Supporting Information

checkHNMR: an open-source tool for checking the consistency of ^{1}H NMR descriptions before publication

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Section S1. Reproducing the report in Figure 1

The report in **Figure 1** was produced on the *checkHNMR* website (https://checkhnmr.org/v2.1.3-beta/), version V2.1.3-beta, with the One compound tab. To repeat the check, open the website, choose One compound and copy the text of each box below into the field named above it. Do not copy the field names. Leave the ^{19}F and ^{31}P fields empty.

Compound label

```
1
```

SMILES

```
COC(=O)/C=C/c1ccccc1O
```

^{1}H NMR description

```
1H NMR (400 MHz, CDCl3) δ 8.01 (d, J = 16.1 Hz, 1H), 7.47 (dd, J = 7.7
Hz, 1H), 7.27–7.21 (m, 1H), 6.92 (t, J = 7.5 Hz, 1H), 6.85 (d, J = 8.1
Hz, 1H), 6.63 (d, J = 16.1 Hz, 1H), 3.81 (s, 3H).
```

^{19}F NMR description – leave empty

^{31}P NMR description – leave empty

HRMS

```
HRMS (ESI) m/z: [M + H]+ calcd for C10H11O3 179.0703; found 179.0705
```

The report shows one alert of each level and the verification code **9445-9C84-5432**:

A, item 4(a): the signal at 7.47 ppm is reported as a dd with one coupling constant;

B, item 3: the partner of J = 8.1 Hz may be the multiplet at 7.27–7.21 ppm;

C, item 1: the *OH* proton is not reported.

The verification code is computed from the version of the tool and from the entries exactly as entered, including the label; spaces at the start and end of each field are removed. A single changed character gives a different code even when the alerts are the same, for example a hyphen-minus typed instead of the en dash (U+2013) in “7.27–7.21”, or a line break that a PDF viewer inserts

into the description when it is copied. If the copied description breaks into several lines, join them into one line, or copy the entries from Supporting Information File 1. The date of the check and the responses do not enter the code. A later version of the tool gives a different code for the same entries.