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'RESEARCH NEVER STOPS'

info@evotec.com | *www.evotec.com*

COMPOUND LIBRARY SYNTHESIS

Medicinal Chemistry and Early Development

Through the provision of high quality lead finding or focused libraries, delivered in the format of your choice, Evotec will accelerate your lead discovery and medicinal chemistry projects in a cost efficient manner.
Evotec has a strong track record in the design and synthesis of compound libraries using parallel synthesis and autopurification technologies.
Evotec has completed in excess of 200 chemistry projects over the past 10 years for world leading pharmaceutical and biotechnology companies. As a result, Evotec scientists have completed the preparation of >1,000 compound libraries and >500,000 compounds.

OUR CAPABILITIES, SKILLS AND EXPERTISE

PEOPLE

— Key strengths in communication and project management developed through the successful delivery of >1,000 libraries
— Team includes experience in synthesising >500,000s compound using parallel synthesis

LIBRARY DESIGN AND PROFILING

— Structure and ligand-based design strategies carried out by an experienced team of molecular modellers
— Proprietary software used to design and profile libraries for maximum diversity whilst ensuring favourable drug-like or lead-like criteria are met
— EVOseek™: Proprietary software, used for *in silico* prediction of ADMET properties for compound libraries

SYNTHESIS

— State-of-the-art platform for parallel synthesis, analysis, autopurification and reformatting into multiple plate and vial formats
— Validated parallel synthesis process with stringent QC to ensure high hit rate and close correlation between virtual and supplied libraries

ENABLING TECHNOLOGIES AND ANALYTICAL CAPABILITIES

— Bespoke and customised equipment enabling the effective high throughput synthesis of compound libraries: ▸ Customised Zinsser Lissy systems ▸ Genevac Series II ▸ Biotage Horizons
— State-of-the-art high throughput analytical and purification equipment: ▸ 2 x Waters 4-Way MUX MS ▸ MassLynx software suite ▸ 2 x NMR (400 MHz)

PURIFICATION AND REFORMATTING

— Semi-prep. and prep. systems using Gilson / Waters LC-UV systems, with high, low or neutral pHs
— Automated reformatting and dispatch including high throughput liquid handling and multi-format weighing
— Flexible dispatch formats including vials, plates and tubes

LIBRARY MANAGEMENT

— Reformatting into 96 / 384 well plates
— High throughput HPLC-MS analysis on every sample

A validated high throughput chemistry platform providing high quality and cost effective solutions to your compound library needs

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An enviable track record of success...

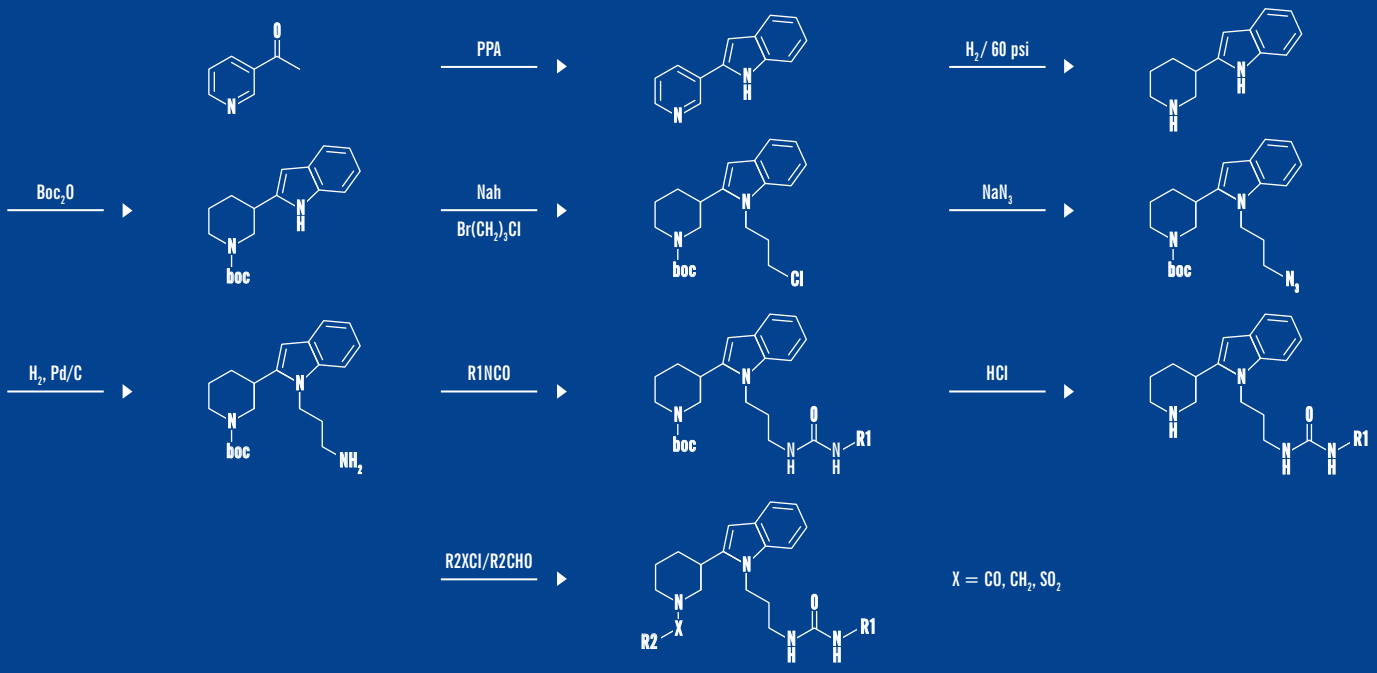
IN THE PAST 12 MONTHS

— 15 projects completed for our biotech, pharmaceutical and agrochemical clients
— >20 libraries completed (10's to 1,000's compounds per library)
— Libraries up to 10 synthetic steps successfully executed
— All clients have returned for additional work
— All work completed to schedule

Case Studies: Challenging chemistries efficiently carried out to produce high quality lead finding and focused libraries

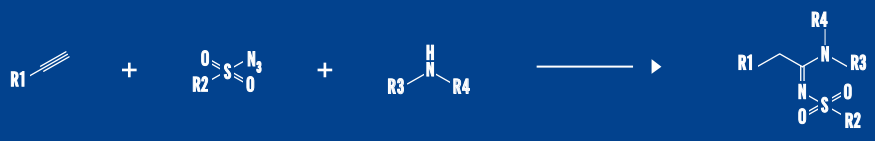
SYNTHESIS OF INDILYL PIPERIDINE LIBRARY

— 9 steps synthesis delivering ca. 700 compounds (>10 mg and >90% purity by HPLC-MS)



SYNTHESIS OF N-SULPHONYL AMIDINE LIBRARY

— Multi-component reactions delivering ca. 850 compounds (>10 mg and >90% purity by HPLC-MS)



EXAMPLE OF FINAL STEP CHEMISTRIES SUCCESSFULLY CARRIED OUT

— Validated final step chemistries in a parallel setting include:

ACYLATION	ARYLATION
ALKYLATION	(THIO)UREA SYNTHESIS
(FUKIYAMA-) MITSUNOBU	AMINATION
AMIDATION	GUANIDINE SYNTHESIS
ESTERIFICATION	SAPONIFICATION
DEPROTECTIONS	[3+2] CYCLOADDITIONS
SULFONYLATION	[2+2] CYCLOADDITIONS