**Sulfated copper oxide catalyzed one-pot synthesis of**

***N*-fused benzimidazolo/benzothiazolo pyrimidines**

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**Synthetic Procedure for various *N*-fused benzimidazolo/benzthiazolo pyrimidines**

***Synthetic procedure for the preparation of 2,4-Diphenylbenzo[4,5]imidazo[1,2-a]pyrimidine (4a)***

A mixture of benzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded the 2,4-Diphenylbenzo[4,5]imidazo[1,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 2-(4-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4b)***

A mixture of 4-nitrobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded the 2-(4-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 4-(4-Phenylbenzo[4,5]imidazo[1,2-a]pyrimidin-2-yl)-benzonitrile (4c)***

A mixture of 4-cyanobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-(4-Phenylbenzo[4,5]imidazo[1,2-*a*]pyrimidin-2-yl)-benzonitrile.

***Synthetic procedure for the preparation of 2-(4-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4d)***

A mixture of 4-bromobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(4-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 2-(4-Chlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4e)***

A mixture of 4-chlorobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(4-Chlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 2-(2-nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]pyrimidine (4f)***

A mixture of 2-nitrobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(2-nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]pyrimidine.

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***Synthetic procedure for the preparation of 2-(2,6-Dichlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4g)***

A mixture of 2,6-dichlorobenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(2,6-Dichlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(p-tolyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4h)***

A mixture of 4-methylbenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(*p*-tolyl)benzo[4,5]imidazo[1,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(o-tolyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4i)***

A mixture of 2-methylbenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(*o*-tolyl)benzo[4,5]imidazo[1,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(3,4,5-trimethoxyphenyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4j)***

A mixture of 3,4,5-methoxybenzaldehyde (1 mmol), 2-aminobenzimidazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(3,4,5-trimethoxyphenyl)benzo[4,5]imidazo[1,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 2,4-Diphenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5a)***

A mixture of benzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2,4-Diphenyl-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 2-(4-Nitrophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5b)***

A mixture of 4-nitrobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(4-Nitrophenyl)-4-phenyl-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 4-(4-Phenyl)-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidin-2-yl)benzonitrile (5c)***

A mixture of 4-cyanobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-(4-Phenyl)-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidin-2-yl)benzonitrile.

***Synthetic procedure for the preparation of 2-(4-Bromophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5d)***

A mixture of 4-bromobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(4-Bromophenyl)-4-phenyl-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 2-(4-Chlorophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5e)***

A mixture of 4-chlorobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(4-Chlorophenyl)-4-phenyl-2*H*-benzo[4,5]thiazolo[3,2-a]-pyrimidine.

***Synthetic procedure for the preparation of 2-(2-nitrophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5f)***

A mixture of 2-nitrobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(2-nitrophenyl)-4-phenyl-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

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***Synthetic procedure for the preparation of 2-(2,6-dichlorophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5g)***

A mixture of 2,6-dichlorobenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 2-(2,6-dichlorophenyl)-4-phenyl-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(p-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine (5h)***

A mixture of 4-methylbenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(*p*-tolyl)-2*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(o-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine (5i)***

A mixture of 2-methylbenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(*o*-tolyl)-2*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidine.

***Synthetic procedure for the preparation of 4-phenyl-2-(3,4,5-trimethoxyphenyl)-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5j)***

A mixture of 3,4,5-trimethoxybenzaldehyde (1 mmol), 2-aminobenzothiazole (1 mmol) and acetonitrile (5 ml) were taken in a sealed tube and warmed for 5 minutes. Phenyl acetylene (1.1 mmol) and sulfated copper oxide (prepared according to literature 62) (10 mol %) were added to the reaction mixture and stirred for another 10 minutes under nitrogen atmosphere at room temperature and the reaction mixture was refluxed at 800 C. Upon completion (3 h) of the reaction, as indicated by TLC, the mixture was washed with ethyl acetate and the catalyst was separated by filtration. The solvent was evaporated under reduced pressure to get the crude product. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexane) and afforded 4-phenyl-2-(3,4,5-trimethoxyphenyl)-2*H*-benzo[4,5]thiazolo[3,2-*a*]-pyrimidine.

**SPECTRAL DETAILS**

***2,4-Diphenylbenzo[4,5]imidazo[1,2-a]pyrimidine (4a)*** *(Lit. 31)*

Yellow solid; 1H NMR (400 MHz, DMSO-*d6*): δ 8.27-7.78 (m, 5H, Ar-H), 7.57 (s, 1H, CH), 7.34-6.81 (m, 9H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.6, 160.0, 150.1, 142.2, 138.8, 135.2, 133.3, 129.8, 128.8, 127.9, 123.7, 117.1, 113.2, 103.6 ppm; Anal. Calcd for C22H15N3: C, 82.22; H, 4.70; N, 13.08. Found: C, 82.20; H, 4.67; N, 13.06.

***2-(4-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4b)*** *(Lit. 31)*

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 8.56-7.73 (m, 8H, Ar-H), 7.56 (s, 1H, CH), 7.34 -6.81 (m, 5H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.0, 160.7, 150.6, 147.4, 142.1, 141.5, 139.8, 135.8, 129.7, 128.6, 127.8, 125.4, 124.1, 123.6, 118.3, 113.2, 103.9 ppm; Anal. Calcd for C22H14N4O2: C, 72.12; H, 3.85; N, 15.29. Found: C, 72.09; H, 3.83; N, 15.27.

***4-(4-Phenylbenzo[4,5]imidazo[1,2-a]pyrimidin-2-yl)-benzonitrile (4c)*** *(Lit. 31)*

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 8.22-7.72 (m, 8H, Ar-H), 7.52 (s, 1H, CH), 7.33-6.81 (m, 5H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.5, 160.1, 150.1, 142.6, 139.2, 135.9, 132.1, 129.7, 128.0, 127.7, 126.6, 123.5, 119.4, 118.4, 113.7, 112.8, 103.0 ppm; Anal. Calcd for C23H14N4: C, 79.75; H, 4.07; N, 16.17. Found: C, 79.71; H, 4.03; N, 16.13.

***2-(4-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4d)*** *(Lit. 31)*

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 8.12-7.70 (m, 8H, Ar-H), 7.51 (s, 1H, CH), 7.37-6.89 (m, 5H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.4, 160.1, 151.4, 143.6, 139.6, 136.3, 135.8, 132.5, 129.0, 128.8, 127.3, 126.0, 123.6, 122.3, 119.5, 113.4, 104.0 ppm; Anal. Calcd for C22H14BrN3: C, 66.01; H, 3.53; N, 10.50. Found: C, 65.97; H, 3.51; N, 10.48.

***2-(4-Chlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4e)*** *(Lit. 31)*

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 8.12-7.72 (m, 8H, Ar-H), 7.54 (s, 1H), 7.35-6.94 (m, 5H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.1, 160.5, 151.1, 143.4, 139.4, 134.2, 133.5, 132.7, 130.4, 129.8, 128.1, 127.2, 126.9, 123.8, 120.8, 114.1, 104.2 ppm; Anal. Calcd for C22H14ClN3: C, 74.26; H, 3.97; N, 11.81. Found: C, 74.24; H, 3.95; N, 11.78.

***2-(2-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]pyrimidine (4f)*** *(Lit. 32)*

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.20-7.77 (m, 6H, Ar-H), 7.51 (s, 1H, CH), 7.39-6.95 (m, 7H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 163.3, 161.1, 150.6, 149.9, 143.3, 140.2, 135.1, 133.7, 132.2, 130.8, 129.7, 128.3, 127.6, 123.6, 119.6, 113.9, 105.8 ppm; Anal. Calcd for C22H14N4O2: C, 74.26; H, 3.97; N, 11.81. Found: C, 74.24; H, 3.95; N, 11.78.

***2-(2,6-Dichlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine (4g )*** *(Lit. 31)*

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 8.12-7.67 (m, 5H, Ar-H), 7.53 (s, 1H, CH), 7.49-6.93 (m, 7H, Ar-H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 163.1, 161.3, 149.2, 143.7, 140.2, 135.0, 133.4, 131.2, 130.2, 129.4, 128.4, 127.0, 126.7, 123.2, 119.1, 113.5, 105.3 ppm; Anal. Calcd for C22H13Cl2N3: C, 67.71; H, 3.36; N, 10.77. Found: C, 67.70; H, 3.33; N, 10.74.

***4-Phenyl-2-(p-tolyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4h)*** *(Lit. 32)*

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.27-7.78 (m, 4H, Ar-H), 7.57 (s, 1H, CH), 7.49-6.82 (m, 9H, Ar-H), 2.38 (s, 3H, CH3) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.9, 160.0, 150.7, 143.2 139.6, 135.4, 132.1, 131.4, 130.4, 129.9, 128.1, 127.8, 124.6, 123.1, 119.8, 112.1, 105.1, 21.7 ppm; Anal. Calcd for C23H17N3: C, 82.36; H, 5.11; N, 12.53. Found: 82.34; H, 5.09; N, 12.52.

***4-Phenyl-2-(o-tolyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4i)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.26-7.71 (m, 5H, Ar-H), 7.52 (s, 1H, CH), 7.48-6.94 (m, 8H, Ar-H), 2.35 (s, 3H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 163.3, 161.1, 150.0, 143.7, 140.7, 137.0, 135.0, 131.5, 130.4, 129.4, 128.8, 127.6, 126.2, 123.6, 122.2, 119.0, 117.6, 105.1, 19.2 ppm; Anal. Calcd for C23H17N3: C, 82.36; H, 5.11; N, 12.53. Found: 82.34; H, 5.10; N, 12.51; HRMS:*m/z* Calculated: 335.1422, Found: 336.1507 [M + H] +

***4-Phenyl-2-(3,4,5-trimethoxyphenyl)benzo[4,5]imidazo[1,2-a]pyrimidine (4j)*** *(Lit. 32)*

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.23-7.77 (m, 4H, Ar-H), 7.53 (s, 1H, CH), 7.37-6.51 (m, 7H, Ar-H), 3.89 (s, 9H, 3-OCH3) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 162.3, 160.5, 153.4, 150.0, 143.5, 140.2, 139.0, 135.5, 129.6, 128.1, 127.0, 126.1, 123.4, 119.0, 113.8, 105.0, 100.1, 61.2, 56.2 ppm; Anal. Calcd for C25H21N3O3: C, 72.98; H, 5.14; N, 10.21; O, 11.67. Found: C, 72.96; H, 5.11; N, 10.19; O, 11.66.

***2,4-Diphenyl-2H- benzo[4,5]thiazolo[3,2-a]-pyrimidine (5a)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 7.94-6.92 (m, 14H, Ar-H), 6.01 (d, 8.1 Hz, 1H), 5.54 (d, J = 7.6 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 145.8, 143.2, 141.8, 134.2, 129.9, 128.6, 127.5, 126.0, 125.9, 124.7, 123.8, 122.0, 121.8, 119.4, 101.8, 60.8 ppm; Anal. Calcd for C22H16N2S: C, 77.62; H, 4.74; N, 8.23: S, 9.42. Found: C, 77.60; H, 4.72; N, 8.21: S, 9.38; HRMS:*m/z* Calculated: 340.1034, Found: 341.1119 [M + H] +

***2-(4-Nitrophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5b)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.12-6.91 (m, 13H, Ar-H), 6.02 (d, 8.4 Hz, 1H), 5.53 (d, J = 8.1 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 161.0, 147.1, 146.8, 145.5, 143.9, 134.3, 130.2, 129.2, 128.2, 127.9, 126.6, 124.4, 123.2, 122.5, 121.9, 119.5, 100.2, 60.0 ppm; Anal. Calcd for C22H15N3O2S: C, 68.55; H, 3.92; N, 10.90; S, 8.32; Found: 68.53; H, 3.90; N, 10.87; S, 8.29; HRMS:*m/z* Calculated: 385.0885, Found: 386.0968 [M + H] +

***4-(4-Phenyl)-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidin-2-yl)benzonitrile (5c)***

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 7.93-6.92 (m, 13H, Ar-H), 6.03 (d, 8.1 Hz, 1H), 5.54 (d, J = 8.1 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 146.0, 145.9, 143.1, 134.2, 132.4, 129.5, 128.7, 127.4, 126.1, 125.8, 124.7, 122.1, 121.9, 119.7, 117.8, 110.4, 101.5, 60.7 ppm; Anal. Calcd for C23H15N3S: C, 75.59; H, 4.14; N, 11.50; S, 8.77; Found: C, 75.56; H, 4.11; N, 11.48; S, 8.75; HRMS:*m/z* Calculated: 365.0987, Found: 366.1069 [M + H] +

***2-(4-Bromophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5d)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 7.94-6.91 (m, 13H, Ar-H), 6.04 (d, 8.1 Hz, 1H), 5.53 (d, J = 8.1 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.8, 145.0, 143.1, 141.3, 134.3, 132.6, 131.5, 129.4, 128.8, 127.8, 126.1, 124.7, 122.2, 121.6, 120.0, 119.8, 101.4, 60.8 ppm; Anal. Calcd for C22H15BrN2S: C, 63.01; H, 3.61; N, 6.68; S, 7.65; Found: C, 62.98; H, 3.59; N, 6.66; S, 7.63; HRMS:*m/z* Calculated: 418.0139, Found: 419.0221 [M + H] +

***2-(4-Chlorophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5e)*** *(Lit. 31)*

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 7.95-6.93 (m, 13H, Ar-H), 6.03 (d, 8.1 Hz, 1H), 5.54 (d, J = 8.1 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 145.6, 143.0, 141.2, 135.9, 132.3, 131.6, 130.1, 129.3, 128.4, 127.9, 126.0, 124.2, 122.1, 121.9, 119.6, 101.3, 60.1 ppm; Anal. Calcd for C22H15ClN2S: C, 70.48; H, 4.03 N, 7.47. Found: C, 70.45; H, 4.01 N, 7.45.

***2-(2-Nitrophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5f)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.13-6.91 (m, 13H, Ar-H), 6.03 (d, 8.1 Hz, 1H), 5.53 (d, J = 8.4 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.2, 145.5, 143.1, 140.6, 136.4, 135.3, 134.2, 129.1, 128.8, 127.2, 126.7, 125.4, 124.8, 123.6, 122.7, 121.2, 119.2, 101.6, 50.9 ppm; Anal. Calcd for C22H15N3O2S: C, 68.55; H, 3.92; N, 10.90; S, 8.32; Found: C, 68.53; H, 3.90; N, 10.87; S, 8.30; HRMS:*m/z* Calculated: 385.0885, Found: 386.0969 [M + H] +

***2-(2,6-Dichlorophenyl)-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5g)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.14-7.12 (m, 13H, Ar-H), 6.03 (d, 8.1 Hz, 1H), 5.54 (d, J = 8.1 Hz, 1H) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 145.8, 143.2, 140.2, 136.2, 135.7, 134.1, 129.4, 128.1, 127.4, 126.8, 125.7, 124.4, 123.0, 122.1, 121.9, 120.5, 101.5, 50.0 ppm; Anal. Calcd for C22H14Cl2N2S: C, 64.55; H, 3.45; N, 6.84; S, 7.83 Found: C, 64.53; H, 3.42; N, 6.83; S, 7.81; HRMS:*m/z* Calculated: 408.0255, Found: 409.0338 [M + H] +

***4-Phenyl-2-(p-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine (5h)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.13-7.10 (m, 13H, Ar-H), 6.04 (d, 8.1 Hz, 1H), 5.56 (d, J = 8.1 Hz, 1H), 2.37 (s, 3H, CH3) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 145.7, 143.0, 138.7, 136.7, 133.1, 129.3, 128.3, 127.3, 126.7, 125.4, 124.1, 122.4, 121.9, 119.7, 100.6, 61.8, 21.2 ppm; Anal. Calcd for C23H18N2S: C, 77.93; H, 5.12; N, 7.90; S, 9.05. Found: C, 77.89; H, 5.10; N, 7.89; S, 9.04; HRMS:*m/z* Calculated: 354.1191, Found: 355.1276 [M + H] +

***4-Phenyl-2-(o-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine (5i)***

Yellow solid; 1H NMR(400 MHz, DMSO*-d6*): δ 6.91-8.12 (m, 13H, Ar-H), 6.04 (d, 8.1 Hz, 1H), 5.52 (d, J = 8.1 Hz, 1H), 2.35 (s, 3H, CH3) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.7, 145.6, 143.4, 138.5, 136.9, 134.1, 131.4, 130.0, 129.8, 128.6, 127.3, 126.3, 125.5, 124.9, 122.8, 121.4, 119.1, 101.8, 60.0, 20.0 ppm; Anal. Calcd for C23H18N2S: C, 77.93; H, 5.12; N, 7.90; S, 9.05. Found: C, 77.89; H, 5.10; N, 7.89; S, 9.04; HRMS:*m/z* Calculated: 354.1191, Found: 355.1276 [M + H] +

***4-Phenyl-2-(3,4,5-trimethoxyphenyl)-2H-benzo[4,5]thiazolo[3,2-a]-pyrimidine (5j)***

Yellow solid; 1H NMR (400 MHz, DMSO*-d6*): δ 8.12-7.12 (m, 9H, Ar-H) 6.52 (s, 2H), 6.03 (d, 8.1 Hz, 1H), 5.54 (d, J = 8.1 Hz, 1H), 3.81 (s, 9H, 3-OCH3) ppm; 13C NMR (100 MHz, DMSO*-d6*): δ 160.8, 151.5, 145.2, 143.8, 136.5, 133.8, 129.5, 128.8, 127.5, 126.4, 124.1, 122.3, 121.8, 119.4, 105.5, 100.9, 61.7, 60.8, 55.7 ppm; Anal. Calcd for C25H22N2O3S: C, 69.75; H, 5.15; N, 6.51; S, 7.45; Found: C, 69.73; H, 5.12; N, 6.49; S, 7.43; HRMS:*m/z* Calculated: 430.1351, Found: 431.1436 [M + H] +

**Supporting Information:**

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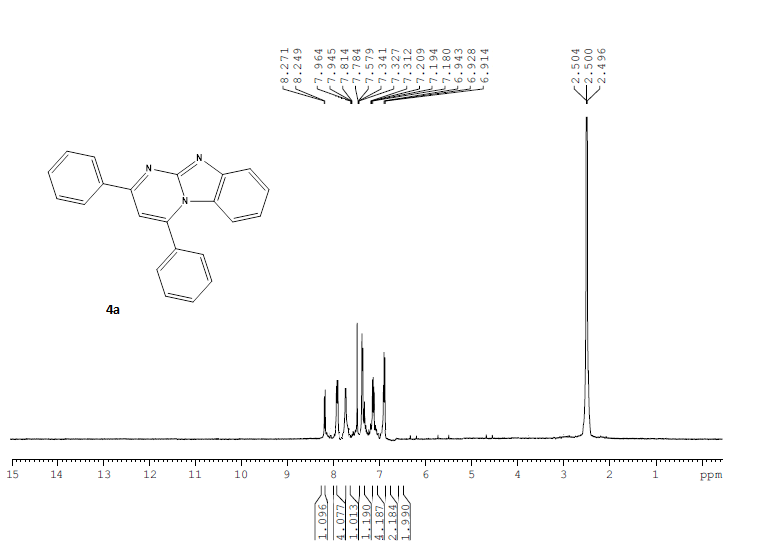
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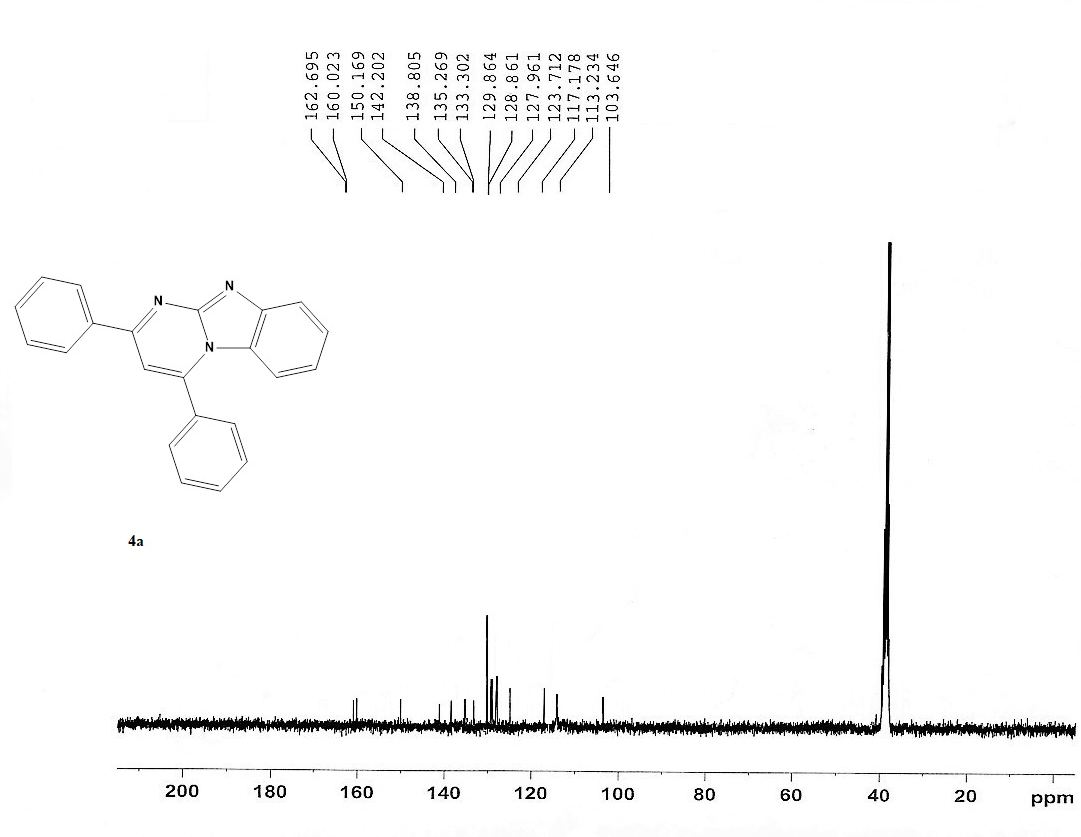
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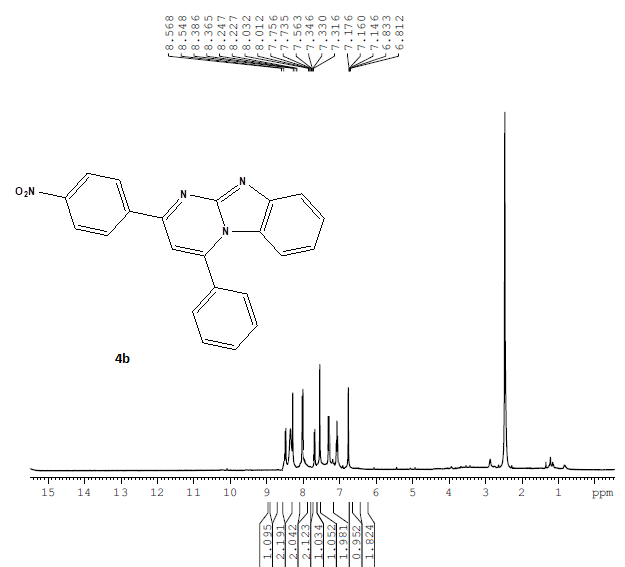
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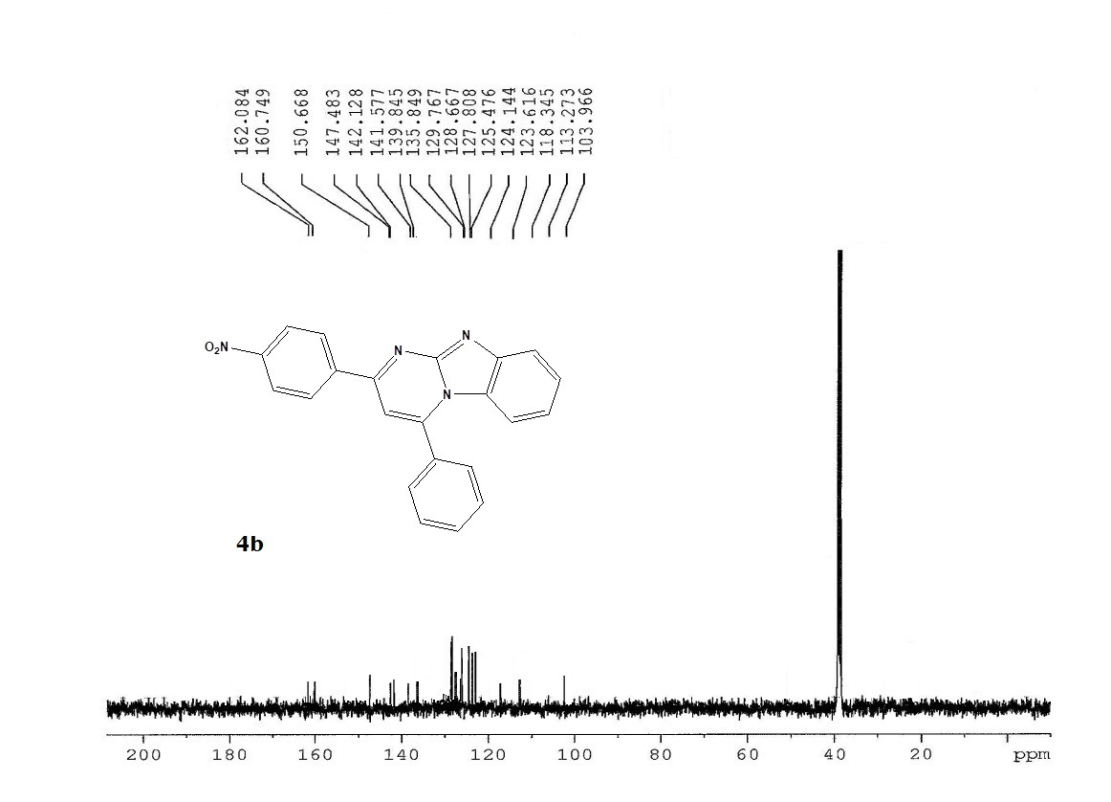
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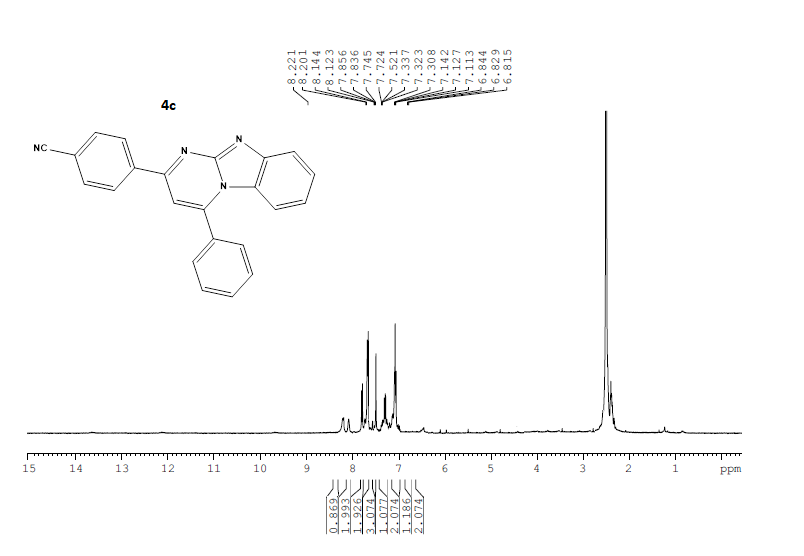
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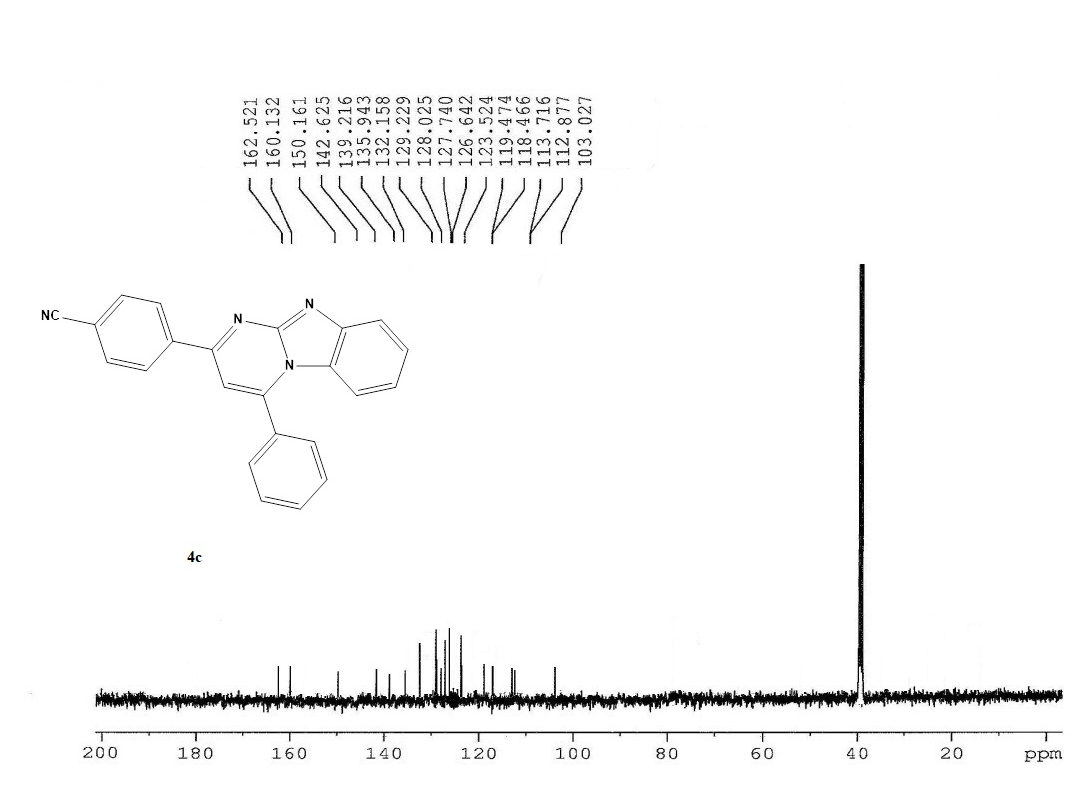
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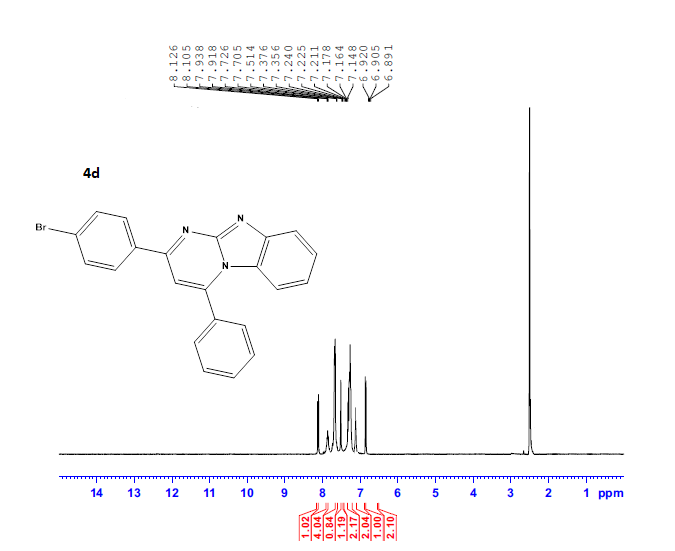
**13C NMR spectra of 4b**

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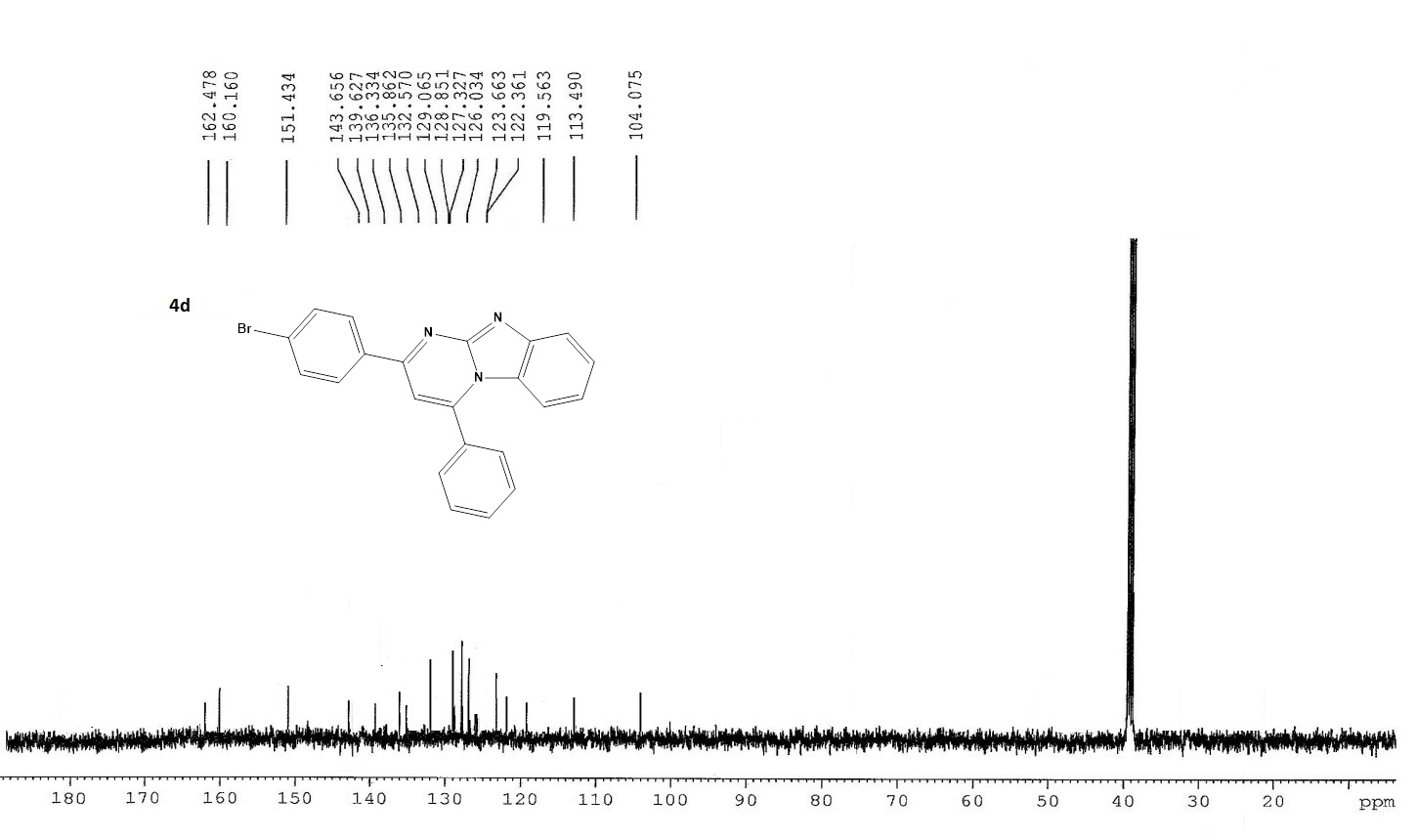
**1H NMR spectra of 4c**

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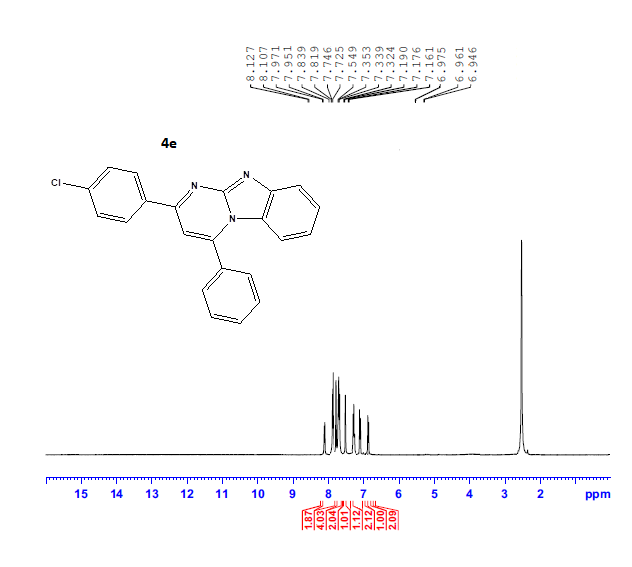
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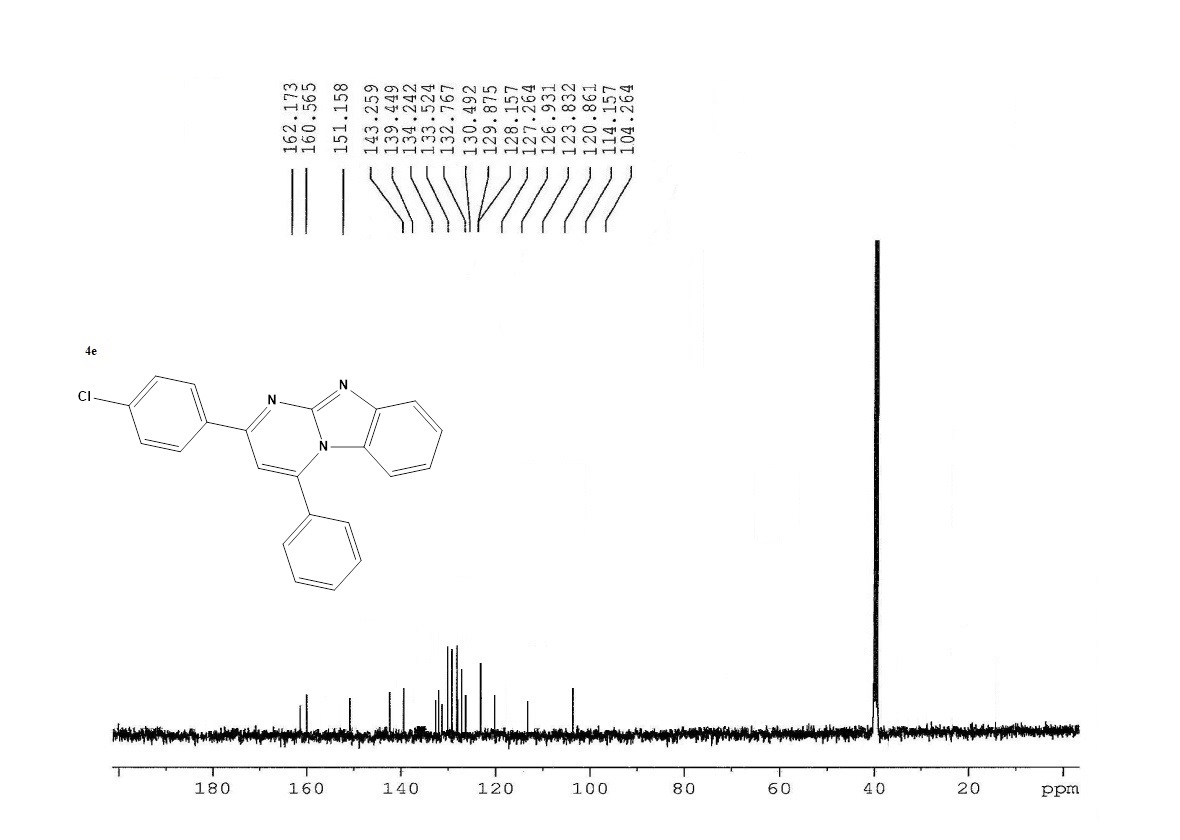
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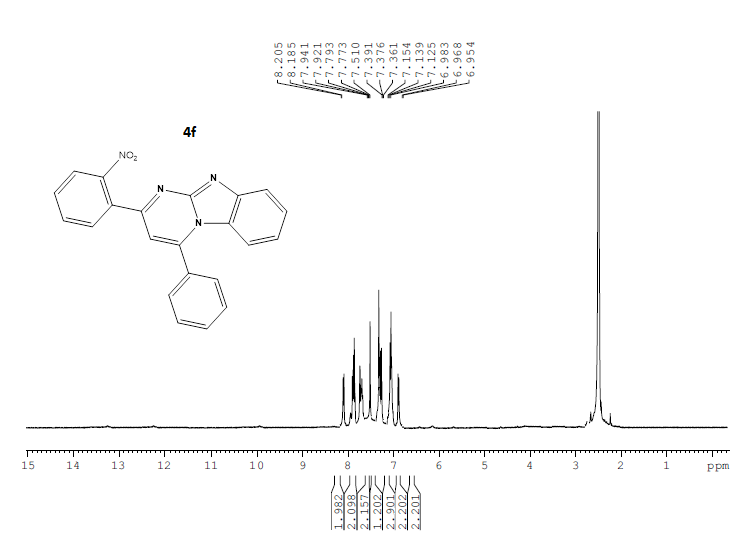
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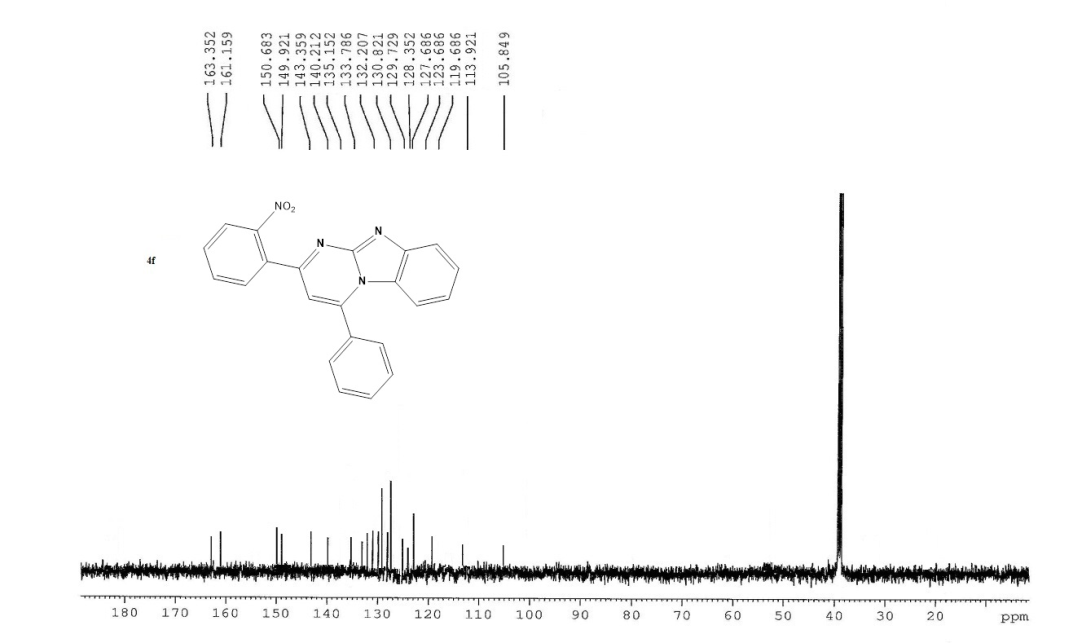
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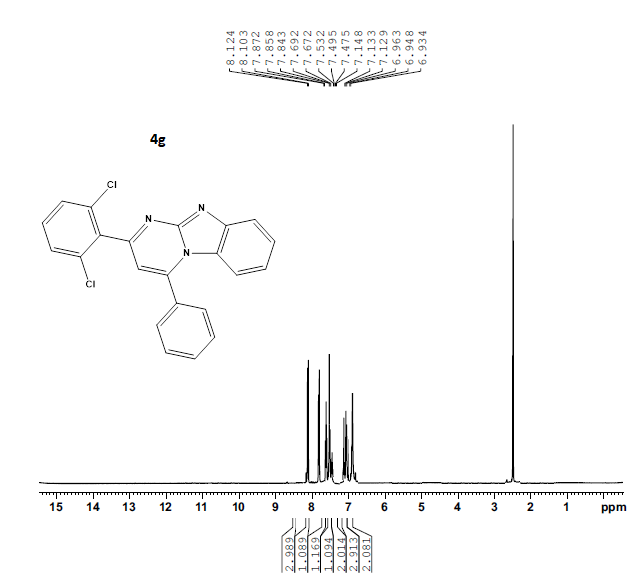
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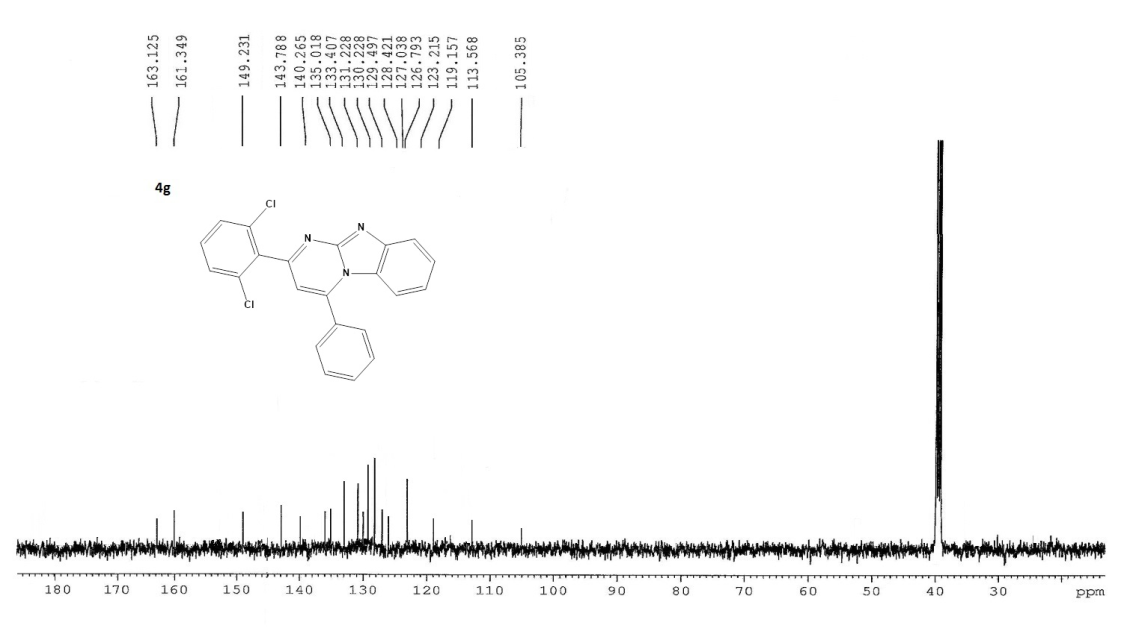
**1H NMR spectra of 4f**

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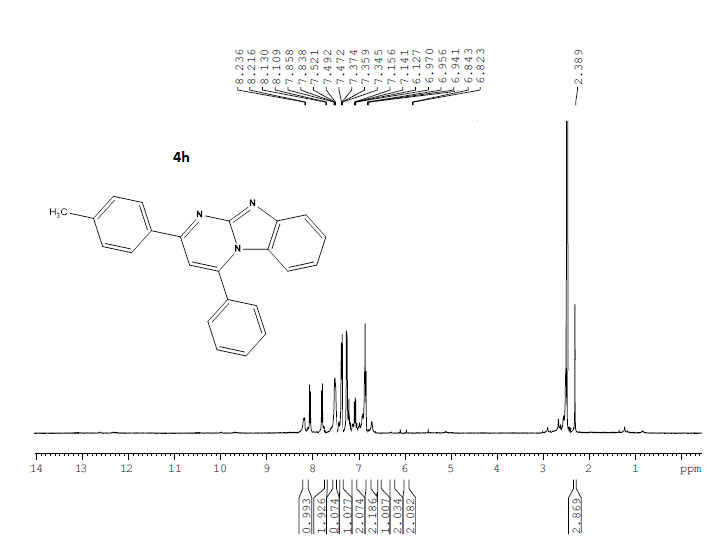
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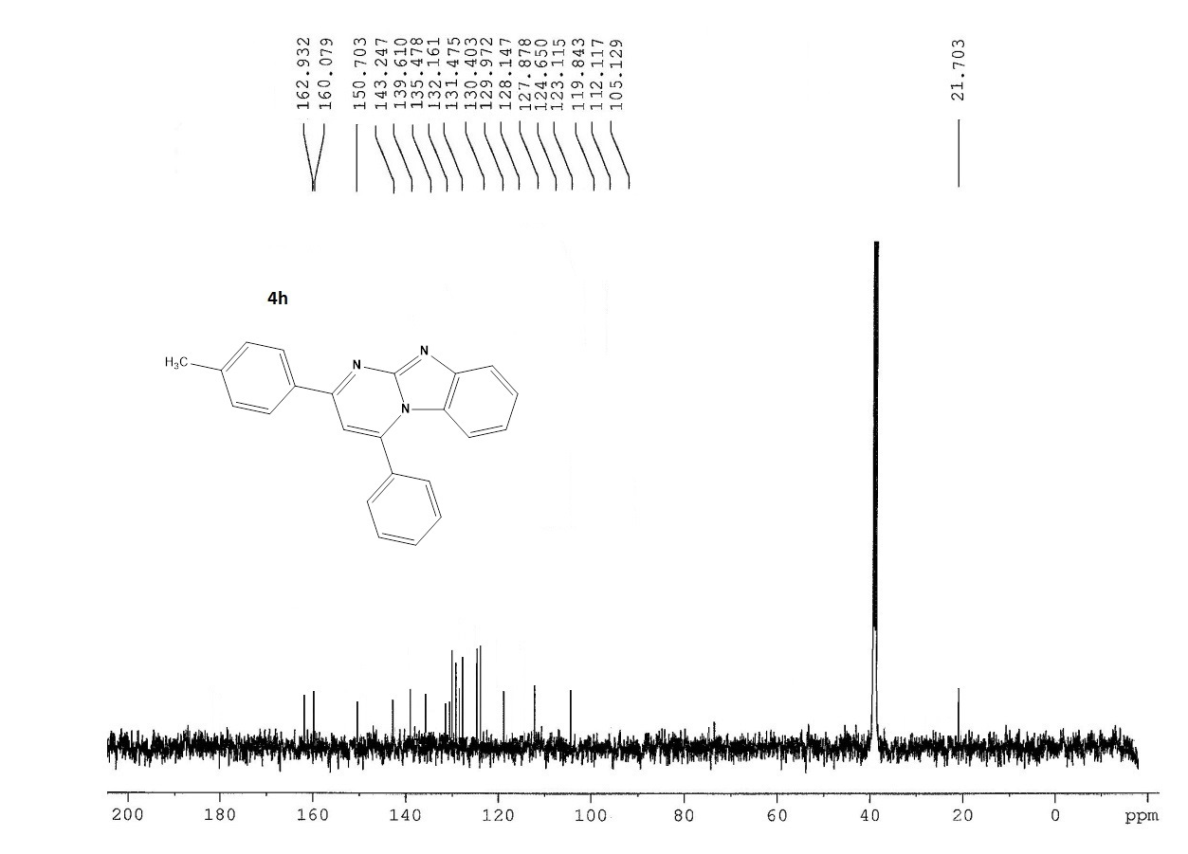
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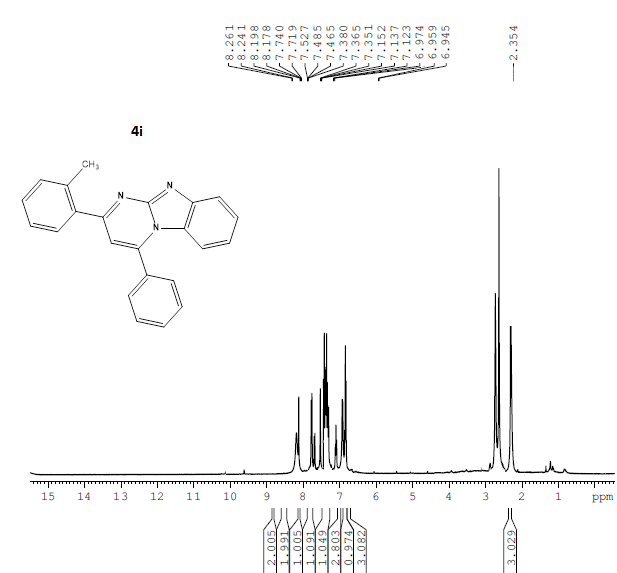
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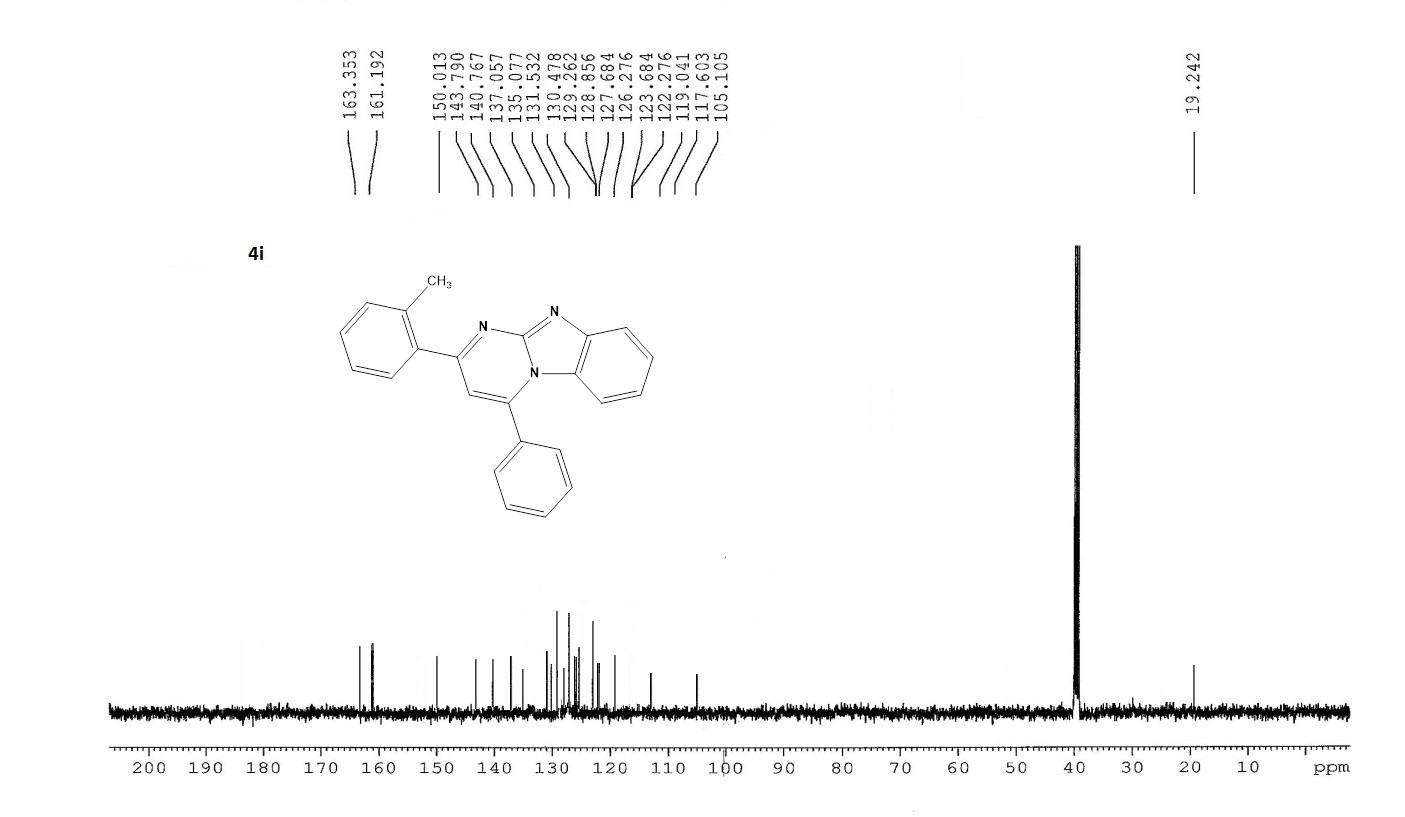
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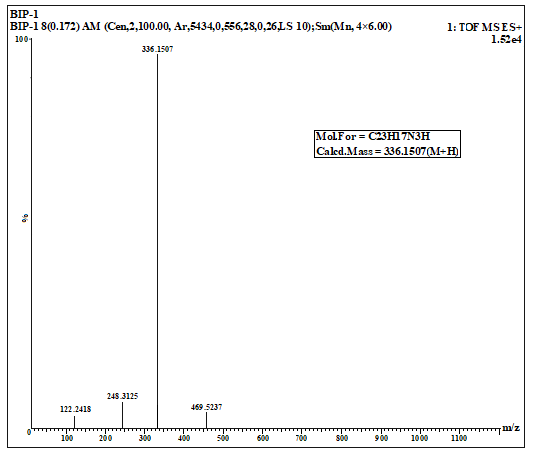
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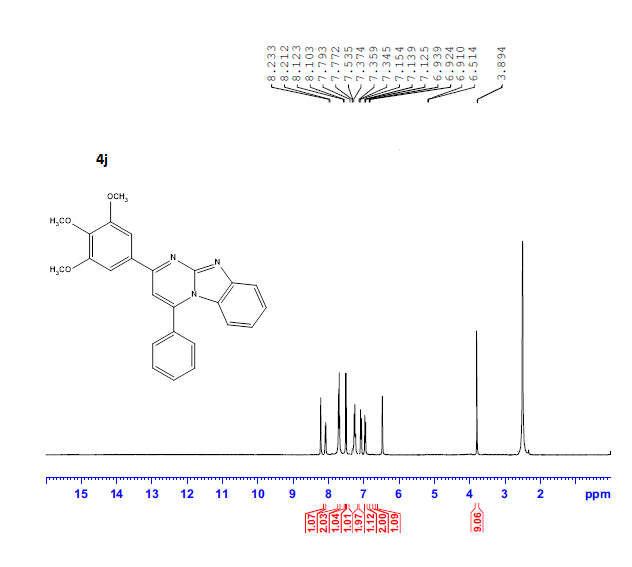
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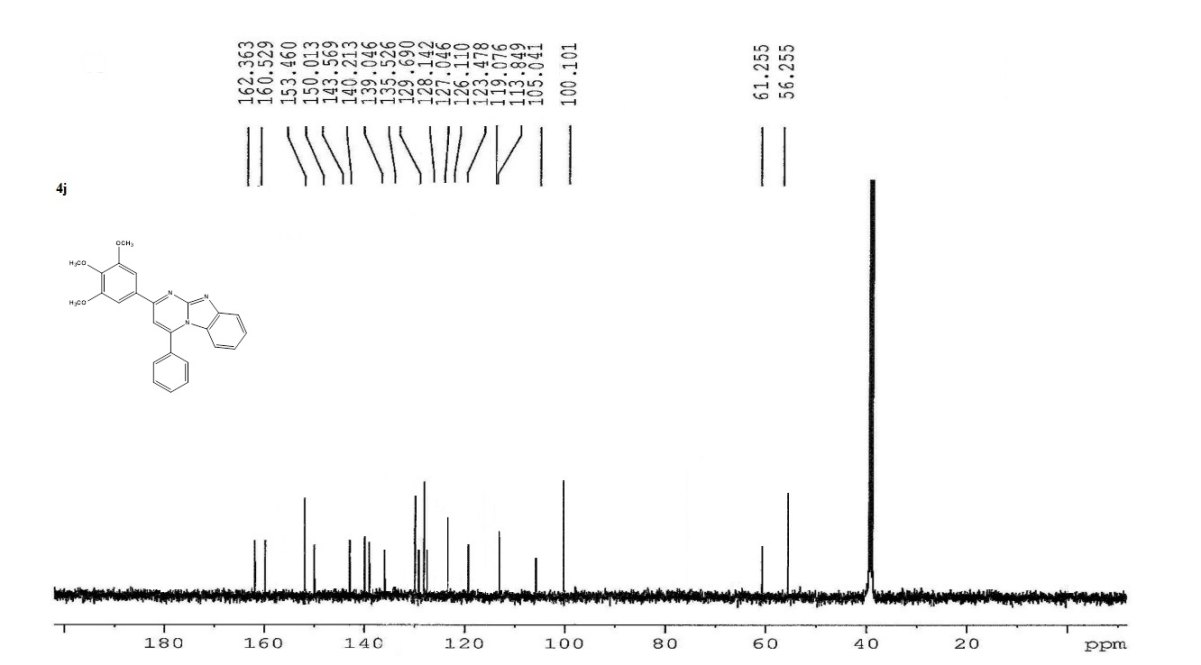
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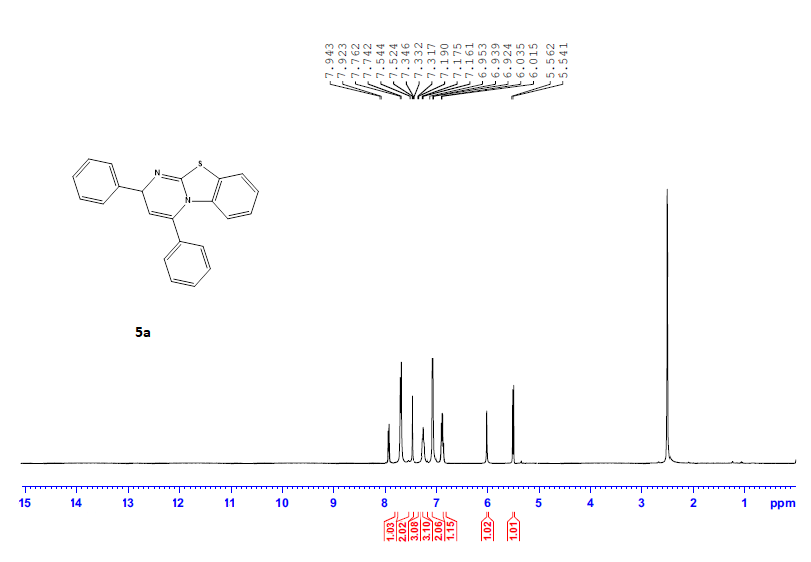
**HRMS spectra of 4i**

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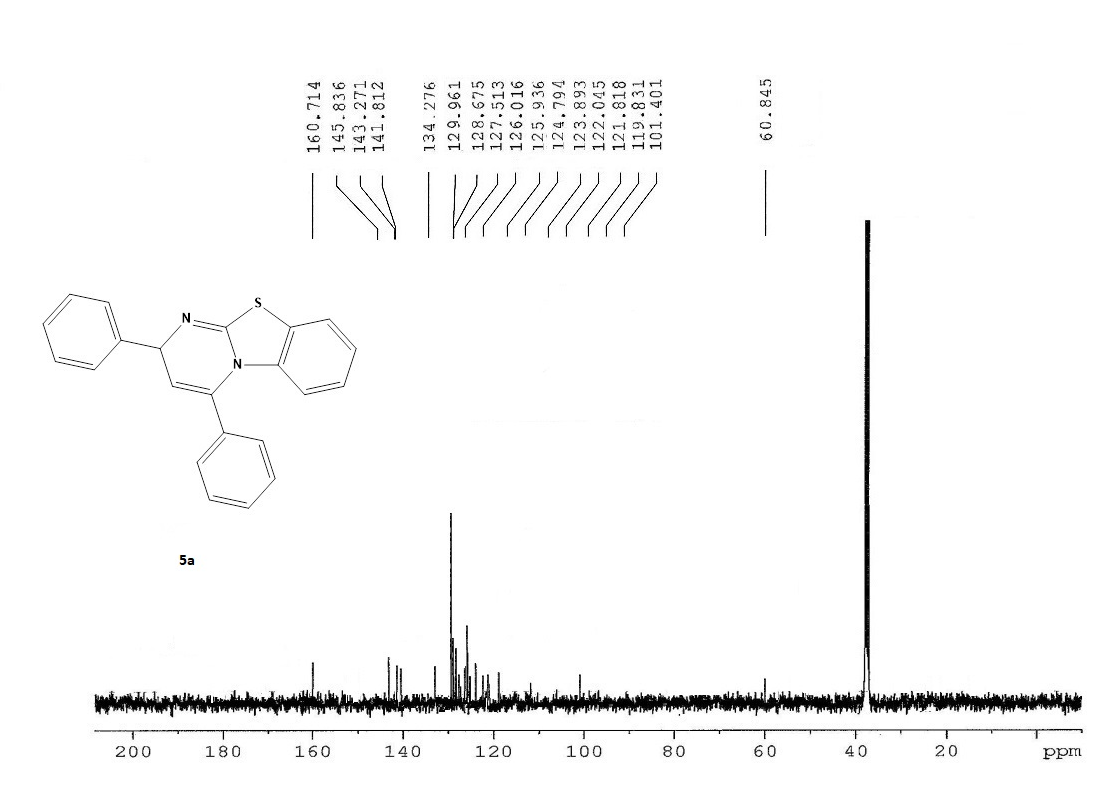
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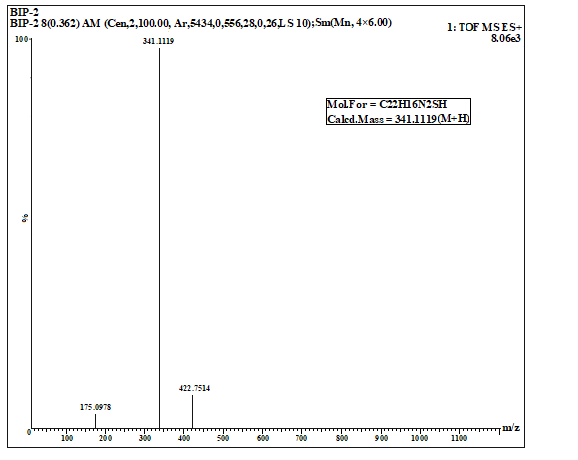
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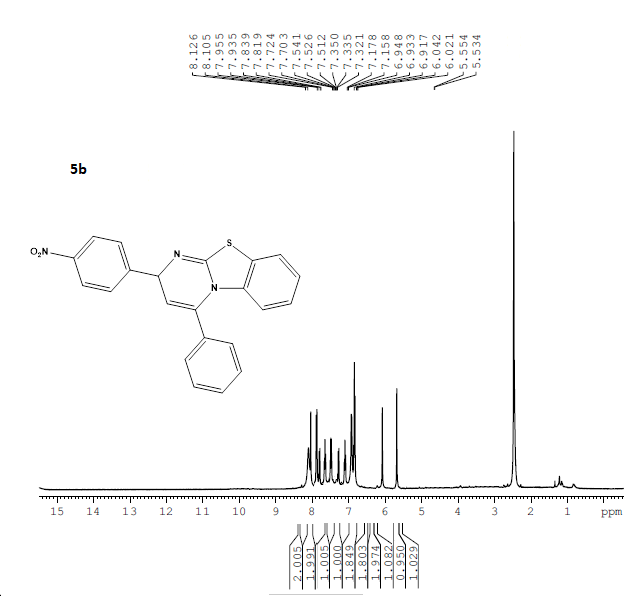
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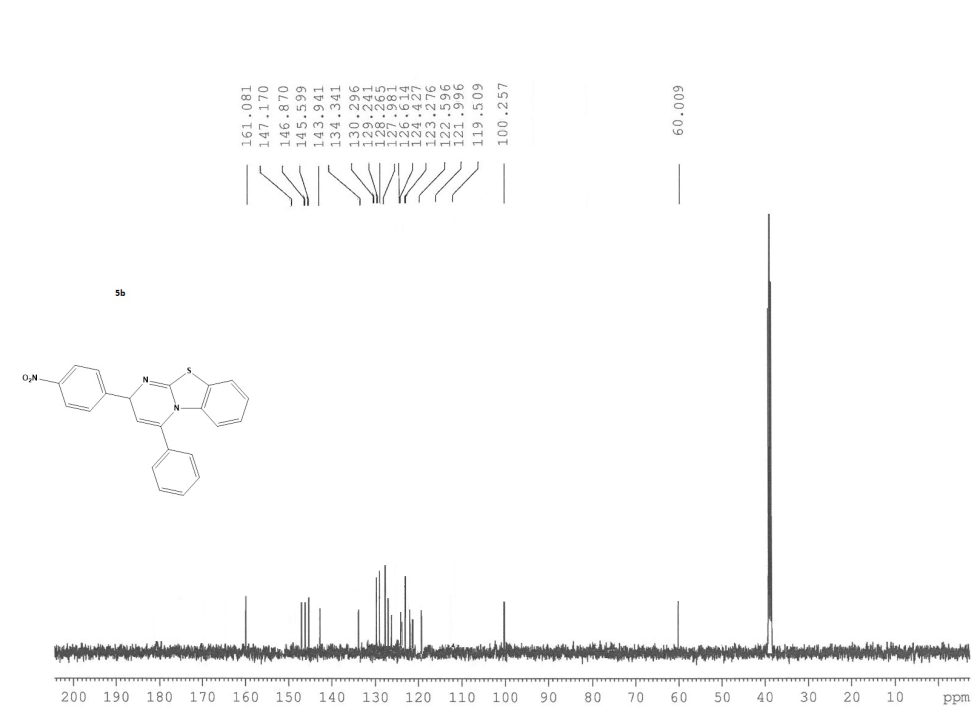
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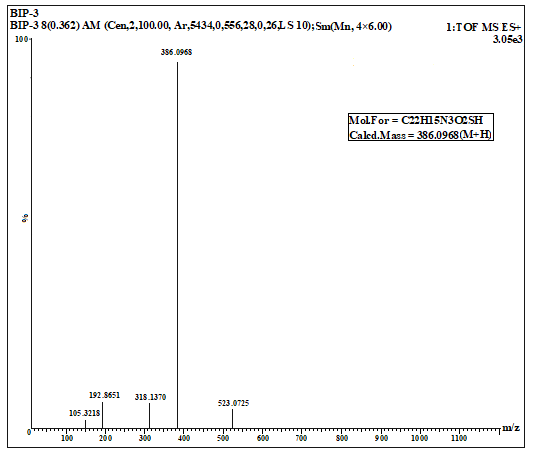
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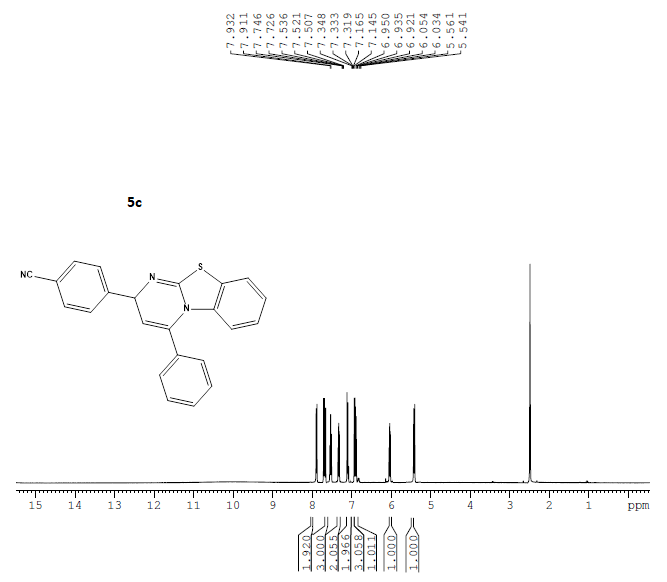
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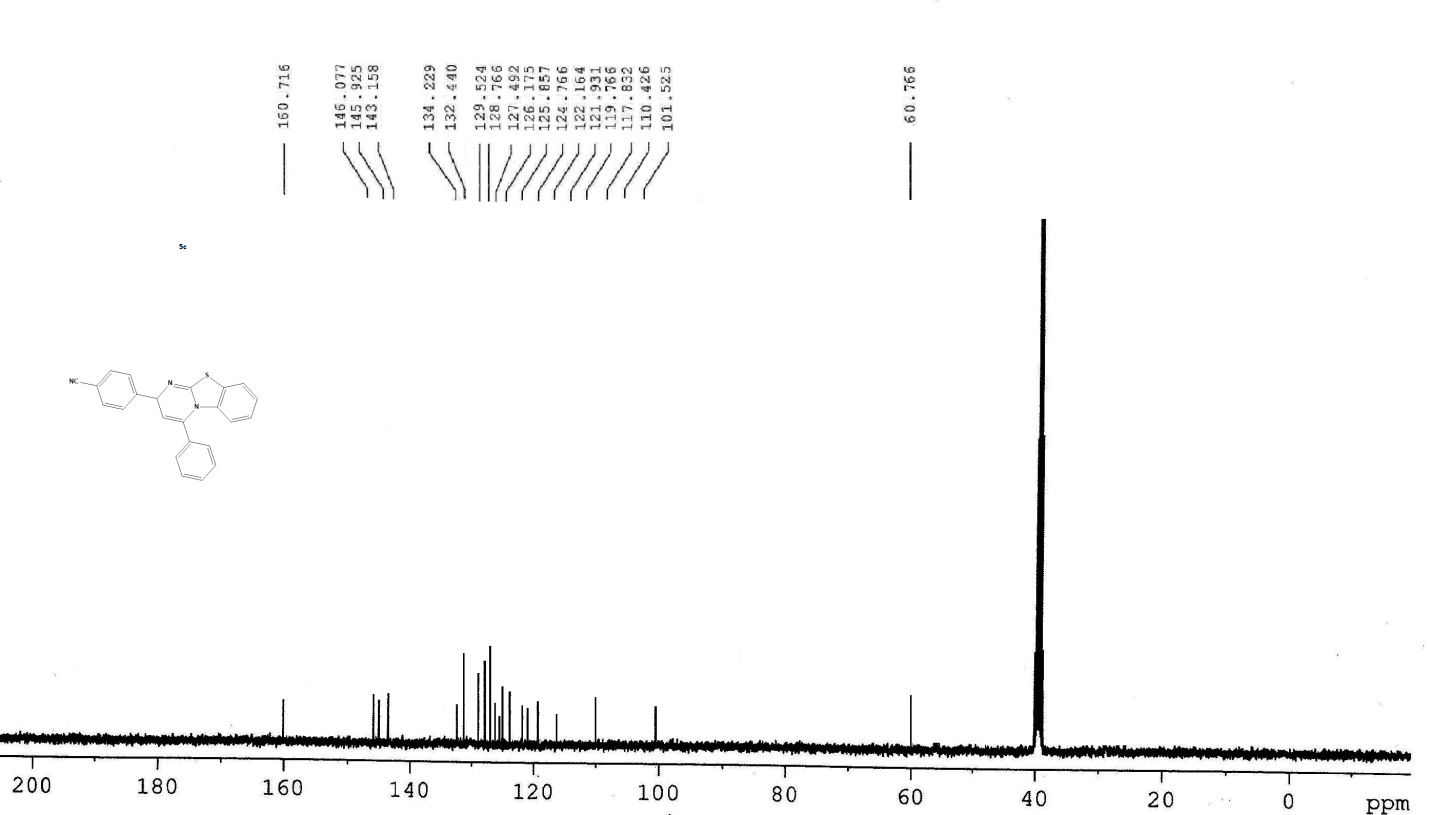
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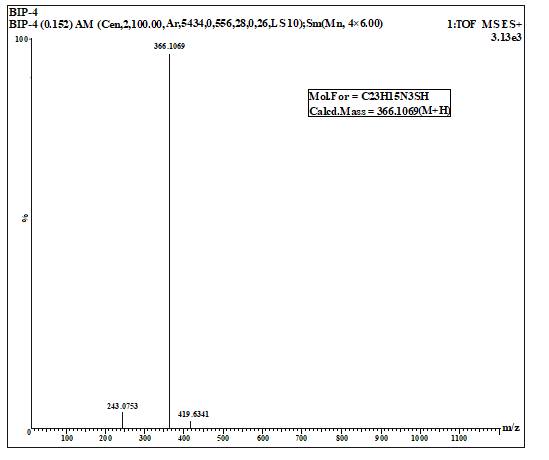
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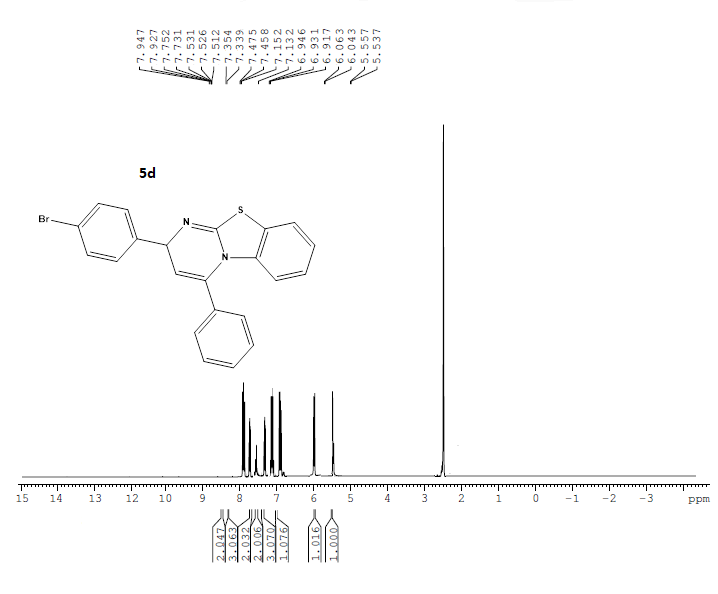
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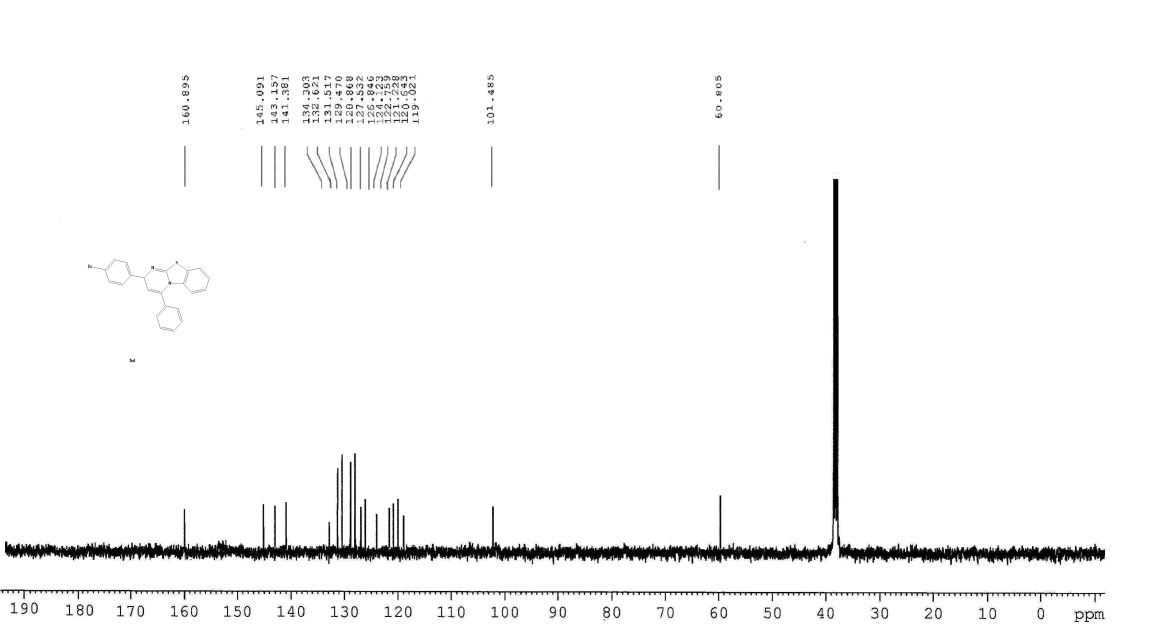
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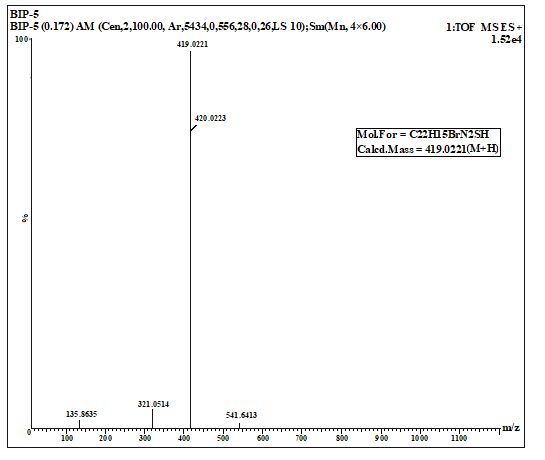
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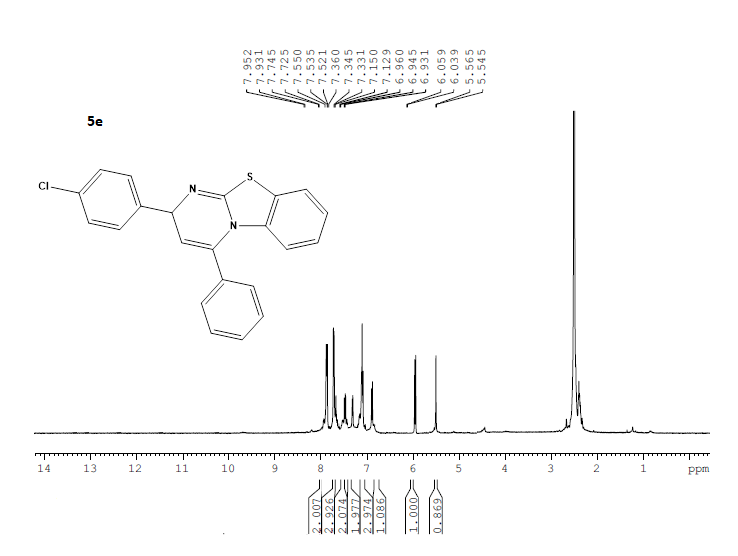
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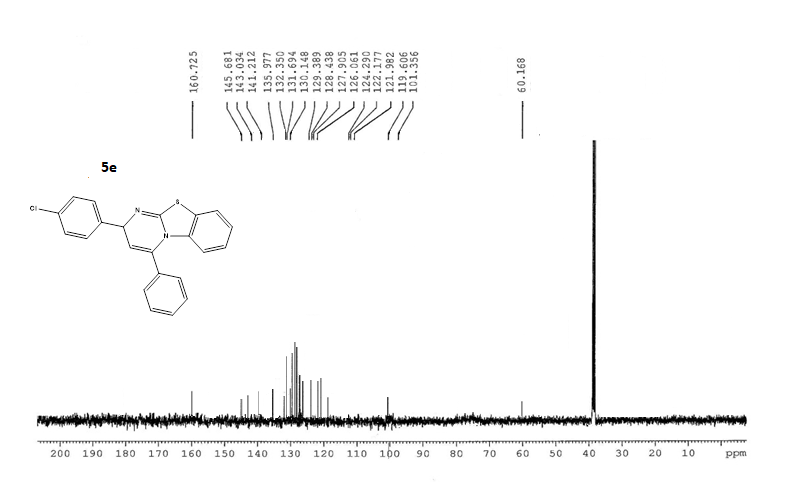
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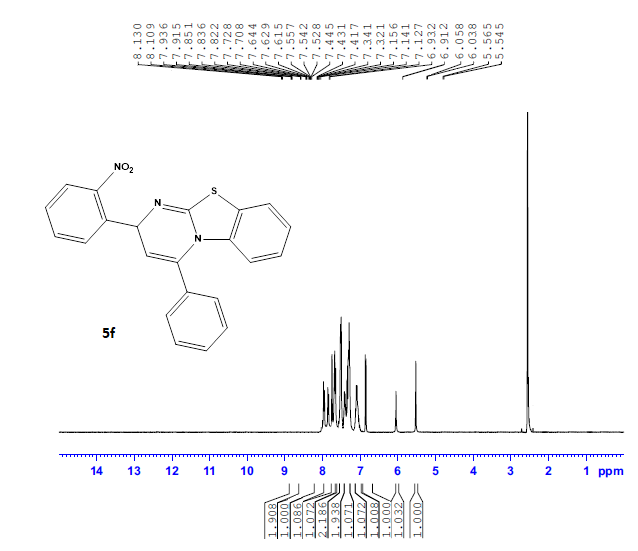
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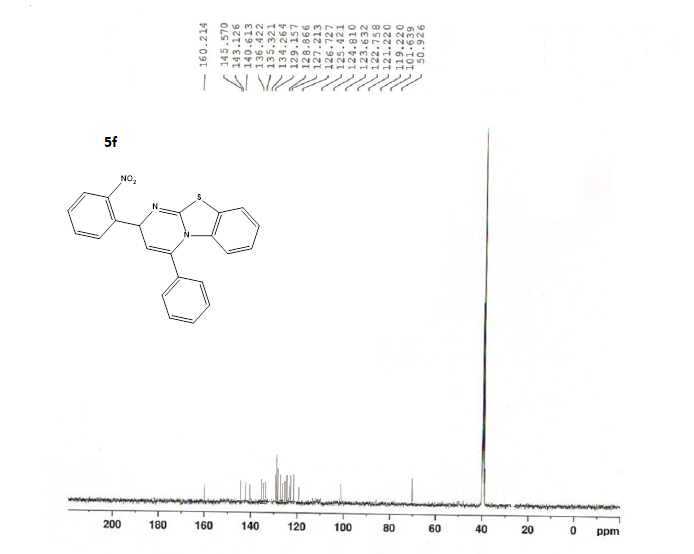
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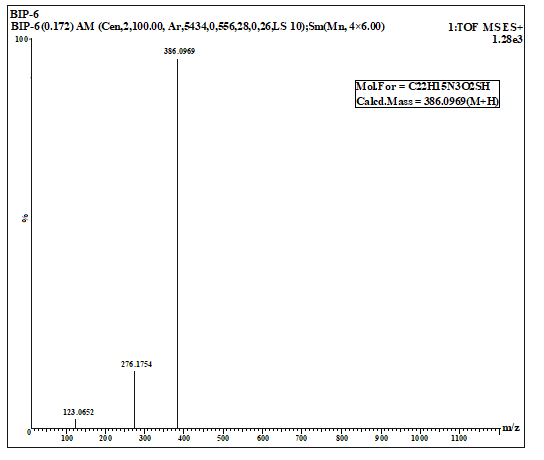
**13C NMR spectra of 5e**

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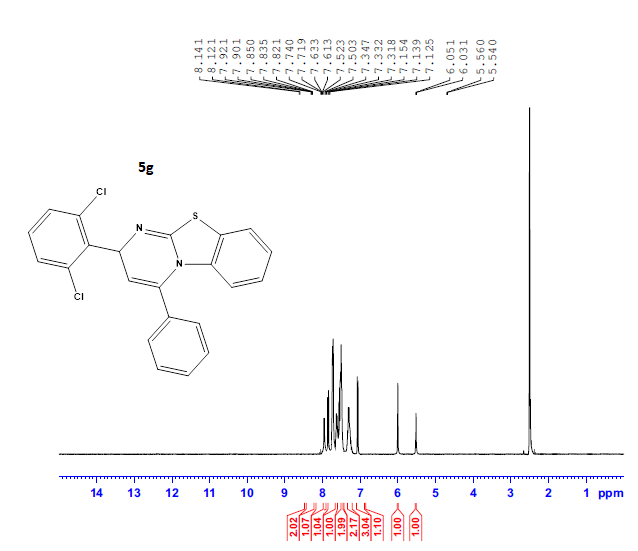
**1H NMR spectra of 5f**

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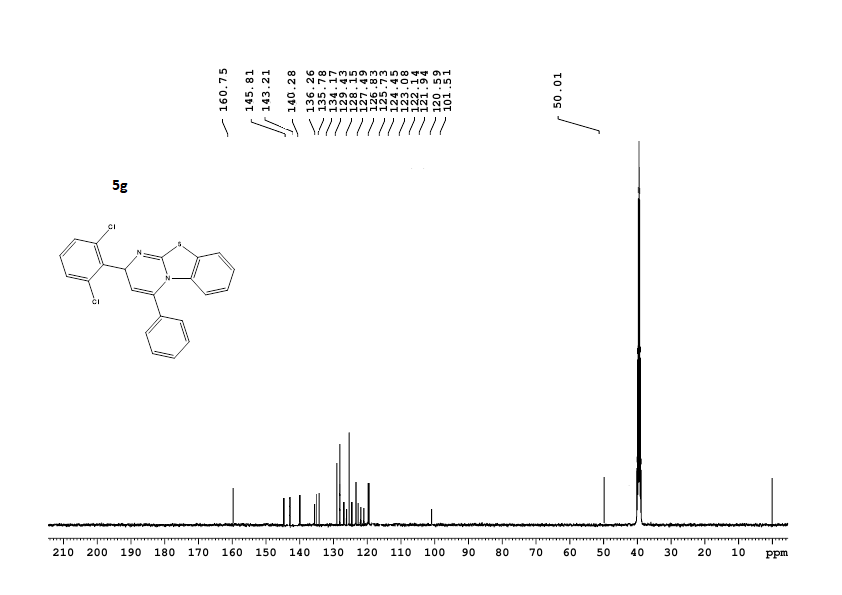
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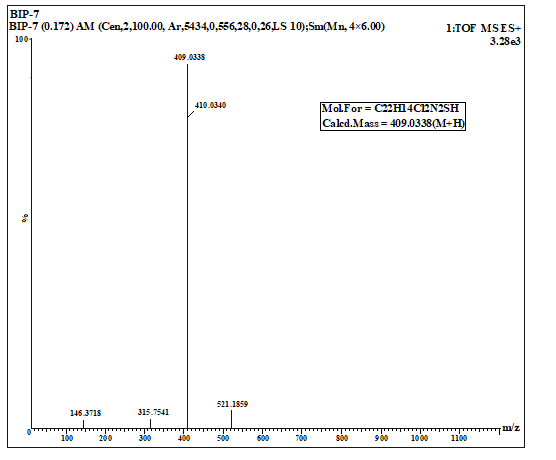
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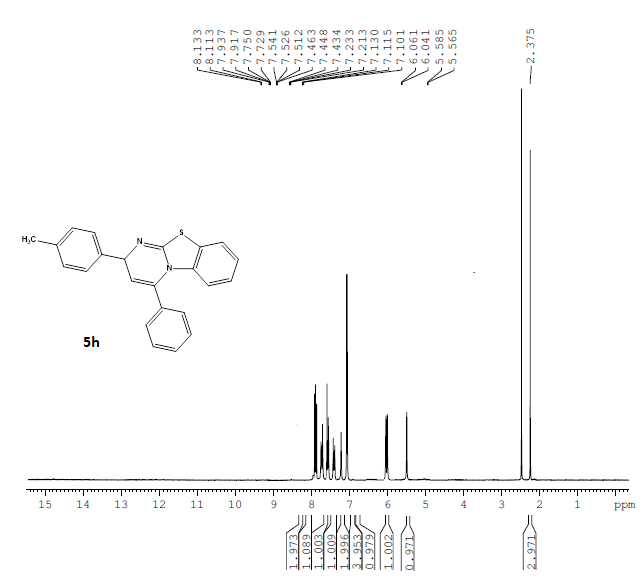
**1H NMR spectra of 5g**



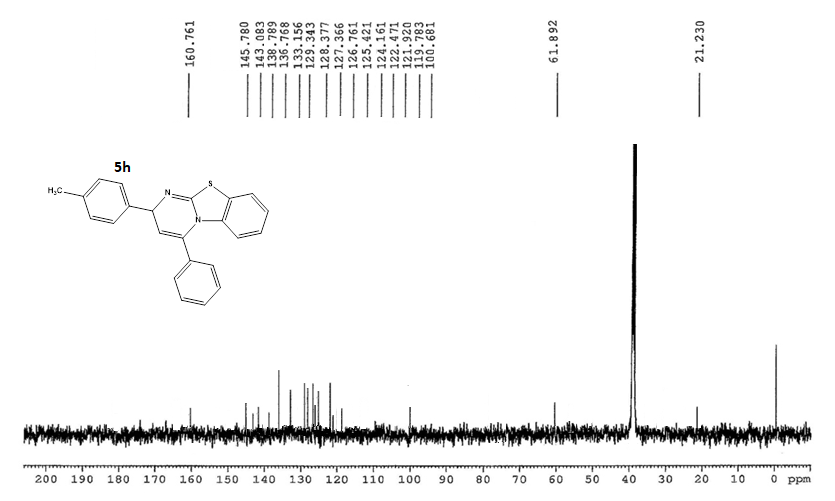
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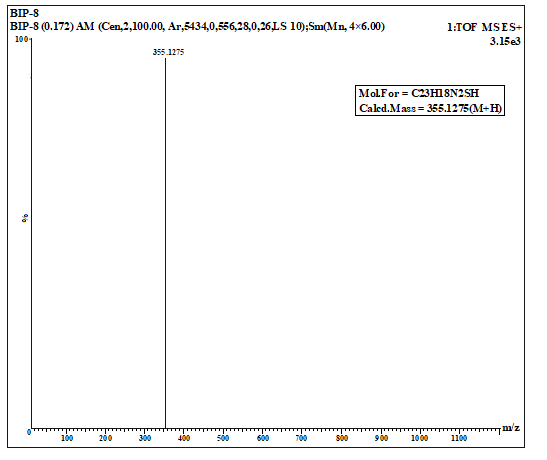
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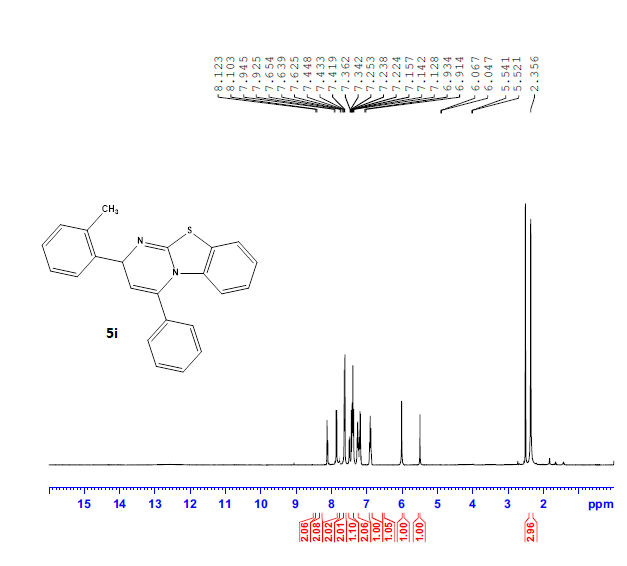
**1H NMR spectra of 5h**

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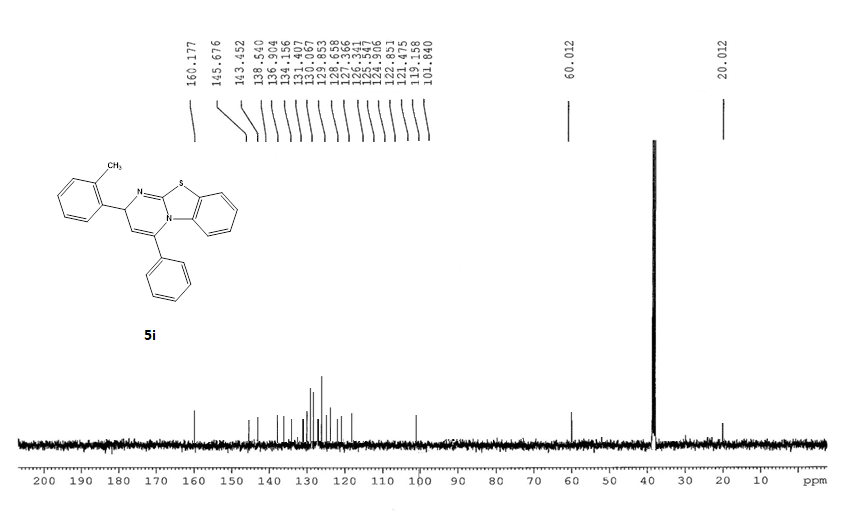
**13C NMR spectra of 5h**

****

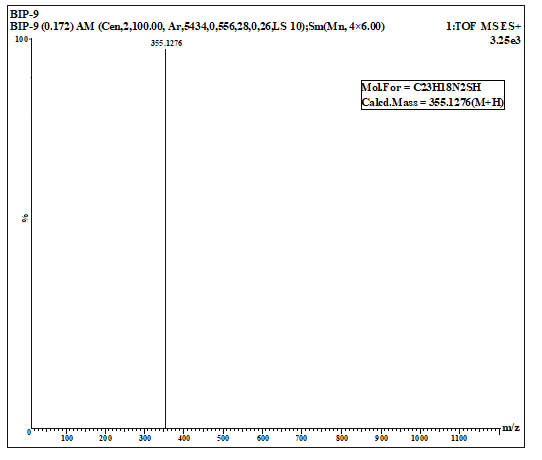
HRMS spectra of 5h

****

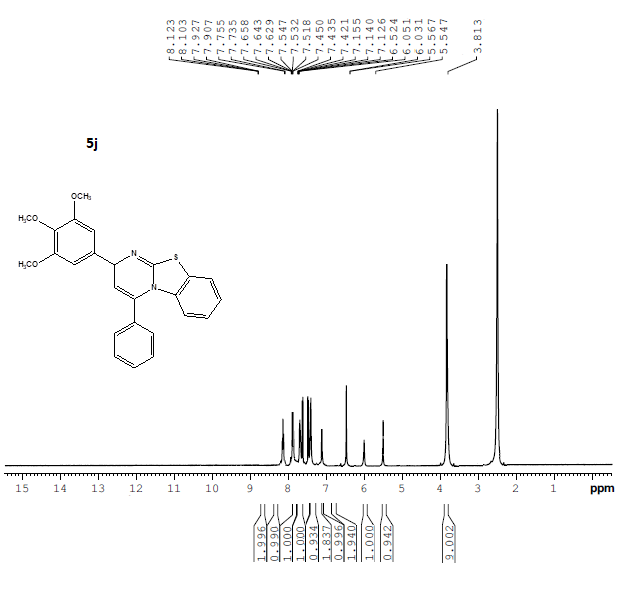
**1H NMR spectra of 5i**

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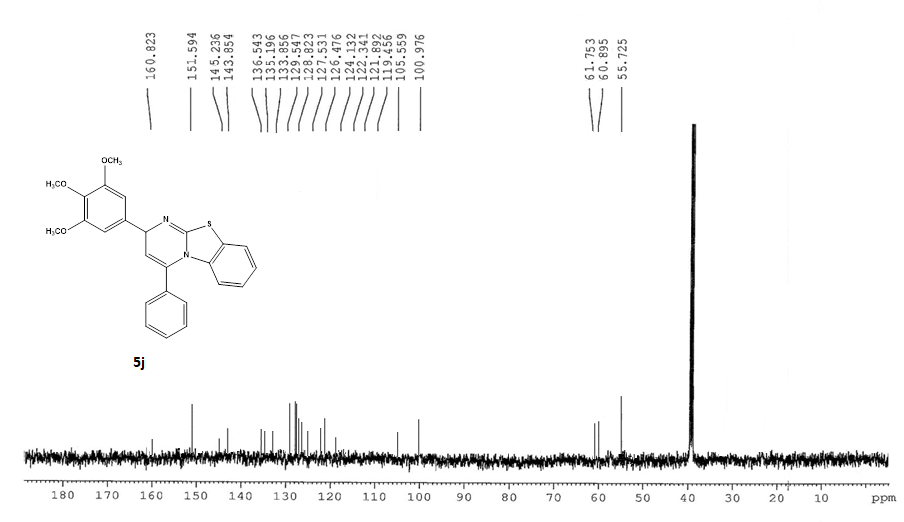
**13C NMR spectra of 5i**



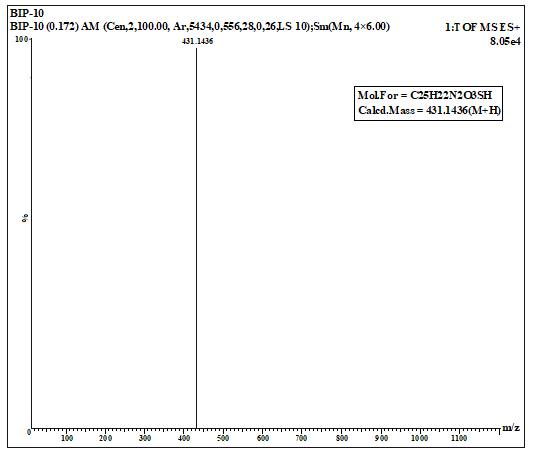
HRMS spectra of 5i

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**1H NMR spectra of 5j**



**13C NMR spectra of 5j**



HRMS spectra of 5j