Table 1. Presents the physicochemical properties of the compounds under study. Important features include a molecular weight below 500 g/mol to enhance bioavailability and heavy atoms that indicate complexity. The Csp^3 fraction affects solubility, while the number of H-bond acceptors/donors impacts permeability. Any potential drug candidate with favorable properties must undergo experimental validation to ensure alignment with drug-likeness principles.

Molecule	**Quinolone**	**Nicotinamide**	**Uracil**	**2-hydroxyquinoline**
Formula	C9H7N	C6H6N2O	C4H4N2O2	C9H7NO
MW	129.16	122.12	112.09	145.16
Heavy atoms	10	9	8	11
Aromatic heavy atoms	10	6	6	10
Fraction Csp3	0.00	0.00	0.00	0.00
Rotatable bonds	0	1	0	0
H-bond acceptors	1	2	2	1
H-bond donors	0	1	2	1
MR (Molar Refractivity)	41.74	32.33	27.68	44.57
TPSA	12.89	55.98	65.72	32.86
iLOGP	1.73	0.70	0.52	1.56
XLOGP3	2.03	-0.37	-1.07	1.26
ESOL Log S	-2.66	-0.79	-0.42	-2.21
ESOL Solubility (mg/ml)	2.83e-01	1.97e+01	4.30e+01	9.02e-01
ESOL Class	Soluble	Very soluble	Very soluble	Soluble

7, 8-benzoquinoline	6-methylquinoline	6-hydroxyquinoline	4-methylquinoline	4-hydroxyquinoline	2-methylquinoline
C13H9N	C10H9N	C9H7NO	C10H9N	C9H7NO	C10H9N
179.22	143.19	145.16	143.19	145.16	143.19
14	11	11	11	11	11
14	10	10	10	10	10
0.00	0.10	0.00	0.10	0.00	0.10
0	0	0	0	0	0
1	1	2	1	2	1
0	0	1	0	1	0
59.25	46.71	43.77	46.71	43.77	46.71
12.89	12.89	33.12	12.89	33.12	12.89
2.15	1.98	1.48	1.97	1.45	2.00
3.43	2.57	1.80	2.61	0.58	2.59
-3.85	-3.02	-2.55	-3.04	-1.78	-3.03
2.52e-02	1.37e-01	4.12e-01	1.29e-01	2.42e+00	1.33e-01
Soluble	Soluble	Soluble	Soluble	Very soluble	Soluble

Cucurbitacin D	Cucurbitacin C	Cucurbitacin B	Cucurbitacin A	Colocynthin	8-methylquinoline	8-hydroxyquinoline
C32H46O8	C32H46O8	C32H46O8	C32H46O9	C38H54O13	C10H9N	C9H7NO
558.70	558.70	558.70	574.70	718.83	143.19	145.16
40	40	40	41	51	11	11
0	0	0	0	0	10	10
0.75	0.75	0.75	0.75	0.74	0.10	0.00
6	6	6	7	9	0	0
8	8	8	9	13	1	2
3	3	3	4	6	0	1
150.94	150.94	150.94	152.10	182.85	46.71	43.77
138.20	138.20	138.20	158.43	217.35	12.89	33.12
3.77	3.77	3.77	3.03	3.59	1.99	1.65
2.64	2.64	2.64	1.97	1.45	2.60	2.02
-4.57	-4.57	-4.57	-4.18	-4.62	-3.04	-2.69
1.50e-02	1.50e-02	1.50e-02	3.78e-02	1.74e-02	1.31e-01	3.00e-01
Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Soluble	Soluble

Cucurbitacin L	Cucurbitacin K	Cucurbitacin J	Cucurbitacin I	Cucurbitacin H	Cucurbitacin F	Cucurbitacin E
C32H46O8	C32H46O8	C32H46O8	C32H46O8	C32H46O8	C32H46O8	C32H46O8
558.70	558.70	558.70	558.70	558.70	558.70	558.70
40	40	40	40	40	40	40
0	0	0	0	0	0	0
0.75	0.75	0.75	0.75	0.75	0.75	0.75
6	6	6	6	6	6	6
8	8	8	8	8	8	8
3	3	3	3	3	3	3
150.94	150.94	150.94	150.94	150.94	150.94	150.94
138.20	138.20	138.20	138.20	138.20	138.20	138.20
3.77	3.77	3.77	3.77	3.77	3.77	3.77
2.64	2.64	2.64	2.64	2.64	2.64	2.64
-4.57	-4.57	-4.57	-4.57	-4.57	-4.57	-4.57
1.50e-02	1.50e-02	1.50e-02	1.50e-02	1.50e-02	1.50e-02	1.50e-02
Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble

3-Epi-Isocucurbitacin D	Khekadaengoside E	23,24-dihydrocucurbitacin E	Iso-cucurbitacin B	Cucurbitacin R	cucurbitacin I 2-O-beta-D-glucopyranoside
C30H44O7	C36H54O12	C32H46O8	C32H46O8	C30H46O7	C36H52O12
516.67	678.81	558.7	558.7	518.68	676.79
37	48	40	40	37	48
0	0	0	0	0	0
0.77	0.78	0.75	0.75	0.83	0.75
4	7	7	6	5	7
7	12	8	8	7	12
4	8	3	3	4	7
141.2	174.07	151.35	150.94	141.68	173.11
132.13	214.44	138.2	138.2	132.13	211.28
2.82	2.78	3.57	3.15	2.81	3.72
1.95	0.55	3.31	2.52	2.12	0.87
-4.01	-3.93	-4.93	-4.5	-4.06	-4.12
5.07E-02	7.92E-02	6.61E-03	1.78E-02	4.50E-02	5.11E-02
Moderately soluble	Soluble	Moderately soluble	Moderately soluble	Moderately soluble	Moderately soluble

β-sitosterol	**alpha-Spinasterol 3-glucoside**	**α-spinasterone**	**6-hydroxy-4-methylchromen-2-one**	**Quercetin**	**Kaempferol**	**Isovitexin**	**Isosaponarin**	**Cianidanol**
C29H50O	C35H58O6	C29H46O	C10H8O3	C15H10O7	C15H10O6	C21H20O10	C27H30O15	C15H14O6
414.71	574.83	410.67	176.17	302.24	286.24	432.38	594.52	290.27
30	41	30	13	22	21	31	42	21
0	0	0	10	16	16	16	16	12
0.93	0.89	0.83	0.1	0	0	0.29	0.44	0.2
6	8	5	0	1	1	3	6	1
1	6	1	3	7	6	10	15	6
1	4	0	1	5	4	7	10	5
133.23	165.14	131.79	49.47	78.03	76.01	106.61	138.73	74.33
20.23	99.38	17.07	50.44	131.36	111.13	181.05	260.2	110.38
5.05	5.14	4.83	1.62	1.63	1.7	1.6	2.87	1.33
9.34	6.71	7.88	1.9	1.54	1.9	0.21	-1.6	0.36
-7.9	-7.1	-7.02	-2.7	-3.16	-3.31	-2.84	-2.4	-2.22
5.23E-06	4.53E-05	3.92E-05	3.53E-01	2.11E-01	1.40E-01	6.29E-01	2.35E+00	1.74E+00
Poorly soluble	Poorly soluble	Poorly soluble	Soluble	Soluble	Soluble	Soluble	Soluble	Soluble

Gallic Acid	**Ferulic acid**	**Chlorogenic Acid**	**Caffeic acid**	**4-(β-D-glucopyranosyloxy)-benzaldehyde**	**4-hydroxybenzyl β-D-glucopyranoside**	**Benzyl beta-d-glucopyranoside**	**Schottenol**
C7H6O5	C16H18O9	C16H18O9	C9H8O4	C13H16O7	C13H18O7	C13H18O6	C29H50O
170.12	354.31	354.31	180.16	284.26	286.28	270.28	414.71
12	25	25	13	20	20	19	30
6	6	6	6	6	6	6	0
0	0.38	0.38	0	0.46	0.54	0.54	0.93
1	5	5	2	4	4	4	6
5	9	9	4	7	7	6	1
4	6	6	3	4	5	4	1
39.47	83.5	83.5	47.16	65.97	66.98	64.95	133.23
97.99	164.75	164.75	77.76	116.45	119.61	99.38	20.23
0.21	0.87	0.87	0.97	1.59	-0.4	0.6	5.11
0.7	-0.42	-0.42	1.15	-0.91	-1.06	-0.7	9.08
-1.64	-1.62	-1.62	-1.89	-0.99	-0.91	-1.04	-7.74
3.90E+00	8.50E+00	8.50E+00	2.32E+00	2.93E+01	3.56E+01	2.44E+01	7.62E-06
Very soluble	Very soluble	Very soluble	Very soluble	Very soluble	Very soluble	Very soluble	Poorly soluble

Tocopherol	3,4-dihydroxyphenylacetic acid	4-Hydroxybenzoic acid	P-coumaric acid	Sinapinic acid	Sinapic acid	Protocatechuic acid	Hydroxycaffeic acid
C29H50O2	C8H8O4	C7H6O3	C9H8O3	C11H12O5	C11H12O5	C7H6O4	C9H8O5
430.71	168.15	138.12	164.16	224.21	224.21	154.12	196.16
31	12	10	12	16	16	11	14
6	6	6	6	6	6	6	6
0.79	0.12	0	0	0.18	0.18	0	0
12	2	1	2	4	4	1	2
2	4	3	3	5	5	4	5
1	3	2	2	2	2	3	4
139.27	42.03	35.42	45.13	58.12	58.12	37.45	48.73
29.46	77.76	57.53	57.53	75.99	75.99	77.76	97.99
6.04	0.81	0.85	0.95	1.63	1.63	0.66	0.93
10.7	0.98	1.58	1.46	1.46	1.46	1.15	1.02
-8.6	-1.74	-2.07	-2.02	-2.16	-2.16	-1.86	-1.88
1.08E-06	3.07E+00	1.18E+00	1.58E+00	1.54E+00	1.54E+00	2.14E+00	2.56E+00
Poorly soluble	Very soluble	Soluble	Soluble	Soluble	Soluble	Very soluble	Very soluble