Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

The challenge of using isopropylamine as amine donor in transaminase catalysed synthesis of chiral amines

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Table ESI-1: Identity matrix of the fold class I ATA, as calculated after alignment with Blosum62 (Geneious 9.1.8).

Source	***A. citreus* CNB05-01**	***B. vietnamiensis***	***C. violaceum***	***H. elongata***	***K. pneumonia***	***O. anthropi***	***P. putida***	***R. sphaeroides***	***Ruegeria sp.***	***S. pomeroyi***	***V. fluvialis***
***A. citreus* CNB05-01**		20.6	24.1	24.3	22.4	22.8	21.5	22.5	23.4	23.2	19.6
B. vietnamiensis	20.6		34.3	36.0	23.2	43.7	31.8	27.5	31.7	34.0	51.4
C. violaceum	24.1	34.3		54.6	20.0	38.6	35.1	31.0	35.2	50.2	36.4
H. elongata	24.3	36.0	54.6		22.9	39.7	38.8	37.5	37.1	56.8	37.2
K. pneumonia	22.4	23.2	20.0	22.9		23.3	24.9	23.5	23.2	25.3	23.0
O. anthropi	22.8	43.7	38.6	39.7	23.3		33.5	32.4	39.0	38.7	40.9
P. putida	21.5	31.8	35.1	38.8	24.9	33.5		41.8	34.4	38.6	31.1
R. sphaeroides	22.5	27.5	31.0	37.5	23.5	32.4	41.8		33.3	36.1	30.3
Ruegeria sp.	23.4	31.7	35.2	37.1	23.2	39.0	34.4	33.3		34.4	31.3
S. pomeroyi	23.2	34.0	50.2	56.8	25.3	38.7	38.6	36.1	34.4		33.5
V. fluvialis	19.6	51.4	36.4	37.2	23.0	40.9	31.1	30.3	31.3	33.5	

Table ESI-2: Similarity matrix of the fold class I ATA, as calculated after alignment with Blosum62 (Geneious 9.1.8).

Source	***A. citreus* CNB05-01**	***B. vietnamiensis***	***C. violaceum***	***H. elongata***	***K. pneumonia***	***O. anthropi***	***P. putida***	***R. sphaeroides***	***Ruegeria sp.***	***S. pomeroyi***	***V. fluvialis***
***A. citreus* CNB05-01**		52.1	53.7	51.5	50.6	54.7	53.0	52.2	51.5	52.6	49.3
B. vietnamiensis	52.1		67.4	70.1	56.3	76.1	66.3	64.9	67.7	66.4	78.2
C. violaceum	53.7	67.4		79.5	51.7	70.0	64.9	63.7	67.7	77.3	66.4
H. elongata	51.5	70.1	79.5		53.0	70.9	67.9	65.7	66.1	79.7	67.3
K. pneumonia	50.6	56.3	51.7	53.0		56.2	55.9	55.3	53.6	54.0	53.6
O. anthropi	54.7	76.1	70.0	70.9	56.2		67.8	65.3	72.9	69.5	73.1
P. putida	53.0	66.3	64.9	67.9	55.9	67.8		70.7	66.9	70.0	62.2
R. sphaeroides	52.2	64.9	63.7	65.7	55.3	65.3	70.7		63.8	66.5	61.6
Ruegeria sp.	51.5	67.7	67.7	66.1	53.6	72.9	66.9	63.8		64.1	67.0
S. pomeroyi	52.6	66.4	77.3	79.7	54.0	69.5	70.0	66.5	64.1		63.3
V. fluvialis	49.3	78.2	66.4	67.3	53.6	73.1	62.2	61.6	67.0	63.3	

Table ESI-3: Identity matrix of the fold class IV ATA, as calculated after alignment with Blosum62 (Geneious 9.1.8).

Source	***Arthrobacter sp.* (3WWH/I306V)**	***Arthrobacter sp.* (5FR9)**	***A. fumigatus***	***C. seiimmersa***	***F. graminearum***	***M. vanbaalenii***
***Arthrobacter sp.* (3WWH/I306V)**		91.8	38.3	36.3	37.5	47.7
***Arthrobacter sp.* (5FR9)**	91.8		36.0	33.1	34.9	47.1
A. fumigatus	38.3	36.0		55.2	62.4	37.4
C. seiimmersa	36.3	33.1	55.2		57.7	37.1
F. graminearum	37.5	34.9	62.4	57.7		38.5
M. vanbaalenii	47.7	47.1	37.4	37.1	38.5	

Table ESI-4: Similarity matrix of the fold class IV ATA, as calculated after alignment with Blosum62 (Geneious 9.1.8).

Source	***Arthrobacter sp.* (3WWH/I306V)**	***Arthrobacter sp.* (5FR9)**	***A. fumigatus***	***C. seiimmersa***	***F. graminearum***	***M. vanbaalenii***
***Arthrobacter sp.* (3WWH/I306V)**		95.5	72.0	63.9	69.5	72.8
***Arthrobacter sp.* (5FR9)**	95.5		69.3	59.8	66.9	71.4
A. fumigatus	72.0	69.3		77.6	84.5	65.7
C. seiimmersa	63.9	59.8	77.6		78.4	59.4
F. graminearum	69.5	66.9	84.5	78.4		64.4
M. vanbaalenii	72.8	71.4	65.7	59.4	64.4	