

Uncertainty of Prebiotic Scenarios: The Case of the Non-Enzymatic Reverse Tricarboxylic Acid Cycle

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Supplementary Information

Computational Results

Cycles found in the rTCA supernetwork that include acetate and/or glyoxylate (content of the file SI.tar.gz)

Folder "SI" contains *graphml* files of 1881 cycles.

ASCII file *cycles_SI* contains the following information:

- label (matching file names in SI folder), number of branching points, number of molecules, "height" (G_high-G_low), "cost" (DG_net), and list of all reactions (reaction sequence). The label of rTCA cycle is 64_4_3.
- In the reaction sequence each equation is followed by the label of the reaction type and Gibbs free energy of the reaction.
- The reaction sequence is followed by the net equation.

File *cycles_Table_SI.pdf* contains the same information except for the reaction sequences in a tabulated form.

Degree distribution in the rTCA supernetwork.

The degree distribution is characterized separately for the partition of molecules within the bi-partite graph and for its projection which is a single-mode graph. The latter is equivalent to the "interaction network" representation of a chemical network. Both distributions are heavy-tailed (Fig. S1); we relied on the methodology introduced in Ref. 21 in order to fit a power law to the dataset, assess the reliability of the fit, and compare the power law to alternative distributions, such as the log-normal, stretched exponential, and a power law with exponential cut-off (Table S1).

Following the methodology of Ref. 21 we conclude that there is a possibility for alternatives, such as the log-normal distribution, but the power-law is a good fit with exponents of 5.7 and 3.82 for the partition in the bi-partite graph and its projection, respectively.

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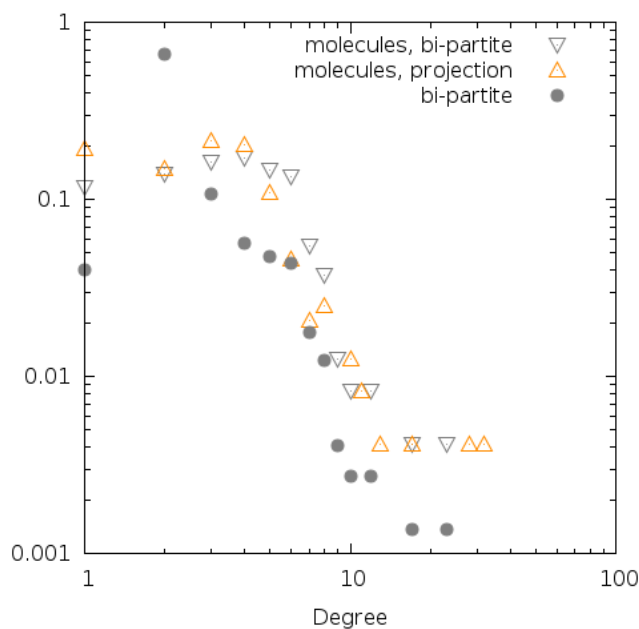


Figure S1. Degree distribution in the M-rTCA network (Fig. 2B). The filled circles represent the degree distribution for both partitions (molecules and reactions) of the bi-partite graph. The empty triangles pointing down represent the degree distribution in the partition of molecules in the bi-partite graph. Finally, the empty triangles pointing down represent the degree distribution in the projected partition of molecules.

Notably, acetate, which served as a starting point of the reconstruction process, has only the second largest degree with 14 incoming and 3 outgoing connections. It is glyoxylate that emerges as the most connected component with 18 incoming and 4 outgoing connections. Both molecules are the most frequent products in the network due to cleavage reactions (Fig. 1B). As far as the molecules undergoing cleavage reactions, hydroxycitrate is involved in 3 of them. This is the the highest number of cleavage reactions for a molecule. Citrate, along with 46 other molecules, has only 1 cleavage channel.

Table S1. Comparison of the fitted power-law behavior against alternatives for degree distribution in the molecular partition and its projection. For the power law, p-value *above 0.1* indicates significance of the fit. For the alternatives, positive log-likelihood ratios LR indicate that power law is favored over the alternative. Significance of the likelihood ratio test is given by p-value that has to be *below 0.1* for LR test to be significant.

| | Power law p | Log-normal LR/p | Exponential LR/p | Stretched exp. LR/p | PL + exp. cutoff LR/p |
|----------------|------------------|----------------------|-----------------------|--------------------------|----------------------------|
| Mol. partition | 0.84 | -1.18/0.24 | 1.08/0.28 | 0.01/0.93 | 0.00/1.0 |
| Projection | 0.78 | -0.63/0.53 | 1.45/0.15 | 0.01/0.93 | - |

Distribution of the “cycle cost” defined as the net change of Gibbs free energy along the cycle

Various approaches can be used to characterize the “uniqueness” of the rTCA cycle; in the following section we consider z-

score as an example. The Z-score is defined as

$$z = \frac{x - \mu}{\sigma} \quad (1)$$

where z is z-score of the datum x in the population with mean μ and standard deviation σ . For the population of cycle cost (see Fig. 3A) the z-score of rTCA cycle is 1.35 meaning that its cost is 1.35 standard deviations above the mean. We assess the modification of z-score in this data-set assuming variability of the redox conditions that translates into the shifts of redox potentials and free energies of redox reactions. The sensitive reaction types are reductive carboxylation (Eq. 1), carbonyl reduction (Eq. 3), and double bond reduction (Eq. 4). The latter two processes are of comparable mechanistic complexity; the former includes multiple steps. Therefore, we introduce one shift parameter to account for the conditions of reductive carboxylation and another shift parameter to account for the conditions of carbonyl and double bond reduction. Cycles have different number of redox reactions of each type, for example there are 2 reductive carboxylation steps in rTCA cycle and total of 3 simple reductive steps, 2 carbonyl and 1 double bond reduction reactions. Distribution of cycle cost will change its shape as redox conditions change, along with the z-score of rTCA cycle (Fig. S2). The “uniqueness” of rTCA cycle increases faster as free energies of simple reduction steps become more positive.

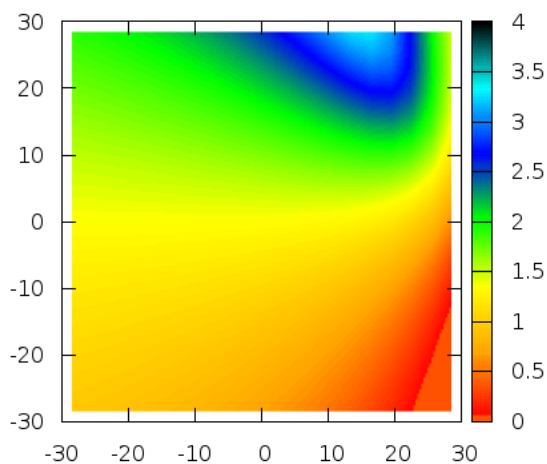
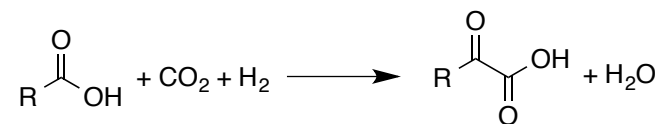


Figure S2. Sensitivity of z-score of rTCA cycle (color map) to the shift of free energies of reactions of reductive carboxylation along the horizontal axis (ΔG , kcal/mol) and double bond and carbonyl reduction along the vertical axis (ΔG , kcal/mol)

References

21. Virkar, Y. & Clauset, A. Power-law distributions in binned empirical data *Ann. Appl. Stat.* **8**, 89-119 (2014).

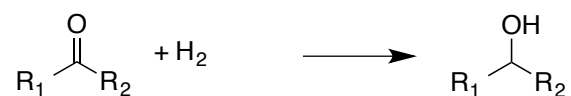
(1) Reductive Carboxylation



(2) Carboxylation



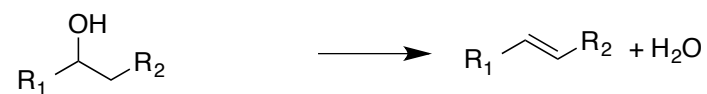
(3) Carbonyl Reduction



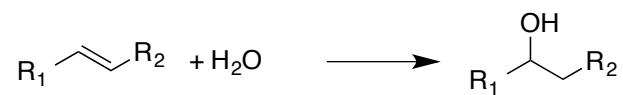
(4) Alkene Reduction



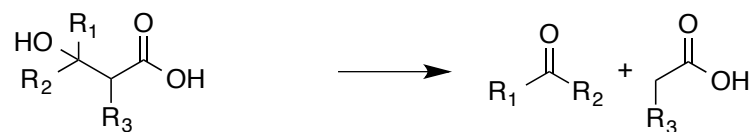
(5) Dehydration



(6) Hydration



(7) Cleavage



Scheme S1: Reaction types of the reverse tricarboxylic acid cycle.

Table S2: Characteristics of reaction cycles consistent with reaction types (1)–(7) of the reverse tricarboxylic acid cycle. n_M : Number of molecules, n_B : number of branching points, E_H : height of the reaction cycle (see main text), kcal/mol, E_C : cost of the reaction cycle (see main text), kcal/mol.

| Label | n_M | n_B | E_C | E_H | Net reaction |
|---------|-------|-------|--------|-------|--|
| 64_4_1 | 11 | 1 | -77.5 | 53.3 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_4_2 | 11 | 1 | -77.5 | 53.3 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_4_3 | 11 | 1 | -77.5 | 43.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_4_4 | 11 | 1 | -77.5 | 43.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_4_5 | 11 | 1 | -77.5 | 40.1 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_4_6 | 11 | 1 | -77.5 | 41.2 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_10_1 | 16 | 0 | -181.7 | 37.8 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_2 | 16 | 0 | -170.9 | 37.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_3 | 16 | 0 | -181.7 | 33.5 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_4 | 16 | 0 | -170.9 | 33.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_5 | 16 | 0 | -181.7 | 34.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_6 | 16 | 0 | -170.9 | 34.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_7 | 16 | 0 | -181.7 | 37.8 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_8 | 16 | 0 | -170.9 | 37.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_9 | 16 | 0 | -181.7 | 33.5 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_10_10 | 16 | 0 | -170.9 | 33.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_11 | 16 | 0 | -181.7 | 34.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_12 | 16 | 0 | -170.9 | 34.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_13 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_14 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_15 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_16 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_17 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_18 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_19 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_20 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_21 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_22 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_23 | 16 | 0 | -181.7 | 39.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_24 | 16 | 0 | -170.9 | 39.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_25 | 16 | 0 | -181.7 | 40.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_26 | 16 | 0 | -170.9 | 40.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_27 | 16 | 0 | -181.7 | 40.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_10_28 | 16 | 0 | -170.9 | 40.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_29 | 16 | 0 | -181.7 | 40.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_30 | 16 | 0 | -170.9 | 40.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_10_31 | 16 | 0 | -181.7 | 40.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 64_10_32 | 16 | 0 | -170.9 | 40.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{OC}=\text{O}$ |
| 64_18_1 | 19 | 0 | -161.2 | 37.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_18_2 | 19 | 0 | -161.2 | 33.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_18_3 | 19 | 0 | -161.2 | 34.0 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_21_1 | 14 | 2 | -113.1 | 50.8 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64_21_2 | 14 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64_21_3 | 14 | 2 | -137.2 | 50.8 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow 2 \text{ CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_21_4 | 14 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow 2 \text{ CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_21_5 | 14 | 2 | -113.1 | 50.8 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64_21_6 | 14 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64_21_7 | 14 | 2 | -137.2 | 50.8 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow 2 \text{ CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_21_8 | 14 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_9 | 13 | 2 | -85.8 | 50.8 | $6 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_10 | 14 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_11 | 13 | 2 | -109.8 | 50.8 | $6 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_12 | 14 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_13 | 13 | 2 | -85.8 | 50.8 | $6 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_14 | 14 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_15 | 13 | 2 | -109.8 | 50.8 | $6 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_16 | 14 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_17 | 13 | 1 | -100.4 | 45.1 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{O=C(C(=O)C(=O)O)C(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_18 | 14 | 1 | -127.7 | 47.0 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_19 | 14 | 2 | -124.4 | 45.1 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_21_20 | 15 | 2 | -151.8 | 47.0 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_21 | 13 | 1 | -100.4 | 45.1 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{O=C(C(=O)C(=O)O)C(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_22 | 14 | 1 | -127.7 | 47.0 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_23 | 14 | 2 | -124.4 | 45.1 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_24 | 15 | 2 | -151.8 | 47.0 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_25 | 13 | 2 | -85.8 | 45.1 | $6 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_26 | 14 | 2 | -113.1 | 47.0 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_27 | 13 | 2 | -115.0 | 45.1 | $6 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_28 | 14 | 2 | -142.3 | 47.0 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_29 | 13 | 2 | -85.8 | 45.1 | $6 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_30 | 14 | 2 | -113.1 | 47.0 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_31 | 13 | 2 | -115.0 | 45.1 | $6 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |

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| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 64_21_32 | 14 | 2 | -142.3 | 47.0 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_33 | 13 | 2 | -85.8 | 45.1 | $6 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_34 | 14 | 2 | -113.1 | 47.0 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_35 | 14 | 3 | -109.8 | 45.1 | $6 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_36 | 15 | 3 | -137.2 | 47.0 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| ∞ 64_21_37 | 12 | 2 | -81.8 | 50.8 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_38 | 13 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_39 | 12 | 2 | -105.8 | 50.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_40 | 13 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_21_41 | 12 | 2 | -81.8 | 50.8 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_42 | 13 | 2 | -113.1 | 52.6 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_43 | 12 | 2 | -105.8 | 50.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64.21.44 | 13 | 2 | -137.2 | 52.6 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64.21.45 | 12 | 1 | -96.4 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.46 | 13 | 1 | -127.7 | 45.7 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.47 | 13 | 2 | -120.4 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.48 | 14 | 2 | -151.8 | 45.7 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.49 | 12 | 1 | -96.4 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.50 | 13 | 1 | -127.7 | 45.7 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.51 | 13 | 2 | -120.4 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.52 | 14 | 2 | -151.8 | 45.7 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.53 | 12 | 2 | -81.8 | 43.9 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.54 | 13 | 2 | -113.1 | 45.7 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.55 | 12 | 2 | -110.9 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_21_56 | 13 | 2 | -142.3 | 45.7 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_57 | 12 | 2 | -81.8 | 43.9 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_58 | 13 | 2 | -113.1 | 45.7 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_59 | 12 | 2 | -110.9 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_60 | 13 | 2 | -142.3 | 45.7 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_61 | 12 | 2 | -81.8 | 43.9 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_62 | 13 | 2 | -113.1 | 45.7 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_63 | 13 | 3 | -105.8 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_21_64 | 14 | 3 | -137.2 | 45.7 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_65 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_66 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_67 | 15 | 2 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64.21.68 | 15 | 2 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.69 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.70 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.71 | 15 | 2 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.72 | 15 | 2 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.73 | 14 | 2 | -113.1 | 45.4 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.74 | 14 | 2 | -113.1 | 47.2 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.75 | 14 | 2 | -142.3 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.76 | 14 | 2 | -142.3 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.77 | 14 | 2 | -113.1 | 45.4 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.78 | 14 | 2 | -113.1 | 47.2 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.79 | 14 | 2 | -142.3 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_21_80 | 14 | 2 | -142.3 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_81 | 14 | 2 | -113.1 | 45.4 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_82 | 14 | 2 | -113.1 | 47.2 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_83 | 15 | 3 | -137.2 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_84 | 15 | 3 | -137.2 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64_21_85 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_86 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_87 | 15 | 1 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64_21_88 | 15 | 1 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64_21_89 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_90 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_21_91 | 15 | 1 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.21.92 | 15 | 1 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64.21.93 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.94 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.95 | 15 | 1 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64.21.96 | 15 | 1 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64.21.97 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.98 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.99 | 15 | 2 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.100 | 15 | 2 | -151.8 | 47.2 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.101 | 14 | 1 | -127.7 | 45.4 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.102 | 14 | 1 | -127.7 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.103 | 15 | 2 | -151.8 | 45.4 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.21.116 | 15 | 3 | -137.2 | 47.2 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 4 \text{ H}_2\text{O}$ |
| 64.21.117 | 14 | 1 | -54.1 | 45.4 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)C(=O)C(C(=O)O)O} + \text{C=O}$ |
| 64.21.118 | 14 | 1 | -54.1 | 47.2 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)C(=O)C(C(=O)O)O} + \text{C=O}$ |
| 64.21.119 | 15 | 1 | -78.1 | 45.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC(=O)C(=O)C(C(=O)O)O} + \text{O=CC(=O)O} + \text{C=O}$ |
| 64.21.120 | 15 | 1 | -78.1 | 47.2 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC(=O)C(=O)C(C(=O)O)O} + \text{O=CC(=O)O} + \text{C=O}$ |
| 64.21.122 | 12 | 2 | -81.8 | 52.6 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.124 | 12 | 2 | -105.8 | 52.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64.21.126 | 12 | 2 | -81.8 | 52.6 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.128 | 12 | 2 | -105.8 | 52.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64.21.130 | 12 | 1 | -96.4 | 45.7 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.132 | 13 | 2 | -120.4 | 45.7 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.134 | 12 | 1 | -96.4 | 45.7 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.21.136 | 13 | 2 | -120.4 | 45.7 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.138 | 12 | 2 | -81.8 | 45.7 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.140 | 12 | 2 | -110.9 | 45.7 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.142 | 12 | 2 | -81.8 | 45.7 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.144 | 12 | 2 | -110.9 | 45.7 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)CC(C(=O)O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.146 | 12 | 2 | -81.8 | 45.7 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.148 | 13 | 3 | -105.8 | 45.7 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow 2 \text{ CC(=O)O} + \text{O=CC(=O)O} + \text{O=C(C(=O)O)C(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.21.149 | 14 | 1 | -127.7 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.150 | 13 | 1 | -127.6 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{OC(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64.21.151 | 15 | 1 | -151.8 | 39.5 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64.21.152 | 14 | 1 | -151.7 | 41.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC(=O)C=C(C(=O)O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OC(C(=O)O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{CC=O}$ |
| 64.21.153 | 14 | 1 | -127.7 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C(C(=O)O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64.21.154 | 13 | 1 | -127.6 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.155 | 15 | 1 | -151.8 | 39.5 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{CC}=\text{O}$ |
| 64.21.156 | 14 | 1 | -151.7 | 41.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{CC}=\text{O}$ |
| 64.21.157 | 14 | 1 | -127.7 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.158 | 13 | 1 | -127.6 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.159 | 15 | 1 | -151.8 | 39.5 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{CC}=\text{O}$ |
| 64.21.160 | 14 | 1 | -151.7 | 41.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{CC}=\text{O}$ |
| 64.21.161 | 14 | 1 | -127.7 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.162 | 13 | 1 | -127.6 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.163 | 15 | 2 | -151.8 | 39.5 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.164 | 14 | 2 | -151.7 | 41.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.165 | 14 | 1 | -127.7 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.21.166 | 13 | 1 | -127.6 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.167 | 15 | 2 | -151.8 | 39.5 | $6 \text{ CO}_2 + 10 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.168 | 14 | 2 | -151.7 | 41.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.21.169 | 14 | 2 | -113.1 | 39.5 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64.21.170 | 13 | 2 | -113.0 | 41.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64.21.171 | 14 | 2 | -142.3 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{CC}(\text{C}(\text{=O})\text{O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64.21.172 | 13 | 2 | -142.2 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{CC}(\text{C}(\text{=O})\text{O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64.21.173 | 14 | 2 | -113.1 | 39.5 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64.21.174 | 13 | 2 | -113.0 | 41.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64.21.175 | 14 | 2 | -142.3 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{CC}(\text{C}(\text{=O})\text{O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64.21.176 | 13 | 2 | -142.2 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC}(\text{=O})\text{C}=\text{C}(\text{C}(\text{=O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{CC}(\text{C}(\text{=O})\text{O})\text{O} + \text{OC}(\text{C}(\text{=O})\text{O})\text{C}(\text{=O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64.21.177 | 14 | 2 | -113.1 | 39.5 | $6 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{OC}(\text{=O})\text{C}(\text{=O})\text{C}(\text{C}(\text{=O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64_21_178 | 13 | 2 | -113.0 | 41.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_21_179 | 15 | 3 | -137.2 | 39.5 | $6 \text{ CO}_2 + 9 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow 2 \text{ CC}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 64_21_180 | 14 | 3 | -137.1 | 41.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow 2 \text{ CC}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OC}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_21_181 | 14 | 1 | -54.1 | 44.4 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_21_182 | 13 | 1 | -54.0 | 46.2 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_21_183 | 15 | 1 | -78.1 | 44.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_21_184 | 14 | 1 | -78.0 | 46.2 | $4 \text{ CO}_2 + 6 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_22_1 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_22_2 | 11 | 1 | -77.3 | 52.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_22_3 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_22_4 | 10 | 1 | -96.2 | 52.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_22_5 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_22_6 | 11 | 1 | -77.3 | 52.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_22_7 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64_22_8 | 10 | 1 | -96.2 | 52.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64_22_9 | 11 | 0 | -91.9 | 43.9 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O} + \text{OC(=O)C(=O)O}$ |
| 64_22_10 | 11 | 0 | -91.9 | 45.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O} + \text{OC(=O)C(=O)O}$ |
| 64_22_11 | 11 | 1 | -110.8 | 43.9 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_22_12 | 11 | 1 | -110.8 | 45.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_22_13 | 11 | 0 | -91.9 | 43.9 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O} + \text{OC(=O)C(=O)O}$ |
| 64_22_14 | 11 | 0 | -91.9 | 45.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O} + \text{OC(=O)C(=O)O}$ |
| 64_22_15 | 11 | 1 | -110.8 | 43.9 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_22_16 | 11 | 1 | -110.8 | 45.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_22_17 | 11 | 1 | -77.3 | 43.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64_22_18 | 11 | 1 | -77.3 | 45.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64_22_19 | 10 | 1 | -101.4 | 43.9 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 64_22_20 | 10 | 1 | -101.4 | 45.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 64_22_21 | 11 | 1 | -77.3 | 43.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64_22_22 | 11 | 1 | -77.3 | 45.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64_22_23 | 10 | 1 | -101.4 | 43.9 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 64_22_24 | 10 | 1 | -101.4 | 45.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 64_22_25 | 11 | 1 | -77.3 | 43.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|-------|-------|---|
| 64_22_26 | 11 | 1 | -77.3 | 45.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64_22_27 | 11 | 2 | -96.2 | 43.9 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_22_28 | 11 | 2 | -96.2 | 45.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64_29.1 | 10 | 1 | -82.5 | 37.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.2 | 10 | 1 | -82.5 | 37.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.3 | 10 | 1 | -82.5 | 37.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.4 | 10 | 1 | -82.5 | 46.0 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.5 | 10 | 1 | -82.5 | 37.8 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.6 | 10 | 1 | -82.5 | 45.5 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.7 | 10 | 1 | -82.5 | 45.5 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.8 | 10 | 1 | -82.5 | 45.5 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.9 | 10 | 1 | -82.5 | 46.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.10 | 10 | 1 | -82.5 | 34.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.11 | 10 | 1 | -82.5 | 34.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.12 | 10 | 1 | -82.5 | 34.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.13 | 10 | 1 | -82.5 | 43.0 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.14 | 10 | 1 | -82.5 | 34.9 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64_29.15 | 10 | 1 | -82.5 | 41.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64.29.16 | 10 | 1 | -82.5 | 48.8 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64.29.17 | 10 | 1 | -82.5 | 40.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{OC(=O)C(=O)C} + 3 \text{ H}_2\text{O}$ |
| 64.48.1 | 18 | 0 | -161.2 | 37.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.2 | 18 | 0 | -161.2 | 33.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.3 | 18 | 0 | -161.2 | 34.0 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.7 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.8 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.9 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.10 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.11 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.12 | 17 | 0 | -151.2 | 39.2 | $5 \text{ CO}_2 + 10 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ $\rightarrow 4 \text{ H}_2\text{O} + \text{CCC(C(=O)O)O} + \text{OCC(=O)O} + \text{CC=O} + \text{C=O}$ |
| 64.48.13 | 16 | 0 | -129.2 | 40.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC=CC(=O)O} \rightarrow$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| | | | | | $\rightarrow 4 \text{H}_2\text{O} + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_48_14 | 16 | 0 | -129.2 | 40.1 | $5 \text{CO}_2 + 9 \text{H}_2 + \text{CC}=\text{CC}(=\text{O})\text{O} \rightarrow$ $\rightarrow 4 \text{H}_2\text{O} + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_48_15 | 16 | 0 | -129.2 | 40.1 | $5 \text{CO}_2 + 9 \text{H}_2 + \text{CC}=\text{CC}(=\text{O})\text{O} \rightarrow$ $\rightarrow 4 \text{H}_2\text{O} + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_48_16 | 15 | 0 | -124.7 | 40.7 | $4 \text{CO}_2 + 8 \text{H}_2 + \text{CC}=\text{CC}(=\text{O})\text{O} \rightarrow$ $\rightarrow 3 \text{H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_49_1 | 10 | 0 | -120.5 | 30.9 | $3 \text{CO}_2 + 7 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_2 | 10 | 0 | -109.6 | 30.6 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow 3 \text{H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_3 | 10 | 0 | -120.5 | 26.6 | $3 \text{CO}_2 + 7 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_4 | 10 | 0 | -109.6 | 26.3 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow 3 \text{H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_5 | 10 | 0 | -120.5 | 27.2 | $3 \text{CO}_2 + 7 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_6 | 10 | 0 | -109.6 | 26.8 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow 3 \text{H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_7 | 10 | 0 | -120.5 | 28.5 | $3 \text{CO}_2 + 7 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_49_8 | 10 | 0 | -109.6 | 28.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow 3 \text{H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_9 | 10 | 0 | -120.5 | 28.5 | $3 \text{CO}_2 + 7 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64_49_10 | 10 | 0 | -109.6 | 28.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow 3 \text{H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64_49_11 | 10 | 1 | -105.9 | 32.1 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 64.49.12 | 10 | 1 | -95.0 | 32.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC=O}$ |
| 64.49.13 | 10 | 1 | -105.9 | 36.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.49.14 | 10 | 1 | -95.0 | 36.8 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC=O}$ |
| 64.49.15 | 10 | 1 | -105.9 | 36.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.49.16 | 9 | 1 | -84.1 | 36.8 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.69.1 | 10 | 1 | -105.9 | 39.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.69.2 | 10 | 1 | -105.9 | 37.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.69.4 | 9 | 1 | -84.1 | 39.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.69.5 | 9 | 1 | -84.1 | 37.5 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.71.1 | 4 | 0 | -13.8 | 29.0 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64.79.2 | 4 | 0 | -13.8 | 33.7 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{O=CC(=O)O}$ |
| 64.81.1 | 3 | 0 | -12.6 | 21.3 | $\text{CO}_2 + \text{H}_2 \rightarrow \text{OC=O}$ |
| 64.85.1 | 8 | 0 | -36.1 | 32.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C=O} + \text{OC(=O)C(O)O}$ |
| 64.87.1 | 5 | 0 | -23.4 | 29.0 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C=O}$ |
| 64.90.1 | 10 | 0 | -120.5 | 30.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 64.90.2 | 10 | 0 | -120.5 | 29.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 64.90.4 | 10 | 0 | -109.6 | 30.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O}$ |
| 64.90.5 | 10 | 0 | -109.6 | 28.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|--|
| 64.90.7 | 10 | 0 | -120.5 | 30.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64.90.8 | 10 | 0 | -120.5 | 29.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 64.90.10 | 10 | 0 | -109.6 | 30.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64.90.11 | 10 | 0 | -109.6 | 28.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O}$ |
| 64.90.13 | 10 | 1 | -105.9 | 34.4 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.90.14 | 10 | 1 | -105.9 | 32.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.90.16 | 10 | 1 | -95.0 | 34.4 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.90.17 | 10 | 1 | -95.0 | 32.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.90.19 | 10 | 1 | -105.9 | 39.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.90.20 | 10 | 1 | -105.9 | 37.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.90.22 | 10 | 1 | -95.0 | 39.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.90.23 | 10 | 1 | -95.0 | 37.5 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.92.1 | 7 | 0 | -37.2 | 27.4 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.92.2 | 7 | 0 | -97.1 | 25.0 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.92.3 | 7 | 0 | -97.1 | 29.3 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.95.1 | 5 | 0 | -23.4 | 32.0 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.107.2 | 7 | 0 | -37.2 | 32.4 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.113.1 | 7 | 0 | -23.4 | 42.3 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_113_2 | 7 | 0 | -23.4 | 42.3 | $\text{CO}_2 + 2 \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_113_4 | 7 | 0 | -23.4 | 42.3 | $\text{CO}_2 + 2 \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_1 | 14 | 1 | -105.9 | 39.0 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_2 | 14 | 1 | -95.0 | 39.0 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_3 | 14 | 1 | -105.9 | 34.7 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_4 | 14 | 1 | -95.0 | 34.7 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_5 | 14 | 1 | -105.9 | 35.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_6 | 14 | 1 | -95.0 | 35.2 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_7 | 14 | 1 | -105.9 | 32.5 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_8 | 14 | 1 | -95.0 | 32.5 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_9 | 14 | 1 | -105.9 | 35.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_10 | 14 | 1 | -95.0 | 35.2 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_11 | 14 | 1 | -105.9 | 35.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_12 | 14 | 1 | -95.0 | 35.2 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_13 | 14 | 1 | -105.9 | 31.8 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_14 | 14 | 1 | -95.0 | 31.8 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |
| 64_115_15 | 14 | 1 | -105.9 | 35.2 | $3 \text{CO}_2 + 6 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64_115_16 | 14 | 1 | -95.0 | 35.2 | $3 \text{CO}_2 + 5 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{H}_2\text{O} + \text{OC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64.115.17 | 14 | 1 | -105.9 | 35.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.115.18 | 14 | 1 | -95.0 | 35.2 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.115.19 | 13 | 1 | -105.9 | 35.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.115.20 | 14 | 1 | -95.0 | 35.2 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}=\text{O}$ |
| 64.115.21 | 12 | 1 | -83.7 | 32.0 | $3 \text{ CO}_2 + 5 \text{ H}_2 + \text{OCCC}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{CC}(=\text{O})\text{O} + \text{OC}=\text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 64.132.3 | 7 | 0 | -97.1 | 25.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.134.1 | 7 | 0 | -27.5 | 41.4 | $4 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.134.2 | 7 | 0 | -27.5 | 41.4 | $4 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.145.4 | 7 | 0 | -23.4 | 34.2 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.145.5 | 7 | 0 | -23.4 | 34.2 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.154.1 | 9 | 0 | -58.0 | 26.7 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.2 | 9 | 0 | -58.0 | 28.1 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.3 | 9 | 0 | -37.2 | 29.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.154.4 | 9 | 0 | -97.1 | 35.4 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.5 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.6 | 9 | 0 | -97.1 | 24.8 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.8 | 9 | 0 | -37.2 | 29.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|-------|-------|--|
| 64.154.9 | 9 | 0 | -37.2 | 29.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.154.11 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.12 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.13 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.154.14 | 9 | 0 | -97.1 | 35.4 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.15 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.16 | 9 | 0 | -97.1 | 27.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.18 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.154.19 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.154.21 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.22 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.154.23 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.154.24 | 9 | 0 | -97.1 | 35.4 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.25 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.26 | 9 | 0 | -97.1 | 27.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.27 | 9 | 0 | -97.1 | 29.8 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.154.28 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.154.29 | 8 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_154_30 | 9 | 0 | -37.2 | 32.4 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_160_1 | 9 | 0 | -97.1 | 36.1 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_166_15 | 11 | 0 | -91.9 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_16 | 11 | 0 | -110.8 | 39.5 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_166_17 | 11 | 0 | -91.9 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_18 | 11 | 0 | -110.8 | 39.5 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_166_19 | 11 | 0 | -91.9 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_20 | 11 | 0 | -110.8 | 39.5 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_166_21 | 11 | 0 | -91.9 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_22 | 11 | 1 | -110.8 | 39.5 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_166_23 | 11 | 0 | -91.9 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_24 | 11 | 1 | -110.8 | 39.5 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_166_25 | 11 | 1 | -77.3 | 39.5 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_26 | 10 | 1 | -101.4 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_166_27 | 11 | 1 | -77.3 | 39.5 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_28 | 10 | 1 | -101.4 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_166_29 | 11 | 1 | -77.3 | 39.5 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_166_30 | 11 | 2 | -96.2 | 39.5 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.166.31 | 11 | 0 | -18.3 | 44.4 | $3 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.166.32 | 11 | 0 | -37.2 | 44.4 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.171.2 | 7 | 0 | -23.4 | 28.5 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.173.1 | 6 | 0 | -13.8 | 41.1 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.175.1 | 5 | 0 | 0.7 | 45.3 | $3 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{O}=\text{C}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.175.2 | 5 | 0 | 0.7 | 45.3 | $3 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{O}=\text{C}(\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.1 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.2 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.177.3 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.4 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.177.5 | 11 | 0 | -91.9 | 45.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.6 | 11 | 1 | -110.8 | 45.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.177.7 | 11 | 0 | -91.9 | 45.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.8 | 11 | 1 | -110.8 | 45.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.177.9 | 11 | 1 | -77.3 | 45.1 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.10 | 10 | 1 | -101.4 | 45.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64.177.11 | 11 | 1 | -77.3 | 45.1 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.177.12 | 10 | 1 | -101.4 | 45.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64.177.13 | 11 | 1 | -77.3 | 45.1 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OC(=O)C(=O)O}$ |
| 64.177.14 | 11 | 2 | -96.2 | 45.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{O=CC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 64.185.1 | 13 | 0 | -133.0 | 42.9 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{OC=O}$ |
| 64.185.2 | 13 | 0 | -133.0 | 41.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{OC=O}$ |
| 64.185.3 | 13 | 0 | -133.0 | 40.6 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{OC=O}$ |
| 64.185.4 | 13 | 0 | -122.2 | 42.9 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.5 | 13 | 0 | -122.2 | 41.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.6 | 13 | 0 | -122.2 | 40.6 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.7 | 13 | 1 | -118.4 | 50.6 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.8 | 13 | 1 | -118.4 | 49.0 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.9 | 13 | 1 | -118.4 | 48.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.10 | 13 | 1 | -107.6 | 50.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.11 | 13 | 1 | -107.6 | 49.0 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.12 | 13 | 1 | -107.6 | 48.3 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.13 | 13 | 1 | -118.4 | 50.6 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.14 | 13 | 1 | -118.4 | 49.0 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.15 | 13 | 1 | -118.4 | 48.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.16 | 13 | 1 | -107.6 | 50.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64.185.17 | 13 | 1 | -107.6 | 49.0 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.18 | 13 | 1 | -107.6 | 48.3 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.19 | 12 | 0 | -133.0 | 43.7 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.20 | 12 | 0 | -133.0 | 42.1 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.21 | 12 | 0 | -133.0 | 41.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.22 | 12 | 0 | -122.2 | 43.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.23 | 12 | 0 | -122.2 | 42.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.24 | 12 | 0 | -122.2 | 41.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.25 | 12 | 0 | -133.0 | 43.7 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.26 | 12 | 0 | -133.0 | 42.1 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.27 | 12 | 0 | -133.0 | 41.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{OC=O}$ |
| 64.185.28 | 12 | 0 | -122.2 | 43.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.29 | 12 | 0 | -122.2 | 42.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.30 | 12 | 0 | -122.2 | 41.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ OC=O} + \text{CC=O}$ |
| 64.185.31 | 12 | 1 | -118.4 | 43.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.32 | 12 | 1 | -118.4 | 42.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.33 | 12 | 1 | -118.4 | 41.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.34 | 12 | 1 | -107.6 | 43.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64.185.35 | 12 | 1 | -107.6 | 42.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.36 | 12 | 1 | -107.6 | 41.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.37 | 12 | 1 | -118.4 | 43.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.38 | 12 | 1 | -118.4 | 42.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.39 | 12 | 1 | -118.4 | 41.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{OC=O}$ |
| 64.185.40 | 12 | 1 | -107.6 | 43.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.41 | 12 | 1 | -107.6 | 42.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.42 | 12 | 1 | -107.6 | 41.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ OC=O}$ |
| 64.185.43 | 12 | 2 | -118.4 | 43.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC=O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.185.44 | 12 | 2 | -118.4 | 42.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC=O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.185.45 | 12 | 2 | -118.4 | 41.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{OC=O} + 3 \text{ H}_2\text{O} + \text{C=O}$ |
| 64.185.46 | 11 | 2 | -96.6 | 43.7 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC=O} + 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.185.47 | 11 | 2 | -96.6 | 42.1 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC=O} + 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.185.48 | 11 | 2 | -96.6 | 41.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC=O} + 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O}$ |
| 64.190.3 | 6 | 0 | -3.7 | 41.4 | $4 \text{ CO}_2 + 3 \text{ H}_2 + \text{OC(=O)CC(C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)CC(=O)C(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O=CC(=O)O}$ |
| 64.190.4 | 6 | 0 | -3.7 | 41.4 | $4 \text{ CO}_2 + 3 \text{ H}_2 + \text{OC(=O)CC(C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)CC(=O)C(=O)O} + 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O=CC(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|-------|-------|---|
| 64.198.1 | 10 | 0 | -44.9 | 28.2 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}=\text{CC}=\text{O}$ |
| 64.198.2 | 10 | 0 | -44.9 | 32.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}=\text{CC}=\text{O}$ |
| 64.215.1 | 9 | 0 | -97.1 | 35.7 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.220.1 | 9 | 0 | -23.4 | 46.8 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.228.1 | 9 | 0 | -58.0 | 34.6 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.228.2 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.228.4 | 9 | 0 | -58.0 | 30.3 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.228.5 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.228.7 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.228.8 | 9 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.235.6 | 7 | 0 | -23.4 | 35.2 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 64.237.10 | 9 | 0 | -37.2 | 42.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.237.11 | 9 | 0 | -37.2 | 42.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.237.12 | 9 | 0 | -37.2 | 42.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.237.13 | 9 | 0 | -37.2 | 34.2 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.237.14 | 9 | 0 | -37.2 | 34.2 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.237.15 | 8 | 0 | -37.2 | 34.2 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.239.2 | 11 | 1 | -96.2 | 54.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_239_4 | 11 | 1 | -96.2 | 54.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_241_5 | 6 | 0 | -3.7 | 41.1 | $4 \text{ CO}_2 + 3 \text{ H}_2 + \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_241_6 | 6 | 0 | -3.7 | 41.1 | $4 \text{ CO}_2 + 3 \text{ H}_2 + \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_243_1 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_2 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_243_3 | 11 | 1 | -77.3 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_4 | 10 | 1 | -96.2 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_243_33 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_34 | 11 | 1 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_243_35 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_36 | 11 | 1 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_243_37 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_38 | 10 | 1 | -101.4 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_39 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_40 | 10 | 1 | -101.4 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_41 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_243_42 | 11 | 2 | -96.2 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_43 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_44 | 11 | 0 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_243_45 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_46 | 11 | 0 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_243_47 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_48 | 11 | 0 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{CC}=\text{O}$ |
| 64_243_49 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_50 | 11 | 1 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_243_51 | 11 | 0 | -91.9 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_52 | 11 | 1 | -110.8 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_243_53 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_54 | 10 | 1 | -101.4 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_55 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_56 | 10 | 1 | -101.4 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_57 | 11 | 1 | -77.3 | 45.4 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 64_243_58 | 11 | 2 | -96.2 | 45.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 64_243_59 | 11 | 0 | -18.3 | 45.4 | $3 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.243.60 | 11 | 0 | -37.2 | 45.4 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64.255.1 | 10 | 0 | -90.3 | 36.4 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 64.255.2 | 10 | 0 | -90.3 | 41.2 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 64.267.4 | 9 | 0 | -58.0 | 30.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.267.5 | 9 | 0 | -58.0 | 32.0 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 64.282.1 | 6 | 0 | -3.3 | 45.3 | $4 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{C}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.282.2 | 6 | 0 | -3.3 | 45.3 | $4 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{C}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{C}(=\text{O})\text{O}$ |
| 64.322.1 | 11 | 0 | -109.6 | 41.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}=\text{O}$ |
| 64.322.2 | 12 | 0 | -109.6 | 48.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}=\text{O}$ |
| 64.322.3 | 12 | 0 | -109.6 | 40.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OC}=\text{O}$ |
| 64.338.1 | 7 | 0 | -30.7 | 45.3 | $4 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O}$ |
| 64.338.2 | 7 | 0 | -30.7 | 45.3 | $4 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(=\text{O})\text{C}(\text{C}(=\text{O})\text{O})\text{O}$ |
| 64.387.2 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.4 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.6 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.8 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.10 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.12 | 11 | 0 | -97.1 | 46.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64.387.14 | 11 | 0 | -97.1 | 47.7 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.16 | 11 | 0 | -97.1 | 47.7 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.18 | 11 | 0 | -97.1 | 47.7 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.387.20 | 11 | 0 | -97.1 | 48.4 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64.400.1 | 13 | 1 | -110.8 | 40.6 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}=\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.400.2 | 13 | 1 | -110.8 | 40.6 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}=\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64.407.1 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.2 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.3 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.4 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.5 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.6 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.7 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.8 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.9 | 15 | 0 | -148.5 | 45.1 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.10 | 15 | 0 | -137.6 | 45.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.11 | 15 | 0 | -148.5 | 45.1 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64.407.12 | 15 | 0 | -137.6 | 45.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_407_13 | 15 | 1 | -133.9 | 45.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_14 | 15 | 1 | -123.0 | 45.1 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_15 | 15 | 1 | -133.9 | 45.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_16 | 15 | 1 | -123.0 | 45.1 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_17 | 15 | 1 | -133.9 | 45.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_18 | 14 | 1 | -112.1 | 45.1 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O} + \text{O=CC(O)O}$ |
| 64_407_19 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_20 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_21 | 15 | 1 | -133.9 | 50.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_22 | 15 | 1 | -123.0 | 50.8 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_23 | 15 | 0 | -148.5 | 43.9 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_24 | 15 | 0 | -137.6 | 43.9 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_25 | 15 | 0 | -148.5 | 43.9 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_26 | 15 | 0 | -137.6 | 43.9 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_27 | 15 | 1 | -133.9 | 43.9 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_28 | 15 | 1 | -123.0 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_29 | 15 | 1 | -133.9 | 43.9 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_30 | 15 | 1 | -123.0 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64_407_31 | 15 | 1 | -133.9 | 43.9 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_32 | 14 | 1 | -112.1 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O} + \text{O=CC(O)O}$ |
| 64_407_33 | 14 | 0 | -148.5 | 45.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_34 | 14 | 0 | -137.6 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_35 | 14 | 0 | -148.5 | 45.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_36 | 14 | 0 | -137.6 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_37 | 14 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_38 | 14 | 1 | -123.0 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_39 | 14 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_40 | 14 | 1 | -123.0 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_41 | 14 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_42 | 13 | 1 | -112.1 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O} + \text{O=CC(O)O}$ |
| 64_407_43 | 13 | 0 | -142.5 | 45.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_44 | 13 | 0 | -131.6 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_45 | 13 | 0 | -142.5 | 45.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_407_46 | 13 | 0 | -131.6 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_47 | 13 | 0 | -142.5 | 45.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_48 | 13 | 0 | -131.6 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_49 | 13 | 0 | -142.5 | 45.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_50 | 13 | 0 | -131.6 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_51 | 13 | 0 | -142.5 | 45.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_52 | 13 | 0 | -131.6 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_53 | 13 | 1 | -127.9 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_54 | 13 | 1 | -117.0 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{O=CC(O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_407_55 | 13 | 1 | -127.9 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_56 | 13 | 1 | -117.0 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + 2 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_57 | 13 | 1 | -127.9 | 45.4 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC(=O)O} + \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_58 | 12 | 1 | -106.1 | 45.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 2 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O} + \text{OCC(=O)O} + \text{O=CC(O)O}$ |
| 64_407_61 | 15 | 1 | -133.9 | 52.6 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_62 | 15 | 1 | -123.0 | 52.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_63 | 15 | 1 | -133.9 | 52.6 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_64 | 15 | 1 | -123.0 | 52.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_65 | 15 | 0 | -148.5 | 45.7 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_66 | 15 | 0 | -137.6 | 45.7 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_67 | 15 | 0 | -148.5 | 45.7 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_68 | 15 | 0 | -137.6 | 45.7 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_69 | 15 | 1 | -133.9 | 45.7 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_70 | 15 | 1 | -123.0 | 45.7 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_407_71 | 15 | 1 | -133.9 | 45.7 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_72 | 15 | 1 | -123.0 | 45.7 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_73 | 15 | 1 | -133.9 | 45.7 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_74 | 14 | 1 | -112.1 | 45.7 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(CC(=O)O)O} + \text{O=CC(O)O}$ |
| 64_407_75 | 14 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_76 | 14 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_77 | 14 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_78 | 14 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_79 | 14 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_80 | 14 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_81 | 14 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_82 | 14 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_83 | 14 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_84 | 14 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC=O} + \text{CC=O} + \text{O=CC(O)O}$ |
| 64_407_85 | 14 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_86 | 14 | 1 | -123.0 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |
| 64_407_87 | 14 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{O=CC(O)O}$ |
| 64_407_88 | 14 | 1 | -123.0 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_407_89 | 14 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_407_90 | 13 | 1 | -112.1 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(\text{CC}(=\text{O})\text{O})\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_407_91 | 12 | 0 | -74.8 | 44.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_407_92 | 11 | 0 | -64.0 | 44.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_425_1 | 10 | 0 | -54.5 | 32.3 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 64_425_4 | 11 | 0 | -37.2 | 29.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_6 | 10 | 0 | -54.5 | 34.0 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 64_425_9 | 10 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_11 | 10 | 0 | -54.5 | 34.0 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 64_425_14 | 9 | 0 | -34.3 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + \text{H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_15 | 9 | 0 | -37.2 | 34.0 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_16 | 10 | 0 | -54.5 | 42.3 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 64_425_19 | 10 | 0 | -37.2 | 42.3 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_21 | 10 | 0 | -54.5 | 34.2 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 64_425_24 | 9 | 0 | -34.3 | 34.2 | $3 \text{ CO}_2 + 4 \text{ H}_2 + \text{OC}(=\text{O})\text{C}=\text{C} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + \text{H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_425_25 | 9 | 0 | -37.2 | 34.2 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 64_458_33 | 15 | 0 | -148.5 | 45.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_34 | 15 | 0 | -137.6 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_35 | 15 | 0 | -148.5 | 45.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_36 | 15 | 0 | -137.6 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_37 | 15 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_38 | 15 | 1 | -123.0 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_39 | 15 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_40 | 15 | 1 | -123.0 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_41 | 15 | 1 | -133.9 | 45.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_42 | 14 | 1 | -112.1 | 45.4 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(\text{CC}(=\text{O})\text{O})\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_75 | 15 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_76 | 15 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_77 | 15 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_78 | 15 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_79 | 15 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_80 | 15 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_81 | 15 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_82 | 15 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64_458_83 | 15 | 0 | -148.5 | 39.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_84 | 15 | 0 | -137.6 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_85 | 15 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_86 | 15 | 1 | -123.0 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_87 | 15 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_88 | 15 | 1 | -123.0 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_89 | 15 | 1 | -133.9 | 39.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_90 | 14 | 1 | -112.1 | 39.5 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(\text{CC}(=\text{O})\text{O})\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_91 | 13 | 0 | -74.8 | 44.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_458_92 | 12 | 0 | -64.0 | 44.4 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 64_465_1 | 16 | 1 | -119.7 | 36.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_465_2 | 16 | 1 | -119.7 | 41.3 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_465_3 | 16 | 1 | -119.7 | 39.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_465_4 | 16 | 1 | -108.8 | 36.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_465_5 | 16 | 1 | -108.8 | 41.3 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_465_6 | 16 | 1 | -108.8 | 39.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{O}=\text{CC}(=\text{O})\text{O}$ |
| 64_465_7 | 16 | 1 | -119.7 | 36.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 64_465_8 | 16 | 1 | -119.7 | 41.3 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{O}=\text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64_465_9 | 16 | 1 | -119.7 | 39.6 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC(=O)O} + 4 \text{ H}_2\text{O} + \text{O=CC(=O)O} + \text{C=O}$ |
| 64_465_10 | 16 | 1 | -108.8 | 36.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(=O)O}$ |
| 64_465_11 | 16 | 1 | -108.8 | 41.3 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(=O)O}$ |
| 64_465_12 | 16 | 1 | -108.8 | 39.6 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CC(=O)O} + 3 \text{ H}_2\text{O} + \text{OC=O} + \text{O=CC(=O)O}$ |
| 64_471_7 | 18 | 0 | -181.7 | 37.8 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 64_471_8 | 18 | 0 | -170.9 | 37.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC=O} + \text{OC=O}$ |
| 64_471_9 | 18 | 0 | -181.7 | 33.5 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 64_471_10 | 18 | 0 | -170.9 | 33.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC=O} + \text{OC=O}$ |
| 64_471_11 | 18 | 0 | -181.7 | 34.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 64_471_12 | 18 | 0 | -170.9 | 34.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CCC=O} + \text{OC=O}$ |
| 64_484_4 | 11 | 0 | -97.1 | 34.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_5 | 11 | 0 | -97.1 | 31.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_6 | 11 | 0 | -97.1 | 31.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_7 | 11 | 0 | -97.1 | 31.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_8 | 11 | 0 | -97.1 | 31.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_9 | 11 | 0 | -97.1 | 31.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_10 | 11 | 0 | -97.1 | 30.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |
| 64_484_11 | 11 | 0 | -97.1 | 30.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 64_484_12 | 11 | 0 | -97.1 | 30.6 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_484_13 | 11 | 0 | -97.1 | 30.1 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_484_14 | 11 | 0 | -97.1 | 36.5 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_2 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_4 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_6 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_8 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_10 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_12 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_14 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_16 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_18 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_20 | 11 | 0 | -97.1 | 34.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 64_496_22 | 11 | 0 | -97.1 | 39.4 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_5_1 | 15 | 0 | -164.9 | 53.3 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC}(=\text{O})\text{O}$ |
| 90_5_3 | 15 | 0 | -164.9 | 53.3 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC}(=\text{O})\text{O}$ |
| 90_5_5 | 15 | 0 | -164.9 | 53.3 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC}(=\text{O})\text{O}$ |
| 90_5_7 | 15 | 0 | -164.9 | 53.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|---------|-------|-------|--------|-------|--|
| 90_5_9 | 15 | 0 | -164.9 | 53.3 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_11 | 15 | 0 | -164.9 | 53.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_13 | 15 | 0 | -164.9 | 47.4 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_15 | 15 | 0 | -164.9 | 47.4 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_17 | 15 | 0 | -164.9 | 47.1 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_19 | 15 | 0 | -164.9 | 45.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_21 | 15 | 0 | -164.9 | 43.7 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_23 | 15 | 0 | -164.9 | 45.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_25 | 15 | 0 | -164.9 | 47.4 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_27 | 15 | 0 | -164.9 | 47.4 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_29 | 15 | 0 | -164.9 | 47.1 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_31 | 15 | 0 | -164.9 | 45.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_33 | 15 | 0 | -164.9 | 41.5 | $8 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_5_35 | 15 | 0 | -164.9 | 45.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ CC(=O)O}$ |
| 90_10_1 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC=O} + \text{ C=O}$ |
| 90_10_2 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC=O} + \text{ C=O}$ |
| 90_10_3 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{ OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{ OCC(=O)O} + \text{ CCC=O} + \text{ C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|--|
| 90_10_4 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_5 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_6 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_7 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_8 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_9 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_10 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_11 | 15 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_12 | 14 | 0 | -175.7 | 40.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_13 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_14 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_15 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_16 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_17 | 15 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|--|
| 90_10_18 | 14 | 0 | -175.7 | 40.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_19 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_20 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_21 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_22 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_23 | 15 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_24 | 14 | 0 | -175.7 | 40.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_25 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_26 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_27 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_28 | 16 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_29 | 15 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_10_30 | 14 | 0 | -175.7 | 41.1 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|--|
| 90_10_31 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_32 | 15 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_33 | 14 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_34 | 16 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_35 | 15 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_36 | 14 | 0 | -175.7 | 41.1 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_37 | 16 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_38 | 15 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_39 | 14 | 0 | -175.7 | 41.7 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_40 | 16 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_41 | 15 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_10_42 | 14 | 0 | -175.7 | 41.7 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_18_73 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_18_76 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_18_79 | 21 | 2 | -207.3 | 45.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_18_82 | 21 | 1 | -207.3 | 45.5 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_85 | 21 | 1 | -207.3 | 45.5 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_88 | 21 | 2 | -207.3 | 45.5 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_18_91 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_94 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_97 | 21 | 2 | -207.3 | 45.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_18_100 | 21 | 1 | -207.3 | 45.5 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_103 | 21 | 1 | -207.3 | 45.5 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_106 | 21 | 2 | -207.3 | 45.5 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_18_109 | 20 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_112 | 20 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_115 | 20 | 2 | -202.8 | 46.1 | $11 \text{ H}_2 + 5 \text{ CO}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + 2 \text{ CCC(=O)O} + \text{C=O}$ |
| 90_18_118 | 20 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_18_121 | 20 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_18_124 | 20 | 2 | -202.8 | 46.1 | $11 \text{ H}_2 + 5 \text{ CO}_2 + \text{CCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + 2 \text{ CCC(=O)O} + \text{C=O}$ |
| 90_21_1 | 9 | 0 | -82.5 | 45.4 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC(=O)O}$ |
| 90_21_2 | 9 | 0 | -82.5 | 45.4 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC(=O)O}$ |
| 90_21_3 | 9 | 0 | -82.5 | 45.1 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC(=O)O}$ |
| 90_21_5 | 9 | 0 | -82.5 | 39.5 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC(=O)O}$ |
| 90_48_1 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_2 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_3 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_4 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_5 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_6 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_7 | 21 | 2 | -207.3 | 45.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_8 | 21 | 2 | -207.3 | 40.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_9 | 21 | 2 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_10 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|--|
| 90_48_11 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_12 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_13 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_14 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_15 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_16 | 21 | 2 | -207.3 | 45.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_17 | 21 | 2 | -207.3 | 40.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_18 | 21 | 2 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_19 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_20 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_21 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_22 | 21 | 1 | -207.3 | 45.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_23 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_24 | 21 | 1 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |
| 90_48_25 | 21 | 2 | -207.3 | 45.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_26 | 21 | 2 | -207.3 | 40.7 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_27 | 21 | 2 | -207.3 | 40.7 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC(=O)O} + \text{C=O}$ |
| 90_48_28 | 21 | 1 | -207.3 | 44.6 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC(=O)O} + \text{OCC(=O)O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_48_101 | 21 | 1 | -207.3 | 40.4 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_102 | 21 | 1 | -207.3 | 40.4 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_103 | 20 | 1 | -207.3 | 45.5 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_104 | 21 | 1 | -207.3 | 40.4 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_105 | 21 | 1 | -207.3 | 40.4 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_106 | 20 | 2 | -207.3 | 45.5 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_107 | 21 | 2 | -207.3 | 40.4 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_108 | 21 | 2 | -207.3 | 40.4 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_109 | 19 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_110 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_111 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_112 | 19 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_113 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_114 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_115 | 19 | 2 | -202.8 | 46.1 | $11 \text{ H}_2 + 5 \text{ CO}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_48_116 | 20 | 2 | -207.3 | 41.1 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_117 | 20 | 2 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_118 | 19 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_119 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_120 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_121 | 19 | 1 | -202.8 | 46.1 | $5 \text{ CO}_2 + 11 \text{ H}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_122 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_123 | 20 | 1 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O} + \text{OCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_124 | 19 | 2 | -202.8 | 46.1 | $11 \text{ H}_2 + 5 \text{ CO}_2 + \text{CCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + 2 \text{ CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_125 | 20 | 2 | -207.3 | 41.1 | $12 \text{ H}_2 + 6 \text{ CO}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_48_126 | 20 | 2 | -207.3 | 41.1 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_49_1 | 3 | 0 | -23.4 | 36.4 | $2 \text{ H}_2 + \text{CO}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 90_65_1 | 10 | 0 | -105.9 | 38.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_2 | 10 | 0 | -105.9 | 38.9 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_3 | 10 | 0 | -105.9 | 37.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|----------|-------|-------|--------|-------|---|
| 90_65_4 | 10 | 0 | -105.9 | 37.2 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_5 | 10 | 0 | -105.9 | 36.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_6 | 10 | 0 | -105.9 | 36.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_7 | 10 | 0 | -105.9 | 35.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_8 | 10 | 0 | -105.9 | 35.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_9 | 10 | 0 | -105.9 | 33.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_10 | 10 | 0 | -105.9 | 33.7 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_11 | 10 | 0 | -105.9 | 33.0 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_65_12 | 10 | 0 | -105.9 | 33.0 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O} + \text{C}=\text{O}$ |
| 90_69_1 | 4 | 1 | -13.8 | 31.3 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}$ |
| 90_81_1 | 7 | 0 | -82.5 | 30.5 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_81_2 | 7 | 0 | -82.5 | 28.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_81_3 | 7 | 0 | -82.5 | 28.2 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_87_1 | 7 | 0 | -97.1 | 32.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_87_2 | 7 | 0 | -97.1 | 32.9 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_87_3 | 7 | 0 | -97.1 | 32.9 | $5 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_1 | 9 | 0 | -97.1 | 36.1 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_3 | 9 | 0 | -97.1 | 36.1 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_99_5 | 9 | 0 | -97.1 | 36.1 | $5 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_7 | 9 | 0 | -97.1 | 33.5 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_8 | 9 | 0 | -97.1 | 32.1 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_9 | 9 | 0 | -97.1 | 31.8 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_10 | 9 | 0 | -97.1 | 30.5 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_11 | 9 | 0 | -97.1 | 31.1 | $5 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_99_12 | 9 | 0 | -97.1 | 29.8 | $5 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_107_1 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_2 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_3 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_4 | 11 | 1 | -108.1 | 38.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_107_5 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_6 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_7 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_8 | 11 | 1 | -108.1 | 38.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_107_9 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_10 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |
| 90_107_11 | 12 | 1 | -111.8 | 38.7 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_107_12 | 11 | 1 | -108.1 | 38.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_115_1 | 13 | 0 | -107.2 | 38.9 | $4 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC}(\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{O}=\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 4 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_115_2 | 13 | 0 | -129.3 | 37.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_115_3 | 12 | 0 | -123.3 | 36.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_116_1 | 6 | 0 | -46.8 | 38.7 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + 2 \text{ C}=\text{O}$ |
| 90_119_1 | 7 | 0 | -82.5 | 45.4 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_119_2 | 7 | 0 | -82.5 | 45.4 | $4 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_119_3 | 7 | 0 | -82.5 | 45.1 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_119_4 | 7 | 0 | -82.5 | 43.9 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_119_5 | 7 | 0 | -82.5 | 39.5 | $4 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_119_6 | 7 | 0 | -82.5 | 45.7 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_130_1 | 13 | 0 | -143.9 | 38.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_130_2 | 12 | 0 | -143.9 | 38.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_130_3 | 11 | 0 | -137.9 | 38.8 | $3 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_130_4 | 13 | 0 | -133.0 | 38.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_130_5 | 12 | 0 | -133.0 | 38.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_130_6 | 11 | 0 | -127.1 | 38.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_134_1 | 12 | 1 | -100.9 | 46.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_2 | 12 | 1 | -100.9 | 45.1 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_3 | 12 | 1 | -100.9 | 44.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_4 | 12 | 1 | -90.1 | 46.8 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_134_5 | 12 | 1 | -90.1 | 45.1 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_134_6 | 12 | 1 | -90.1 | 44.4 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_134_7 | 12 | 1 | -100.9 | 46.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_8 | 12 | 1 | -100.9 | 45.1 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_9 | 12 | 1 | -100.9 | 44.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_10 | 12 | 1 | -100.9 | 46.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_11 | 12 | 1 | -100.9 | 45.1 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_12 | 12 | 1 | -100.9 | 44.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_13 | 12 | 1 | -100.9 | 46.8 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_14 | 12 | 1 | -100.9 | 45.1 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |
| 90_134_15 | 12 | 1 | -100.9 | 44.4 | $5 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_134_16 | 12 | 1 | -90.1 | 46.8 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_134_17 | 12 | 1 | -90.1 | 45.1 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_134_18 | 12 | 1 | -90.1 | 44.4 | $5 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O} + \text{OC}=\text{O}$ |
| 90_137_1 | 3 | 0 | -23.4 | 37.1 | $\text{CO}_2 + 2 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{C}=\text{O}$ |
| 90_145_1 | 10 | 0 | -110.9 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_2 | 10 | 0 | -110.9 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_3 | 10 | 0 | -110.9 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_4 | 10 | 1 | -110.9 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_5 | 10 | 1 | -110.9 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_6 | 10 | 1 | -110.9 | 40.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_7 | 10 | 1 | -110.9 | 37.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_8 | 10 | 1 | -110.9 | 36.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_9 | 10 | 1 | -110.9 | 35.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{C}=\text{C} + 4 \text{ H}_2\text{O}$ |
| 90_145_10 | 10 | 0 | -110.9 | 38.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_11 | 10 | 0 | -110.9 | 37.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_12 | 10 | 0 | -110.9 | 36.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_13 | 10 | 0 | -110.9 | 35.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_145_14 | 10 | 0 | -110.9 | 33.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_145_15 | 10 | 0 | -110.9 | 33.0 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_154_4 | 9 | 0 | -97.1 | 33.5 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_154_5 | 9 | 0 | -97.1 | 31.8 | $2 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_154_6 | 9 | 0 | -97.1 | 31.1 | $5 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_160_1 | 11 | 1 | -143.2 | 46.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_2 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_3 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_4 | 11 | 1 | -143.2 | 46.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_5 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_6 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_7 | 11 | 1 | -143.2 | 46.1 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_8 | 11 | 1 | -143.2 | 41.1 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_9 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_10 | 11 | 1 | -143.2 | 46.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_11 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_12 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_13 | 11 | 1 | -143.2 | 46.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_14 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_160_15 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_16 | 11 | 1 | -143.2 | 46.1 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_17 | 11 | 1 | -143.2 | 41.1 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_160_18 | 11 | 1 | -143.2 | 41.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{CCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O}$ |
| 90_166.1 | 4 | 1 | -13.8 | 37.0 | $2 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}$ |
| 90_166.3 | 4 | 1 | -13.8 | 45.7 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}$ |
| 90_173.1 | 8 | 0 | -72.6 | 46.6 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O}$ |
| 90_173.2 | 8 | 0 | -72.6 | 46.6 | $4 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O}$ |
| 90_173.3 | 8 | 0 | -72.6 | 46.6 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O}$ |
| 90_173.4 | 8 | 0 | -72.6 | 46.6 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O}$ |
| 90_173.5 | 8 | 0 | -72.6 | 46.6 | $4 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_173.6 | 8 | 0 | -72.6 | 48.5 | $3 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_175.1 | 9 | 0 | -77.5 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_175.2 | 9 | 0 | -82.5 | 50.8 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_175.4 | 9 | 0 | -77.5 | 50.8 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_175.5 | 9 | 0 | -82.5 | 50.8 | $4 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_175.7 | 9 | 0 | -77.5 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_175.8 | 9 | 0 | -82.5 | 50.8 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{CC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_175_10 | 9 | 0 | -77.5 | 50.8 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_175_13 | 9 | 0 | -77.5 | 50.8 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_175_14 | 9 | 0 | -82.5 | 50.8 | $4 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 2 \text{ H}_2\text{O}$ |
| 90_175_16 | 9 | 0 | -77.5 | 52.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_177_1 | 4 | 1 | -13.8 | 43.0 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}$ |
| 90_177_3 | 4 | 1 | -13.8 | 41.8 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{O}=\text{CC}(=\text{O})\text{O} + \text{O}$ |
| 90_182_2 | 5 | 0 | -46.8 | 37.1 | $2 \text{ CO}_2 + 4 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + 2 \text{ C}=\text{O}$ |
| 90_182_3 | 4 | 0 | -40.9 | 36.4 | $3 \text{ H}_2 + \text{CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + \text{H}_2\text{O} + 2 \text{ C}=\text{O}$ |
| 90_185_1 | 3 | 0 | -12.6 | 31.3 | $\text{CO}_2 + \text{H}_2 \rightarrow \text{OC}=\text{O}$ |
| 90_187_1 | 10 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_187_2 | 9 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_187_3 | 8 | 0 | -114.5 | 41.3 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_190_1 | 9 | 0 | -77.5 | 46.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_190_2 | 9 | 0 | -77.5 | 46.9 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_190_3 | 9 | 0 | -77.5 | 46.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_190_4 | 9 | 0 | -77.5 | 46.9 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_190.5 | 9 | 0 | -77.5 | 46.9 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_190.6 | 9 | 0 | -77.5 | 48.7 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CC}(=\text{O})\text{C}(=\text{O})\text{O}$ |
| 90_215.1 | 15 | 0 | -143.9 | 42.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_215.3 | 14 | 0 | -143.9 | 41.3 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_215.5 | 13 | 0 | -137.9 | 40.6 | $3 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + 2 \text{ C}=\text{O} + \text{CC}=\text{O}$ |
| 90_215.7 | 15 | 0 | -133.0 | 42.9 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_215.9 | 14 | 0 | -133.0 | 41.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_215.11 | 13 | 0 | -127.1 | 40.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 3 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{OC}=\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_218.1 | 10 | 0 | -95.0 | 45.4 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_218.2 | 10 | 0 | -95.0 | 45.4 | $5 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_218.3 | 10 | 0 | -95.0 | 45.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_218.4 | 10 | 0 | -95.0 | 43.9 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_218.5 | 10 | 0 | -95.0 | 39.5 | $5 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_218.6 | 10 | 0 | -95.0 | 45.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{OC}=\text{O} + \text{CC}(=\text{O})\text{O}$ |
| 90_228.4 | 12 | 0 | -120.5 | 38.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |
| 90_228.5 | 11 | 0 | -120.5 | 37.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_228_6 | 10 | 0 | -114.5 | 36.4 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_7 | 12 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_8 | 11 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_9 | 10 | 0 | -114.5 | 41.3 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_10 | 12 | 0 | -120.5 | 38.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_11 | 11 | 0 | -120.5 | 37.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_12 | 10 | 0 | -114.5 | 36.4 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_13 | 12 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_14 | 11 | 0 | -120.5 | 41.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_15 | 10 | 0 | -114.5 | 41.3 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_16 | 12 | 0 | -120.5 | 38.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_17 | 11 | 0 | -120.5 | 37.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |
| 90_228_18 | 10 | 0 | -114.5 | 36.4 | $6 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{OCC(=O)O} + 3 \text{ H}_2\text{O} + \text{CC=O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_233_13 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_14 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_15 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_16 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_17 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_18 | 11 | 0 | -143.2 | 48.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_19 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_20 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_21 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_22 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_23 | 11 | 0 | -143.2 | 40.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_24 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_25 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_26 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_27 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_28 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_29 | 11 | 0 | -143.2 | 40.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_233_30 | 11 | 0 | -143.2 | 40.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_233_31 | 11 | 0 | -143.2 | 41.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_32 | 11 | 0 | -143.2 | 41.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_33 | 11 | 0 | -143.2 | 41.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_34 | 11 | 0 | -143.2 | 41.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_35 | 11 | 0 | -143.2 | 41.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_36 | 11 | 0 | -143.2 | 41.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_37 | 11 | 0 | -143.2 | 38.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_38 | 11 | 0 | -143.2 | 38.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_39 | 11 | 0 | -143.2 | 38.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_40 | 11 | 0 | -143.2 | 38.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_41 | 11 | 0 | -143.2 | 38.2 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_233_42 | 11 | 0 | -143.2 | 38.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_237_1 | 10 | 0 | -110.9 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_237_2 | 10 | 0 | -110.9 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_237_3 | 10 | 0 | -110.9 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_237_4 | 10 | 0 | -110.9 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_237_5 | 10 | 0 | -110.9 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |
| 90_237_6 | 10 | 0 | -110.9 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{C}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_237.7 | 10 | 1 | -110.9 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_237.8 | 10 | 1 | -110.9 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_237.9 | 10 | 1 | -110.9 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_237.10 | 10 | 1 | -110.9 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_237.11 | 10 | 1 | -110.9 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_237.12 | 10 | 1 | -110.9 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC(=O)C=C} + 4 \text{ H}_2\text{O}$ |
| 90_241.7 | 9 | 0 | -77.5 | 46.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_241.8 | 9 | 0 | -77.5 | 46.6 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_241.9 | 9 | 0 | -77.5 | 46.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_241.10 | 9 | 0 | -77.5 | 46.6 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_241.11 | 9 | 0 | -77.5 | 46.6 | $5 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_241.12 | 9 | 0 | -77.5 | 48.5 | $4 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC(=O)CC(=O)C(=O)O}$ |
| 90_243.1 | 4 | 1 | -13.8 | 43.6 | $2 \text{ CO}_2 + 2 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + \text{O}$ |
| 90_243.3 | 4 | 1 | -13.8 | 42.9 | $2 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{O=CC(=O)O} + \text{O}$ |
| 90_255.1 | 12 | 1 | -135.3 | 47.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.2 | 12 | 1 | -135.3 | 47.4 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.3 | 12 | 1 | -135.3 | 47.4 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.4 | 12 | 1 | -135.3 | 47.4 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_255.5 | 12 | 1 | -135.3 | 47.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.6 | 12 | 1 | -135.3 | 47.1 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.7 | 12 | 1 | -135.3 | 45.8 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.8 | 12 | 1 | -135.3 | 45.8 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.9 | 12 | 1 | -135.3 | 43.7 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.10 | 12 | 1 | -135.3 | 41.5 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.11 | 12 | 1 | -135.3 | 45.8 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_255.12 | 12 | 1 | -135.3 | 45.8 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow \text{OC(=O)CCC(=O)O} + 4 \text{ H}_2\text{O}$ |
| 90_258.1 | 11 | 0 | -143.2 | 45.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.2 | 11 | 0 | -143.2 | 45.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.3 | 11 | 0 | -143.2 | 45.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.4 | 11 | 0 | -143.2 | 45.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.5 | 11 | 0 | -143.2 | 45.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.6 | 11 | 0 | -143.2 | 45.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.7 | 11 | 0 | -143.2 | 45.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.8 | 11 | 0 | -143.2 | 45.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.9 | 11 | 0 | -143.2 | 45.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258.10 | 11 | 0 | -143.2 | 45.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_258_11 | 11 | 0 | -143.2 | 45.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_258_12 | 11 | 0 | -143.2 | 45.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_269_1 | 16 | 2 | -134.3 | 41.3 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC=O} + \text{O=CC(=O)O} + 5 \text{ H}_2\text{O} + \text{C=O}$ |
| 90_269_2 | 15 | 1 | -119.7 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC(=O)O}$ |
| 90_269_3 | 15 | 2 | -134.3 | 41.3 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC=O} + \text{O=CC(=O)O} + 5 \text{ H}_2\text{O} + \text{C=O}$ |
| 90_269_4 | 14 | 1 | -92.0 | 43.9 | $5 \text{ CO}_2 + 7 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{O=CC(=O)O} + \text{O=CC(=O)C(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC(=O)O}$ |
| 90_269_5 | 14 | 2 | -128.3 | 41.3 | $4 \text{ CO}_2 + 8 \text{ H}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow \text{CC=O} + \text{O=CC(=O)O} + \text{OCC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O}$ |
| 90_269_6 | 15 | 1 | -119.7 | 43.9 | $5 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{O=CC(=O)O} + 4 \text{ H}_2\text{O} + \text{C=O} + \text{CC(=O)O}$ |
| 90_312_19 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_20 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_21 | 11 | 0 | -143.2 | 40.3 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_22 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_23 | 11 | 0 | -143.2 | 36.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_24 | 11 | 0 | -143.2 | 35.4 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_25 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_312_26 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_312_27 | 11 | 0 | -143.2 | 40.3 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_28 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_29 | 11 | 0 | -143.2 | 36.1 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_30 | 11 | 0 | -143.2 | 35.4 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_31 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_32 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_33 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_34 | 11 | 0 | -143.2 | 40.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_35 | 11 | 0 | -143.2 | 40.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_36 | 11 | 0 | -143.2 | 40.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_37 | 11 | 0 | -143.2 | 37.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_38 | 11 | 0 | -143.2 | 36.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_39 | 11 | 0 | -143.2 | 35.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_40 | 11 | 0 | -143.2 | 38.9 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_41 | 11 | 0 | -143.2 | 37.2 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_42 | 11 | 0 | -143.2 | 36.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_43 | 11 | 0 | -143.2 | 35.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_312_44 | 11 | 0 | -143.2 | 33.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_312_45 | 11 | 0 | -143.2 | 33.0 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC(=O)O}$ |
| 90_318_1 | 13 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_2 | 12 | 0 | -190.3 | 32.9 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_3 | 14 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_4 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_5 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_6 | 13 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_7 | 12 | 0 | -190.3 | 32.9 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_8 | 14 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_9 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_10 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_11 | 13 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_12 | 12 | 0 | -190.3 | 32.9 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_318_13 | 14 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_318_14 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_318_15 | 14 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_2 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_3 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_4 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_5 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_6 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_8 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_9 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_10 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_11 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_12 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_14 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_15 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_16 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_17 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_320_18 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_20 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_21 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_22 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_23 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_24 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_26 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_27 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_28 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_29 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_30 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_32 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_33 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_34 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_35 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_36 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_38 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_39 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| | | | | | $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_40 | 16 | 1 | -179.5 | 37.0 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_41 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_42 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_44 | 15 | 0 | -194.1 | 35.6 | $4 \text{CO}_2 + 10 \text{H}_2 \rightarrow 6 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_45 | 14 | 0 | -190.3 | 35.6 | $3 \text{CO}_2 + 9 \text{H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_46 | 16 | 1 | -179.5 | 37.0 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_47 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_48 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_50 | 15 | 0 | -194.1 | 35.6 | $4 \text{CO}_2 + 10 \text{H}_2 \rightarrow 6 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_51 | 14 | 0 | -190.3 | 35.6 | $3 \text{CO}_2 + 9 \text{H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_52 | 16 | 1 | -179.5 | 37.0 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_53 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_54 | 16 | 1 | -179.5 | 41.7 | $4 \text{CO}_2 + 9 \text{H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_56 | 16 | 0 | -194.1 | 34.6 | $4 \text{CO}_2 + 10 \text{H}_2 \rightarrow 6 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |
| 90_320_57 | 16 | 0 | -194.1 | 34.6 | $4 \text{CO}_2 + 10 \text{H}_2 \rightarrow 6 \text{H}_2\text{O} + 2 \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_320_58 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_59 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_60 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_62 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_63 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_64 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_65 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_66 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_68 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_69 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_70 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_71 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_72 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_74 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_75 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_76 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_77 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_78 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_320_80 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_81 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_82 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_83 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_84 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_86 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_87 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_88 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_89 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_90 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_92 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_93 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_94 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_95 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_96 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_98 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_99 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_100 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90.320.101 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.102 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.104 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.105 | 16 | 0 | -194.1 | 34.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.106 | 16 | 1 | -179.5 | 35.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.107 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.108 | 16 | 1 | -179.5 | 40.6 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.110 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.111 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.112 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.113 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.114 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.116 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.117 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.320.118 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.320.119 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_320_120 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_122 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_123 | 14 | 0 | -190.3 | 35.6 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_124 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_125 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_126 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_128 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_129 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_130 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_131 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_132 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_134 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_135 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_136 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_137 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_138 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_140 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_320_141 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_142 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_143 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_144 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_146 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_147 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_148 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_149 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_150 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_152 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_153 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_154 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_155 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_156 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_158 | 16 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_159 | 15 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_160 | 16 | 1 | -179.5 | 37.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_161 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_320_162 | 16 | 1 | -179.5 | 41.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_164 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_165 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_166 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_167 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_168 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_170 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_171 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_172 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_173 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_174 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_176 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_177 | 16 | 0 | -194.1 | 35.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_178 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_179 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_180 | 16 | 1 | -179.5 | 41.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_182 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_183 | 15 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_320_184 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_185 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_186 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_188 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_189 | 15 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_190 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_191 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_192 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_194 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_195 | 15 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_196 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_197 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_198 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_200 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_201 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_320_202 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_203 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_320_204 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_320_206 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_207 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_208 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_209 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_210 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_212 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_213 | 16 | 0 | -194.1 | 36.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_320_214 | 16 | 1 | -179.5 | 37.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_215 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_320_216 | 16 | 1 | -179.5 | 42.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_327_1 | 5 | 0 | -40.7 | 45.4 | $2 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 90_327_2 | 5 | 1 | -40.7 | 45.4 | $3 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{OCC}(=\text{O})\text{O} + \text{O}$ |
| 90_327_3 | 5 | 0 | -40.7 | 45.1 | $2 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 90_327_4 | 5 | 0 | -40.7 | 43.9 | $2 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 90_327_5 | 5 | 1 | -40.7 | 39.5 | $3 \text{ H}_2 + 2 \text{ CO}_2 \rightarrow \text{OCC}(=\text{O})\text{O} + \text{O}$ |
| 90_327_6 | 5 | 0 | -40.7 | 45.7 | $2 \text{ CO}_2 + 3 \text{ H}_2 \rightarrow \text{H}_2\text{O} + \text{OCC}(=\text{O})\text{O}$ |
| 90_338_1 | 10 | 1 | -101.4 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_338_2 | 10 | 1 | -101.4 | 50.8 | $6 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{CC}(\text{C}(=\text{O})\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_338_3 | 10 | 1 | -101.4 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 90_338_4 | 10 | 1 | -101.4 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 90_338_5 | 10 | 1 | -101.4 | 50.8 | $6 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 90_338_6 | 10 | 1 | -101.4 | 52.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC(=O)CC(C(=O)O)O} + 3 \text{ H}_2\text{O}$ |
| 90_355_1 | 14 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_6 | 14 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_11 | 14 | 0 | -194.1 | 32.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_16 | 16 | 0 | -194.1 | 30.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_17 | 16 | 0 | -194.1 | 30.2 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_18 | 16 | 1 | -179.5 | 34.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_19 | 16 | 1 | -179.5 | 39.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_20 | 16 | 1 | -179.5 | 39.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_21 | 16 | 0 | -194.1 | 28.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_22 | 16 | 0 | -194.1 | 28.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_355_23 | 16 | 1 | -179.5 | 32.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_24 | 16 | 1 | -179.5 | 37.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_25 | 16 | 1 | -179.5 | 37.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_355_26 | 16 | 0 | -194.1 | 27.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_355_27 | 16 | 0 | -194.1 | 27.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_355_28 | 16 | 1 | -179.5 | 32.1 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_355_29 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_355_30 | 16 | 1 | -179.5 | 36.8 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_358_2 | 14 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_358_8 | 14 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_358_14 | 14 | 0 | -194.1 | 35.6 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_370_1 | 14 | 0 | -155.0 | 34.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_2 | 14 | 0 | -155.0 | 34.5 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_3 | 14 | 1 | -140.5 | 34.5 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_4 | 14 | 1 | -140.5 | 39.1 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_5 | 14 | 1 | -140.5 | 39.1 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_7 | 14 | 0 | -155.0 | 32.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_8 | 14 | 0 | -155.0 | 32.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_9 | 14 | 1 | -140.5 | 32.9 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_10 | 14 | 1 | -140.5 | 37.5 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_11 | 14 | 1 | -140.5 | 37.5 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_12 | 12 | 0 | -120.5 | 37.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_370_13 | 14 | 0 | -155.0 | 32.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_14 | 14 | 0 | -155.0 | 32.2 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow 5 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{OCC}=\text{O}$ |
| 90_370_15 | 14 | 1 | -140.5 | 32.2 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_16 | 14 | 1 | -140.5 | 36.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_370_17 | 14 | 1 | -140.5 | 36.8 | $4 \text{ CO}_2 + 8 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 4 \text{ H}_2\text{O} + \text{OCC}=\text{O}$ |
| 90_373_1 | 11 | 0 | -103.9 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_373_2 | 11 | 0 | -103.9 | 50.8 | $6 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_373_3 | 11 | 0 | -103.9 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_373_4 | 11 | 0 | -103.9 | 50.8 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_373_5 | 11 | 0 | -103.9 | 50.8 | $6 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_373_6 | 11 | 0 | -103.9 | 52.6 | $4 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}=\text{CC}(=\text{O})\text{O}$ |
| 90_387_2 | 18 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_3 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_4 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_6 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_8 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_10 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90.387.12 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.13 | 16 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.14 | 17 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.15 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.16 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.18 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.20 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.22 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.24 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.26 | 16 | 0 | -175.7 | 48.0 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.27 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.28 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.30 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC}(\text{C}(=\text{O})\text{C}(=\text{O})\text{O})\text{O} \rightarrow$ $\rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 5 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.32 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.34 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_387_36 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_38 | 18 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_40 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_42 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_44 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_46 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_48 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_49 | 16 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_50 | 17 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_52 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_54 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_56 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_58 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_60 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_62 | 16 | 0 | -175.7 | 46.9 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_64 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_66 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90.387.68 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.70 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.72 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.74 | 18 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.75 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.76 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.78 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.80 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.82 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.84 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.85 | 16 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.86 | 17 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.87 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.88 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.90 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.92 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_94 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_96 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_98 | 16 | 0 | -175.7 | 48.0 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_99 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_100 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_102 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_104 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_106 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_108 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_110 | 18 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_112 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_114 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_116 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_118 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_120 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_121 | 16 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90.387.122 | 17 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.124 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.126 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.128 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.130 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.132 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.134 | 16 | 0 | -175.7 | 46.9 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.136 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.138 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.140 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.142 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.144 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90.387.146 | 18 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90.387.148 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.149 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.150 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90.387.152 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_154 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_156 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_157 | 16 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_158 | 17 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_160 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_161 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_162 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_164 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_166 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_168 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_170 | 16 | 0 | -175.7 | 48.0 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_172 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_173 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_174 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_176 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_178 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_180 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_182 | 18 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_184 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_186 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_188 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_190 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_192 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_193 | 16 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_194 | 17 | 0 | -181.7 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_196 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_198 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_200 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_202 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_204 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_206 | 16 | 0 | -175.7 | 46.9 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_208 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_210 | 18 | 0 | -194.1 | 46.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_212 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90.387.214 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.216 | 18 | 1 | -179.5 | 46.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.218 | 18 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.219 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.220 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.222 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.224 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.226 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.228 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.229 | 16 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.230 | 17 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.231 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.232 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.234 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.236 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.238 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90.387.240 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.242 | 16 | 0 | -175.7 | 48.0 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.243 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.244 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.246 | 16 | 0 | -190.3 | 48.0 | $3 \text{ CO}_2 + 9 \text{ H}_2 + \text{CC(C(=O)C(=O)O)O} \rightarrow$ $\rightarrow \text{OC(=O)C(O)C} + 5 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.248 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.250 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.252 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.254 | 18 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.256 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.258 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90.387.260 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.262 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.264 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90.387.265 | 16 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90.387.266 | 17 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_268 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_270 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_272 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_274 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_276 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_278 | 16 | 0 | -175.7 | 47.7 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_280 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_282 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_284 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_286 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_288 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_290 | 18 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_292 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_293 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_294 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_296 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_298 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_300 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_301 | 16 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_302 | 17 | 0 | -181.7 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_304 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_305 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_306 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_308 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_310 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_312 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_314 | 16 | 0 | -175.7 | 48.0 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_316 | 18 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_317 | 16 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_318 | 17 | 0 | -194.1 | 48.0 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_320 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_322 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_324 | 18 | 1 | -179.5 | 48.0 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_326 | 18 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_328 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_330 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_332 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_334 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_336 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_337 | 16 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_338 | 17 | 0 | -181.7 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_340 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_342 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_344 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_346 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_348 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_350 | 16 | 0 | -175.7 | 47.7 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_352 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_354 | 18 | 0 | -194.1 | 47.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_356 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_358 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_360 | 18 | 1 | -179.5 | 47.7 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_362 | 18 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_364 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_365 | 16 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_366 | 17 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_368 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_370 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_372 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_373 | 16 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_374 | 17 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_376 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_377 | 16 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_378 | 17 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_380 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_382 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_384 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_386 | 16 | 0 | -175.7 | 48.4 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_388 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_389 | 16 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_390 | 17 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_392 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_394 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_396 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_398 | 18 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_400 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_402 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_404 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_406 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_408 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_409 | 16 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_410 | 17 | 0 | -181.7 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_387_412 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_414 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_387_416 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_387_418 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|--|
| 90_387_420 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_422 | 16 | 0 | -175.7 | 48.4 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC(=O)C(=O)O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC(=O)O} + \text{CCC=O} + \text{C=O}$ |
| 90_387_424 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_426 | 18 | 0 | -194.1 | 48.4 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_387_428 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_430 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_387_432 | 18 | 1 | -179.5 | 48.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC(=O)O} + 5 \text{ H}_2\text{O} + \text{CC=O}$ |
| 90_400_1 | 19 | 2 | -208.9 | 40.6 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow \text{CC=O} + \text{CC(C(=O)C(=O)O)O} + 7 \text{ H}_2\text{O}$ |
| 90_400_2 | 18 | 2 | -205.1 | 40.6 | $5 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC=O} + \text{OC(=O)C(O)C} + 6 \text{ H}_2\text{O}$ |
| 90_400_3 | 20 | 3 | -193.3 | 40.6 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |
| 90_400_4 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |
| 90_400_5 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |
| 90_400_6 | 19 | 2 | -208.9 | 40.6 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow \text{CC=O} + \text{CC(C(=O)C(=O)O)O} + 7 \text{ H}_2\text{O}$ |
| 90_400_7 | 18 | 2 | -205.1 | 40.6 | $5 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC=O} + \text{OC(=O)C(O)C} + 6 \text{ H}_2\text{O}$ |
| 90_400_8 | 20 | 3 | -193.3 | 40.6 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |
| 90_400_9 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |
| 90_400_10 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC(=O)O} + \text{CC=O} + \text{O=CC(=O)O} + 6 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_400_11 | 19 | 2 | -208.9 | 40.6 | $6 \text{ CO}_2 + 12 \text{ H}_2 \rightarrow \text{CC}=\text{O} + \text{CC}(\text{C}(\text{=O})\text{C}(\text{=O})\text{O})\text{O} + 7 \text{ H}_2\text{O}$ |
| 90_400_12 | 18 | 2 | -205.1 | 40.6 | $5 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC}=\text{O} + \text{OC}(\text{=O})\text{C}(\text{O})\text{C} + 6 \text{ H}_2\text{O}$ |
| 90_400_13 | 20 | 3 | -193.3 | 40.6 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + 6 \text{ H}_2\text{O}$ |
| 90_400_14 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + 6 \text{ H}_2\text{O}$ |
| 90_400_15 | 20 | 3 | -193.3 | 43.7 | $6 \text{ CO}_2 + 11 \text{ H}_2 \rightarrow \text{CC}(\text{=O})\text{O} + \text{CC}=\text{O} + \text{O}=\text{CC}(\text{=O})\text{O} + 6 \text{ H}_2\text{O}$ |
| 90_402_1 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_2 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_3 | 11 | 0 | -143.2 | 40.3 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_4 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_5 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_6 | 11 | 0 | -143.2 | 37.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_7 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_8 | 11 | 0 | -143.2 | 40.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_9 | 11 | 0 | -143.2 | 40.3 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_10 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_11 | 11 | 0 | -143.2 | 37.7 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_12 | 11 | 0 | -143.2 | 37.7 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |
| 90_402_13 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(\text{=O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_402_14 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_15 | 11 | 0 | -143.2 | 48.6 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_16 | 11 | 0 | -143.2 | 40.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_17 | 11 | 0 | -143.2 | 40.5 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_18 | 11 | 0 | -143.2 | 40.5 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_19 | 11 | 0 | -143.2 | 37.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_20 | 11 | 0 | -143.2 | 37.8 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_21 | 11 | 0 | -143.2 | 37.8 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_22 | 11 | 0 | -143.2 | 38.9 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_23 | 11 | 0 | -143.2 | 38.9 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_24 | 11 | 0 | -143.2 | 38.9 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_25 | 11 | 0 | -143.2 | 35.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_26 | 11 | 0 | -143.2 | 35.3 | $3 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_402_27 | 11 | 0 | -143.2 | 35.3 | $7 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{CCC}(=\text{O})\text{O}$ |
| 90_407_1 | 7 | 0 | -51.4 | 45.4 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 90_407_2 | 6 | 0 | -45.4 | 45.4 | $4 \text{ H}_2 + 2 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow \text{OCC}(=\text{O})\text{O} + \text{H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 90_407_3 | 8 | 0 | -51.4 | 45.1 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_407.4 | 8 | 0 | -51.4 | 43.9 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 90_407.5 | 7 | 0 | -51.4 | 39.5 | $5 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 90_407.6 | 8 | 0 | -51.4 | 45.7 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{C}=\text{O} + \text{O}=\text{CC}(\text{O})\text{O}$ |
| 90_412.1 | 17 | 0 | -187.3 | 47.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.2 | 17 | 0 | -187.3 | 47.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.3 | 16 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.4 | 16 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.5 | 17 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.6 | 17 | 0 | -187.3 | 47.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.7 | 17 | 0 | -187.3 | 47.4 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.8 | 16 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.9 | 16 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.10 | 17 | 1 | -172.7 | 47.4 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.11 | 17 | 0 | -187.3 | 47.1 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.12 | 17 | 0 | -187.3 | 47.1 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.13 | 16 | 1 | -172.7 | 47.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.14 | 16 | 1 | -172.7 | 47.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412.15 | 17 | 1 | -172.7 | 47.1 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_412_16 | 17 | 0 | -187.3 | 45.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_17 | 17 | 0 | -187.3 | 45.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_18 | 16 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_19 | 16 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_20 | 17 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_21 | 17 | 0 | -187.3 | 41.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_22 | 17 | 0 | -187.3 | 41.5 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_23 | 16 | 1 | -172.7 | 41.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_24 | 16 | 1 | -172.7 | 41.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_25 | 17 | 1 | -172.7 | 41.5 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_26 | 17 | 0 | -187.3 | 45.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_27 | 17 | 0 | -187.3 | 45.8 | $5 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CC}=\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_28 | 16 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_29 | 16 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_412_30 | 17 | 1 | -172.7 | 45.8 | $5 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{O}=\text{CCC}(=\text{O})\text{O}$ |
| 90_425_1 | 11 | 1 | -108.1 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_2 | 11 | 1 | -108.1 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_3 | 11 | 1 | -108.1 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_425_4 | 11 | 0 | -108.1 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_5 | 11 | 0 | -108.1 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_6 | 11 | 0 | -108.1 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_7 | 11 | 1 | -108.1 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_8 | 11 | 1 | -108.1 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_9 | 11 | 1 | -108.1 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_10 | 11 | 0 | -108.1 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_11 | 11 | 0 | -108.1 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_12 | 11 | 0 | -108.1 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_13 | 11 | 1 | -108.1 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_14 | 11 | 1 | -108.1 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_15 | 11 | 1 | -108.1 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_16 | 11 | 1 | -108.1 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_17 | 11 | 1 | -108.1 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_18 | 11 | 1 | -108.1 | 40.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OC}(=\text{O})\text{C}(\text{O})\text{C} + 3 \text{ H}_2\text{O}$ |
| 90_425_19 | 11 | 0 | -108.1 | 37.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_20 | 11 | 0 | -108.1 | 36.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_21 | 11 | 0 | -108.1 | 35.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|---|
| 90_425_22 | 11 | 0 | -108.1 | 38.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_23 | 11 | 0 | -108.1 | 37.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_24 | 11 | 0 | -108.1 | 36.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_25 | 11 | 0 | -108.1 | 35.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_26 | 11 | 0 | -108.1 | 33.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_425_27 | 11 | 0 | -108.1 | 33.0 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{C}(\text{O})\text{C}$ |
| 90_428_1 | 11 | 0 | -107.5 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_2 | 11 | 0 | -107.5 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_3 | 11 | 0 | -107.5 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_4 | 11 | 1 | -107.5 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_428_5 | 11 | 1 | -107.5 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_428_6 | 11 | 1 | -107.5 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_428_7 | 11 | 0 | -107.5 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_8 | 11 | 0 | -107.5 | 40.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_9 | 11 | 0 | -107.5 | 40.3 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC}(=\text{O})\text{O}$ |
| 90_428_10 | 11 | 1 | -107.5 | 37.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_428_11 | 11 | 1 | -107.5 | 36.1 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |
| 90_428_12 | 11 | 1 | -107.5 | 35.4 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OCCC}(=\text{O})\text{O} + 3 \text{ H}_2\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_428_13 | 11 | 0 | -107.5 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_14 | 11 | 0 | -107.5 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_15 | 11 | 0 | -107.5 | 48.6 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_16 | 11 | 0 | -107.5 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_17 | 11 | 0 | -107.5 | 40.5 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_18 | 11 | 0 | -107.5 | 40.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_19 | 11 | 1 | -107.5 | 37.8 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_20 | 11 | 1 | -107.5 | 36.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_21 | 11 | 1 | -107.5 | 35.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_22 | 11 | 1 | -107.5 | 38.9 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_23 | 11 | 1 | -107.5 | 37.2 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_24 | 11 | 1 | -107.5 | 36.5 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow \text{OCCC(=O)O} + 3 \text{ H}_2\text{O}$ |
| 90_428_25 | 11 | 0 | -107.5 | 35.3 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_26 | 11 | 0 | -107.5 | 33.7 | $3 \text{ CO}_2 + 6 \text{ H}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_428_27 | 11 | 0 | -107.5 | 33.0 | $6 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 3 \text{ H}_2\text{O} + \text{OCCC(=O)O}$ |
| 90_447_218 | 15 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |
| 90_447_223 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC=O} + \text{C=O}$ |
| 90_447_224 | 15 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC=O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_447_230 | 15 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_236 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_241 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_242 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_248 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_259 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_272 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_277 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_278 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_284 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_295 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_309 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_313 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_315 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_321 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_331 | 16 | 0 | -181.7 | 40.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_344 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_349 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|------------|-------|-------|--------|-------|---|
| 90_447_350 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_356 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_367 | 16 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_381 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_385 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_387 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_393 | 16 | 0 | -194.1 | 38.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_403 | 16 | 0 | -181.7 | 41.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_417 | 16 | 0 | -194.1 | 39.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_421 | 16 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_447_423 | 16 | 0 | -194.1 | 39.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_429 | 16 | 0 | -194.1 | 39.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_447_439 | 16 | 0 | -181.7 | 41.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_458_1 | 8 | 0 | -51.4 | 45.4 | $3 \text{ CO}_2 + 5 \text{ H}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{ C}=\text{O} + \text{ O}=\text{CC}(\text{O})\text{O}$ |
| 90_458_5 | 8 | 0 | -51.4 | 39.5 | $5 \text{ H}_2 + 3 \text{ CO}_2 \rightarrow 2 \text{ H}_2\text{O} + \text{ C}=\text{O} + \text{ O}=\text{CC}(\text{O})\text{O}$ |
| 90_471_2 | 16 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_471_4 | 18 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |
| 90_471_5 | 17 | 0 | -181.7 | 41.3 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{ CCC}=\text{O} + \text{ C}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_471.6 | 16 | 0 | -175.7 | 41.3 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_471.7 | 18 | 0 | -181.7 | 38.7 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_471.8 | 17 | 0 | -181.7 | 37.1 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_471.9 | 16 | 0 | -175.7 | 36.4 | $9 \text{ H}_2 + 3 \text{ CO}_2 + \text{OCC}(=\text{O})\text{C}(=\text{O})\text{O} \rightarrow$ $\rightarrow 5 \text{ H}_2\text{O} + \text{OCC}(=\text{O})\text{O} + \text{CCC}=\text{O} + \text{C}=\text{O}$ |
| 90_486.1 | 12 | 0 | -135.3 | 53.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_486.2 | 12 | 0 | -135.3 | 53.3 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_486.3 | 12 | 0 | -135.3 | 53.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_486.4 | 12 | 0 | -135.3 | 53.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_486.5 | 12 | 0 | -135.3 | 53.3 | $7 \text{ H}_2 + 4 \text{ CO}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_486.6 | 12 | 0 | -135.3 | 53.3 | $4 \text{ CO}_2 + 7 \text{ H}_2 \rightarrow 4 \text{ H}_2\text{O} + \text{OC}(=\text{O})\text{CCC}(=\text{O})\text{O}$ |
| 90_496.2 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_496.4 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_496.6 | 16 | 1 | -179.5 | 34.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496.8 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496.10 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496.12 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |

| Label | n_M | n_B | E_C | E_H | Net reaction |
|-----------|-------|-------|--------|-------|--|
| 90_496_14 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_496_16 | 16 | 1 | -179.5 | 34.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496_18 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496_20 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496_22 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_496_24 | 16 | 0 | -194.1 | 34.9 | $4 \text{ CO}_2 + 10 \text{ H}_2 \rightarrow 6 \text{ H}_2\text{O} + 2 \text{ CC}=\text{O}$ |
| 90_496_26 | 16 | 1 | -179.5 | 34.9 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496_28 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |
| 90_496_30 | 16 | 1 | -179.5 | 39.4 | $4 \text{ CO}_2 + 9 \text{ H}_2 \rightarrow \text{CC}(=\text{O})\text{O} + 5 \text{ H}_2\text{O} + \text{CC}=\text{O}$ |