

Supplementary data

[1] Construction of in house library from Plants (105 Compounds)

The world is rich in medicinal plants. Man cannot survive on this earth for long life without plant because the plant products and their active constituents have always been playing an important role. These include Gamma-Asarone, cis-asarone, Trans-asarone, Isoeugenol methyl ether, Acoramone, asarylaldehyde, Shyobunone, Epishyobunone, Isocalamendiol, Acoragermacrone, Preisocalamendiol, Thujane, Limonene, Myrcene, Cymene-Para, Beta pinenes, Terpinolene, Galangin, Acoradin, Beta-sitosterol, 29-tetrahydroxyolean-12-en-3-O-Beta-D-arabinosyl, 1,3-Beta-D Arabinopyranoside, 2,6-diepishyobunone, Calamusenone, Aspargamine A, Racemosol, Racemofuran, Quercitin, Shatavarin V, Sarsasapogenin, Niazimicin, Pterygospermin, Withaferin A, Viscosalactone B, Withanolide D, Lanosterin Anaferine, Epipodophyllotoxins, Etoposide, Teniposide, Daunorubicin, Doxorubicin, Idarubicin, Epirubicin, Anthracyclines, Sabarubicin, Nemorubicin, Rohitukine, flavopiridol, Beta lapachone, Paclitaxel, Cisplatin, Curcumin, Resveratrol, Bisindole alkaloids, Taxanes, Combretastatin A4 phosphate, Stilbenoid, Homoharringtonine, Mepesuccinate, Cephalotaxine A, Homoharringtonine, Benzopyran, Daidzein, Isoflavone, Phenoxodiol, Ingenol 3-O-angelate, Genistein, Diterpines [Pub chem], p-Sitosterol, a-Amyrin, Lupeol, Kaempferol, Rutin, Hexacosanol, P-Dglucoside, p-Sitosterol, Cleomin, 5,7-Dihydroxychromone, 5-hydroxy-3,7,4'-trimethoxyflavone, Lupeolin, Glucocapparine, Viscosic acid, flavone-viscosin, P-carotene, Methyl glucosinolate, Glucoiberine, Neoglucobrassicin, 5,7-dihydroxychromone, 5, Hydroxy-3,7,4'-trimethoxy flavone, Lupeolin, Cleogynol (*Cleome gynandra* Linn.), Beta-ocimene, Gamma-terpinene, cis-sabinene hydrate, Alpha-terpinolene, trans-sabinene hydrate, Linalool, Camphor, Terpinen-4-ol, Myrtenol, trans-caryophyllene, Germacrene D (*Ocimum kilimandscharicum*). In this study 105 natural compounds from different plants were selected through searching scientific literature and deposited in to in houses libraries for further screening.

[2] Compounds from vegetables (51 Compounds)

Glucoerucin, ERUCIN, Sulphoraphen, Docetaxel, Paclitaxel, Gemcitabine, Depocyt, Cytarabine, [Pub Chem], Oxalic acid, Glucoraphanin, Folic acid, Phytic acid, Chlorogenic acid, Epigallocatechin 3-gallate, Resveratrol, Lycopene, Flavonols, Sulforaphane, Caffeic acid, Ferulic Acid, Xylitol, Sorbitol, Mannitol, Lactitol, Daidzein, Genistein, Dithiolthiones, omega-3 fatty acids, Glucosinolates, Kaempferol, Quercetin, Isorhamnetin, 4-Methoxyindol-3-ylmethyl, 1-Methoxyindol-3-ylmethyl, Indol-3-ylmethyl, 4-Hydroxy-3-indolylmethyl, 3-Butenyl, 5-Methylthio pentyl, 4-Methylsulphinyl butyl,

Glucoberteroin, Glucoputranjivin isopropyl, Glucochlearin, Glucojiabutin, Desulpho-glucosinolates, Quercetin-O-sophorotrioside-7-O-sophoroside, Tetradecanoic acid, Octadecanoic acid, Eicosanoic acid, Kaempferol-O-tetraglucoside-7-O-sophoroside, Kaempferol 3-O-sophoroside-7-O-(caffeoyl)-rhamnoside, Isorhamnetin-3-sophorotrioside-7-sophoroside, Hydroxycinnamic acids, 3-caffeoyl quinic acid Decanoic acid.

[3] Construction of in house library from Lichen (50 Compounds)

Lichens are considered one of the rich sources of bio medically useful compounds likes Chloratranorin, D-Arabinitol, Lichesterol, Methyl haematommate, Atranorin, Glutanol, Vulpinic acid (2), 6Alpha-acetoxypentane-16Beta, 22-diol, 16Beta-acetoxypentane-6Alpha, 22-diolzeorin, Connorstictic acid, Salazinic acid, Norstictic acid, Chloroatranoric acid, Constipatic acid, Atranorin, Chloroatranorin (*Heterodermia appendiculata*), Stictic acid, Constictic acid, Consalazinic acid, Atranorin (*Bulbothrix isidiza*), Confumarprotocetraric acid, Protocetraric acid, fumarprotocetraric acid, Sekikaic acid, Homosekikaic acid, Atranorin, Hyperhomosekikaic acid (*Cladonia adspersa*), Beta-alectoronic acid, Alpha-collatolic acid, Skyrin (*Parmotrema rampoddense*), Isonephrosterinic acid, Protolichesterinic acid, Lichesterinic acid, (*Hypotrachyna ikomae*), Norobtusatic acid, 4-O-demethylbarbatic acid, Obtusatic acid, Barbatic acid (*Hypotrachyna imbricatula*) (3) Diffractaic acid, Protocetric acid, Lecanoric acid, Orsellinic acid (*Ramalina lacera*), (8) Gyrophoric acid, Usnic acid (17) flavo-obscurin A-B, oxolobaric acid, Lobaric acid.

[4] Bacteria derived compounds for in house library (60 Compounds)

Around 23,000 bioactive secondary metabolites from microorganisms have been reported and over 10,000 of these are from actinomycetes, representing 45% of all bioactive microbial metabolites and submit in house library for further screening. Actinomycin D, Bleomycin, L-asparaginase, Ecteinasidin 743, Aureolic acid, Dactinomycin, Idarubicin, Laxaphycins A, Laxaphycins B (*Streptomyces* spp.), (*Streptomyces verticillus*), Daunomycin (*Streptomyces coeruleorubidus*), Epirubicin (*Streptomyces pneuceticus*), Mitomycin C (*Streptomyces caespitosus*), Geldanamycin, Rapamicin (*Streptomyces hygrosopicus*), Wortamannin (*Talaromyces wortmanni* (9), Dolastatin 10, Dolastatin 15, Macrocylic polyethers, Halichondrin B, Didemnin B, Cyclic Depsipeptide, Aplidine, Bryostatins, Synthadotin, Kahalalide F, Squalamine, Dehydrodidemnin B, Cemadotin, Didemnin, Soblidotin, Discodermodide, Bengamide B, Curacin A, Salinosporamide A, Lulimalide, Vitilevuamide, Diazonamide, Eleutherobin, Sarcodictyin, Peloruside A, Salicylhalimides A

and B, Thiocoraline, Ascidiemin, Variolins, Lamellarin D, Dictyodendrins, Psammaphin A-F, Bromotyrosine disulfide, Biprasin, Laxaphycins A and B, Epirubicin, Daunomycin, Aeropylsinin.

[5] Ligand library from Fungus (51 Compounds)

Natural compounds produced by fungus have been great potential and useful in safety and human health. There is significant demand of fungal compounds in drug industry for synthetic products due to economic and time reducing reasons. Brefeldin A, Irofulven, Lodamin A, Aculeatins A, Aculeatins B, Lodamin B, Aculeatols A-E, Cytotoxic dioxadispiroketal, Silvestrol, Amomol A, Episilvestrol, Methyl rocaglate, Camptothecin, Gliotoxin, Illudin S, Leptomycins, Palmarumycin, Terrecyclic acid, Wortmannin, Lovastatin, Pravastatin, Griseofulvin, Compactin, Simvastatin, Tricitrinol A-C, Terrein, Brefeldin A, Asperlin, Griseofulvin, Sequoiamonascin, Phaeosphaerin B, Hypocrellin, Calphostin C, Diketopiperazine, Fumitremorgin C, Asperphenamate, Notoamide A, Oxo tryprostatin A, Stephacidin A, Xanthocillin, Phenylahistin, Aurantiamine, Leucinostatin A, Taxol, Trichothecene A, 3-Hydroxyroridin E, Caffeic acid, p-coumaric acid, Hyperoside, Ellagic acid, Quercetin of fungus through searching scientific literature and submit in house library for further screening.

[6] Nutritional and Functional Food for preparation of in house library (51 Compounds)

Anticancer activities from many functional food sources have been reported. Some dietary factors now known to promote cancer development like polished grain, foods and low intake of fresh vegetables. Lycopene, Beta-glucan, Conjugated linoleic acid (CLA), Flavones, Catechins, Anthocyanidins, Lignans, Daidzein, Genistein, Balsamita, Parsley, Parsnips, Epigallocatechin 3-gal, Alpha-linolenic acid, Docosapentaenoic acid, Epigallocatechin gallate, Phytosteryl oleates, Docosahexaenates, Phytosteryl caffeates, Ferulates, Sinapates, Phytosteryl phenolates, Malvidin, Cyanidin, Delphinidin, Pelargoidin, Peonidin, Peltunidin, Apigenin, Luteolin, Myricetin, Quercetin, Catechin, Epicatechin, Gallic acid,

Epigallocatechin, Daidzein, Genistein, Gallic acid, Phydroxybenzoic, Vanillic acid, Genistein, Caffeic acid, Ferulic acid, p-coumaric acid, Sinapic acid, Pinoresinol, Podophyllotoxin, Steganacin, Castalin, Pentagalloyl glucose, Procyanidins, Phytic acid, Secoisolariciresinol diglucoside (SDG), Enterodiol, Enterolactone, Vanillin, Syringic acid, Tocotrienols (*T. durum*). In this study we extract 50-50 chemical compounds from 6 different foods and drink (brown rice, barley, wheat, green tea and coffee) as well some vegetables (bitter melon, garlic, onions, broccoli, and cabbage) through searching scientific literature and deposited in to in houses libraries for further screening.

[7] Compounds from marine and terrestrial cyanobacteria (52 Compounds)

The majority of species are found in the oceans, which constitute 70% of the world's surface. Marine organisms are a rich source of chemical products. Overall, more than 3000 new substances have been identified from marine organisms that demonstrate the great potential as a source of novel chemical classes. Grenadamed B-C, Curacin A, Grenadadiene, Lyngbyabellin A -B, Tanikolide, Kalkitoxin, Isomalnyngamide A-B, Barbamide (Lyngbya majuscula), Guineamide G, Semiplenamide A-G, Pahayokolide A (*Lyngbya semiplena*), Phormidolide (*Phormidium sp.*), Comnostin A-E (*Nostoc commune*), Cyanolide A (*Lyngbya bouillonii*), Aerucyclamide A-B (*Microcystis aeruginosa*), Oscillapeptin J (*Planktothrix rubescens*) (4 Rif), Caylobolide A- B, Desmethoxy majusculamide C, Apratoxins A-C, Cocosamides A, Curacin A, Grassypeptolides F -G, Pitipeptolides A-B, Hectochlorin, Jamaicamides A-C, Palmyramide A, Dolabellin, Tanikolide dimer (Lyngbya majuscula), Palau'imide, Bisebromoamide, Lyngbyacyclamides A-D, Ulongamides A-F, Ulongapeptin (*Lyngbya sp.*), Guamamide, Tasiptepsins, Apramides A-G, Dolastatin, Belamide A, Symplostatin, Tasiamide B, Micromide (*Symploca sp.*) (6) Apratoxin D-E, Aurilide B-C, Biselyngbyaside, Coibamide A, Cryptophycin 1, Dolastatin 10, Ethyl Tumonoate A, Hoiamide A, Dragonamide, Kalkitoxin, Largazole, Malnyngolide dimer