

Pyridinium Trifluoro Acetate Mediated Synthesis of 3,4-Dihydropyrimidin-2(1H)-ones and Tetrazolo[1,5-a]pyrimidine-6-carboxylates

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ABSTRACT

A simple and economic synthesis of 3,4-dihydropyrimidin-2(1H)-ones using pyridinium triflate as catalyst under microwave condition was attempted with an easy work-up protocol. Further tetrazolo [1,5-a] pyrimidine-6-carboxylates were synthesized by three-component coupling reaction of β -ketoesters with a mixture of aromatic aldehyde and 5-aminotetrazole. The products were well characterized with IR, NMR (1H and 13C NMR) and mass spectrometry.

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1. Introduction

Three component coupling reactions are long known as an efficient and simple method for the synthesis of dihydropyridines¹, dihydropyrimidine derivatives² and tetrazolopyrimidines³. Biginelli compounds and its analogues have wide applications because of their pharmaceutical and therapeutic properties⁴. Though research on Biginelli reaction is time tested, still active molecules are emerging with dihydropyrimidine core because of their medicinal importance as antihypertensive agents and calcium channel blockers⁵. Further, monastrol with dihydropyrimidine core moiety is much explored owing to its wide application as a cell-permeable small molecule inhibitor of the mitotic kinesin, Eg5⁶. Several of the marine alkaloids also found to contain the dihydropyrimidine core unit by nature and were found to show interesting biological activities such as antiviral, antibacterial and anti-inflammatory activity^{7, 8}. Thus the synthesis of the dihydropyrimidine core unit gains much

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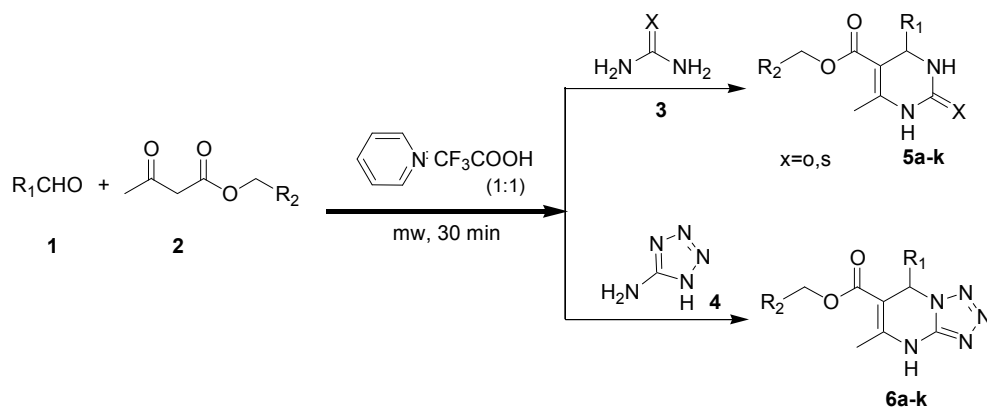
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importance. Purine derivatives which are well-known for its wide range of biological activities, such as antimicrobial activity⁹, fungicidal activity³, antihypertensive¹⁰, K(ATP) channel opening¹¹, central nervous system stimulating¹² *etc.*, has interestingly the fundamental dihydropyrimidine core.

There exist a number of conditions for the synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones using Lewis acid catalysts such as InCl₃¹³, Cu(OTf)₂¹⁴, CF₃COONH₄¹⁵, organo catalyst¹⁶, Trifluoro Acetic Acid¹⁷, Metal triflimide¹⁸, acid catalyst¹⁹ *etc.* Tetrazolopyrimidines were synthesised using iodine²⁰, mineral acid²¹, sulfamic acid²² and strontium chloride hexahydrate²³. Our interest was to further explore the interesting dihydropyrimidine core and its synthesis. With an equal interest towards the synthesis of tetrazolopyrimidines, which still remain unexplored in terms of its synthesis and biological activity. According to our extensive literature survey we understood that the available synthetic protocols include high temperatures, prolonged reaction time, drastic reaction conditions, low yields and the use of often expensive acid catalysts. In order to develop a simpler protocol for the synthesis of these biologically important compounds, we optimized and herein report pyridinium trifluoroacetate catalysed synthetic method. Further to our interest the catalyst is readily available from commercial sources and is an economic catalyst.

2. Results and Discussion

Because of its favourable acidity, pyridinium triflate catalyses biginelli three component coupling reaction between aldehyde, urea or 5-amino tetrazole and the β -keto ester. Further the microwave irradiation at 90°C effectively reduces the reaction completion time from 4 hours (reflux) to for 40 min with good to excellent yields (**Scheme 1**). The method is worked and well optimized for both aromatic aldehydes and functional hetero-aromatic aldehydes. Wide range of aldehydes with electron withdrawing and electron donating substituents are experimented under the pyridinium triflate catalysed reaction condition.



Scheme 1. Representative triflate salt (TFA: pyridine) mediated synthesis of dihydropyrimidines and Tetrazolo pyrimidines

It was observed longer reaction time in the case of the electron withdrawing substituent in the aldehyde phenyl ring that further affected the yield (**5g** in **Table 1**) of product. The positive mesomeric effect of *p*-Chloro substituent enhanced the reaction yield (**5e**) with the reduction in the reaction completion time. The steric hindrance at *ortho* position reduced the reaction yield (**5f**). The nature and position of the substituents in the aromatic aldehydes affected the course of the reaction and product yield.

Heteroaromatic aldehydes were also undergone the biginelli reaction with the pyridinium triflate mediated protocol so as to generalize the reaction condition for all the aromatic systems. Compared to the aromatic systems it was observed that the heteroaromatic systems produced less yield.

Table 1
General synthesis of pyridinium triflate mediated dihydropyrimidines

Compound	R ₁	R ₂	X	Time (min)	Yield (%) ^a	Mp (°C)
5a	phenyl	CH ₃	O	10	98	201-203
5b	Phenyl	CH ₃	S	15	83	207-208
5c	Phenyl	H	O	14	96	190-191
5d	3-Methoxy phenyl	CH ₃	O	38	90	220-222
5e	4-Chloro phenyl	H	S	15	97	138-139
5f	2-hydroxy-5- <i>t</i> -butyl phenyl	CH ₃	O	35	70	222-225
5g	3,5-Bis trifluoromethyl phenyl	CH ₃	O	40	65	209-210
5h	2-Thienyl	CH ₃	O	28	75	204-205
5i	2-Imidazolyl	CH ₃	O	30	70	249-251
5j	2-Pyridyl	CH ₃	O	32	84	180-182
5k	2-Thiazolyl	CH ₃	O	38	60	211-213

^a Isolated yield

^b All the target molecules were characterized with IR, LCMS, ¹H NMR, ¹³C NMR.

Similar trend with respect to the substituents in the aldehydic groups was observed during the synthesis of tetrazolopyrimidines also (**Table 2**). Thus the versatility of pyridinium trifluoroacetate mediated route was clear from the good to excellent yields of dihydropyrimidines and tetrazolopyrimidines under microwave assisted reaction conditions. Further we have achieved the synthesis of the title compounds with commercially available and economic catalyst with reduced reaction times.

Table 2
General synthesis of pyridinium triflate mediated tetrazolo [1,5*a*] pyrimidines.

Compound	R ₁	R ₂	Time (min)	Yield (%) ^{a,b}	Mp (°C)
6a	Phenyl	CH ₃	25	98	196-198
6b	3-Methoxy phenyl	H	28	83	184-185
6c	3-phenyl propinal	CH ₃	30	95	165-166
6d	2-Fluoro	CH ₃	30	89	180-183
6e	2-Pyridyl	CH ₃	27	90	256-257
6f	3-Thiophenyl	CH ₃	35	85	197-198
6g	3-Thiophenyl	H	25	89	183-184
6h	5-Br-2-thiophenyl	CH ₃	35	68	180-181
6i	2-Furyl	CH ₃	34	75	189-192
6j	phenyl ^c	dimedone	25	93	268-273
6k	4-biphenyl ^c	dimedone	20	95	287-288

^a Isolated yield,

^b All the target molecules were characterized with IR, LCMS, ¹H NMR, ¹³C NMR.

^c All reactions were carried out using Dimedone instead of Ethyl aceto acetate.

We have compared the reactivity of the pyridinium triflate catalysed biginelli reaction with the ammonium trifluoroacetate catalysed condition. It was observed from the comparison experiments (**Table 3**) that the pyridinium catalyst has improved the yield of the reaction when compared to other catalyst.

Table 3
Catalyst optimization for the synthesis of 5a, 6a under solvent- media

Entry	Triflate salt ^{a,b}	Temp (°C)	Time (min)	Yield (%)
1	CF ₃ COONH ₄ ^c	90	40	89 (5a) & 85 (6a)
2	Pyridinium trifluoroacetate	90	25	95 (5a) & 93 (6a)

^a All the reaction were carried out in 1:1 ratio.

^b All the reaction were carried out in both acetonitrile and ethanol.

^c Ammonium Trifluoroacetate

3. Conclusions

A new method of synthesis for dihydropyrimidines and tetrazolopyrimidines was accomplished mediated by pyridinium triflate catalyst. In general the reaction time for the synthesis has been reduced with the utility of microwave assisted synthesis. The evaluation of anticancer and antioxidant activity of the synthesized novel tetrazolopyrimidines will be of our future interest.

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4. Experimental

4.1 Materials and Methods

Common reagents and solvents were purchased from commercial sources. ^1H NMR (300 or 400 MHz) and ^{13}C NMR (75 or 100 MHz) spectra were recorded in DMSO- d_6 on a Bruker DPX 300 and 400 MHz spectrometer with chemical shifts being reported in parts per million (δ) relative to internal standard tetramethylsilane. IR spectra were obtained as mineral- oil mulls on a Spekord N80 spectrophotometer in the frequency of absorption (cm^{-1}). Low resolution mass spectra were recorded at ionizing voltage (eV) by electron impact. Melting points were determined with Buchi melting B-545.

4.2 General procedure

A mixture of aldehyde (1 mmol), β -diketo ester/ dimedone (1 mmol), Urea (1.5 mmol) / thiourea (1.5 mmol) / 5-amino tetrazole (1 mmol) and pyridinium Trifluoroacetate (0.5 mmol) was taken in a microwave vial and irradiated at 90°C for 30 to 40min. After cooling, solid formed was filtered and washed with cold water ($2 \times 10\text{ml}$) followed by diethyl ether, if necessary recrystallised from ethanol or ethyl acetate to afford pure product.

4.3 Physical and Spectral Data

Compound- 5b: ^1H NMR (300 MHz, DMSO- d_6): δ 10.33 (s, 1H), 9.65 (brs, 1H), 7.36-7.19 (m, 5H), 5.16 (d, 1H, $J = 3.6$ Hz), 4.03 (q, 2H), 2.28 (s, 3H), 1.10 (t, 3H). ^{13}C NMR (75 MHz, DMSO- d_6): 174.7, 165.6, 145.5, 143.9, 129.0, 128.1, 126.8, 101.2, 60.0, 54.5, 17.6, 14.5. IR (KBr): 3328, 3174, 3106, 2982, 1671, 1573, 1467, 1422, 1327, 1197, 1117, 1026, 722 cm^{-1} . LC/MS: m/z 277 ($\text{M}+\text{H}^+$).

Compound- 5c: ^1H NMR (300 MHz, DMSO- d_6): δ 9.20 (s, 1H), 7.74 (brs, 1H), 7.31-7.20 (m, 5H), 5.13 (d, 1H, $J = 3.42$ Hz), 3.51 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (75 MHz, DMSO- d_6): 166.3, 152.6, 149.1, 145.1, 128.9, 127.7, 126.6, 99.5, 54.2, 51.2, 18.3. IR (KBr): 3446, 3333, 3222, 2950, 1696, 1667, 1437, 1349, 1239, 1094, 792, 698, 520, 458 cm^{-1} LC/MS: m/z 247 ($\text{M}+\text{H}^+$).

Compound-5d : ^1H NMR (300 MHz, DMSO- d_6): δ 9.19 (s, 1H), 7.73 (brs, 1H), 7.23 (t, 1H), 6.81-6.76 (m, 3H), 5.10 (s, 1H), 3.99 (q, 2H, $J = 7\text{Hz}$), 3.70 (s, 3H), 2.22 (s, 3H), 1.11 (t, 3H, $J = 7.08$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): δ 165.8, 159.7, 152.6, 148.9, 146.8, 130.0, 118.7, 112.8, 112.6, 99.6, 59.7, 55.4, 54.2, 18.2, 14.6. IR (KBr): 3240, 3104, 2931, 1704, 1649, 1330, 1091 cm^{-1} . LC/MS: m/z 291 ($\text{M}+\text{H}^+$).

Compound-5e : ^1H NMR (300 MHz, DMSO- d_6): δ 10.40 (s, 1H), 9.68 (s, 1H), 7.43-7.40 (d, 2H, $J = 9$ Hz) 7.23-7.20 (d, 2H, $J = 9$ Hz), 5.16 (s, 1H), 3.54 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (75 MHz, DMSO- d_6): δ 174.7, 166.0, 146.1, 142.6, 132.8, 129.1, 128.7, 100.5, 53.8, 51.6, 17.7. IR (KBr): 3313, 3169, 2995, 2947, 1715, 1570, 1190, 1113, 827 cm^{-1} LC/MS: m/z 297 ($\text{M}+\text{H}^+$).

Compound-5f : ^1H NMR (300 MHz, DMSO- d_6): δ 9.33 (s, 1H), 9.07 (s, 1H), 7.04-7.00 (m, 3H), 6.70-6.67 (d, 1H, $J = 8.34$ Hz), 5.37 (brs, 1H), 3.93-3.89 (q, 2H, $J = 7$ Hz), 2.23 (s, 1H), 1.17 (s, 9H), 1.05-1.00 (t, 3H, $J = 7$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): δ 166.0, 152.9, 152.7, 148.7, 140.9, 129.4, 125.3, 124.5, 115.5, 98.2, 59.3, 50.8, 33.9, 31.8, 18.1, 14.6. IR (KBr): 3382, 3283, 2958, 1678, 1629, 1219, 1003, 876, 605 cm^{-1} LC/MS: m/z 331 ($\text{M}-\text{H}^+$).

Compound-5g : ^1H NMR (300 MHz, DMSO- d_6): δ 9.41 (s, 1H), 80.5 (s, 1H), 7.91-7.84 (m, 3H), 5.37 (brs, 1H), 3.99-3.96 (q, 2H), 2.26 (s, 3H), 1.07-1.02 (t, 3H). ^{13}C NMR (75 MHz, DMSO- d_6): δ 165.4, 152.0, 150.3, 148.7, 131.0, 130.7, 127.5, 125.1, 98.3, 59.9, 54.0, 18.3, 14.3. IR (KBr): 3441, 3321, 1654, 1543, 1275, 1118, 896, 676 cm^{-1} . LC/MS: m/z 395 ($\text{M}-\text{H}^+$).

Compound-5h : ^1H NMR (300 MHz, DMSO- d_6): δ 9.33 (brs, 1H), 7.91 (brs, 1H), 7.35 (d, 1H, $J = 4.98$ Hz), 6.94-6.88 (m, 2H), 5.26 (s, 1H), 4.08 (q, 2H, $J = 7.08$ Hz), 2.20 (s, 3H), 1.17 (t, 3H, $J = 7.11$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): 165.5, 160.0, 152.7, 149.2, 127.1, 125.1, 123.9, 100.3, 59.8, 49.8, 18.1, 14.6. IR (KBr): 3446, 3336, 2983, 1628, 1457, 1315, 1231, 1157, 1025, 710, 556 cm^{-1} LC/MS: m/z 267.1 ($\text{M}+\text{H}^+$).

Compound-5i : ^1H NMR (300 MHz, DMSO- d_6): δ 11.2 (brs, 1H), 8.96 (s, 1H), 6.72 (s, 2H), 4.93 (s, 1H), 4.05-3.98 (q, 2H, $J = 7$ Hz), 2.19 (s, 3H), 1.14-1.09 (t, 3H, $J = 7$ Hz). IR (KBr): 3358, 3165, 3039, 2980, 2900, 2810, 1654, 1511, 1207, 1016, 818, 657 cm^{-1} LC/MS: m/z 251 ($\text{M}+\text{H}^+$).

Compound-5j : ^1H NMR (300 MHz, DMSO- d_6): δ 9.25 (s, 1H), 8.59-8.57 (d, 1H, $J = 4.5$ Hz), 7.96-7.91 (t, 1H, $J = 7.6$ Hz), 7.70 (s, 1H), 7.44-7.40 (m, 2H), 5.28 (brs, 1H), 3.97-3.91 (q, 2H, $J = 7$ Hz), 2.22 (s, 3H), 1.09-1.01 (t, 3H, $J = 7$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): δ 165.6, 161.7, 152.3, 149.9, 147.8, 139.5, 123.9, 122.4, 97.6, 59.6, 55.6, 18.4, 14.5. IR (KBr): 3209, 3081, 2947, 1698, 1650, 1068, 814 cm^{-1} LC/MS: m/z 262 ($\text{M}+\text{H}^+$).

Compound- 5k : ^1H NMR (300 MHz, DMSO- d_6): δ 9.39 (brs, 1H), 7.99 (brs, 1H), 7.72-7.71 (d, 1H, $J = 3.21$ Hz), 7.62-7.61 (d, 1H, $J = 3.21$ Hz), 5.47 (brs, 1H), 4.08-4.01 (q, 2H, $J = 7$ Hz), 2.22 (s, 3H), 1.15-1.09 (t, 3H, $J = 7$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): δ 173.3, 165.3, 152.5, 150.4, 142.9, 120.7, 98.5, 59.9, 52.0, 18.2, 14.6. IR (KBr): 3204, 3074, 2855, 1692, 1632, 1214, 1088, 944, 752 cm^{-1} LC/MS: m/z 268 ($\text{M}+\text{H}^+$).

Compound- 6a : ^1H NMR (300 MHz, DMSO- d_6): δ 11.33 (s, 1H), 7.34-7.28 (m, 5H), 6.64 (s, 1H), 3.97-3.92 (q, 2H, $J = 7$ Hz), 2.44 (s, 3H), 1.02 (t, 3H, $J = 7$ Hz). ^{13}C NMR (100 MHz, DMSO- d_6): 164.5, 148.4, 146.6, 140.9, 128.7, 128.5, 127.2, 97.7, 59.6, 58.7, 18.4, 13.8. IR (KBr): 3224, 3162, 3053, 2986, 2946, 1696, 1656, 1569, 1299, 1230, 1099, 1019, 655 cm^{-1} . LC/MS: m/z 286 ($\text{M}+\text{H}^+$).

Compound- 6b: ^1H NMR (400 MHz, DMSO- d_6): δ 14.33 (brs, 1H), 11.31 (1H, s), 7.28-7.24 (m, 1H), 6.89-6.81 (m, 3H), 6.64 (1H, s), 6.48 (2H, s), 3.73 (s, 3H), 3.53 (s, 3H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6): 165.2, 159.3, 156.4, 148.5, 146.8, 142.3, 130.1, 119, 113.4, 113.3, 97.5, 58.5, 55.1, 51.1, 18.5. IR (KBr): 3474, 3335, 3260, 3187, 2950, 1661, 1575, 1431, 1298, 1158, 1034, 772 cm^{-1} .LC/MS: m/z 301 ($\text{M}+\text{H}^+$).

Compound- 6c: ^1H NMR (300 MHz, DMSO- d_6): δ 11.3 (brs, 1H), 7.26-7.10 (m, 5H), 6.42 (s, 1H), 5.62 (1H, s), 4.12-4.05 (q, 2H, $J = 7$ Hz), 2.48 (m, 2H), 2.32 (3H, s), 2.09 (2H, m), 1.16 (t, 3H, $J = 7$ Hz). ^{13}C NMR (100 MHz, DMSO- d_6): 165.2, 149.7, 148, 140.7, 128.7, 128.6, 126.4, 97.1, 60.2, 55.2, 37.7, 30.8, 18.9, 14.5. IR (KBr): 3384, 3184, 3057, 2980, 2854, 1698, 1562, 1451, 1220, 1097, 698 cm^{-1} . LC/MS: m/z 312 (M- H^+).

Compound- 6d: ^1H NMR (300MHz, DMSO- d_6): δ 1.00 (3H, t, $J=7.08$ Hz), 2.50 (3H, s), 3.94 (2H, q, $J=7.08$ Hz), 6.88 (1H, s), 7.21-7.16 (2H, m), 7.40-7.34 (2H, m), 11.36 (1H, brs, NH). ^{13}C NMR: (75 MHz, DMSO- d_6): δ 14.2, 18.9, 53.8, 60.1, 96.7, 116, 116.2, 125.2, 125.3, 128.2, 128.3, 130.1, 130.2, 131.2, 131.3, 147.7, 148.9, 158.9, 161.4, 164.8. IR (KBr): 3227, 3057, 2986, 2945, 1657, 1569, 1491, 1333, 1270, 1126, 1021, 855, 754. cm^{-1} . LC/ MS: m/z 303 (M+ H^+).

Compound- 6e: ^1H NMR (300 MHz, DMSO- d_6): δ 11.2 (brs, 1H), 8.42-8.41 (m, 1H), 7.81 (t, 1H), 7.59-7.56 (1H, t, $J = 7.6$ Hz), 7.24 (1H, t), 6.74 (1H, s), 3.97-3.92 (q, 2H, $J = 7$ Hz), 2.44 (s, 3H), 1.02 (t, 3H, $J = 7$ Hz). ^{13}C NMR (100 MHz, DMSO- d_6): 165.1, 158.8, 150.2, 149.6, 147.6, 137.3, 124.1, 123, 97.5, 60.1, 60, 19, 14.3. IR (KBr): 3179, 3052, 2946, 1702, 1566, 1277, 1224, 1068, 755 cm^{-1} . LC/MS: m/z 287 (M+ H^+).

Compound- 6f: ^1H NMR (400 MHz, DMSO- d_6): δ 11.3 (brs, 1H), 7.49-7.41 (m, 1H), 7.25-7.1 (m, 3H), 6.70 (1H, s), 4.1- 3.8 (2H, m, $J = 7$ Hz), 2.51 (s, 3H), 1.02 (t, 3H, $J = 7$ Hz). ^{13}C NMR (100 MHz, DMSO- d_6): 164.9, 163.7, 161.3, 148.7, 147.6, 144.1, 144, 131.3, 131.2, 123.9, 123.8, 115.9, 115.7, 114.8, 114.6, 97.5, 60.1, 58.6, 18.9, 14.2. IR (KBr): 3179, 3052, 2946, 1702, 1566, 1277, 1224, 1068, 755 cm^{-1} . LC/MS: m/z 290 (M- H^+).

Compound- 6g: ^1H NMR (400 MHz, DMSO- d_6): δ 11.3 (brs, 1H), 7.48-7.45 (m, 2H), 6.96-6.94 (d, 1H), 6.78 (1H, s), 3.57 (3H, s), 2.49 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6): 165.1, 148.5, 146.7, 141.4, 127.3, 126, 123.8, 97.4, 53.6, 51.1, 18.4. IR (KBr): 3163, 3079, 2942, 1710, 577, 1434, 1269, 1213, 1140, 1065, 763 cm^{-1} . LC/MS: m/z 276 (M- H^+).

Compound- 6h: ^1H NMR (300 MHz, DMSO- d_6): δ 11.5 (brs, 1H), 7.09 (m, 1H), 6.95-6.91 (m, 2H), 6.44 (1H, s), 4.04 (q, 2H, $J = 7$ Hz), 2.43(3H, s), 1.08 (t, 3H, $J = 7$ Hz). ^{13}C NMR (75 MHz, DMSO- d_6): 164.8, 148.6, 147.9, 146, 130.9, 127.7, 112.5, 97.3, 60.4, 53.9, 18.9, 14.4. IR (KBr): 3470, 3336, 3186, 2931, 1642, 1566, 1432, 1297, 1217, 1058, 774. cm^{-1} . LC/MS: m/z 367 (M-2 H^+).

Compound- 6i: ^1H NMR (300MHz, DMSO- d_6): δ 1.12 (3H, t, $J=7.08$ Hz). 2.40 (3H, s), 4.08 (2H, q, $J=7.08$ Hz), 6.30 (1H, s), 6.67 (1H, s), 7.56 (1H, s), 7.69 (1H, s), 11.3 (1H, brs). ^{13}C NMR: (75 MHz, DMSO- d_6): δ 14.4, 18.8, 51.1, 60.2, 97.4, 109.4, 126.2, 141.1, 144.5, 147.1, 149.1, 165.1. IR (KBr): 3787, 3157, 3086, 2935, 1707, 1567, 1383, 1273, 1069, 778. cm^{-1} . LC/MS: m/z 275 (M- H^+).

Compound- 6j: ^1H NMR (300MHz, DMSO- d_6): δ 0.98 (3H, s), 1.05 (3H, s), 2.20-2.14 (2H, m), 2.58 (2H, s), 6.58 (1H, s), 7.31-7.25 (5H, m), 11.6 (1H, s). ^{13}C NMR: (75 MHz, DMSO- d_6): δ 27.5, 28.7, 32.7, 50.3, 57.9, 106.1, 127.6, 128.8, 129.1, 140.9, 148.9, 150.9, 193.5. IR (KBr): 3166, 3058, 2958, 2930, 1647, 1577, 1364, 1314, 734 cm^{-1} . LC/MS: m/z 296 (M+ H^+).

Compound- 6k: ^1H NMR (300MHz, DMSO- d_6): δ 1.1 (6H, s), 2.21-2.09 (2H, m), 2.48 (1H, s), 2.6 (1H, m), 6.64 (1H, s), 7.61-7.58 (4H, m), 7.43-7.34 (5H, m), 11.6 (1H, s). ^{13}C NMR: (100 MHz, DMSO- d_6): δ 27.1, 27.8, 28.2, 32.3, 32.4, 41.2, 49.9, 57.2, 105.5, 126.7, 126.9, 127.6, 127.8, 128.9, 139.5, 140.3, 148.4, 150.6, 193.1. IR (KBr): 3385, 3191, 3048, 2921, 2336, 1644, 1578, 1370, 1051 cm^{-1} . LC/MS: m/z 372 (M+ H^+).

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