	The six main Monascus pigments	are highlighted in yellow
	Name	Canonical SMILES
yellow	monascin	CCCCCC(=O)C1C(=O)OC2(C1CC1=C(C2=O)COC(=C1)/C=C/C)C
yellow	ankaflavin	CCCCCCCC(=O)C1C(=O)OC2(C1CC1=C(C2=O)COC(=C1)/C=C/C)C
orange	rubropunctatin	CCCCCC(=O)C1=C2C=C3C=C(/C=C/C)OC=C3C(=O)C2(OC1=O)C
orange	monascorubrin	CCCCCCCC(=O)C1=C2C=C3C=C(/C=C\C)OC=C3C(=O)C2(OC1=O)C
red	rubropunctamine	CCCCCC(=O)C1=C2C=C3C=C(NC=C3C(=O)C2(C)OC1=O)\C=C\C
red	monascorubramine	CCCCCCCC(=O)C1=C2C=C3C=C(NC=C3C(=O)C2(C)OC1=O)\C=C\C
yellow	xanthomonasin A	CCCCCC(=O)C1=C2c3oc(c(c3C[C@@]([C@]2(OC1=O)C)(O)/C=C/(
yellow	xanthomonasin B	CCCCCCCC(=O)C1=C(O)O[C@]2(C1=C1OC(=O)C(=C1C[C@@]2(O
yellow	yellow Ⅱ	CCCCCCCC(=O)C1=C(O)OC2(C1=CC1=C/C(=C/C)/OCC1C2=O)C
yellow	monankarin A	C[C@@H]1CC(=O)C=C(O1)c1cc2c(oc1=O)cc(c(c2[C@H]([C@H](C
yellow	monankarin B	C[C@@H]1CC(=O)C=C(O1)c1cc2c(oc1=O)cc(c(c2[C@@H]([C@H
yellow	monankarin C	CC1CC(=O)C=C(O1)c1cc2c([C@H]([C@H](O)C)C)c(C)c(c(c2oc1=O
yellow	monankarin D	CC1CC(=O)C=C(O1)c1cc2c([C@@H]([C@@H](O)C)C)c(C)c(c(c2oc
yellow	monankarin E	CC(Cc1cc(O)c(c2c1cc(C1=CC(=O)CC(O1)C)c(=O)o2)C)O
yellow	monankarin F	CC1CC(=O)C=C(O1)c1cc2c(CC(O)C)c(C)c(c(c2oc1=O)C)O
yellow	monascusone A	C[C@@H](CC1=CC2=C(CO1)C(=O)[C@]([C@H](C2)O)(C)O)O
yellow	monascusone B	C/C=C/C1=CC2=C(CO1)C(=O)[C@]1([C@H](C2)[C@@H](C(=O)C)
yellow	FK17-P2B2	C/C=C/C1=CC2=C(CO1)C(=O)[C@]([C@H](C2)O)(C)O
yellow	Y3	CC(CC(C(CC(=O)O)(O)C)(c1c(OC(=S)CC(O)C)cc(c(c1O)C)O)O)C
yellow	monaphilone A	CCCCCCCC(=O)C[C@H]1CC2=C(C(=O)[C@]1(C)O)COC(=C2)/C=C/
yellow	monaphilone B	CCCCCC(=O)C[C@H]1CC2=C(C(=O)[C@]1(C)O)COC(=C2)/C=C/C
yellow	monaphilone C	CCCCCC(=O)C[C@@H]1CC(=C(C(=O)[C@]1(C)O)C)CC(=O)CCC
yellow	monapurone A	CCCCCC(=O)C[C@@H]1C2=COC(=CC2=CC(=O)[C@]1(C)O)/C=C/(
yellow	monapurone B	CCCCC[C@@]1(OC)C[C@H]2[C@](O1)(C)C(=O)C=C1C2=COC(=C1
yellow	monapurone C	CCCCC[C@]1(OC)C[C@H]2[C@](O1)(C)C(=O)C=C1C2=COC(=C1)/
yellow	monarubrin	CCCCCC(=O)CC1C=C2C=C(/C=C/C)OC=C2C(=O)C1(C)O
yellow	rubropunctin	CCCCCCCC(=O)CC1C=C2C=C(/C=C/C)OC=C2C(=O)C1(C)O
orange	monapilol A	CCCCCCCC(=O)C1=C2C=C3C=C(/C=C/C)OC=C3[C@@H]([C@@]2
orange	monapilol B	CCCCCC(=O)C1=C2C=C3C=C(/C=C/C)OC=C3[C@@H]([C@@]2(O(
orange	monapilol C	CCCCCCCC(=O)C1=C2C=C3C=C(/C=C/C)OC=C3[C@]([C@@]2(OC
orange	monapilol D	CCCCCC(=O)C1=C2C=C3C=C(/C=C/C)OC=C3[C@]([C@@]2(OC1=(
red	N-glucosylrubropunctamine	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=O)C
red	N-glucosylmonascorubramine	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=C
red	N-glutarylrubropunctamine	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)C2(OC1=O)C)C(C(=
red	N-glutarylmonascorubramine	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)C2(OC1=O)C)C((
red	Red Derivat 1	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=C
red	Red Derivat 2	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=O)C
red	Red Derivat 3	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=C
red	Red Derivat 4	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=O)C
red	Red Derivat 5	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=C
red	Red Derivat 6	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=O)C
red	Red Derivat 7	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=C
red	Red Derivat 8	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)[C@@]2(OC1=O)C
red	R3	CCCCCC(=O)C1C(=O)OC2(C1C1=COC(=CC1=CC2=O)CC(O)C)C
red	Unamed	C/C=C/C1=CC2=CC3=[O+]NOC3(C(C2CN1C(C(=O)O)CCCCN)O)C
red	PP-V	CCCCCCCC(=O)C1=C2C=C3C=C(/C=C\C(=O)[O-])[NH2+]C=C3C(=C
red	New Red Pigment	CCCCCC(C1C(=O)OC2(C1c1c[nH]c(cc1=CC2=O)CC(O)C)C)O

red	Isolate MPs 1	CCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)C2(OC1=O)C)C(C(=
red	Isolate MPs 2	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)C2(OC1=O)C)C((
red	Isolate MPs 3	CCCCCCCC(=O)C1=C2C=c3cc(/C=C/C)n(cc3C(=O)C2(OC1=O)C)CC
red	glycyl-rubropunctatin	CCCCCC(=O)C1=C2CC3=C(C(=O)[C@@]2(OC1=O)C)CN(C(=C3)/C=
red	Isolate MPs 4	CCCCCCCC(=O)C1=C2CC3=C(C(=O)[C@@]2(OC1=O)C)CN(C(=C3)/
red	Monascopyridine A	CCCCCC(=O)[C@@H]1C(=O)O[C@]2([C@H]1Cc1cc(/C=C/C)ncc1(
red	Monascopyridine B	CCCCCCCC(=O)[C@@H]1C(=O)O[C@]2([C@H]1Cc1cc(/C=C/C)nc
red	Monascopyridine C	CCCCCC(=O)C[C@@H]1Cc2cc(/C=C/C)ncc2C(=O)[C@@]1(C)O
red	Monascopyridine D	CCCCCCCC(=O)C[C@@H]1Cc2cc(/C=C/C)ncc2C(=O)[C@@]1(C)O
yellow	Monasfluore A	CCCCCC(=O)C1C(=O)OC2(C1C1=COC(=CC1=CC2=O)/C=C/C)C
yellow	Monasfluore B	CCCCCCCC(=O)C1C(=O)OC2(C1C1=COC(=CC1=CC2=O)/C=C/C)C
yellow	purpureusone	CCCCCCCC(=O)[C@H]1C(=O)O[C@@]2(C1CC(=C(C2=O)C)CC(=O)
red	Red Shandong 1	C=CCCCC(C1=CC2=C/C(=C/C=C)/NCC2C(C1O)O)O
red	Red Shandong 2	C=CCCCCCC(C1=CC2=C/C(=C/C=C)/NCC2C(C1O)O)O

Formula	MW	#Heavy atoms	#Aromatic	Fraction Cs	#Rotatable	#H-bond a	#H-bond d	MR
C21H26O5	358.43	26	0	0.57	6	5	0	98.11
C23H30O5	386.48	28	0	0.61	8	5	0	107.72
C21H22O5	354.4	26	0	0.38	6	5	0	97.16
C23H26O5	382.45	28	0	0.43	8	5	0	106.77
C21H23NO4	353.41	26	6	0.38	6	4	1	100.33
C23H27NO4	381.46	28	6	0.43	8	4	1	109.94
C21H24O7	388.41	28	5	0.48	7	7	2	101.69
C23H28O7	416.46	30	0	0.52	9	7	2	110.02
C22H28O5	372.45	27	0	0.55	7	5	1	103.81
C20H22O6	358.39	26	10	0.4	3	6	2	98.51
C20H22O6	358.39	26	10	0.4	3	6	2	98.51
C21H24O6	372.41	27	10	0.43	3	6	2	103.48
C21H24O6	372.41	27	10	0.43	3	6	2	103.48
C19H20O6	344.36	25	10	0.37	3	6	2	93.7
C20H22O6	358.39	26	10	0.4	3	6	2	98.67
C13H18O5	254.28	18	0	0.62	2	5	3	64.24
C17H18O5	302.32	22	0	0.47	2	5	0	78.88
C13H16O4	236.26	17	0	0.46	1	4	2	62.6
C20H30O8S	430.51	29	6	0.6	10	8	6	112.76
C22H32O4	360.49	26	0	0.64	9	4	1	104.9
C20H28O4	332.43	24	0	0.6	7	4	1	95.29
C20H32O4	336.47	24	0	0.75	10	4	1	97.47
C20H26O4	330.42	24	0	0.5	7	4	1	94.81
C21H28O4	344.44	25	0	0.57	6	4	0	98.35
C21H28O4	344.44	25	0	0.57	6	4	0	98.35
C20H26O4	330.42	24	0	0.5	7	4	1	94.81
C22H30O4	358.47	26	0	0.55	9	4	1	104.43
C23H28O5	384.47	28	0	0.48	8	5	1	107.73
C21H24O5	356.41	26	0	0.43	6	5	1	98.12
C26H32O6	440.53	32	0	0.5	10	6	1	122.39
C24H28O6	412.48	30	0	0.46	8	6	1	112.78
C27H33NO9	515.55	37	6	0.52	8	9	4	132.88
C29H37NO9	543.61	39	6	0.55	10	9	4	142.5
C26H29NO8	483.51	35	6	0.42	11	8	2	128
C28H33NO8	511.56	37	6	0.46	13	8	2	137.62
C26H31NO6	453.53	33	6	0.46	10	6	1	126.23
C24H27NO6	425.47	31	6	0.42	8	6	1	116.62
C27H31NO8	497.54	36	6	0.44	12	8	2	132.81
C25H27NO8	469.48	34	6	0.4	10	8	2	123.2
C26H31NO6	453.53	33	6	0.46	10	6	1	126.23
C24H27NO6	425.47	31	6	0.42	8	6	1	116.62
C27H31NO8	497.54	36	6	0.44	12	8	2	132.81
C25H27NO8	469.48	34	6	0.4	10	8	2	123.2
C21H26O6	374.43	27	0	0.57	7	6	1	99.27
C19H28N3O5	378.44	27	0	0.58	7	6	4	107.23
C23H25NO6	411.45	30	0	0.39	9	7	1	113.19
C21H29NO5	375.46	27	6	0.62	7	5	3	102.39

C27H34N4O6	510.58	37	6	0.44	13	7	4	140.14
C29H38N4O6	538.64	39	6	0.48	15	7	4	149.75
C25H29NO6	439.5	32	6	0.44	10	6	1	121.42
C23H27NO6	413.46	30	0	0.48	8	6	1	114.74
C25H31NO6	441.52	32	0	0.52	10	6	1	124.36
C21H25NO4	355.43	26	6	0.52	6	5	0	99.66
C23H29NO4	383.48	28	6	0.57	8	5	0	109.27
C20H27NO3	329.43	24	6	0.55	7	4	1	96.84
C22H31NO3	357.49	26	6	0.59	9	4	1	106.46
C21H24O5	356.41	26	0	0.48	6	5	0	97.63
C23H28O5	384.47	28	0	0.52	8	5	0	107.25
C23H34O5	390.51	28	0	0.74	11	5	0	109.9
C18H25NO3	303.4	22	0	0.44	6	3	4	92.24
C20H29NO3	331.45	24	0	0.5	8	3	4	101.86

TPSA	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT L	Consensus	ESOL Log S
69.67	2.72	3.2	3.44	1.94	4.49	3.16	-3.68
69.67	3.23	4.28	4.22	2.38	5.3	3.88	-4.4
69.67	3.32	3.23	3.63	1.78	4.46	3.29	-3.68
69.67	3.99	4.31	4.41	2.22	5.27	4.04	-4.4
76.23	3.26	3.24	2.96	1.71	5.32	3.3	-3.85
76.23	3.64	4.32	3.74	2.14	6.14	4	-4.56
114.04	2.08	2.6	2.88	0.88	4.4	2.57	-3.56
110.13	1.59	2.72	3.49	1.09	4.59	2.7	-3.54
72.83	3.65	4.31	4.46	1.75	4.57	3.75	-4.4
96.97	2.52	2.37	3.01	1.25	3.94	2.62	-3.64
96.97	2.55	2.37	3.01	1.25	3.94	2.62	-3.64
96.97	2.91	2.74	3.32	1.47	4.46	2.98	-3.95
96.97	2.93	2.74	3.32	1.47	4.46	2.98	-3.95
96.97	2.6	2.04	2.45	1.02	3.71	2.36	-3.36
96.97	2.51	2.41	2.76	1.25	4.24	2.63	-3.67
86.99	2.24	-0.82	0.05	-0.54	1.07	0.4	-0.77
69.67	1.95	1.29	1.88	1.02	2.9	1.81	-2.4
66.76	2.4	0.18	0.86	0.19	1.67	1.06	-1.35
179.77	2.65	1.89	2.23	0.6	3.44	2.16	-3.19
63.6	3.43	3.7	4.43	2.26	5.39	3.84	-3.81
63.6	3.62	2.62	3.65	1.82	4.57	3.26	-3.09
71.44	3.23	2.37	3.94	1.9	5.24	3.34	-2.76
63.6	2.85	2.26	3.78	1.74	4.16	2.96	-2.85
44.76	4.02	3.53	4.59	2.45	4.48	3.81	-3.8
44.76	4.07	3.53	4.59	2.45	4.48	3.82	-3.8
63.6	3.49	2.71	3.78	1.74	4.16	3.18	-3.13
63.6	4.12	3.8	4.56	2.18	4.98	3.93	-3.86
72.83	4.17	3.32	4.2	2.3	4.68	3.73	-3.79
72.83	3.5	2.23	3.42	1.86	3.87	2.98	-3.06
89.9	4.23	3.35	4.55	2.03	5.59	3.95	-4.02
89.9	3.35	2.26	3.77	1.62	4.76	3.15	-3.29
155.52	3.43	1.25	0.08	-0.58	2.27	1.29	-3.42
155.52	3.17	2.33	0.86	-0.18	3.09	1.85	-4.13
139.97	2.83	2.86	2.92	1.06	4.23	2.78	-4.04
139.97	3.28	3.95	3.7	1.46	5.07	3.49	-4.76
102.67	3.8	4.46	3.86	1.89	5.26	3.85	-4.94
102.67	3.17	3.37	3.08	1.48	4.43	3.1	-4.22
139.97	3.14	3.59	3.31	1.27	4.65	3.19	-4.52
139.97	2.58	2.5	2.53	0.86	3.81	2.46	-3.8
102.67	3.79	4.46	3.86	1.89	5.26	3.85	-4.94
102.67	3.03	3.37	3.08	1.48	4.43	3.08	-4.22
139.97	3.07	3.59	3.31	1.27	4.65	3.18	-4.52
139.97	2.77	2.5	2.53	0.86	3.81	2.49	-3.8
89.9	3.07	1.84	2.76	1.13	3.49	2.46	-2.86
125.12	-2.7	-1.37	-0.19	0.8	-0.6	-0.81	-0.86
117.18	2.3	3.27	0.31	-2.34	5.1	1.73	-3.86
99.62	3.07	2.29	1.54	1.13	4.03	2.41	-3.31

164.57	2.28	2.55	2.32	0.9	3.78	2.37	-3.87
164.57	3.33	3.64	3.1	1.3	4.62	3.2	-4.6
102.67	3.4	4.06	3.3	1.69	5.01	3.49	-4.6
100.98	2.72	2.71	2.5	1.42	3.88	2.64	-3.58
100.98	3.63	3.79	3.28	1.84	4.71	3.45	-4.31
73.33	3.06	3.68	3.44	1.86	4.92	3.39	-4.14
73.33	3.46	4.76	4.22	2.3	5.73	4.09	-4.85
67.26	2.99	3.1	3.65	1.74	5	3.3	-3.56
67.26	3.35	4.18	4.43	2.18	5.82	3.99	-4.27
69.67	3.16	2.84	3.57	1.86	4.08	3.1	-3.44
69.67	3.12	3.92	4.35	2.3	4.89	3.72	-4.17
77.51	3.66	4.03	4.51	2.46	6.01	4.14	-4.07
72.72	2.97	1.82	1.2	1.36	2.29	1.93	-2.47
72.72	3.32	2.91	1.98	1.82	3.1	2.63	-3.2

ESOL Solubility (mg/ml)	ESOL Solut	ESOL Class	Ali Log S	Ali Solubili	Ali Solubili
7.45E-02	2.08E-04	Soluble	-4.33	1.66E-02	4.62E-05
1.52E-02	3.94E-05	Moderatel	-5.46	1.35E-03	3.50E-06
7.47E-02	2.11E-04	Soluble	-4.37	1.53E-02	4.30E-05
1.53E-02	3.99E-05	Moderatel	-5.49	1.25E-03	3.26E-06
5.03E-02	1.42E-04	Soluble	-4.51	1.08E-02	3.06E-05
1.06E-02	2.77E-05	Moderatel	-5.63	8.84E-04	2.32E-06
1.08E-01	2.78E-04	Soluble	-4.64	8.82E-03	2.27E-05
1.20E-01	2.87E-04	Soluble	-4.69	8.57E-03	2.06E-05
1.47E-02	3.96E-05	Moderatel	-5.55	1.04E-03	2.80E-06
8.18E-02	2.28E-04	Soluble	-4.05	3.22E-02	8.98E-05
8.18E-02	2.28E-04	Soluble	-4.05	3.22E-02	8.98E-05
4.17E-02	1.12E-04	Soluble	-4.43	1.38E-02	3.71E-05
4.17E-02	1.12E-04	Soluble	-4.43	1.38E-02	3.71E-05
1.51E-01	4.38E-04	Soluble	-3.7	6.80E-02	1.97E-04
7.72E-02	2.15E-04	Soluble	-4.09	2.92E-02	8.16E-05
4.34E+01	1.71E-01	Very solub	-0.53	7.56E+01	2.97E-01
1.22E+00	4.03E-03	Soluble	-2.35	1.34E+00	4.44E-03
1.05E+01	4.44E-02	Very solub	-1.14	1.71E+01	7.25E-02
2.76E-01	6.41E-04	Soluble	-5.29	2.22E-03	5.16E-06
5.56E-02	1.54E-04	Soluble	-4.73	6.77E-03	1.88E-05
2.70E-01	8.13E-04	Soluble	-3.61	8.24E-02	2.48E-04
5.86E-01	1.74E-03	Soluble	-3.51	1.04E-01	3.08E-04
4.66E-01	1.41E-03	Soluble	-3.23	1.94E-01	5.86E-04
5.42E-02	1.57E-04	Soluble	-4.15	2.41E-02	7.01E-05
5.42E-02	1.57E-04	Soluble	-4.15	2.41E-02	7.01E-05
2.43E-01	7.35E-04	Soluble	-3.7	6.61E-02	2.00E-04
4.92E-02	1.37E-04	Soluble	-4.83	5.30E-03	1.48E-05
6.27E-02	1.63E-04	Soluble	-4.53	1.15E-02	2.98E-05
3.11E-01	8.74E-04	Soluble	-3.39	1.44E-01	4.03E-04
4.19E-02	9.51E-05	Moderatel	-4.92	5.35E-03	1.22E-05
2.10E-01	5.09E-04	Soluble	-3.78	6.78E-02	1.64E-04
1.98E-01	3.84E-04	Soluble	-4.11	3.96E-02	7.69E-05
4.01E-02	7.38E-05	Moderatel	-5.23	3.16E-03	5.82E-06
4.41E-02	9.11E-05	Moderatel	-5.46	1.68E-03	3.48E-06
8.85E-03	1.73E-05	Moderatel	-6.59	1.32E-04	2.57E-07
5.25E-03	1.16E-05	Moderatel	-6.34	2.10E-04	4.62E-07
2.59E-02	6.08E-05	Moderatel	-5.2	2.66E-03	6.25E-06
1.51E-02	3.04E-05	Moderatel	-6.22	3.03E-04	6.08E-07
7.50E-02	1.60E-04	Soluble	-5.08	3.86E-03	8.23E-06
5.25E-03	1.16E-05	Moderatel	-6.34	2.10E-04	4.62E-07
2.59E-02	6.08E-05	Moderatel	-5.2	2.66E-03	6.25E-06
1.51E-02	3.04E-05	Moderatel	-6.22	3.03E-04	6.08E-07
7.50E-02	1.60E-04	Soluble	-5.08	3.86E-03	8.23E-06
5.18E-01	1.38E-03	Soluble	-3.35	1.68E-01	4.48E-04
5.21E+01	1.38E-01	Very solub	-0.76	6.62E+01	1.75E-01
5.72E-02	1.39E-04	Soluble	-5.41	1.62E-03	3.93E-06
1.83E-01	4.86E-04	Soluble	-4.02	3.59E-02	9.56E-05

6.82E-02	1.34E-04	Soluble	-5.65	1.13E-03	2.22E-06
1.36E-02	2.53E-05	Moderatel	-6.78	8.85E-05	1.64E-07
1.10E-02	2.50E-05	Moderatel	-5.92	5.28E-04	1.20E-06
1.08E-01	2.61E-04	Soluble	-4.48	1.36E-02	3.28E-05
2.19E-02	4.95E-05	Moderatel	-5.6	1.10E-03	2.49E-06
2.59E-02	7.30E-05	Moderatel	-4.91	4.37E-03	1.23E-05
5.45E-03	1.42E-05	Moderatel	-6.03	3.57E-04	9.32E-07
9.11E-02	2.76E-04	Soluble	-4.18	2.17E-02	6.60E-05
1.93E-02	5.41E-05	Moderatel	-5.3	1.79E-03	5.00E-06
1.29E-01	3.61E-04	Soluble	-3.96	3.90E-02	1.09E-04
2.63E-02	6.83E-05	Moderatel	-5.08	3.18E-03	8.28E-06
3.29E-02	8.43E-05	Moderatel	-5.36	1.70E-03	4.36E-06
1.02E+00	3.38E-03	Soluble	-2.97	3.27E-01	1.08E-03
2.09E-01	6.31E-04	Soluble	-4.1	2.64E-02	7.98E-05

Ali Class	Silicos-IT L	Silicos-IT S	Silicos-IT S	Silicos-IT cl	GI absorption	BBB permeant
Moderately soluble	-4.21	2.21E-02	6.17E-05	Moderatel	High	Yes
Moderately soluble	-5	3.88E-03	1.00E-05	Moderatel	High	Yes
Moderately soluble	-4.18	2.36E-02	6.67E-05	Moderatel	High	Yes
Moderately soluble	-4.96	4.16E-03	1.09E-05	Moderatel	High	Yes
Moderately soluble	-5.71	6.91E-04	1.95E-06	Moderatel	High	Yes
Moderately soluble	-6.5	1.21E-04	3.18E-07	Poorly solu	High	Yes
Moderately soluble	-4.4	1.55E-02	4.00E-05	Moderatel	High	No
Moderately soluble	-4.24	2.39E-02	5.73E-05	Moderatel	High	No
Moderately soluble	-4.47	1.27E-02	3.41E-05	Moderatel	High	Yes
Moderately soluble	-4.6	9.00E-03	2.51E-05	Moderatel	High	No
Moderately soluble	-4.6	9.00E-03	2.51E-05	Moderatel	High	No
Moderately soluble	-4.98	3.93E-03	1.05E-05	Moderatel	High	No
Moderately soluble	-4.98	3.93E-03	1.05E-05	Moderatel	High	No
Soluble	-4.58	9.08E-03	2.64E-05	Moderatel	High	No
Moderately soluble	-4.96	3.97E-03	1.11E-05	Moderatel	High	No
Very soluble	-0.99	2.58E+01	1.01E-01	Soluble	High	No
Soluble	-2.62	7.19E-01	2.38E-03	Soluble	High	Yes
Very soluble	-1.21	1.46E+01	6.19E-02	Soluble	High	No
Moderately soluble	-2.03	4.04E+00	9.38E-03	Soluble	Low	No
Moderately soluble	-4.9	4.56E-03	1.26E-05	Moderatel	High	Yes
Soluble	-4.11	2.60E-02	7.82E-05	Moderatel	High	Yes
Soluble	-5.24	1.92E-03	5.71E-06	Moderatel	High	Yes
Soluble	-3.64	7.57E-02	2.29E-04	Soluble	High	Yes
Moderately soluble	-4.26	1.89E-02	5.48E-05	Moderatel	High	Yes
Moderately soluble	-4.26	1.89E-02	5.48E-05	Moderatel	High	Yes
Soluble	-3.64	7.57E-02	2.29E-04	Soluble	High	Yes
Moderately soluble	-4.43	1.33E-02	3.71E-05	Moderatel	High	Yes
Moderately soluble	-4.27	2.07E-02	5.40E-05	Moderatel	High	Yes
Soluble	-3.48	1.18E-01	3.31E-04	Soluble	High	Yes
Moderately soluble	-5.18	2.92E-03	6.64E-06	Moderatel	High	No
Soluble	-4.39	1.66E-02	4.03E-05	Moderatel	High	No
Moderately soluble	-2.81	7.98E-01	1.55E-03	Soluble	Low	No
Moderately soluble	-3.59	1.41E-01	2.59E-04	Soluble	Low	No
Moderately soluble	-4.37	2.06E-02	4.26E-05	Moderatel	Low	No
Poorly soluble	-5.15	3.63E-03	7.10E-06	Moderatel	Low	No
Poorly soluble	-5.42	1.74E-03	3.84E-06	Moderatel	High	No
Moderately soluble	-4.63	9.88E-03	2.32E-05	Moderatel	High	No
Poorly soluble	-4.76	8.65E-03	1.74E-05	Moderatel	Low	No
Moderately soluble	-3.98	4.89E-02	1.04E-04	Soluble	Low	No
Poorly soluble	-5.42	1.74E-03	3.84E-06	Moderatel	High	No
Moderately soluble	-4.63	9.88E-03	2.32E-05	Moderatel	High	No
Poorly soluble	-4.76	8.65E-03	1.74E-05	Moderatel	Low	No
Moderately soluble	-3.98	4.89E-02	1.04E-04	Soluble	Low	No
Soluble	-3.52	1.14E-01	3.03E-04	Soluble	High	No
Very soluble	-1.48	1.25E+01	3.30E-02	Soluble	High	No
Moderately soluble	-5.46	1.43E-03	3.48E-06	Moderatel	High	No
Moderately soluble	-4.58	9.99E-03	2.66E-05	Moderatel	High	No

Moderately soluble	-5.16	3.55E-03	6.95E-06	Moderatel	Low	No
Poorly soluble	-5.93	6.27E-04	1.16E-06	Moderatel	Low	No
Moderately soluble	-5.4	1.75E-03	3.99E-06	Moderatel	High	No
Moderately soluble	-3.97	4.42E-02	1.07E-04	Soluble	High	No
Moderately soluble	-4.75	7.78E-03	1.76E-05	Moderatel	High	No
Moderately soluble	-5.51	1.11E-03	3.11E-06	Moderatel	High	Yes
Poorly soluble	-6.29	1.94E-04	5.07E-07	Poorly solu	High	Yes
Moderately soluble	-5.4	1.30E-03	3.94E-06	Moderatel	High	Yes
Moderately soluble	-6.2	2.28E-04	6.38E-07	Poorly solu	High	Yes
Soluble	-3.74	6.44E-02	1.81E-04	Soluble	High	Yes
Moderately soluble	-4.53	1.13E-02	2.94E-05	Moderatel	High	Yes
Moderately soluble	-6.13	2.87E-04	7.36E-07	Poorly solu	High	No
Soluble	-1.69	6.22E+00	2.05E-02	Soluble	High	No
Moderately soluble	-2.48	1.09E+00	3.30E-03	Soluble	High	Yes

Pgp substrate	CYP1A2 inh	CYP2C19 in	CYP2C9 inh	CYP2D6 inh	CYP3A4 inh	log Kp (cm/s)
No	No	Yes	Yes	No	No	-6.21
No	No	Yes	Yes	Yes	No	-5.62
No	Yes	Yes	Yes	No	No	-6.17
No	Yes	Yes	Yes	Yes	No	-5.57
No	Yes	Yes	Yes	No	Yes	-6.16
No	Yes	Yes	Yes	Yes	Yes	-5.56
Yes	No	No	Yes	No	No	-6.82
Yes	No	No	Yes	No	No	-6.91
No	No	Yes	Yes	Yes	Yes	-5.51
Yes	No	No	No	No	Yes	-6.8
Yes	No	No	No	No	Yes	-6.8
Yes	No	No	No	No	Yes	-6.63
Yes	No	No	No	No	Yes	-6.63
Yes	No	No	No	No	No	-6.95
Yes	No	No	No	No	Yes	-6.78
No	No	No	No	No	No	-8.43
No	No	No	No	No	No	-7.23
No	No	No	No	No	No	-7.61
Yes	No	No	No	No	No	-7.58
Yes	No	Yes	Yes	Yes	No	-5.87
Yes	No	Yes	No	Yes	No	-6.47
Yes	No	No	No	Yes	No	-6.67
Yes	No	Yes	No	No	No	-6.71
No	No	Yes	Yes	Yes	Yes	-5.89
No	No	Yes	Yes	Yes	Yes	-5.89
No	Yes	Yes	Yes	Yes	No	-6.39
Yes	Yes	Yes	Yes	Yes	Yes	-5.79
Yes	Yes	Yes	Yes	Yes	Yes	-6.29
No	No	Yes	Yes	No	No	-6.89
Yes	No	Yes	Yes	No	No	-6.61
Yes	No	Yes	Yes	No	No	-7.21
Yes	No	No	No	No	No	-8.56
Yes	No	No	No	No	No	-7.96
No	No	No	Yes	No	No	-7.22
Yes	No	No	Yes	No	No	-6.62
No	Yes	Yes	Yes	Yes	Yes	-5.9
No	Yes	Yes	Yes	Yes	No	-6.5
Yes	No	No	Yes	No	No	-6.79
No	No	No	Yes	No	No	-7.39
No	Yes	Yes	Yes	Yes	Yes	-5.9
No	Yes	Yes	Yes	Yes	No	-6.5
Yes	No	No	Yes	No	No	-6.79
No	No	No	Yes	No	No	-7.39
No	No	No	No	No	No	-7.28
No	No	No	No	No	No	-9.58
No	No	No	Yes	No	No	-6.49
Yes	No	No	No	No	Yes	-6.96

Yes	No	No	No	No	No	-7.6
Yes	No	No	Yes	No	No	-7
No	Yes	Yes	Yes	Yes	No	-6.1
No	No	Yes	Yes	No	No	-6.9
Yes	No	Yes	Yes	No	No	-6.3
No	Yes	Yes	Yes	No	Yes	-5.86
No	Yes	Yes	Yes	Yes	Yes	-5.26
No	No	No	No	No	No	-6.11
No	No	No	No	Yes	Yes	-5.51
No	No	Yes	Yes	No	No	-6.46
No	No	Yes	Yes	Yes	No	-5.86
Yes	Yes	Yes	Yes	Yes	No	-5.82
Yes	No	No	No	No	No	-6.86
Yes	No	No	Yes	No	No	-6.26

Lipinski #violations	Ghose #violations	Veber #vio	Egan #viol	Muegge #v
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	0	1	1	2
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	2	1	1	1
1	3	1	1	1
0	1	1	1	0
1	2	1	1	0
0	0	0	0	0
0	0	0	0	0
0	2	1	1	0
0	0	0	1	0
0	0	0	0	0
0	0	0	0	0
0	2	1	1	0
0	0	0	1	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

1	3	2	1	1
1	3	2	1	1
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	1	0	0
0	0	0	0	0
0	0	0	0	0

Bioavailability Score	PAINS #ale	Brenk #ale	Leadlikene	Synthetic Accessibility
0.55	0	1	1	5.37
0.55	0	1	3	5.6
0.56	0	1	1	4.82
0.56	0	1	3	5.05
0.55	0	1	1	4.27
0.55	0	1	3	4.5
0.55	0	3	1	4.94
0.56	0	3	2	5.52
0.56	0	0	2	5.57
0.56	0	1	1	4.9
0.56	0	1	1	4.9
0.56	0	1	1	5.01
0.56	0	1	1	5.01
0.56	0	1	0	4.61
0.56	0	1	1	4.72
0.55	0	0	0	4.92
0.55	0	1	0	4.93
0.55	0	0	1	4.64
0.11	0	1	2	4.57
0.55	0	0	3	5.54
0.55	0	0	0	5.31
0.55	0	0	1	4.71
0.55	0	0	0	5.08
0.55	0	0	1	5.44
0.55	0	0	1	5.44
0.56	0	0	0	5.2
0.56	0	0	3	5.42
0.55	0	1	2	5.27
0.55	0	1	1	5.04
0.55	0	1	2	5.62
0.55	0	1	2	5.38
0.55	0	1	2	6.05
0.55	0	1	2	6.29
0.56	0	1	2	5.15
0.56	0	1	3	5.39
0.56	0	1	3	5.15
0.56	0	1	2	4.92
0.56	0	1	3	5.29
0.56	0	1	2	5.06
0.56	0	1	3	5.15
0.56	0	1	2	4.92
0.56	0	1	3	5.29
0.56	0	1	2	5.06
0.55	0	1	1	5.35
0.55	0	1	1	5.53
0.55	0	2	2	4.98
0.55	0	0	1	4.96

0.55	0	3	2	5.41
0.55	0	3	3	5.65
0.56	0	1	3	4.77
0.56	0	1	2	4.94
0.56	0	1	3	5.17
0.55	0	1	2	4.27
0.55	0	1	3	4.49
0.55	0	0	0	3.95
0.55	0	0	3	4.18
0.55	0	1	1	5.15
0.55	0	1	3	5.37
0.55	0	1	3	5.08
0.55	0	1	0	5.19
0.55	0	1	1	5.41