

1

2 **Electronic Supplementary Information**

3

4

5 **A new route for the synthesis of methacrylic acid from 2-methyl-**
6 **1,3-propanediol by integrating biotransformation and catalytic**
7 **dehydration**

8

9 Sang-Hyun Pyo^{a,*}, Tarek Dishisha^a, Secil Dayankac^a, Jargalan Gerelsaikhan^a,
10 Stefan Lundmark^b, Nicola Rehnberg^c, and Rajni Hatti-Kaul^a

11

12 ^a Department of Biotechnology, Center for Chemistry and Chemical Engineering, Lund
13 University, Box 124, SE-221 00 Lund, Sweden

14

15 ^b Perstorp AB, 284 80 Perstorp, Sweden

16

17 ^c Strategic R&D, Bona AB, Box 210 74, 200 21 Malmö, Sweden

18

19

20

21

22

23

24

25

26

27

28

29

*Corresponding Author

30

31

Tel: +46-46-222-4838; Fax: +46-46-222-4713

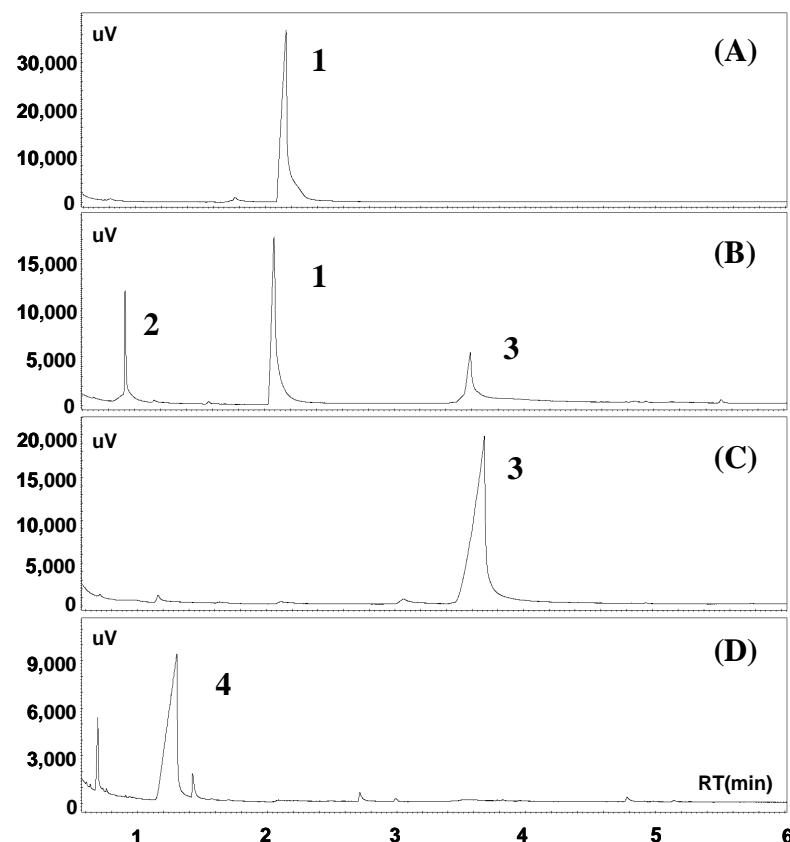
32

E-mail: Sang-Hyun.Pyo@biotek.lu.se (S.-H. Pyo)

33

34 Fig. S1. Gas chromatograms of (A) 2-methyl-1,3-propanediol (1), (B) reaction mixture
35 containing 3-hydroxy-2-methylpropanal (2), 2-methyl-1,3-propanediol and 3-hydroxy-2-
36 methylpropionic acid (3), (C) 3-hydroxy-2-methylpropionic acid, and (D) methacrylic
37 acid (4). Experimental details are provided in the text.

38



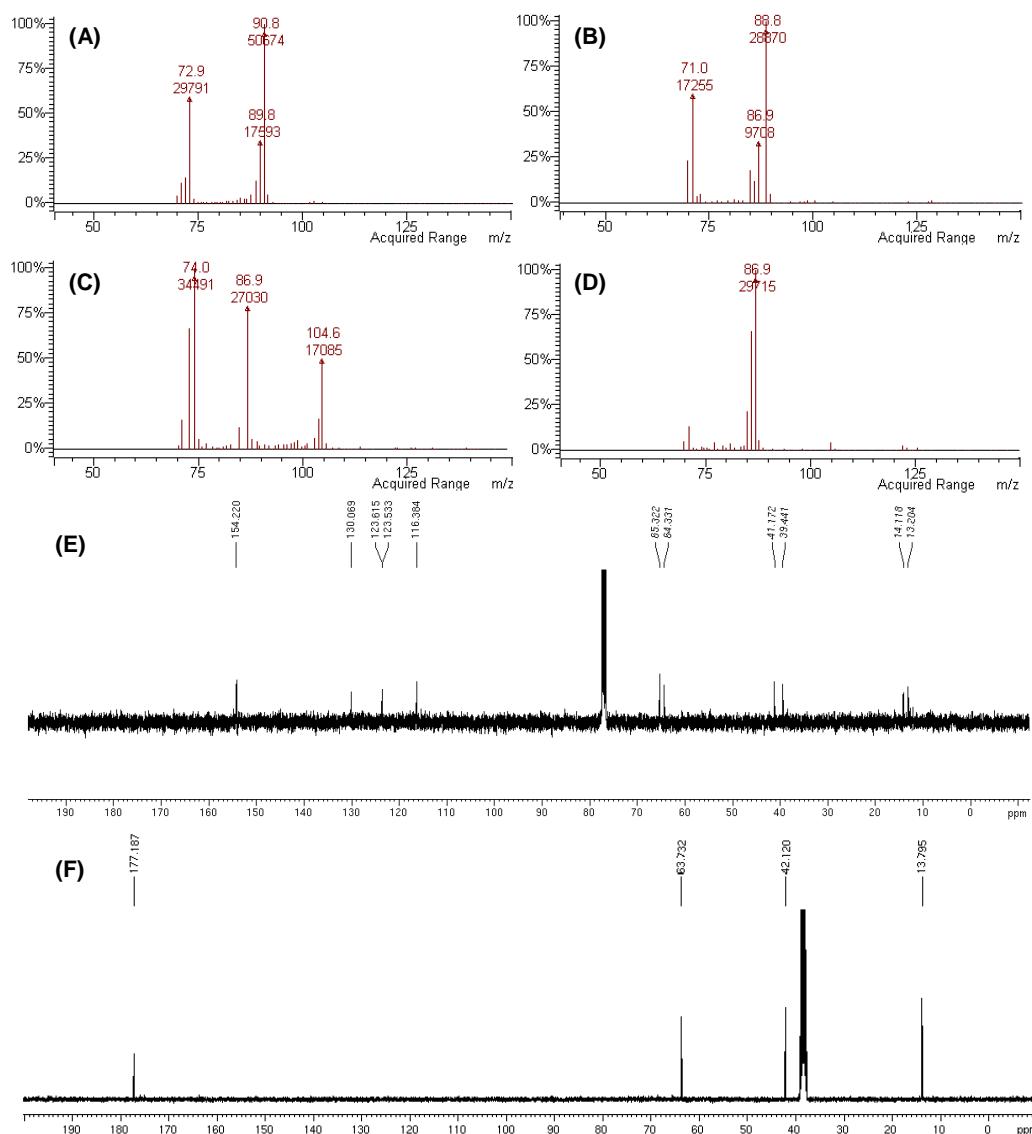
39

40

41

42 Fig. S2. GC-MS and NMR data of reaction components. Mass spectrum of 2-methyl-1,3-
43 propandiol (A, cal. MW 90.12), 3-hydroxy-2-methylpropnal (B, cal. MW 88.10), 3-
44 hydroxy-2-methylpropionic acid (C, cal. MW 104.10), and methacrylic acid (D, cal. MW
45 86.09). ^{13}C -NMR spectrum; (E) derivatized 3-hydroxy-2-methylpropanal (CDCl_3), (F) 3-
46 hydroxy-2-methylpropionic acid and its ^1H -NMR (DMSO-d_6): 0.98 (d, 3H), 2.38(m, 1H),
47 3.39(m, 1H), 3.50(m, 1H).

48



49

50