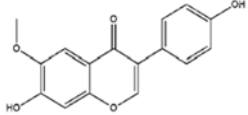
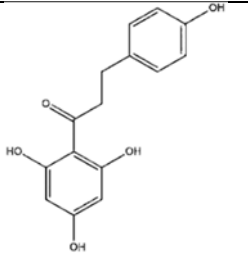
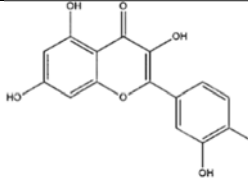
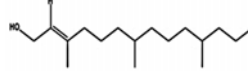
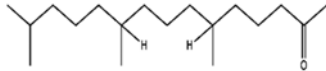
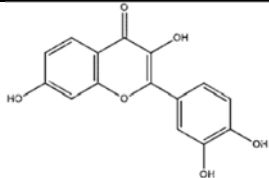
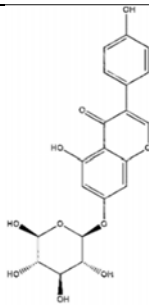
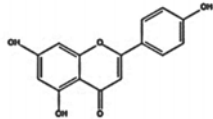
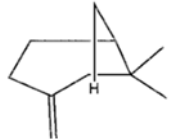
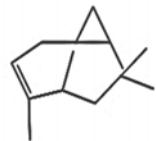
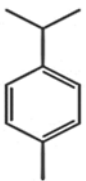
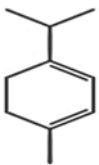
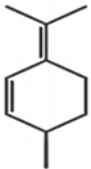


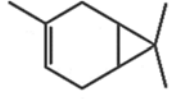
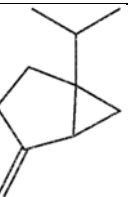


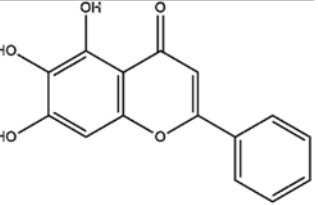
Supporting information

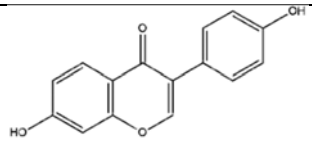
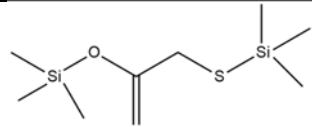
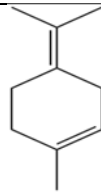
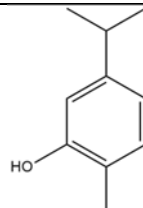
S1 Table. Docking results of 31 selected compounds against SdiA receptor protein of *K. pneumoniae* (PDB: 4LFU)

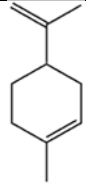
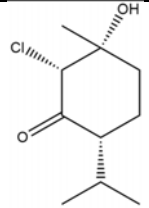
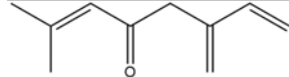
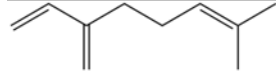
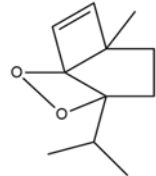
Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction
Glycitein		Flavonoids	C ₁₆ H ₁₂ O ₅	284.26	-9.752	Ala110, Trp95, Leu115, Tyr63, Cys45, Tyr71, Leu83, Val82, Pro81, Leu106, Trp107, Phe100
Phloretin		Flavonoids	C ₁₅ H ₁₄ O ₅	274.27	-9.722	Leu115, Leu106, Ala109, Ala110, Tyr63, Phe76, Leu77, Phe59, Val57, Leu83, Cys45, Tyr71, Tyr70, Val68, Trp67
Quercetin		Flavonoids	C ₁₅ H ₁₀ O ₇	302,236	-9.290	Ala109, Ala110, Leu106, Phe76, Trp67, Val68, Tyr70, Tyr71, Phe59, Tyr63, Cys45
3,7,11,15-Tetramethyl-2-hexadecen-1-OL (phytol)		Terpenes	C ₁₀ H ₁₆	296.5	-9.205	Leu115, Ala110, Ala109, Leu106, Tyr63, Phe59, Ala58, Val57, Cys45, Leu77, Leu83, Phe76, Tyr71, Tyr70, Val68, Trp67

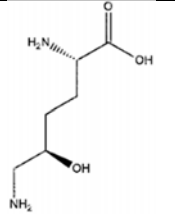
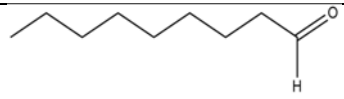

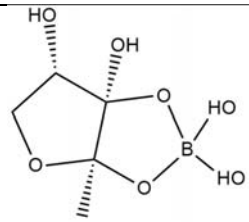
6,10,14-Trimethylpentadecan-2-one		sesquiterpenoids	C ₁₈ H ₃₆ O	268.5	-8.977	Trp67, Val68, Tyr70, Tyr71, Tyr63, Phe59, Val57, Cys45, Leu106, Ala109, Leu83, Leu77, Ala110, Phe76, Leu115
Fisetin		Flavonoids	C ₁₅ H ₁₀ O ₆	286.24	-8.364	Ala110, Trp107, Leu106, Phe100, Leu115, Trp95, Tyr63, Tyr71, Leu83, Val82, Pro81, Phe100, Leu106, Trp107
Genistin		Flavonoids	C ₂₁ H ₂₀ O ₁₀	432.4	-8.337	Phe100, Trp95, Met94, Ala100, Val82, Trp107, Leu106, Tyr63, Tyr71, Leu115
Apigenin		Flavonoids	C ₁₅ H ₁₀ O ₅	270,0528	-8.222	Ala110, Ala109, Leu106, Phe76, Tyr63, Phe59, Cys45, Tyr71, Tyr70, Val68, Trp67
Beta-pinene		Terpenes	C ₁₀ H ₁₆	136,23	-7.473	Leu115, Ala110, Ala109, Leu106, Phe76, Tyr63, Tyr71, Tyr70, Val68, Trp67

Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction
Alpha-pinene		Terpenes	C ₁₀ H ₁₆	136,23	-7.343	Ala109, Ala110, Leu106, Phe76, Tyr63, Tyr71, Tyr70, Val68, Trp67, Leu115
P-cymene		Terpenes	C ₁₀ H ₁₄	134,22	-7.277	Ala110, Ala109, Leu106, Tyr71, Tyr70, Val68, Trp67, Tyr63, Phe76, Trp95, Leu115
Alpha-terpinene		Terpenes	C ₁₀ H ₁₆	136.23	-7.245	Leu115, Ala110, Ala109, Leu106, Tyr71, Tyr70, Phe76, Val68, Trp67, Tyr63, Trp95
Isoterpinolene		Terpenes	C ₁₀ H ₁₆	136.23	-7.235	Tyr71, Tyr70, Val68, Trp67, Ala110, Ala109, Phe76, Leu106, Leu115, Tyr63
Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction

3-Carene		Terpenes	C ₁₀ H ₁₆	136.23	-7.226	Ala110, Ala109, Leu106, Phe76, Tyr71, Tyr70, Val68, Trp67, Tyr63, Leu115
Sabinene		Terpenes	C ₁₀ H ₁₆	136.23	-7.209	Leu115, Ala110, Ala109, Trp67, Val68, Leu106, Tyr70, Tyr71, Phe76, Tyr63
Octadecane		Alkanes	C ₁₈ H ₃₈	254.494	-7.179	Leu77, Phe76, Leu106, Ala109, Ala110, Leu115, Leu77, Phe76, Trp67, Val68, Tyr70, Tyr71, Tyr63, Phe59, Val57, Cys45, Leu83
Camphene		Terpenes	C ₁₀ H ₁₆	136.24	-7.039	Ala110, Ala109, Leu106, Tyr71, Tyr70, Val68, Trp67, Phe76, Leu115, Tyr63
Baicalein		Flavonoids	C ₁₅ H ₁₀ O ₅	270.24	-6.996	Ala110, Phe100, Trp107, Leu106, Val82, Trp95, Tyr63, Leu115

Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction
Daidzein		Flavonoids	C ₁₅ H ₁₀ O ₄	254.24	-6.969	Leu115, Ala110, Trp95, Trp107, Leu106, Phe100, Val82, Leu83, Cys45, Tyr71, Tyr63
Acetic acid, [(trimethylsilyl)thio]-, trimethylsilyl ester		Carboxylic acid	C ₈ H ₂₀ O ₂ SSi ₂	132.233	-6.896	Ala110, Ala109, Leu106, Phe76, Leu77, Leu83, Phe59, Tyr63, Tyr71, Cys45, Tyr70, Val68, Trp67, Leu115
Terpinolene		Terpenes	C ₁₀ H ₁₆	136,23	-6.812	Ala110, Ala109, Leu106, Phe76, Leu115, Trp67, Val68, Tyr70, Tyr71, Tyr63
Carvacrol		Terpenes	C ₁₀ H ₁₄ O	150.22	-6.633	Phe76, Ala110, Ala109, Leu106, Trp67, Val68, Tyr70, Tyr71, Tyr63, Leu115
Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction

Limonene		Terpenes	C ₁₀ H ₁₆	136.23	-6.633	Tyr63, Ala110, Ala109, Leu106, Phe76, Tyr71, Tyr70, Val68, Trp67
Longifone		Terpenes	C ₁₀ H ₁₇ ClO ₂	204.69	-6.301	Phe76, Ala110, Ala109, Leu106, Trp67, Val68, Tyr70, Tyr71, Trp95, Tyr63, Leu115
Ipsdienone		Terpenes	C ₁₀ H ₁₄ O	150.22	-6.237	Leu106, Ala109, Ala110, Phe76, Leu115, Tyr71, Tyr70, Val68, Trp67, Pro64, Tyr63
Myrcene		Terpenes	C ₁₀ H ₁₆	136,23	-5.768	Leu115, Tyr63, Pro64, Trp67, Val68, Tyr70, Tyr71, Phe76, Leu106, Ala110, Ala109
Ascaridole		Terpenes	C ₁₀ H ₁₆ O ₂	168.23	-5.385	Trp95, Trp67, Val68, Tyr70, Tyr71, Leu115, Ala110, Ala109, Leu106, Tyr63
Compound name	Chemical structure	Class	Molecular formula	Molecular weight (g/mol)	Docking score (Kcal/mol)	Hydrophobic interaction

5-Hydroxylysine		L-alpha amino acid	$C_6H_{14}N_2O_3$	162,187	-5.098	Leu115, Ala110, Tyr63, Phe59, Leu83, Cys45, Tyr71, Val68, Trp67, Phe76, Leu106
Nonanal		Aldehydes	$C_9H_{18}O$	142,2386	-4.879	Leu106, Ala109, Ala110, Leu115, Trp67, Val68, Phe76, Tyr70, Tyr71, Phe59, Tyr63
1-Octanol		Fatty alcohols	$C_8H_{18}O$ or $CH_3(CH_2)_6CH_2OH$	130,23	-4.676	Tyr71, Tyr70, Trp67, Trp95, Tyr63, Trp67, Leu115, Ala110, Ala109, Leu106, Phe76
Reference compound						
Furanosylborate diester (AI-2 molecule)		Borates	$C_5H_{10}BO_7$	192.940	-6.081	Leu115, Ala110, Trp107, Leu106, Phe100, Trp95

S2 Table. MM/GBSA-based binding free energy profile of SdiA bonded terpenes and flavonoids

S/N	Terpenes	Energy components (kcal/mol)					Flavonoids	Energy components (kcal/mol)				
		ΔE_{vdw}	ΔE_{ele}	ΔG_{gas}	ΔG_{sol}	ΔG_{bind}		ΔE_{vdw}	ΔE_{ele}	ΔG_{gas}	ΔG_{sol}	ΔG_{bind}
1	P-cymene	-24.7764	0.6310	-24.1454	5.7552	-18.3902	Fisetin	-23.8535	-22.5346	-46.3881	24.1463	-22.2418
2	3,7,11,15-Tetramethyl-2-hexadecen-1-OL (phytol)	-48.8645	-4.6792	-53.5437	10.2756	-43.2680	Genistin	-24.8153	-34.2254	-59.0407	36.5112	-22.5295
3	Alpha-pinene	-24.8209	0.0145	-24.8064	4.4408	-20.3656	Diadzein	-28.5005	-14.3454	-42.8459	18.0030	-24.8429
4	Terpinene	-25.1307	0.5571	-24.5736	4.5242	-20.0495	Quercetin	-42.3552	-12.2763	-54.6315	22.4873	-32.1442
5	3 - Carene	-23.7216	-1.0117	-24.7333	4.8996	-19.8336	Glycitein	-31.2432	-19.8918	-51.1351	24.2802	-26.8549
6	Camphene	-22.5031	-22.5031	-22.9386	4.7237	-18.2148	Phloretin	-37.0394	-21.3957	-58.4350	26.5341	-31.9010
7	Sabinene	-6.6711	-0.0279	-6.6990	1.8893	-4.8097	Apigenin	-22.7803	-11.3078	-34.0881	15.0348	-19.0533
8	Beta-pinene	-13.1169	-0.3701	-13.4871	3.1648	-10.3223	Biacalein	-30.0588	-33.4847	-63.5436	29.2440	-34.2996
9	Isoterpinolene	-24.5669	-0.2579	-24.8248	5.1453	-19.6795						

All energies are in kcal/mol.

ΔE_{ele} = electrostatic energy; ΔE_{vdw} = van der Waals energy; ΔG_{bind} = total binding free energy; ΔG_{sol} = solvation free energy ΔG = gas phase free energy

S3 Table. Water Solubility

Compounds	Log S (ESOL)	Solubility (mg/mL)	class	Log S (Ali)	Solubility (mg/mL)	Class	Log S (SILICOS-IT)	Solubility (mg/mL)	class
3,7,11,15-Tetramethyl-2-hexadecen-1-OL(Phytol)	-5.98	3.10e-04	Moderately soluble	-8.47	9.94e-07	Poorly soluble	-5.51	9.06e-04	Moderately soluble
Beta-pinene	-3.31	6.74e ⁻⁰²	soluble	-3.87	1.85e ⁻⁰²	Soluble	-2.48	4.55e-01	soluble
Alpha-pinene	-3.51	4.24e-02	soluble	-4.20	8.59e-03	Moderately soluble	-2.23	8.06e-01	soluble
P-cymene	-3.63	3.12e-02	soluble	-3.81	2.10e-02	Soluble	-3.57	3.58e-02	soluble
Alpha-terpinene	-3.30	6.89e-02	soluble	-3.96	1.49e-02	Soluble	-2.23	8.06e-01	soluble
Isoterpinolene	-2.90	1.73e-01	soluble	-3.19	8.72e-02	Soluble	-2.01	1.33e+00	soluble
3-Carene	-3.44	4.90e-02	soluble	-4.10	1.09e-02	Moderately soluble	-2.33	8.06e-01	soluble
Sabinene	-2.57	3.71e-01	soluble	-2.76	2.38e-01	Soluble	-2.48	2.38e-01	soluble
Camphene	-3.34	6.18e-02	soluble	-3.93	1.60e-02	Soluble	-2.48	4.55e-01	soluble
Glycitein	-3.57	7.63e-02	Soluble	-3.76	4.93e-02	Soluble	-5.10	2.25e-03	Moderately soluble

Phloretin	-3.38	1.15e-01	soluble	-4.34	1.26e-02	Moderately soluble	-3.37	1.16e-01	soluble
Fisetin	-3.35	1.27e-01	soluble	-3.93	3.37e-02	Soluble	-3.82	4.29e-02	soluble
Genistin	-3.18	2.85e-01	soluble	-4.01	4.18e-02	Moderately soluble	-2.69	8.77e-01	soluble
Apigenin	-3.94	3.07e-02	soluble	-4.59	6.88e-03	Moderately soluble	-4.40	1.07e-02	Moderately soluble
Baicalein	-4.03	2.51e-02	Moderately soluble	-4.74	4.93e-03	Moderately soluble	-4.40	1.07e-02	Moderately soluble
Compounds	Log S (ESOL)	Solubility (mg/mL)	class	Log S (Ali)	Solubility (mg/mL)	Class	Log S (SILICOS-IT)	Solubility (mg/mL)	class
Daidzein	-3.53	7.51e-02	Soluble	-3.60	6.41e-02	Soluble	-4.98	2.64e-03	Moderately soluble
Quercetin	-3.16	2.11e-01	Soluble	-3.91	3.74e-02	Soluble	-3.24	1.73e-01	Soluble
Furanosylboratediester	0.48	5.77e+02	Highly soluble	0.66	8.79e+02	Highly soluble	1.91	1.58e+04	Soluble

S4 Table. Pharmacokinetics

Compounds	GI absorption	BBB permeation	P-gp substrate	CYP1A2 Inhibitor	CYP2C19 Inhibitor	CYP2C9 Inhibitor	CYP2D6 Inhibitor	CYP3A4 Inhibitor	Log Kp (Skin permeation) (cm/s)
Phytol	Low	No	Yes	No	No	Yes	No	No	-2.29
Beta-pinene	Low	Yes	No	No	No	Yes	No	No	-4.18
Alpha-pinene	Low	Yes	No	No	No	Yes	No	No	-3.95
P-cymene	Low	Yes	No	No	No	No	Yes	No	-4.21
Alpha-terpinene	Low	Yes	No	No	No	No	No	No	-4.11
Isoterpinolene	Low	Yes	No	No	No	Yes	No	No	-4.64
3-Carene	Low	Yes	No	No	No	Yes	No	No	-4.02
Sabinene	Low	Yes	No	No	No	No	No	No	-4.94
Camphene	Low	Yes	No	No	No	Yes	No	No	-4.13
Glycitein	High	No	No	Yes	No	No	Yes	Yes	-6.30
Phloretin	High	No	No	Yes	No	Yes	No	Yes	-6.11
Fisetin	High	No	No	Yes	No	No	Yes	Yes	-6.65
Genistin	Low	No	Yes	No	No	No	No	No	-8.33
Apigenin	High	No	No	Yes	No	No	Yes	Yes	-5.80
Baicalein	High	No	No	Yes	No	No	Yes	Yes	-5.70
Daidzein	High	Yes	No	Yes	No	No	Yes	Yes	-6.10
Quercetin	High	No	No	Yes	No	No	Yes	Yes	-7.05
Furanosylborate diester	Low	No	No	No	No	No	No	No	-9.18

S5 Table. Drug-likeness

Compounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability score
3,7,11,15-Tetramethyl-2-hexadecen-1-OL(Phytol)	Yes; 1 violation: MLOGP>4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
Beta-pinene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Alpha-pinene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
P-cymene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Alpha-terpinene	Yes; 0 violation	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Isoterpinolene	Yes; 0 violation	No; 1 violation: MW<160	Yes	Yes	No; 2 violations:	0.55

					MW<200, Heteroatoms<2	
3-Carene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Sabinene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Camphene	Yes; 1 violation: MLOGP>4.15	No; 1 violation: MW<160	Yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
Glycitein	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Phloretin	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Fisetin	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Genistin	Yes; 1 violation: NH _{or} OH>5	Yes	No; 1 violation: TPSA>140	No; 1 violation: TPSA>131.6	No; 2 violations: TPSA>150, H- don>5	0.55
Apigenin	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Baicalein	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55

Daidzein	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Quercetin	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Furanosylboratediester	Yes; 0 violation	No; 2 violations: WLOGP<-0.4, MR<40	Yes	Yes	No; 2 violations: MW<200, XLOGP3<-2	0.56

S6 Table. Medicinal Chemistry

Compounds	PAINS	Brenk	Leadlikeness	Synthetic accessibility
3,7,11,15-Tetramethyl-2-hexadecen-1-OL (phytol)	0 alert	1 alert: isolated_alkene	No; 2 violations: Rotors>7, XLOGP3>3.5	4.30
Beta-pinene	0 alert	1 alert: isolated_alkene	No; 2 violations: MW<250, XLOGP3>3.5	3.73
Alpha-pinene	0 alert	1 alert: isolated_alkene	No; 2 violations: MW<250, XLOGP3>3.5	4.44
P-cymene	0 alert	0 alert	No; 2 violations: MW<250, XLOGP3>3.5	1.00
Alpha-terpinene	0 alert	0 alert	No; 2 violations: MW<250, XLOGP3>3.5	3.63
Isoterpinolene	0 alert	0 alert	No; 2 violations: MW<250, XLOGP3>3.5	3.72
3-Carene	0 alert	1 alert: isolated_alkene	No; 2 violations: MW<250, XLOGP3>3.5	3.84
Sabinene	0 alert	1 alert: isolated_alkene	No; 1 violation: MW<250	2.87
Camphene	0 alert	1 alert: isolated_alkene	No; 2 violations: MW<250, XLOGP3>3.5	3.50
Glycitein	0 alert	0 alert	Yes	2.95
Phloretin	0 alert	0 alert	Yes	1.88
Fisetin	1 alert: catechol_A	1 alert: catecho	Yes	3.16
Genistin	0 alert	0 alert	No; 1 violation: MW>350	5.12
Apigenin	0 alert	0 alert	Yes	2.96
Baicalein	1 alert: catechol_A	1 alert: catechol_A	Yes	3.02
Daidzein	0 alert	0 alert	Yes	2.79
Quercetin	1 alert: catechol_A	1 alert: catechol_A	Yes	3.23
Furanosylboratediester	0 alert	1 alert: heavy_metal	No; 1 violation: MW<250	3.63