Supporting Information for:

A versatile biobased continuous flow strategy for the production of 3-butene-1,2-diol and vinyl ethylene carbonate from erythritol

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1. Continuous flow setups

1.1 Description of reactor elements

All continuous flow reactors were assembled with commercially available parts.

1.1.1 Pumps

Chemicals were pumped with ThalesNano microHPLC® pumps (wetted parts: SS 316, ruby and sapphire) or with Chemyx Fusion 6000® High Force syringe pumps equipped with stainless steel syringes with Dupont™ Kalrez® Spectrum™ AS-568 O-rings (0.549 x 0.103”).

1.1.2 SS coil reactors

SS coil reactors were constructed with deburred-end, steam-cleaned and acid-passivated 316 SS tubing (1.58 mm outer diameter, 500 µm internal diameter) of fixed internal volumes for both the DODH and the heating or cooling loops.

1.1.3 SS packed-bed reactor

A SS column (10 cm × 7 mm o.d. × 3.5 mm i.d.) was utilized for the packed-bed reactor (carbonation step).

1.1.4 PEEK tubing

The sections of the reactor that were not subjected to high temperatures were constructed from PEEK tubing (green striped, 1.58 mm outer diameter, 750 µm internal diameter).

1.1.5 PFA tubing and coils

The sections of the reactor not subjected to high pressure and temperature were constructed from PFA tubing (high purity PFA; 1.58 mm outer diameter, 750 µm internal diameter), including the section of tubing connecting the BPR to the collection flask, the in- and outlets of the on-line IR spectrometer and the reaction coil utilized for the homogeneous carbonation trials.

1.1.6 Connectors, ferrules and mixers

Sections of the reactor that were not subjected to high temperature were equipped with coned PEEK fittings and micromixers. Sections of the reactor that were subjected to high temperature were equipped Valco SS fittings, ferrules and unions. Connectors, ferrules and unions were purchased from IDEX/Upchurch (details in Table S1).

1.1.7 Check-valves

The check-valves inserted between the pumps and the reactors were purchased from IDEX/Upchurch Scientific, and were installed in a SS check-valve holder (IDEX/Upchurch Scientific).

1.1.8 Back-pressure regulators

A standard spring-loaded BPR (IDEX/Upchurch Scientific) set at 100 psi was installed in a SS BPR holder (IDEX/Upchurch Scientific). Dome-type BPRs were purchased from Zaiput Flow Technologies. The dome-type BPR was connected to a compressed gas cylinder (nitrogen or argon) to set the working pressure (150 psi).

1.1.9 Thermoregulatory devices

The DODH SS coil was hosted in a modified Thermo Finnigan© (Intersciences) thermoregulated oven. Additional thermocouples and temperature sensors were inserted in the setup. PFA coils, low temperature SS coils (carbonation) and packed-bed reactors were operated in thermoregulated oil baths (Heidolph™ MR Hei-Tec® equipped with a Pt-1000 temperature sensors).

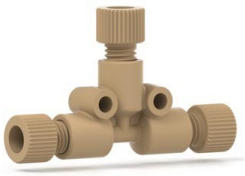
1.1.10 On-line IR spectrometer

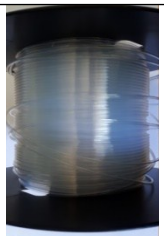
On-line reaction monitoring was carried out with a FlowIR™ (SN# 2964) from Mettler-Toledo equipped with a DTGS detector using HappGenzel apodization, a Silicon probe connected via a FlowIR™ sensor and a high pressure heated 10 µL cell. Sampling was performed from 4000 to 650 cm^{-1} at 8 wavenumber resolution with 128 scans.

1.2 Part numbers & vendors

The reactor coils were constructed from standard fluidic elements purchased from IDEX/Upchurch Scientific and Valco Instruments Co. Inc (Table S1).

Table S1. Connectors, ferules and unions

Item	Details	Picture	Vendor	Reference
Connectors	One-Piece Fingertight, PEEK, 10-32 Coned, for 1/16" OD		IDEX/ Upchurch Scientific	F-120X
	Super Flangeless Nuts, natural PEEK 1/4-28 thread for 1/16" OD tubing		IDEX/ Upchurch Scientific	P-255X
	Super Flangeless Ferrule Tefzel (ETFE) and SS ring 1/4-28 thread for 1/16" OD tubing		IDEX/ Upchurch Scientific	P-259X
	SS Nut, standard, for 1/16" OD tubing		VICI (Valco Ins. Co. Inc.)	ZN1-10
	SS ferrule, 303, for 1/16" OD tubing		VICI (Valco Ins. Co. Inc.)	ZF1-10
Unions	Natural polypropylene standard low pressure union 1/4-28		IDEX/ Upchurch Scientific	P-620
	SS ZDV union Valco type for 1/16" OD, tubing		IDEX/ Upchurch Scientific	U-322
Mixers	T-mixer, natural PEEK 1/4-28 thread for 1/16" o.d. tubing, 0.02" through hole		IDEX/ Upchurch Scientific	P-712
Check-valve	Check-valve inline cartridge 1.5 psi		IDEX/ Upchurch Scientific	CV-3001
Spring-loaded BPR	BPR cartridge 100 psi with gold coating		IDEX/ Upchurch	P-763

			Scientific	
Cartridge holder	BPR and check-valve cartridge holder, SS		IDEX/ Upchurch Scientific	U-469
Dome-type BPR	Dome-type BPR, metal-free, with adjustable set point		Zaiput Flow Techn.	BPR-10
Tubing	316 SS tubing (1.58 mm outer diameter, 500 µm internal diameter)		VICI (Valco Ins. Co. Inc.)	TSS120
	PEEK tubing (green striped, 1.58 mm outer diameter, 750 µm internal diameter).		VICI (Valco Ins. Co. Inc.)	JR-T-6003-M3
	High-purity PFA tubing, 1.58 mm outer diameter, 750 µm internal diameter		VICI (Valco Ins. Co. Inc.)	JR-T-4002-M25

1.3 Detailed continuous flow setups

1.3.1 Continuous flow setup for the DODH of erythritol

The reader is referred to the main manuscript for experimental details (Feed concentrations, flow rates, counter-pressures).

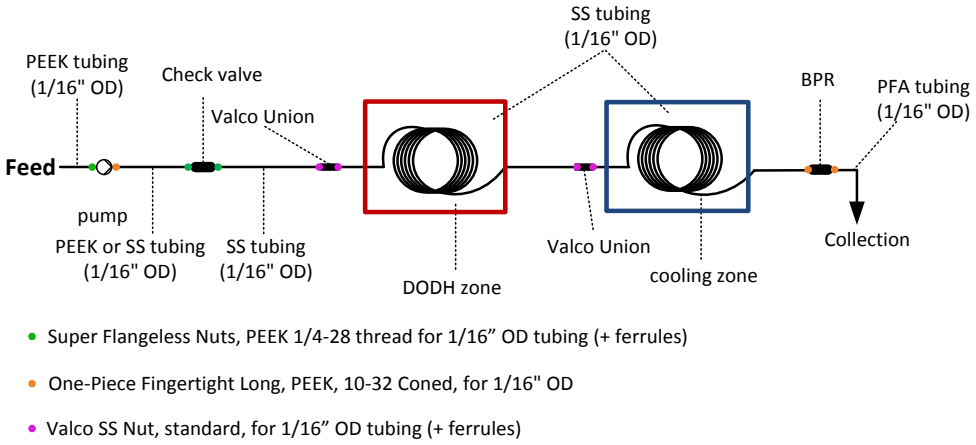


Figure S1. Continuous flow setup for the DODH of erythritol

1.3.2 Continuous flow setup for the homogeneous carbonation of 3-butene-1,2-diol

The reader is referred to the main manuscript for experimental details (Feed concentrations, flow rates, counter-pressures).

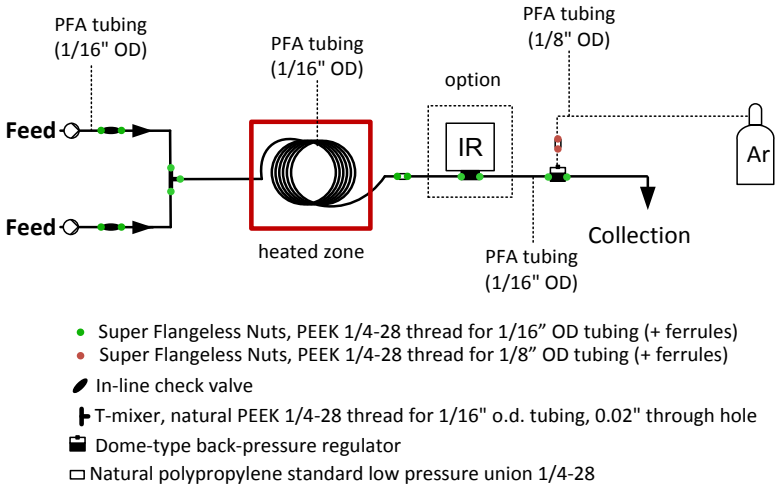


Figure S2. Continuous flow setup for the homogeneous carbonation of 3-butene-1,2-diol

1.3.3 Continuous flow setup for the heterogeneous carbonation of 3-butene-1,2-diol

The reader is referred to the main manuscript for experimental details (Feed concentrations, flow rates, counter-pressures).

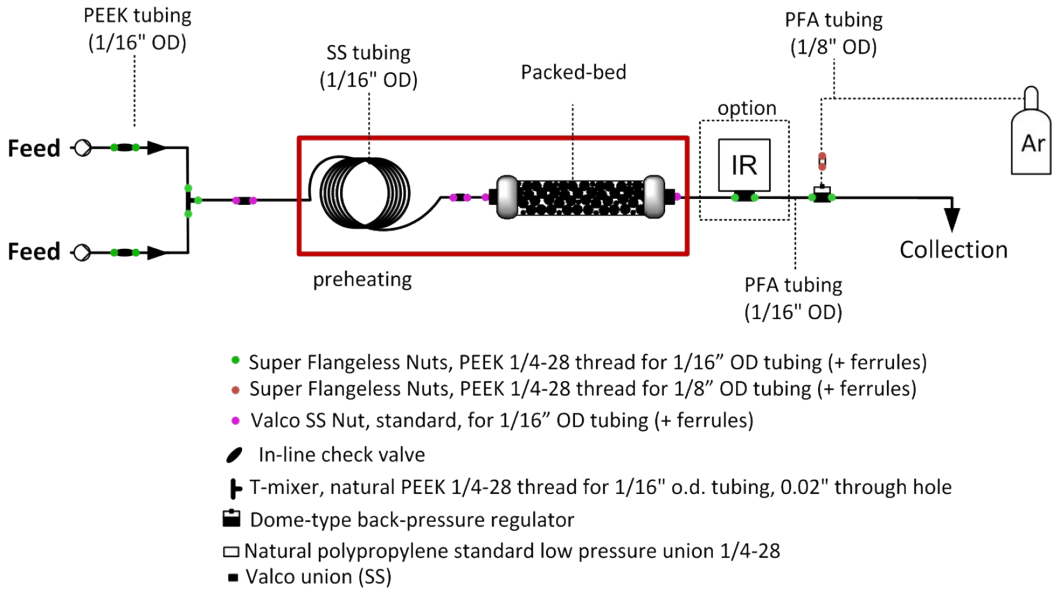


Figure S3. Continuous flow setup for the heterogeneous carbonation of 3-butene-1,2-diol

1.3.4 Concatenated continuous flow setup

The reader is referred to the main manuscript for experimental details (Feed concentrations, flow rates, counter-pressures).

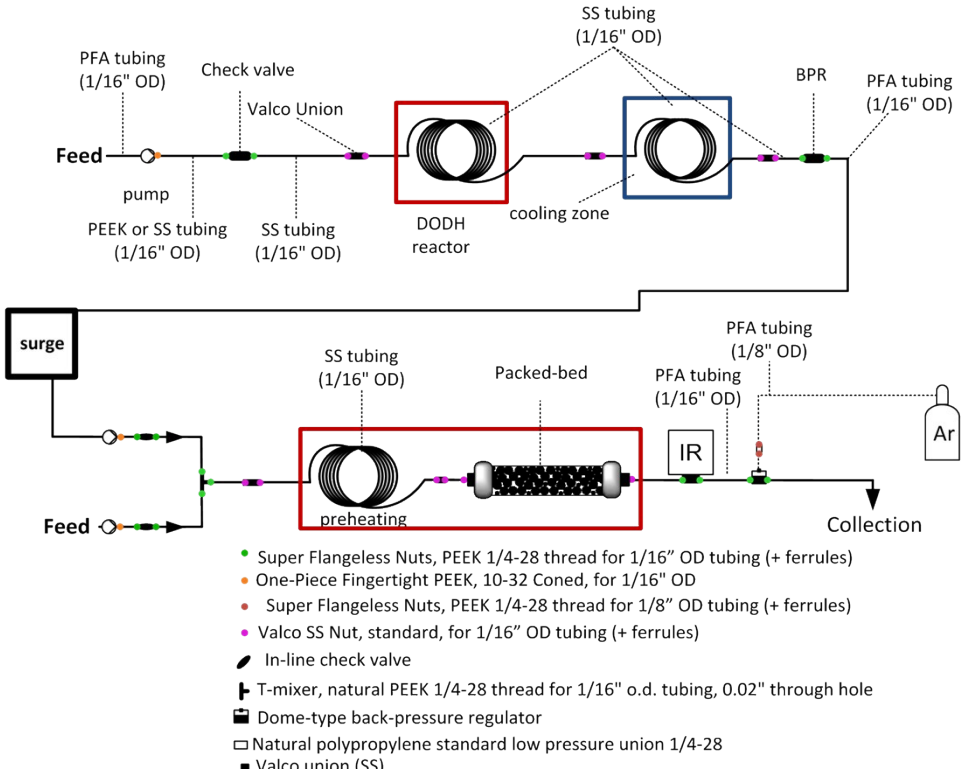


Figure S4. Concatenated continuous flow setup

1.4 DODH standard operating procedures

1.4.1 Operation to steady state

The reactor was stabilized for 3 residence times before collection. Steady state was experimentally determined by collecting and analyzing successive fractions.

1.4.2 Start-up procedure

The reactor was thoroughly flushed with DMSO or [EMIM][ES] at room temperature for 5 min. Then, the feed was connected to the HPLC pump, and the erythritol dynamic mixture was fed into the reactor at room temperature. The temperature was next set to the desired process temperature, and system was equilibrated for 3 residence times.

1.4.3 Shut-down procedure

The reactor was flushed with DMSO, and then the temperature was progressively decreased to room temperature.

1.4.4 In case of clogging

Formation of solid material was noticed at high temperature (> 300 °C), eventually leading to reactor clogging. The SS coil was removed from the setup and left at 500 °C for 10 hours, and next thoroughly flushed with DMSO and isopropanol.

2. Additional experimental details

2.1 Chemicals

Chemicals, purity, CAS numbers and suppliers are listed in Table S2.

Table S2. Chemicals and suppliers

Products	Purity (%)	CAS Number	Supplier
DMSO	>99	67-68-5	Merck/Sigma-Aldrich
[EMIM][ES] 1-Ethyl-3-methylimidazolium ethyl sulfate	99	342573-75-5	ABCR
meso-Erythritol	> 99	149-32-6	TCI
Formic acid	97	64-18-6	ABCR
Triethyl orthoformate (TEOF)	> 98	122-51-0	TCI
Glycerol	99	56-81-5	ABCR
1,3-Butadiene	99	106-99-0	TCI
2,5-Dihydrofuran	> 98	1708-29-8	TCI
Furan	> 99	110-00-9	TCI
3-Butene-1,2-diol	≥ 99	497-06-3	Merck/Sigma-Aldrich
cis-2-Butene-1,4-diol	> 94	6117-80-2	TCI

trans-2-Butene-1,4-diol	95	821-11-4	ABCR
1,4-Anhydro-Erythritol	98	4358-64-9	ABCR
trans-1,2-Cyclohexanediol	>99	1460-57-7	TCI
cis-1,2-Cyclohexanediol	>98	1792-81-0	TCI
trans-But-2-enal	>99	123-73-9	Merck/Sigma-Aldrich
1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	>99	6674-22-2	Merck/Sigma-Aldrich
DBU, polystyrene-bound, 100-200 mesh, 1 % cross-linked with DVB, 1.5-2.5 mmol g^{-1} loading	/	/	Merck/Sigma-Aldrich
4-Vinyl-1,3-dioxolan-2-one (vinyl ethylene carbonate)	99	4427-96-7	Merck/Sigma-Aldrich
3,4-Epoxy-1-butene	98	930-22-3	Merck/Sigma-Aldrich

2.2 Preparation and storage of the DODH feed solutions

In a typical procedure, a feed solution (500 mL total volume) of erythritol was prepared by mixing dissolving erythritol in DMSO (2.4 M in DMSO), then by adding 1 equiv. of triethyl orthoformate and 0.1 equiv. of formic acid. No particular precautions were taken to keep the solution from air and moisture. The feed solution was utilized over 19 days without any alteration of the results.

2.3 Off-line Gas Chromatography quantitative analysis

2.3.1 Generalities

Gas Chromatography (GC) was performed for the analysis of the volatile fraction (b.p. < 70 °C) of the reactor effluent. GC was performed with a Trace-GC 2000 (Thermo-Scientific, Waltham, MA, USA) oven equipped with a Programmable Temperature Vaporization (PTV) injector used in split mode (volatile fraction) or in splitless mode (liquid fraction) and kept at 250 ˚C. Chromatographic separation was achieved on a PoraBond-Q (25 m x 0.32 mm x 5 µm) capillary column (Varian, Palo Alto, CA, USA) for the volatile fraction and on a VF-5ms (50 m x 0.20 mm x 0.33 µm) capillary column (Varian, Palo Alto, CA, USA) for the liquid fraction after derivatization (see below) with He as carrier (Alpha gas 2, Air Liquide, Belgium). Mass spectrometric detection was performed with a PolarisQ ion-trap (Thermo-Scientific, Waltham, MA, USA). Ions were produced by a 70 eV positive Electronic Ionisation (EI), with the ion source kept at 200 ˚C. The acquisition was recorded in full scan mode with a 30-200 (volatiles) or 50-600 (liquid fraction) *m/z* mass range. The quantification was achieved using external calibration curves prepared daily using pure commercial standards. Gas chromatography coupled with flame ionization detection (GC/FID) was performed to monitor the carbonation reaction of 3-butene-1,2-diol.

2.3.2 Headspace-Solid Phase Micro Extraction

Headspace-Solid Phase Micro Extraction technique (HS-SPME) with Carboxen-PDMS fibers was carried out for the analysis of the volatile fraction and the quantification of 2,5-dihydrofuran, furan and butadiene. HS-SPME is an appropriate method to extract Volatiles and Very Volatiles Organic Compounds (VOC, VVOC),[1] and consists in adsorbing volatiles from the headspace onto a thin polymeric fiber. In a typical procedure, a sample of the reactor effluent (~10 mg) was collected in a 20 mL SPME air-tight sealed vial. The vials were then weighted, 1 mL of Milli-Q® water was added and the samples was homogenized at 750 rpm for 1 min and sent to the analysis in HS. The extraction of molecules in the headspace was performed at low temperature (15 ˚C) for 10 min with Carboxen-PDMS fiber.[2] Carboxen-PDMS fibers were used as they exhibit a high selectivity toward furan family.[3] Volatiles were then thermally desorbed from the fiber in the GC injection port for 1 min with a split ratio of 29. After each extraction-desorption cycle, the fiber was cleaned in a conditioning station for 15 min at 275 ˚C. Fiber blanks were run daily to insure the absence of carryover.

2.3.3 Derivatization

Some compounds in the liquid fractions (b.p. > 70 °C) not directly quantifiable by ^{1}H NMR were derivatized for GC analysis (residual erythritol and anhydroerythritol, see Figures S7 and S8). In a typical derivatization procedure, a sample of reactor effluent (80 mg) was diluted in 1 mL of methanol (picograde, LGC-Promochem, Wesel). Next, 10 µL of the solution were weighted and concentrated under Nitrogen flow in a 1 mL GC-vial. Pyridine (50 µL) was added as a solvent, and the resulting homogeneous solution was treated with 50 µL of *N,O*-bis(trimethylsilyl)trifluoroacetamide as a derivatization agent (Sigma-Aldrich) at 60 ˚C (1 h) in a sealed GC-vial.

2.3.4 Reference chromatograms

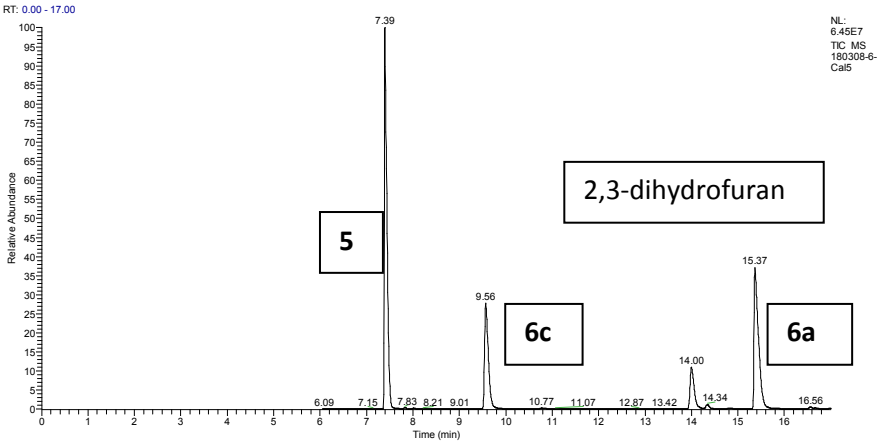


Figure S5. Retention times of commercial pure samples: butadiene (**5**, 7.39 min), furan (**6c**, 9.56 min), 2,3-dihydrofuran (not detected in this study, 14 min) and 2,5-dihydrofuran (**6a**, 15.37 min).

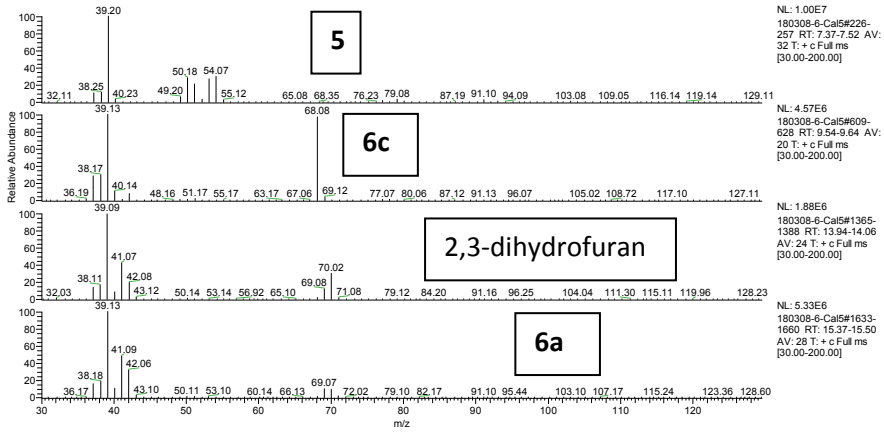


Figure S6. Mass spectrograms for commercial pure samples: butadiene (**5**), furan (**6c**), 2,3-dihydrofuran (not detected in this study) and 2,5-dihydrofuran (**6a**)

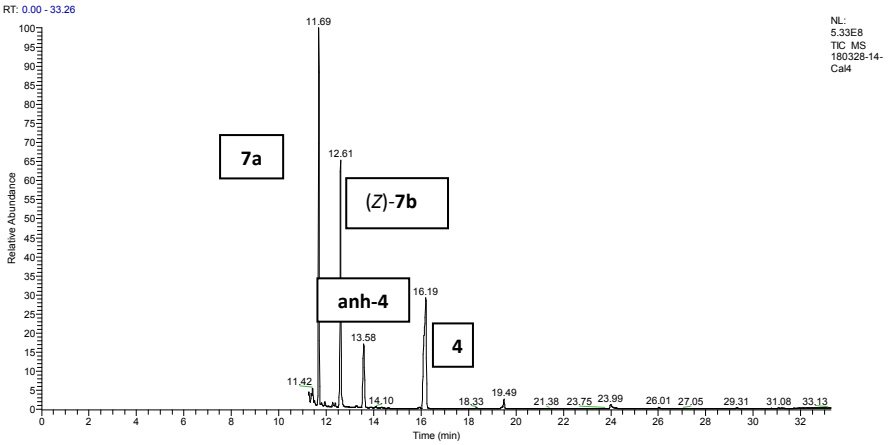


Figure S7. Retention times of commercial pure samples after derivatization: 3-butene-1,2-diol (**7a**, 11.59 min), *cis*-2-butene-1,4-diol ((*Z*)-**7b**, 12.61 min), 1,4-anhydroerythritol (**anh-4**, 13.58 min) and erythritol (**4**, 16.19 min).

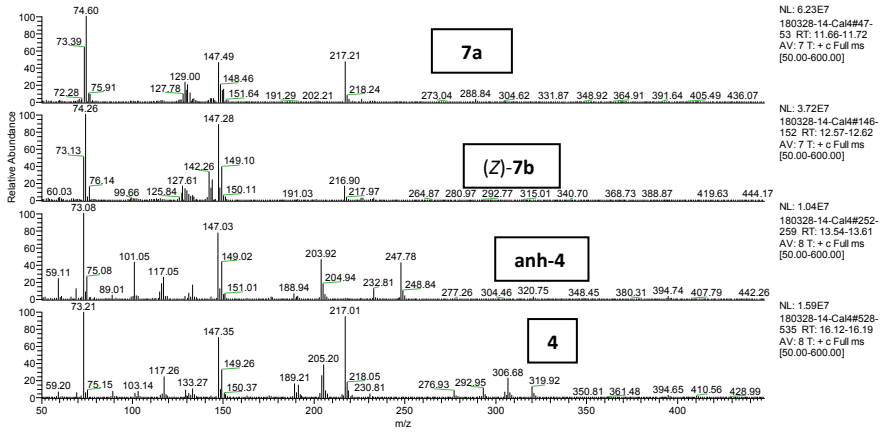


Figure S8. Mass spectrograms for commercial pure samples: 3-butene-1,2-diol (**7a**), *cis*-2-butene-1,4-diol ((*Z*)-**7b**), 1,4-anhydroerythritol (**anh-4**) and erythritol (**4**).

2.3.5 Representative results

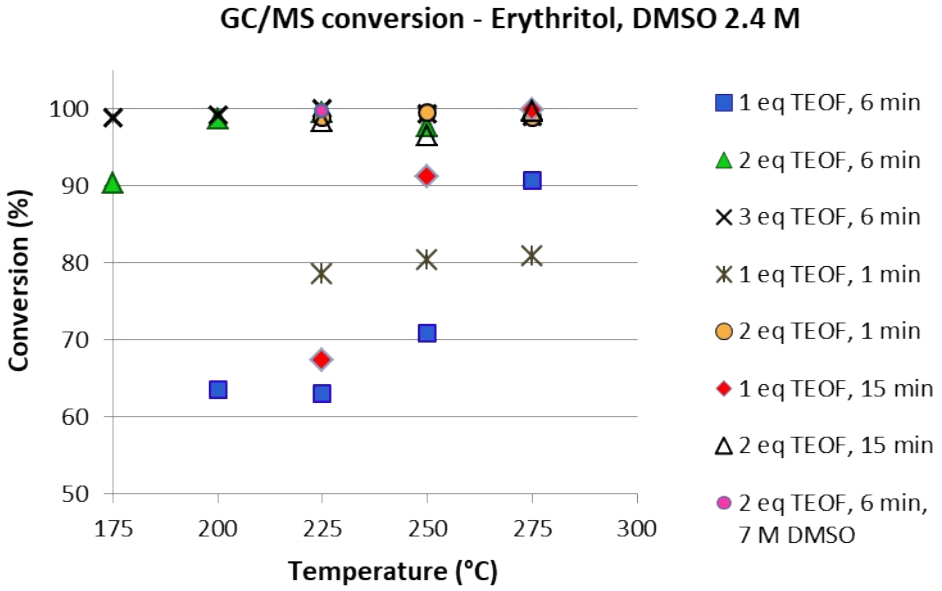


Figure S9. Conversion of erythritol (**4**) in DMSO determined by GC/MS after derivatization

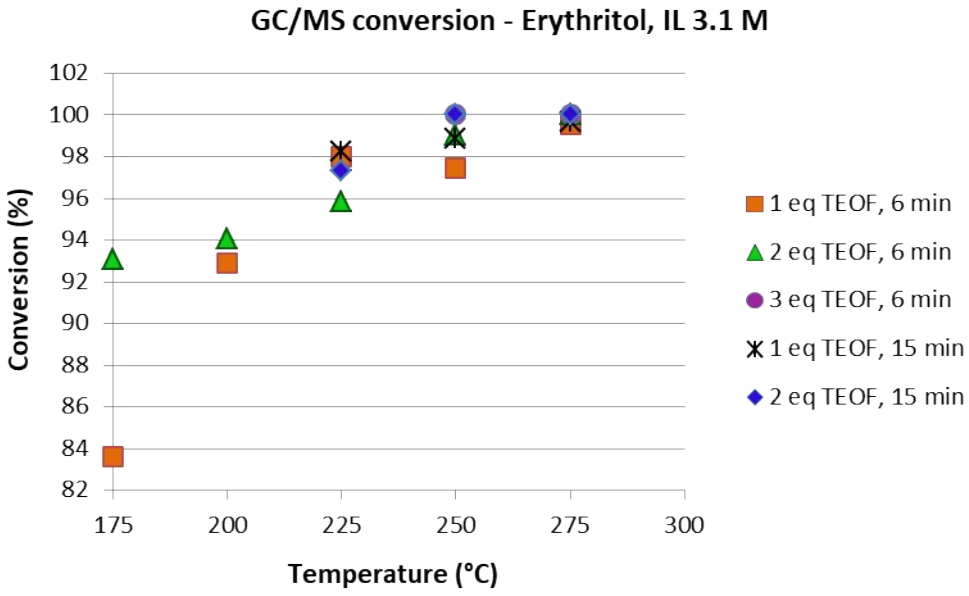


Figure S10. Conversion of erythritol (**4**) in [EMIM][ES] determined by GC/MS after derivatization

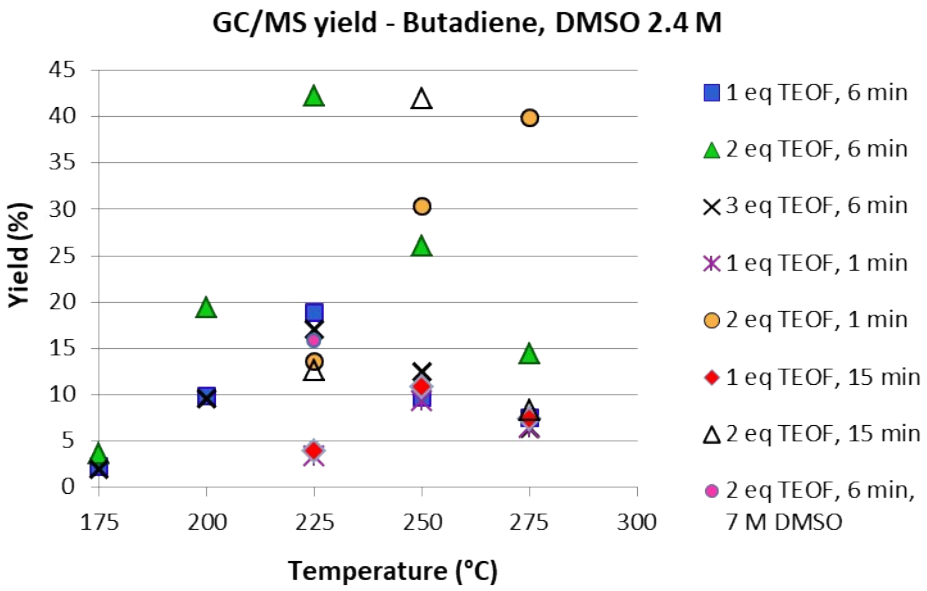


Figure S11. Yield of butadiene (**5**) in DMSO determined by GC/MS after HS-SPME

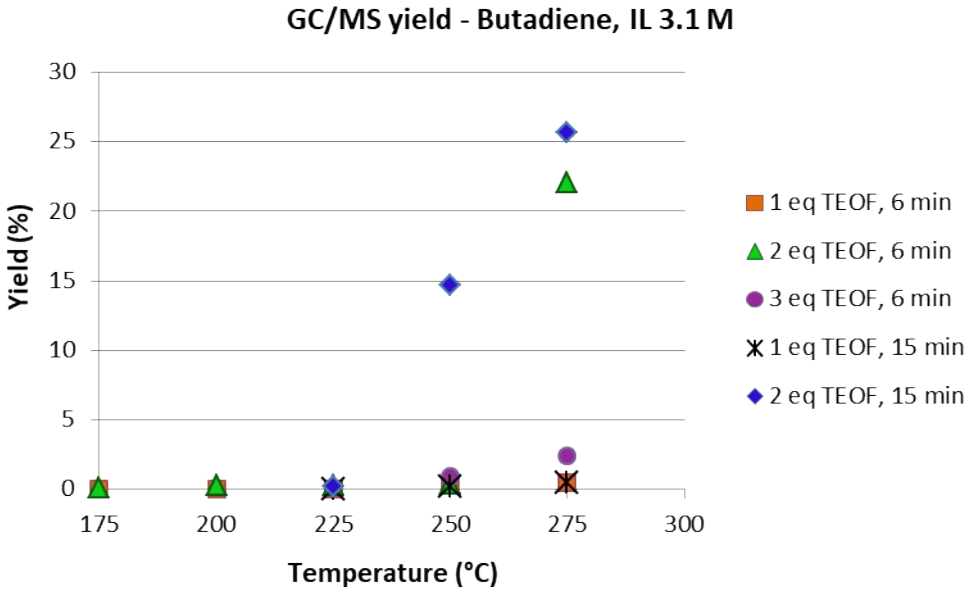


Figure S12. Yield of butadiene (**5**) in [EMIM][ES] determined by GC/MS after HS-SPME

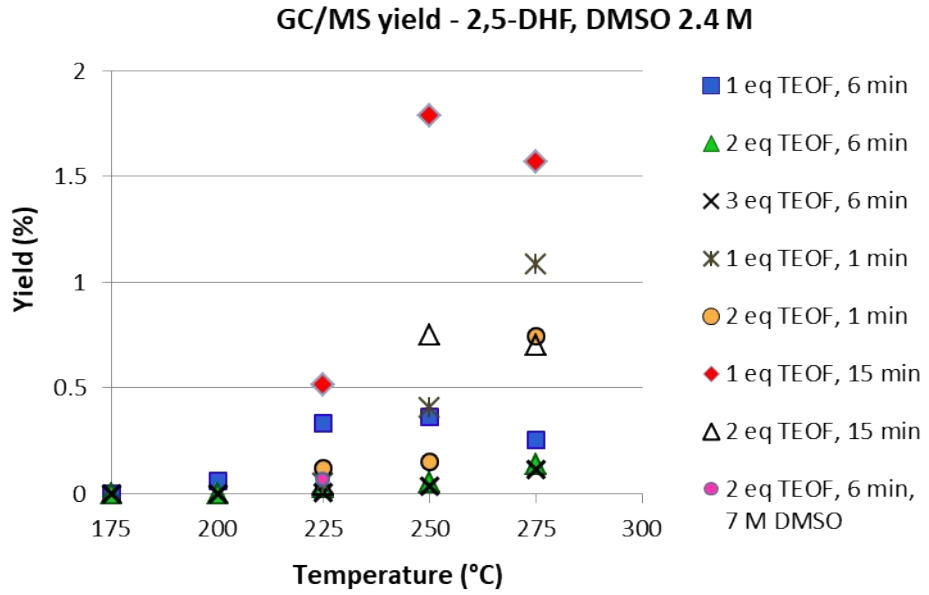


Figure S13. Yield of 2,5-dihydrofuran (**6a**) in DMSO determined by GC/MS after HS-SPME

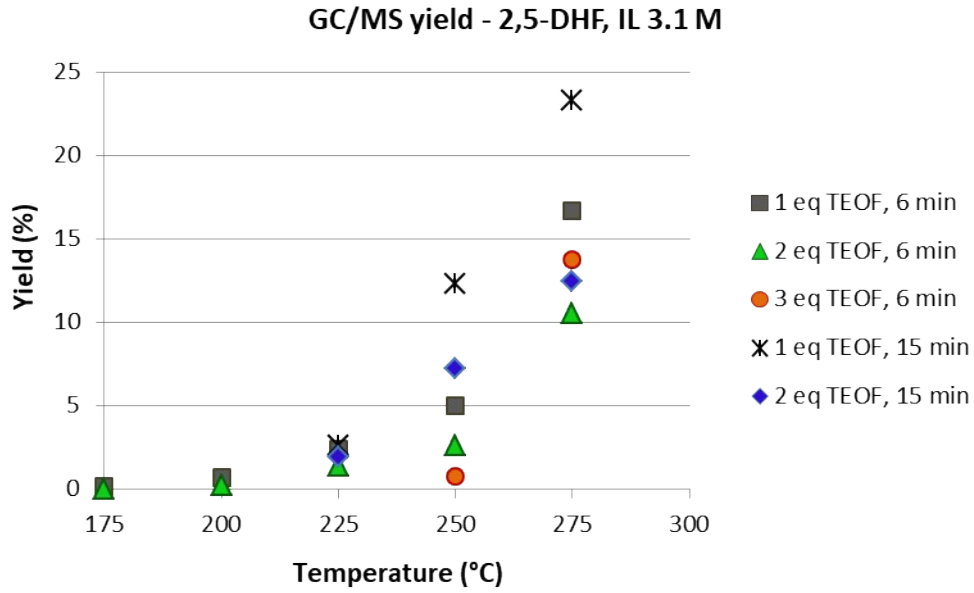


Figure S14. Yield of 2,5-dihydrofuran (**6a**) in [EMIM][ES] determined by GC/MS after HS-SPME

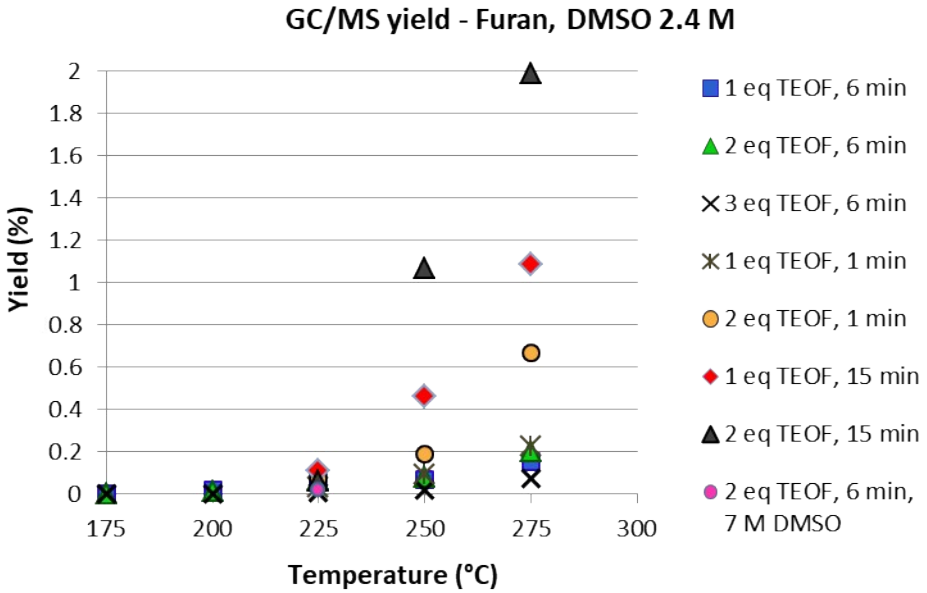


Figure S14. Yield of furan (**6c**) in DMSO determined by GC/MS after HS-SPME

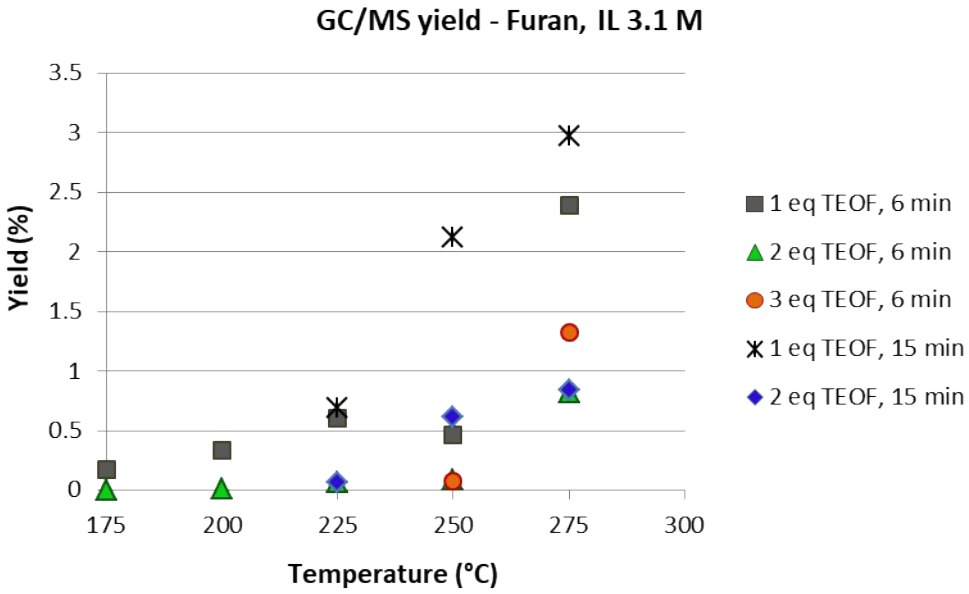


Figure S16. Yield of furan (**6c**) in [EMIM][ES] determined by GC/MS after HS-SPME

2.4 Off-line NMR quantitative analysis

2.4.1 General procedure

The samples were prepared by adding 600 µL of stock solution of mesitylene (0.04 M) in d_6-acetone to 10 µL of untreated crude reactor effluent. The reactor effluents were collected in closed vials under an inert atmosphere (argon), and kept at 4 °C before analysis. Analytical ^{1}H NMR spectra were recorded at 400 MHz on a Bruker Avance III HD spectrometer (9.4 Tesla) equipped with a high-resolution multinuclear probe that operated in the range of 40-400 MHz. Spectra were recorded in 5 mm NMR tube (Norell). Free induction decays were acquired at 298 K using a standard pulse sequence (Bruker, zg30). The spectral width was 20 ppm (8012.820 Hz). A 30 ° excitation pulse and a 4 s relaxation delay were used to collect 64 scans.

2.4.2 Spectral libraries

The chemical shifts are reported in ppm relative to TMS as internal standard or to solvent residual peak. Figure S17 regroups ^{1}H NMR spectra (400 MHz, d_6-acetone) of the main reagents and products reported in this study.

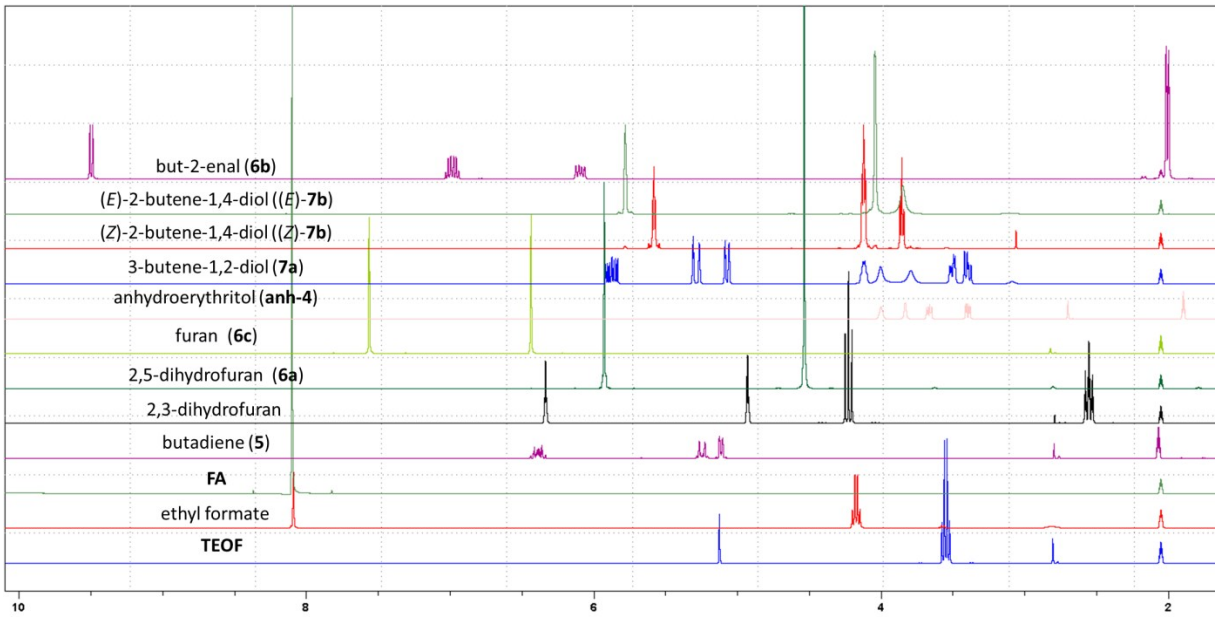


Figure S17. ^{1}H NMR (400 MHz) spectral library in d_6-acetone (from 2 to 10 ppm)

2.4.3 Representative examples

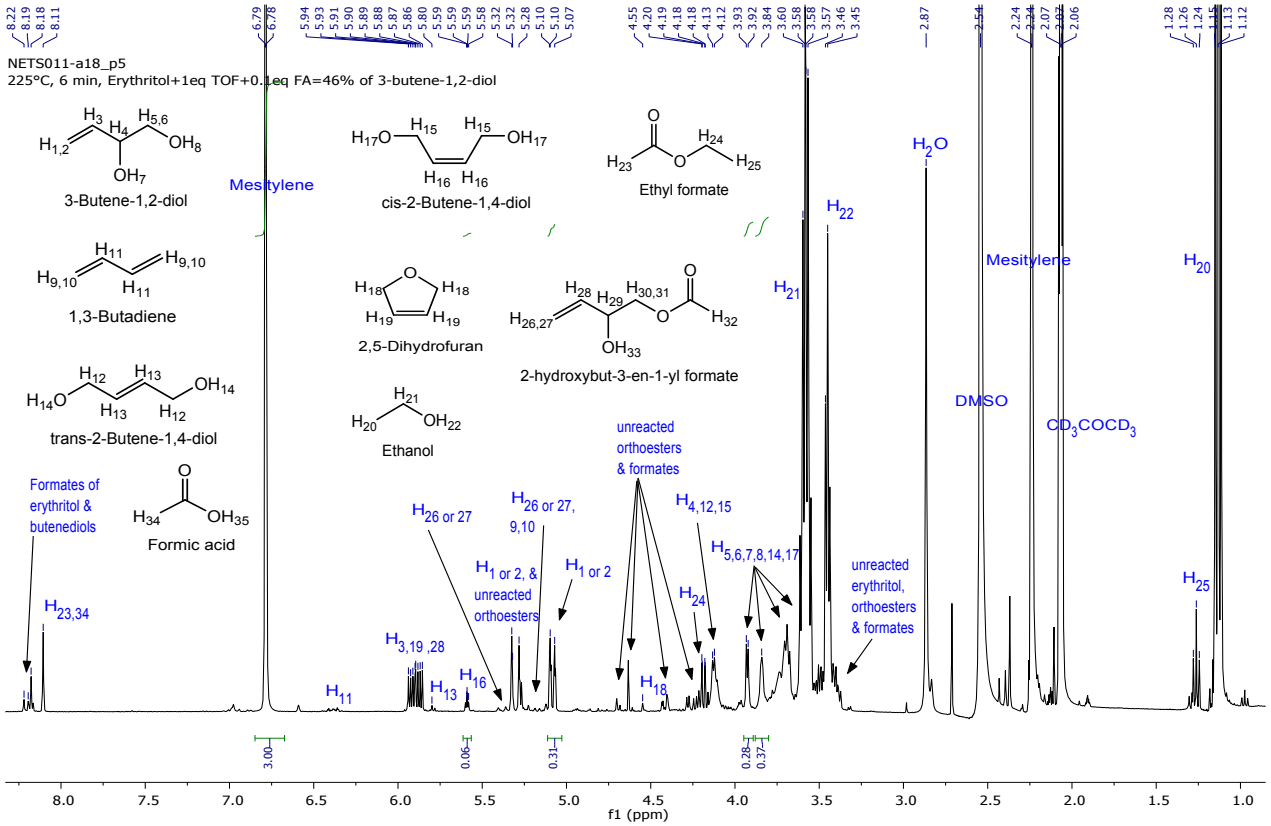


Figure S18. ^{1}H NMR of a crude reactor effluent in CD_3COCD_3: deoxydehydration of erythritol (2.4 M in DMSO) in the presence of triethyl orthoformate (1 equiv.) and formic acid (10 mol%) at 225 °C (6 min residence time, 6.9 bar) (46% yield for 3-butene-1,2-diol)

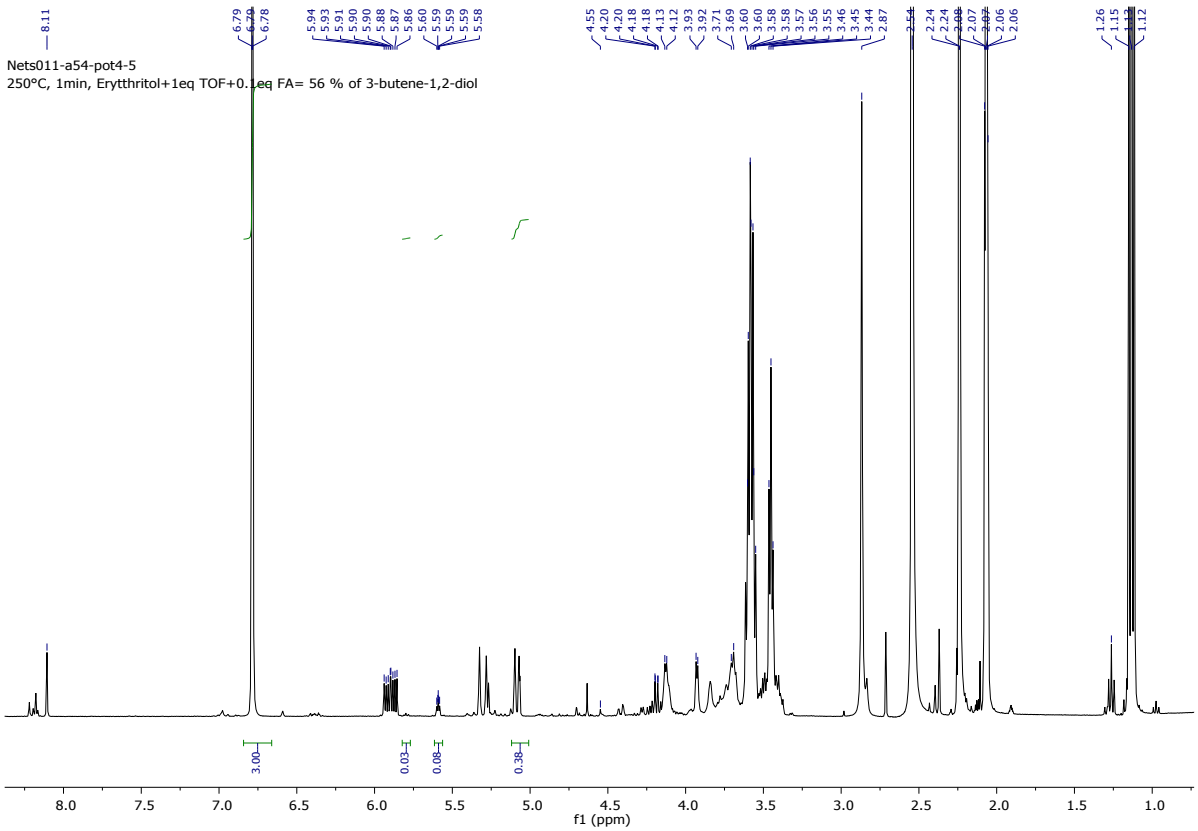


Figure S19. ^{1}H NMR of a crude reactor effluent in CD_3COCD_3: deoxydehydration of erythritol (2.4 M in DMSO) in the presence of triethyl orthoformate (1 equiv.) and formic acid (10 mol%) at 250 °C (1 min residence time, 6.9 bar) (56% yield for 3-butene-1,2-diol).

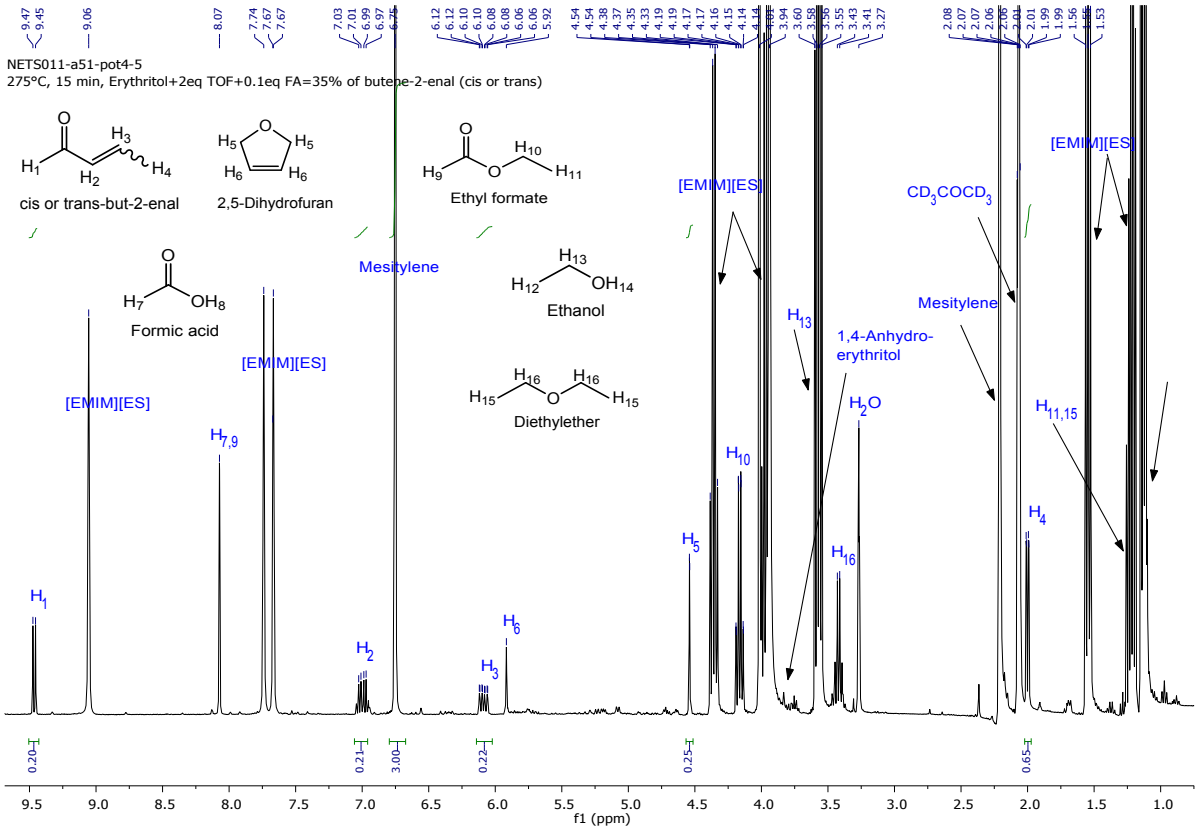


Figure S20. ^{1}H NMR of a crude reactor effluent in CD_3COCD_3/CD_3OD, 4/1 and: deoxydehydration of erythritol (3.1 M in [EMIM][ES]) in the presence of triethyl orthoformate (2 equiv.) and formic acid (10 mol%) at 275 °C (15 min residence time, 6.9 bar) (35% yield for *cis* or *trans*-but-2-enal).

2.4.4 Representative results

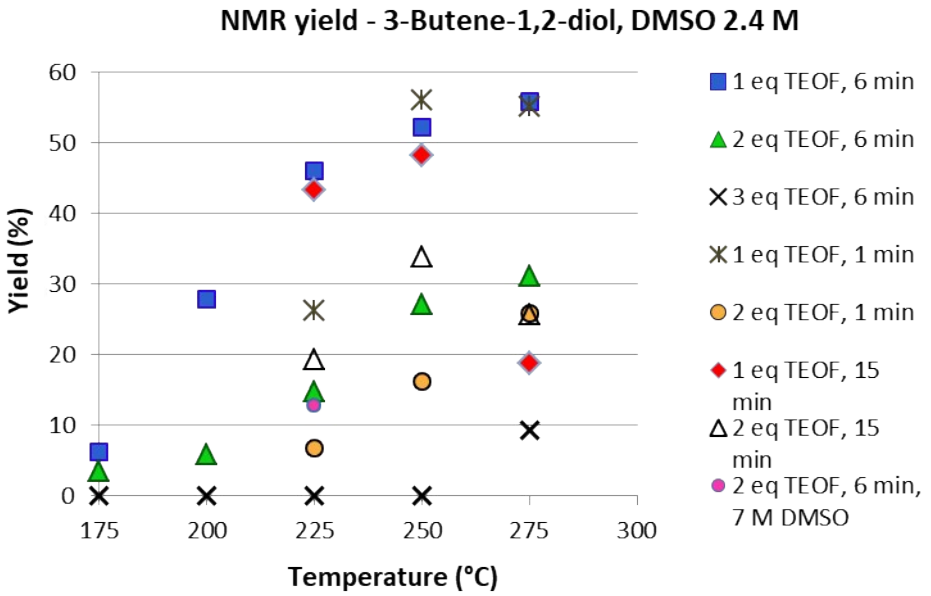


Figure S21. Yield of 3-butene-1,2-diol (**7a**) in DMSO determined by ^{1}H NMR

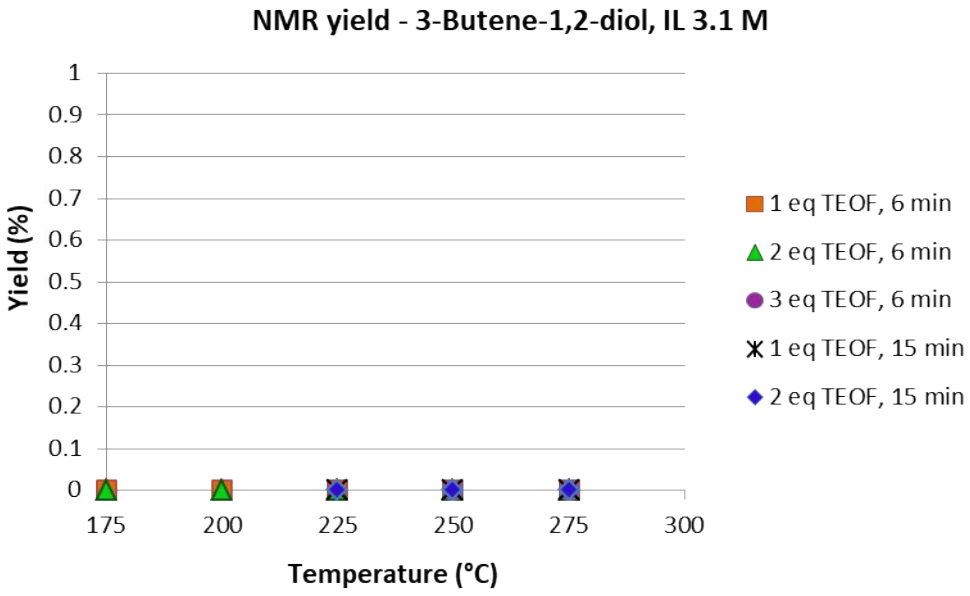


Figure S22. Yield of 3-butene-1,2-diol (**7a**) in [EMIM]ES] determined by ^{1}H NMR

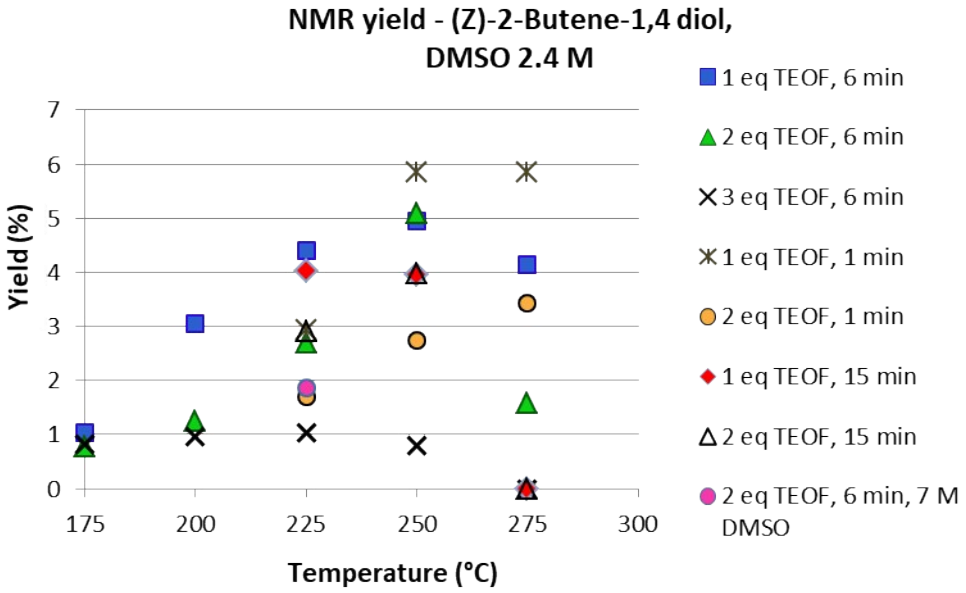


Figure S23. Yield of (*Z*)-2-butene-1,4 diol, ((*Z*)-**7b**) in DMSO determined by ^{1}H NMR

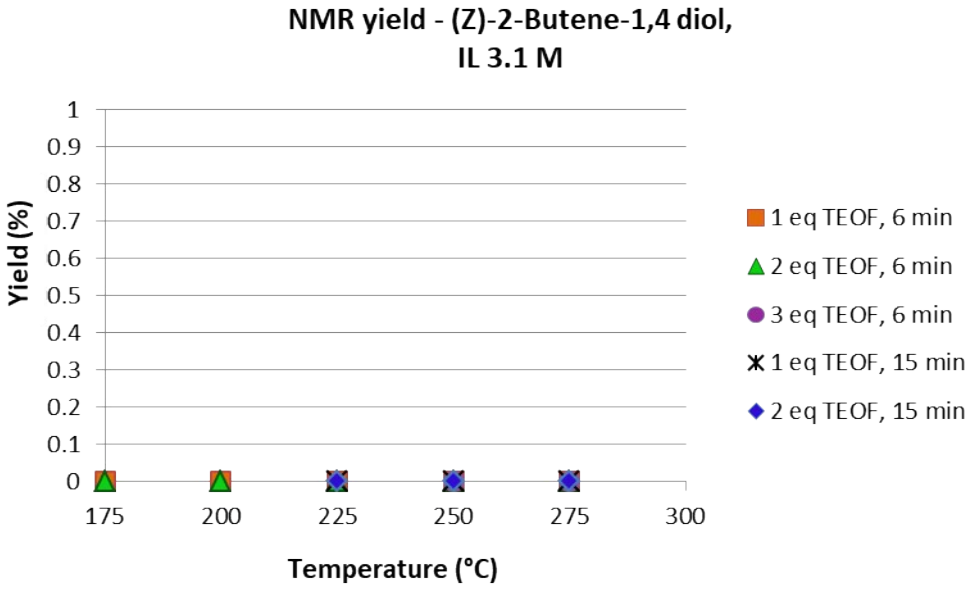


Figure S24. Yield of (*Z*)-2-butene-1,4 diol, ((*Z*)-**7b**) in [EMIM][ES] determined by ^{1}H NMR

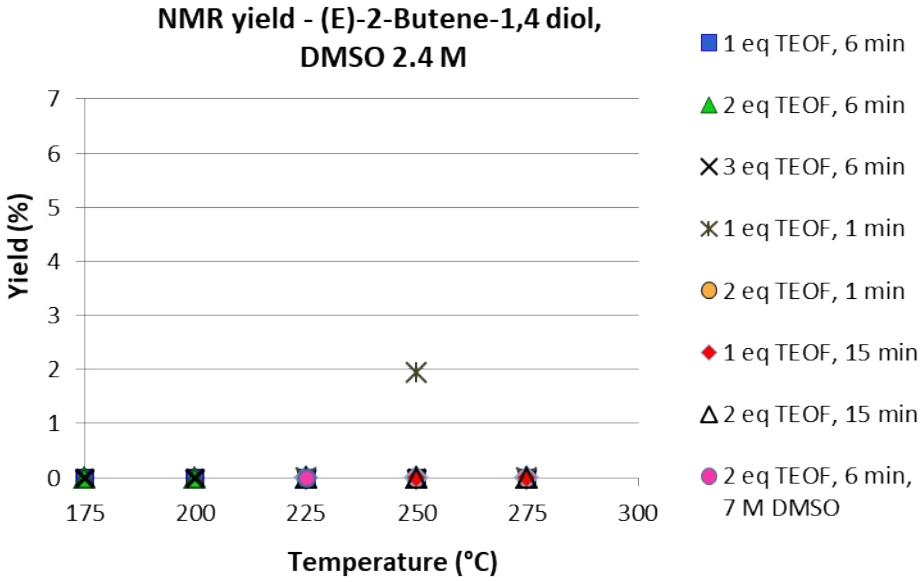


Figure S24. Yield of (*E*)-2-butene-1,4 diol, ((*E*)-**7b**) in DMSO determined by ^{1}H NMR

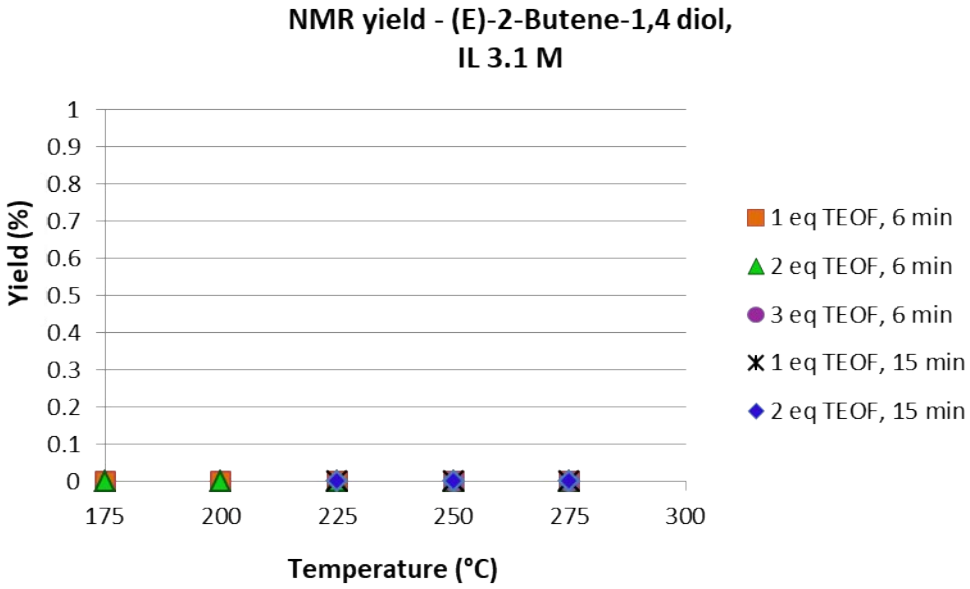


Figure S26. Yield of (*E*)-2-butene-1,4 diol, ((*E*)-**7b**) in [EMIM][ES] determined by ^{1}H NMR

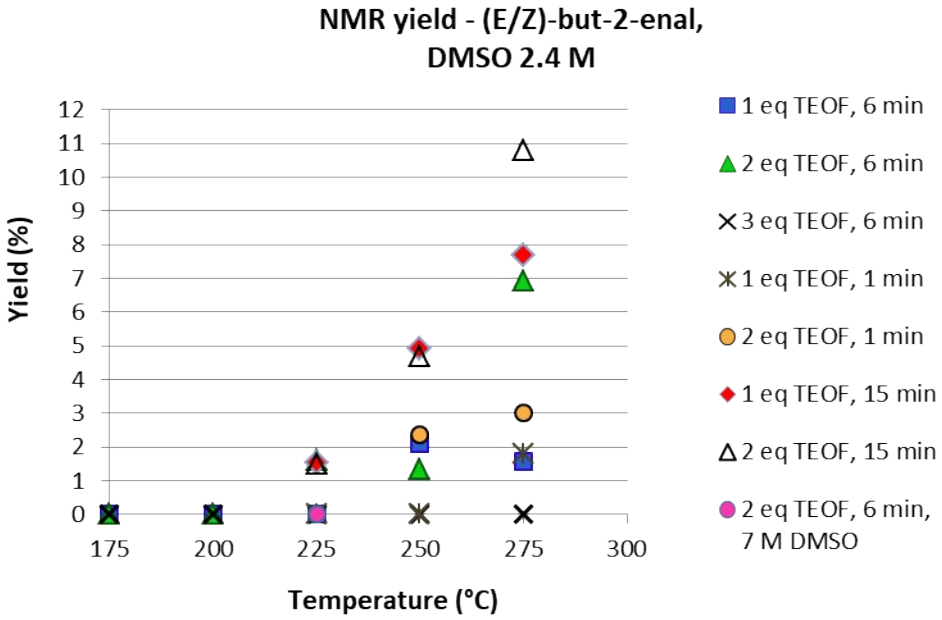


Figure S27. Yield of (*E/Z*)-but-2-enal, ((*E/Z*)-**6b**) in DMSO determined by ^{1}H NMR

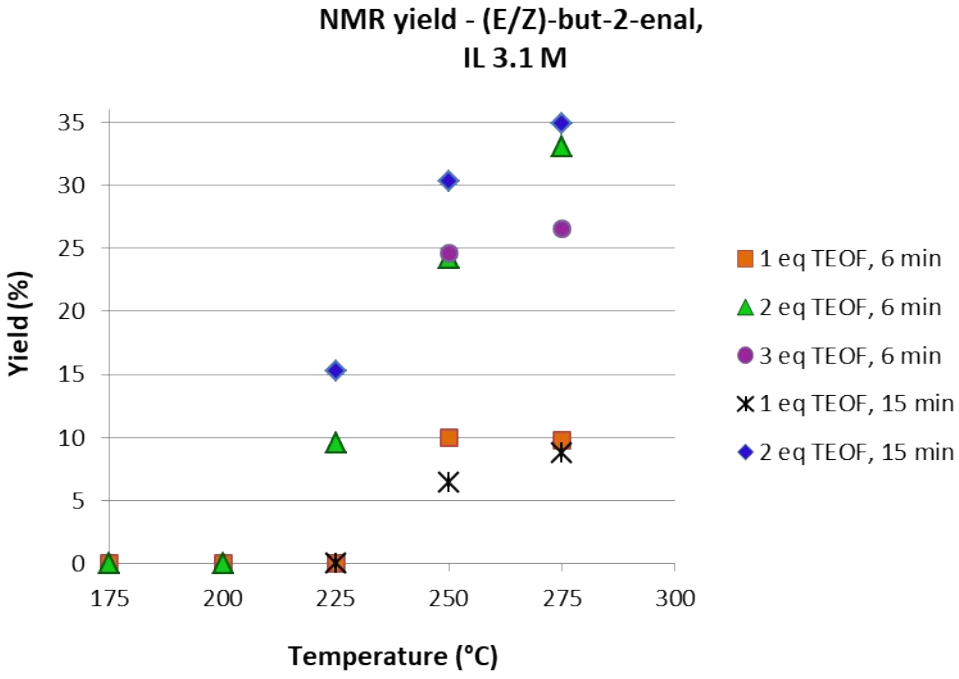


Figure S28. Yield of (*E/Z*)-but-2-enal, ((*E/Z*)-**6b**) in [EMIM][ES] determined by ^{1}H NMR

2.5 Optimization of the preparation of 4-vinyl-1,3-dioxolan-2-one from 3-butene-1,2-diol under homogeneous conditions

Table S3 Process optimization for the homogeneous continuous flow carbonation of purified 3-butene-1,2-diol.

Entry	Residence time (min)	T (°C)	DMC (equiv.)	DBU [a] (mol%)	Conv. [b] (%)	Selec. [b] (%)
1[c]	3	100	2	2	23	84
2[c]	3	120	2	2	31	83
3[c]	3	140	2	2	44	81
4[c]	3	160	2	2	70	80
5[c]	4	160	2	2	77	81
6[c]	5	160	2	2	83	74
7[c]	6	160	2	2	83	76
8[c]	4	160	2	1	52	78
9[c]	4	160	2	3	80	80
10[c]	4	160	2	4	80	73
11[c]	4	160	2.5	2	85	75
12[c]	4	160	3	2	86	80
13[c]	4	160	3.5	2	87	79
14[c]	4	150	3	3	84	78
15[c]	4	170	3	2	85	76
16[d]	4	160	3	2	95	80
17[d]	4	160	3	0	9	0

P = 11 bar. [a] The loading of organocatalyst is relative to the number of moles of 3-butene-1,2-diol. [b] Conversion and yield were determined by GC-FID. [c] 3-Butene-1,2-diol was pumped as a neat solution. [d] 3-Butene-1,2-diol was pumped as a 1.5 M solution in DMSO.

2.6 On-line IR qualitative analysis

2.6.1 Spectral libraries

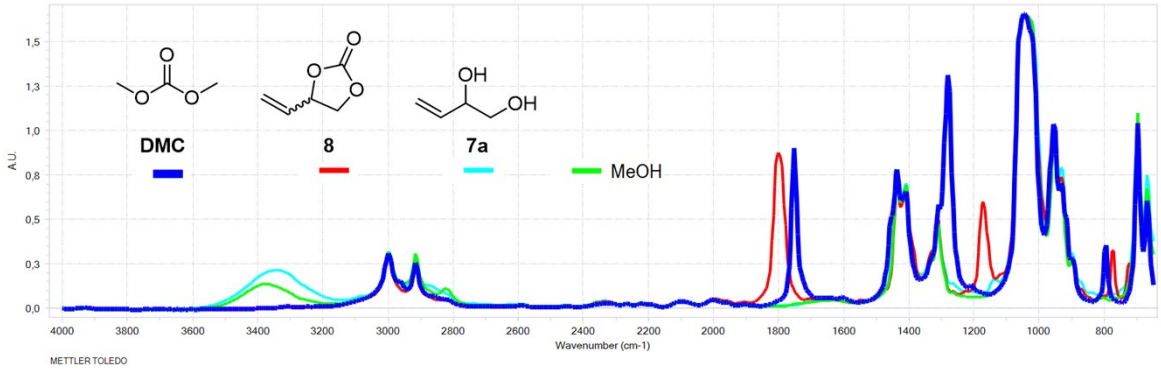


Figure S29. Spectral library of compounds **DMC**, **8**, **7a** and methanol in DMSO

2.6.2 On-line reaction monitoring for the carbonation of 3-butene-1,2-diol (**7a**)

On-line reaction monitoring was recorded with the iC IR® software (version 4.3). The outcome of the reaction was monitored in real time by following the decrease of the characteristic vibration bands of DMC ($\nu_{C=O}$ at 1750 cm^{-1}) and the increase of the characteristic vibration bands of vinyl ethylene carbonate (**8**, $\nu_{C=O}$ at 1810 cm^{-1}). Figure S30

shows the evolution of the conversion to **8** as a function of the temperature, using homogeneous DBU.

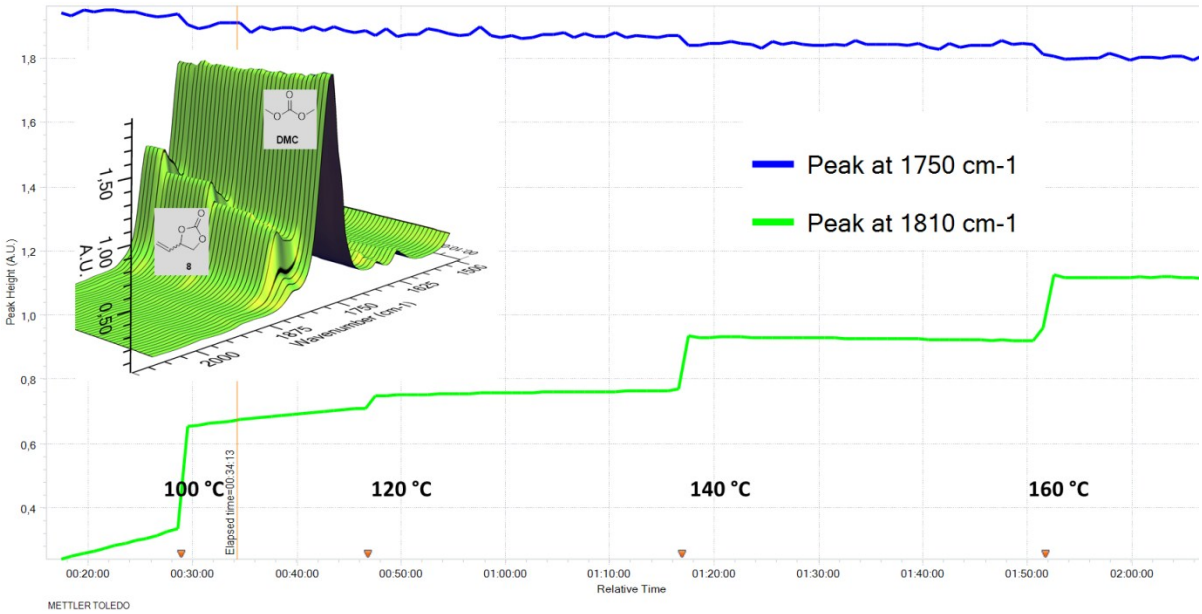


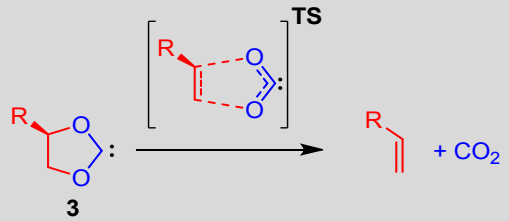
Figure S30. On-line IR reaction monitoring for the carbonation of neat 3-butene-1,2-diol (**7a**) in the presence of 2 equiv. of dimethyl carbonate and 2 mol% DBU (homogeneous conditions) showing the impact of the temperature on the conversion of **7a** toward **8** ($\nu_{C=O}$ at 1810 cm^{-1}, green series).

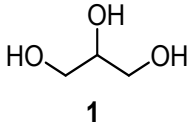
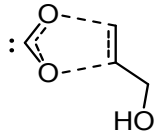
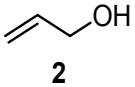
3. Computations

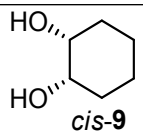
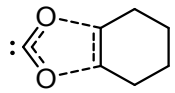
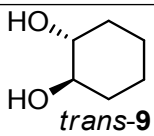
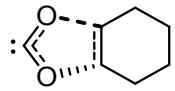
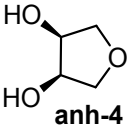
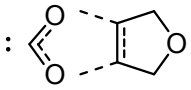
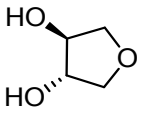
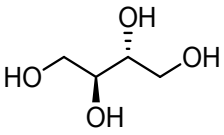
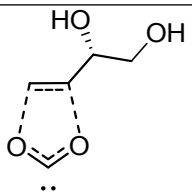
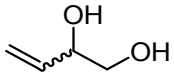
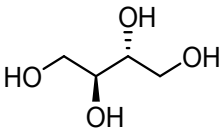
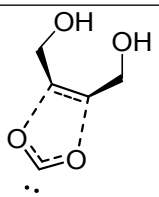
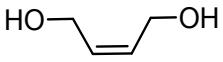
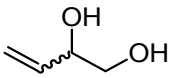
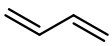
3.1 CO_2 extrusion from dioxolidin-2-ylidene species

The most representative results are summarized in Table S4 (MP2/6-31+G**, kcal mol^{-1}). $\Delta\Delta G^{\neq}$ values are calculated for isomeric TS and given as indicative values. The reader is redirected to reference[4] for more details.

Table S4. Activation parameters



Substrate	TS	Product	**DMSO** (ε = 46.83) $\Delta G^{\neq}$ ($\Delta\Delta G^{\neq}$)
 **1**		 **2**	10.7

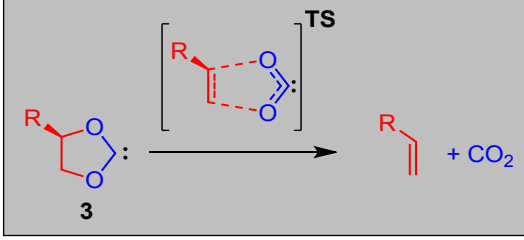
 *cis*-**9**		 **10**	11.1
 *trans*-**9**		 **10**	(30.5)
 **anh-4**		 **6a**	11.6
 **anhydrothreitol**	**No TS structure compatible with a DODH process**	/	/
 **4**		 **7a**	10.2
 **4**		 (*Z*)-**7b**	(3.1)
 **7a**		 **5**	7.8

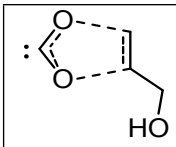
3.2 Cartesian coordinates

Cartesian coordinates and absolute energies for representative stationary points are listed below (Table S5).

Table S5. Cartesian coordinates and absolute energies for representative stationary points

CO_2 extrusion from dioxolidin-2-ylidene species





from **1**

MP2/6-31+G** (Hartree)

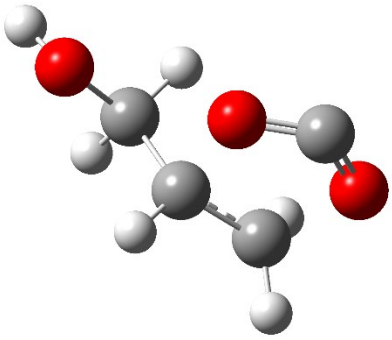
13

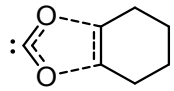
scf done: -380.577271

C	0.030220	-0.028248	0.037717
O	0.073603	0.023082	1.292799
C	1.796402	0.014469	1.762058
C	2.443512	0.005133	0.481417
O	1.083975	-0.056282	-0.649642
H	1.804460	0.950418	2.310798
H	2.905764	0.923083	0.144223
H	2.954679	-0.901702	0.179735
C	1.894535	-1.212604	2.621278
H	2.922616	-1.305206	2.984210
H	1.654489	-2.100174	2.029186
O	0.990293	-1.063730	3.720424
H	1.148439	-1.793739	4.335496

H = -380.469545

G = -380.508573





from *cis*-**9**

MP2/6-31+G** (Hartree)

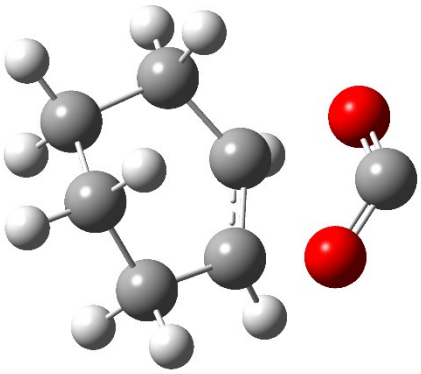
19

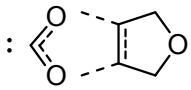
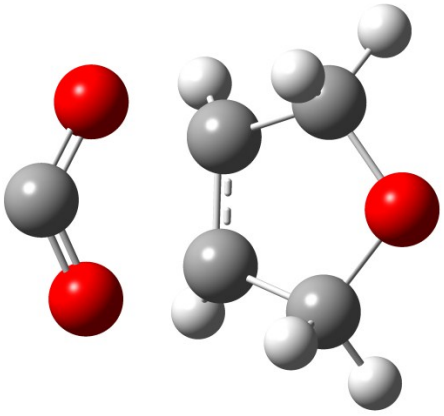
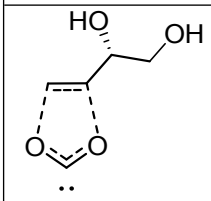
scf done: -421.909854

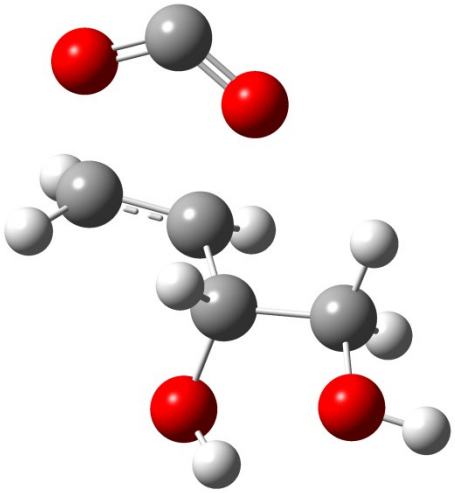
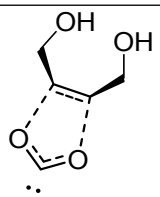
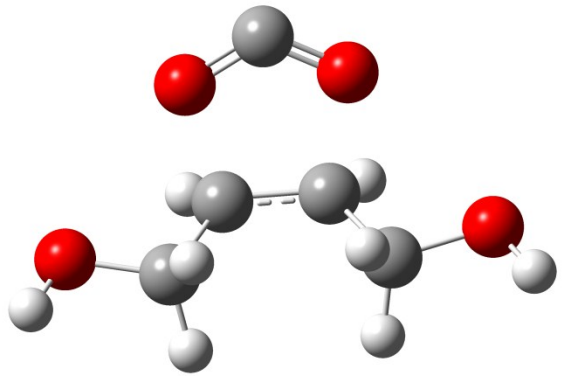
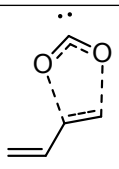
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.242899
C	1.796194	0.000000	1.793045
C	2.488828	-0.122698	0.537553
O	1.034779	-0.013998	-0.685851
C	1.828070	-1.117012	2.813085
C	2.147118	-2.484210	2.196642
C	3.399961	-2.384118	1.317487
C	3.174167	-1.422174	0.136053
H	2.934895	0.790834	0.157974
H	1.750922	1.003429	2.207005
H	0.884534	-1.134543	3.368840
H	2.607203	-0.861410	3.545995
H	1.297050	-2.834982	1.595970
H	2.294966	-3.218255	2.996248
H	3.684945	-3.368109	0.929525

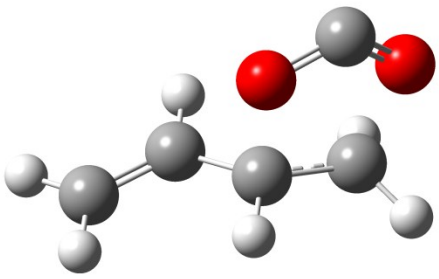
H = -421.738948

G = -421.779795



H 4.239592 -2.030157 1.930857 H 4.126336 -1.183087 -0.349002 H 2.564095 -1.925901 -0.622646	
 from **anh-4**	**MP2/6-31+G**** (Hartree)
14 scf done: -418.558176 C -0.024342 0.000000 -0.013759 O 0.041276 0.000000 1.276830 C 1.647523 -0.004233 1.777265 C 2.373101 0.011556 0.494157 O 1.113889 0.018723 -0.624005 C 1.941860 -1.358122 2.417524 O 3.093297 -1.876066 1.725477 C 3.091498 -1.330828 0.391773 H 1.679626 0.878833 2.406770 H 2.916901 0.907648 0.213509 H 4.126418 -1.238867 0.071836 H 2.551851 -1.988103 -0.293784 H 2.195544 -1.286695 3.472017 H 1.082704 -2.022894 2.290347	H = -418.443111 G = -418.481474 
 from **4** to **7a**	**MP2/6-31+G**** (Hartree)
17 scf done: -494.808218 C 0.036150 -0.002214 -0.011974 O 0.050543 0.026646 1.245976 C 1.759608 0.001150 1.749616 C 2.436140 -0.000894 0.483528 O 1.106380 -0.026028 -0.671791 H 1.778254 0.930059 2.312188 H 2.939382 -0.913656 0.188045 H 2.921791 0.913144 0.168114 C 1.819578 -1.250731 2.586324 O 3.171467 -1.345905 3.064123	H = -494.664498 G = -494.709271

C 0.866370 -1.224828 3.766778 O 1.160117 -2.413949 4.520288 H 1.588965 -2.120017 1.957950 H 3.145198 -1.995463 3.787683 H 1.055421 -0.333287 4.369925 H -0.168925 -1.225997 3.425127 H 0.769568 -2.326321 5.400662	
 from **4** to (*Z*)-**7b**	**MP2/6-31+G**** (Hartree)
17 scf done: -494.802527 C 0.003592 -0.002081 0.024304 O -0.035201 -0.012758 1.281876 C 1.645766 0.001278 1.864272 C 2.393961 0.008700 0.632720 O 1.101332 0.004100 -0.590419 H 1.623764 -0.946055 2.393436 H 2.856220 -0.934580 0.359755 C 1.656615 1.192992 2.779024 O 0.747623 0.914628 3.848862 C 3.208183 1.206620 0.233428 O 3.746491 0.940255 -1.065777 H 1.360246 2.097095 2.241589 H 2.670466 1.335564 3.167538 H 0.806647 1.641392 4.485026 H 2.591379 2.108651 0.221801 H 4.016345 1.346514 0.959122 H 4.335738 1.671851 -1.298170	H = -494.658881 G = -494.704254 
 from **7a** to **5**	**MP2/6-31+G**** (Hartree)

13 scf done: -343.508330 C 0.034849 -0.014231 -0.038578 O 0.020796 0.034075 1.215009 C 1.754773 0.001813 1.763166 C 2.413925 0.007695 0.478882 O 1.134597 -0.045940 -0.667252 H 1.736689 0.942827 2.303981 H 2.952168 -0.889764 0.198566 H 2.890424 0.930294 0.173729 C 1.820501 -1.204033 2.596829 C 1.757396 -1.167637 3.940790 H 1.919470 -2.153484 2.079591 H 1.661735 -0.228868 4.472065 H 1.808748 -2.073616 4.528114	H = -343.4008320 G = -343.4392340 

4. References

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