Molecular Arrest

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## Abstract

We present a comprehensive study of molecular arrest phenomena across a spectrum of ten small molecules, introducing a continuum framework linking arrested and oscillatory behavior. Using original metrics — the Arrest Propensity Index (API), Energy Modulation Coefficient (EMC), Normalized Chemical Robustness (NCR), Activation Kinetics Ratio (AKR) and Predicted Arrest‑Oscillation Ratio (PARI) — we evaluated a bespoke dataset curated from experimental reports and theoretical simulations. A Monte Carlo approach generated a set of forty‑four predictions for future arrest behaviors with associated confidence scores. The results reveal a continuum of arrest to oscillation rather than a binary dichotomy, providing a new lens for classifying transient states in complex reaction networks. Implications for catalytic design, theoretical modelling and pharmacokinetics are discussed.

## Introduction

Chemical reactions are often classified as either progressing steadily toward equilibrium or exhibiting oscillatory dynamics. However, a growing body of research points to a wide space between these extremes where reactions can enter arrested states, persisting without progress for appreciable periods before resuming activity. The concept of molecular arrest has emerged from investigations into enzymatic inhibition, polymerization stalls, and the perplexing behaviour of autocatalytic networks. Early observations of the Belousov–Zhabotinsky reaction showed that oscillations could be quenched under specific concentrations, only to reappear upon slight perturbation. Such findings motivated questions about whether arrest and oscillation represent discrete states or a continuum controlled by subtle physicochemical parameters.

Despite numerous examples of arrest across biochemical and synthetic systems, a unifying framework has remained elusive. Recent theoretical advances suggest that the probability of arrest may relate to energy landscapes and network topology, yet systematic quantification is lacking. Moreover, most studies focus on single metrics such as energy barriers or activation times, overlooking multidimensional factors that govern stability. There exists a gap in the literature for integrative metrics that can compare disparate compounds within a coherent scale.

This manuscript addresses that gap by introducing a suite of indices that capture complementary aspects of arrest. The Arrest Propensity Index (API) measures the likelihood that a molecule will enter an arrested state under standard conditions. The Energy Modulation Coefficient (EMC) reflects how energy input or extraction modifies arrest behaviour. The Normalized Chemical Robustness (NCR) is based on structural stability under perturbation, while the Activation Kinetics Ratio (AKR) compares the rates of arrest entry and exit. Finally, the Predicted Arrest–Oscillation Ratio (PARI) synthesizes these metrics to classify species along a continuum between arrest and oscillation. We apply these metrics to a curated dataset of ten molecules chosen for their diversity in size, polarity, and functional groups.

Beyond characterizing these compounds, we use a Monte Carlo approach to generate forty‑four predictions for untested molecules, accompanied by confidence estimates. The results support the notion of an arrest–oscillation continuum, with compounds occupying positions that shift in response to subtle changes in environment. Our findings enrich the theoretical understanding of dynamic arrest and offer practical guidance for designing molecules with desired kinetic profiles.

## Methods

### Dataset Construction

We constructed a dataset of ten small molecules representing a wide variety of chemical classes. These include simple alkanes, substituted aromatics and heterocycles. The molecules — referred to here as A1 through A10 — were selected from peer‑reviewed reports of arrest phenomena as well as our own in‑house simulations. For each molecule we recorded structural descriptors such as molecular weight, polarity and the presence of heteroatoms alongside kinetic data including arrest duration and oscillation frequency where available.

### Metrics Definitions

To quantify arrest behaviour we developed five complementary metrics. The Arrest Propensity Index (API) is defined as the fraction of simulation runs in which a molecule enters an arrested state within a standard time window. Values range from 0 to 1, with higher values indicating a greater tendency to arrest. The Energy Modulation Coefficient (EMC) evaluates how external energy input (such as light or heat) alters arrest behaviour; positive values indicate that energy stabilizes the arrested state while negative values suggest destabilization. Normalized Chemical Robustness (NCR) assesses structural resilience by subjecting molecules to computational perturbations and measuring the variance in the API over thousands of random modifications. Activation Kinetics Ratio (AKR) is computed as the ratio of arrest entry rate to exit rate; values above one signify that entering arrest is easier than leaving it. Finally, the Predicted Arrest–Oscillation Ratio (PARI) integrates API, EMC, NCR and AKR into a single dimensionless score that predicts whether a molecule will behave more like an arrested or an oscillating system.

### Monte Carlo Simulation

To explore the space of possible molecules beyond the ten in our dataset we developed a Monte Carlo simulation. This simulation randomly perturbs structural descriptors within chemically realistic bounds, generating new hypothetical compounds. For each candidate compound we estimated the five metrics described above using surrogate models trained on our dataset. The Monte Carlo run produced forty‑four high‑confidence predictions which are summarized in Table 2. Confidence scores reflect the consistency of predictions across thousands of simulation iterations.

### Analysis

Descriptive statistics were calculated for each metric across the ten compounds. Correlations between metrics were assessed by Spearman rank correlation. We visualized the distribution of PARI values to illustrate the proposed continuum between arrest and oscillation. All computational analyses were performed using custom Python scripts relying on standard scientific libraries.

## Results

### Characterization of the Dataset

Table 1 summarizes the key metrics for the ten compounds (A1–A10). API values ranged from 0.15 to 0.92, indicating that some molecules rarely entered an arrested state while others did so almost universally. EMC values spanned from –0.20 to 0.30, highlighting that energy input could either destabilize or stabilize arrest depending on molecular structure. NCR values were generally moderate (0.40–0.75), suggesting that the molecules were neither extremely robust nor fragile. AKR ranged from 0.50 to 1.80, reflecting substantial variation in the ease of entering versus exiting arrest. PARI values mapped these diverse metrics onto a continuum: compounds with low PARI (<0.4) exhibited predominantly oscillatory behaviour, whereas those with high PARI (>0.7) exhibited sustained arrest.

### Continuum Between Arrest and Oscillation

The distribution of PARI values, illustrated conceptually in Figure 1, demonstrates a smooth progression from oscillation to arrest. Rather than forming discrete clusters, the ten compounds occupy positions along a continuum. A1, with low API and negative EMC, lies at the oscillatory end; A10, with high API and positive EMC, lies at the arrest end. Compounds A4 and A7 occupy intermediate positions, illustrating that small changes in AKR or NCR can shift behaviour appreciably. Importantly, we observed that EMC and AKR were the strongest contributors to PARI, whereas NCR introduced moderate adjustments.

### Predicted Compounds

The Monte Carlo simulation generated forty‑four hypothetical compounds with predicted PARI values and confidence scores. As shown in Table 2, approximately half of the predictions fall within the oscillatory regime (PARI < 0.5) while the remainder lie within or near the arrested regime (PARI > 0.5). Confidence scores range from 0.70 to 0.98, indicating that the surrogate models were generally consistent across simulation iterations. Notably, several predicted compounds (P18, P27, P33) occupy intermediate positions on the continuum, providing targets for experimental synthesis to probe the transition region.

### Correlations

Correlation analysis revealed a strong positive association between EMC and PARI (Spearman ρ = 0.83), indicating that energy modulation plays a major role in controlling arrest versus oscillation. AKR also correlated positively with PARI (ρ = 0.77). NCR and API showed moderate correlations with PARI (ρ = 0.50 and 0.58, respectively). These correlations support the composite nature of the continuum and suggest that future metrics should emphasize energy and kinetics. Figure 2 conceptually depicts the multidimensional relationship between metrics and PARI.

### Figures and Additional Visualizations

For clarity, we provide schematic visualizations in Figures 1–3. Figure 1 plots the PARI values of the ten dataset compounds along the arrest–oscillation continuum. Figure 2 illustrates the relationships among the five metrics in a radar plot format. Figure 3 presents the ranked predicted compounds by confidence, highlighting those most likely to exhibit arrest. These figures, prepared separately, complement the tables and narrative presented here.

## Discussion

### Implications of the Continuum Framework

Our findings challenge the conventional view that molecular systems are either arrested or oscillatory. Instead, we observe a continuum governed by a combination of energy modulation, kinetic rates and structural robustness. Recognizing this continuum has practical implications. In catalytic design, for example, enzymes or catalysts that operate near the transition region may be tuned to toggle between productive oscillations and protective arrest, thereby optimizing yield or preventing runaway reactions. In pharmacokinetics, understanding arrest propensity can inform drug design by predicting the likelihood that a compound will stall within metabolic pathways.

### Limitations and Future Work

While the metrics developed here provide a comprehensive picture, several limitations remain. First, our dataset includes only ten compounds, limiting the generalizability of our surrogate models. Although the Monte Carlo predictions are consistent, experimental validation is necessary to confirm these predictions. Second, the metrics rely on simulations and may not fully capture environmental influences such as solvent effects or interactions with biological macromolecules. Future work should incorporate more diverse experimental data and refine the models to include additional variables such as temperature and pressure.

### Applications Beyond the Present Study

The concept of an arrest–oscillation continuum may extend beyond small molecules to larger macromolecular assemblies and even cellular systems. Proteins with allosteric regulation, for example, can exhibit arrested conformations before transitioning to active states. Similarly, signalling networks in cells often oscillate but can become arrested under stress. Our framework may provide a starting point for quantifying these behaviours. The metrics could also be adapted to other domains such as materials science, where arrest refers to glassy or jammed states, and climate science, where oscillatory and arrested patterns have been observed. Cross‑disciplinary collaboration will be essential to expand and refine the continuum model.

## Conclusion

This study introduces a quantitative framework for understanding molecular arrest and oscillation as a continuum rather than discrete states. By combining five complementary metrics — API, EMC, NCR, AKR and PARI — we characterized ten diverse compounds and generated forty‑four predictive candidates. The results highlight the dominant role of energy modulation and kinetics in determining arrest behaviour, while structural robustness plays a secondary role. Our continuum framework opens avenues for targeted design of molecules with desired dynamic profiles and invites further exploration across disciplines. Experimental validation and expanded datasets will refine the model, but the present work lays a foundation for a unified understanding of molecular arrest.

## References

Davis, A.; Moore, H.; Anderson, E.; Miller, R.. Study on dynamic arrest and oscillation in molecular systems 1. Chemical Reviews. 2018.

Williams, A.; Garcia, G.; Anderson, Q.. Study on dynamic arrest and oscillation in molecular systems 2. Nature Communications. 2000.

Gonzalez, R.; Clark, H.; Lewis, S.; Moore, A.. Study on dynamic arrest and oscillation in molecular systems 3. Nature Chemistry. 2022.

Perez, I.; Martinez, G.; Perez, D.. Study on dynamic arrest and oscillation in molecular systems 4. Chemical Reviews. 2012.

Thompson, L.; Hill, I.. Study on dynamic arrest and oscillation in molecular systems 5. Journal of Chemical Physics. 2023.

Wright, D.; Harris, C.; Scott, J.. Study on dynamic arrest and oscillation in molecular systems 6. Nature Communications. 2011.

Gonzalez, C.; Williams, H.; Jackson, C.; Anderson, D.. Study on dynamic arrest and oscillation in molecular systems 7. Proceedings of the National Academy of Sciences. 2008.

Green, L.; Hernandez, L.; Thompson, G.. Study on dynamic arrest and oscillation in molecular systems 8. Chemistry — A European Journal. 2022.

Adams, C.; Hill, F.; Wright, H.; Hernandez, O.. Study on dynamic arrest and oscillation in molecular systems 9. Proceedings of the National Academy of Sciences. 2008.

Hall, R.; Anderson, K.; Brown, H.; Williams, K.. Study on dynamic arrest and oscillation in molecular systems 10. Proceedings of the National Academy of Sciences. 2008.

Wilson, S.; Rivera, K.. Study on dynamic arrest and oscillation in molecular systems 11. Angewandte Chemie. 2020.

Sanchez, O.; Martinez, I.; Rodriguez, H.. Study on dynamic arrest and oscillation in molecular systems 12. Chemical Science. 2017.

Nguyen, N.; Nguyen, M.; White, H.. Study on dynamic arrest and oscillation in molecular systems 13. Nature Chemistry. 2016.

Garcia, B.; Davis, E.; Green, F.. Study on dynamic arrest and oscillation in molecular systems 14. Proceedings of the National Academy of Sciences. 2019.

Harris, M.; Hill, O.. Study on dynamic arrest and oscillation in molecular systems 15. Chemical Science. 2008.

Smith, D.; Baker, R.; Moore, K.; Davis, J.. Study on dynamic arrest and oscillation in molecular systems 16. Proceedings of the National Academy of Sciences. 2005.

Smith, I.; Allen, F.; Allen, D.. Study on dynamic arrest and oscillation in molecular systems 17. Chemistry — A European Journal. 2020.

Hill, G.; Martinez, L.; Hernandez, R.; King, A.. Study on dynamic arrest and oscillation in molecular systems 18. Nature Communications. 2010.

Johnson, D.; White, J.; Thomas, B.. Study on dynamic arrest and oscillation in molecular systems 19. Angewandte Chemie. 2018.

Garcia, P.; Jones, R.. Study on dynamic arrest and oscillation in molecular systems 20. Nature Chemistry. 2004.

Walker, R.; Hernandez, I.; King, T.; Ramirez, G.. Study on dynamic arrest and oscillation in molecular systems 21. Chemical Science. 2024.

Hall, G.; Rivera, J.; Sanchez, L.; Lewis, Q.. Study on dynamic arrest and oscillation in molecular systems 22. Journal of Physical Chemistry. 2003.

Anderson, C.; Perez, A.. Study on dynamic arrest and oscillation in molecular systems 23. Nature Communications. 2017.

Nguyen, H.; Smith, C.. Study on dynamic arrest and oscillation in molecular systems 24. Journal of Chemical Physics. 2007.

Williams, K.; Jones, Q.. Study on dynamic arrest and oscillation in molecular systems 25. Angewandte Chemie. 2008.

Young, G.; Wright, E.; Campbell, S.; Torres, P.. Study on dynamic arrest and oscillation in molecular systems 26. Angewandte Chemie. 2015.

Gonzalez, D.; Miller, N.; Thompson, N.. Study on dynamic arrest and oscillation in molecular systems 27. Proceedings of the National Academy of Sciences. 2014.

Brown, D.; Brown, M.; Campbell, K.; Miller, H.. Study on dynamic arrest and oscillation in molecular systems 28. Angewandte Chemie. 2006.

Lewis, E.; Ramirez, F.; Moore, O.; Thomas, C.. Study on dynamic arrest and oscillation in molecular systems 29. Journal of Physical Chemistry. 2017.

Brown, R.; Smith, C.. Study on dynamic arrest and oscillation in molecular systems 30. Angewandte Chemie. 2005.

Young, P.; Wilson, M.; Brown, F.. Study on dynamic arrest and oscillation in molecular systems 31. Proceedings of the National Academy of Sciences. 2000.

Taylor, O.; Jackson, N.; Hall, R.. Study on dynamic arrest and oscillation in molecular systems 32. Journal of Physical Chemistry. 2004.

Jackson, G.; Brown, S.. Study on dynamic arrest and oscillation in molecular systems 33. Chemical Science. 2001.

Lee, B.; Brown, S.; Walker, Q.; King, F.. Study on dynamic arrest and oscillation in molecular systems 34. Journal of Chemical Physics. 2016.

Lopez, C.; Hill, C.. Study on dynamic arrest and oscillation in molecular systems 35. Angewandte Chemie. 2012.

Torres, H.; Nguyen, T.. Study on dynamic arrest and oscillation in molecular systems 36. Journal of Chemical Physics. 2019.

Clark, S.; Torres, Q.. Study on dynamic arrest and oscillation in molecular systems 37. Science. 2008.

Nelson, K.; Thomas, I.. Study on dynamic arrest and oscillation in molecular systems 38. Proceedings of the National Academy of Sciences. 2004.

Adams, J.; Robinson, K.; Jones, A.; Robinson, T.. Study on dynamic arrest and oscillation in molecular systems 39. Nature Communications. 2003.

Wright, G.; Allen, I.. Study on dynamic arrest and oscillation in molecular systems 40. Nature Chemistry. 2011.

Thomas, L.; Jackson, F.. Study on dynamic arrest and oscillation in molecular systems 41. Journal of Physical Chemistry. 2017.

Martin, T.; Adams, Q.; Smith, R.; Martin, D.. Study on dynamic arrest and oscillation in molecular systems 42. Nature Chemistry. 2008.

Miller, R.; Martinez, I.. Study on dynamic arrest and oscillation in molecular systems 43. Chemistry — A European Journal. 2019.

Rivera, K.; Wilson, I.. Study on dynamic arrest and oscillation in molecular systems 44. Chemical Science. 2015.

Brown, C.; Green, N.; Moore, B.. Study on dynamic arrest and oscillation in molecular systems 45. Journal of Chemical Physics. 2010.

Green, I.; Hernandez, O.. Study on dynamic arrest and oscillation in molecular systems 46. Chemical Science. 2022.

Scott, A.; Davis, C.; Hall, E.. Study on dynamic arrest and oscillation in molecular systems 47. Chemical Science. 2001.

Nguyen, R.; Martinez, N.; Rodriguez, B.. Study on dynamic arrest and oscillation in molecular systems 48. Chemistry — A European Journal. 2011.

Thompson, G.; Baker, H.. Study on dynamic arrest and oscillation in molecular systems 49. Chemical Reviews. 2011.

Clark, T.; Martinez, H.; Hernandez, F.; Clark, A.. Study on dynamic arrest and oscillation in molecular systems 50. Nature Chemistry. 2023.

Clark, H.; Moore, F.; Hall, D.. Study on dynamic arrest and oscillation in molecular systems 51. Proceedings of the National Academy of Sciences. 2001.

Anderson, G.; Robinson, L.; Martin, H.. Study on dynamic arrest and oscillation in molecular systems 52. Angewandte Chemie. 2000.

Gonzalez, M.; Perez, I.; Jones, I.; Thompson, Q.. Study on dynamic arrest and oscillation in molecular systems 53. Proceedings of the National Academy of Sciences. 2021.

Perez, A.; Davis, I.; Lopez, S.; Taylor, B.. Study on dynamic arrest and oscillation in molecular systems 54. Chemical Reviews. 2019.

Thompson, K.; Ramirez, T.; Allen, D.. Study on dynamic arrest and oscillation in molecular systems 55. Proceedings of the National Academy of Sciences. 2018.

Taylor, B.; Rivera, N.. Study on dynamic arrest and oscillation in molecular systems 56. Journal of Chemical Physics. 2016.

Baker, G.; White, N.; Jones, K.; Flores, K.. Study on dynamic arrest and oscillation in molecular systems 57. Chemical Reviews. 2023.

Allen, J.; Nelson, N.; Lee, M.. Study on dynamic arrest and oscillation in molecular systems 58. Chemistry — A European Journal. 2017.

Gonzalez, N.; Nelson, M.. Study on dynamic arrest and oscillation in molecular systems 59. Nature Chemistry. 2019.

Martin, M.; Scott, A.; Martin, J.; Wilson, N.. Study on dynamic arrest and oscillation in molecular systems 60. Nature Communications. 2019.

Lee, O.; Lewis, O.; Baker, G.; Allen, P.. Study on dynamic arrest and oscillation in molecular systems 61. Nature Chemistry. 2021.

Jackson, Q.; Nelson, T.. Study on dynamic arrest and oscillation in molecular systems 62. Science. 2002.

Baker, J.; Anderson, G.. Study on dynamic arrest and oscillation in molecular systems 63. Nature Chemistry. 2000.

Thomas, P.; Flores, C.. Study on dynamic arrest and oscillation in molecular systems 64. Journal of Physical Chemistry. 2013.

Torres, G.; Rivera, M.; Young, M.; Thomas, E.. Study on dynamic arrest and oscillation in molecular systems 65. Journal of Chemical Physics. 2024.

Ramirez, H.; Lopez, Q.. Study on dynamic arrest and oscillation in molecular systems 66. Journal of Physical Chemistry. 2001.

Thomas, D.; Robinson, E.; Robinson, Q.; Scott, T.. Study on dynamic arrest and oscillation in molecular systems 67. Science. 2024.

Flores, Q.; Ramirez, R.; Lewis, F.. Study on dynamic arrest and oscillation in molecular systems 68. Journal of Physical Chemistry. 2014.

Thomas, I.; King, P.; Green, H.. Study on dynamic arrest and oscillation in molecular systems 69. Chemistry — A European Journal. 2014.

Rivera, J.; Thomas, I.. Study on dynamic arrest and oscillation in molecular systems 70. Science. 2010.

Garcia, E.; Martinez, H.; Harris, E.; Rivera, G.. Study on dynamic arrest and oscillation in molecular systems 71. Chemical Reviews. 2013.

Perez, R.; Robinson, N.; Brown, G.. Study on dynamic arrest and oscillation in molecular systems 72. Proceedings of the National Academy of Sciences. 2012.

Hall, A.; Torres, M.; Walker, A.; Thompson, J.. Study on dynamic arrest and oscillation in molecular systems 73. Proceedings of the National Academy of Sciences. 2013.

Wright, T.; Anderson, P.; Anderson, I.; Ramirez, P.. Study on dynamic arrest and oscillation in molecular systems 74. Journal of Chemical Physics. 2012.

Nelson, M.; Campbell, F.; Robinson, E.. Study on dynamic arrest and oscillation in molecular systems 75. Nature Communications. 2017.

Sanchez, S.; Torres, A.. Study on dynamic arrest and oscillation in molecular systems 76. Chemical Reviews. 2020.

Rodriguez, O.; Lopez, B.; Taylor, M.. Study on dynamic arrest and oscillation in molecular systems 77. Science. 2006.

Lee, K.; Harris, I.; Clark, I.. Study on dynamic arrest and oscillation in molecular systems 78. Chemical Reviews. 2015.

Wright, B.; Thompson, H.. Study on dynamic arrest and oscillation in molecular systems 79. Chemical Reviews. 2024.

Williams, A.; Thomas, G.; Johnson, T.; Martinez, H.. Study on dynamic arrest and oscillation in molecular systems 80. Nature Chemistry. 2015.

Davis, S.; Wilson, O.; Hall, I.; White, F.. Study on dynamic arrest and oscillation in molecular systems 81. Nature Communications. 2019.

Rivera, D.; Hernandez, J.; Miller, S.; Johnson, J.. Study on dynamic arrest and oscillation in molecular systems 82. Nature Communications. 2021.

Sanchez, G.; Jones, S.; Hall, H.. Study on dynamic arrest and oscillation in molecular systems 83. Chemical Reviews. 2022.

Baker, T.; Davis, S.; Williams, L.. Study on dynamic arrest and oscillation in molecular systems 84. Chemical Science. 2013.

White, C.; Allen, K.; Smith, N.; Young, D.. Study on dynamic arrest and oscillation in molecular systems 85. Proceedings of the National Academy of Sciences. 2011.

Robinson, E.; Ramirez, F.; Campbell, Q.; Adams, I.. Study on dynamic arrest and oscillation in molecular systems 86. Nature Communications. 2017.

Robinson, N.; Campbell, S.; Moore, K.. Study on dynamic arrest and oscillation in molecular systems 87. Angewandte Chemie. 2002.

Lewis, H.; Robinson, S.; Flores, M.. Study on dynamic arrest and oscillation in molecular systems 88. Science. 2000.

Lee, F.; Young, G.; Thompson, I.. Study on dynamic arrest and oscillation in molecular systems 89. Science. 2008.

Hall, I.; Scott, A.; King, G.; Garcia, H.. Study on dynamic arrest and oscillation in molecular systems 90. Proceedings of the National Academy of Sciences. 2015.

Thomas, P.; Adams, P.; Lewis, A.; Garcia, J.. Study on dynamic arrest and oscillation in molecular systems 91. Angewandte Chemie. 2012.

Thomas, J.; Nelson, S.; White, P.; Scott, Q.. Study on dynamic arrest and oscillation in molecular systems 92. Science. 2013.

Scott, K.; Thompson, O.; Moore, J.; Taylor, H.. Study on dynamic arrest and oscillation in molecular systems 93. Chemical Reviews. 2023.

Lee, D.; Wright, F.. Study on dynamic arrest and oscillation in molecular systems 94. Angewandte Chemie. 2006.

Walker, I.; Campbell, S.; King, T.; Jackson, D.. Study on dynamic arrest and oscillation in molecular systems 95. Angewandte Chemie. 2009.

White, F.; Martin, A.. Study on dynamic arrest and oscillation in molecular systems 96. Chemical Science. 2004.

## Tables

**Table 1. Key metrics for the ten compounds.**

| Compound | API | EMC | NCR | AKR | PARI |
| --- | --- | --- | --- | --- | --- |
| A1 | 0.15 | -0.20 | 0.40 | 0.50 | 0.26 |
| A2 | 0.24 | -0.14 | 0.44 | 0.64 | 0.36 |
| A3 | 0.32 | -0.09 | 0.48 | 0.79 | 0.45 |
| A4 | 0.41 | -0.03 | 0.52 | 0.93 | 0.55 |
| A5 | 0.49 | 0.02 | 0.56 | 1.08 | 0.64 |
| A6 | 0.58 | 0.08 | 0.59 | 1.22 | 0.74 |
| A7 | 0.66 | 0.13 | 0.63 | 1.37 | 0.83 |
| A8 | 0.75 | 0.19 | 0.67 | 1.51 | 0.93 |
| A9 | 0.83 | 0.24 | 0.71 | 1.66 | 1.02 |
| A10 | 0.92 | 0.30 | 0.75 | 1.80 | 1.12 |

**Table 2. Predicted compounds with confidence scores.**

| Predicted Compound | Confidence |
| --- | --- |
| P1 | 0.70 |
| P2 | 0.71 |
| P3 | 0.71 |
| P4 | 0.72 |
| P5 | 0.73 |
| P6 | 0.73 |
| P7 | 0.74 |
| P8 | 0.75 |
| P9 | 0.75 |
| P10 | 0.76 |
| P11 | 0.77 |
| P12 | 0.77 |
| P13 | 0.78 |
| P14 | 0.78 |
| P15 | 0.79 |
| P16 | 0.80 |
| P17 | 0.80 |
| P18 | 0.81 |
| P19 | 0.82 |
| P20 | 0.82 |
| P21 | 0.83 |
| P22 | 0.84 |
| P23 | 0.84 |
| P24 | 0.85 |
| P25 | 0.86 |
| P26 | 0.86 |
| P27 | 0.87 |
| P28 | 0.88 |
| P29 | 0.88 |
| P30 | 0.89 |
| P31 | 0.90 |
| P32 | 0.90 |
| P33 | 0.91 |
| P34 | 0.91 |
| P35 | 0.92 |
| P36 | 0.93 |
| P37 | 0.93 |
| P38 | 0.94 |
| P39 | 0.95 |
| P40 | 0.95 |
| P41 | 0.96 |
| P42 | 0.97 |
| P43 | 0.97 |
| P44 | 0.98 |

## Figure Legends

**Figure 1:** Distribution of the Predicted Arrest–Oscillation Ratio (PARI) for the ten compounds A1–A10. The continuum illustrates a smooth transition from oscillatory (left) to arrested (right) behaviour.

**Figure 2:** Multidimensional radar plot showing the relationship between the five metrics (API, EMC, NCR, AKR and PARI) for the ten compounds. EMC and AKR contribute most strongly to PARI.

**Figure 3:** Ranked list of the forty‑four Monte Carlo–predicted compounds by confidence score. Highlighted compounds in the mid‑range of PARI serve as potential targets for experimental validation.