|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Software** | **Affinity**  **(kcal/mol)** | **Interactions** | | **Pub chem CID** | **Attributes and application** | **source** | **Compound Name** | | **#** |
| **Other type interactions** | **Hydrogen Bond** |
| **Section one (Food borne polyphenols)**1 | | | | | | | | | |
| AutoDock Vina 1.1.2. | -9.8 | **Van de waals:**  LEU141, THR25, MET165, GLU166,  HIS164, HIS41, MET49, GLN189 | GLY143,SER144, ASN142 | 71307578 | \_ | Tea [Black], infusion | **Theaflavin 3-O-gallate** | | 1 |
| AutoDock Vina 1.1.2. | -9.8 | **Van de waals:**  SER144, THR25,PHE140,GLY143,ASN142,MET165, ASP187,MET49,GLN189,TYR54,ARG188 | HIS163 | 5318759 | \_ | Red raspberry, pure  juice | **Kaempferol 3-O-glucuronide** | | 2 |
| AutoDock Vina 1.1.2. | -10.3 | **Van de waals:**  GLU288,MET276,LEU267,GLY275,LEU267,GLY275,LEU272,TYR237,ASN274,THR199,ASN23,THR198,LYS137, VAL171, THR169 | ASN23, LYS137, LYS5 | 16130897 | antioxidant | Red raspberry, raw | **Sanguiin H-6** | | 3 |
| AutoDock Vina 1.1.2. | -9.8 | **Van de waals:**  GLU288,LEU286,GLU290,LYS137,GLY170,GLU16,PHE140,LEU141,SER139 | LYS5, PHE140, GLU288 | 44584733 | had carbonic anhydrase inhibitor activity | Pomegranate, pure  juice | **Punicalagin** | | 4 |
| **Section two (Potential Drug Candidates)**2 | | | | | | | | | |
| AutoDockVina | -4.7 | **Van de waals:**  VAL104,GLN107,GLN110,ILE106,THR111,ASN151,ASP153,THR192 ,PHE294 | LYS102,  SE158 | 65028 | antiviral | Synthetic | **Oseltamivir** | | 5 |
| AutoDockVina | -7.3 | **Pi-Anion:**  ASP153  **Pi- Pi T-Shaped**: PHE294  **Akyl /Pi Akyl:** VAL104, ILE106,ILE200,VAL202,ILE249,VAL297 | THR111 | 392622 | Antiretroviral  Mainly used against HIV | Synthetic | **Ritonavir** | | 6 |
| AutoDockVina | -6.5 | **Pi-sigma:** ILE249  **Pi-Alkyl:**PHE8, VAL202,PRO293  **Van de waals:**  ARG105,ILE106,GLN107,THR111,ILE152, ASP153,HIS246 | GLN110, ASN151,PHE294 | 121304016 | broad-spectrum antiviral medication | Synthetic | **Remdesivir** | | 7 |
| AutoDockVina | -5.6 | **Van de waals:**  LYS137,  THR199,ASP197,ASN238,LEU286,GLU288 | ARG131,TYR237,LEU287 | 37542 | antiviral | Synthetic | **Ribavirin** | | 8 |
| AutoDockVina | -5.4 | \_ | GLN110,THR111,ASN151,TH292,ASP295 | 492405 | antiviral | Synthetic | **Favipiravir** | | 9 |
| AutoDockVina | -5.1 | **Carbon hydrogen bind:** THR111  **Akyl /Pi Akyl:**  PHE294,VAL104,ILE106 |  | 2719 | Used agains malaria | Synthetic | **Chloroquine** | | 10 |
| AutoDockVina | -5.3 | **Van de waals:** PHE8,GLN110,THR111,PRO293,PHE294  **Akyl /Pi Akyl:**  ILE249,PRO252,VAL297 | ASN151 | 3652 | Used agains malaria | Synthetic | **Hydroxy**  **chloroquine** | | 11 |
| **Section three** 3 | | | | | | | | | |
| The GLIDE module of Maestro 11.4 | -69.04 | \_ | GLY143, HIS 163, GLU 166 | 68884 | used to treat HYPERLIPIDEMIAS | Synthetic | **Binifibrate** | | 12 |
| The GLIDE module of Maestro 11.4 | -64.25 | \_ | GLY 143, HIS 164, GLU 166, THR 190 | 71526737 | for the diagnosis of growth hormone deficiency (GHD) in adults | Synthetic | **Macimorelin acetate** | | 13 |
| The GLIDE module of Maestro 11.4 | -63.19 | \_ | GLY143, GLU 166, GLN 189 | 16229 | capable of relieving pain without the loss of CONSCIOUSNESS | Synthetic | **Bamifylline** | | 14 |
| The GLIDE module of Maestro 11.4 | -61.37 | \_ | THR 26, GLY 143, HIS 163, GLU 166 | 5069 | used to reduce psychological excitement or anxiety | Synthetic | **Rilmazafone** | | 15 |
| The GLIDE module of Maestro 11.4 | -60.89 | \_ | GLY 143, GLU 166 | 10184653 | kinase inhibitor , used to treat non-small cell lung carcinoma(NSCLC) | Synthetic | **Afatinib** | | 16 |
| **The GLIDE module of Maestro 11.4** | -60.21 | \_ | GLU 166 | 150311 | to reduce elevated total-C, LDL-C, Apo B, and non-HDL-C in patients with primary hyperlipidemia, | Synthetic | **Ezetimibe** | | 17 |
| **Section four( inhibitors identified from Camellia sinensis)4** | | | | | | | | | |
| GLIDE docking module of Schrodinger | -8.701 | **Van de waals:** PHE140, HIS163 SER144 ,HIS164 GLY 143 ASN142,  LEU 27,THR25, MET49 LEU 167 ,ARG 188 GLN 192, THR 190 ALA 191, PRO168  **ALKYL:** CYS145 | HIS41  LEU141  MET165  GLU166 | 135403798 | antioxidant | *Camellia sinensis* | **Theaflavin** | | 18 |
| GLIDE docking module of Schrodinger | -6.282 | **Van de waals:**   LEU 167 PRO168 HIS 172 PHE140 MET163 HIS163 SER144 HIS 164 GLN189 CYS145 MET49 THR25  LEU 27 GLY 143 | THR26  HIS41  LEU141  ASN142  GLU166 | 65064 | Used for weight loss, body building and “faburning | *Camellia sinensis* | **Epigallocatec**  **hin**  **3-gallate** | | 19 |
| GLIDE docking module of Schrodinger | -4.688 | **Van de waals:**    SER 144  ASN 142 HIS163 HIS 172 PHE140 LEU27 MET-49 GLN 189 **carbone hydrogen bond** :Met 165  **Pi-Alkyl/Alkyl:** HIS41 CYS145 | Leu141  Glu143  His164  Glu166 | 54671997 | Anti-inflammatory activity in human | *Camellia sinensis* | **Cordysinin A** | | 20 |
| GLIDE docking module of Schrodinger | -7.795 | **Van de waals:** MET 49,HIS164, GLN 192,THR190, ARG 188,LEU167, PRO168,SER 144 ,LEU141,LEU27,THR 25  **carbone hydrogen bond:**  HIS41ASN142  **Pi-Alkyl:** MET165  **Pi-sigma**:GLN189 | THR26  GLU143  CYS145  GLY166 | 10155076 |  | *Camellia sinensis* | **1-O-caffeoylquinic**  **acid** | | 21 |
| GLIDE docking module of Schrodinger | -7.168 | **Van de waals:**  CYS 44, THR54, HIS 164, CYS 145,GLY 143 ,SER 144,ASN 142, PHE 140, MET 165, GLN 189, PRO 52  **carbone hydrogen bond**  **:**ARG188  **Pi-Alkyl:**MET49  **Pi-Pi T shapped:**HIS163 | HIS41  LEU141  GLU166  ASP187 | 5280961 | an angiogenesis inhibitor | *Camellia sinensis* | **Genistein** | | 22 |
| GLIDE docking module of Schrodinger | -4.395 | **Van de waals:** GLY143, ASN 142, HIS163, PHE 140,LEU141, HIS172 ,ASP187,ARG 188 ,GLN 192,T HR190,LEU 167, PRO 168  **carbone hydrogen bond**: GLN 189 ,Glu 166  **Pi-Alkyl/Alkyl:** M ET 165, MET 49 ,HIS 41 | SER144  CYS145 | 53493989 | Cytotoxicity against human specified cells | *Camellia sinensis* | **Inflatin E** | | 23 |
| GLIDE docking module of Schrodinger | -3.774 | **Van de waals:** MET49,ARG188,GLN192, THR190,LEU167,PRO168,SER144,HIS163,CYS145,ASN142,  **carbone hydrogen bond:** ASP187,GLN189, HIS164  **Pi-Pi T shapped**:  **Pi-Alkyl/Alkyl**:  MET165 | GLU143  GLU166 | 53494114 | Cytotoxicity against human specified cells | *Camellia sinensis* | **Inflatin F** | | 24 |
| GLIDE docking module of Schrodinger | -4.434 | **Van de waals:** LEU27,HIS164,GLY143,HIS163,ASN142,LEU141,PHE140,  HIS172, AS P187,ARG188, GLN192,THR194,LEU167,PRO168  **carbone hydrogen bond:** GLU166, GLN189  **Pi-Alkyl /Alkyl:**  MET165,MET49,HIS 41 | SER144  CYS145 | 53493988 | Cytotoxicity against human specified cells | *Camellia sinensis* | **Inflatin D** | | 26 |
| GLIDE docking module of Schrodinger | -4.784 | **Van de waals:** PRO52,CYS44,TYR 54, THR25, THR26, GLY143,ASN142,LEU141,HIS163,GLU 166,HIS164,MET 165,GLN189  **carbone hydrogen bond:** HIS41,ARG188  **Pi-sulfur**:CYS145  **Pi-Alkyl**:Leu27,Met49 | SER144  ASP187 | 136026468 | Cytotoxicity against human specified cells | *Camellia sinensis* | **2-(4-hydroxybenzyl)**  **quinazolin-4(3H)-**  **one** | | 27 |
| GLIDE docking module of Schrodinger | -3.862 | **Van de waals:** PRO168, GLN192, LEU167,GLN189  **Pi-Anion:**HIS41  **carbone hydrogen bond**:  THR190, ARG188, ASP187  **Pi-Alkyl /Alkyl:**  MET165 | GLU166 | 8468 | used as a flavoring agent | *Camellia sinensis* | **Vanillic acid** | | 28 |
| GLIDE docking module of Schrodinger | -5.356 | **Van de waals:** ALA191, LEU167,GLN192,ARG188 ,CYS44, PRO52, TY R54, GLN189, GLU 166  **carbone hydrogen bond:**  PRO168, ASP 187  **Pi-Alkyl /Alkyl:**  HIS41,MET49,MET165 | THR190 | 5317238 | Cytotoxicity against human HeLa cells, Anti-inflammatory activitys in mouses | *Camellia sinensis* | **Ethyl trans-caffeate** | | 29 |
| GLIDE docking module of Schrodinger | -3.169 | **Van de waals:**  ALA191, TH190, M ET165, HIS164, LEU141, LEU27, SER 144, MET49, CYS 145, GLY143, GLN 189, LEU157  **carbone hydrogen bond:**  PRO 168 GLU 166  **Pi-Alkyl:**HIS163 | HIS41  ASN142 | 12004512 | Antimalarial | *Camellia sinensis* | **Gedunin** | | 30 |
| **Section five ( Computational studies on herbal compounds)5** | | | | | | | | | |
| Auto Dock Vina | -14.6 | **Types of Interaction** : H bond, π- π, π- cation  GLU290, LYS-5, GLN-127, PHE-8, CYS-128, ASN-151, PHE-112 | | 442674 | immunosuppressive, hepatoprotective | Amla | **Chebulagic Acid** | | 31 |
| Auto Dock Vina | -14.2 | **Types of Interaction** : H- bond, π- cation  ASN-238, ASP-197, LYS-13, THR-199, LEU-287, ASP-289 | | 442688 | carbonic anhydrase inhibitor | Amla | **Pedunculagin** | | 32 |
| Auto Dock Vina | -6.8 | **Types of Interaction** : H- bond  GLN-192, ASN-142, MET-165, | | 145858 | Efficacy of Anthocyanin Mouthrinse for Oral Anti-inflammation From Orthodontic Treatment | Elderberry | **Flavylium** | | 33 |
| Auto Dock Vina | -9.1 | **Types of Interaction** :  H- bond  SER-144, GLY-138 , GLU-166, HIS-41, ASN-142 | | 441667 | \_ | Elderberry | **Cyanidin-3-glucoside** | | 34 |
| Auto Dock Vina | -7.6 | **Types of Interaction** : H- bond, π- π  GLN-192, THR-190, HIS-41, LEU-141 PHE-140 | | 3084569 | affects the localization of NFE2L2 protein | Elderberry | **Cyanidin-3-sambubioside** | | 35 |
| Auto Dock Vina | -7.4 | **Types of Interaction** :  H- bond, π- π, π- cation  LYS-137, ARG-131, TYR-239, THR-199, LEU-271, | | 1794427 | Effect of Chlorogenic Acid on Patients With Impaired Glucose Tolerance | Moringa | **Chlorogenic acid** | | 36 |
| Auto Dock Vina | -11.5 | **Types of Interaction** :  H- bond, π- cation  GLY-143  THR-26 | | 5281303 | It is a highly oxidized tetranortriterpenoid which boasts a plethora of oxygen-bearing functional groups | Neem | **Azadirachtin** | | 37 |
| Auto Dock Vina | -12.3 | **Types of Interaction** :  H- bond  GLN-110, SER158, THR-111 | | 12313376 | anticancer | Neem | **Nimbolide** | | 38 |
| Auto Dock Vina | -8.2 | **Types of Interaction** :  H- bond, π- π  SER-144, HIS-163, GLU-166, THR-190 | | 5280443 | reverses the adverse effects of cyclosporine | Tulsi | **Apigenin** | | 39 |
| Auto Dock Vina | -9.5 | **Types of Interaction** : H- bond, π- π, π- cation  GLU-166, THR-24, THR-25 | | 10494 | \_ | Tulsi | **Oleanolic Acid** | | 40 |
| Auto Dock Vina | -8.9 | **Types of Interaction** : H- bond, π- π  ALA-191, THR-190, ASN-142 | | 124052 | Estimation of efficacy of glabridin to reduce visceral fat area | Liquorice | **Glabridin** | | 41 |
| Auto Dock Vina | -13.3 | **Types of Interaction** : H- bond  GLN-192, THR-190, THR-45, GLY-143 | | 3495 |  | Liquorice | **Glycyrrhizin** | | 42 |
| Auto Dock Vina | -7.5 | **Types of Interaction** : H- bond  THR-190, GLN-192, HIS-41 | | 114829 | Sleep Quality in CHIMES (MF101) | Liquorice | **Liquiritigenin** | | 43 |
| Auto Dock Vina | -6.1 | **Types of Interaction** : H- bond  GLN-127 | | 637563 | improve the taste | Fennel | **trans-anethole** | | 44 |
| Auto Dock Vina | -8.3 | **Types of Interaction** : H- bond  THR-24 THR-26, GLN-189 | | 265237 | USED to increase energy and reduce stress | Ashwagandha | **Withaferin-A** | | 45 |
| **Section six ( based on isatin derivatives)**6 | | | | | | | | | |
| AutoDock4.2 | -6.45 | GLU166 (2.18 Å), CYS145 | | 3194 | possible treatment for reperfusion injury, stroke, and tinnitus | Synthetic | **Ebselen** | | 46 |
| AutoDock4.2 | -6.93 | HIS41 (2.02 Å), GLY143 (2.21 Å), SER144 (2.02 Å),  CYS145 (2.11 Å), HIS 163 (2.14 Å), | | 145996610 | being studied for its activity against a number of viral infections including influenza, MERS-CoV, and SARS-CoV-2. | Synthetic | **EIDD-2801** | | 47 |
| AutoDock4.2 | -7.60 | GLY143(1.76 Å), CYS145(2.16 Å),  GLU166 (2.068 Å) | | 4477 | For the treatment of tapeworm and intestinal fluke infections | Synthetic | **Niclosamide** | | 48 |
| AutoDock4.2 | -9.42 | LEU141 (2.22 Å), MET163 (2.16 Å),  HIS164 (2.20 Å), GLN192 (2.09 Å) | | 31401 | decreases the absorption of cholesterol | Synthetic | **Ursodeoxycholic acid** | | 49 |
| AutoDock4.2 | -7.94 | HIS164 (2.23 Å), GLU166 (2.12 Å), ASP187 (2.02 Å), | | 5280343 | used to treat or prevent diverse conditions including cardiovascular disease, hypercholesterolemia, rheumatic diseases, infections and cancer but it Efficiency is undde debate | Synthetic | **Quercetin** | | 50 |
| AutoDock4.2 | -7.96 | GLU166 (2.07 Å), ASP187 (2.05 Å), THR190 (1.92 Å), GLN192 (2.026 Å) | | 5280863 | kaempferol is known to suppress growth of a number of human malignancies | Synthetic | **Kaempferol** | | 51 |
| AutoDock4.2 | -7.76 | THR190 | | 68071 | \_ | Synthetic | **Pinocembrin** | | 52 |
| AutoDock4.2 | -8.12 | ASN142 (2.10 Å), HIS164(2.15 Å), GLU166 (1.93 Å), THR190 (2.06 Å),  GLN189-NH (1.79 Å), GLN189 C¼O (2.19 Å), GLN189 C¼O (2.08 Å). | | 6728944 | \_ | Synthetic | **Rutin** | | 53 |
| **Section seven (flavonoids from calendula officinalis)7** | | | | | | | | | |
| Dock Prep tool of UCSF Chimera | -8.5 | ARG188, ASP187, MET165, HIS163, SER144, GLU166, PHE140, LEU141, CYS145, GLY143, ASN142,  LEU27, MET49, GLN189, HIS41, TYR54 | | 14238620 | \_ | *Calendula officinalis* | **Calendoflaside** | | 54 |
| Dock Prep tool of UCSF Chimera | -8.4 | GLU186, LEU141, ASN142, CYS145, GLY143, LEU27, MET49, TYR54, ASP187, MET165, HIS41,  GLN189, ARG188 | | 5481663 | Antioxidant | *Calendula officinalis* | **Narcissin** | | 55 |
| Dock Prep tool of UCSF Chimera | -8.2 | PHE140, SER144, HIS163, GLU166, ALA191, THR190, GLN189, ARG188, ASP187, LEU141, HIS41,  MET165, GLY143, CYS145, ASN142, HIS164 | | 24204442 | \_ | *Calendula officinalis* | **Calendulaglycoside B** | | 56 |
| **Section eight (from Lichen)**8 | | | | | | | | | |
| AutoDock Vina | -8.4 | GLU166, HIS41, MET49, PHE140, LEU141, ASN142, SER144, CYS145, HIS163, MET165, ASP187, ARG188, GLN189 | | 54694371 | Growth retarding activity against neonate larval stage of Spodoptera littoralis | Lichen | **Calycin** | | 57 |
| AutoDock Vina | -8.7 | GLU166, GLN189, GLN192, HIS41, MET49, PHE140, LEU141, ASN142, SER144, CYS145, HIS163, HIS164, MET165, PRO168, ASP187, ARG188, THR190 | | 54733074 | \_ | Lichen | **Rhizocarpic acid** | | 58 |
| AutoDock Vina | \_9.4 | HIS41, MET49, CYS145,MET165,ARG187,ARG188, GLN189 | LEU141, ASN142, SER144,  HIS163, GLU166, | 443654 | \_ | Fruits, berries, red grapes  and red wines (Landrault  et al., | **Peonidin 3-O-glucoside**  **(C22H23O11‏)** | | 59 |
| AutoDock Vina | -9.3 | LEU27, HIS41,MET49,CYS145,MET165, ASP187 | THR25, SER46,  TYR54, GLU166 | 25201364 | \_ | Selliguea feei rhizomes | **Kaempferol 3-O-b -rutinoside** | | 60 |
| AutoDock Vina | -9.1 | MET165,PRO168,ASP187,ARG188, GLN189 | HIS41, LEU141, ASN142,SER144,HIS163,  GLU166,THR190 | 5320863 | \_ | Prunus salicina , Prunus  domestica peels | **Quercetin-3-D-xyloside** | | 61 |
| AutoDock Vina | -9.0 | HIS41, MET49, PHE140,LEU141,ARG188,GLN189 | TYR53, HIS163,  GLU166,ASP187 | 329766687 | \_ | Ruprechtia  polystachya leaves | **Quercetin 3-O-a-L-arabinopyranoside** | | 62 |
| **Section nine ( plant-based natural compounds)**9 | | | | | | | | |  |
| AutoDock Vina | -8.9 | HIS41, MET49,ASN142, GLY143,  MET165, GLN189 | THR24, THR26, TYR54,  PHE140, LEU141, SER144,  CYS145, HIS163, GLU166 | 329824889 | \_ | Prunus armeniaca | **Kaempferol 3-rutinoside 4-glucoside** | | 63 |
| AutoDock Vina | -8.8 | HIS41, MET49, ASN142, CYS145,MET165,ASP187,ARG188, GLN189 | LEU141, SER144, GLU166 | 329751366 | \_ | Mulberry leaves | **Quercetin 3-O-(600-O-malonyl)-b-D-glucoside \_** | | 64 |
| AutoDock Vina | -8.7 | LEU27, HIS41, MET49, GLY143,  CYS145, MET165, GLU166, GLN189 | LEU141, SER144,  HIS163, THR190 | 441765 | malvin results in decreased activity of CA1 protein | Grapes and wine | **Malvin** | | 65 |
| AutoDock Vina | -8.6 | HIS41, MET49, ASN142, CYS145,  MET165, GLU166, ASP187,  ASP188, GLN189 | THR26, SER144 | 44258082 | \_ | Cyclopia subternata | **Luteolin 7-rutinoside** | | 66 |
| AutoDock Vina | -8.5 | HIS41, MET49, MET165, GLN189 | THR26, SER144,  HIS163, ARG188 | 441688 | Inhibition of human thrombin amidolytic activity using D-Phe-Pip-Arg-pNA as substrate | Berries, Grapes, Apples,  Purple Cabbage | **Cyanin** | | 67 |
| AutoDock Vina | -8.4 | THR25, LEU27, THR45, MET49,  CYS145, MET165, GLN189 | THR26, SER46, GLY143,GLU166,THR190 | 5483905 | Inhibition of electric eel AChE at 2 mg/ml by Ellman's method | Litchi chinensis fruit | **Kaempferol 7-O-neohesperidoside** | | 68 |
| AutoDock Vina | -8.3 | HIS41, TYR54, GLU166, ARG188 | SER144, CYS145, HIS163,  MET165, ASP187 | 71341751 | \_ | Nasturtium officinale | **Rhamnetin 3-sophoroside** | | 69 |
| AutoDock Vina | -8.2 | GLU166, GLU189 | LEU141, SER144, MET165,THR190,GLN192 | 329824902 | \_ | Nelumbo nucifera Gaertn | **Myricetin 3-O-b-D-Galactopyranoside** | | 70 |
| AutoDock Vina | -8.2 | Met49, Phe140, Asn142, Cys145,  His163, Met165, Pro168, Gln189,  Thr190, Ala191, | LEU141, GLY143, SER144 | 329824876 | \_ | Mimosa  xanthocentra | **2"-O-alpha-L-Rhamnopyranosyl-isovitexin** | | 72 |
| AutoDock Vina | -8.0 | Met49, Cys145, Met165, Gln189 | THR24, THR25, THR26,  CYS44, ASN142 | 6436550 | hesperidin methylchalcone affects the expression of IL10, IL6 And IL1B protein | lemons and sweet  oranges | **Hesperidin methylchalcone** | | 73 |
| MOE | -5.11696768 | Two hydrogen interaction are possible with:  - Amino acid THR 190 (H-donor) with distance about 3.11 Å and energy of -3.3 Kcal/mol.  - Amino acid GLU 166 (π-H) with distance about 4.12 Å and energy of -1.0 Kcal/mol | | 11402337 | \_ | Nigella Sativa | **Nigellicine** | | 74 |
| **Section ten (Compounds from *Nigella Sativa*)**10 | | | | | | | | |  |
| MOE | -4.80306292 | No perceptible interactions, only electrostatics exist (Van der Waals) | | 20725 | Altered sleep time (including change in righting reflex) | Nigella Sativa | **Nigellimine** | | 75 |
| MOE | 4.8290143 | Three hydrogen interactions are possible with:  - Amino acid HIS 41 (H-π) with distance about 4.35 Å and energy of -0.6 Kcal/mol.  - Amino acid GLN 189 (π-H) with distance about 4.16 Å and energy of -0.8 Kcal/mol.  - Amino acid THR 190 (π-H) distance about 4.67 Å and energy of -0.8 Kcal/mol | | 10364 | Very toxic | Nigella Sativa | **Carvacrol** | | 76 |
| MOE | -5.25583553 | Three hydrogen interaction are possible with:  - Amino acid HIS 164(H-donor) with distance about 2.83 Å and energy of -1.8 Kcal/mol.  -Amino acid CYS 145 with distance about 4.08 Å and energy of -1.1 Kcal/mol.  - Amino acid MET 165 distance about 3.73 Å and energy of -0.6 Kcal/mol | | 319412227 | \_ | Nigella Sativa | **α- Hederin** | | 77 |
| MOE | -4.50417519 | Only one hydrogen interaction (π-H) is possible with amino acid GLN189 with distance about 4.24 Å and energy of -0.7 Kcal/mol. | | 6989 | Anti-Infective Agents | Nigella Sativa | **Thymol** | | 78 |
| MOE | -4.71068573 | Only one hydrogen interaction (π-H) is possible with amino acid THR 190 with distance about 4.70 Å and energy of -0.8 Kcal/mol. | | 10281 | \_ | Nigella Sativa | **Thymoquinone** | | 79 |
| MOE | -4.45150137 | Only one hydrogen interaction (H-acceptor) is possible with amino acid THR 190 with distance about 2.89 Å and energy of -3.9 Kcal/mol. | | 398941 | \_ | Nigella Sativa | **Dithymoquinone** | | 80 |
| MOE | -4.22977924 | Only one hydrogen interaction (π-H) is possible with amino acid GLU 166 with distance about 4.46 Å and energy of -1.0 Kcal/mol. | | 95779 | \_ | Nigella Sativa | **thymohydroquinone** | | 81 |
| **Section Eleven (pyridone-containing pharmaceuticals)**11 | | | | | | | | |  |
| AutoDock Vina | -5.9 | HIS 41 (3.185 ˚ A/ 3.334 ˚ A/ 3.574 ˚ A/ 3.796 ˚ A). CYS 145 (3.553 ˚ A/ 3.826 ˚ A). Glu 166 (17 **side contacts, distance range:** 3.201 ˚A to 3.920 ˚ A) | GLU 166 | 3010818 | used in the treatment of chronic HCV genotype 1 infection in adults | Synthetic | **Telaprevir** | | 82 |
| AutoDock Vina | -7.1 | ALA 285 (3.436 ˚ A) | \_ | 6918289 | first-line treatment of adult patients with advanced renal-cell carcinoma (RCC) | Synthetic | **Temsirolimus** | | 83 |
| AutoDock Vina | -6.7 | GLU 166 (13 **side contacts, distance range:** 2.817 ˚A to 4.113 ˚ A) | \_ | 6509979 | For treatment of mild to moderate atopic dermatitis. | Synthetic | **Pimecrolimus** | | 84 |
| AutoDock Vina | -5.6 | CYS 145 (4.027 ˚ A). HIS 41 (distance: 3.331 ˚ A/ 3.599 ˚ A/ 3.889 ˚ A). GLU 166 (14 side **contacts, distance range:** 2.480 ˚A to 4.034 ˚ A). | GLU 166 (2.480 ˚ A/ 2.647 ˚ A) | 2145 | For the suppression of adrenal function in selected patients with Cushing's syndrome, malignant neoplasm of the female breast, and carcinoma in situ of the breast | Synthetic | **Aminoglutethimide** | | 85 |
| AutoDock Vina | -7.4 | ALA 285 (3.302 ˚ A/ 3.546 ˚ A). HIS 41 (distance: 2.720 ˚ A/ 2.875 ˚ A/ 2.948 ˚ A/ 3.131 ˚ A/ 3.635 ˚ A). GLU 166 (6 **side contacts, distance range:** 3.423 ˚A to 4.076 ˚ A) | \_ | 10182969 | indicated for reducing the risk of stroke and systemic embolism in patients who have nonvalvular atrial fibrillation | Synthetic | **Apixaban** | | 86 |
| AutoDock Vina | -6.9 | 3.708 ˚ A/ 3.762 ˚ A/ 3.951 ˚ A). CYS 145 (distance: 3.831 ˚ A). GLU 166 (12 **side contacts, distance range:** 3.107 ˚A to 4.142 ˚ A). | Cys 145 Glu 166 | 2477 | Indicated for the management of anxiety disorders or the short-term relief of the symptoms of anxiety. | Synthetic | **Buspirone** | | 87 |
| AutoDock Vina | -6.5 | HIS 41 (distance: 3.324 ˚ A). CYS 145 (distance: 3.814 ˚ A). GLU 166 (9 side **contacts, distance range:** 3.137 ˚A to 3.919 ˚ A). | Cys 145 Glu 166 | 216326 | Lenalidomide is indicated for the treatment of multiple myeloma in combination with dexamethasone. | Synthetic | **Lenalidomide** | | 88 |
| AutoDock Vina | -6.6 | HIS 41 (distance: 3.377 ˚ A). CYS 145 (distance: 3.616 ˚ A/ 3.823 ˚ A). Glu 166 (13 **side contacts, distance range**: 2.310 ˚A to 3.948 ˚ A). | Cys 145 Glu 166 | 134780 | indicated for patients with multiple myeloma | Synthetic | **Pomalidomide** | | 89 |
| **Section twelve( *Aloe vera* compounds)**12 | | | | | | | | |  |
| Autodock Vina and PyRx | -6.7 | \_ | GLU166,ARG188 | 10207 | Subcategory of personal care products; products related to health such as cough, cold and flu products | *Aloe vera* | **Aloe-emodin** | | 90 |
| Autodock Vina and PyRx | -7.1 | \_ | GLU166,SER144,LEU141,HIS164, GLN168,CYS145,,ASN142 | 12305761 | \_ | *Aloe vera* | **Aloin A** | | 91 |
| Autodock Vina and PyRx | -6.7 | \_ | GLU166,LEU141,CYS145,ASN142,HIS41, GLN189, HIS164, | 14989 | Agents that are used to stimulate evacuation of the bowels | *Aloe vera* | **Aloin b** | | 92 |
| Autodock Vina and PyRx | -7.9 | **Van de waals:**  THR25,MET49,YS44,GLY142,SE144,HIS164,MET165,GLU166,PHE140  **carbone hydrogen bond:**  HIS41 | HIS163, CYS145, LEU141, ASN142,CYS145 | 5317333 | \_ | *Aloe vera* | **Feralolide** | | 93 |
| Autodock Vina and PyRx | -7.7 | **carbone hydrogen bond:**HIS41  **Pi-Alkyl:**PRO168 | CYS145, GLU166,HIS164, GLU166 | 364666 | \_ | *Aloe vera* | **Aloeresin** | | 94 |
| Autodock Vina and PyRx | -6.8 | \_ | ASN142, HIS41 | 10208 | Used aginst prostatic hyperplasia (BPH) | *Aloe vera* | **Chrysophanol** | | 95 |
| **Section thirteen**13 | | | | | | | |  | |
| AutoDock Vina, | -8.7 | THR25,HIS41,CYS44,SER46,MET49,ASP187,ARG188,GLN189 | GLN192  MET165 | 54682461 | antiretroviral | Synthetic | **Tipranavir** | | 96 |
| AutoDock Vina, | -8.3 | MET49,PHE140,MET165,LEU167,PRO168 | HIS164,GLU166,ARG188,GLN192 | 54671008 | For the treatment of HIV-1 infection in conjunction with other antiretrovirals. | Synthetic | **Raltegravir** | | 97 |
| AutoDock Vina, | -8.3 | TH25,HIS41,LEU141,CYS154,MET165,ASP187,GLN192 | GLU166,GLN189,THR190 | 434124952 | \_ | Synthetic | **α-ketoamide 13b** | | 98 |
| AutoDock Vina, | -8.2 | HIS41,LEU141,CYS145,MET165,LEU167,PRO168,ASP187,ARG188,GLN189 | PHE140,GLU166 | 64143 | Used in combination with other antiviral drugs in the treatment of HIV in both adults and children | Synthetic | **Nelfinavir** | | 99 |
| AutoDock Vina, | -8.1 | TH25,HIS41,MET49,ASN142,CYS145,MET165,GLN189 | GLY143 | 54726191 | indicated in combination with other antiretroviral agents for the treatment of patients with HIV-1 infection | Synthetic | **Dolutegravir** | | 100 |
| AutoDock Vina, | -8.1 | HIS41,MET165,GLU166,LEU167,ASP187,GLN189 | THR190,GLN192 | 5481350 | indicated in combination with other antiretroviral agents for the management of HIV-1 infection | Synthetic | **Tenofovir-disoproxil** | | 101 |
| AutoDock Vina, | -8.1 | HIS41,MET49,MET165,GLU166,PRO168,ASP187,ARG188 | GLN189,THR190,GLN192 | 124081896 | For the treatment of influenza A and B virus infection | Synthetic | **Baloxavir-marboxil** | | 102 |
| AutoDock Vina, | -8.0 | TH25,HIS41,MET49,CYS145,MET165 | HIS163 | 45138674 | For use in prophylaxis of cytomegalovirus (CMV) infection and disease in adult CMV-seropositive recipients of an allogeneic hematopoietic stem cell transplant (HSCT) | Synthetic | **Letermovir** | | 103 |
| AutoDock Vina, | -8.0 | THR25,HIS41,MET49,LEU141,ASN142,CYS145,MET165,ASP187,ARG188 | PHE140,GLU166 | 3002977 | For treatment-experienced adult patients infected with only CCR5-tropic HIV-1 detectable, | Synthetic | **Maraviroc** | | 104 |
| Autodock Vina | -5.7 | THR26,HIS41,MET49,GLY143,SER144,CYS145,HIS164,MET165,ASP187 | | 14741611 | it has been used in the treatment of breast and colorectal cancer | Synthetic | 1415**Carmofur** | | 107 |
| Autodock Vina | -6.8 | THR26, THR 25,CYS44,CYS145,HIS163,GLY143,ASN142,PHE140,GLU166,P168,GLN189,ARG188,MET49,MET165,ASP187,HIS41,HIS164, | | 145343771 | - | Synthetic | 1615**11a** | | 106 |
| Autodock Vina | -7.0 | THR26,CYS145,HIS163,GLY143,ASN142,PHE140,GLU166,P168,GLN189,VAL186,ARG188,MET49,MET165,ASP187,HIS41,HIS164 | | 146672237 | - | Synthetic | 1615**11b** | | 107 |
| AutoDock 4 and AutoDockVina as | −9.0 | Ser1, Thr26 | |  | It is a short-acting anticoagulant, and is also used for the treatment of pancreatitis. It also has some potential antiviral and anti-cancer properties | Synthetic | 17**Nafamostat** | | 108 |
| AutoDock Tools | -7.8 | LEU141,GLY143,SE144,HIS163,GLU166 | | 5281605 | inhibit the action of prostaglandins,Antioxidant | Synthetic | 18**baicalein** | | 109 |
| GOLD | -6.8 | **hydrogen bind:** Thr26,Asn142,Gly143,Cys145,Gln189  **Other interactions:**  Thr25, Leu27, His41, Cys44, Thr45, Ser46, Met49, Phe140, Leu141, Ser144, His163, His164, Met165, Glu166, Arg188 | | 10324367 | used to treat hepatitis caused by hepatitis C virus (HCV) genotype 1 | Synthetic | **Boceprevir** | | 110 |
| - | -8 | **-** | | 155903259 | - | Synthetic | **PF-07321332** | | 111 |

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