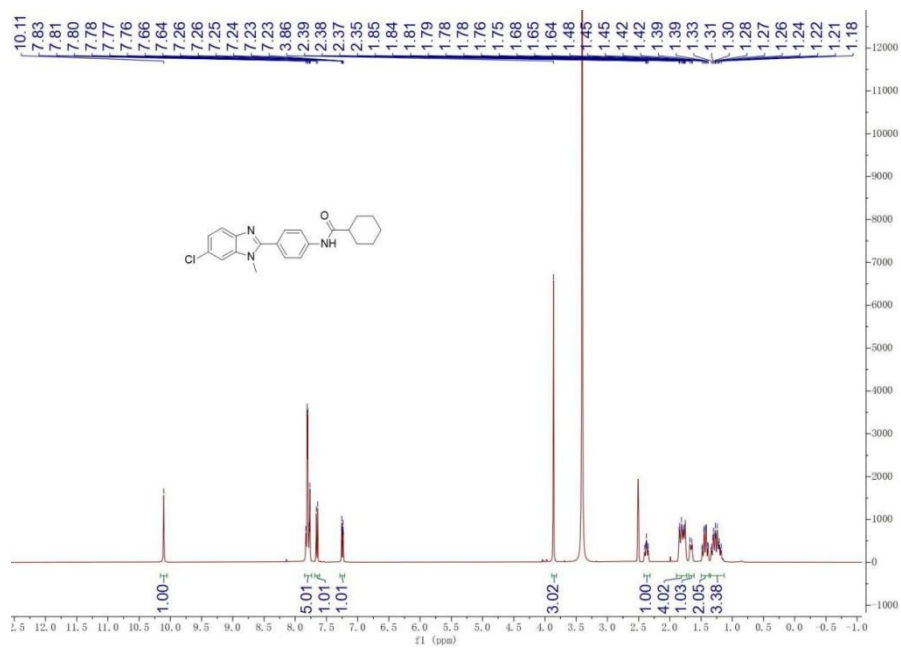


¹³C NMR of compound 39

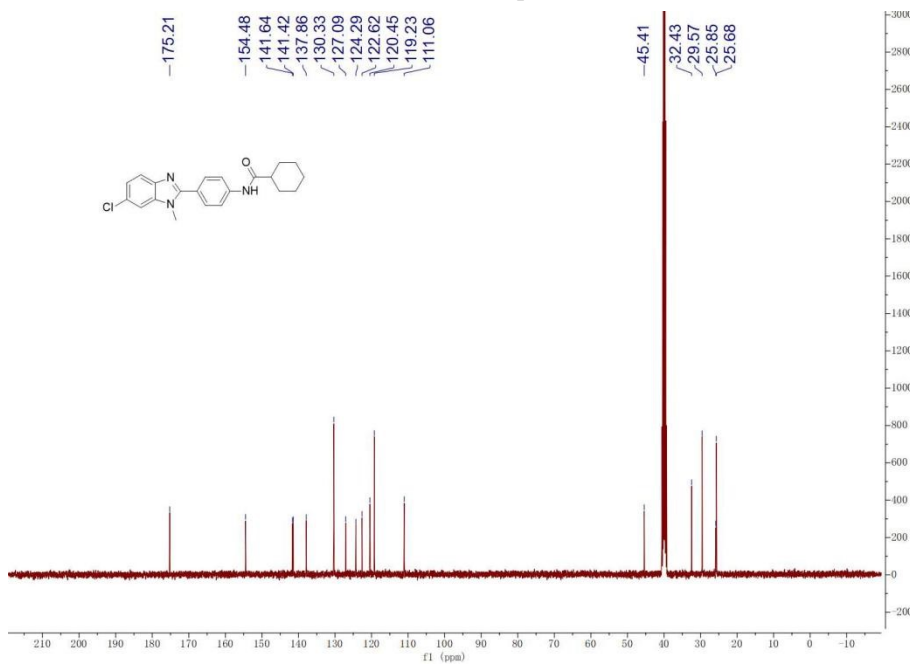


HR-MS of compound 39

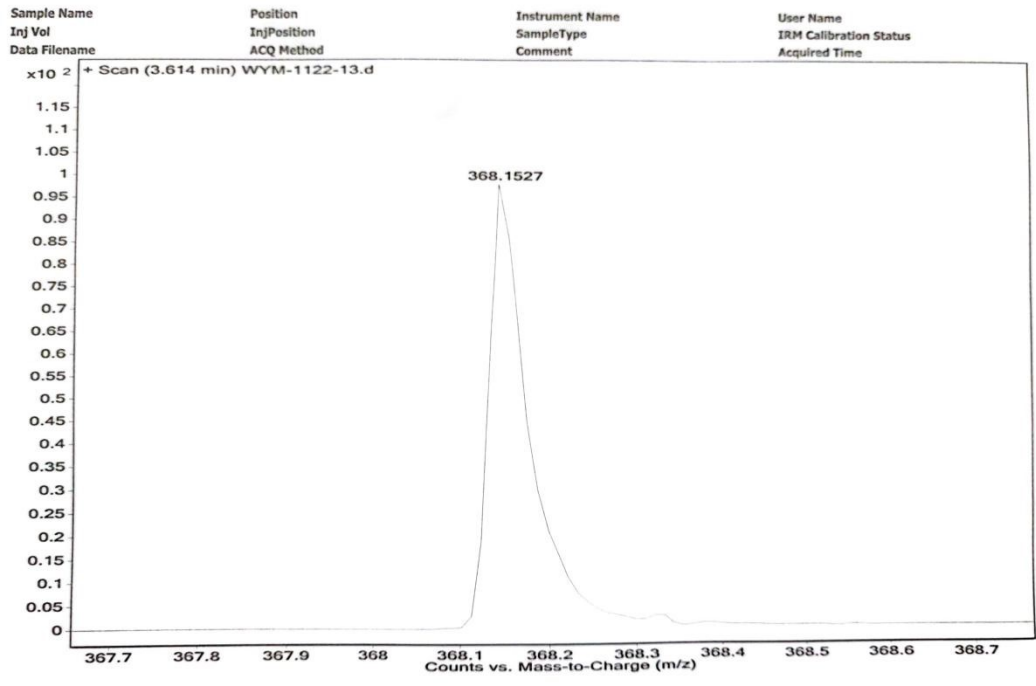
N-(4-(6-chloro-1-methyl-1H-benzo[d]imidazol-2-yl)phenyl)cyclohexanecarboxamide (40)



¹H NMR of compound 40

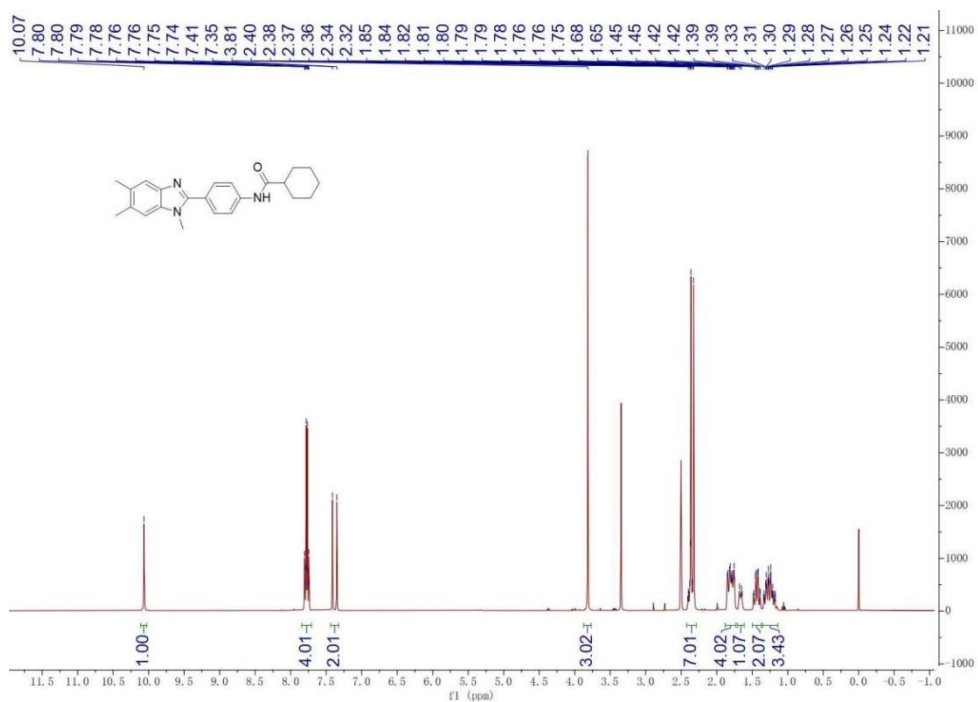


¹³C NMR of compound 40

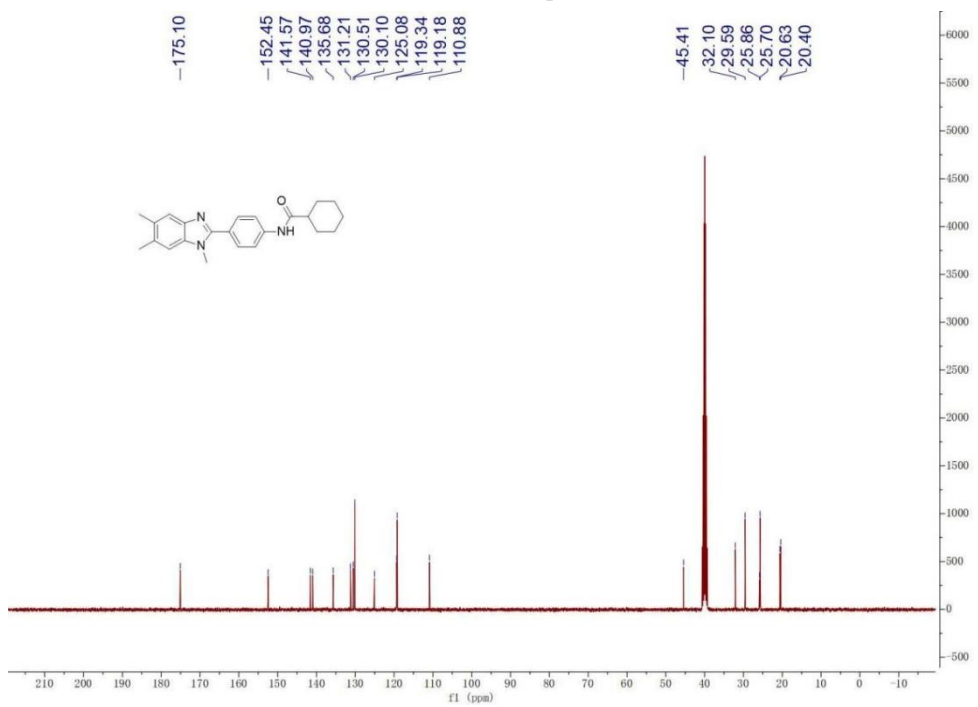


HR-MS of compound 40

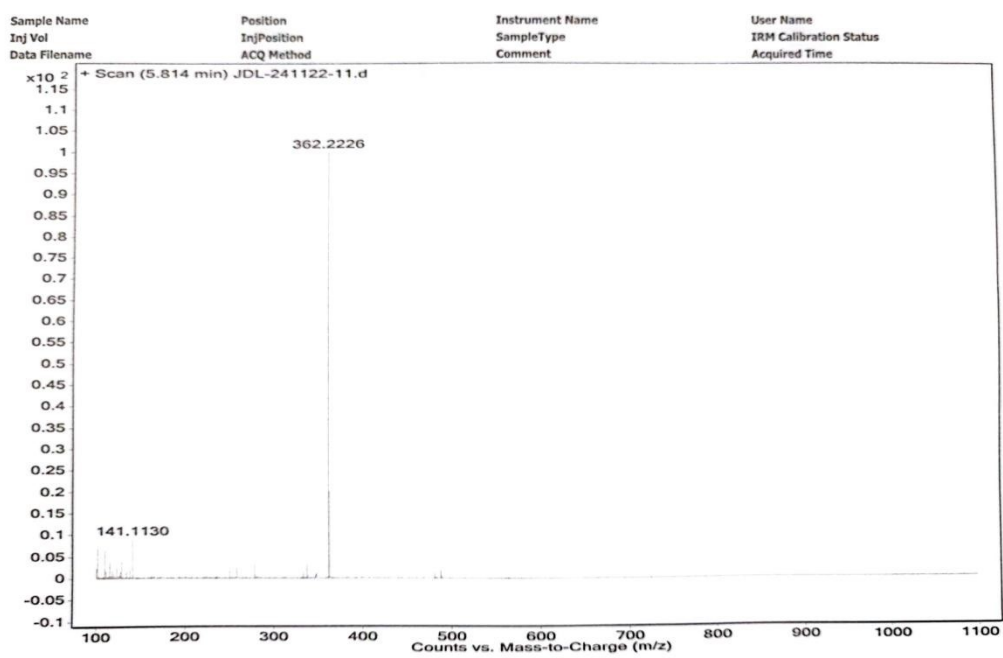
N-(4-(1,5,6-trimethyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)cyclohexanecarboxamide (**41**)



¹H NMR of compound **41**

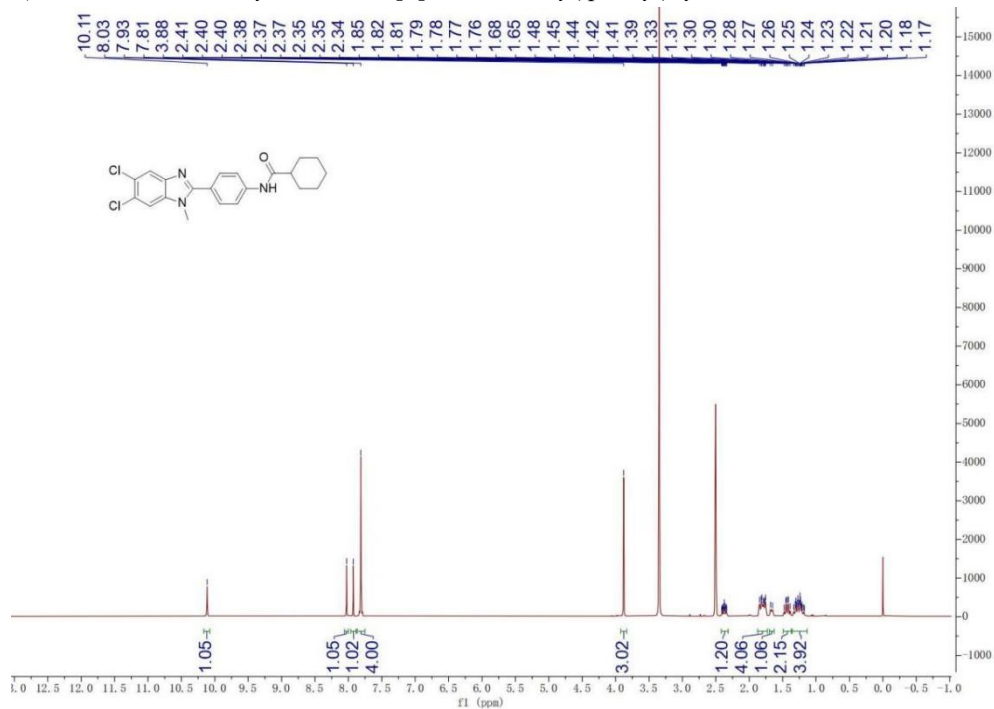


¹³C NMR of compound **41**

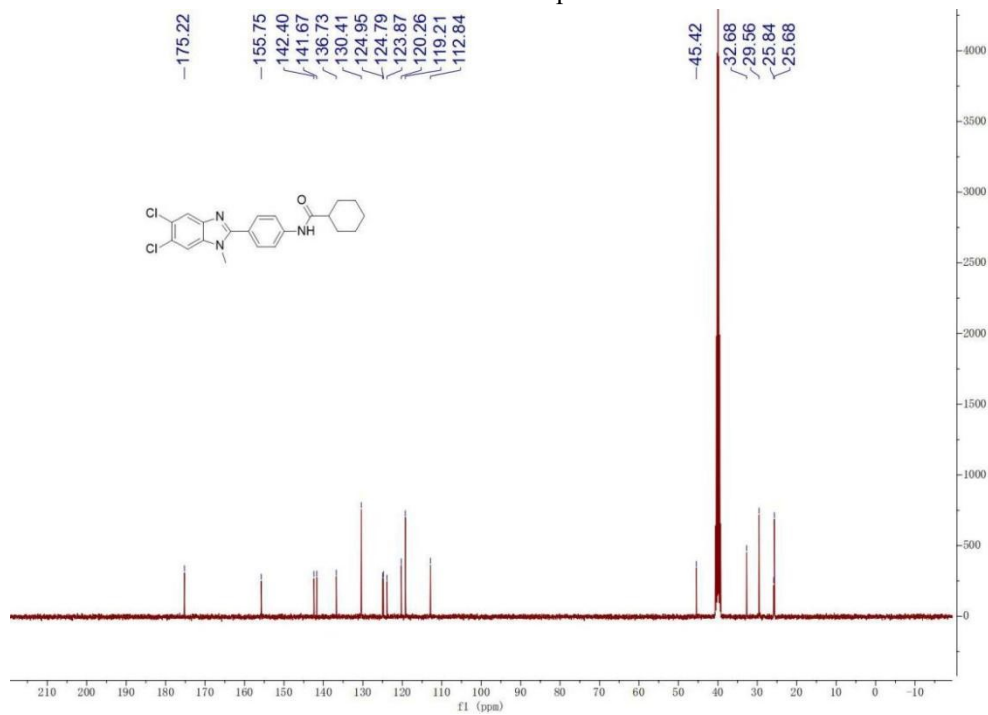


HR-MS of compound 41

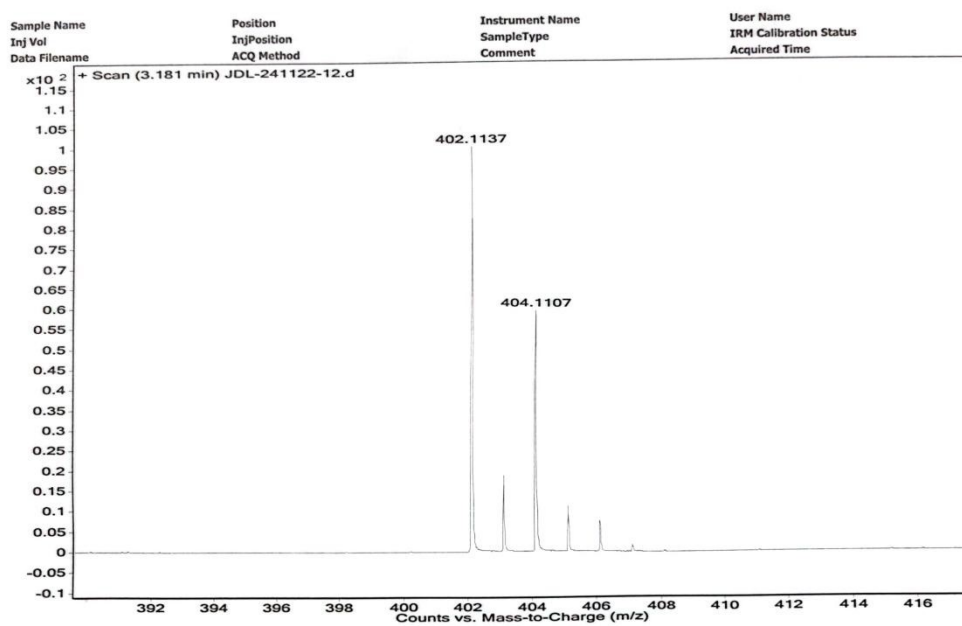
N-(4-(5,6-dichloro-1-methyl-1*H*-benzo[d]imidazol-2-yl)phenyl)cyclohexanecarboxamide (42)



¹H NMR of compound 42

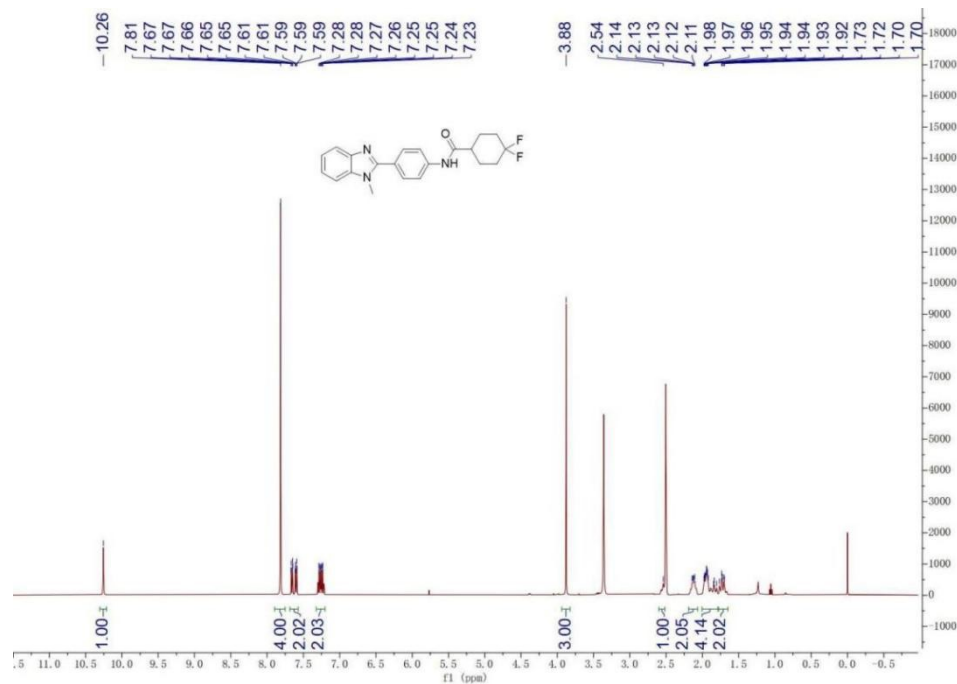


¹³C NMR of compound 42

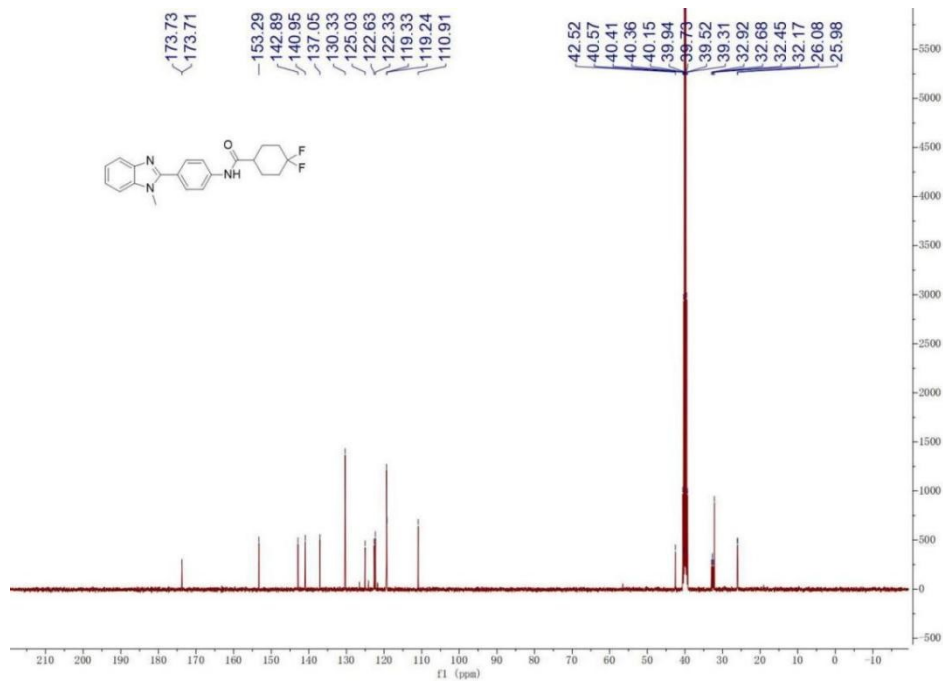


HR-MS of compound 42

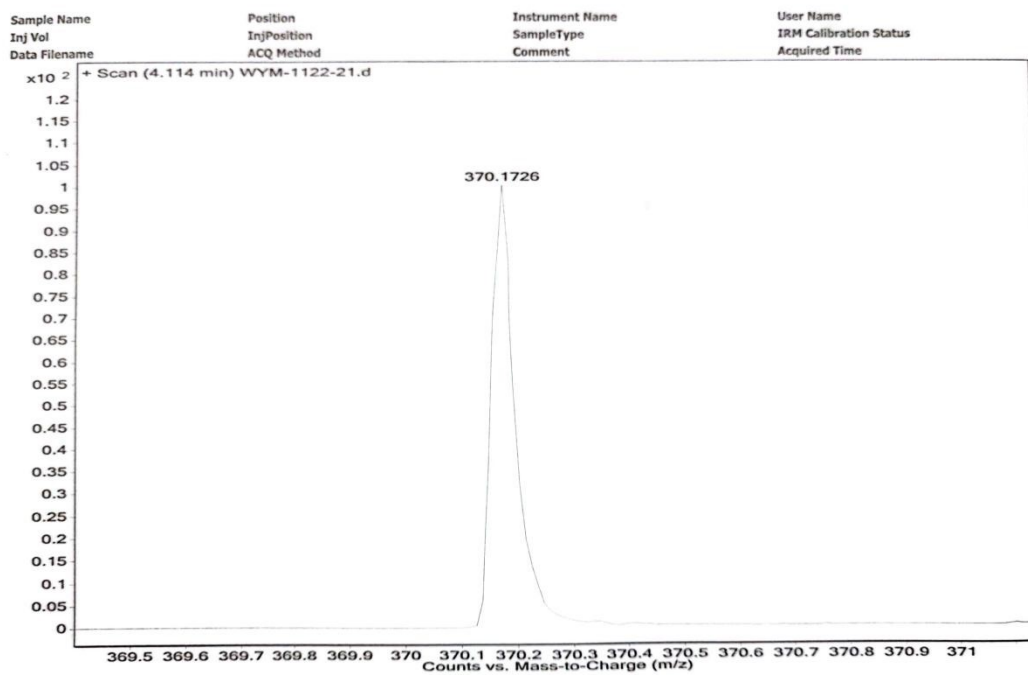
4,4-difluoro-N-(4-(1-methyl-1H-benzo[d]imidazol-2-yl)phenyl)cyclohexane-1-carboxamide (43)



¹H NMR of compound 43

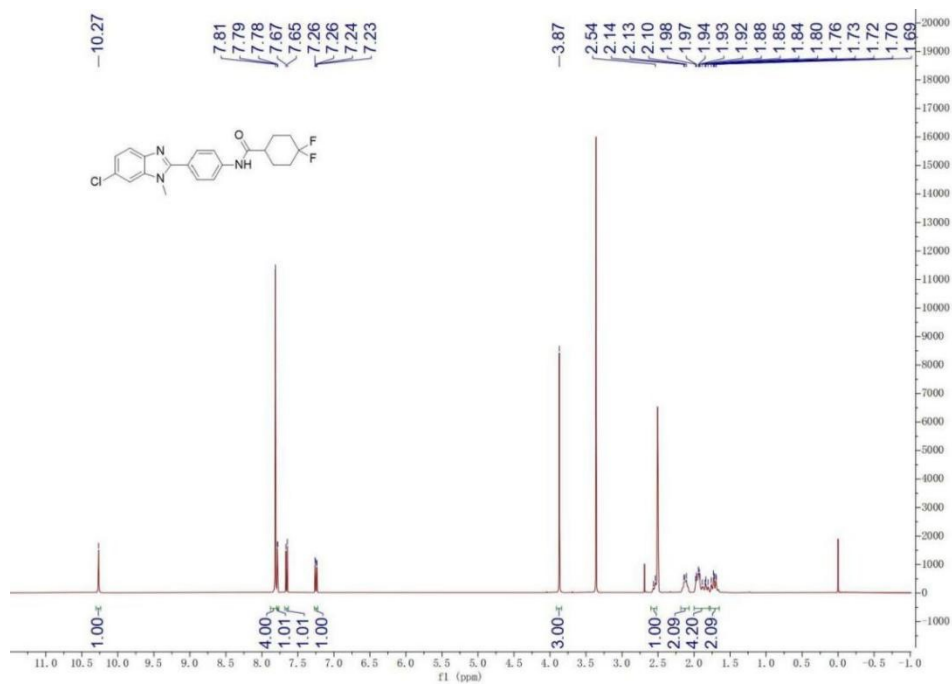


¹³C NMR of compound 43

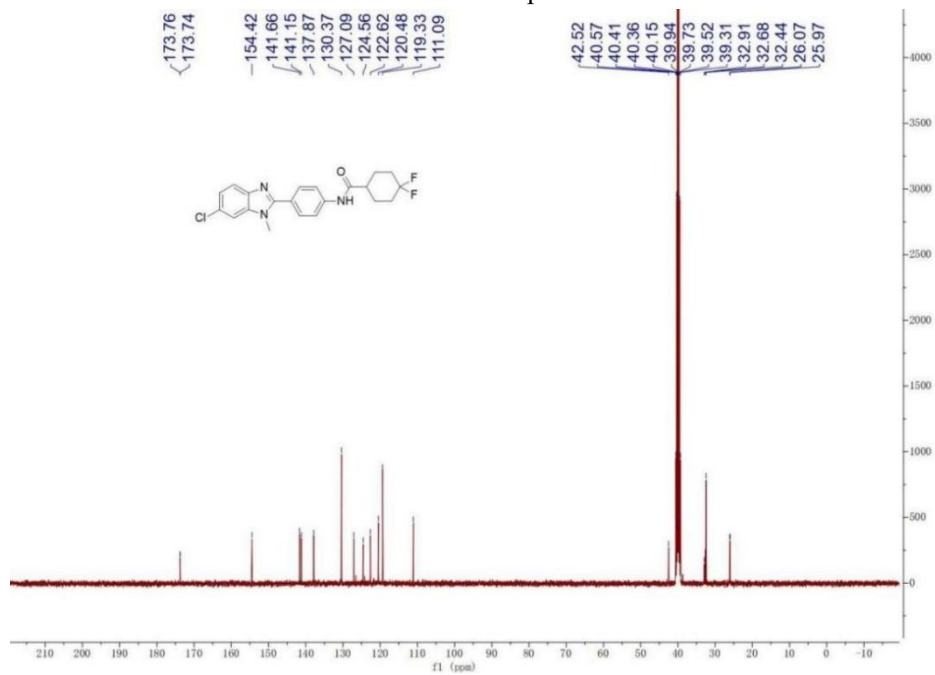


HR-MS of compound 43

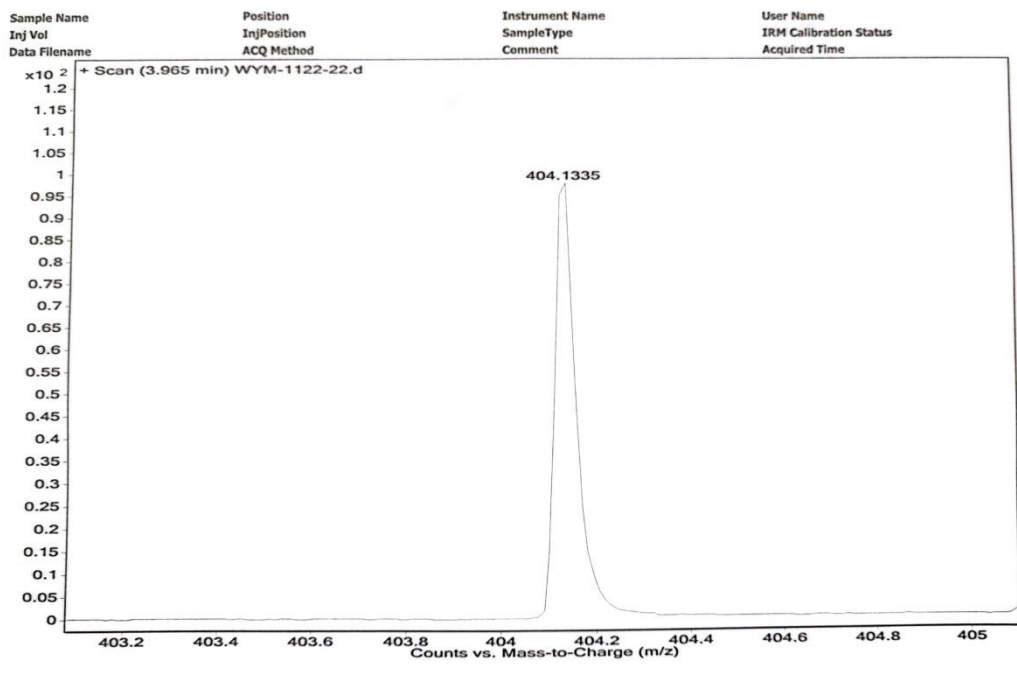
N-(4-(6-chloro-1-methyl-1*H*-benzo[d]imidazol-2-yl)phenyl)-4,4-difluorocyclohexane-1-carboxamide (**44**)



¹H NMR of compound **44**



¹³C NMR of compound **44**



HR-MS of compound 44