Additional Chemistry Services

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QC

ChemDiv supports comprehensive QC of all compounds; by NMR, HPLC/MS/UV and other options. ChemDiv provides 100% quality control for all compounds and guarantee more than 90% purity (+/- 5% accuracy). The purity accuracy is confirmed by 1H NMR and/or LC (UV)/ MS spectra in electronic format (MS TIF files) for all stock available compounds.

Logistics and Formatting Solutions

With its extensive experience derived from establishing, maintaining and building the largest commercial compound collection in the world, ChemDiv is the partner of choice for global logistics. This guarantees a smooth and fast progression for every project serviced. ChemDiv provides solutions for both compound acquisition and logistics support, including:

- Ordering of compounds from multiple suppliers (including thousands of sources in our global research network)
- High throughput QC, analytical and purification
- IT platform integration, data base procurement, mining and selection
- Library formatting, liquid and neat sample handling; dry / inert atmosphere
- Storage of chemical inventory; both automated and manual.
- Inventory and order tracking online, global in time distribution.

ChemDiv’s network in this area includes over 1,500 academic, biotechnology and pharmaceutical companies worldwide. The compounds can be formatted as a dry powder, dry film or frozen DMSO solution. The weighing can be done in umol or mg. Any handling solutions – multiple copies formatting, storage and dispensing on demand, partial shipments are available. All formats to be individually packed in bar-coded plates or vials. 96well plates with detachable tubes, 384 well microplates, 4 ml Amber glass vials are available is a standard tare. Customized tare is also welcome. Barcodes format 39/128 is to be confirmed by the customer. Delivery within 2-5 weeks for orders of any size. 2-3 bussiness days for orders below 500 compounds. Post synthetic manipulation of compounds such as preparation of screening ready plates, dilution, storage and shipping can all be handled through CDI to make a seamless transition from concept to biological data.

Follow-Up

Analog series

At ChemDiv we have developed a strategy combining the rigor of single compound synthesis in liquid phase with the high throughput of parallel synthesis and purification of

combinatorial methods. One promising method enhancing the efficiency of compound synthesis is the use of multicomponent reactions, in which several building blocks are brought together in a single step. We applied this method for the Ugi, Biginelli, Passerini, Tsuge, and other reactions and developed several significant modifications of known multicomponent reactions. This approach gives our customers the opportunity to perform direct hit analogs search from stock available compounds.

Computational Chemistry

Our strategy for lead generation (focused) libraries design includes:

- Gathering project data (reference compounds, X-ray structure if available, literature patents)
- Computational chemistry (methods depends on target)
- Chemistry evaluation (investigate parallel feasibility)
- CCE database. Library ideas. Synthesis

The computational tool that we use on regular basis to narrow down large chemical space to a more relevant chemical space are listed here.

- ChemoSoftTM (CDI) www.chemosoft.com
- Smart Mining (CDRI)
- Cerius2 (Accelrys)
- Discovery Studio (Accelrys)
- NeuroSolution (NeuroDimension)
- ISIS Base (MDL)
- AutoDock (Scripps)
- Surflex (Biopharmics)
- MolSoft ICM (MolSoft LLC)

The first two programs have been created here at ChemDiv/CDRI. The last one is our partner. All of these tools help maximize

the chance of your finding an active compound using such familiar approaches as docking, searches based on 3D pharmacophore models and shape similarity (target-based strategy) and 2D fingerprint similarity, QSAR models, and substructure searches (in the ligand-based franchise). We also actively use a Neural Networks (NN) approach to assess libraries' various parameters influencing ADME/PK characteristics such as potential interactions with P450, blood-brain barrier permeability, DMSO solubility, probability of being modulators of particular target classes, etc. For such libraries, using ChemoSoftTM, we can efficiently calculate prediction of their major physiochemical parameters, which are routinely used for the assessment of the compounds' drug-likeness based on the Lipinski rules of 5 and certain ADME predictions.

Re-Supply/Re-Synthesis

All products can be supported by adequate replenishing, scale up. Re-supply is subject to ChemDiv's current stock availability. Compounds re-synthesis (subject to the Customer's confirmation) will be offered by ChemDiv if no adequate sample quantity is available for re-supply.

CDI comprehensive chemistry skill set includes:

- Pd-catalyzed coupling reactions (Sonogashira, Buchwald, Heck, Suzuki, Grubbs metathesis, etc.)
- Large-scale (100-150 g per run) (organometallic reactions, lithiation of aromatics and heteroaromatics , Cu, Mg, Zn, SM chemistry)
- Modern protective group strategies
- High-pressure and high-temperature reactions
- Microwave-assisted organic synthesis (Set of Biotage and CEM automated reactors)
- Solid phase supported library synthesis (Teabag technology)

- Liquid phase parallel synthesis (Solid phase catalysts, Scavenger resins, SPE purification)