

## **Supporting Information**

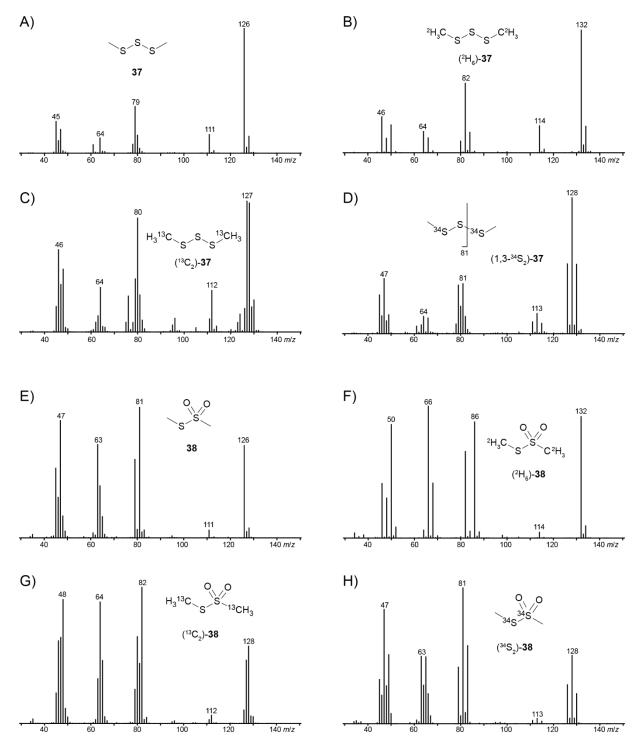
for

## Identification of volatiles from six marine Celeribacter strains

Anuj Kumar Chhalodia, Jan Rinkel, Dorota Konvalinkova, Jörn Petersen and Jeroen S. Dickschat

Beilstein J. Org. Chem. 2021, 17, 420-430. doi:10.3762/bjoc.17.38

DMSP demethylation pathway in *Celeribacter* spp. and copies of spectra



**Figure S1:** El mass spectra of A) unlabeled dimethyl trisulfide (**37**) and of labeled **37** after feeding of B) [*methyl*-<sup>2</sup>H<sub>3</sub>]methionine, C) [*methyl*-<sup>13</sup>C]methionine and D) [<sup>34</sup>S]DMSP, E) unlabeled S-methyl methanethiosulfonate (**38**) and of labeled **38** after feeding of F) [*methyl*-<sup>2</sup>H<sub>3</sub>]methionine, G) [*methyl*-<sup>13</sup>C]methionine, and H) [<sup>34</sup>S]DMSP. The structures of labeled compounds show the isotopomers of maximum incorporation of labeling.

 Table S1: The DMSP demethylation pathway in Celeribacter spp.

Strain	DmdA <sup>a</sup>	DmdB <sup>a</sup>	DmdC <sup>a</sup>	DmdDa
C. marinus DSM 100036 <sup>™</sup>	WP_062220065 (21%)	WP_062217242 (22%)	WP_062219918 (38%)	WP_062217896 (30%)
C. neptunius DSM 26471 <sup>⊤</sup>	WP_090061255 (26%)b	WP_090061186 (25%)	WP_090062142 (40%)	WP_090062168 (43%)
C. manganoxidans DSM 27541 <sup>™</sup>	WP_097373155 (21%)b	WP_097373111 (31%)	WP_097372585 (41%)	WP_088662863 (30%)
C. baekdonensis DSM 27375 <sup>T</sup>	WP_074644298 (28%) <sup>b</sup>	WP_107720993 (32%)	WP_107720980 (46%)	WP_074641224 (43%)
C. halophilus DSM 26270 <sup>T</sup>	WP_066599093 (25%) <sup>b</sup>	WP_066604139 (26%)	WP_066603281 (39%)	WP_066601109 (31%)
C. indicus DSM 27257 <sup>™</sup>	_	WP_139267207 (27%)	WP_043868654 (40%)	WP_043869106 (42%)

<sup>&</sup>lt;sup>a</sup>NCBI accession numbers and % identity of the closest homologs of the functionally characterized enzymes DmdABCD from *Ruegeria* pomeroyi DSS-3 obtained by BLAST search; <sup>b</sup>identity by comparison to C-terminal domain.

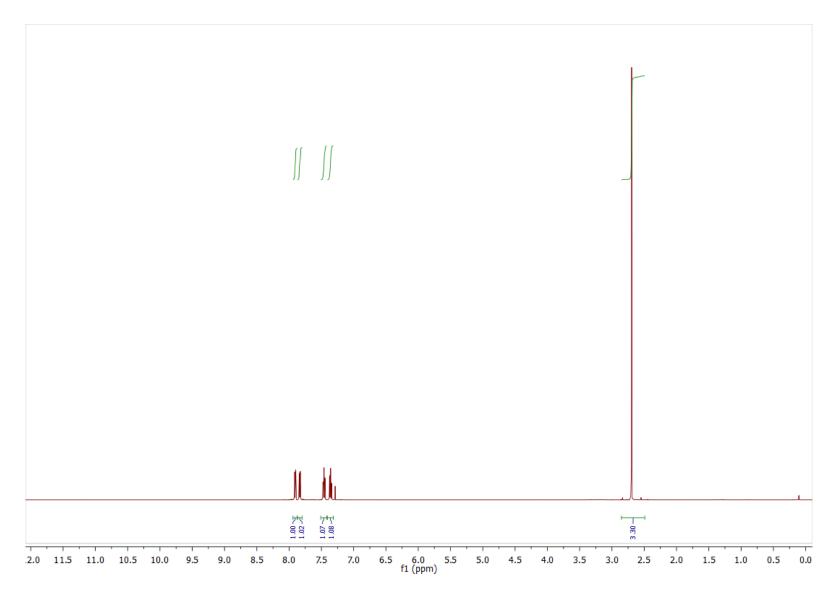


Figure S2: <sup>1</sup>H NMR spectrum (CDCI<sub>3</sub>, 500 MHz) of 41.

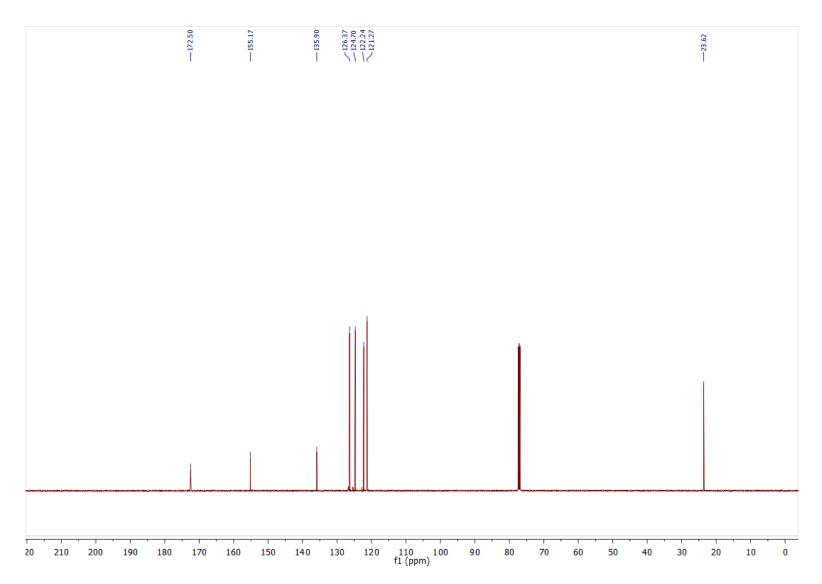


Figure S3: <sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>, 125 MHz) of 41.

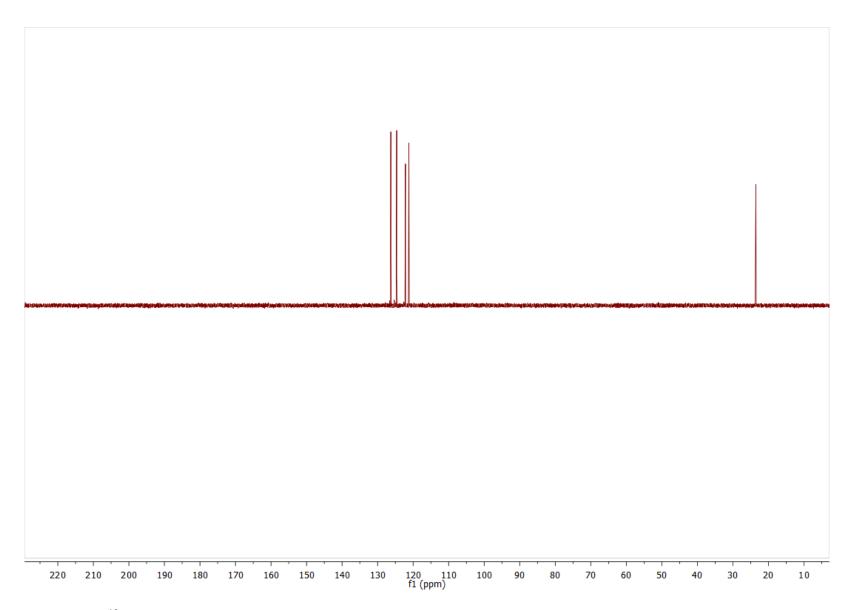


Figure S4: <sup>13</sup>C-DEPT spectrum (CDCI<sub>3</sub>, 125 MHz) of **41**.

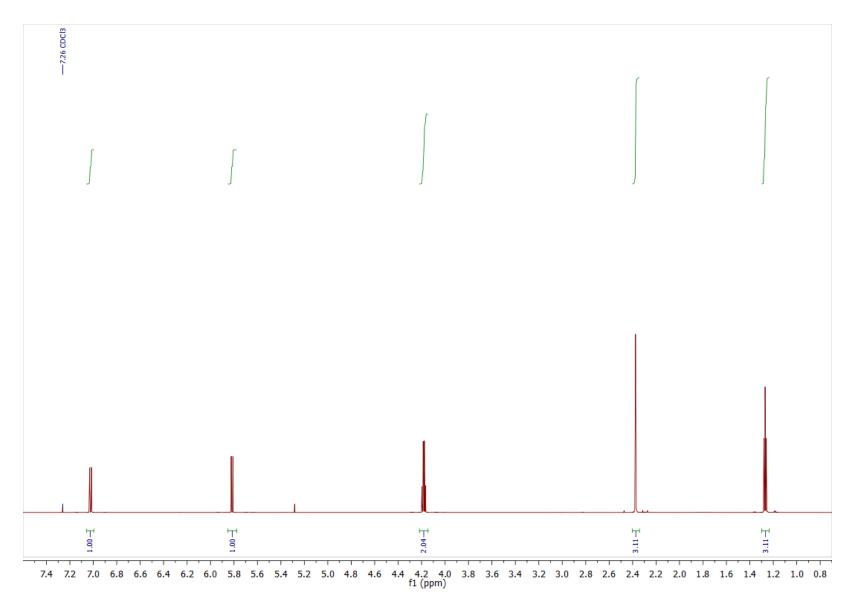


Figure S5: <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 700 MHz) of (*Z*)-42.

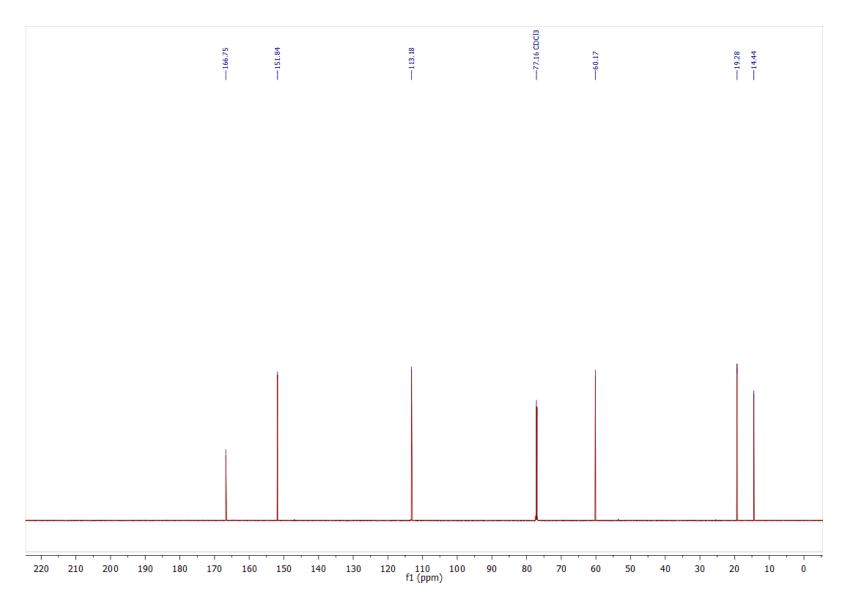


Figure S6:  $^{13}$ C NMR spectrum (CDCl<sub>3</sub>, 175 MHz) of (Z)-42.

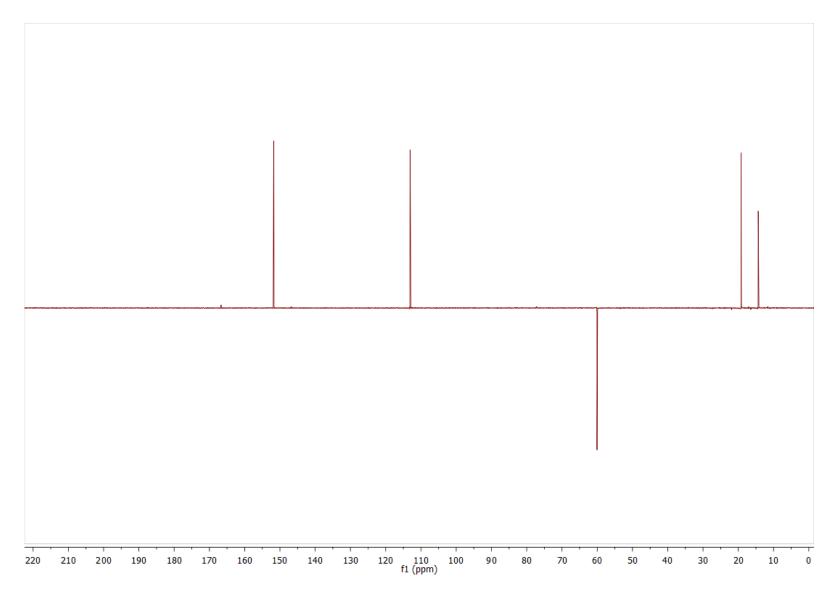
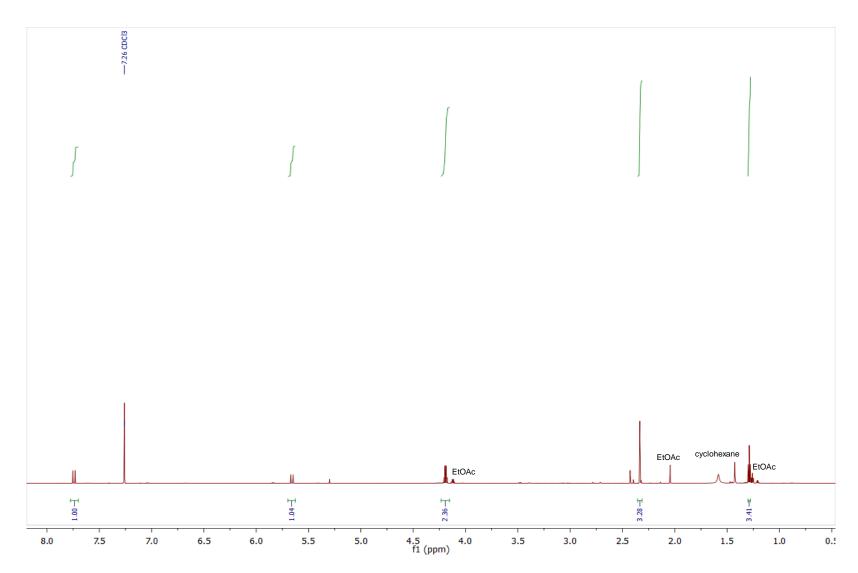


Figure S7:  $^{13}$ C-DEPT spectrum (D<sub>2</sub>O, 175 MHz) of (Z)-42.



**Figure S8:** <sup>1</sup>H NMR spectrum (CDCI<sub>3</sub>, 700 MHz) of (*E*)-**42**. Minor impurities originate from solvents which were not rigorously removed, because the compound was obtained in small amounts and is volatile.

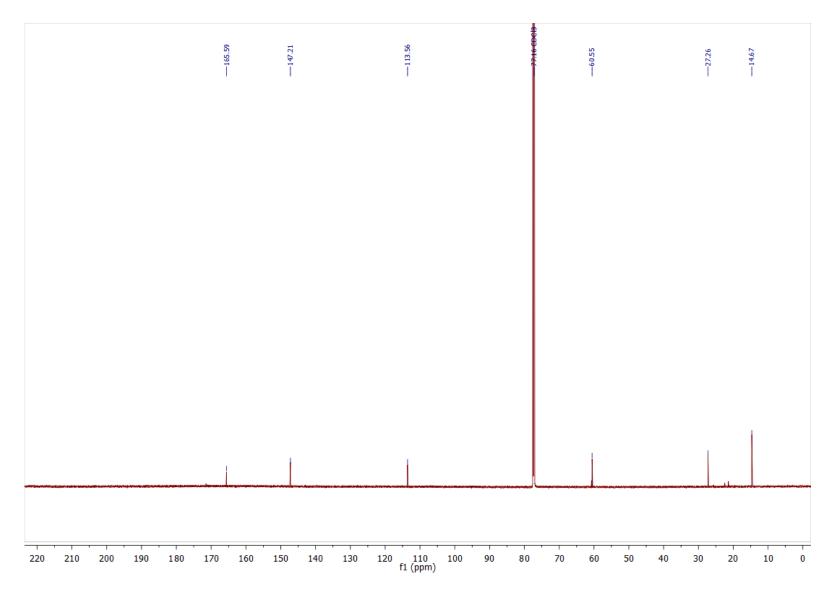


Figure S9:  $^{13}$ C NMR spectrum (CDCl<sub>3</sub>, 175 MHz) of (*E*)-42.

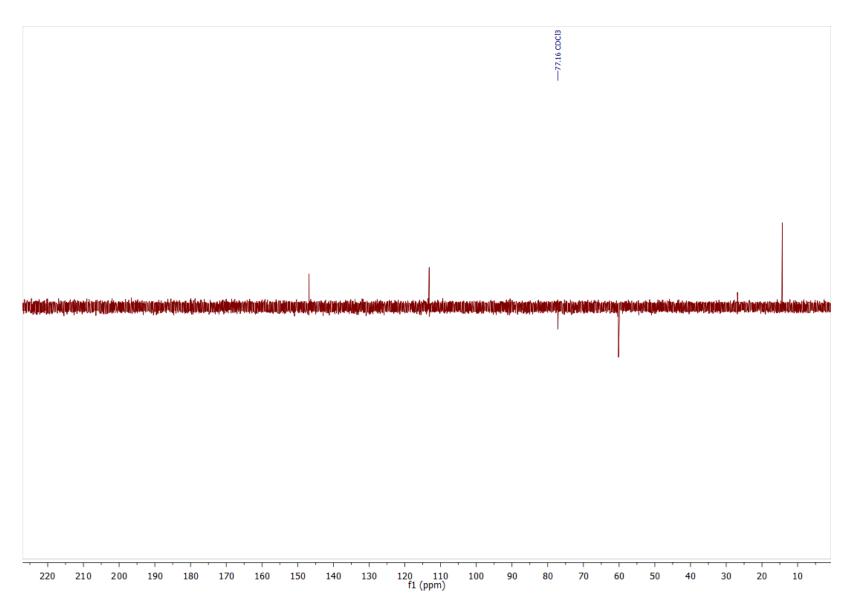


Figure S10:  $^{13}$ C-DEPT spectrum (CDCl<sub>3</sub>, 175 MHz) of (*E*)-42.