Supporting Information

"Unveiling the Reaction Pathways of Hydrocarbon via Experiment, Computations and Data Science"

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Molecule	**In/Out Degrees**	**Degree**
[H+]	218 / 218	436
[CH3+]	126 / 126	252
[CH2+]C	53 / 53	106
C=C	38 / 38	76
C=CC	34 / 34	68
C[C+](CC)C(C)CC	33 / 33	66
C[C+](CCC)C(C)C	32 / 32	64
CC[CH+]C(C)C(C)C	32 / 32	64
CC1C(C)C1C[CH+]C	29 / 29	58
[CH2+]CC1CC1CCC	29 / 29	58

Table S1. Top 10 nodes with the highest degrees of the network illustrated in Figure 1.

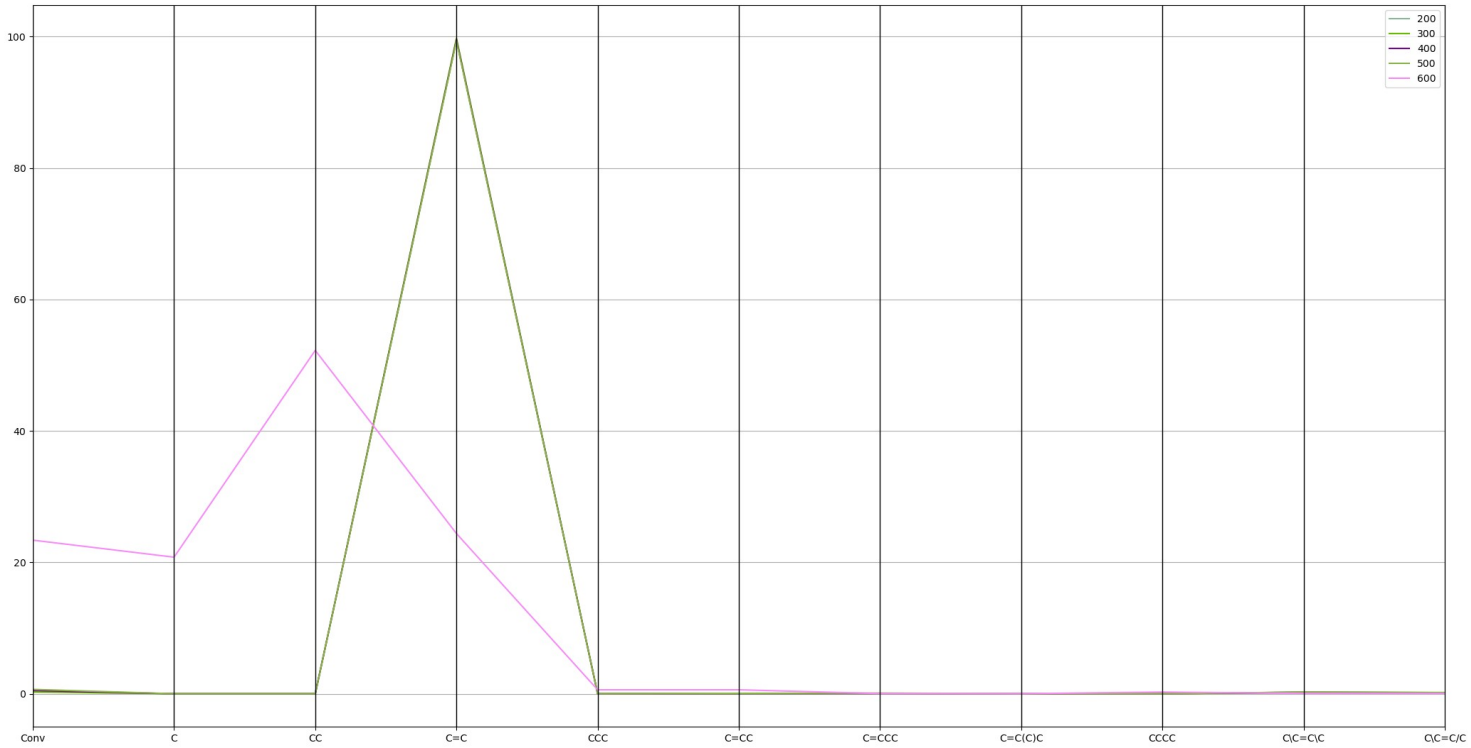

Figure S1. Parallel coordinate of C_2H_4 (C=C) conversion and percentage of molecules from C_2H_4 after the reaction out of a total percentage of 100 for all products. Color indicates the temperature in °C.

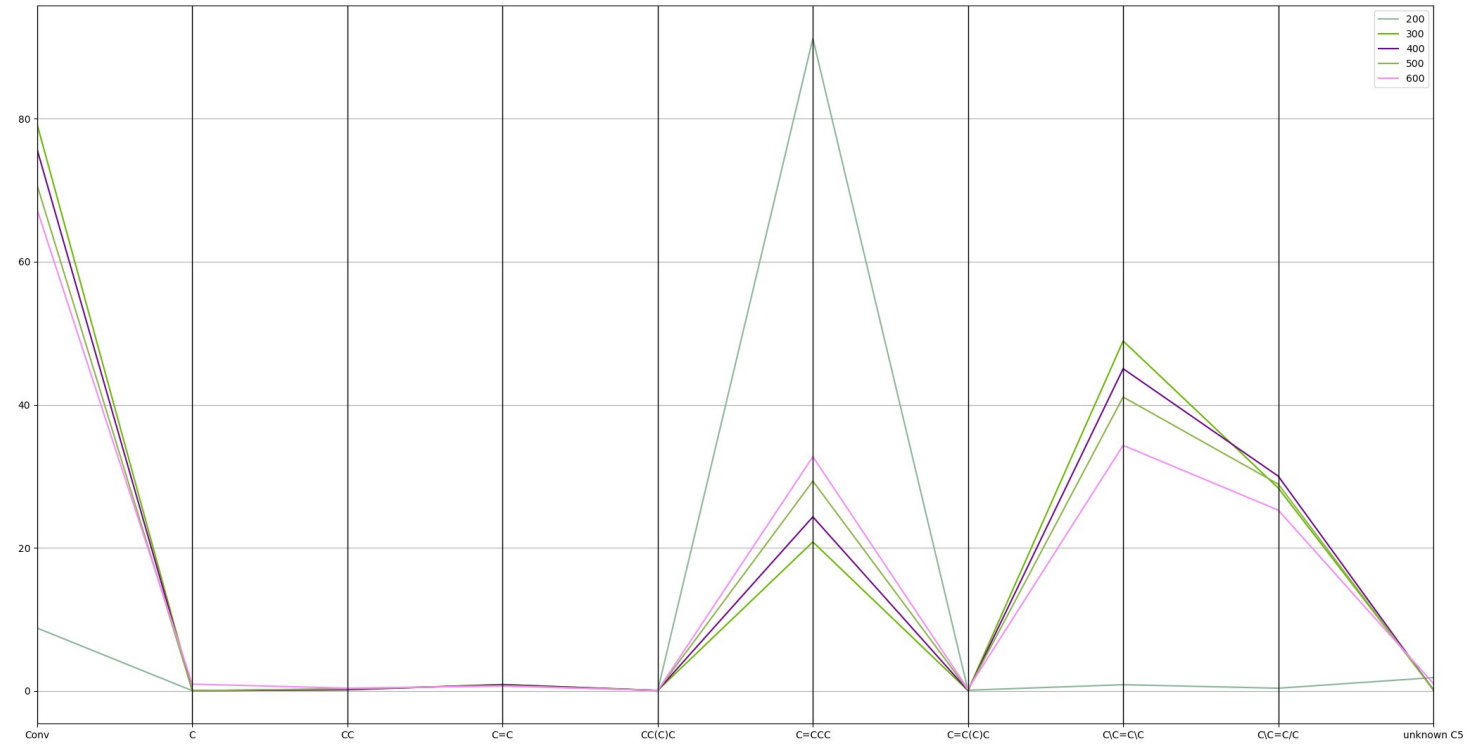

Figure S2. Parallel coordinate of 1-C_4H_8 (C=CCC) conversion and percentage of molecules from 1-C_4H_8 after the rreaction out of a total percentage of 100 for all products . Color indicates the temperature in ℃.

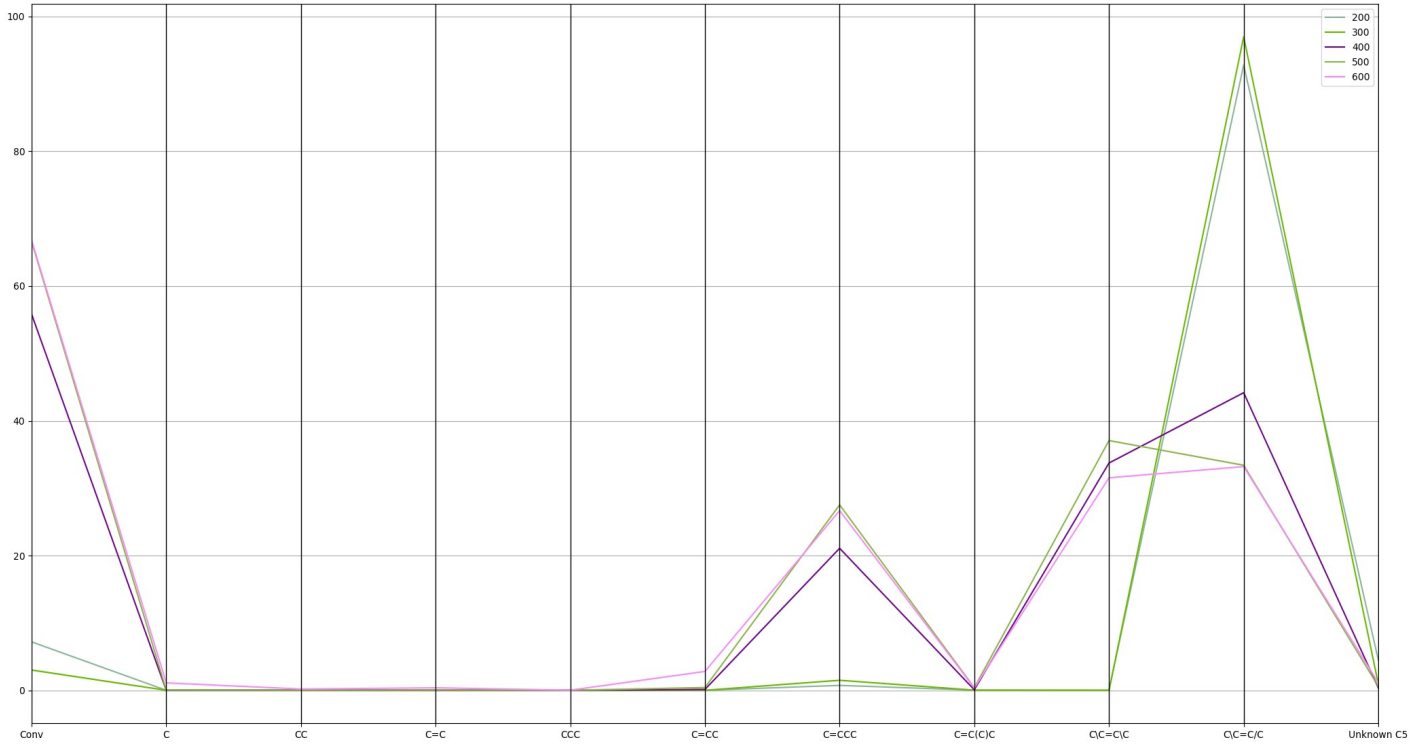

Figure S3. Parallel coordinate of cis-2-C_4H_8 (C\C=C/C) conversion and percentage of molecules from cis-2-C_4H_8 after the reaction out of a total percentage of 100 for all products. Color indicates the temperature in ℃.

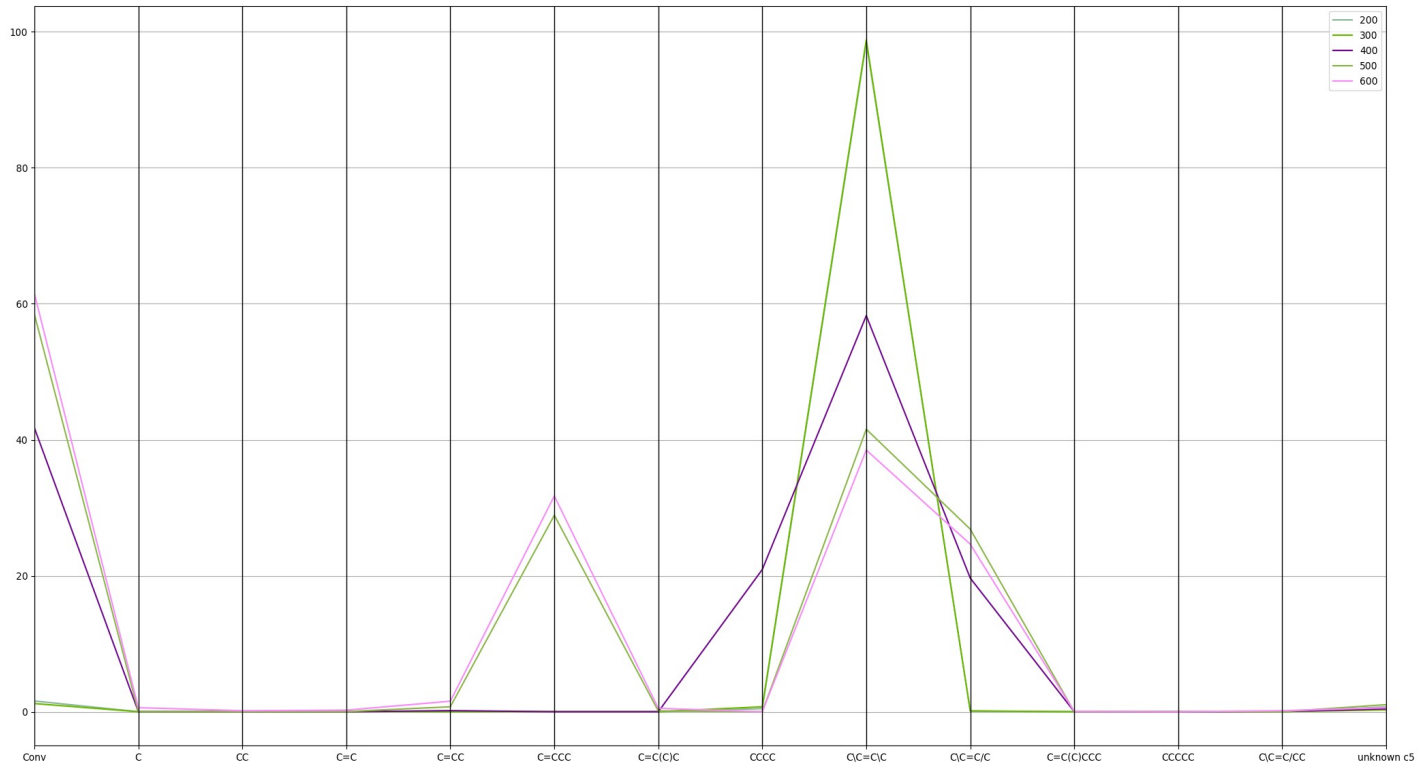

Figure S4. Parallel coordinate of trans-2-C_4H_8 (C\C=C\C) conversion and percentage of molecules from trans-2-C_4H_8 after the reaction out of a total percentage of 100 for all products. Color indicates the temperature in ℃.

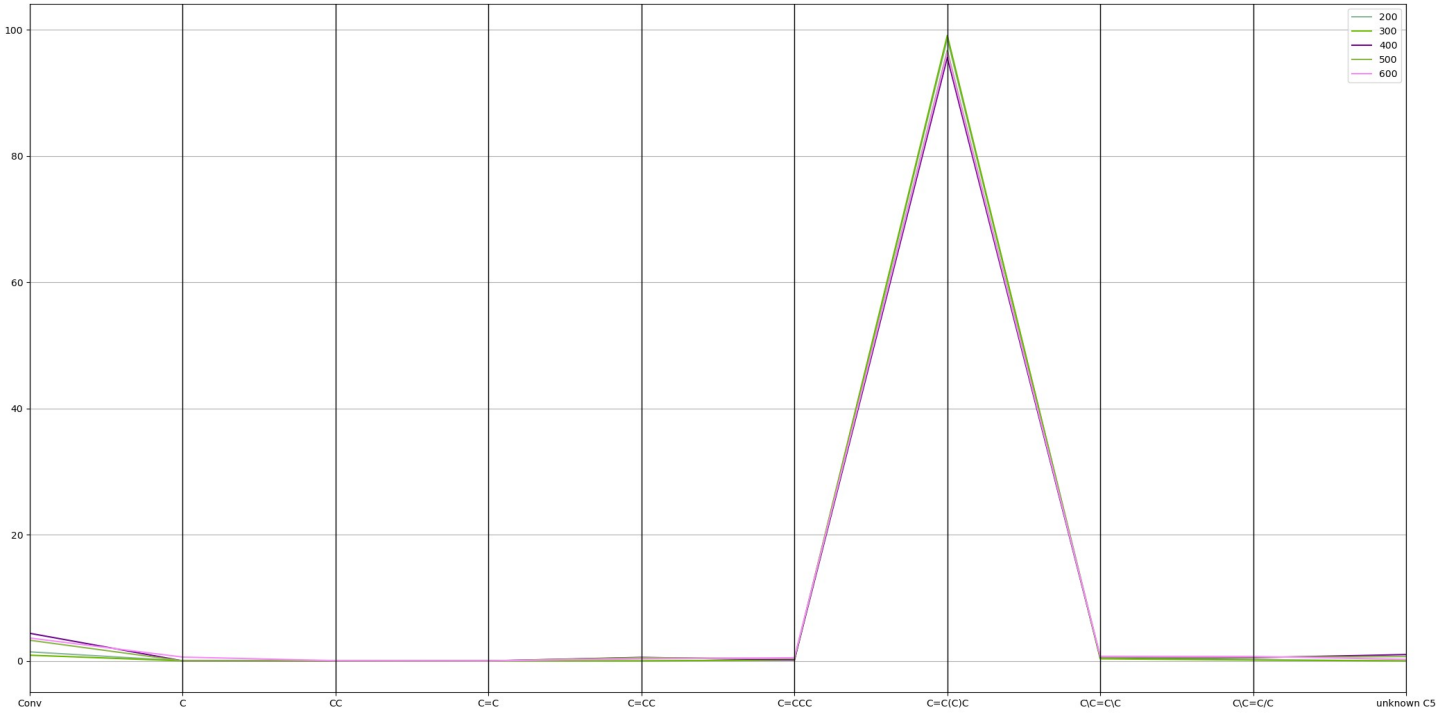

Figure S5. Parallel coordinate of iso-C_4H_8 (C=C(C)C) conversion and percentage of molecules from iso-C_4H_8 after the reaction out of a total percentage of 100 for all products. Color indicates the temperature in ℃.

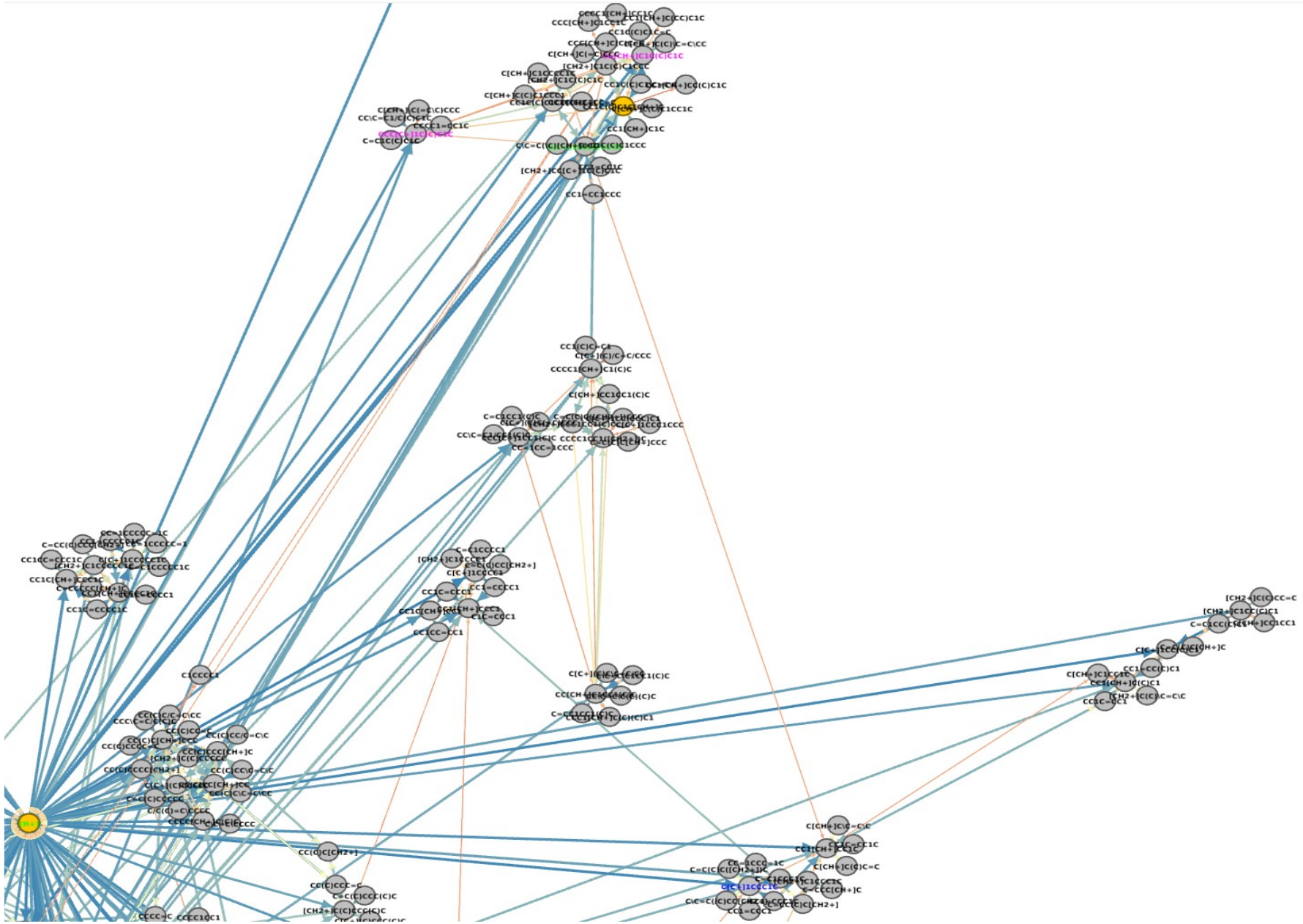

Figure S6. A zoomed-in portion of the reaction network illustrated in Figure 1.

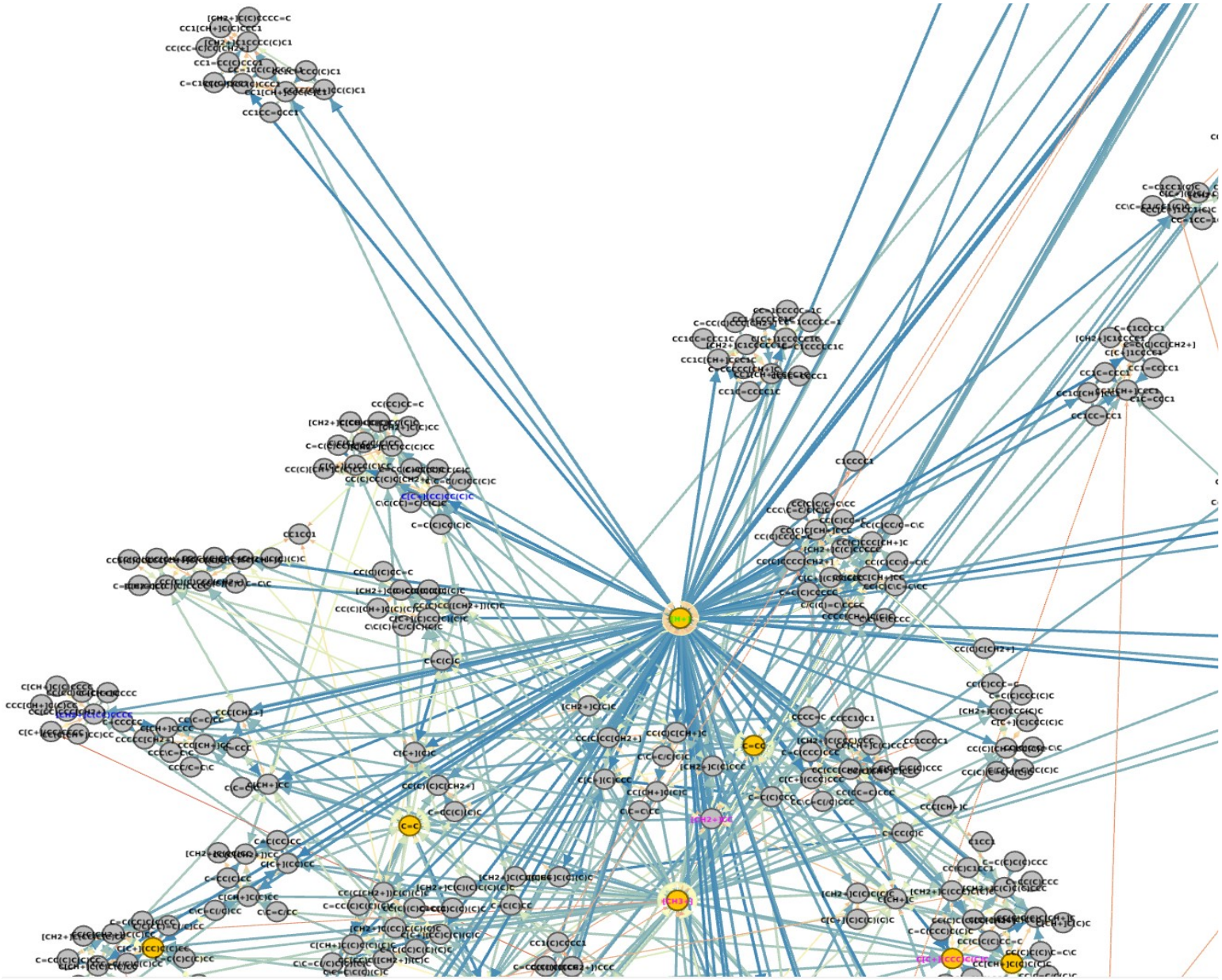

Figure S7. A zoomed-in portion of the reaction network illustrated in Figure 1.

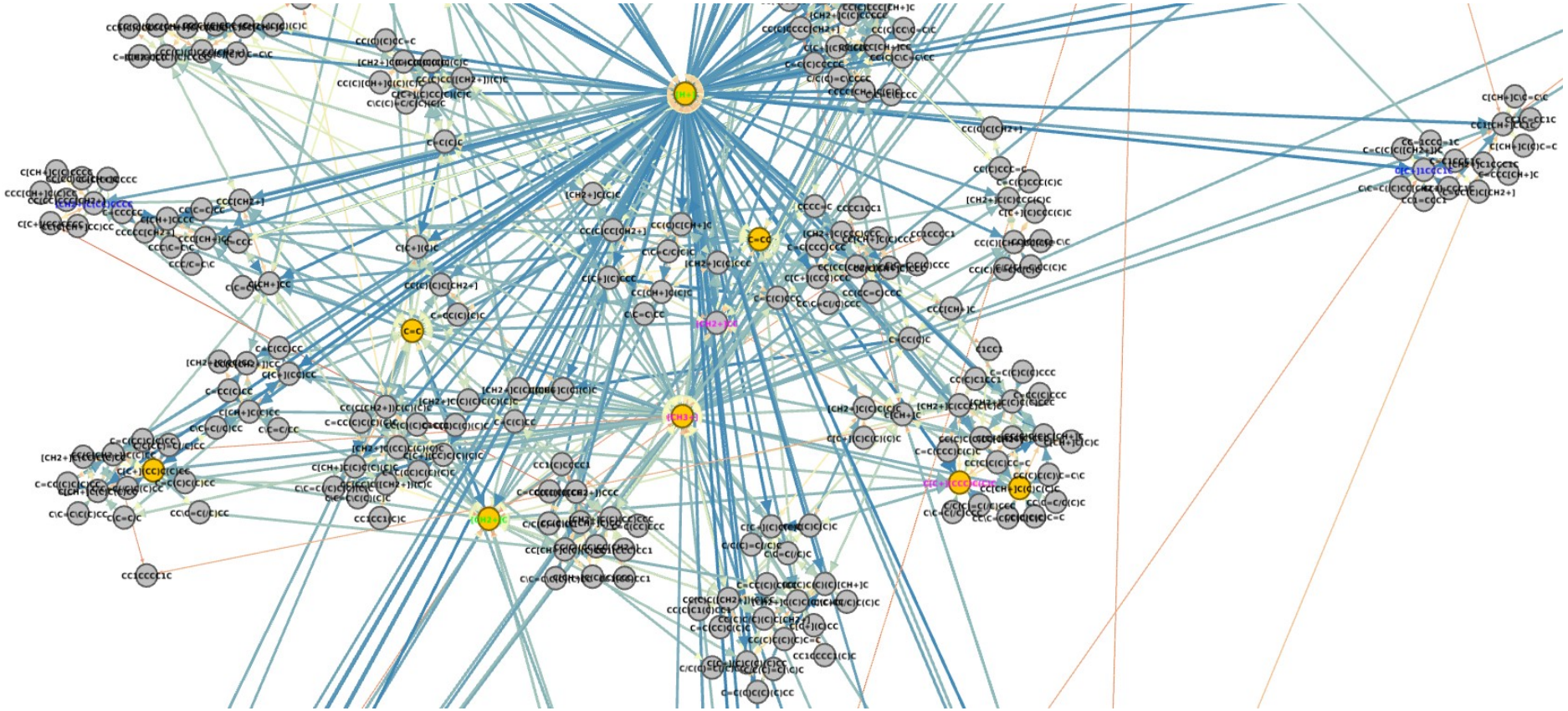

Figure S8. A zoomed-in portion of the reaction network illustrated in Figure 1.

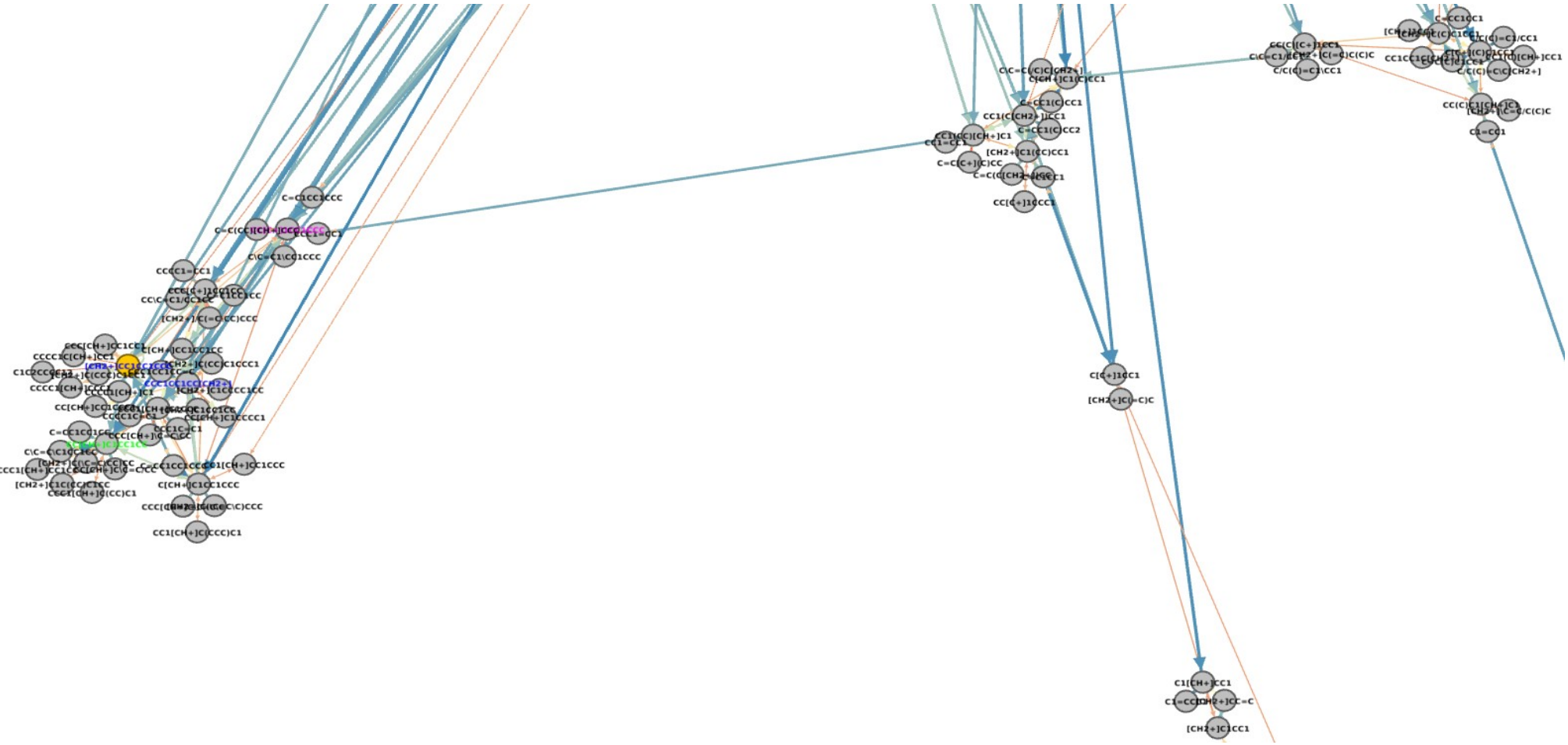

Figure S9. A zoomed-in portion of the reaction network illustrated in Figure 1.

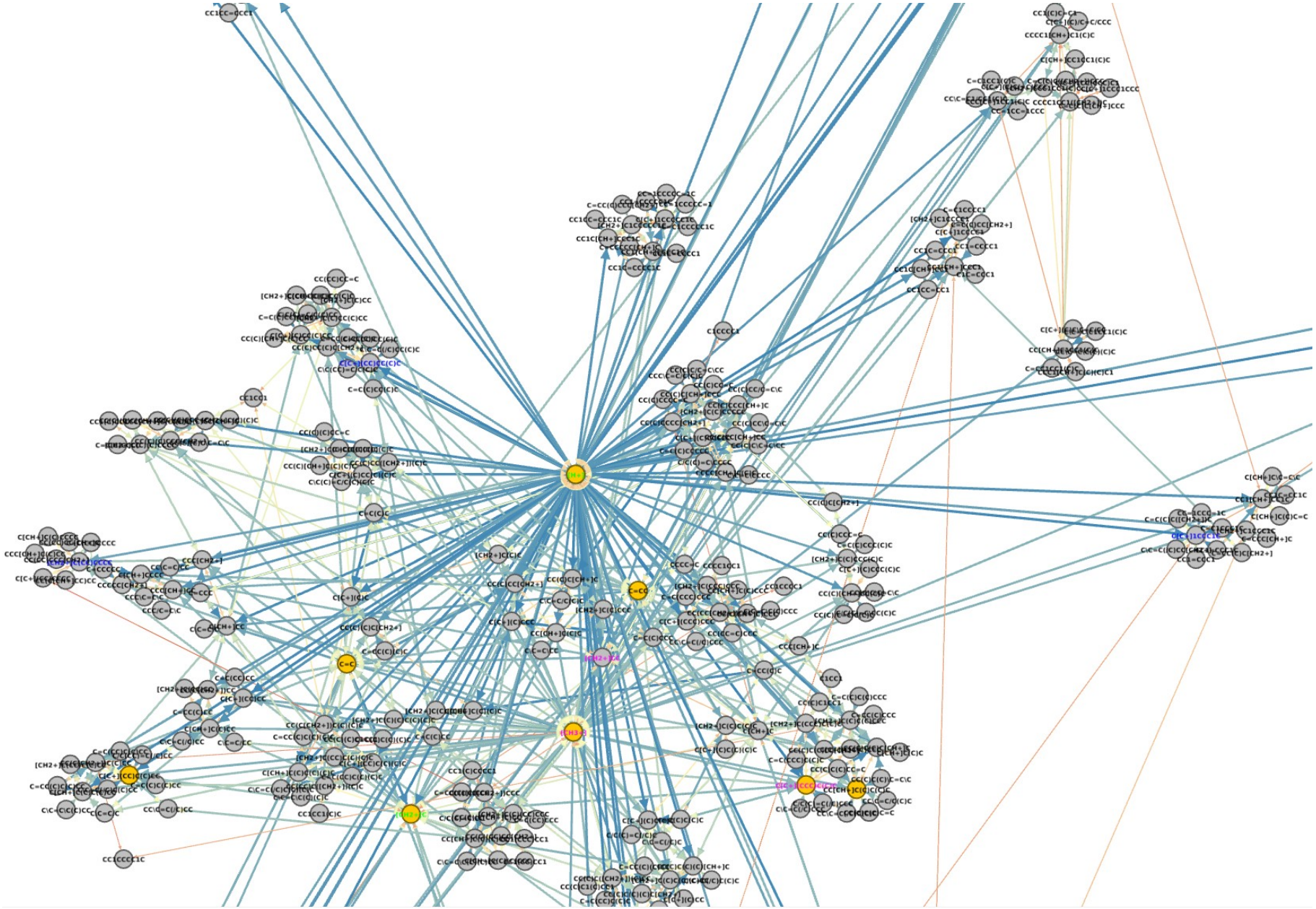

Figure S10. A zoomed-in portion of the reaction network illustrated in Figure 4.