

Table S1. ProtParam and Self Optimized Prediction from Multiple Alignment (SOPMA) computed parameters for cellulases and ligninases from *Alternaria arborescens*, *Paecilomyces variotii*, *Trichocladium griseum*, *Penicillium chrysogenum*, *Penicillium crustosum*, *Aspergillus flavus*, *Fusarium solani*, *Penicillium citrinum*, and *Fusarium equiseti*

Fungus	Accession	Designation	Length (a.a)	MW	EC	pI	<i>In vivo</i> HL (> hours)	Ii	Ai	GRAVY	R−	R+	α -Helix %	Extended strand %	β -Turn %	Random coil %
<i>Alternaria arborescens</i>	XP_028512170.1	Endoglucanase	421	43508.55	63090	6.05	20	30.39	69.07	−0.092	33	29	34.44	16.63	6.65	42.28
	RYO67414.1	Endoglucanase	421	43508.55	63090	6.05	20	30.39	69.07	−0.092	33	29	34.44	16.63	6.65	42.28
	RYN41850.1	Endoglucanase	421	43508.55	63090	6.05	20	30.39	69.07	−0.092	33	29	34.44	16.63	6.65	42.28
	XP_028500248.1	Endoglucanase 1	420	44668.08	79965	4.78	20	29.3	61.4	−0.333	47	30	16.9	22.86	7.38	52.86
	RYO69679.1	Endoglucanase 1	420	44668.08	79965	4.78	20	29.3	61.4	−0.333	47	30	16.9	22.86	7.38	52.86
	XP_028501869.1	Beta-glucosidase	479	54735.39	124720	5.34	20	32.83	66.83	−0.619	75	61	36.12	15.87	6.89	41.13
	XP_028505045.1	Beta-glucosidase	731	77985.83	130665	6.87	20	28.73	77.15	−0.258	70	69	26.54	22.3	6.29	44.87
	RYO56859.1	Beta-glucosidase	753	80125.15	132280	7.17	20	28.89	76.22	−0.252	70	70	26.03	21.91	6.77	45.29
	XP_028501739.1	Beta-glucosidase B	733	80299.58	82070	5.65	20	34.27	78.23	−0.389	98	80	23.47	24.28	6.68	45.57
	RYO18646.1	Beta-glucosidase B	733	80299.58	82070	5.65	20	34.27	78.23	−0.389	98	80	23.47	24.28	6.68	45.57
	XP_028501087.1	Laccase	616	66979.26	128270	6.96	20	35.75	75.86	−0.226	43	42	10.23	26.3	5.19	58.28
	XP_028510645.1	Laccase	603	66669.74	126655	5.62	20	32.06	78.09	−0.359	60	41	8.62	26.87	6.14	58.37
	RYO69350.1	Laccase	603	66681.79	126655	5.62	20	32.06	78.74	−0.351	60	41	8.79	26.2	5.8	59.2
	RYO39750.1	Laccase	616	66964.33	126780	6.96	20	34.45	77.13	−0.197	43	42	11.36	26.14	6.01	56.49
	RYO39394.1	Laccase	603	66669.74	126655	5.62	20	32.06	78.09	−0.359	60	41	8.62	26.87	6.14	58.37

<i>Paecilomyces variotii</i>	XP_028485664.1	Endoglucanase	300	32331.07	51505	6.48	20	33.5	56.27	−0.334	20	18	8	22.67	5	64.33
	RWQ96019.1	Endoglucanase	300	32331.07	51505	6.48	20	33.5	56.27	−0.334	20	18	8	22.67	5	64.33
	GAD94262.1	Endoglucanase	298	32175.92	44515	5.8	20	27.28	57.92	−0.353	24	18	8.05	22.15	3.36	66.44
	RWQ99350.1	Beta-glucosidase M	806	86879.95	136640	4.98	20	31.49	81.94	−0.174	78	55	28.78	19.11	6.82	45.29
	XP_028487745.1	Beta-1,4-glucosidase	861	92721.34	173080	4.69	20	25.99	77.02	−0.265	92	58	25.32	19.28	5.69	49.71
	GAD99276.1	Beta-glucosidase 1	861	92853.45	170100	4.67	20	26.21	74.99	−0.300	97	58	24.97	19.4	5.34	50.29
	GAD93537.1	Beta-glucosidase J	840	91812.84	131250	5.98	20	37.12	83.57	−0.241	96	85	28.21	24.64	7.02	40.12
	GAD98731.1	Beta-glucosidase 1B	474	53117.78	114165	5.59	20	28.38	74.73	−0.388	61	52	37.34	15.61	7.38	39.66
	XP_028484177.1	Multicopper oxidase-domain-containing protein	622	68988.32	141790	5.44	20	35.36	78.83	−0.347	66	44	9.16	24.92	6.27	59.65
	RWQ94532.1	Multicopper oxidase-domain-containing protein	622	68988.32	141790	5.44	20	35.36	78.83	−0.347	66	44	9.16	24.92	6.27	59.65
	A0A443HK79.1	Multicopper oxidase VdtB (precursor)	685	78142.47	202055	5.44	20	40.00	73.75	−0.427	84	60	16.64	26.13	6.72	50.51
	A0A443HK11.1	FAD-binding monooxygenase VdtE	571	64947.35	128270	6.35	20	41.70	69	−0.435	69	65	31.87	19.96	7.53	40.63
	GAD97601.1	Extracellular dihydrogeodin oxidase/laccase	558	62250.84	127240	4.7	20	31.17	75.82	−0.341	66	28	11.83	28.85	6.09	53.23

<i>Trichocladium griseum</i>	AAM77714.2	Endoglucanase	254	28883.26	90090	5.92	20	16.62	69.92	−0.458	25	23	19.69	27.95	4.33	48.03
	1W2U_A	Chain A, ENDOGLUCANASE	224	25864.89	90090	5.61	20	14.27	61.83	−0.598	24	21	11.61	26.79	4.02	57.59
<i>Penicillium chrysogenum</i>	KZN87403.1	Endo-beta-1,4- glucanase A	401	42850.6	101675	5	20	28.1	67.26	−0.124	29	21	28.43	17.21	5.74	48.63
	KZN89060.1	Endoglucanase B	574	61626.61	123090	4.6	20	30.47	84.13	−0.001	54	31	31.36	19.16	5.4	44.08
	KZN84919.1	Endoglucanase C	469	54797.68	125040	5.51	20	36.58	67.4	−0.59	72	56	45.2	13.65	5.97	35.18
	KZN90305.1	Beta-glucosidase B	846	92078.7	103205	5.18	20	40.81	86.87	−0.102	96	71	24.82	22.81	5.91	46.45
	KZN93408.1	Beta-glucosidase 1B	483	54514.17	115655	4.9	20	30.26	75.16	−0.425	73	50	37.68	14.49	6.42	41.41
	KZN93114.1	Beta-glucosidase 1B	852	95463.96	149825	5.2	20	35.43	76.48	−0.41	119	86	36.62	18.66	8.33	36.38
	KZN91501.1	Beta-glucosidase 1A	566	63935	109795	5.34	20	37.32	76.31	−0.273	62	46	34.81	15.72	5.12	44.35
<i>Penicillium crustosum</i>	AHA15977.1	Endo-1,4-beta-D- glucanase, partial	459	48609.49	92165	4.53	20	38.28	65.14	−0.234	42	23	25.27	16.78	5.23	52.72
	XP_056725833.1	Glycoside hydrolase superfamily	410	44478.34	93655	5.08	20	28.93	64.78	−0.352	41	31	30.24	15.61	5.37	48.78
	XP_056725118.1	Beta-glucosidase	259	28456.19	41495	5.34	20	42.11	89.5	−0.063	25	19	24.71	28.19	6.18	40.93
	KAJ5394428.1	Beta-glucosidase	259	28456.19	41495	5.34	20	42.11	89.5	−0.063	25	19	24.71	28.19	6.18	40.93
<i>Aspergillus flavus</i>	RMZ37468.1	Cellulase	569	63032.31	137975	4.85	20	34.23	76.78	−0.259	61	42	30.4	18.63	5.62	45.34
	RAQ66523.1	Cellulase	569	63032.31	137975	4.85	20	34.04	76.78	−0.26	61	42	31.11	17.4	5.45	46.05
	RAQ63436.1	Cellulase	569	63032.31	137975	4.85	20	34.04	76.78	−0.26	61	42	30.05	19.51	5.8	44.64
	RMZ41992.1	Cellulase	503	55560.45	110935	5.6	20	33.23	74.08	−0.282	51	39	30.02	19.88	5.37	44.73

	RMZ37535.1	Cellulase	481	56002.12	125165	5.75	20	37.83	71.64	−0.587	68	55	43.04	14.97	5.2	36.8
	KAJ1715357.1	Endoglucanase	239	26025.58	67505	4.36	20	21.41	66.81	−0.256	22	9	19.33	26.47	4.62	49.58
	KAJ1715009.1	Endoglucanase	328	34908.02	64330	5.74	20	33.63	63.35	−0.3	28	24	9.45	26.52	4.57	59.45
	KAJ1713444.1	Endoglucanase	250	26117.99	43110	4.36	20	25.83	82	−0.106	29	11	12.4	25.2	6.4	56
	KAJ1711735.1	Endoglucanase	240	25594.92	61545	4.04	20	29.72	64.71	−0.206	25	8	19.17	28.75	2.92	49.17
	KAJ1709640.1	Endoglucanase	283	30926.63	50100	8.18	20	26.36	51.06	−0.528	31	33	7.07	27.92	5.65	59.36
	RMZ41167.1	Beta-glucosidase	779	85093.2	132380	4.97	20	29.24	89.46	−0.117	93	64	38.51	15.92	6.8	38.77
	RMZ38224.1	Beta-glucosidase	861	93414.85	177535	4.82	20	27.67	75.57	−0.331	102	66	25.78	18.82	5.34	50.06
	RMZ37309.1	Beta-glucosidase	807	86611.5	148100	5.06	20	37.06	77.77	−0.243	78	57	29.49	18.09	6.69	45.72
	RAQ79441.1	Beta-glucosidase	807	86621.54	148100	5.06	20	37.29	77.77	−0.244	78	57	27.88	18.46	6.69	46.96
	RAQ77926.1	Beta-glucosidase	827	90797.34	123690	5.97	20	36.15	87.03	−0.154	92	78	28.54	24.67	7.01	39.78
	KAJ1710886.1	Laccase	588	65575.04	110950	5.67	20	40.05	82.76	−0.176	57	40	15.31	26.02	6.29	52.38
	KAJ1705330.1	Laccase	583	64821.77	92040	5.18	20	46.65	84.75	−0.272	61	32	8.58	27.1	6	58.32
	RMZ45971.1	Laccase	593	66014.16	86665	5.48	20	46.73	82.18	−0.354	62	41	7.08	25.46	4.89	62.56
	RMZ39576.1	Laccase	589	65706.23	110950	5.67	20	39.95	82.61	−0.172	57	40	15.28	26.32	6.62	51.78
	RAQ73286.1	Laccase	588	65575.04	110950	5.67	20	40.05	82.76	−0.176	57	40	15.31	26.02	6.29	52.38
<i>Fusarium solani</i>	KAH7250822.1	1, 4-beta cellobiohydrolase	468	49814.33	105365	5.18	20	26.24	68.38	−0.294	38	29	36.11	11.54	5.13	47.22
	XP_046129634.1	Endoglucanase	244	26027.35	64525	4.12	20	25.29	68.81	−0.238	29	9	18.03	28.28	4.1	49.59

	XP_046126616.1	Beta-glucosidase	484	55397.99	153460	5.75	20	30.15	66.14	−0.566	65	56	36.78	15.29	6.61	41.32
	KAJ4232191.1	Beta-glucosidase	832	90407.45	128730	5.29	20	25.64	82.67	−0.221	108	87	28.12	24.88	6.73	40.26
	KAJ4211136.1	Beta-glucosidase	880	95537.54	181670	4.97	20	29.64	75.94	−0.342	97	66	24.55	18.41	5.57	51.48
	AGT80114.1	Laccase	583	64873.05	111185	5.71	20	29.43	78.39	−0.41	64	49	9.43	26.76	7.2	6.6
	AHD26939.1	Laccase	588	65326.41	111185	5.77	20	28.82	80.2	−0.387	62	46	8.67	27.55	6.8	56.97
	AHZ65142.1	Laccase 1	622	68374.92	95480	4.88	20	28.46	79.07	−0.236	75	44	19.13	26.05	7.07	47.75
	AHZ65141.1	Laccase 2	651	74233.33	157845	5.62	20	35.28	73.96	−0.477	79	59	7.22	24.88	4.76	63.13
	AHZ65140.1	Laccase 3	599	66337.7	88030	5.02	20	34.88	79.43	−0.302	74	46	15.69	29.22	7.35	47.75
<i>Penicillium citrinum</i>	XP_056497110.1	Beta-glucosidase	494	54139.06	86415	5.45	20	43.1	80.59	−0.2	49	36	42.51	10.53	5.67	41.3
	XP_056501835.1	Beta-glucosidase	259	30002.72	35005	9.36	20	52.29	83.24	−0.326	25	38	42.86	5.41	2.32	49.42
	XP_056501834.1	Beta-glucosidase	853	93292.75	120250	5.38	20	34.46	87.6	−0.203	106	84	29.31	24.15	6.92	39.62
	XP_056498616.1	Beta-glucosidase M	809	87423.76	132170	5.38	20	35.68	78.74	−0.323	89	69	28.18	18.29	6.55	46.97
	XP_056495445.1	Beta-glucosidase A	862	93307.35	155200	5.28	20	26.54	75.05	−0.332	96	73	26.33	18.68	5.22	49.77
<i>Fusarium equiseti</i>	AAM77703.1	Endoglucanase	238	26363.18	68535	4.72	20	17.49	66.43	−0.398	25	15	18.91	28.15	4.2	48.74
	KAJ4127785.1	Endoglucanase gh5-1	382	42495.45	108205	6.31	20	21.14	56.99	−0.497	33	31	31.94	15.45	6.28	46.34
	KAJ4141610.1	Beta-glucosidase	891	96609.56	173065	5.15	20	34.24	71.8	−0.385	97	72	25.14	18.86	5.61	50.39
	KAJ4133747.1	Beta-glucosidase	832	90898.82	126335	5.21	20	32.58	82.64	−0.278	113	87	28	25	6.97	40.02

Table S2. Tridimensional structure modeling of selected enzymes using SWISS MODEL server and quality verification

Fungus	Accession	Template	Sequence Id	GMQE	QMEAN
<i>Alternaria arborescens</i>	XP_028512170.1	3qr3.1.A	58.65	0.66	−1.49
	XP_028500248.1	6yp1.1.A	59.38	0.82	−0.47
	XP_028501869.1	4mdo.1.A	72.84	0.92	0.1
	XP_028505045.1	3zyz.1.A	63.3	0.86	−0.96
	RYO56859.1	3zyz.1.A	63.48	0.84	−0.83
	XP_028501739.1	3abz.1.A	39.15	0.72	−2.53
	XP_028501087.1	6f5k.1.A	45.32	0.7	−2.16
	XP_028510645.1	6f5k.1.A	43.05	0.72	−1.41
	RYO69350.1	6f5k.1.A	43.05	0.72	−1.4
	RYO39750.1	6f5k.1.A	44.94	0.7	−2.22
<i>Paecilomyces variotii</i>	XP_028485664.1	7p3u.1.A	37.89	0.48	−6.08
	GAD94262.1	7p3u.1.A	38.1	0.48	−5.9
	RWQ99350.1	5fji.1.A	44.06	0.69	−3.03
	XP_028487745.1	4iic.1.A	69.38	0.88	−0.72
	GAD99276.1	4iic.1.A	69.74	0.88	−0.69
	GAD93537.1	3abz.1.A	48.67	0.81	−1.77
	GAD98731.1	4mdo.1.A	67.75	0.88	−0.87
	XP_028484177.1	3sqr.1.A	43.11	0.67	−3.39
	GAD97601.1	5lwx.1.A	51.08	0.79	−1.54
<i>Trichocladium griseum</i>	AAM77714.2	1uu4.1.A	100	0.88	0.99
<i>Penicillium chrysogenum</i>	KZN87403.1	6tpc.1.A	65.81	0.71	−1.27
	KZN89060.1	4yzp.1.A	35.2	0.65	−3.85
	KZN84919.1	6jyz.1.A	21.8	0.41	−7.31
	KZN93408.1	4mdo.1.A	74.74	0.92	0.69
	KZN93114.1	4mdo.1.A	54.66	0.46	−1.1
	KZN91501.1	6m4e.1.A	30.99	0.63	−4.96
<i>Penicillium crustosum</i>	AHA15977.1	5i79.1.A	65.2	0.57	−1.02
	XP_056725833.1	6tpc.1.A	64.08	0.68	−1.78
<i>Aspergillus flavus</i>	RMZ37468.1	4yzp.1.A	33.98	0.68	−3.52
	RAQ66523.1	4yzp.1.A	33.79	0.68	−3.43
	RMZ41992.1	5jl4.1.A	25.96	0.53	−5.41
	RMZ37535.1	6zb9.1.A	20.39	0.37	−3.62
	KAJ1715357.1	1ks4.1.A	76.92	0.84	−1.54
	KAJ1715009.1	8b7p.1.A	44.55	0.51	−1.96
	KAJ1713444.1	6ha5.1.A	72.05	0.86	−0.43
	KAJ1711735.1	3vl8.1.A	63.96	0.85	−0.63
	KAJ1709640.1	8b7p.1.A	46.19	0.58	−3.13
	RMZ41167.1	7eap.1.A	99.6	0.95	0.15
	RMZ38224.1	5fji.1.A	99.64	0.92	−0.25
	RMZ37309.1	6sz6.1.A	44.24	0.68	−4.23

	RAQ79441.1	6sz6.1.A	44.24	0.68	−4.23
	RAQ77926.1	3abz.1.A	45.82	0.81	−1.98
	RMZ39576.1	7zn6.1.A	49.82	0.79	−2.96
<i>Fusarium solani</i>	KAH7250822.1	1qjw.1.A	73.48	0.72	−0.94
	XP_046129634.1	4npr.1.A	53.18	0.8	−0.6
	XP_046126616.1	3ahy.1.A	51.84	0.82	−0.86
	KAJ4232191.1	3abz.1.A	50.18	0.83	−2.01
	KAJ4211136.1	5nbs.1.A	66.35	0.85	−1.16
	AGT80114.1	5lwx.1.A	36.87	0.7	−1.61
	AHD26939.1	5lwx.1.A	37.16	0.7	−1.57
	AHZ65142.1	1zpu.1.A	53.24	0.75	−1.74
	AHZ65141.1	3v9e.1.A	43.31	0.66	−2.96
	AHZ65140.1	1zpu.1.A	49.52	0.77	−0.74
<i>Penicillium citrinum</i>	XP_056501834.1	3abz.1.A	46.05	0.79	−2.07
	XP_056498616.1	5fjj.1.A	39.92	0.67	−4.24
	XP_056495445.1	5fjj.1.A	71.22	0.88	−0.44
<i>Fusarium equiseti</i>	AAM77703.1	5m2d.1.A	56.9	0.85	−0.35
	KAJ4127785.1	1gzj.1.A	63.58	0.72	−2.42
	KAJ4141610.1	5nbs.1.A	66.87	0.83	−1.2
	KAJ4133747.1	3abz.1.A	50.12	0.83	−2.07

Table S3. Best model search and validation of tridimensional structure using PROCHECK, ERRAT and ProSA servers. MFR, AAR, GAR, DS refer to most favored, additional allowed, generously allowed, and disallowed regions

Fungus	Accession	Best-fit Template	PROCHECK				ERRAT Quality factor	ProSA Z-score
			MFR	AAR	GAR	DS		
<i>A. arborescens</i>	XP_028501869.1	4mdo.1.A	89.2	9.8	0.7	0.2	98.5075	−10.79
	RYO56859.1	3zyz.1.A	91	8.5	0.5	0	91.0256	−10.67
<i>P. variotii</i>	GAD99276.1	4iic.1.A	90.9	8.6	0.5	0	92.963	−10.48
	GAD98731.1	4mdo.1.A	89.2	9.8	0.7	0.2	98.5075	−10.79
	GAD97601.1	5lwx.1.A	86.9	12.1	1.1	0	91.8669	−9.14
<i>T. griseum</i>	AAM77714.2	1uu4.1.A	88.3	11.7	0	0	92.9907	−6.96
<i>P. chrysogenum</i>	KZN87403.1	6tpc.1.A	89.2	10	0.4	0.4	96.4587	−8.07
	KZN93408.1	4mdo.1.A	89.2	9.8	0.7	0.2	98.5075	−10.79
<i>P. crustosum</i>	XP_056725833.1	6tpc.1.A	89.2	10	0.4	0.4	96.4587	−8.07
<i>A. flavus</i>	KAJ1715357.1	1ks4.1.A	84	14.9	0.5	0.5	89.5238	−6.51
	KAJ1713444.1	6ha5.1.A	87.9	11.5	0	0.5	93.9252	−6.48
	KAJ1711735.1	3vl8.1.A	92.1	7.9	0	0	89.604	−5.64
	RMZ41167.1	7eap.1.A	89.1	9.6	0.2	0.2	95.9459	−11.07
	RMZ38224.1	5fjj.1.A	89.1	10.3	0.7	0	93.0233	−10.3
<i>F. solani</i>	KAH7250822.1	1qjw.1.A	86.3	13.7	0	0	97.3126	−9.28
	XP_046129634.1	4npr.1.A	88.6	11.4	0	0	90.8654	−6.25
	XP_046126616.1	3ahy.1.A	90.6	8.6	0.8	0.1	95.1807	−9.99
	KAJ4211136.1	5nbs.1.A	89.5	9.2	0.3	0	94.2389	−10.67
	AHZ65142.1	1zpu.1.A	85.3	12.9	1.3	0.4	86.7144	−8.69
<i>P. citrinum</i>	XP_056495445.1	5fjj.1.A	89.1	10.3	0.7	0	93.0233	−10.3
<i>F. equiseti</i>	AAM77703.1	5m2d.1.A	89	11	0	0	89.6135	−5.87
	KAJ4127785.1	1gzj.1.A	89.8	8.8	0	0.4	96.7851	−8.48
	KAJ4141610.1	5nbs.1.A	90.5	9.2	0.3	0	94.2389	−10.67

Table S4. Predicted binding energies and interacting residues identified through molecular docking of cellobiose with four β -glucosidases from Moroccan fungal species using AutoDock. Bond distances (Å) refer to hydrogen bonding observed in Discovery Studio Visualizer

Protein PDB ID	Binding energy (kcal/mol)	Interacting residue	Bond distance (Å)
3zyz	-4.97	Asp61	2.08
		Arg67	1.80, 2.67
		Arg125	2.12
		Lys158	2.14
		Glu441	1.69
		Trp237	3.54
4iic	-0.85	Arg150	2.18
		Asn157	1.89, 2.70, 2.80, 2.94
		Phe161	1.77
		Val551	1.59
		Tyr607	2.92
		Asp633	1.76
3ahy	-4.67	Glu165	2.15
		Cys168	2.24
		Asn225	2.21
		Asp227	2.01
		Arg246	1.86
		Asn301	4.57
5nbs	-5.32	Trp339	2.04
		Asp88	1.95, 2.07
		Arg94	1.96
		Arg152	6.31
		Lys185	2.49
		Gln197	2.26
		Asp276	2.25
		Gln278	2.58