Supplementary Material

Systematic *In Silico* Screening of Nigerian Medicinal Plant Phytoconstituents Against Six Breast Cancer-Associated Proteins

Table S1. Phytoconstituents identified from the 21 included Nigerian medicinal plant species, by plant part, extraction solvent, and reference.

Plant Name	Plant Part	Solvent used for extraction	Compound(s) identified	Reference
Allium sativum L.	Clove	Hydroethanol (40% ethanol)	Allicin **(1)**, Allyl methyl sulfide **(2)**, Dimethyl disulfide **(3)**, Diallyl Sulfide **(4)**, 1,1'-Thiobis-1-propene **(5)**, Allyl(prop-1-en-1-yl)sulfane **(6)**, 3,4-Dimethyl thiophene **(7)**, Methyl-2-propenyl disulfide **(8)**, Methyl-1-propenyl disulfide **(9)**, 1,3-Dithiane **(10)**, Methyl isothiocyanate **(11)**, Diallyl disulfide **(12)**, 1-Propenyl allyl disulfide **(13)**, Dipropenyl disulfide **(14)**, Allyl methyl trisulfide **(15)**, 3-Vinyl-1,2-dithiacyclohex-4-ene **(16)**, 3-Vinyl-1,2-dithiacyclohex-5-ene **(17)**, Di-2-propenyl trisulfide **(18)**	[1]
Mangifera indica L	Pulp	Ethanol, methanol, and acetone (1:1:1)	Gallic acid **(19)**, Mono-galloyl glucoside **(20)**, Tetra–galloyl glucoside **(21)**, Penta-galleo glucoside **(22)**, Hydroxybenzoic acid hexoside **(23)**	[2]
Zingiber officinale Roscoe	Rhizome	Ethanol	[6]-Gingerol **(24)**, [8]-Gingerol **(25)**, [10]-Gingerol **(26)**	[3,4]
Annona muricata L.	Pulp	Ethyl acetate	15–acetyl guanacone **(27)**	[5]
Cola lepidota K.Schum	Seed	Hydromethanol (25% methanol)	Triethylammoniumyl-acetate monohydrate **(28)**	[6]
Cajanus cajan (L.) Huth	Leaf	Hydroethanol (50% ethanol)	Tryptophan **(29)**, Orientin **(30)**, Vitexin **(31)**, Pinosylvin monomethylether **(32)**, Pinostrobin **(33)**, Cajaninstilbene acid **(34)**	[7]
		Methanol	Hexadecanoic acid methyl ester **(35)**, α-Amyrin **(36)**, β-Sitosterol **(37)**, Pinostrobin **(33)**, Longistylin A **(38)**, Longistylin C **(39)**	[8]
		Ethanol	Cajanstilbenoid A **(40)**, Cajanstilbenoid B **(41)**	[9]
Camellia sinensis (L.) Kuntze	Leaf	Ethanol (95%), water (1:1)	(+)-gallocatechin **(42)**, (–)-epicatechin **(43)**, (–)-epigallocatechin **(44)**, (–)-epicatechin gallate **(45)**, (–)-epigallocatechin gallate **(46)**, caffeine **(47)**	[10]
Chromolaena odorata (L.) R.M.King & H.Rob.	Leaf	Ethanol (90%)	5-hydroxy-7,4`-dimethoxyflavanone **(48)**, 2`-hydroxy-4,4`,5`,6`-tetramethoxychalcone **(49)**, 1,6-dimethyl-4-(1-methylethyl)naphthalene (cadalene) **(50)**	[11]
Curcuma longa L.	Rhizome	Ethanol (50%)	Curcumin **(51)**	[12]
Khaya senegalensis (Desr.) A.Juss.	Stem bark	Methanol	3α,7α-dideacetylkhivorin **(52)**, 1-*O*-acetylkhayanolide B **(53)**	[13]
Ocimum gratissimum L.	Leaf	Ethanol (95%)	Oleanolic acid **(54)**	[14]
Terminalia chebula Retz.	Fruit	Water	Gallic acid **(19)**, Punicalagin **(55)**, Isoterchebulin **(56),** 1,3,6-Tri-*O*-galloyl-β-D-glucopyranose **(57)**, Chebulagic acid **(58)**, Chebulinic acid **(59)**	[15]
Psidium guajava L.	Leaf	Methanol	Guajadial C **(60)**, Guajadial D **(61)**, Guajadial E **(62)**, Guajadial F **(63)**	[16]
	Fruit	Ethanol	*E*-lycopene **(64)**, 5-*cis*-lycopene **(65)**, 13-*cis*-lycopene **(66)**	[17]
Detarium microcarpum Guill. & Perr.	Stem bark	Water	Serpyllin **(67)**, 6,8-Di-rhamnosylapigenin **(68)**, Phloionolic acid **(69)**, Tetracosatetraenoic acid n-6 **(70)**, Amorphaquinone **(71)**, Gallic acid **(19)**, Violanthin **(72)**, Syringin **(73)**, Isoderrone **(74)**, Procyanidin B3 **(75)**, Alpinumisoflavone **(76)**, Epifisetinidol-(4β->8)-catechin **(77)**, 3-Hydroxy-1-phenyl-1-eicosanone **(78)**	[18]

		Methanol	Cyclomammein **(79)**, Calabaxanthone **(80)**, Justicidin A **(81)**, Demethylnobiletin **(82)**	
Guiera senegalensis J.F.Gmel.	Stem bark	Water	Phloionolic acid **(69)**, Tetracosatetraenoic acid n-6 **(70)**, Isorhamnetin **(83)**, 1,3,4,5-Tetra-*O*-galloylquinic acid **(84)**, Gallic acid **(19)**, Eupatorin **(85)**, 3,4-Di-*O*-galloylquinic acid **(86)**, 7,7-Dihydroxy-6,8'-bicoumarin **(87)**, 2,3-Dihydroxybenzoic acid **(88)**, Rothindin **(89)**, Trifolirhizin-6'-monoacetate **(90)**, 3-Hydroxy-1-phenylicosan-1-one **(78)**	
		Methanol	Cumanin **(91)**, Jamaicin **(92)**, Gancaonin X **(93)**, Isorhamnetin **(83)**, 1,3,4,5-Tetra-*O*-galloylquinic acid **(84)**, Hypericin **(94)**, Glucosyl passiflorate **(95)**	
Senna siamea (Lam.) H.S.Irwin & Barneby (*syn. Cassia siamea*)	Stem bark	Methanol	Serpyllin **(67)**, Lusitanicoside **(96)**, Phloionolic acid **(69)**, Tetracosatetraenoic acid n-6 **(70)**, Cumanin **(91)**	
Caesalpinia pulcherrima (L.) Sw.	Root	Chloroform	Vouacapen-5α-ol **(97)**, 8,9,11,14-Didehydrovouacapen-5α-ol **(98)**, 6β-cinnamoyl-7β-hydroxyvouacapen-5α-ol **(99)**, Pulcherrin A **(100)**, Pulcherrin B **(101)**, Pulcherrin J **(102)**, Pulcherrimin A **(103)**, Pulcherrimin B **(104)**, Pulcherrimin C **(105)**, Pulcherrimin E **(106)**, 6β-Hydroxyisovouacapenol C **(107)**, 6β-Cinnamoyl-7β-acetoxyvouacapen-5α-ol **(108)**, Pulcherrimin D **(109)**	[19]
Conyza sumatrensis (S.F.Blake) Pruski & G.Sancho	Leaf	Chloroform	Stigmast-5, 22-dien-3- *O*-β-D-glucopyranoside **(110)**, 2, 3-Dihydroxylpropyl hexacosanoate **(111)**	[20]
Citrus aurantium L.	Stem bark	Methanol	Citrusinine-I **(112)**, Citracridone-I **(113)**, 5-Hydroxynoracronycine **(114)**, Natsucitrine-I **(115)**, Glycofolinine **(116)**, Citracridone-III **(117)**	[21]
Hymenocardia acida Tul. (syn. *Hymenocardia acida* var. acida)	Stem bark	Methanol	Lupeol **(118)**	[22]
Vernonia amygdalina Del.	Leaf	Ethyl acetate fraction	Diosmetin **(119)**, 4-Methylumbelliferyl glucuronide **(120)**, Chlorogenic acid **(121)**, 4-Methylumbelliferone **(122)**, Scutellarin **(123)**, Rhoifolin **(124)**, 7-Hydroxycoumarine **(125)**, Apigetrin **(126)**, Apigenin **(127)**, Baicalin **(128)**, Luteolin **(129)**, Ingenol-3-angelate **(130)**, 4-Methoxycinnamic acid **(131)**	[23]
		n-butanol fraction	Vernodalinol **(132)**	[24]
Mangifera indica L.	Stem bark	Water	Mangiferin **(133)**	[25]
	Kernel	Ethanol (95%)	1-Butanol, 3-methyl-, acetate **(134)**, Butane, 1,1-diethoxy-3-methyl- **(135)**, Propane, 1,1,3-triethoxy- **(136)**, Ethaneperoxoic acid, 1-cyano-1-(2-methylphenyl) ethyl ester **(137)**, Apigenin 7-glucoside (Apigetrin) **(126)**, 1,4-Diamino-2-methoxyanthraquinone **(138)**, Phenol, 4,6-di (1,1-dimethylethyl)-2-methyl- **(139)**, Chlorazanil **(140)**, Isoheptadecanol (1-Hexadecanol,2-methyl) **(141)**, *cis*-5-Dodecenoic acid, (3-cyanopropyl) dimethylsilyl ester **(142)**, Fumaric acid, 2-decyl undecyl ester **(143)**, Phthalic acid, hept-2-yl isohexyl ester **(144)**	[26]
	Leaf	Ethanol	Gallic acid **(19)**, Iriflophenone-3-C-β-D-glucoside **(145)**, Iriflophenone-3-C-(2-*O*-p-hydroxybenzoyl)-β-D-glucoside **(146)**, Mangiferin **(133)**, Iriflophenone-3-C-(2-*O*-galloyl)-β-D-glucoside **(147)**, 2,3,4,6-Tetra-*O*-galloyl-D-glucose (Tetra–galloyl glucoside) **(21)**, Quercetin-3-D-galactoside	[27]

			(148), Quercetin-3-β-D-glucoside **(149)**, Quercetin-3-*O*-xyloside **(150)**, Quercetin-3-*O*-α-L arabinopyranoside **(151)**, Penta-*O*-galloyl-glucose (Penta-galleo glucoside) **(22)**	
		Hydroethanol (50%)	Gallic acid **(19)**, Iriflophenone-3-C-β-D-glucoside **(145)**, Iriflophenone-3-C-(2-*O*-p-hydroxybenzoyl)-β-D-glucoside **(146)**, Mangiferin **(133)**, Iriflophenone-3-C-(2-*O*-galloyl)-β-D-glucoside **(147)**, 2,3,4,6-Tetra-*O*-galloyl-D-glucose (Tetra–galloyl glucoside) **(21)**, Quercetin-3-D-galactoside **(148)**, Quercetin-3-β-D-glucoside **(149)**, Quercetin-3-*O*-xyloside **(150)**, Quercetin-3-*O*-α-L arabinopyranoside **(151)**, Penta-*O*-galloyl-glucose (Penta-galleo glucoside) **(22)**	
	Peel	Ethanol (80%)	Chlorogenic acid **(121)**, Caffeic acid **(152)**, 3,4-Dicaffeoyl quinic acid **(153)**, 4,5-Dicaffeoyl quinic acid **(154)**, Catechin **(155)**, Gallic acid **(19)**, Quercetin **(156)**	[28]
	Pulp	Methanol, acetone (1:1)	Monogalloyl glucoside **(20)**, Gallic acid **(19)**, *p*-Hydroxybenzoic acid glycoside **(23)**	[29]

Table S2. SwissADME/ProTox-3.0 drug-likeness and toxicity screening parameters for the 156 catalogued phytoconstituents. Compounds shaded orange are the 50 compounds advanced to docking

Compounds	**MW (g/mol)**	**LP**	**LVN**	**BBP**	**PgpS**	**CYP_{2C9} Inb.**	**CYP_{2D6} Inb.**	**CYP_{3A4} Inb.**
Allicin	162.27	1.18	0	Yes	No	Active	Inactive	Inactive
Allyl methyl sulfide	88.17	1.67	0	Yes	No	Active	Inactive	Inactive
Dimethyl disulfide	94.20	0.84	0	Yes	No	Active	Inactive	Inactive
Diallyl Sulfide	114.21	2.35	0	Yes	No	Active	Inactive	Inactive
1,1'-Thiobis-1-propene	114.21	2.35	0	Yes	No	Active	Inactive	Inactive
Allyl(prop-1-en-1-yl)sulfane	114.21	2.35	0	Yes	No	Active	Inactive	Inactive
3,4-Dimethyl thiophene	112.19	1.91	0	Yes	No	Active	Inactive	Inactive
Methyl-2-propenyl disulfide	162.32	2.81	0	Yes	No	Active	Inactive	Inactive
Methyl-1-propenyl disulfide	120.24	1.67	0	Yes	No	Active	Inactive	Inactive
1,3-Dithiane	120.24	1.42	0	Yes	No	Active	Inactive	Inactive
Methyl isothiocyanate	73.12	1.10	0	Yes	No	Inactive	Inactive	Inactive
Diallyl disulfide	146.27	2.35	0	Yes	No	Active	Inactive	Inactive
1-Propenyl allyl disulfide	146.27	2.35	0	Yes	No	Active	Inactive	Inactive
Dipropenyl disulfide	146.27	2.35	0	Yes	No	Active	Inactive	Inactive
Allyl methyl trisulfide	152.30	1.67	0	Yes	No	Active	Inactive	Inactive
3-Vinyl-1,2-dithiacyclohex-4-ene	144.26	1.96	0	Yes	No	Active	Inactive	Inactive
3-Vinyl-1,2-dithiacyclohex-5-ene	144.26	1.96	0	Yes	No	Active	Inactive	Inactive
Di-2-propenyl trisulfide	178.34	2.35	0	Yes	No	Active	Inactive	Inactive
Gallic acid	170.12	-0.16	0	No	No	Active	Inactive	Inactive
Mono-galloyl glucoside	332.26	-2.29	1	No	No	Inactive	Inactive	Inactive
Tetra-galleo glucoside	788.57	-2.60	3	No	Yes	Inactive	Inactive	Inactive
Penta-galleo glucoside	940.68	-2.83	3	No	Yes	Inactive	Inactive	Active
Hydroxybenzoic acid hexoside	300.26	-1.28	0	No	No	Inactive	Inactive	Inactive
[6]-Gingerol	249.39	2.14	0	Yes	No	Inactive	Inactive	Inactive
[8]-Gingerol	322.44	2.61	0	Yes	No	Inactive	Inactive	Inactive
[10]-Gingerol	350.49	3.06	0	Yes	No	Inactive	Inactive	Inactive
Acetyl guanacone	662.94	4.00	0	No	Yes	Inactive	Inactive	Inactive
Triethylammoniumyl-acetate monohydrate	179.26	-3.46	0	No	No	Inactive	Inactive	Inactive
Tryptophan	204.23	-1.66	0	No	No	Inactive	Inactive	Inactive

Orientin	448.38	-2.51	2	No	No	Inactive	Inactive	Inactive
Vitexin	432.38	-2.02	1	No	No	Inactive	Inactive	Inactive
Pinosylvin monomethylether	226.27	3.13	0	Yes	No	Active	Inactive	Inactive
Pinostrobin	270.28	1.52	0	Yes	No	Active	Inactive	Inactive
Cajaninstilbene acid	338.40	3.73	0	Yes	No	Active	Inactive	Inactive
Hexadecanoic acid methyl ester	270.45	4.44	0	Yes	No	Inactive	Inactive	Inactive
α-Amyrin	426.72	6.92	1	No	No	Active	Inactive	Inactive
β-Sitosterol	414.71	6.73	1	No	No	Active	Inactive	Inactive
Longistylin A	294.39	4.24	1	Yes	No	Active	Inactive	Inactive
Longistylin C	294.39	4.24	1	Yes	No	Active	Inactive	Inactive
Cajanstilbenoid A	588.77	6.09	2	No	Yes	Active	Inactive	Inactive
Cajanstilbenoid B	520.66	5.35	2	No	No	Active	Inactive	Inactive
(+)-Gallocatechin	306.27	-0.29	1	No	No	Inactive	Inactive	Inactive
(-)-Epicatechin	290.27	0.24	0	No	Yes	Inactive	Inactive	Inactive
(-)-Epigallocatechin	306.27	-0.29	1	No	No	Inactive	Inactive	Inactive
(-)-Epicatechin gallate	442.37	0.05	1	No	No	Inactive	Inactive	Inactive
(-)-Epigallocatechin gallate	458.37	-0.44	2	No	No	Inactive	Inactive	Inactive
Caffeine	194.19	0.22	0	No	No	Inactive	Inactive	Inactive
5-hydroxy-7,4`-dimethoxyflavanone	300.31	1.20	0	Yes	No	Active	Inactive	Inactive
1,6-Dimethyl-4-(1-methylethyl)naphthalene (cadalene)	198.30	5.62	1	No	No	Active	Inactive	Inactive
Curcumin	368.38	1.47	0	No	No	Active	Inactive	Active
3-α,7-α-dideacetylkhivorin	488.61	2.00	0	No	Yes	Inactive	Inactive	Active
1-*O*-acetylkhayanolide B	546.61	0.58	1	No	Yes	Inactive	Inactive	Inactive
Oleanolic acid	456.70	5.82	1	No	No	Inactive	Inactive	Inactive
Punicalagin	1084.72	-3.76	3	No	Yes	Inactive	Inactive	Inactive
Isoterchebulin	1084.72	-3.02	3	No	Yes	Inactive	Inactive	Inactive
1,3,6-Tri-*O*-galloyl-β-D-glucopyranose	636.47	-2.42	3	No	Yes	Inactive	Inactive	Inactive
Chebulagic acid	954.66	-2.64	3	No	Yes	Inactive	Inactive	Inactive
Chebulinic acid	956.68	-2.64	3	No	Yes	Inactive	Inactive	Inactive
Guajadial C	474.59	3.55	0	No	No	Active	Inactive	Inactive
Guajadial D	474.59	3.55	0	No	No	Active	Inactive	Inactive
Guajadial E	474.59	3.55	0	No	No	Active	Inactive	Inactive
Guajadial F	474.59	3.55	0	No	No	Active	Inactive	Inactive
All *E*-lycopene	536.87	9.21	2	No	Yes	Active	Inactive	Inactive
5-*cis*-lycopene	536.87	9.21	2	No	Yes	Active	Inactive	Inactive
13-*cis*-lycopene	536.87	9.21	2	No	Yes	Active	Inactive	Inactive
Serpyllin	388.37	0.11	0	No	No	Active	Inactive	Active
6,8-Di-rhamnosyl apigenin	562.52	-3.02	3	No	No	Active	Inactive	Inactive
Phloionolic acid	332.48	2.11	0	No	Yes	Inactive	Inactive	Inactive
Tetracosatetraenoic acid n-6	360.57	5.62	1	No	No	Inactive	Inactive	Inactive
Amorphaquinone	346.33	-0.44	0	No	No	Active	Inactive	Inactive
Violanthin	578.52	-3.77	3	No	No	Inactive	Inactive	Inactive
Syringin	372.37	-1.59	0	No	No	Inactive	Inactive	Inactive
Isoderrone	336.34	1.64	0	No	No	Active	Inactive	Inactive
Procyanidin B3	578.52	-0.26	3	No	No	Inactive	Inactive	Inactive
Alpinumisoflavone	336.34	1.64	0	No	No	Active	Inactive	Inactive
Epifisetinidol-(4β-8)-catechin	562.52	0.23	3	No	No	Inactive	Inactive	Inactive
3-Hydroxy-1-phenyl-1-eicosanone	388.63	5.31	1	No	No	Inactive	Inactive	Inactive
Cyclomammein	388.45	2.03	0	No	Yes	Active	Inactive	Inactive
Calabaxanthone	392.44	2.73	0	No	No	Active	Inactive	Inactive

Justicidin A	394.37	2.29	0	Yes	Yes	Active	Active	Active
Demethylnobiletin	388.37	0.11	0	No	No	Active	Inactive	Active
Isorhamnetin	316.26	-0.31	0	No	No	Active	Inactive	Inactive
1,3,4,5-Tetra-*O*-galloylquinic acid	800.58	-2.08	3	No	Yes	Active	Inactive	Inactive
Eupatorin	344.32	0.17	0	No	No	Active	Inactive	Inactive
3,4-Di-*O*-galloylquinic acid	496.38	-1.75	2	No	No	Active	Inactive	Inactive
7,7-Dihydroxy-6,8-bicoumarin	322.27	1.81	0	No	Yes	Inactive	Inactive	Inactive
2,3-Dihydroxybenzoic acid	154.12	0.40	0	No	No	Active	Inactive	Inactive
Rothindin	444.39	-0.99	0	No	No	Inactive	Inactive	Inactive
Trifolirhizin-6-monoacetate	488.44	-0.05	1	No	No	Inactive	Inactive	Inactive
Cumanin	266.33	1.71	0	Yes	No	Inactive	Inactive	Inactive
Jamaicin	378.37	1.94	0	Yes	Yes	Active	Active	Active
Gancaonin X	338.40	2.95	0	Yes	Yes	Active	Inactive	Inactive
Hypericin	504.44	1.36	2	No	No	Active	Active	Active
Glucosyl passiflorate	696.87	0.88	3	No	Yes	Inactive	Inactive	Inactive
Lusitanicoside	442.46	-1.57	1	No	No	Active	Inactive	Inactive
Vouacapen-5-α-ol	302.45	3.77	0	Yes	No	Active	Inactive	Inactive
Didehydrovouacapen-5-α-ol	298.42	3.82	0	Yes	No	Active	Inactive	Inactive
6-β-cinnamoyl-7-β-hydroxyvouacapen-5-α-ol	464.59	3.47	0	No	No	Active	Inactive	Inactive
Pulcherrin A	464.59	3.47	0	No	No	Active	Inactive	Inactive
Pulcherrin B	438.56	4.43	0	No	Yes	Active	Inactive	Inactive
Pulcherrin J	448.59	4.30	1	No	No	Active	Inactive	Inactive
Pulcherrimin A	588.64	3.10	1	No	Yes	Active	Inactive	Inactive
Pulcherrimin B	570.63	3.81	1	No	Yes	Active	Inactive	Inactive
Pulcherrimin C	572.64	3.88	1	No	Yes	Active	Inactive	Inactive
Pulcherrimin E	680.68	3.43	1	No	Yes	Active	Inactive	Inactive
6-β-Hydroxyisovouacapenol C	334.45	2.04	0	Yes	Yes	Inactive	Inactive	Inactive
6-β-Cinnamoyl-7-β-acetoxyvouacapen-5-α-ol	506.63	3.78	1	No	Yes	Active	Inactive	Inactive
Pulcherrimin D	630.68	3.43	1	No	Yes	Active	Inactive	Inactive
Stigmast-5, 22-dien-3- *O*-β-D-glucopyranoside	544.81	5.29	2	No	No	Inactive	Inactive	Inactive
2, 3-Dihydroxylpropyl hexacosanoate	414.66	4.48	1	No	No	Inactive	Inactive	Inactive
Citrusinine-I	301.29	0.53	0	No	No	Inactive	Inactive	Inactive
Citracridone-I	353.37	1.39	0	No	No	Inactive	Inactive	Inactive
5-Hydroxynoracronycine	323.34	1.71	0	Yes	No	Inactive	Inactive	Inactive
Natsucitrine-I	301.29	0.53	0	No	No	Inactive	Inactive	Inactive
Glycofolinine	331.32	0.24	0	No	No	Inactive	Inactive	Inactive
Citracridone-III	339.34	1.17	0	No	No	Inactive	Inactive	Inactive
Lupeol	426.72	6.92	1	No	No	Active	Inactive	Inactive
Diosmetin	300.26	0.22	0	No	No	Active	Inactive	Inactive
Methylumbelliferyl glucuronide	352.29	-0.77	0	No	No	Inactive	Inactive	Inactive
Chlorogenic acid	354.31	-1.05	1	No	No	Inactive	Inactive	Inactive
4-Methylumbelliferone	176.17	1.34	0	Yes	No	Inactive	Inactive	Inactive
Scutellarin	462.36	-2.12	2	No	No	Active	Inactive	Inactive
Rhoifolin	578.52	-2.96	3	No	Yes	Inactive	Inactive	Inactive
7-Hydroxycoumarine	162.14	1.04	0	Yes	No	Inactive	Inactive	Inactive
Apigetrin	432.38	-1.61	1	No	No	Inactive	Inactive	Inactive
Apigenin	270.24	0.52	0	No	No	Active	Inactive	Active
Baicalin	446.36	-1.63	2	No	No	Active	Inactive	Inactive
Luteolin	286.24	-0.03	0	No	No	Active	Inactive	Inactive
Ingenol-3-angelate	430.53	2.06	0	No	Yes	Inactive	Inactive	Inactive

Methoxycinnamic acid	178.18	1.32	0	Yes	No	Active	Inactive	Inactive
Vernodalinol	378.37	0.63	0	No	No	Active	Active	Inactive
Mangiferin	422.34	-2.66	2	No	No	Inactive	Inactive	Inactive
1-Butanol, 3-methyl-, acetate	130.18	1.63	0	Yes	No	Inactive	Inactive	Inactive
Butane, 1,1-diethoxy-3-methyl-	160.25	2.02	0	Yes	No	Inactive	Inactive	Inactive
Propane, 1,1,3-triethoxy-	176.25	1.14	0	Yes	No	Inactive	Inactive	Inactive
Ethaneperoxoic acid, 1-cyano-1-(2-methylphenyl) ethyl ester	219.24	1.85	0	Yes	No	Inactive	Inactive	Inactive
1,4-Diamino-2-methoxyanthraquinone	268.27	0.36	0	No	No	Active	Active	Active
Phenol, 4,6-di (1,1-dimethylethyl)-2-methyl-	220.35	4.12	0	Yes	No	Active	Inactive	Inactive
Chlorazanil	221.65	1.05	0	No	No	Inactive	Active	Inactive
Isoheptadecanol	256.47	4.70	1	Yes	No	Inactive	Inactive	Inactive
cis-5-Dodecenoic acid, (3-cyanopropyl) dimethylsilyl ester	323.55	3.59	0	Yes	No	Inactive	Inactive	Inactive
Fumaric acid, 2-decyl undecyl ester	410.63	5.09	1	No	No	Inactive	Inactive	Inactive
Phthalic acid, hept-2-yl isohexyl ester	348.48	4.59	1	Yes	No	Inactive	Inactive	Inactive
Iriflophenone-3-C-β-D-glucoside	408.36	-2.28	1	No	Yes	Inactive	Inactive	Inactive
Iriflophenone-3-C-(2-*O*-p-hydroxybenzoyl)-β-D-glucoside	560.46	-2.86	3	No	No	Active	Inactive	Inactive
Iriflophenone-3-C-(2-*O*-galloyl)-β-D-glucoside	592.46	-3.79	3	No	No	Active	Inactive	Inactive
Quercetin-3-D-galactoside	464.38	-2.59	2	No	No	Inactive	Inactive	Inactive
Quercetin-3-β-D-glucoside	464.38	-2.59	2	No	No	Inactive	Inactive	Inactive
Quercetin-3-*O*-xyloside	434.35	-2.06	2	No	No	Inactive	Inactive	Inactive
Quercetin-3-*O*-α-L arabinopyranoside	434.35	-2.06	2	No	No	Inactive	Inactive	Inactive
Caffeic acid	180.16	0.70	0	No	No	Active	Inactive	Inactive
3,4-Dicaffeoyl quinic acid	516.45	-0.35	3	No	Yes	Active	Inactive	Inactive
4,5-Dicaffeoyl quinic acid	516.45	-0.35	3	No	Yes	Active	Inactive	Inactive
Catechin	290.27	0.24	0	No	Yes	Inactive	Inactive	Inactive
Quercetin	302.24	-0.56	0	No	No	Active	Inactive	Inactive

Compounds with red font were selected to be used for the *in silico* analysis due to their fit based on the parameter used. MW: molecular weight; LP: lipophilicity (MLogP); LVN: Lipinski number of violations; BBP: blood-brain barrier permeant; PgpS: P-glycoprotein substrate; Inb: inhibitor.

Table S3. Docking score and MM-GBSA binding free energy of all 50 screened compounds against BRCA1 (4Y2G), BRCA2 (3EU7), and CDK-1 (4Y72).

Compound	**BRCA1**		**BRCA2**		**CDK-1**	
	Docking score	**MM-GBSA**	**Docking score**	**MM-GBSA**	**Docking score**	**MM-GBSA**
Gallic acid	N/A	N/A	-6.01	-9.90	-6.62	-26.08
Mono-galloyl glucoside	N/A	N/A	-10.76	-54.63	-11.88	-40.83
Hydroxybenzoic acid hexoside	N/A	N/A	-8.58	-33.03	-9.18	-15.40
Acetyl guanacone	-2.02	-36.41	-5.42	-47.58	-6.59	-31.17
Triethylammoniumyl-acetate monohydrate	N/A	N/A	-4.33	-18.68	-1.75	-16.69
Tryptophan	N/A	N/A	-7.02	-23.24	-5.48	-24.91
Vitexin	N/A	N/A	-10.00	-47.38	-12.23	-55.94
(+)-Gallocatechin	N/A	N/A	-7.69	-38.01	-9.95	-48.53
(-)-Epicatechin	-3.38	-10.32	-8.20	-37.31	-9.03	-38.65

(-)-Epigallocatechin	N/A	N/A	-7.69	-38.01	-9.95	-48.53
(-)-Epicatechin gallate	N/A	N/A	-11.30	-58.65	-10.73	-45.53
Caffeine	N/A	N/A	-3.53	-20.22	-4.48	-29.32
Cadalene	-2.35	-28.29	-3.91	-29.83	-6.27	-31.47
Oleanolic acid	-2.09	-20.52	-3.59	-2.56	-3.58	-23.45
Guajadial C	-2.89	-18.07	-5.01	-10.53	-3.64	-23.45
Guajadial D	-2.72	-23.74	-4.96	-4.34	-3.37	9.61
Guajadial E	-2.47	-16.82	-5.18	-14.97	-3.49	-7.18
Guajadial F	-1.46	-18.89	-4.88	-12.61	-3.55	37.18
Phloionolic acid	-4.65	-40.47	-7.74	-28.19	-8.73	-28.64
Tetracosatetraenoic acid n-6	-2.02	-25.00	-2.04	-26.17	-5.24	-34.90
Amorphaquinone	N/A	N/A	-5.57	-39.30	-6.77	-23.47
Syringin	-5.99	-37.62	-9.52	-34.50	-11.11	-38.49
Isoderrone	-2.11	-24.27	-3.94	-30.22	-6.73	-35.74
Alpinumisoflavone	N/A	N/A	-4.31	-15.77	-6.20	-32.69
3-Hydroxy-1-phenyl-1-eicosanone	-0.42	-35.04	-5.10	-28.14	-6.80	-50.52
Calabaxanthone	N/A	N/A	-0.24	-22.74	-6.36	-32.36
Isorhamnetin	N/A	N/A	-6.77	-43.15	-8.90	-36.13
Eupatorin	N/A	N/A	-4.96	-29.43	-7.18	-32.52
7,7-Dihydroxy-6,8-bicoumarin	N/A	N/A	-5.70	-14.51	-6.80	-33.64
2,3-Dihydroxybenzoic acid	-3.44	-18.73	-4.55	-11.53	-6.61	-13.39
Rothindin	-2.42	-28.71	-7.65	-53.01	-9.14	-32.88
Trifolirhizin-6-monoacetate	-2.63	-27.79	-7.91	-30.97	-7.94	-47.23
6-β-cinnamoyl-7-β-hydroxyvouacapen-5-α-ol	-2.14	-24.97	-6.94	-32.73	-4.26	-33.91
Pulcherrin A	-3.15	-26.77	-5.33	-37.82	-5.58	-19.76
2,3-Dihydroxylpropyl hexacosanoate	-1.74	-28.87	-4.09	-43.56	-5.62	-41.39
Citrusinine-I	N/A	N/A	-4.15	-23.65	-7.03	-9.29
Citracridone-I	N/A	N/A	-4.93	-3.80	-6.32	-32.19
Natsucitrine-I	N/A	N/A	-3.98	-7.54	-5.20	-6.91
Glycofolinine	N/A	N/A	-5.06	-22.15	-6.49	-28.90
Citracridone-III	N/A	N/A	-5.51	10.74	-6.69	-35.48
Diosmetin	N/A	N/A	-7.11	-46.96	-7.78	-36.62
4-Methylumbelliferyl glucuronide	-2.46	-24.47	-7.99	-31.79	-9.93	-45.48
Chlorogenic acid	N/A	N/A	-9.38	-32.49	-8.92	-28.90
Apigetrin	-5.76	-30.19	-9.80	-41.34	-11.26	-56.98
Luteolin	N/A	N/A	-7.18	-43.68	-8.34	-39.41
Ingenol-3-angelate	-4.01	-33.97	-6.38	-32.58	-7.95	13.42
Chlorazanil	N/A	N/A	-4.74	-24.87	-6.40	-37.58
Fumaric acid, 2-decyl undecyl ester	-0.07	-41.12	-3.03	-39.75	-4.58	-29.75
Caffeic acid	-2.37	-16.83	-5.42	-25.04	-6.81	-27.02
Catechin	-3.46	-10.42	-8.27	-37.33	-9.14	-44.55
Quercetin	N/A	N/A	-7.90	-45.49	-8.98	-42.77

Table S4. Docking score and MM-GBSA binding free energy of all 50 screened compounds against CDK-2 (2XMY), ERK5 (5O7I), and estrogen receptor-alpha (1G5O).

Compound	CDK-2		ERK5		ERα	
	Docking score	MM-GBSA	Docking score	MM-GBSA	Docking score	MM-GBSA
Gallic acid	-5.65	-4.05	-7.26	-17.70	-5.84	-24.84
Mono-galloyl glucoside	-9.75	-47.01	-10.42	-50.80	-9.38	-30.39
Hydroxybenzoic acid hexoside	-9.03	-16.91	-8.80	-34.29	-7.95	-18.61
Acetyl guanacone	-6.59	-25.02	-6.51	-49.86	N/A	N/A
Triethylammoniumyl-acetate monohydrate	0.53	-17.19	0.80	-21.11	-2.59	-31.57
Tryptophan	-5.91	-22.22	-6.37	-31.97	-7.85	-30.44
Vitexin	-10.24	-32.20	-11.83	-54.90	N/A	N/A
(+)-Gallocatechin	-8.98	-39.69	-9.14	-46.77	-10.18	-32.90
(-)-Epicatechin	-7.83	-43.96	-8.40	-40.70	-10.48	-39.94
(-)-Epigallocatechin	-8.98	-39.69	-9.14	-46.77	-10.18	-32.90
(-)-Epicatechin gallate	-10.21	-53.61	-10.62	-65.98	N/A	N/A
Caffeine	-3.57	-24.67	-4.37	-31.60	-4.69	-32.79
Cadalene	-4.51	-21.98	-4.25	-29.39	-8.10	-32.88
Oleanolic acid	-3.94	-21.73	-4.65	-14.27	N/A	N/A
Guajadial C	-3.53	-10.43	-5.37	-20.97	N/A	N/A
Guajadial D	-3.40	12.11	-5.38	-20.85	N/A	N/A
Guajadial E	-3.56	-5.37	-5.47	-27.78	N/A	N/A
Guajadial F	-3.75	-16.89	-5.91	-27.78	N/A	N/A
Phloionolic acid	-6.94	-22.00	-8.43	-46.61	-8.15	23.25
Tetracosatetraenoic acid n-6	-4.24	-25.36	-3.89	-35.57	N/A	N/A
Amorphaquinone	-5.12	-39.72	-7.27	-45.80	N/A	N/A
Syringin	-8.36	-37.72	-8.53	-51.83	-8.16	6.31
Isoderrone	-5.41	-23.90	-5.56	-46.41	N/A	N/A
Alpinumisoflavone	-7.35	-34.29	-5.84	-38.30	N/A	N/A
3-Hydroxy-1-phenyl-1-eicosanone	-4.97	-38.83	-5.31	-47.55	N/A	N/A
Calabaxanthone	-5.24	-28.74	-4.51	-44.96	N/A	N/A
Isorhamnetin	-7.15	-30.70	-8.95	-37.95	N/A	N/A
Eupatorin	-6.58	-32.68	-6.81	-36.92	N/A	N/A
7,7-Dihydroxy-6,8-bicoumarin	-4.51	-0.41	-6.31	-45.26	N/A	N/A
2,3-Dihydroxybenzoic acid	-5.12	-11.68	-5.63	-22.70	-5.48	-16.51
Rothindin	-7.98	-40.94	-8.42	-45.63	N/A	N/A
Trifolirhizin-6-monoacetate	-7.62	-45.69	-8.09	-58.59	N/A	N/A
6-β-cinnamoyl-7-β-hydroxyvouacapen-5-α-ol	-4.42	-31.03	-5.03	-32.70	N/A	N/A
Pulcherrin A	-5.58	-34.40	-5.88	-41.54	N/A	N/A
2,3-Dihydroxylpropyl hexacosanoate	-1.65	-31.07	-5.73	-58.43	N/A	N/A
Citrusinine-I	-5.19	-21.72	-5.49	-37.43	-6.14	2.26
Citracridone-I	-4.12	-16.22	-5.21	-25.96	N/A	N/A
Natsucitrine-I	-5.16	17.29	-5.58	-16.97	-2.89	12.49
Glycofolinine	-4.99	29.54	-5.13	-17.91	N/A	N/A
Citracridone-III	-4.82	-3.96	-5.62	-11.69	N/A	N/A

Diosmetin	-7.01	-31.32	-7.18	-39.33	-6.70	0.01
4-Methylumbelliferyl glucuronide	-6.83	-24.18	-8.69	-31.44	-2.59	42.00
Chlorogenic acid	-8.26	-31.95	-8.69	-31.44	-7.73	34.16
Apigetrin	-10.76	-40.42	-11.23	-45.40	N/A	N/A
Luteolin	-7.42	-37.78	-8.76	-41.87	-7.97	-19.68
Ingenol-3-angelate	-5.55	-29.33	-6.27	-33.65	N/A	N/A
Chlorazanil	-5.31	-28.93	-4.77	-26.38	-5.96	-37.38
Fumaric acid, 2-decyl undecyl ester	0.14	-19.10	-3.18	-45.51	N/A	N/A
Caffeic acid	-5.43	-15.78	-6.32	-27.44	-6.47	-27.49
Catechin	-8.20	-36.72	-8.33	-40.80	-10.41	-40.00
Quercetin	-7.88	-38.97	-8.93	-34.24	-0.71	22.99

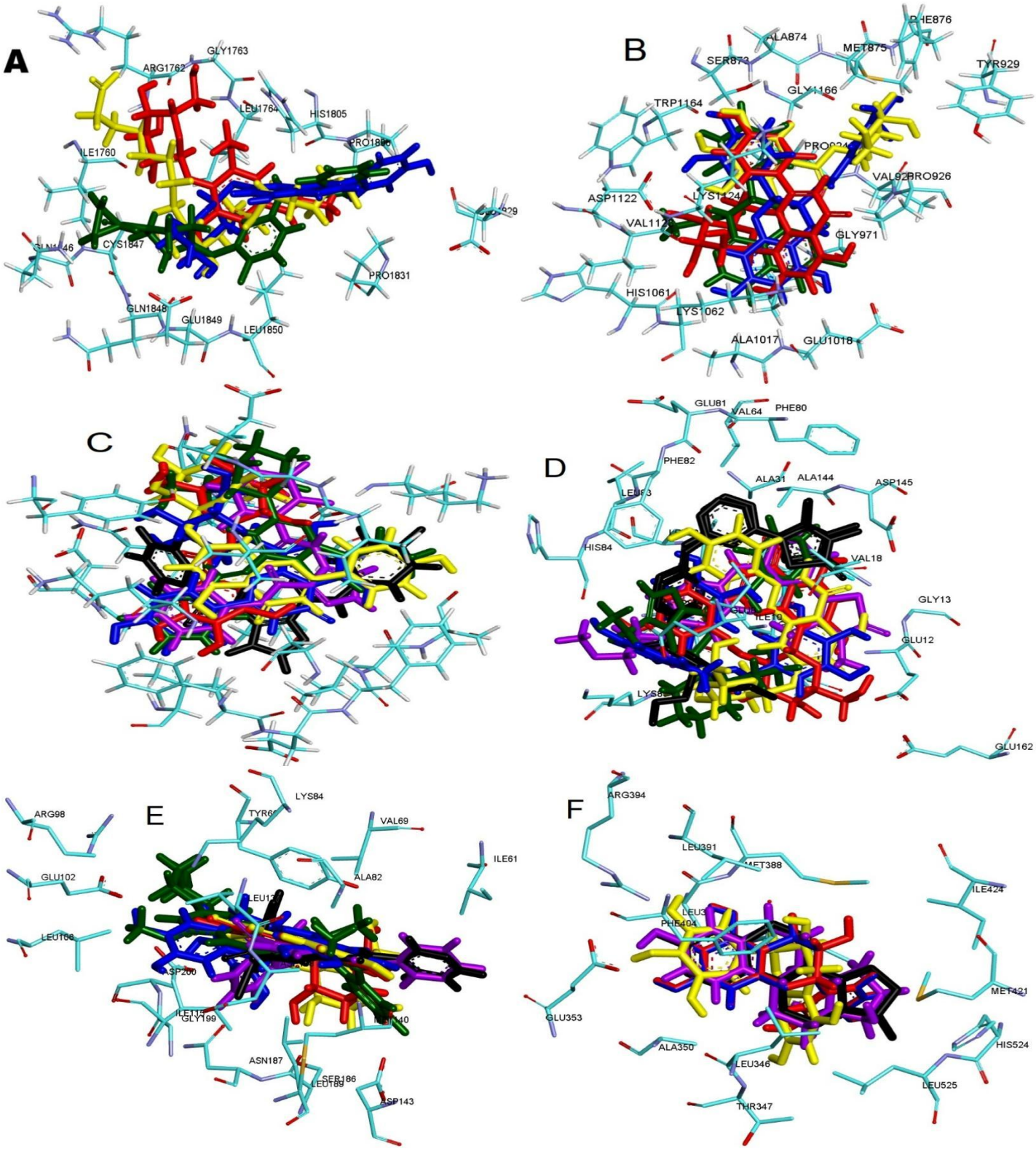

Fig. S1. Superimposed docked poses of the top-ranked compounds for each target on their native co-crystallised ligand (black), used for docking-protocol validation: (A) BRCA1, (B) BRCA2, (C) CDK-1, (D) CDK-2, (E) ERK5, (F) estrogen receptor-alpha. All compounds and standard drugs superimposed with RMSD ≤ 2.0 Å (colour code in Table S3). All top-ranked compounds and standard drugs superimposed with the native/redocked co-crystallised ligand (CCL) with RMSD ≤ 2.0 Å (CDK-1: 1.57 Å; CDK-2: 1.89 Å; ERK5: 0.414 Å; estrogen receptor-alpha: 0.197 Å). BRCA1 and BRCA2 have no native co-crystallised ligand; validation for these two targets used binding-site residue conservation.

Table S5. Colour-code key for compounds shown in the docking-validation superimposition figure (Fig. S1).

Compound	BRCA1	BRCA2	CDK-1	CDK-2	ERK5	Estrogen Receptor
Syringin	Red	N/A	N/A	N/A	N/A	N/A
Apigetrin	Blue	N/A	Yellow	Yellow	Yellow	N/A
Phloionolic acid	Yellow	N/A	N/A	N/A	N/A	N/A
Vitexin	N/A	Red	Blue	Red	Red	N/A
(-)-Epicatechin gallate	N/A	Blue	N/A	Blue	Blue	N/A
Mono-galloyl glucoside	N/A	Yellow	Red	N/A	N/A	N/A
Catechin	N/A	N/A	N/A	N/A	N/A	Red
(-)-Epicatechin	N/A	N/A	N/A	N/A	N/A	Blue
(+)-Gallocatechin	N/A	N/A	N/A	N/A	N/A	Yellow
Olaparib (standard drug)	Green	N/A	N/A	N/A	N/A	N/A
Talazoparib (standard drug)	N/A	Green	N/A	N/A	N/A	N/A
Dinaciclib (standard drug)	N/A	N/A	Green	Green	N/A	N/A
JWG-045 (standard drug)	N/A	N/A	N/A	N/A	Green	N/A
Native ligand (CCL)	N/A	N/A	Black	Black	Black	Black
Redocked CCL	N/A	N/A	Purple	Purple	Purple	Purple

Molecular Surface Representations

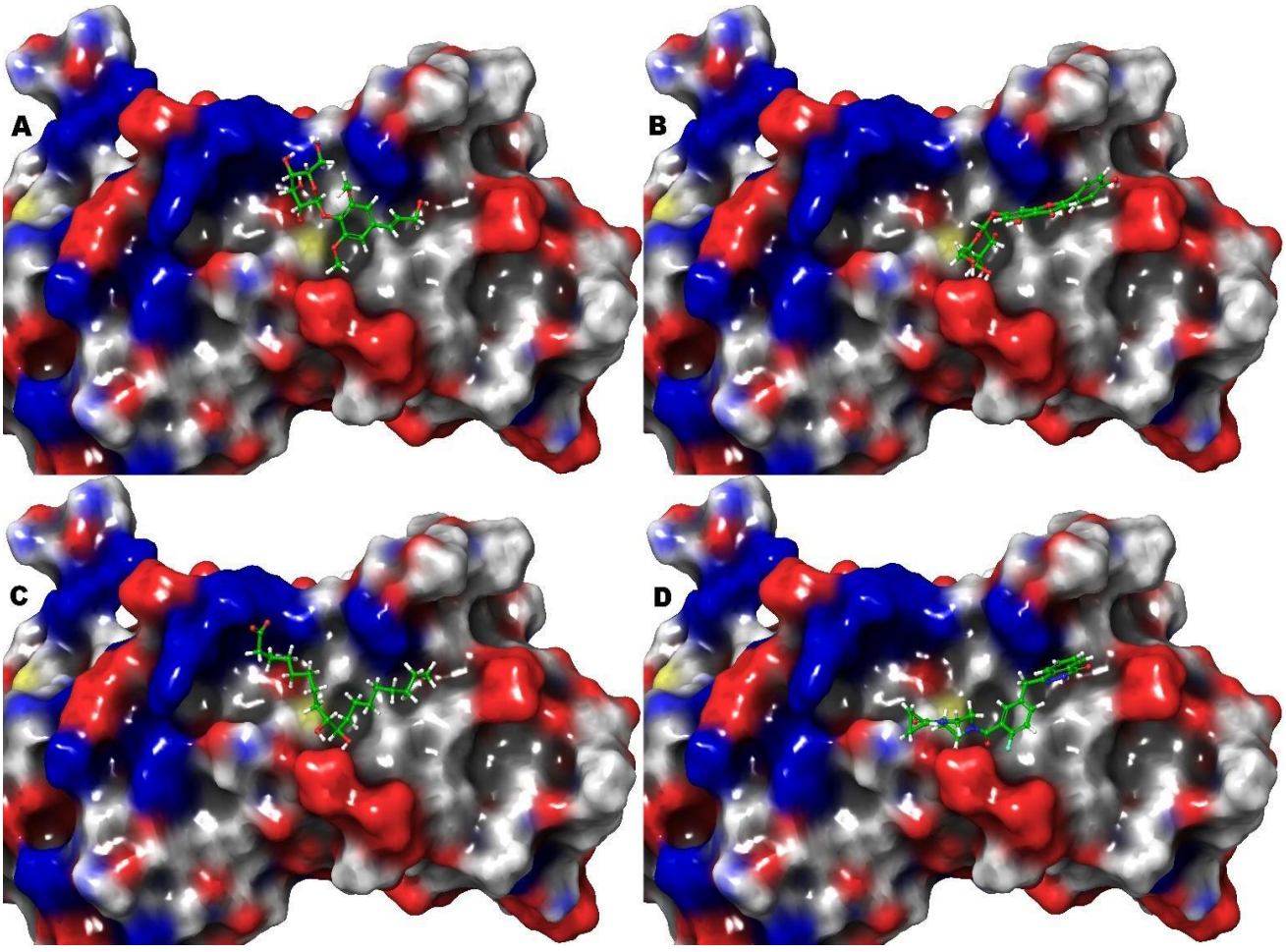

Fig. S2. Molecular surface representations (coloured by residue charge) of (A) syringin, (B) apigetrin, (C) phloionolic acid, and (D) olaparib (standard drug) at the binding pocket of BRCA1 (4Y2G). Red = negatively charged residues; blue = positively charged residues; white/grey = hydrophobic/neutral residues; yellow = sulfur residues.

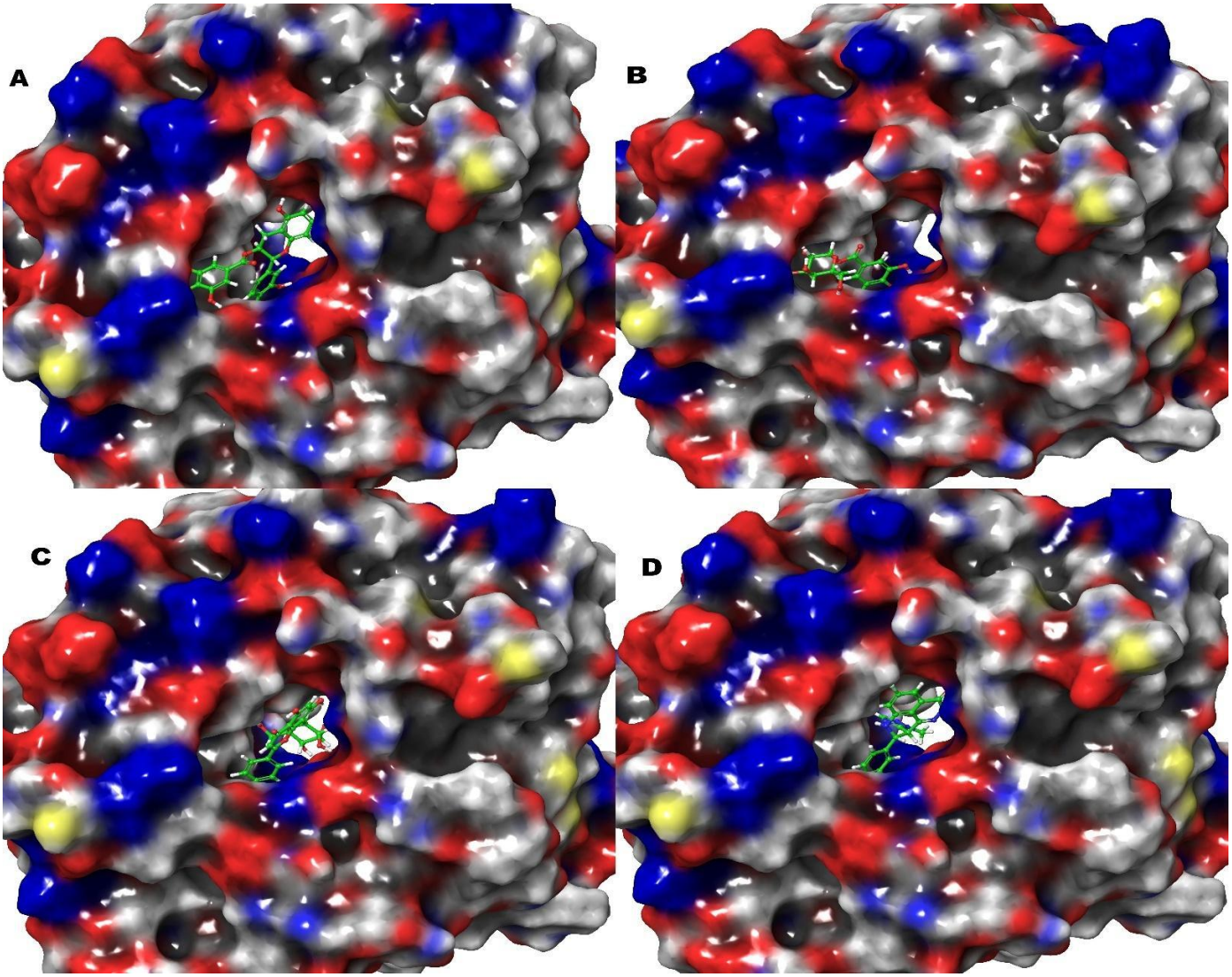

Fig. S3. Molecular surface representations (coloured by residue charge) of (A) (-)-epicatechin gallate, (B) mono-galloyl glucoside, (C) vitexin, and (D) talazoparib (standard drug) at the binding pocket of BRCA2 (3EU7). Red = negatively charged residues; blue = positively charged residues; white/grey = hydrophobic/neutral residues; yellow = sulfur residues.

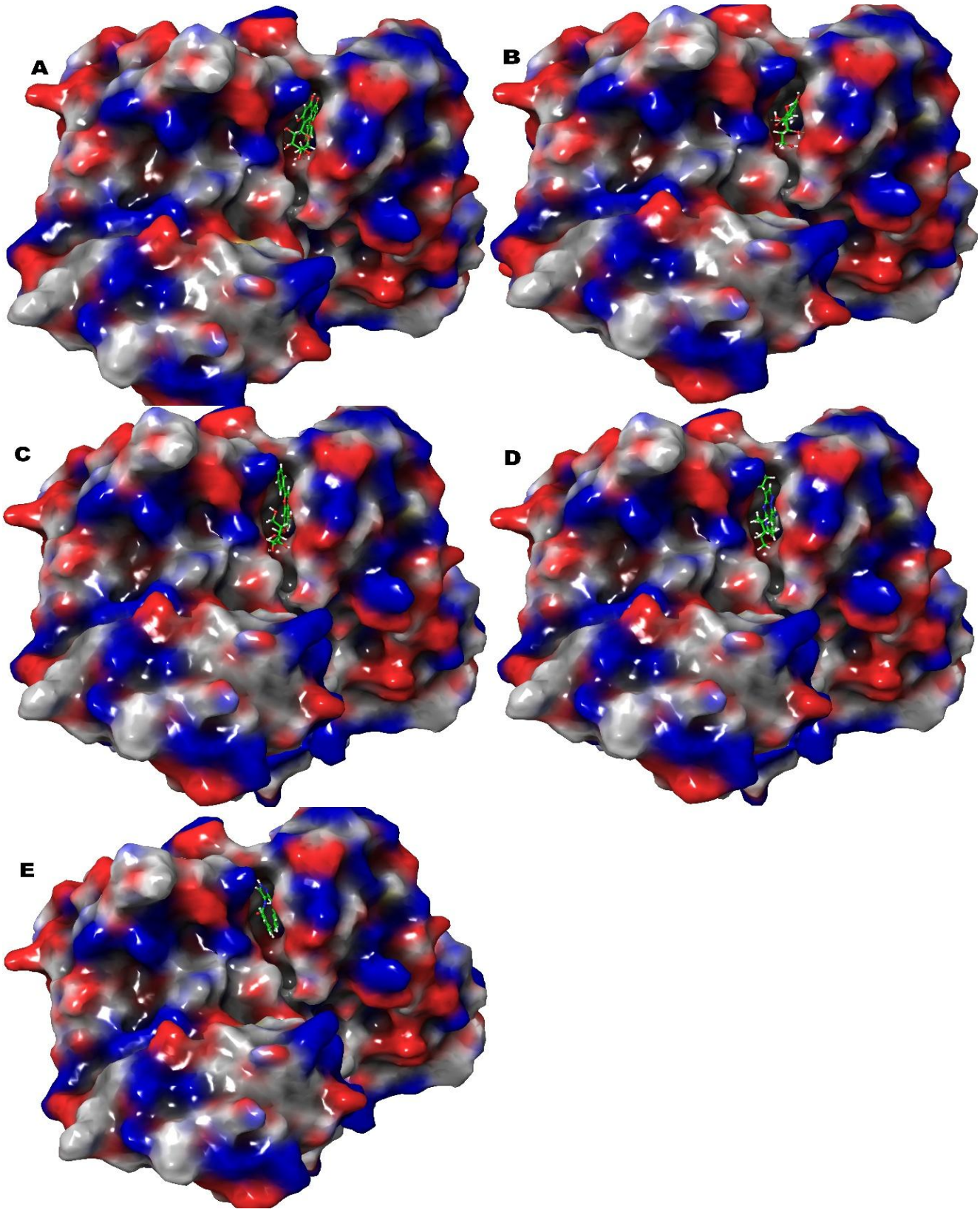

Fig. S4. Molecular surface representations (coloured by residue charge) of (A) vitexin, (B) mono-galloyl glucoside, (C) apigetrin, (D) dinaciclib (standard drug), and (E) the pyrazole-3-carboxamide co-crystallised ligand (CCL) at the binding pocket of CDK-1 (4Y72). Red = negatively charged residues; blue = positively charged residues; white/grey = hydrophobic/neutral residues.

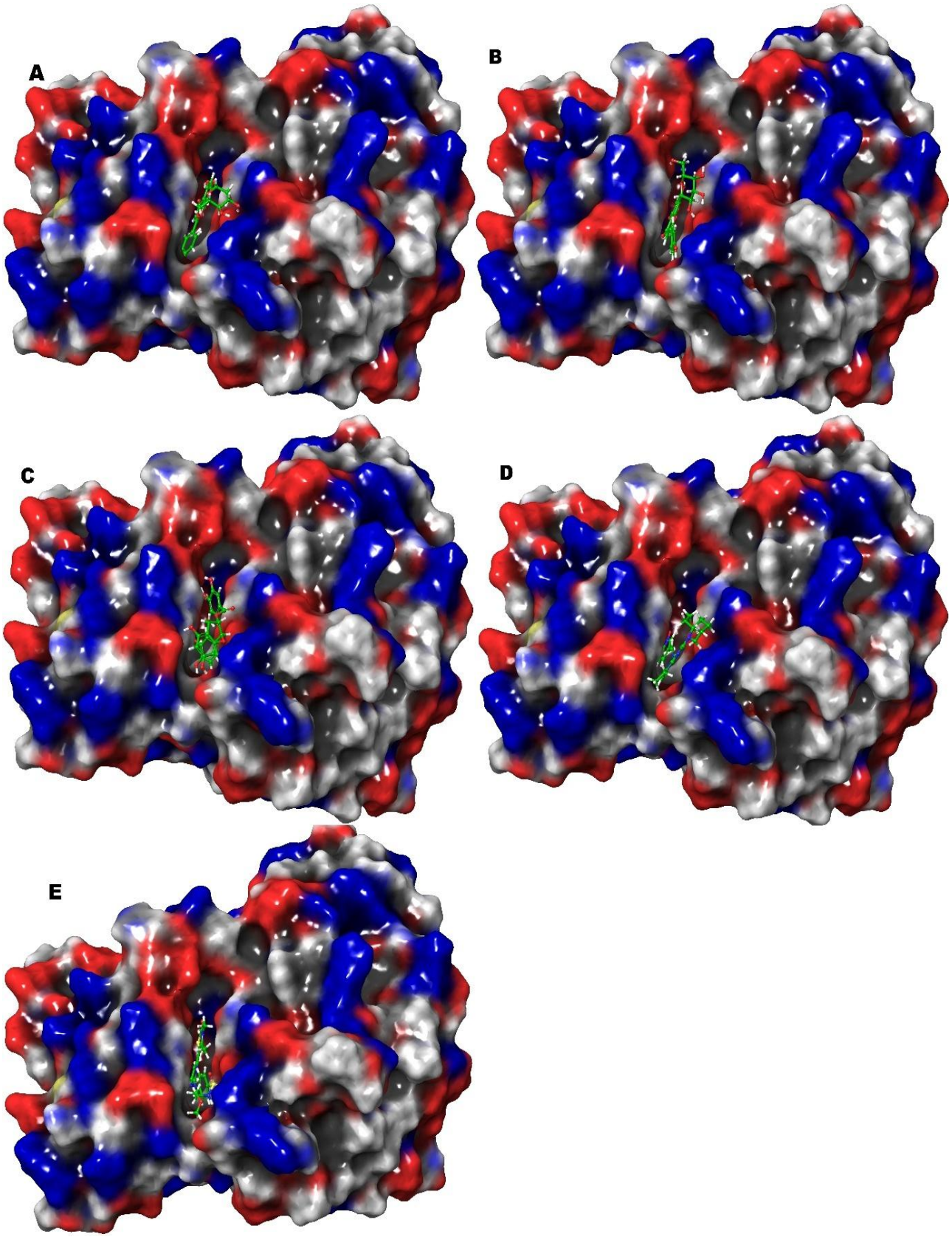

Fig. S5. Molecular surface representations (coloured by residue charge) of (A) apigetrin, (B) vitexin, (C) (-)-epicatechin gallate, (D) dinaciclib (standard drug), and (E) CDK inhibitor 11 (CCL) at the binding pocket of CDK-2 (2XMY). Red = negatively charged residues; blue = positively charged residues; white/grey = hydrophobic/neutral residues

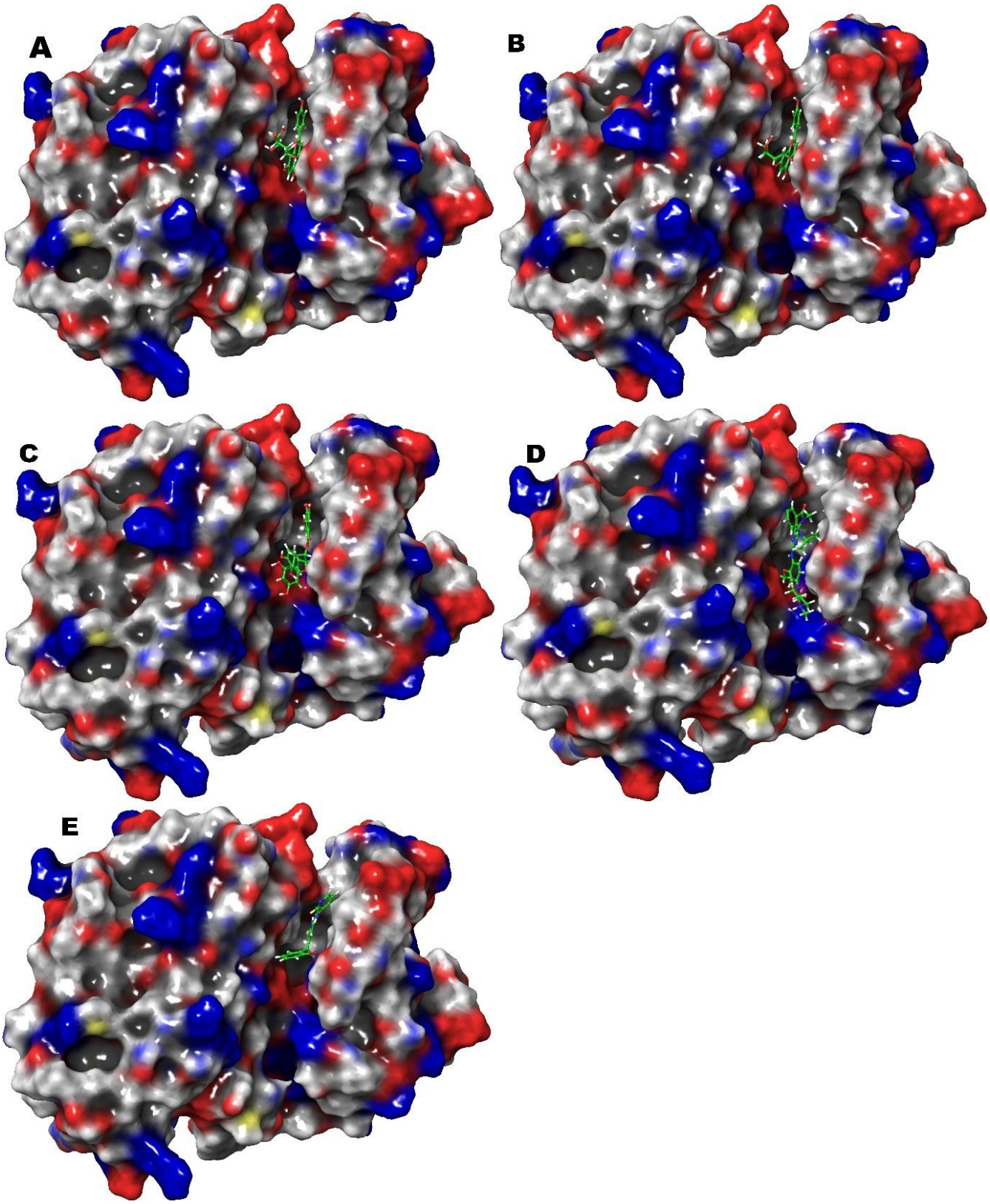

Fig. S6. Molecular surface representations (coloured by residue charge) of (A) vitexin, (B) apigetrin, (C) (-)-epicatechin gallate, (D) JWG-045 (standard drug), and (E) the pyrrole-based co-crystallised ligand (CCL) at the binding pocket of ERK5 (5O7I). Red = negatively charged residues; blue = positively charged residues; white/grey = hydrophobic/neutral residues; yellow = sulfur residues.

No corresponding molecular surface figure was generated for estrogen receptor-alpha, as its active site lies at the protein core and is not accessible for surface visualisation (see main text, Section 3.3.6).

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