Table 1 List of chemical constituents reported in *Pinus roxburghii*

S.No	Chemical constituent	CHEMSPIDER ID	LOG P	H BOND Acceptor	H BOND donor	Mol wt	No of violation	TPSA
	Resin acid							
1.	Pimaric acid	16735968	4.957	2	1	302.458	0	37.299
2.	Abietic acid	10127	5.007	2	1	302.458	1	37.299
3.	Sandracopimaric acid	192262	4.957	2	1	302.458	0	37.299
4.	Dehydroabietic acid	85184	5.67	2	1	300.442	1	37.299
5.	Neoabietic acid	191824	5.312	2	1	302.458	1	37.299
	Sterols							
6.	Campesterol	151215	8.305	1	1	400.691	1	20.228
7.	Sitosterol	192962	8.62	1	1	414.718	1	20.228
8.	Stigmasterol	4444352	7.869	1	1	412.702	1	20.228
	Simple acid							
9.	3,4 dihyroxybenzoic acid	71	0.88	4	3	154.121	0	77.755
10.	3,4 dihyroxycinnamic acid	1266077	0.941	4	3	180.159	0	
	Ferulates							
11.	Hexacosyferrulate	----------	10.107	3	1	558.932	2	46.533
	Lignans							
12.	Pinoresinol	204822	2.587	6	2	358.39	0	77.392
13.	secoisoresinol	58845	2.075	6	4	362.422	0	99.38
	Stilbens							
14.	Pinosylvin	11286912	3.437	2	2	226.275	0	40.456
	Flavonoids							
15.	Catechin	8711	1.369	6	5	290.271	0	110.374
16.	Taxifoiln	621332	0.712	7	5	304.251	0	127.445
17.	Quercitin	4444051	1.683	7	5	302.238	0	131.351
18.	Rutin	4444362	-1.063	16	10	610.521	3	269.427
19.	Cedeodarin	158323	1.349	7	5	318.281	0	127.445
20.	Kaempferol	4444395	2.172	6	4	286.239	0	111.123
21.	Rhamnetin	4445008	2.219	7	4	316.265	0	120.357
22.	Isorhamnetin	4444973	1.99	7	4	316.265	0	120.357
23.	Xanthone	6753	3.57	2	0	196.205	0	30.211
	Triterpenoid							
24.	Friedelin	82597	7.854	1	0	426.729	1	17.071
	Fatty alcohol							
25.	Ceryl alcohol	61478	9.655	1	1	382.717	1	20.228

Table 2 Docking scores of Chemical constituents from *Pinus roxburghii* using PDB ID: 1IR3

S.no	Compound	MolDock Score	Amino acid residue	Atom of the ligand	H-boond length (A^0)
1.	**ANP**	**-268.525**	**Ser 1006** **Lys 1030** **Asp 1083** **Ser 1006** **Met 1079** **Glu 1077**	**O of SO_2** **3-OH of furan** **N of NH_2** **O of SO_2** **O of Pyranose** **O of 4-OH**	**2.80** **2.79** **2.02** **3.40** **3.10** **3.07**
2.	3,4 dihyroxybenzoic acid	-82.7528	Ser 1006 Ser1006 Gln 1004	O of CO2 O of CO2 O of ligand	2.82 3.12 2.99
3.	Catechin	-90.1103	Met 1079 Met 1079 Asp 1083 Lys 1030	O of 4-OH O of 4-OH O of 4-OH O of OH	3.14 3.32 2.99 3.23
4.	**Secoisoresinol**	**-123.346**	**Glu 1077** **Met 1079** **Asp1083** **Lys 1030**	**O of 4-OH** **O of 4-OH** **O of -OH** **O of 4-OH**	**3.29** **3.04** **2.97** **3.12**
5.	Sandracopimaric acid	-104.622	Lys 1030	O of -CO	3.03
6.	**Pinoresinol**	**-122.854**	**Met 1079** **Met 1079**	**O of 4-OH** **O of 4-OH**	**3.12** **2.91**
7.	Taxifoiln	-96.0355	Leu 1002 Asp 1083 Asp 1083 Lys 1030 Lys 1030	O of 4-OH O of 3-OH O of 3-OH O of –OH O of 4-OH	3.12 2.37 2.64 3.10 2.50
8.	Caffeic acid	-98.7362	Lys 1030 Lys 1030	O of 3-OH O of 4-OH	2.60 2.75
9.	Quercitin	-95.4304	Leu 1002 Gln 1004 Met 1079 Met 1079 Met 1079	O of 4-OH O of 4-OH O of 2-OH O of 2-OH O of 4-OH	2.94 2.85 2.56 2.60 3.23
10.	Kaempferol	-97.722	Leu 1002 Lys 1030 Lys 1030	O of 4-OH O of 5-OH of quinoline O of 5-OH of	3.39 3.11 2.67

				quinoline	
11.	Isorhamnetin	-101.084	Lys 1030 Lys 1030 Leu 1002	O of 4-OH of quinoline O of 5-OH of quinoline O of 4-OH	2.72 3.13 3.13
12.	Rhamnetin	-97.8341	Lys 1030 Lys 1030 Leu 1002	O of 4-OH O of 5-OH O of 4-OH	2.65 3.13 3.10
13.	Pinosylvin	-90.5397	Lys 1030 Ser 1006	O of 3-OH O of 5-OH	2.88 3.37
14.	Pimaric acid	-96.3319	No interaction		
15.	Hexacosyferrulate	-5.52251	No interaction		
16.	Xanthone	-70.433	Met1079	4-OH pyranose	2.82
17.	Cedeodarin	-173.749	No interaction		

Table 3 Docking scores of Chemical constituents from *Pinus roxburghii* using PDB ID: 1USO

S.no	**Compound**	**MolDock Score**	**Amino acid residue**	**Atom of the ligand**	**H-boond length (A^0)**
1.	IDD594	-155.639	Tyr48 Tyr48 Tyr209 Ser210	O of COOH N of C=N O of 2-OCH_2 S of SH	3.09 2.66 3.41 3.30
2.	3,4 dihyroxybenzoic acid	-95.9973	Ser 214 Leu 212 Lys 262 Ile 260	O of C=O O of C=O O of C=O O of -OH	3.14 3.10 3.10 2.83
3.	Catechin	-134.751	Cys 303 Tyr 309 Ala 299 Cys 298 Tyr 209 His 110 Tyr 309	O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH	3.02 2.51 3.10 2.60 3.15 2.79 3.44

4.	Secoisoresinol	-180.947	Trp111 His110 Asn160 Cys298 Tyr48 Ser210 Ser210 Asp216 Leu212 Asp43 Thr19 Trp20	O of -4OH O of -4OH O of -4OH O of -4OH O of -4OH O of –OH O of –OH O of -4OH O of 3-OCH_3 O of -OH O of –OH O of -OH	2.98 3.03 2.60 3.13 3.36 2.65 3.48 3.25 3.12 3.10 2.92 3.04
5.	Sandracopimaric acid	-125.402	Tyr 48	O of -OH	2.60
6.	Pinoresinol	-146.801	Ser 210 Ser 159 Gln 183 Pro 215	O of -O- O of -OH O of -OH O of -4-OH	2.78 3.52 2.83 2.38
7.	Taxifoiln	-140.194	Asp 43 Gln 183 Lys 77 Cys 298 Tyr 209 Ser 210 Ile 260 Leu 212 Pro 211 Ser 210	O of -OH O of -OH O of -OH O of -OH O of -OH O of Pyranose O of -OH O of -OH O of -OH O of Pyranose	3.04 2.63 3.27 2.80 3.47 2.92 2.99 2.74 3.15 3.55
8.	Caffeic acid	-115.197	Ser 214 Leu 212 Lys 262 Ile 260 Ser 210 Asp 43	O of C=O O of C=O O of C=O O of -OH O of -OH O of -OH	3.04 3.02 3.00 3.03 3.00 3.49
9.	Quercitin	-141.885.067	Ile 260 Ser 210 Tyr 209 Cys 298 Lys 77 Gln 183 Asp 43 Pro 211 Leu 212	N of Quinoloine N of Quinoloine O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH	2.62 3.01 3.42 2.82 3.10 2.70 2.88 3.26 2.73

10.	Kaempferol	-138.548	Ile 260 Asp 43 Lys 77 Ser 210 Ser 210 Cys 298 Tyr 209 Gln 183	O of -OH O of -OH O of -OH N of Quinoline N of Quinoline O of -OH O of -OH O of -OH	2.59 3.10 3.20 2.94 3.55 2.87 3.48 2.93
11.	Isorhamnetin	-145.042	Lys 77 Gln 183 Asp 43 Tyr 209 Cys 298 Ser 210 Ile 260 Leu 212	O of -OH O of -OH O of -OH O of -OH O of -OH N of Quinoloine O of -OH O of $-OCH_3$	3.07 2.61 2.84 3.33 2.84 2.99 2.77 3.17
12.	Rhamnetin	-150.026	Asp 43 Lys 77 Gln 183 Cys 298 Asp 216 Tyr 209 Ser 210 Ser 210 Ile 260	O of 3-OH O of 5-OH O of 5-OH O of 5-OH O of 3-OH O of 3-OH O of 8-OH N of Quinoloine O of –OH	3.00 3.10 2.84 2.95 2.51 3.56 3.53 3.03 2.48
13.	Pinosylvin	-134.563	Asp 43 Tyr 48 Asp 43 Thr 19 Trp 20	O of -OH O of -OH O of -OH O of -OH O of –OH	3.46 3.10 3.10 2.60 3.05
14.	Pimaric acid	-132.033	Tyr 48	O of -C=O	2.60
15.	Hexacosyferrulate	-190.717	Tyr 309 Cys 303	O of -C=O O of -C=O	3.34 3.06
16.	Xanthone	-109.842	Ser210 Trp20 Lys21	O of pyranose 4-OH pyranose 4-OH pyranose	2.96 2.88 2.50
17.	Cedeodarin	-198.027	Asp43 Lys262 Ser214 Leu212	N of NH O of CO_2 O of CO_2 O of CO_2	2.90 2.75 3.43 3.25

			Asp216 Ser214 Ser210	N of NH_2 N of NH_2 N of CONH	3.54 3.38 3.22

Table 4 Docking scores of Chemical constituents from *Pinus roxburghii* using PDB ID: 2f70

S.no	**Compound**	**MolDock Score**	**Amino acid residue**	**Atom of the ligand**	**H-boond length (A^0)**
1.	**UN608**	**-70.6666**	**Arg 221** **Arg 221** **Ser 216** **Gly 218** **Ser 216** **Ile 219** **Gly 220** **Asp 181** **Arg 221** **Gly 86** **His 214**	**-O of SO_2** **-O of SO_2** **-O of SO_2** **-O of SO_2** **-O of SO_2** **-O of SO_2** **-O of SO_2** **-O of Ether** **-O of SO_2** **-O of SO_2** **-O of SO_2**	**2.85** **2.65** **2.65** **3.10** **3.08** **2.89** **1.94** **3.22** **2.60** **2.79** **2.88**
2.	3,4 dihyroxybenzoic acid	-93.2968	Ile 219 Gly 220 Gly 218 Arg 221 Arg 221 Tyr 46 Cys 215	O of C=O O of C=O O of C=O O of C=O O of C=O O of 3-OH O of C=O	2.94 2.60 3.27 3.11 3.10 2.91 2.60
3.	Catechin	-83.535	Arg 221 Gly 220 Tyr 46 Arg 221	O of 4-OH O of 5-OH O of pyranose O of 4-OH	3.08 2.95 3.17 3.27

4.	Secoisoresinol	19.1388	Gln 218 Gly 220 Cys 215 Ile 219 Arg 221 Arg 221 Arg 221 Gly 259	O of 3 -OH O of 4 OH O of CH_3 O of 4OH O of OCH_3 O of OCH_3 O of OCH_3 O of 4OH	3.15 2.55 2.99 2.66 3.29 2.46 3.20 3.57
5.	Sandracopimaric acid	-87.863	Ile 219 Gly 218 Ala 217 Arg 221 Arg 221	O of C=O O of C=O O of C=O O of C=O O of C=O	3.28 2.84 3.01 2.76 3.10
6.	Pinoresinol	-84.4847	Arg 221 Ser 216 Ala 217 Cys 215	O of 4-OH O of 4-OH O of OCH_3 O of OCH_3	2.91 2.95 3.51 3.40
7.	Taxifoiln	-88.3651	Arg 221 Asp 181 Arg 221 Ser 216 Cys 215 Gly 220 Arg 221 Asp 48 Ile 219	O of 4-OH O of 4-OH O of 3-OH O of 4-OH O of 4-OH O of 3-OH O of 4-OH O of 3-OH O of 3-OH	2.99 3.46 3.48 3.91 3.26 2.42 2.60 3.41 3.29
8.	**Caffeic acid**	**-101.897**	**Tyr 46** **Gly 2220** **Ile 219** **Arg 221** **Arg 221** **Ser 216** **Cys 215** **Arg 221** **Cys 215**	**3-OH** **O of 3-OH** **C=O** **O of 4 -OH** **O of 4** **O of 4** **O of 4** **O of 3-OH** **O of 3-OH**	**3.20** **2.59** **3.28** **2.67** **3.39** **3.40** **3.30** **3.34** **2.46**

9.	Quercitin	49.6707	Tyr 46 Arg 221 Gly 262 Arg 221 Ser 216 Tyr 46 Pro 180 Trp 179 Asp 181	O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH O of -OH	3.17 3.01 2.93 3.39 3.51 3.26 310 2.96 2.74
10.	**Kaempferol**	**-104.744**	**Try 46** **Asp 181** **Arg 221** **Gly 220** **Cys 215**	**4-OH of Quinoline** **5-OH of Quinoline** **7-OH of Quinoline** **7-OH of Quinoline** **7-OH of Quinoline**	**3.04** **2.95** **3.07** **2.80** **2.61**
11.	Isorhamnetin	-89.1876	Arg 221 Ser 216 Gly 220 Asp 181 Asp 48	3-OH 3-OH 4-OH 3-OH 3-OH of Quinoline	2.94 3.48 3.22 3.10 3.08
12.	Rhamnetin	17.7531	Asp181 Lys 120 Tyr 46 Arg 221 Met 258	3-OH of Quinoline 3-OH of OCH_3 3-OH of Quinoline O of OCH_3 O of 4-OH	3.18 4.95 3.47 3.06 3.10
13.	Pinosylvin	-88.6779	Arg 221 Arg 221 Ser 216 Gly 220 Cys 215	O of OH O of OH O of OH O of -OH -OH	3.16 2.57 2.60 2.61 3.09
14.	Pimaric acid	-68.8936	No interaction		
15.	Hexacosyferrulate	291.3442	Ser 270	O of $–OCH_3$	2.66
16.	Xanthone	-83.1765	Gln262	4-OH pyranose	3.18
17.	Cedeodarin	95.3797	Lys116	O of CO_2	2.78

			Gln262 Gly220	O of CO_2 N of CONH	2.73 3.34

Table 5 Docking scores of Chemical constituents from *Pinus roxburghii* using PDB ID: 3F8S

S.no	**Compound**	**MolDock Score**	**Amino acid residue**	**Atom of the ligand**	**H-boond length (A^0)**
1.	**Pf2**	**-107.94**	**Asn 710** **Tyr 662** **Ser 630** **Ser 630**	**O of –OH** **O of Furan** **O of Furan** **O of Furan**	**3.31** **3.50** **3.17** **3.40**
2.	3,4 dihyroxybenzoic acid	-71.4059	Arg 125 Arg 125 Asp 709 Lys 122 Asp 793	O of C=O O of C=O O of OH O of OH O of OH	3.06 3.06 2.60 2.93 3.00
3.	Catechin	-112.972	Tyr 585 Glu 361 Ile 407 Glu 361 Arg 358 Arg 356 Arg 356	O of –OH O of –OH O of -OH O of -OH O of –Oh O of -OH O of Pyranose	3.17 3.09 3.18 3.10 3.48 3.03 2.85
4.	Secoisoresinol	-106.909	Tyr 585 Arg 429 Arg 358 Ile 405	OCH3 OCH3 O of OH O of OH	3.10 3.47 2.60 3.08
5.	Sandracopimaric acid	-98.5671	No interaction		
6.	Pinoresinol	-114.634	Phe 357 Arg 358 Arg 358 Arg 358 Trp 215	3 –OH O og OCH_3 O of Furan O of Furan O of OH	3.10 3.54 3.06 3.22 3.51
7.	Taxifoiln	-91.4079	Asp 739 Glu 205 Asp 739 Lys 122	O of -OH O of -OH O of -OH O of -OH	3.10 2.91 3.10 2.81

8.	Caffeic acid	-86.569	Asp 709 Asp 709 Arg 125	O of –OH O of -OH O of –C=O	2.87 2.76 2.60
9.	Quercitin	-88.291	Arg 358 Arg 358 Glu 361 Pro 359 Asp 302 Val 303	N of quinoline N of quinoline O of 4 OH quinoline O of 4 OH quinoline O of 3OH quinoline O of 3 OH	3.12 2.78 2.81 2.60 2.98 2.94
10.	Kaempferol	-99.4805	Asp 739 Asp 739 Lys 122 Glu 205 Glu 205	4 OH of quinoline 5 OH of quinoline 5 OH of quinoline 7 OH of quinoline 7 OH of quinoline	2.85 3.10 2.77 2.93 2.93
11.	Isorhamnetin	-97.2701	Glu 408 Ile 407 Ile 407 Ile 407 Arg 356 Arg 356 Arg 382	4 OH quinoline 3 OH quinoline 3 OH quinoline 4 OH quinoline O of –OCH_3 O of –OCH_3 O of -OH	2.96 2.90 3.37 3.54 3.09 2.73 3.38
12.	Rhamnetin	-96.9684	Arg 358 Arg 356 Arg 356 Arg 382 Ile 407 Ile 407 Ile 407 Ile 407 Glu 408	O of -OH O of -OH O of -OH O of -OH O of –OH O of –OH O of –OH O of –OH O of -OH	2.53 2.97 2.76 3.18 3.49 3.00 3.49 2.60 3.14
13.	Pinosylvin	-97.9143	Ser 630 His 740	O of -OH	2.87 3.31

				O of -OH	
14.	Pimaric acid	-91.6603	Arg 356 Arg 356	O of C=O O of C=O	3.03 3.23
15.	Hexacosyferrulate	-59.1203	Arg 356 Arg 356	O of C=O O of C=O	3.12 2.60
16.	Xanthone	-81.6503	Phe713 Thr706 Ser239 Tyr241	O of 4-OH pyranose O of 4-OH pyranose O of pyranose O of pyranose	3.29 2.60 2.60 2.75
17.	Cedeodarin	-100.132	Thr736 Thr706 Tyr241 Ser239 Gln714 Phe713 Ser239 Thr706 Glu237	O of C=O O of C=O N of CONH O of C=O O of C=O O of C=O O of CONH N of NH_2 O of 4-OH cyclohexane	3.01 3.13 3.02 3.40 3.10 3.53 3.17 3.09 3.36