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Perspective

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Characterizing emerging companies in computational drug development

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Supplementary Tables

Supplementary Table 1: **Company selection criteria.** Ordered list of criteria used curate a dataset of emerging computational drug development companies for analysis.

Criteria #	Description
1	Computational techniques should be a major aspiration / ethos of the company, with the biopharma industry as core focus.
2	Small to medium market capitalization (market capitalization below 10 billion)
3	Has received more than $25 million in private funding or is a public company.
4	The company has a dataset, tool, or product that can directly support any part of the drug development process.
5	Companies focused only on diagnosis, life science tools, wearables, devices, or lab automation are excluded, unless they aim to support drug development as a business component.
6	We distinguish between companies with a drug pipeline (partnered or proprietary) versus companies operating as service providers, see Figure 1.

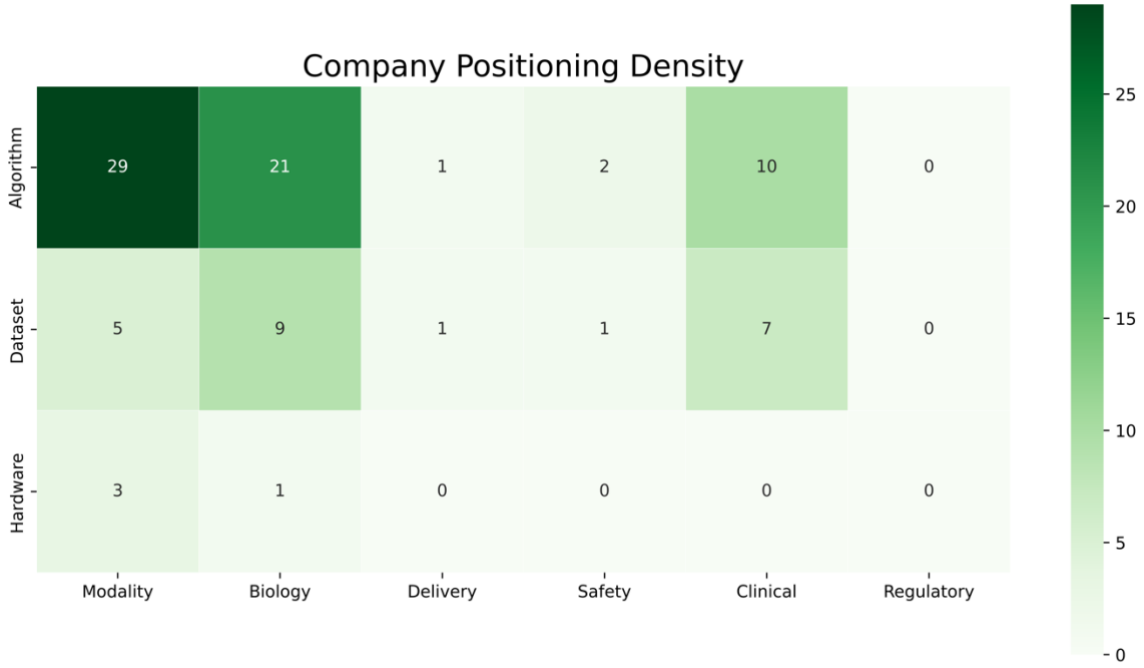
Supplementary Table 2: **Drug R&D and computational dimensions.** Definitions used to classify computational drug R&D companies by drug R&D focus and computational advantage.

Dimension	Description
Drug R&D Axis	
Therapeutic modality design	Design, selection, and optimization of the drug candidate. The modality can be a small molecule, antibody, gene editing, etc. Docking and protein structural information also falls into this category.
Biological insight	Functional validation of the relationship between a disease and a biological target. This includes phenotypic characterization of a living system, understanding of signaling pathways, and roles of mutations.
Tissue & delivery	Ability to target the tissue or cell type of interest, including formulation delivery mechanism, such as nano-particle or viral vector.
Toxicology and safety	Safety in animal model and human, ADMET, hERG interaction, and carcinogenesis.
Clinical trial and patient profiling	Clinical trial design, synthetic arms, biomarkers for patient selection, diagnosis, and personalized treatment.
Commercialization & regulatory	Market access and reimbursement, pricing, post-market monitoring, advertisement, and sales.
Computational Axis	
Computing hardware advantage	Exceptional hardware to be differentiated, cloud computing democratized access to big computing power.
Dataset advantage	Proprietary dataset, unique collection about a biomedical topic, not publicly available. Dataset should be difficult to replicate by competitors.
Algorithm & analytics advantage	Unique software developed by the company, or special techniques to mine datasets, generate insights, or make predictions.

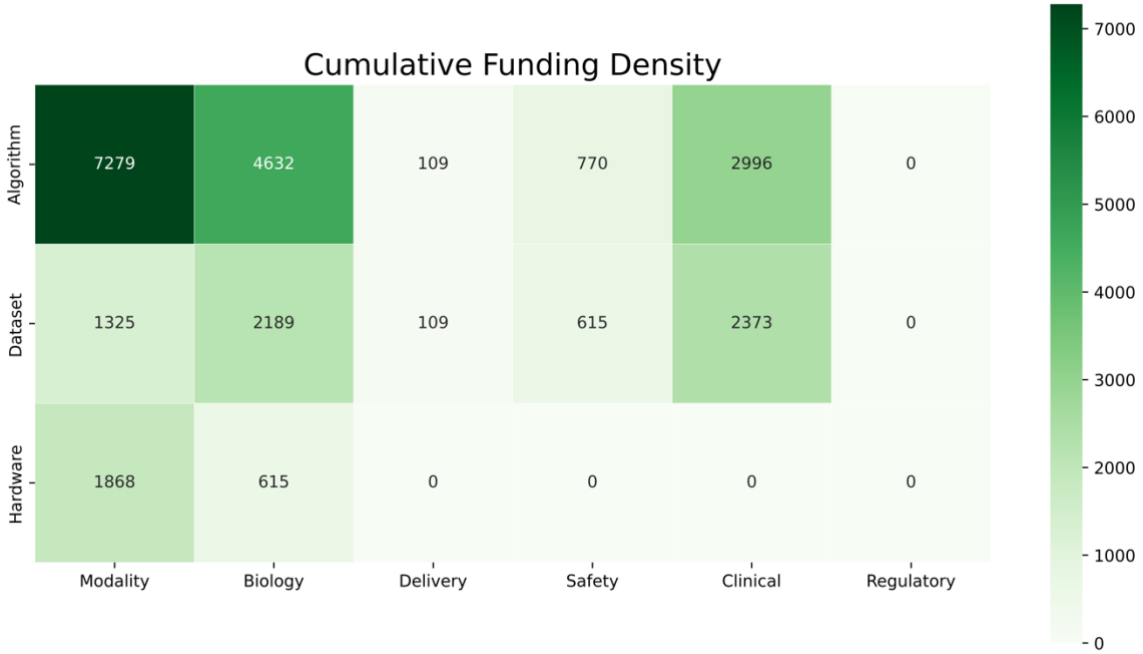
Supplementary Table 3: Deal types. Descriptions of types of deals completed by computational drug R&D companies and partners, with larger theme of deal indicated.

Deal type	Description
Drug – CRADA	Principal and Partner (US federal agency) establish a Cooperative Research and Development Agreement (CRADA).
Drug – Funding	Principal receives (or receives commitment) from Partner for funding to direct to development of drug(s). This type of agreement usually occurs between a pharma or biotech company and a charity, a non-profit organization, or a government agency. The Principal company is the one receiving the funds.
Drug – Asset Divestment	Principal sells to Partner assets associated with drug(s).
Drug – Discovery/Design	Principal and Partner agree to jointly or individually discover and design a drug candidate(s), with a business strategy to develop the drug(s) further.
Drug – Screening/Evaluation	Principal agrees to screen or evaluate a drug candidate(s) against potential targets or in a particular model for Partner.
Drug – Early Research/Development	Principal and Partner form an alliance to jointly use expertise/resources to develop drug candidates.
Drug – Development/ Commercialization License	Partner acquires a license from Principal to develop and commercialize (sell) drug(s).
Drug – Commercialization License	Partner acquires a license from Principal to market drug(s) OR Principal agrees to promote drug(s) in collaboration with Partner.
Drug – Manufacturing/Supply	Principal agrees to manufacture or supply drug(s) for Partner.
Drug – Development Services	Principal agrees to perform drug development services for Partner.
Drug – Authorized Generic	Partner acquires a license from Principal to sell a repackaged version of brand drug as authorized generic.
Technology – Asset Divestment	Principal sells to Partner assets associated with technology (or technologies).
Technology – Delivery/Formulation	Partner acquires a license to use Principal's delivery/formulation technology with drug(s) OR Principal agrees to work with Partner to formulate drug(s).
Technology – Target Validation	Partner acquires a license to use Principal's technology to validate or verify a target, which a developed drug would be directed against.
Technology – Other Proprietary	Partner acquires a license to use Principal's technology with drug(s) OR Principal agrees to use its technology with Partner's drug.
Patent – Asset Divestment	Principal sells to Partner patent rights.
Patent – Exclusive Rights	Partner acquires an exclusive license to use patent(s) belonging to Principal. Exclusive means that no other company has (or will have) the same rights to the patent(s).
Patent – Non-Exclusive Rights	Partner acquires a non-exclusive license to use patent(s) belonging to Principal. Non-exclusive means that the Principal retains rights to license the same rights to other companies.
Patent – Litigation Settlement	Principal resolves patent litigation with Partner. Principal may grant Partner a license to begin marketing its own generic version of brand drug on a specified date.
Company – Joint Venture	Principal and Partner establish a joint venture company/branch.
Company – M&A (in whole or part)	All Partner operating units, assets, and liabilities are transferred to Principal.

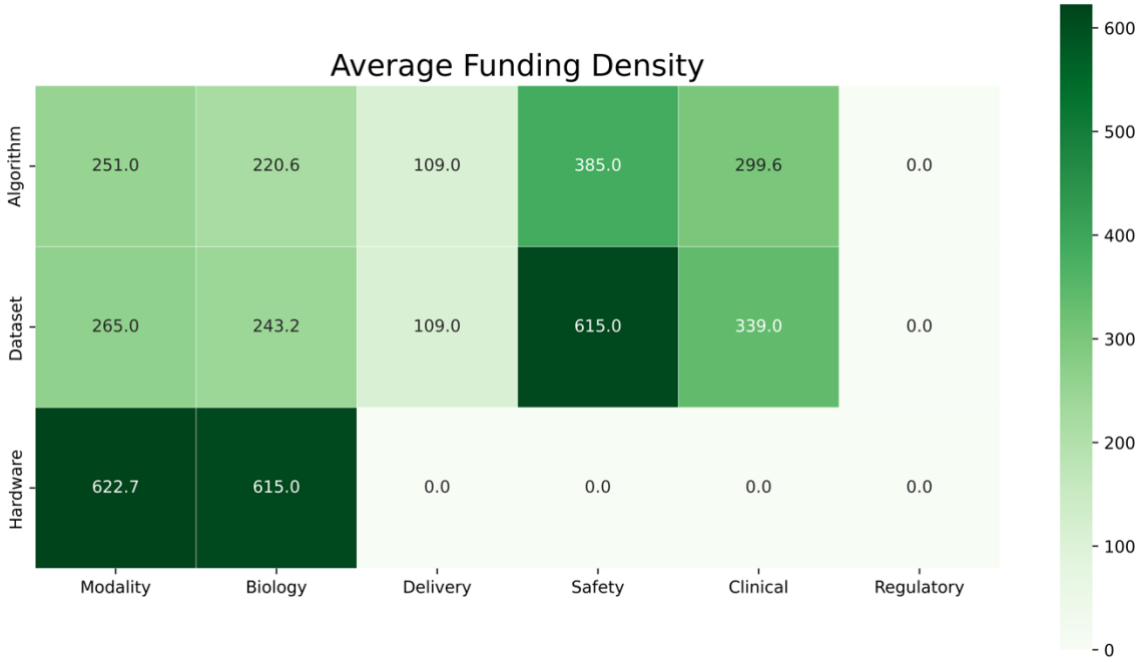
Supplementary Figures



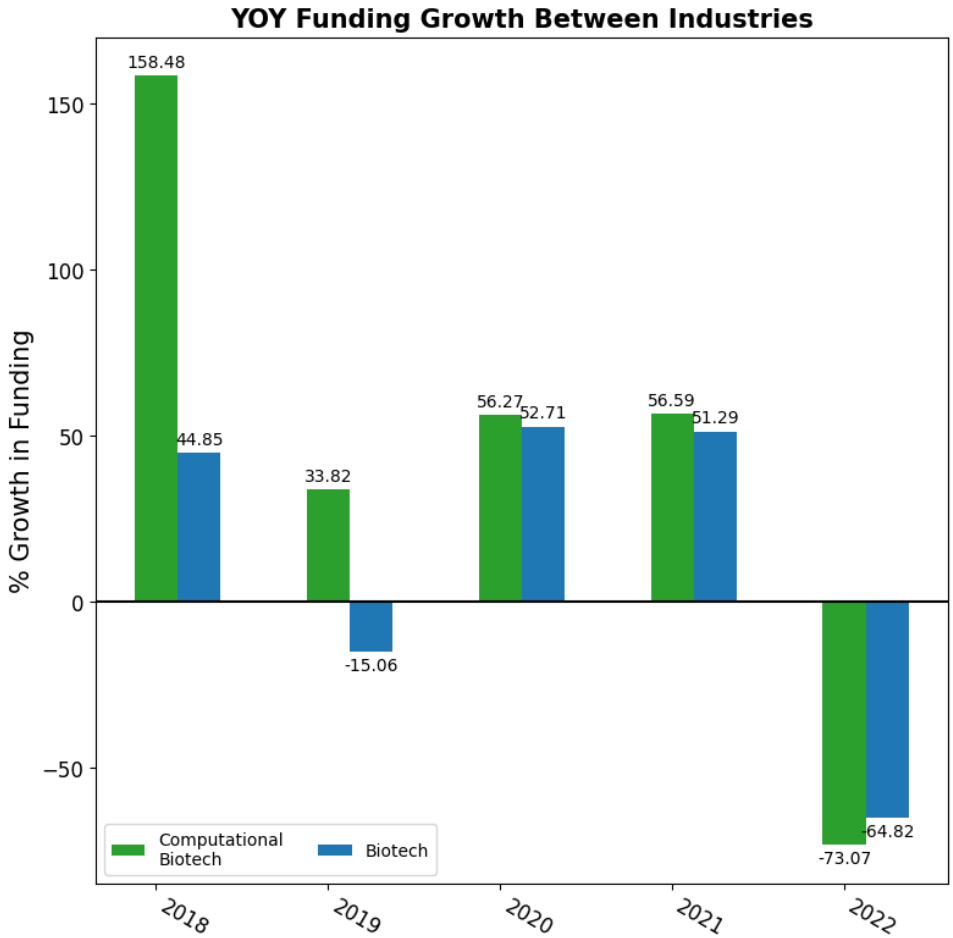
Supplementary Figure 1: Company positioning based on drug R&D focus and computational capabilities. The cell value reflects the number of companies with indicated profile. A company can be present in more than one cell.



Supplementary Figure 2: Heatmap of cumulative funding raised by companies in each sector. If a company appears in multiple cells, the total amount raised will be used for all cells.



Supplementary Figure 3: Heatmap of average funding raised per company in each sector. If a company appears in multiple cells, the total amount raised will be used for all cells.



Supplementary Figure 4: Recent funding growth comparison of overall biotech industry and subset of computational drug R&D companies. Funding growth represented as percent growth year over year.