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# Configuration at the Transannular Centre: Uniformity of the Selected Branch over the Structure Series, and the Descriptor Pattern of the Twenty

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**Abstract.** The corpus establishes that the installation of the $\alpha$-nitrogen at C6$\alpha$ admits two local approach branches forming a torsor under $\mathbb{Z}/2$, that an oriented cage condition excluding one of them is a section-supplying datum, and that the section so obtained is not a name: identifying the selected configuration with the $L$ series requires the substituent ordering together with a convention adopted outside the architecture. This paper does not repair that separation and does not claim to. It works on the near side of it.

The selection is uniform. The side chain begins at C5, a framework carbon, while the stereogenic centre is C6$\alpha$, the first arm carbon; at sixteen of the nineteen chiral structures the retained subgraph meets the reactive subgraph only at its root. At three it does not — two retain the arm-bearing carbon and one closes onto the backbone nitrogen — and those are reached instead if the canonical word installs the nitrogen before the excision, the branch being selected on a substrate that does not yet distinguish the residues. The corpus permits that order and does not force it. Fixing the configuration at one structure fixes it over the domain of uniformity, so the external input falls from nineteen namings to one bit.

Substituent-priority evaluation over the series is finite and is performed and audited here. The descriptor at C6$\alpha$ is constant with a single inversion, at the sulfur-bearing structure, and is unchanged by liberation. At the two structures rendering C5 stereogenic the severance record gives two distinct attachment modes, so a reading on which they present the same arrangement is unavailable; one face datum nonetheless fixes both descriptors, at 3$S$ and 3$R$, the opposite face fixing neither.

Residues made together are treated at the junction cell, whose even vessel count yields two rather than one. Both arise by the same transannular route on their own units, so every statement above applies at each centre unamended, and only the parity of the relation between the carriers bears on the hand. That relation is face inversion with the order of sites kept, which presents the other face of a planar unit and is therefore proper. The pair is homochiral, and under the same anchor both residues are of the $L$ series, their descriptors $R$ and $S$.

At cluster level the argument becomes a condition on the symmetry group of the assembly: an assembly is homochiral exactly when no operation relating two of its vessels is improper. The carrier's own datum does not settle it. An orientation marker records which of two orientations a unit is in and not how the two are related in space, and no statement about the pattern can see a determinant. That realisation is what remains between the architecture and homochirality over a cluster.

**Keywords:** Chrysene Formalism; homochirality; torsor section; transannular centre; substituent priority; structure series; uniformity; hypothesis register; falsification register

## 1 Introduction

### 1.1 What the corpus establishes, and what it withholds

The corpus establishes a section and withholds a name. At the installation of the $\alpha$-nitrogen the two local approach branches at C6$\alpha$, distinguished by the sign of the attack scalar against an oriented local frame, form a torsor under $\mathbb{Z}/2$; an oriented cage condition excluding one branch supplies a section; and under strong exclusion the realized configuration is the selected one, written $\chi^\star$. That is homochirality in the strict sense — a mechanism by which the product of the architecture is of one configuration rather than of a mixture — and it is reached from the geometry of the stack rather than assumed.

What the corpus withholds is the identification $\chi^\star = \chi_L$. It withholds it for a reason that is structural and not remediable by a better chemical argument: a torsor admits no canonical naming

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of its own elements, and naming the surviving branch requires the substituent ordering of the completed product composed with the biochemical $L/D$ convention, neither of which the architecture supplies. Article 54 twice declines the universal identification and takes $\chi^\star = \chi_L$ as a supposition where it is used. The coordinating paper carries that refusal forward and records that a sentence of the form *the formalism explains why the residues are of the L series* is not available to it.

## 1.2 What this paper addresses

Between a section at one centre and a series of twenty there is a question the corpus has not put: whether the section is the *same* section at every structure. Nothing stated so far excludes a cage condition whose sense of exclusion varies with the side chain, and if it did vary, the architecture would deliver twenty independent configurations rather than one, and homochirality would fail even though a section exists at each centre separately. The corpus has assumed uniformity without isolating it.

Section 6 isolates it and proves it twice, by two arguments that cover different parts of the series. The first turns on a structural fact: the side chain begins at C5, a framework carbon, while the stereogenic centre is C6$\alpha$, the first arm carbon, so that the handedness question and the side-chain question are about different atoms. That argument reaches sixteen of the nineteen chiral structures and is refuted at three, where the side chain runs back through the arm-bearing carbon or closes onto the backbone nitrogen. The second turns on the order of two generators of the canonical word: if the nitrogen is installed before the excision, the branch is selected on a substrate that does not yet distinguish the residues, and uniformity is total. The corpus does not fix that order, and Section 6 is where its freedom acquires a cost.

## 1.3 What is established here, by kind

**Recovered.** The branch torsor at C6$\alpha$, the cage condition as section-supplying datum, and the separation of selection from naming, all imported unamended at Section 5.

**Proved here.** Uniformity of the section over the structure series, in two forms: at sixteen structures with no premise about the canonical word (Theorem 6.11), and at all nineteen under a premise about its generator order (Proposition 6.9). With them the corollary that one anchor fixes the configuration over the domain of uniformity (Corollary 6.14).

**Found.** That the order of two generators of the canonical word, left open in the corpus on methodological grounds, decides whether the account of homochirality is exceptionless (Remark 13.2). And that the hand of a co-synthesised pair depends on the relation between its two carriers through the parity of that relation alone, so that the junction's face inversion — proper, being a rotation about an in-plane axis — delivers both residues of one hand (Theorem 9.5, Corollary 9.7).

**Computed here.** The substituent-priority evaluation at C6$\alpha$ over all twenty structures, and at C5 over the two structures at which it is stereogenic (Appendix B). The decoration record on which the computation runs is the record the coordinating paper reported as held in supplement and not printed, and one result there was demoted on that account; printing and auditing it here is a by-product of this paper and is entered as such.

**Supposed.** $\chi^\star = \chi_L$ at one reference structure (Supposition 8.4), stated where used, in the manner of Article 54.

**Not claimed.** Everything in Section 3.

## 1.4 Organization

Section 2 fixes status and nomenclature and scopes the paper to one substitution context. Section 3 refuses six readings before any construction. Section 4 states the reference architecture. Section 5 imports the selection. Section 6 is the paper's theorem. Section 7 treats the second centre. Section 8 computes the descriptor over the series and states the supposition. Section 9 asks the question the preceding sections do not, whether the selection agrees at two vessels making their residues together, and answers it at the junction cell. Section 10 states the same argument at cluster level, where it becomes a condition on the symmetry group of the assembly. Section 11 is the consolidated register and is the paper's centre of gravity; Section 12 is the falsification register for the middle sections, those of Sections 9 and 10 being carried there. Section 13 is the precedence entry and Section 14 aggregates the targets and concludes. Appendix A is the hypothesis register, Appendix B the verification, Appendix C the conformational commentary, isolated, and Appendix D the record of what was withdrawn in preparing this paper.

# 2 Status, nomenclature, scope

**Convention 2.1** (Status labels)**. [A]** As in the coordinating paper. **[A]** finite or axiom-free; **[D]** derived under named hypotheses, which are registered in Appendix A; **[C]** imported, with the source named; **[E]** molecular reading, which enters no proof. Scholia carry no label and enter no proof.

**Notation 2.2** (Locants)**. [C]** Notation 10.7 of the coordinating paper governs and is restated. The two carbons of the substitution arm are C6$\alpha$ and C6$\beta$. Greek locants without a numeric prefix are residue nomenclature: C′ is the carboxyl carbon and equals C6$\beta$; C$\alpha$ is the $\alpha$ carbon and equals C6$\alpha$; and C$\beta$, the first side-chain carbon, is C5. Statements written in the other convention are restated, not reconciled by context.

**Remark 2.3** (The two carbons of the chirality question)**. [A]** The consequence of the notation for this paper should be stated once and plainly. The stereogenic centre formed at the installation of the nitrogen is C6$\alpha$, an arm carbon. The side chain begins at C5, a framework carbon of the vessel graph $\mathcal{X}$. These are different atoms, and the whole of Section 6 is an argument about that difference.

**Convention 2.4** (Scope)**. [A]** The reference substitution context is the 6, 12-disubstituted unit. Transport of any statement below to the contexts $\{3, 6, 12\}$ and $\{3, 6, 9, 12\}$ is governed by Theorem 10.15 of the coordinating paper: the chemical half is exact under local concordance of the reactive subgraph, the cage half is conditional on supplied candidate lifts meeting a margin condition, and persistence of the selected branch requires the transported amino-installation lift to meet that condition. No transported statement is asserted here.

**Convention 2.5** (Strong exclusion)**. [C]** Two realizations are admitted by the source: strong exclusion of one branch, and an energetic discrimination supporting preferential rather than deterministic selection. Every statement below is written under strong exclusion. Under the weaker realization each conclusion weakens from a section to an enrichment, and Remark 6.20 says how far.

# 3 Non-implications

**Proposition 3.1** (Non-implications of this paper)**. [A]** *None of the following is asserted anywhere below.*

*(i)* ***That the architecture produces the L series.*** *What is established is the exclusion of one branch and the uniformity of that exclusion. The naming of the surviving branch is a separate datum, is supplied at Supposition 8.4 as a supposition, and is not derived here.*

*(ii)* ***That the descriptor pattern is evidence for the L series.*** *The pattern — one descriptor at nineteen structures with a single inversion at the sulfur-bearing one — is* entailed *by the L assignment and is a consequence of the priority rules, not an independent observation. Its role here is as an audit of the decoration record, and Scholium 3.2 says so at length because this is the clause a reader is most likely to over-read.*

*(iii)* ***That any conformational statement enters a proof.*** *Rotameric descriptions of the liberated residue — anti, gauche, intramolecular hydrogen bonding at the hydroxyl — describe interconverting states about a bond and do not fix a configuration. They appear in Appendix C, are labelled* **[E]** *, and enter no numbered statement.*

*(iv)* ***That the realization is decided.*** *Nothing here distinguishes strong exclusion from energetic bias.*

*(v)* ***That glycine is in scope.*** *The structure of empty retained set carries no stereogenic centre and is outside every uniformity statement below. It is counted where counting is done and is excluded where configuration is asserted.*

*(vi)* ***That handedness is generated rather than transferred.*** *Theorem 10.6 satisfies the parity criterion by the configuration of the ribose, which the carrier already has. The account is one of transfer from the sugar to the residue, and nothing here says why the sugar is of the series it is. Remark 10.10 states the distinction at length.*

*(vii)* ***That the transformation occurs.*** *Reachability is the non-emptiness of a hom-set. Convention 10.2 of the coordinating paper — connectivity, chemical admissibility, geometric accessibility, physical realization kept apart — is adopted here as this paper's.*

**Scholium 3.2** (Why (ii) is stated so early)**.** A paper that computes the descriptor at twenty structures and finds nineteen of one sign and one of the other is under pressure to present that as a result about the architecture. It is not one, and the reason is worth stating positively.

For any residue of the *L* series the priority rules return the same descriptor except where the side chain carries an atom of higher atomic number than oxygen at the first point of difference, which occurs at exactly one of the twenty. The pattern is therefore true of the *L* series by the definition of the descriptor, and would be recovered by any account whatever that produced the *L* series, including an account with no architecture in it at all. It discriminates nothing.

What the computation does discriminate is the corpus's own structure series. The series is a list of subgraphs with decorations, and whether those decorations constitute the twenty canonical residues has, until now, been asserted in interpretive appendices that enter no proof. Running the priority evaluation over the printed record is a check on *that* identification: if a row fails to return the descriptor its residue requires, the decoration record is wrong at that row, not the architecture. The computation is an audit instrument pointed inward, and its value is entirely in what it would catch.

# 4 The reference architecture

**Proposition 4.1** (The reference transformation)**. [C]** *The resting motif is the saturated tether*

$$\mathrm{C6-O-C6}\alpha\mathrm{H_2-C6}\beta\mathrm{H_2} \\ -\mathrm{OP(=O)(O)CH_2CH_2O}\text{–}\mathit{Ado},$$

*and the target connectivity is*

$$\mathrm{C5-C6}\alpha\mathrm{(H)(NH_2)-C6}\beta\mathrm{(=O)-O2'Ado},$$

*reached while preserving the inherited* C5–C6 *framework bond and complete atom provenance. The transformation is transannular in the strict sense: the arm borne at* C6 *reaches across to the adjacent framework carbon* C5*, which lies in the bay region, and the framework bond between the two is retained rather than broken.*

**Proposition 4.2** (The residue)**. [C]** *The residue formed at a vessel is*

$$\mathrm{C6}\alpha\mathrm{(NH_2)}(R)-\mathrm{C6}\beta\mathrm{(=O)O-C2'},$$

*in which* C6$\beta$ *is oxidised and transferred onto the* 2′*-hydroxyl of the adenosine ribose as an ester,* C6$\alpha$ *bears the* $\alpha$*-nitrogen and is the stereogenic centre, and R is the side chain. For every residue except the one of empty retained set, R begins at* C5*.*

**Definition 4.3** (The chiral series)**. [D]** Let $\Sigma$ be the structure space of the coordinating paper and let $\Sigma^{\times} \subset \Sigma$ be the structures of non-empty retained set. Write $n = |\Sigma^{\times}|$.

**Lemma 4.4** (The count)**. [A]** $|\Sigma| = 20$ *and* $n = 19$*, the structure of empty retained set being the one whose residue carries no side chain. Two rows require separate treatment below: the one whose retained set contains* C6 *in two instances, and the one carrying a closure onto the backbone nitrogen.*

*Proof.* Finite, over the retained sets; Appendix B, block V1, computed. □

# 5 The selection at C6$\alpha$

**Proposition 5.1** (Selection, and naming, separated)**. [C]** *Installation of the nitrogen at* C6$\alpha$ *produces a stereogenic centre there. The two local approach branches, distinguished by the sign of the attack scalar against an oriented local frame, form a torsor under* $\mathbb{Z}/2$*. An oriented cage condition excluding one branch is a section-supplying datum, and under strong exclusion the realized configuration is the selected one,*

$$\chi(\mathrm{C6}\alpha) \;=\; \chi^{\star}.$$

*The identification* $\chi^{\star} = \chi_L$ *is not part of this statement.*

**Recovery Lemma 5.2** (Article 54 and the coordinating paper)**. [A]** *Proposition 5.1 asserts neither more nor less than Proposition 10.12 of the coordinating paper, which in turn asserts neither more nor less than Article 54. Nothing is added and no hypothesis is amended.*

**Remark 5.3** (What has and has not been fixed by this point)**. [A]** At the end of this section the architecture has fixed one configuration at one centre of one structure. It has not fixed which configuration, and it has not said that the same fixing holds at any other structure. The second of these is the gap Section 6 closes; the first it does not close.

# 6 Uniformity of the section

The section of Proposition 5.1 is supplied at one centre of one structure. Nothing stated so far says it is the *same* section at another, and if it were not, the architecture would deliver a section at each centre separately and a mixture over the series, which is not homochirality and is not what the arc claims. This section isolates the missing statement and proves it.

The proof divides on a question the corpus leaves open, and the division is the section's second result: under one order of the canonical word uniformity is total and needs no hypothesis about side chains at all, and under the other it is general but not exceptionless.

## 6.1 The reactive subgraph

**Definition 6.1** (Reactive subgraph)**. [D]** The reactive subgraph of the nitrogen-installation generator is

$$W \;=\; \{\,\mathrm{C6}\alpha,\ \mathrm{N},\ \mathrm{C6}\beta,\ \mathrm{C5},\ \mathrm{C6}\,\},$$

comprising the incipient stereocentre, the incoming nitrogen, the carboxyl carbon of the arm, the framework carbon attacked, and the framework carbon bearing the arm, together with the bonds among them and the oriented local frame against which the attack scalar is signed.

**Remark 6.2** (Why C6 is in $W$)**. [A]** The arm is borne at C6 and the framework bond C5–C6 is retained through the transformation, so the approach of C6$\alpha$ to C5 is a motion across that bond and the geometry of the selection is stated against it. A definition of $W$ omitting C6 would make the disjointness lemma below vacuously easier and would misdescribe the geometry.

**Lemma 6.3** (Disjointness, and its three exceptions)**. [A]** *Let $x \in \Sigma^{\times}$ and let $S_x$ be its retained set. Then $S_x \cap W = \{\mathrm{C5}\}$ at sixteen of the nineteen structures. At three it is larger: at two the retained set contains* C6*, and at one the structure carries a closure from its retained set onto the backbone nitrogen.*

*Proof.* Finite, over the retained sets and the closure field; Appendix B, block V6, computed. □

**Hypothesis 6.4** (Side-chain independence)**. [D]** $S_x \cap W = \{\mathrm{C5}\}$, and the selection at C6$\alpha$ is a function of $W$ alone.

**Remark 6.5** (The hypothesis is false at three rows, and this is not fatal)**. [A]** Hypothesis 6.4 is refuted as a universal statement by Lemma 6.3, and a draft asserting it over the whole series would have been wrong. What follows is written so that the three rows are visible throughout rather than absorbed.
The two rows retaining C6 are the ones whose side chain runs back through the arm-bearing carbon: C6 is at once a vertex of $W$ and a carbon of the product's side chain. The third is the row whose retained set closes onto the nitrogen, so that the side chain and the incoming nitrogen are not independent objects there. In all three the failure is structural and not marginal.
Proposition 6.9 reaches all three without the hypothesis, at the cost of a premise about the order of the canonical word.

## 6.2 The order of the canonical word

**Remark 6.6** (An open premise, and why it becomes load--bearing here)**. [A]** The reference transformation is a composite of six generators. The reaction category is free by construction, and the source declines to select one route as the route, distinct rules, matches and generator orderings remaining distinguishable; a coordinating paper is under pressure to smooth that over and does not.
The freedom is not free here. Two generators are the installation of the nitrogen at C6$\alpha$ and the excision that carves the retained subgraph, and whichever of them runs first determines what the substrate looks like when the branch is selected. The two cases are stated separately below and they do not agree on the three rows of Lemma 6.3.

**Supposition 6.7** (Amination first)**. [D]** In the canonical word, the nitrogen-installation generator precedes the excision generator.
Adopted here as the best case. The reaction-cell development places the amination at a tether carbon, orders it against no stage, and records that a reader wishing to place it early may do so; nothing in the corpus forbids the placement and nothing forces it. It is therefore stated as a supposition, in the manner of Article 54, rather than left as an open target, and the account proceeds under it. Remark 6.8 states what the paper becomes if it fails.

**Remark 6.8** (What fails with it)**. [A]** Nothing outside Proposition 6.9. Under the failure, Corollary 6.13 stands at sixteen of nineteen and the three rows of Lemma 6.3 are unresolved; the descriptor computation, the second centre and the junction pair are untouched, none of them referring to the order of the word. The cost of the supposition failing is three rows, not the account.

**Proposition 6.9** (Uniformity by common intermediate)**. [D]** *Assume Hypothesis 6.7 and strong exclusion. Then the selection at* C6$\alpha$ *is made on a substrate that is the same for every $x \in \Sigma^{\times}$, and the section is the same section at all nineteen structures, the three rows of Lemma 6.3 included.*

*Proof.* Under Hypothesis 6.7 no excision has occurred when the nitrogen is installed. The substrate at that point carries the intact vessel graph and the resting tether, neither of which is a function of $x$: by Proposition 4.1 the resting motif is one motif, and by Proposition 4.2 the structures differ only in the retained subgraph, which does not yet exist. The cage condition of Proposition 5.1 is a condition on that substrate in the stack, and a condition on an object independent of $x$ selects independently of $x$. The section is therefore formed once, before the series branches, and every structure inherits it. □

**Remark 6.10** (What the proposition costs and what it buys)**. [A]** It buys the whole series, exceptions included, and it buys it by an argument with no chemistry in it beyond the order of two generators: if the stereocentre is set before the residues are distinguished, they cannot differ in it. It costs a premise the corpus has not asserted and has deliberately left open.
The premise is also chemically substantive rather than

bookkeeping. It says the architecture fixes handedness first and identity second, which is a claim about what kind of object the carrier is — a machine that makes one chiral backbone and then decorates it, rather than twenty syntheses that happen to agree.

**Theorem 6.11** (Uniformity by disjointness)**. [D]** *Assume Hypothesis 6.4 and strong exclusion, and make no assumption on the order of the word. Then the cage condition excluding one approach branch at* C6$\alpha$ *is the same condition at every structure at which the hypothesis holds, and the map*

$$\Sigma^{\times} \supseteq \{x : S_x \cap W = \{\mathrm{C5}\}\} \longrightarrow \{\text{ branches at } \mathrm{C6}\alpha\},$$
$$x \longmapsto \chi(\mathrm{C6}\alpha; x),$$

*is constant. By Lemma 6.3 its domain is sixteen of the nineteen.*

*Proof.* Three steps.
*(a) The approach geometry is carrier data.* By Proposition 4.1 the bond formed is C5–C6$\alpha$ across the retained framework bond C5–C6, and the tether length and the stack orientation are properties of the unit and of the cluster. None is a function of $x$.
*(b) The side chain is outside $W$.* By hypothesis $S_x$ meets $W$ only at C5, which is the root and is common to all $x$. The situation is that of Theorem 10.15 of the coordinating paper with $x$ in the role of the remote substitution: local concordance of the reactive subgraph holds identically, since $W$ does not depend on $x$ at all, and the external context is reaction-inert at the installation step by hypothesis. The chemical half of the transport is therefore exact, not merely concordant.
*(c) The cage condition is a condition on the stack.* The oriented cage condition of Proposition 5.1 is stated against the stack, which is invariant over $\Sigma^{\times}$; by (a) and (b) it is evaluated on data independent of $x$; hence it excludes the same branch. The section supplied is therefore the same section, and $\chi(\mathrm{C6}\alpha; \cdot)$ is constant on the domain stated. □

**Remark 6.12** (Where the cage half still bites)**. [A]** Step (b) delivers the chemical half exactly, and the geometric half is inherited rather than proved: Theorem 10.15 makes cage-level persistence conditional on supplied candidate lifts meeting a margin condition, and persistence of the selected branch requires the transported installation lift to meet the same condition. Within one substitution context the lift is the same lift and the condition is trivial, which is why this section is scoped to the 6, 12-disubstituted unit. A reader who grants Theorem 6.11 in that context has not thereby granted it in another.

## 6.3 What holds under either order

**Corollary 6.13** (The floor, and the ceiling)**. [D]** *Uniformity of the section holds at sixteen of the nineteen chiral structures under either order of the canonical word, by Theorem 6.11. At the remaining three it holds under Hypothesis 6.7, by Proposition 6.9, and is unresolved without it.*

**Corollary 6.14** (One bit fixes the series)**. [D]** *On the domain of uniformity, a datum fixing $\chi$*(C6$\alpha$) *at any single structure fixes it at every structure of that domain. The external input required to name the series is one bit and not n bits.*

**Remark 6.15** (The order, as far as the corpus fixes it)**. [C]** The reaction-cell development stages its transformation and orders the first three stages totally, by valence and by what must exist before what. On the two generators at issue here it is explicit: the amination at the tether $\alpha$ carbons is ordered against no stage, its site lying at distance from every sulfur site and from every edge destroyed, and no valence argument constrains it; a reader wishing to place the amination early may do so, while a reader placing the transannular bond early may not.
So Hypothesis 6.7 is admissible and unconstrained, and is not forced. Proposition 6.9 is therefore available as a reading of the word rather than as a consequence of it, and Corollary 6.13 stands as stated: sixteen unconditionally, nineteen under a premise the corpus permits and does not supply.

**Remark 6.16** (A parameter the early amination introduces)**. [D]** If the nitrogen is installed before the transannular bond forms, then at the moment of installation C6$\alpha$ carries the ether oxygen to C6, the nitrogen, a hydrogen and C6$\beta$ — four distinct substituents, so the centre is stereogenic already — and the bond to C5 is formed later by substitution at that centre. The stereochemical course of that substitution, retention or inversion, is then a further datum.
It does not disturb uniformity. The substitution is the same substitution at every structure, so whatever its course it acts alike on all of them and Proposition 6.9 is unaffected. It disturbs only the naming, by composing one more binary operation between the selected branch and the descriptor, and the naming is carried by Supposition 8.4, which absorbs it.

**Remark 6.17** (The closure structure keeps its letter)**. [A]** Evaluated separately, with the amine secondary and the side

chain re-entrant, the closure structure returns the descriptor its residue requires; Appendix B, block V3, computed. This bears on the letter and not on Hypothesis 6.4, which fails at that row whatever the letter is. The two are easy to run together and are kept apart here for that reason.

**Target 6.18.** (Aggregated at Target 14.2.) Determine whether the canonical word runs the amination before the excision as a matter of fact and not merely of admissibility. The reaction-cell development permits the placement and does not force it, and the question decides whether the account of homochirality is exceptionless or holds at sixteen of nineteen.

**Scholium 6.19** (What the division shows about the corpus)**.** The freedom of the reaction category is a methodological virtue and the source is right to keep it: target existence should be separated from reaction-word uniqueness, and a paper that named one route as the route would be assigning physical probability without grounds.
But a freedom that costs nothing where it was introduced can cost something downstream, and this is where it does. The order of two generators is unobservable from the target connectivity, which is why the source could leave it open; it is not unobservable from the handedness statement, because the stereocentre is set by one of them and the side chain is carved by the other. Fixing the order is not a matter of selecting a route for its own sake. It is the difference between an account of homochirality that covers the series and one that covers most of it.
The finding is entered at Section 13. It is not a correction to any article; it is a place where two articles' silences meet and produce a question neither was asked.

**Remark 6.20** (Under the weaker realization)**. [A]** If the cage supplies an energetic discrimination rather than an exclusion, then Proposition 6.9 and Theorem 6.11 state that the same discrimination obtains throughout: the enrichment is of one sense and one magnitude, both being properties of the cage rather than of $x$. That is weaker than a section and is not nothing — it is the statement that the series is enriched coherently rather than residue by residue, which is what an origins account requires of it. Corollary 6.14 survives with *configuration* read as *sense of enrichment*.

# 7 The second centre, at C5

## 7.1 Where the second centre is, and how the arm attaches to it

**Proposition 7.1** (Two attachment modes)**. [D]** *Let $x \in \Sigma^{\times}$ be a structure retaining* C5*. In the resting state* C5 *carries two framework bonds, to* C6 *and to* C4b*, and one hydrogen; dearomatisation creates a fourth position. The transannular bond to* C6$\alpha$ *consumes one severance at* C5 *where there is one. Hence exactly two modes occur:*

*(a)* C5 *loses no framework bond. Both framework directions are retained, and the bond to* C6$\alpha$ *occupies the position created by dearomatisation.*

*(b)* C5 *loses one framework bond, at* C6*. The bond to* C6$\alpha$ *occupies the direction so vacated, and the position created by dearomatisation is filled by a decoration.*

*The mode is read off the severance record and is not a free choice.*

*Proof.* Finite, from the per-vertex loss at C5 and the rule that the transannular bond consumes one severance there; Appendix B, block V4, computed against block R9 of the coordinating paper. □

**Remark 7.2** (The two structures with a second centre fall in different modes)**. [A]** Of the structures of $\Sigma^{\times}$, exactly two render C5 stereogenic, and they fall one in each mode: the structure of the branched hydrocarbon side chain has no severance at C5 and is in mode (a), while the structure carrying a hydroxyl at C5 loses one and is in mode (b), the hydroxyl occupying the new position. Block V4 exhibits both.
A reading on which these two present the same spatial arrangement at C5 is therefore not available, and none is asserted below. An earlier draft of this section asserted one, and the assertion is withdrawn in Appendix D.

**Hypothesis 7.3** (The face datum)**. [D]** The position created by dearomatisation at C5 is filled from the exposed face of the chrysene plane, and the exposed face is a datum of the stack.

**Target 7.4.** Decide whether the exposed face of Hypothesis 7.3 and the sign of the attack scalar at C6$\alpha$ are the same datum. The question is geometric and is finite once the stack orientation is written down. It is taken up at Section 7.3 and is answered there in part and in the negative.

## 7.2 Two modes, two descriptors

**Theorem 7.5** (The relative configuration is forced)**. [D]** *Assume Hypothesis 7.3. Then the descriptors at* C5 *of the two structures of Remark 7.2 are determined together by the face, and the two values so determined are opposite: one face yields* 3*S at the mode-(a) structure and* 3*R at the mode-(b) structure, and the other face yields the two reversed. No face yields like descriptors.*

*Proof.* Finite. The priority ordering at C5 is computed for each structure on the hierarchical digraph, the four substituents are placed at the framework directions and the new position according to Proposition 7.1, and the descriptor is read from the sign of the triple product. Both faces are evaluated. Appendix B, block V4, computed. □

**Corollary 7.6** (The pair, under the anchor)**. [D]** *Under Hypothesis 7.3 anchored so that the mode-(a) structure carries* 3*S, the mode-(b) structure carries* 3*R, and the pair is* $(2S, 3S)$ *and* $(2S, 3R)$ *respectively.*

**Scholium 7.7** (Why this is the paper's sharpest check)**.** Every other statement in this paper predicts sameness — the same branch, the same section, the same configuration. Sameness is cheap to predict and hard to falsify, since a mechanism that did nothing at all would predict it too.
Theorem 7.5 predicts a difference, and it predicts the difference from a single datum rather than from two. One face is chosen; two descriptors come out, at two structures, by two different routes — one because the transannular bond sits at the new position and one because a hydroxyl does — and they come out opposite. The computation that produces them runs over a priority ordering that knows nothing of the architecture, and the comparand is fixed independently by the naming of the two residues.
Three outcomes would have refuted it and one confirmed it. Had the two come out alike under both faces, the mode distinction of Proposition 7.1 would be doing no work. Had one face given one comparand and the other face the other, the pair would cost two bits rather than one and the section would have no theorem. Had a face given the comparands reversed, the attachment modes would be assigned to the wrong structures. What block V4 returns is the fourth case.

## 7.3 Target 7.4, resolved in part

**Proposition 7.8** (The face of an arm)**. [D]** *Each arm of a unit departs toward one face of the skeleton, and the two arms of a* 6, 12*-disubstituted unit depart toward opposite faces. A position filled by the chemistry of a given arm is filled from that arm's face. In particular the position created by dearomatisation at* C5 *is filled from the face of the arm at* C6*.*

**Remark 7.9** (A stronger form, withdrawn)**. [A]** An earlier form of this proposition argued that one face of each unit is buried in the stack and unavailable, so that every arm lies on a single exposed face. The reaction-cell development states the contrary: the two arms of a unit leave toward *opposite* faces, and the conformation in which both leave toward one face is the alternative it excludes. The weaker form above is what survives, and it is enough for Section 7, which concerns one arm. What it no longer supplies is a single face common to the whole unit, and Section 9 is where that loss is felt.

**Corollary 7.10** (Hypothesis 7.3 is not an independent premise)**. [D]** *Proposition 7.8 derives Hypothesis 7.3 from the conformation. What remains free is not whether the new position is filled from the arm's face, but which face the arm at* C6 *departs toward, and that is the same datum the cage condition of Proposition 5.1 is stated against.*

**Proposition 7.11** (What the burial argument does not reach)**. [D]** *The burial argument does not by itself fix the branch at* C6$\alpha$*. With the exposed face given, the nitrogen is installed anti to the ring and* C5 *lies toward it, which places* N *and* C5 *but leaves* C6$\beta$ *and the hydrogen in the two remaining positions about the* C5–C6$\alpha$ *axis. The branch is fixed only once the disposition of* C6$\beta$ *about that axis is fixed, and* C6$\beta$ *is the carbon carrying the ester to the ribose, so its disposition is set by the anchoring of the adenosine in the cluster.*

**Supposition 7.12** (Lattice-constrained cage)**. [D]** The cage is lattice-constrained: the vessels of an assembly occupy congruent sites, related to one another by operations of the assembly's own symmetry group, and no vessel sits in an environment peculiar to itself.
Adopted here as the best case, and adopted in place of a stronger hypothesis this paper earlier required. What it supplies is stated at Proposition 7.13.

**Proposition 7.13** (Congruence makes the azimuth uniform, without fixing it)**. [D]** *Under Supposition 7.12 the disposition of* C6$\beta$ *about the* C5–C6$\alpha$ *axis is the same at every vessel of an assembly, being a consequence of a site geome-*

*try that is the same at every vessel. Its value is not thereby determined.*

**Remark 7.14** (Why the weaker premise is enough)**. [A]** This paper never needed the value of the azimuth. It needed the azimuth to be the same wherever a residue is made, so that the branch parameter is one parameter and not one per vessel; the value itself is absorbed, with the face, into the single composite that Supposition 8.4 names.
So the account is restored to one external input. The two geometric parameters of block V7 are uniform by Proposition 7.13 and forced in their relation to the arm by Proposition 7.8; their joint value is the one bit the anchor fixes; and no second naming is required anywhere. What was two parameters at Remark 7.15 is one composite under a premise about the assembly rather than about a rotamer, which is the better place for it to sit.

**Remark 7.15** (The answer to Target 7.4, stated plainly)**. [A]** The target asked whether the face datum and the attack scalar are one datum. The answer is no, and the correction runs against this paper's earlier framing rather than for it.
Block V7 enumerates the four combinations of the two parameters and finds that exactly one reproduces the record — which is not evidence of coupling but the opposite. Each of the two mixed combinations is internally consistent, and each is excluded only by the comparands, which are supplied from outside. Nothing in the retained sets, the severance counts or the priority orderings relates the two.
What Proposition 7.8 achieves is a reduction of a different kind: the face parameter is not a free bit at all, being forced by the arm. What Proposition 7.11 concedes is that the branch parameter is not thereby forced with it, a further datum being required.
That datum is supplied, in the only form the paper needs, by Supposition 7.12 and Proposition 7.13: not the value of the azimuth but its uniformity, which is what makes the two parameters one composite. Under that supposition the account returns to a single external input, the naming convention, and Remark 7.14 states the reduction.

**Remark 7.16** (What the reaction-cell development supplies, and what it does not)**. [C]** That development specifies the tether in full — ether-linked at C6, through a phosphodiester, to the C2 position of an adenosine — and states that the linkage leaves the pairing edge of the base unobstructed and that the two nucleosides of a unit present their edges on opposite sides of the skeleton. That fixes the face toward which each arm departs. It does not fix the disposition of C6$\beta$ about the C5–C6$\alpha$ axis, which is a rotamer of the arm and not a face, and Hypothesis 7.12 therefore stands undischarged.
It also corrects Proposition 7.8 of this paper, and the correction is recorded at Appendix D.

**Target 7.17.** (Aggregated at Target 14.3.) Establish that the cage is lattice-constrained in the sense of Supposition 7.12, or exhibit a vessel whose site is not congruent to the others. The question belongs to the cage literature. What it does *not* require is the value of the azimuth, which Proposition 7.13 shows the account can do without.

**Remark 7.18** (What is still declared)**. [A]** Two things in this section are read from the record rather than derived, and a reader should know which. The attachment modes are read from the severance counts at C5 in block R9, which this paper does not recompute from the excision. The assignment of side-chain branches to the two framework directions — which retained vertex carries which substituent — is read from the retained sets. Both are entered in the hypothesis register as H5 and both are audited for consistency at block V5, which is weaker than deriving them.

# 8 The descriptor over the series

## 8.1 The computation

**Theorem 8.1** (The descriptor at C6$\alpha$ is constant with one inversion)**. [A]** *Substituent-priority evaluation at* C6$\alpha$ *over the printed decoration record of* $\Sigma^{\times}$ *returns the same descriptor at every structure save one. The exception is the structure whose side chain carries sulfur at the first point of difference, at which the side chain outranks the carboxyl carbon and the descriptor is the opposite letter for the same spatial arrangement.*

*Proof.* Finite: Appendix B, block V2, which constructs the ordering at each row from the decoration record and emits the descriptor, together with the comparand column and a disagreement count, which is zero. □

**Corollary 8.2** (Liberation does not move the descriptor)**. [A]** *The descriptor at* C6$\alpha$ *is the same in the tethered product, where* C6$\beta$ *carries the ester to the ribose* 2′*-oxygen, as in the liberated residue, at every row. Excision therefore introduces no clause here.*

*Proof.* Finite, the two evaluations run side by side; Appendix B, block V2b, computed. The carboxyl branch presents

the same three oxygens at sphere two under either reading, and every comparison against it is decided by sphere two. □

**Remark 8.3** (The letter is not the configuration)**. [A]** Theorem 8.1 is a statement about *letters*, and the letters change at one row while the configuration, by Theorem 6.11, does not change anywhere. That the two disagree at one row is the whole content of the theorem and is a fact about the naming convention. A reader who takes the inversion as a chemical exception has read a convention as a mechanism.

## 8.2 The anchor

**Supposition 8.4** (The reference identification)**. [D]** Let $x_0 \in \Sigma^{\times}$ be the reference structure of minimal retained set. Suppose

$$\chi^{\star} = \chi_L \quad \text{at } x_0.$$

This is a supposition and is stated where it is used, in the manner of Article 54. It is not derived here, is not derived anywhere in the corpus, and is registered as H1 in Appendix A. It is the single external bit of Corollary 6.14.

**Corollary 8.5** (The series under the supposition)**. [D]** *Assume Theorem 6.11, Theorem 8.1, Theorem 7.5 and Supposition 8.4. Then every structure of* $\Sigma^{\times}$ *realizes the configuration of the L series at* C6$\alpha$*; the descriptor is S at every such structure except the sulfur-bearing one, at which it is R; and and, under Hypothesis 7.3 anchored as at Corollary 7.6, the two structures with a second centre realize* $(2S, 3S)$ *and* $(2S, 3R)$ *respectively.*

**Scholium 8.6** (What the corollary is worth)**.** Corollary 8.5 is conditional and the condition is one supposition, which is either the strongest or the weakest thing about it depending on what the reader came for.

A reader who came for a derivation of the *L* series does not get one, and the corpus has said three times now that none is available from an architecture of this kind. A reader who came for an account of *homochirality* — of why the products should be of one hand rather than of a mixture, which is the question the origins literature actually poses — gets that unconditionally from Theorem 6.11, with the letter supplied afterwards by convention and by one supposition. The distance between the two is one bit for the $\alpha$ series, and the contribution of this paper is to have shown that it is one bit and not nineteen. That is a smaller claim than the one the arc is liable to be summarised as making, and it is the one that holds.

The second centre is not covered by that bit, and Remark 7.15 says why: the parameter fixing it is forced by the stack, but its coupling to the branch at C6$\alpha$ is not established here and may not be establishable without the cluster geometry. A summary of this paper should say one bit for the series and a second, conditional, for the pair.

# 9 The junction pair, and the parity of the relation

Sections 6 to 8 establish that the selection is the same across the twenty structures at one vessel. They do not ask whether it is the same at two vessels that make their residues together, and the question arises at exactly one place in the corpus: the junction cell, which yields two residues rather than one.

The answer is favourable and is obtained by an argument with one moving part.

## 9.1 Both residues take the same route

**Proposition 9.1** (The atom map of the junction pair)**. [C]** *At a junction two strands meet chrysene to chrysene, the two facing units stacked* $\pi$*-face to* $\pi$*-face. The junction cell comprises six vessels; six being even, the cell has no central vessel but a central pair, falls outside the localisation rule rather than excepting it, and yields two residues, one on each facing unit. Writing* X3 *and* X4 *for the facing units, the map is*

| | | | |
|---|---|---|---|
| *first:* | C′ = C6$\beta$@X3, | C6$\alpha$@X3, | C$\beta$ = C5@X3, |
| *second:* | C′ = C6$\beta$@X4, | C6$\alpha$@X4, | C$\beta$ = C5@X4. |

*Both retained sets and both cut lists are the corpus's published rows, used unamended. The two residues share no atom and no bond.*

**Corollary 9.2** (The preceding sections apply twice, unamended)**. [D]** *Each residue of the junction pair is formed by the transannular attack of* C6$\alpha$ *on* C5 *from the arm of its own unit. Every statement of Sections 5 to 8 is therefore a statement about each of the two centres separately, with no amendment and no new premise. In particular the selection at each is the selection of Proposition 5.1, and the descriptor at each is the descriptor of Theorem 8.1.*

**Remark 9.3** (The second arm does not enter)**. [A]** The arm at C12 supplies no $\alpha$ carbon of this cell, and C12$\alpha$ is not a stereocentre of it. A reading on which the two residues of the pair are borne by the two arms of one unit is a different cell, and Section 9.3 says what becomes of the question there.

## 9.2 Only the parity of the relation matters

**Definition 9.4** (The relation between the facing units)**. [D]** Let $\tau$ be the spatial operation carrying the first facing unit, with its arm and tether, onto the second.

**Theorem 9.5** (Parity decides the hand of the pair)**. [D]** *Assume that the selection at* C6$\alpha$ *is stated intrinsically at each unit, as Proposition 5.1 states it, and that $\tau$ carries the datum supplying the selection at the first unit to the datum supplying it at the second. Then the two residues are of the same hand if $\tau$ is proper, and of opposite hands if $\tau$ is improper. No other feature of $\tau$ bears on the question.*

*Proof.* A configuration is read from the sign of a triple product of three substituent directions. A proper operation has determinant $+1$ and preserves that sign; an improper operation has determinant $-1$ and reverses it. The hypothesis makes the second selection the $\tau$-image of the first, so the two signs agree or disagree according as $\det \tau$ is $+1$ or $-1$, and nothing else in $\tau$ enters. □

**Proposition 9.6** (The junction relation is proper)**. [D]** *At a junction the two strands are related by face inversion with the order of sites kept, the order-reversing alternatives failing at the discriminating case. Face inversion presents the other face of a unit, and presenting the other face of a planar object is a rotation by $\pi$ about an axis lying in its plane. That operation is proper. Hence* $\det \tau = +1$.

**Corollary 9.7** (The junction pair is homochiral)**. [D]** *By Theorem 9.5 and Proposition 9.6 the two residues of a junction cell are of the same hand. Under Supposition 8.4 both are of the L series, and their descriptors are R and S respectively, the first carrying the sulfur side chain that inverts the letter.*

*Proof.* Finite, given the parity; Appendix B, block V8, computed at both parities. □

**Remark 9.8** (Which case the letters would betray)**. [A]** Block V8 records a circumstance worth keeping in view. The homochiral pair carries *unlike* letters at its two centres, *R* and *S*, because the sulfur side chain of the first inverts its letter and the side chain of the second does not. An antipodal pair would carry *like* letters, *R* and *R*.

A table recording letters alone would therefore read the racemic case as the tidy one and the correct one as the anomaly. This is the sharpest instance in the paper of Scholium 3.2, and it is the reason that scholium refuses the descriptors as evidence rather than merely cautioning about them.

## 9.3 What the improper case was, and where it belongs

**Remark 9.9** (The single-unit arrangement, and why it does not arise here)**. [A]** There is an arrangement in which the two sulfur residues are formed on one unit, from its two arms. On that reading the second $\alpha$ carbon is C12$\alpha$, the two centres are related by the skeleton's unique automorphism, and that automorphism is stated to be realised as a *point inversion* — an improper operation. Theorem 9.5 then gives an antipodal pair, and homochirality on such a cell would require a datum breaking the symmetry that the cell is stated not to carry.

That arrangement is not the junction cell and is not the arrangement this paper treats. At a junction the two residues occupy different molecules, both are formed at C6$\alpha$–C5 by the route of Section 4, the published rows are used unamended, and the relation is proper. The single-unit reading is a distinct cell whose own development states the premise placing both residues on one unit as its own and as underived.

The consequence is recorded because it is a consequence and not because this paper adopts the premise: on the single-unit reading, handedness joins the list of things that premise carries, alongside the amended retained set and the ring distortion its own development records. Nothing in Sections 6 to 8 is affected either way, those sections concerning one vessel and twenty structures.

**Scholium 9.10** (What the junction supplies that this paper could not)**.** The result of this section is not one this paper's own apparatus could have reached, and it is worth saying where it comes from.

Sections 6 to 8 establish uniformity across structures at a vessel, and reduce the external input for the series to one naming convention. They say nothing about two vessels, because at one vessel there is nothing to say. The junction supplies a case where two residues are made together, and it supplies with it the one fact the question turns on: that the two strands are related by face inversion with the order kept, and not by either operation involving a reversal.

That fact is established there for a different purpose — it is what relates the two codons and what makes the pair complementary of necessity — and its bearing on handedness appears not to have been drawn. Drawn, it says that the architecture makes its two co-synthesised residues of one hand by the same route and under the same anchor as it makes the other eighteen. The account of homochirality

therefore extends from the twenty structures to the pair without a further premise, which is the strongest statement this paper is able to make.

### 9.4 Falsification register for this section

**Corollary 9.2**
A junction residue formed otherwise than by the attack of C6$\alpha$ on C5 of its own unit; or an atom map placing either $\alpha$ carbon on the arm at C12.

**Theorem 9.5**
Nothing chemical: the statement is that a determinant decides a sign. It is refuted only by a selection rule not stated intrinsically at a unit, so that the second selection is not the image of the first.

**Proposition 9.6**
A spatial realisation of the strand relation as an improper operation; or a junction at which the two strands are related by one of the order-reversing operations, which that development excludes at the discriminating case.

**Corollary 9.7**
An exhibited junction pair of opposite hands, which would refute Proposition 9.6 or the intrinsic statement of the selection.

**Corollary 10.3**
A development of the corpus whose co-synthesised pair is related by an operation that is neither proper nor improper, which is impossible, or one whose hand does not follow the parity, which would refute Theorem 9.5.

**Remark 9.8**
A recomputation at block V8 giving like letters in the proper row.

## 10 The cluster, and the parity of the assembly

Section 9 decides the hand of two residues made at one junction. The same argument decides the hand of a cluster, and stating it at that level is worth doing, because it produces the paper's most general statement and locates the one thing still capable of breaking homochirality.

### 10.1 The statement

**Definition 10.1** (Assembly relations)**. [D]** Let an assembly carry vessels $v_1, \dots, v_m$. For each pair, let $\tau_{ij}$ be the spatial operation carrying $v_i$, with its arm and tether, onto $v_j$, which Supposition 7.12 supplies. Write $\det \tau_{ij} \in \{+1, -1\}$ for its parity.

**Theorem 10.2** (Cluster homochirality is a parity condition)**. [D]** *Assume Supposition 7.12, and that the selection at* C6$\alpha$ *is stated intrinsically at each vessel. Then*

$$\chi(v_j) \;=\; \det(\tau_{1j}) \cdot \chi(v_1),$$

*so the assembly is homochiral if and only if every operation relating two of its vessels is proper. If some $\tau_{ij}$ is improper, the vessels it relates are antipodal, and the hand of the assembly partitions its vessels into two classes according to the parity of the relation carrying each to the first.*

*Proof.* By Supposition 7.12 the site geometry is the same at every vessel, so the datum supplying the selection at $v_j$ is the $\tau_{1j}$-image of the datum at $v_1$; by Theorem 9.5 the configuration is preserved or reversed according to the parity of that operation. Composition of parities along any path gives the same result, det being a homomorphism, so the partition is well defined. □

**Corollary 10.3** (The two developments are the two values)**. [D]** *Theorem 10.2 takes both values in the corpus. At a junction the two facing units are related by face inversion with the order kept, which is proper (Proposition 9.6), and the pair is homochiral. On the arrangement placing two residues on one unit, the two centres are related by a point inversion, which is improper, and the pair is antipodal (Remark 9.9). Neither is an exception to the other; they are the two values of one parameter.*

### 10.2 What the orientation marker does not record

**Remark 10.4** (Parity is not in the carrier's datum)**. [A]** The carrier's only datum is the orientation pattern of its units, one binary marker per site. Block V9 records what that datum does and does not settle.

It does not settle the hand. An alternation of orientation realised as a flip about an axis in the plane is proper and leaves the cluster homochiral; the same alternation realised as a point inversion is improper and makes it alternately handed. The two are the same pattern of markers. A marker records which of two orientations a unit is in; it does not record how the two orientations are related in space, and the parity lives entirely in that realisation.

This is worth stating plainly because the formalism's treatment of the marker is complete, and its silence here is not a gap in that treatment but a feature of what a marker is. The registry, the coboundary, the class count and the capacity are all statements about the pattern, and none of them can see a determinant.

## 10.3 The parity is fixed by the ribose

**Proposition 10.5** (Every vessel carries the same sugar)**. [C]** *Each unit of the assembly bears its arm through a phosphodiester to an adenosine, and the residue's carboxyl carbon* C6$\beta$ *is esterified to the* 2′*-oxygen of that adenosine's ribose. The ribose is of the D series, and is of the D series at every unit of the assembly.*

**Theorem 10.6** (No improper operation relates two vessels)**. [D]** *Let $\tau_{ij}$ be as in Definition 10.1, carrying $v_i$ together with its arm and tether onto $v_j$. An improper operation carries a D ribose to an L ribose. By Proposition 10.5 the ribose of $v_j$ is of the D series, so $\tau_{ij}$ is not improper. Hence* $\det \tau_{ij} = +1$ *for every pair, and by Theorem 10.2 the assembly is homochiral.*

*Proof.* The tether is part of the object transported, by Definition 10.1; the ribose is part of the tether, by Proposition 4.1. An operation of determinant $-1$ carries a configuration to its opposite at every centre of the object it carries, the ribose centres included. A $\tau_{ij}$ of determinant $-1$ would therefore present $v_j$ with a ribose of the $L$ series, contradicting Proposition 10.5. □

**Corollary 10.7** (The criterion of Theorem 10.2 is met)**. [D]** *The condition under which an assembly is homochiral is satisfied by every assembly of the architecture. Homochirality over the cluster is therefore not conditional on a datum the corpus has yet to supply.*

**Proposition 10.8** (The junction relation, reached a second way)**. [D]** *Both strands of a junction are poly-adenosine complexes and their riboses are of the D series. By Theorem 10.6 the operation relating the two facing units is proper, so Proposition 9.6 holds whatever the spatial realisation of face inversion turns out to be, and Corollary 9.7 does not depend on that realisation.*

**Remark 10.9** (A second proof, and why it is worth having)**. [A]** Proposition 9.6 argues from face inversion presenting the other face of a planar unit, hence from a rotation about an axis in the plane. That argument passes from an operation on orientation values to a spatial motion, and Remark 10.4 is at pains to say that the orientation datum does not record the motion. Proposition 10.8 reaches the same conclusion without that passage. Where a result is carried by two arguments and one of them crosses a step the paper elsewhere refuses, the other should be the one cited.

## 10.4 What this is, and what it is not

**Remark 10.10** (Transfer, not generation)**. [A]** The reading a reader will want to put on Corollary 10.7 is not the one available, and the difference should be stated before anyone states it for us.

On this argument the architecture does not produce handedness from an achiral beginning. It transfers handedness it already carries: the parity condition is met because every vessel bears a sugar of one series, and the amino-acid configuration is inherited from the nucleoside configuration through the tether that joins them. A carrier assembled from $L$ riboses would make the antipodal series by every argument in this paper, and nothing here says why the sugar is $D$.

That is a respectable position and it is not a small one — transfer of configuration from the sugar to the residue is a recognised shape of account in the origins literature, and this paper supplies a mechanism for it rather than a correlation. But an account of transfer is not an account of origin, and a summary of this paper that says the cage makes the residues one-handed, full stop, says more than the paper holds. Proposition 3.1(vii) refuses that reading where refusals belong.

**Remark 10.11** (Where the anchor now sits)**. [A]** Supposition 8.4 is not discharged by any of this and is not weakened. What changes is that it acquires an address. The one external bit naming the selected branch is plausibly a function of the ribose configuration composed with the tether geometry, both of which are carrier data rather than conventions; and a supposition about the carrier is a different object from a supposition about a naming, even when neither is established. Whether the composite can be computed is Target 14.1 as it now reads.

**Remark 10.12** (Uniform assembly, and the congruence of sites)**. [D]** The specification encodes the cluster so that the aromatic systems of adjacent substituted units align, the adenine of each unit stacking against the tethered chrysene of its neighbour throughout. A pairing whose units are not so aligned does not yield a tethered adenosine–chrysene unit at all and does not enter the architecture; base stacking then holds the aligned assembly in place.

This is the ground Supposition 7.12 asked for. Units assembled by one encoding into one registered stack occupy congruent sites, so the disposition of C6$\beta$ about the C5–C6$\alpha$ axis is the same at every vessel, which is what Proposition 7.13 requires and all that it requires.

It is worth being exact about what the alignment does *not* give. Alignment is a statement about positions, and parity

is not a function of positions: a column of planar molecules in perfect registry may be related by an inversion centre, and its registry does not reveal the inversion. The exclusion of misaligned pairings excludes misaligned assemblies and not improper ones. So the alignment argument grounds Supposition 7.12 and leaves Theorem 10.6 to do the other work.

**Target 10.13.** (Aggregated at Target 14.1.) Determine whether the one external bit of Supposition 8.4 is computable from the ribose configuration together with the tether geometry. A positive answer would discharge the last supposition of the paper and would make the *L* series a consequence of the *D* sugar; a negative answer would say which further datum the composite needs. The question is geometric and is finite once the tether is written down.

**Scholium 10.14** (Where the account now stands, and where it can still fail)**.** It is worth setting out, once, what carries the account and what would break it, since the premises have moved twice in the drafting.

Homochirality across the twenty structures at one vessel rests on the disjointness of the side chain from the reactive subgraph, with three rows carried by Supposition 6.7. Homochirality across two vessels making their residues together rests on the parity of the relation between them, and at a junction that parity is favourable. Homochirality across a cluster rests on Theorem 10.2, and reduces to a single question about the assembly's symmetry group. The naming of the common configuration rests on Supposition 8.4 alone, one bit, as Remark 7.14 restores it.

What can still break it is one thing and it is not a chemical one. If any operation relating two vessels of an assembly is improper, the assembly is alternately handed, and no feature of the residues, the excisions or the descriptors would repair it or reveal it: the letters, as Remark 9.8 shows, would read tidier in the broken case than in the sound one. An architecture that produced residues of one hand by an argument at each vessel and mixed hands by the relation between vessels would look correct at every point at which the corpus currently looks.

That is the value of stating the account at cluster level rather than at vessel level, and it is the reason this section exists.

## 10.5 Falsification register for this section

**Supposition 7.12**
A vessel whose site is not congruent to the others; or an assembly in which the arm's disposition differs between vessels of the same orientation.

**Proposition 7.13**
Falsified with the supposition and not independently.

**Theorem 10.2**
A selection at C6$\alpha$ not stated intrinsically at a vessel — one depending on the assembly's global frame rather than on the vessel's own — which would break the transport and with it the parity argument.

**Theorem 10.6**
An assembly whose vessels do not all bear a ribose of one series; a tether from which the ribose is absent, so that the transported object carries no configuration to be reversed; or a reading of Definition 10.1 on which the tether is not carried with the vessel.

**Corollary 10.7, Proposition 10.8**
Falsified with Theorem 10.6 and not independently.

**Remark 10.12**
An encoding admitting a registered stack whose vessels are not congruent; or a misaligned pairing that nonetheless yields a tethered unit. Note that no alignment finding refutes Theorem 10.6, the two arguments bearing on different premises.

**Remark 10.10**
A derivation, from the architecture alone, of the series of the ribose. That would refute the remark by establishing more than it allows, and would convert the account from transfer to generation.

**Remark 10.4**
A derivation of the parity of an assembly relation from the orientation pattern alone, which would place the question inside the registry.

# 11 Consolidated register

This section states, in one place, what the account answers and on what. It adds nothing. Its purpose is that a reader who has followed the argument should be able to see, without reassembling it, which answers are finite, which rest on a supposition, and which are open — and the three are not alike.

## 11.1 What is answered, and on what

**Is the product at one vessel of one configuration rather than a mixture?**
Yes: an oriented cage condition excludes one approach branch and supplies a section. *Rests on:* H1. Imported unamended (Prop. 5.1). *Standing:* **[C]** Established in the corpus; weakens to an enrichment under the bias reading.

**Is it the same configuration at every structure of the series?**
Yes at sixteen of nineteen without a premise about the word; at all nineteen with one. *Rests on:* H2 at sixteen; H2b for the

remaining three. *Standing:* **[D]** Established at sixteen; supposed at nineteen.

**Can the side chain affect the selection?**
No at sixteen rows, where the retained subgraph meets $W$ only at its root. At three it does. *Rests on:* Finite, from the retained sets (Lem. 6.3). *Standing:* **[A]** Established, exceptions named.

***Which* configuration is selected?**
Not determined by the architecture, and not determinable by an argument of its kind. *Rests on:* Sup. 8.4, one bit, supplied from outside. *Standing:* **[D]** Refused as a derivation; supposed where used.

**What is the descriptor at** C6$\alpha$ **over the series?**
One letter at eighteen rows and its opposite at the sulfur-bearing row; the structure of empty retained set has none. *Rests on:* Finite, over the decoration record (Thm. 8.1). *Standing:* **[A]** Computed, block V2; entailed by the naming and not evidence for it.

**Does excision change the descriptor?**
No. The ester and the liberated acid give the same letter at every row. *Rests on:* Finite (block V2b). *Standing:* **[A]** Computed.

**Is there a second stereogenic centre?**
At two structures, and there it is C5, a framework carbon. *Rests on:* Finite, by distinctness of the four branches. *Standing:* **[A]** Computed, block V4.

**Is its configuration fixed, and how?**
Yes. The transannular bond attaches in two modes, and one face datum fixes both descriptors, at 3$S$ and 3$R$. *Rests on:* Prop. 7.1, Hyp. 7.3; the face by Prop. 7.8. *Standing:* **[D]** Relative configuration forced; absolute on the same composite as the $\alpha$ series.

**Are two residues made together of one hand?**
At a junction yes; on a single unit no. The two are the values of one parameter. *Rests on:* Thm. 9.5; the junction parity by Prop. 9.6. *Standing:* **[D]** Established given the parity, which is imported at the junction.

**Is a cluster homochiral?**
Exactly when no operation relating two of its vessels is improper. Whether that holds is not settled. *Rests on:* Thm. 10.2, under H6; the parity itself is H8. *Standing:* **[D]** Criterion established; the criterion's value open (Target 10.13).

**Does the carrier's own datum settle the hand?**
No. An orientation marker records which orientation, not how two orientations are related in space. *Rests on:* Finite (Rem. 10.4, block V9). *Standing:* **[A]** Established, and it is a limitation of the datum rather than of the formalism.

**Is the $L$ series derived?**
No, and no argument of this kind can derive it. *Rests on:* — *Standing:* **[A]** Refused at Prop. 3.1(i), before every construction.

## 11.2 How much is finite

> **Remark 11.1** (The three kinds, counted)**. [A]** Of the twelve entries above, five are finite computations over the record and stand whatever becomes of any hypothesis: the disjointness and its exceptions, the two descriptor computations, the second centre, and the indifference of the marker to parity. Five are derived under named premises. One is a supposition and one is a refusal.
> The distribution is worth noting because it runs against the shape of the subject. Handedness arguments are usually conformational throughout; here the conformational content is confined to two premises about the cage, H1 and H6, and everything else is either a finite check over a graph or a determinant.

## 11.3 What the account would look like at each failure

**H1, the cage condition**
The strongest loss. No section at any vessel, and the architecture yields a mixture. The finite content survives — the structures, the descriptors, the attachment modes — and describes a racemic synthesis. Under the weaker reading, in which the cage discriminates energetically rather than excluding, every statement of this paper holds with *configuration* read as *sense of enrichment*.

**H2, side-chain independence**
A section at each vessel, and no statement relating the vessels. Homochirality across the series fails. Recoverable in full through H2b.

**H2b, amination first**
Three rows. Uniformity at sixteen of nineteen; the descriptor work, the second centre and the junction pair untouched.

**H3, the face at** C5
The second centre, at two structures. The $\alpha$ series entire is unaffected.

**H4, the anchor**
The letter, and nothing else. Under its failure the series is uniformly $D$ rather than failing piecewise, which is Corollary 6.14 read from the other side.

**H5, the decoration record**
The audit value of blocks V2 to V5, and the identification of the structures with named residues. The architectural statements are about subgraphs and survive.

**H6, the lattice constraint**
The reduction to one external input. The branch becomes a second input, named separately; every per-vessel result stands, and Theorem 10.2 loses its hypothesis.

**H8, assembly parity**
Homochirality over the cluster, and nothing below it. Each

vessel still produces one configuration, the series is still uniform, and the cluster is alternately handed. This is the failure that no observation at the residue level would reveal.

> **Scholium 11.2** (The asymmetry of the table)**.** The right-hand column is not uniform in kind, and the difference matters more than the entries.
> Most failures cost a statement and leave a smaller account that is still an account. H2b costs three rows; H3 costs two structures; H4 costs a letter and substitutes another. A reader who denies several of these still has an architecture that makes one configuration at a vessel.
> Two are different. H1 failing removes the section, and with it the subject of the paper. H8 failing leaves every statement of the paper standing and the conclusion false — a cluster of alternately handed residues, produced by an architecture that is doing everything this paper says it does at every vessel. The second is the more dangerous because it is the one that leaves no trace where anyone is looking.

# 12 Falsification register for Sections 6 to 8

**Lemma 6.3**
A recount at block V6 disagreeing at any row; or a reading of Definition 6.1 on which C6 is outside $W$, which would move two rows into the general argument and is to be argued rather than assumed.

**Proposition 6.9**
A canonical word running the excision first, which refutes Hypothesis 6.7 and leaves Corollary 6.13 at sixteen; or an excision-independent substrate that nonetheless admits an $x$-dependent cage condition.

**Theorem 6.11**
A substitution or decoration outside $W$ at which the excluded branch reverses; or a cage condition whose sense depends on the retained subgraph. Either yields a mixture over the series while preserving a section at each centre, and is the most informative negative result available to this paper.

**Corollary 6.13, Corollary 6.14**
Falsified with the two statements above and not independently.

**Proposition 7.1**
A structure retaining C5 whose severance count there is neither zero nor one; or a transannular bond not consuming a severance where one exists.

**Proposition 7.8**
A new position at C5 filled from the buried face; an arm reaching the buried face; or a cluster geometry leaving both faces available, which would return Hypothesis 7.3 to the status of a free premise.

**Hypothesis 7.12**
A cluster in which the adenosine anchor admits two dispositions of C6$\beta$ about the C5–C6$\alpha$ axis, or in which the disposition differs between vessels; either leaves the branch parameter free and the account at two external inputs.

**Theorem 7.5**
A recomputation at block V4 returning like descriptors at the two structures under either face; or returning the two comparands under *different* faces, which would cost the pair a second bit and leave the section without a theorem; or returning them reversed, which would misassign the attachment modes.

**Theorem 8.1**
A recomputation at block V2 disagreeing at any row; or a second row of the series at which the side chain outranks the carboxyl carbon, which the decoration record would then be wrong to have printed.

**Lemma 4.4**
A recount at block V1 disagreeing; or a second structure of empty retained set.

**Corollary 8.2**
A row at which the ester and the liberated acid give different letters, which block V2b would show and which would require a clause at Section 8.

**Corollary 7.6**
Falsified with Theorem 7.5 and not independently; or a decoration record giving the two comparands under different faces.

**Proposition 7.11**
A cage geometry in which the exposed face alone determines the branch at C6$\alpha$, which would establish more than the proposition allows and make Supposition 7.12 unnecessary rather than false.

**Corollary 8.5**
Falsified by any of the above, or by the failure of Supposition 8.4, under which the corollary reverses to the $D$ series entire rather than failing piecewise — which is itself a statement worth recording, and is Corollary 6.14 seen from the other side.

# 13 Precedence

> **Ruling 13.1** (Disposition against the coordinating paper and Article 54)**. [A]** *Consistent, strengthening.* This paper supplies the substituent ordering named at Scholium 10.14 of the coordinating paper as the missing composite, and reduces the external input from a naming at each structure to a single supposition. It does not supply the convention, does not derive the supposition, and does not amend Scholium 10.14, which stands. No statement of Article 54 is superseded.

**Remark 13.2** (A coordination finding: the order of the canonical word)**. [A]** The reachability development leaves the ordering of the generators of the canonical word undetermined, deliberately and on a stated methodological ground. The structure development classifies retained subgraphs and does not speak to the word at all. Neither silence is a defect where it stands.
They meet here. The stereocentre is set by one generator and the side chain is carved by another, so the order of those two decides whether the uniformity statement is exceptionless or holds at sixteen of nineteen (Corollary 6.13). The question is put to the reachability development by Target 6.18; it is not a correction to any article and no published statement changes on its account.

**Ruling 13.3** (Disposition against the junction development)**. [A]** *Consistent; one consequence added.* Nothing of that paper is superseded. Its atom map, its vessel-parity theorem and its frame relation are imported unamended at Section 9, and Corollary 9.7 is a consequence of them together with the parity argument of Theorem 9.5, which that paper does not draw. It belongs in that paper's own account of what the junction delivers.

**Remark 13.4** (And against the single-unit development)**. [A]** *Consistent; one consequence added, conditionally.* On the arrangement placing both residues on one unit, the two $\alpha$ centres are related by a point inversion and Theorem 9.5 makes the pair antipodal. The consequence attaches to that development's co-synthesis premise, which it states as its own and as its weakest joint, and joins the list of things that premise carries. It bears on no result obtained independently of the premise, and Remark 9.9 bounds it.

**Remark 13.5** (What the coordinating paper may now cite)**. [A]** Three entries. That the section of Proposition 10.12 is uniform over the structure series, which that paper assumed without isolating; and that the decoration record of Section 14, reported there as held in supplement and unprinted, is printed and audited at Appendix B of this paper. The second bears on Target 14.13 and the bearing should be stated when that target is next taken up. And third, the finding of Remark 13.2, which belongs in that paper's coordination ledger rather than in its arc.

# 14 Targets, and conclusion

## 14.1 Targets, aggregated

**Target 14.1** (The address of the anchor)**.** Determine whether the one external bit of Supposition 8.4 is computable from the ribose configuration together with the tether geometry. This is the paper's last supposition and the only one whose discharge would change what the account claims rather than how much of it holds: a positive answer makes the $L$ series a consequence of the $D$ sugar and turns Remark 10.10's transfer into a derivation of one series from the other.
It replaces the target this paper carried through drafting, which asked for the spatial realisation of the orientation alternation. That question is answered by Theorem 10.6 without being settled: the parity is fixed by the ribose whatever the realisation, so the realisation is no longer load-bearing here, though it remains of interest to the cage literature for its own reasons.

**Target 14.2** (The generator order)**.** Establish, as a matter of fact rather than of admissibility, that the canonical word installs the nitrogen before the excision. The corpus permits the placement and does not force it, and the paper proceeds under Supposition 6.7. Settling it moves three rows from supposed to established.

**Target 14.3** (The lattice constraint)**.** Establish that the cage is lattice-constrained in the sense of Supposition 7.12, or exhibit a vessel whose site is not congruent to the others. What the account requires is the congruence and not the value of any rotamer, and Proposition 7.13 states the difference.

**Target 14.4** (The closure structure)**.** Decide whether the selection persists at the structure whose retained set closes onto the backbone nitrogen, independently of Supposition 6.7. It is one row and a finite question.

**Target 14.5** (The decoration record)**.** Print the decoration record in full, so that blocks V2 to V5 audit the corpus's own data rather than a declaration made here. The record is the input to every computed block of this paper and is the one place where the paper reads rather than derives.

**Target 14.6** (The mode-(b) geometry)**.** Determine whether a transannular arm can reach a framework direction at C5 rather than a face, as mode (b) of Proposition 7.1 requires. The question belongs to the certification layer and bears on

two structures.

## 14.2 Conclusion

**Proposition 14.7** (What is established)**. [A]** *Subject to the register of Appendix A, and distinguished by kind:*

*(i) The selection at* C6α *is uniform over the structure series. The side chain lies outside the reactive subgraph at sixteen of the nineteen chiral structures (Lemma 6.3, Theorem 6.11), and at all nineteen under Supposition 6.7, where the branch is selected on a substrate that does not yet distinguish the residues (Proposition 6.9).*

*(ii) The external input required to name the series is one bit and not nineteen (Corollary 6.14), and under the lattice supposition it remains one bit for the paper entire (Remark 7.14).*

*(iii) The descriptor at* C6α *is constant over the series with a single inversion, at the sulfur-bearing structure, and is unchanged by liberation (Theorem 8.1, blocks V2, V2b). The pattern is entailed by the naming and is used here as an audit of the decoration record and not as evidence.*

*(iv) The transannular bond attaches at* C5 *in two modes, read from the severance record (Proposition 7.1), and one face datum fixes the descriptors of both structures with a second centre, at* 3*S and* 3*R respectively, the opposite face fixing neither (Theorem 7.5).*

*(v) The hand of two residues made together is decided by the parity of the relation between their carriers and by nothing else (Theorem 9.5). At a junction that relation is face inversion with the order kept, which is proper, so the pair is homochiral and both residues are of the L series under the same anchor (Corollary 9.7).*

*(vi) An assembly is homochiral exactly when no operation relating two of its vessels is improper (Theorem 10.2). The corpus's two co-synthesis developments are the two values of that parameter (Corollary 10.3).*

*(vii) The criterion is met. An improper operation would carry the ribose of one vessel to the opposite series, and every vessel of an assembly bears a ribose of the same series; hence no operation relating two vessels is improper and the cluster is homochiral (Theorem 10.6, Corollary 10.7). The handedness of the residues is thereby transferred from the sugar and not generated, and why the sugar is of its series is not addressed here (Remark 10.10).*

*(viii) The carrier's orientation datum does not settle the hand. A marker records which of two orientations a unit is in and not how the two are related in space, and the registry, the class count and the capacity are statements about the pattern (Remark 10.4, block V9).*

**Remark 14.8** (What is not established, restated)**. [A]** The architecture produces one configuration and not the letter *L*. The identification is a naming, is supposed at Supposition 8.4, and is derived nowhere in this paper or in the corpus. Proposition 3.1 states this before every construction and Scholium 3.2 states why the descriptor computation does not weaken it.

**Scholium 14.9** (What would overturn the paper)**.** Three findings would do it and they are of quite different weights. A cage condition excluding neither branch would remove the section and with it the subject. What remained would be a finite account of twenty structures, their descriptors and their attachment modes, describing a racemic synthesis, and it would be sound.

An improper operation relating two vessels of an assembly would leave every statement of this paper standing and make its conclusion false. Each vessel would produce one configuration, the series would be uniform, the junction pair would be homochiral, and the cluster would be alternately handed. Nothing at the residue level would show it, and the descriptors would read tidier in that case than in this one.

A derivation of the *L* assignment from the architecture alone would refute the paper in the other direction, by establishing more than Proposition 5.1 allows. It is worth naming because a reader who wanted the architecture to produce the letter would take such a derivation as a success, and it would be a refutation of the account's own statement of what a torsor can supply.

# A Hypothesis register

| | **premise** | **what rests on it** | **what survives its failure** |
|---|---|---|---|
| H1 | The oriented cage condition excludes one branch at C6$\alpha$ (strong exclusion). | Prop. 5.1, and through it everything. | The bias reading of Remark 6.20: enrichment of one sense, coherent over the series. |
| H2 | Side-chain independence of the selection (Hyp. 6.4). False at three rows by Lem. 6.3; assumed at the other sixteen. | Thm. 6.11, and through it Cor. 6.13, Cor. 6.14, Cor. 8.5. | Section at each centre separately; no statement about the series. Homochirality fails. |
| H2b | Amination precedes excision in the canonical word (Sup. 6.7, adopted as best case). | Prop. 6.9, and with it the three rows of Lem. 6.3. | Uniformity at sixteen of nineteen; the three rows unresolved, and the account of homochirality no longer exceptionless. |
| H3 | The new position at C5 is filled from the exposed face (Hyp. 7.3). | Thm. 7.5, Cor. 7.6. | The $\alpha$ results entire, and the relative statement of Thm. 7.5 in the form *opposite, face unknown*; the absolute descriptors at the two structures are lost. |
| H7 | The relation between the two facing units of a junction is proper (Prop. 9.6), and the selection is stated intrinsically at each. | Cor. 9.7 only. | The pair of a junction cell is of opposite hands. Nothing in Sections 6–8 is affected, those concerning one vessel. |
| H6 | The cage is lattice-constrained, vessels occupying congruent sites (Sup. 7.12). | Prop. 7.13, the reduction to one external input, and Thm. 10.2. | The branch becomes a second external input, named separately; the per-vessel results stand. |
| H8 | Every operation relating two vessels of an assembly is proper (Target 10.13). | Homochirality over the cluster (Thm. 10.2). | Homochirality at each vessel and across the twenty structures, with the cluster alternately handed. Nothing in Sections 6–8 is affected. |
| H4 | $\chi^\star = \chi_L$ at $x_0$ (Sup. 8.4). | Cor. 8.5 only. | Everything except the letter. Under its failure the series is uniformly $D$, which is Cor. 6.14 unchanged. |
| H5 | The printed decoration record is the corpus's record of the twenty, and the attachment modes and branch assignments at C5 are as its severance counts and retained sets give them. | Thm. 8.1, Prop. 7.1, and the audit value of both. | The architectural statements, which are about $\Sigma^\times$ as a set of subgraphs and not about which residues they are. |

**Remark A.1** (The dependency, in one sentence)**. [A]** H1 carries the paper; H9 carries the cluster through H8 and nothing below it; H2 and H2b carry the series jointly and in the alternative, the first at sixteen rows without a premise about the word and the second at all nineteen with one; H3 carries one section; H4 carries one letter; H5 carries the audit. A reader who denies H4 loses the title's second clause and keeps the first, and a reader who denies both H2 and H2b has no account of the series at all.

# B Verification

Each block recomputes its claim from an explicit structure and emits its own numbers. Nothing quantitative in the body of this paper is asserted; every such statement is transcribed from a block below.

Block V0 is the exception. It emits the *decoration record*: the retained sets, the cut lists and the heteroatom assignments that every subsequent block runs on. Until now those were declared in the script and audited against nothing; printing them here discharges Target 14.5 and converts blocks V2 to V5 and V7 to V8 from declarations into audits. A reader may check the record against the coordinating paper's block R9 and the structure series of Article 57.

**V0** [COMPUTED] **The decoration record**

The retained sets, cut lists, consumed edges and side-chain heteroatom assignments for all twenty structures, together with the vessel graph topology and the product molecular formulae that cross-check the SMILES record.

```
This block prints the decoration record: the retained set,
the cut list, the consumed-edge list, and the side-chain
heteroatom assignments for every structure of the series.
This is the record the computed blocks V2-V5 and V7-V8 run on.
A reader may check it against the coordinating paper's block R9
and the structure series of Article 57.

VESSEL GRAPH TOPOLOGY
18-cycle: 1-2-3-4-4a-4b-5-6-6a-7-8-9-10-10a-10b-11-12-12a-1
Chords: C4a-C12a, C4b-C10b, C6a-C10a
Degree-3 (chord endpoints): C10a, C10b, C12a, C4a, C4b, C6a

ARM LOCANTS (every structure, fixed)
  C6alpha = C6alpha  (stereogenic centre, alpha-amine installed here)
  C6beta = C6beta   (carboxyl carbon, esterified to ribose 2'-O)
  C5  = Cbeta       (first side-chain carbon, transannular target)

CARRIER SOURCES (every structure)
  carboxyl O(1): phosphate O at C6beta
  carboxyl O(2): ribose 2'-O of tethered adenosine (ester)
  remnant O:     ether O at C6 (carrier)

====================================================================
str   retained set               cut list                          consumed edges
--------------------------------------------------------------------
Ala   {C5}                       C4b-C5, C5-C6
Arg   {C10b,C11,C4b,C5}          C10a-C10b, C11-C12, C4a-C4b, C5-C6
Asn   {C4b,C5}                   C10b-C4b, C4a-C4b, C5-C6
Asp   {C4b,C5}                   C10b-C4b, C4a-C4b, C5-C6
Cys   {C5}                       C4b-C5, C5-C6
Gln   {C10b,C4b,C5}              C10a-C10b, C10b-C11, C4a-C4b, C5-C6
Glu   {C4a,C4b,C5}               C10b-C4b, C12a-C4a, C4-C4a, C5-C6
Gly   {{}}                        (none)
His   {C10b,C11,C4b,C5}          C10a-C10b, C11-C12, C4a-C4b, C5-C6
Ile   {C10b,C4b,C5,C6}           C10a-C10b, C10b-C11, C4a-C4b, C6-C6a
Leu   {C10b,C4a,C4b,C5}          C10a-C10b, C10b-C11, C12a-C4a, C4-C4a, C5-C6
Lys   {C10b,C11,C4b,C5}          C10a-C10b, C11-C12, C4a-C4b, C5-C6
Met   {C10b,C4b,C5}              C10a-C10b, C10b-C11, C4a-C4b, C5-C6 C10b-C4b
Phe   {C10b,C11,C12,C12a,C4a,C4b,C5} C1-C12a, C10a-C10b, C4-C4a, C5-C6
Pro   {C10b,C4b,C5}              C10a-C10b, C10b-C11, C4a-C4b, C5-C6
Ser   {C5}                       C4b-C5, C5-C6
Thr   {C4b,C5}                   C10b-C4b, C4a-C4b, C5-C6
Trp   {C1,C10b,C12a,C2,C3,C4,C4a,C4b,C5} C10a-C10b, C10b-C11, C12-C12a, C5-C6
Tyr   {C10b,C11,C12,C12a,C4a,C4b,C5} C1-C12a, C10a-C10b, C4-C4a, C5-C6
Val   {C4b,C5,C6}                C10b-C4b, C4a-C4b, C6-C6a
--------------------------------------------------------------------

SIDE-CHAIN HETEROATOM DECORATIONS
Sources: alpha-nitrogen and the two carboxyl oxygens are arm/tether
atoms, not ring decorations.  The entries below record only
decorations of the retained framework vertices.

str   S source   N source                              side-chain decoration
--------------------------------------------------------------------------
Ala   --          medium (alpha-amine from tether C6alpha)
Arg   --          medium x3 side-chain N               Ndelta(CH2), Nepsilon(guanidinium) at C11-end
Asn   --          medium x1 side-chain N               C=O.NH2 amide at C4b
Asp   --          medium (alpha-amine from tether C6alpha)     carboxyl OO at C4b
Cys   medium (terminal thiol) medium (alpha-amine from tether C6alpha)     S--H terminal at C5
Gln   --          medium x1 side-chain N               C=O.NH2 amide at C10b
Glu   --          medium (alpha-amine from tether C6alpha)     carboxyl OO at C4a
Gly   --          medium (alpha-amine from tether C6alpha)     --
His   --          medium x2 side-chain N               imidazole N at C10b, C11
Ile   --          medium (alpha-amine from tether C6alpha)     --
Leu   --          medium (alpha-amine from tether C6alpha)     --
Lys   --          medium x1 side-chain N               Nzeta--NH2 at C11-end
Met   medium (bridging disulfide, thioether) medium (alpha-amine from tether C6alpha)     S internal in edge C4b--C10b; thioether
Phe   --          medium (alpha-amine from tether C6alpha)     --
Pro   --          medium; closes onto backbone N (secondary amine) ring closure N$\to$C6alpha (secondary amine, backbone N)
Ser   --          medium (alpha-amine from tether C6alpha)     O--H hydroxyl at C5
Thr   --          medium (alpha-amine from tether C6alpha)     O--H hydroxyl at new position on C5 (mode b); C5 loses C6 bond
Trp   --          medium x1 side-chain N               indole N--H at C1
Tyr   --          medium (alpha-amine from tether C6alpha)     phenol O--H at C11
```

```
Val   --          medium (alpha-amine from tether C6alpha)     --
------------------------------------------------------------------------

PRODUCT MOLECULAR FORMULAE (from the declared SMILES record)
A disagreement with the corpus is a defect in the SMILES, not
in the architecture.  Formulae include the freed alpha-amino group
and the carboxyl as the liberated acid.

str    formula
------------------------------------------------------------------------
Ala    C3H7NO2
Arg    C6H14N4O2
Asn    C4H8N2O3
Asp    C4H7NO4
Cys    C3H7NO2S
Gln    C5H10N2O3
Glu    C5H9NO4
Gly    C2H5NO2
His    C6H9N3O2
Ile    C6H13NO2
Leu    C6H13NO2
Lys    C6H14N2O2
Met    C5H11NO2S
Phe    C9H11NO2
Pro    C5H9NO2
Ser    C3H7NO3
Thr    C4H9NO3
Trp    C11H12N2O2
Tyr    C9H11NO3
Val    C5H11NO2
------------------------------------------------------------------------
```

**V1** [COMPUTED] **The chiral series**

Enumerate $\Sigma$ from the retained-set record; partition by emptiness of the retained set; emit $|\Sigma|$, $|\Sigma^{\times}|$, and the row identifiers of each part. Flag the row carrying a closure onto the backbone nitrogen and the row exceeding the retention classification.

```
Partition of Sigma by emptiness of the retained set, from R9.

|Sigma|            = 20
|Sigma^x|          = 19   (non-empty retained set)
empty retained set : Gly

Rows requiring separate treatment (Remark 6.4):
  closure onto the backbone nitrogen : Pro
    -- retained subgraph meets the reactive subgraph of H2;
       carried as a separate row throughout, block V3.
  retained set exceeding the retention classification : Trp
    -- retained set of size 9, rooted at C5, disjoint from the
       reactive subgraph; H2 holds, no separate treatment.

n as used in Theorem 6.2 and Corollary 6.3 = 19, of which Pro is
carried conditionally pending Target 6.5.
```

**V2** [COMPUTED] **Priority evaluation at** C6$\alpha$

For each row of $\Sigma^{\times}$: construct the four substituents at C6$\alpha$ from the decoration record — the $\alpha$-nitrogen, the carboxyl carbon C6$\beta$, the side chain rooted at C5, and the hydrogen — and order them by the hierarchical-digraph rules, emitting the first point of difference at each comparison. Emit the ordering and the descriptor under the branch fixed by Supposition 8.4.
Emit a comparand column carrying the descriptor the named residue requires, and a disagreement count. A non-zero disagreement count is a defect in the decoration record and is to be reported as such, not reconciled.

```
Substituents at C6alpha in the architecture order
    ( N , C' , R , H )
with R the side chain rooted at C5.  The ordering below is by
the sequence rules, computed on the hierarchical digraph; the
descriptor follows from the permutation parity against the
architecture order together with the anchor.

ANCHOR (Supposition 8.2): chi* = chi_L at Ala, descriptor S.
         solved: epsilon = +1
```

```
        (epsilon is the one external bit of Corollary 6.3)

str   priority order         desc   comparand agree
-------------------------------------------------------------------------
Ala   N > C' > R > H         S      S         yes
Arg   N > C' > R > H         S      S         yes
Asn   N > C' > R > H         S      S         yes
Asp   N > C' > R > H         S      S         yes
Cys   N > R > C' > H         R      R         yes
Gln   N > C' > R > H         S      S         yes
Glu   N > C' > R > H         S      S         yes
Gly   not stereogenic        -      -         n/a
His   N > C' > R > H         S      S         yes
Ile   N > C' > R > H         S      S         yes
Leu   N > C' > R > H         S      S         yes
Lys   N > C' > R > H         S      S         yes
Met   N > C' > R > H         S      S         yes
Phe   N > C' > R > H         S      S         yes
Pro   N > C' > R > H         S      S         yes
Ser   N > C' > R > H         S      S         yes
Thr   N > C' > R > H         S      S         yes
Trp   N > C' > R > H         S      S         yes
Tyr   N > C' > R > H         S      S         yes
Val   N > C' > R > H         S      S         yes
-------------------------------------------------------------------------
disagreements against comparand: 0

The inversion, located:
  Ala  R vs C' : (8,8,8,6) > (6,1,1,1) at sphere 2
  Cys  R vs C' : (16,6,1,1) > (8,8,8,6) at sphere 2
  Ser  R vs C' : (8,8,8,6) > (8,6,1,1) at sphere 2

Cys is the only row at which the side chain outranks the carboxyl
carbon, and it is the only row whose descriptor differs.  The
configuration is the same at every row (Theorem 6.2); only the
letter moves.

SURROGATE NOTE.  The evaluation above is run on the liberated
residue.  In the tethered product C6beta carries an ester to the
ribose 2'-oxygen rather than a hydroxyl.  At C6alpha the carboxyl
branch presents (O,O,O) at sphere 2 under either reading, and
every comparison against it is decided at sphere 1 or 2; the
ester therefore cannot move the ordering.  Block V2b confirms.
```

**V2b** [COMPUTED] **Descriptor invariance under liberation**

The same evaluation with C6$\beta$ carrying the ester to the ribose 2′-oxygen, the ribose truncated at a methyl surrogate. If any row moved, excision would change the descriptor and Section 8 would need a clause.

```
The same evaluation with C6beta carrying an ester, the ribose
truncated at a methyl surrogate.  If any row moved, excision
would change the descriptor and Section 8 would need a clause.

str   free     ester    same
-------------------------------------------------------------------------
Ala   S        S        yes
Arg   S        S        yes
Asn   S        S        yes
Asp   S        S        yes
Cys   R        R        yes
Gln   S        S        yes
Glu   S        S        yes
Gly   -        -        n/a
His   S        S        yes
Ile   S        S        yes
Leu   S        S        yes
Lys   S        S        yes
Met   S        S        yes
Phe   S        S        yes
Pro   S        S        yes
Ser   S        S        yes
Thr   S        S        yes
Trp   S        S        yes
Tyr   S        S        yes
Val   S        S        yes
```

```
------------------------------------------------------------------------
rows moving under liberation: 0
```

**V3** [COMPUTED] **The closure structure, evaluated separately**

Repeat V2 at the row carrying the closure onto the backbone nitrogen, with the amine secondary and the side chain re-entrant. Emit the ordering explicitly, since the re-entrant branch is compared against the carboxyl carbon along a path returning to the nitrogen and the first point of difference is not where the other rows put it.

```
Pro carries a closure from its retained set onto the backbone
nitrogen.  Its amine is secondary and its side chain is
re-entrant, so the branch at R and the branch at N traverse the
same ring in opposite senses and the first point of difference
is not where the other rows put it.

  ring:            N - C6alpha - C5 - C(10b) - C(4b) - N
  priority order:  N > C' > R > H
  N  vs C' :       Z 7 > 6 at sphere 1
  C' vs R  :       (8,8,8,6) > (6,6,1,1) at sphere 2
  descriptor:      S     comparand: S     agree

The descriptor agrees.  This is a statement about the letter and
not about H2: whether the selection at C6alpha persists when the
retained subgraph closes onto the nitrogen is Target 6.5 and is
not settled by this block.
```

**V4** [COMPUTED] **Priority evaluation and geometry at** C5

Decide which rows render C5 stereogenic, by distinctness of the four branches. For each, read the attachment mode from the severance count at C5 in block R9. Place the four substituents at the two framework directions, the exocyclic hydrogen position and the new position, evaluate the priority ordering on the digraph, and emit the descriptor from the sign of the triple product — *at both faces*, so that the reader sees which face is anchored and what the other would give. Emit the comparand pair with the assignment of each to its row.

```
C5 is stereogenic at the rows below and at no other.  Tested by
distinctness of the four branches at C5 in the product graph.

  stereogenic at C5: Ile, Thr
  (Val is excluded: two methyls at C5 are indistinguishable)

ATTACHMENT MODE, from block R9 of the coordinating paper.
R9 gives the framework-bond loss at C5 and states that the
transannular bond to C6alpha consumes one severance at C5 in
every entry retaining C5.  Hence:

  Ile  loss at C5 = 0   ->  no severance at C5, so C6alpha occupies the new position
  Thr  loss at C5 = 1   ->  C6alpha at the vacated C6 direction; the new position is filled by a decoration

The two modes are different, and this is the content of
Proposition 7.1.  A reading on which Ile and Thr present the
same spatial arrangement at C5 is not available.

FACE ANCHOR (Hypothesis H3).  One datum: the position created by
dearomatisation is filled from the exposed face.  Its sense is
anchored at Ile and Thr is then a prediction.

  face = +1
    Ile   newbond > inplane_C4b > inplane_C6 > exo_H      R   comparand S   DISAGREE
    Thr   newbond > inplane_C6 > inplane_C4b > exo_H      S   comparand R   DISAGREE

  face = -1
    Ile   newbond > inplane_C4b > inplane_C6 > exo_H      S   comparand S   agree
    Thr   newbond > inplane_C6 > inplane_C4b > exo_H      R   comparand R   agree

RESULT.  One and the same face gives both comparands, and the
other face gives neither.  The relative configuration of the two
is therefore predicted outright; the absolute configuration costs
one bit, which is the face, and Target 7.4 asks whether that bit
is the same datum as the attack scalar of Proposition 5.1.
```

### V6 [COMPUTED] Disjointness against the reactive subgraph

For each row: the retained set, whether it contains C6, and whether it carries a closure onto the backbone nitrogen. Emit the rows at which Hypothesis 6.4 fails, and the uniformity count under each order of the canonical word.

```
The reactive subgraph of the nitrogen-installation generator is
taken to be

    W = { C6alpha, N, C6beta, C5, C6 }

comprising the incipient stereocentre, the incoming nitrogen, the
carboxyl carbon of the arm, the framework carbon attacked, and the
framework carbon bearing the arm.  Hypothesis H2 asserts that the
retained subgraph of a structure lies outside W apart from its root
at C5.  This block tests that assertion structure by structure.

Two ways to meet W other than at the root:
  (i)  the retained set contains C6, which bears the tether;
  (ii) the retained set closes onto the backbone nitrogen.

str   retained set                has C6   closure  H2
-------------------------------------------------------------------------
Ala   5                           no       no       holds
Arg   10b,11,4b,5                 no       no       holds
Asn   4b,5                        no       no       holds
Asp   4b,5                        no       no       holds
Cys   5                           no       no       holds
Gln   10b,4b,5                    no       no       holds
Glu   4a,4b,5                     no       no       holds
Gly   (empty)                     no       no       holds
His   10b,11,4b,5                 no       no       holds
Ile   10b,4b,5,6                  yes      no       FAILS
Leu   10b,4a,4b,5                 no       no       holds
Lys   10b,11,4b,5                 no       no       holds
Met   10b,4b,5                    no       no       holds
Phe   10b,11,12,12a,4a,4b,5       no       no       holds
Pro   10b,4b,5                    no       yes      FAILS
Ser   5                           no       no       holds
Thr   4b,5                        no       no       holds
Trp   1,10b,12a,2,3,4,4a,4b,5     no       no       holds
Tyr   10b,11,12,12a,4a,4b,5       no       no       holds
Val   4b,5,6                      yes      no       FAILS
-------------------------------------------------------------------------
rows at which H2 fails as stated: 3  ['Ile', 'Pro', 'Val']

These rows are not counterexamples to uniformity.  They are rows
at which the disjointness argument does not reach, and which the
common-intermediate argument reaches instead whenever the
canonical word installs the nitrogen before the excision.  Under
that order the retained subgraph does not yet exist when the
branch is selected, and W is the whole of the substrate that does.

Count under each order of the canonical word:
  amination before excision : uniformity at 19 of 19
  excision before amination : uniformity at 16 of 19, with Ile, Pro, Val
                              carried separately and unresolved

The order of the two generators is therefore not a matter of
indifference, and the corpus does not fix it.  This is entered as
a coordination finding in the precedence section.
```

### V7 [COMPUTED] The two geometric parameters, jointly

Enumerate the four combinations of the branch parameter and the face parameter. For each, emit agreement against the $\alpha$ comparands at all chiral rows and against the $\beta$ pair. Emit the count of combinations reproducing the record, and state what the count does and does not show about coupling.

```
Two binary parameters enter the paper:

  epsilon   the branch selected at C6alpha (the attack scalar)
  face      the face from which the new position at C5 is filled

This block enumerates all four combinations and reports, for each,
agreement against the comparands: the alpha descriptor at all
```

```
nineteen chiral rows, and the beta pair at the two rows with a
second centre.  The question it settles is not which combination
is right -- that is the anchor -- but whether the two parameters
are coupled by anything computed here.  They are not.

epsilon   face   alpha agree  beta agree   all agree
-------------------------------------------------------------------------
+1        +1     19/19        0/2          no
+1        -1     19/19        2/2          yes
-1        +1     0/19         0/2          no
-1        -1     0/19         2/2          no
-------------------------------------------------------------------------
combinations reproducing every comparand: 1 of 4   [(1, -1)]

READING.  Exactly one combination reproduces the record, so the
comparands fix both parameters.  But they fix them jointly and
from outside: nothing in the structure record, the retained sets
or the priority orderings couples epsilon to face.  Each of the
two mixed combinations is internally consistent and is excluded
only by the comparands.

Consequently the account as computed here costs TWO parameters and
not one.  The reduction to one is a geometric claim and not a
computation: it holds if and only if the branch at C6alpha and the
filling at C5 are both consequences of the burial of one face of
the unit in the stack.  The burial argument reaches the C5 filling
directly, since the arm cannot reach the buried face.  It does not
reach the branch at C6alpha without a further datum, namely the
disposition of C6beta about the C5-C6alpha axis, which the cluster
supplies through the anchoring of the adenosine and which no block
of this paper computes.
```

**V8** [COMPUTED] **The junction pair, and the parity of the relation**

For the two residues of the junction cell, both formed at C6$\alpha$–C5 on their own units: the descriptor at each $\alpha$ carbon under a proper relation between the carriers and under an improper one, with the $L/D$ reading of each. Emit the letters in both cases, so that the masking of Remark 9.8 is on the record.

```
At a junction two strands meet chrysene to chrysene, the two
facing units stacked pi-face to pi-face.  The junction cell has
six vessels; six is even, so the cell has no central vessel but a
central pair, and it yields two residues instead of one -- one on
each facing unit.  The atom map of that cell is

   first residue,  on X3:  C' = C6beta@X3  Calpha = C6alpha@X3  Cbeta = C5@X3
   second residue, on X4:  C' = C6beta@X4  Calpha = C6alpha@X4  Cbeta = C5@X4

Both residues therefore arise by the SAME transannular route,
C6alpha attacking C5, each on its own unit and from its own arm.
C12alpha is not a stereocentre of this cell and does not appear.
Every statement of the preceding sections applies at each of the
two centres without amendment.

What remains is the relation between the two units, and only its
PARITY matters.  A configuration is preserved by a proper
operation (determinant +1) and reversed by an improper one (-1).

  relation PROPER   (flip about an in-plane axis)   det = +1
    Cys at C6alpha@X3 : R  (L)
    Met at C6alpha@X4 : S  (L)
    pair: HOMOCHIRAL   letters: R, S

  relation IMPROPER (point inversion / reflection)   det = -1
    Cys at C6alpha@X3 : R  (L)
    Met at C6alpha@X4 : R  (D)
    pair: one of each hand   letters: R, R

READING.  Turning a planar unit over -- presenting its other
face -- is a rotation by pi about an axis lying in the plane.
That is a PROPER operation, determinant +1, and it preserves
configuration.  Face inversion with the order of sites kept is
that operation, and it is the relation the junction development
establishes between the two strands, the order-reversing
alternatives failing at the discriminating case.  The junction
pair is therefore homochiral, and under the anchor both residues
```

```
are of the L series.

The improper row is retained for contrast and is not the junction.
It is the arrangement in which two residues form on ONE unit from
its two arms, where the relation is a point inversion about the
centre of the skeleton -- improper, and antipodal in consequence.

Note which case the letters would betray.  Homochiral gives R and
S, unlike letters at the two centres; antipodal gives R and R,
alike.  A table recording letters alone would read the racemic
case as the tidy one.
```

**V9** [COMPUTED] **Hand as a function of assembly parity**

For each of four assemblies, given as a word of relation parities over six vessels with the first anchored: emit the hand at each vessel and the number of distinct hands. Emit the two assemblies that share an orientation pattern and differ in parity, so that the indifference of the marker to the determinant is on the record.

```
A cluster is six units.  Let the operation relating each unit to
the next be given as a word over {proper, improper}.  By the
parity theorem the configuration at a unit is that of the first
unit reversed once for each improper relation along the way, so
the hand at unit i is the hand at unit 1 times the product of the
determinants of the relations preceding it.

Four assemblies, with the anchor fixing unit 1 at L:

  pure translation (all proper)                 L L L L L L   hands: 1
  alternation by in-plane flip (all proper)     L L L L L L   hands: 1
  alternation by point inversion (all improper) L D L D L D   hands: 2
  one improper relation, at the third step      L L L D D D   hands: 2

READING.  The hand of the cluster is decided by the parity of the
assembly relations and by nothing else: not by the orientation
pattern as such, not by the letters, not by the side chains.  An
orientation alternation realised as a flip about an in-plane axis
is proper and leaves the cluster homochiral; the same alternation
realised as a point inversion is improper and makes it
alternately handed.  The two are indistinguishable as patterns of
an orientation marker, which carries one bit per site and records
no parity.

Which row the architecture is in is NOT settled by the orientation
datum, and is not settled by this block either.  It is settled in
the body by the ribose: every vessel bears its arm through a
nucleoside whose sugar is of one series, an improper relation
would present the next vessel with the other series, and so no
relation between two vessels is improper.  The assembly is
therefore in one of the two all-proper rows above, whichever
orientation pattern it carries.

Note what that does and does not establish.  The hand of the
residues is inherited from the hand of the sugar.  This block
computes the transfer and says nothing about its source.
```

**V5** [COMPUTED] **Record audit**

Cross-check every row used in V2–V4 against the coordinating paper's blocks R9 and R17: molecular formula, valence at each retained vertex, and severance count at C5. Emit disagreements by row and by field.

```
Each product graph is checked against block R9: the carbon count
of the side chain must equal the size of the retained set, since
every retained vertex is a framework carbon and every side-chain
carbon is retained.  Heteroatoms are decorations and are counted
separately.

str   |S|      side C     side het   agree  formula
-------------------------------------------------------------------------
Ala   1        1          0          yes    C3H7NO2
Arg   4        4          3          yes    C6H14N4O2
Asn   2        2          2          yes    C4H8N2O3
Asp   2        2          2          yes    C4H7NO4
```

```
Cys   1        1          1          yes    C3H7NO2S
Gln   3        3          2          yes    C5H10N2O3
Glu   3        3          2          yes    C5H9NO4
Gly   0        0          0          yes    C2H5NO2
His   4        4          2          yes    C6H9N3O2
Ile   4        4          0          yes    C6H13NO2
Leu   4        4          0          yes    C6H13NO2
Lys   4        4          1          yes    C6H14N2O2
Met   3        3          1          yes    C5H11NO2S
Phe   7        7          0          yes    C9H11NO2
Pro   3        3          1          yes    C5H9NO2
Ser   1        1          1          yes    C3H7NO3
Thr   2        2          1          yes    C4H9NO3
Trp   9        9          1          yes    C11H12N2O2
Tyr   7        7          1          yes    C9H11NO3
Val   3        3          0          yes    C5H11NO2
------------------------------------------------------------------------
rows disagreeing with R9: 0

A disagreement here is a defect in the declared product graph or
in the retained-set record, and is to be reported as such rather
than reconciled.
```

# C Conformational commentary, isolated

**Remark C.1** (Status of this appendix)**. [A]** Nothing in this appendix enters a numbered statement of this paper, and no statement of this paper is weakened by its removal. It is retained because the observations are natural ones for a reader to make at the point where the residue is liberated, and a paper that omitted them would invite a reader to supply them in a load-bearing place.

**Remark C.2** (Rotamer and configuration)**. [E]** Once the residue is excised and liberated, rotation about the C6$\alpha$–C5 bond interconverts staggered arrangements freely at ordinary temperatures. Statements to the effect that one such arrangement relieves steric compression along a branched side chain, or that another places a hydroxyl in range of the backbone for intramolecular hydrogen bonding, are statements about populations over an interconverting ensemble. They describe the residue after formation and say nothing about which configuration was formed, the configuration being fixed by the attachment mode of Proposition 7.1 together with Hypothesis 7.3, and not by any subsequent preference.
The appendix records them because they are true of the liberated residues and because their relation to the configurational argument is exactly the relation this paper needs a reader not to invert.

**Remark C.3** (The hydroxyl, and where it points)**. [E]** At the structure whose branch substituent carries oxygen, the hydroxyl occupies the position created by dearomatisation and therefore stands on the exposed face, while the transannular bond to C6$\alpha$ lies at the vacated framework direction. This is the molecular reading of mode (b) of Proposition 7.1 under Hypothesis 7.3; the configurational content is in the body, and the reading adds nothing to it.
It is worth saying that this is the one place where the architecture asks something of a reader's chemical intuition that the intuition may resist: at mode-(b) structures the arm reaches a framework direction rather than a face. Whether that is geometrically comfortable in the cage is not settled here and is a question for the certification layer.

# D What was withdrawn in preparing this paper

**Remark D.1** (The same-arrangement reading of the second centre)**. [A]** An earlier draft of Section 7 asserted that the two structures with a second centre present the same spatial arrangement at C5, and derived their opposite descriptors from a transposition of priorities alone — the branch substituent ranking below C6$\alpha$ at one structure and the oxygen-bearing substituent ranking above it at the other.
The reading is not available. Block R9 of the coordinating paper gives the framework-bond loss at C5 as zero at one of the two and one at the other, and states that the transannular bond consumes a severance at C5 wherever one exists. The arm therefore attaches at the new position in one case and at a vacated framework direction in the other, and the arrangements are not the same.

Worse for the withdrawn reading, its own arithmetic fails: carried out with the branch substituents placed where the retained sets put them, the transposition argument returns *like* relative configurations, which is the allo pair and not the pair the residues require.
What replaced it is stronger and is Theorem 7.5. The withdrawal is recorded here rather than absorbed, and the two attachment modes it exposed are now Proposition 7.1.

**Remark D.2** (The antipodal reading of the co-synthesised pair)**. [A]** An earlier form of Section 9 was written against the arrangement placing both sulfur residues on a single unit, and concluded that the pair is antipodal. The conclusion is correct of that arrangement and was stated of the wrong one.
At a junction the two residues occupy different molecules, both are formed at C6$\alpha$–C5 from the arm of their own unit, and the second $\alpha$ carbon is not C12$\alpha$ at all. The relation between the carriers is then face inversion with the order kept, which is proper, and the pair is homochiral. What survives of the earlier form is Theorem 9.5, which is indifferent to which arrangement is meant and decides both; the antipodal statement is retained at Remark 9.9 as the value that theorem takes on the single-unit reading.
The error was not in the parity argument but in which pair of centres it was applied to, and it was found by reading the junction atom map rather than by recomputing anything.

**Remark D.3** (The buried-face argument)**. [A]** An earlier form of Section 7.3 argued that one face of each unit is buried in the stack and unavailable to the arm, so that every arm lies on a single exposed face common to the unit. The reaction-cell development states that the two arms of a unit leave toward opposite faces, and excludes the conformation placing both on one face. The argument is withdrawn and replaced by Proposition 7.8, which speaks of the face of an arm rather than of the unit. It was found by reading an imported conformation rather than by recomputing anything, and the loss it entails is the subject of Section 9.

**Remark D.4** (A conformational justification, withdrawn before drafting)**. [A]** The secondary centres were at one point to be justified by conformational preference in the liberated residue — a staggered arrangement relieving steric compression at one, an intramolecular hydrogen bond at the other. Rotamers about the C6$\alpha$–C5 bond interconvert freely and fix no configuration, so the justification was of the wrong kind for the statement it was to support. The observations are retained, without that role, at Appendix C.

# E Sources, by use

**Remark E.1** (Status of this appendix)**. [A]** A concordance. It establishes nothing and enters no proof. It is included because this paper imports at four points and a reader is owed an exact account of which statement comes from where, without reading the corpus to find out.

| source | used at | what is taken |
|---|---|---|
| [Sch26a] | Prop. 5.1, Rem. 6.12 | The branch torsor at C6$\alpha$, the cage condition as section-supplying datum, the separation of selection from naming, and local transformation invariance with its margin condition. Also the stacking of units, on which Prop. 7.8 rests. |
| [Sch26c] | Prop. 4.1, Prop. 4.2, App. B | The vessel graph and its locant registry; the reference transformation and the target connectivity; the structure series, the retained sets and the severance record against which every computed block here is checked. |
| [Sch26d] | Rem. 6.15, Rem. 9.9 | That the amination is ordered against no stage and may be placed early; and the single-unit arrangement, with its point-inversion realisation, which Cor. 10.3 takes as the improper value. |

| source | used at | what is taken |
|---|---|---|
| [Sch26e] | Sec. 9 | The junction cell and its even vessel count; the atom map placing both residues at C6$\alpha$–C5 on their own units; and that the two strands are related by face inversion with the order of sites kept, the order-reversing alternatives failing at the discriminating case. |
| [Sch26b] | Sec. 2, Sec. 13 | The locant ruling, the status labels, the four-level convention, and the statement of what the cage does and does not deliver, which this paper does not amend. |
| [Sch25a, Sch25b] | Sec. 4, Sec. 10 | The substituted family as encoding material; the tether and the exhibited integrated product; the ribose of the nucleoside to which each arm runs, which carries Thm. 10.6; and the encoding of the cluster into a registered stack of aligned aromatic systems, which grounds Sup. 7.12 at Rem. 10.12. |
| [Sch20] | — | Prior art for the substituted family and for the residue-from-aromatic hypothesis. No inference is drawn here from them. |

**Remark E.2** (What is not used)**. [A]** The seeding and refinement apparatus, the assignment machinery, the capacity theorem and the parity obstruction are not drawn on. This paper takes a configuration at a centre and says what happens to it; nothing here turns on which assignment the registry supports, and no statement of this paper is affected by the corpus's undecided dilemma between the selected assignment and the observed mapping.

# References

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