

A metagenomics approach for new biocatalyst discovery: Application to Class III transaminases and the synthesis of valuable amine synthons

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Supporting information

CONTIG ID	Numerical ID	pQR number
1707	1	pQR1108
5460	2	pQR1109
5556	3	pQR1110
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29279	9	pQR1116
12630	10	pQR1117
2889	11	pQR1118

DNA sequences of the retrieved enzymes and their corresponding *in silico* sequences

pQR1108 (1707)

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1707 contig

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pQR1109 (5460)

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5460 contig

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pQR1110 (5556)

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>5556 contig

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pQR1111 (6798)

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6798 contig

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pQR1112 (35373)

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35373 contig

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pQR1113 (28681)

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28681 contig

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pQR1114 (27491)

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TTATGATGGTGTATCATCCTTGTGGGTTAATATTCATGGCCATAATCATCCTGTGCTTAATCAAGCGTTGAAGGACCAA
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TACCAATACCGTCAATTAGTAGGTCAAACGAAGAAAACGAAGTTTATCGCACTCAATGCGGGCTATCATGGTGATACA
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27491 contig

ATGATGGCAGAGAAACAACCTTTCACAAATTGCACAATGGGACCACGAATTTGTATGGCATCCATTTACGCAAATGCAA
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pQR1115 (29297)

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29297 contig

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pQR1116 (29279)

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29279 contig

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pQR1117 (12630)

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12630 contig

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pQR1118 (2889)

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2889 contig

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Primer s for enzyme retrieval

>pQR1108fwd	AAGGTCATATGTTATATAATAACG
>pQR1108rvr	CGCCTTCCATGGGCTGTGTTC
>pQR1109fwd	GAATTGCATATGAACCGTAATGAAAGC
>pQR1109rvr	AGCTTCTCGAGCGCCATTCTTG
>pQR1110fwd	TTTCATATGAAGGTAGCCGTG
>pQR1110rvr	GCGGTTGGCTACTCGAGCTGAG
>pQR1111fwd	AGGCACCGATCATATGACTCGC
>pQR1111rvr	CTCGCGTCTCGAGGGCTGCGGC
>pQR1112fwd	TTCGGAGGATCATATGAGTAATACAATCG
>pQR1112rvr	TATCTACGCCACTCGAGAACGTAGCC
>pQR1113fwd	AGGTGACCATATGGCAGAGAAACAGC
>pQR1113rvr	CGTAAATCGCTCGAGAATAATTGGC
>pQR1114fwd	GTATGAGGTCATATGATGGCAGAG
>pQR1114rvr	TTTAAACCATGGAATGATTGGTTTCAAATCTTC
>pQR1115fwd	AAGGAGTGCATATGTTACAAC TAGG
>pQR1115rvr	AATACCTCGAGTGTTTCACTG
>pQR1116fwd	TGGTTACAAAAGTAAGGAGAACATATGTTCC
>pQR1116rvr	AATAATGCATCTCGAGATTCTTTAATGTATCAC
>pQR1117fwd	GATTTAACATATGTTTTTTCACCCTTGTGC
>pQR1117rvr	TACAAGCCTCGAGCATTTTATC
>pQR1118fwd	GGATTAAAACATATGACAAAATCAACCG
>pQR1118rvr	TTGTCCATGGAGCAACTGCTGC

Amino acid sequences of the retrieved enzymes and TAm
s from Cv, Pp, Vf and Kp

pQR1108

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RGYHGDTWNAMSVCDPETGMHHIFGSALPQRSFVDNPKSRFNDEWDGTDLQPVRALFEAHHADIAAFILEPVVQGAGG
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CVAQGIWVRPFGRLVYLMPPYIISDDLLEADKTVQILKEHSPW

pQR1109

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pQR1110

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pQR1111

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pQR1112

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GIEPDVVSTAKGLAGGLPMGATLFNEKMQYVLNAGAHATTFGGNPICAAAGNTIINRLTPEFLDSVKAKGDYVKATLAGKP
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pQR1113

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GNALACAVALASLVFREEKVIEGLPKKIEFTNALKPIEKLKHVKEVRQRGLIVGIELEKDVATHEAYRPNDVAGAKVAILAR
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pQR1114

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RELTAKHDVFLIVDEVATGFGRTGKFFACEHEGVSPDFMTLSKGITGGYLPLAATLTTRVFDALGTFEKKTFYHGHSTG
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pQR1115

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pQR1116

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pQR1117

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E

pQR1118

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Cv

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Vf

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Pp

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Kp

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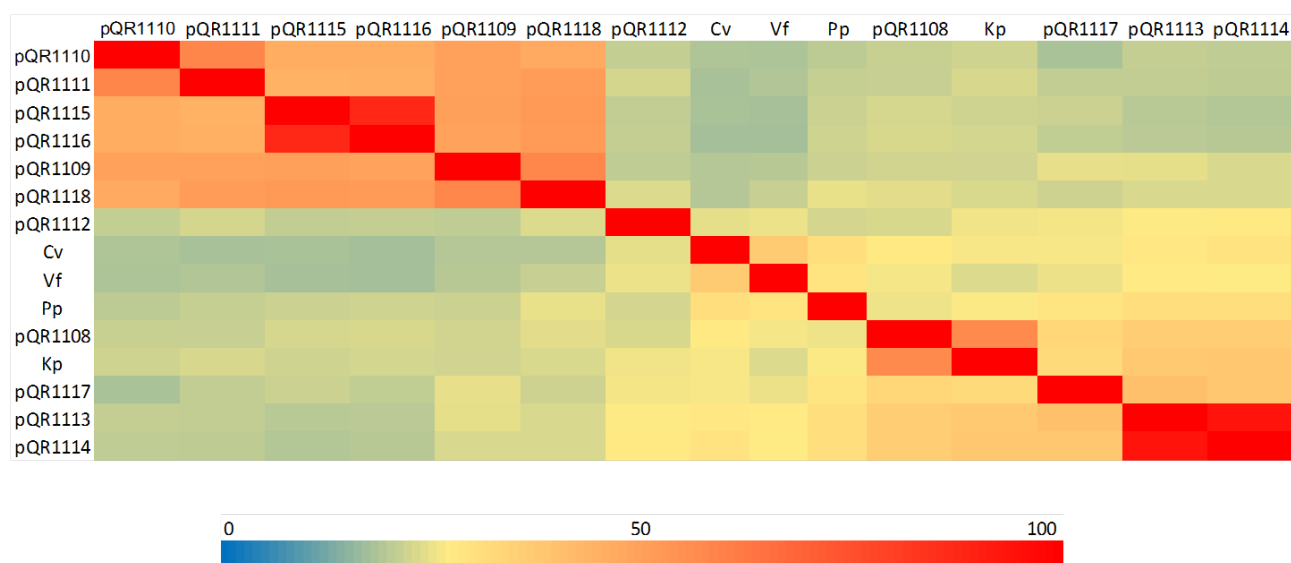
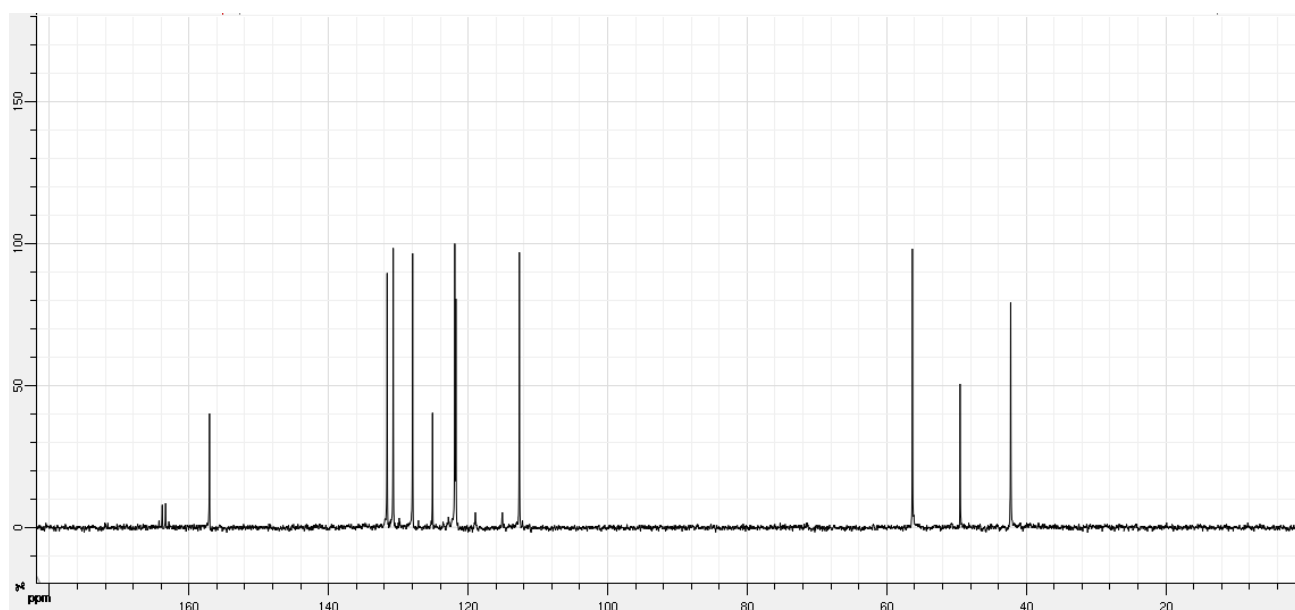
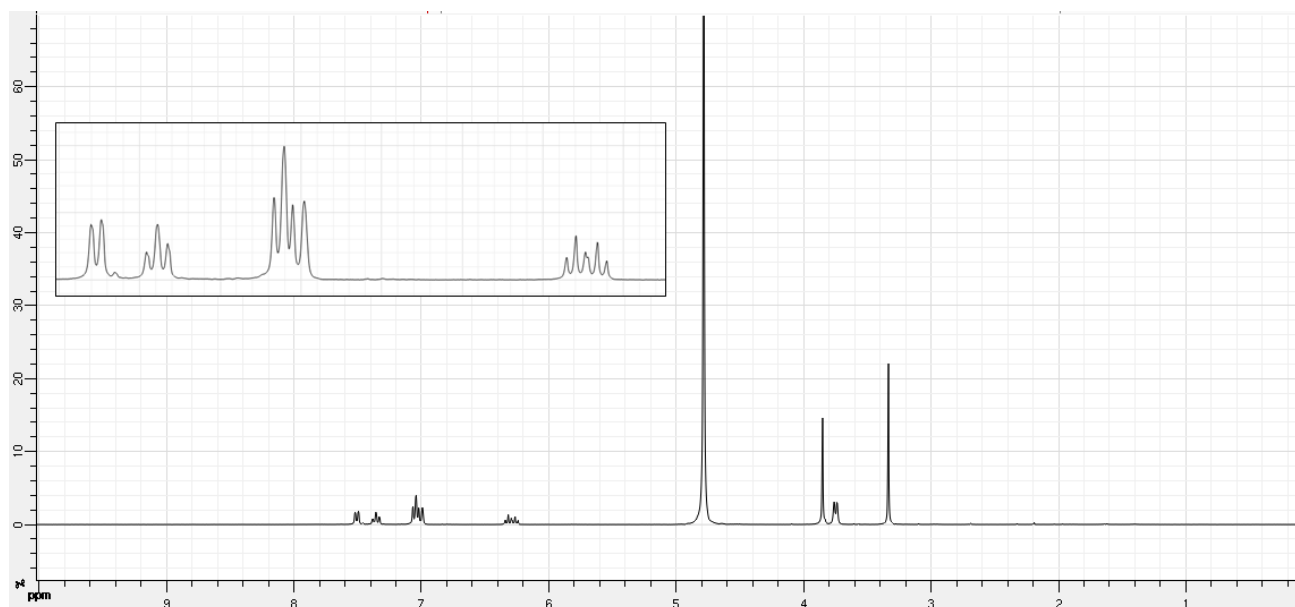
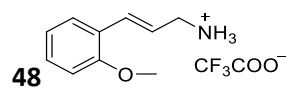


Fig 1. Percentage identity matrix of the 11 metagenomic TAmS and 4 previously identified TAmS

Table 1. Sequence identity and similarity to Cv-TAm (CV2025). The comparisons were carried out in a pairwise manner using the ALIGN programme at Uniprot and each new transaminase was compared with Cv-TAm (CV2025).

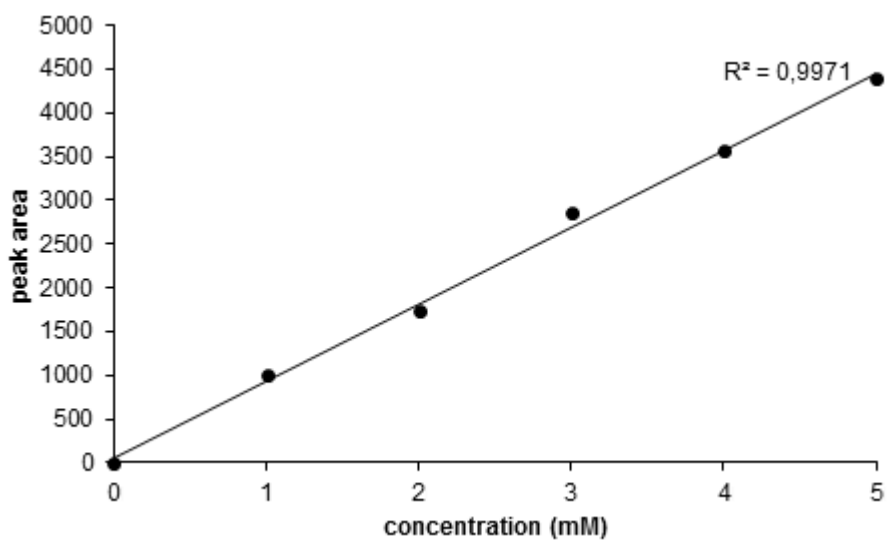
Cv-TAm (CV2025)		
Name of clone	%Identity	%Similarity
pQR1108	25%	32%
pQR1109	19%	36%
pQR1110	17%	32%
pQR1111	20%	40%
pQR1112	22%	32%
pQR1113	26%	40%
pQR1114	28%	38%
pQR1115	19%	37%
pQR1116	18%	38%
pQR1117	24%	38%
pQR1118	21%	33%

NMR spectra

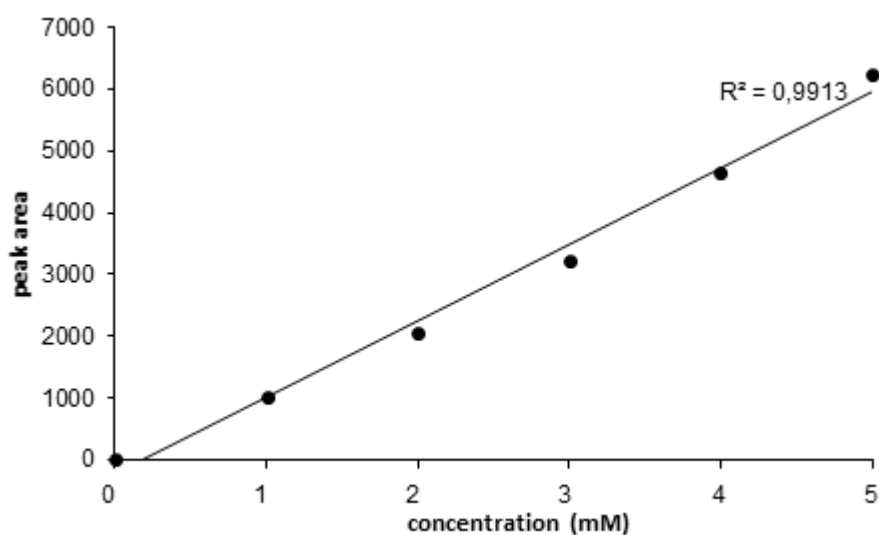


Calibration curves

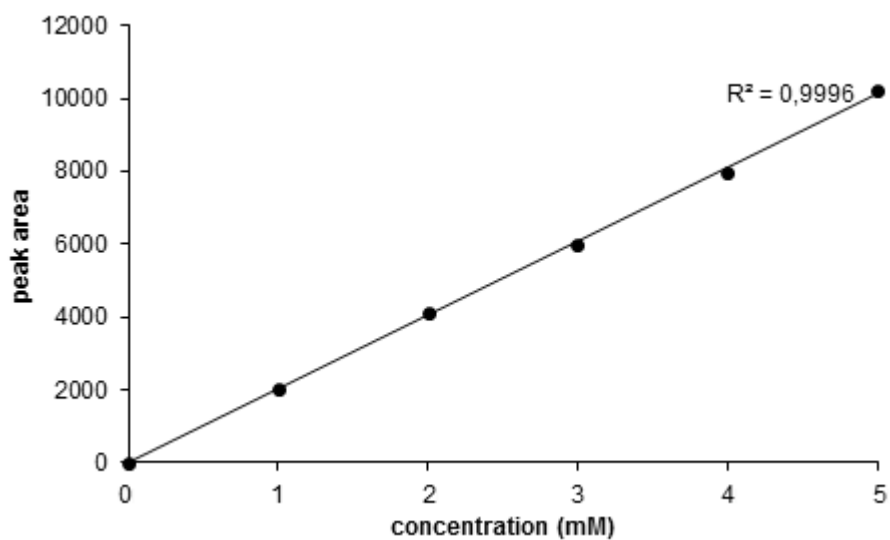
Acetophenone (@ 250 nm)



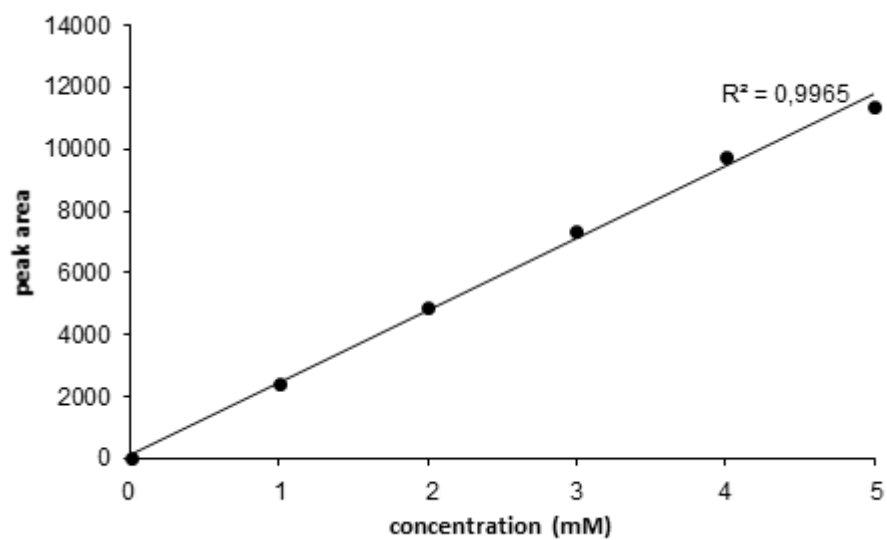
Benzylamine (@ 210 nm)



(E)-3-(2-Methoxyphenyl)prop-2-en-1-amine 2,2,2-trifluoroacetate (@ 210 nm)



(E)-3-Phenylprop-2-en-1-amine (@ 210 nm)



3-Phenylpropan-1-amine (@ 210 nm)

