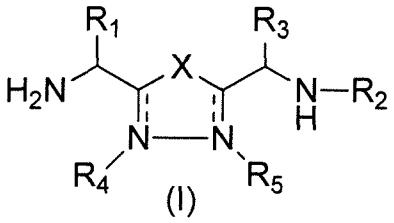
# CLAIMS

1. A compound of formula (I)




(I)

wherein,

$R_1$ represents a side chain of an amino acid selected from Ser, Thr, Phe, Ala and Asn;

X is S or O;

$R_2$ is hydrogen or -CO-Aaa;

Aaa is an amino acid residue selected from Ser, Asn and Thr; wherein a C-terminus thereof is a free terminus, is amidated or is esterified;

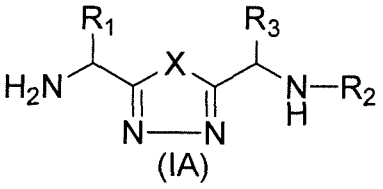
$R_3$ represents a side chain of an amino acid selected from Ser, Ala, Glu, Gln, Asn and Asp;

---- is an optional bond;

$R_4$ and $R_5$ independently are hydrogen or absent;

or a pharmaceutically acceptable salt thereof.

2. The compound according to claim 1, having a structure of formula (IA):



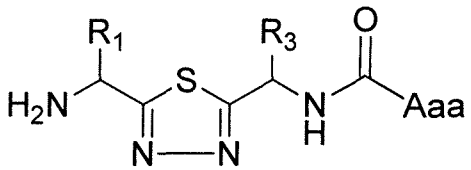

(IA)

3. The compound according to claim 1 or 2, wherein X is S.

4. The compound according to claim 1 or 2, wherein X is O.

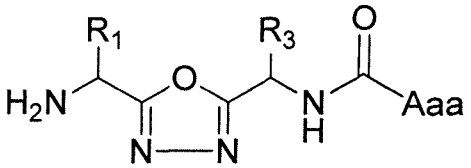
5. The compound according to any one of claims 1 to 4, wherein $R_2$ is hydrogen.

6. The compound according to claim 1 or 2, having the structure of formula (IB):




(IB)

7. The compound according to claim 1 or 2, having the structure of formula (IC):




(IC)

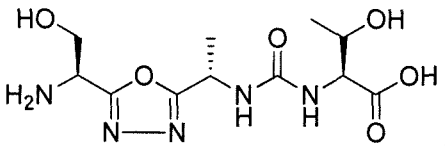
8. The compound according to any one of claims 1 to 4, 6, and 7, wherein $R_2$ is -CO-Aaa.

9. The compound according to any one of claims 1 to 4 and 6 to 8, wherein Aaa is an amino acid residue Ser or Thr; wherein the C-terminus is a free terminus.

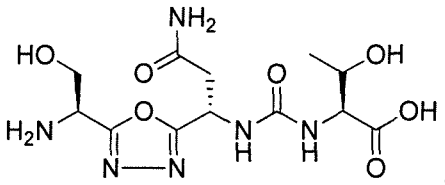
10. The compound according to any one of claims 1 to 9, wherein $R_1$ represents the side chain of an amino acid residue Ser or Thr.

11. The compound according to any one of claims 1 to 10, wherein $R_3$ represents the side chain of the amino acid residue selected from Glu, Gln, Asn, and Asp.

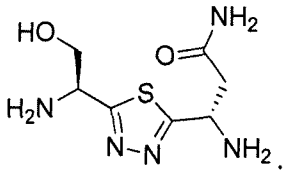
12. The compound according to claim 1, having the following structure:



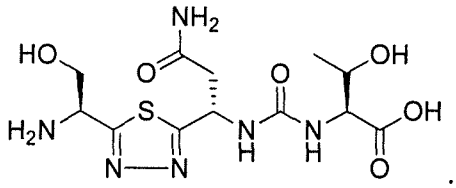

13. The compound according to claim 1, having the following structure:



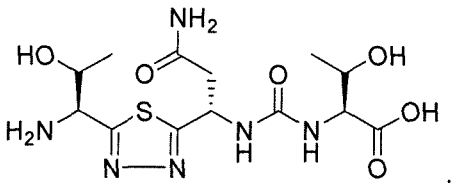
14. The compound according to claim 1, having the following structure:



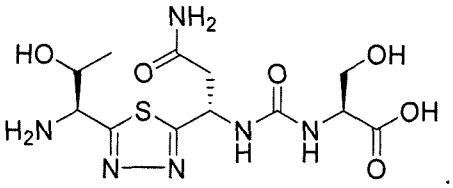
15. The compound according to claim 1, having the following structure:



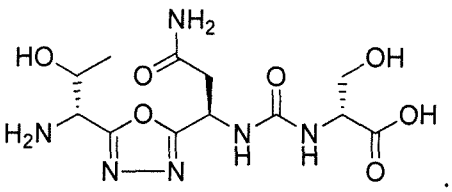
16. The compound according to claim 1, having the following structure:



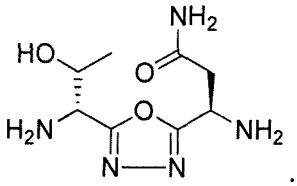
17. The compound according to claim 1, having the following structure:



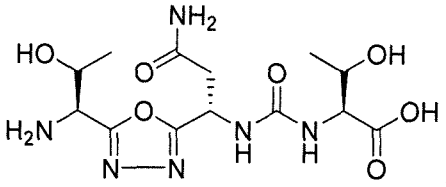
18. The compound according to claim 1, having the following structure:



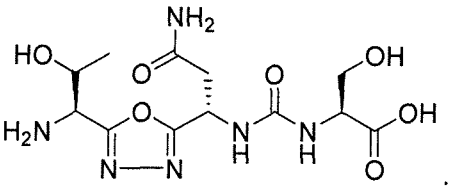
19. The compound according to claim 1, having the following structure:



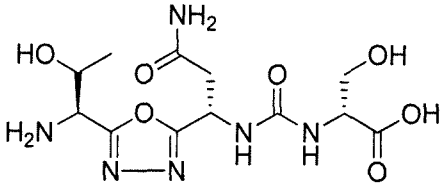
20. The compound according to claim 1, having the following structure:



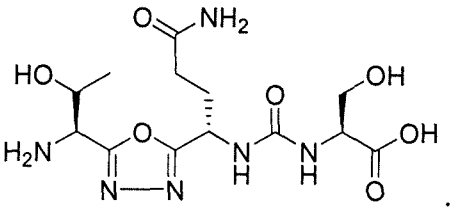
21. The compound according to claim 1, having the following structure:



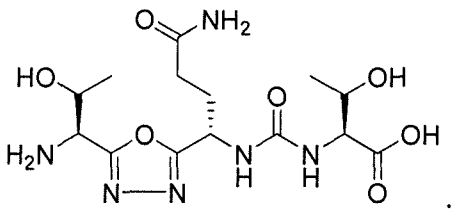
22. The compound according to claim 1, having the following structure:



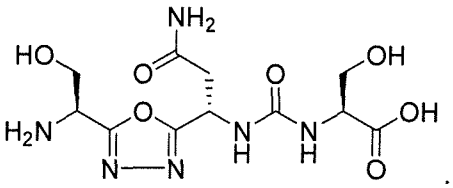
23. The compound according to claim 1, having the following structure:



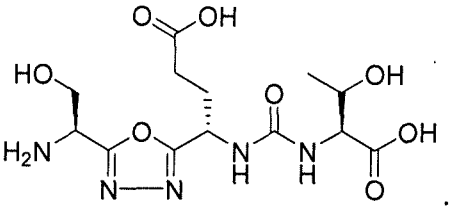
24. The compound according to claim 1, having the following structure:



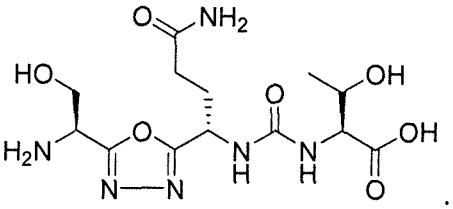
25. The compound according to claim 1, having the following structure:



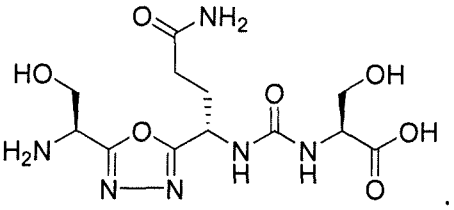
26. The compound according to claim 1, having the following structure:



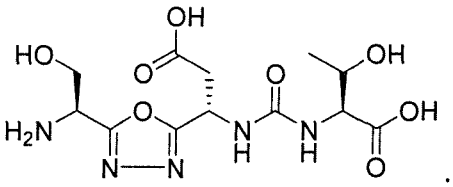
27. The compound according to claim 1, having the following structure:



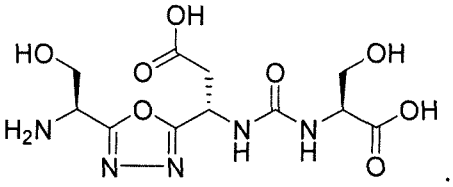
28. The compound according to claim 1, having the following structure:



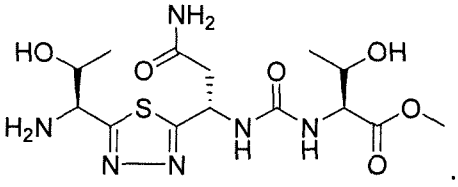
29. The compound according to claim 1, having the following structure:



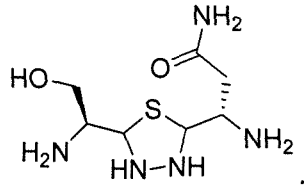
30. The compound according to claim 1, having the following structure:



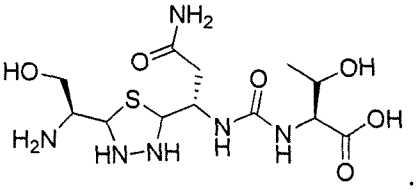
31. The compound according to claim 1, having the following structure:



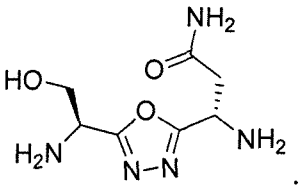
32. The compound according to claim 1, having the following structure:



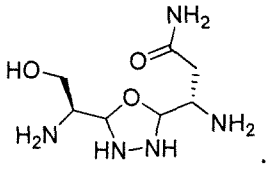
33. The compound according to claim 1, having the following structure:



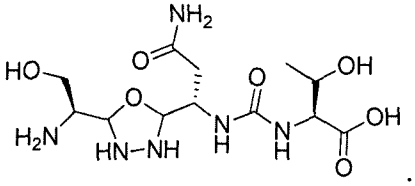
34. The compound according to claim 1, having the following structure:



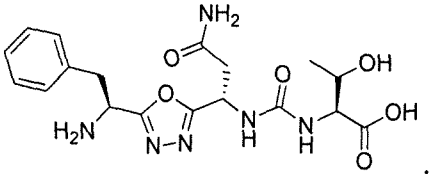
35. The compound according to claim 1, having the following structure:



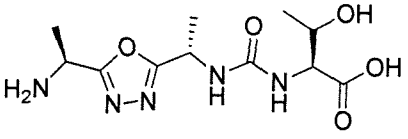
36. The compound according to claim 1, having the following structure:



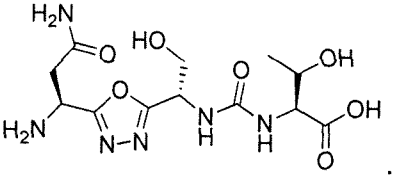
37. The compound according to claim 1, having the following structure:



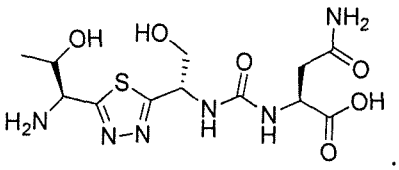
38. The compound according to claim 1, having the following structure:



39. The compound according to claim 1, having the following structure:



40. The compound according to claim 1, having the following structure:



41. A pharmaceutical composition comprising a pharmaceutically acceptable carrier or excipient and at least one compound according to any one of claims 1 to 40 or a pharmaceutically acceptable salt thereof.

42. The pharmaceutical composition according to claim 41, further comprising at least one agent selected from an anticancer agent, a chemotherapy agent, and an antiproliferative compound.

43. Use of a compound according to any one of claims 1 to 40 or a pharmaceutically acceptable salt thereof, for the manufacture of a medicament for modulating an immune response mediated by PD-1 signaling pathway in a cancer.

44. Use of a compound according to any one of claims 1 to 40 or a pharmaceutically acceptable salt thereof, for the manufacture of a medicament for the treatment of cancer.

45. Use according to claim 44, wherein the cancer is selected from breast cancer, colon cancer, lung cancer, melanoma, prostate cancer, and renal cancer.

46. Use according to claim 44, wherein the cancer is selected from bone cancer, cancer of the head or neck, pancreatic cancer, skin cancer, cutaneous or intraocular malignant melanoma, carcinoma of the endometrium, carcinoma of the cervix, carcinoma of the vagina, carcinoma of the vulva, Hodgkin's Disease, non-Hodgkin's lymphoma, cancer of the esophagus, cancer of the small intestine, cancer of the endocrine system, cancer of the thyroid gland, cancer of the parathyroid gland, cancer of the adrenal gland, sarcoma of soft tissue, cancer of the urethra, cancer of the penis, chronic or acute leukemias including acute myeloid leukemia, chronic myeloid leukemia, acute lymphoblastic leukemia, chronic lymphocytic leukemia, solid tumors of

childhood, lymphocytic lymphoma, cancer of the bladder, cancer of the kidney or ureter, carcinoma of the renal pelvis, neoplasm of the central nervous system (CNS), primary CNS lymphoma, tumor angiogenesis, spinal axis tumor, brain stem glioma, pituitary adenoma, Kaposi's sarcoma, epidermoid cancer, squamous cell cancer, T-cell lymphoma, environmentally induced cancers including those induced by asbestos, and combinations of said cancers.

47. Use of a compound according to any one of claims 1 to 40 or a pharmaceutically acceptable salt thereof, for the manufacture of a medicament for modulating an immune response mediated by PD-1 signaling pathway in an infectious disease.

48. Use of a compound according to any one of claims 1 to 40 or a pharmaceutically acceptable salt thereof, for the manufacture of a medicament for modulating an immune response mediated by PD-1 signaling pathway in a bacterial infectious disease, a viral infectious disease or a fungal infectious disease.

49. Use according to claim 47, wherein the infectious disease is selected from HIV, Influenza, Herpes, *Giardia*, Malaria, *Leishmania*, the pathogenic infection by the virus Hepatitis (A, B, & C), herpes virus (e.g., VZV, HSV-I, HAV-6, HSV-II, and CMV, Epstein Barr virus), adenovirus, influenza virus, flaviviruses, echovirus, rhinovirus, coxsackie virus, cornovirus, respiratory syncytial virus, mumps virus, rotavirus, measles virus, rubella virus, parvovirus, vaccinia virus, HTLV virus, dengue virus, papillomavirus, molluscum virus, poliovirus, rabies virus, JC virus and arboviral encephalitis virus, pathogenic infection by the bacteria *chlamydia*, rickettsial bacteria, mycobacteria, staphylococci, streptococci, pneumonococci, meningococci and conococci, *klebsiella, proteus, serratia, pseudomonas, E. coli, legionella*, diphtheria, *salmonella*, bacilli, cholera, tetanus, botulism, anthrax, plague, leptospirosis, and Lyme's disease bacteria, pathogenic infection by the fungi *Candida* (*albicans, krusei, glabrata, tropicalis*, etc.), *Cryptococcus neoformans, Aspergillus* (*fumigatus, niger*, etc.), Genus *Mucorales* (*mucor, absidia, rhizophus*), *Sporothrix schenkii, Blastomyces dermatitidis, Paracoccidioides brasiliensis, Coccidioides immitis* and *Histoplasma capsulatum*, and pathogenic infection by the parasites *Entamoeba histolytica,*

*Balantidium coli, Naegleria fowleri, Acanthamoeba* sp., *Giardia lambia, Cryptosporidium* sp., *Pneumocystis carinii, Plasmodium vivax, Babesia microti, Trypanosoma brucei, Trypanosoma cruzi, Leishmania donovani, Toxoplasma gondi,* or *Nippostrongylus brasiliensis.*