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A REVIEW ON HETEROCYCLIC RINGS PRESENT IN DRUGS USED IN CANCER TREATMENT

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ABSTRACT
Cancer which is an uncontrollable cell division that can occur in any part of the body, As our Human body is made up of no of billions of cells, depending upon place of origin there are several types of cancer, The drugs used in treatment of cancer has contain Heterocycles in them where the heteroatoms Sulphur, Oxygen and Nitrogen present in the structure are responsible for different modes of action like Tyrosine kinase Inhibitor, Protein Kinase Inhibitor, Epidermal Growth Factor receptor inhibitor, FLT3 Inhibitor, Alkylating agent, Topoisomerase-I inhibitor, Microtubule formation inhibitor and increase in pharmacodynamic and pharmacokinetic properties of the lead molecule like lipohilicity, Hydrogen bonding In this review we summarize current drugs used in cancer treatment, along with their mechanism of action and chemical structures.

KEYWORDS: Cancer, Heterocyclic ring, Pharmacokinetic, Pharmacodynamic, Mechanism of action.

INTRODUCTION
Heterocyclic compounds are inevitable part of many naturally occurring compounds which have therapeutic efficacy like alkaloids, carbohydrates, proteins hemoglobin, vitamins, In Humans they have significant contribution in many biological functions, one of them is formation of DNA and RNA where these heterocyclic rings are present as Nitrogen bases and contribute in cell division. So these nitrogen bases serve as molecular targets in treatment of Cancer.[1] The aim of our present review is to consolidate different types of heterocyclic motifs used in the treatment of cancer.

Cancer can be lucidly defined as Uncontrollable cell division of cells which leads to abnormal cell growth. Its incidence has been increased in recent times According to Indian Council of Medical Research – National Institute of Cancer Prevention and Research in India, estimated number of people living with Cancer is around 2.5 million with new cancer patients registered over 7 lakh annually and cancer related deaths account up to 5,56,400 annually.[2]

The treatments of cancer involve clinical trials, chemotherapy, hormone therapy, personalized and targeted therapies, surgery, maintenance therapy, bone marrow/stem cell transplantation, immunotherapy and vaccination, radiation therapy and integrative medication.[3] In cancer therapy and medications, heterocycle moieties play an important role in drug design due to their biological activity and versatility. Especially oxygen, nitrogen and sulphur-containing heterocyclic scaffolds were found in these types of anticancer drugs.[4][5]

Anti-cancer drugs with Oxygen heterocycles

The oxygen contusing heterocycles are important due to their natural abundance in various forms one such important derivative is Taxol which is an Anticancer drug, other include Benzofuran, Coumarin, chromane Xanthene and all these belonged to fused heterocycles where the hetereocyclic ring fused with other ring systems.

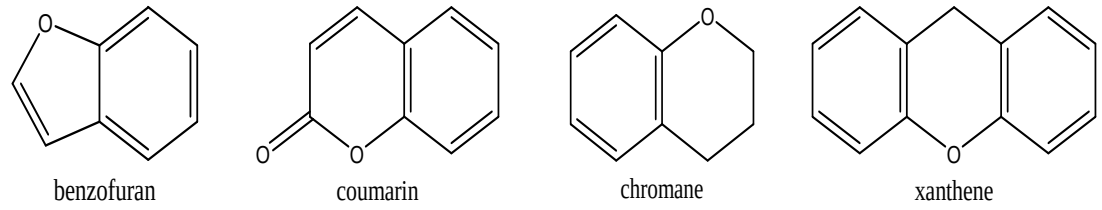

Fig. 1: Heterocycles with oxygen as Hetero atom.

Some of the other oxygen containing ring systems used in cancer treatment are three membered e.g, cryptophycins, Triptolide.

Cryptophycins are a class of dioxadiazacyclohexadecenetetrone cytotoxins with a potent ability to induce tubulin depolymerization. The cryptophycins were first isolated from the cultures of the *Nostoc* cyanobacteria in the early 1990s.[6]

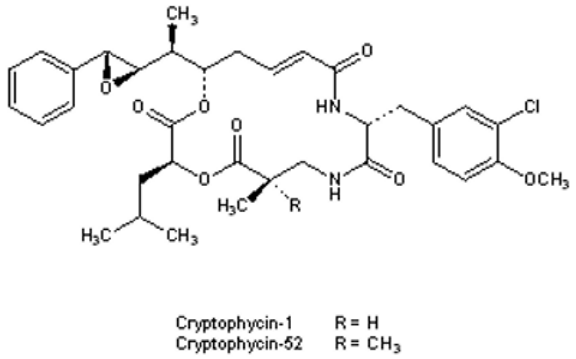

Fig. 2: Cryptophycins.

Triptolide is an important diterpene active compound in *T. wilfordii*. Since 1972, when Kupchan et al. first isolated triptolide and found its significant anti-leukaemic effects.[7]

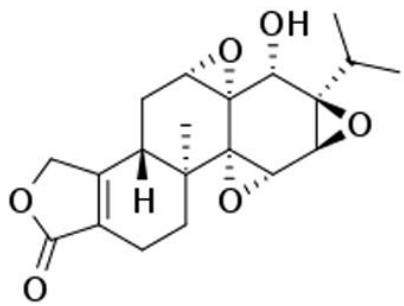

Fig. 3: Triptolide.

Four membered Oxygen containing heterocyclic ring known as Oxetane is found in anti cancer drugs like Paclitaxel, Docetaxel, cabazitaxel, crenolanib.

Paclitaxel, initially named taxol, is a naturally occurring diterpenoid compound extracted from the Pacific yew tree, *Taxus brevifolia*.[8]

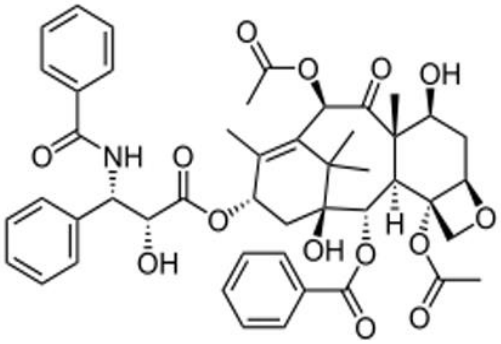

Fig 4: Paclitaxel.

Docetaxel is a complex diterpenoid molecule and a semis synthetic analogue of Paclitaxel.[9]

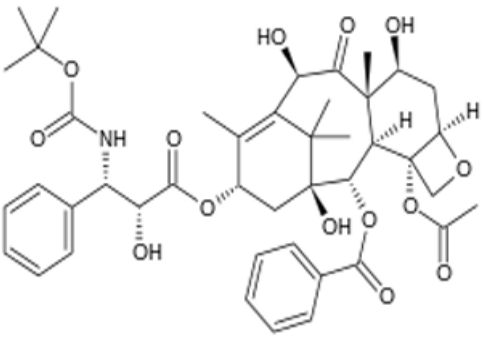

Fig. 5: Docetaxel.

Cabazitaxel is a taxoid synthesized from 10-decacetylbaccatin-iii, a compound found in *Taxas buccata*, It is a second generation semisynthetic microtubule inhibitor.[10]

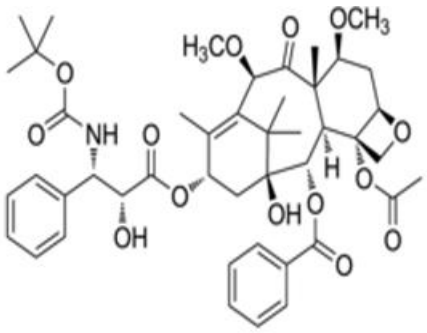

Fig. 6: Cabazitaxel.

Eight membered oxygen containing heterocyclic ring system known as oxocane is found in drugs like Laurencin, Octalactin B. Laurencin is cyclic bromoether isolated from Laurencia species (Laurencia glandulifera) of Rhodomelaceae family in 1965 by Irie et al.[11]

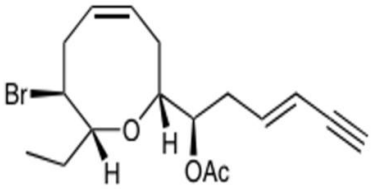

Fig. 7: Laurencin.

Octalactin B belongs to class of β-lactones isolated from marine derived actinomycetes (streptomyces) along with Octalactin A.[12].[13]

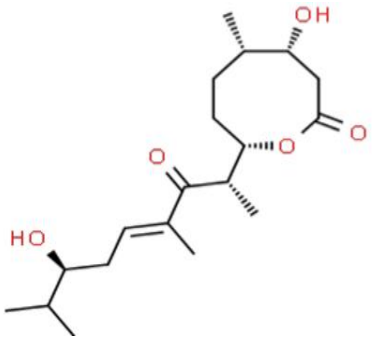

Fig. 8: Octalactin.

Anti-Cancer drugs with Nitrogen Heterocycles

Most of the biologically active compounds in their chemical structure contains pentacyclic or hexacyclic ring structures with atleast one or two nitrogen atoms as hetero atoms[14] like Adennine, Guanine, Cytosine, Thymine, Uracil, Nicotine, Trytamine, thiamine, Riboflavin, Pyridoxal[17] According to US FDA more than 50% of drugs have Nitrogen containing heterocycles in their structures.[15] [16],

Current research for anti cancer drugs mainly focusses on development of the Pyrimidines, Quinoline, Carbazole, Pyridine, Imidazole, Benzimidazole, Triazole, beta lactams, Indole, Pyrazole, quinazoline, Quinaoxaline, isatins.

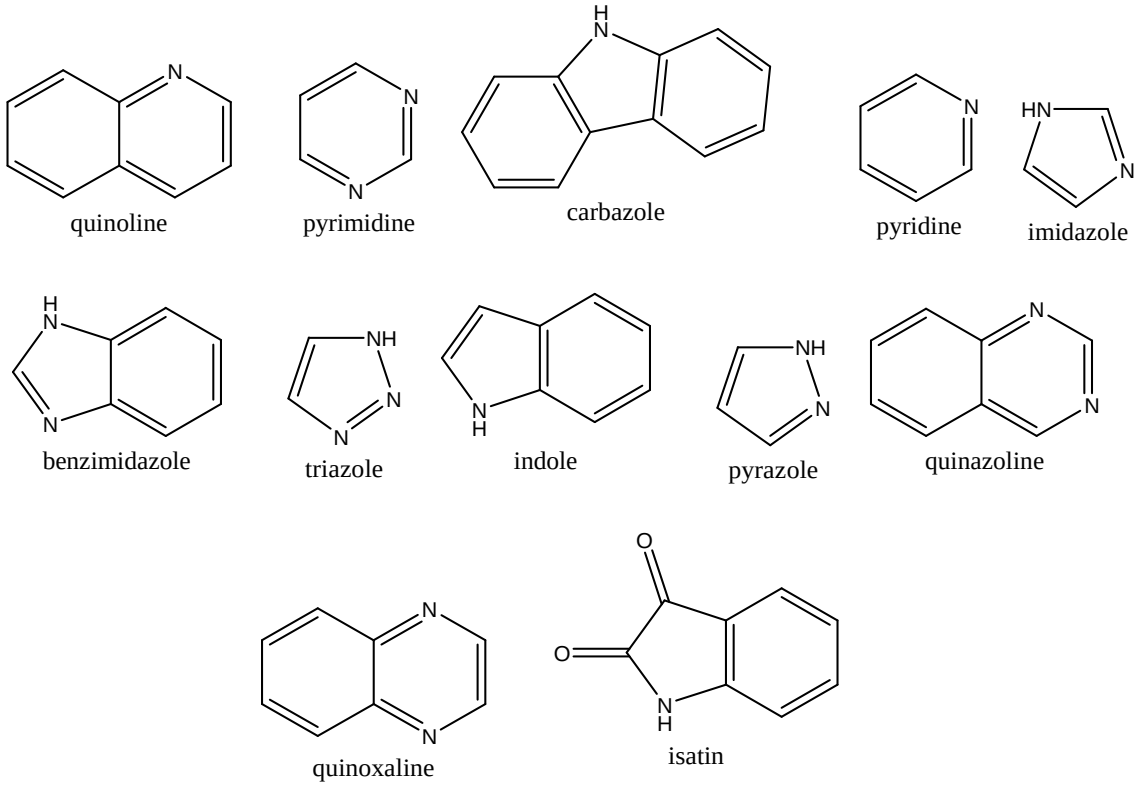

Fig. 9: Heterocycles with Nitrogen as hetero atom.

Aziridine is a three membered nitrogen containing heterocyclic ring and widely found in natural products mainly alkaloids with antimicrobial and anti-cancer properties like mitomycin.

Pyridine is a six membered nitrogen containing heterocyclic compound found in campothecin an anti-cancer agent, following drugs approved by FDA as anti-cancer agents with nitrogen in their structure.

Alectinib Hydrochloride (2015)[19], Brigatinib (2017)[20], Lorlatinib (2018)[21], Entrectinib (2019)[22] are Anaplastic lymphoma kinase inhibitors primarily used I treatment of non-small cell lung cancer.

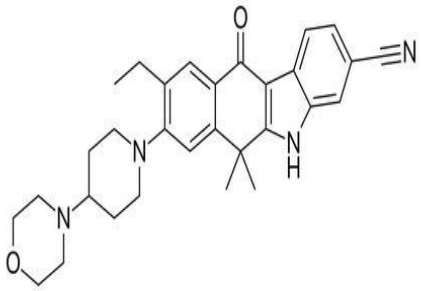

Fig. 10: Alectinib.

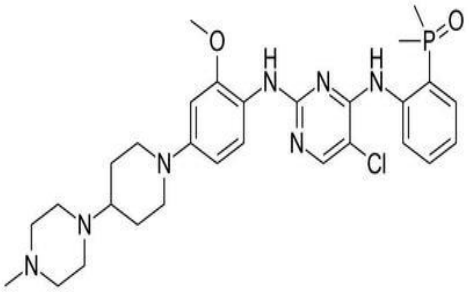

Fig. 11: Brigatinib.

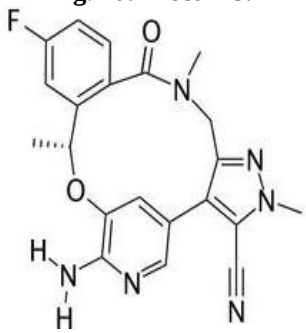

Fig 12: Lorlatinib.

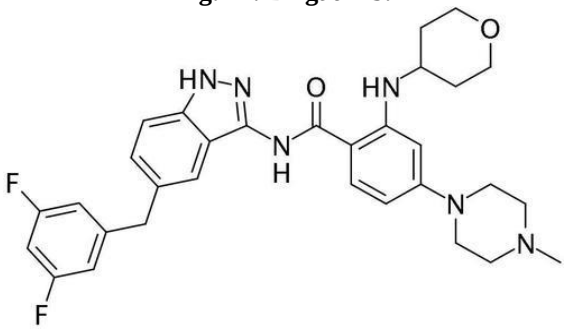

Fig 13: Entrectinib.

Midostaurin (2017)[23,24], Gilteritinib fumarate (2018)[25], Quizartinib (2018)[26] are FMS like tyrosine kinase inhibitor used in various stages of acute myeloid leukemia.

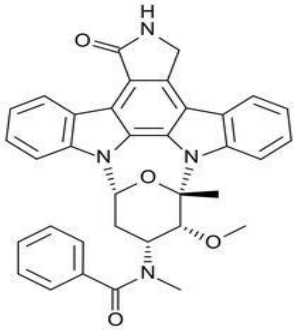

Fig. 14: Midostaurin.

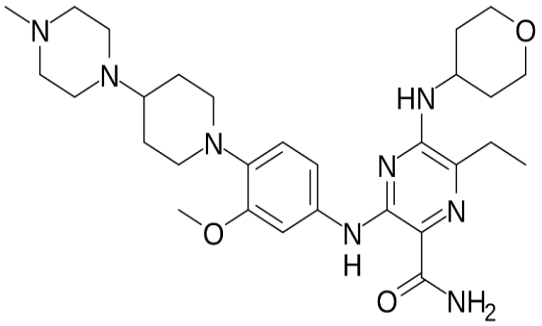

Fig 15: Gilteritinib.

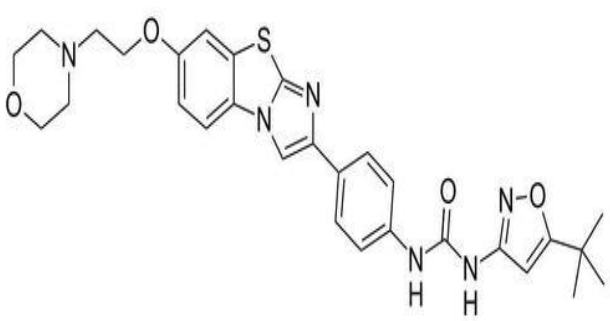

Fig. 16: Quizartinib.

Osimertinib (2018).[28] Olmutinib 2015[29], Neratinib (2017)[30], Dacomitinib (2018)[31], Pyrotinib (2018)[32], Almonertinib (2020)[33] are Epidermal growth factor (EGF) receptor inhibitors used in treatment of non-small lung cancer, pancreatic cancer, breast cancer and colon cancer.

Fig. 17: Osimertinib.

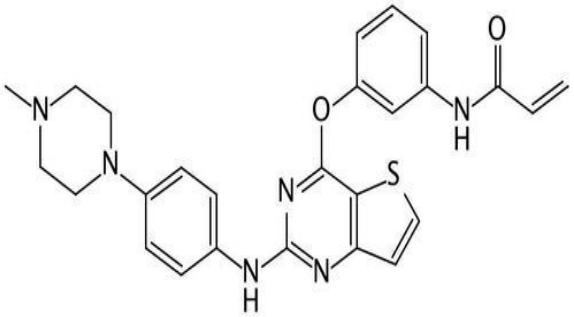

Fig. 18: Olmutinib.

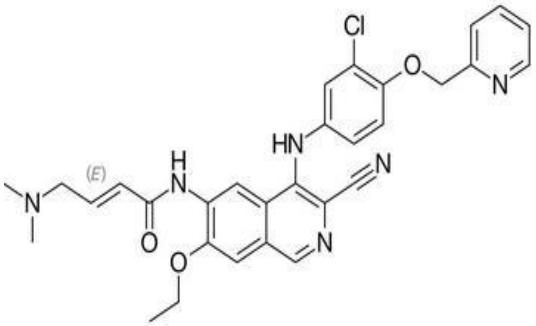

Fig. 19: Neratinib.

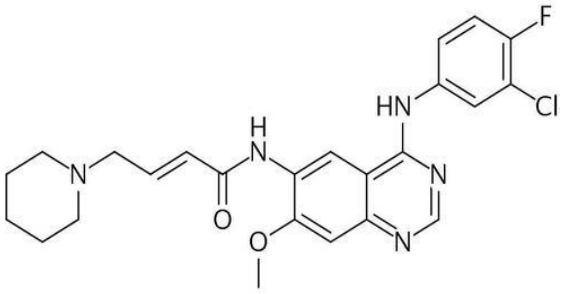

Fig. 20: Dacomitinib.

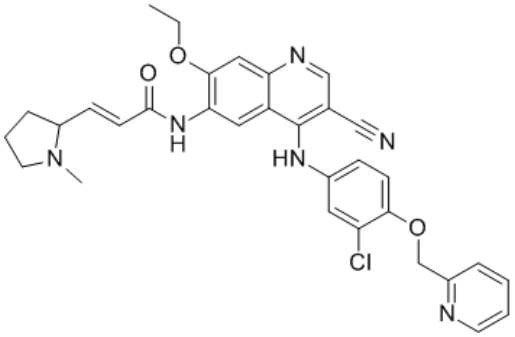

Fig 21: Pyrotinib.

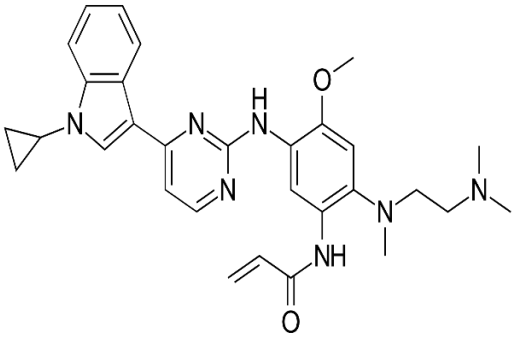

Fig 22: Almonertinib.

Lenvatinib (2015)[34], Tivozanib (2021)[35], Fruquintinib (2020)[36], Anlotinib (2020)[37] are Vascular endothelial growth factor (VEGF) inhibitors used in treatment of cancer which block the growth of blood vessels that support tumor growth.

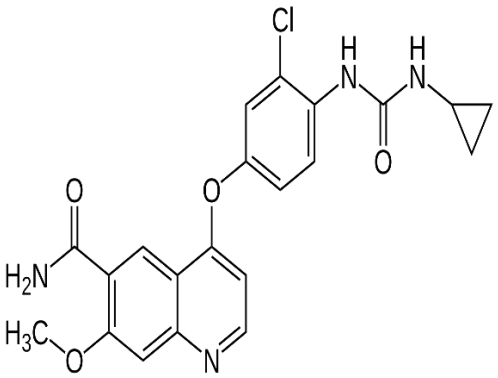

Fig 23: Lenvatinib.

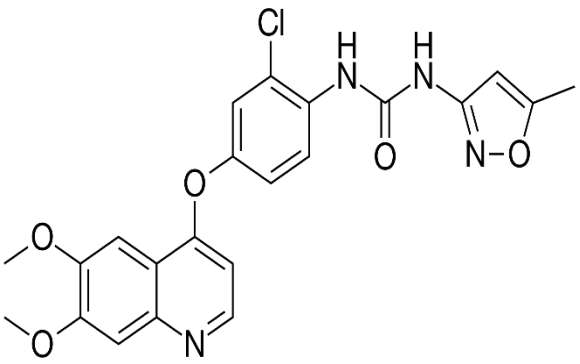

Fig 24: Tivozanib.

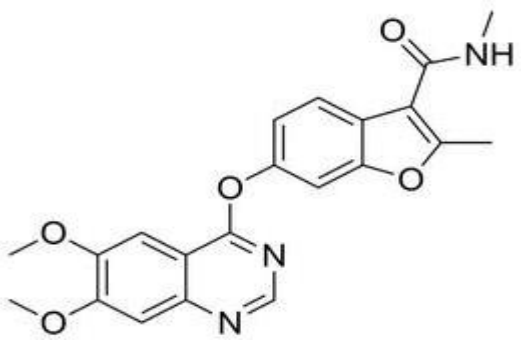

Fig 25: Fruquintinib.

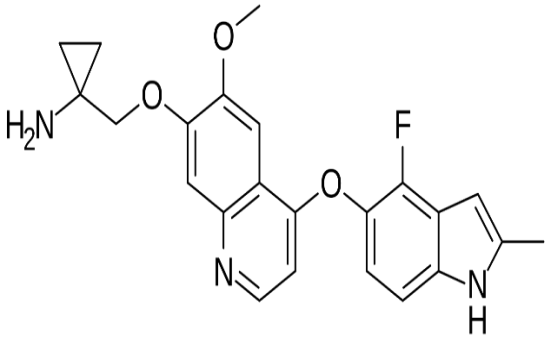

Fig 26: Anlotinib.

Acalabrutinib (2017)[38], Zanubrutinib (2021)[39] and Nilotinib (2007)[104] are Tyrosine kinase inhibitors used in treatment of lung, breast and colon cancer.

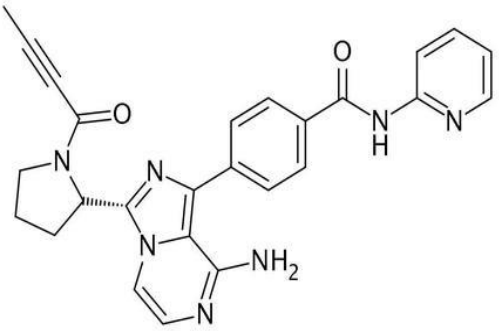

Fig 27: Acalabrutinib.

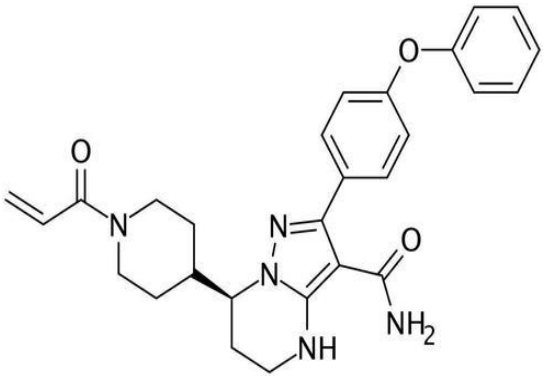

Fig 28: Zanubrutinib.

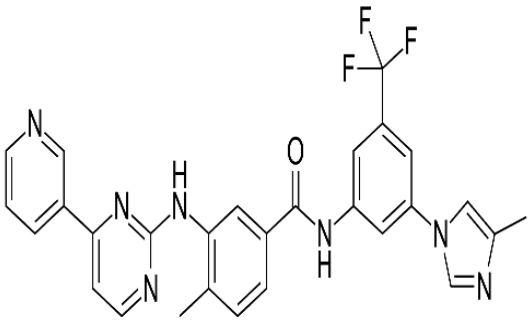

Fig 29: NIlotinib.

Fedratinib (2019)[40] is Janus kinase 2 (JAK2) inhibitor which is used in treatment of myeloproliferative neoplasm a rare type of Blood cancer.

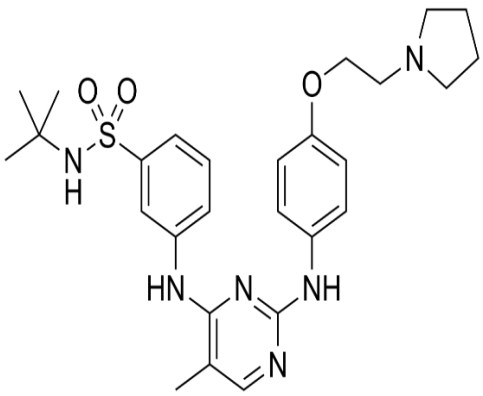

Fig 30: Fedratinib.

Copanlisib (2014)[41,42], Duvelisib (2018)[45], Alpelisib (2019)[89], and Idelalisib (2014)[71,72] are Phosphatidylinositol 3-hydroxy kinase inhibitors used in treatment of breast cancer, colorectal cancer, and hematologic malignancies like chronic lymphocytic leukemia and non-Hodgkin lymphoma.

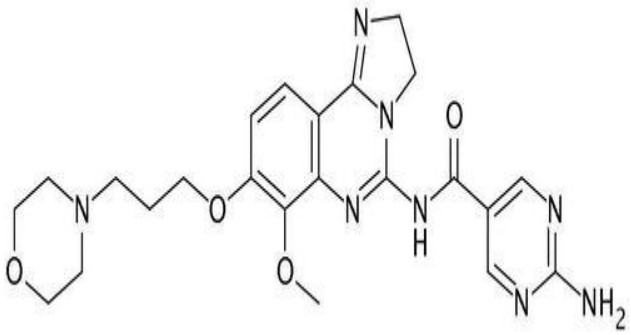

Fig 31: Copanlisib.

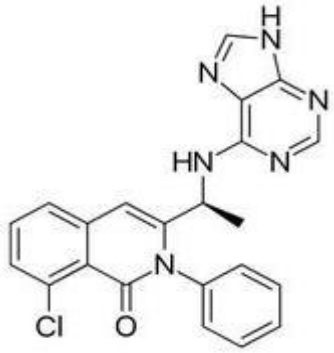

Fig 32: Duvelisib.

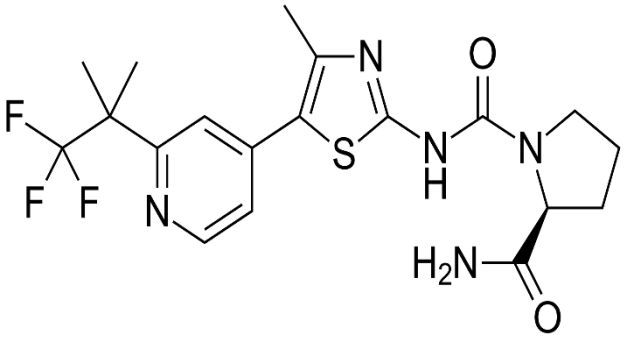

Fig 33: Alpelisib.

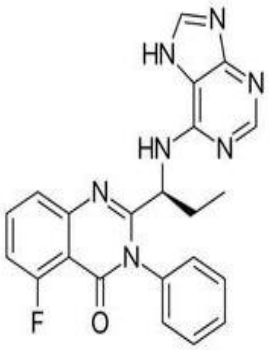

Fig 34: Idelilasib.

Mocetinostat (2014)[43,44] is Hydroxamic acid-based Histone deacetylase Inhibitor used in treatment of follicular lymphoma, Hodgkins lymphoma.

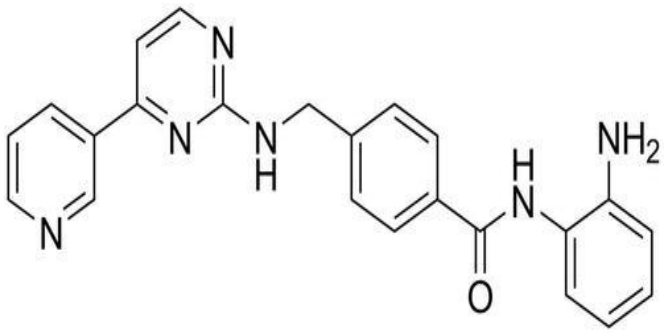

Fig. 35: Mocetinostat.

Oxaliplatin (2004)[46,47] inhibits transcription of DNA used in treatment of colon and colorectal cancer.

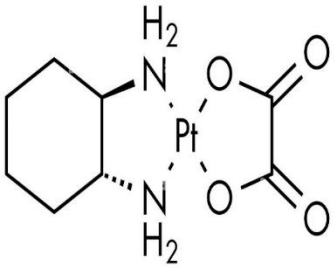

Fig. 36: Oxaliplatin.

Irinotecan (2000)[48,49] and Topotecan (1996)[70] are Topoisomerase I inhibitors used in treatment of ovarian cancer, small cell lung cancer, cervical cancer and cancer of colon and rectum.

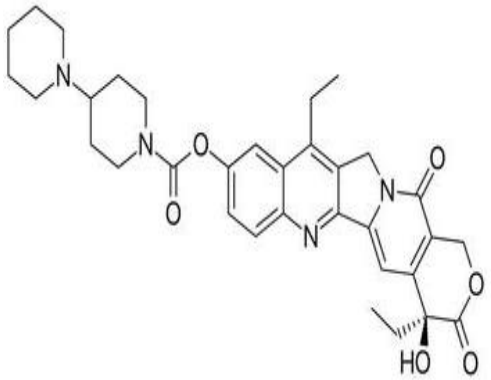

Fig. 37: Irinotecan.

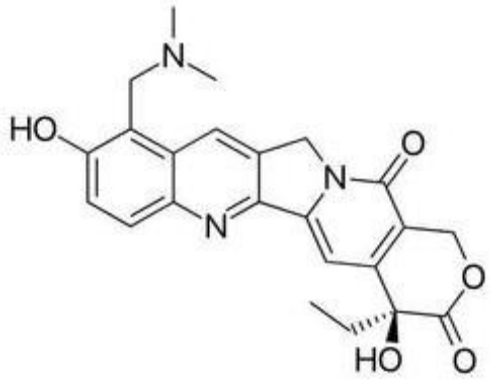

Fig. 38: Topotecan.

Cytarabine (1999)[50,51], Gemcitabine (1996)[52,53] are Pyrimidine nucleoside antimetabolite which are used in treatment of leukemia, pancreatic cancer; non-small-cell lung cancer; breast, bladder, and ovarian cancers; and small-cell lung cancer.

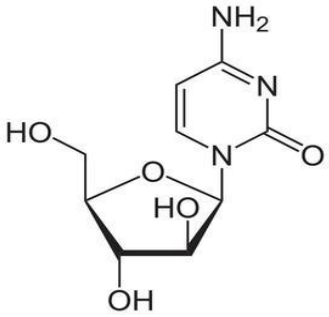

Fig 39: Cytarabine

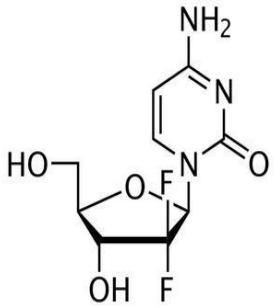

Fig 40: Gemcitabine

Trabectedin (2015)[54,55], Bendamustine (2008)[63] are alkylating agents, used in treatment of sickle cell anemia, prostate cancer, blood cancer (acute lymphocytic leukemia), soft tissue sarcoma and Hodgkin's disease.

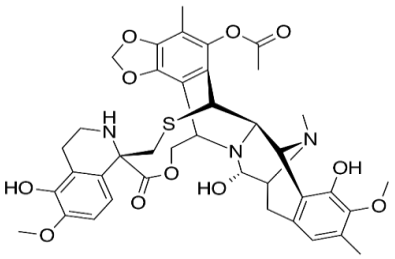

Fig 41: Trabectedin

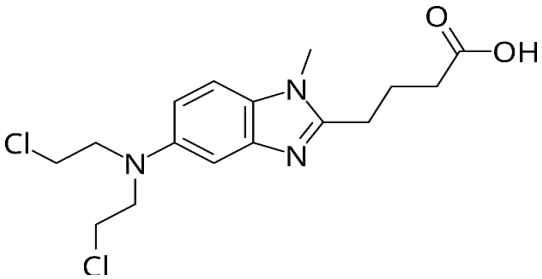

Fig 42: Bendamustine

Kahalalide F (2004)[56,57] is a lysosomal membrane disruptor, which is used in treatment of Prostate cancer, breast cancer, colon cancer and under trials for other cancer types.

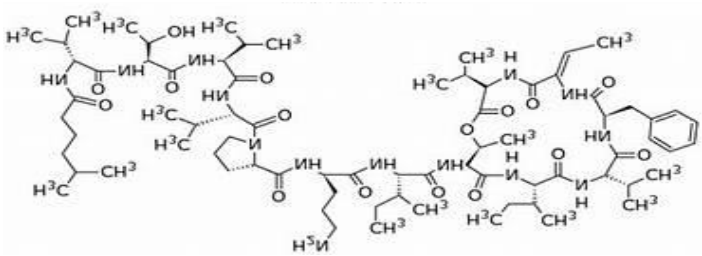

Fig. 43: Kahalide F.

Salinosporamide A (2004)[58] an Inhibitor of the 20S proteasomes, used in treatment of Breast Cancer.

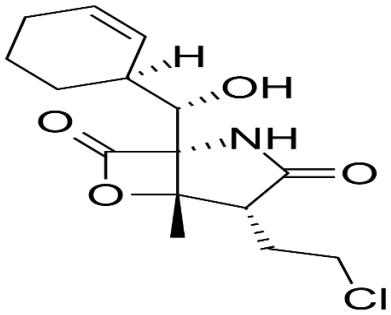

Fig. 44: Salinosporamide A.

Osimertinib (2015)[59], Erlotinib (2004)[95] and Gefitinib (2003)[64] are Epidermal Growth Factor Receptor and tyrosine kinase inhibitor and are used to treat Breast, Colon and Lung cancer.

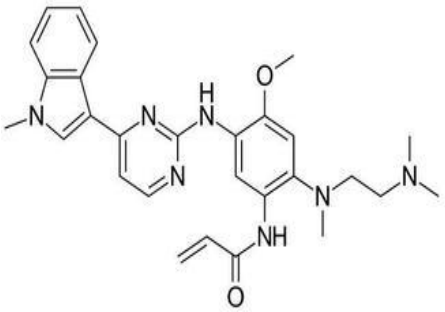

Fig. 45: Osimertinib

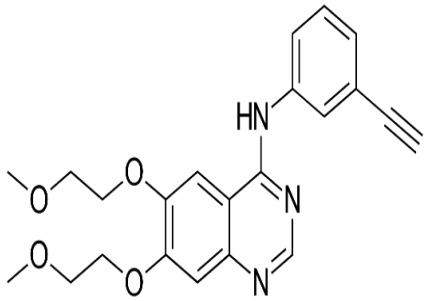

Fig. 46: Erlotinib

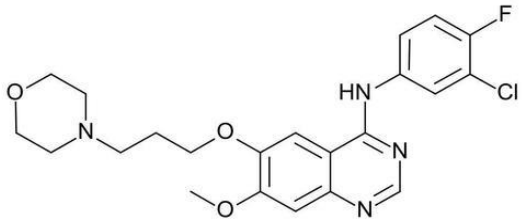

Fig. 47: Geftinib.

Soblidotin (2011)[60] inhibits microtubule polymerisation used in treatment of sarcoma and lung cancer

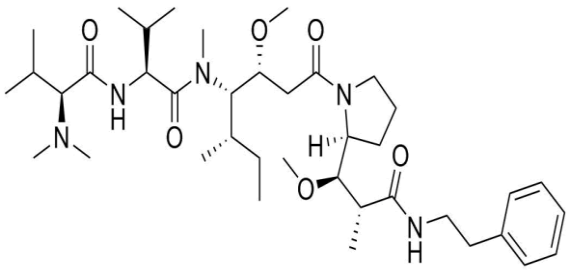

Fig. 48: Soblidotin.

Selinexor (42) (2019)[61,62] tumor suppressing protein activator, and used in treatment of multiple myeloma

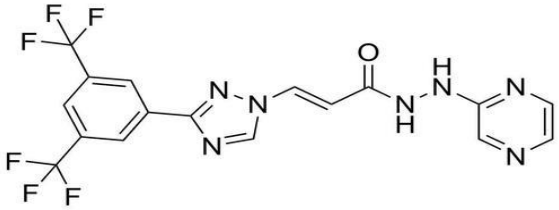

Fig 49: Selinexor.

Abemaciclib (2017)[65,66], Ribociclib (2018)[67], Palbociclib (2016)1[78,79] are CDK 4 and CDK 6 inhibitor, currently used in treatment of metastatic breast cancer.

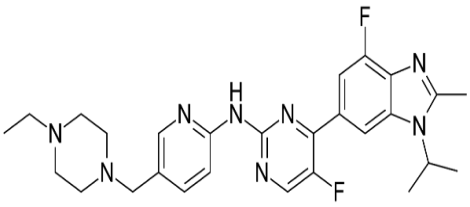

Fig. 50: Abemaciclib.

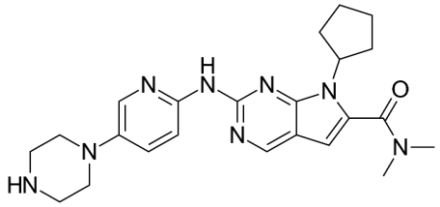

Fig. 51: Ribociclib.

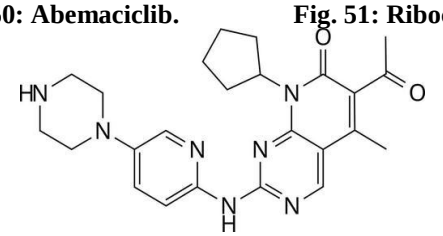

Fig. 52: Palbociclib.

Mitomycin C (1974)[68] double stranded DNA alkylating agent,

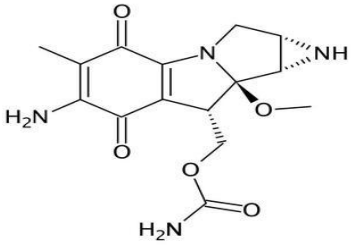

Fig. 53: Mitomycin C.

Porfimer (2002)[69] Photodynamic therapy agent High-affinity immunoglobulin gamma Fc receptor I antagonist,

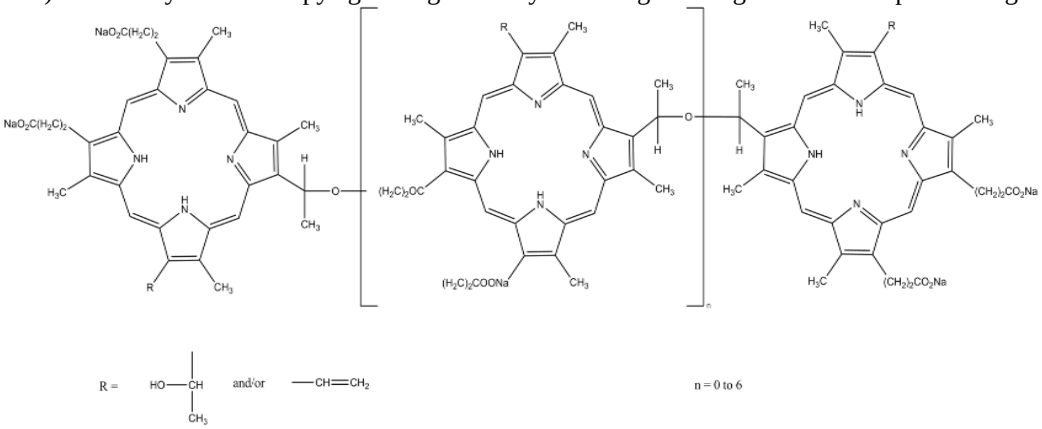

Fig. 54: Porfimer.

Acalabrutinib (2017)[73] and Cabozantinib (2016)[74,75] are tyrosine kinase inhibitor, used in treatment of leukemia

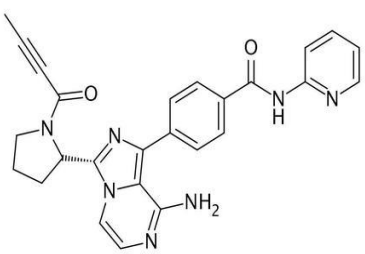

Fig. 55: Acalabrutinib.

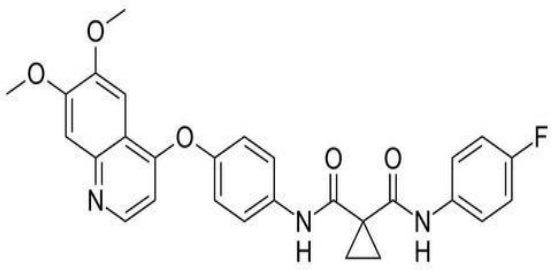

Fig. 56: cabozantinib.

Lenvatinib (2018)[76,77], Afatinib (2016)[83,84], Gilteritinib (2018)[87,88] are tyrosine kinase inhibitor and Trametinib (2013)[80,81,82] are protein kinase inhibitor are used in treatment of Acute myeloid leukemia and Non-small cell lung cancer.

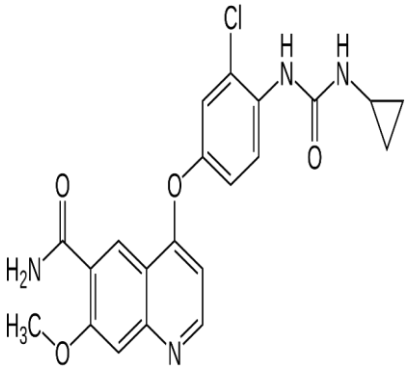

Fig 57: Lenvatinib

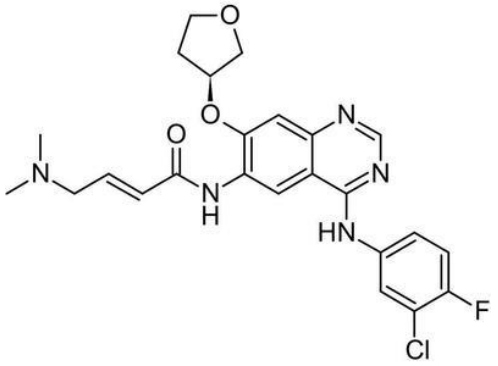

Fig 58: Afatinib

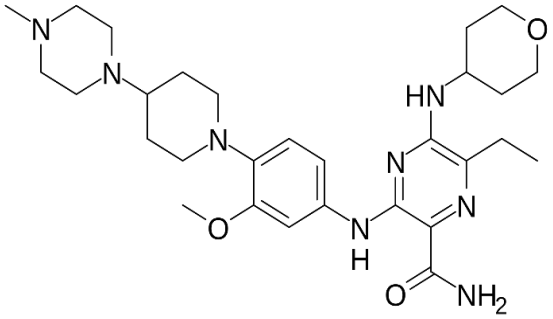

Fig 59: Gilteritinib

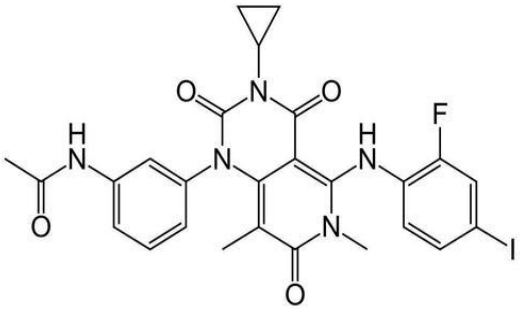

Fig 60: Trametinib

Dabrafenib (2013)[85,86] BRAF protein kinase inhibitor, used in treatment of metastatic melanoma.

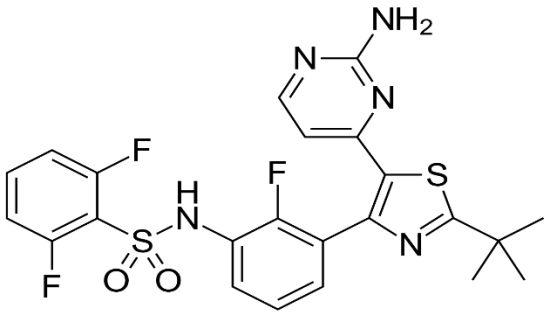

Fig. 61: Dabrafenib.

Binimetinib (2018)[90,91] and Crizotinib (2022)[92,93] Small-molecule kinase inhibitor melanoma and non-small lung cancer treatment respectively.

Fig 62: Binimetinib

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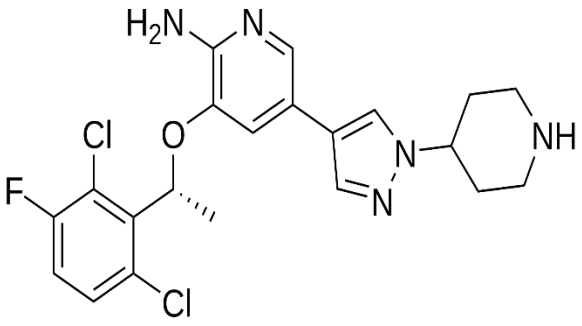

Fig 63: Crizotinib

Dactinomycin (2009)[94] is a transcription inhibitor used in treatment of testicular cancer, Wilms' tumor, gestational trophoblastic neoplasia and Ewing's sarcoma.

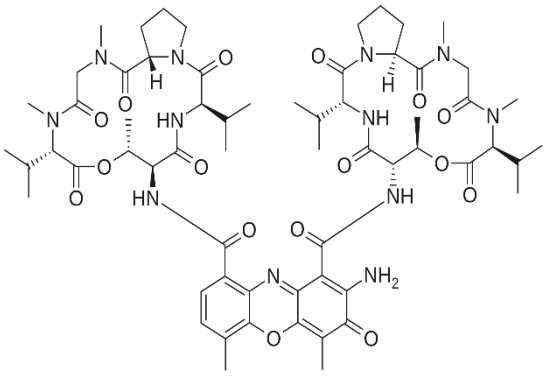

Fig. 64: Dactinomycin.

Ibrutinib (2022)[96,97] is a Bruton Tyrosine kinase inhibitor is used in B-cell lymphoma.

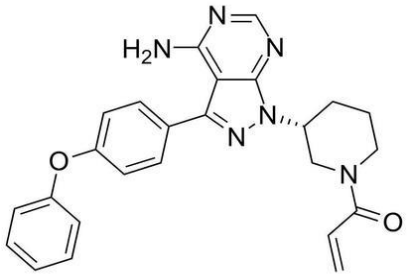

Fig. 65: Ibrutinib.

Lapatinib (2007)[98] HER 2 and E.G.F.R antagonist used in treatment of metastatic breast cancer.

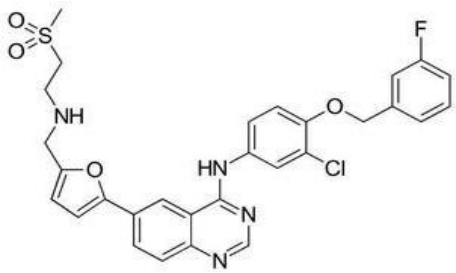

Fig. 66: Lapatinib.

Larotrectinib (2018)[99,100] T.R.K. (Tropomyosin Receptor Kinase) inhibitor,

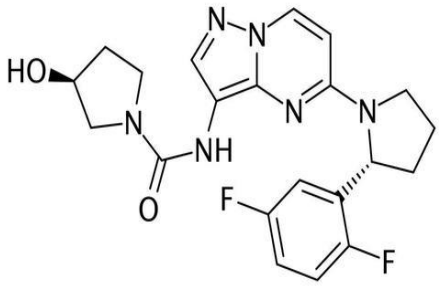

Fig. 67: Larotrectinib.

Mercaptopurine (2014)[101] Hypoxanthine-guanine phospho ribosyl transferase, Amido phospho ribosyl transferase, Inosine-5′-monophosphate dehydrogenase Inhibitor used mainly in acute lymphoblastic leukemia.

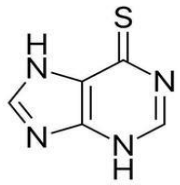

Fig. 68: Mercaptopurine.

Methotrexate (1999)[102,103] is a Thymidylate synthase and Dihydrofolate reductase Inhibitors used in treatment of leukemia, breast, skin, lung, head and neck cancers.

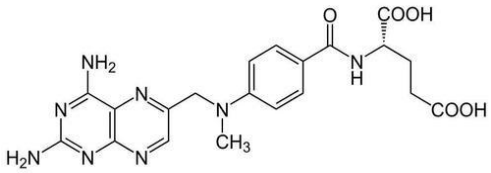

Fig. 69: Methotrexate.

Nilutamide (2016)[105] is an Androgen receptor antagonist, used in treatment of Prostate cancer.

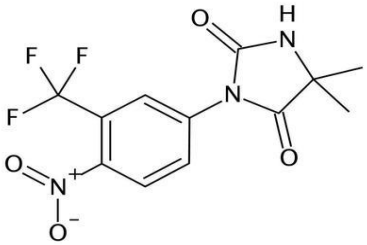

Fig. 70: Nilutamide.

Olaparib (2014)[106,107] Poly (ADP-ribose) polymerase (*PARP*) inhibitor used in treatment of breast and ovarian cancer.

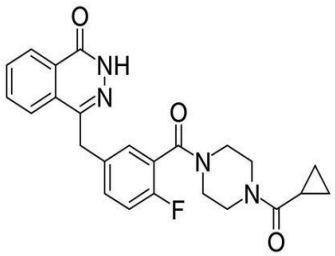

Fig. 71: Olaparib.

Anti-Cancer drugs with Sulphur Heterocycles

Sulphur containing Heterocycles are widely known for their anticancer properties as they can neutralise the drug resistance usually observed in chemotherapy with other drugs, Recent research shows that Sulforaphane found in cruciferous vegetables have significant anti-cancer property.[108,109]

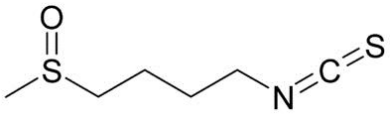

Fig. 72: Sulforaphane.

Some of the sulphur containing heterocycles are Thiophenes, Thiazoles, Thiazolidines, Benzothiazoles, Dibenzothiophenes are under investigation for anti-cancer activities.[113,114,115]

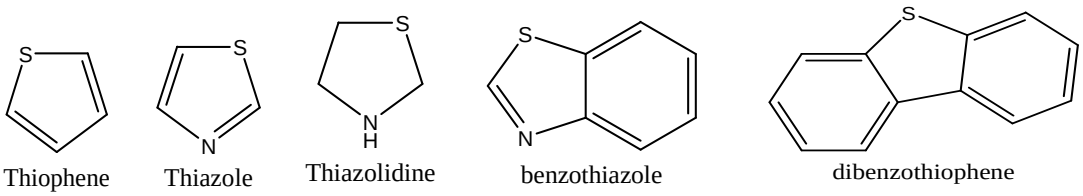

Fig. 73: Heterocycles with sulphur as hetero atom.

Alpelisib is a phosphatidylinositol 3-kinase (PI3K) inhibitor developed by Novartis Pharmaceuticals[110] in 2019.

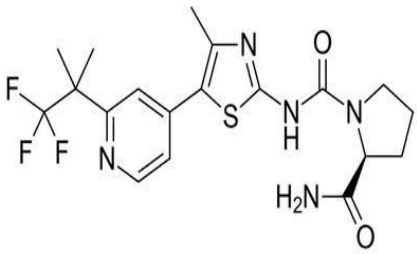

Fig. 74: Alpelisib.

Quizartinib is a FLT3(a cytokine receptor) inhibitor, developed ambit biosciences (2019) approved by FDA to use in combination with standard cytarabine and anthracycline induction and cytarabine consolidation, and as maintenance monotherapy following consolidation chemotherapy, for the treatment of adult patients with newly diagnosed acute myeloid leukemia (AML) that is FLT3 internal tandem duplication (ITD)-positive in 2023.[111]

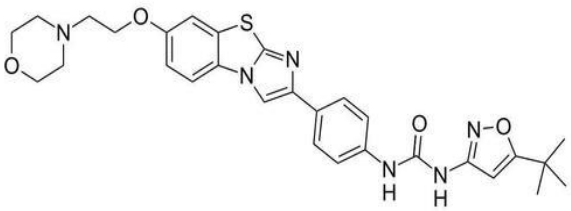

Fig 75: Quizartinib.

Encorafenib was first approved by the FDA in 2018, in combination with another drug called Binimetinib, to treat unresectable or metastatic melanoma with a specific genetic mutation, Encorafenib is a small molecule kinase inhibitor that was developed by Novartis.[112]

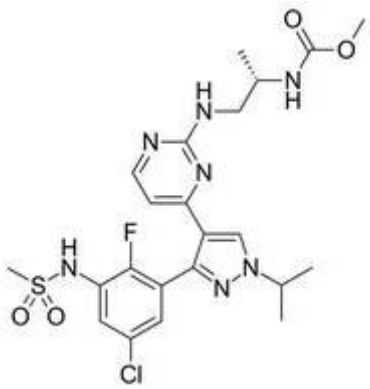

Fig. 76: Encorafenib.

CONCLUSION

Inspite the advances in Modern drug discovery one of the major challenges in treatment of cancer is development of resistance to current medications along with increase in day to day cases of cancer. Heterocyclic compounds being a diverse class of compounds with wide range of heterocycles like three, four, five, six and seven membered and sulphur, nitrogen and oxygen as heteroatoms offer lead molecules or those which can be used in combination with other medicines.

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