

Supporting Information

***in vivo* and *in silico* evaluation of jasmonoyl-L-isoleucine analogs having a pyrazolidin-3-one ring**

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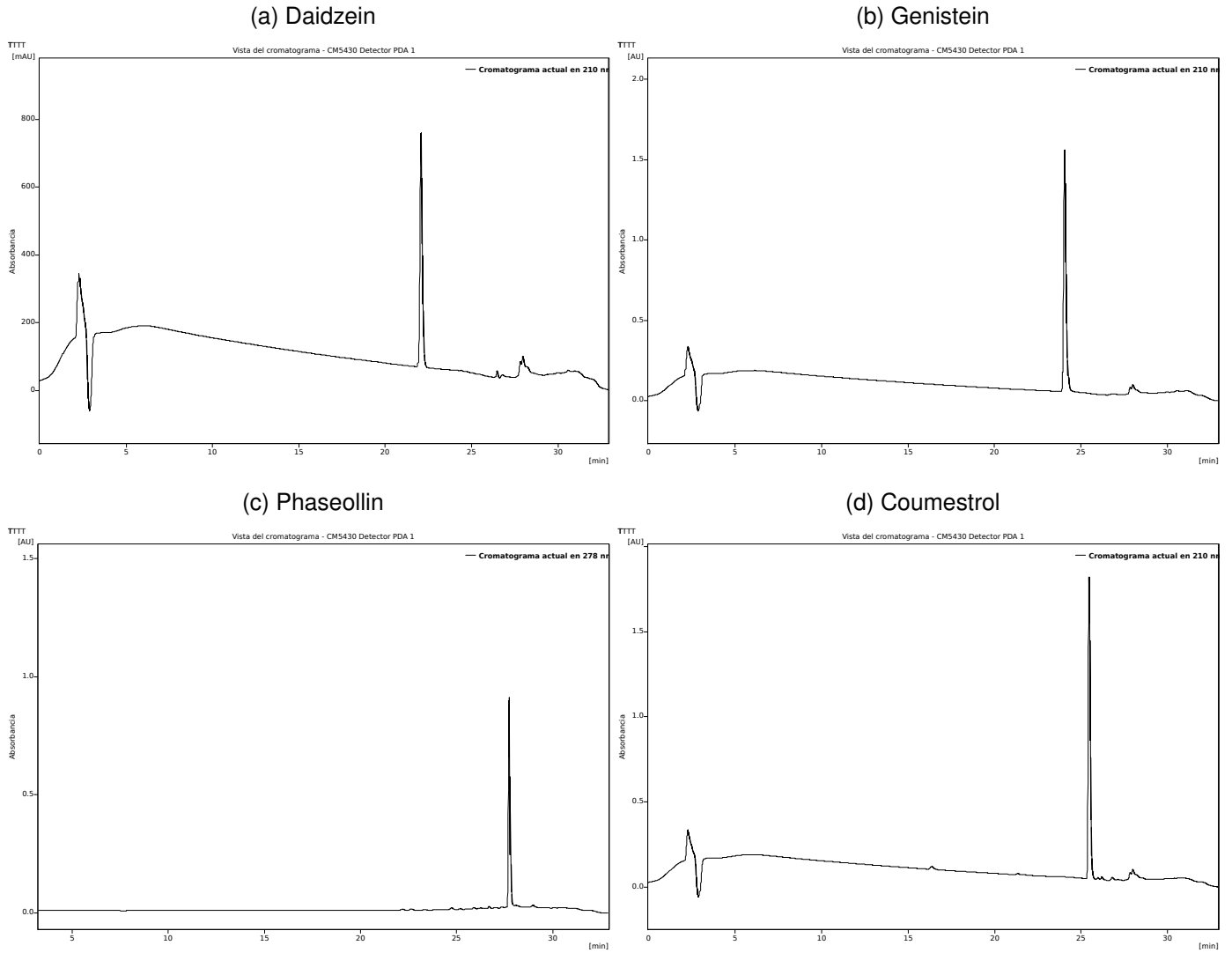
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1 Chromatograms

Figure S1: Chromatograms of the standards of phytoalexins Daidzein, Genistein, Phaseollin and Coumestrol.



2 Quantitative data from phytoalexin elicitor activity

Table S1: Phytoalexins quantifications for treatments at 0.05 mM

Treatment	Sample	g f. w.	EtOH ext. [g]	Yield (%)	Daidzein [µg/mL]	Coumestrol [µg/mL]	Genistein [µg/mL]	Phaseollin [µg/mL]	Daidzein	Coumestrol	Genistein	Phaseollin
6@0.5 mM	1	4.7928	0.2288	4.8	0.508	2.124	0.167	24.922	0.530	2.216	0.174	25.999
6@0.5 mM	2	4.5379	0.2267	5.0	0.236	1.599	0.305	19.241	0.260	1.762	0.336	21.200
7a	1	5.1080	0.1987	3.9	1.309	4.221	0.275	17.905	1.281	4.132	0.269	17.526
7a	2	5.6658	0.2092	3.7	1.002	3.694	0.225	19.089	0.884	3.260	0.199	16.846
7b	1	4.5965	0.0806	1.8	2.558	5.192	0.481	16.935	2.783	5.648	0.523	18.422
7b	2	4.6229	0.1688	3.7	0.382	4.191	0.243	17.532	0.413	4.533	0.263	18.962
7c	1	7.0260	0.2014	2.9	0.813	4.418	0.181	19.605	0.579	3.144	0.129	13.952
7c	2	6.2709	0.2027	3.2	0.810	4.014	0.147	20.759	0.646	3.200	0.117	16.552
7d	1	5.8097	0.2015	3.5	0.380	2.716	0.111	17.301	0.327	2.337	0.096	14.890
7d	2	4.3860	0.1712	3.9	0.477	2.089	0.099	18.699	0.544	2.381	0.113	21.317
7e	1	5.0047	0.2373	4.7	2.977	4.325	0.296	38.112	2.974	4.321	0.296	38.076
7e	2	4.0713	0.1514	3.7	1.234	3.218	0.184	23.765	1.515	3.952	0.226	29.186
7f	1	3.2649	0.1509	4.6	0.511	2.193	0.250	12.983	0.783	3.358	0.383	19.883
7f	2	4.5961	0.1883	4.1	0.808	5.108	0.169	16.807	0.879	5.557	0.184	18.284
7g	1	7.3280	0.1877	2.6	1.315	2.322	0.195	5.970	0.897	1.584	0.133	4.073
7g	2	4.9641	0.1392	2.8	0.356	1.718	0.070	3.427	0.359	1.730	0.071	3.452
7h	1	6.5057	0.1631	2.5	1.337	3.728	0.269	10.801	1.028	2.865	0.207	8.301
7h	2	5.1764	0.1455	2.8	0.800	2.048	0.286	9.504	0.773	1.978	0.276	9.180
7i	1	4.3087	0.1229	2.9	0.968	1.284	0.533	9.980	1.123	1.490	0.619	11.581
7i	2	5.7297	0.2081	3.6	0.633	1.408	0.274	9.694	0.552	1.229	0.239	8.459
(-)Blank	1	6.0340	0.1685	2.8	0.632	3.073	0.194	9.630	0.524	2.546	0.161	7.980
(-)Blank	2	4.7474	0.1701	3.6	0.529	2.156	0.174	5.075	0.557	2.271	0.183	5.345

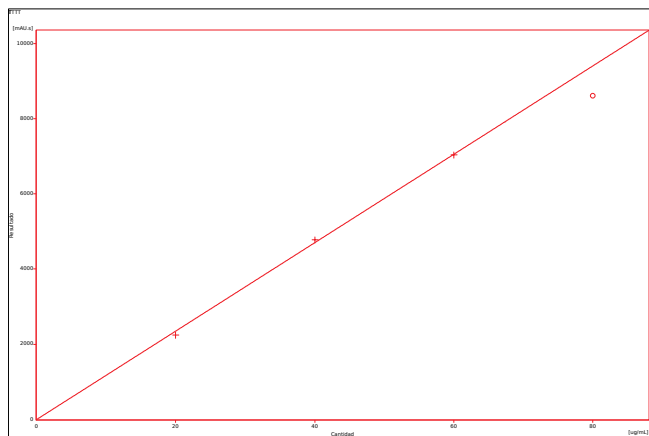
Table S2: Phytoalexins quantifications for treatments at 0.05 mM

Treatment	Sample	g f. w.	EtOH ext. [g]	Yield (%)	Daidzein [µg/mL]	Coumestrol [µg/mL]	Genistein [µg/mL]	Phaseollin [µg/mL]	Daidzein	Coumestrol	Genistein	Phaseollin
6@0.5 mM	1	4.7928	0.2288	4.8	0.508	2.124	0.167	24.922	0.530	2.216	0.174	25.999
6@0.5 mM	2	4.5379	0.2267	5.0	0.236	1.599	0.305	19.241	0.260	1.762	0.336	21.200
7a	1	5.0657	0.1896	3.7	3.871	6.221	0.447	49.622	3.821	6.140	0.441	48.978
7a	2	4.3521	0.1536	3.5	1.552	6.350	0.169	38.918	1.783	7.295	0.194	44.712
7b	1	2.9062	0.1349	4.6	0.853	5.531	0.294	40.777	1.468	9.516	0.506	70.155
7b	2	4.0362	0.1826	4.5	0.916	6.480	0.250	44.921	1.135	8.027	0.310	55.648
7c	1	5.3999	0.1812	3.4	0.984	5.682	0.126	40.451	0.911	5.261	0.117	37.455
7c	2	2.6408	0.0977	3.7	1.813	2.506	0.198	19.944	3.433	4.745	0.375	37.761
7d	1	3.9616	0.1256	3.2	0.526	3.225	0.180	29.026	0.664	4.070	0.227	36.634
7d	2	5.7544	0.2076	3.6	0.759	5.102	0.169	44.173	0.659	4.433	0.147	38.382
7e	1	5.1854	0.1814	3.5	0.734	4.268	0.195	40.578	0.708	4.115	0.188	39.127
7e	2	5.6788	0.1783	3.1	0.462	5.801	0.121	60.065	0.407	5.108	0.107	52.885
7f	1	2.7148	0.1062	3.9	0.723	4.634	0.175	23.102	1.332	8.535	0.322	42.548
7f	2	3.3656	0.1781	5.3	0.948	5.094	0.222	26.641	1.408	7.568	0.330	39.578
7g	1	4.4878	0.1871	4.2	1.988	6.183	0.385	20.801	2.215	6.889	0.429	23.175
7g	2	3.7168	0.1717	4.6	0.337	4.225	0.192	14.791	0.453	5.684	0.258	19.897
7h	1	8.1951	0.2160	2.6	0.555	4.110	0.164	11.881	0.339	2.508	0.100	7.249
7h	2	7.4306	0.1710	2.3	0.550	3.756	0.107	11.101	0.370	2.527	0.072	7.470
7i	1	6.7301	0.2252	3.3	0.652	1.162	0.136	11.652	0.484	0.863	0.101	8.657
7i	2	9.2051	0.3307	3.6	2.794	2.081	0.335	10.789	1.518	1.130	0.182	5.860
(-)Blank	1	6.0340	0.1685	2.8	0.632	3.073	0.194	9.630	0.524	2.546	0.161	7.980
(-)Blank	2	4.7474	0.1701	3.6	0.529	2.156	0.174	5.075	0.557	2.271	0.183	5.345

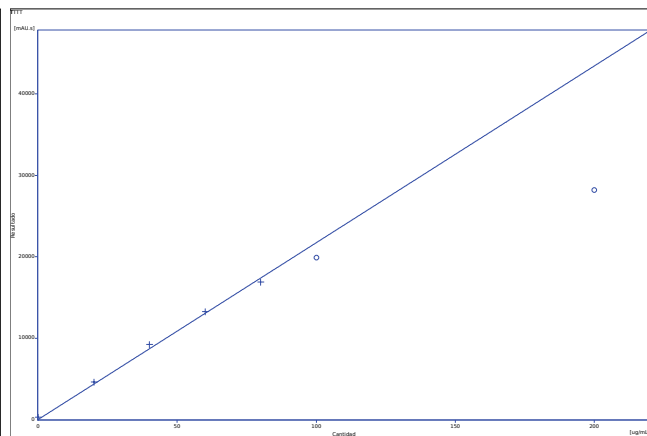
4 Calibration curves

Figure S2: Calibration curves of the standards.

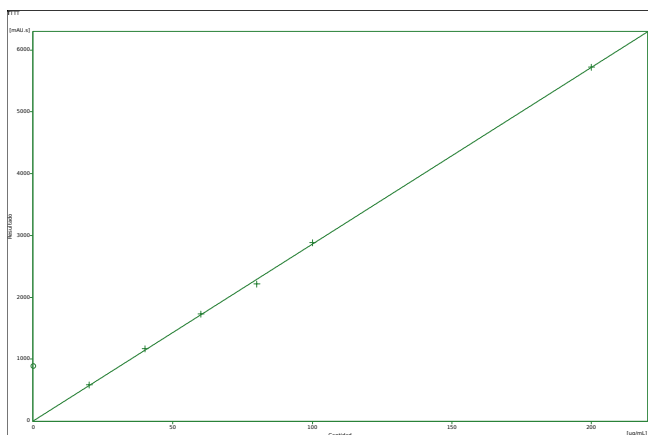
(a) Daidzein. $R = 0.99974$



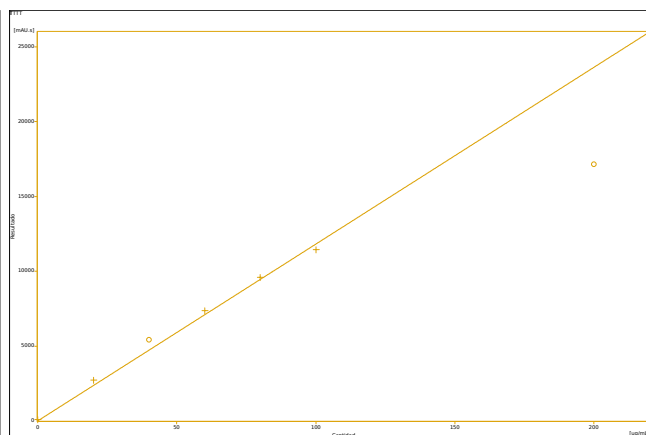
(b) Genistein. $R = 0.99867$



(c) Phaseollin. $R = 0.99986$

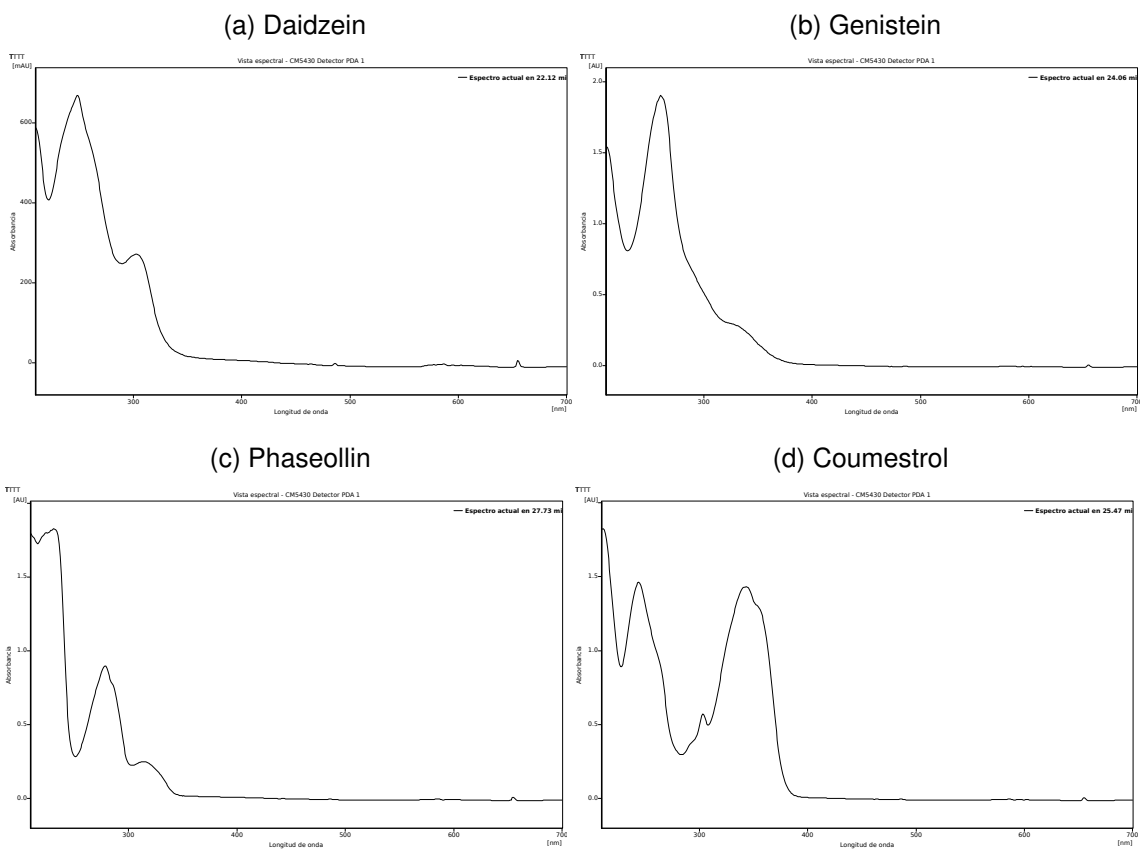


(d) Coumestrol. $R = 0.99862$



5 UV-Vis spectra

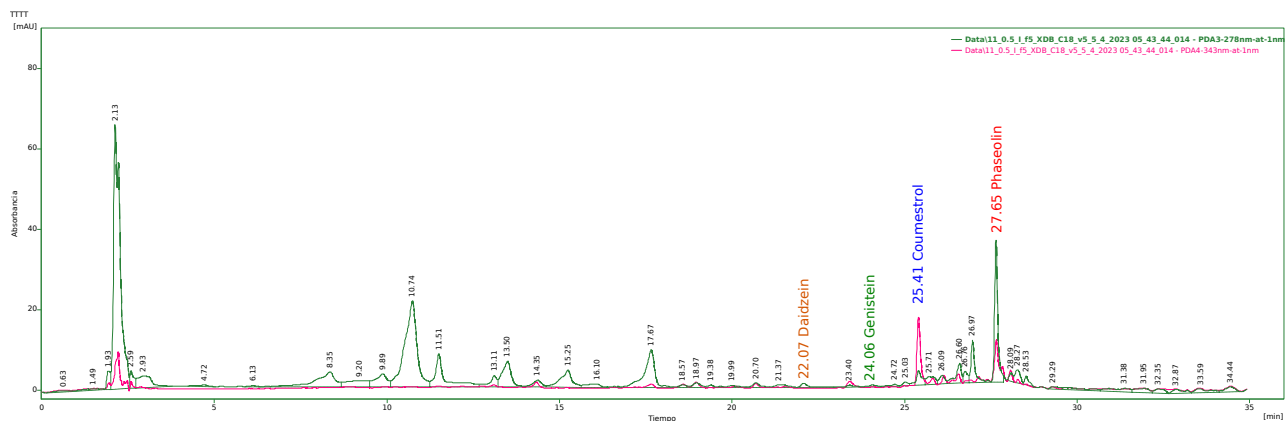
Figure S3: UV-Vis spectra of the standards.



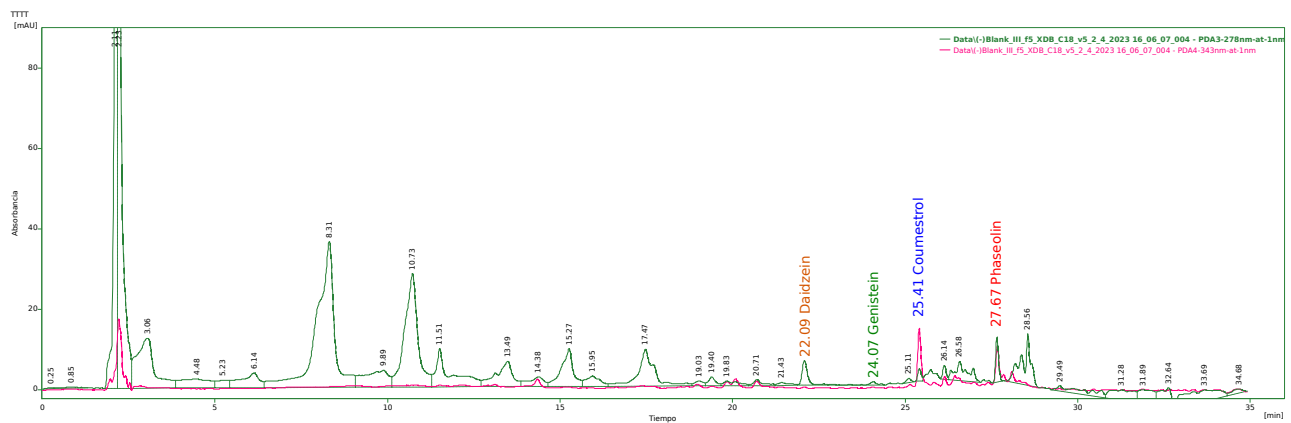
6 Example chromatograms

Figure S4: Chromatograms at 278 nm (green) and 343 nm (pink) after the induction with **7i** at 0.5 mM (a), and from a negative blank (b).

(a) **7i** at 0.5 mM

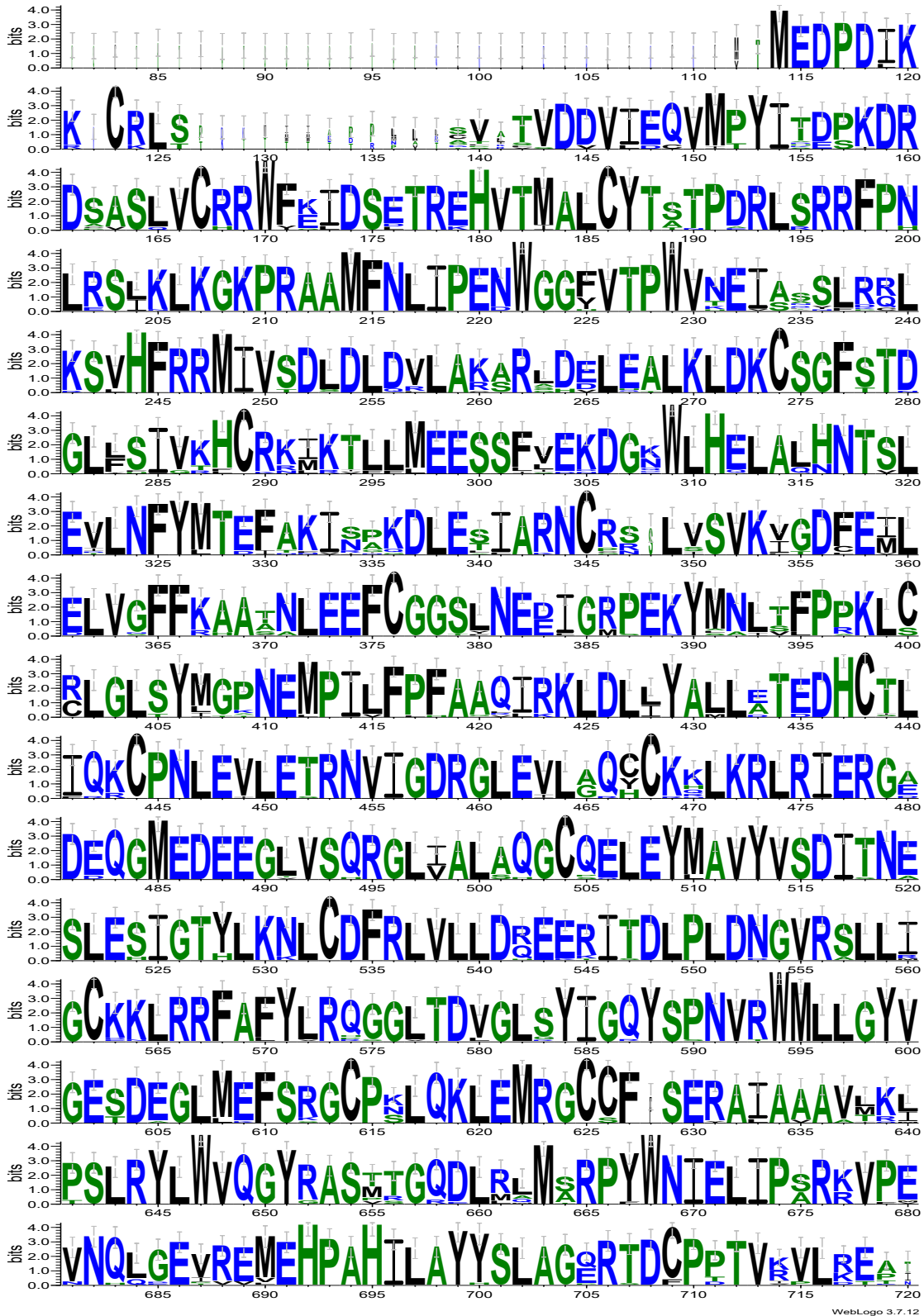


(b) Negative blank



7 Consensus logo of COI1 proteins

Figure S5: Logo of sequence conservation in COI1 proteins.



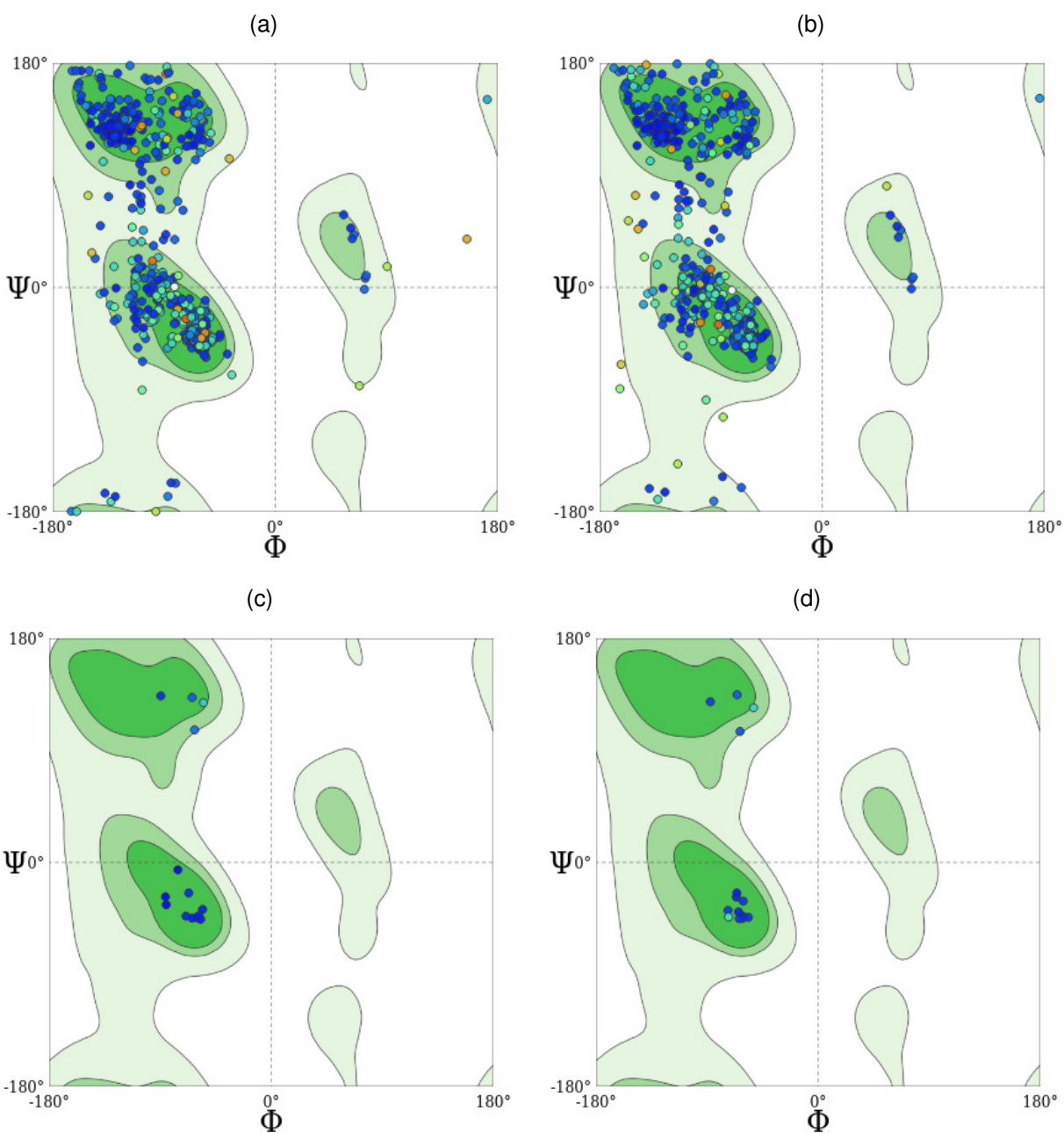
8 Consensus logo of JAZ proteins

Figure S6: Logo of sequence conservation in JAZ proteins.



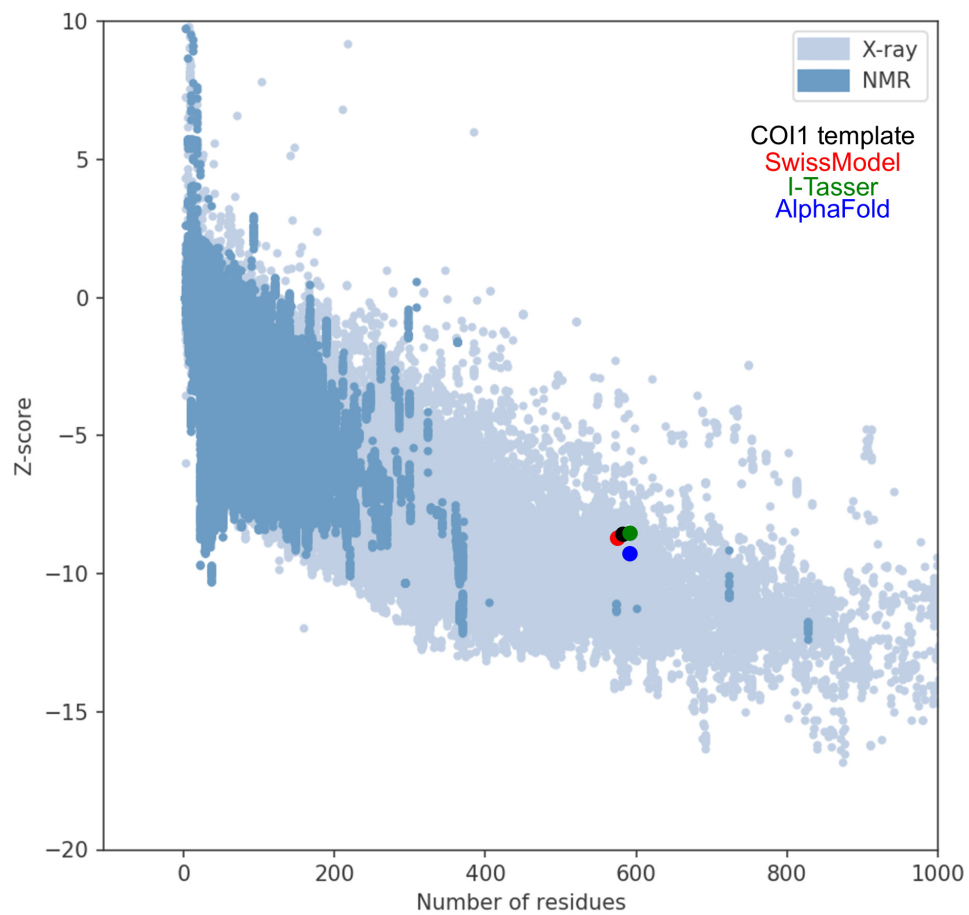
9 Ramachandran plots of SM models

Figure S7: Ramachandran plots for V7CZF7 (a), V7BBE9 (b), V7CCD0 (c), V7AYI4 (d).



10 Z-plots of protein models

Figure S8: Z-scores for COI1 protein models.



11 Tukey HSD analysis of docking results

Table S5: Matrix of significant differences of binding energies from docking. Value of 1 represents significant differences.

	7a-ARATH	7a-PHAVU	7b-ARATH	7b-PHAVU	7c-ARATH	7c-PHAVU	7d-ARATH	7d-PHAVU	7e-ARATH	7e-PHAVU	7f-ARATH	7f-PHAVU	7g-ARATH	7g-PHAVU	7h-ARATH	7h-PHAVU	7i-ARATH	7i-PHAVU	8-ARATH	8-PHAVU	9-ARATH	9-PHAVU
7a-ARATH	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	1	1	1	1	1	0	0
7a-PHAVU	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	1
7b-ARATH	0	0	0	0	0	1	0	1	0	0	0	1	0	1	0	1	1	1	1	1	0	0
7b-PHAVU	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	0
7c-ARATH	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	0
7c-PHAVU	1	0	1	0	0	0	0	0	0	0	0	1	1	0	0	1	0	1	1	1	1	1
7d-ARATH	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	0
7d-PHAVU	1	0	1	0	0	0	0	0	1	0	0	1	1	0	0	1	0	1	1	1	1	1
7e-ARATH	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	1	1	1	1	1	0	0
7e-PHAVU	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	1	1	1	1	1	1	0
7f-ARATH	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	1	1	1	1	0	0
7f-PHAVU	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	0	0	1	1	1	1	1
7g-ARATH	0	1	0	1	1	1	1	1	0	0	0	1	0	1	1	1	1	1	1	1	1	0
7g-PHAVU	1	0	1	0	0	0	0	0	1	1	0	1	1	0	0	1	0	1	1	1	1	1
7h-ARATH	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	1	1	1	1	1	0
7h-PHAVU	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	0	0	1	1	1	1	1
7i-ARATH	1	1	1	1	1	0	1	0	1	1	1	0	1	0	1	0	0	1	1	1	1	1
7i-PHAVU	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	1
8-ARATH	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1
8-PHAVU	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1
9-ARATH	0	1	0	1	1	1	1	1	0	0	0	1	0	1	1	1	1	1	1	1	0	0
9-PHAVU	0	1	0	0	0	1	0	1	0	0	0	1	0	1	0	1	1	1	1	1	0	0

12 Linear correlation of the binding energies between receptors

Figure S9: Pearson's correlation coefficient from the binding energies of the docked molecules in receptors of *A. thaliana* (ARATH) and *P. vulgaris* (PHAVU).

