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Structure and Biological Activities: Steroid Moieties

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ABSTRACT

A steroid is a type of organic compound that contains a characteristic arrangement of four cycloalkane rings that are joined to each other. The core of steroids is composed of twenty carbon atoms bonded together that take the form of four fused rings, three cyclohexane rings and one cyclopentane ring. The steroids vary by the functional groups attached to this four-ring core and by the oxidation state of the rings. Steroid derivatives have occupied a unique place in the field of medicinal chemistry for their therapeutic values. This articles aims to review the work reported, their chemistry and biological activities of Steroid derivatives during past years.

Keywords: Cyclopentanoperhydrophenanthrene nucleus, Clinical trials, neoplastic drugs, contraceptive, pharmaceutical drugs.

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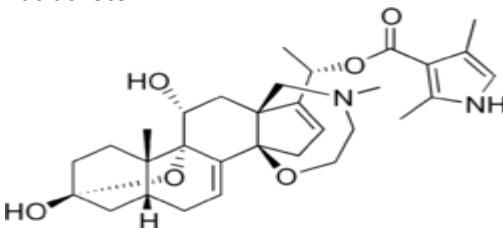
INTRODUCTION

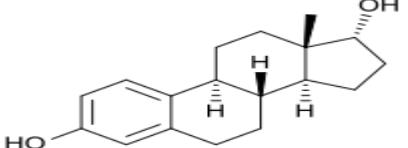
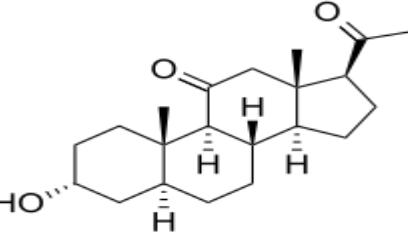
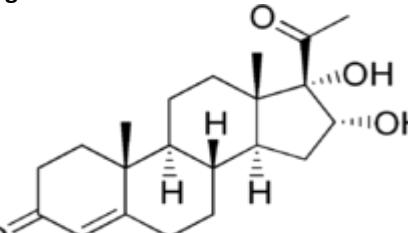
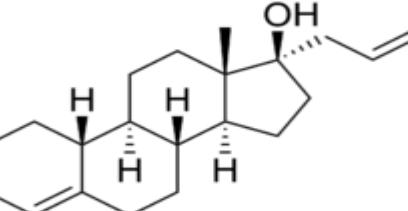
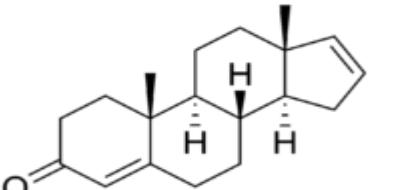
Sterols are special forms of steroids, with a hydroxyl group at position-3 and a skeleton derived from cholestane. Examples of steroids include the dietary fat cholesterol, the sex hormones estradiol and testosterone, and the anti-inflammatory drug dexamethasone. Hundreds of distinct steroids are found in plants, animals, and fungi. All steroids are made in cells either from the sterols lanosterol (animals and fungi) or from cycloartenol (plants). Both lanosterol and cycloartenol are derived from the cyclization of the triterpene squalene. Steroid may be divided in the following manner:

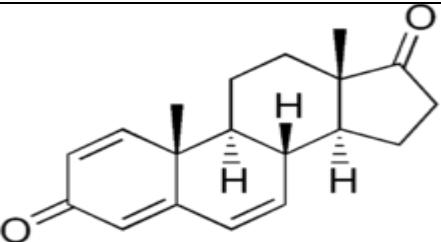
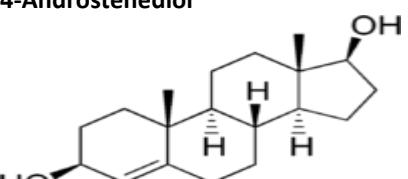
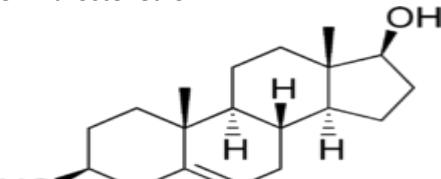
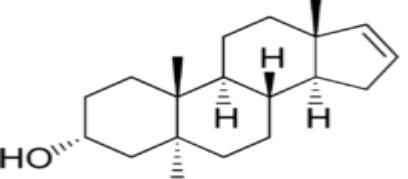
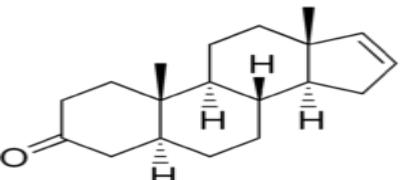
- Sterols- cholesterol, ergosterol, coprosterol
- Bile acids - glycholic acid, taurocholic acid
- Sex hormone- testosterone, estradiol
- Vitamin D- vitamin D₂&D₃
- Adrenocortical hormone- corticosterone
- Cardiac glycoside- strophanthine
- Saponin- digitonin

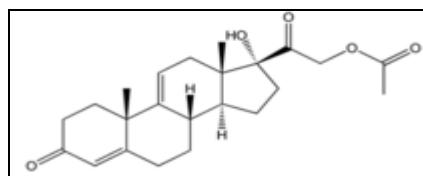
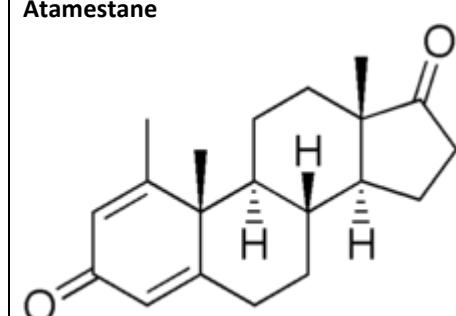
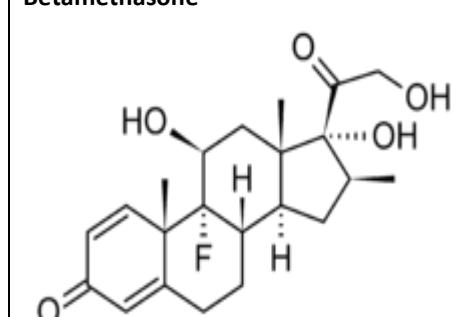
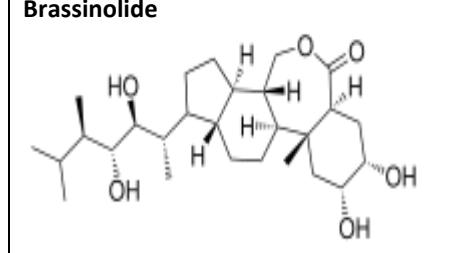
Medicinal chemistry is the discipline concerned with determining the influence of chemical structure on biological activity and in the practice of medicinal chemistry developed from an empirical one involving organic synthesis of new compound based largely on the modification of structure and then identifies their biological activity. Medicinal chemistry concerns with the discovery, development, interpretation and the identification of mechanism of action of biologically active compounds at the molecular level. Various type of steroid are synthesizes till now & are numerous compound are under clinical trials which are found to be most promising in the health care system. Few examples are given below along with their pharmacological effect in table-1.

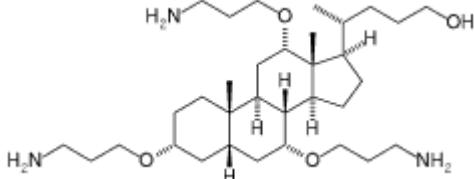
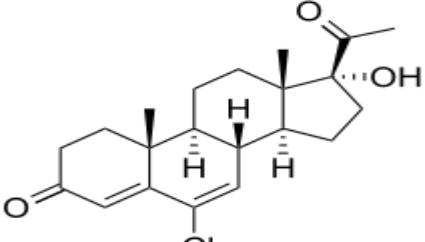
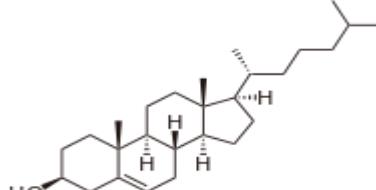
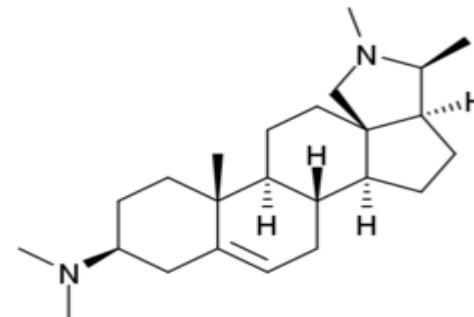
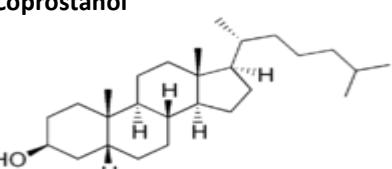
Table-1

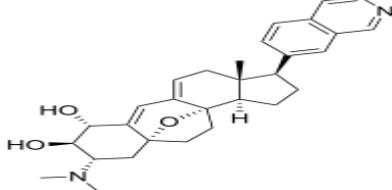
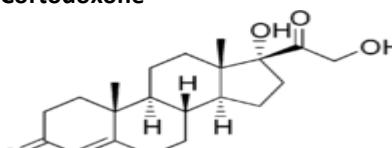
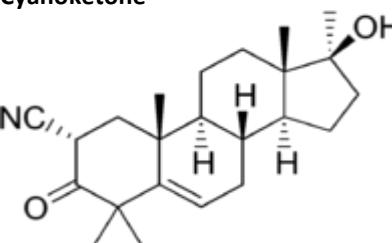
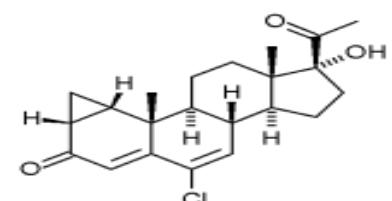
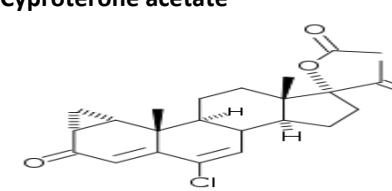
Name of compound	Pharmacological Uses	References
Batrachotoxin 	It is a potent cardiotoxic and neurotoxic steroid alkaloids	Tokuyama, T. et.al [1]

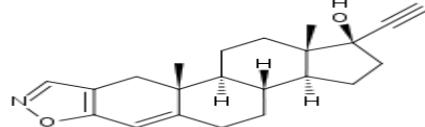
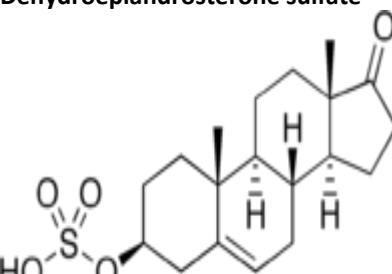
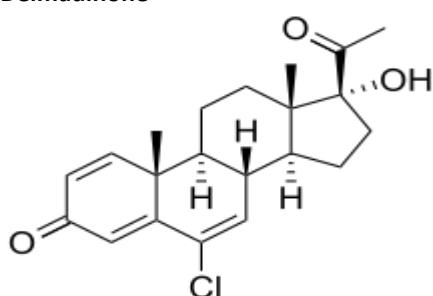
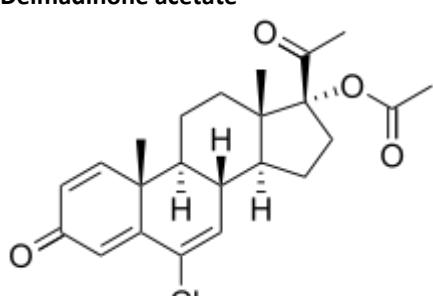
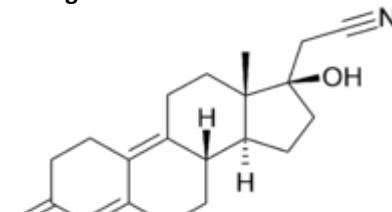
Alfatradiol  Estra-1,3,5(10)-triene-3,17 α -diol	Used for the treatment of androgenic alopecia (hair loss) in men and women	Berger.et.al [2]
Alfaxolone/alfadolone 	Used as anaesthetic agent	Clarke, R. S.et.al [3]
Algestone  16 α ,17 α -dihydroxypregn-4-ene-3,20-dione	Used as a contraceptive drug	A. D. Roberts.et.al [4]
Allylestrenol  (17 β)-17-(prop-2-en-1-yl)estr-4-en-17-ol	Used to prevent threatened miscarriage, recurrent pregnancy loss and premature labor.	Sweetman.et.al [5]
Androstadienone  (8S,9S,10R,13S)-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15-decahydrocyclopenta[a]phenanthren-3-one	Androstadienone is commonly sold in male fragrances, it is purported, to increase sexual attraction.	Wyart C.et.al [6]
1,4,6-Androstatriene-3,17-dione	It is used to control estrogen synthesis	Adkins-Regan.et.al [7]

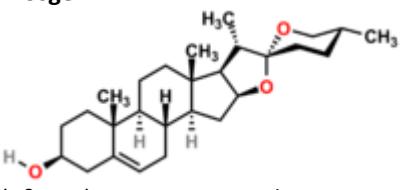
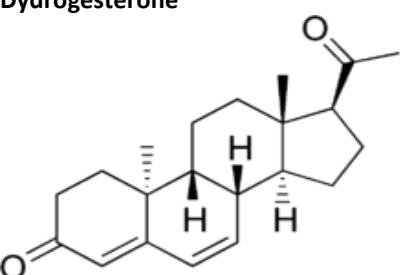
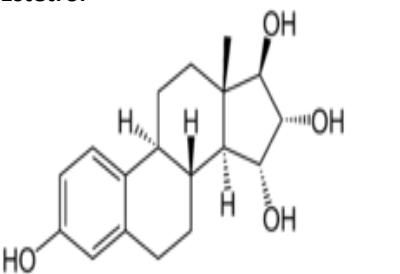
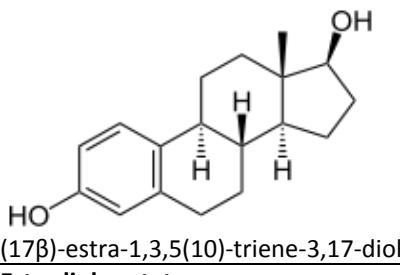
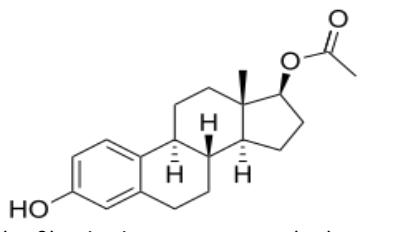
 <p>(8R,9S,10R,13S,14S)-10,13-dimethyl-9,11,12,14,15,16-hexahydro-8H-cyclopenta[a]phenanthrene-3,17-dione</p>		
<p>4-Androstenediol</p>  <p>(3S,8R,9S,10R,13S,14S,17S)-10,13-dimethyl-2,3,6,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,17-diol</p>	<p>It has androgenic effects</p>	Chen F.et.al [8]
<p>5-Androstenediol</p>  <p>(3S,8R,9S,10R,13S,14S,17S)-10,13-Dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,17-diol</p>	<p>Its potential use as a radiation countermeasure</p>	Whitnall MH.et.al [9]
<p>Androstenol</p>  <p>(2R,5R,7S,15R)-2,15-dimethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-13-en-5-ol</p>	<p>It is analogous to sex hormones</p>	Kirk-Smith.et.al [10]
<p>Androstenone</p>  <p>(5S,8R,9S,10S,13R,14S)-10,13-dimethyl-1,2,4,5,6,7,8,9,11,12,14,15-dodecahydrocyclopenta[a]phenanthren-3-one</p>	<p>Androstenone is the active ingredient in 'Boarmate', a commercial product made by DuPont sold to pig farmers to test sows for timing of artificial insemination.</p>	Kirk-Smith.et.al [11]
<p>Anecortave</p>	<p>It is used in the treatment of the exudative (wet) form of age-related macular degeneration</p>	Reid J.G et.al [12]

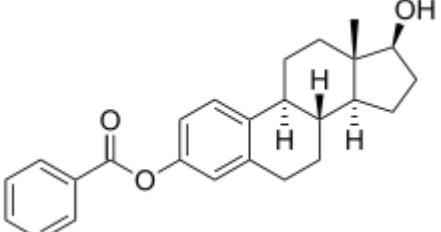
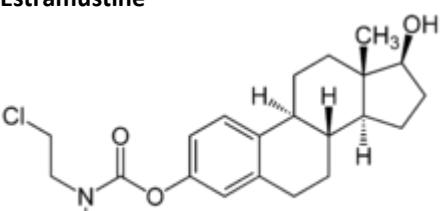
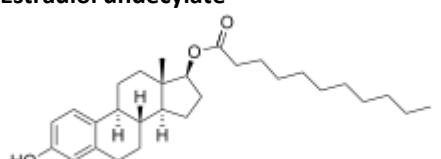
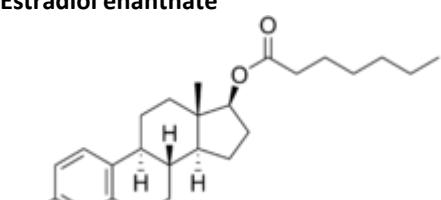
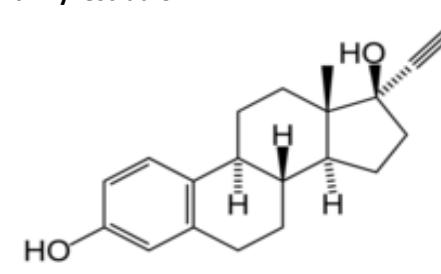
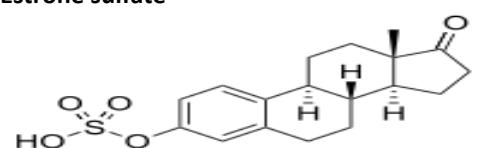
 <p>[2-[(8R,10S,13S,14R,17R)-17-hydroxy-10,13-dimethyl-3-oxo-2,6,7,8,12,14,15,16-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-oxo-ethyl] acetate</p>		
<p>Atamestane</p>  <p>(8R,9S,10S,13S,14S)-1,10,13-Trimethyl-7,8,9,11,12,14,15,16-octahydro-6H-cyclopenta[a]phenanthrene-3,17-dione</p>	<p>Atamestane is an aromatase inhibitor that is being studied in the treatment of cancer.</p>	Etreby MF.et.al [13]
<p>Betamethasone</p>  <p>(8S,9R,10S,11S,13S,14S,16S,17R)-9-fluoro-11,17-dihydroxy-17-(2-hydroxyacetyl)-10,13,16-trimethyl-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-3H-cyclopenta[a]phenanthren-3-one</p>	<p>It has anti-inflammatory and immunosuppressive properties</p>	Chu C.C.et.al [14]
<p>Brassinolide</p>  <p>(3aS,5S,6R,7aR,7bS,9aS,10R,12aS,12bS)-10-[(2S,3R,4R,5S)-3,4-Dihydroxy-5,6-dimethyl-2-heptanyl]-5,6-dihydroxy-7a,9a-dimethylhexadecahydro-3H-benzo[c]indeno[5,4-e]oxepin-3-one</p>	<p>Brassinolide is a plant hormone.</p>	Grove.et.al [15]
<p>Ceragenin</p>	<p>It shows road spectrum</p>	Savage P.B.et.al

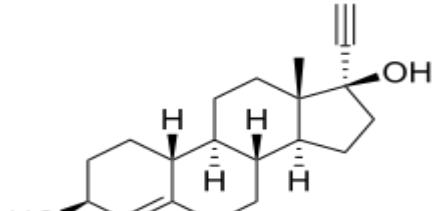
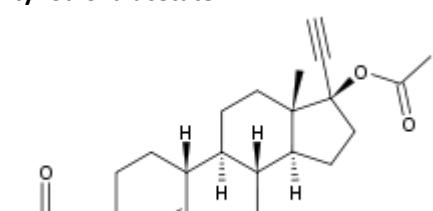
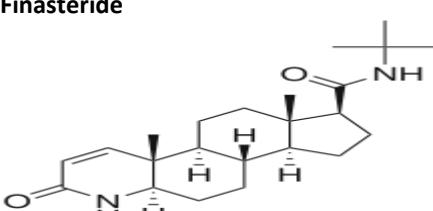
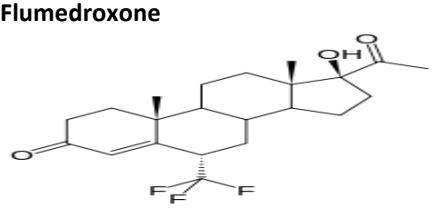
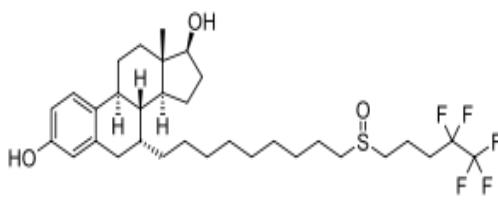
	antibacterial activity.	[16]
Chlormadinone  6-chloro-17 α -hydroxypregna-4,6-diene-3,20-dione	clinically used as a pharmaceutical drug	Macdonald.et.al [17]
Cholesterol  (3 β)-cholest-5-en-3-ol	It serves as a precursor for the biosynthesis of steroid hormones, bile acids, and vitamin D	Hanukoglu I.et.al [18]
Conessine  N,N-Dimethyl-con-5-enin-3-amine	Used for treatment of amoebic dysentery	Garg S.et.al [19]
Coprostanol  5 β -cholest-3 β -ol	This compound has frequently been used as a biomarker for the presence of human faecal matter in the environment.	Mudge S.M.et.al [20]
Cortistatins	Represses viral replication in cells infected with HIV via binding to the Tat protein	Aoki S.et.al [21]

 <p>(1<i>R</i>,2<i>R</i>,3<i>S</i>,5<i>R</i>,8<i>β</i>,17<i>β</i>)-3-(Dimethylamino)-17-(isoquinolin-7-yl)-5,8-epoxy-9,19-cyclo-9,10-secoandrosta-9(11),10-diene-1,2-diol</p>		
<p>Cortodoxone</p>  <p>(8<i>R</i>,9<i>S</i>,10<i>R</i>,13<i>S</i>,14<i>S</i>,17<i>R</i>)-17-hydroxy-17-(2-hydroxyacetyl)-10,13-dimethyl-2,6,7,8,9,11,12,14,15,16-decahydro-1<i>H</i>-cyclopenta[<i>a</i>]phenanthren-3-one</p>	<p>Cortodoxone functions as a mineralocorticoid</p>	<p>Peterson DH.et.al [22]</p>
<p>Cyanoketone</p>  <p>(2<i>S</i>,8<i>R</i>,9<i>S</i>,10<i>R</i>,13<i>S</i>,14<i>S</i>,17<i>S</i>)-17-hydroxy-4,4,10,13,17-pentamethyl-3-oxo-1,2,7,8,9,11,12,14,15,16-decahydrocyclopenta[<i>a</i>]phenanthrene-2-carbonitrile</p>	<p>It has been shown to inhibit steroidogenesis</p>	<p>Di Prisco [23]</p>
<p>Cyproterone</p>  <p>6-chloro-17-hydroxy-1<i>α</i>,2<i>α</i>-methylenepregna-4,6-diene-3,20-dione</p>	<p>It is a steroidal antiandrogen</p>	<p>Taylor.et.al [24]</p>
<p>Cyproterone acetate</p>  <p>6-chloro-17-hydroxy-1<i>α</i>,2<i>α</i>-methylenepregna-4,6-diene-3,20-dione</p>	<p>it can also be used to treat acne and hirsutism in females</p>	<p>Neumann F.et.al [25]</p>
<p>Danazol</p>	<p>Its role as a treatment for endometriosis has been largely replaced by the GnRH agonists.</p>	<p>Dmowski W.P.et.al [26]</p>

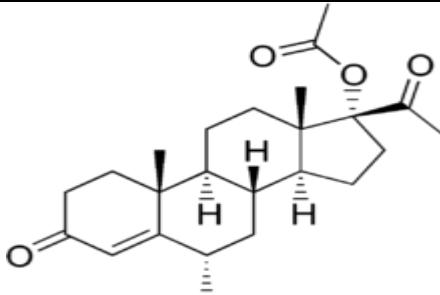
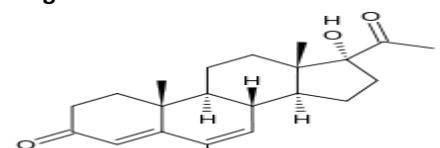
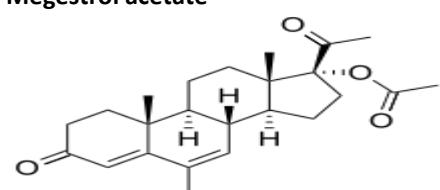
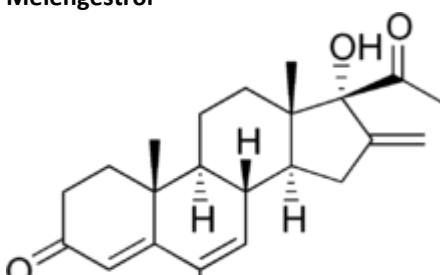
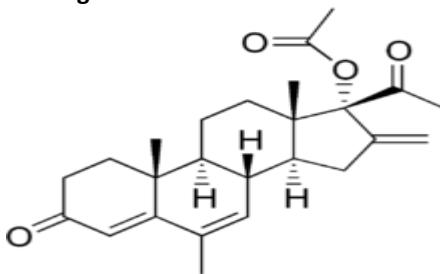
 <p>(1S,2R,13R,14S,17R,18S)-17-ethynyl-2,18-dimethyl-7-oxa-6-azapentacyclo[11.7.0.0^{2,10}.0^{4,8}.0^{14,18}]icos-4(8),5,9-trien-17-ol</p>		
Dehydroepiandrosterone sulfate  <p>[(3S,8R,9S,10R,13S,14S)-10,13-Dimethyl-17-oxo-1,2,3,4,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthren-3-yl] hydrogen sulfate</p>	<p>Use as biomarker</p>	Rainey W.E.et.al [27]
Delmadinone  <p>6-chloro-17-hydroxypregna-1,4,6-triene-3,20-dione</p>	<p>It is used in veterinary medicine.</p>	Macdonald.et.al [28]
Delmadinone acetate  <p>6-chloro-3,20-dioxopregna-1,4,6-trien-17-yl acetate</p>	<p>It is used to treat androgen-associated conditions in veterinary medicine</p>	Macdonald.et.al [28]
Dienogest 	<p>It is available for use as an oral contraceptive in combination with ethinylestradiol</p>	Foster R.H.et.al [29]

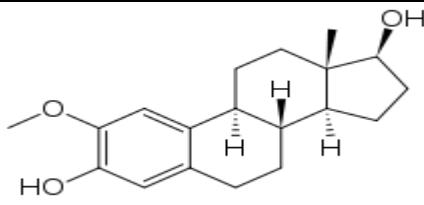
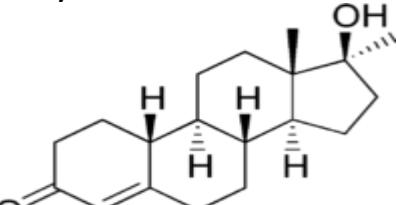
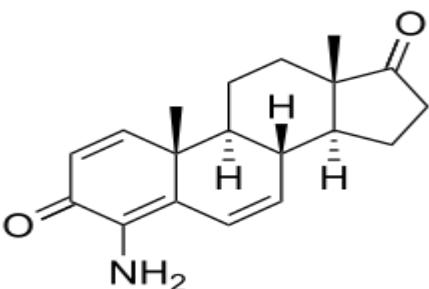
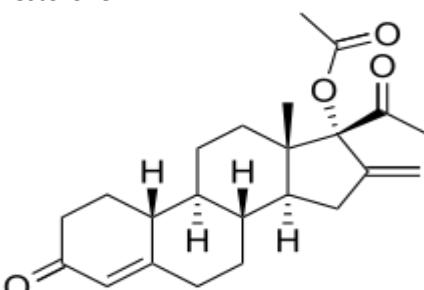
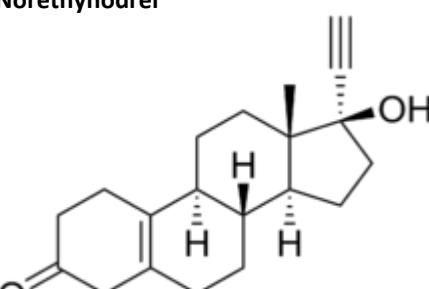
17-hydroxy-3-oxo-19-nor-17 α -pregna-4,9-diene-21-nitrile Diosgenin  (3 β ,25R)-spirost-5-en-3-ol	Diosgenin is used for the commercial synthesis of cortisone, pregnenolone, progesterone, and other steroid products. Djerassi C.et.al [30]	
Dydrogesterone  (9 β ,10 α)-pregna-4,6-diene-3,20-dione	Effective against menstrual disorders, infertility, threatened and habitual abortion. Davis S.et.al [31]	
Estetrol  (8R,9S,13S,14S,15R,16R,17R)-13-methyl-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthrene-3,15,16,17-tetrol	Use of E4 as a marker for fetal well-being Hagen A.A.et.al [32]	
Estradiol  (17 β)-esta-1,3,5(10)-triene-3,17-diol	Used in combined oral contraceptive pills Wu CH.et.al [33]	
Estradiol acetate  (17 β)-3-hydroxyestra-1,3,5(10)-trien-17-yl acetate	Used to treat and prevent symptoms of menopause such as osteoporosis in postmenopausal women Speroff L.et.al [34]	
Estradiol benzoate	It was the first form of estrogen to be marketed	Roberts A. D.et.al [35]

 (17 β)-17-hydroxyestra-1,3,5(10)-tri엔-3-yl benzoate		
Estramustine  (17 β)-17-Hydroxyestra-1(10),2,4-trien-3-yl bis(2-chloroethyl)carbamate	Used to treat prostate cancer	H. J.et.al [36]
Estradiol undecylate  (17 β)-3-hydroxyestra-1,3,5(10)-tri엔-17-yl undecanoate	Formerly used to treat prostate cancer	Christoph Zink .et.al [37]
Estradiol enanthate  (17 β)-3-hydroxyestra-1,3,5(10)-tri엔-17-yl heptanoate	Used as injectable hormonal contraceptive	Roberts A.D.et.al [38]
Ethinyl estradiol  19-nor-17 α -pregna-1,3,5(10)-tri엔-20-yne-3,17-diol	Used in many formulations of combined oral contraceptive pills	Walter .et.al [39]
Estrone sulfate  [(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,14,15,16-	Used as a prognosis indicator for prostate cancer.	Horne C.et.al [40]

octahydro-6H-cyclopenta[<i>a</i>]phenanthren-3-yl] hydrogen sulfate Etynodiol  (3 β ,17 β)-17-ethynylestr-4-ene-3,17-diol	Used in hormonal contraceptives	Macdonald.et.al [41]
Etynodiol diacetate  (3 β ,17 β)-17-ethynylestr-4-ene-3,17-diyil diacetate	Used in hormonal contraceptives	Macdonald.et.al [41]
Finasteride  N-(1,1-dimethylethyl)-3-oxo-(5 α ,17 β)-4-azaandrost-1-ene-17-carboxamide	It is approved for the treatment of benign prostatic hyperplasia (BPH) and male pattern baldness (MPB).	Edwards.et.al [42]
Flumadroxone  (2 <i>R</i> ,8 <i>S</i> ,14 <i>S</i> ,15 <i>S</i>)-14-acetyl-14-hydroxy-2,15-dimethyl-8-(trifluoromethyl)tetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]heptadec-6-en-5-one	Used to treat migraines	Bradley W.G.et.al [43]
Fulvestrant  (7 α ,17 β)-7-{9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl}estra-1,3,5(10)-triene-3,17-diol	Used treatment of hormone receptor-positive metastatic breast cancer in postmenopausal women	S. Kansra.et.al [44]
Fusidic acid	bacteriostatic antibiotic	Falagas ME.et.al [45]

<p>2-[(1S,2S,5R,6S,7S,10S,11S,13S,14Z,15R,17R)-13-(acetoxy)-5,17-dihydroxy-2,6,10,11-tetramethyltetracyclo[8.7.0.0^2,7.0^11,15]heptadecan-14-ylidene]-6-methylhept-5-enoic acid</p>		
<p>Gestrinone</p> <p>13-ethyl-17alpha-hydroxy-18,19-dinorpregna-4,9,11-trien-20-yn-3-one</p>	<p>Used for treatment of endometriosis</p>	<p>Tamaya T.et.al [46]</p>
<p>Guggulsterone</p> <p>(8R,9S,10R,13S,14S)-17-Ethylidene-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15-decahydrocyclopenta[a]phenanthrene-3,16-dione</p>	<p>Guggulsterone is an ingredient in many nutritional supplements.</p>	<p>Szapary P.O.et.al [47]</p>
<p>Lumisterol</p> <p>(3S,9R,10S,13R,14R,17R)-17-[(E,2R,5R)-5,6-Dimethylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,9,11,12,14,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-ol</p>	<p>Lumisterol is a compound that is part of the vitamin D family of steroid compounds</p>	<p>Dewick.et.al [48]</p>
<p>Medrogestone</p> <p>6,17-dimethylpregna-4,6-diene-3,20-dione</p>	<p>A hormone involved in the menstrual cycle and pregnancy</p>	<p>Goodman.et.al [49]</p>
<p>Medroxyprogesterone acetate</p>	<p>It is used as a contraceptive, in hormone replacement therapy and for the treatment of endometriosis</p>	<p>Schindler A.E.et.al [50]</p>

 <p>17α-hydroxy-6α-methylpregn-4-ene-3,20-dione acetate</p>		
Megestrol  <p>17-hydroxy-6-methylpregna-4,6-diene-3,20-dione</p>	Used as a pharmaceutical drug.	Macdonald.et.al [41]
Megestrol acetate  <p>17-(acetoxy)-6-methyl-pregna-4,6-diene-3,20-dione</p>	Used as an antineoplastic agent in the treatment of breast, endometrial, and prostate cancers	Schindler A.E.et.al [50]
Melengestrol  <p>17-hydroxy-6-methyl-16-methylenepregna-4,6-diene-3,20-dione</p>	Used as a growth promoter in animals	Macdonald.et.al [41]
Melengestrol acetate  <p>17-hydroxy-6-methyl-16-methylenepregna-4,6-diene-3,20-dione acetate</p>	Used as a feed additive to promote growth in cattle	David J.et.al [51]
2-Methoxyestradiol	It has undergone Phase 1 clinical trials against breast cancer.	Lakhani N.et.al [52]

 <p>(8R,9S,13S,14S,17S)-2-methoxy-13-methyl-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthrene-3,17-diol</p>		
Methylestrenolone 	It is an anabolic steroid	Calvet D.et.al [53]
Minamestane  4-aminoandrosta-1,4,6-triene-3,17-dione	Act as antineoplastic agent	Macdonald.et.al [41]
Nestorone  (17 α)-17-acetyl-16-methylene-3-oxoestr-4-en-17-yl acetate	Used as a hormonal contraceptive	Lippincott.et.al [54]
Norethynodrel  (8S,9S,13S,14S,17S)-17-ethynyl-17-hydroxy-13-methyl-	Used as oral contraceptive	R. A.et.al [55]

1,2,4,6,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthren-3-one Norethisterone acetate		
(8R,9S,10R,13S,14S,17S)-17-ethynyl-13-methyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl acetate	Used as a hormonal contraceptive	Macdonald et.al [41]
Nomegestrol (17 α)-17-acetyl-17-hydroxy-6-methylestra-4,6-dien-3-one	hormonal contraceptive	Macdonald et.al [41]
Olesoxime (NZ)-N-[(8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R)-6-methylheptan-2-yl]-1,2,6,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-ylidene]hydroxylamine	Undergoing a phase II clinical trial as treatment for spinal muscular atrophy.	Martin L.J .et.al [56]
Plomestane 10H-(2-propynyl)-estr-4-ene-3,17-dione	antineoplastic agent for the treatment of breast cancer.	Macdonald et.al [41]
Prednimustine	Prednimustine is a drug used in	Monnerat C.et.al

<p>(11β)-11,17-dihydroxy-3,20-dioxopregna-1,4-dien-21-yl 4-[bis(2-chloroethyl)amino]phenyl}butanoate</p>	chemotherapy	[57]
Quingestanol acetate <p>(17β)-3-(Cyclopentyloxy)-17-ethynylestra-3,5-dien-17-yl acetate</p>	Used as postcoital hormonal contraceptive	Giannina T.et.al [58]
Rubrosterone <p>2β,3β,14α-trihydroxy-5β-androst-7-ene-6,17-dione</p>	hypolipidemic agent in rats	Geetha.et.al [59]
Testolactone <p>(4aS,4bR,10aR,10bS,12aS)-10a,12a-dimethyl-3,4,4a,5,6,10a,10b,11,12,12a-decahydro-2H-naphtho[2,1-f]chromene-2,8(4bH)-dione</p>	Antineoplastic agent	Dunkel L.et.al [60]
Telapristone <p>[(8S,11R,13S,14S,17R)-11-[4-(Dimethylamino)phenyl]-17-(2-methoxyacetyl)-13-methyl-3-oxo-</p>	Tested for treatment of progesterone sensitive myomata	Attardi B.J.et.al [61]

1,2,6,7,8,11,12,14,15,16-decahydrocyclopenta[<i>a</i>]phenanthren-17-yl] acetate Spirolactone 7 α -acetylthio-3-oxo-17 α -pregn-4-ene-21,17-carbolactone	Used as a diuretic and antihypertensive Brittain.et.al [62]	
Squalamine (1 <i>S</i> ,2 <i>S</i> ,5 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> ,11 <i>S</i> ,14 <i>R</i> ,15 <i>R</i>)-N-[3-[(4-aminobutyl)amino]propyl]-9-hydroxy-2,15-dimethyl- 14-[(2 <i>R</i> ,5 <i>R</i>)-6-methyl-5-(sulfoxy)heptan-2-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan-5-aminium	Broad-spectrum antibiotic Moore K .S.et.al [63]	

CONCLUSION

The reviewed Steroid moiety has shown a wide spectrum of biological activities. The various substitute steroid are having significant antihypertensive activity., Significant ,antineoplastic and veterinary drugs. some modified steroid are found to be effective as oral contraceptive, hormonal contraceptive, whereas some of the derivatives of steroid are found to be effective as nutritional supplement, broad spectrum antibiotic, treatment of breast cancer, endometrial, and prostate cancers, used as a contraceptive, in hormone replacement therapy and for the treatment of endometriosis, growth promoter in animals. Recently it was proven that, some of the important marketed steroid nucleolus containing drug having different biological or pharmacological activity were discussed in table. The steroid nucleolus based pharmaceutical are rapidly becoming very important class of therapeutic agents and are likely to replace many existing organic based pharmaceuticals in the very near future. The steroid based pharmaceuticals will be produced on a large scale by modern drug Discovery Company by different research development processes and will become available commercially for therapeutic use. With the key benefits including favorable time to market and high rate of success in clinical trial compared with traditional pharmaceuticals due to diverse biological action with less toxicity, so in future therapeutic steroid drug will play vital role in the treatment of different diseases. The biological profiles of this new generation of steroid represent much progress with regard to the older compounds.

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