

Table S1 The list of NPs screened from PharmMapper server.

No.	UNPD ID	Chemical_Name	CAS_NO.	PubChem CID
1	UNPD133185	Coniferyl alcohol	32811-40-8 458-35-5	1549095
2	UNPD27847	Pseudoprotodioscinbeta	102115-79-7 117557-44-5	N/A
3	UNPD36432	Pseudoprotodioscin	102115-79-7	N/A
4	UNPD43533	Nyasol	230292-85-0	6438674
5	UNPD60722	(25S)-5beta-spirostan-3beta-yl-O-[O-alpha-L-rhamnosyl (1->4)]-beta-D-glucopyranoside	58881-26-8	N/A
6	UNPD77220	Asparenydiol	166762-98-7	10084256
7	UNPD11158	Asparacoside	N/A	21575006
8	UNPD126821	Pseudoprotodioscin	N/A	N/A
9	UNPD130293	Asp-VI	N/A	N/A
10	UNPD135865	3'-Hydroxy-4'-methoxy-4'-dehydroxynyasol	N/A	21575014
11	UNPD136991	Asparacosin A	N/A	11385250
12	UNPD14125	Asparacoside	N/A	21575006
13	UNPD143968	1,3-bis(4-hydroxyphenyl)pent-4-en-1-one	N/A	N/A
14	UNPD174302	Asparacosin B	N/A	21575013
15	UNPD206348	Aspachioside C	N/A	N/A
16	UNPD206349	Aspachioside D	N/A	N/A
17	UNPD68648	3''-Methoxyasparenydiol	N/A	N/A
18	UNPD96599	3''-Methoxynyasol	N/A	25218067
19	UNPD96816	Asp-V	N/A	N/A

Table S2 The list of FDA approved intestinal anti-inflammatory agents.

No.	Drug name	Drug ID	CAS NO.	Molecular Formula	Molecular Weight	ALogP	Num H Acceptors	Num H Donors	Num Rotatable Bonds	Num Rings
1	Sulfasalazine	DB00795	599-79-1	C ₁₈ H ₁₄ N ₄ O ₅ S	398.393	2.92	8	3	5	3
2	Balsalazide	DB01014	80573-04-2	C ₁₇ H ₁₅ N ₃ O ₆	357.3175	3.37	8	4	7	2
3	Olsalazine	DB01250	15722-48-2	C ₁₄ H ₁₀ N ₂ O ₆	302.239	2.77	8	4	4	2
4	Mesalazine	DB00244	89-57-6	C ₇ H ₇ NO ₃	153.1354	0.75	4	3	1	1
5	Cromoglicic Acid	DB01003	16110-51-3	C ₂₃ H ₁₆ O ₁₁	468.3665	1.84	11	3	8	4
6	Prednisone	DB00635	1953-3-2	C ₂₁ H ₂₆ O ₅	358.4281	2.07	5	2	2	4
7	Beclomethasone	DB00394	5534-9-8	C ₂₈ H ₃₇ ClO ₇	521.042	3.69	5	1	8	4
8	Budesonide	DB01222	51333-22-3	C ₂₅ H ₃₄ O ₆	430.5339	2.42	6	2	4	5
9	Prednisolone	DB00860	50-24-8	C ₂₁ H ₂₈ O ₅	360.444	1.66	5	3	2	4
10	Betamethasone	DB00443	378-44-9	C ₂₂ H ₂₉ FO ₅	392.4611	1.93	5	3	2	4
11	Hydrocortisone	DB00741	50-23-7	C ₂₁ H ₃₀ O ₅	362.4599	1.79	5	3	2	4

Table S3 The list of NPs accorded with Lipinski's rule of five.

No.	UNPD ID	Chemical Name	Molecular Weight	ALogP	Num H Acceptors	Num H Donors	Num Rotatable Bonds	Num Rings
1	UNPD133185	Coniferyl alcohol	180.2	1.434	3	2	3	1
2	UNPD135865	3'-Hydroxy-4'-methoxy-4'-	282.334	4.089	3	2	5	2
3	UNPD43533	Nyasol	252.308	4.105	2	2	4	2
4	UNPD68648	3''-Methoxyasparennydiol	296.317	3.954	4	2	6	2
5	UNPD77220	Asparennydiol	266.291	3.971	3	2	5	2
6	UNPD96599	3''-Methoxynyasol	282.334	4.089	3	2	5	2