Distilling System Complexity to Enable Unbiased and Predictive Computational Reaction Investigations - Supporting Information

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1 Additional Analyses

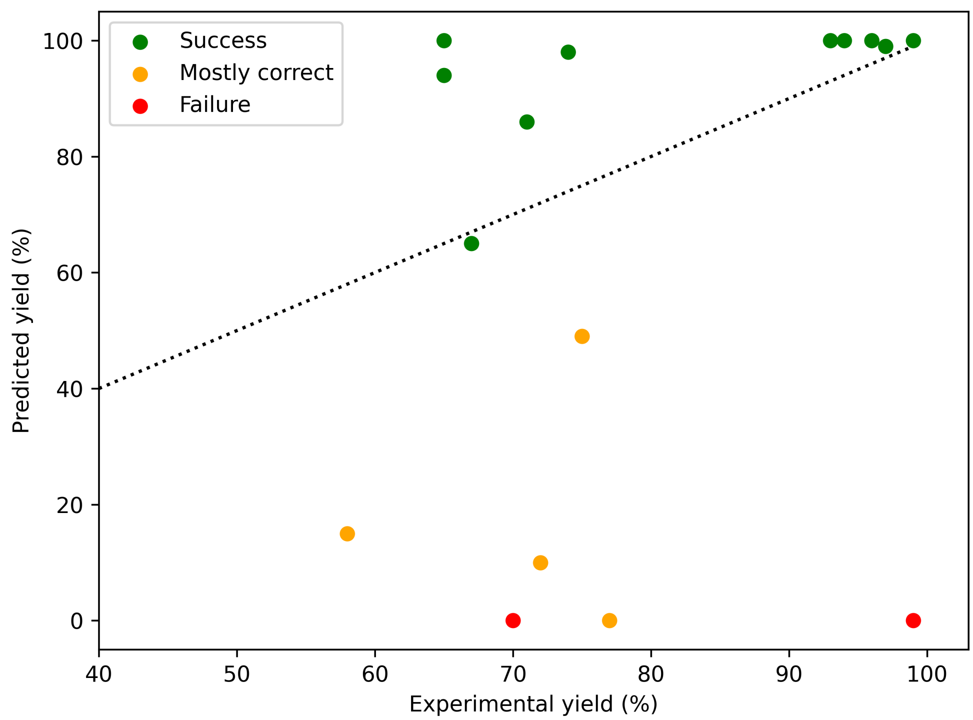

Figure S1: Predicted *versus* experimental yields of major products.[a]

[a]A6 is excluded from this analysis due to the influence of the methodology on the results.

Figure S1 shows the correlation between the predicted and the experimental yields of major reaction products. Naturally, failures are associated with a predicted yield of 0%. Reaction explorations identified as "mostly correct" resulted generally in underestimated predicted yields, while the reaction networks contain most or all significant pathways. In the case of reaction C1, the yield of the major product is null, but the major product identified with methodology B differs only by the alkene's position. In the case of correct predictions, the predicted yields are generally higher than the experimental yields due to the absence of miscellaneous losses during isolation and purification. The experimental mass balance is very rarely perfect, which slightly complicates the quantitative comparison between experimental and predicted yields. Nevertheless, all reactions have yields high enough to unambiguously validate the predictions.

Table S1: Confusion matrix between predicted and experimental product significance.[a]
[a]A6 is excluded from this analysis due to the influence of the methodology on the results. Methodology A is assumed for C1.

		Experimental outcome		
		Major	Minor	Unidentified
	Major	10	0	5
Predicted	Minor	3	2	4
outcome	Trace ($< 5\%$)	0	0	3
	Unidentified	3	1	–

Table S1 displays the confusion matrix between predicted and experimental product significances. It is worth noting that incorrect major product predictions add two off-diagonal entries, one for the missing correct product and one for the incorrect predicted product.

10 major products and 2 minor products were correctly identified, while 3 major products were predicted to be minor products. 3 major products and 1 minor product were not discovered by the computational reaction explorations (false negatives), and 5 incorrect major products were predicted (false positives). It is also interesting to note that the reaction explorations yielded 4 unidentified minor products and 3 unidentified trace products. While these predictions might be incorrect, it is also possible that some of those products were formed but simply not isolated experimentally, as discussed in the manuscript.

2 Additional Methodological Details

2.1 Reaction Modeling

While GFN2-xTB produced geometries sufficiently correct in almost all cases, we did notice one particular shortcoming in cyclopropanation reactions involving an alkyne and an alkene. Namely, the GFN2-xTB potential energy surface (PES) contains two saddle points leading to the cyclopropane, while the DFT PES contains only one (except with very polarized alkenes). We found that both saddle points could have sufficiently different Gibbs free energies in order to change the outcome of the reaction if only one is considered. Since this kind of reaction is common in gold(I) chemistry, this shortcoming could not be ignored.

After considering several possibilities, we decided to explicitly detect cyclopropanation reactions and search for the complementary transition state. This approach is admittedly not elegant, but does yield cyclopropanation barriers much closer to computed reference values in problematic cases. The transition states of those reaction possibilities are followed by "_alt" in our reaction networks.

This shortcoming likely stems from the small size of the basis set used in the GFN2-xTB method. The true transition state is too high in energy due to the long forming C-C distances, and thus poor overlap of the tight basis functions. Using another accurate semi-empirical method with somewhat larger basis sets should improve accuracy at the cost of longer computing time. Such a method that can also be applied to transition metals also might not currently exist, although pTB[1], which uses a polarized double-ζ basis set, is arguably the most likely candidate once it is more mature.

2.1.1 Determination of pruning energetic thresholds

As explained earlier, each reaction possibility goes through several steps before it yields the final (reagent, transition state, product) group. When preliminary energetic values are obtained during this process, they can be used to prematurely end reaction possibilities which no longer seem reasonable (*i.e.*, with a barrier below the exploration threshold).

To determine the ideal thresholds, we have used our preliminary exploration data as representative sample of reaction possibilities at different stages. For each of those stages, we compare the (Gibbs) energy of the (approximate) transition state to the same quantity in the scan parent.

The relevant structures we obtain are the following:

- Stage 1: The relaxed scan maximal point (E, GFN2-xTB)
- Stage 2: The Growing String approximate transition state (E, GFN2-xTB)
- Stage 3: The optimized transition state (G, GFN2-xTB)
- Stage 4: The optimized transition state (G, DFT//GFN2-xTB)
- Stage 5: The optimized transition state with the complete ligand (G, GFN2-xTB)
- Stage 6: The optimized transition state with the complete ligand (G, DFT//GFN2-xTB)

The first two barriers show poor correlation with the final barrier (derived from stage 6), as could be expected. They are typically significantly greater than the final barrier, which warrants a certain tolerance.

Using our preliminary exploration data, we explored the influence of each preliminary threshold on the "miss rate", meaning the rate of reasonable reactions ($\Delta G^{\ddagger} \leq 120$ kJ/mol) which are erroneously eliminated. We also evaluated the proportion of all scans which would be evaluated with each threshold in order to estimate the computational cost.

We used the final barriers as reference to determine which reactions were reasonable. All the reactions which did not have the scan parent as reagent (meaning that the initial reaction converged to a different reaction) were not included in our dataset.

The acceptable failure rate for a single scan was chosen as 0.5%. It should be noted, however, that the remaining redundancy in the reactions scans results in reactions being sometimes discovered more than once. Thus, the few reasonable reactions that have been screened out will likely be found anyway.

We note the high threshold for stages 1 and 2. While the exploration rate in stage 1 is almost 100%, this rate is somewhat biased, since a tolerance of 280 kJ/mol was used in stage 1 while collecting this data.

Stage 4, namely the DFT//GFN2-xTB barrier with the model ligand, is very discriminating, with a required tolerance of only 30 kJ/mol. While this barrier is not used in the final results, it is computed in order to reduce the number of subsequent calculations. In particular, the final DFT SP calculation on the complete system (stage 6) is an order of magnitude more costly than stage 4. This means that adding stage 4 lowers the overall computational cost of the exploration.

Table S2: Pruning thresholds for each stage of the reaction refinement process

Stage	Tolerance @ 0.5% failure rate	Exploration rate @ 0.5% failure rate	N
1	265 kJ/mol	98.7 %	1067
2	240 kJ/mol	98.3 %	1067
3	45 kJ/mol	75.5 %	1067
4	30 kJ/mol	72.1 %	387
5	50 kJ/mol	75.4 %	1067

2.2 Complexation isomers, conformers and tautomers

Especially in large, flexible systems, conformational sampling is important to obtain representative Gibbs free energies. Analogously, the catalyst can bind to different sites of the substrate (*e.g.*, Lewis basic groups), which significantly influences the atomic reactivities. The catalyst can also form covalent bonds with the substrate, which requires a different treatment. In order to take into account these aspects, the vertical catalyst decomplexation energy is calculated in a vacuum at the GFN2-xTB level of theory:

$$E_{decomplexation\ X} = E_{adduct\ X} - (E_{catalyst} + E_{unoptimized\ substrate\ X})$$

where $E_{adduct\ X}$ is the energy associated with the stationary point of adduct X and $E_{unoptimized\ substrate\ X})$ is the energy of this system with the same geometry, but with the catalyst removed. The substrate without catalyst is not reoptimized. In the case of a non-covalent adduct, the decomplexation energy will be reasonably small, as the substrate is stable by itself. In the case of a covalent adduct (*i.e.*, with the catalyst covalent bonded to the substrate), removing the catalyst will produce an unstable intermediate with a pure anionic charge at the former position of the catalyst. Thus, the decomplexation energy will be large. By looking at a series of covalent and non-covalent adducts, the threshold of 160 kJ/mol was determined.

In the case of covalent adducts, conformational sampling is identical to that of organic molecules. Conformational sampling is thus carried out using the procedure implemented in CREST.[2–4] The catalyst is fixed and excluded for the metadynamic simulations, as well as the atom(s) bonded to the gold atom. This ensures that the correct geometry is kept for that part and enables the use of the very fast GFN-FF level of theory. Without any constraint, the atoms around the gold atom adopt incorrect geometries (*e.g.*, the L$\cdots$Au$\cdots$R angle greatly deviates from 180°).

Following the initial conformer generation, the structures are clustered based on their symmetry-aware geometric root mean square deviations (RMSD) using the DBSCAN algorithm. This is achieved by calculating the distance matrix between the structures with the psyrmsd package.[5] Based on the number of structures considered unique with a default clustering threshold, this threshold is adjusted following a binary search procedure until either the number of conformers is within the desired range (between 5 and 20 structures for covalent isomers) or the search ends unsuccessfully. This was added after observing that a single threshold often found too many unique structures when those were large and too few when those were small, thus either producing duplicate conformers or eliminating unique conformers.

Then, structures whose connectivity has changed during the conformational search are filtered out and the remaining structures are optimized. Conformers possessing equivalent R values are deduplicated.

In order to generate complexation isomers of non-covalent adducts, the catalyst is first removed from the structure and conformers of the substrate are found and clustered in the same manner. For each substrate conformer, complexation isomers are generated using the docking procedure of the quantum cluster growth[6] (QCG), as implemented in CREST. Each ensemble is reclustered using symmetry-aware RMSD, then all structures are merged and reclustered. After removed structures with different connectivities, the set of structures is pruned one last time based on atomic reactivities.

As discussed previously, the position of the catalyst influences the calculated R values of distant, unactivated atoms. In this pruning procedure, the atomic activations only are considered. Moreover, we found that the number of unique sets of activated atoms was generally quite large for average-sized substrates due to the sheer number of combinations of activated atoms. For example, if the catalyst at one position can activate up to 5 atoms, there will be $\sum_{i=0}^{5}\binom{5}{i} = 32$ unique sets of activated atoms. Of course, not all possibilities are relevant to consider. Adducts whose set of activated atoms is contained in the set of another adduct can be eliminated, as the latter will be at least as reactive. In practice, this is not enough to make the number of adducts manageable. Instead, only the adducts with at least one unique *strongest* activation are kept. This ensures that all possible activations will be considered at least once, and in their most extreme form, which should lead to the discovery of all reactions that this activation can promote.

While this does not ensure the consideration of each *pair* of most extreme activations (nor triplet, quadruplet, *etc.*), it seems extremely unlikely that one adduct with the greatest activation of atom A will have such a low activation of nearby atom B that reasonable reaction possibilities will be missed. Moreover, as the reaction possibilities are first evaluated through relaxed scans, the catalyst is free to reposition itself in order to better catalyse the reaction process.

Both conformers and complexation isomers are added to the reaction network as "isomers" of the initial intermediate and do not have a transition state.

Organic mechanisms often involve proton transfers promoted by weak acids or bases found in the reaction mixture. Among other reasons, geometric constraints can prevent intramolecular proton transfers, while they are possible when a proton transfer agent is involved. Modelling this possibly ill-defined process is challenging, although a reasonable approximation can be made from first principles. Gold(I)-catalyzed reactions rarely contain added acids or bases, and so the most likely proton transfer agent is the substrate itself. Explicitly modelling proton transfers automatically appears very challenging. However, it is possible to approximate the proton transfer transition states Gibbs energies using the transient species formed after adding or removing a proton. By coupling this reaction with an opposite proton transfer to the substrate molecule, a relative

Gibbs energy is obtained for the transient species. As such, both the basicity/acidity of the proton transfer agent (the initial substrate) and of the considered intermediate will be represented in the tautomerization barrier.

In practice, the tautomerizations are generated by using CREST's protonation and deprotonation procedures.[7] Reasonable protonation sites are determined through the Foster-Boys orbital localization method, which yields localized lone pairs and π orbitals. Deprotonations simply involve removing in turn each possible proton and identifying energetically reasonable intermediates. While CREST possesses a complete tautomerization procedure, we instead used each subprocedure individually. Both the protonation-deprotonation and the deprotonation-protonation pathways are evaluated and structures whose skeleton changes are removed.

Tautomerizations are added to the reaction network like "true" reactions, with the only difference that the transition state is also a stable intermediate and can lead to multiple products.

2.2.1 Identifying relevant complexation isomers and conformers by R

In order to consider all the relevant reactions of the substrate, it is necessary to consider the different complexation isomers which differ only by the complexation site of the catalyst. Similarly, conformational changes are expected to change the reactivity of the substrate, albeit to a lesser extent on average.

This is a challenging issue to handle in the context of automated reaction explorations. While ensembles of complexation isomers and conformers can be generated automatically (for example with the CREST package[2–4]), they can contain duplicate structures from the point of view of chemical reactivity. The standard approach to eliminate duplicate structures is to use a minimal root mean square deviation (RMSD) between the atomic positions of two structures considered to be non-equivalent. While this approach does work to eliminate nearly identical structures, small variations in dihedral angles can greatly increase the RMSD between two nearly identical conformers of large, flexible molecules. Similarly, a small different in the complexation angle of the catalyst will greatly increase the RMSD, while the differences in internal coordinates and in chemical reactivity are negligible.

While internal coordinates could be used to attempt to compute a more representative deviation metric, this approach is not trivial either and still has no direct connection to chemical reactivity.

Thus, the atomic reactivity R was used to identify unique complexation isomers and conformers. We first envisioned to directly cluster the generated structure ensemble in terms of R in order to obtain the smallest number of structures which fully represent the range of possible reactivities. However, due to its charge, the catalyst influenced the computed GFN2-xTB partial charges at an unreasonable long range (up to 10 $\AA$). Namely, the electronic density was attracted towards the cationic catalyst. This effect was of the same magnitude as the expected activations at close range, which introduced significant noise. It is possible that this is an artifact from the tight-binding method.

In order to reduce the long-range influence of the catalyst on partial charges, the purely coulombic influence of the catalyst was used as baseline. This means that activations ΔR were used instead of R values directly. The activations were calculated as the variations between the system and a fictitious system where each atom of the catalyst is replaced by an analogous point charge:

$$\Delta R = R_{sub+cat} - R_{sub+charges} \tag{S1}$$

For the substrate-catalyst adduct, this formulation is exact. In subsequent intermediates, however, only currently activated atoms will be detected, and not other atoms whose reactivity has changed with respect to the substrate because of bond changes. Thus, reactions which involve *only* these atoms will be ignored. In practice, these cases seem rare or are found anyway through scans of other reaction coordinates, as no such failure was identified. If it did become a problem, one could consider using as reference the reactivities in the starting material under perturbation of point charges. These reactivities might however change depending on the position of the catalyst/point charges. Another approach would be to use DFT-derived atomic reactivities, which are likely to be more robust and not display such artifact. This would mean systematically carrying out DFT single-point energies, increasing the computational cost, or missing out on atomic reactivities in cases where those calculations don't seem useful enough. pTB[1]-derived atomic reactivities are also plausibly more robust, although this was not evaluated. In this work, we have preferred to use GFN2-xTB-derived atomic reactivities despite this possible shortcoming.

After calculating the activations of the generated complexation isomers, they are filtered in order to eliminate redundancy. More specifically, a structure is only kept if it is associated with the strongest activation of at least one atom. In other words, structures featuring moderate activation of multiple atoms are not kept, while structures featuring strong activations for those atoms are kept. What constitutes "moderate" or "strong" entirely depends on the activations in the set. The only parameters are the R equivalence criteria, which determine if there is a meaningful activation or difference in activation.

2.3 Atomic reactivity

2.3.1 Formulating an Approximation of R

In the main text, the atomic reactivity R has been kept abstract and exact. However, it is necessary to implement a concrete descriptor that can easily be calculated. Let us consider the energy of a system perturbed by a small change $\delta v(\boldsymbol{r})$ in external potential (e.g., atoms approaching each other). Following the conventional expansion to the second order in the framework of conceptual DFT,[8,9] we obtain:

$$
\begin{aligned}
E[v(\boldsymbol{r}) + \delta v(\boldsymbol{r})] \approx E[v(\boldsymbol{r})] &+ \int \left(\frac{\delta E}{\delta v(\boldsymbol{r})}\right) \delta v(\boldsymbol{r}) d\boldsymbol{r} \\
&+ \int\int \left(\frac{\delta^2 E}{\delta v(\boldsymbol{r}_1)\delta v(\boldsymbol{r}_2)}\right) \delta v(\boldsymbol{r}_1)\delta v(\boldsymbol{r}_2) d\boldsymbol{r}_1 d\boldsymbol{r}_2 + \mathcal{O}(\delta v^3) \\
&= E[v(\boldsymbol{r})] + \int \rho(\boldsymbol{r})\delta v(\boldsymbol{r}) d\boldsymbol{r} + \int\int \chi(\boldsymbol{r}_1, \boldsymbol{r}_2)\delta v(\boldsymbol{r}_1)\delta v(\boldsymbol{r}_2) d\boldsymbol{r}_1 d\boldsymbol{r}_2
\end{aligned}
\tag{S2}
$$

with $\rho(\boldsymbol{r})$ being the electron density and $\chi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ being the linear response function.

In order to derive a more convenient form of this expression, we use the response of molecular fragment (RMF) approach.[10] In short, we will condense the fundamental properties of system into discrete atoms before calculating its derived properties. For the equation above, we will condense the total electronic density ρ into N nucleus-centered point charges of charge $Z_I - q_I$, where Z_I is the atomic number of atom I and q_I is its partial charge (as obtained from QM calculations). The linear response function χ is also condensed and becomes discrete, meaning that it expresses the change in atomic partial charge as the electrostatic potential changes at atomic positions. This has already been explored in more depth by Geerlings and coworkers.[11]

The expression of the perturbed energy thus becomes:

$$
E[v(\boldsymbol{r}) + \delta v(\boldsymbol{r})] - E[v(\boldsymbol{r})] \approx \sum_I^N (Z_I - q_I)\delta v(\boldsymbol{r}_I) + \sum_I^N \sum_J^N \chi'(\boldsymbol{r}_I, \boldsymbol{r}_J)\delta v_1(\boldsymbol{r}_I)\delta v_2(\boldsymbol{r}_J) \tag{S3}
$$

Our goal was not to obtain a quantitatively accurate equation to predict the reaction barriers, but simply to have well-grounded descriptors of atomic reactivities.

We thus use the partial charges q and the atomic polarizabilities α as the two components the atomic reactivity parameter R. The linear response function χ has been shown to be highly linked to atomic polarizability.[11] These two properties are conveniently already computed by the *xtb* package and do not require any additional calculation.

However, this formulation has two obvious shortcomings: it does not represent steric hindrance nor geometrical constraints such as ring strain. These two factors certainly influence the reaction barriers, but they are not as simple to quantify. While some formulations of steric hindrance exist within the framework of conceptual DFT, such as Liu and coworkers' steric charge,[12] none appears reasonable to compute, numerically robust as well as well correlated with the influence of steric hindrance on reaction barriers. Geometrical constraints are complex to represent in a simple way (such as a scalar) without losing a lot of information and introducing noise. The size of the ring in which each atom is (if any) is not directly correlated to reaction barrier height and fails to account for complex skeletons.

In order to circumvent this issue, error cancellation was maximized by only allowing comparisons between "the same" atoms in the different intermediates. Based on their numbers in the structures, it is possible to determine which atoms correspond to each other and can be compared. This prevents cases where two atoms with equivalent atomic reactivities yet different steric environments and/or geometrical constraints are considered equivalent. Thus, failure to react with one will not cause the pruning of the equivalent reaction with the other.

In terms of R correlations, it is not trivial to directly modify the R value of an atom in order to measure its effect on other R values. This is because the polarizability α is difficult to control. As first approach, we explored the calculation of R correlations by only influencing the partial charges q, more specifically by introducing a single point charge centered on the atom. The correlated atoms could then be identified as those with a change in R greater than a certain threshold. While this approach worked, there some shortcomings that lead us to abandon it.

Firstly, point charges in the GFN2-xTB level of theory (used through the *xtb* software) requires a hardness parameter, which the atoms possess. We found that the hardness had a considerable influence on the R fluctuations of neighboring atoms, yet no value seemed more justified than the other. Using the same hardness as the main atom resulted in great differences in R fluctuations depending on the element, which would throw off the correlation detection. Moreover, the magnitude of the point charge and the ΔR threshold indicating a correlation are both parameters that had to be determined without concrete reference point. We also noticed that point charges could induce R fluctuations in atoms which are relatively far and very unlikely to be truly influenced (this artifact is discussed in more detail in subsection 2.2.1).

Thus, we assume that each atom is only correlated to its neighboring (*i.e.*, directly connected) atoms. It is certain that these pairs of atoms strongly influence each other, so this assumption serves a basis for further improvements.

2.3.2 Clustering reactions by R

With this definition, R is a continuous property with two subcomponents. When comparing two such atomic reactivities, it is necessary to define specific difference thresholds above which the two reactivities are considered different. In order to determine these thresholds, we used our preliminary exploration data to simulate how different reactions will be clustered. In particular, we clustered together all reactions with equivalent R values, with equivalence being defined as absolute differences less than $(\Delta q; \Delta\alpha)$ from each other (Fig. S2). The standard deviation within each cluster quantifies the variability of the reaction barriers. With a perfect definition of R, we would expect the standard deviations to tend toward zero as the thresholds are decreased.

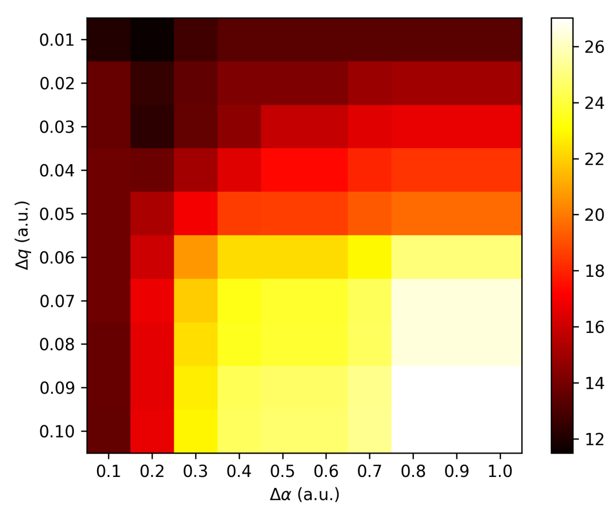

Figure S2: Standard deviation within clusters of equivalent reactions (kJ/mol)

As can be seen in Fig. S2, increasing the thresholds greatly increases the average barrier standard deviation, up to 27.0 kJ/mol with $\Delta q = 0.10$ and $\Delta\alpha = 1.0$. The lowest standard deviation is found with

$\Delta q = 0.01$ and $\Delta\alpha = 0.2$, at only 11.5 kJ/mol. However, the tightest thresholds ((0.01; 0.1)) give a sensibly equivalent result, with a standard deviation of 12.1 kJ/mol.

We chose (0.02; 0.2) for our explorations, as it offers a low standard deviation of 13 kJ/mol while allowing more clustering than very tight thresholds.

2.3.3 Pseudocode

```
def calculate_activations(
    xyz, # Input structure
    xtb_config, # xtb calculation parameters, including molecular charge
):
    # Run the xtb calculation, parse the atomic partial charges (q) and atomic polarizabilities (alpha).
    # R = ((q1, alpha1), ...)
    R_cat = run_xtb_calculation(
        xyz, xtb_config
    )

    xyz_substrate = xyz[:catalyst_ind]
    point_charges = []

    for ind, atom in xyz[catalyst_ind:]:
        point_charges.append(
            [R_cat[ind][0], atom.pos, 0.1], # Point charge with same charge as the atom, at the same
                ↪ position, and with very low hardness (eta=0.1)
        )

    R_sub = run_xtb_calculation(
        xyz_substrate, xtb_config, point_charges
    )

    activations = R_cat[:catalyst_ind] − R_sub

    # Atoms are considered activated if either abs(dq) > 0.02 or abs(dalpha) > 0.2 (see subsection 2.3.2 of
      ↪ the ESI)

    return (
        R_cat,
        activations,
    )

def reaction_possibility_to_explore(intermediate, pos):
    # ‘pos‘ contains the reaction coordinates to consider
    # e.g., pos = ((’F’, 1, 2), (’B’, 4, 5))
    # This function decides if the possibility should be evaluated for this intermediate

    ### Basic criteria go here (valence checks, etc.)

    # Substrate−based activation principle
    if not involves_activated_atom(intermediate, p):
        return False

    # R correlation principle
    if not correlated_coordinates(intermediate, p):
        return False
```

```
    # Data-driven pruning
    if is_unlikely_possibility(intermediate, p):
        return False

    return True

def involves_activated_atom(intermediate, p):
    if len(intermediate.activated_atoms) == 0:
        return False

    # Gather all activated atoms indices in the intermediate
    act_atoms = []
    for act in intermediate.activated_atoms:
        if act[0] not in act_atoms:
            act_atoms.append(act[0])

    # Check if at least one atom of the reaction possibility is activated
    for f_or_b, num1, num2 in p:
        if num1 in act_atoms or num2 in act_atoms:
            return True

    return False

def correlated_coordinates(intermediate, p):
    if len(p) == 1:
        return True

    # In the current formulation, only bonded atoms are considered to be "correlated" (see subsection 2.3.1
        ↪ of the ESI)
    corr = intermediate.correlations

    # Get the indices of the two atoms in the first coordinate
    pool = p[0][1:]

    def corr_with_pool(i):
        for j in pool:
            if (
                i == j
                or are_connected(i, j)
            ):
                return True
        return False

    # For every other coordinate
    for pp in p[1:]:
        # For each of the two atoms in the coordinate
        for i in pp[1:]:
            # Check if it is correlated with an atom from the pool
            if corr_with_pool(i):
                break
        else:
            # None of the two atoms in this coordinate are correlated with the pool.
            # This means that we are considering two independent reactions in this possibility.
```

```
            # Reject this possibility.
            return False

        for i in pp[1:]:
            if i not in pool:
                pool.append(i)
    return True

def equivalent_reactions(rx1, rx2):
    # Reactions can only equivalent if they involve the same number of bond formations and breakages,
    # and each atom in both reactions must have equivalent R values.
    # Additionally, we add the constraint of equivalent atom numberings, taking into account molecular
        ↪ symmetry (see subsection 3.3 of the manuscript)

    if rx1.coordinates != rx2.coordinates:
        return False

    diff = rx1.reactivities − rx2.reactivities

    # If either the partial charges of polarizabilities of any atom pair is too different, the reactions are not
        ↪ equivalent
    if max(abs(diff[:,0])) > 0.02 or max(abs(diff[:,1])) > 0.2:
        return False

    return True


def is_unlikely_possibility(intermediate, p):
    matches = []

    # Get the reactivities of all atoms involved in this reaction possibility
    test_rx = intermediate.as_reaction(p)

    for rx in all_known_reactions:
        if equivalent_reactions(rx, test_rx):
            matches.append(rx)

    return predict_possibility_unlikeliness(matches)


def predict_possibility_unlikeliness(matches):

    # Thresholds from Table S2 (kJ/mol)
    STAGE_THRESHOLDS = {
        1: 265,
        2: 240,
        3: 45,
        4: 30,
        5: 50,
    }

    TOLERANCE = 70 # To account for imperfect sampling

    # For each stage (see subsection 2.1.1 in the ESI), compile the (approximate) barriers of the matches
```

```
for stage in 1..6:
    stage_barriers = []
    for match in matches:
        stage_barriers.append(match.barriers[stage])

    if mean(stage_barriers) − TOLERANCE > STAGE_THRESHOLDS[stage]:
        # The reaction is unlikely based on prior data
        return True
return False
```

2.4 Preliminary Modelling Benchmark

We performed a preliminary theory level benchmark in order to determine the most cost-efficient modelling approach. The results are shown below. We used reaction barriers calculated with DLPNO-CCSD(T)/def2-TZVP/SMD(DCM) // B97-D3/def2-SVP/CPCM(DCM) and the experimental ligand (4-SP1) as references. The dataset included 13 transition states from 3 different reaction networks, leading to 10 relative reaction barriers. A reduced grid (keyboard "defgrid1" in ORCA) was used to further reduce the computational cost.

The double-hybrid functional B2K-PLYP-D3 produced energies deviating only by 6 kJ/mol from DLPNO-CCSD(T) on average (4-SP2). While GFN2-xTB energies proved to be inadequate for accurate reaction barriers (entries 1 and 2), geometries and thermochemical corrections calculated with it enabled the calculation of reaction barriers deviating by only 7 kJ/mol from the references on average, when combined with B2K-PLYP-D3 energies (entry 2-SP). Entry 3-SP shows that using the experimental ligand is more significant than using DFT geometries with Me_3P as model ligand.

Table S3: Preliminary benchmark of relative free energies depending on modelling parameters

Label	Geometry	Energy	Ligand	Mean average error (kJ/mol)
4-SP1	B97-D3/def2-SVP/CPCM(DCM)	DLPNO-CCSD(T)/def2-TZVP/SMD(DCM)	exp.	–
4-SP2	B97-D3/def2-SVP/CPCM(DCM)	B2K-PLYP-D3/def2-TZVP/SMD(DCM)	exp.	6
4	B97-D3/def2-SVP/CPCM(DCM)	B97-D3/def2-SVP/CPCM(DCM)	exp.	19
1	GFN2-xTB/ALPB(DCM)	GFN2-xTB/ALPB(DCM)	min.	28
2	GFN2-xTB/ALPB(DCM)	GFN2-xTB/ALPB(DCM)	exp.	33
2-SP	GFN2-xTB/ALPB(DCM)	B2K-PLYP-D3/def2-TZVP/SMD(DCM)	exp.	7
3	B97-D3/def2-SVP/CPCM(DCM)	B97-D3/def2-SVP/CPCM(DCM)	min.	23
3-SP	B97-D3/def2-SVP/CPCM(DCM)	B2K-PLYP-D3/def2-TZVP/SMD(DCM)	min.	14

2.5 Kinetic Simulations

2.5.1 Kinetic Modelling Details

The automatically obtained transition states (TSs) might not be "well behaved" in terms of Gibbs free energy, despite all measures in place to detect erroneous transition states. A barrier may be negative (the TS being lower in Gibbs free energy than the reactant), especially in the case of proton transfers pseudo-transition states. This will be problematic for the kinetic model, as the reaction rate will be incredibly large, which can cause numerical issues. Simply taking a fixed value as the lowest possible barrier does address the issue, but ignores the relative orders of reaction barriers and thus eliminates any selectivity in those reactions. Instead, we modify the Gibbs free energy of the reactant such that it is 10 kJ/mol below the lowest directly connected TSs, restoring the selectivity while introducing negligible error in the final results. Positive barriers below 10 kJ/mol will be taken as 10 kJ/mol in order to avoid extremely large speed constants, which can cause numerical issues.

Neophile kinetic simulations use a simulation time of one hour, while kinetic simulations to determine the final product distribution uses a simulation time of 10 hours (except when specified otherwise in the text).

2.5.2 Neophile Kinetic Simulation Details

In order to choose the new intermediates whose reactions will be evaluated, relative effective Gibbs energy are computed for all intermediates. This quantity is defined based on the final concentrations of the intermediates in the network:

$$\Delta G_{eff\ i} = -RTln\left(\frac{C_i}{C_{max}}\right) \tag{S4}$$

For every intermediate i, we calculate the ratio between its final concentration and the maximal final concentration found in the network. In order to make comparisons easier, we treat the ratio as an equilibrium ratio and transform it into the molar energy dimension. It represents the relative Gibbs energy of the intermediates if they were intermediates in thermodynamic equilibrium. This effective relative Gibbs energy, however, captures the essence of how products are formed preferably, regardless of the separate kinetic and thermodynamic factors.

We have determined that a threshold of 15 kJ/mol included all intermediates that were susceptible to influence the exploration direction. As such, we only considered intermediates where $\Delta G_{eff\ i} \leq 15\ kJ/mol$.

2.5.3 Simulation Efficiency

Analysis of large reaction networks can be challenging. Different approaches have been developed to tackle this issue.[13,14]

Neophile kinetic simulations use the LSODA algorithm[15] as implement in the Python package SciPy for numerical integrations, which can be greatly sped up by providing an exact Jacobian matrix. Since we are considering only (pseudo)unimolecular reactions, the matrix elements of the Jacobian end up being trivial to compute.

The matrix element $J_{i,j}$ of the Jacobian is given by $\partial C_i/\partial C_j$, which we can derive from the definition of dC_i:

$$\frac{\partial(dC_i)}{\partial C_j} = \begin{cases} -\sum_l k_{i\to l} & \text{if } j = i \\ k_{j\to i} & \text{otherwise} \end{cases} \tag{S5}$$

The Jacobian is thus constant throughtout the kinetic simulation and only needs to be computed once. It speeds up the overall kinetic simulation by a couple orders of magnitude, making it a negligible computational cost of the overall exploration process.

2.5.4 Pseudocode

```
def rate_constant(barrier, temperature):
    if barrier < 10 kJ/mol:
        barrier = 10 kJ/mol

    return (
        (Boltzmann constant ∗ temperature) / Plank constant
        ∗ exp(−barrier / (R ∗ temperature))
    )
```

```
def run_neophile_kinetic_simulation(
    reaction_graph,
    temperature,
    t_max,
    neophile,
    KINETIC_G_THRESHOLD = 15 kJ/mol,
):
    # 'neophile' is True during the network exploration, False for the final product distribution calculation
    # 'KINETIC_G_THRESHOLD' is the relative effective Gibbs energy threshold (Eq. S4)

    # Build list of kinetic states
    state_names = [node.name for node in reaction_graph.nodes]

    num_states = len(state_names)

    # Initialize concentrations
    C = array of zeros with length num_states
    reagent_index = index of "reagents" in state_names
    C[reagent_index] = 100

    # Initialize reaction dictionary
    # reactions[i] = list of (j, k) meaning reaction of i to j with rate k
    reactions = {i: [] for i in 0 .. num_states−1}

    # Compile reactions
    for product_node in reaction_graph.nodes:

        product_index = index of product_node.name in state_names

        for substrate_node in product_node.incoming_neighbors:

            substrate_index = index of substrate_node.name in state_names
            barrier_f = barrier from substrate_node to product_node
            barrier_b = barrier from product_node to substrate_node

            # Forward reaction
            if (
                neophile is False
                or substrate_node.group == "scanned"
            ):
                k_f = rate_constant(barrier_f, temperature)
                reactions[substrate_index].append(
                    (product_index, k_f)
                )

            # Backward reaction
            if (
                neophile is False
                or product_node.group != "scanned"
            ):
                k_b = rate_constant(barrier_b, temperature)
                reactions[product_index].append(
                    (substrate_index, k_b)
                )
```

```
# Build Jacobian matrix
J = zero matrix of size (num_states, num_states)

for i in reactions:
    for (j, k) in reactions[i]:
        J[i, i] −= k
        J[j, i] += k

# Define kinetic ODE system
def dC_dt(t, C):
    dC = zero vector of length num_states

    for i in reactions:
        for (j, k) in reactions[i]:
            flux = C[i] ∗ k

            dC[i] −= flux
            dC[j] += flux

    return dC

# Integrate concentrations in time
solution = integrate dC_dt from t = 0 to t = t_max
           using stiff ODE solver with Jacobian J

# Calculate relative effective Gibbs energies (Eq. S4)
final_C = concentrations at t_max
C_max = max(final_C)

kinetic_free_energies = []
partition_sum = 0

for i in 0 .. num_states−1:

    if final_C[i] == C_max:
        dG = 0
        partition_sum += 1
    else:
        dG = (R ∗ temperature) ∗ ln(C_max / final_C[i])
        partition_sum += exp(−dG / (R ∗ temperature))

    kinetic_free_energies.append(
        (state_names[i], dG)
    )

final_concentrations = []

# Identify kinetically significant unscanned intermediates
to_scan = []

for (state_name, dG) in kinetic_free_energies:

    node = reaction_graph.node_with_name(state_name)
```

```
        final_concentrations.append(exp(−dG/(R ∗ temperature)) / partition_sum)

        if dG < KINETIC_G_THRESHOLD and node.group == "unscanned":
            to_scan.append(node)

    # Outputs
    return (
        to_scan, # Nodes to consider next
        final_concentrations
    )
```

2.6 Overall process

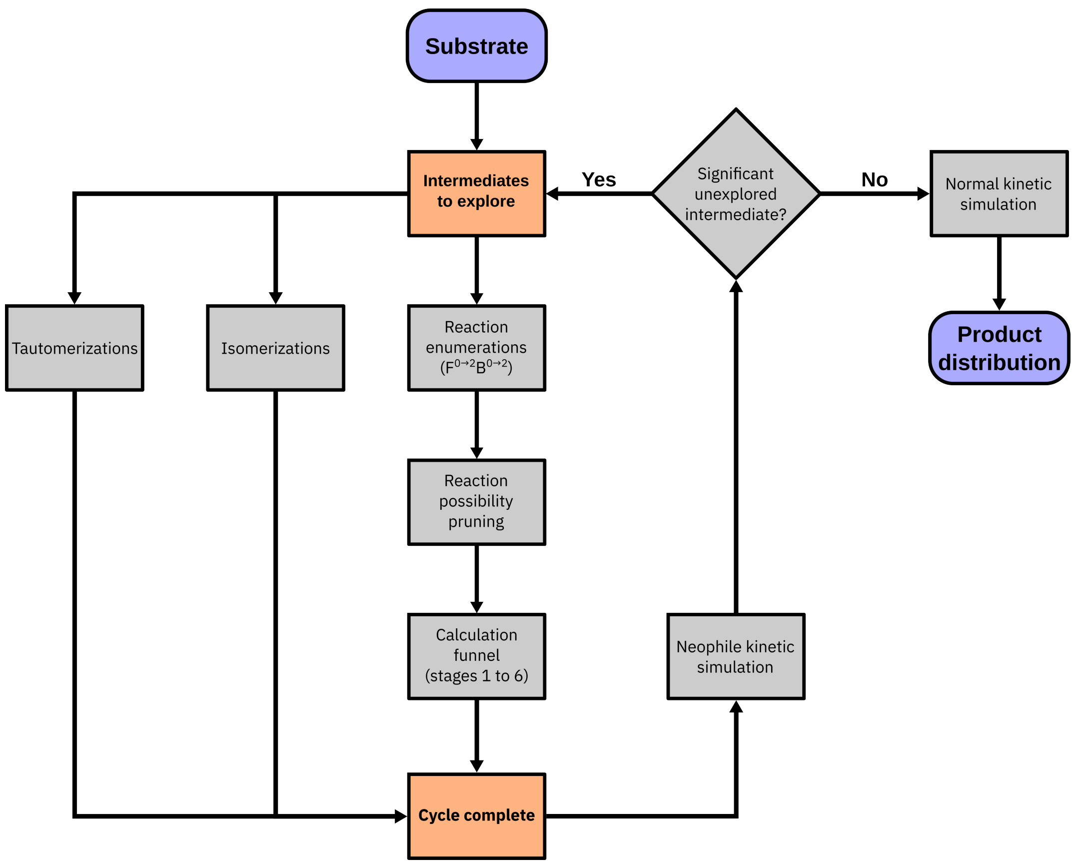

Figure S3: Flowchart of the overall exploration process

2.7 Software Details

DFT and coupled-cluster quantum calculations were carried out with ORCA 5.0.4.[16–19] GFN2-xTB calculations were performed with xtb 6.7.0 and 6.7.1.[20–22] Conformational sampling, automated protonation and deprotonation procedures, as well as complexation isomer generation made use of CREST 3.0.1.[2–4,6,7,23] Growing string method (GSM) calculations and transition state searches were performed through their implementations in the Pysisyphus[24] Python package combined with the xtb package as QM engine.

3 Raw Kinetic Simulation Results

The following lists the final relative free Gibbs energy (ΔG_{eff} in Eq. S4) and final concentration (as percentage of the reactant) for each intermediate in the network. All reaction networks with labeled nodes can be found in the Supplementary Data.

3.1 A1

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
a8cce183: 0.0 kJ/mol (91.70%)
5c94eca2_iso1: 9.0 kJ/mol (2.43%)
5c94eca2_iso3: 9.0 kJ/mol (2.43%)
5c94eca2_iso4: 9.0 kJ/mol (2.43%)
b538fd9d: 12.5 kJ/mol (0.60%)
8d0443bc_iso1: 13.5 kJ/mol (0.40%)
8d0443bc_iso2: 22.5 kJ/mol (0.01%)
5c94eca2_iso2: 34.0 kJ/mol (0.00%)
38bfaf08: 34.9 kJ/mol (0.00%)
056ca758: 35.0 kJ/mol (0.00%)
8d0443bc_iso3: 35.5 kJ/mol (0.00%)
1408d6fc: 38.0 kJ/mol (0.00%)
115d19dc: 52.2 kJ/mol (0.00%)
547882f8: 64.7 kJ/mol (0.00%)
b208ca24: 69.6 kJ/mol (0.00%)
50b57bf6: 75.3 kJ/mol (0.00%)
983949df: 79.1 kJ/mol (0.00%)
6920780b_iso1: 79.8 kJ/mol (0.00%)
600e41e5: 84.7 kJ/mol (0.00%)
1f01669b: 87.7 kJ/mol (0.00%)
887d9147: 89.3 kJ/mol (0.00%)
8115ed60: 92.5 kJ/mol (0.00%)
8f7d0836: 98.9 kJ/mol (0.00%)
58459b36: 100.0 kJ/mol (0.00%)
3792f50b: 100.2 kJ/mol (0.00%)
9c3ef451: 102.5 kJ/mol (0.00%)
f5121ea5: 102.8 kJ/mol (0.00%)
a7481388: 103.4 kJ/mol (0.00%)
2ecb4018: 106.7 kJ/mol (0.00%)
reagents: 107.3 kJ/mol (0.00%)
reagents_iso1: 107.3 kJ/mol (0.00%)
c97d1242: 107.3 kJ/mol (0.00%)
678b143c_iso1: 107.8 kJ/mol (0.00%)
678b143c: 107.8 kJ/mol (0.00%)
reagents_iso4: 109.3 kJ/mol (0.00%)
564f7f74: 109.3 kJ/mol (0.00%)
77be0984: 109.5 kJ/mol (0.00%)
6920780b_iso2: 109.8 kJ/mol (0.00%)
ffc0e6d7_iso1: 110.5 kJ/mol (0.00%)
d59266e0: 110.5 kJ/mol (0.00%)
db68e6d6_iso1: 110.5 kJ/mol (0.00%)
5f54dd91: 112.3 kJ/mol (0.00%)
81b7acf3_iso1: 114.2 kJ/mol (0.00%)
c3a4c632: 121.4 kJ/mol (0.00%)
```

```
a32fcd57_iso1: 122.3 kJ/mol (0.00%)
3b9a539a: 125.0 kJ/mol (0.00%)
reagents_iso5: 126.3 kJ/mol (0.00%)
4ffc3408: 127.1 kJ/mol (0.00%)
93944bc1_iso1: 128.7 kJ/mol (0.00%)
reagents_iso2: 131.3 kJ/mol (0.00%)
reagents_iso6: 131.3 kJ/mol (0.00%)
a710442b: 133.5 kJ/mol (0.00%)
f9cff75e_iso1: 133.8 kJ/mol (0.00%)
8bc57dcb: 136.7 kJ/mol (0.00%)
a1f73ef0: 138.7 kJ/mol (0.00%)
29a489ac: 140.0 kJ/mol (0.00%)
5eb68c1f: 143.5 kJ/mol (0.00%)
675c251e: 146.7 kJ/mol (0.00%)
e4c8c478: 147.3 kJ/mol (0.00%)
03debeef: 148.9 kJ/mol (0.00%)
560f4363: 153.5 kJ/mol (0.00%)
cbb3fc11: 154.1 kJ/mol (0.00%)
cbb3fc11_iso1: 154.1 kJ/mol (0.00%)
b51f0774: 154.1 kJ/mol (0.00%)
bc2075ff: 154.8 kJ/mol (0.00%)
604bcd88: 161.1 kJ/mol (0.00%)
ec733408: 162.5 kJ/mol (0.00%)
18e49115: 163.2 kJ/mol (0.00%)
292abac5: 165.4 kJ/mol (0.00%)
993566ec: 168.1 kJ/mol (0.00%)
6b4caad4: 175.7 kJ/mol (0.00%)
470fc556_iso1: 176.7 kJ/mol (0.00%)
599ae476: 178.2 kJ/mol (0.00%)
7a9915fe: 180.5 kJ/mol (0.00%)
a10bfc16: 183.3 kJ/mol (0.00%)
01f77307: 184.2 kJ/mol (0.00%)
710293d1: 186.8 kJ/mol (0.00%)
3af7a9ab: 188.9 kJ/mol (0.00%)
bb311480: 193.0 kJ/mol (0.00%)
25321d0a: 193.8 kJ/mol (0.00%)
8ce10944: 209.3 kJ/mol (0.00%)
a1d99ce1: 211.3 kJ/mol (0.00%)
be9a9601: 214.3 kJ/mol (0.00%)
ed3d0130: 215.0 kJ/mol (0.00%)
d79e2258: 217.1 kJ/mol (0.00%)
6a7a8fa3: 217.3 kJ/mol (0.00%)
8d4ce852: 220.4 kJ/mol (0.00%)
b683f7ce: 221.1 kJ/mol (0.00%)
91e51121: 224.7 kJ/mol (0.00%)
5bb612d9: 225.4 kJ/mol (0.00%)
0f15d6d3: 227.3 kJ/mol (0.00%)
3f0cec21: 258.3 kJ/mol (0.00%)
a6baf94b: 999.0 kJ/mol (0.00%)
d8fe0fde: 999.0 kJ/mol (0.00%)
53d9f1a9: 999.0 kJ/mol (0.00%)
cf31ade3: 999.0 kJ/mol (0.00%)
110d67ef: 999.0 kJ/mol (0.00%)
49a9e039: 999.0 kJ/mol (0.00%)
```

4289e526: 999.0 kJ/mol (0.00%)

3.2 A2

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
8de2fc2f_iso1: 0.0 kJ/mol (59.44%)
78f8e40d: 3.2 kJ/mol (16.04%)
fc700346_iso1: 3.2 kJ/mol (16.04%)
3a3ac607: 6.0 kJ/mol (5.28%)
fc700346_iso2: 7.2 kJ/mol (3.19%)
11efdbb2: 25.0 kJ/mol (0.00%)
8de2fc2f_iso3: 32.0 kJ/mol (0.00%)
8e98811d: 42.7 kJ/mol (0.00%)
d64aded1: 66.8 kJ/mol (0.00%)
db63e90a: 69.5 kJ/mol (0.00%)
846aa24e: 74.0 kJ/mol (0.00%)
reagents: 118.9 kJ/mol (0.00%)
reagents_iso3: 118.9 kJ/mol (0.00%)
10cf7daf: 125.9 kJ/mol (0.00%)
e6c048a7: 128.0 kJ/mol (0.00%)
fe3397f1: 130.0 kJ/mol (0.00%)
099b17d7: 133.2 kJ/mol (0.00%)
reagents_iso2: 135.2 kJ/mol (0.00%)
f861e985: 135.2 kJ/mol (0.00%)
30522a08_iso1: 137.2 kJ/mol (0.00%)
reagents_iso8: 138.2 kJ/mol (0.00%)
26ebcdf6: 140.8 kJ/mol (0.00%)
reagents_iso1: 140.9 kJ/mol (0.00%)
24f79f58: 141.5 kJ/mol (0.00%)
972e75a6: 142.6 kJ/mol (0.00%)
423ab989: 142.7 kJ/mol (0.00%)
e6b0f0d7_iso1: 142.8 kJ/mol (0.00%)
804ea2db_iso1: 142.8 kJ/mol (0.00%)
804ea2db_iso2: 142.8 kJ/mol (0.00%)
reagents_iso6: 143.9 kJ/mol (0.00%)
reagents_iso4: 144.2 kJ/mol (0.00%)
reagents_iso7: 146.2 kJ/mol (0.00%)
2597e63d: 146.3 kJ/mol (0.00%)
0fe7f62e: 146.7 kJ/mol (0.00%)
aab5bdbc: 146.7 kJ/mol (0.00%)
reagents_iso5: 146.9 kJ/mol (0.00%)
e0877c7f: 148.0 kJ/mol (0.00%)
449fec5c: 151.2 kJ/mol (0.00%)
1cfc596d_iso1: 153.1 kJ/mol (0.00%)
83b512ec: 156.2 kJ/mol (0.00%)
95cc0943: 156.2 kJ/mol (0.00%)
7fc1588f_iso1: 156.7 kJ/mol (0.00%)
b8438762: 157.7 kJ/mol (0.00%)
c943a440: 158.0 kJ/mol (0.00%)
cf1deb50: 162.2 kJ/mol (0.00%)
062b5ad3: 170.2 kJ/mol (0.00%)
80f6e60d: 174.0 kJ/mol (0.00%)
64ea0d8c: 179.7 kJ/mol (0.00%)

4e91ccf0: 180.0 kJ/mol (0.00%)
5ee54b45: 188.9 kJ/mol (0.00%)
5061e4fb: 194.7 kJ/mol (0.00%)
36e71276: 195.0 kJ/mol (0.00%)
305634d4: 195.5 kJ/mol (0.00%)
ad0e2197: 196.8 kJ/mol (0.00%)
7ed9f08c: 200.8 kJ/mol (0.00%)
295b4be7: 202.3 kJ/mol (0.00%)
7f0715d0: 211.7 kJ/mol (0.00%)
95bb8972: 212.8 kJ/mol (0.00%)
1df5f2a3: 222.7 kJ/mol (0.00%)
c4919dd0: 224.6 kJ/mol (0.00%)
b93d1c34: 232.4 kJ/mol (0.00%)
6de7a325: 235.2 kJ/mol (0.00%)
90758f92: 236.2 kJ/mol (0.00%)
47039c75: 253.8 kJ/mol (0.00%)
5dec1457: 267.9 kJ/mol (0.00%)
78441fb8: 999.0 kJ/mol (0.00%)
40df0bdb: 999.0 kJ/mol (0.00%)
4f00de2b: 999.0 kJ/mol (0.00%)
788b1bed: 999.0 kJ/mol (0.00%)
3ff34af9: 999.0 kJ/mol (0.00%)
9619bf48: 999.0 kJ/mol (0.00%)
8e412abf: 999.0 kJ/mol (0.00%)

3.3 A3

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
57bfba80: 0.0 kJ/mol (98.21%)
6444ca0f: 10.0 kJ/mol (1.74%)
73254260: 20.3 kJ/mol (0.03%)
cc4b57ca_iso1: 23.0 kJ/mol (0.01%)
4f14b345: 24.6 kJ/mol (0.00%)
2e2e130f: 25.4 kJ/mol (0.00%)
5de491ce: 26.2 kJ/mol (0.00%)
116b675a: 30.2 kJ/mol (0.00%)
f914a25a: 32.2 kJ/mol (0.00%)
5f56e3e9: 36.3 kJ/mol (0.00%)
cc4b57ca_iso2: 38.0 kJ/mol (0.00%)
6d96cd3b: 40.3 kJ/mol (0.00%)
d1b08818: 43.0 kJ/mol (0.00%)
c88111fb: 45.8 kJ/mol (0.00%)
88b7d777: 46.0 kJ/mol (0.00%)
4e1b1dd2: 46.6 kJ/mol (0.00%)
bafb8b3d: 47.3 kJ/mol (0.00%)
902f7f6b: 55.2 kJ/mol (0.00%)
afe46e4a: 55.7 kJ/mol (0.00%)
reagents: 60.7 kJ/mol (0.00%)
reagents_iso3: 60.7 kJ/mol (0.00%)
b483dfac: 65.9 kJ/mol (0.00%)
528b8544: 68.0 kJ/mol (0.00%)
e48999c4: 74.3 kJ/mol (0.00%)
f1dc03a3: 75.4 kJ/mol (0.00%)

cbb552f3: 77.0 kJ/mol (0.00%)
cc4b57ca_iso3: 78.0 kJ/mol (0.00%)
reagents_iso1: 78.7 kJ/mol (0.00%)
89ec696d: 80.2 kJ/mol (0.00%)
6fe7bac3: 85.7 kJ/mol (0.00%)
9295b464: 86.2 kJ/mol (0.00%)
8bd153d6: 86.7 kJ/mol (0.00%)
17aa42c1: 89.5 kJ/mol (0.00%)
reagents_iso4: 90.0 kJ/mol (0.00%)
reagents_iso2: 93.0 kJ/mol (0.00%)
d4ade357: 95.9 kJ/mol (0.00%)
4b4e9aa9: 100.1 kJ/mol (0.00%)
reagents_iso5: 100.4 kJ/mol (0.00%)
38018f4a: 101.0 kJ/mol (0.00%)
4454828a: 103.0 kJ/mol (0.00%)
a1a156bf: 104.0 kJ/mol (0.00%)
5eea21b1: 105.6 kJ/mol (0.00%)
a7e5c295: 106.7 kJ/mol (0.00%)
3b805624: 108.9 kJ/mol (0.00%)
010eafc1: 111.5 kJ/mol (0.00%)
5f2a83f3: 111.8 kJ/mol (0.00%)
31e8e845: 114.4 kJ/mol (0.00%)
28513034_iso1: 115.8 kJ/mol (0.00%)
1d99908b: 118.1 kJ/mol (0.00%)
68ae9c44: 122.0 kJ/mol (0.00%)
3b9d48c5: 125.8 kJ/mol (0.00%)
d3269085: 127.9 kJ/mol (0.00%)
31e8e845_iso1: 130.2 kJ/mol (0.00%)
4ed94b09_iso1: 130.9 kJ/mol (0.00%)
2d94a46d: 132.4 kJ/mol (0.00%)
7fc91b37: 135.8 kJ/mol (0.00%)
37705a77: 138.5 kJ/mol (0.00%)
4cf1355f: 139.4 kJ/mol (0.00%)
5ab3e7b6: 139.9 kJ/mol (0.00%)
cc4b57ca_iso4: 146.0 kJ/mol (0.00%)
577392a0: 152.8 kJ/mol (0.00%)
9c7e6eed: 153.7 kJ/mol (0.00%)
fa384f9a: 160.8 kJ/mol (0.00%)
31d3afaf: 162.6 kJ/mol (0.00%)
965e5bd6: 164.0 kJ/mol (0.00%)
14455a00: 166.8 kJ/mol (0.00%)
03c6fb9d: 173.4 kJ/mol (0.00%)
25780274: 175.7 kJ/mol (0.00%)
14b5d00d: 177.0 kJ/mol (0.00%)
c4316361: 178.7 kJ/mol (0.00%)
8c2af412: 185.0 kJ/mol (0.00%)
37705a77_iso1: 186.5 kJ/mol (0.00%)
d4c53ecc: 187.7 kJ/mol (0.00%)
392ac938: 190.7 kJ/mol (0.00%)
a7b2c85c: 193.0 kJ/mol (0.00%)
97f553f4: 206.0 kJ/mol (0.00%)
2f5813db: 208.5 kJ/mol (0.00%)
a6d56839: 209.9 kJ/mol (0.00%)
3e161196: 211.0 kJ/mol (0.00%)

```
4e4f7a25: 234.0 kJ/mol (0.00%)
aca4d6a0: 236.0 kJ/mol (0.00%)
7eb100a7: 243.0 kJ/mol (0.00%)
49e084a2: 249.8 kJ/mol (0.00%)
3fdfd5e1: 999.0 kJ/mol (0.00%)
d05bd13e: 999.0 kJ/mol (0.00%)
2c07923d: 999.0 kJ/mol (0.00%)
32c46c08: 999.0 kJ/mol (0.00%)
7f4fec64: 999.0 kJ/mol (0.00%)
0ba9c6ea: 999.0 kJ/mol (0.00%)
81db197e: 999.0 kJ/mol (0.00%)
84e9a1d9: 999.0 kJ/mol (0.00%)
a9aebc32: 999.0 kJ/mol (0.00%)
ee1dfe50: 999.0 kJ/mol (0.00%)
23cefa80: 999.0 kJ/mol (0.00%)
61572af4: 999.0 kJ/mol (0.00%)
a7a90156: 999.0 kJ/mol (0.00%)
8e813a90: 999.0 kJ/mol (0.00%)
3fdfd5e1_iso1: 999.0 kJ/mol (0.00%)
3fdfd5e1_iso6: 999.0 kJ/mol (0.00%)
3fdfd5e1_iso2: 999.0 kJ/mol (0.00%)
020b8424: 999.0 kJ/mol (0.00%)
60a4e69f: 999.0 kJ/mol (0.00%)
d065f975: 999.0 kJ/mol (0.00%)
592e0c35: 999.0 kJ/mol (0.00%)
f3a97212: 999.0 kJ/mol (0.00%)
f621746f: 999.0 kJ/mol (0.00%)
529b20ba: 999.0 kJ/mol (0.00%)
f92ca188: 999.0 kJ/mol (0.00%)
17d076be: 999.0 kJ/mol (0.00%)
070660c2: 999.0 kJ/mol (0.00%)
```

3.4 A4

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
01da7603: 0.0 kJ/mol (64.70%)
dd072602_iso2: 2.0 kJ/mol (28.88%)
446c2eef: 7.7 kJ/mol (2.91%)
446c2eef_iso2: 7.7 kJ/mol (2.91%)
af070acc: 12.5 kJ/mol (0.42%)
dd072602_iso1: 15.0 kJ/mol (0.15%)
446c2eef_iso1: 20.7 kJ/mol (0.02%)
cbd696cd: 23.0 kJ/mol (0.01%)
473b6d42: 28.3 kJ/mol (0.00%)
d8d5b769: 41.2 kJ/mol (0.00%)
5493bcdb: 49.1 kJ/mol (0.00%)
793739bd: 52.5 kJ/mol (0.00%)
f02245a8: 54.6 kJ/mol (0.00%)
f834ea36: 60.0 kJ/mol (0.00%)
211eb739: 60.7 kJ/mol (0.00%)
0b678781: 66.9 kJ/mol (0.00%)
a9cd4464: 68.1 kJ/mol (0.00%)
b8acc2be_iso1: 78.2 kJ/mol (0.00%)
```

4751f759: 79.4 kJ/mol (0.00%)
dea1816d: 80.2 kJ/mol (0.00%)
c6a73485: 89.7 kJ/mol (0.00%)
reagents: 93.8 kJ/mol (0.00%)
reagents_iso2: 93.8 kJ/mol (0.00%)
18697be2: 93.8 kJ/mol (0.00%)
761ca47e: 94.9 kJ/mol (0.00%)
f3b914ad: 95.4 kJ/mol (0.00%)
b8ea956b: 97.1 kJ/mol (0.00%)
2e890c28: 99.3 kJ/mol (0.00%)
reagents_iso3: 99.5 kJ/mol (0.00%)
cf18f83c: 100.1 kJ/mol (0.00%)
7d33bfc9: 100.9 kJ/mol (0.00%)
dcc8a32e: 103.1 kJ/mol (0.00%)
3ba10da9_iso1: 104.1 kJ/mol (0.00%)
50d2865d: 112.4 kJ/mol (0.00%)
bb29a260: 115.6 kJ/mol (0.00%)
4c28d4c2: 119.2 kJ/mol (0.00%)
ad9235ed: 127.2 kJ/mol (0.00%)
0cd66ed5_iso1: 129.1 kJ/mol (0.00%)
5ac124b2_iso1: 132.4 kJ/mol (0.00%)
b0c6b332: 133.2 kJ/mol (0.00%)
0eb2e5d5: 136.3 kJ/mol (0.00%)
79b6f051: 136.5 kJ/mol (0.00%)
fd764783: 140.5 kJ/mol (0.00%)
954beb3d: 143.2 kJ/mol (0.00%)
cffba098_iso1: 145.4 kJ/mol (0.00%)
5b20d09d: 145.5 kJ/mol (0.00%)
b459934a: 147.5 kJ/mol (0.00%)
bd579444: 149.4 kJ/mol (0.00%)
fb1ca922: 153.4 kJ/mol (0.00%)
87788e05: 158.5 kJ/mol (0.00%)
cba4fade: 163.2 kJ/mol (0.00%)
9c2adddf_iso1: 163.5 kJ/mol (0.00%)
57233625: 167.8 kJ/mol (0.00%)
4ee1e7b4: 172.1 kJ/mol (0.00%)
345e9481: 177.5 kJ/mol (0.00%)
42964292: 199.3 kJ/mol (0.00%)
c116c190: 200.4 kJ/mol (0.00%)
f0452349: 202.4 kJ/mol (0.00%)
f2061ae5: 206.5 kJ/mol (0.00%)
d496a55e: 208.2 kJ/mol (0.00%)
ed10e443: 220.7 kJ/mol (0.00%)
d01120b7: 222.5 kJ/mol (0.00%)
ec6b01ed: 245.2 kJ/mol (0.00%)
6dc1f740: 999.0 kJ/mol (0.00%)
99405421: 999.0 kJ/mol (0.00%)
5d94340d: 999.0 kJ/mol (0.00%)
5ba4305f: 999.0 kJ/mol (0.00%)
f5bebe69: 999.0 kJ/mol (0.00%)
a0021073: 999.0 kJ/mol (0.00%)
fecf2f3d: 999.0 kJ/mol (0.00%)
c0784f87: 999.0 kJ/mol (0.00%)

3.5 A5

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
91d8d8b7: 0.0 kJ/mol (94.32%)
6701c574_iso1: 7.0 kJ/mol (5.60%)
47072b3e: 20.8 kJ/mol (0.02%)
7c6557fd_iso2: 21.8 kJ/mol (0.01%)
6701c574_iso3: 22.0 kJ/mol (0.01%)
d66e85ab_iso3: 22.8 kJ/mol (0.01%)
fc401f6f_iso1: 22.8 kJ/mol (0.01%)
6701c574_iso2: 23.0 kJ/mol (0.01%)
14741fc7: 25.1 kJ/mol (0.00%)
0c4125c4_iso1: 26.1 kJ/mol (0.00%)
fc401f6f_iso2: 30.8 kJ/mol (0.00%)
7c6557fd_iso3: 30.8 kJ/mol (0.00%)
d66e85ab_iso1: 30.8 kJ/mol (0.00%)
888cb9c1: 34.1 kJ/mol (0.00%)
162f6f59: 35.1 kJ/mol (0.00%)
4a22f18b: 35.1 kJ/mol (0.00%)
0c4125c4_iso2: 40.1 kJ/mol (0.00%)
fc401f6f_iso3: 45.8 kJ/mol (0.00%)
fc401f6f_iso4: 45.8 kJ/mol (0.00%)
7c6557fd_iso1: 48.8 kJ/mol (0.00%)
f270e058: 49.3 kJ/mol (0.00%)
d66e85ab_iso2: 49.8 kJ/mol (0.00%)
0c6c417f: 50.1 kJ/mol (0.00%)
d66e85ab_iso4: 50.8 kJ/mol (0.00%)
0c4125c4_iso3: 53.1 kJ/mol (0.00%)
2cd05f25: 53.1 kJ/mol (0.00%)
6355911f: 57.0 kJ/mol (0.00%)
0c4125c4_iso4: 60.1 kJ/mol (0.00%)
1488d965: 64.6 kJ/mol (0.00%)
6b481e8d: 72.3 kJ/mol (0.00%)
8d3b9490: 74.5 kJ/mol (0.00%)
0ca15791: 74.5 kJ/mol (0.00%)
044742e3: 77.1 kJ/mol (0.00%)
8bc43330_iso1: 79.2 kJ/mol (0.00%)
b260541f_iso1: 80.2 kJ/mol (0.00%)
8bc43330_iso5: 92.2 kJ/mol (0.00%)
8bc43330_iso4: 92.2 kJ/mol (0.00%)
307325e2: 92.2 kJ/mol (0.00%)
b260541f_iso3: 96.2 kJ/mol (0.00%)
b260541f_iso2: 96.2 kJ/mol (0.00%)
8bc43330_iso2: 100.2 kJ/mol (0.00%)
reagents: 104.0 kJ/mol (0.00%)
cfa318f9: 104.0 kJ/mol (0.00%)
8bc43330_iso3: 105.2 kJ/mol (0.00%)
reagents_iso3: 106.9 kJ/mol (0.00%)
b260541f_iso4: 111.2 kJ/mol (0.00%)
a99d7e92: 111.5 kJ/mol (0.00%)
b260541f_iso5: 113.2 kJ/mol (0.00%)
a2f27c82: 115.2 kJ/mol (0.00%)
42104479: 117.2 kJ/mol (0.00%)
reagents_iso4: 119.3 kJ/mol (0.00%)

reagents_iso2: 124.3 kJ/mol (0.00%)
2f34313d: 131.8 kJ/mol (0.00%)
33514eaf: 137.8 kJ/mol (0.00%)
24c544b4: 137.9 kJ/mol (0.00%)
198c6fe5: 139.8 kJ/mol (0.00%)
511af874: 144.2 kJ/mol (0.00%)
0c4125c4_iso5: 145.1 kJ/mol (0.00%)
3d886ebd: 150.8 kJ/mol (0.00%)
10fcbd86: 160.3 kJ/mol (0.00%)
7ca71d1c: 165.1 kJ/mol (0.00%)
6028981d: 165.8 kJ/mol (0.00%)
262aa3af_iso1: 165.8 kJ/mol (0.00%)
36e3cc00: 181.8 kJ/mol (0.00%)
1f9cb48b: 185.8 kJ/mol (0.00%)
430a65d9: 210.5 kJ/mol (0.00%)
d66abaca: 215.8 kJ/mol (0.00%)
a054c51a: 219.2 kJ/mol (0.00%)
d471dc2f: 224.9 kJ/mol (0.00%)
17ffd5f0: 237.7 kJ/mol (0.00%)
8127bc51: 262.6 kJ/mol (0.00%)
28af747c: 999.0 kJ/mol (0.00%)
1fec04ae: 999.0 kJ/mol (0.00%)
7799cb00: 999.0 kJ/mol (0.00%)
fa077ee1: 999.0 kJ/mol (0.00%)
7e1b0f73: 999.0 kJ/mol (0.00%)
8333d351: 999.0 kJ/mol (0.00%)

3.6 A6

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
ab5d30e7: 0.0 kJ/mol (96.17%)
f95599fd: 9.4 kJ/mol (2.13%)
37457ed7_iso1: 10.0 kJ/mol (1.70%)
54b2f4b9_iso4: 30.0 kJ/mol (0.00%)
af9684de: 30.6 kJ/mol (0.00%)
2073ffb6: 30.9 kJ/mol (0.00%)
54b2f4b9_iso3: 35.0 kJ/mol (0.00%)
54b2f4b9: 36.0 kJ/mol (0.00%)
3b2eadda: 40.9 kJ/mol (0.00%)
a15c0b81: 42.5 kJ/mol (0.00%)
54b2f4b9_iso5: 46.0 kJ/mol (0.00%)
7623e443: 52.3 kJ/mol (0.00%)
54b2f4b9_iso1: 54.0 kJ/mol (0.00%)
54b2f4b9_iso2: 54.0 kJ/mol (0.00%)
305cb32f: 55.8 kJ/mol (0.00%)
672fb362: 60.6 kJ/mol (0.00%)
reagents: 62.4 kJ/mol (0.00%)
reagents_iso1: 62.4 kJ/mol (0.00%)
d0743158: 67.3 kJ/mol (0.00%)
7f1c512f: 72.8 kJ/mol (0.00%)
4c25cf9e: 74.2 kJ/mol (0.00%)
37a7cbf1: 78.0 kJ/mol (0.00%)
db1bfbb4: 78.8 kJ/mol (0.00%)

```
46ef33f1: 79.0 kJ/mol (0.00%)
61cc4787_iso3: 80.0 kJ/mol (0.00%)
8237ac40: 81.0 kJ/mol (0.00%)
61cc4787_iso5: 85.0 kJ/mol (0.00%)
2affba97: 86.0 kJ/mol (0.00%)
61cc4787_iso4: 91.0 kJ/mol (0.00%)
7ecff0d4: 92.4 kJ/mol (0.00%)
23d06e0c: 93.6 kJ/mol (0.00%)
61cc4787_iso2: 94.0 kJ/mol (0.00%)
61cc4787_iso1: 94.0 kJ/mol (0.00%)
4a80e8b8: 94.1 kJ/mol (0.00%)
034cb6a8: 96.0 kJ/mol (0.00%)
reagents_iso2: 96.4 kJ/mol (0.00%)
fd9f619e: 98.8 kJ/mol (0.00%)
d56dc1d7: 99.0 kJ/mol (0.00%)
78bf226d: 99.0 kJ/mol (0.00%)
b643dced: 99.1 kJ/mol (0.00%)
345a25c9: 99.2 kJ/mol (0.00%)
461b5c55: 99.5 kJ/mol (0.00%)
47de74ae: 99.7 kJ/mol (0.00%)
f877d62b: 100.2 kJ/mol (0.00%)
19adce57_iso2: 100.7 kJ/mol (0.00%)
19adce57_iso1: 101.2 kJ/mol (0.00%)
3f2ba683: 103.5 kJ/mol (0.00%)
9a9976a9: 105.0 kJ/mol (0.00%)
c728763d: 106.1 kJ/mol (0.00%)
23fdc73c: 106.8 kJ/mol (0.00%)
23fdc73c_iso1: 106.8 kJ/mol (0.00%)
19adce57_iso4: 107.2 kJ/mol (0.00%)
e20c2c7a: 107.9 kJ/mol (0.00%)
19adce57_iso3: 108.7 kJ/mol (0.00%)
233a83fe: 110.4 kJ/mol (0.00%)
413cc2f8: 111.0 kJ/mol (0.00%)
f6756754: 111.7 kJ/mol (0.00%)
9d531ec8: 112.1 kJ/mol (0.00%)
66b321ae: 113.4 kJ/mol (0.00%)
5ce76e7a: 114.0 kJ/mol (0.00%)
bd9930ed: 114.2 kJ/mol (0.00%)
1652606c: 114.5 kJ/mol (0.00%)
reagents_iso3: 116.4 kJ/mol (0.00%)
ace0e44c: 117.8 kJ/mol (0.00%)
1292247e: 121.1 kJ/mol (0.00%)
ce1ea67a: 122.2 kJ/mol (0.00%)
f36dc79f: 124.1 kJ/mol (0.00%)
b52c29f5: 124.4 kJ/mol (0.00%)
1a79bf3d: 125.0 kJ/mol (0.00%)
0826e5f4: 125.0 kJ/mol (0.00%)
ffcd9754: 126.8 kJ/mol (0.00%)
bfc7dc60: 127.3 kJ/mol (0.00%)
f57d550e: 127.5 kJ/mol (0.00%)
f6e01a05: 128.3 kJ/mol (0.00%)
a6c0a54e: 128.4 kJ/mol (0.00%)
47b173d7: 129.7 kJ/mol (0.00%)
f70b595e: 129.9 kJ/mol (0.00%)
```

315bd041: 130.2 kJ/mol (0.00%)
f8775867: 131.0 kJ/mol (0.00%)
d28c6608: 132.9 kJ/mol (0.00%)
bbe571c9: 134.5 kJ/mol (0.00%)
29c3d92b: 134.7 kJ/mol (0.00%)
3bf1207d: 135.0 kJ/mol (0.00%)
d1076c42: 138.2 kJ/mol (0.00%)
fedb4ef7: 138.6 kJ/mol (0.00%)
eda4b3c3: 139.0 kJ/mol (0.00%)
23b0dfa3_iso1: 139.6 kJ/mol (0.00%)
1accfa05: 140.0 kJ/mol (0.00%)
b76b2b75: 141.0 kJ/mol (0.00%)
7c258b49: 141.3 kJ/mol (0.00%)
23b0dfa3: 141.9 kJ/mol (0.00%)
83abe782: 143.3 kJ/mol (0.00%)
d8bc4e50: 144.6 kJ/mol (0.00%)
e23c31ec: 147.0 kJ/mol (0.00%)
df69bcd1: 148.0 kJ/mol (0.00%)
19aaf50d: 151.0 kJ/mol (0.00%)
dbb469f2: 154.7 kJ/mol (0.00%)
b684dad3: 156.0 kJ/mol (0.00%)
7c80a0e7: 157.4 kJ/mol (0.00%)
28ea44c0: 157.6 kJ/mol (0.00%)
3809b166: 158.5 kJ/mol (0.00%)
f77dd049: 160.0 kJ/mol (0.00%)
77deedce: 161.4 kJ/mol (0.00%)
87a84479: 165.0 kJ/mol (0.00%)
4e38e9bc: 167.0 kJ/mol (0.00%)
105deec0: 167.0 kJ/mol (0.00%)
4b14fb0d: 168.7 kJ/mol (0.00%)
5a2d38ba: 170.7 kJ/mol (0.00%)
6a1e289e: 174.8 kJ/mol (0.00%)
9489d247: 176.3 kJ/mol (0.00%)
b1ee5063: 182.8 kJ/mol (0.00%)
aa3029f1: 184.4 kJ/mol (0.00%)
4439e770: 184.4 kJ/mol (0.00%)
4ccb7578: 189.2 kJ/mol (0.00%)
e8da34ed: 192.2 kJ/mol (0.00%)
8021c342: 192.7 kJ/mol (0.00%)
7db4ed75: 193.4 kJ/mol (0.00%)
1a1b31b2: 194.1 kJ/mol (0.00%)
2d68d357: 194.9 kJ/mol (0.00%)
bbb02a8f: 195.5 kJ/mol (0.00%)
21f7a27c: 198.4 kJ/mol (0.00%)
37ffdaa7: 198.5 kJ/mol (0.00%)
71216363: 208.3 kJ/mol (0.00%)
306c6369: 208.4 kJ/mol (0.00%)
c8263420: 209.3 kJ/mol (0.00%)
fbcc3721: 209.5 kJ/mol (0.00%)
c1a02e5f: 210.9 kJ/mol (0.00%)
2fb8052a: 211.0 kJ/mol (0.00%)
ff365f89: 212.3 kJ/mol (0.00%)
e4a6a0c2: 212.5 kJ/mol (0.00%)
d0a5566b: 213.0 kJ/mol (0.00%)

```
7487e2ae: 213.0 kJ/mol (0.00%)
3bd45fa2: 218.7 kJ/mol (0.00%)
5726caa3: 220.0 kJ/mol (0.00%)
a1445a37: 222.7 kJ/mol (0.00%)
983652b3: 224.5 kJ/mol (0.00%)
6a01bc5f: 226.2 kJ/mol (0.00%)
7f5ec639: 227.0 kJ/mol (0.00%)
2ad50a98: 230.0 kJ/mol (0.00%)
122ebe72: 233.2 kJ/mol (0.00%)
47bfd287: 235.3 kJ/mol (0.00%)
7b4a104b: 236.7 kJ/mol (0.00%)
c218ea2e: 237.0 kJ/mol (0.00%)
c28ef96c: 237.4 kJ/mol (0.00%)
97093fa0: 239.3 kJ/mol (0.00%)
a390599c: 241.2 kJ/mol (0.00%)
2004f8b9: 241.5 kJ/mol (0.00%)
0a5741c5: 247.4 kJ/mol (0.00%)
ae026747: 258.3 kJ/mol (0.00%)
43dd5257: 279.7 kJ/mol (0.00%)
525ceb4b: 288.1 kJ/mol (0.00%)
301a51d4: 295.2 kJ/mol (0.00%)
cd190874: 999.0 kJ/mol (0.00%)
7b00e45a: 999.0 kJ/mol (0.00%)
72110785: 999.0 kJ/mol (0.00%)
4eda8e4c: 999.0 kJ/mol (0.00%)
10592db4: 999.0 kJ/mol (0.00%)
f791fb22: 999.0 kJ/mol (0.00%)
e7206e9f: 999.0 kJ/mol (0.00%)
b088eaa6: 999.0 kJ/mol (0.00%)
cad8416c: 999.0 kJ/mol (0.00%)
6fc4adbf: 999.0 kJ/mol (0.00%)
4e99572d: 999.0 kJ/mol (0.00%)
fc7341bf: 999.0 kJ/mol (0.00%)
63eaa7b6: 999.0 kJ/mol (0.00%)
a5370bd6: 999.0 kJ/mol (0.00%)
5f2c6aba: 999.0 kJ/mol (0.00%)
6b206b71: 999.0 kJ/mol (0.00%)
d7465917: 999.0 kJ/mol (0.00%)
b01d8185: 999.0 kJ/mol (0.00%)
024b04d1: 999.0 kJ/mol (0.00%)
144e44ba: 999.0 kJ/mol (0.00%)
e9e589ba: 999.0 kJ/mol (0.00%)
afcca4cd: 999.0 kJ/mol (0.00%)
e0ea883f: 999.0 kJ/mol (0.00%)
fe285a80: 999.0 kJ/mol (0.00%)
5740c778: 999.0 kJ/mol (0.00%)
c458d44e: 999.0 kJ/mol (0.00%)
8528d8ad: 999.0 kJ/mol (0.00%)
8d4f86af: 999.0 kJ/mol (0.00%)
a819f726: 999.0 kJ/mol (0.00%)
e29eab8c: 999.0 kJ/mol (0.00%)
e10e7743: 999.0 kJ/mol (0.00%)
539f0417: 999.0 kJ/mol (0.00%)
412c00f4: 999.0 kJ/mol (0.00%)
```

```
0c0d56b2: 999.0 kJ/mol (0.00%)
ed0d5373: 999.0 kJ/mol (0.00%)
9579290c: 999.0 kJ/mol (0.00%)
0bec3ecb: 999.0 kJ/mol (0.00%)
959d67fc: 999.0 kJ/mol (0.00%)
e2d24130: 999.0 kJ/mol (0.00%)
c4b503b8: 999.0 kJ/mol (0.00%)
149f7fc6: 999.0 kJ/mol (0.00%)
e3e5a15f: 999.0 kJ/mol (0.00%)
6f05e8f3: 999.0 kJ/mol (0.00%)
```

3.7 A6 (no tautomerization)

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
61cc4787_iso3: 0.0 kJ/mol (52.88%)
b0228c33: 1.0 kJ/mol (35.33%)
2f5b5ca7: 4.0 kJ/mol (10.53%)
61cc4787_iso4: 11.0 kJ/mol (0.63%)
61cc4787_iso2: 14.0 kJ/mol (0.19%)
61cc4787_iso1: 14.0 kJ/mol (0.19%)
86908d8a: 14.2 kJ/mol (0.17%)
e4970827: 16.0 kJ/mol (0.08%)
2073ffb6: 29.4 kJ/mol (0.00%)
3b2eadda: 39.4 kJ/mol (0.00%)
32374caa: 40.3 kJ/mol (0.00%)
bfc7dc60: 48.0 kJ/mol (0.00%)
1ff50f69: 49.0 kJ/mol (0.00%)
f70b595e: 49.3 kJ/mol (0.00%)
877f0155: 49.9 kJ/mol (0.00%)
23d06e0c: 52.0 kJ/mol (0.00%)
f6e01a05: 56.0 kJ/mol (0.00%)
a6c0a54e: 56.0 kJ/mol (0.00%)
eda4b3c3: 59.4 kJ/mol (0.00%)
reagents: 60.7 kJ/mol (0.00%)
reagents_iso1: 60.7 kJ/mol (0.00%)
ed7db0a6: 61.0 kJ/mol (0.00%)
83abe782: 64.0 kJ/mol (0.00%)
e14f7514: 65.1 kJ/mol (0.00%)
d0743158: 65.8 kJ/mol (0.00%)
9ead1ba3: 67.0 kJ/mol (0.00%)
7c258b49: 67.8 kJ/mol (0.00%)
dbb469f2: 73.9 kJ/mol (0.00%)
5fe54bec: 75.0 kJ/mol (0.00%)
d3d8ae3b: 84.0 kJ/mol (0.00%)
32c4cef5: 89.0 kJ/mol (0.00%)
b261f9aa: 90.4 kJ/mol (0.00%)
29c3d92b: 93.0 kJ/mol (0.00%)
reagents_iso2: 94.7 kJ/mol (0.00%)
e56b101e: 96.7 kJ/mol (0.00%)
39b41426: 98.0 kJ/mol (0.00%)
d8bc4e50: 102.0 kJ/mol (0.00%)
02fc4b6e: 106.0 kJ/mol (0.00%)
75015f34: 108.3 kJ/mol (0.00%)
```

beab5701: 109.1 kJ/mol (0.00%)
eab1d806: 110.0 kJ/mol (0.00%)
8021c342: 112.9 kJ/mol (0.00%)
b003404c: 113.3 kJ/mol (0.00%)
reagents_iso3: 114.7 kJ/mol (0.00%)
28ea44c0: 116.0 kJ/mol (0.00%)
25fb9c6d: 116.0 kJ/mol (0.00%)
7b00e45a: 116.9 kJ/mol (0.00%)
523e57a3: 121.0 kJ/mol (0.00%)
7487e2ae: 133.0 kJ/mol (0.00%)
ff360b85: 133.5 kJ/mol (0.00%)
a1445a37: 141.9 kJ/mol (0.00%)
c8263420: 143.5 kJ/mol (0.00%)
6a01bc5f: 145.6 kJ/mol (0.00%)
7f5ec639: 147.0 kJ/mol (0.00%)
7b4a104b: 155.9 kJ/mol (0.00%)
c2b8890d: 159.0 kJ/mol (0.00%)
a390599c: 161.2 kJ/mol (0.00%)
0a5741c5: 167.4 kJ/mol (0.00%)
6f24d3c5: 173.0 kJ/mol (0.00%)
242fe6da: 173.0 kJ/mol (0.00%)
ae026747: 178.3 kJ/mol (0.00%)
60b20899: 193.3 kJ/mol (0.00%)
43dd5257: 198.9 kJ/mol (0.00%)
649b435b: 227.0 kJ/mol (0.00%)
cd190874: 999.0 kJ/mol (0.00%)
72110785: 999.0 kJ/mol (0.00%)
4eda8e4c: 999.0 kJ/mol (0.00%)
10592db4: 999.0 kJ/mol (0.00%)
8528d8ad: 999.0 kJ/mol (0.00%)
5740c778: 999.0 kJ/mol (0.00%)
c458d44e: 999.0 kJ/mol (0.00%)
d1a5f897: 999.0 kJ/mol (0.00%)
053ec129: 999.0 kJ/mol (0.00%)
ff229fbd: 999.0 kJ/mol (0.00%)
d1398c4b: 999.0 kJ/mol (0.00%)

3.8 B1

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
b7a6f195: 0.0 kJ/mol (98.80%)
0fe73bb0: 11.2 kJ/mol (1.09%)
dc749f8c: 17.2 kJ/mol (0.10%)
7f509b56_iso1: 25.1 kJ/mol (0.00%)
533bd493: 25.1 kJ/mol (0.00%)
0201e043: 25.2 kJ/mol (0.00%)
50ddcfa3: 28.7 kJ/mol (0.00%)
61b1ea36_iso1: 36.7 kJ/mol (0.00%)
356cabb8: 39.8 kJ/mol (0.00%)
edd74c85: 39.9 kJ/mol (0.00%)
0d590032: 41.8 kJ/mol (0.00%)
ed351c3d_iso1: 43.2 kJ/mol (0.00%)
ed351c3d_iso4: 43.2 kJ/mol (0.00%)

ed351c3d_iso2: 46.2 kJ/mol (0.00%)
ed351c3d_iso5: 48.2 kJ/mol (0.00%)
ed351c3d_iso3: 50.2 kJ/mol (0.00%)
5ae83ec3: 57.9 kJ/mol (0.00%)
ed351c3d_iso6: 61.2 kJ/mol (0.00%)
9f7a2bc6: 62.2 kJ/mol (0.00%)
f843680c: 62.7 kJ/mol (0.00%)
347c28e5: 70.4 kJ/mol (0.00%)
cd58e5da: 70.7 kJ/mol (0.00%)
b96222f1: 73.8 kJ/mol (0.00%)
c3578d73: 75.4 kJ/mol (0.00%)
cd58e5da_iso6: 76.7 kJ/mol (0.00%)
fa47b8d9: 79.2 kJ/mol (0.00%)
cd58e5da_iso3: 80.7 kJ/mol (0.00%)
49418bf6_iso1: 81.2 kJ/mol (0.00%)
e2ad8d5c: 86.2 kJ/mol (0.00%)
74e49a7e: 87.3 kJ/mol (0.00%)
a7202e4d: 88.0 kJ/mol (0.00%)
21c00fea: 90.0 kJ/mol (0.00%)
cd58e5da_iso2: 90.7 kJ/mol (0.00%)
f892f214: 92.0 kJ/mol (0.00%)
1f6a5bbf_iso1: 93.0 kJ/mol (0.00%)
a16317c9: 94.1 kJ/mol (0.00%)
6b9fb67d: 95.0 kJ/mol (0.00%)
b5c91dfd: 95.0 kJ/mol (0.00%)
e7372992: 95.0 kJ/mol (0.00%)
21299b4c: 96.1 kJ/mol (0.00%)
fb21b4b0: 96.8 kJ/mol (0.00%)
reagents: 97.0 kJ/mol (0.00%)
reagents_iso2: 97.0 kJ/mol (0.00%)
cd58e5da_iso1: 100.7 kJ/mol (0.00%)
reagents_iso4: 101.0 kJ/mol (0.00%)
74d00d13: 102.3 kJ/mol (0.00%)
cd58e5da_iso4: 103.7 kJ/mol (0.00%)
1eedb326: 108.1 kJ/mol (0.00%)
reagents_iso1: 109.0 kJ/mol (0.00%)
cd58e5da_iso5: 109.7 kJ/mol (0.00%)
977db1ab: 111.1 kJ/mol (0.00%)
c15da9c5: 111.2 kJ/mol (0.00%)
8da9c6bd: 112.5 kJ/mol (0.00%)
f81d07d0: 112.5 kJ/mol (0.00%)
835c7b6d: 113.1 kJ/mol (0.00%)
baa1f1db: 114.1 kJ/mol (0.00%)
f3b23776: 115.4 kJ/mol (0.00%)
d71155da: 115.7 kJ/mol (0.00%)
df63dde4: 117.3 kJ/mol (0.00%)
1c23390c: 117.8 kJ/mol (0.00%)
reagents_iso5: 117.8 kJ/mol (0.00%)
e536e23a: 119.0 kJ/mol (0.00%)
85fdf4b6_iso1: 122.3 kJ/mol (0.00%)
8bcafb13: 125.3 kJ/mol (0.00%)
a640bdc8: 126.6 kJ/mol (0.00%)
043068ba: 127.1 kJ/mol (0.00%)
00019670_iso1: 130.3 kJ/mol (0.00%)

d6f57e77: 131.0 kJ/mol (0.00%)
62b1135e: 132.3 kJ/mol (0.00%)
fb5c7f7f: 134.0 kJ/mol (0.00%)
200f8c23: 134.9 kJ/mol (0.00%)
00019670: 140.3 kJ/mol (0.00%)
f6795a86: 142.0 kJ/mol (0.00%)
a108855e: 142.2 kJ/mol (0.00%)
f9c1a766_iso1: 144.2 kJ/mol (0.00%)
f9c1a766: 144.3 kJ/mol (0.00%)
e6c874bb: 147.2 kJ/mol (0.00%)
06afe465: 148.7 kJ/mol (0.00%)
6eb4f8f1: 150.5 kJ/mol (0.00%)
ed281f37: 151.0 kJ/mol (0.00%)
40ef751f: 151.9 kJ/mol (0.00%)
bf63a043: 151.9 kJ/mol (0.00%)
79fcc143_iso1: 152.2 kJ/mol (0.00%)
ad4cf74e: 152.5 kJ/mol (0.00%)
6727d743: 154.1 kJ/mol (0.00%)
a2ad9a63: 154.2 kJ/mol (0.00%)
156495f9: 156.3 kJ/mol (0.00%)
b0eae757: 157.1 kJ/mol (0.00%)
b8b3cc89: 158.1 kJ/mol (0.00%)
1e1af0af: 160.1 kJ/mol (0.00%)
b9fa2e0e: 162.1 kJ/mol (0.00%)
d2091b2a: 162.7 kJ/mol (0.00%)
b353946c: 163.2 kJ/mol (0.00%)
8a7923d0_iso1: 164.8 kJ/mol (0.00%)
c105fa5d: 165.0 kJ/mol (0.00%)
0d08615c: 168.3 kJ/mol (0.00%)
7ac78d9a: 168.8 kJ/mol (0.00%)
8d2c3381: 168.9 kJ/mol (0.00%)
83d423b8: 170.5 kJ/mol (0.00%)
2c27feeb: 170.6 kJ/mol (0.00%)
bb6543eb: 173.8 kJ/mol (0.00%)
18e30ad7: 174.4 kJ/mol (0.00%)
184b443f: 174.9 kJ/mol (0.00%)
8f78347b: 175.3 kJ/mol (0.00%)
0505c076: 176.5 kJ/mol (0.00%)
a244f1dc: 177.8 kJ/mol (0.00%)
0491b7a0: 182.7 kJ/mol (0.00%)
07514ddf: 183.7 kJ/mol (0.00%)
542dd5f8: 184.6 kJ/mol (0.00%)
14c0445d: 184.9 kJ/mol (0.00%)
c46e4ad4: 185.7 kJ/mol (0.00%)
bc5c804a: 187.7 kJ/mol (0.00%)
dd9c0f95: 187.7 kJ/mol (0.00%)
b509c032: 195.9 kJ/mol (0.00%)
bbcaf7f5: 197.0 kJ/mol (0.00%)
0ab8e564: 198.9 kJ/mol (0.00%)
4eacf5d4: 200.0 kJ/mol (0.00%)
b8302c1a: 204.4 kJ/mol (0.00%)
1929650f: 209.7 kJ/mol (0.00%)
9e18007a: 210.1 kJ/mol (0.00%)
759e9970: 214.1 kJ/mol (0.00%)

62f37a7f: 230.3 kJ/mol (0.00%)
676c6b0e: 250.2 kJ/mol (0.00%)
97f99ed1: 265.0 kJ/mol (0.00%)
45c3e742: 276.2 kJ/mol (0.00%)
e04fb83f: 280.2 kJ/mol (0.00%)
fc38788e: 286.3 kJ/mol (0.00%)
a9971ab4: 999.0 kJ/mol (0.00%)
f521d06e: 999.0 kJ/mol (0.00%)
25f232d6: 999.0 kJ/mol (0.00%)
a0fd9aa7: 999.0 kJ/mol (0.00%)
e8fc9500: 999.0 kJ/mol (0.00%)
6ed85bdf: 999.0 kJ/mol (0.00%)
4fc0e350: 999.0 kJ/mol (0.00%)
f98a4aeb: 999.0 kJ/mol (0.00%)
5058b9c1: 999.0 kJ/mol (0.00%)
92591272: 999.0 kJ/mol (0.00%)
35294520: 999.0 kJ/mol (0.00%)
afcbb99f: 999.0 kJ/mol (0.00%)
c6af3beb: 999.0 kJ/mol (0.00%)
d552cd5f: 999.0 kJ/mol (0.00%)
2bf1bce3: 999.0 kJ/mol (0.00%)
019697ca: 999.0 kJ/mol (0.00%)
9cb08683: 999.0 kJ/mol (0.00%)
0472380b: 999.0 kJ/mol (0.00%)
d95d0c66: 999.0 kJ/mol (0.00%)
bbc4e9bd: 999.0 kJ/mol (0.00%)
a7342653: 999.0 kJ/mol (0.00%)
85f37e88: 999.0 kJ/mol (0.00%)
2257e828: 999.0 kJ/mol (0.00%)
fe5458e6: 999.0 kJ/mol (0.00%)
8e8ed15c: 999.0 kJ/mol (0.00%)
346d4f24: 999.0 kJ/mol (0.00%)
d4066f09: 999.0 kJ/mol (0.00%)
32bae2df: 999.0 kJ/mol (0.00%)
c3876980: 999.0 kJ/mol (0.00%)
f06e4bd1: 999.0 kJ/mol (0.00%)
809c8f9d: 999.0 kJ/mol (0.00%)
c02f8c41: 999.0 kJ/mol (0.00%)
b160672f: 999.0 kJ/mol (0.00%)
c5d0dfec: 999.0 kJ/mol (0.00%)
55117819: 999.0 kJ/mol (0.00%)
d509340b: 999.0 kJ/mol (0.00%)

3.9 B2

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
6048d13b: 0.0 kJ/mol (59.62%)
1690e605: 2.0 kJ/mol (26.75%)
b4cd04c9: 4.5 kJ/mol (9.59%)
08b81e96_iso1: 7.5 kJ/mol (2.86%)
3b801ef5_iso1: 10.6 kJ/mol (0.84%)
761b0946_iso1: 14.5 kJ/mol (0.17%)
2abaa90b: 16.6 kJ/mol (0.07%)

761b0946: 17.5 kJ/mol (0.05%)
94131469: 17.7 kJ/mol (0.05%)
b04c2c48: 25.5 kJ/mol (0.00%)
cb9239c9: 25.5 kJ/mol (0.00%)
3e97b4ad: 26.6 kJ/mol (0.00%)
5dded2f2: 27.6 kJ/mol (0.00%)
da6c6138: 27.7 kJ/mol (0.00%)
18c3e5f5: 28.8 kJ/mol (0.00%)
761b0946_iso2: 30.5 kJ/mol (0.00%)
e7e6b8d1: 36.8 kJ/mol (0.00%)
226c0c5d: 37.8 kJ/mol (0.00%)
3b801ef5_iso3: 39.6 kJ/mol (0.00%)
aea1d626: 43.6 kJ/mol (0.00%)
9cc4e746_iso4: 43.8 kJ/mol (0.00%)
5ba51183: 44.7 kJ/mol (0.00%)
56c633eb: 46.1 kJ/mol (0.00%)
9cc4e746_iso2: 50.8 kJ/mol (0.00%)
ccc5698d_iso1: 51.0 kJ/mol (0.00%)
3b801ef5_iso2: 51.6 kJ/mol (0.00%)
e71382e4: 52.5 kJ/mol (0.00%)
9cc4e746_iso3: 52.8 kJ/mol (0.00%)
651d5686: 54.4 kJ/mol (0.00%)
d912ea99: 57.3 kJ/mol (0.00%)
9cc4e746_iso5: 58.8 kJ/mol (0.00%)
c1c7d96c_iso3: 60.5 kJ/mol (0.00%)
cc79d38d: 63.8 kJ/mol (0.00%)
b2aa87a5: 66.5 kJ/mol (0.00%)
e0ff3318: 67.4 kJ/mol (0.00%)
0fa002a6_iso1: 72.0 kJ/mol (0.00%)
701c2a69: 73.2 kJ/mol (0.00%)
0fa002a6: 74.0 kJ/mol (0.00%)
5b20cd8e: 74.5 kJ/mol (0.00%)
9cc4e746_iso1: 75.8 kJ/mol (0.00%)
b8f43053: 77.2 kJ/mol (0.00%)
bf8e8823: 77.4 kJ/mol (0.00%)
de19bfec: 77.4 kJ/mol (0.00%)
31c2beb9: 79.0 kJ/mol (0.00%)
a5e6a091: 79.5 kJ/mol (0.00%)
c1c7d96c_iso5: 82.5 kJ/mol (0.00%)
c1c7d96c_iso4: 83.5 kJ/mol (0.00%)
15a6978e_iso2: 84.3 kJ/mol (0.00%)
94e0f805: 85.5 kJ/mol (0.00%)
2a43e444: 86.7 kJ/mol (0.00%)
df141210: 89.3 kJ/mol (0.00%)
0f0b6add: 89.7 kJ/mol (0.00%)
0fa002a6_iso2: 90.0 kJ/mol (0.00%)
c1c7d96c_iso2: 90.5 kJ/mol (0.00%)
c1c7d96c_iso1: 91.5 kJ/mol (0.00%)
d319c8cb: 93.8 kJ/mol (0.00%)
9a1b0962: 95.3 kJ/mol (0.00%)
c52521be: 95.9 kJ/mol (0.00%)
24d647ae_iso4: 96.1 kJ/mol (0.00%)
55b00a80: 96.3 kJ/mol (0.00%)
1ef6672c: 96.6 kJ/mol (0.00%)

9f08edcf: 96.9 kJ/mol (0.00%)
reagents: 97.1 kJ/mol (0.00%)
5f4f0b8b: 97.2 kJ/mol (0.00%)
reagents_iso1: 98.1 kJ/mol (0.00%)
1ad74151: 100.2 kJ/mol (0.00%)
ff7fe025: 100.2 kJ/mol (0.00%)
5d269ba4: 100.3 kJ/mol (0.00%)
72003bba: 100.3 kJ/mol (0.00%)
fde75714: 100.5 kJ/mol (0.00%)
60253096: 100.5 kJ/mol (0.00%)
24d647ae: 101.1 kJ/mol (0.00%)
24d647ae_iso1: 101.1 kJ/mol (0.00%)
ce66cf57: 101.3 kJ/mol (0.00%)
1a532df3: 101.3 kJ/mol (0.00%)
e9e26ae9: 101.5 kJ/mol (0.00%)
reagents_iso2: 101.9 kJ/mol (0.00%)
46f6214b: 102.6 kJ/mol (0.00%)
d6802aa7_iso1: 102.8 kJ/mol (0.00%)
24d647ae_iso6: 103.1 kJ/mol (0.00%)
24d647ae_iso2: 104.1 kJ/mol (0.00%)
0e0d38f8: 104.8 kJ/mol (0.00%)
f514f331: 105.4 kJ/mol (0.00%)
8208c5b9: 106.5 kJ/mol (0.00%)
f892c612: 106.9 kJ/mol (0.00%)
994d245d: 109.0 kJ/mol (0.00%)
24d647ae_iso3: 111.1 kJ/mol (0.00%)
0d1e752b: 111.5 kJ/mol (0.00%)
0d950e0c: 112.1 kJ/mol (0.00%)
d0502505: 112.1 kJ/mol (0.00%)
15a6978e_iso1: 114.3 kJ/mol (0.00%)
1eed9ea7: 114.9 kJ/mol (0.00%)
d6802aa7_iso2: 115.2 kJ/mol (0.00%)
35b68a66: 115.6 kJ/mol (0.00%)
23bbd974: 116.6 kJ/mol (0.00%)
f6695f01: 117.2 kJ/mol (0.00%)
24d647ae_iso5: 118.1 kJ/mol (0.00%)
57cfc8b9: 118.5 kJ/mol (0.00%)
0fa002a6_iso3: 119.0 kJ/mol (0.00%)
53aa5b71: 119.3 kJ/mol (0.00%)
47046269: 120.3 kJ/mol (0.00%)
b4971053_iso1: 120.3 kJ/mol (0.00%)
23aee4b0: 120.3 kJ/mol (0.00%)
2759dc4e: 120.6 kJ/mol (0.00%)
dad9d745: 121.5 kJ/mol (0.00%)
9be6e13e: 121.6 kJ/mol (0.00%)
528c903f: 121.7 kJ/mol (0.00%)
2be02dcd_iso1: 122.8 kJ/mol (0.00%)
35fc18f2: 123.6 kJ/mol (0.00%)
2870f7c4: 124.5 kJ/mol (0.00%)
95743de9: 125.9 kJ/mol (0.00%)
dfddc32e: 127.6 kJ/mol (0.00%)
5778de93: 127.9 kJ/mol (0.00%)
d9c3eed6: 129.2 kJ/mol (0.00%)
9e42914f: 129.5 kJ/mol (0.00%)

90e49c96_iso1: 130.8 kJ/mol (0.00%)
8d562a46: 131.2 kJ/mol (0.00%)
8ab37ca1: 131.5 kJ/mol (0.00%)
00c932fb: 131.7 kJ/mol (0.00%)
50bd4458: 132.4 kJ/mol (0.00%)
5ff934cc: 132.9 kJ/mol (0.00%)
51b6ccf8: 134.0 kJ/mol (0.00%)
6caeba07_iso1: 134.2 kJ/mol (0.00%)
68e73e9c: 134.3 kJ/mol (0.00%)
8faf3275: 135.0 kJ/mol (0.00%)
5deb0ec8_iso1: 135.5 kJ/mol (0.00%)
7a085e63: 136.3 kJ/mol (0.00%)
d81a0996: 136.3 kJ/mol (0.00%)
2a823292: 137.0 kJ/mol (0.00%)
dacd210f: 137.0 kJ/mol (0.00%)
7ac4ffac: 137.1 kJ/mol (0.00%)
0ae1af6b: 138.0 kJ/mol (0.00%)
328cddd1: 138.6 kJ/mol (0.00%)
cab1cba7: 140.5 kJ/mol (0.00%)
2f793bee: 140.9 kJ/mol (0.00%)
3bc1edd1_iso4: 141.0 kJ/mol (0.00%)
3bc1edd1_iso2: 141.0 kJ/mol (0.00%)
e793275e_iso1: 141.0 kJ/mol (0.00%)
479f2c07: 141.3 kJ/mol (0.00%)
c62546f8_iso1: 141.5 kJ/mol (0.00%)
4d7ca987: 142.5 kJ/mol (0.00%)
5edf005e: 143.7 kJ/mol (0.00%)
69fdd4a9: 144.1 kJ/mol (0.00%)
f24e9523: 145.5 kJ/mol (0.00%)
5888f655: 146.9 kJ/mol (0.00%)
5db11f60: 147.1 kJ/mol (0.00%)
e0dca851: 148.7 kJ/mol (0.00%)
64f4cda3: 148.8 kJ/mol (0.00%)
9ce68efc: 149.5 kJ/mol (0.00%)
e196bfe4: 149.5 kJ/mol (0.00%)
ba3b9b5d: 150.5 kJ/mol (0.00%)
86cedca9: 151.0 kJ/mol (0.00%)
ea78578a: 151.0 kJ/mol (0.00%)
c9a49326: 151.3 kJ/mol (0.00%)
70427249: 151.3 kJ/mol (0.00%)
f3a0415d: 151.7 kJ/mol (0.00%)
7217992f: 152.4 kJ/mol (0.00%)
02fd0712: 152.8 kJ/mol (0.00%)
cd2d12f0: 153.4 kJ/mol (0.00%)
ae0fe9f7: 154.0 kJ/mol (0.00%)
2f468c76: 155.5 kJ/mol (0.00%)
3c8b8283: 156.7 kJ/mol (0.00%)
a66e0b06: 157.0 kJ/mol (0.00%)
2f7c3266: 158.6 kJ/mol (0.00%)
9d2d4364: 158.8 kJ/mol (0.00%)
c899d28f: 159.2 kJ/mol (0.00%)
bb8241a4: 161.5 kJ/mol (0.00%)
76500621_iso1: 161.7 kJ/mol (0.00%)
15623a5e: 161.9 kJ/mol (0.00%)

1f264fed: 162.0 kJ/mol (0.00%)
3767b9fe: 162.1 kJ/mol (0.00%)
76500621: 162.7 kJ/mol (0.00%)
f6c28ab4: 163.0 kJ/mol (0.00%)
c43da37b: 163.0 kJ/mol (0.00%)
3882688a: 163.0 kJ/mol (0.00%)
e58b01c4: 163.5 kJ/mol (0.00%)
64a8b890: 163.8 kJ/mol (0.00%)
32dabdd7_iso1: 164.3 kJ/mol (0.00%)
a509fddc: 164.4 kJ/mol (0.00%)
de289e41: 164.5 kJ/mol (0.00%)
c62546f8_iso3: 164.5 kJ/mol (0.00%)
4320c423: 165.3 kJ/mol (0.00%)
1b6a26de: 165.7 kJ/mol (0.00%)
7e30a7b1: 165.8 kJ/mol (0.00%)
c3f9a05d: 166.0 kJ/mol (0.00%)
3bc1edd1_iso3: 167.0 kJ/mol (0.00%)
0dd8da87: 170.8 kJ/mol (0.00%)
348494de: 171.3 kJ/mol (0.00%)
9ea5216a: 171.8 kJ/mol (0.00%)
3a451801: 173.3 kJ/mol (0.00%)
2bb2ccd3: 173.3 kJ/mol (0.00%)
d672c4cc: 173.6 kJ/mol (0.00%)
e9eda72c: 174.4 kJ/mol (0.00%)
9b6740e9: 174.5 kJ/mol (0.00%)
63f5cae4: 174.5 kJ/mol (0.00%)
599badee: 175.6 kJ/mol (0.00%)
92274d66: 176.5 kJ/mol (0.00%)
a6e633ed: 176.8 kJ/mol (0.00%)
67d0bb59: 177.0 kJ/mol (0.00%)
33025e01_iso1: 177.7 kJ/mol (0.00%)
b251b7cd: 178.8 kJ/mol (0.00%)
2d3d9a8f: 179.0 kJ/mol (0.00%)
aef6502c: 179.6 kJ/mol (0.00%)
a20c1ac7: 180.3 kJ/mol (0.00%)
428d20d6: 180.8 kJ/mol (0.00%)
b5df76b0: 182.7 kJ/mol (0.00%)
d79d49d4: 182.8 kJ/mol (0.00%)
8929753a: 183.3 kJ/mol (0.00%)
b6668bce: 188.3 kJ/mol (0.00%)
355fe34c: 189.0 kJ/mol (0.00%)
6a0d5865: 189.5 kJ/mol (0.00%)
54ee6070: 190.5 kJ/mol (0.00%)
e5a61aa2: 190.5 kJ/mol (0.00%)
3bc1edd1_iso5: 192.0 kJ/mol (0.00%)
fbc41a53: 192.3 kJ/mol (0.00%)
c686f6ad: 192.8 kJ/mol (0.00%)
3bc1edd1_iso1: 193.0 kJ/mol (0.00%)
e9d840f4: 193.5 kJ/mol (0.00%)
a4ccab25: 196.5 kJ/mol (0.00%)
aace1dbe: 196.5 kJ/mol (0.00%)
210d26ac: 196.8 kJ/mol (0.00%)
47dff39d: 197.3 kJ/mol (0.00%)
7cc6e751: 197.7 kJ/mol (0.00%)

051b2a08: 197.7 kJ/mol (0.00%)
eeba8970: 200.7 kJ/mol (0.00%)
fd6e83f8: 203.3 kJ/mol (0.00%)
37dbc871: 204.3 kJ/mol (0.00%)
4b0a87f4: 204.8 kJ/mol (0.00%)
910714e9: 205.0 kJ/mol (0.00%)
93f83c42: 206.7 kJ/mol (0.00%)
8c605cbe: 208.0 kJ/mol (0.00%)
513a93ae: 211.0 kJ/mol (0.00%)
95341f96: 212.2 kJ/mol (0.00%)
62e46de0: 215.0 kJ/mol (0.00%)
df19f662: 215.0 kJ/mol (0.00%)
3f73fc1a: 217.8 kJ/mol (0.00%)
27a914b6: 219.8 kJ/mol (0.00%)
e4e31fb7: 221.9 kJ/mol (0.00%)
a2312e4c: 222.2 kJ/mol (0.00%)
d3ecfc07: 222.7 kJ/mol (0.00%)
0108cd23: 223.3 kJ/mol (0.00%)
36405c2a: 223.5 kJ/mol (0.00%)
f8774749: 224.7 kJ/mol (0.00%)
a860a220: 225.2 kJ/mol (0.00%)
644d9caf: 225.3 kJ/mol (0.00%)
85a8705f: 226.0 kJ/mol (0.00%)
524ed1f2: 226.6 kJ/mol (0.00%)
9c41a981: 226.7 kJ/mol (0.00%)
d8309ac5: 227.1 kJ/mol (0.00%)
b938b385: 227.6 kJ/mol (0.00%)
d227e2e7: 230.7 kJ/mol (0.00%)
0ff57bc5: 230.9 kJ/mol (0.00%)
477f9dc8: 231.1 kJ/mol (0.00%)
d5bd9095: 232.7 kJ/mol (0.00%)
74ac8a8a: 233.7 kJ/mol (0.00%)
480ee447: 234.1 kJ/mol (0.00%)
ffde5ba4: 234.7 kJ/mol (0.00%)
751c99af: 235.0 kJ/mol (0.00%)
d4c79206: 236.3 kJ/mol (0.00%)
e8525521: 236.9 kJ/mol (0.00%)
30df7b09: 237.0 kJ/mol (0.00%)
324b82e1: 238.0 kJ/mol (0.00%)
c62546f8_iso2: 238.5 kJ/mol (0.00%)
e1a69b7b: 239.7 kJ/mol (0.00%)
0a37b69a: 244.9 kJ/mol (0.00%)
68eebe35: 246.1 kJ/mol (0.00%)
edc232e1: 250.4 kJ/mol (0.00%)
ec035bde: 252.3 kJ/mol (0.00%)
85a03087: 254.3 kJ/mol (0.00%)
13a8ee0c: 258.7 kJ/mol (0.00%)
79085ebd: 260.1 kJ/mol (0.00%)
ad08e693: 260.5 kJ/mol (0.00%)
52166a81: 265.6 kJ/mol (0.00%)
736eb929: 267.2 kJ/mol (0.00%)
3c1869b2: 269.0 kJ/mol (0.00%)
b7c5fcc4: 269.0 kJ/mol (0.00%)
ee521f85: 272.9 kJ/mol (0.00%)

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0f0689f3: 273.0 kJ/mol (0.00%)
6891ee05: 275.3 kJ/mol (0.00%)
945536ea: 285.0 kJ/mol (0.00%)
3f79070c: 293.0 kJ/mol (0.00%)
1cae8ac1: 298.9 kJ/mol (0.00%)
9c6a9128: 302.0 kJ/mol (0.00%)
1c5ad5ae: 314.7 kJ/mol (0.00%)
2fb87b7b: 321.0 kJ/mol (0.00%)
a84baec2: 326.0 kJ/mol (0.00%)
cdf835a8: 354.3 kJ/mol (0.00%)
b35b85c5: 999.0 kJ/mol (0.00%)
e7c3fdf5: 999.0 kJ/mol (0.00%)
a1cf521c: 999.0 kJ/mol (0.00%)
3ddb9733: 999.0 kJ/mol (0.00%)
d998d8e2: 999.0 kJ/mol (0.00%)
94a1b2c3: 999.0 kJ/mol (0.00%)
d2935729: 999.0 kJ/mol (0.00%)
5dcffaef: 999.0 kJ/mol (0.00%)
c191085d: 999.0 kJ/mol (0.00%)
1ab82546: 999.0 kJ/mol (0.00%)
275cedbc: 999.0 kJ/mol (0.00%)
80255c57: 999.0 kJ/mol (0.00%)
880a2d3a: 999.0 kJ/mol (0.00%)
332cf907: 999.0 kJ/mol (0.00%)
750dccb5: 999.0 kJ/mol (0.00%)
9540e912: 999.0 kJ/mol (0.00%)
4b65ef81: 999.0 kJ/mol (0.00%)
58a15e37: 999.0 kJ/mol (0.00%)
bec2b087: 999.0 kJ/mol (0.00%)
b2c227dc: 999.0 kJ/mol (0.00%)
46acd229: 999.0 kJ/mol (0.00%)
28d4ef26: 999.0 kJ/mol (0.00%)
684da5df: 999.0 kJ/mol (0.00%)
f7ce8f53: 999.0 kJ/mol (0.00%)
ad2e2fd3: 999.0 kJ/mol (0.00%)
9f323aa8: 999.0 kJ/mol (0.00%)
187a9e97: 999.0 kJ/mol (0.00%)
e4045d59: 999.0 kJ/mol (0.00%)
15a3d090: 999.0 kJ/mol (0.00%)
9de4da23: 999.0 kJ/mol (0.00%)
7a0884d5: 999.0 kJ/mol (0.00%)
784652ca: 999.0 kJ/mol (0.00%)
a80d9d2a: 999.0 kJ/mol (0.00%)
6c1f3ad4: 999.0 kJ/mol (0.00%)
2273a5ec: 999.0 kJ/mol (0.00%)
6dcefbe0: 999.0 kJ/mol (0.00%)
ce6b197c: 999.0 kJ/mol (0.00%)
b4237607: 999.0 kJ/mol (0.00%)
faefb867: 999.0 kJ/mol (0.00%)
c59949c8: 999.0 kJ/mol (0.00%)
d1f44f17: 999.0 kJ/mol (0.00%)
9fcfb85c: 999.0 kJ/mol (0.00%)
5873050d: 999.0 kJ/mol (0.00%)
559c6d33: 999.0 kJ/mol (0.00%)
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ffd6afd7: 999.0 kJ/mol (0.00%)
3981dbf1: 999.0 kJ/mol (0.00%)
ce63d039: 999.0 kJ/mol (0.00%)
b6db1419: 999.0 kJ/mol (0.00%)
2d444ba4: 999.0 kJ/mol (0.00%)
c542ce44: 999.0 kJ/mol (0.00%)
e71154ad: 999.0 kJ/mol (0.00%)
479a2c94: 999.0 kJ/mol (0.00%)
072472d2: 999.0 kJ/mol (0.00%)
1d73e579: 999.0 kJ/mol (0.00%)
7b1a8dce: 999.0 kJ/mol (0.00%)
63df11f1: 999.0 kJ/mol (0.00%)
b07ad4e5: 999.0 kJ/mol (0.00%)
75c0cb22: 999.0 kJ/mol (0.00%)
6e72d28f: 999.0 kJ/mol (0.00%)
60045ee8: 999.0 kJ/mol (0.00%)
724a0f25: 999.0 kJ/mol (0.00%)
bc65f05e: 999.0 kJ/mol (0.00%)
5dc2fe62: 999.0 kJ/mol (0.00%)
f67d2d7a: 999.0 kJ/mol (0.00%)
999e5ed6: 999.0 kJ/mol (0.00%)
94a22aac: 999.0 kJ/mol (0.00%)
b4446ea2: 999.0 kJ/mol (0.00%)
a7706ab2: 999.0 kJ/mol (0.00%)
18ce8da8: 999.0 kJ/mol (0.00%)
11eaa956: 999.0 kJ/mol (0.00%)
7158cab5: 999.0 kJ/mol (0.00%)
2f25a8f7: 999.0 kJ/mol (0.00%)
e4243f75: 999.0 kJ/mol (0.00%)
c5ac8994: 999.0 kJ/mol (0.00%)
e9806dfa: 999.0 kJ/mol (0.00%)
45655813: 999.0 kJ/mol (0.00%)
638e708d: 999.0 kJ/mol (0.00%)
507bada7: 999.0 kJ/mol (0.00%)
6dcd7f3e: 999.0 kJ/mol (0.00%)
f28fa8ff: 999.0 kJ/mol (0.00%)
5a0ab907: 999.0 kJ/mol (0.00%)
39c75f6c: 999.0 kJ/mol (0.00%)
936e1d98: 999.0 kJ/mol (0.00%)
b12adde5: 999.0 kJ/mol (0.00%)
8d529d63: 999.0 kJ/mol (0.00%)
ec236753: 999.0 kJ/mol (0.00%)
3a3904ee: 999.0 kJ/mol (0.00%)
ef2ef76e: 999.0 kJ/mol (0.00%)
3b69070e: 999.0 kJ/mol (0.00%)
da8e7465: 999.0 kJ/mol (0.00%)
1f1351d0: 999.0 kJ/mol (0.00%)
27867885: 999.0 kJ/mol (0.00%)
34c24559: 999.0 kJ/mol (0.00%)
7e77d489: 999.0 kJ/mol (0.00%)
68de5eb4: 999.0 kJ/mol (0.00%)
c2649713: 999.0 kJ/mol (0.00%)
bb91da5f: 999.0 kJ/mol (0.00%)
da7ac152: 999.0 kJ/mol (0.00%)

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a9d52e44: 999.0 kJ/mol (0.00%)
9c547dd2: 999.0 kJ/mol (0.00%)
80d8f7e6: 999.0 kJ/mol (0.00%)
9d9269b2: 999.0 kJ/mol (0.00%)
0fcf3c90: 999.0 kJ/mol (0.00%)
0c600bd6: 999.0 kJ/mol (0.00%)
8e60a072: 999.0 kJ/mol (0.00%)
72bc8c3e: 999.0 kJ/mol (0.00%)
81476e20: 999.0 kJ/mol (0.00%)
d0908e88: 999.0 kJ/mol (0.00%)
ce40d643: 999.0 kJ/mol (0.00%)
75e4c7c9: 999.0 kJ/mol (0.00%)
6101d109: 999.0 kJ/mol (0.00%)
4b1ef08b: 999.0 kJ/mol (0.00%)
ad024314: 999.0 kJ/mol (0.00%)
5b821e2f: 999.0 kJ/mol (0.00%)
463ec39e: 999.0 kJ/mol (0.00%)
b7295273: 999.0 kJ/mol (0.00%)
636b3386: 999.0 kJ/mol (0.00%)
e84ebdcd: 999.0 kJ/mol (0.00%)
138b737d: 999.0 kJ/mol (0.00%)
88fcff50: 999.0 kJ/mol (0.00%)
b988ceee: 999.0 kJ/mol (0.00%)
8693e2ef: 999.0 kJ/mol (0.00%)
d501ea04: 999.0 kJ/mol (0.00%)
cf3df8ad: 999.0 kJ/mol (0.00%)
bdd2cdd5: 999.0 kJ/mol (0.00%)
2b1c7934: 999.0 kJ/mol (0.00%)
6ced10bb: 999.0 kJ/mol (0.00%)
b85381af: 999.0 kJ/mol (0.00%)
eec9d2ae: 999.0 kJ/mol (0.00%)
a0d44409: 999.0 kJ/mol (0.00%)
da79d4ca: 999.0 kJ/mol (0.00%)
e1b9e250: 999.0 kJ/mol (0.00%)
d32f3bec: 999.0 kJ/mol (0.00%)
99dfe66f: 999.0 kJ/mol (0.00%)
a531104c: 999.0 kJ/mol (0.00%)
310a7773: 999.0 kJ/mol (0.00%)
acd501f5: 999.0 kJ/mol (0.00%)
c7281a0d: 999.0 kJ/mol (0.00%)
39ac8d2a: 999.0 kJ/mol (0.00%)
dcacf7d9: 999.0 kJ/mol (0.00%)
843762b7: 999.0 kJ/mol (0.00%)
b92ccacb: 999.0 kJ/mol (0.00%)
6fa7480f: 999.0 kJ/mol (0.00%)
6e8313bb: 999.0 kJ/mol (0.00%)
f65a984c: 999.0 kJ/mol (0.00%)
f022e75b: 999.0 kJ/mol (0.00%)
54549654: 999.0 kJ/mol (0.00%)
07569789: 999.0 kJ/mol (0.00%)
f1e11ff5: 999.0 kJ/mol (0.00%)
4f7086ea: 999.0 kJ/mol (0.00%)
971d4c73: 999.0 kJ/mol (0.00%)
c8f364f3: 999.0 kJ/mol (0.00%)
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d10fd475: 999.0 kJ/mol (0.00%)
f612db12: 999.0 kJ/mol (0.00%)
1d2fe2ff: 999.0 kJ/mol (0.00%)
815be6af: 999.0 kJ/mol (0.00%)
902c2fc8: 999.0 kJ/mol (0.00%)
e63ffac0: 999.0 kJ/mol (0.00%)
060f621d: 999.0 kJ/mol (0.00%)
2fb633c5: 999.0 kJ/mol (0.00%)
936fe20f: 999.0 kJ/mol (0.00%)
b875a3dc: 999.0 kJ/mol (0.00%)
3ed3bb29: 999.0 kJ/mol (0.00%)
ec5f76be: 999.0 kJ/mol (0.00%)
3e56bf34: 999.0 kJ/mol (0.00%)
ae1fd8d1: 999.0 kJ/mol (0.00%)
32c3c4f8: 999.0 kJ/mol (0.00%)
41d2da2a: 999.0 kJ/mol (0.00%)
e24635d0: 999.0 kJ/mol (0.00%)
fdfed845: 999.0 kJ/mol (0.00%)
51cc39da: 999.0 kJ/mol (0.00%)
9b51ff2a: 999.0 kJ/mol (0.00%)
2d2357e1: 999.0 kJ/mol (0.00%)
e45dab5e: 999.0 kJ/mol (0.00%)
b8297ca8: 999.0 kJ/mol (0.00%)
62817fe0: 999.0 kJ/mol (0.00%)
680ad1ed: 999.0 kJ/mol (0.00%)
812665d9: 999.0 kJ/mol (0.00%)
780e3f64: 999.0 kJ/mol (0.00%)
11a85bad: 999.0 kJ/mol (0.00%)
5697e09c: 999.0 kJ/mol (0.00%)
157997ad: 999.0 kJ/mol (0.00%)
eff0f521: 999.0 kJ/mol (0.00%)
596e16ac: 999.0 kJ/mol (0.00%)
76208488: 999.0 kJ/mol (0.00%)
2a69683a: 999.0 kJ/mol (0.00%)
0d14d0d8: 999.0 kJ/mol (0.00%)
fc63ce74: 999.0 kJ/mol (0.00%)
d18b8fb5: 999.0 kJ/mol (0.00%)
060c25fd: 999.0 kJ/mol (0.00%)
0a4ba1dd: 999.0 kJ/mol (0.00%)
221e5d94: 999.0 kJ/mol (0.00%)
6798992b: 999.0 kJ/mol (0.00%)
93db0385: 999.0 kJ/mol (0.00%)
4438e58a: 999.0 kJ/mol (0.00%)
d4d48c87: 999.0 kJ/mol (0.00%)
d5409c01: 999.0 kJ/mol (0.00%)
903e7534: 999.0 kJ/mol (0.00%)
6873e980: 999.0 kJ/mol (0.00%)
6ea6223c: 999.0 kJ/mol (0.00%)
fde8c838: 999.0 kJ/mol (0.00%)
f65e4fe1: 999.0 kJ/mol (0.00%)
5b0af647: 999.0 kJ/mol (0.00%)
4701f68c: 999.0 kJ/mol (0.00%)
eb1ec4d8: 999.0 kJ/mol (0.00%)
2d75ea13: 999.0 kJ/mol (0.00%)
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f032be8d: 999.0 kJ/mol (0.00%)
db293d16: 999.0 kJ/mol (0.00%)
711970b1: 999.0 kJ/mol (0.00%)
d7116cd5: 999.0 kJ/mol (0.00%)
eeb4f10c: 999.0 kJ/mol (0.00%)
b80fa049: 999.0 kJ/mol (0.00%)
80d0e0ca: 999.0 kJ/mol (0.00%)
0a372bae: 999.0 kJ/mol (0.00%)
57123cae: 999.0 kJ/mol (0.00%)
ae2b3a16: 999.0 kJ/mol (0.00%)
c07b2b3f: 999.0 kJ/mol (0.00%)
f794b662: 999.0 kJ/mol (0.00%)
61ec6d81: 999.0 kJ/mol (0.00%)
bda7c39f: 999.0 kJ/mol (0.00%)
4b9774da: 999.0 kJ/mol (0.00%)
3c3db374: 999.0 kJ/mol (0.00%)
54ea3a14: 999.0 kJ/mol (0.00%)
52c97787: 999.0 kJ/mol (0.00%)
eb80f3e8: 999.0 kJ/mol (0.00%)
1211da4b: 999.0 kJ/mol (0.00%)
68ae37b5: 999.0 kJ/mol (0.00%)
07439e66: 999.0 kJ/mol (0.00%)
e8f61b6e: 999.0 kJ/mol (0.00%)
2323845e: 999.0 kJ/mol (0.00%)
476437a9: 999.0 kJ/mol (0.00%)
e14ef519: 999.0 kJ/mol (0.00%)
60b8f9e1: 999.0 kJ/mol (0.00%)
6f171c68: 999.0 kJ/mol (0.00%)
023f7168: 999.0 kJ/mol (0.00%)
3d70ae5a: 999.0 kJ/mol (0.00%)

3.10 B3

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
79301047_iso8: 0.0 kJ/mol (30.78%)
4004c885: 0.6 kJ/mol (24.21%)
17de874b_iso2: 2.4 kJ/mol (11.76%)
48341f3f: 3.0 kJ/mol (9.18%)
17de874b_iso1: 3.4 kJ/mol (7.86%)
17de874b: 4.4 kJ/mol (5.25%)
79301047_iso7: 5.0 kJ/mol (4.10%)
79301047_iso1: 6.0 kJ/mol (2.74%)
79301047_iso6: 6.0 kJ/mol (2.74%)
0183f6dd: 10.5 kJ/mol (0.44%)
0183f6dd_iso1: 10.5 kJ/mol (0.44%)
0183f6dd_iso2: 10.5 kJ/mol (0.44%)
d0101c6d: 17.8 kJ/mol (0.02%)
79301047_iso2: 18.0 kJ/mol (0.02%)
79301047_iso4: 18.0 kJ/mol (0.02%)
79301047_iso5: 21.0 kJ/mol (0.01%)
79301047_iso3: 23.0 kJ/mol (0.00%)
6abdbd19: 33.5 kJ/mol (0.00%)
a8737464: 34.8 kJ/mol (0.00%)

283f123c: 40.9 kJ/mol (0.00%)
efcd7ad1: 52.5 kJ/mol (0.00%)
9c319a6b: 57.1 kJ/mol (0.00%)
44eaab55: 60.5 kJ/mol (0.00%)
36fc9278: 62.1 kJ/mol (0.00%)
f43e363e_iso5: 65.0 kJ/mol (0.00%)
6180fd8c: 65.5 kJ/mol (0.00%)
4693dd32: 67.5 kJ/mol (0.00%)
f43e363e: 73.0 kJ/mol (0.00%)
f43e363e_iso1: 73.0 kJ/mol (0.00%)
cc6d7404: 78.6 kJ/mol (0.00%)
f43e363e_iso2: 79.0 kJ/mol (0.00%)
reagents: 84.7 kJ/mol (0.00%)
reagents_iso1: 84.7 kJ/mol (0.00%)
f43e363e_iso4: 85.0 kJ/mol (0.00%)
f43e363e_iso3: 89.0 kJ/mol (0.00%)
7913ba37: 91.9 kJ/mol (0.00%)
044f74f6: 93.3 kJ/mol (0.00%)
reagents_iso3: 96.7 kJ/mol (0.00%)
reagents_iso2: 97.7 kJ/mol (0.00%)
88de0727_iso1: 99.3 kJ/mol (0.00%)
2e0d2603: 101.8 kJ/mol (0.00%)
88de0727_iso4: 104.3 kJ/mol (0.00%)
88de0727_iso3: 106.3 kJ/mol (0.00%)
bb839ea1: 110.3 kJ/mol (0.00%)
2e131f35: 113.5 kJ/mol (0.00%)
88de0727_iso2: 116.3 kJ/mol (0.00%)
ff931d4c: 118.8 kJ/mol (0.00%)
88de0727_iso7: 119.1 kJ/mol (0.00%)
88de0727_iso5: 119.9 kJ/mol (0.00%)
88de0727_iso6: 120.3 kJ/mol (0.00%)
0dbbdeb0: 122.8 kJ/mol (0.00%)
3a99da1d: 124.0 kJ/mol (0.00%)
719a60d4: 130.3 kJ/mol (0.00%)
cc629e5f: 133.0 kJ/mol (0.00%)
b3653e74: 143.0 kJ/mol (0.00%)
ecc38206: 143.3 kJ/mol (0.00%)
8a35e400: 145.0 kJ/mol (0.00%)
b63a79a9: 147.2 kJ/mol (0.00%)
7711f81a: 149.8 kJ/mol (0.00%)
bafe3772: 155.6 kJ/mol (0.00%)
f27e0e2d: 164.8 kJ/mol (0.00%)
9f0dfa37: 167.3 kJ/mol (0.00%)
0f9ee42e: 169.3 kJ/mol (0.00%)
e8a2e8f7: 186.0 kJ/mol (0.00%)
3ae690dd: 186.7 kJ/mol (0.00%)
8301f9b7: 188.0 kJ/mol (0.00%)
2e261323: 221.9 kJ/mol (0.00%)
36855c5b: 227.0 kJ/mol (0.00%)
df7f432b: 236.0 kJ/mol (0.00%)
1a4e26d8: 236.1 kJ/mol (0.00%)
f417c9e6: 999.0 kJ/mol (0.00%)
d2ce363b: 999.0 kJ/mol (0.00%)
1810856b: 999.0 kJ/mol (0.00%)

c0766450: 999.0 kJ/mol (0.00%)
d2a02fbd: 999.0 kJ/mol (0.00%)
92617375: 999.0 kJ/mol (0.00%)
c5cf9c2e: 999.0 kJ/mol (0.00%)
c9ffd176: 999.0 kJ/mol (0.00%)
af62e0f4: 999.0 kJ/mol (0.00%)
cba7c60d: 999.0 kJ/mol (0.00%)
d854988c: 999.0 kJ/mol (0.00%)
33fb09e0: 999.0 kJ/mol (0.00%)
eb42d506: 999.0 kJ/mol (0.00%)
a65dedf9: 999.0 kJ/mol (0.00%)
4a485713: 999.0 kJ/mol (0.00%)
269cd9e5: 999.0 kJ/mol (0.00%)
96218453: 999.0 kJ/mol (0.00%)
28f4c9b5: 999.0 kJ/mol (0.00%)
b805183a: 999.0 kJ/mol (0.00%)
b6a22de8: 999.0 kJ/mol (0.00%)
bbb28a06: 999.0 kJ/mol (0.00%)
81a983ad: 999.0 kJ/mol (0.00%)
99f60dea: 999.0 kJ/mol (0.00%)

3.11 B4

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
7d63dbc2: 0.0 kJ/mol (84.54%)
44b3fbea: 4.5 kJ/mol (13.65%)
0b20af27_iso1: 10.5 kJ/mol (1.21%)
0b20af27_iso2: 14.5 kJ/mol (0.24%)
f35163ec_iso1: 17.0 kJ/mol (0.09%)
9ab473e6: 17.4 kJ/mol (0.08%)
e7c68fa0: 18.1 kJ/mol (0.06%)
e38705eb: 18.1 kJ/mol (0.06%)
645fde71: 18.6 kJ/mol (0.05%)
55f891e8: 22.0 kJ/mol (0.01%)
383dc84a: 22.8 kJ/mol (0.01%)
d87c81ce: 24.8 kJ/mol (0.00%)
83820d6f: 24.8 kJ/mol (0.00%)
0a82d5ae: 26.4 kJ/mol (0.00%)
0b20af27_iso3: 30.5 kJ/mol (0.00%)
cd398528: 31.7 kJ/mol (0.00%)
99d5d682: 33.8 kJ/mol (0.00%)
069f5763: 34.2 kJ/mol (0.00%)
825a383f: 35.0 kJ/mol (0.00%)
faf381e8: 40.5 kJ/mol (0.00%)
4121b711: 40.5 kJ/mol (0.00%)
reagents: 41.6 kJ/mol (0.00%)
reagents_iso4: 41.6 kJ/mol (0.00%)
448fb495: 41.6 kJ/mol (0.00%)
4eacf931: 42.5 kJ/mol (0.00%)
reagents_iso1: 42.6 kJ/mol (0.00%)
d9493da8: 43.9 kJ/mol (0.00%)
a24bebe1: 45.6 kJ/mol (0.00%)
44779f65: 46.4 kJ/mol (0.00%)

11704a84: 48.0 kJ/mol (0.00%)
57915a23: 49.6 kJ/mol (0.00%)
0ec99548: 55.8 kJ/mol (0.00%)
b35dbb48: 56.6 kJ/mol (0.00%)
08c61e2d: 56.7 kJ/mol (0.00%)
ae4df090: 57.5 kJ/mol (0.00%)
d460845d: 60.5 kJ/mol (0.00%)
8313e49d: 60.6 kJ/mol (0.00%)
821bfdd3: 61.4 kJ/mol (0.00%)
1528c35a: 62.5 kJ/mol (0.00%)
13dd579a: 63.2 kJ/mol (0.00%)
53bde0ec: 64.6 kJ/mol (0.00%)
5e360fe7: 65.3 kJ/mol (0.00%)
35106e77: 66.1 kJ/mol (0.00%)
df5fd731: 66.1 kJ/mol (0.00%)
703920bd_iso1: 68.5 kJ/mol (0.00%)
c64396b1: 70.8 kJ/mol (0.00%)
703920bd_iso2: 71.4 kJ/mol (0.00%)
6fa60ecb: 74.0 kJ/mol (0.00%)
c9ef3630_iso2: 74.1 kJ/mol (0.00%)
ef992d8f_iso1: 74.4 kJ/mol (0.00%)
e6ad8239: 75.6 kJ/mol (0.00%)
ecfecf5f: 76.0 kJ/mol (0.00%)
25c968dc: 76.2 kJ/mol (0.00%)
8eca7057: 76.8 kJ/mol (0.00%)
d0164dd3: 77.0 kJ/mol (0.00%)
6099f25e: 77.0 kJ/mol (0.00%)
c9ef3630_iso3: 78.2 kJ/mol (0.00%)
805b763e: 78.8 kJ/mol (0.00%)
ef992d8f_iso2: 79.4 kJ/mol (0.00%)
c43bc9af: 80.0 kJ/mol (0.00%)
d2bb93b4: 80.7 kJ/mol (0.00%)
f108fa3b: 80.8 kJ/mol (0.00%)
733a7e09_iso1: 81.0 kJ/mol (0.00%)
c9ef3630_iso5: 85.7 kJ/mol (0.00%)
c9ef3630_iso4: 85.7 kJ/mol (0.00%)
c9ef3630_iso1: 85.7 kJ/mol (0.00%)
252f1154: 86.3 kJ/mol (0.00%)
7785139c: 86.4 kJ/mol (0.00%)
1dafab5d: 88.0 kJ/mol (0.00%)
60c25592: 91.9 kJ/mol (0.00%)
703920bd_iso3: 95.5 kJ/mol (0.00%)
de0fc377: 96.5 kJ/mol (0.00%)
703920bd_iso4: 99.5 kJ/mol (0.00%)
c09c0ae8: 103.2 kJ/mol (0.00%)
659d5d7a: 107.5 kJ/mol (0.00%)
c6446001: 107.6 kJ/mol (0.00%)
8e930666: 109.7 kJ/mol (0.00%)
fce9bf08: 114.0 kJ/mol (0.00%)
84845f77: 123.0 kJ/mol (0.00%)
f4a79a8a: 123.7 kJ/mol (0.00%)
3c4e9b35: 125.5 kJ/mol (0.00%)
9f38b128: 125.7 kJ/mol (0.00%)
be95ff29_iso1: 126.7 kJ/mol (0.00%)

```
d502202a: 127.3 kJ/mol (0.00%)
266c139a: 127.5 kJ/mol (0.00%)
7edc1e61: 134.2 kJ/mol (0.00%)
7565dabb: 134.9 kJ/mol (0.00%)
6ab80909: 136.6 kJ/mol (0.00%)
997be6ee: 140.4 kJ/mol (0.00%)
a176f71d: 144.5 kJ/mol (0.00%)
0c789d48: 145.8 kJ/mol (0.00%)
6b7de07c_iso1: 145.8 kJ/mol (0.00%)
e708dfd7: 152.6 kJ/mol (0.00%)
4d97b7ba: 156.1 kJ/mol (0.00%)
bbf6d694: 158.5 kJ/mol (0.00%)
683426a3: 167.0 kJ/mol (0.00%)
d7d12080: 208.0 kJ/mol (0.00%)
a6ee78ce: 218.0 kJ/mol (0.00%)
502568a4: 999.0 kJ/mol (0.00%)
50c6ec00: 999.0 kJ/mol (0.00%)
a8ce9f3f: 999.0 kJ/mol (0.00%)
55cf2e94: 999.0 kJ/mol (0.00%)
e518f1ad: 999.0 kJ/mol (0.00%)
b031b2aa: 999.0 kJ/mol (0.00%)
d6fb70e5: 999.0 kJ/mol (0.00%)
0d51b9e6: 999.0 kJ/mol (0.00%)
81c724c8: 999.0 kJ/mol (0.00%)
d1768900: 999.0 kJ/mol (0.00%)
ed93ff2c: 999.0 kJ/mol (0.00%)
b5475e30: 999.0 kJ/mol (0.00%)
```

3.12 C1 (standard parameters)

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
ce3fb896_iso1: 0.0 kJ/mol (64.02%)
95bd421f: 4.0 kJ/mol (12.93%)
95bd421f_iso2: 4.0 kJ/mol (12.93%)
b2322e34_iso1: 4.9 kJ/mol (8.75%)
3966abce: 11.0 kJ/mol (0.76%)
1dbf89ab: 13.0 kJ/mol (0.33%)
95bd421f_iso1: 16.0 kJ/mol (0.10%)
ce3fb896_iso2: 17.0 kJ/mol (0.07%)
1dbf89ab_iso3: 17.0 kJ/mol (0.07%)
1dbf89ab_iso2: 20.0 kJ/mol (0.02%)
1dbf89ab_iso1: 21.0 kJ/mol (0.01%)
ce3fb896_iso3: 22.0 kJ/mol (0.01%)
e1fe10a2: 24.9 kJ/mol (0.00%)
b2322e34_iso2: 27.9 kJ/mol (0.00%)
b2322e34_iso3: 34.9 kJ/mol (0.00%)
df552d15: 35.0 kJ/mol (0.00%)
df552d15_iso2: 35.0 kJ/mol (0.00%)
df552d15_iso3: 36.0 kJ/mol (0.00%)
df552d15_iso1: 39.0 kJ/mol (0.00%)
906d3a5f: 41.0 kJ/mol (0.00%)
36db918b: 43.0 kJ/mol (0.00%)
9e521008: 47.3 kJ/mol (0.00%)
```

```
ad7229f3: 47.6 kJ/mol (0.00%)
0703cba8: 55.0 kJ/mol (0.00%)
e2464e9c: 55.1 kJ/mol (0.00%)
b6b3f22e: 55.3 kJ/mol (0.00%)
53e7bc7b: 57.0 kJ/mol (0.00%)
8b00999d: 58.0 kJ/mol (0.00%)
65dcd307: 60.0 kJ/mol (0.00%)
d5ab9c5b: 61.0 kJ/mol (0.00%)
6ecee2de: 62.3 kJ/mol (0.00%)
61b89b99: 64.6 kJ/mol (0.00%)
87b9d6cb: 65.8 kJ/mol (0.00%)
reagents_iso2: 73.4 kJ/mol (0.00%)
reagents: 73.4 kJ/mol (0.00%)
a05f477a: 73.4 kJ/mol (0.00%)
f27da291: 76.9 kJ/mol (0.00%)
0a881e76: 78.4 kJ/mol (0.00%)
41ee2bb7: 78.5 kJ/mol (0.00%)
6e120bcf: 78.9 kJ/mol (0.00%)
0ae3c339: 79.5 kJ/mol (0.00%)
1f40d877: 95.0 kJ/mol (0.00%)
7d710a9f: 97.0 kJ/mol (0.00%)
ceab3138: 98.0 kJ/mol (0.00%)
f301e060: 100.3 kJ/mol (0.00%)
7cca303b: 101.9 kJ/mol (0.00%)
59023ac6: 103.3 kJ/mol (0.00%)
5f22a0ec_iso1: 106.1 kJ/mol (0.00%)
bffca0df: 106.4 kJ/mol (0.00%)
6c84106c: 108.7 kJ/mol (0.00%)
ba589370: 108.9 kJ/mol (0.00%)
11cadd6b: 110.9 kJ/mol (0.00%)
436ef9de: 112.9 kJ/mol (0.00%)
4982d558: 114.0 kJ/mol (0.00%)
34274188: 114.9 kJ/mol (0.00%)
e4df749d: 115.1 kJ/mol (0.00%)
023fcb0d_iso1: 115.4 kJ/mol (0.00%)
ac9bd1ed: 122.4 kJ/mol (0.00%)
e9b4463c: 122.9 kJ/mol (0.00%)
9e8cf8a7: 125.0 kJ/mol (0.00%)
6c05cf72: 125.9 kJ/mol (0.00%)
7a364f3c: 128.0 kJ/mol (0.00%)
ff9b7bea: 131.0 kJ/mol (0.00%)
5c5013b0: 131.0 kJ/mol (0.00%)
757de2e1: 132.4 kJ/mol (0.00%)
a83b483e: 143.3 kJ/mol (0.00%)
a1848c8a: 146.9 kJ/mol (0.00%)
dc46bdd3: 152.1 kJ/mol (0.00%)
acf27d1a: 155.0 kJ/mol (0.00%)
8244c12e: 155.4 kJ/mol (0.00%)
50f34a6e: 156.0 kJ/mol (0.00%)
44955a0a: 162.4 kJ/mol (0.00%)
dfa995d7: 164.3 kJ/mol (0.00%)
2db09390: 167.0 kJ/mol (0.00%)
c202aab9: 168.3 kJ/mol (0.00%)
987d0eaf: 170.0 kJ/mol (0.00%)
```

```
1d5c4e85: 173.4 kJ/mol (0.00%)
c4b4716c: 175.0 kJ/mol (0.00%)
926141b1: 177.0 kJ/mol (0.00%)
3eea2215: 181.1 kJ/mol (0.00%)
dc840b13: 186.0 kJ/mol (0.00%)
2f82c142: 195.0 kJ/mol (0.00%)
8c349b1b: 196.1 kJ/mol (0.00%)
09ffed19: 199.0 kJ/mol (0.00%)
6e11ddd1: 999.0 kJ/mol (0.00%)
72c93b9f: 999.0 kJ/mol (0.00%)
27ae2c57: 999.0 kJ/mol (0.00%)
64e57191: 999.0 kJ/mol (0.00%)
3ed971dd: 999.0 kJ/mol (0.00%)
37f8c646: 999.0 kJ/mol (0.00%)
c43c9380: 999.0 kJ/mol (0.00%)
2bd43ff2: 999.0 kJ/mol (0.00%)
73694f35: 999.0 kJ/mol (0.00%)
6dee931b: 999.0 kJ/mol (0.00%)
46321695: 999.0 kJ/mol (0.00%)
3afef2e5: 999.0 kJ/mol (0.00%)
```

3.13 C1 (traces of water)

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
c0218d9d: 0.0 kJ/mol (72.33%)
be5954a3: 5.3 kJ/mol (8.57%)
476a2dbd_iso4: 6.4 kJ/mol (5.41%)
a1614b5a_iso4: 6.6 kJ/mol (4.99%)
82a25b8a: 9.0 kJ/mol (1.94%)
a7fa0755: 9.4 kJ/mol (1.61%)
c3aaa925_iso4: 10.0 kJ/mol (1.29%)
3452703f: 11.1 kJ/mol (0.82%)
a1614b5a_iso2: 11.6 kJ/mol (0.66%)
b2322e34_iso1: 12.3 kJ/mol (0.51%)
4af77da0: 13.0 kJ/mol (0.38%)
8d9c1f0c: 13.0 kJ/mol (0.38%)
36efe39f_iso1: 13.0 kJ/mol (0.38%)
c3aaa925_iso3: 15.0 kJ/mol (0.17%)
476a2dbd_iso2: 15.4 kJ/mol (0.14%)
ca3b990f: 15.6 kJ/mol (0.13%)
12785316: 16.0 kJ/mol (0.11%)
8c65ba6a_iso1: 18.0 kJ/mol (0.05%)
36efe39f: 19.0 kJ/mol (0.03%)
c3aaa925_iso5: 20.0 kJ/mol (0.02%)
476a2dbd_iso3: 20.4 kJ/mol (0.02%)
36efe39f_iso2: 21.0 kJ/mol (0.02%)
87b9d6cb_iso5: 23.6 kJ/mol (0.01%)
1516324e: 26.6 kJ/mol (0.00%)
87b9d6cb_iso1: 28.6 kJ/mol (0.00%)
ce3fb896_iso1: 28.6 kJ/mol (0.00%)
dd0fd152: 29.0 kJ/mol (0.00%)
0fa40cba: 29.6 kJ/mol (0.00%)
c3aaa925_iso6: 30.0 kJ/mol (0.00%)
```

6ddb7f90: 30.0 kJ/mol (0.00%)
745cd4e1: 31.3 kJ/mol (0.00%)
c3aaa925_iso1: 32.0 kJ/mol (0.00%)
c3aaa925_iso2: 32.0 kJ/mol (0.00%)
220c8f16: 32.0 kJ/mol (0.00%)
41ee2bb7_iso1: 33.1 kJ/mol (0.00%)
87b9d6cb_iso2: 33.6 kJ/mol (0.00%)
1dbf89ab: 34.9 kJ/mol (0.00%)
25f972c0: 34.9 kJ/mol (0.00%)
2ee85692_iso4: 35.0 kJ/mol (0.00%)
b2322e34_iso2: 35.3 kJ/mol (0.00%)
2ee85692_iso3: 36.0 kJ/mol (0.00%)
87b9d6cb_iso4: 36.6 kJ/mol (0.00%)
a1614b5a_iso3: 36.6 kJ/mol (0.00%)
41ee2bb7_iso2: 38.1 kJ/mol (0.00%)
1dbf89ab_iso3: 38.9 kJ/mol (0.00%)
2ee85692_iso5: 39.0 kJ/mol (0.00%)
87b9d6cb_iso3: 39.6 kJ/mol (0.00%)
a170560c: 39.8 kJ/mol (0.00%)
a1614b5a_iso6: 40.6 kJ/mol (0.00%)
2ee85692_iso2: 41.0 kJ/mol (0.00%)
1dbf89ab_iso2: 41.9 kJ/mol (0.00%)
a7863635_iso1: 42.2 kJ/mol (0.00%)
b2322e34_iso3: 42.3 kJ/mol (0.00%)
1dbf89ab_iso1: 42.9 kJ/mol (0.00%)
43bba2fb: 43.4 kJ/mol (0.00%)
54bcd596: 43.6 kJ/mol (0.00%)
52aba1a7: 44.8 kJ/mol (0.00%)
a7863635: 45.2 kJ/mol (0.00%)
40511f99: 45.4 kJ/mol (0.00%)
a1614b5a_iso1: 45.6 kJ/mol (0.00%)
69309741_iso4: 46.2 kJ/mol (0.00%)
c1791410: 46.2 kJ/mol (0.00%)
95bd421f: 46.5 kJ/mol (0.00%)
95bd421f_iso2: 46.5 kJ/mol (0.00%)
ce3fb896_iso2: 46.6 kJ/mol (0.00%)
4aaeec87_iso1: 46.7 kJ/mol (0.00%)
36db918b: 46.9 kJ/mol (0.00%)
11cadd6b: 47.2 kJ/mol (0.00%)
a67dc816: 47.6 kJ/mol (0.00%)
2ee85692_iso1: 48.0 kJ/mol (0.00%)
94ae675f: 48.1 kJ/mol (0.00%)
fdd1f0e4: 49.8 kJ/mol (0.00%)
d1814d03: 50.8 kJ/mol (0.00%)
b1d67439: 51.5 kJ/mol (0.00%)
ce3fb896_iso3: 51.6 kJ/mol (0.00%)
4aaeec87_iso5: 51.7 kJ/mol (0.00%)
6e3a95b4: 52.2 kJ/mol (0.00%)
476a2dbd_iso1: 52.4 kJ/mol (0.00%)
70400aa5: 52.8 kJ/mol (0.00%)
9e521008: 54.1 kJ/mol (0.00%)
bc6e217b: 54.2 kJ/mol (0.00%)
af58a8d5: 54.3 kJ/mol (0.00%)
a1614b5a_iso5: 54.6 kJ/mol (0.00%)

69309741_iso3: 55.2 kJ/mol (0.00%)
a1614b5a_iso7: 56.6 kJ/mol (0.00%)
69309741_iso1: 57.2 kJ/mol (0.00%)
44c9cfc7: 57.4 kJ/mol (0.00%)
278d5221: 58.1 kJ/mol (0.00%)
94993670: 58.2 kJ/mol (0.00%)
95bd421f_iso1: 58.5 kJ/mol (0.00%)
8af48ddb: 58.7 kJ/mol (0.00%)
939a29c5: 58.7 kJ/mol (0.00%)
05410936_iso1: 58.8 kJ/mol (0.00%)
69309741_iso2: 59.2 kJ/mol (0.00%)
4aaeec87_iso2: 59.7 kJ/mol (0.00%)
41ace24f: 59.8 kJ/mol (0.00%)
b734f0ac: 60.0 kJ/mol (0.00%)
b6b3f22e: 60.0 kJ/mol (0.00%)
4f5e9580: 60.0 kJ/mol (0.00%)
f81b17d2: 62.0 kJ/mol (0.00%)
4aaeec87_iso9: 62.7 kJ/mol (0.00%)
1355eeb0: 62.9 kJ/mol (0.00%)
906d3a5f: 63.0 kJ/mol (0.00%)
7d9a1d79: 63.0 kJ/mol (0.00%)
b518aef4_iso2: 64.1 kJ/mol (0.00%)
438d416f: 65.1 kJ/mol (0.00%)
afc8c127: 65.7 kJ/mol (0.00%)
4aaeec87_iso3: 66.7 kJ/mol (0.00%)
d857ca42: 66.7 kJ/mol (0.00%)
dfedb5d7: 68.1 kJ/mol (0.00%)
4aaeec87_iso6: 68.7 kJ/mol (0.00%)
a1614b5a_iso8: 69.6 kJ/mol (0.00%)
b518aef4_iso4: 70.1 kJ/mol (0.00%)
3c867405: 70.6 kJ/mol (0.00%)
96460a49: 71.2 kJ/mol (0.00%)
4aaeec87_iso8: 71.7 kJ/mol (0.00%)
reagents: 71.9 kJ/mol (0.00%)
f265c733: 71.9 kJ/mol (0.00%)
baedaf73: 73.0 kJ/mol (0.00%)
57c94a9c: 73.1 kJ/mol (0.00%)
70fe1301: 73.5 kJ/mol (0.00%)
4aaeec87_iso4: 73.7 kJ/mol (0.00%)
892705fb: 73.9 kJ/mol (0.00%)
reagents_iso1: 74.8 kJ/mol (0.00%)
21aa385b: 75.1 kJ/mol (0.00%)
68e8f9a3: 75.2 kJ/mol (0.00%)
90f695db: 75.5 kJ/mol (0.00%)
0e6eb35d: 75.7 kJ/mol (0.00%)
b518aef4_iso3: 76.1 kJ/mol (0.00%)
df552d15_iso2: 76.2 kJ/mol (0.00%)
3998e699: 76.7 kJ/mol (0.00%)
2b949d61: 76.8 kJ/mol (0.00%)
e4d7c463: 77.0 kJ/mol (0.00%)
fc10d716: 77.0 kJ/mol (0.00%)
20645107: 77.5 kJ/mol (0.00%)
578abfc8: 77.7 kJ/mol (0.00%)
df552d15_iso3: 78.2 kJ/mol (0.00%)

e0b3f5ee_iso1: 78.3 kJ/mol (0.00%)
4aaeec87_iso7: 78.7 kJ/mol (0.00%)
feab3da5: 79.1 kJ/mol (0.00%)
df552d15_iso1: 80.2 kJ/mol (0.00%)
42c72480: 80.7 kJ/mol (0.00%)
cf8fc539: 81.6 kJ/mol (0.00%)
22c092b0: 81.7 kJ/mol (0.00%)
5c5013b0: 82.0 kJ/mol (0.00%)
5c5013b0_iso1: 82.0 kJ/mol (0.00%)
0347fa47: 83.8 kJ/mol (0.00%)
53e7bc7b: 84.0 kJ/mol (0.00%)
c64f7f05: 85.7 kJ/mol (0.00%)
ff838b34: 86.5 kJ/mol (0.00%)
72c93b9f_iso1: 86.7 kJ/mol (0.00%)
84d8b88d: 87.4 kJ/mol (0.00%)
30fa467b: 87.7 kJ/mol (0.00%)
787ed27f: 87.7 kJ/mol (0.00%)
ad7229f3: 87.8 kJ/mol (0.00%)
b1e046a7: 87.9 kJ/mol (0.00%)
d5ab9c5b: 88.0 kJ/mol (0.00%)
6658ad8e: 88.5 kJ/mol (0.00%)
6e120bcf: 89.1 kJ/mol (0.00%)
dbec1675: 89.3 kJ/mol (0.00%)
0a3e0bfe: 89.8 kJ/mol (0.00%)
a5dd6fe2: 90.3 kJ/mol (0.00%)
6b736b5a: 91.3 kJ/mol (0.00%)
7a8e931b: 92.0 kJ/mol (0.00%)
f24b0713: 92.1 kJ/mol (0.00%)
581ceada: 93.0 kJ/mol (0.00%)
392b5e92: 94.0 kJ/mol (0.00%)
39334313_iso1: 94.1 kJ/mol (0.00%)
39334313_iso5: 94.1 kJ/mol (0.00%)
2ae7d181: 94.8 kJ/mol (0.00%)
0b6ab3a6: 95.6 kJ/mol (0.00%)
a5657d37: 97.0 kJ/mol (0.00%)
8b00999d: 97.3 kJ/mol (0.00%)
0d68203f: 98.1 kJ/mol (0.00%)
75024d16: 98.2 kJ/mol (0.00%)
810d8f44: 98.4 kJ/mol (0.00%)
47a5f542: 98.6 kJ/mol (0.00%)
446ffc72: 99.0 kJ/mol (0.00%)
e0154dc8: 99.2 kJ/mol (0.00%)
515b53b5: 100.6 kJ/mol (0.00%)
9a7c0865: 101.0 kJ/mol (0.00%)
0733a3d3: 101.4 kJ/mol (0.00%)
c2259bcc: 101.4 kJ/mol (0.00%)
7177e7d0: 101.5 kJ/mol (0.00%)
347799b3: 104.0 kJ/mol (0.00%)
2274e5fc: 105.1 kJ/mol (0.00%)
32eb6f11: 105.6 kJ/mol (0.00%)
1c199b0d: 106.0 kJ/mol (0.00%)
947defdb_iso1: 106.1 kJ/mol (0.00%)
cfd6dc35: 106.2 kJ/mol (0.00%)
532a1d21: 107.8 kJ/mol (0.00%)

95015706: 108.1 kJ/mol (0.00%)
39334313_iso3: 108.1 kJ/mol (0.00%)
b518aef4_iso1: 108.1 kJ/mol (0.00%)
ea53d0b0: 108.3 kJ/mol (0.00%)
410a47f3: 108.8 kJ/mol (0.00%)
0eaee174: 109.0 kJ/mol (0.00%)
73694f35: 109.5 kJ/mol (0.00%)
f9547974: 110.2 kJ/mol (0.00%)
bffca0df: 110.6 kJ/mol (0.00%)
2cbd2222: 110.6 kJ/mol (0.00%)
c9f57ad8: 111.2 kJ/mol (0.00%)
6903cd01: 111.4 kJ/mol (0.00%)
f61c2df8: 112.3 kJ/mol (0.00%)
53da1ba2: 113.1 kJ/mol (0.00%)
baecbb7c: 115.0 kJ/mol (0.00%)
14f21aa0: 116.0 kJ/mol (0.00%)
3405a7ac: 116.7 kJ/mol (0.00%)
f27da291: 117.1 kJ/mol (0.00%)
f3e9e02d: 119.1 kJ/mol (0.00%)
f67d0032: 119.6 kJ/mol (0.00%)
7d710a9f: 120.6 kJ/mol (0.00%)
b84ba48e: 120.7 kJ/mol (0.00%)
411241f2: 120.8 kJ/mol (0.00%)
453d9a17: 121.0 kJ/mol (0.00%)
422a0446: 121.1 kJ/mol (0.00%)
50ae04c1: 123.5 kJ/mol (0.00%)
d959b760: 124.1 kJ/mol (0.00%)
16191336: 124.2 kJ/mol (0.00%)
6a15d6f6: 124.4 kJ/mol (0.00%)
7daf51d1: 125.8 kJ/mol (0.00%)
e54cb6ff: 126.0 kJ/mol (0.00%)
1c165b5d: 126.0 kJ/mol (0.00%)
39334313_iso2: 126.1 kJ/mol (0.00%)
da4d5915: 126.3 kJ/mol (0.00%)
cdff053a: 127.0 kJ/mol (0.00%)
1cce89bd: 127.0 kJ/mol (0.00%)
f301e060: 127.2 kJ/mol (0.00%)
bc13ae15: 129.6 kJ/mol (0.00%)
591f1ea5: 129.8 kJ/mol (0.00%)
a839722f: 130.0 kJ/mol (0.00%)
b842f01d: 130.2 kJ/mol (0.00%)
5f22a0ec_iso1: 130.5 kJ/mol (0.00%)
34274188: 131.0 kJ/mol (0.00%)
635042c4: 131.4 kJ/mol (0.00%)
5413467b: 131.5 kJ/mol (0.00%)
d94636a5: 131.6 kJ/mol (0.00%)
067c9ee1: 132.2 kJ/mol (0.00%)
c9e0d854: 132.5 kJ/mol (0.00%)
6c05cf72: 133.3 kJ/mol (0.00%)
3a26336e: 133.6 kJ/mol (0.00%)
757de2e1: 133.8 kJ/mol (0.00%)
7b02d57a: 133.8 kJ/mol (0.00%)
fd4ccd88: 133.8 kJ/mol (0.00%)
75cffb95: 133.9 kJ/mol (0.00%)

6a06f3ef: 134.6 kJ/mol (0.00%)
5f831297: 135.0 kJ/mol (0.00%)
08062113: 135.2 kJ/mol (0.00%)
1f40d877: 136.2 kJ/mol (0.00%)
67f876a8: 136.2 kJ/mol (0.00%)
e4df749d: 136.6 kJ/mol (0.00%)
8e1268d4: 137.5 kJ/mol (0.00%)
4982d558: 137.6 kJ/mol (0.00%)
7c37c3b1: 139.1 kJ/mol (0.00%)
54376309: 139.2 kJ/mol (0.00%)
7cca303b: 139.4 kJ/mol (0.00%)
5e377f9a: 140.1 kJ/mol (0.00%)
39334313_iso4: 140.1 kJ/mol (0.00%)
14c3e6d9: 140.8 kJ/mol (0.00%)
5849cce1: 142.0 kJ/mol (0.00%)
c397d33e: 142.4 kJ/mol (0.00%)
eb854929: 142.6 kJ/mol (0.00%)
023fcb0d_iso1: 143.2 kJ/mol (0.00%)
46fb02ce: 143.7 kJ/mol (0.00%)
e9b4463c: 144.9 kJ/mol (0.00%)
535bc507: 145.8 kJ/mol (0.00%)
bfcc09e9: 146.0 kJ/mol (0.00%)
0c47afee: 146.0 kJ/mol (0.00%)
ac9bd1ed: 146.2 kJ/mol (0.00%)
37ce1508: 146.3 kJ/mol (0.00%)
f6e5b2dc: 147.3 kJ/mol (0.00%)
b9733653: 148.1 kJ/mol (0.00%)
fdb89dd9: 148.2 kJ/mol (0.00%)
ce54be14: 148.3 kJ/mol (0.00%)
097c517d: 148.4 kJ/mol (0.00%)
0283b665: 149.9 kJ/mol (0.00%)
8f8276aa: 149.9 kJ/mol (0.00%)
80f0ac98: 150.0 kJ/mol (0.00%)
8406c9a5: 150.3 kJ/mol (0.00%)
f4a80253: 150.4 kJ/mol (0.00%)
7e7f1f73: 150.4 kJ/mol (0.00%)
a7672b7a: 150.6 kJ/mol (0.00%)
7acc35a6: 151.6 kJ/mol (0.00%)
7a364f3c: 151.6 kJ/mol (0.00%)
2f640941: 152.6 kJ/mol (0.00%)
c462b46c: 153.6 kJ/mol (0.00%)
943e6937: 153.7 kJ/mol (0.00%)
8244c12e: 153.9 kJ/mol (0.00%)
a1848c8a: 154.3 kJ/mol (0.00%)
436ef9de: 155.1 kJ/mol (0.00%)
a2da6e32: 155.6 kJ/mol (0.00%)
82776c1f: 156.3 kJ/mol (0.00%)
3b55347e: 156.6 kJ/mol (0.00%)
398aef58: 157.2 kJ/mol (0.00%)
5cf6225a: 158.2 kJ/mol (0.00%)
f67ea77d: 158.6 kJ/mol (0.00%)
395f2d10: 159.4 kJ/mol (0.00%)
adb79a04: 159.7 kJ/mol (0.00%)
fc6b6aec: 159.9 kJ/mol (0.00%)

9ece2004: 161.0 kJ/mol (0.00%)
0792445b: 161.1 kJ/mol (0.00%)
7136999b: 161.4 kJ/mol (0.00%)
e9a3ffb1: 162.0 kJ/mol (0.00%)
c37c38f8: 162.2 kJ/mol (0.00%)
b1a0fb72: 163.1 kJ/mol (0.00%)
0186079b: 164.0 kJ/mol (0.00%)
d52965bc: 164.5 kJ/mol (0.00%)
f9a0a034: 165.4 kJ/mol (0.00%)
ea2852e0: 165.6 kJ/mol (0.00%)
dffbaef0: 165.6 kJ/mol (0.00%)
9e8cf8a7: 167.5 kJ/mol (0.00%)
f7bf459c: 168.0 kJ/mol (0.00%)
eadafa4c: 168.6 kJ/mol (0.00%)
a83b483e: 170.2 kJ/mol (0.00%)
02983091: 170.3 kJ/mol (0.00%)
46032e4a: 171.6 kJ/mol (0.00%)
86892d71: 172.0 kJ/mol (0.00%)
a171daf2: 172.1 kJ/mol (0.00%)
638b86f4: 172.1 kJ/mol (0.00%)
e77f7be9: 172.6 kJ/mol (0.00%)
278b4b9c: 172.6 kJ/mol (0.00%)
dc46bdd3: 173.6 kJ/mol (0.00%)
b19da941: 173.7 kJ/mol (0.00%)
23fdc73c: 173.9 kJ/mol (0.00%)
bf5730a6: 174.0 kJ/mol (0.00%)
0343779c: 174.2 kJ/mol (0.00%)
c2248ebc: 175.2 kJ/mol (0.00%)
6d5c9250: 175.2 kJ/mol (0.00%)
6122975b: 176.6 kJ/mol (0.00%)
b69b36af: 178.6 kJ/mol (0.00%)
1be46151: 180.0 kJ/mol (0.00%)
50f34a6e: 180.6 kJ/mol (0.00%)
92e589ac: 182.0 kJ/mol (0.00%)
5f2ec45d: 182.2 kJ/mol (0.00%)
3639f23f: 187.3 kJ/mol (0.00%)
c1878f8b: 190.7 kJ/mol (0.00%)
b5eb8b85: 191.8 kJ/mol (0.00%)
7a37d27b: 194.2 kJ/mol (0.00%)
4e45f0f7: 195.0 kJ/mol (0.00%)
c202aab9: 195.2 kJ/mol (0.00%)
15b1254c: 195.2 kJ/mol (0.00%)
f6eecd3d: 197.0 kJ/mol (0.00%)
987d0eaf: 197.0 kJ/mol (0.00%)
404e5494: 202.1 kJ/mol (0.00%)
ccee0a18: 205.0 kJ/mol (0.00%)
3eea2215: 205.5 kJ/mol (0.00%)
949b671b: 207.5 kJ/mol (0.00%)
2db09390: 208.2 kJ/mol (0.00%)
79cf8467: 211.7 kJ/mol (0.00%)
2f82c142: 212.9 kJ/mol (0.00%)
8813ab1a: 213.7 kJ/mol (0.00%)
95c66d2c: 214.1 kJ/mol (0.00%)
c4b4716c: 216.2 kJ/mol (0.00%)

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8c349b1b: 217.6 kJ/mol (0.00%)
926141b1: 218.2 kJ/mol (0.00%)
59aba0ba: 218.2 kJ/mol (0.00%)
97012c1c: 219.1 kJ/mol (0.00%)
969fe2ae: 220.1 kJ/mol (0.00%)
a52d56fd: 223.7 kJ/mol (0.00%)
c0bf44fb: 224.2 kJ/mol (0.00%)
dc840b13: 227.2 kJ/mol (0.00%)
c6510534: 231.1 kJ/mol (0.00%)
1bf7dd8c: 234.7 kJ/mol (0.00%)
f3a56696: 234.9 kJ/mol (0.00%)
7ec957c7: 238.6 kJ/mol (0.00%)
09ffed19: 240.2 kJ/mol (0.00%)
7b501832: 244.1 kJ/mol (0.00%)
daed7e98: 249.1 kJ/mol (0.00%)
6d628c82: 253.1 kJ/mol (0.00%)
bdcccd9a: 267.0 kJ/mol (0.00%)
b1fda6c5: 999.0 kJ/mol (0.00%)
21e32d31: 999.0 kJ/mol (0.00%)
15e28628: 999.0 kJ/mol (0.00%)
c43c9380: 999.0 kJ/mol (0.00%)
64e57191: 999.0 kJ/mol (0.00%)
3ed971dd: 999.0 kJ/mol (0.00%)
37f8c646: 999.0 kJ/mol (0.00%)
ac0c4b1c: 999.0 kJ/mol (0.00%)
1dbeaba0: 999.0 kJ/mol (0.00%)
ee067efc: 999.0 kJ/mol (0.00%)
7c2ceea6: 999.0 kJ/mol (0.00%)
50edc79f: 999.0 kJ/mol (0.00%)
9f7be429: 999.0 kJ/mol (0.00%)
e170e11e: 999.0 kJ/mol (0.00%)
2bd43ff2: 999.0 kJ/mol (0.00%)
3afef2e5: 999.0 kJ/mol (0.00%)
6dee931b: 999.0 kJ/mol (0.00%)
46321695: 999.0 kJ/mol (0.00%)
0a77af16: 999.0 kJ/mol (0.00%)
46fffcb4: 999.0 kJ/mol (0.00%)
112bdaf1: 999.0 kJ/mol (0.00%)
32aa8df6: 999.0 kJ/mol (0.00%)
9331ed71: 999.0 kJ/mol (0.00%)
7a253077: 999.0 kJ/mol (0.00%)
56a9f817: 999.0 kJ/mol (0.00%)
2fcd870a: 999.0 kJ/mol (0.00%)
5dee0072: 999.0 kJ/mol (0.00%)
b583471a: 999.0 kJ/mol (0.00%)
6412f19a: 999.0 kJ/mol (0.00%)
f3037298: 999.0 kJ/mol (0.00%)
27995094: 999.0 kJ/mol (0.00%)
9fe198aa: 999.0 kJ/mol (0.00%)
406fb383: 999.0 kJ/mol (0.00%)
d30e2f97: 999.0 kJ/mol (0.00%)
984dc95b: 999.0 kJ/mol (0.00%)
92375b24: 999.0 kJ/mol (0.00%)
6d48a909: 999.0 kJ/mol (0.00%)
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db0b882a: 999.0 kJ/mol (0.00%)
e3757d4c: 999.0 kJ/mol (0.00%)
783405e3: 999.0 kJ/mol (0.00%)
59791eb4: 999.0 kJ/mol (0.00%)
ba8cb57d: 999.0 kJ/mol (0.00%)
44a2c490: 999.0 kJ/mol (0.00%)
25991442: 999.0 kJ/mol (0.00%)
e36bd0a2: 999.0 kJ/mol (0.00%)
749e5ca8: 999.0 kJ/mol (0.00%)
c434fe19: 999.0 kJ/mol (0.00%)
ebcf843e: 999.0 kJ/mol (0.00%)
16a6a891: 999.0 kJ/mol (0.00%)
555fd62d: 999.0 kJ/mol (0.00%)
1acb8195: 999.0 kJ/mol (0.00%)
88e320fc: 999.0 kJ/mol (0.00%)
4616e782: 999.0 kJ/mol (0.00%)
7cd76dcd: 999.0 kJ/mol (0.00%)
5e520afd: 999.0 kJ/mol (0.00%)
9f5a5834: 999.0 kJ/mol (0.00%)
c9d5f61e: 999.0 kJ/mol (0.00%)
57637b54: 999.0 kJ/mol (0.00%)
a98388f4: 999.0 kJ/mol (0.00%)
1d7a5a46: 999.0 kJ/mol (0.00%)
ef3a3aea: 999.0 kJ/mol (0.00%)
966ff4e0: 999.0 kJ/mol (0.00%)
44927097: 999.0 kJ/mol (0.00%)
07d8c325: 999.0 kJ/mol (0.00%)
360d6b17: 999.0 kJ/mol (0.00%)
33412408: 999.0 kJ/mol (0.00%)
369d40c9: 999.0 kJ/mol (0.00%)
1715ee02: 999.0 kJ/mol (0.00%)
49d2f023: 999.0 kJ/mol (0.00%)
a80e00a7: 999.0 kJ/mol (0.00%)
5edcb3d8: 999.0 kJ/mol (0.00%)
0b032a8c: 999.0 kJ/mol (0.00%)
45402207: 999.0 kJ/mol (0.00%)
8efe316c: 999.0 kJ/mol (0.00%)
59a3afdd: 999.0 kJ/mol (0.00%)
5c16a4f6: 999.0 kJ/mol (0.00%)
9320cb51: 999.0 kJ/mol (0.00%)
4dc7e2d2: 999.0 kJ/mol (0.00%)
7d2626db: 999.0 kJ/mol (0.00%)
f50f8fe2: 999.0 kJ/mol (0.00%)
2caa03f3: 999.0 kJ/mol (0.00%)
5ab9bd11: 999.0 kJ/mol (0.00%)
731744be: 999.0 kJ/mol (0.00%)
d889abd0: 999.0 kJ/mol (0.00%)
c89a2689: 999.0 kJ/mol (0.00%)
ea2d06a8: 999.0 kJ/mol (0.00%)
e37334f4: 999.0 kJ/mol (0.00%)
d5f75275: 999.0 kJ/mol (0.00%)
922ad16f: 999.0 kJ/mol (0.00%)
e53757e4: 999.0 kJ/mol (0.00%)
0dec5fcc: 999.0 kJ/mol (0.00%)

f0be6721: 999.0 kJ/mol (0.00%)
d36fd241: 999.0 kJ/mol (0.00%)
58a0cc11: 999.0 kJ/mol (0.00%)
a31eea09: 999.0 kJ/mol (0.00%)
a1901afc: 999.0 kJ/mol (0.00%)
0894e093: 999.0 kJ/mol (0.00%)
6f2ab934: 999.0 kJ/mol (0.00%)
370642c8: 999.0 kJ/mol (0.00%)
b80e07f5: 999.0 kJ/mol (0.00%)

3.14 C2

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
49da4c4a: 0.0 kJ/mol (53.23%)
8736a284_iso4: 1.0 kJ/mol (35.56%)
c91a59af: 4.0 kJ/mol (10.60%)
8736a284_iso3: 12.0 kJ/mol (0.42%)
8736a284_iso1: 16.0 kJ/mol (0.08%)
8736a284_iso2: 16.0 kJ/mol (0.08%)
19849d71: 21.2 kJ/mol (0.01%)
e70324d0: 27.0 kJ/mol (0.00%)
06e4ff22: 55.7 kJ/mol (0.00%)
6ea85867: 56.0 kJ/mol (0.00%)
138d32c9: 56.0 kJ/mol (0.00%)
bf3081d8_iso1: 70.8 kJ/mol (0.00%)
69540273: 77.5 kJ/mol (0.00%)
reagents: 86.3 kJ/mol (0.00%)
18257f2f: 86.3 kJ/mol (0.00%)
reagents_iso2: 86.3 kJ/mol (0.00%)
c5507a5f: 91.5 kJ/mol (0.00%)
ec6fe9ca: 95.3 kJ/mol (0.00%)
3821a10d: 97.3 kJ/mol (0.00%)
78a5b243: 97.8 kJ/mol (0.00%)
6ea5f370: 99.8 kJ/mol (0.00%)
d7f6a7dd: 101.0 kJ/mol (0.00%)
35745ff9: 104.3 kJ/mol (0.00%)
b13a6013_iso2: 105.3 kJ/mol (0.00%)
c7d02437: 107.3 kJ/mol (0.00%)
74f0d9fc: 111.0 kJ/mol (0.00%)
e10826d0: 111.1 kJ/mol (0.00%)
3c771357: 112.3 kJ/mol (0.00%)
7274189d: 118.3 kJ/mol (0.00%)
b13a6013_iso3: 118.3 kJ/mol (0.00%)
b13a6013_iso1: 120.3 kJ/mol (0.00%)
f2b2b674_iso1: 123.9 kJ/mol (0.00%)
8fb8e04d: 125.3 kJ/mol (0.00%)
6500ce9c: 127.3 kJ/mol (0.00%)
7f048c00: 128.0 kJ/mol (0.00%)
b43a7a83: 129.4 kJ/mol (0.00%)
4a285dd1_iso4: 131.3 kJ/mol (0.00%)
069632db: 137.0 kJ/mol (0.00%)
422141ec: 142.5 kJ/mol (0.00%)
27ad6ce4: 144.0 kJ/mol (0.00%)

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f99e3f27: 147.4 kJ/mol (0.00%)
fc63f822: 149.3 kJ/mol (0.00%)
d65a839c: 149.3 kJ/mol (0.00%)
4a285dd1_iso2: 154.3 kJ/mol (0.00%)
10edc4b2: 155.3 kJ/mol (0.00%)
8906c711: 159.9 kJ/mol (0.00%)
a268959f: 161.0 kJ/mol (0.00%)
18acd33d: 161.3 kJ/mol (0.00%)
6bd4cc19: 162.3 kJ/mol (0.00%)
f534c371: 166.3 kJ/mol (0.00%)
4a285dd1_iso5: 171.3 kJ/mol (0.00%)
3192b068: 171.5 kJ/mol (0.00%)
f038bcde: 179.0 kJ/mol (0.00%)
reagents_iso1: 184.6 kJ/mol (0.00%)
7ad9f8b1_iso1: 185.3 kJ/mol (0.00%)
4a285dd1_iso3: 192.3 kJ/mol (0.00%)
88520ad9: 193.0 kJ/mol (0.00%)
34899522: 194.3 kJ/mol (0.00%)
4a285dd1_iso1: 219.3 kJ/mol (0.00%)
139fad6b: 233.6 kJ/mol (0.00%)
38ca76b1: 238.9 kJ/mol (0.00%)
079bd2e4: 304.1 kJ/mol (0.00%)
491d179e: 320.7 kJ/mol (0.00%)
5ea1b842: 999.0 kJ/mol (0.00%)
8d694653: 999.0 kJ/mol (0.00%)
35c1f05f: 999.0 kJ/mol (0.00%)
94f9c28a: 999.0 kJ/mol (0.00%)
b5598cef: 999.0 kJ/mol (0.00%)
069d9fc3: 999.0 kJ/mol (0.00%)
7fd12e7b: 999.0 kJ/mol (0.00%)
ff9f192a: 999.0 kJ/mol (0.00%)
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3.15 C3 (standard parameters)

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Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=363K)
9ad545b5: 0.0 kJ/mol (52.76%)
reagents: 2.0 kJ/mol (27.20%)
3ac3eb0f: 3.0 kJ/mol (19.52%)
reagents_iso4: 14.0 kJ/mol (0.51%)
reagents_iso6: 26.3 kJ/mol (0.01%)
6accacb2: 29.0 kJ/mol (0.00%)
reagents_iso1: 35.0 kJ/mol (0.00%)
09e92f90_iso3: 67.0 kJ/mol (0.00%)
dc5148f7: 91.9 kJ/mol (0.00%)
b0797263: 102.0 kJ/mol (0.00%)
5fd05bf8: 111.2 kJ/mol (0.00%)
df520d7e: 112.0 kJ/mol (0.00%)
b775fa8f: 121.0 kJ/mol (0.00%)
6495822d: 125.4 kJ/mol (0.00%)
8908508d: 128.0 kJ/mol (0.00%)
c5deb41c: 133.7 kJ/mol (0.00%)
847924d6: 147.0 kJ/mol (0.00%)
25b0f5e6: 153.0 kJ/mol (0.00%)
```

```
09e92f90_iso2: 153.9 kJ/mol (0.00%)
b0797263_iso1: 156.0 kJ/mol (0.00%)
8d3fa798: 159.3 kJ/mol (0.00%)
09e92f90_iso1: 188.9 kJ/mol (0.00%)
b0137998: 206.0 kJ/mol (0.00%)
```

3.16 C3 (traces of water, $\Delta G^{\ddagger}_{max} = 150\,\mathrm{kJ/mol}$)

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=363K)
9ad545b5: 0.0 kJ/mol (40.93%)
reagents: 2.0 kJ/mol (21.10%)
reagents_iso3: 2.0 kJ/mol (21.10%)
3ac3eb0f: 3.0 kJ/mol (15.14%)
b563628d: 11.1 kJ/mol (1.05%)
reagents_iso4: 14.0 kJ/mol (0.40%)
16cdbb8d: 19.3 kJ/mol (0.07%)
905113d7: 19.7 kJ/mol (0.06%)
e169c493: 20.0 kJ/mol (0.05%)
064a1f19_iso3: 20.3 kJ/mol (0.05%)
064a1f19_iso1: 20.3 kJ/mol (0.05%)
reagents_iso6: 26.3 kJ/mol (0.01%)
2c6110fc_iso2: 35.1 kJ/mol (0.00%)
539cd49f: 40.1 kJ/mol (0.00%)
fb3965cf: 40.1 kJ/mol (0.00%)
5e9e4c04: 40.7 kJ/mol (0.00%)
745c9807: 54.1 kJ/mol (0.00%)
15df2eb0_iso1: 57.9 kJ/mol (0.00%)
09e92f90_iso3: 58.7 kJ/mol (0.00%)
513cb349: 64.1 kJ/mol (0.00%)
2c6110fc_iso1: 64.1 kJ/mol (0.00%)
55d48758: 71.8 kJ/mol (0.00%)
2c6110fc_iso3: 76.1 kJ/mol (0.00%)
15df2eb0_iso4: 80.3 kJ/mol (0.00%)
fea18223: 82.9 kJ/mol (0.00%)
5d6932f3: 83.1 kJ/mol (0.00%)
73c07021: 84.3 kJ/mol (0.00%)
8f2ad513: 84.4 kJ/mol (0.00%)
fc7fcf6c: 87.1 kJ/mol (0.00%)
515fcf5e: 89.0 kJ/mol (0.00%)
81d9ca48: 89.3 kJ/mol (0.00%)
064a1f19_iso2: 90.3 kJ/mol (0.00%)
19bb6f07: 91.3 kJ/mol (0.00%)
dc5148f7: 91.9 kJ/mol (0.00%)
85a37158: 92.3 kJ/mol (0.00%)
e2349175: 93.8 kJ/mol (0.00%)
82cb38b4: 94.3 kJ/mol (0.00%)
6534b186: 95.3 kJ/mol (0.00%)
2d422d28: 97.1 kJ/mol (0.00%)
abfa30a6: 97.1 kJ/mol (0.00%)
df520d7e: 98.7 kJ/mol (0.00%)
1d946d7b: 103.2 kJ/mol (0.00%)
b0797263: 103.6 kJ/mol (0.00%)
6c58cbd1: 103.8 kJ/mol (0.00%)
```

0608a5c9: 108.7 kJ/mol (0.00%)
afd04b4a: 111.3 kJ/mol (0.00%)
81caa516: 113.3 kJ/mol (0.00%)
f36f0080: 114.3 kJ/mol (0.00%)
7ccfdc70: 115.0 kJ/mol (0.00%)
15df2eb0_iso2: 116.0 kJ/mol (0.00%)
b775fa8f: 116.8 kJ/mol (0.00%)
b3cbc1c2: 120.4 kJ/mol (0.00%)
6495822d: 125.4 kJ/mol (0.00%)
1d946d7b_iso1: 127.2 kJ/mol (0.00%)
8908508d: 128.9 kJ/mol (0.00%)
2edf108d: 130.1 kJ/mol (0.00%)
f8d2c3dc: 130.1 kJ/mol (0.00%)
bb5197b2: 132.7 kJ/mol (0.00%)
8b097074: 133.0 kJ/mol (0.00%)
066a7d8e: 133.3 kJ/mol (0.00%)
c5deb41c: 133.7 kJ/mol (0.00%)
874b00d8: 134.1 kJ/mol (0.00%)
64f74bb7: 135.7 kJ/mol (0.00%)
1277f734: 136.1 kJ/mol (0.00%)
6cd81b04: 136.4 kJ/mol (0.00%)
ae2d9e99_iso1: 137.8 kJ/mol (0.00%)
84447ea3: 139.2 kJ/mol (0.00%)
d3e77fcc: 139.3 kJ/mol (0.00%)
82fd8e8e: 140.9 kJ/mol (0.00%)
cdebbeb6: 145.8 kJ/mol (0.00%)
5541c583: 146.0 kJ/mol (0.00%)
847924d6: 147.0 kJ/mol (0.00%)
00c97be6: 149.0 kJ/mol (0.00%)
27a9abca: 150.7 kJ/mol (0.00%)
09e92f90_iso2: 153.9 kJ/mol (0.00%)
b0797263_iso1: 157.6 kJ/mol (0.00%)
8d3fa798: 159.2 kJ/mol (0.00%)
0fdcbbf8: 160.1 kJ/mol (0.00%)
b05c30e8: 160.3 kJ/mol (0.00%)
2eabdcbc: 163.3 kJ/mol (0.00%)
c1741033: 169.3 kJ/mol (0.00%)
fe03f7ab: 184.3 kJ/mol (0.00%)
09e92f90_iso1: 188.9 kJ/mol (0.00%)
59011572: 197.1 kJ/mol (0.00%)
128f3e88: 198.1 kJ/mol (0.00%)
1598521f: 203.3 kJ/mol (0.00%)
52fc36ec: 205.3 kJ/mol (0.00%)
b0137998: 207.6 kJ/mol (0.00%)
a277d61d: 229.0 kJ/mol (0.00%)
971d889a: 235.3 kJ/mol (0.00%)
c3f6dd6f: 272.4 kJ/mol (0.00%)
fe3db213: 999.0 kJ/mol (0.00%)
bd930cde: 999.0 kJ/mol (0.00%)
cc8e6f8c: 999.0 kJ/mol (0.00%)
16ced70b: 999.0 kJ/mol (0.00%)
d3d422f9: 999.0 kJ/mol (0.00%)

3.17 C4

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=373K)
3f62e740: 0.0 kJ/mol (99.70%)
49342575_iso1: 18.0 kJ/mol (0.30%)
3295b5d2: 40.4 kJ/mol (0.00%)
013e8090: 42.9 kJ/mol (0.00%)
08a061f6: 50.3 kJ/mol (0.00%)
a7386600: 58.0 kJ/mol (0.00%)
170ab091: 58.5 kJ/mol (0.00%)
a8a74f3c: 59.5 kJ/mol (0.00%)
441f3533: 88.0 kJ/mol (0.00%)
60daf09c: 95.7 kJ/mol (0.00%)
reagents: 105.7 kJ/mol (0.00%)
reagents_iso1: 105.7 kJ/mol (0.00%)
ae665732: 105.7 kJ/mol (0.00%)
9c552afb: 108.6 kJ/mol (0.00%)
reagents_iso3: 113.7 kJ/mol (0.00%)
1786d68c: 116.3 kJ/mol (0.00%)
reagents_iso4: 120.7 kJ/mol (0.00%)
f55e61f0: 128.0 kJ/mol (0.00%)
1b7ad146: 133.5 kJ/mol (0.00%)
f9fdcb74: 162.7 kJ/mol (0.00%)
80a0b97e: 173.0 kJ/mol (0.00%)
40661807: 174.0 kJ/mol (0.00%)
bfae37f5: 178.5 kJ/mol (0.00%)
439e97a3: 181.0 kJ/mol (0.00%)
047b0ed9: 183.0 kJ/mol (0.00%)
2d5d51b9: 202.1 kJ/mol (0.00%)
bf9aff94: 206.3 kJ/mol (0.00%)
a355339c: 210.7 kJ/mol (0.00%)
f82648fe: 215.1 kJ/mol (0.00%)
e20041cd: 216.3 kJ/mol (0.00%)
75e0854e: 231.3 kJ/mol (0.00%)
191ec5c0: 999.0 kJ/mol (0.00%)
330e8cbe: 999.0 kJ/mol (0.00%)
67d7d76b: 999.0 kJ/mol (0.00%)
345ee4c9: 999.0 kJ/mol (0.00%)
da1442d2: 999.0 kJ/mol (0.00%)
```

3.18 C5

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
71678f28_iso3: 0.0 kJ/mol (59.66%)
c4a684f0: 2.0 kJ/mol (26.63%)
71678f28_iso1: 4.0 kJ/mol (11.88%)
71678f28_iso2: 10.0 kJ/mol (1.06%)
71678f28_iso5: 11.0 kJ/mol (0.71%)
c4ba4b5c_iso3: 17.5 kJ/mol (0.05%)
b269c4ef: 23.2 kJ/mol (0.01%)
c4ba4b5c: 24.5 kJ/mol (0.00%)
c4ba4b5c_iso1: 24.5 kJ/mol (0.00%)
c4ba4b5c_iso4: 24.5 kJ/mol (0.00%)
```

2386d14f: 34.8 kJ/mol (0.00%)
c4ba4b5c_iso2: 36.5 kJ/mol (0.00%)
923cda4b: 44.7 kJ/mol (0.00%)
1a627e1b: 46.0 kJ/mol (0.00%)
35d4ee84: 54.1 kJ/mol (0.00%)
2aab54de: 54.5 kJ/mol (0.00%)
3433012f: 55.7 kJ/mol (0.00%)
522dee4c: 66.4 kJ/mol (0.00%)
cc3d25d1: 66.8 kJ/mol (0.00%)
9001f558: 67.8 kJ/mol (0.00%)
deb3343e: 68.9 kJ/mol (0.00%)
71678f28_iso4: 70.0 kJ/mol (0.00%)
c2cd5837: 71.1 kJ/mol (0.00%)
9f95bb85: 72.4 kJ/mol (0.00%)
f1755cee: 73.6 kJ/mol (0.00%)
68f20511: 75.9 kJ/mol (0.00%)
fde78aa0: 76.6 kJ/mol (0.00%)
1e379a5d: 77.0 kJ/mol (0.00%)
fc61b09a: 77.7 kJ/mol (0.00%)
b5918a7d: 79.0 kJ/mol (0.00%)
f446b1a3: 88.0 kJ/mol (0.00%)
f859e8e3: 88.4 kJ/mol (0.00%)
c4541344_iso1: 88.7 kJ/mol (0.00%)
c4cbae7d: 89.5 kJ/mol (0.00%)
f580d69b: 89.5 kJ/mol (0.00%)
07b35b7b: 89.5 kJ/mol (0.00%)
0a8f1556: 90.0 kJ/mol (0.00%)
65eedd5f: 91.2 kJ/mol (0.00%)
115781e1: 96.0 kJ/mol (0.00%)
7c12b600: 97.1 kJ/mol (0.00%)
7c12b600_iso1: 97.1 kJ/mol (0.00%)
e1935770: 99.4 kJ/mol (0.00%)
f446b1a3_iso1: 100.0 kJ/mol (0.00%)
4698be2f: 106.5 kJ/mol (0.00%)
6d0c9bd7: 107.5 kJ/mol (0.00%)
fa4384d2: 109.3 kJ/mol (0.00%)
943d61b7: 109.5 kJ/mol (0.00%)
b2cc6ed1: 109.8 kJ/mol (0.00%)
8c7629cf: 114.1 kJ/mol (0.00%)
aa31948e: 114.2 kJ/mol (0.00%)
8ef52498: 116.4 kJ/mol (0.00%)
292431bb: 118.0 kJ/mol (0.00%)
dd2115f4: 118.6 kJ/mol (0.00%)
8a4e3726: 121.4 kJ/mol (0.00%)
ef0007fe: 124.0 kJ/mol (0.00%)
5a6d5700: 128.2 kJ/mol (0.00%)
4b114049_iso1: 129.5 kJ/mol (0.00%)
aa31948e_iso1: 130.2 kJ/mol (0.00%)
9ab7ff52: 130.2 kJ/mol (0.00%)
0c5fab1e: 131.0 kJ/mol (0.00%)
dc6cae83: 134.1 kJ/mol (0.00%)
e1165af6: 138.5 kJ/mol (0.00%)
7cf09cb2_iso1: 141.2 kJ/mol (0.00%)
0b35598c: 143.1 kJ/mol (0.00%)

3c087106: 143.2 kJ/mol (0.00%)
d4abfb96: 144.1 kJ/mol (0.00%)
2a1bf5ad: 146.2 kJ/mol (0.00%)
53a0b519: 147.0 kJ/mol (0.00%)
f112ded6: 148.2 kJ/mol (0.00%)
reagents: 150.0 kJ/mol (0.00%)
reagents_iso3: 150.0 kJ/mol (0.00%)
12b17c6a: 151.2 kJ/mol (0.00%)
9db58a26: 153.1 kJ/mol (0.00%)
da2e945a: 156.0 kJ/mol (0.00%)
reagents_iso1: 157.0 kJ/mol (0.00%)
574b46e2_iso2: 157.0 kJ/mol (0.00%)
f5ca4284_iso2: 157.2 kJ/mol (0.00%)
2b5ca702: 157.6 kJ/mol (0.00%)
4c6df61a_iso2: 158.1 kJ/mol (0.00%)
2084e746: 158.3 kJ/mol (0.00%)
f5ca4284_iso4: 160.2 kJ/mol (0.00%)
fa50c01b: 160.6 kJ/mol (0.00%)
4c6df61a_iso1: 161.1 kJ/mol (0.00%)
767caffc_iso1: 161.4 kJ/mol (0.00%)
reagents_iso2: 163.0 kJ/mol (0.00%)
5abf7d78: 163.5 kJ/mol (0.00%)
2bcd7cc2: 164.4 kJ/mol (0.00%)
574b46e2_iso3: 165.0 kJ/mol (0.00%)
9bcb1411: 165.4 kJ/mol (0.00%)
98ed8ea1: 166.4 kJ/mol (0.00%)
f5ca4284_iso1: 168.0 kJ/mol (0.00%)
9ecebe4b_iso1: 168.6 kJ/mol (0.00%)
4fe83467: 171.4 kJ/mol (0.00%)
df36a3b2: 172.2 kJ/mol (0.00%)
a1ab2490: 172.4 kJ/mol (0.00%)
fc3f6b48: 172.9 kJ/mol (0.00%)
574b46e2_iso5: 173.0 kJ/mol (0.00%)
574b46e2_iso6: 174.0 kJ/mol (0.00%)
f5ca4284_iso3: 177.2 kJ/mol (0.00%)
574b46e2_iso4: 179.0 kJ/mol (0.00%)
13c890c8: 181.1 kJ/mol (0.00%)
5336edd9: 182.6 kJ/mol (0.00%)
0407b74a: 182.7 kJ/mol (0.00%)
e0aa3a05: 185.6 kJ/mol (0.00%)
574b46e2_iso1: 192.0 kJ/mol (0.00%)
dbb28e6c: 201.0 kJ/mol (0.00%)
de28c7c1: 202.1 kJ/mol (0.00%)
126d453e: 205.0 kJ/mol (0.00%)
89980cc0: 205.1 kJ/mol (0.00%)
3d70645e: 209.0 kJ/mol (0.00%)
4c6df61a_iso3: 210.8 kJ/mol (0.00%)
3313f20d: 213.1 kJ/mol (0.00%)
32842253: 213.4 kJ/mol (0.00%)
dc5229c9: 215.0 kJ/mol (0.00%)
cb6810fa: 217.0 kJ/mol (0.00%)
f05c97dc: 223.5 kJ/mol (0.00%)
bc0c01a8: 226.0 kJ/mol (0.00%)
81baa9b0: 226.8 kJ/mol (0.00%)

f2e0d7d7: 227.1 kJ/mol (0.00%)
dcb3f840: 230.7 kJ/mol (0.00%)
836fc8c8: 234.0 kJ/mol (0.00%)
25221ea2: 240.7 kJ/mol (0.00%)
c8f4c43f: 243.0 kJ/mol (0.00%)
deaf92c3: 247.5 kJ/mol (0.00%)
26dd96d8: 251.6 kJ/mol (0.00%)
9b3acf93: 259.1 kJ/mol (0.00%)
f003a8a4: 259.3 kJ/mol (0.00%)
d030947d: 271.6 kJ/mol (0.00%)
80df7717: 291.1 kJ/mol (0.00%)
a4b2016d: 999.0 kJ/mol (0.00%)
bd8b3c69: 999.0 kJ/mol (0.00%)
78e144e5: 999.0 kJ/mol (0.00%)
7dd50ce8: 999.0 kJ/mol (0.00%)
f4e03666: 999.0 kJ/mol (0.00%)
4464b3bc: 999.0 kJ/mol (0.00%)
bb5d2a62: 999.0 kJ/mol (0.00%)
91fb0fe2: 999.0 kJ/mol (0.00%)
1166d08f: 999.0 kJ/mol (0.00%)
6ec7e8c0: 999.0 kJ/mol (0.00%)
ad31aaee: 999.0 kJ/mol (0.00%)
39c4d16c: 999.0 kJ/mol (0.00%)
c7a0e4fd: 999.0 kJ/mol (0.00%)
4c7324ef: 999.0 kJ/mol (0.00%)
315127fb: 999.0 kJ/mol (0.00%)
ec312a73: 999.0 kJ/mol (0.00%)
bfe490ad: 999.0 kJ/mol (0.00%)
4c456776: 999.0 kJ/mol (0.00%)
7e20537e: 999.0 kJ/mol (0.00%)
a8603042: 999.0 kJ/mol (0.00%)
110e0676: 999.0 kJ/mol (0.00%)
a51ef2c8: 999.0 kJ/mol (0.00%)
1ea155ff: 999.0 kJ/mol (0.00%)
a2e27a7c: 999.0 kJ/mol (0.00%)
ab977756: 999.0 kJ/mol (0.00%)
83ea126b: 999.0 kJ/mol (0.00%)

3.19 C6

Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=383K)
1ecf72ae: 0.0 kJ/mol (89.82%)
26c6dee3_iso1: 10.2 kJ/mol (3.66%)
972aced2: 12.7 kJ/mol (1.68%)
2170a2ff_iso1: 13.8 kJ/mol (1.16%)
2170a2ff_iso2: 13.8 kJ/mol (1.16%)
4bf60607_iso1: 14.7 kJ/mol (0.90%)
4a43b082_iso2: 15.7 kJ/mol (0.65%)
3887220e: 17.2 kJ/mol (0.41%)
ac71abb0: 17.7 kJ/mol (0.35%)
4a43b082_iso1: 19.7 kJ/mol (0.18%)
c7753bfd: 27.0 kJ/mol (0.02%)
70409b09: 29.0 kJ/mol (0.01%)

2170a2ff: 30.8 kJ/mol (0.01%)
4c7db559: 31.7 kJ/mol (0.00%)
bc25aecf: 32.8 kJ/mol (0.00%)
c0721f99: 35.7 kJ/mol (0.00%)
6f463b5f: 37.4 kJ/mol (0.00%)
fbea3018: 45.1 kJ/mol (0.00%)
9a6506d2_iso3: 45.8 kJ/mol (0.00%)
0da56300: 49.5 kJ/mol (0.00%)
154a75e1: 53.3 kJ/mol (0.00%)
119b689f: 55.0 kJ/mol (0.00%)
9655210a: 56.0 kJ/mol (0.00%)
52d502e5: 56.9 kJ/mol (0.00%)
21f99c68_iso1: 56.9 kJ/mol (0.00%)
1fb6ac13: 58.7 kJ/mol (0.00%)
f9f0836b: 58.9 kJ/mol (0.00%)
9032f632: 62.2 kJ/mol (0.00%)
f2ad33fc_iso1: 62.9 kJ/mol (0.00%)
d55ba9b8_iso1: 62.9 kJ/mol (0.00%)
84fc0d4e: 63.8 kJ/mol (0.00%)
d881e6c1_iso1: 65.3 kJ/mol (0.00%)
b89dc451: 67.7 kJ/mol (0.00%)
ec2a2696_iso1: 68.3 kJ/mol (0.00%)
26724122_iso1: 70.2 kJ/mol (0.00%)
b1471680: 71.9 kJ/mol (0.00%)
b60c4f17: 71.9 kJ/mol (0.00%)
5654b31d: 71.9 kJ/mol (0.00%)
4762da6a_iso1: 72.3 kJ/mol (0.00%)
d2102e80: 73.0 kJ/mol (0.00%)
d2102e80_iso1: 73.0 kJ/mol (0.00%)
d2102e80_iso2: 73.0 kJ/mol (0.00%)
da3993e8: 77.0 kJ/mol (0.00%)
0ec8b90f_iso1: 77.1 kJ/mol (0.00%)
f3b33200: 77.5 kJ/mol (0.00%)
d881e6c1_iso4: 78.9 kJ/mol (0.00%)
77034d82: 79.6 kJ/mol (0.00%)
d881e6c1_iso3: 79.9 kJ/mol (0.00%)
ec2a2696_iso3: 79.9 kJ/mol (0.00%)
26724122_iso2: 79.9 kJ/mol (0.00%)
8d15ddfc: 80.3 kJ/mol (0.00%)
df61f8d0: 80.7 kJ/mol (0.00%)
eb052611: 80.8 kJ/mol (0.00%)
c221ff19: 81.7 kJ/mol (0.00%)
68143172: 82.9 kJ/mol (0.00%)
866a6a02: 83.3 kJ/mol (0.00%)
4862f8c0: 84.5 kJ/mol (0.00%)
060dddca: 84.9 kJ/mol (0.00%)
9472028f: 85.5 kJ/mol (0.00%)
752ee838: 85.8 kJ/mol (0.00%)
d56b8585: 85.8 kJ/mol (0.00%)
f27bc214: 86.3 kJ/mol (0.00%)
21b97d75: 88.1 kJ/mol (0.00%)
528198f6: 88.2 kJ/mol (0.00%)
ab33a5f6: 88.7 kJ/mol (0.00%)
reagents: 89.4 kJ/mol (0.00%)

reagents_iso3: 89.4 kJ/mol (0.00%)
9a6506d2_iso2: 89.7 kJ/mol (0.00%)
0a60546e: 89.9 kJ/mol (0.00%)
reagents_iso2: 90.4 kJ/mol (0.00%)
reagents_iso5: 92.4 kJ/mol (0.00%)
9a6506d2_iso1: 92.8 kJ/mol (0.00%)
4762da6a: 93.7 kJ/mol (0.00%)
ddfcd209_iso1: 94.8 kJ/mol (0.00%)
f4e7bbc4: 95.2 kJ/mol (0.00%)
16dcd359: 96.0 kJ/mol (0.00%)
46f43c77: 96.0 kJ/mol (0.00%)
f2d44a6c: 96.7 kJ/mol (0.00%)
f9227462: 97.2 kJ/mol (0.00%)
6c4942b9: 97.8 kJ/mol (0.00%)
d55ba9b8_iso2: 97.9 kJ/mol (0.00%)
ce079e38: 98.6 kJ/mol (0.00%)
7afc098f: 100.8 kJ/mol (0.00%)
reagents_iso6: 102.4 kJ/mol (0.00%)
reagents_iso7: 103.4 kJ/mol (0.00%)
c9ba5710: 104.5 kJ/mol (0.00%)
6aa1ef93: 105.9 kJ/mol (0.00%)
reagents_iso10: 106.4 kJ/mol (0.00%)
ec2a2696_iso2: 107.2 kJ/mol (0.00%)
91882478: 107.5 kJ/mol (0.00%)
2f61c7ac: 107.8 kJ/mol (0.00%)
reagents_iso8: 108.4 kJ/mol (0.00%)
310dbc65: 110.0 kJ/mol (0.00%)
310dbc65_iso1: 110.0 kJ/mol (0.00%)
bd9c8288: 110.9 kJ/mol (0.00%)
reagents_iso4: 112.1 kJ/mol (0.00%)
558a5f5d: 113.2 kJ/mol (0.00%)
f825f1b2: 113.4 kJ/mol (0.00%)
reagents_iso11: 114.4 kJ/mol (0.00%)
d881e6c1_iso2: 114.9 kJ/mol (0.00%)
84419486: 116.0 kJ/mol (0.00%)
ceb34f44: 118.9 kJ/mol (0.00%)
32a9af0e: 119.5 kJ/mol (0.00%)
7564877a: 120.0 kJ/mol (0.00%)
24346392: 120.0 kJ/mol (0.00%)
7d13f7f6: 120.6 kJ/mol (0.00%)
5b2f1c81: 120.8 kJ/mol (0.00%)
332f426b: 121.0 kJ/mol (0.00%)
1707a82f: 121.8 kJ/mol (0.00%)
35b848ae: 122.0 kJ/mol (0.00%)
333415ee: 122.8 kJ/mol (0.00%)
ca338eec: 123.0 kJ/mol (0.00%)
34c00e17: 123.1 kJ/mol (0.00%)
a61cb4e0: 123.4 kJ/mol (0.00%)
b4f51433: 125.0 kJ/mol (0.00%)
reagents_iso1: 125.4 kJ/mol (0.00%)
eddad56a_iso1: 126.1 kJ/mol (0.00%)
22c52650: 127.8 kJ/mol (0.00%)
4762da6a_iso2: 128.3 kJ/mol (0.00%)
1968ec4e: 128.7 kJ/mol (0.00%)

```
cecea50f: 129.0 kJ/mol (0.00%)
9b792e1c: 129.3 kJ/mol (0.00%)
reagents_iso9: 129.4 kJ/mol (0.00%)
3671ff6e: 130.0 kJ/mol (0.00%)
6ddc1a5f: 131.1 kJ/mol (0.00%)
7fc03b3c: 136.1 kJ/mol (0.00%)
319823b8: 138.9 kJ/mol (0.00%)
cb1a0269: 144.2 kJ/mol (0.00%)
75574133: 148.6 kJ/mol (0.00%)
56d196ac: 149.2 kJ/mol (0.00%)
e6ab7d77: 150.9 kJ/mol (0.00%)
c286b35a: 151.3 kJ/mol (0.00%)
6c282fc6: 154.9 kJ/mol (0.00%)
c81da2b2: 155.0 kJ/mol (0.00%)
ac76f1e4: 155.8 kJ/mol (0.00%)
9294bb7e: 156.2 kJ/mol (0.00%)
9a184ff4: 156.3 kJ/mol (0.00%)
df9cd29a: 156.4 kJ/mol (0.00%)
fe261a1e: 159.0 kJ/mol (0.00%)
90b17a81: 159.5 kJ/mol (0.00%)
a46ba2e8: 160.0 kJ/mol (0.00%)
536e0ef5: 166.0 kJ/mol (0.00%)
2e970413: 170.8 kJ/mol (0.00%)
5c26cfb2: 171.5 kJ/mol (0.00%)
55702e7e: 172.4 kJ/mol (0.00%)
5eb19351: 173.1 kJ/mol (0.00%)
18f03425_iso1: 181.0 kJ/mol (0.00%)
76e87d1b: 181.8 kJ/mol (0.00%)
46e9ee11: 181.9 kJ/mol (0.00%)
f2e87a6a: 183.9 kJ/mol (0.00%)
cf5b59ca: 186.9 kJ/mol (0.00%)
e62c29ef: 187.9 kJ/mol (0.00%)
3862504f: 187.9 kJ/mol (0.00%)
50aa277f: 190.8 kJ/mol (0.00%)
ade856ff: 191.9 kJ/mol (0.00%)
54ad3f25: 193.0 kJ/mol (0.00%)
20a874f9: 196.2 kJ/mol (0.00%)
d7d8cba1: 197.8 kJ/mol (0.00%)
673fc4be: 199.9 kJ/mol (0.00%)
a3fe264f: 205.5 kJ/mol (0.00%)
b4ab59bf: 211.8 kJ/mol (0.00%)
6b6342dd: 215.0 kJ/mol (0.00%)
a4477a70: 216.1 kJ/mol (0.00%)
064cefbe: 216.8 kJ/mol (0.00%)
99ac3bf6: 222.3 kJ/mol (0.00%)
7f1e510f: 225.0 kJ/mol (0.00%)
1e5607a1: 227.0 kJ/mol (0.00%)
102f99a1: 227.3 kJ/mol (0.00%)
c37fde5e: 236.3 kJ/mol (0.00%)
ee71a191: 236.7 kJ/mol (0.00%)
ffa99591: 242.0 kJ/mol (0.00%)
f072be79: 242.9 kJ/mol (0.00%)
184ea981: 254.0 kJ/mol (0.00%)
7068c3a1: 254.9 kJ/mol (0.00%)
```

```
54ca7fdc: 255.1 kJ/mol (0.00%)
7dd6226e: 999.0 kJ/mol (0.00%)
90173ede: 999.0 kJ/mol (0.00%)
7d4bd280: 999.0 kJ/mol (0.00%)
a17f307c: 999.0 kJ/mol (0.00%)
481a85ad: 999.0 kJ/mol (0.00%)
c22bc576: 999.0 kJ/mol (0.00%)
14aee9cf: 999.0 kJ/mol (0.00%)
a64c25c4: 999.0 kJ/mol (0.00%)
617704cc: 999.0 kJ/mol (0.00%)
453d6c84: 999.0 kJ/mol (0.00%)
1a41ab7a: 999.0 kJ/mol (0.00%)
7bbecf2d: 999.0 kJ/mol (0.00%)
74fcf165: 999.0 kJ/mol (0.00%)
2aedaa64: 999.0 kJ/mol (0.00%)
6b5b20ac: 999.0 kJ/mol (0.00%)
b95d7390: 999.0 kJ/mol (0.00%)
ee9326e7: 999.0 kJ/mol (0.00%)
86e64484: 999.0 kJ/mol (0.00%)
4f9d1aa1: 999.0 kJ/mol (0.00%)
d7cc4484: 999.0 kJ/mol (0.00%)
dec63516: 999.0 kJ/mol (0.00%)
7c03b912: 999.0 kJ/mol (0.00%)
643caa55: 999.0 kJ/mol (0.00%)
865096d6: 999.0 kJ/mol (0.00%)
5d96908d: 999.0 kJ/mol (0.00%)
5d4f128d: 999.0 kJ/mol (0.00%)
4e45a912: 999.0 kJ/mol (0.00%)
9af5abc9: 999.0 kJ/mol (0.00%)
b84adb70: 999.0 kJ/mol (0.00%)
0d2beb5e: 999.0 kJ/mol (0.00%)
94da3e2f: 999.0 kJ/mol (0.00%)
513e94c2: 999.0 kJ/mol (0.00%)
```

3.20 C7

```
Product distribution according to the kinetic simulation
(t=36000s, neophile=False, T=298K)
795894b2: 0.0 kJ/mol (99.80%)
6700576a_iso3: 16.0 kJ/mol (0.16%)
55c8fd91: 19.0 kJ/mol (0.05%)
6700576a_iso1: 30.0 kJ/mol (0.00%)
382484fe: 35.5 kJ/mol (0.00%)
5b1dfc16: 41.5 kJ/mol (0.00%)
6700576a_iso2: 42.0 kJ/mol (0.00%)
84cd30dd: 45.5 kJ/mol (0.00%)
a41a3883: 46.4 kJ/mol (0.00%)
04ddc8e2: 57.2 kJ/mol (0.00%)
f32afc31: 58.3 kJ/mol (0.00%)
4fff478b: 59.6 kJ/mol (0.00%)
d5302c0d: 61.3 kJ/mol (0.00%)
eafd3db3: 64.0 kJ/mol (0.00%)
c93f838d: 67.9 kJ/mol (0.00%)
0ea82eb2: 68.0 kJ/mol (0.00%)
```

2cc4da48: 68.1 kJ/mol (0.00%)
e628609b: 68.3 kJ/mol (0.00%)
8a3d3e83: 68.5 kJ/mol (0.00%)
e9327bd9: 71.5 kJ/mol (0.00%)
8533c9f9: 72.6 kJ/mol (0.00%)
a3325c4a: 73.1 kJ/mol (0.00%)
f6167aea_iso4: 76.0 kJ/mol (0.00%)
64f0365c: 77.6 kJ/mol (0.00%)
045ac38d_iso4: 78.0 kJ/mol (0.00%)
045ac38d_iso3: 79.0 kJ/mol (0.00%)
abafa662_iso7: 79.1 kJ/mol (0.00%)
dcbd60c9: 79.5 kJ/mol (0.00%)
cf968b37_iso1: 79.6 kJ/mol (0.00%)
abafa662_iso6: 80.1 kJ/mol (0.00%)
abafa662_iso5: 80.1 kJ/mol (0.00%)
abafa662_iso8: 80.1 kJ/mol (0.00%)
abafa662_iso1: 80.1 kJ/mol (0.00%)
f6167aea_iso3: 81.0 kJ/mol (0.00%)
61136ea8: 81.1 kJ/mol (0.00%)
045ac38d_iso1: 83.0 kJ/mol (0.00%)
e7df4ff3: 83.0 kJ/mol (0.00%)
255dcf4d: 84.0 kJ/mol (0.00%)
abafa662_iso9: 84.1 kJ/mol (0.00%)
cd4d1dfc: 84.2 kJ/mol (0.00%)
abafa662_iso4: 86.1 kJ/mol (0.00%)
89bdf3ee: 86.4 kJ/mol (0.00%)
045b4923: 87.0 kJ/mol (0.00%)
abafa662_iso2: 87.1 kJ/mol (0.00%)
c8f24449: 88.0 kJ/mol (0.00%)
5dc83cb6: 88.0 kJ/mol (0.00%)
045ac38d_iso2: 89.0 kJ/mol (0.00%)
b21c109b: 90.0 kJ/mol (0.00%)
f6167aea_iso2: 90.0 kJ/mol (0.00%)
172d1312: 92.0 kJ/mol (0.00%)
f6167aea_iso1: 92.0 kJ/mol (0.00%)
a3a0c727: 92.3 kJ/mol (0.00%)
f8475f90: 92.5 kJ/mol (0.00%)
8eae9fff: 93.0 kJ/mol (0.00%)
8e1e4df2: 93.5 kJ/mol (0.00%)
f6167aea_iso5: 94.0 kJ/mol (0.00%)
2cf94bbf: 95.5 kJ/mol (0.00%)
365c06e3: 95.9 kJ/mol (0.00%)
045ac38d_iso7: 96.0 kJ/mol (0.00%)
b709858b: 96.0 kJ/mol (0.00%)
79fc3fc2: 96.9 kJ/mol (0.00%)
0700d32c: 97.0 kJ/mol (0.00%)
631b4cd4: 97.4 kJ/mol (0.00%)
a5878db0: 97.8 kJ/mol (0.00%)
045ac38d_iso5: 98.0 kJ/mol (0.00%)
045ac38d_iso6: 98.0 kJ/mol (0.00%)
f6167aea_iso6: 99.0 kJ/mol (0.00%)
193253d9: 99.3 kJ/mol (0.00%)
bb4c8ecb_iso2: 99.9 kJ/mol (0.00%)
52ebd70a_iso3: 101.9 kJ/mol (0.00%)

ddfcf432: 102.8 kJ/mol (0.00%)
abafa662_iso3: 103.1 kJ/mol (0.00%)
1eee23fd_iso2: 106.0 kJ/mol (0.00%)
1eee23fd_iso1: 106.0 kJ/mol (0.00%)
1eee23fd_iso4: 106.0 kJ/mol (0.00%)
e4f3aac9: 107.0 kJ/mol (0.00%)
1769f1c3: 110.3 kJ/mol (0.00%)
08bfdeb5: 110.5 kJ/mol (0.00%)
b3d69e8d: 110.5 kJ/mol (0.00%)
1eee23fd_iso3: 111.0 kJ/mol (0.00%)
2be8cbab: 111.3 kJ/mol (0.00%)
7069153b: 111.4 kJ/mol (0.00%)
4a84451e: 111.4 kJ/mol (0.00%)
63036c19: 111.6 kJ/mol (0.00%)
29f66e21: 111.6 kJ/mol (0.00%)
3cf3605b: 111.7 kJ/mol (0.00%)
8c395ee3: 111.8 kJ/mol (0.00%)
d89514d4: 111.9 kJ/mol (0.00%)
f7154b62: 112.0 kJ/mol (0.00%)
53f7fe23: 112.0 kJ/mol (0.00%)
8d7cf113: 112.5 kJ/mol (0.00%)
aeb08ef2: 112.8 kJ/mol (0.00%)
938a3c76: 113.5 kJ/mol (0.00%)
5c4abf8b: 115.9 kJ/mol (0.00%)
8ed847e5_iso1: 116.0 kJ/mol (0.00%)
e6fee49f: 116.8 kJ/mol (0.00%)
4413fe87: 117.3 kJ/mol (0.00%)
52ebd70a_iso1: 118.9 kJ/mol (0.00%)
ebcb2134: 122.5 kJ/mol (0.00%)
bb4c8ecb_iso1: 124.4 kJ/mol (0.00%)
957fae3f_iso1: 124.8 kJ/mol (0.00%)
8ed847e5: 127.0 kJ/mol (0.00%)
5c4abf8b_iso1: 127.9 kJ/mol (0.00%)
0a04a46a: 128.0 kJ/mol (0.00%)
58f4682d: 128.6 kJ/mol (0.00%)
138c6ba8: 130.9 kJ/mol (0.00%)
ffbceeec: 131.3 kJ/mol (0.00%)
49a84a9e: 134.5 kJ/mol (0.00%)
957fae3f_iso2: 137.0 kJ/mol (0.00%)
957fae3f_iso3: 137.0 kJ/mol (0.00%)
2f440199: 137.7 kJ/mol (0.00%)
f99f0198: 138.5 kJ/mol (0.00%)
ed974708: 142.4 kJ/mol (0.00%)
4b5a0c9f: 145.9 kJ/mol (0.00%)
a796c048: 148.4 kJ/mol (0.00%)
8f86a77a: 150.5 kJ/mol (0.00%)
516e4d1e: 153.0 kJ/mol (0.00%)
bb4c8ecb_iso3: 153.1 kJ/mol (0.00%)
49915f9c: 153.3 kJ/mol (0.00%)
2541f7ee: 154.5 kJ/mol (0.00%)
1a81fd74: 155.5 kJ/mol (0.00%)
52ebd70a_iso2: 155.9 kJ/mol (0.00%)
89b0c304: 160.9 kJ/mol (0.00%)
reagents: 166.9 kJ/mol (0.00%)

```
5d6068a6: 166.9 kJ/mol (0.00%)
reagents_iso3: 166.9 kJ/mol (0.00%)
28391a91: 167.9 kJ/mol (0.00%)
367c87c5: 168.9 kJ/mol (0.00%)
8c1d238a: 168.9 kJ/mol (0.00%)
d776dc20: 169.0 kJ/mol (0.00%)
2b271df6: 169.6 kJ/mol (0.00%)
reagents_iso6: 171.9 kJ/mol (0.00%)
a9b1c823: 172.0 kJ/mol (0.00%)
329c5bb0: 172.8 kJ/mol (0.00%)
reagents_iso8: 172.9 kJ/mol (0.00%)
4a2173a4: 173.6 kJ/mol (0.00%)
354d45c2: 173.9 kJ/mol (0.00%)
f09e55d7: 174.0 kJ/mol (0.00%)
a12dec12: 176.0 kJ/mol (0.00%)
16a9ff47: 176.8 kJ/mol (0.00%)
6da589d8: 178.0 kJ/mol (0.00%)
reagents_iso4: 178.9 kJ/mol (0.00%)
bef39e9c: 180.0 kJ/mol (0.00%)
c9a229ed: 181.0 kJ/mol (0.00%)
c3a8f8f4: 182.0 kJ/mol (0.00%)
0f479ba4: 182.0 kJ/mol (0.00%)
0457262e: 185.1 kJ/mol (0.00%)
dfa93ece: 186.8 kJ/mol (0.00%)
2255e9f8: 186.9 kJ/mol (0.00%)
899c6151: 191.8 kJ/mol (0.00%)
efeafa70: 193.1 kJ/mol (0.00%)
045ae978: 195.4 kJ/mol (0.00%)
82e65018: 196.0 kJ/mol (0.00%)
7b61e9a1: 197.8 kJ/mol (0.00%)
73101e9a: 197.9 kJ/mol (0.00%)
39d79219: 200.0 kJ/mol (0.00%)
5a7b36b3: 200.5 kJ/mol (0.00%)
c288321c: 200.6 kJ/mol (0.00%)
reagents_iso1: 200.9 kJ/mol (0.00%)
ff95a319: 202.0 kJ/mol (0.00%)
c9f694f0_iso10: 202.9 kJ/mol (0.00%)
564dd2e6: 204.0 kJ/mol (0.00%)
326815d8: 204.1 kJ/mol (0.00%)
2af112a9: 204.7 kJ/mol (0.00%)
ddb47fec_iso1: 204.9 kJ/mol (0.00%)
dbbdb820: 205.9 kJ/mol (0.00%)
53d80b73: 205.9 kJ/mol (0.00%)
ddb47fec_iso4: 206.9 kJ/mol (0.00%)
c9f694f0_iso1: 206.9 kJ/mol (0.00%)
da5e758e: 208.8 kJ/mol (0.00%)
ddb47fec_iso9: 208.9 kJ/mol (0.00%)
b22ed421: 209.0 kJ/mol (0.00%)
87f5574b: 209.8 kJ/mol (0.00%)
fcad84b7: 210.0 kJ/mol (0.00%)
c9f694f0_iso3: 210.9 kJ/mol (0.00%)
6d1f2ccc: 212.0 kJ/mol (0.00%)
c4105938: 212.1 kJ/mol (0.00%)
ca522139: 212.8 kJ/mol (0.00%)
```

80854742: 212.8 kJ/mol (0.00%)
ddb47fec_iso7: 212.9 kJ/mol (0.00%)
c9f694f0_iso4: 212.9 kJ/mol (0.00%)
c9f694f0_iso9: 212.9 kJ/mol (0.00%)
ddb47fec_iso5: 212.9 kJ/mol (0.00%)
726e5785: 213.0 kJ/mol (0.00%)
ddb47fec_iso11: 213.9 kJ/mol (0.00%)
09c5a54a: 214.8 kJ/mol (0.00%)
ddb47fec_iso2: 214.9 kJ/mol (0.00%)
dc449bd4: 214.9 kJ/mol (0.00%)
88b3d4c1: 215.0 kJ/mol (0.00%)
ddb47fec_iso10: 216.4 kJ/mol (0.00%)
280051be: 217.5 kJ/mol (0.00%)
51147d79: 217.9 kJ/mol (0.00%)
d12a7c11: 218.7 kJ/mol (0.00%)
f4a50a69: 218.9 kJ/mol (0.00%)
ddb47fec_iso12: 218.9 kJ/mol (0.00%)
c9f694f0_iso8: 219.9 kJ/mol (0.00%)
fcb187d3: 220.4 kJ/mol (0.00%)
c9f694f0_iso6: 220.9 kJ/mol (0.00%)
2aab5c6d: 222.8 kJ/mol (0.00%)
c9f694f0_iso5: 222.9 kJ/mol (0.00%)
4eb03ddf: 224.1 kJ/mol (0.00%)
8883ba32: 225.0 kJ/mol (0.00%)
c9f694f0_iso2: 226.9 kJ/mol (0.00%)
02331aee: 227.0 kJ/mol (0.00%)
ddb47fec_iso13: 227.9 kJ/mol (0.00%)
beb740bf: 228.0 kJ/mol (0.00%)
b25ccfbd: 228.0 kJ/mol (0.00%)
63d41865: 230.0 kJ/mol (0.00%)
e9467b1a: 231.0 kJ/mol (0.00%)
72134ad8: 232.9 kJ/mol (0.00%)
7f51324f: 233.0 kJ/mol (0.00%)
2a62ce5d_iso1: 233.1 kJ/mol (0.00%)
a57eea2b: 234.0 kJ/mol (0.00%)
0ba93a55: 234.7 kJ/mol (0.00%)
6417085f: 235.2 kJ/mol (0.00%)
545e9511: 236.8 kJ/mol (0.00%)
434f714b: 237.0 kJ/mol (0.00%)
b7becd49: 238.0 kJ/mol (0.00%)
8f039680: 238.8 kJ/mol (0.00%)
6501edfe: 239.0 kJ/mol (0.00%)
c32a6511: 240.0 kJ/mol (0.00%)
1df07cc9: 241.0 kJ/mol (0.00%)
ef690888: 241.5 kJ/mol (0.00%)
320703a9: 242.0 kJ/mol (0.00%)
38ae4108: 242.1 kJ/mol (0.00%)
9acf31a3: 242.9 kJ/mol (0.00%)
bd98ddeb: 243.3 kJ/mol (0.00%)
ddb47fec_iso3: 243.9 kJ/mol (0.00%)
ddb47fec_iso14: 243.9 kJ/mol (0.00%)
262ac738: 244.0 kJ/mol (0.00%)
cf0d8e81: 244.0 kJ/mol (0.00%)
b2602522: 244.3 kJ/mol (0.00%)

fd25f7a7: 245.7 kJ/mol (0.00%)
ddb47fec_iso6: 245.9 kJ/mol (0.00%)
d9166232: 246.4 kJ/mol (0.00%)
cd60bc57: 247.0 kJ/mol (0.00%)
1b0d6713: 247.9 kJ/mol (0.00%)
f7a34902: 248.9 kJ/mol (0.00%)
c9f694f0_iso7: 252.9 kJ/mol (0.00%)
d9cb627c: 252.9 kJ/mol (0.00%)
3d7d3faf: 254.0 kJ/mol (0.00%)
a7b1c783: 257.8 kJ/mol (0.00%)
51147d79_iso1: 257.9 kJ/mol (0.00%)
18530657: 257.9 kJ/mol (0.00%)
ddb47fec_iso8: 258.9 kJ/mol (0.00%)
bb3fda2c: 261.0 kJ/mol (0.00%)
3efa3122: 261.1 kJ/mol (0.00%)
d38a0aeb: 262.2 kJ/mol (0.00%)
9afc8aeb: 264.9 kJ/mol (0.00%)
268582d2: 268.0 kJ/mol (0.00%)
9b424ec6: 271.2 kJ/mol (0.00%)
10076e91: 275.1 kJ/mol (0.00%)
dd882c09: 275.7 kJ/mol (0.00%)
86e9ed9b: 278.0 kJ/mol (0.00%)
fabd278f: 283.1 kJ/mol (0.00%)
14fe1440: 292.1 kJ/mol (0.00%)
1b649690: 302.0 kJ/mol (0.00%)
dbb9fafd: 314.9 kJ/mol (0.00%)
b6e9701b: 317.9 kJ/mol (0.00%)
6133e055: 325.6 kJ/mol (0.00%)
f5520c35: 335.9 kJ/mol (0.00%)
29e3b899: 358.9 kJ/mol (0.00%)
11355b01: 999.0 kJ/mol (0.00%)
b2f49b5d: 999.0 kJ/mol (0.00%)
39836ff6: 999.0 kJ/mol (0.00%)
342a724e: 999.0 kJ/mol (0.00%)
f6b53235: 999.0 kJ/mol (0.00%)
618ff760: 999.0 kJ/mol (0.00%)
7b9e869d: 999.0 kJ/mol (0.00%)
8b29a966: 999.0 kJ/mol (0.00%)
cbfd62b4: 999.0 kJ/mol (0.00%)
ec7650cb: 999.0 kJ/mol (0.00%)
c4d3e42f: 999.0 kJ/mol (0.00%)
3dcd68cc: 999.0 kJ/mol (0.00%)
c39a30fd: 999.0 kJ/mol (0.00%)
26a86cf1: 999.0 kJ/mol (0.00%)
9df906ec: 999.0 kJ/mol (0.00%)
dd5ec3f1: 999.0 kJ/mol (0.00%)
b501d4ed: 999.0 kJ/mol (0.00%)
b9e7f508: 999.0 kJ/mol (0.00%)
8438ef2b: 999.0 kJ/mol (0.00%)
dc63e82c: 999.0 kJ/mol (0.00%)
eaab9a57: 999.0 kJ/mol (0.00%)
5911f6b3: 999.0 kJ/mol (0.00%)
22aaa38a: 999.0 kJ/mol (0.00%)
4de4ecfc: 999.0 kJ/mol (0.00%)

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1da6f8e4: 999.0 kJ/mol (0.00%)
235fa464: 999.0 kJ/mol (0.00%)
fc58944d: 999.0 kJ/mol (0.00%)
0063e535: 999.0 kJ/mol (0.00%)
cff98039: 999.0 kJ/mol (0.00%)
0a3d7a9f: 999.0 kJ/mol (0.00%)
1d52e517: 999.0 kJ/mol (0.00%)
a7d9e581: 999.0 kJ/mol (0.00%)
eb623cff: 999.0 kJ/mol (0.00%)
f9955d9d: 999.0 kJ/mol (0.00%)
74792298: 999.0 kJ/mol (0.00%)
2d88aaf0: 999.0 kJ/mol (0.00%)
a4878302: 999.0 kJ/mol (0.00%)
bc91482d: 999.0 kJ/mol (0.00%)
77cdb1eb: 999.0 kJ/mol (0.00%)
6c72850d: 999.0 kJ/mol (0.00%)
7912683a: 999.0 kJ/mol (0.00%)
f538226e: 999.0 kJ/mol (0.00%)
830777a3: 999.0 kJ/mol (0.00%)
9792f640: 999.0 kJ/mol (0.00%)
99be9160: 999.0 kJ/mol (0.00%)
1ec436d6: 999.0 kJ/mol (0.00%)
20d6c35e: 999.0 kJ/mol (0.00%)
5f7fe253: 999.0 kJ/mol (0.00%)
ee6a42c7: 999.0 kJ/mol (0.00%)
4494b148: 999.0 kJ/mol (0.00%)
82e3fa67: 999.0 kJ/mol (0.00%)
9000592f: 999.0 kJ/mol (0.00%)
059bfcbe: 999.0 kJ/mol (0.00%)
794de38c: 999.0 kJ/mol (0.00%)
2efdc93d: 999.0 kJ/mol (0.00%)
c8c1b5bc: 999.0 kJ/mol (0.00%)
2298857d: 999.0 kJ/mol (0.00%)
0557f084: 999.0 kJ/mol (0.00%)
5e0fb550: 999.0 kJ/mol (0.00%)
bbf6ddae: 999.0 kJ/mol (0.00%)
fb1e20d8: 999.0 kJ/mol (0.00%)
dd3038b3: 999.0 kJ/mol (0.00%)
8d0606cb: 999.0 kJ/mol (0.00%)
7cd57a56: 999.0 kJ/mol (0.00%)
f1174135: 999.0 kJ/mol (0.00%)
ab571705: 999.0 kJ/mol (0.00%)
17f15d2b: 999.0 kJ/mol (0.00%)
05dd2506: 999.0 kJ/mol (0.00%)
495c6101: 999.0 kJ/mol (0.00%)
1f2abf59: 999.0 kJ/mol (0.00%)
6755df2a: 999.0 kJ/mol (0.00%)
ba537bfc: 999.0 kJ/mol (0.00%)
e8a41bee: 999.0 kJ/mol (0.00%)
c8577488: 999.0 kJ/mol (0.00%)
03efbd66: 999.0 kJ/mol (0.00%)
b788255c: 999.0 kJ/mol (0.00%)
ee4b8899: 999.0 kJ/mol (0.00%)
ea81562d: 999.0 kJ/mol (0.00%)
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24927428: 999.0 kJ/mol (0.00%)
f2e8e3dd: 999.0 kJ/mol (0.00%)
b2ac821a: 999.0 kJ/mol (0.00%)
35709258: 999.0 kJ/mol (0.00%)
9efcbd82: 999.0 kJ/mol (0.00%)
b8a2a490: 999.0 kJ/mol (0.00%)
d63d2e1b: 999.0 kJ/mol (0.00%)
cd116924: 999.0 kJ/mol (0.00%)
3b196cf4: 999.0 kJ/mol (0.00%)
ee60c244: 999.0 kJ/mol (0.00%)
065cbaf4: 999.0 kJ/mol (0.00%)
a826aa87: 999.0 kJ/mol (0.00%)
83d00cfc: 999.0 kJ/mol (0.00%)
776b63b3: 999.0 kJ/mol (0.00%)
c92425fe: 999.0 kJ/mol (0.00%)
9d565393: 999.0 kJ/mol (0.00%)
0657f301: 999.0 kJ/mol (0.00%)
821dff49: 999.0 kJ/mol (0.00%)
bf807363: 999.0 kJ/mol (0.00%)
34fc1500: 999.0 kJ/mol (0.00%)
6d63f314: 999.0 kJ/mol (0.00%)
70cea3f5: 999.0 kJ/mol (0.00%)
b957b2f0: 999.0 kJ/mol (0.00%)
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3ef78290: 999.0 kJ/mol (0.00%)
4b20c8a2: 999.0 kJ/mol (0.00%)
15fdc0bb: 999.0 kJ/mol (0.00%)
3c119761: 999.0 kJ/mol (0.00%)
a749e50f: 999.0 kJ/mol (0.00%)
c57ba612: 999.0 kJ/mol (0.00%)
cbc0b331: 999.0 kJ/mol (0.00%)
907acdac: 999.0 kJ/mol (0.00%)
0f42879f: 999.0 kJ/mol (0.00%)
2d2abd4b: 999.0 kJ/mol (0.00%)
a7f23819: 999.0 kJ/mol (0.00%)
0a0f479f: 999.0 kJ/mol (0.00%)
ec70ae5f: 999.0 kJ/mol (0.00%)
505a61be: 999.0 kJ/mol (0.00%)
15c3cf7e: 999.0 kJ/mol (0.00%)
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