Provisional MSI Token Roadmap

- **Phase 1 (complete in Q3/2022)**: Proof of Concept for token utility: Distributed, compensated scientific compute for <u>virtual screening</u>

  - Engineering / Product

    - Token Whitepaper

    - Virtual Screen Job (VS Job) Spec

    - Distributed Compute Backend

      - Smart contract for VS Job lifecycle management

        - Publishes requested VS Jobs to blockchain

        - After VS Job deadline, reward mechanism evaluates candidate ligand poses and sends tokens to validators and qualifying workers

      - Node V1

        - Worker

          - Executes VS Jobs and submits candidate ligand poses to blockchain

          - Receives tokens from smart contract upon qualifying reward step

        - Validator

          - Uses a novel Proof-of-Affinity method to evaluate candidate ligand poses using <u>QM/MM</u> simulation and scoring functions

          - Sybil-resistant consensus scheme includes reputation staking system and escrow for robust verification

          - Receives tokens from smart contract for validating work performed by other worker nodes

- Distributed storage layer implementation for input/output datasets
  - Web Frontend V1: Publicly accessible web frontend MVP for building, submitting, and monitoring virtual screening jobs and workflows
    - Supports uploading custom compound / protein libraries (free or proprietary)
    - Supports posting VS Jobs funded by connected wallet
    - Supports building discovery pipelines with basic process types
      - Ligand preparation
      - Protein preparation
      - Conformer generators
      - Cavity detection
      - Docking engines
    - Submits pipelines to Compute Backend for execution
    - Supports previewing and exporting pipeline result datasets
- Finance
  - Evaluate application-specific blockchains/sidechains based on technical requirements required for compute result publication
  - Smart contract audit
- Marketing
  - Token rebrand
  - Launch official website with mailing list
  - Social media presence
  - CoinMarketCap listing
- Operations
  - Begin building a target user group for the platform (researchers, industry employees, students, testers)

- Start product steering committee with selected candidates from target user group

- Begin building partnerships with wet-labs and CROs interested in future platform integration

- **Phase 2 (complete in Q1/2023):** Enhanced platform capability

  - Engineering / Product

    - Web Frontend V2: Additional tooling

      - AlphaFold protein source

      - Molecular dynamics integration

      - Fragment-based screeners

      - Protein sequence analysis tools

      - Homology modeling suite

      - Isostere generation

      - QSAR + pharmacophore filtering

      - ADMET modeling

      - Additional FF, QM/MM, and GPU-accelerated screeners

      - SMILES/structure search for compound libraries

    - Node V2

      - Support for worker pooling

      - GPU platform support

      - Better task selection filters allow workers to determine contribution to individual projects

  - Cross-functional

    - Workflow Specification V2

      - Engineering and ops teams work with CRO/web-lab candidates to add in-vivo assay tools and support to the Job spec

- **Phase 3 (tentative)**