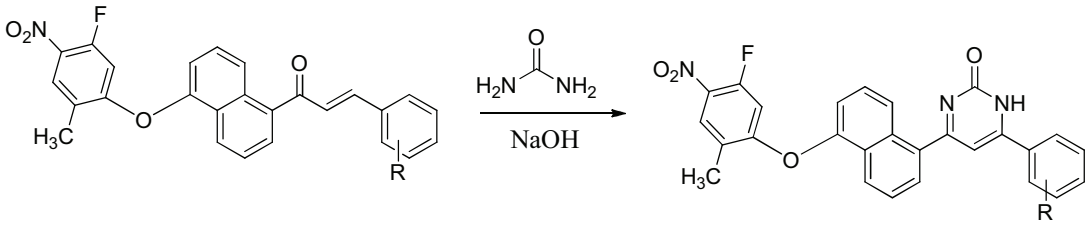
CHAPTER – IV

SYNTHESIS AND CHARACTERIZATION OF PYRIMIDINES

CONTENTS

4.1 REACTION SCHEME

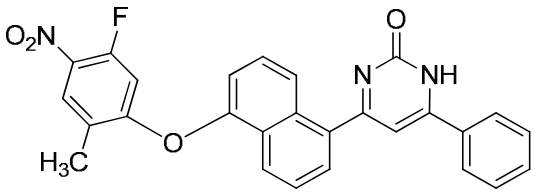
Pyrimidines **B1-B19** planned to prepare by reaction between chalcones **A1-A19** and urea in the presence of ethanol and 40% NaOH (**Scheme 4.1)**.



Scheme 4.1 Synthesis of Pyrimidines B1-B19

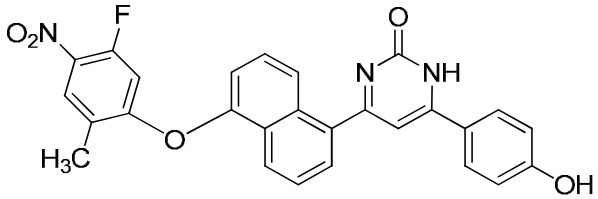
4.2 STRUCTURE OF COMPOUNDS B1 TO B19

Compound B1:



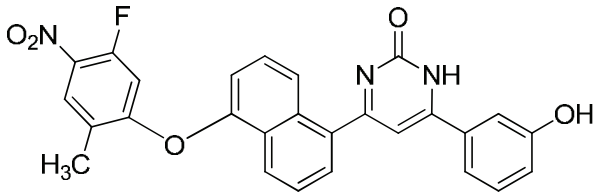
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-phenylpyrimidin-2(1*H*)-one

Compound B2:



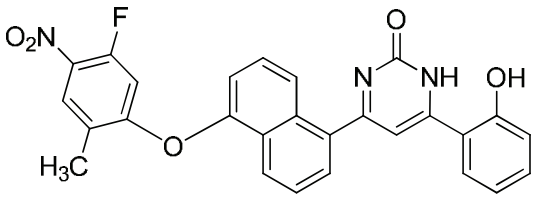
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-hydroxyphenyl)pyrimidin-2(1*H*)-one

Compound B3:



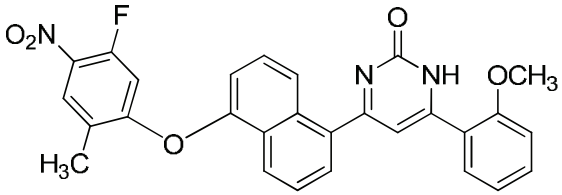
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-hydroxyphenyl)pyrimidin-2(1*H*)-one

Compound B4:



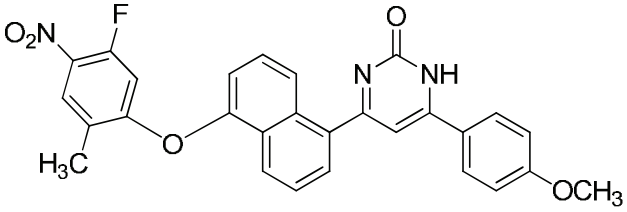
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-hydroxyphenyl)pyrimidin-2(1*H*)-one

Compound B5:



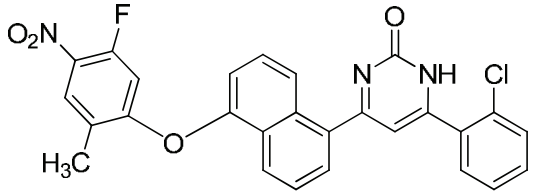
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-methoxyphenyl)pyrimidin-2(1*H*)-one

Compound B6:



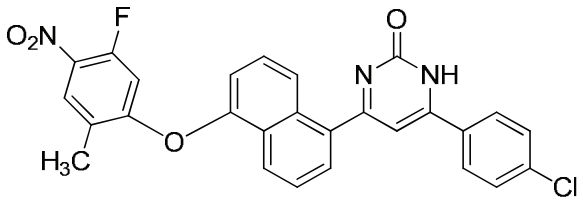
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-methoxyphenyl)pyrimidin-2(1*H*)-one

Compound B7:



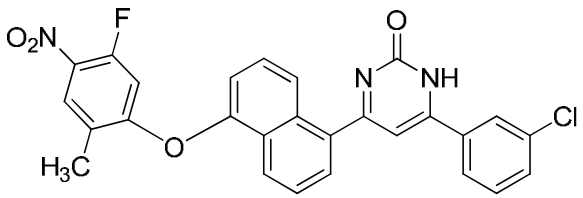
6-(2-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B8:



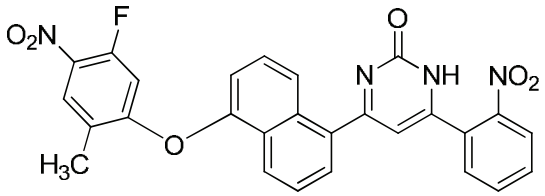
6-(4-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B9:



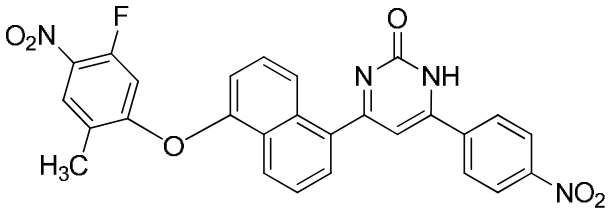
6-(3-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B10:



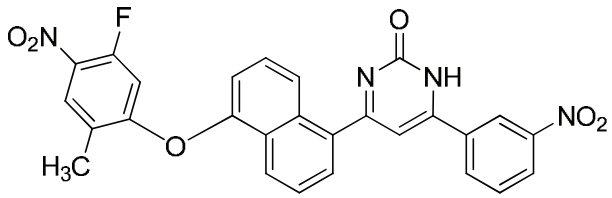
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-nitrophenyl)pyrimidin-2(1*H*)-one

Compound B11:



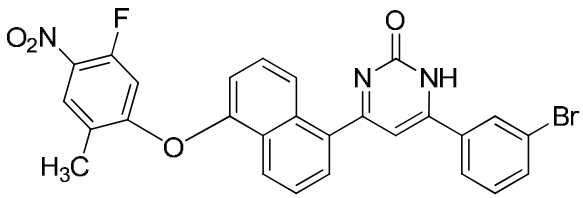
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-nitrophenyl)pyrimidin-2(1*H*)-one

Compound B12:



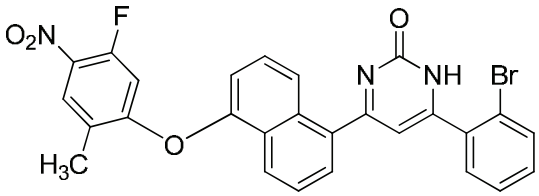
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-nitrophenyl)pyrimidin-2(1*H*)-one

Compound B13:



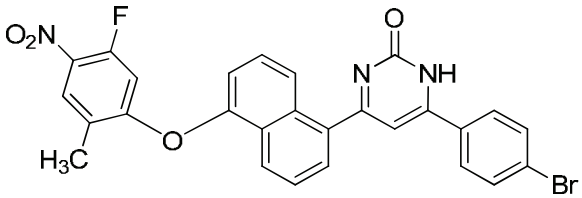
6-(3-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B14:



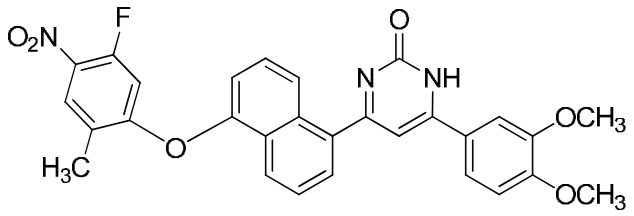
6-(2-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B15:



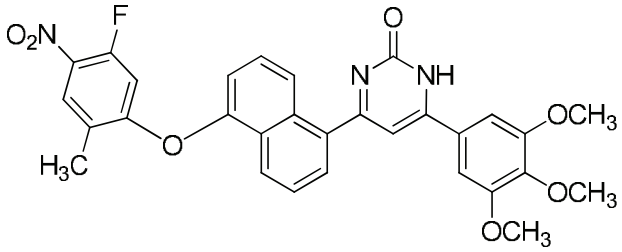
6-(4-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B16:



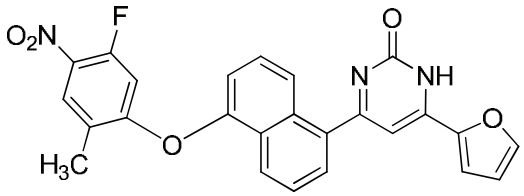
6-(3,4-dimethoxyphenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

Compound B17:



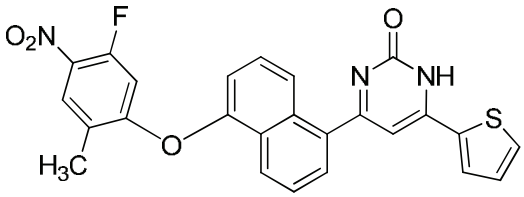
4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3,4,5-trimethoxyphenyl)pyrimidin-2(1*H*)-one

Compound B18:



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(furan-2-yl)pyrimidin-2(1*H*)-one

Compound B19:



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(thiophen-2-yl)pyrimidin-2(1*H*)-one

4.3. EXPERIMENTAL

4.3.1 Chemicals and Reagents

All chemicals used were of laboratory reagent grade and used without further purification**.** NaOH, urea and ethanol were used as received from Merck, Mumbai, India.

4.3.2 Analytical Methods

Bruker Avance-400 MHz instrument was used for Proton NMR study and 100 MHz frequency instrument was used for ^{13}C NMR. Parts per million (ppm) unit was used to express chemical shift values. ABB Bomem Inc. FT-IR 3000 Spectrophotometer was used for Infrared Spectral study. Data obtained were expressed in cm^{-1} unit. Shimadzu LCMS-2010 was used for MASS spectral analysis.Perkin Elmer-2400 Series II CHNS/O Elemental Analyzer was used for Composition measurements.

4.3.3 General Experimental procedure

4.3.3.1 Synthesis of Pyrimidine B1

Chalcone **A1** (0.01 ml) was taken in 250 ml RBF, and to this 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC. Completion of reaction was checked by TLC. The pyrimidine obtained is called **B1**.

4.3.3.2 Synthesis of Pyrimidine B2

Chalcone **A2** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine so obtained was called **B2**.

4.3.3.3 Synthesis of Pyrimidine B3

Chalcone **A3** (0.01 mol) was taken in 250 ml RBF, and to this 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hour to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was checked by TLC. The pyrimidine so obtained was termed as **B3**.

4.3.3.4 Synthesis of Pyrimidine B4

Chalcone **A4** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of reaction was also checked by TLC. The pyrimidine obtained is termed as **B4**.

4.3.3.5 Synthesis of Pyrimidine B5

Chalcone **A5** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of the reaction was checked by TLC. The pyrimidine so obtained was called **B5**.

4.3.3.6 Synthesis of Pyrimidine B6

Chalcone **A6** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of the reaction was also checked by TLC. The pyrimidine so obtained was called **B6**.

4.3.3.7 Synthesis of Pyrimidine B7

Chalcone **A7** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of the reaction was also checked by TLC. The pyrimidine so obtained was called **B7**.

4.3.3.8 Synthesis of Pyrimidine B8

Chalcone **A8** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol Urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion of the reaction was also checked by TLC. The pyrimidine so obtained was called **B8**.

4.3.3.9 Synthesis of Pyrimidine B9

Chalcone **A9** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The reaction was monitored by TLC and completion was also checked by TLC. The pyrimidine so obtained was called **B9**.

4.3.3.10 Synthesis of Pyrimidine B10

Chalcone **A10** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine so obtained was called **B10**.

4.3.3.11 Synthesis of Pyrimidine B11

Chalcone **A11** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine so obtained was called **B11**.

4.3.3.12 Synthesis of Pyrimidine B12

Chalcone **A12** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B12**.

4.3.3.13 Synthesis of Pyrimidine B13

Chalcone **A13** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B13**.

4.3.3.14 Synthesis of Pyrimidine B14

Chalcone **A14** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B14**.

4.3.3.15 Synthesis of Pyrimidine B15

Chalcone **A15** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B15**.

4.3.3.16 Synthesis of Pyrimidine B16

Chalcone **A16** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B16**.

4.3.3.17 Synthesis of Pyrimidine B17

Chalcone **A17** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B17**.

4.3.3.18 Synthesis of Pyrimidine B18

Chalcone **A18** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B18**.

4.3.3.19 Synthesis of Pyrimidine B19

Chalcone **A19** (0.01 mol) was taken in 250 mL RBF, and to it 0.01 mol urea, 40 mL ethanol and 40 mL 40% NaOH were added. The entire mixture was refluxed for 1-2 hours to produce Primidone**.** The progress of reaction was monitored by TLC and its completion was also checked by TLC. The pyrimidine obtained was called **B19**.

4.4 CHARACTERSTICS DATA SHOWING SYNTHESIS OF PYRIMIDINE B1-B19.

Table 4.1 Synthesis of Pyrimidine B1-B19

Sr. No.	Compounds	R	Reaction Time (h)	% Yield[b]
1	**B1**	-H	3	72
2	**B2**	4-OH	3	72
3	**B3**	3-OH	3	68
4	**B4**	2-OH	3	75
5	**B5**	2- OCH_3	3.5	68
6	**B6**	4-OCH_3	3.5	67
7	**B7**	2-Cl	2.5	80
8	**B8**	4-Cl	2.5	80
9	**B9**	3-Cl	2.5	75
10	**B10**	2-NO_2	2.5	83
11	**B11**	4-NO_2	2.5	83
12	**B12**	3-NO_2	2.5	82
13	**B13**	3-Br	3	78
14	**B14**	2- Br	3	75
15	**B15**	4- Br	3	78
16	**B16**	3, 4-$(OCH_3)_2$	3.5	72
17	**B17**	3,4,5-$(OCH_3)_3$	3.5	72
18	**B18**	2-furfuryl[c]	2.5	82
19	**B19**	2-Thineyl[c]	2.5	80

[a]Reaction is monitored by TLC, [b]Isolated yield and [c]Names of aldehyde groups

4.5 RESULTS AND DISCUSSION

Table 4.1 shows the data for various condensation products of reaction between various chalcones andurea. It clearly indicates that the compounds bearing electron withdrawing groups are synthesized in shorter reaction time as compared to compounds bearing electron donating group. Compounds **B7-B15** bearing electron withdrawing groups were synthesized in **2.5 to 3 h** as compared to compounds bearing electron donating group. Compounds **B5, B6, B16** and **B17** which have electron donating groups were synthesized in **3.5 h**.

4.6 PHYSICAL DATA OF SYNTHESIZED DERIVATIVES

Table 4.2 Physical data of compounds B1 to B19.

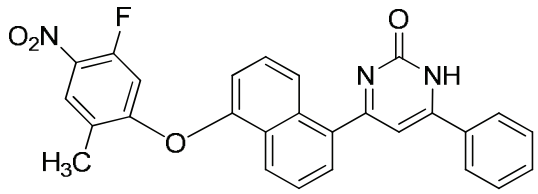
Comp.	R	Molecular Formula	Mol. Wt. (g/m)	% Yield	M.P. °C	% Carbon		% Hydrogen		% Nitrogen	
						Found	Calcd.	Found	Calcd.	Found	Calcd.
B1	-H	$C_{27}H_{18}FN_3O_4$	467.4	72	234	69.30	69.37	3.80	3.88	8.85	8.99
B2	4-OH	$C_{27}H_{18}FN_3O_5$	483.4	72	210	67.10	67.08	3.70	3.75	8.60	8.69
B3	3-OH	$C_{27}H_{18}FN_3O_5$	483.4	68	215	67.12	67.08	3.78	3.75	8.62	8.69
B4	2-OH	$C_{27}H_{18}FN_3O_5$	483.4	75	250	67.08	67.08	3.80	3.75	8.64	8.69
B5	2- OCH_3	$C_{28}H_{20}FN_3O_5$	494.7	68	240	67.70	67.60	4.10	4.05	8.40	8.45
B6	4-OCH_3	$C_{28}H_{20}FN_3O_5$	494.7	67	230	67.72	67.60	4.12	4.05	8.38	8.45
B7	2-Cl	$C_{27}H_{17}FClN_3O_4$	501.8	80	225	64.65	64.61	3.45	3.41	8.42	8.37
B8	4-Cl	$C_{27}H_{17}FClN_3O_4$	501.8	80	230	64.69	64.61	3.47	3.41	8.30	8.37
B9	3-Cl	$C_{27}H_{17}FClN_3O_4$	501.8	75	242	64.66	64.61	3.48	3.41	8.43	8.37

B10	2-NO_2	$C_{27}H_{17}FN_4O_6$	512.4	83	223	63.22	63.28	3.28	3.34	10.85	10.93
B11	4-NO_2	$C_{27}H_{17}FN_4O_6$	512.4	83	225	63.24	63.28	3.29	3.34	10.86	10.93
B12	3-NO_2	$C_{27}H_{17}FN_4O_6$	512.4	82	224	63.20	63.28	3.30	3.34	10.87	10.93
B13	3-Br	$C_{27}H_{17}FBrN_3O_4$	546.3	78	235	59.28	59.36	3.10	3.14	7.62	7.69
B14	2- Br	$C_{27}H_{17}FBrN_3O_4$	546.3	75	240	59.22	59.36	3.12	3.14	7.65	7.69
B15	4- Br	$C_{27}H_{17}FBrN_3O_4$	546.3	78	245	59.29	59.3	3.09	3.14	7.63	7.69
B16	3, 4-$(OCH_3)_2$	$C_{29}H_{22}FN_3O_6$	527.5	72	245	66.10	66.03	4.10	4.20	7.90	7.97
B17	3,4,5-$(OCH_3)_3$	$C_{30}H_{24}FN_3O_7$	557.5	72	260	64.68	64.63	4.39	4.34	7.45	7.54
B18	2-furfuryl	$C_{25}H_{16}FN_3O_5$	457.4	82	255	65.60	65.65	3.58	3.53	9.10	9.19
B19	2-Thineyl	$C_{25}H_{16}FSN_3O_4$	473.4	80	225	63.48	63.42	3.45	3.41	8.83	8.87

4.7 SPECTROSCOPIC CHARACTERIZATION OF COMPOUNDS B1-B19.

For characterization,**compound B1** was taken as the model compound from the series and it was characterized by various spectroscopic methods such as ^{1}H NMR, ^{13}C NMR, MASS and IR spectroscopy. Its structure was decided by these spectroscopic technique. (as shown in Fig. 4.1 to Fig. 4.4)

Compound B1



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-phenylpyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound gives singlet at δ 2.5 ppm in downfield region. All 14 aromatic protons appeared in aromatic region between δ 6.8 to 8.3 ppm. Singlet due to NH proton appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 128.9, 129.4, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 ppm and carbonyl carbon of amide group comes at δ 165.2 ppm.

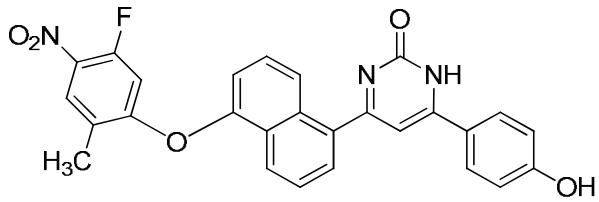
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3311 cm^{-1} indicates the N-H stretching. The bands at 3120 cm^{-1} indicates thearomatic C-H stretching, and at 2950 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1611, 1592 and 1569 cm^{-1} and due to the C=C and N=O stretching. The band at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 467.4, which indicates the molecular weight of the compound.

Compound B2



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-hydroxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.4 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.7 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.8 to 8.3 ppm. Singlet due to NH proton is shown at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 128.9, 130.3, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 ppm and carbonyl carbon of amide group at δ 164.2 ppm.

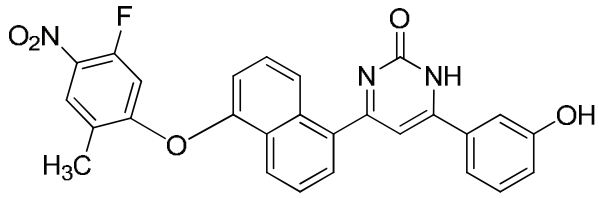
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3415 and 3310 cm^{-1} indicates the O-H and N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. The band at 2950 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1592 and 1569 cm^{-1} and due to the C=C and N=O stretching. The band at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 483.4, which indicates the molecular weight of the compound.

Compound B3



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-hydroxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.4 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.7 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.6 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 129.4, 130.4, 131.6, 140.2, 146.6, 151.7, 153.7, 155.1 ppm and signal due to carbonyl carbon of amide group appeared at 164.2 δ ppm.

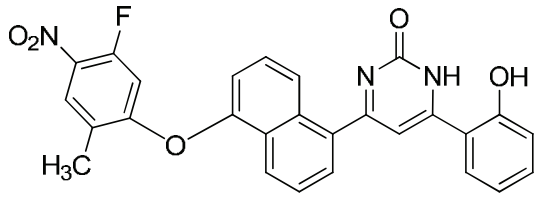
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3419 and 3310 cm^{-1} indicates the O-H and N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2951 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1611, 1592 and 1569 cm^{-1} and due to the C=C and N=O stretching. The band at 746 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 483.4, which indicates the molecular weight of the compound.

Compound B4



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-hydroxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. Singlet due to one –OH proton appeared at δ 2.6 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 128.9, 130.4, 131.6, 140.2, 146.6, 151.7, 154.7, 156.1 ppm and signal due to carbonyl carbon of amide group appeared at 165.2 δ ppm.

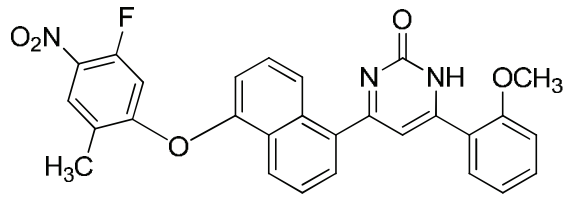
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3420 and 3312 cm^{-1} indicates the O-H and N-H stretching, respectively. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2952 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1611, 1590 and 1565 cm^{-1} and due to the C=C and N=O stretching. The band at 750 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 483.4, which indicates the molecular weight of the compound.

Compound B5



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-methoxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. Singlet due to $–OCH_3$ proton appeared at δ 3.4 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. Signal due to $–OCH_3$ group is comes at 39.0 δ ppm. All aromatic carbons give signals at δ 127.9, 129.4, 131.6, 140.2, 146.6, 151.7, 154.7, 156.1 ppm and signal due to carbonyl carbon of amide group appeared at 164.2 δ ppm.

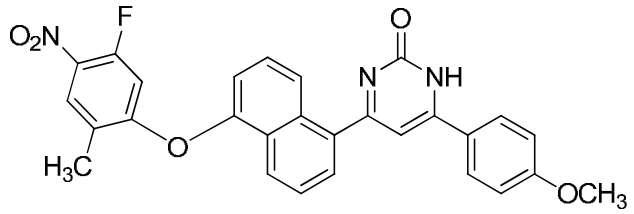
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3312 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2951 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1612, 1590 and 1568 cm^{-1} and due to the C=C and N=O stretching. The band at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 494.7, which indicates the molecular weight of the compound.

Compound B6



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-methoxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. Singlet due to $–OCH_3$ proton appeared at δ 3.4 ppm. All 13 aromatic protons appeared in aromatic region between δ 6.4 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.6 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.1 ppm. Signal due to $–OCH_3$ group is comes at 39.0 δ ppm. All aromatic carbons give signals at δ 127.9, 129.4, 131.4, 131.6, 140.2, 146.6, 152.7, 154.7, 156.1 ppm and signal due to carbonyl carbon of amide group appeared at 164.2 δ ppm.

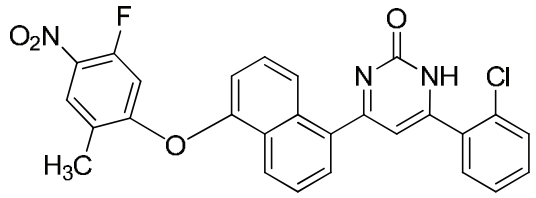
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3316 cm^{-1} indicates the N-H stretching. The band at 3132 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2971 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1612, 1590 and 1568 cm^{-1} and due to the C=C and N=O stretching. The band at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 494.7, which indicates the molecular weight of the compound.

Compound B7



6-(2-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 33.0 ppm. All aromatic carbons give signals at δ 129.4, 130.3, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 ppm and signal due to carbonyl carbon of amide group appeared at 164.2 δ ppm.

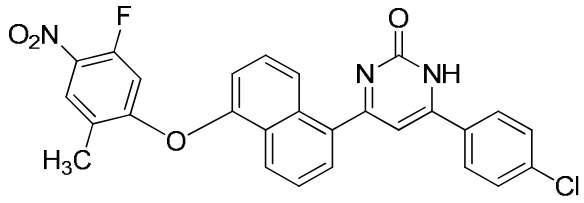
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3311 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1610, 1592 and 1567 cm^{-1} and due to the C=C and N=O stretching. The band at 744 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 501.8, which indicates the molecular weight of the compound.

Compound B8



6-(4-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 31.5 ppm. All aromatic carbons give signals at δ 128.5, 130.2, 131.6, 140.2, 146.6, 151.9, 153.6, 155.1 ppm and signal due to carbonyl carbon of amide group appeared at 165.2 δ ppm.

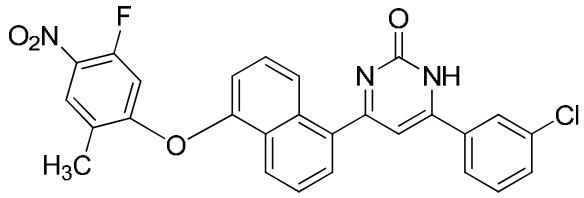
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that absorption at 3370 cm^{-1} indicates the N-H stretching. The band at 3121 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2980 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1610, 1595 and 1567 cm^{-1} and due to the C=C and N=O stretching. The band at 746 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 501.8, which indicates the molecular weight of the compound.

Compound B9



6-(3-chlorophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.6 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.4 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.1 ppm. All aromatic carbons give signals at δ 129.4, 130.3, 133.6, 140.2, 146.6, 151.9, 152.6, 155.1 ppm and signal due to carbonyl carbon of amide group appeared at 164.2 δ ppm.

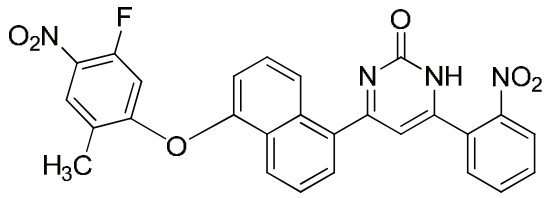
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that the absorption band at 3320 cm^{-1} indicates the N-H stretching. The band at 3121 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2985 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1609, 1595 and 1567 cm^{-1} indicates the C=C and N=O stretching. Band at 746 cm^{-1} attributed to C-H bending vibrations disubstituted benzene ring.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 501.8, which indicates the molecular weight of the compound.

Compound B10



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(2-nitrophenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at 32.2 δ ppm. All aromatic carbons give signals at δ 128.4, 130.4, 131.6, 140.2, 146.6, 155.8, 155.6, 155.2 ppm and carbonyl carbon of amide group appeared at 164.1 δ ppm.

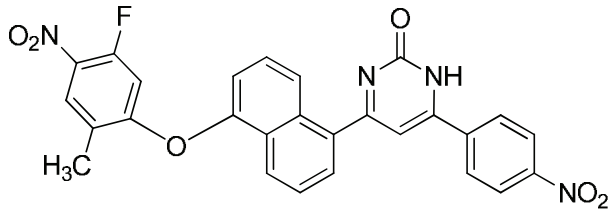
IR Spectroscopy (KBr)

Infrared spectra recorded in KBr reveals that the absorption band at 3311 cm^{-1} indicates the N-H stretching. The band at 3120 cm^{-1} indicates the aromatic C-H stretching. Absorption at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. The band at 1610, 1592 and 1567 cm^{-1} indicates the C=C and N=O stretching. Band at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 512.4, which indicates the molecular weight of the compound.

Compound B11



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(4-nitrophenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.6 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.2 ppm. All aromatic carbons give signals at δ 129.4, 130.3, 131.6, 140.2, 146.6, 151.9, 153.6, 155.1 ppm and carbonyl carbon of amide group appeared at δ 165.2 ppm.

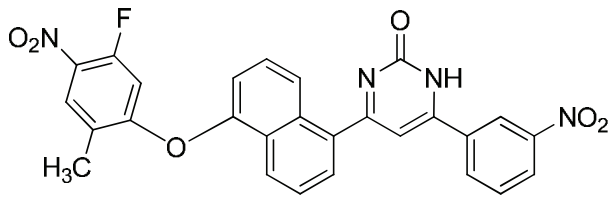
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3310 cm^{-1} indicates the N-H stretching. Absorption at 3120 cm^{-1} indicates the aromatic C-H stretching. Band at 2982 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1590 and 1567 cm^{-1} indicates the C=C and N=O stretching. Band at 746 cm^{-1} is due to C-H bending vibrations mono and disubstituted benzene ring.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 512.4, which indicates the molecular weight of the compound.

Compound B12



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3-nitrophenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.2 ppm. All aromatic carbons give signals at δ 126.4, 130.3, 131.6, 141.2, 146.6, 151.8, 153.6, 154.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

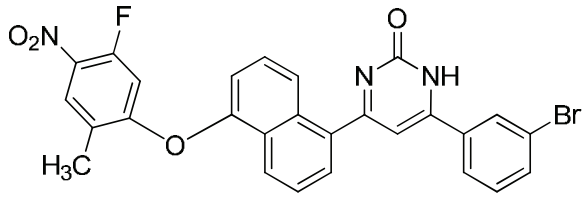
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3411 cm^{-1} indicates the N-H stretching. Absorption at 3020 cm^{-1} indicates the aromatic C-H stretching. Band at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1590 and 1567 cm^{-1} indicates the C=C and N=O stretching. Band at 744 cm^{-1} is due to C-H bending vibrations mono and disubstituted benzene ring.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 512.4, which indicates the molecular weight of the compound.

Compound B13



6-(3-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.4 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 31.1 ppm. All aromatic carbons give signals at δ 129.4, 130.3, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

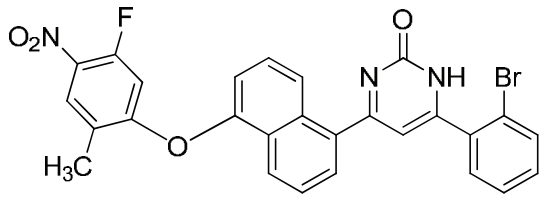
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3316 cm^{-1} indicates the N-H stretching. Absorption at 3121 cm^{-1} indicates the aromatic C-H stretching. Band at 2930 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1591 and 1565 cm^{-1} indicates the C=C and N=O stretching. Band at 740 cm^{-1} is due to C-H bending vibrations mono and disubstituted benzene ring.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 546.3, which indicates the molecular weight of the compound.

Compound B14



6-(2-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 129.4, 130.4, 131.6, 140.2, 146.6, 151.9, 153.6, 155.1 ppm and carbonyl carbon of amide group appeared at δ 165.2 ppm.

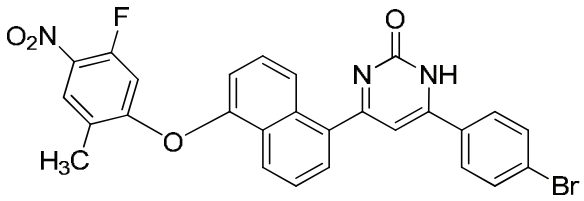
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3360 cm^{-1} indicates the N-H stretching. Absorption at 3121 cm^{-1} indicates the aromatic C-H stretching. Band at 2980 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1593 and 1560 cm^{-1} indicates the C=C and N=O stretching. Band at 750 cm^{-1} is due to C-H bending vibrations mono and disubstituted benzene ring.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 546.3, which indicates the molecular weight of the compound.

Compound B15



6-(4-bromophenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.4 ppm in downfield region. All 13 aromatic protons appeared in aromatic region between δ 6.5 to 8.3 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.1 ppm. All aromatic carbons give signals at δ 128.9, 130.3, 131.6, 140.2, 146.6, 151.8, 153.6, 155.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

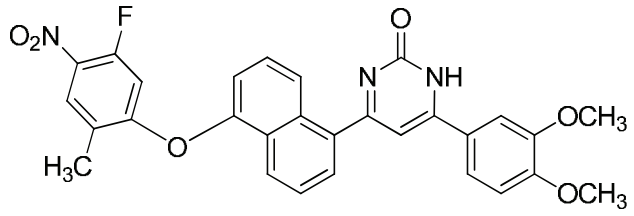
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3310 cm^{-1} indicates the N-H stretching. Absorption at 3105 cm^{-1} indicates the aromatic C-H stretching. Band at 2960 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1610, 1590 and 1550 cm^{-1} indicates the C=C and N=O stretching. Band at 750 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 546.3, which indicates the molecular weight of the compound.

Compound B16



6-(3,4-dimethoxyphenyl)-4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. Singlet due to two $–OCH_3$ proton appeared at δ 3.5 ppm. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 31.2 ppm. Signal due to two $–OCH_3$ group is appeared at 39.0 and 40.1 δ ppm. All aromatic carbons give signals at δ 127.9, 131.4, 131.6, 140.2, 146.6, 152.7, 154.7, 157.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

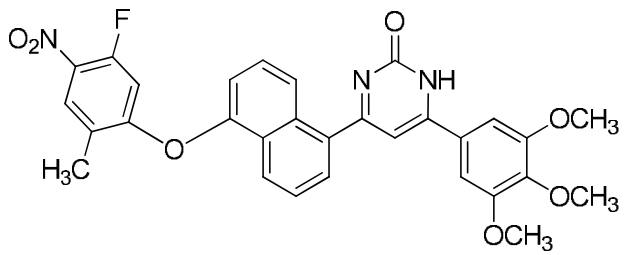
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3320 cm^{-1} indicates the N-H stretching. Absorption at 3130 cm^{-1} indicates the aromatic C-H stretching. Band at 2970 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1612, 1592 and 1568 cm^{-1} indicates the C=C and N=O stretching. Band at 741 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 527.5, which indicates the molecular weight of the compound.

Compound B17



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(3,4,5-trimethoxyphenyl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. Singlet due to two –OCH_3 proton appeared at δ 3.4 ppm. All 11 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. Signal due to three –OCH_3 group is appeared at 38.6, 39.0 and 40.1 δ ppm. All aromatic carbons give signals at δ 127.9, 131.4, 131.6, 140.2, 146.6, 152.7, 154.7, 157.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

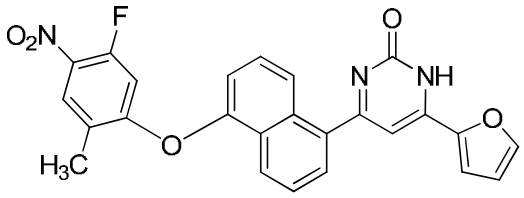
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3312 cm^{-1} indicates the N-H stretching. Absorption at 3130 cm^{-1} indicates the aromatic C-H stretching. Band at 2972 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1612, 1590 and 1565 cm^{-1} indicates the C=C and N=O stretching. Band at 740 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 557.5, which indicates the molecular weight of the compound.

Compound B18



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(furan-2-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.7 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 128.9, 130.4, 131.6, 131.6.2, 142.6, 146.6, 153.7, 154.7, 157.1 ppm and carbonyl carbon of amide group appeared at δ 164.3 ppm.

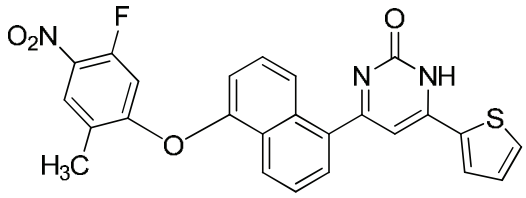
IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3315 cm^{-1} indicates the N-H stretching. Absorption at 3130 cm^{-1} indicates the aromatic C-H stretching. Band at 2929 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1613, 1590 and 1560 cm^{-1} indicates the C=C and N=O stretching. Band at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 557.4, which indicates the molecular weight of the compound.

Compound B19



4-(5-(5-fluoro-2-methyl-4-nitrophenoxy)naphthalen-1-yl)-6-(thiophen-2-yl)pyrimidin-2(1*H*)-one

^{1}H NMR Spectroscopy

400 MHz apparatus was used to record ^{1}H NMR spectra. Deuterated chloroform was used as the solvent. Three protons of the CH_3 of the compound give singlet at δ 2.5 ppm in downfield region. All 12 aromatic protons appeared in aromatic region between δ 6.5 to 8.4 ppm. Singlet due to NH proton is appeared at δ 9.8 ppm.

^{13}C NMR Spectroscopy

100 MHz apparatus was used to record ^{13}C NMR spectra. Deuterated chloroform ($CDCl_3$) was used as the solvent. Signal due to carbon of methyl group attached to aryl ring appeared at δ 32.0 ppm. All aromatic carbons give signals at δ 129.4, 131.4, 131.6, 142.2, 146.6, 152.7, 154.7, 157.1 ppm and carbonyl carbon of amide group appeared at δ 164.2 ppm.

IR Spectroscopy (KBr)

Infrared spectra was recorded using KBr reveals that the absorption band at 3315 cm^{-1} indicates the N-H stretching. Absorption at 3130 cm^{-1} indicates the aromatic C-H stretching. Band at 2973 cm^{-1} shows aliphatic C-H stretching of the methyl group. Absorption at 1612, 1590 and 1565 cm^{-1} indicates the C=C and N=O stretching. Band at 745 cm^{-1} is due to mono and disubstituted benzene ring C-H bending vibrations.

Mass Spectroscopy

In the Mass spectrum of the given compound, molecular ion peak appeared at M+ 473.4, which indicates the molecular weight of the compound.

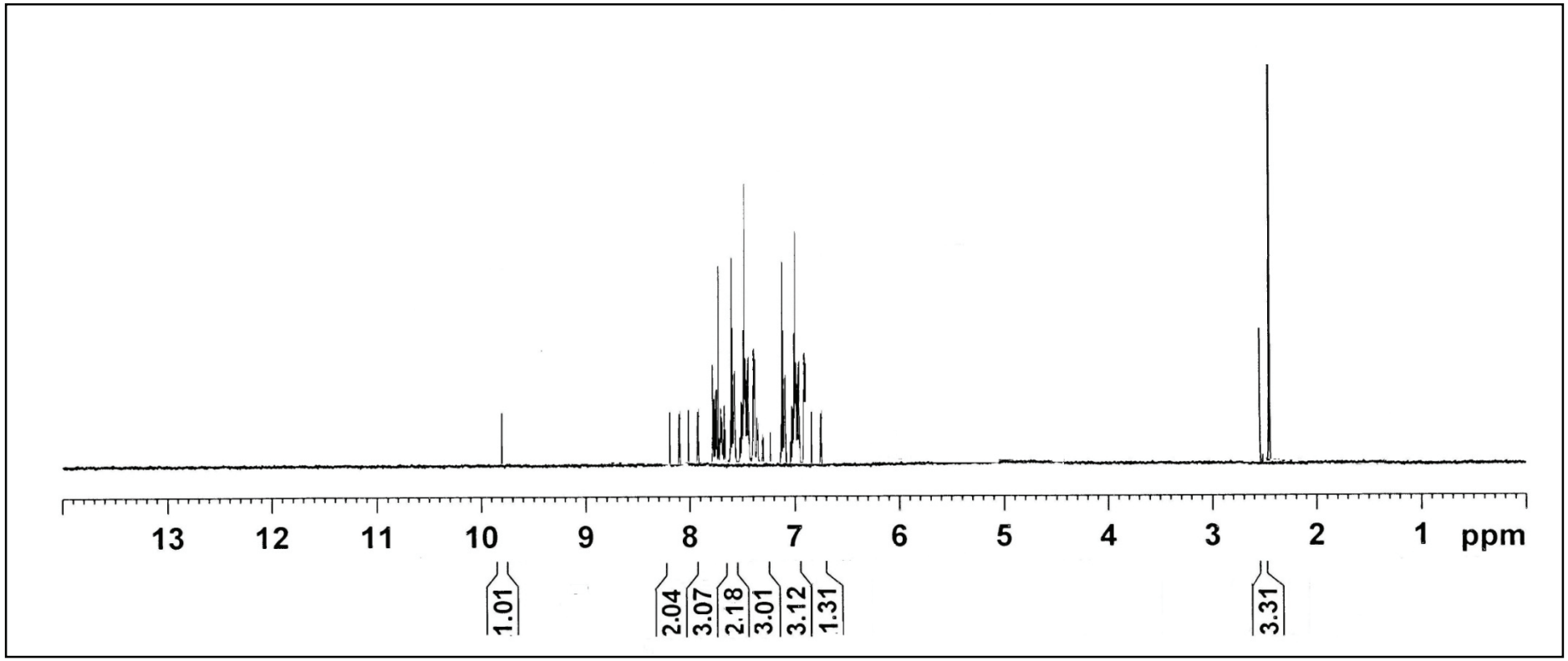


Fig. 4.1: ^{1}H NMR spectrum of B1

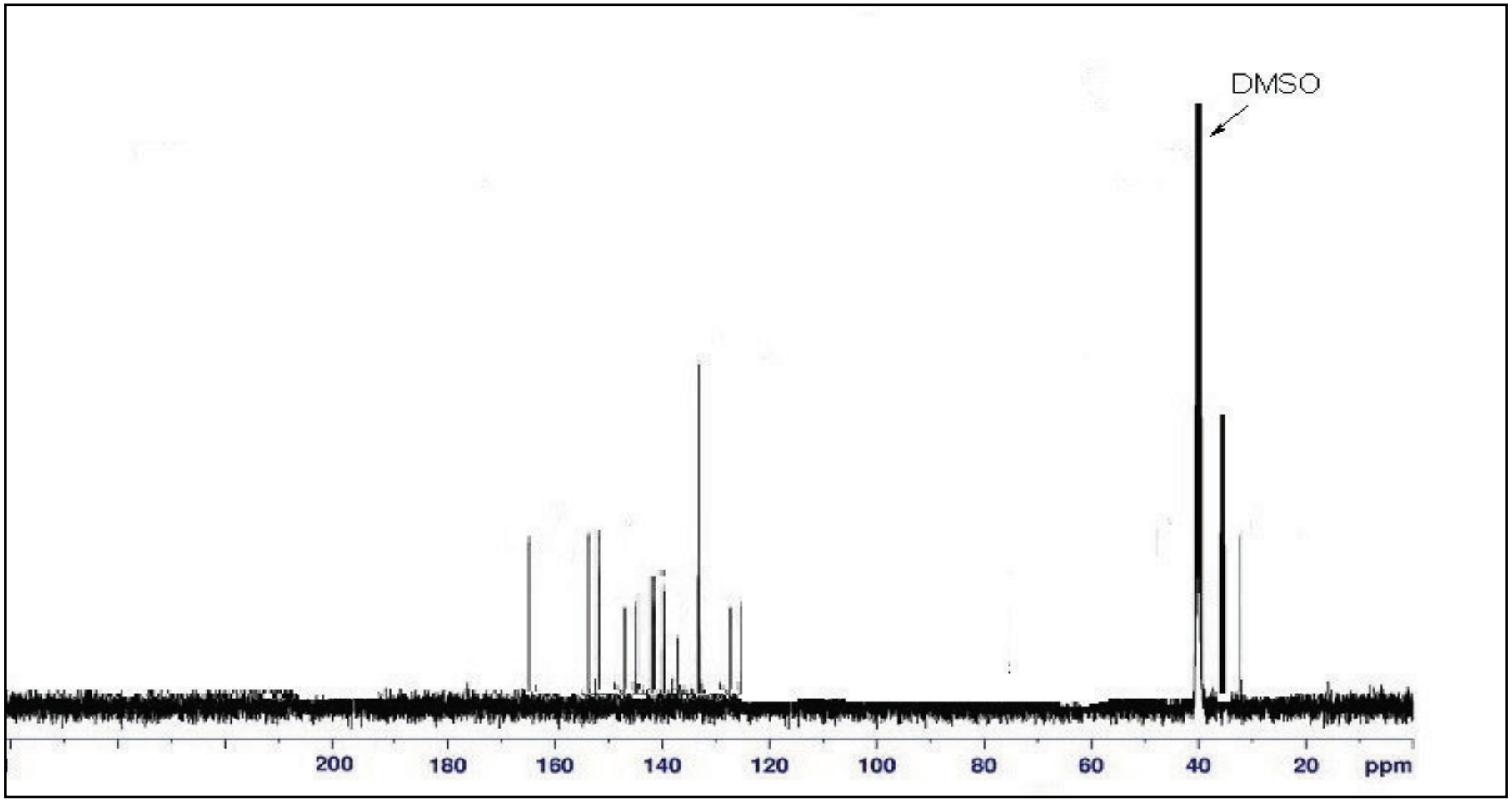


Fig. 4.2: ^{13}C NMR spectrum of B1

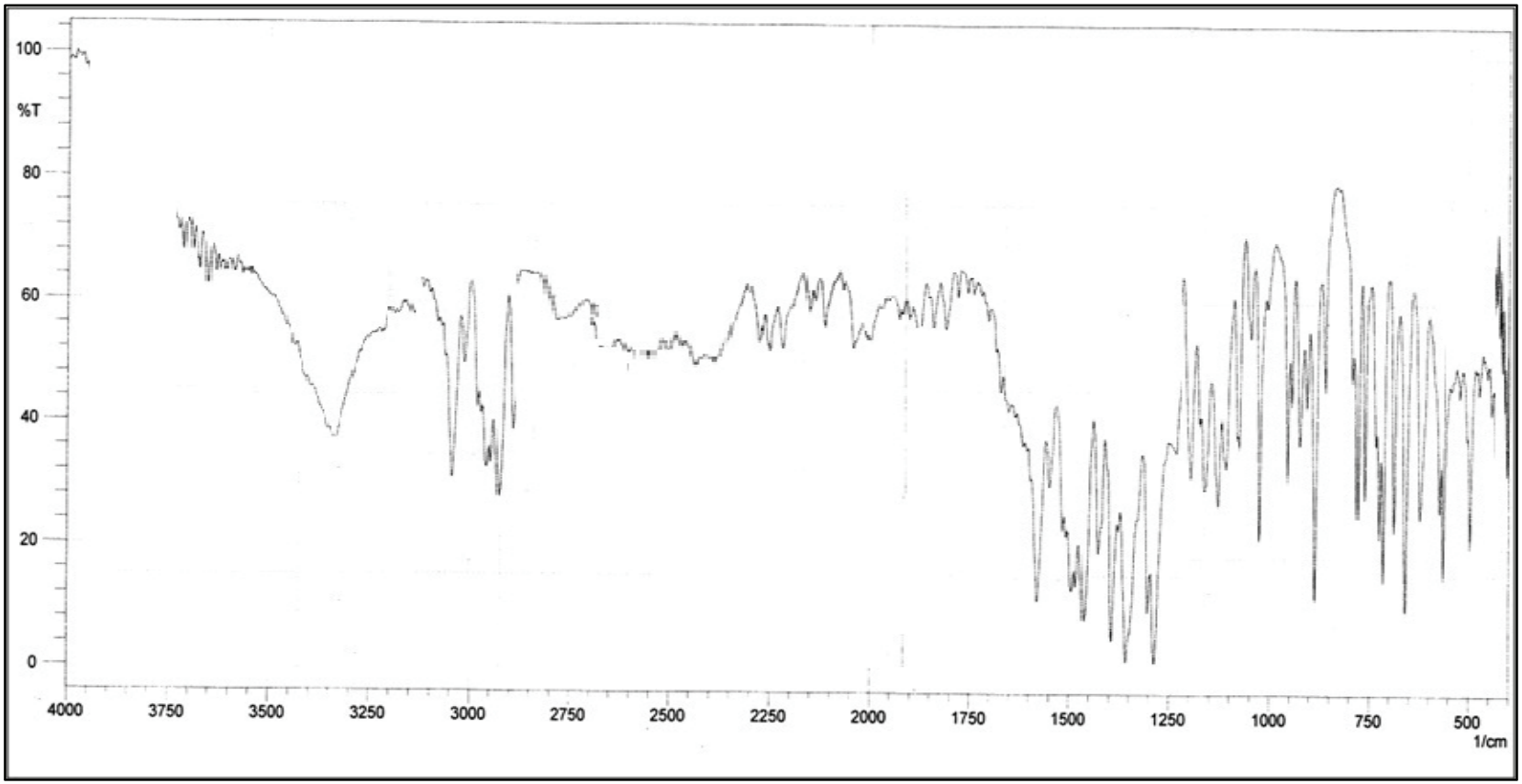


Fig. 4.3: IR spectrum of B1

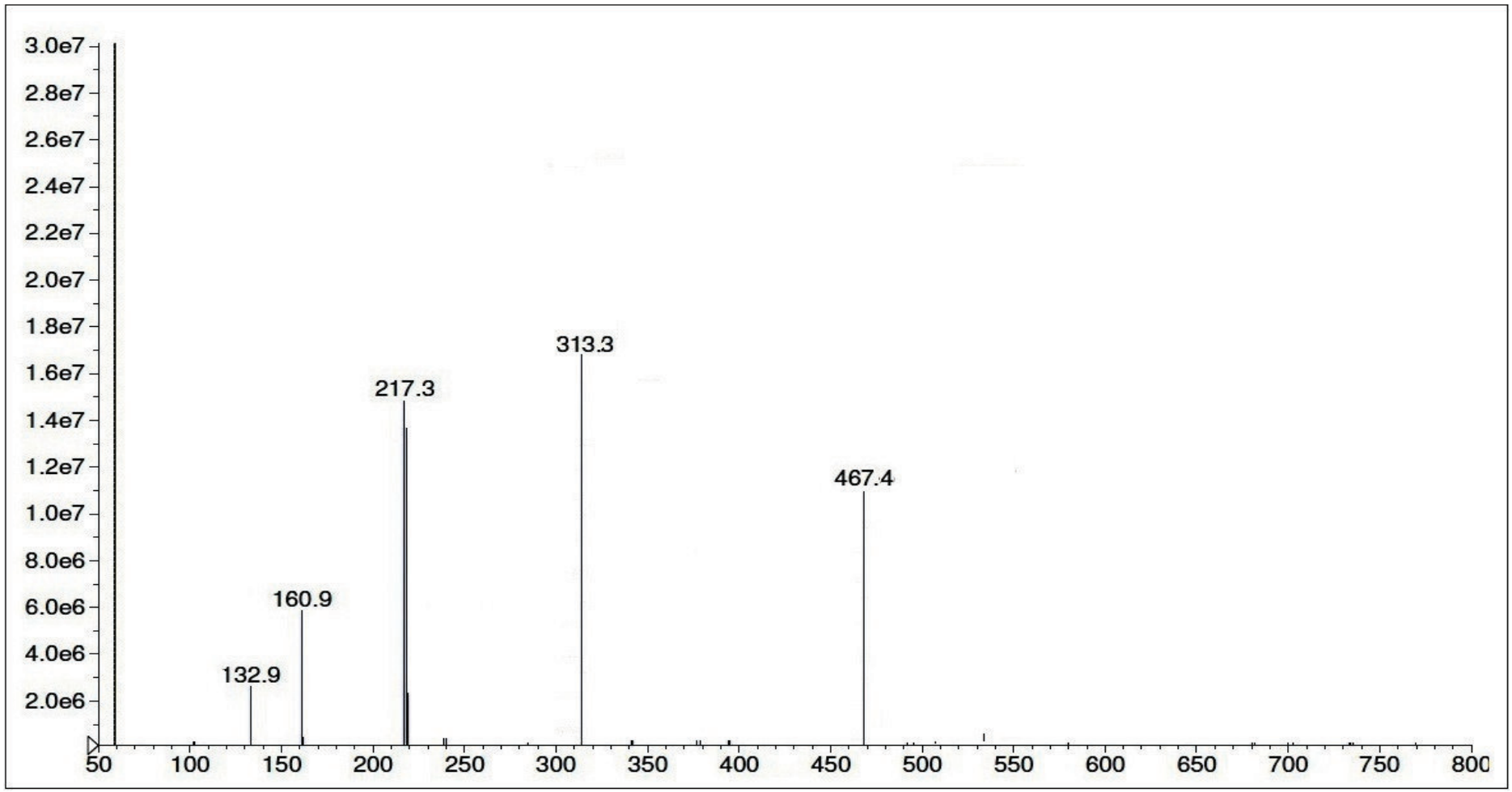


Fig. 4.4: Mass spectrum of B1

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