Electronic Supplementary Material (ESI) for Green Chemistry.

Catalytic conversion of glycerol with co-feeds (fatty acids, alcohols, and alkanes) to bio-based aromatics: remarkable and unprecedented synergetic effects on catalyst performance

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Contents

An example of calculation for the data shown in Table 2 and Figs. 5 and S13

The following general calculation equation was used:

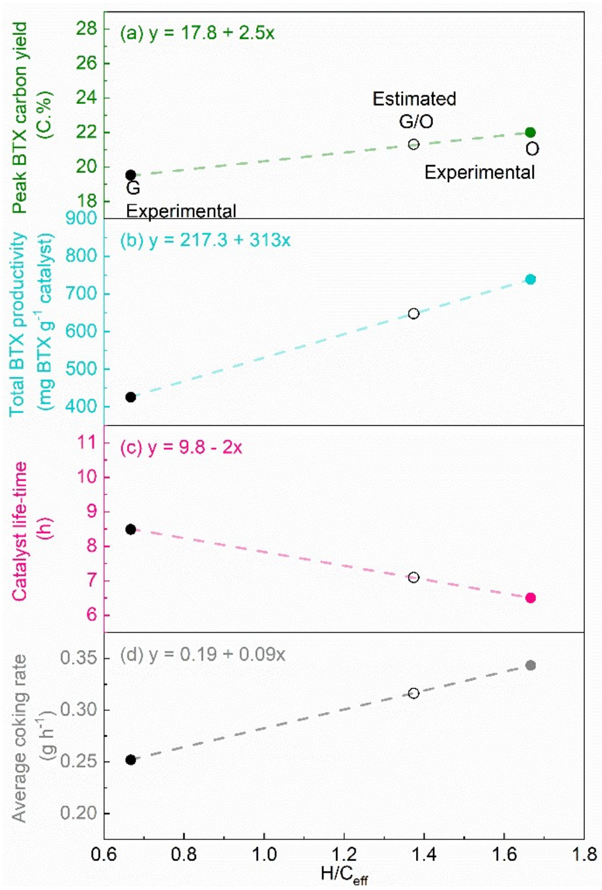
Calculated performance data of the co-feed = Experimental performance data of Feed A * carbon fraction (%) of Feed A in the total feed + Experimental performance data of Feed B * carbon fraction (%) of Feed B in the total feed

The results for the calculation procedure for the data provided for the catalytic co-conversion of glycerol and oleic acid (G/O) at a 45/55 wt.% feed intake, which corresponds to a carbon fraction of G of 0.3 and a carbon fraction of O of 0.7, are given below.

	G (Experimental)	O (Experimental)	G/O (Calculated)
Peak BTX carbon yield (C.%)	19.5	22.0	19.5*0.3+22.0*0.7=21.3
Total BTX productivity (mg_{BTX} g^{-1}_{cat})	426	739	426*0.3+739*0.7=645
BTX carbon selectivity (%)	35.0	25.9	35.0*0.3+25.9*0.7=28.6
Other aromatics carbon selectivity (%)	3.9	4.0	3.9*0.3+4.0*0.7=4.0
CO & CO_2 carbon selectivity (%)	7.8	9.6	7.8*0.3+9.6*0.7=9.1
C_1 - C_3 carbon selectivity (%)	33.1	53.0	33.1*0.3+53.0*0.7=47.0
Coke on the spent catalyst carbon selectivity (%)	20.2	7.5	20.2*0.3+7.5*0.7=11.3

An example of calculation of estimated (theoretical) results shown in Figs. 2 and 4

The performance data (peak BTX carbon yield, total BTX productivity, catalyst life-time, and average coking rate) for the individual glycerol and oleic acid *versus* H/C_{eff} were plotted and modeled using linear relations.



Peak BTX carbon yield = 17.8 + 2.5*H/C_{eff}

Total BTX productivity = 217.3 + 313*H/C_{eff}

Catalyst life-time = 9.8 - 2*H/C_{eff}

Average coking rate = 0.19 + 0.09*H/C_{eff}

With this information, the estimated (theoretical) results were determined. A calculation procedure for the catalytic co-conversion of glycerol and oleic acid (G/O, 45/55 wt.%, H/C_{eff} of 1.37) is as follows:

Estimated peak BTX carbon yield = 17.8 + 2.5*1.37 = 21.2 C.%

Estimated total BTX productivity = 217.3 + 313*1.37 = 646 $mg_{BTX}\ g_{catalyst}^{-1}$

Estimated catalyst life-time = 9.8 - 2*1.37 = 7 h

Estimated average coking rate = 0.19 + 0.09*1.37 = 0.3 g h^{-1}

An example of calculation for the data shown in Figs. 3 and S14

The following general calculation equation was used:

Calculated performance data of the co-feed = Experimental performance data of Feed A * carbon fraction (%) of Feed A in the total feed + Experimental performance data of Feed B * carbon fraction (%) of Feed B in the total feed

The results for the calculation procedure for the data provided for the catalytic co-conversion of glycerol and oleic acid (G/O) at a 45/55 wt.% feed intake, which corresponds to a carbon fraction of G of 0.3 and a carbon fraction of O of 0.7, at a TOS of 3 h are given below.

(TOS of 3 h)	G (Experimental)	O (Experimental)	G/O (Calculated)
Benzene carbon yield (C.%)	3.2	4.1	3.2*0.3+4.1*0.7=3.9
Toluene carbon yield (C.%)	9.0	8.2	9.0*0.3+8.2*0.7=8.4
m,p-Xylene carbon yield (C.%)	4.7	3.5	4.7*0.3+3.5*0.7=3.9
o-Xylene carbon yield (C.%)	1.2	1.1	1.2*0.3+1.1*0.7=1.1
Ethylbenzene carbon yield (C.%)	0.3	0.3	0.3*0.3+0.3*0.7=0.3
Naphthalene carbon yield (C.%)	0.6	1.1	0.6*0.3+1.1*0.7=1.0
2-Methyl naphthalene carbon yield (C.%)	0.8	1.1	0.8*0.3+1.1*0.7=1.0
1-Methyl naphthalene carbon yield (C.%)	0.2	0.3	0.2*0.3+0.3*0.7=0.3
CO_2 carbon yield (C.%)	3.5	1.7	3.5*0.3+1.7*0.7=2.2
Ethylene carbon yield (C.%)	7.4	6.2	7.4*0.3+6.2*0.7=6.6
Ethane carbon yield (C.%)	1.4	6.6	1.4*0.3+6.6*0.7=5.0
Propylene carbon yield (C.%)	2.0	6.2	2.2*0.3+6.2*0.7=5.0
Propane carbon yield (C.%)	5.1	15.0	5.1*0.3+15.0*0.7=12.0
Methane carbon yield (C.%)	0.5	4.3	0.5*0.3+4.3*0.7=3.2
CO carbon yield (C.%)	5.4	2.6	5.4*0.3+2.6*0.7=3.4

An example of calculation for the data shown in Fig. 6

The calculation procedure for the calculated amount of D in benzene for the catalytic co-conversion of $C_3\mathbf{D}_8O_3$ and $C_{18}\mathbf{H}_{34}O_2$ is as follows:

For an experiment using pure $C_3\mathbf{D}_8O_3$, the D amount in benzene is 37% (by experiment). For an experiment using pure $C_3\mathbf{D}_8O_3/C_{18}\mathbf{H}_{34}O_2$, the molar ratio of $C_3\mathbf{D}_8O_3/C_{18}\mathbf{H}_{34}O_2$ is 2.8 (mol./mol.). Thus the amount of D in the feed is 2.8*8/(2.8*8+1*34) = 39.7%. Assuming no synergetic effects, the amount of D in benzene is calculated to be 37%*39.7% = 14.7%.

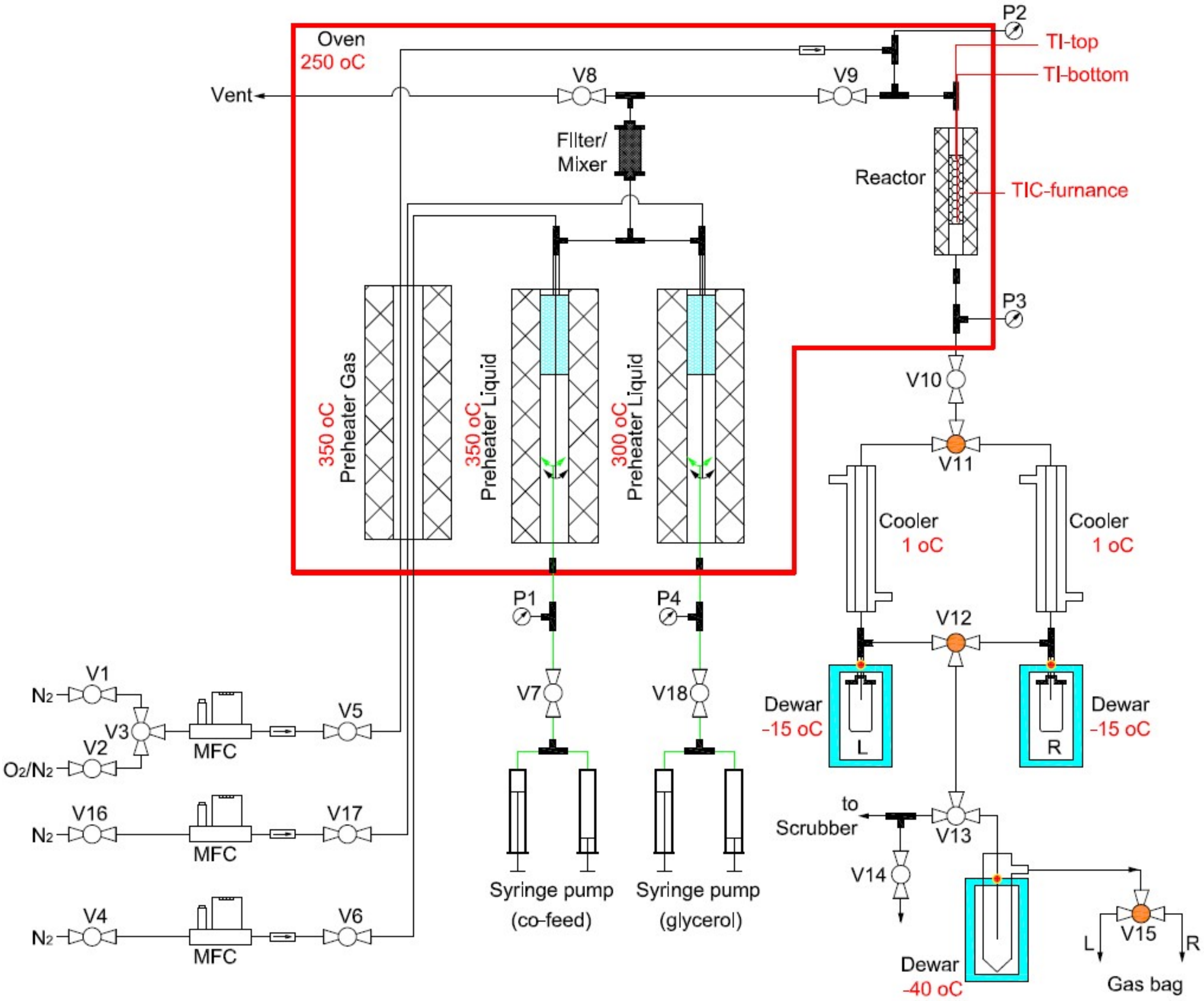


Figure S1. Schematic representative of the setup for catalytic co-conversion of glycerol and the other feedstocks to bio-based aromatics.

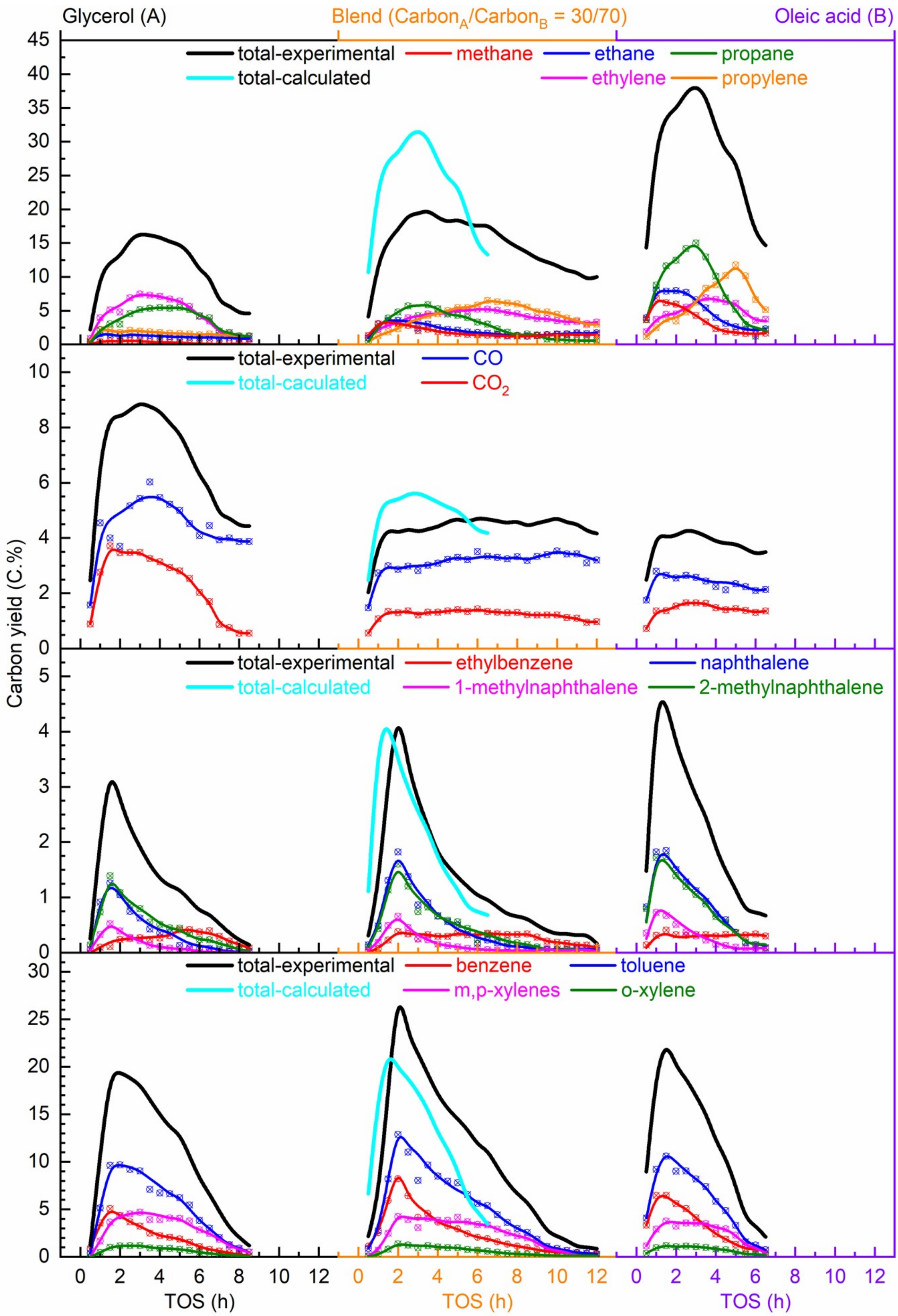


Figure S2. Carbon yields of the gas and liquid products *versus* TOS for the catalytic (co-) conversion of glycerol, oleic acid, and their blend (G/O 45/55 wt.%).

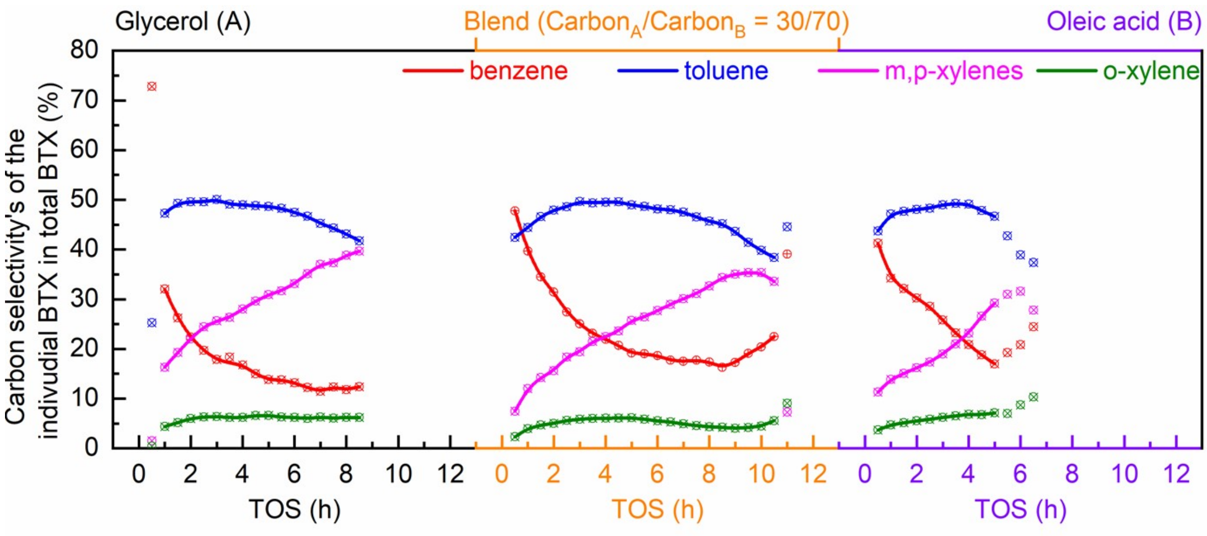


Figure S3. Carbon selectivity's of the individual BTX in total BTX *versus* TOS for the catalytic (co-) conversion of glycerol, oleic acid, and their blend (G/O 45/55 wt.%).

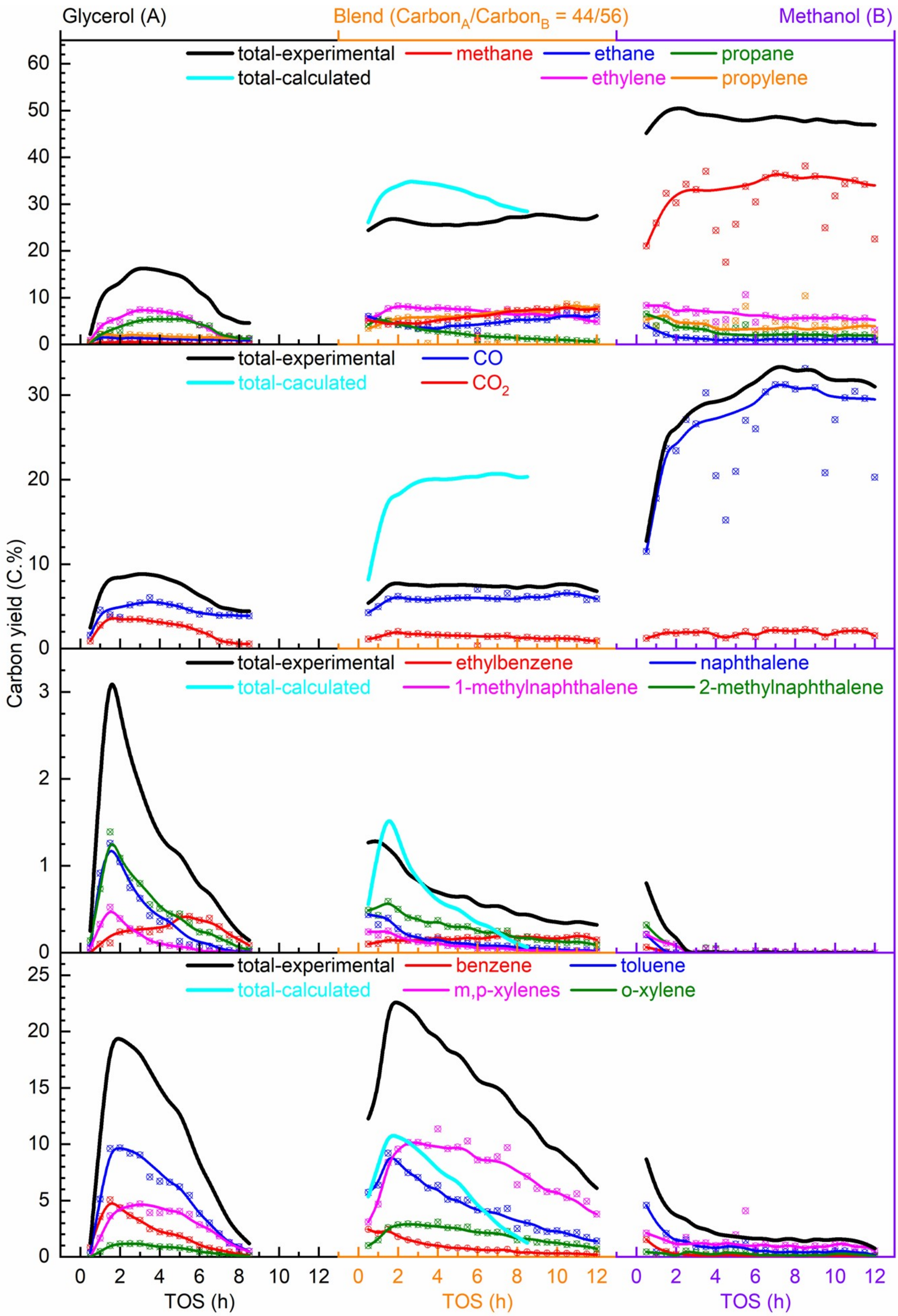


Figure S4. Carbon yields of the gas and liquid products *versus* TOS for the catalytic (co-) conversion of glycerol, methanol, and their blend (G/M 43/57 wt.%).

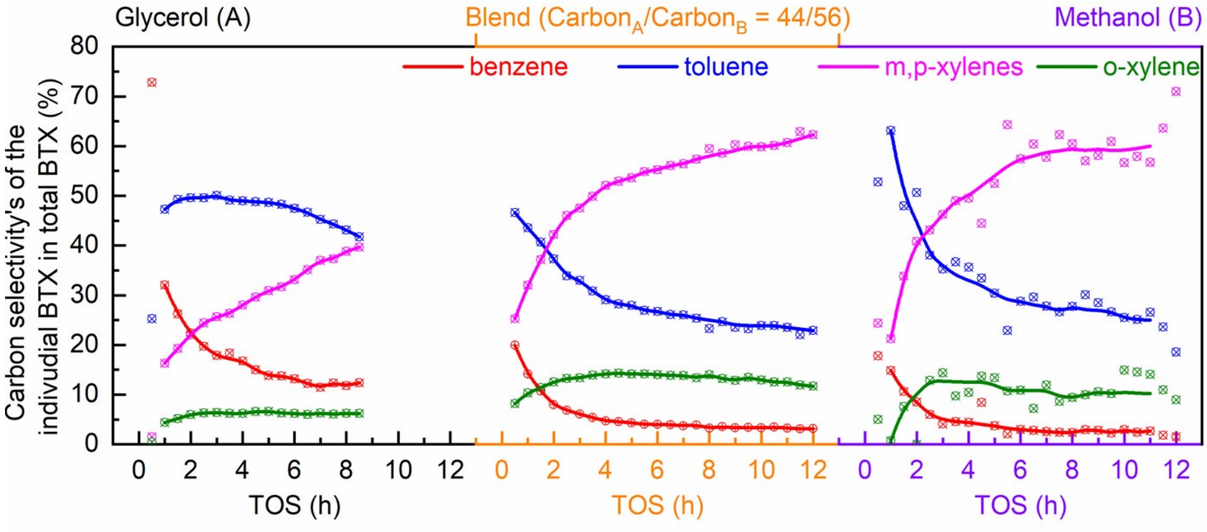


Figure S5. Carbon selectivity's of the individual BTX in total BTX *versus* TOS for the catalytic (co-) conversion of glycerol, methanol, and their blend (G/M 43/57 wt.%).

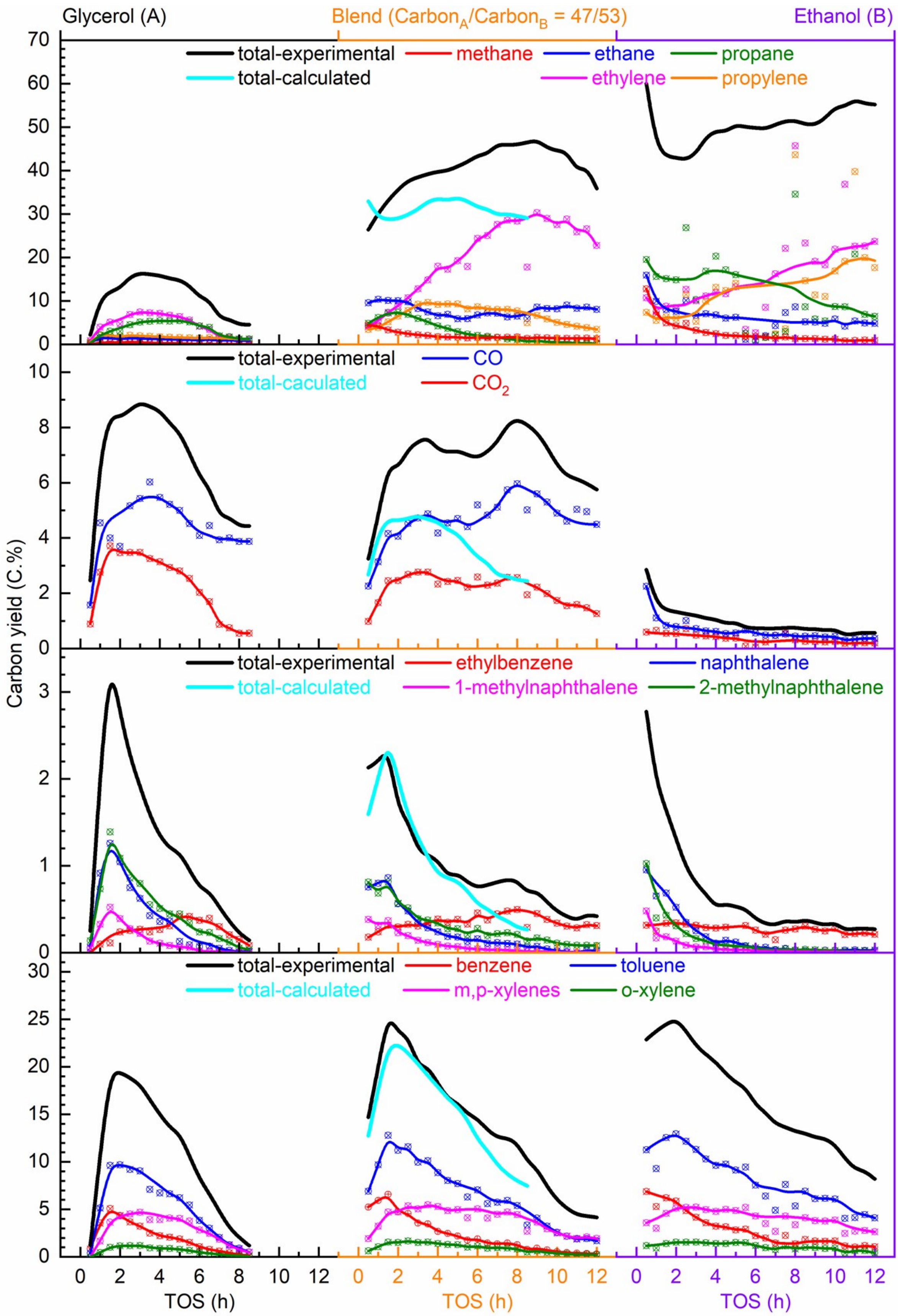


Figure S6. Carbon yields of the gas and liquid products *versus* TOS for the catalytic (co-) conversion of glycerol, ethanol, and their blend (G/E 54/46 wt.%).

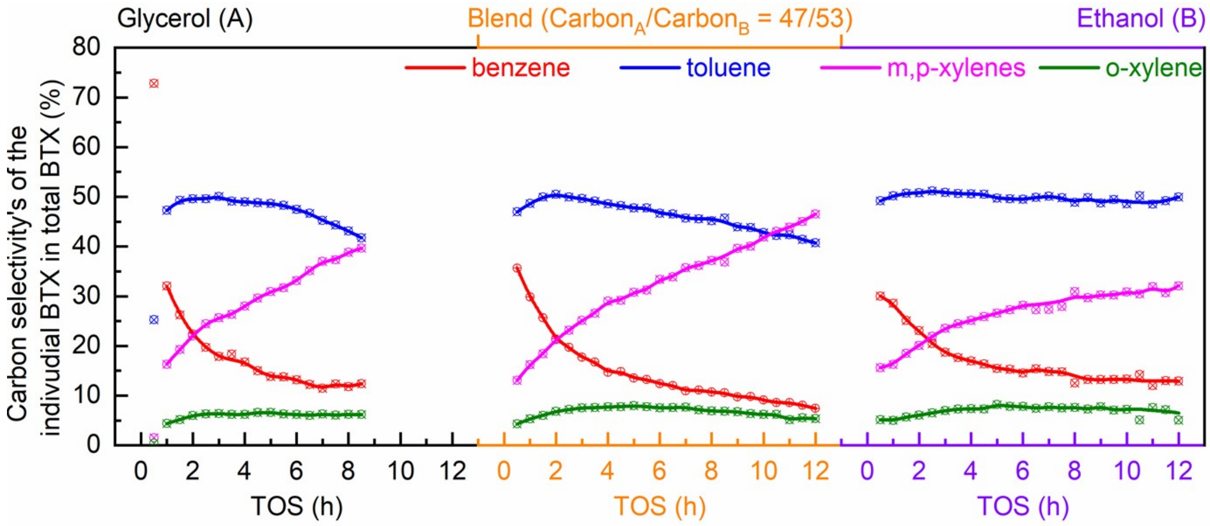


Figure S7. Carbon selectivity's of the individual BTX in total BTX *versus* TOS for the catalytic (co-) conversion of glycerol, ethanol, and their blend (G/E 54/46 wt.%).

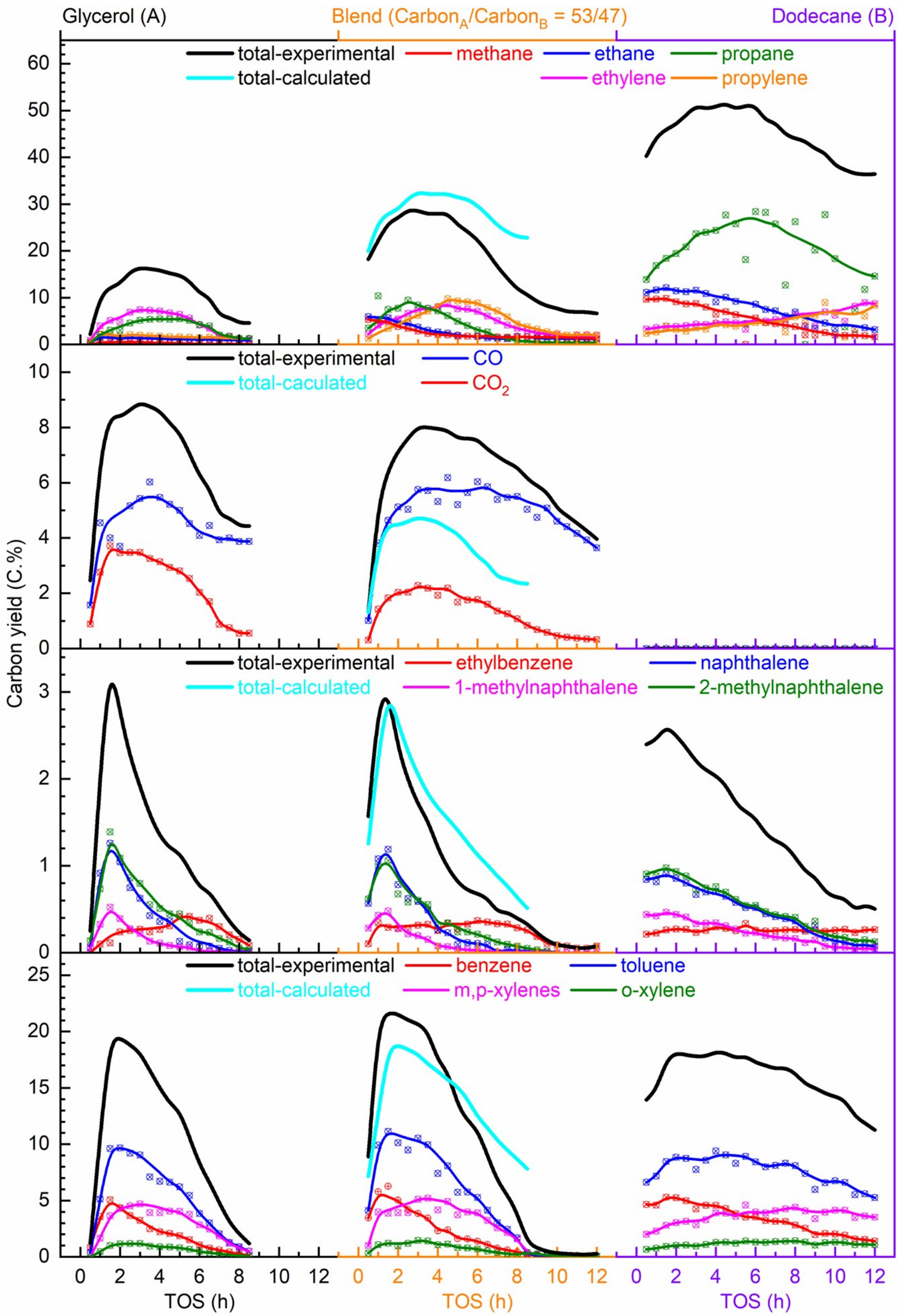


Figure S8. Carbon yields of the gas and liquid products *versus* TOS for the catalytic (co-) conversion of glycerol, dodecane, and their blend (G/D 71/29 wt.%).

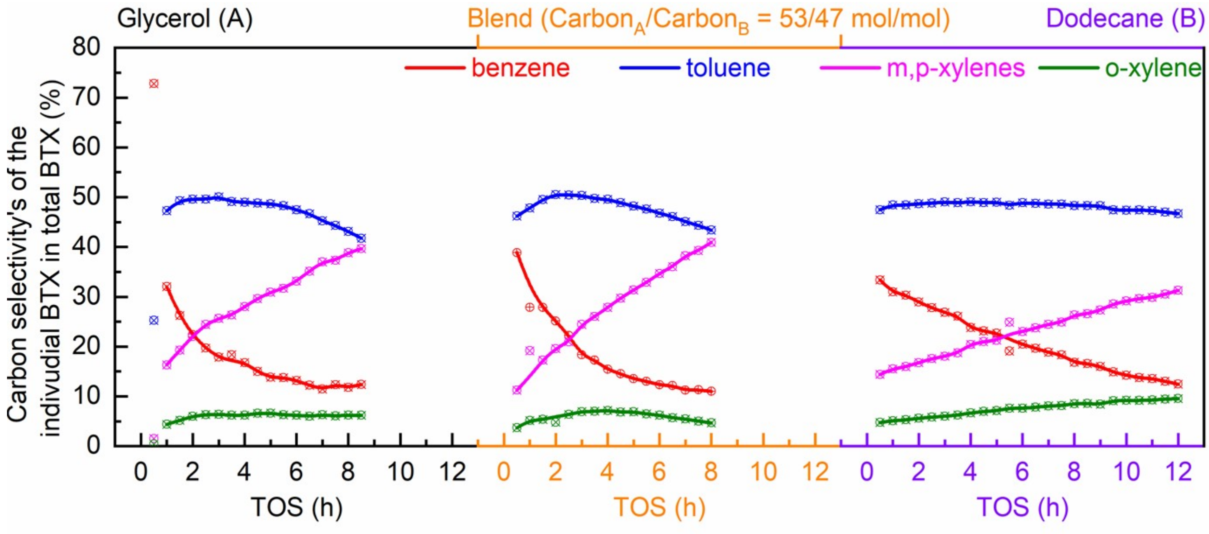


Figure S9. Carbon selectivity's of the individual BTX in total BTX *versus* TOS for the catalytic (co-) conversion of glycerol, dodecane, and their blend (G/D 71/29 wt.%).

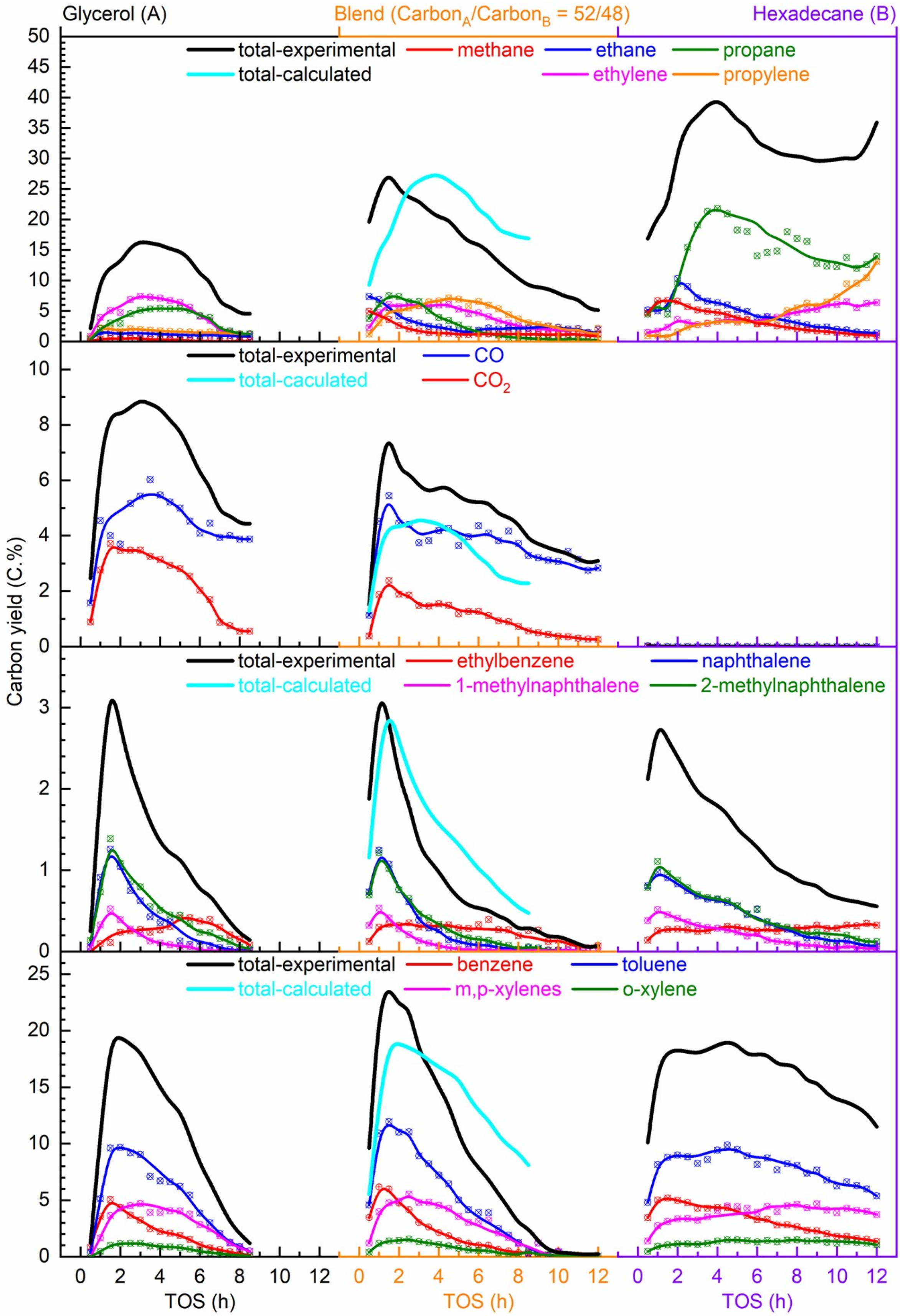


Figure S10. Carbon yields of the gas and liquid products *versus* TOS for the catalytic (co-) conversion of glycerol, hexadecane, and their blend (G/H 71/30 wt.%).

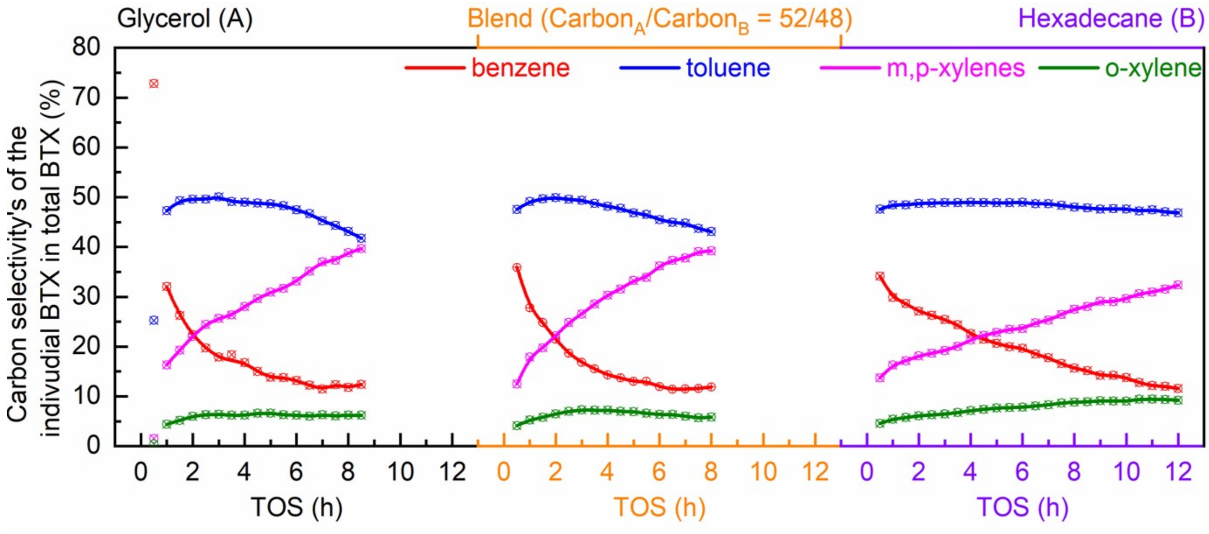


Figure S11. Carbon selectivity's of the individual BTX in total BTX *versus* TOS for the catalytic (co-) conversion of glycerol, hexadecane, and their blend (G/H 71/30 wt.%).

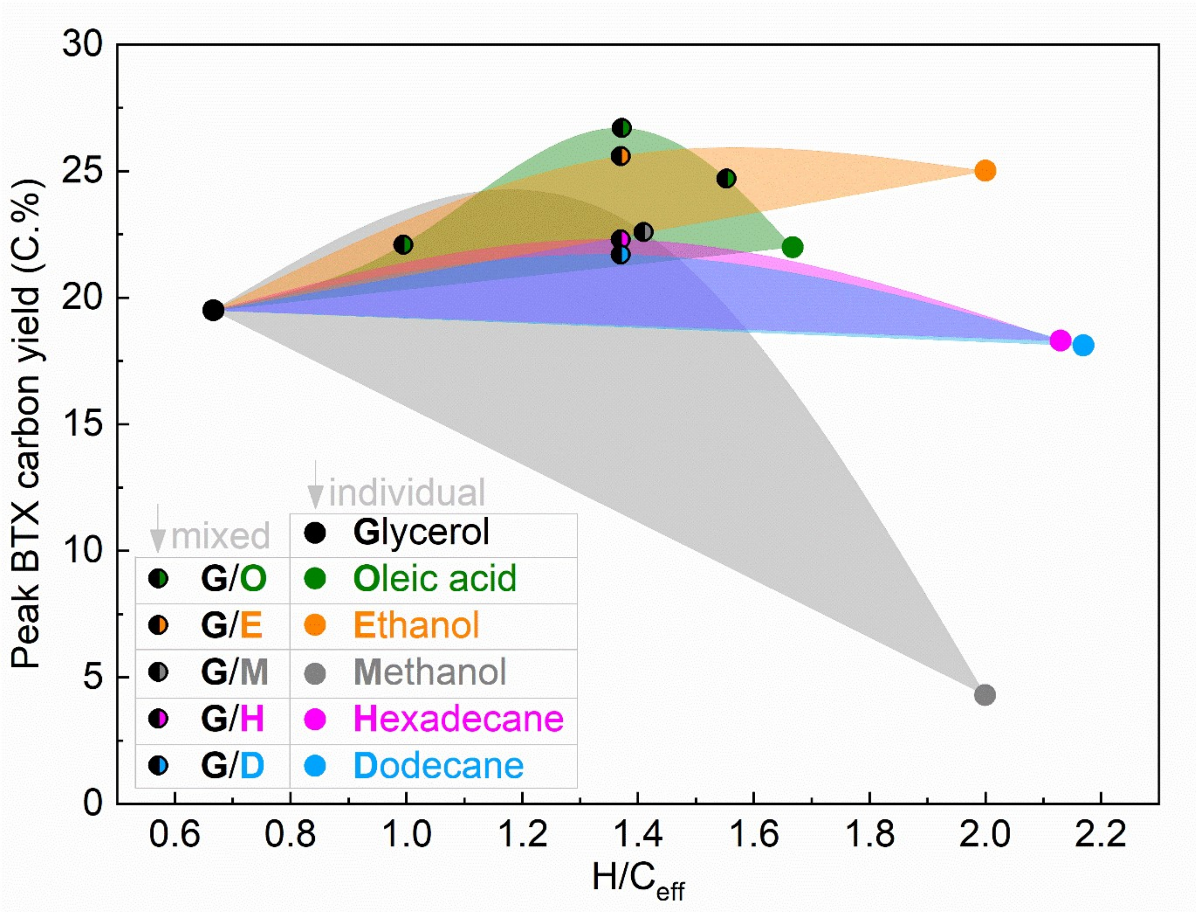


Figure S12. The peak BTX carbon yield *versus* the hydrogen to carbon effective ratio of the (co-)feed. Reaction conditions: H-ZSM-5/Al_2O_3 (60/40 wt.%) catalyst of 10 g, WHSV of the (co-)feed of 1 h^{-1}, N_2 flow of 50 ml min^{-1}, reactor temperature of 550 °C, and atmospheric pressure.

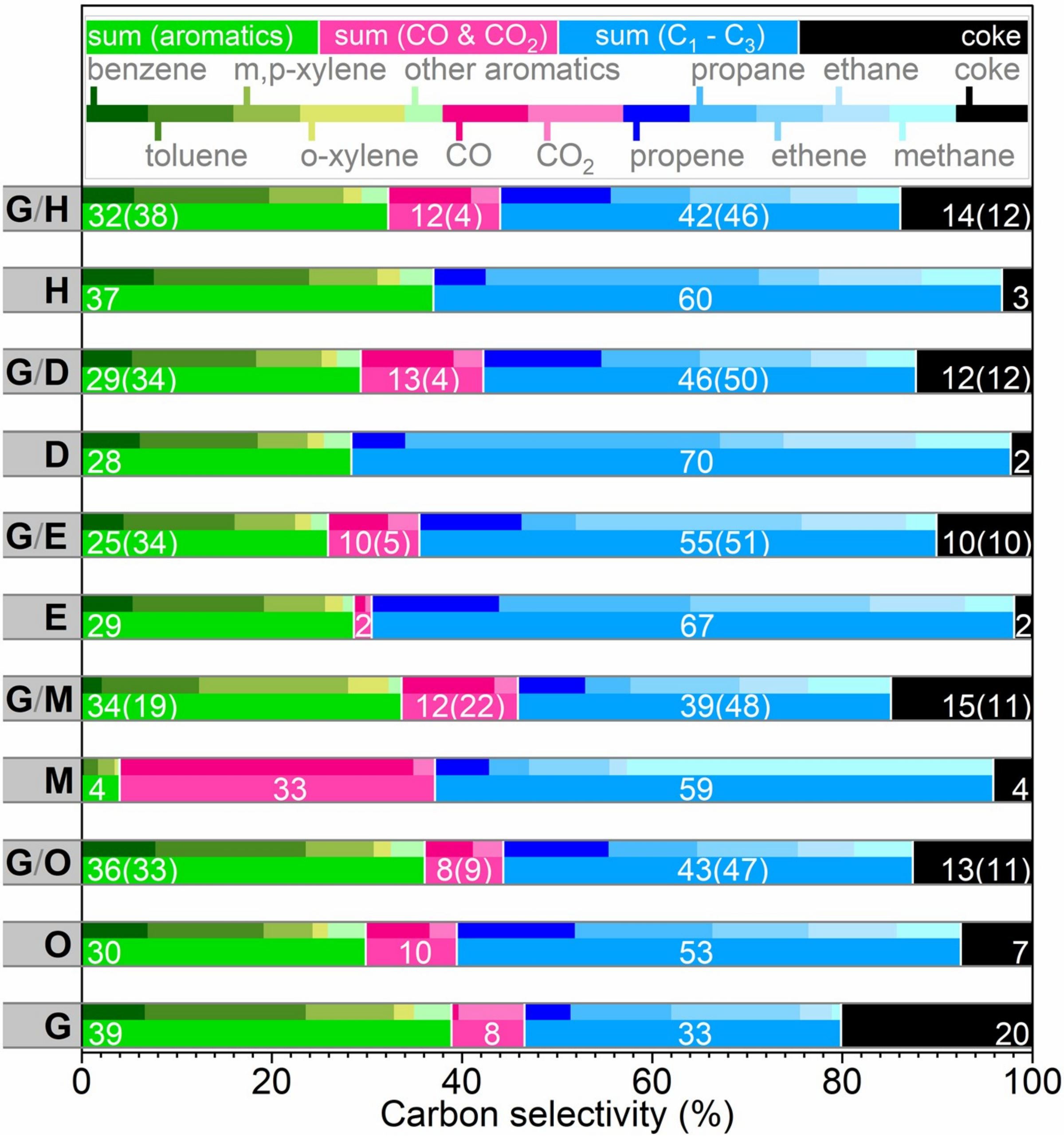


Figure S13. Carbon selectivity's of the major products. Reaction conditions: H-ZSM-5/Al_2O_3 (60/40 wt.%) catalyst of 10 g, WHSV of the (co-)feed of 1 h^{-1}, N_2 flow of 50 ml min^{-1}, reactor temperature of 550 °C, and atmospheric pressure. (The numbers in brackets are calculated according to the feed ratios of the individual feeds (Table 1, Entries 7 - 11) and their corresponding carbon selectivities.)

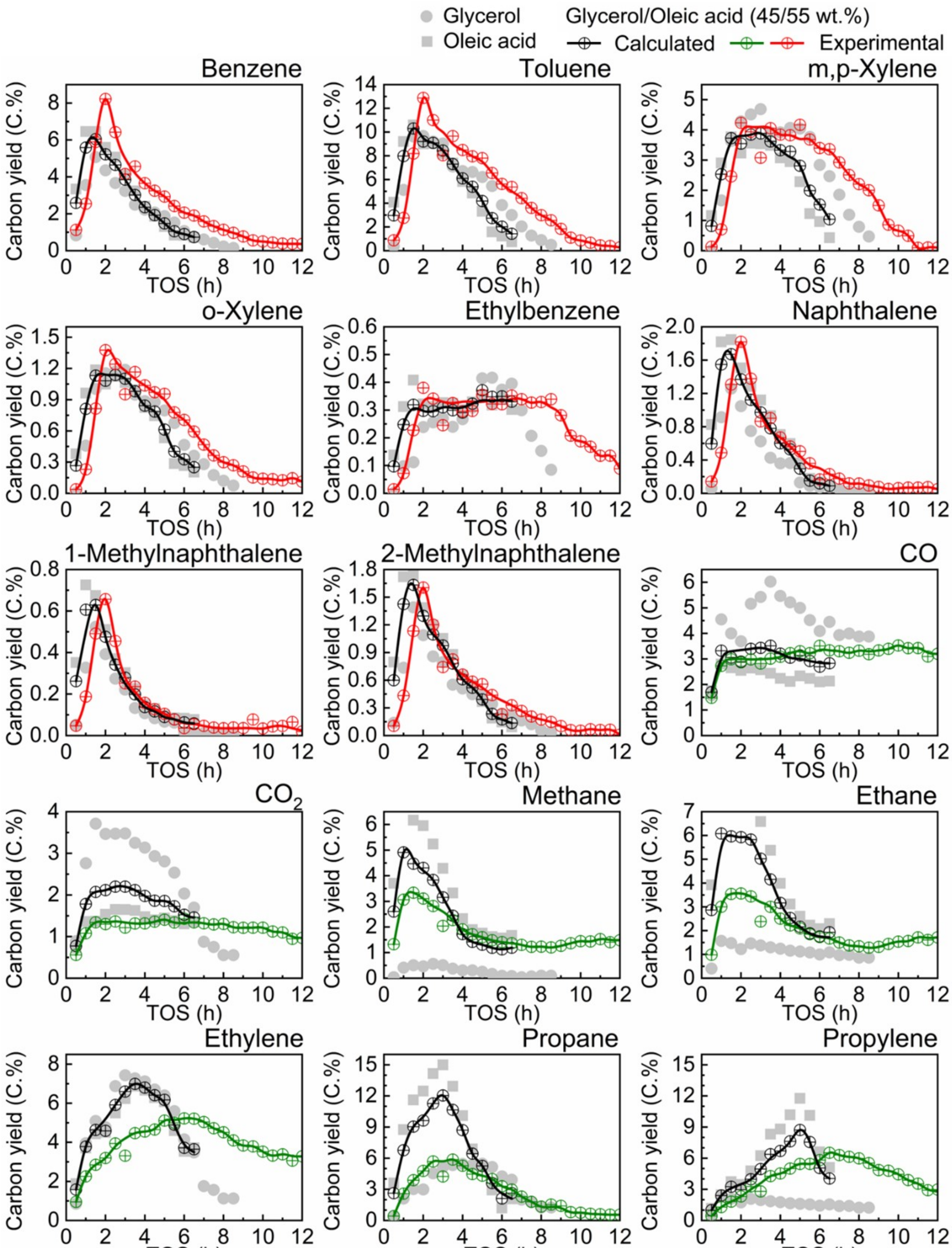


Figure S14. The experimental and calculated carbon yields of the gaseous and liquid products *versus* TOS for the catalytic co-conversion of glycerol and oleic acid (45/55 wt.%). Reaction conditions: H-ZSM-5/Al_2O_3 (60/40 wt.%) catalyst of 10 g, WHSV of the (co-)feed of 1 h^{-1}, N_2 flow of 50 ml min^{-1}, reactor temperature of 550 °C, and atmospheric pressure. (The calculated carbon yields are based on the feed ratios of the individual feeds (Table 1, Entry 11) and and their corresponding carbon yields.)

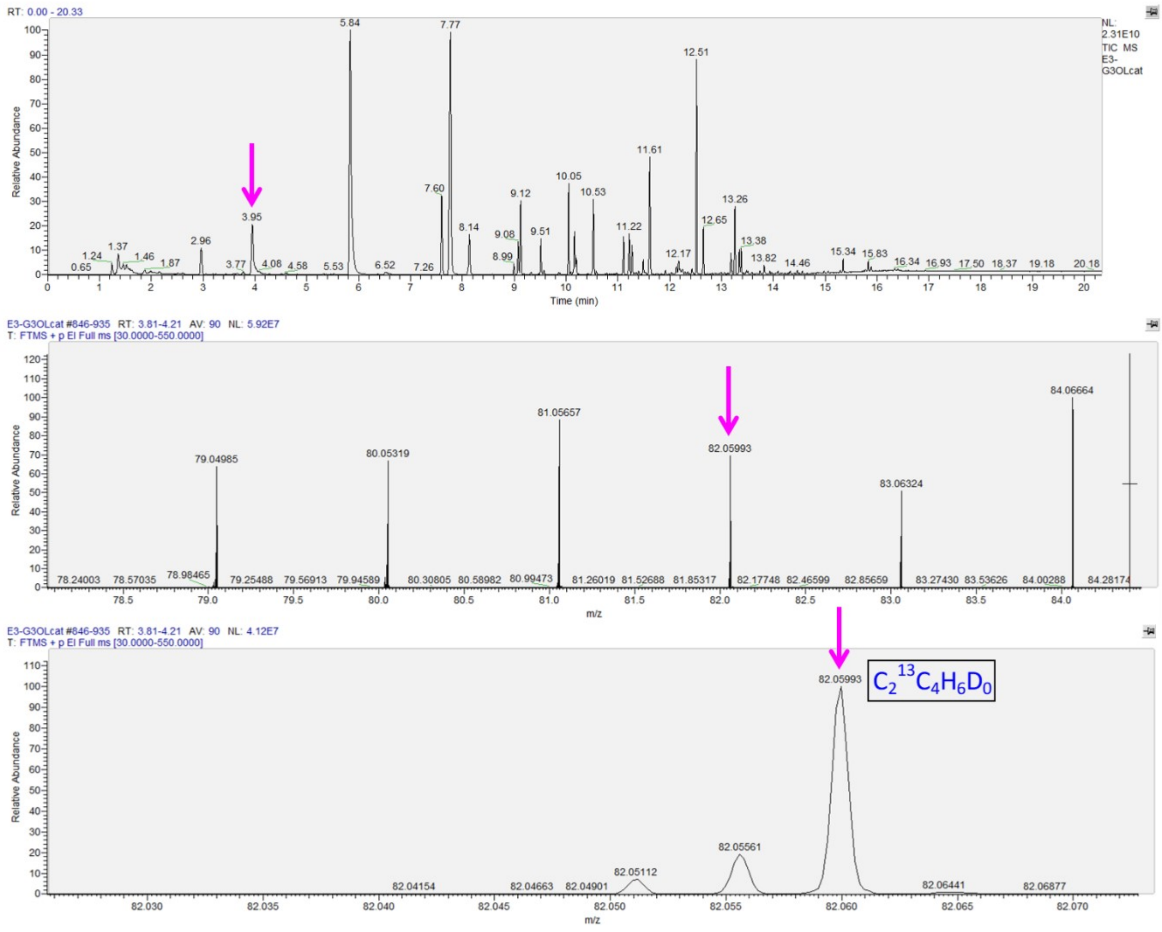


Figure S15. An example of the pyrolysis/GC-Orbitrap MS analysis for the conversion of the mixed $^{13}C_3H_8O_3$ and oleic acid over the H-ZSM-5/Al_2O_3 catalyst.

Table S1. The molecular weight of the BTX with various labeled D and 13C atom(s)

^{12}C	^{13}C	H	D		Benzene		^{12}C	^{13}C	H	D		Toluene		^{12}C	^{13}C	H	D		Xylene
6	0	6	0	$C_6{}^{13}C_0H_6D_0$	78.04640		7	0	8	0	$C_7{}^{13}C_0H_8D_0$	92.06205		8	0	10	0	$C_8{}^{13}C_0H_{10}D_0$	106.07770
5	1	6	0	$C_5{}^{13}C_1H_6D_0$	79.04976		6	1	8	0	$C_6{}^{13}C_1H_8D_0$	93.06541		7	1	10	0	$C_7{}^{13}C_1H_{10}D_0$	107.08106
6	0	5	1	$C_6{}^{13}C_0H_5D_1$	79.05268		7	0	7	1	$C_7{}^{13}C_0H_7D_1$	93.06833		8	0	9	1	$C_8{}^{13}C_0H_9D_1$	107.08398
4	2	6	0	$C_4{}^{13}C_2H_6D_0$	80.05311		5	2	8	0	$C_5{}^{13}C_2H_8D_0$	94.06876		6	2	10	0	$C_6{}^{13}C_2H_{10}D_0$	108.08441
5	1	5	1	$C_5{}^{13}C_1H_5D_1$	80.05603		6	1	7	1	$C_6{}^{13}C_1H_7D_1$	94.07168		7	1	9	1	$C_7{}^{13}C_1H_9D_1$	108.08733
6	0	4	2	$C_6{}^{13}C_0H_4D_2$	80.05895		7	0	6	2	$C_7{}^{13}C_0H_6D_2$	94.07460		8	0	8	2	$C_8{}^{13}C_0H_8D_2$	108.09025
3	3	6	0	$C_3{}^{13}C_3H_6D_0$	81.05647		4	3	8	0	$C_4{}^{13}C_3H_8D_0$	95.07212		5	3	10	0	$C_5{}^{13}C_3H_{10}D_0$	109.08777
4	2	5	1	$C_4{}^{13}C_2H_5D_1$	81.05939		5	2	7	1	$C_5{}^{13}C_2H_7D_1$	95.07504		6	2	9	1	$C_6{}^{13}C_2H_9D_1$	109.09069
5	1	4	2	$C_5{}^{13}C_1H_4D_2$	81.06231		6	1	6	2	$C_6{}^{13}C_1H_6D_2$	95.07796		7	1	8	2	$C_7{}^{13}C_1H_8D_2$	109.09361
6	0	3	3	$C_6{}^{13}C_0H_3D_3$	81.06523		7	0	5	3	$C_7{}^{13}C_0H_5D_3$	95.08088		8	0	7	3	$C_8{}^{13}C_0H_7D_3$	109.09653
2	4	6	0	$C_2{}^{13}C_4H_6D_0$	82.05982		3	4	8	0	$C_3{}^{13}C_4H_8D_0$	96.07547		4	4	10	0	$C_4{}^{13}C_4H_{10}D_0$	110.09112
3	3	5	1	$C_3{}^{13}C_3H_5D_1$	82.06274		4	3	7	1	$C_4{}^{13}C_3H_7D_1$	96.07839		5	3	9	1	$C_5{}^{13}C_3H_9D_1$	110.09404
4	2	4	2	$C_4{}^{13}C_2H_4D_2$	82.06566		5	2	6	2	$C_5{}^{13}C_2H_6D_2$	96.08131		6	2	8	2	$C_6{}^{13}C_2H_8D_2$	110.09696
5	1	3	3	$C_5{}^{13}C_1H_3D_3$	82.06859		6	1	5	3	$C_6{}^{13}C_1H_5D_3$	96.08424		7	1	7	3	$C_7{}^{13}C_1H_7D_3$	110.09989
6	0	2	4	$C_6{}^{13}C_0H_2D_4$	82.07151		7	0	4	4	$C_7{}^{13}C_0H_4D_4$	96.08716		8	0	6	4	$C_8{}^{13}C_0H_6D_4$	110.10281
1	5	6	0	$C_1{}^{13}C_5H_6D_0$	83.06318		2	5	8	0	$C_2{}^{13}C_5H_8D_0$	97.07883		3	5	10	0	$C_3{}^{13}C_5H_{10}D_0$	111.09448
2	4	5	1	$C_2{}^{13}C_4H_5D_1$	83.06610		3	4	7	1	$C_3{}^{13}C_4H_7D_1$	97.08175		4	4	9	1	$C_4{}^{13}C_4H_9D_1$	111.09740
3	3	4	2	$C_3{}^{13}C_3H_4D_2$	83.06902		4	3	6	2	$C_4{}^{13}C_3H_6D_2$	97.08467		5	3	8	2	$C_5{}^{13}C_3H_8D_2$	111.10032
4	2	3	3	$C_4{}^{13}C_2H_3D_3$	83.07194		5	2	5	3	$C_5{}^{13}C_2H_5D_3$	97.08759		6	2	7	3	$C_6{}^{13}C_2H_7D_3$	111.10324
5	1	2	4	$C_5{}^{13}C_1H_2D_4$	83.07486		6	1	4	4	$C_6{}^{13}C_1H_4D_4$	97.09051		7	1	6	4	$C_7{}^{13}C_1H_6D_4$	111.10616

^{12}C	^{13}C	H	D		Benzene		^{12}C	^{13}C	H	D		Toluene		^{12}C	^{13}C	H	D		Xylene
6	0	1	5	$C_6{}^{13}C_0H_1D_5$	83.07779		7	0	3	5	$C_7{}^{13}C_0H_3D_5$	97.09344		8	0	5	5	$C_8{}^{13}C_0H_5D_5$	111.10909
0	6	6	0	$C_0{}^{13}C_6H_6D_0$	84.06653		1	6	8	0	$C_1{}^{13}C_6H_8D_0$	98.08218		2	6	10	0	$C_2{}^{13}C_6H_{10}D_0$	112.09783
1	5	5	1	$C_1{}^{13}C_5H_5D_1$	84.06945		2	5	7	1	$C_2{}^{13}C_5H_7D_1$	98.08510		3	5	9	1	$C_3{}^{13}C_5H_9D_1$	112.10075
2	4	4	2	$C_2{}^{13}C_4H_4D_2$	84.07237		3	4	6	2	$C_3{}^{13}C_4H_6D_2$	98.08802		4	4	8	2	$C_4{}^{13}C_4H_8D_2$	112.10367
3	3	3	3	$C_3{}^{13}C_3H_3D_3$	84.07530		4	3	5	3	$C_4{}^{13}C_3H_5D_3$	98.09095		5	3	7	3	$C_5{}^{13}C_3H_7D_3$	112.10660
4	2	2	4	$C_4{}^{13}C_2H_2D_4$	84.07822		5	2	4	4	$C_5{}^{13}C_2H_4D_4$	98.09387		6	2	6	4	$C_6{}^{13}C_2H_6D_4$	112.10952
5	1	1	5	$C_5{}^{13}C_1H_1D_5$	84.08114		6	1	3	5	$C_6{}^{13}C_1H_3D_5$	98.09679		7	1	5	5	$C_7{}^{13}C_1H_5D_5$	112.11244
6	0	0	6	$C_6{}^{13}C_0H_0D_6$	84.08406		7	0	2	6	$C_7{}^{13}C_0H_2D_6$	98.09971		8	0	4	6	$C_8{}^{13}C_0H_4D_6$	112.11536
0	6	5	1	$C_0{}^{13}C_6H_5D_1$	85.07281		0	7	8	0	$C_0{}^{13}C_7H_8D_0$	99.08554		1	7	10	0	$C_1{}^{13}C_7H_{10}D_0$	113.10119
1	5	4	2	$C_1{}^{13}C_5H_4D_2$	85.07573		1	6	7	1	$C_1{}^{13}C_6H_7D_1$	99.08846		2	6	9	1	$C_2{}^{13}C_6H_9D_1$	113.10411
2	4	3	3	$C_2{}^{13}C_4H_3D_3$	85.07865		2	5	6	2	$C_2{}^{13}C_5H_6D_2$	99.09138		3	5	8	2	$C_3{}^{13}C_5H_8D_2$	113.10703
3	3	2	4	$C_3{}^{13}C_3H_2D_4$	85.08157		3	4	5	3	$C_3{}^{13}C_4H_5D_3$	99.09430		4	4	7	3	$C_4{}^{13}C_4H_7D_3$	113.10995
4	2	1	5	$C_4{}^{13}C_2H_1D_5$	85.08450		4	3	4	4	$C_4{}^{13}C_3H_4D_4$	99.09722		5	3	6	4	$C_5{}^{13}C_3H_6D_4$	113.11287
5	1	0	6	$C_5{}^{13}C_1H_0D_6$	85.08742		5	2	3	5	$C_5{}^{13}C_2H_3D_5$	99.10015		6	2	5	5	$C_6{}^{13}C_2H_5D_5$	113.11580
0	6	4	2	$C_0{}^{13}C_6H_4D_2$	86.07908		6	1	2	6	$C_6{}^{13}C_1H_2D_6$	99.10307		7	1	4	6	$C_7{}^{13}C_1H_4D_6$	113.11872
1	5	3	3	$C_1{}^{13}C_5H_3D_3$	86.08201		7	0	1	7	$C_7{}^{13}C_0H_1D_7$	99.10599		8	0	3	7	$C_8{}^{13}C_0H_3D_7$	113.12164
2	4	2	4	$C_2{}^{13}C_4H_2D_4$	86.08493		0	7	7	1	$C_0{}^{13}C_7H_7D_1$	100.09181		0	8	10	0	$C_0{}^{13}C_8H_{10}D_0$	114.10454
3	3	1	5	$C_3{}^{13}C_3H_1D_5$	86.08785		1	6	6	2	$C_1{}^{13}C_6H_6D_2$	100.09473		1	7	9	1	$C_1{}^{13}C_7H_9D_1$	114.10746
4	2	0	6	$C_4{}^{13}C_2H_0D_6$	86.09077		2	5	5	3	$C_2{}^{13}C_5H_5D_3$	100.09766		2	6	8	2	$C_2{}^{13}C_6H_8D_2$	114.11038
0	6	3	3	$C_0{}^{13}C_6H_3D_3$	87.08536		3	4	4	4	$C_3{}^{13}C_4H_4D_4$	100.10058		3	5	7	3	$C_3{}^{13}C_5H_7D_3$	114.11331
1	5	2	4	$C_1{}^{13}C_5H_2D_4$	87.08828		4	3	3	5	$C_4{}^{13}C_3H_3D_5$	100.10350		4	4	6	4	$C_4{}^{13}C_4H_6D_4$	114.11623

^{12}C	^{13}C	H	D		**Benzene**		^{12}C	^{13}C	H	D		**Toluene**		^{12}C	^{13}C	H	D		**Xylene**
2	4	1	5	$C_2{}^{13}C_4H_1D_5$	87.09121		5	2	2	6	$C_5{}^{13}C_2H_2D_6$	100.10642		5	3	5	5	$C_5{}^{13}C_3H_5D_5$	114.11915
3	3	0	6	$C_3{}^{13}C_3H_0D_6$	87.09413		6	1	1	7	$C_6{}^{13}C_1H_1D_7$	100.10934		6	2	4	6	$C_6{}^{13}C_2H_4D_6$	114.12207
0	6	2	4	$C_0{}^{13}C_6H_2D_4$	88.09164		7	0	0	8	$C_7{}^{13}C_0H_0D_8$	100.11227		7	1	3	7	$C_7{}^{13}C_1H_3D_7$	114.12499
1	5	1	5	$C_1{}^{13}C_5H_1D_5$	88.09456		0	7	6	2	$C_0{}^{13}C_7H_6D_2$	101.09809		8	0	2	8	$C_8{}^{13}C_0H_2D_8$	114.12792
2	4	0	6	$C_2{}^{13}C_4H_0D_6$	88.09748		1	6	5	3	$C_1{}^{13}C_6H_5D_3$	101.10101		0	8	9	1	$C_0{}^{13}C_8H_9D_1$	115.11082
0	6	1	5	$C_0{}^{13}C_6H_1D_5$	89.09792		2	5	4	4	$C_2{}^{13}C_5H_4D_4$	101.10393		1	7	8	2	$C_1{}^{13}C_7H_8D_2$	115.11374
1	5	0	6	$C_1{}^{13}C_5H_0D_6$	89.10084		3	4	3	5	$C_3{}^{13}C_4H_3D_5$	101.10686		2	6	7	3	$C_2{}^{13}C_6H_7D_3$	115.11666
0	6	0	6	$C_0{}^{13}C_6H_0D_6$	90.10419		4	3	2	6	$C_4{}^{13}C_3H_2D_6$	101.10978		3	5	6	4	$C_3{}^{13}C_5H_6D_4$	115.11958
							5	2	1	7	$C_5{}^{13}C_2H_1D_7$	101.11270		4	4	5	5	$C_4{}^{13}C_4H_5D_5$	115.12251
							6	1	0	8	$C_6{}^{13}C_1H_0D_8$	101.11562		5	3	4	6	$C_5{}^{13}C_3H_4D_6$	115.12543
							0	7	5	3	$C_0{}^{13}C_7H_5D_3$	102.10437		6	2	3	7	$C_6{}^{13}C_2H_3D_7$	115.12835
							1	6	4	4	$C_1{}^{13}C_6H_4D_4$	102.10729		7	1	2	8	$C_7{}^{13}C_1H_2D_8$	115.13127
							2	5	3	5	$C_2{}^{13}C_5H_3D_5$	102.11021		8	0	1	9	$C_8{}^{13}C_0H_1D_9$	115.13419
							3	4	2	6	$C_3{}^{13}C_4H_2D_6$	102.11313		0	8	8	2	$C_0{}^{13}C_8H_8D_2$	116.11709
							4	3	1	7	$C_4{}^{13}C_3H_1D_7$	102.11605		1	7	7	3	$C_1{}^{13}C_7H_7D_3$	116.12002
							5	2	0	8	$C_5{}^{13}C_2H_0D_8$	102.11898		2	6	6	4	$C_2{}^{13}C_6H_6D_4$	116.12294
							0	7	4	4	$C_0{}^{13}C_7H_4D_4$	103.11064		3	5	5	5	$C_3{}^{13}C_5H_5D_5$	116.12586
							1	6	3	5	$C_1{}^{13}C_6H_3D_5$	103.11357		4	4	4	6	$C_4{}^{13}C_4H_4D_6$	116.12878
							2	5	2	6	$C_2{}^{13}C_5H_2D_6$	103.11649		5	3	3	7	$C_5{}^{13}C_3H_3D_7$	116.13170
							3	4	1	7	$C_3{}^{13}C_4H_1D_7$	103.11941		6	2	2	8	$C_6{}^{13}C_2H_2D_8$	116.13463
							4	3	0	8	$C_4{}^{13}C_3H_0D_8$	103.12233		7	1	1	9	$C_7{}^{13}C_1H_1D_9$	116.13755

^{12}C	^{13}C	H	D		Benzene		^{12}C	^{13}C	H	D		Toluene		^{12}C	^{13}C	H	D		Xylene
							0	7	3	5	$C_0{}^{13}C_7H_3D_5$	104.11692		8	0	0	10	$C_8{}^{13}C_0H_0D_{10}$	116.14047
							1	6	2	6	$C_1{}^{13}C_6H_2D_6$	104.11984		0	8	7	3	$C_0{}^{13}C_8H_7D_3$	117.12337
							2	5	1	7	$C_2{}^{13}C_5H_1D_7$	104.12276		1	7	6	4	$C_1{}^{13}C_7H_6D_4$	117.12629
							3	4	0	8	$C_3{}^{13}C_4H_0D_8$	104.12569		2	6	5	5	$C_2{}^{13}C_6H_5D_5$	117.12922
							0	7	2	6	$C_0{}^{13}C_7H_2D_6$	105.12320		3	5	4	6	$C_3{}^{13}C_5H_4D_6$	117.13214
							1	6	1	7	$C_1{}^{13}C_6H_1D_7$	105.12612		4	4	3	7	$C_4{}^{13}C_4H_3D_7$	117.13506
							2	5	0	8	$C_2{}^{13}C_5H_0D_8$	105.12904		5	3	2	8	$C_5{}^{13}C_3H_2D_8$	117.13798
							0	7	1	7	$C_0{}^{13}C_7H_1D_7$	106.12947		6	2	1	9	$C_6{}^{13}C_2H_1D_9$	117.14090
							1	6	0	8	$C_1{}^{13}C_6H_0D_8$	106.13240		7	1	0	10	$C_7{}^{13}C_1H_0D_{10}$	117.14383
							0	7	0	8	$C_0{}^{13}C_7H_0D_8$	107.13575		0	8	6	4	$C_0{}^{13}C_8H_6D_4$	118.12965
														1	7	5	5	$C_1{}^{13}C_7H_5D_5$	118.13257
														2	6	4	6	$C_2{}^{13}C_6H_4D_6$	118.13549
														3	5	3	7	$C_3{}^{13}C_5H_3D_7$	118.13841
														4	4	2	8	$C_4{}^{13}C_4H_2D_8$	118.14134
														5	3	1	9	$C_5{}^{13}C_3H_1D_9$	118.14426
														6	2	0	10	$C_6{}^{13}C_2H_0D_{10}$	118.14718
														0	8	5	5	$C_0{}^{13}C_8H_5D_5$	119.13593
														1	7	4	6	$C_1{}^{13}C_7H_4D_6$	119.13885
														2	6	3	7	$C_2{}^{13}C_6H_3D_7$	119.14177
														3	5	2	8	$C_3{}^{13}C_5H_2D_8$	119.14469
														4	4	1	9	$C_4{}^{13}C_4H_1D_9$	119.14761

^{12}C	^{13}C	H	D		Benzene		^{12}C	^{13}C	H	D		Toluene		^{12}C	^{13}C	H	D		Xylene
														5	3	0	10	$C_5{}^{13}C_3H_0D_{10}$	119.15054
														0	8	4	6	$C_0{}^{13}C_8H_4D_6$	120.14220
														1	7	3	7	$C_1{}^{13}C_7H_3D_7$	120.14512
														2	6	2	8	$C_2{}^{13}C_6H_2D_8$	120.14805
														3	5	1	9	$C_3{}^{13}C_5H_1D_9$	120.15097
														4	4	0	10	$C_4{}^{13}C_4H_0D_{10}$	120.15389
														0	8	3	7	$C_0{}^{13}C_8H_3D_7$	121.14848
														1	7	2	8	$C_1{}^{13}C_7H_2D_8$	121.15140
														2	6	1	9	$C_2{}^{13}C_6H_1D_9$	121.15432
														3	5	0	10	$C_3{}^{13}C_5H_0D_{10}$	121.15725
														0	8	2	8	$C_0{}^{13}C_8H_2D_8$	122.15476
														1	7	1	9	$C_1{}^{13}C_7H_1D_9$	122.15768
														2	6	0	10	$C_2{}^{13}C_6H_0D_{10}$	122.16060
														0	8	1	9	$C_0{}^{13}C_8H_1D_9$	123.16103
														1	7	0	10	$C_1{}^{13}C_7H_0D_{10}$	123.16396
														0	8	0	10	$C_0{}^{13}C_8H_0D_{10}$	124.16731