A New Hierarchy of Phylogenetic Models Consistent with Heterogeneous Substitution Rates - Supplementary Material

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1 Renaming of Basis Matrices

The translation between basis matrix names in Fernández-Sánchez et al. [2014] and this paper are as follows:

F-S *et al*	This paper	F-S *et al*	This paper	F-S *et al*	This paper
$B^{\texttt{id}}$	A	$B_1^{\texttt{id}}$	A_1	$B^{\texttt{sgn}}$	B
B^{ζ_1}	C	B^{ζ_2}	D	$B_1^{\zeta_2}$	D_1
B_1^{ξ}	E_1	B_3^{ξ}	F_1	B_5^{ξ}	G_1
B_2^{ξ}	E_2	B_4^{ξ}	F_2	B_6^{ξ}	G_2

2 Equilibrium Base Frequencies

A rate matrix Q in a Lie Markov model is a weighted sum of basis matrices, with weights $(a, a_1, b, c, d, d_1, e_1, e_2, f_1, f_2, g_1, g_2)$. (Depending on the model, some of these weights may be constrained to be zero.) Define

$$
\begin{aligned}
p &= 4a^3 + 4a^2a_1 + aa_1^2 - ab^2 + ac^2 - ad_1^2 + 2af_1g_1 + a_1f_1g_1 - d_1f_1g_1 \\
&\quad + bf_2g_1 + cf_2g_1 - bf_1g_2 + cf_1g_2 - 2af_2g_2 - a_1f_2g_2 - d_1f_2g_2 \\
q &= 4a^2d + 4aa_1d + a_1^2d - b^2d + c^2d - dd_1^2 - 2ae_1g_1 - a_1e_1g_1 + d_1e_1g_1 \\
&\quad - be_2g_1 - ce_2g_1 + be_1g_2 - ce_1g_2 + 2ae_2g_2 + a_1e_2g_2 + d_1e_2g_2 \\
r &= 4a^2e_1 + 2aa_1e_1 - 2ad_1e_1 + 2abe_2 + 2ace_2 + 4adf_1 \\
&\quad + 2a_1df_1 - 2dd_1f_1 + 2bdf_2 + 2cdf_2 + 2e_2f_1g_2 - 2e_1f_2g_2 \\
s &= 2abe_1 - 2ace_1 + 4a^2e_2 + 2aa_1e_2 + 2ad_1e_2 + 2bdf_1 \\
&\quad - 2cdf_1 + 4adf_2 + 2a_1df_2 + 2dd_1f_2 + 2e_2f_1g_1 - 2e_1f_2g_1
\end{aligned}
$$

then the equilibrium base frequencies are given by

$$
\begin{aligned}
\pi_A &= \frac{1}{4} + \frac{q+r}{4p} \\
\pi_G &= \frac{1}{4} + \frac{q-r}{4p} \\
\pi_C &= \frac{1}{4} + \frac{-q+s}{4p} \\
\pi_T &= \frac{1}{4} + \frac{-q-s}{4p}
\end{aligned}
$$

3 Nesting Diagram

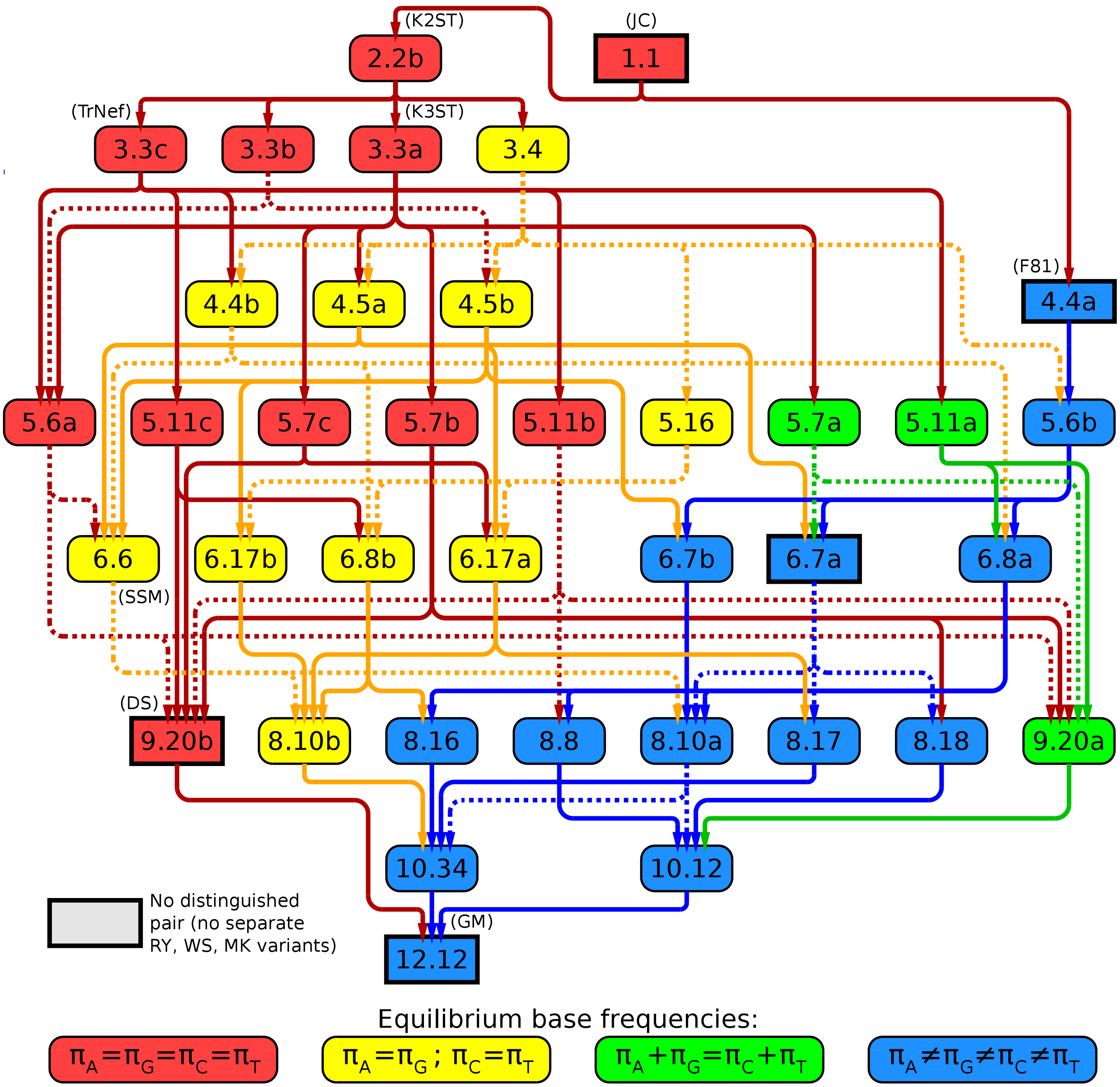

Figure S1: Nesting relationships of the RY Lie Markov models. (Colour version of paper figure 1.) Box colour indicates the degrees of freedom in equilibrium base frequencies. Solid or dotted connecting lines are to reduce visual confusion and have no additional significance.

4 AICc Rank Summary

Table S1: Summary of rankings of models under AICc for the 7 data sets. Models marked "*" are time reversible, non-Lie Markov models. EBF DF = Equilibrium frequency degrees of freedom. AICc penalizes high dimensional models less strongly than BIC.

Model	Median rank	Best rank	EBF DF	Model	Median rank	Best rank	EBF DF	Model	Median rank	Best rank	EBF DF
12.12	1	1	3	9.20b	39	5	0	WS8.8	73	8	3
RY10.12	4	2	3	*SYM	41	4	0	WS8.16	74	10	3
RY8.8	4	1	3	RY8.10b	41	33	1	MK6.7b	75	42	3
RY8.18	7	1	3	WS4.5a	42	26	1	WS6.7b	76	27	3
*GTR	9	2	3	MK8.10b	43	7	1	MK8.8	76	39	3
MK10.34	9	2	3	RY6.8b	43	38	1	MK8.16	77	38	3
WS10.34	9	6	3	RY6.6	47	39	1	WS6.8a	78	2	3
*TVM	10	4	3	WS6.6	48	7	1	MK6.8a	79	41	3
WS10.12	11	3	3	*TVMef	49	24	0	WS5.6b	79	31	3
WS8.10a	13	3	3	MK6.6	50	18	1	WS6.17b	82	39	1
RY9.20a	15	2	2	RY5.11b	50	1	0	WS5.11a	82	50	2
*K81uf	15	9	3	RY5.11c	50	34	0	MK5.6b	84	41	3
*TIM	16	8	3	WS5.7a	51	25	2	WS6.8b	87	20	1
MK8.17	17	5	3	RY6.17a	51	34	1	WS5.16	87	40	1
*TrN	18	4	3	RY5.16	52	40	1	MK5.11a	88	43	2
*HKY	18	5	3	MK6.17a	53	36	1	WS5.11b	88	64	0
MK10.12	19	7	3	RY6.17b	53	36	1	WS4.5b	89	29	1
MK8.10a	19	10	3	RY4.4b	54	25	1	MK4.5b	89	68	1
RY8.16	20	3	3	MK5.6a	57	37	0	WS4.4b	91	6	1
RY10.34	21	2	3	RY4.5a	58	44	1	MK6.8b	91	67	1
WS8.10b	21	10	1	RY5.7b	59	8	0	MK4.4b	91	65	1
WS8.17	22	15	3	WS5.6a	60	40	0	WS3.4	92	36	1
RY8.10a	23	12	3	RY5.6a	60	29	0	MK6.17b	93	69	1
RY6.8a	23	18	3	*TIMef	61	22	0	WS3.3b	93	77	0
MK8.18	24	16	3	RY5.7c	61	43	0	WS5.11c	94	67	0
RY8.17	25	8	3	MK4.5a	62	36	1	MK5.16	96	71	1
MK9.20a	27	20	2	WS5.7c	62	35	0	WS3.3c	97	58	0
6.7a	28	23	3	MK5.7c	64	31	0	MK5.11b	97	82	0
WS8.18	28	20	3	MK5.7b	66	44	0	MK3.4	98	70	1
RY5.11a	32	15	2	RY4.5b	66	47	1	WS2.2b	98	75	0
RY6.7b	33	26	3	RY3.3c	67	20	0	4.4a	99	49	3
RY5.6b	34	27	3	RY3.4	68	48	1	MK5.11c	99	79	0
RY5.7a	35	23	2	WS5.7b	69	51	0	MK3.3c	99	86	0
MK5.7a	36	22	2	3.3a	70	62	0	MK3.3b	100	85	0
WS9.20a	38	25	2	RY3.3b	71	65	0	MK2.2b	106	86	0
WS6.17a	38	17	1	RY2.2b	72	58	0	*JC	108	97	0

5 BIC Scores and Ranks

Table S2: Relative Bayesian Information Criterion (BIC) scores for all models for a range of data sets. The ***bold italic*** entry is the BIC score for the optimal model, all other entries in the column are relative to this. (Lower values are better, values below 2 indicate the model is not significantly worse than the optimal model).

Clade:	Human	Angiosperms	Cormorants	Yeast	Teleost Fish	Buttercups	Ratites
Approx range:	Species	Class	Family	Genus	mult. orders	Genus	Order
DNA type	mitoch	chlorop	mito/nuc	mostly nuc	nuclear	chlorop	mitoch
taxa×sites	53×202	15×89436	33×1141	8×127026	11×2178	14×4135	27×7324
Site rate model	$+\Gamma + I$	$+\Gamma$	$+\Gamma + I$	$+\Gamma + I$	$+\Gamma$	$+I$	$+\Gamma + I$
JC	3051.5	22001.2	1452.7	67394.1	640.8	548.3	4913.6
TVMef	1644.6	6554.4	308.0	17193.7	12.9	531.6	667.7
TIMef	1658.2	6837.5	313.0	17894.0	6.7	535.7	900.7
SYM	1654.3	6523.9	287.5	16044.0	9.5	539.8	489.7
HKY	8.9	1886.4	***12790.7***	2840.4	17.5	55.3	121.7
TrN	***58370.3***	1896.3	6.5	1640.5	19.6	63.2	119.5
K81uf	18.6	903.2	6.8	2794.0	23.8	14.4	101.8
TVM	29.9	615.5	19.3	1518.7	25.6	24.7	8.6
TIM	9.7	913.0	13.3	1613.4	25.9	22.3	99.5
GTR	21.3	626.6	25.4	79.8	28.6	32.6	15.2
RY2.2b	1642.2	7436.1	340.8	19109.1	3.4	555.2	1131.2
WS2.2b	2559.7	15064.3	975.3	53685.9	477.9	521.4	3329.4
MK2.2b	2565.1	19735.7	1167.6	49359.0	432.0	540.0	4077.4
3.3a	1651.9	6862.3	333.3	19032.7	10.0	527.5	1083.3
RY3.3b	1651.4	7438.0	343.1	19058.9	11.1	562.9	1108.1
WS3.3b	2560.3	14560.1	970.4	51362.2	465.4	528.4	3178.1
MK3.3b	2565.0	19745.6	1018.2	49239.4	432.8	547.5	3600.7
RY3.3c	1651.8	7411.2	320.7	17969.0	0.1	563.4	948.2
WS3.3c	2565.4	14818.8	979.4	52886.6	481.6	517.2	3114.4
MK3.3c	2554.1	19677.0	1142.7	48282.1	432.1	548.4	3889.1
RY3.4	1408.6	7348.9	328.2	19065.8	8.5	561.1	635.2
WS3.4	2391.5	10330.8	975.8	41248.8	479.9	0.0	2995.3
MK3.4	1593.8	19690.4	1017.2	49026.3	439.5	546.6	3845.3
4.4a	1469.4	17487.5	1278.4	57328.3	643.7	50.4	3569.3
RY4.4b	1418.3	7351.9	315.0	17696.5	7.5	569.2	584.7
WS4.4b	2372.3	8995.5	981.9	37817.6	487.3	0.0	3001.6
MK4.4b	1498.4	19677.1	924.3	48275.5	435.7	554.9	3835.5
RY4.5a	1418.3	6772.4	319.7	18991.0	15.1	533.2	572.5
WS4.5a	1500.7	2875.5	323.9	6743.0	11.1	5.1	822.3
MK4.5a	780.8	6824.2	207.0	18771.5	17.2	534.2	837.3
RY4.5b	1417.9	7346.4	328.7	19017.6	16.2	568.6	599.2
WS4.5b	2369.5	10221.3	974.5	35049.5	470.9	6.0	2945.8
MK4.5b	1593.9	19701.5	761.3	48999.9	439.6	554.2	3098.4
RY5.6a	1670.7	6842.4	318.7	17844.8	14.3	543.7	877.8
WS5.6a	1668.1	6020.3	329.7	18344.7	16.9	530.1	832.6
MK5.6a	1651.3	6817.0	315.7	17885.1	15.3	543.7	898.4
RY5.6b	338.3	3644.1	196.2	6464.1	17.4	57.9	100.9
WS5.6b	1096.1	10184.2	910.2	41261.3	488.2	12.4	2216.1
MK5.6b	1110.8	15677.2	980.6	39734.4	436.5	38.2	2847.8
RY5.7a	582.3	2848.2	207.8	6532.9	18.2	10.7	547.7
WS5.7a	435.9	6752.4	185.7	18762.5	22.1	537.6	240.1
MK5.7a	1147.4	2801.9	305.2	6735.0	16.1	10.3	260.3
RY5.7b	1656.2	6835.6	327.0	17919.1	6.4	538.6	866.6

Clade:	Human	Angiosperms	Cormorants	Yeast	Teleost Fish	Buttercups	Ratites
WS5.7b	1661.4	6855.1	331.7	17869.2	23.4	543.6	1066.5
MK5.7b	1670.4	6037.2	342.8	18823.0	22.9	530.7	780.8
RY5.7c	1661.4	6030.0	330.3	18127.6	25.0	530.7	835.4
WS5.7c	1657.8	6847.5	337.9	18320.3	14.7	543.8	820.3
MK5.7c	1668.1	6858.0	321.3	18028.1	14.9	538.5	1010.8
RY5.11a	521.0	3712.9	182.1	5647.6	9.6	60.2	412.5
WS5.11a	1211.7	14679.0	899.6	52898.0	489.8	528.8	2324.4
MK5.11a	2024.7	15630.1	1082.6	39206.5	428.8	40.0	2945.7
RY5.11b	1656.6	7297.2	296.5	16692.0	***27905.0***	579.2	672.5
WS5.11b	2584.4	14817.4	914.9	52094.1	491.7	533.2	2877.7
MK5.11b	2568.5	19168.8	1134.4	47079.0	440.6	561.9	3567.1
RY5.11c	1664.1	6607.5	308.8	17183.5	14.5	578.1	749.2
WS5.11c	2582.8	14803.1	984.0	52669.4	484.3	533.5	2980.0
MK5.11c	2573.2	19218.5	1154.2	47887.7	434.6	564.2	3820.6
RY5.16	1421.3	6547.6	317.6	18132.2	23.3	575.8	457.6
WS5.16	2402.8	10301.5	980.4	41177.5	482.5	16.2	2885.7
MK5.16	1613.1	19230.1	1026.2	48424.3	443.6	562.4	3774.8
RY6.6	1437.3	6783.1	313.0	17571.7	21.8	549.5	517.3
WS6.6	1474.5	131.7	335.9	2332.9	23.9	13.1	729.2
MK6.6	595.7	6817.0	51.9	17866.6	19.0	550.2	832.7
6.7a	347.9	2746.7	192.6	6475.5	23.2	17.4	92.2
RY6.7b	347.9	3643.5	197.3	6377.0	25.1	64.8	101.5
WS6.7b	1080.3	10076.1	915.6	35057.9	479.6	18.2	2222.8
MK6.7b	1105.0	15687.9	727.6	39728.1	438.2	46.2	2150.9
RY6.8a	297.7	3646.1	175.9	5389.6	17.0	66.1	65.0
WS6.8a	1016.8	8868.8	903.1	37817.7	495.5	11.5	2223.0
MK6.8a	967.1	15632.1	850.9	39216.3	432.6	46.5	2853.8
RY6.8b	1431.1	6548.4	303.0	16851.7	21.9	583.9	426.9
WS6.8b	2389.5	8976.8	986.5	37685.6	490.0	16.2	2893.7
MK6.8b	1517.4	19219.9	937.2	47869.2	438.8	570.7	3764.6
RY6.17a	1428.6	5939.8	318.4	18050.1	29.8	536.1	392.8
WS6.17a	1508.9	2838.5	334.7	6380.4	15.9	21.2	689.2
MK6.17a	794.5	6820.1	217.7	17903.4	21.6	545.3	780.8
RY6.17b	1431.0	6551.3	323.9	18055.7	31.0	583.4	406.4
WS6.17b	2382.8	10194.7	980.4	35043.1	473.5	22.1	2846.5
MK6.17b	1613.1	19240.0	774.6	48404.7	444.9	570.2	3098.5
RY8.8	13.5	717.0	10.8	946.5	20.2	74.4	68.3
WS8.8	1010.6	8856.0	842.9	37273.1	508.4	26.2	2060.0
MK8.8	961.0	15475.6	822.2	37354.1	442.3	60.9	2681.0
RY8.10a	312.5	2756.0	177.8	5308.8	30.6	32.4	63.9
WS8.10a	248.2	27.3	205.1	2008.8	35.9	24.4	34.7
MK8.10a	106.3	2724.7	17.3	5770.1	25.2	31.5	101.5
RY8.10b	1448.0	5952.0	311.6	16697.6	36.0	552.5	348.4
WS8.10b	1481.4	108.5	344.4	1878.3	28.4	29.2	608.7
MK8.10b	611.3	6813.8	51.4	17171.5	22.3	561.3	781.2
RY8.16	306.7	3210.7	176.7	4812.5	31.5	77.6	***89371.1***
WS8.16	982.0	8886.9	880.8	37653.5	501.1	26.3	2152.9
MK8.16	940.1	14635.2	833.3	38609.4	444.4	60.5	2733.5
RY8.17	354.7	2667.6	205.1	5663.8	38.0	27.9	30.5
WS8.17	106.7	2753.1	21.6	6329.0	26.3	31.4	102.6
MK8.17	246.6	26.9	205.2	2189.9	34.3	25.0	72.3
RY8.18	15.4	16.0	16.2	2297.9	23.5	24.0	67.1
WS8.18	359.4	2747.4	205.7	5962.2	37.1	31.0	101.7
MK8.18	344.5	2674.8	200.6	6134.7	37.2	28.7	70.0
RY9.20a	265.7	89.5	26.3	1156.6	25.1	34.3	421.8
WS9.20a	448.9	5918.2	211.5	17202.3	42.3	556.3	116.0

Clade:	Human	Angiosperms	Cormorants	Yeast	Teleost Fish	Buttercups	Ratites
MK9.20a	1179.4	2666.6	299.1	4884.5	36.2	37.7	108.8
9.20b	1686.1	5963.2	292.4	16048.2	26.9	562.7	485.0
RY10.12	30.5	29.8	20.1	912.0	32.5	40.1	64.1
WS10.12	259.6	28.3	217.1	1450.6	49.3	39.1	18.6
MK10.12	122.0	2666.9	31.3	4886.6	39.9	44.2	42.3
RY10.34	323.1	2680.5	188.9	4686.8	44.8	44.0	7.8
WS10.34	33.5	36.1	26.2	1823.4	38.7	39.3	44.6
MK10.34	31.1	***861748.3***	22.9	1663.0	35.4	40.1	80.8
12.12	48.2	16.9	30.1	***1365233.1***	46.0	55.4	14.0

Table S3: For each data set, the models ranked by BIC score, from best to worst.

Human $+\Gamma+I$	Angiosperms $+\Gamma$	Cormorants $+\Gamma+I$	Yeast $+\Gamma+I$	Teleost Fish $+\Gamma$	Buttercups $+I$	Ratites $+\Gamma+I$
TrN	MK10.34	HKY	12.12	RY5.11b	WS4.4b	RY8.16
HKY	RY8.18	TrN	GTR	RY3.3c	WS3.4	RY10.34
TIM	12.12	K81uf	RY10.12	RY2.2b	WS4.5a	TVM
RY8.8	MK8.17	RY8.8	RY8.8	RY5.7b	WS4.5b	12.12
RY8.18	WS8.10a	TIM	RY9.20a	TIMef	MK5.7a	GTR
K81uf	WS10.12	RY8.18	WS10.12	RY4.4b	RY5.7a	WS10.12
GTR	RY10.12	MK8.10a	TVM	RY3.4	WS6.8a	RY8.17
TVM	WS10.34	TVM	TIM	SYM	WS5.6b	WS8.10a
RY10.12	RY9.20a	RY10.12	TrN	RY5.11a	WS6.6	MK10.12
MK10.34	WS8.10b	WS8.17	MK10.34	3.3a	K81uf	WS10.34
WS10.34	WS6.6	MK10.34	WS10.34	RY3.3b	WS5.16	RY8.10a
12.12	TVM	GTR	WS8.10b	WS4.5a	WS6.8b	RY10.12
MK8.10a	GTR	WS10.34	WS8.10a	TVMef	6.7a	RY6.8a
WS8.17	RY8.8	RY9.20a	MK8.17	RY5.6a	WS6.7b	RY8.18
MK10.12	K81uf	12.12	RY8.18	RY5.11c	WS6.17a	RY8.8
MK8.17	TIM	MK10.12	WS6.6	WS5.7c	WS6.17b	MK8.18
WS8.10a	HKY	MK8.10b	K81uf	MK5.7c	TIM	MK8.17
WS10.12	TrN	MK6.6	HKY	RY4.5a	RY8.18	MK10.34
RY9.20a	MK9.20a	RY6.8a	RY10.34	MK5.6a	WS8.10a	6.7a
RY6.8a	MK10.12	RY8.16	RY8.16	WS6.17a	TVM	TIM
RY8.16	RY8.17	RY8.10a	MK9.20a	MK5.7a	MK8.17	RY5.6b
RY8.10a	MK8.18	RY5.11a	MK10.12	RY4.5b	WS8.8	RY6.7b
RY10.34	RY10.34	WS5.7a	RY8.10a	WS5.6a	WS8.16	MK8.10a
RY5.6b	MK8.10a	RY10.34	RY6.8a	RY6.8a	RY8.17	WS8.18
MK8.18	6.7a	6.7a	RY5.11a	MK4.5a	MK8.18	K81uf
RY6.7b	WS8.18	RY5.6b	RY8.17	RY5.6b	WS8.10b	WS8.17
6.7a	WS8.17	RY6.7b	MK8.10a	HKY	WS8.18	MK9.20a
RY8.17	RY8.10a	MK8.18	WS8.18	RY5.7a	WS8.17	WS9.20a
WS8.18	MK5.7a	RY8.17	MK8.18	MK6.6	MK8.10a	TrN
WS5.7a	WS6.17a	WS8.10a	WS8.17	TrN	RY8.10a	HKY
WS9.20a	RY5.7a	MK8.17	RY6.7b	RY8.8	GTR	WS5.7a
RY5.11a	WS4.5a	WS8.18	WS6.17a	MK6.17a	RY9.20a	MK5.7a

Human	Angiosperms	Cormorants	Yeast	Teleost Fish	Buttercups	Ratites
RY5.7a	RY8.16	MK4.5a	RY5.6b	RY6.6	MK9.20a	RY8.10b
MK6.6	RY6.7b	RY5.7a	6.7a	RY6.8b	MK5.6b	RY6.17a
MK8.10b	RY5.6b	WS9.20a	RY5.7a	WS5.7a	WS10.12	RY6.17b
MK4.5a	RY6.8a	WS10.12	MK5.7a	MK8.10b	WS10.34	RY5.11a
MK6.17a	RY5.11a	MK6.17a	WS4.5a	MK5.7b	MK5.11a	RY9.20a
MK8.16	WS9.20a	SYM	SYM	6.7a	MK10.34	RY6.8b
MK8.8	RY6.17a	9.20b	9.20b	RY5.16	RY10.12	RY5.16
MK6.8a	RY8.10b	RY5.11b	RY5.11b	WS5.7b	RY10.34	9.20b
WS8.16	9.20b	MK9.20a	RY8.10b	RY8.18	MK10.12	SYM
WS8.8	WS5.6a	RY6.8b	RY6.8b	K81uf	MK6.7b	RY6.6
WS6.8a	RY5.7c	MK5.7a	MK8.10b	WS6.6	MK6.8a	RY5.7a
WS6.7b	MK5.7b	TVMef	RY5.11c	RY5.7c	4.4a	RY4.5a
WS5.6b	SYM	RY5.11c	TVMef	RY9.20a	HKY	RY4.4b
MK6.7b	RY5.16	RY8.10b	WS9.20a	RY6.7b	12.12	RY4.5b
MK5.6b	RY6.8b	TIMef	RY6.6	MK8.10a	RY5.6b	WS8.10b
MK5.7a	RY6.17b	RY6.6	RY4.4b	TVM	RY5.11a	RY3.4
MK9.20a	TVMef	RY4.4b	RY5.6a	TIM	MK8.16	TVMef
WS5.11a	RY5.11c	MK5.6a	MK6.6	WS8.17	MK8.8	RY5.11b
RY3.4	WS5.7a	RY5.16	WS5.7b	9.20b	TrN	WS6.17a
RY4.5b	RY4.5a	RY6.17a	MK5.6a	WS8.10b	RY6.7b	WS6.6
RY4.5a	RY6.6	RY5.6a	TIMef	GTR	RY6.8a	RY5.11c
RY4.4b	MK8.10b	RY4.5a	MK6.17a	RY6.17a	RY8.8	MK6.17a
RY5.16	MK5.6a	RY3.3c	RY5.7b	RY8.10a	RY8.16	MK5.7b
RY6.17a	MK6.6	MK5.7c	RY3.3c	RY6.17b	WS3.3c	MK8.10b
RY6.17b	MK6.17a	WS4.5a	MK5.7c	RY8.16	WS2.2b	WS5.7c
RY6.8b	MK4.5a	RY6.17b	RY6.17a	RY10.12	3.3a	WS4.5a
RY6.6	RY5.7b	RY5.7b	RY6.17b	MK8.17	WS3.3b	WS5.6a
RY8.10b	TIMef	RY3.4	RY5.7c	MK10.34	WS5.11a	MK6.6
4.4a	RY5.6a	RY4.5b	RY5.16	WS8.10a	WS5.6a	RY5.7c
WS6.6	WS5.7c	WS5.6a	WS5.7c	RY8.10b	RY5.7c	MK4.5a
WS8.10b	WS5.7b	RY5.7c	WS5.6a	MK9.20a	MK5.7b	RY5.7b
MK4.4b	MK5.7c	WS5.7b	WS5.7a	WS8.18	TVMef	RY5.6a
WS4.5a	3.3a	3.3a	MK4.5a	MK8.18	WS5.11b	MK5.6a
WS6.17a	RY5.11b	WS6.17a	MK5.7b	RY8.17	RY4.5a	TIMef
MK6.8b	RY4.5b	WS6.6	RY4.5a	WS10.34	WS5.11c	RY3.3c
MK3.4	RY3.4	WS5.7c	RY4.5b	MK10.12	MK4.5a	MK5.7c
MK4.5b	RY4.4b	RY2.2b	3.3a	WS9.20a	TIMef	WS5.7b
MK5.16	RY3.3c	MK5.7b	RY3.3b	RY10.34	RY6.17a	3.3a
MK6.17b	RY2.2b	RY3.3b	RY3.4	12.12	WS5.7a	RY3.3b
RY2.2b	RY3.3b	WS8.10b	RY2.2b	WS10.12	MK5.7c	RY2.2b
TVMef	WS8.8	MK6.7b	WS6.17b	MK5.11a	RY5.7b	WS8.8
MK5.6a	WS6.8a	MK4.5b	WS4.5b	MK2.2b	SYM	MK6.7b
RY3.3b	WS8.16	MK6.17b	WS6.7b	MK3.3c	MK2.2b	WS8.16
RY3.3c	WS6.8b	MK8.8	WS8.8	MK6.8a	WS5.7b	WS5.6b
3.3a	WS4.4b	MK8.16	MK8.8	MK3.3b	MK5.6a	WS6.7b
SYM	WS6.7b	WS8.8	WS8.16	MK5.11c	RY5.6a	WS6.8a

Human	Angiosperms	Cormorants	Yeast	Teleost Fish	Buttercups	Ratites
RY5.7b	WS5.6b	MK6.8a	WS6.8b	MK4.4b	WS5.7c	WS5.11a
RY5.11b	WS6.17b	WS8.16	WS4.4b	MK5.6b	MK6.17a	MK8.8
WS5.7c	WS4.5b	WS5.11a	WS6.8a	MK6.7b	MK3.4	MK8.16
TIMef	WS5.16	WS6.8a	MK8.16	MK6.8b	MK3.3b	WS6.17b
RY5.7c	WS3.4	WS5.6b	MK5.11a	MK3.4	JC	MK5.6b
WS5.7b	WS3.3b	WS5.11b	MK6.8a	MK4.5b	MK3.3c	MK6.8a
RY5.11c	MK8.16	WS6.7b	MK6.7b	MK5.11b	RY6.6	WS5.11b
WS5.6a	WS5.11a	MK4.4b	MK5.6b	MK8.8	MK6.6	WS5.16
MK5.7c	WS5.11c	MK6.8b	WS5.16	MK5.16	RY8.10b	WS6.8b
MK5.7b	WS5.11b	WS3.3b	WS3.4	MK8.16	MK4.5b	MK5.11a
RY5.6a	WS3.3c	WS4.5b	WS5.6b	MK6.17b	MK4.4b	WS4.5b
9.20b	WS2.2b	WS2.2b	MK5.11b	WS3.3b	RY2.2b	WS5.11c
MK5.11a	MK8.8	WS3.4	MK6.8b	WS4.5b	WS9.20a	WS3.4
WS4.5b	MK5.11a	WS3.3c	MK5.11c	WS6.17b	RY3.4	WS4.4b
WS4.4b	MK6.8a	WS5.16	MK4.4b	WS2.2b	MK8.10b	MK4.5b
WS6.17b	MK5.6b	WS6.17b	MK3.3c	WS6.7b	MK5.11b	MK6.17b
WS6.8b	MK6.7b	MK5.6b	MK6.17b	WS3.4	MK5.16	WS3.3c
WS3.4	4.4a	WS4.4b	MK5.16	WS3.3c	9.20b	WS3.3b
WS5.16	MK5.11b	WS5.11c	MK4.5b	WS5.16	RY3.3b	WS2.2b
MK3.3c	MK5.11c	WS6.8b	MK3.4	WS5.11c	RY3.3c	MK5.11b
WS2.2b	MK6.8b	MK3.4	MK3.3b	WS4.4b	MK5.11c	4.4a
WS3.3b	MK5.16	MK3.3b	MK2.2b	WS5.6b	RY4.5b	MK3.3b
MK3.3b	MK6.17b	MK5.16	WS3.3b	WS5.11a	RY4.4b	MK6.8b
MK2.2b	MK3.3c	MK5.11a	WS5.11b	WS6.8b	MK6.17b	MK5.16
WS3.3c	MK4.4b	MK5.11b	WS5.11c	WS5.11b	MK6.8b	MK5.11c
MK5.11b	MK3.4	MK3.3c	WS3.3c	WS6.8a	RY5.16	MK4.4b
MK5.11c	MK4.5b	MK5.11c	WS5.11a	WS8.16	RY5.11c	MK3.4
WS5.11c	MK2.2b	MK2.2b	WS2.2b	WS8.8	RY5.11b	MK3.3c
WS5.11b	MK3.3b	4.4a	4.4a	JC	RY6.17b	MK2.2b
JC	JC	JC	JC	4.4a	RY6.8b	JC

6 Fourier-Motzkin Parameterizations

In tables S4 to S8, the parameters A, B, C, D, D_1, E_1, E_2, F_1, F_2, G_1, G_2 are all constrained to have absolute value less than or equal to 1. (These parameters are real numbers, not the basis matrices of the same name in the main paper.) The parameterizations listed here constrain the resulting rate matrix to have trace of -4. (I.e. when constructing a Markov matrix by $M = e^{Qt}$, the units of time t will approximately be expected number of mutations per site.) The formulæ are derived in a *Mathematica* notebook, also included in the supplementary material. These parameterizations are not unique, as they depend on the order in which variables are chosen for elimination.

Model	Fourier-Motzkin Parameterization
2.2b (K2ST)	$a = (A+1)/4$
	$a_1 = 1-3a$
3.3a (K3ST)	$a = (A+1)/4$
	$a_1 = 1-3a$
	$b = Ba$
3.3b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$c = Ca$
3.3c (TrNef)	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d_1 = D_1 a$
3.4	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d = D\min(a_1+a, a)$
4.4a (F81)	$a = 1/3$
	$d = Da$
	$e_1 = E_1(a+d)$
	$e_2 = E_2(a-d)$
4.4b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d = Da$
	$d_1 = D_1(a_1+a)-d$
4.5a	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d = D\min(a_1+a, a)$
	$b = B(a-\lvert d\rvert)$
4.5b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d = D\min(a_1+a, a)$
	$c = C(a-\lvert d\rvert)$
5.6a	$a = (A+1)/4$
	$a_1 = 1-3a$
	$c = Ca$
	$b = B(a-\lvert c\rvert)$
	$d_1 = D_1(a_1+a)$

Model	Fourier-Motzkin Parameterization
5.6b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d = D\min(a_1+a, a)$
	$e_1 = E_1\min(a_1+a+d, a+d)$
	$e_2 = E_2\min(a_1+a-d, a-d)$
5.7a	$a = (A+1)/4$
	$a_1 = 1-3a$
	$b = Ba$
	$e_1 = E_1\min(a_1+a, a-\lvert b\rvert)$
	$e_2 = E_2\min(a_1+a, a-\lvert b\rvert)$
5.7b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$b = Ba$
	$f_1 = K\min(a_1+a, a-\lvert b\rvert)$
	$f_2 = L\min(a_1+a, a-\lvert b\rvert)$
5.7c	$a = (A+1)/4$
	$a_1 = 1-3a$
	$b = Ba$
	$g_1 = G_1\min(a_1+a, a-\lvert b\rvert)$
	$g_2 = G_2\min(a_1+a, a-\lvert b\rvert)$
5.11a	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d_1 = D_1(a_1+a)$
	$e_1 = E_1\min(a_1+a+d_1, a)$
	$e_2 = E_2\min(a_1+a-d_1, a)$
5.11b	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d_1 = D_1(a_1+a)$
	$f_1 = F_1\min(a_1+a+d_1, a)$
	$f_2 = F_2\min(a_1+a-d_1, a)$
5.11c	$a = (A+1)/4$
	$a_1 = 1-3a$
	$d_1 = D_1(a_1+a)$
	$g_1 = G_1\min(a_1+a+d_1, a)$
	$g_2 = G_2\min(a_1+a-d_1, a)$

Table S4: Fourier-Motzkin parameterizations, up to 5.11c

Model	Fourier-Motzkin Parameterization
5.16	$a = (A+1)/4$ $a_1 = 1-3a$ $d = D\min(a_1+a, a)$ $g_1 = G_1\min(a_1+a+d, a-d)$ $g_2 = G_2\min(a_1+a-d, a+d)$
6.6	$a = (A+1)/4$ $a_1 = 1-3a$ $c = Ca$ $b = Ba$ $d = \frac{1-D}{2}(-a+\lvert c+b\rvert) + \frac{1+D}{2}(a-\lvert c-b\rvert)$ $d_1 = D_1(a_1+a) - d$
6.7a	$a = (A+1)/4$ $a_1 = 1-3a$ $b = Ba$ $d = D\min(a-\lvert b\rvert, a_1+a)$ $e_1 = E_1\min(a+d-\lvert b\rvert, a_1+a+d)$ $e_2 = E_2\min(a-d-\lvert b\rvert, a_1+a-d)$
6.7b	$a = (A+1)/4$ $a_1 = 1-3a$ $c = Ca$ $d = D\min(a-\lvert b\rvert, a_1+a)$ $e_1 = E_1\min(a+d-\lvert b\rvert, a_1+a+d)$ $e_2 = E_2\min(a-d-\lvert b\rvert, a_1+a-d)$
6.8a	$a = (A+1)/4$ $a_1 = 1-3a$ $d = Da$ $d_1 = D_1(a_1+a) - d$ $e_1 = E_1\min(a+d, a_1+a+d_1+d)$ $e_2 = E_2\min(a-d, a_1+a-d_1-d)$
6.8b	$a = (A+1)/4$ $a_1 = 1-3a$ $d = Da$ $d_1 = D_1(a_1+a) - d$ $g_1 = G_1\min(a-d, a_1+a+d_1+d)$ $g_2 = G_2\min(a+d, a_1+a-d_1-d)$
6.17a	$a = (A+1)/4$ $a_1 = 1-3a$ $b = Ba$ $d = D\min(a-\lvert b\rvert, a_1+a)$ $g_1 = G_1\min(a-d-\lvert b\rvert, a_1+a+d)$ $g_2 = G_2\min(a+d-\lvert b\rvert, a_1+a-d)$

Table S5: Fourier-Motzkin parameterizations, 5.16 to 6.17a

Model	Fourier-Motzkin Parameterization
6.17b	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ c &= Ca \\ d &= D\min(a-\lvert c\rvert, a_1+a) \\ g_1 &= G_1\min(a-d-\lvert c\rvert, a_1+a+d) \\ g_2 &= G_2\min(a+d-\lvert c\rvert, a_1+a-d) \end{aligned}$
8.8	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ d &= Da \\ d_1 &= D_1(a_1+a)-d \\ e_1 &= E_1(\tfrac{a_1}{2}+a+\tfrac{d_1}{2}+d) \\ e_2 &= E_2(\tfrac{a_1}{2}+a-\tfrac{d_1}{2}-d) \\ f_1 &= \tfrac{1-F_1}{2}\max(-a-d+e_1, -a_1-a-d_1-d-e_1) \\ &+ \tfrac{1+F_1}{2}\min(a+d+e_1, a_1+a+d_1+d-e_1) \\ f_2 &= \tfrac{1-F_2}{2}\max(-a+d-e_2, -a_1-a+d_1+d+e_2) \\ &+ \tfrac{1+F_2}{2}\min(a-d-e_2, a_1+a-d_1-d+e_2) \end{aligned}$
8.10a	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ d_1 &= (a_1+2a) \\ d &= \tfrac{1-D}{2}\max(-a_1-a-d_1, -a)+\tfrac{1+D}{2}\min(a_1+a-d_1, a) \\ e_1 &= E_1\min(a+d, a_1+a+d_1+d) \\ e_2 &= E_2\min(a-d, a_1+a-d_1-d) \\ c &= C(a-\tfrac{\lvert e_1\rvert}{2}-\tfrac{\lvert e_2\rvert}{2}) \\ b &= \tfrac{1-B}{2}\max(-a+c+d+\lvert e_2\rvert, -a-c-d+\lvert e_1\rvert) \\ &+ \tfrac{1+B}{2}\min(a-c+d-\lvert e_1\rvert, a+c-d-\lvert e_2\rvert) \end{aligned}$
8.10b	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ d_1 &= D_1(a_1+2a) \\ d &= \tfrac{1-D}{2}\max(-a_1-a-d_1, -a)+\tfrac{1+D}{2}\min(a_1+a-d_1, a) \\ g_1 &= G_1\min(a-d, a_1+a+d_1+d) \\ g_2 &= G_2\min(a+d, a_1+a-d_1-d) \\ c &= (a-\tfrac{\lvert g_1\rvert}{2}-\tfrac{\lvert g_2\rvert}{2}) \\ b &= \tfrac{1-B}{2}\max(-a+c+d+\lvert g_1\rvert, -a-c-d+\lvert g_2\rvert) \\ &+ \tfrac{1+B}{2}\min(a-c+d-\lvert g_2\rvert, a+c-d-\lvert g_1\rvert) \end{aligned}$
8.16	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ d_1 &= D_1(a_1+2a) \\ d &= \tfrac{1-D}{2}\max(-a_1-a-d_1, -a)+\tfrac{1+D}{2}\min(a_1+a-d_1, a) \\ e_1 &= E_1\min(a+d, a_1+2a, a_1+2a+d_1) \\ e_2 &= E_2\min(a-d, a_1+2a-\lvert d_1\rvert-\lvert e_1\rvert) \\ g_1 &= \tfrac{1-G_1}{2}\max(-a_1-a-d_1-d-e_1, -a+d+\lvert e_2\rvert) \\ &+ \tfrac{1+G_1}{2}\min(a_1+a+d_1+d-e_1, a-d-\lvert e_2\rvert) \\ g_2 &= \tfrac{1-G_2}{2}\max(-a_1-a+d_1+d-e_2, -a-d+\lvert e_1\rvert) \\ &+ \tfrac{1+G_2}{2}\min(a_1+a-d_1-d-e_2, a+d-\lvert e_1\rvert) \end{aligned}$

Table S6: Fourier-Motzkin parameterizations, 6.17b to 8.16

Model			Fourier-Motzkin Parameterization
	a	$=$	$(A+1)/4$
	a_1	$=$	$1-3a$
	b	$=$	Ba
	d	$=$	$D\min(a_1+a, a-\lvert b\rvert)$
	e_1	$=$	$E_1(a+d)$
8.17	e_2	$=$	$\frac{1-E_2}{2}\max(-a_1-2a+\lvert b-e_1\rvert, -a+d)$
		$+$	$\frac{1+E_2}{2}\min(a_1+2a-\lvert b+e_1\rvert, a-d)$
	g_1	$=$	$\frac{1-G_1}{2}\max(-a+d+\lvert b+e_2\rvert, -a_1-a-d-e_1)$
		$+$	$\frac{1+G_1}{2}\min(a-d-\lvert b-e_2\rvert, a_1+a+d-e_1)$
	g_2	$=$	$\frac{1-G_2}{2}\max(-a-d+\lvert b+e_1\rvert, -a_1-a+d-e_2)$
		$+$	$\frac{1+G_2}{2}\min(a+d-\lvert b-e_1\rvert, a_1+a-d-e_2)$
	a	$=$	$(A+1)/4$
	a_1	$=$	$1-3a$
	b	$=$	Ba
	d	$=$	$D\min(a-\lvert b\rvert, a_1+a)$
8.18	e_1	$=$	$E_1(\frac{a_1}{2}+a+d-\frac{\lvert b\rvert}{2})$
	e_2	$=$	$E_2(\frac{a_1}{2}+a-d-\frac{\lvert b\rvert}{2})$
	f_1	$=$	$\frac{1-F_1}{2}\max(-a-d+e_1+\lvert b\rvert, -a_1-a-d-e_1)$
		$+$	$\frac{1+F_1}{2}\min(a+d+e_1-\lvert b\rvert, a_1+a+d-e_1)$
	f_2	$=$	$\frac{1-F_2}{2}\max(-a+d-e_2+\lvert b\rvert, -a_1-a+d+e_2)$
		$+$	$\frac{1+F_2}{2}\min(a-d-e_2-\lvert b\rvert, a_1+a-d+e_2)$
	a	$=$	$(A+1)/4$
	a_1	$=$	$1-3a$
	c	$=$	Ca
	b	$=$	$B(a-\lvert c\rvert)$
	d_1	$=$	$D_1(a_1+a$
9.20a	e_1	$=$	$E_1(\frac{a_1}{2}+a+\frac{d_1}{2}-\frac{\lvert c+b\rvert}{2})$
	e_2	$=$	$E_2(\frac{a_1}{2}+a-\frac{d_1}{2}-\frac{\lvert c-b\rvert}{2})$
	f_1	$=$	$\frac{1-F_1}{2}\max(-a+e_1+\lvert c+b\rvert, -a_1-a-d_1-e_1)$
		$+$	$\frac{1+F_1}{2}\min(a+e_1-\lvert c+b\rvert, a_1+a+d_1-e_1)$
	f_2	$=$	$\frac{1-F_2}{2}\max(-a-e_2+\lvert c-b\rvert, -a_1-a+d_1+e_2)$
		$+$	$\frac{1+F_2}{2}\min(a-e_2-\lvert c-b\rvert, a_1+a-d_1+e_2)$

Table S7: Fourier-Motzkin parameterizations, 8.17 to 9.20a

Model	Fourier-Motzkin Parameterization
9.20b	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ d_1 &= D_1(a_1+a) \\ c &= C\min(a_1+2a, a) \\ b &= B\min(a_1+2a, a-\lvert c\rvert) \\ g_1 &= G_1\min(a, a_1+2a-\lvert c\rvert) \\ g_2 &= \tfrac{1-G_2}{2}\max(-a, -a_1-2a+c+\lvert b-d_1+g_1\rvert, -a_1-2a-c+\lvert b+d_1+g_1\rvert) \\ &+ \tfrac{1+G_2}{2}\min(a, a_1+2a+c-\lvert b+d_1-g_1\rvert, a_1+2a-c-\lvert b-d_1-g_1\rvert) \\ f_1 &= \tfrac{1-F_1}{2}\max(-a+\lvert c+b-g_2\rvert, -a_1-a-d_1-g_1) \\ &+ \tfrac{1+F_1}{2}\min(a-\lvert c+b+g_2\rvert, a_1+a+d_1-g_1) \\ f_2 &= \tfrac{1-F_2}{2}\max(-a+\lvert c-b-g_1\rvert, -a_1-a+d_1+g_2) \\ &+ \tfrac{1+F_2}{2}\min(a-\lvert c-b+g_1\rvert, a_1+a-d_1+g_2) \end{aligned}$
10.12	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ c &= Ca \\ d &= Da \\ b &= \tfrac{1-B}{2}(-a+\lvert c+d\rvert)+\tfrac{1+B}{2}(a-\lvert c-d\rvert) \\ d_1 &= D_1(a_1+a)-d \\ e_1 &= E_1(\tfrac{a_1}{2}+a+\tfrac{d_1}{2}+d-\tfrac{\lvert c+b\rvert}{2}) \\ e_2 &= E_2(\tfrac{a_1}{2}+a-\tfrac{d_1}{2}-d-\tfrac{\lvert c-b\rvert}{2}) \\ f_1 &= \tfrac{1-F_1}{2}\max(-a-d+e_1+\lvert c+b\rvert, -a_1-a-d_1-d-e_1) \\ &+ \tfrac{1+F_1}{2}\min(a+d+e_1-\lvert c+b\rvert, a_1+a+d_1+d-e_1) \\ f_2 &= \tfrac{1-F_2}{2}\max(-a+d-e_2+\lvert c-b\rvert, -a_1-a+d_1+d+e_2) \\ &+ \tfrac{1+F_2}{2}\min(a-d-e_2-\lvert c-b\rvert, a_1+a-d_1-d+e_2) \end{aligned}$
10.34	$\begin{aligned} a &= (A+1)/4 \\ a_1 &= 1-3a \\ c &= Ca \\ b &= Ba \\ d &= \tfrac{1-D}{2}(\lvert c+b\rvert-a)+\tfrac{1+D}{2}(a-\lvert c-b\rvert) \\ d_1 &= D_1(a_1+a)-d \\ e_1 &= E_1\min(a+d, a_1+2a-\lvert c\rvert, a_1+2a+d_1, a_1+3a-c-b-d_1-d, a_1+3a+c+b-d_1-d) \\ e_2 &= \tfrac{1-E_2}{2}\max(-a+d, -a_1-2a+c+\lvert b+d_1-e_1\rvert, -a_1-2a-c+\lvert b-d_1-e_1\rvert) \\ &+ \tfrac{1+E_2}{2}\min(a-d, a_1+2a-c-\lvert b+d_1+e_1\rvert, a_1+2a+c-\lvert b-d_1+e_1\rvert) \\ g_1 &= \tfrac{1-G_1}{2}\max(-a+d+\lvert c-b-e_2\rvert, -a_1-a-d_1-d-e_1) \\ &+ \tfrac{1+G_1}{2}\min(a-d-\lvert c-b+e_2\rvert, a_1+a+d_1+d-e_1) \\ g_2 &= \tfrac{1-G_2}{2}\max(-a-d+\lvert c+b+e_1\rvert, -a_1-a+d_1+d-e_2) \\ &+ \tfrac{1+G_2}{2}\min(a+d-\lvert c+b-e_1\rvert, a_1+a-d_1-d-e_2) \end{aligned}$

Table S8: Fourier-Motzkin parameterizations, 9.20b to 10.34

References

J. Fernández-Sánchez, J. G. Sumner, P. D. Jarvis, and M. D. Woodhams. Lie Markov models with purine/pyrimidine symmetry. *J Math Biol*, pages 1–37, 2014. ISSN 0303-6812. doi: 10.1007/s00285-014-0773-z. URL http://dx.doi.org/10.1007/s00285-014-0773-z.