**Supplemental Figure Captions**

**Fig. S1:** Active Compound **1**1-(1-benzyl-1H-indol-3-y1)-2, 3, 4, 11-tetrahydro-1H-pyrido[2,1-b] quinazoline exhibiting cytotoxic, anti-clonogenic and G0/G1 cell cycle phase inhibitory properties.

**Figure S2:** Active Coumarin-pyridine/ fused pyridine hybrids (compound **1**, **2** and **3**) demonstrating growth inhibitory activity at G2/M phase and apoptotic cell death.

**Figure S3:** Active pyridine-chalcone analogue (compound **1**) possessing G2/M phase inhibitory and anti-cancerous properties.

**Figure S4:** Active pyrazolo[3,4-b] pyridine-bridged derivative of combretastatin A-4 which acquiring anti-proliferative activity *via* G2/M cell cycle stage arrest.

**Figure S5:** Active pyridylacrylic- and nicotinic-based hydroxamates and 2'-aminoanilides which perform anti-proliferative actions *via* G2/M stage inhibition.

**Figure S6**: Active Thieno[2,3-b] pyridine analogues (compound **1**, **2**, **3** and **4**) acquiring anti-tumorigenic activity.

**Figure S7:** BTPT [2-(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)-6-methoxy-4-(thiophen-2-yl) pyridine] having anti-proliferative property

**Figure S8:** Active picolinamide derivatives (compound **1**, **2** and **3**) acquiring anti-tumorigenic property.

**Figure S9:** Active pyridine and fused pyridine (Compounds **1- 6**) having anti-tumorigenic property.

**Figure S10:** Substituted 6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]pyridine analogues (compounds **1-10**) exhibiting cytotoxic action.

**Figure S11:** Active thiazole-imidazopyridine derivative (Compound **1**) demonstrating cytotoxicity actions.

**Figure S12:** Active pyridopyrazolopyrimidine and pyridopyrazolotriazine derivatives (Compounds **1** and **2**)having cytotoxic attributes.

**Figure S28:** Active thieno[2,3-e][1,2,3]triazolo[1,5-a] pyrimidines and thieno[3,2e][1,2,3]triazolo[1,5-a] pyrimidines backbone with anti-tumorigenic properties.

**Figure S29:** Active 6,7-dihydro-5H-cyclopenta[d]pyrimidine analogues (Compounds **1** and **2**) exhibiting vascular endothelial growth factor receptor (VEGFR) inhibitory action.

**Figure S30:** Active camphor-derived pyrimidine analogue (Compound **1**) which performs cytotoxic action by a ROS- arbitrated mitochondrial apoptosis pathway

**Figure S31:** Active chalcone 3 analogue exhibiting anti-cancer property in association with the active site of DHFR (dihydrofolate reductase).

**Figure S32:** Active thiazolopyrimidine derivatives (Compounds **1** and **2**) with anti-tumor activity

**Figure S33:** Active 2-fpyrano[2,3-c]pyrazoles-4-ylidenegmalononitrile derivatives (Compounds **1** and **2**)displayingstrong cytotoxic actions.

**Figure S34:** Active pyrimidine derived JAK3 inhibitor (Compound **1**)

**Figure S35:** Active pyrimidinone ring analogues (Compounds **1-5**) having cytotoxic properties.

**Figure S36:** Active azacalix [2] arene [2] pyrimidine backbone exhibiting anti-cancer property *via* showing affinity towards the CK2 protein kinase.

**Figure S37:** Active DHPM (3,4-dihydropyrimidine-2(1H)-one) and 2,6-diaryl-substituted pyridine analogues (Compounds **1-4**) with anti-tumorigenic properties.

**Figure S38:** Active [1,2,3] triazolo[4,5-d] pyrimidine analogue (compound **1**) having LSD1 inhibitory action

**Figure S39:** Active 5-methylpyrazolo[1,5-a] pyrimidine analogues (Compounds **1-4**) exhibiting cytotoxic action.

**Figure S40:** Active oxazolopyrimidines analogues (Compounds **1-3**) demonstrating cytotoxic property.

**Figure S41:** Active thiazolo[3,2-a]pyrimidine hydrobromide analogues (Compounds **2-4**) acquiring cytotoxic properties.

**Figure S42:** Active halogen- and/or nitrogen-containing pyrimidine analogues (Compounds **1** and **2**) correspondingly as ABC transporter inhibitor and ABC transporters-arbitrated MDR reverser.

**Figure S43:** Active compound 2-Amino-8-(2-chlorobenzylidene)-4-(2-chlorophenyl)-5,6,7,8- tetrahydro-4H-chromene-3-carbonitrile (compound **1**) possessing cytotoxic properties.

**Figure S44:** Active 1,2,4-oxadiazole derivatives (Compounds **1-10**) displaying antiproliferative action.

**Figure S45:** Active pyrazole (Compounds **1-4**) and pyrazolo[1,5-a] pyrimidine (Compounds **5- 10**) exhibiting anti-tumorigenic activity.

**Figure S46**: Active triazole- fused pyrimidine analogue having anti-proliferative property.

**Figure S47:** Active chromeno[2,3-d] pyrimidine and chromeno triazolo[1,5-c] pyrimidine analogues (Compounds **1-3**) displaying anti-tumor properties.

**Figure S48:** Active pyrrolo[2,3-d]pyrimidine, the thieno[2,3-d]pyrimidine (compound **1**) revealed to be a RET inhibitor to check tumor cells movement

**Figure S49:** Active diphenyl-4-thioxo-1,4-dihydropyrimidin-5-yl)ethan-1-one analogues backbone possessing anti-tumorigenic action.

**Figure S50:** Active ring-fused pyrazoloamino pyridine/pyrimidine analogue (compound **1**) as potent FAK inhibitor.

**Figure S51:** Active thieophene derivatives (Compounds **1-18**) acquiring anti-tumor property.

**Figure S52:** Active 6-aryl-5-cyano-py pyrimidine-based benzothiazole analogue (Compound **1**) acquiring potent CDK2/cyclin A2 inhibitory properties.

**Figure S53:** Active triazolopyrimidines and sulfanylpyrimidines derivatives (Compounds **1** and **2**) which impede growth *via* COX-2 inhibition.

**Figure S54:** Active indole/isatin conjugated phenyl-amino-pyrimidine derivative which acts as BCR-ABL inhibitor.

**Table Captions**

**Table 1. Synthetic Pyridine Derivatives with Anticancer activity**

**Table 2. Synthetic Pyrimidine Derivatives with Anticancer activity**



**Figure 1.** Basic ring structures of pyridine and pyrimidine









  

**Figure 2:** Marketed anticancer drugs with pyridine **(a-d)** and pyrimidine **(e-f)** moieties.



**Fig. S1:** Active Compound **1**1-(1-benzyl-1H-indol-3-y1)-2, 3, 4, 11-tetrahydro-1H-pyrido[2,1-b] quinazoline exhibiting cytotoxic, anti-clonogenic and G0/G1 cell cycle phase inhibitory properties.

  

**Figure S2:** Active Coumarin-pyridine/ fused pyridine hybrids (compound **1**, **2** and **3**) demonstrating growth inhibitory activity at G2/M phase and apoptotic cell death.



**Figure S3:** Active pyridine-chalcone analogue (compound **1**) possessing G2/M phase inhibitory and anti-cancerous properties.



R = 3-HO,4-CH3OC6H

**Figure S4:** Active pyrazolo[3,4-b] pyridine-bridged derivative of combretastatin A-4 which acquiring anti-proliferative activity *via* G2/M cell cycle stage arrest.



 



**Figure S5:** Active pyridylacrylic- and nicotinic-based hydroxamates and 2'-aminoanilides which perform anti-proliferative actions *via* G2/M stage inhibition.

  

**Figure S6**: Active Thieno[2,3-b] pyridine analogues (compound **1**, **2**, **3** and **4**) acquiring anti-tumorigenic activity.



**Figure S7:** BTPT [2-(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)-6-methoxy-4-(thiophen-2-yl) pyridine] having anti-proliferative property







**Figure S8:** Active picolinamide derivatives (compound **1**, **2** and **3**) acquiring anti-tumorigenic property.

 

 

 

**Figure S9:** Active pyridine and fused pyridine (Compounds **1- 6**) having anti-tumorigenic property.

 

 

 

 

 

**Figure S10:** Substituted 6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]pyridine analogues (compounds **1-10**) exhibiting cytotoxic action.



**Figure S11:** Active thiazole-imidazopyridine derivative (Compound **1**) demonstrating cytotoxicity actions.

 

X=Y=H X=CN, Y=NH2

**Figure S12:** Active pyridopyrazolopyrimidine and pyridopyrazolotriazine derivatives (Compounds **1** and **2**)having cytotoxic attributes.



Compound **1** (R=OH) and Compound **2** (R= )



**Figure S13:** Active pyrazole and pyrazolo[1,5-a] pyrimidine derivatives (Compounds **1-4**) responsible for G0-G1 stage cell-cycle detention.

 



**Figure S14:** Active thieno[2,3-d]pyrimidine analogues (Compounds **4,14, 17**) induce apoptosis *via* apoptosis stimulation while compounds **1, 2, 3** exhibited anti-tumorigenic property through G2/ M stage inhibition.

 

**Figure S15:** Active pyrazolo[1,5-a] pyrimidines analogues displaying cytotoxicity action *via* cell cycle detention at G2/M stage.

 



**Figure S16:** Active pyrazolopyrimidine derivatives (Compounds **1-3**) which inhibit cell cycle at metaphase.

 

**Figure S17:** Active HDAC and PI3K dual inhibitors (Compounds **1** and **2**) demonstrating anti-tumorigenic activity



**Figure S18:** Active 1,5-dihydropyrido-triazolo-pyrimidine analogues backbone which targets CK2 (Human Cyclin-defendant Kinase 2) for human cell cycle and meiosis regulation.

  





**Figure S19:** Active pyrimidine-5-carbonitrile analogues (Compounds **1-5**) which seize the cell cycle at G2/M stage and stimulate apoptosis.



**Figure S20:** Active adenine guanine analogue (compound **1**) which inhibits cancer development by cell cycle regulation and DNA replication

 

 

**Figure S21:** Active hetaryl thiazoles and thiazolyl chalcones (Compounds **1-4**) acquiring anti-tumorigenic actions



**Figure S22:** Active 2,7-disubstituted-thieno[3,2-d]pyrimidine derivative (compound **1**) as active suppressor of MDA-MB-231 cells migration



**Figure S23:** Active triazolo-pyridazine/-pyrimidine derivative (compound **1**) as a potent class II c-Met inhibitor.





**Figure S24:** Active pyrimidine pyrazoline-anthracene analogues (Compounds **1-4**) which induced apoptosis *via* caspase 3/7 activation.



**Figure S25:** Active 6-aryl-5-cyano-pyrimidine analogue (Compound **7**) responsible for caspase 3 activation during pro-apoptosis.

 

a (R=H); b (R=Ph)

  



**Figure S26:** Active pyrazole, diaminopyrimidine, pyrazolo[1,5-a] pyrimidines, triazolo [4,3- a]pyrimidines and imidazo[1,2-a]pyrimidine analogues acquiring anti-tumorigenic property.



**Figure S27:** Active oxacalix[2]arene[2]pyrimidine analogue demonstrating cytotoxic and apoptotic actions.

 

**Figure S28:** Active thieno[2,3-e][1,2,3]triazolo[1,5-a] pyrimidines and thieno[3,2e][1,2,3]triazolo[1,5-a] pyrimidines backbone with anti-tumorigenic properties.



**Figure S29:** Active 6,7-dihydro-5H-cyclopenta[d]pyrimidine analogues (Compounds **1** and **2**) exhibiting vascular endothelial growth factor receptor (VEGFR) inhibitory action.



**Figure S30:** Active camphor-derived pyrimidine analogue (Compound **1**) which performs cytotoxic action by a ROS- arbitrated mitochondrial apoptosis pathway



**Figure S31:** Active chalcone 3 analogue exhibiting anti-cancer property in association with the active site of DHFR (dihydrofolate reductase).





**Figure S32:** Active thiazolopyrimidine derivatives (Compounds **1** and **2**) with anti-tumor activity

 

**Figure S33:** Active 2-fpyrano[2,3-c]pyrazoles-4-ylidenegmalononitrile derivatives (Compounds **1** and **2**)displayingstrong cytotoxic actions.



**Figure S34:** Active pyrimidine derived JAK3 inhibitor (Compound **1**)

 

 



**Figure S35:** Active pyrimidinone ring analogues (Compounds **1-5**) having cytotoxic properties.



**Figure S36:** Active azacalix [2] arene [2] pyrimidine backbone exhibiting anti-cancer property *via* showing affinity towards the CK2 protein kinase.

 

**Figure S37:** Active DHPM (3,4-dihydropyrimidine-2(1H)-one) and 2,6-diaryl-substituted pyridine analogues (Compounds **1-4**) with anti-tumorigenic properties.



**Figure S38:** Active [1,2,3] triazolo[4,5-d] pyrimidine analogue (compound **1**) having LSD1 inhibitory action

 

 

**Figure S39:** Active 5-methylpyrazolo[1,5-a] pyrimidine analogues (Compounds **1-4**) exhibiting cytotoxic action.



**Figure S40:** Active oxazolopyrimidines analogues (Compounds **1-3**) demonstrating cytotoxic property.



**Figure S41:** Active thiazolo[3,2-a]pyrimidine hydrobromide analogues (Compounds **2-4**) acquiring cytotoxic properties.

 

**Figure S42:** Active halogen- and/or nitrogen-containing pyrimidine analogues (Compounds **1** and **2**) correspondingly as ABC transporter inhibitor and ABC transporters-arbitrated MDR reverser.



**Figure S43:** Active compound 2-Amino-8-(2-chlorobenzylidene)-4-(2-chlorophenyl)-5,6,7,8- tetrahydro-4H-chromene-3-carbonitrile (compound **1**) possessing cytotoxic properties.



**Figure S44:** Active 1,2,4-oxadiazole derivatives (Compounds **1-10**) displaying antiproliferative action.

 

 













**Figure S45:** Active pyrazole (Compounds **1-4**) and pyrazolo[1,5-a] pyrimidine (Compounds **5- 10**) exhibiting anti-tumorigenic activity.



**Figure S46**: Active triazole- fused pyrimidine analogue having anti-proliferative property.

 



**Figure S47:** Active chromeno[2,3-d] pyrimidine and chromeno triazolo[1,5-c] pyrimidine analogues (Compounds **1-3**) displaying anti-tumor properties.



**Figure S48:** Active pyrrolo[2,3-d]pyrimidine, the thieno[2,3-d]pyrimidine (compound **1**) revealed to be a RET inhibitor to check tumor cells movement



**Figure S49:** Active diphenyl-4-thioxo-1,4-dihydropyrimidin-5-yl)ethan-1-one analogues

backbone possessing anti-tumorigenic action.



**Figure S50:** Active ring-fused pyrazoloamino pyridine/pyrimidine analogue (compound **1**) as potent FAK inhibitor.

 

 

 

**Figure S51:** Active thieophene derivatives (Compounds **1-18**) acquiring anti-tumor property.



**R1=Cl; R2=H; R3=NH2**

**Figure S52:** Active 6-aryl-5-cyano-py pyrimidine-based benzothiazole analogue (Compound **1**) acquiring potent CDK2/cyclin A2 inhibitory properties.

 

**Figure S53:** Active triazolopyrimidines and sulfanylpyrimidines derivatives (Compounds **1** and **2**) which impede growth *via* COX-2 inhibition.



**Figure S54:** Active indole/isatin conjugated phenyl-amino-pyrimidine derivative which acts as BCR-ABL inhibitor.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table 1. Synthetic Pyridine Derivatives with Anticancer activity** | | | | | |
| **Year** | **Author** | **Compound** | ***In vitro studies*** | ***In silico studies/ Possible targets*** | **Cell lines** |
| **Cell cycle regulatory activity** | | | | | |
| 2019 | Bathula et al. | 11-(1-Benzyl-1H-indol-3-y1)-2, 3, 4, 11-tetrahydro-1H-pyrido[2,1-b] quinazoline | Cytotoxic, anti-clonogenic; G0/G1 cell cycle phase inhibitor | EGFR kinase | NCI-H460, A549, HCT-15, HT-29, HFL, and DU-145 |
| 2019 | Fayed et al. | Coumarin-pyridine/ fused pyridine hybrids | Growth inhibitors at G2/M phase, apoptotic cell death |  | HCT-116, MCF-7, A549, and HepG-2 |
| 2019 | Xu et al. | Pyridine-chalcone analogues | G2/M phase inhibition; anticancer | Anti-tubulin compounds | H22 xenograft models |
| 2020 | Jian et al | Pyrazolo[3,4-b]pyridine-bridged derivatives of combretastatin A-4 acquiring 3,4,5-trimethoxylphenyl groups | Anti-proliferative actions, G2/M stage arrest | Tubulin polymerization inhibition | HeLa |
| 2021 | Zwergel et al. | Aza-analogues like the regioisomers from the N-hydroxy-3-(4-(2-phenylbutanoyl)amino)phenyl)acrylamide comprising pyridine nucleus | G2/M stage inhibition | HDACs | U937, K562, HCT116, A549 |
| **Anti-tumorigenic activity** | | | | | |
| 2019 | Hassan et al. | Thieno[2,3-b]pyridine analogues | Anti-tumor activity |  | HepG‐2 and MCF‐7 cell |
| 2019 | Murugavel et al. | Heterocyclic sulfur thiophene analogue including pyridine and 1,2,3-triazole components | Anti-proliferative | Human topoisomerase IIα targeting ATP binding site | PC-3, A549 and MDAMB-231 |
| 2019 | Zeidan et al. | Picolinamide derivatives acquiring dithiocarbamate and (thio)urea moieties | Anti-tumor action | VEGFR-2 kinase inhibitors | A549, OVCAR-3, Panc-1, HT29, 786-O |
| 2021 | Hassan et al. | Pyridine and fused pyridine derivatives | Anti-tumor action |  | HepG2, MCF-7 |
| **Cytotoxic activity** | | | | | |
| 2020 | Behbehani et al. | Substituted 6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-b]pyridine and 5,6-dihydrobenzo[h]quinoline systems | Cytotoxicity |  | A549, MCF-7, HCT-116 |
| 2020 | Suma et al. | Chalcone linked thiazole-imidazopyridine analogues library | Cytotoxicity |  | MCF-7, A549, DU-145, MDA MB-231 |
| 2021 | Keshk and Izzularab | Cyanopyridines, pyridopyrazolotriazines and pyridopyrazolopyrimidines | Cytotoxicity |  | HepG-2, PANC-1, A-549 |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table 2. Synthetic Pyrimidine Derivatives with Anticancer activity** | | | | | |
| **Year** | **Author** | **Compound** | ***In vitro studies*** | ***In silico studies/ Possible targets*** | **Cell lines** |
| **Cell cycle regulatory activity** | | | | | |
| 2019 | Ali et al. | Pyrazole and pyrazolo[1,5-a] pyrimidine derivatives | G0-G1 stage cell-cycle detention | CDK2/ cyclin A2 enzyme inhibition | MCF-7, A549, HepG2 and Caco2 |
| 2019 | El-Metwally et al. | 4-(3,5-Dimethyl-1H-pyrazol-1-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidine cyclic and acyclic analogues | Cytotoxicity, cell cycle inhibition, apoptosis stimulation | caspase 3, p53, TopoII | MCF-7, HepG2 |
| 2019 | El-Metwally et al. | 16 Thieno[2,3-d]pyrimidine analogues | G2/ M stage inhibition | Tyrosine Kinase, HER2 and EGFR | HepG2, HCT-116, A431 and MCF-7 |
| 2019 | Metwally et al. | Derivatives of pyrazolo[1,5-a]pyrimidines | Cytotoxicity, cell cycle detention at G2/M stage | PDB-ID: 5IVE | Hela, breast cancer |
| 2019 | Muthuraja et al. | Pyrazolopyrimidine derivatives | Cell cycle inhibition at metaphase | Eg5 inhibitor; ATPase allosteric sites | HeLa |
| 2019 | Yang et al. | Combretastatin A-4 (CA-4) analogues | G2/M phase, anti-tubulin action | Tubulin polymerization inhibitors | A549, HeLa, HEK-293 |
| 2019a | Zhang et al. | Camphor-derived pyrimidine analogues | Anti-tumor action, G0/G1 stage, ROS- arbitrated mitochondrial apoptosis |  | MDA-MB-231, RPMI-8226, A549 |
| 2020 | Abdelrazek et al. | 1,5-Dihydropyrido-triazolo-pyrimidine analogues | Cell cycle regulation and meiosis | CK2 |  |
| 2020 | Eissa et al. | Pyrimidine-5-carbonitrile analogues | Anti-proliferative action at G2M stage | Tyrosine kinase inhibitors of EGFR | HCT-116, HepG-2, MCF-7, A549 |
| 2020 | El-Saidi et al. | Adenine 1 and Guanine 6 analogues | Cell cycle regulation | CDK-2 (cyclin-dependent protein kinase 2), BCL-2 | BCL-2 |
| 2020 | Farghaly et al. | 4-Hetarylthiazoles (rigid chalcones) and thiazole-based chalcones | Cell cycle detention at the G2/M stage, increase in the pre-G1 apoptotic cells | Upregulation of Bax and downregulation of BCL-2 | A549, HepG-2 and MCF-7 |
| 2020 | Wang et al. | 2,7-Disubstituted-thieno[3,2-d]pyrimidine derivatives | G0/G1 stage | Focal adhesion kinase (FAK) inhibitors | A-549, U-87MG and MDA-MB-231 |
| 2020 | Zhang et al. | Triazolo-pyridazine/-pyrimidine derivatives | Cytotoxicity, G0/G1 phase | c-Met kinase | A549, HeLa, and MCF-7 |
| **Cytotoxic activity** | | | | | |
| 2019 | Naagla et al. | Pyrimidine pyrazoline-anthracene analogues | Cell viability / cytotoxicity | Caspase 3/7 | HepG2, Huh-7 |
| 2019 | Amin et al. | 6-Aryl-5-cyano-pyrimidine analogues |  | TS inhibitory activity, Bax/ BCL2 | HePG-2, MCF-7 and HCT-116 |
| 2019 | Farag and Fahim | Enaminonitriles based pyrazole analogues | Anticancer activity |  | MCF-7 |
| 2019 | Huang et al. | Oxacalix[2]arene[2]pyrimidine analogues | Cytotoxicity and apoptosis |  | MCF7, HeLa, A549 and HepG2 |
| 2019 | Salem et al. | Pyrimidine analogues via Cerium (IV) ammonium nitrate | Anti-tumor potential, cytotoxic activity |  | HePG-2, MCF-7, HCT-116 and PC3 |
| 2019 | Shyyka et al. | Thieno[2,3-e][1,2,3]triazolo[1,5-a] pyrimidines and thieno[3,2-e][1,2,3]triazolo[1,5‑a] pyrimidines | Cytotoxicity |  | NCI-60, SK-MEL-5 |
| 2019 | Sobhy et al. | 6,7-Dihydro-5H-cyclopenta[d]pyrimidine analogues |  | VEGFR 2 inhibition | |
| 2019b | Zhang et al. | Hydroxamic acid moiety in a quinazoline-dependent PI3K pharmacophore | In vivo anti-tumor property | HDAC and PI3K dual inhibitors | HGC-27 and HCT116 xenograft models |
| 2020 | Ahmed et al. | Pyrimidine derivatives through polarized (e.g., Chalcone) heterocyclization |  | DHFR | HePG-2 and MCF-7 |
| 2020 | Al-Rashood et al. | Thiazolopyrimidine derivatives |  | DNA binding | 60 diverse cell lines |
| 2020 | Bakhotmah et al. | 2-Fpyrano[2,3-c]pyrazoles-4-ylidenegmalononitrile backbone with pyridine, pyrazole, pyrimidine, chromone, diazepine, pyrano[2,3- d]pyrimidine, and pyrano[2,3-c]pyrazole systems | Cytotoxic actions |  | HCT-116, Hep-G2, and MCF-7 |
| 2020 | Balupuri et al. | Pyrimidine-derived JAK3 inhibitors |  | Active sites of TYK2, JAK1 and JAK2, JAK3 | |
| 2020 | Shakila Banu et al. | Pyrimidine analogues comprising pyrrole nucleus | Cytotoxicity |  | A549 |
| 2020 | Ghoneim et al. | Analogues of pyrimidinone ring with five-membered heterocycles | Cytotoxicity | EGFR | PC-3, HepG-2, HCT116 |
| 2020 | Goudzal et al. | Chain of azacalix [2] arene [2] pyrimidines analogues |  | CK2 protein kinase | |
| 2020 | Hosseinzadeh et al. | DHPM (3,4-dihydropyrimidine-2(1H)-one) and 2,6-diaryl-substituted pyridine analogues | Cytotoxicity | Kinesin Eg5 inhibition | MCF-7, AGS , HEK293 |
| 2020 | Khalaf et al. | Substituted pyrimidines through glycosylation | Cytotoxicity |  | MCF-7, HepG2, RPE-1 |
| 2020 | Li et al. | [1,2,3]Triazolo[4,5-d]pyrimidine derivatives | Cytotoxicity | LSD1 (Lysine specific demethylase 1), MAO-A/-B, kinases like BTK and CDK | |
| 2020 | Luo et al. | 5-Methylpyrazolo[1,5-a]pyrimidine analogues | Cytotoxicity | c-Met kinase | MDA-MB-231, SH-SY5Y, HepG2 and A549 |
| 2020 | Nolan et al. | Oxazolopyrimidines |  | VEGFR2 inhibitors | MDA-MB-231,OVCAR-3 and HCT-116 |
| 2020 | Sekhar et al. | Thiazolo[3,2-a]pyrimidine hydrobromide analogues | Cytotoxicity | Topoisomerase-II | A549, MCF-7, HeLa and SKNSH |
| 2020 | Silbermann et al. | Pyrimidine analogues accompanying (a) halogen- and/or nitrogen-containing residues |  | ABCC1/ ABCG2 inhibitors, ABCG2-mediated MDR | SN-38 |
| 2020 | Yousif et al. | 2-Amino-8-(2-chlorobenzylidene)-4-(2-chlorophenyl)-5,6,7,8- tetrahydro-4H-chromene-3-carbonitrile 1 derivatives | Cytotoxicity |  | HT-29 and A-549 |
| 2021 | Bommera et al. | 1,2,4-Oxadiazole derivatives | Cytotoxicity |  | MCF-7, MDA MB-231, A549 and DU-145 |
| **Anti-tumorigenic activity** | | | | | |
| 2019 | Fouda et al. | Pyrazole and pyrazolo[1,5-a] pyrimidine analogues | Anti-tumor activity |  | HCT-116, MCF-7, and HepG-2 |
| 2019 | Li et al. | Triazole- fused pyrimidine analogues | Anti-proliferative action | LSD1/ KDM1A inhibitors; CD11b and CD86 | OCL-AML3, THP-1, K562 and U937, Raji |
| 2020 | Fatma et al. | Substituted chromeno[2,3-d]pyrimidine and chromenotriazolo[1,5-c]pyrimidine analogues | Anti-tumor action |  | MCF-7, HepG2 |
| 2020 | Lakkaniga et al. | Pyrrolo[2,3-d]pyrimidine derivatives | Tumor cells migration | RET kinase | LC-2/ad cells |
| 2020 | Sakr et al. | Diphenyl-4-thioxo-1,4-dihydropyrimidin-5-yl)ethan-1-one | Antitumorgenic |  | MRC-5, A549 |
| 2020 | Xie et al. | Ring-fused pyrazoloamino pyridine/pyrimidine analogues | Anti-proliferative action | Focal adhesion kinase (FAK) inhibitors | BXPC-3, MDA-MB-231, DU145, NCI-H1975 and 786O |
| 2021 | Singh et al. | Pyrimidine-based cationic amphiphiles (PCAms) | Anti-proliferative and anti-tubercular activity | MDR591 | HeLa and KB-V1 |
| 2021 | El-Sharkawy et al. | Thiophene, thienopyridine, Isooxazole, 2-pyridone analogues | Antitumorigenic |  | SF-268, MCF-7 and NCI-H460 |
| **Derivatives having inhibitory actions** | | | | | |
| 2019 | Diao et al. | Pyrimidine-based benzothiazole analogues | CDK2 Binding | CDK2/ cyclin A2 inhibition | HeLa, PC-3, HCT116, and MDA-MB-231 |
| 2019 | Omar et al. | Triazolopyrimidines and sulfanylpyrimidines | Growth inhibitor | COX-2 inhibition | MCF-7 |
| 2019 | Rahim et al. | Indole/isatin conjugated phenyl-amino-pyrimidine derivatives | BCR-ABL inhibition |  | K-562 |
| 2020 | Asati et al. | Pyrazolo-pyrimidine derivatives | Serine/ threonine kinase inhibition | PIM kinase barriers | |