EvoluChem Reagent Screen & prices



your distributor









Table of contents

| EvoluChem Reagent Screen System | 3 |
|---|----|
| General Kit Protocols | 6 |
| Amide Coupling Kits | 8 |
| Suzuki-Miyaura Coupling Kits | 12 |
| Pd Catalyzed Amination Kits | 14 |
| Palladium Precatalysts Kits | 20 |
| Ullmann Reaction Kit | 21 |
| Lead Diversification Tool Box | 22 |
| Alkoxylation and Acetoxylation Kits | 23 |
| Salt Effect on C-H functionalization | 24 |
| Sulfinate Alkylation Diversification Kit | 25 |
| Photocatalytic Alkylation Diversification Kit | 26 |
| Photocatalytic Methylation Array | 27 |
| Fluorination Kit | 28 |
| Iridium/Nickel Photoredox Kits | 29 |
| Biomimetic Oxidation Kits | 31 |
| Glucuronidation Kits | 32 |
| Pre-Filled Reaction Vials | 33 |
| EvoluChem Supplies | 34 |
| Legal information | 35 |

EvoluChem

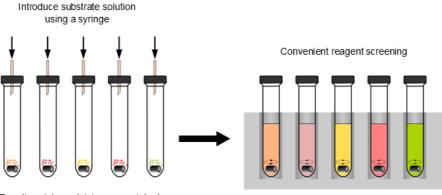


EvoluChem™ Reagent Screen System

Description:

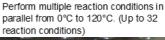
The EvoluChemTM kits are chemistry screening kits. They are the ideal tools for the investigation of chemical reaction conditions. These kits enable you to conveniently screen multiple reaction conditions simultaneously using pre-weighed catalysts and reagents. Most of our kits contain all reagents required to perform the reaction conditions.

EvoluChem™ Reagent Screen System



Reaction vials containing pre-weighed reagents and a stirring bar









EvoluChem™ Reagent Screen System









Benefits

- Facilitate screen of reaction conditions
- Perform up to 96 reaction conditions simultaneously
- Save your substrate using low scale reaction conditions
- Save time on optimization

Features

- 0.3 ml crimped vial with stirring bar
- Specifically designed reaction block
- Pre-weighed reagents and catalysts
- Temperature from 0°C to 120°C
- Pre-designed or custom arrays available
- Reagents are packaged under inert atmosphere
- Solvents are sparged

EvoluChem¹



EvoluChem™ Reagent Screen System



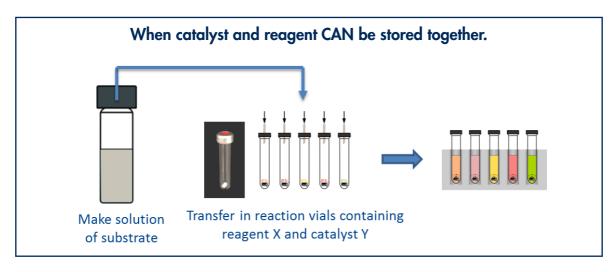
Available Chemistry

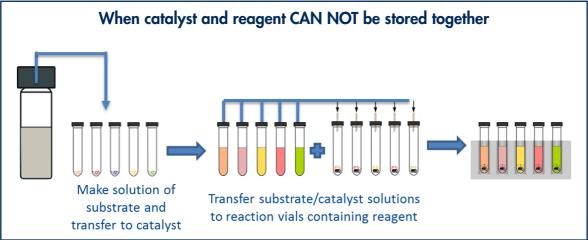
- Cross coupling chemistry
 - Suzuki
 - Pd Precatalysts
 - Copper mediated
- Amide coupling

- Biomimetic Oxidation
- Glucuronidation
- C-H Functionalization
- Photoredox
- Pre-filled Reaction Vials



General Kit Protocols





Starter Kit

• Each kit is designed to perform 2-4 sets of reaction conditions.

 To perform a kit we offer a starter kit (HCK1006-01-001) that contains a reaction block, syringe and decapper. This reaction block is compatible with any EvoluChemTM kit. (Patent

Pending)

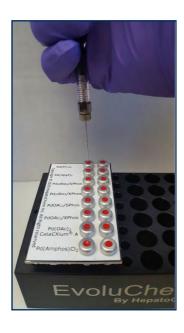


EvoluChem TM By HepatoChem



General Kit Protocols

- 1. Prepare the substrate solution.
- 2. Add to reaction vials containing the pre-weighed reagents and catalysts using a syringe.





3. Place the reaction block on a standard stir/heat plate and set your reaction temperature.









Fast screening of amide coupling reagents

Product overview:

The amide coupling kits are ideal tools for the optimization of amide bond formation. This enables to conveniently screen multiple reaction conditions simultaneously using pre-weighed reagents. We offer pre-selected arrays of reagents and salts or custom arrays depending on your needs.

Standard Protocol: The vials are loaded with 10 µmol of reagent and a stirring bar. Reaction can be performed from 0.2 M in 50 µl to 0.05 M in 200 µl at 1/1 ratio acid and coupling reagent.

Available kits:

Carbodiimide coupling reagent kit

Catalog Ref# HCK1005-01-002: This kit contains the most common DCC derivatives and ethyl(hydroxyimino) cyanoacetate as a safe alternative to HOBt

| Name | CAS Number | Quantity | Amount |
|---------------------------------|------------|----------|---------|
| DCC | 538-75-0 | 4x vial | 10 μmol |
| DIC | 693-13-0 | 4x vial | 10 μmol |
| EDC, HCl | 25952-53-8 | 4x vial | 10 μmol |
| ethyl(hydroxyimino)cyanoacetate | 3849-21-6 | 2x vial | 50 μmol |



9

Aminium coupling reagent kit

Catalog Ref# HCK1005-01-004: This kit contains the most common derivatives of HATU and ethyl(hydroxyimino) cyanoacetate as a safe alternative to HOBt.

| Name | CAS Number | Quantity | Amount |
|----------------------------------|--------------|----------|---------|
| HATU | 148893-10-1 | 2x vial | 10 µmol |
| НВТИ | 94790-37-1 | 2x vial | 10 µmol |
| НСТИ | 330645-87-9 | 2x vial | 10 µmol |
| COMU® | 1075198-30-9 | 2x vial | 10 µmol |
| HDMC | 1082951-62-9 | 2x vial | 10 µmol |
| HDMA | 958029-37-3 | 2x vial | 10 µmol |
| ethyl(hydroxyimino)cyanoacetate* | 3849-21-6 | 2x vial | 70 µmol |

^{*} in kit HCK1005-01-004 only

COMU is a registered trademark of Luxembourg Bio Technologies Ltd.







Phosphonium coupling reagent kit

Catalog Ref# HCK1005-01-006: This kit contains the most common derivatives of PyBOP and ethyl(hydroxyimino)cyanoacetate as a safe alternative to HOBt.

| Name | CAS Number | Quantity | Amount |
|--------------------------------------|-------------|----------|---------|
| PyBOP® | 128625-52-5 | 2x vial | 10 µmol |
| РуАОР | 156311-83-0 | 2x vial | 10 μmol |
| TPTDP | 893413-42-8 | 2x vial | 10 μmol |
| BroP | 50296-37-2 | 2x vial | 10 μmol |
| РуВгор | 132705-51-2 | 2x vial | 10 μmol |
| DEPBT | 56602-33-6 | 2x vial | 10 μmol |
| ethyl(hydroxyimino) Cyanoacetate* | 3849-21-6 | 2x vial | 70 µmol |

^{*} in kit HCK1005-01-006 only

PyBOP is a registered trademark of Merck KGaA.





11

First choice array kit

Catalog Ref# HCK1005-01-007: The first choice array contains a selection of the most representative coupling reagents from the 3 reagent classes; Carboddimide, Aminium and Phosphonium salts. We included ethyl (hydroxyimino)cyanoacetate) as a safe alternative to HOBt. We can also create any custom array that would fit your needs.

| Name | CAS Number | Quantity | Amount |
|-------------------------------------|--------------|----------|---------|
| DIC | 693-13-0 | 2x vial | 10 µmol |
| EDC, HCl | 25952-53-8 | 2x vial | 10 µmol |
| HATU | 148893-10-1 | 2x vial | 10 µmol |
| COMU® | 1075198-30-9 | 2x vial | 10 µmol |
| PyBOP® | 128625-52-5 | 2x vial | 10 µmol |
| DEPBT | 56602-33-6 | 2x vial | 10 µmol |
| ethyl(hydroxyimino) cyanoacetate | 3849-21-6 | 2x vial | 70 μmol |

PyBOP is a registered trademark of Merck KGaA. COMU is a registered trademark of Luxembourg Bio Technologies Ltd.







Suzuki-Miyaura Coupling Kits

Fast screening of cross coupling catalysts, solvents and bases

Product overview:

The Suzuki-Miyaura coupling kits are ideal tools for the investigation of chemical reaction conditions. These kits enable you to conveniently screen multiple reaction simultaneously using pre-weighed catalysts and reagents. The kit contains all reagents to perform the reaction conditions.

Standard Protocol: Substrates solution at 0.15M concentration with 10% catalyst, 2 equivalents of base. 100 µl reaction volume. Additional conditions can be investigated by changing substrate concentration, amount of base.

Available kits:

HCK1003-01-001: Includes 1 set of reagents and solvents with 6 catalysts & 4 bases HCK1003-01-002: Includes 1 set of reagents and solvents with 8 catalysts & 4 bases

Kit contents: 4 reaction vials of each catalysts, 4 bases in aqueous solution at 1M concentration and 4 solvents.

Catalysts available: Pd(PPh₃)₄, Pd(dppf)₂Cl₂, PdOAc₂/SPhos, PdOAc₂/XPhos, Pd₂(dba)₃/SPhos,

Pd₂(dba)₃/XPhos, PdOAc₂/CataCXium® A and Pd(Amphos)Cl₂

Bases: 1M aqueous solutions of Na₂CO₃, K₂CO₃, K₃PO₄ and Cs₂CO₃ **Solvents:** Dioxane, n-Butanol, DMF and acetonitrile (sparged with Nitrogen)

Reaction Conditions

| | | | | Ca | talysts | | | |
|---------------------------------|------------------------------------|---------------------------------------|-----------------------------|-----------------------------|---|---|------------------------------------|-------------------------------|
| | Pd(PPh ₃) ₄ | Pd(dppf) ₂ Cl ₂ | PdOAc ₂ SPhos | PdOAc ₂ XPhos | Pd ₂ (dba) ₃ SPhos | Pd ₂ (dba) ₃ XPhos | PdOAc ₂ CataCXium ®A | Pd(Amphos) Cl ₂ |
| Na_2CO_3 | | | | | | | | |
| K ₂ CO ₃ | | | | ry array | | | Extende | |
| K ₃ PO ₄ | | | | 3-01-001 s & 4 bases | | | HCK1003 8 catalysts | |
| Cs ₂ CO ₃ | | | o cultiysi. | 5 G 1 B0303 | | | o cultifysis | Q 1 50303 |

cataCXium is a registered trademark of Evonik Degussa GmbH.





Suzuki-Miyaura Coupling Kits

13

Test reaction:

Test reaction has been performed using 4-methoxyphenylboronic acid and 4-bromoacetophenone as substrates.

| Catalyst | Base | Solvent | Conversion |
|---|------------|---------|------------|
| Pd(Ph ₃) ₄ | Na_2CO_3 | dioxane | >95% |
| Pd(dppf) ₂ | Na_2CO_3 | dioxane | >95% |
| Pd ₂ dba ₃ /SPhos | K_3PO_4 | dioxane | >95% |
| Pd ₂ dba ₃ /XPhos | K_3PO_4 | dioxane | >95% |
| PdOAc ₂ /SPhos | K_3PO_4 | dioxane | >95% |
| PdOAc ₂ /XPhos | K_3PO_4 | dioxane | >95% |

Protocol using kit HCK1003-01-001

Prepare required volume of a 0.15 mol/L solution of combined substrates (of 4-methoxy phenylboronic acid and 4-bromoacetophenone) in dioxane. Using a clean and dry syringe, add 100μ l of substrates solution to a reaction vial and mix with the catalysts using the syringe. Add 30μ l of the selected base solution. (2 equivalents) Stir the reaction vials in the reaction block at 80° C for 5 hours. Remove the vial caps using a decapper. Prepare analytical sample for each reaction condition with 5μ l sample diluted into 200μ l in DMSO . Analyze resulting analytical samples by LC/MS.









Pd Catalyzed Amination Kits



Fast screening of cross coupling catalysts and bases

Product overview:

The Pd catalyzed amination kits are ideal tools for the investigation of most common precatalysts and bases. These kits enable you to conveniently screen multiple reaction conditions simultaneously using pre-weighed catalysts and reagents. The kit contains all reagents and supplies to perform the reaction conditions. We offer pre-selected arrays of precatalysts and salts or custom arrays depending on your needs.

Palladium catalyzed amination (Buchwald-Hartwig amination) can be performed using a wide variety of palladium sources, ligands, bases and solvents. We designed 2 kits using a combination of palladium precatalysts with either strong bases or weak bases.

$$\begin{array}{c|c} X & & & R & \\ \hline & & & & R & \\ \hline & & & & H & \\ \hline \end{array}$$

Key variables

- Pd Source: Pd(OAc), Pd(dppf), Cl, Pd-Precatalysts...
- Ligand: Phosphine derivatives, BrettPhos, RuPhos, XPhos...
- Base: Na₂CO₃, Cs₂CO₃, K₃PO₄, LHMDS, NaOtBu, P2-Et...
- Solvent: Dioxane, nBuOH, tBuOH, Toluene, DMF, CH₂CN...
- Temperature: rt -> 120C



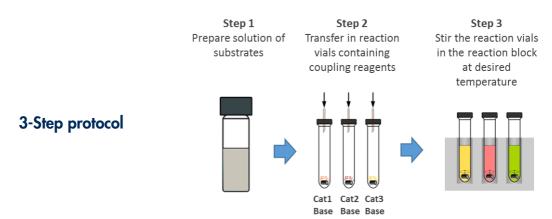
EvoluChem TN By HepatoChem

Pd Catalyzed Amination Kits

15

Weak base arrays

High temperature reaction, compatibility with functional group



Pd Amination weak bases kits (Includes 2 set of reagents)

HCK1004-01-002: 5 Catalysts and 3 bases combinations premixed in same vial. **HCK1004-01-004:** 8 Catalysts and 3 bases combinations premixed in same vial.

| Substrate 15µmol | Weak Bases 30µmol (2 eq) | | | | |
|---|--|--------------------------------|--|--|--|
| Precatalysts 1.5 µmol (10%) | K ₂ CO ₃ | K_2CO_3 Cs_2CO_3 K_3PO_4 | | | |
| BrettPhosG2 | Primary array HCK1004-01-002 5 catalysts & 3 bases | | | | |
| RuPhosG2 | | | | | |
| XPhosG2 | | | | | |
| tBuXPhosG3 | | | | | |
| tBuBrettG3 | - | | | | |
| Pd ₂ dba ₃ / dppf | Extended array | | | | |
| Pd(PtBu ₃) ₂ | HCK1004-01-004 8 catalysts & 3 bases | | | | |
| Pd(OAc) ₂ /CataCXium® A | | | | | |





Pd Catalyzed Amination Kits

Additional weak base arrays

Pd Amination weak bases kits (Includes 2 set of reagents)

HCK1004-01-006: 8 Catalysts and 3 bases combinations premixed in same vial. HCK1004-01-007: 8 Catalysts and 4 bases combinations premixed in same vial. HCK1004-01-008: 8 Catalysts and 3 bases combinations premixed in same vial. HCK1004-01-009: 8 Catalysts and 4 bases combinations premixed in same vial.

| Substrate 15µmol | | Weak Bases 30µmol (2 eq) | | |
|-----------------------------|--------------------------------|---------------------------------|--------------------------------|-------------------------|
| Precatalysts 1.5 µmol (10%) | K ₂ CO ₃ | Cs ₂ CO ₃ | K ₃ PO ₄ | KOAc |
| BrettPhosG2 | | | | |
| RuPhosG2 | | | | |
| XPhosG2 | | | | Extended |
| tBuXPhosG3 | | Primary array HCK1004-01-006 | | array HCK1004-01-007 |
| tBuBrettG3 | | 8 catalysts & 3 bases | | 8 catalysts |
| AmphosG3 | | , | | & 4 bases |
| AdBrettPhosG3 | | | | + buses |
| CataCXium® A G3 | | | | |
| DavePhosG3 | | | | 7 |
| JackiePhosG3 | | | | |
| JosiphosG3 | | | | Extended |
| P(t-Bu)3G4 | | Primary array HCK1004-01-008 | | array HCK1004-01-009 |
| PCy3G4 | | 8 catalysts & 3 bases | | 8 catalysts |
| RockPhosG3 | | • | | & 4 bases |
| SPhosG3 | | | | 4 มนวชว |
| XantphosG3 | | | | |



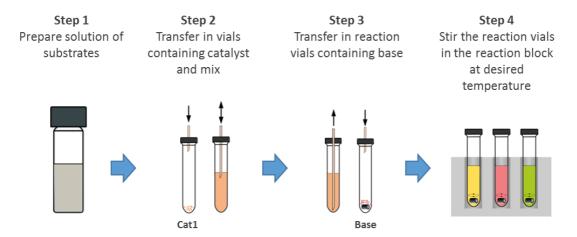
EvoluChem By HepatoChem

Pd Catalyzed Amination Kits

17

Strong base arrays

No need to handle strong bases. Simple protocol.



Pd Amination strong bases kits (Includes 2 sets of reagents) **HCK1004-01-003:** 5 Catalysts and 2 bases in separated vials. **HCK1004-01-005:** 8 Catalysts and 3 bases in separated vials. **HCK1004-01-014:** 8 Catalysts and 2 bases in separated vials.

| Substrate 15µmol | Strong Bases 22.5µmol (1.5 eq) | | | |
|-------------------------------------|----------------------------------|---------|-------------------------|--|
| Precatalysts 1.5µmol (10%) | NaOtBu | LHMDS | P2-Et | |
| BrettPhosG2 | | | | |
| RuPhosG2 | Primary a | rrav | | |
| XPhosG2 | 5 catalysts & 2 bases | | Extended | |
| tBuXPhosG3 | | | array HCK1004-01-005 | |
| tBuBrettG3 | | | 8 catalysts | |
| Pd2dba3/ dppf | Extended array HCK1004-01-014 | | 8 | |
| Pd(PtBu ₃) ₂ | | | 3 bases | |
| Pd(OAc) ₂ /CataCXium® A | 8 catalysts & | 2 bases | | |





Pd Catalyzed Amination Kits

Additional strong base arrays

Pd Amination strong bases kits (Includes 2 sets of reagents)

HCK1004-01-010: 8 Catalysts and 2 bases combinations premixed in same vial. HCK1004-01-011: 8 Catalysts and 3 bases combinations premixed in same vial. HCK1004-01-012: 8 Catalysts and 2 bases combinations premixed in same vial. HCK1004-01-013: 8 Catalysts and 3 bases combinations premixed in same vial.

| Substrate 15µmol | Si | trong Bases 22.5µmol (1. | .5 eq) | |
|----------------------------|---------------------------|--------------------------|-------------------------|--|
| Precatalysts 1.5µmol (10%) | NaOtBu | LHMDS | P2-Et | |
| BrettPhosG2 | | | | |
| RuPhosG2 | | | | |
| XPhosG2 | D.: | | Extended | |
| tBuXPhosG3 | Primary arr HCK1004-01 | | array HCK1004-01-011 | |
| tBuBrettG3 | 8 catalysts & 2 | | 8 catalysts | |
| AmphosG3 | | | & 3 bases | |
| AdBrettPhosG3 | | | 2 nazez | |
| CataCXium® A G3 | | | | |
| DavePhosG3 | | | | |
| JackiePhosG3 | | | | |
| JosiphosG3 | | | Extended | |
| P(t-Bu)3G4 | Primary arr HCK1004-01 | | array HCK1004-01-013 | |
| PCy3G4 | 8 catalysts & 2 | | 8 catalysts | |
| RockPhosG3 | | | 8 | |
| SPhosG3 | | | 3 bases | |
| XantphosG3 | | | | |





Pd Catalyzed Amination Kits



Weak & strong base array

Pd Amination weak 7 strong bases kits (Includes 2 set of reagents)

HCK1004-01-015: 8 Catalysts and Cs_2CO_3 combinations premixed in same vial and 8 Catalysts and NaOtBu in separated vials

| Substrate 15µmol | Strong Bases 22.5µmol (1.5 eq) | Weak Bases 30µmol (2 eq) |
|---|--------------------------------|--|
| Precatalysts 1.5µmol (10%) | NaOtBu | C s ₂ CO ₃ |
| BrettPhosG2 | | |
| RuPhosG2 | | |
| XPhosG2 | | |
| tBuXPhosG3 | Arro HCK1004 | · I |
| tBuBrettG3 | 8 catalysts | |
| Pd ₂ dba ₃ / dppf | | |
| Pd(PtBu3) ₂ | | |
| Pd(OAc) ₂ /CataCXium® A | | |







Pd XPhos/SPhos Precatalysts Kits



Fast screening of cross coupling catalysts, solvents and bases

Product overview:

The palladium precatalysts kits are ideal tools for the investigation of cross-coupling reaction conditions. These kits enable you to conveniently screen multiple reaction conditions simultaneously using pre-weighed catalysts and reagents. The kit contains both precatalysts and bases to perform the reaction conditions. We offer pre-selected arrays of precatalysts and salts or custom arrays depending on your needs.

Standard Protocol: The vials are loaded with 1.5 µmol of precatalyst, 30 µmol of base and a stirring bar. The bases are K₃PO₄ and K₂CO₃ (solid and anhydrous).

| Precatalysts 1.5 µmol | Ligand | Bases 30 µmol |
|--|----------------|--|
| NH | SPhos or XPhos | K ₂ CO ₃ or K ₃ PO ₄ |
| NH Pd L OMs | SPhos or XPhos | K ₂ CO ₃ or K ₃ PO ₄ |
| N CH ₃ Pd L OMS 4 th Generation | SPhos or XPhos | K ₂ CO ₃ or K ₃ PO ₄ |



Ullmann Reaction Kit



21

Fast screening of cross coupling catalysts, solvents and bases

Product overview:

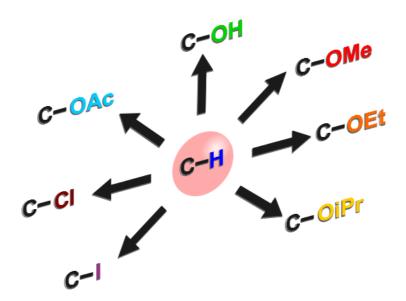
The Ullmann reaction is a interesting alternative to palladium based cross-coupling chemistry. These reactions conditions work with amide, aromatic amine or indole. The Ullmann reaction kit enables to conveniently screen multiple ligands and bases simultaneously using pre-weighed catalysts and reagents.

Standard Protocol: 2ml vial with screw cap and stirring bar, 50µmol of substrates in 500µl solvent (DMF, DMSO, dioxane or acetonitrile, 0.1 mol/L concentration) with 0.1 equivalent of Cul, 0.2 equivalent of ligand and 1.1 equivalent of base.

Kit contents: 2 reaction vials of each catalyst system and base, 36 reaction vials total

| | Copper Iodide / Ligand | | | | | | | | |
|---|------------------------|---|-----------|---|---------------------------------------|-----------------------------|--|--|--|
| | No Ligand | Phenanthroline | S-Proline | 1,2-cyclohexane diamine | N,N'-Dimethyl ethylene diamine | Isobutyryl cyclohexanone | | | |
| | | | NH OH | $\bigcap_{\stackrel{\bullet}{\widehat{\mathbb{N}}}H_2}NH_2$ | H ₃ C NH H CH ₃ | H_3C CH_3 | | | |
| Cs ₂ CO ₃ K ₂ CO ₃ K ₂ PO ₄ | | array HCK1011-01-001 6 catalyst systems & 3 bases | | | | | | | |

Lead Diversification Tool Box



Lead Diversification on your Bench

Lead diversification is becoming an viable alternative to de novo synthesis as C-H functionalization chemistry offers many possible transformations including hydroxylation, acetoxylation, methoxylation, alkylation and fluorination among others. However each desired transformation can quickly become a mini research problem in and of itself, when the end goal is to quickly acquire the analogue for test. A real world drug program does not have the time to develop new reaction conditions in order to make analogues that ultimately may not be active.

Our novel and effective lead diversification tool box addresses all these issues by offering a rapid, practical and cost-effective solution for analogue generation. This approach permits the parallel screening of an selected set of catalytic conditions focusing on generating diversity in an approach which is totally orthogonal and complementary to conventional synthetic methods.





Alkoxylation and Acetoxylation Kits

23

Diversity Kit: 4 different functionalizations

C-H Alkoxylation is one of the most common C-H functionalization described in literature. Our kit is designed to conveniently screen both alkoxylation & acetoxylation reaction conditions using PdOAc₂ as catalyst and several oxidants and additives.

Kit HCK1007-01-001: Includes 2 set of reagents; Catalyst and oxidant are mixed in same vial. Substrate solution is prepared in DMF as one common stock and added to all 4 for solvents. Screen four solvents with three reaction conditions. 10 mol% Pd(OAc)₂, 1 equiv. PhI(OAc)₂.

Kit features:

Vials are filled with 10 mol% Pd(OAc)₂, 1 equiv. PhIOAc₂.

The substrate solution is made in DMF to facilitate the screening of solvents.

Reactions run with 5µmol substrate per reaction. 50 to 200 µl reaction volume (0.025 M to 0.1 M substrate concentration). Reactions from RT to 80 C.

| Transformation | CuOAc ₂ | Ag ₂ CO ₃ | | | | |
|----------------|------------------------------|---------------------------------|--|--|--|--|
| H => 0Me | | | | | | |
| H => 0Et | 10 mol% PdOAc ₂ | | | | | |
| H => 0iPr | 1 equiv. PhIOAc ₂ | | | | | |
| H => OAc | | | | | | |

Test Reaction. (Effect of DMF)

Conversion to mono-substitution

| Transformation | | CuOAc ₂ | Ag ₂ CO ₃ |
|----------------|-----------|--------------------|---------------------------------|
| H => 0Me | 45% (54%) | 57% (70%) | 50%(59%) |
| H => 0Et | 12% (18%) | 22% (24%) | 12% (18%) |
| H => 0iPr | 3% (5%) | 4% (15%) | 5% (11%) |
| H => 0Ac | 7% (17%) | 3% (11%) | 11% (22%) |

In parenthesis without DMF







Salt Effect on C-H functionalization



Optimization Kit: 5 different salts

It has been reported that salt can improved and promote C-H functionalization. Our kit is designed to facilitate the screen of multiple salts simultaneously. These kits contains 5 different salts CuOAc2, Ag₂CO₃, K₂CO₃, Cs₂CO₃ and MgSO₄

Kit HCK1007-01-002: Screen 1 solvent with 12 reaction conditions. 10 mol% PdOAc2, 1 or 2 equivalents of $PhIOAc_2$ with 5 different salts. Prepare one solution in solvent or mixture in $D\overline{M}F$ if solubility

| | Array with 12 reaction conditions | | | | | |
|---------------------------|-----------------------------------|--------------------|---------------------------------|--------------------------------|---------------------------------|----------|
| | | CuOAc ₂ | Ag ₂ CO ₃ | K ₂ CO ₃ | Cs ₂ CO ₃ | $MgSO_4$ |
| 10% Pd(OAc) ₂ | 1 equiv. Ph1(OAc) ₂ | | | | | |
| 10 % Pd(OAc) ₂ | 2 equiv. Phl (OAc) ₂ | | | | | |

Methoxylation of Imatinib

| Catalyst | Oxidant | Salt | % Methoxylation | % Dimethoxylation |
|----------------------|-----------------------|---------------------------------|-----------------|-------------------|
| Pd(OAc) ₂ | PhI(OAc) ₂ | _ | 29.6 | 5.2 |
| Pd(OAc) ₂ | PhI(OAc) ₂ | Cu(OAc) ₂ | 9.6 | 2.5 |
| Pd(OAc) ₂ | PhI(OAc) ₂ | Ag_2CO_3 | 33.5 | 7.6 |
| Pd(OAc) ₂ | PhI(OAc) ₂ | K_2CO_3 | 30.1 | 13.1 |
| Pd(OAc) ₂ | PhI(OAc) ₂ | Cs ₂ CO ₃ | 41.5 | 16.4 |
| Pd(OAc) ₂ | PhI(OAc) ₂ | $MgSO_4$ | 24.0 | 4.5 |

Reaction conditions: 10% Pd(OAc)₂, 1 equiv. PhI(OAc)₂, 0.025 M at 60°C for 18h.

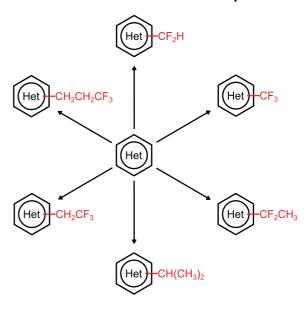
Sulfinate Alkylation Diversification Kit

Product overview: HCK1013-01-001

The sulfinate alkylation reaction described by Prof. Baran is a powerful late stage functionalization tool. Our kit allows to conveniently produce in one step 6 different analogues of a lead compound in mg quantities. Each reaction vial contains 100µmol of sulfinate alkylation reagent (pre-weighed) and a stirring bar to react with 50µmol of substrate. C-H functionalization will primarily occur on electron-deficient heteroarenes at one or several positions.

Standard Protocol: Several solvents or solvent mixtures can be used to perform the reaction (DMSO, DMSO/ H_2O/TFA , CHCl $_3/H_2O/TFA$...). A solution of substrate is made with 300 μ mol of substrate in 2.1ml selected solvent. 350 μ l is added in each vial followed by 20.8 μ l of TBuOOH (70% in water). The reactions are allowed to stir at 50°C for 12-24 hours.

6 Different Diversification Groups



HCK1013-01-001

Kit contents: 2 reaction vials of each reagents (100µmol), 12 reaction vials total.

| | Sulfinate Alkylation Reagents (2 Vials of each) | | | | | | | | | |
|------------|---|---|-----------------------|----------------------------|--|------------------------|--|--|--|--|
| | Zinc difluoro Zinc trifluoro methane sulfinate methane sulfina | | | | nc trifluoro Zinc isopropyl ane sulfinate sulfinate | | | | | |
| | F - S - O - Zn - O - S - F F | F ₃ C ^{-S} O ^{-Zn} O ^{-S} CF ₃ | NaO S CH ₃ | F_3C S Zn S CF_3 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | F ₃ C S ONa | | | | |
| MW (g/mol) | 295.55 | 331.53 | 152.10 | 359.58 | 279.69 | 184.11 | | | | |
| CAS Number | 1355729-38-2 | 39971-65-8 | 1422738-67-7 | 1416821-53-8 | 1416821-55-0 | 1263377-91-8 | | | | |

Literature references:

Ming Yan, Julian C. Lo, Jacob T. Edwards, and Phil S. Baran *J. Am. Chem. Soc.*, **2016**, *138* (39), pp 12692—12714 Fionn O'Hara, Donna G. Blackmond*, and Phil S. Baran *J. Am. Chem. Soc.*, **2013**, *135* (32), pp 12122—12134



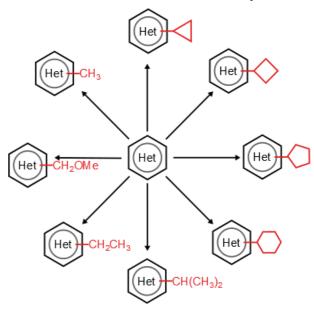
Product overview: HCK1016-01-001

The trifluoroborate alkylation reaction (Minisci reaction) described by Prof. Molander is a powerful late stage functionalization tool. Our kit allows to conveniently produce in one step 8 different analogues of a lead compound in mg quantities. Each reaction vial contains 75µmol of trifluoroborate alkylation reagent (pre-weighed) and a stirring bar to react with 50µmol of substrate. C-H functionalization will primarily occur on electron-deficient heteroarenes at one or several positions.

Kit contents HCK1016-01-001: 2 reaction vials of each BF₃K reagents (75µmol) and $K_2S_2O_8$ (100µmol), 2 vials of photocatalysts and 2 vials of TFA, 16 reaction vials total

Kit Protocol: For each kit, 4mL of a 0.1M solution of substrate (400 µmol total) in DMSO is prepared with 8.98mg photocatalyst Ir(dF-CF₃-ppy)₂(dtbpy) (8µmol, 2 mol%) and trifluoroacetic acid (153µL, 5 equiv) included. The solution is sparged with nitrogen.

8 Different Diversification Groups



HCK1016-01-001

Each vial contains 27.0mg K₂S₂O₈ (100µmol, 2 equiv.) and 1.5 equiv. BF₃K reagent (75µmol) in 2ml vial equipped with stir bar and Teflon septa. Alternatively for methylation, vial contains 39.9µL of TBPA tert-butyl peracetate. Vials are prepared under argon. 500µL of substrate solution added via syringe and vial is placed in PhotoRedox Box equipped with PAR 6200K white light. Reaction is stirred for 2-24 hr.

| | Photocatalytic Alkylation Reagents (2 Vials of each) | | | | | | | | |
|------------|--|--------------|-------------------|-------------------|----------------------|------------------------------------|--|-----------------------|--|
| | Cyclopropyl | Cyclobutyl | Cyclopentyl | Cyclohexyl | Ethyl | Isopropyl | Methoxy methyl | t-Butyl peracetate | |
| | BF ₃ K | BF₃K | \bigcup_{BF_3K} | BF ₃ K | H₃C BF₃K | → BF ₃ - K ⁺ | H ₃ C ^O ✓BF ₃ K | ~~× | |
| MW (g/mol) | 147.98 | 162.00 | 176.03 | 190.06 | 135.97 | 149.99 | 151.97 | 132.16 | |
| CAS Number | 1065010-87-8 | 1065010-88-9 | 1040745-70-7 | 446065-11-8 | 44248-07-9 | 1041642-13-0 | 910251-11-5 | 107-71-1 | |

Literature references:

Jennifer K. Matsui, David N. Primer and Gary A. Molander Chem. Sci., 2017,8, 3512-3522 Tim Cernak, Kevin D. Dykstra, Sriram Tyagarajan, Petr Vachal and Shane W. Krska Chem. Soc. Rev., 2016,45, 546-576





Photocatalytic Methylation Array

Product overview: HCK1009-01-001

With the EvoluChem photomethylation kit, we have demonstrated the reproducibility of both the photomethylation kit and the device.

Kit Protocol: The typical protocol is performed at 0.05mol/l concentration reaction condition using a solution of substrate in 4 different solvents. Each sealed reaction vial contains 0.1 µmol of photocatalyst and 12.5umol of tert-butyl peracetate. Based on the concentration of the substrate stock solution and the volume added, the following reaction stoichiometry can be achieved with the standard photomethylation kit.

| | [Ir{dF(CF3)ppy}2(dtbbpy)]PF6 | [Ir(ppy) ₂ (dtbbpy)]PF ₆ | | | |
|--|------------------------------------|--|--|--|--|
| 50/50 Acetonitrile/TFA | | | | | |
| Acetonitrile (10 equiv. TFA) | 5 equiv. tert-butyl peracetic acid | | | | |
| Acetic acid (10 equiv. TFA) | HCK1009-01-001 | | | | |
| Acetic acid/H ₂ O (10 equiv. TFA) | | | | | |

Kit contents HCK1009-01-001

| Part number | Description | Quantity | Amount |
|---------------|---|----------|----------------------------|
| K-0132-01-001 | ${\rm Ir}[{\rm dF(CF}_3){\rm ppy}]_2({\rm dtbbpy})] {\rm [PF}_6] \ / {\rm tert-butyl} {\rm peracetate}$ | 8x vial | $0.1~\mu mol~/~12.5~u mol$ |
| K-0133-01-001 | $Ir[(ppy)_2(dtbbpy)[PF_6]$ / tert-butyl peracetate | 8x vial | 0.1 µmol / 12.5 umol |
| K-0010-03-001 | 50/50 Acetonitrile/ trifluoroacetic acid | 1x vial | 1 ml |
| K-0011-03-001 | Acetonitrile (10 equiv. trifluoracetic acid*) | 1x vial | 1 ml |
| K-0012-03-001 | Acetic acid (10 equiv. trifluoracetic acid*) | 1x vial | 1 ml |
| K-0012-03-001 | Acetic acid /water (10 equiv. trifluoroacetic acid*) | 1x vial | 1 ml |
| K-0003-04-001 | Substrate stock vial 1 | 1x vial | - |
| K-0003-04-002 | Substrate stock vial 2 | 1x vial | |
| K-0003-04-003 | Substrate stock vial 3 | 1x vial | _ |
| K-0003-04-004 | Substrate stock vial 4 | 1x vial | _ |







Fluorination Kit

Product overview: HCK1008-01-001

Fluorination is one of the most interesting C-H functionalization described in literature. Our kit is designed to conveniently screen fluorination reaction conditions using PdOAc, as catalyst in presence of most common fluorine sources; Silver Fluoride AgF, 1-fluoro-2,4,6-trimethyl-pyridinium triflate (TM-PyF), SelectFluor®, and N-fluorobenzenesulfonimide (NFSI) and oxidant Bis(tert-butylcarbonyloxy iodobenzene (PhIOPiv).

Protocol: The typical protocol is performed at 0.05mol/l concentration of substrate with four different fluorinating agents. When present, reaction includes 10mol% catalyst and 2 equiv. of oxidant. Each kit contains two sets of reagents allowing the screening of two different solvents. Preferred solvents for the fluorination kit include a 5% isobutyronitrile (iPrCN)/dichloroethane mixture, dichloroethane, acetonitrile and dichloromethane. If low solubility of substrate is observed, it is possible to decrease substrate concentration by increasing the reaction volume while maintaining the stoichiometry of the reaction. Maximum volume for reaction vial is 200µl.

12 conditions with AgF, TMPyF, Selectfluor and NFSI

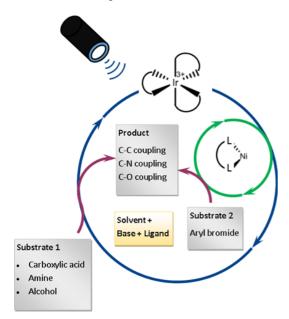
Kit HCK1008-01-001: Includes 2 sets of reagents; Catalyst and oxidant are mixed in the same vial.

| Part number | Part number Vial | | Amount |
|---------------|--|---------|----------------------------------|
| K-0228-01-001 | $Pd(OAc)_2/5$ eq. $AgF/MgSO_4/PhIOPiv$ | 2x vial | 0.25µmol/ 12.5µmol/ 5µmol/ 5µmol |
| K-0229-01-001 | Pd(OAc) ₂ / 5 eq. AgF/ PhIOPiv | 2x vial | 0.25µmol/ 12.5µmol/ 5µmol |
| K-0230-01-001 | Pd(OAc) ₂ / 10 eq. AgF/ PhIOPiv | 2x vial | 0.25µmol/ 25µmol/ 5µmol |
| K-0231-01-001 | Pd(OAc) ₂ / TMPyF | 2x vial | 0.25µmol/ 5µmol |
| K-0232-01-001 | Pd(OAc) ₂ / SelectFluor® | 2x vial | 0.25µmol/ 5µmol |
| K-0233-01-001 | Pd(OAc) ₂ / NFSI | 2x vial | 0.25µmol/ 5µmol |
| K-0234-01-001 | PhIOPiv/ TMPyF | 2x vial | 5µmol/5µmol |
| K-0235-01-001 | PhIOPiv/ SelectFluor® | 2x vial | 5µmol/5µmol |
| K-0236-01-001 | PhIOPiv/ NFSI | 2x vial | 5µmol/5µmol |
| K-0237-01-001 | TMPyF | 2x vial | 5µmol |
| K-0238-01-001 | SelectFluor [®] | 2x vial | 5µmol |
| K-0239-01-001 | NFSI | 2x vial | 5µmol |



Product overview:

In recent years photoredox chemistry has become a powerful tool for chemical synthesis. Many reaction conditions have been reported in the literature using a wide range of catalysts and reagents. However, often these reactions are highly substrate, solvent and base specific. In order to facilitate the screening of common photochemistry reactions, HepatoChem has released a series of kits combining common Iridium, Nickel, ligand and base combinations to achieve successful cross-coupling transformations.



Ir/Ni catalysis versatility

Depending on the ligand, base and solvent, the Ir/Ni catalytic systems can perform different types of cross-coupling reaction.

C-C coupling Ir[dF(CF₃)ppy₂(dtbbpy)]PF₆ NiCt₂-dme / dtbbpy Cs₂CO₃ / DMF blue LED O Ir[dF(CF₃)ppy₂(dtbbpy)]PF₆ NiCt₂-dme / dtbbpy DBU / Ch₃CN blue LED

Iridium catalyst
$$Ir(dF-CF_3-ppy)_2(dtbpy)PF_6$$

$$CF_3$$

$$F$$

$$N$$

$$F$$

$$CF_3$$

$$F-Bu$$

$$F$$

$$CF_3$$



Advion Interchim your distributor HepatoChem



Iridium/Nickel Photoredox Kits



4 Ir/Ni photoredox kits available

Standard Protocol:

5 µmol of substrates in 100µl solvent with Ir catalyst (2 mol %), NiCl₂•dme (10 mol %), ligand (10 mol %), and 3 equivalent of base.

Features

- 0.3 ml vial with crimp cap and stirring bar
- Pre-weighed reagents and catalysts
- Temperature maintained at RT
- Reagents are packaged under inert atmosphere

Ir/Ni base and solvent screen kit 1

With Iridium catalyst Ir(dF-CF₃-ppy)₂(dtbbpy)PF₄ and Ni ligand dtbbpy

| | CS ₂ CO ₃ | K ₃ PO ₄ | K ₂ HPO ₄ | КОН | Li ₂ CO ₃ | K ₂ CO ₃ | DABCO | DBU | |
|-----------|--|--------------------------------|---------------------------------|-----|---------------------------------|--------------------------------|-------|-----|--|
| Solvent A | 2 sets of 8 bases per kit (16 total vials) | | | | | | | | |
| Solvent B | | HCK1009-01-002 | | | | | | | |

Ir/Ni base and ligand screen kit 2 & 3

With Iridium catalyst Ir(dF-CF₃-ppy)₂(dtbbpy)[PF₄]

| | Cs_2CO_3 | K ₃ PO ₄ | K ₂ HPO ₄ | K ₂ CO ₃ | DABCO | DBU |
|------------------------|---|--------------------------------|---------------------------------|--|-------|---------|
| dtbbpy | | | | | 2+{ | / hassa |
| bphen | 2 sets of 4 bases and 4 ligands per kit (32 total vials) HCK1009-01-003 | | | 2 sets of 6 bases and 4 ligands per kit (48 total vials) | | |
| (MeO) ₂ bpy | | | | | | |
| biox | | | | | | |

Ir/Ni base and Ir catalyst screen kit 4

| | Cs ₂ CO ₃ | CsF | DBU |
|--|---------------------------------|---|-----|
| Ir(dF-CF ₃ -ppy) ₂ (dtbbpy)PF ₆ | | | |
| $Ir(dtbbpy)(ppy)_{2}PF_{6}$ | 2 | sets of 3 bases and | |
| Ir(dF-CF ₃ -ppy) ₂ (bpy)PF ₆ | | 6 Ir catalysts per kit (36 total vials) | |
| Ir(dF-ppy) ₃ | | HCK1009-01-005 | |
| Ir(dmppy) ₂ (dtbbpy)PF ₆ | | | |
| Ir(dF-CH ₃ -ppy) ₂ (dtbbpy)PF ₆ | | | |





Biomimetic Oxidation Kits

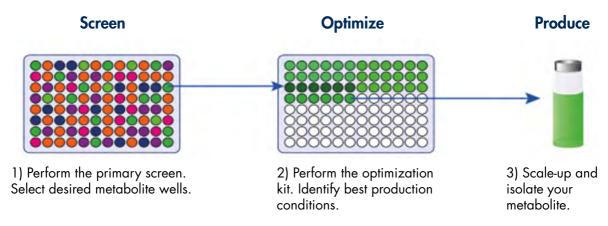
31

Metabolite Production Made Easy

Product overview:

HepatoChem has developed a revolutionary way to screen, optimize, and produce metabolites directly from drug candidates. The BMO Kit exploits an optimized panel of catalytic chemical reaction conditions using organometallic catalysts in a multi-well parallel format. This tool mimics the suite of cytochrome P450 enzymes (CYP) present in human hepatocytes, offering the researcher a unique synthetic chemical liver.

Our BMO kits enable, in three simple steps, synthesis of metabolites directly from the parent drug.



| Available Biomimetic Oxidation Kits BMO Screening Kit Perform the primary screen. Select desired metabolite wells. Order corresponding optimization kit. Complete kit includes all solvents and reagents for 2x25 screening reaction conditions. 2 plates included. | HCK1001-01-001 |
|--|----------------|
| BMO Optimization Kit Perform the optimization kit. Identify best production conditions. Order corresponding production kit. Complete kit includes all solvents and reagents for optimization of selected screening reaction conditions. 1 plate included. | HCK1001-02-xxx |
| BMO Production Kit Scale-up and produce your metabolite. Complete kit includes all solvents and reagents for your metabolite at 12.5 µmol scale or more. | HCK1001-03-xxx |



Glucuronidation Kits

Metabolite Production Made Easy

Product overview:

HepatoChem has developed a revolutionary way to screen, optimize, and produce metabolites directly from drug candidates. The glucuronidation kit exploits an optimized panel of chemical reaction conditions using coupling reagents in a multi-well parallel format. This kit suite is designed to survey chemical reaction conditions that produce O glucuronides. The reaction conditions are derivative of the Koenigs-Knorr reaction.

This is a 2 step process:

1- Coupling with glucuronidation reagent

2- De-protection with base solution

This kit is using 4 different salts (Ag₂CO₃, Ag₂O, Cs₂CO₃ and Na₂CO₃) with 2 different solvents (CH₃CN and CHCl₃), 8 reaction conditions as well as 2 reaction conditions using BF₃.

The first step is performed at 25°C overnight except for BF₃ conditions which are performed at 0°C. Because the reactivity of the substrate may vary, different reaction temperatures or reaction time may be explored. Also we encourage the user to analyze the reaction mixture after the first step, in order to identify the reaction conditions that form the most protected glucuronide product.

The second step consists of de-protecting the intermediate using NaOH/MeOH solution or LiOH/ MeOH solution. The optimum quantity needed for the protection may vary due to the functional groups present on the substrate as well as the stability of the final product.

Available Glucuronidation Kits

Glucuronidation refill kit

HCK1002-01-001

Glucuronidation array kit (10 reaction conditions) to generate O glucuronide metabolite. This kit includes 2 refill of reagents.

Glucuronidation optimization kit

HCK1002-02-XXX

Optimization array kit (4 reaction conditions) to optimize 0 glucuronide metabolite production. This kit includes 4 refill of reagents.

Glucuronidation production kit

HCK1002-03-XXX

Production kit to generate O glucuronide metabolite at 12.5 µmol scale. This kit includes 4 refill of reagents



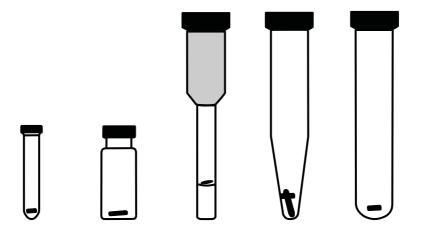
EvoluChem TM By HepatoChem

Pre-Filled Reaction Vials

33

Weak Base Reaction Vials

- Pre-filled reaction vials with base and stir bar
- Easy access to hydroscopic base salts ($Cs_2CO_3 \& K_3PO_4$)
- 5 bases available
- Quick base screen
- Multiformat/scale available



| | Standard H | eating Vials | | Microwave Heating Vials | | |
|---------------------------------|--|----------------|----------------|-------------------------|----------------|--|
| Reaction Volume | 0.05 - 0.2ml | 0.5-1ml | 0.2-0.5ml | 0.5-2ml | 2-5ml | |
| Vial Size | 6x32mm | 12x32mm | 8x83mm | 16x83mm | 16x83mm | |
| Base Amount | 20µmol | 200µmol | 60µmol | 200µmol | 500µmol | |
| | Available base kits (each kit contains 5 reaction vials) | | | | | |
| CS ₂ CO ₃ | HCK1010-01-001 | HCK1010-02-001 | HCK1010-03-001 | HCK1010-04-001 | HCK1010-05-001 | |
| K ₃ PO ₄ | HCK1010-01-002 | HCK1010-02-002 | HCK1010-03-002 | HCK1010-04-002 | HCK1010-05-002 | |
| K ₂ CO ₃ | HCK1010-01-003 | HCK1010-02-003 | HCK1010-03-003 | HCK1010-04-003 | HCK1010-05-003 | |
| Na ₂ CO ₃ | HCK1010-01-004 | HCK1010-02-004 | HCK1010-03-004 | HCK1010-04-004 | HCK1010-05-004 | |
| NaHCO ₃ | HCK1010-01-005 | HCK1010-02-005 | HCK1010-03-005 | HCK1010-04-005 | HCK1010-05-005 | |

EvoluChem Supplies

Available Supplies:

| Item | Reference | Description |
|---------------------------------------|----------------|--|
| Starter Kit | HCK1006-01-001 | 1 reaction block (24x2ml vial, 32x0.3ml vial, 4x2Dram vial), 1 decapper for 8mm crimped vial and 1 syringe Hamilton 81000. |
| EvoluChem Block fits 3 types of vials | HCK1006-01-002 | 1 reaction block (24x2ml vial, 32x0.3ml vial, 4x2Dram vial) |
| EvoluChem Block fits 96x0.3ml vials | HCK1006-01-003 | 1 reaction block (96x0.3ml vial) |
| Micro stir bar 2x2mm | HCK1006-01-012 | 50 stir bars |
| 6mm vials 0.3ml | HCK1006-01-013 | 100 vials |
| Crimp caps for 6mm vial | HCK1006-01-014 | 100 crimp caps |
| Micro stir bar 2x7mm | HCK1006-01-015 | 50 stir bars |



HCK1006-01-001



HCK1006-01-002



HCK1006-01-003



HCK1006-01-012



HCK1006-01-013



HCK1006-01-014



HCK1006-01-015



Legal information

35

All catalysts and reagents are purchased from authorized distributers. cataCXium is a registered trademark of Evonik Degussa GmbH, protected by patent US 7,148,176 Palladium Precatalysts G2 and G3 are protected by patents US 6,395,916 and US 6,307,087 Palladium Precatalysts G4 are protected by patents PCT/US2013/030779, US Serial No. 13/799620

COMU is a registered trademark of Luxembourg Bio Technologies Ltd. PyBOP is a registered trademark of Merck KGaA.

| Catalog number | Kit | Description |
|-------------------|----------------------------------|---|
| HCK1001-01-001 | BMO screen | Perform the primary screen. Select desired metabolite wells. |
| | | Order corresponding optimization kit. |
| HCK1001-02-xxx | BMO optimization | Perform the optimization kit. Identify best production conditions. Order corresponding |
| | | production kit. |
| HCK1001-03-xxx-10 | BMO production 125umol | Scale-up and produce your metabolite. |
| HCK1002-01-001 | Glucuronidation kit refill | This kit allows to identify reaction condition that produces O glucuronide adduct of a |
| 116//1000 00 | | drug compound. |
| HCK1002-02-xxx | Glucuronidation kit optimization | Optimization array kit (4 reaction conditions) to optimize 0 glucuronide metabolite production. |
| HCK1002-03-xxx | Glucuronidation kit Production | Production kit to generate O glucuronide metabolite at 12.5 µmol scale. |
| HCK1003-01-001 | Suzuki array Kit 1 | 1 set of 6 catalysts , 4 base solutions and 4 solvents. 24 reaction vials total |
| HCK1003-01-002 | Suzuki array Kit 2 | 1 set of 8 catalysts , 4 base solutions and 4 solvents. 32 reaction vials total |
| HCK1004-01-002 | Pd amination weak base array 1 | 2 sets of 15 reagent combinations premixed in same vial; 5 Catalysts and 3 bases. 30 reaction vials total |
| HCK1004-01-003 | Pd amination strong base array 1 | 2 sets of 10 reagent combinations in separated vials; 5 Catalysts and 2 bases. 20 reaction vials total |
| HCK1004-01-004 | Pd amination weak base array 2 | 2 sets of 24 reagent combinations premixed in same vial; 8 Catalysts and 3 bases. 48 reaction vials total |
| HCK1004-01-005 | Pd amination strong base array 2 | 2 sets of 24 reagent combinations in separated vials; 8 Catalysts and 3 bases . 48 reaction vials total |
| HCK1004-01-006 | Pd amination weak base array 3 | 2 sets of 24 reagent combinations premixed in same vial; 8 Catalysts and 3 bases.48 reaction vials total |
| HCK1004-01-007 | Pd amination weak base array 4 | 2 sets of 32 reagent combinations premixed in same vial; 8 Catalysts and 4 bases. 64 reaction vials total |
| HCK1004-01-008 | Pd amination weak base array 5 | 2 sets of 24 reagent combinations premixed in same vial; 8 Catalysts and 3 bases. 48 reaction vials total |
| HCK1004-01-009 | Pd amination weak base array 6 | 2 sets of 32 reagent combinations premixed in same vial; 8 Catalysts and 4 bases. 64 reaction vials total |
| HCK1004-01-010 | Pd amination strong base array 3 | 2 sets of 16 reagent combinations in separated vials; 8 Catalysts and 2 bases. 32 reaction vials total |
| HCK1004-01-011 | Pd amination strong base array 4 | 2 sets of 24 reagent combinations in separated vials; 8 Catalysts and 3 bases. 48 reaction vials total |
| HCK1004-01-012 | Pd amination strong base array 5 | 2 sets of 16 reagent combinations in separated vials; 8 Catalysts and 2 bases. 32 reaction vials total |



Legal information

36

| Catalog number | Kit | Description |
|----------------|--|--|
| HCK1004-01-013 | Pd amination strong base array 6 | 2 sets of 24 reagent combinations in separated vials; 8 Catalysts and 3 bases. |
| | | 48 reaction vials total |
| HCK1004-01-014 | Pd amination strong base array 7 | 2 sets of 16 reagent combinations in separated vials; 8 Catalysts and 2 bases. |
| | | 32 reaction vials total |
| HCK1004-01-015 | Pd amination strong and weak base | 2 sets of 16 reagent combinations in separated vial for strong base and premixed |
| | | for weak base; 8 Catalysts and 2 bases 32 reaction vials total |
| HCK1005-01-002 | Carbodiimide coupling reagent kit | 2 sets of 4 reagents. 8 reaction vials total |
| HCK1005-01-004 | Aminium coupling reagent kit 2 | 2 sets of 6 reagents. 12 reaction vials total |
| HCK1005-01-006 | Phosphonium coupling reagent kit 2 | 2 sets of 6 reagents. 12 reaction vials total |
| HCK1005-01-007 | Amide coupling first choice array kit | 2 sets of 6 reagents.1 2 reaction vials total |
| HCK1006-01-001 | Starter Kit | This kit contains 1 reaction block (24x 2ml vial, 32X 0.3ml vial, 4X 2Dram vial), 1 decapper for 8 mm crimped vial and 1 syringe Hamilton 81000. |
| HCK1006-01-002 | Reaction block | 1 reaction block (24x 2ml vial, 32x 0.3ml vial, 4x 2Dram vial) |
| HCK1006-01-003 | Reaction block 96 vials | 1 reaction block (96x 0.3ml vial) |
| HCK1006-01-012 | Micro stir bar 2 X 2mm | 50 Stir bars |
| HCK1006-01-013 | 6 mm vials 0.3 ml | 100 vials |
| HCK1006-01-014 | Crimp caps for 6 mm vial | 100 crimp caps |
| HCK1006-01-015 | Micro stir bar 7 X 2mm | 50 Stir bars |
| HCK1006-01-032 | Reaction block 2 ml vial | 1 reaction block (48x 2 ml vial) |
| HCK1007-01-001 | Alkoxylation & Acetoxylation Kit | 8 sets of 3 reaction conditions. 10 mol% PdOAc ₂ , PhIOAc, with 2 different salts |
| 11007 01 001 | randa flution a rector flution tal | with 4 different solvents. 24 reaction vials total |
| HCK1007-01-002 | Alkoxylation & Acetoxylation Opti. Kit | 2 set of 12 reaction conditions. 10 mol% PdOAc ₂ , 1 or 2 equivalents of PhIOAc ₂ |
| | , , , , | with 5 different salts. 24 reaction vials total |
| HCK1008-01-001 | Fluorination kit | Kit with PdOAc, with either AgF, SelectFluor, NFSI or TMPyF with or without PhIOPiv |
| | | as oxidant 24 reaction vials totals |
| HCK1009-01-001 | Photomethylation kit | 2 sets of photomethylation reaction conditions with 2 iridium catalysts, AcOOtBu |
| | | and 4 different solvent systems 16 reaction vials total |
| HCK1009-01-002 | Ir/Ni base and solvent screen kit 1 | 2 sets of reaction conditions with iridium catalyst, Ni/dtbbpy and 8 bases. 16 reaction vials total |
| HCK1009-01-003 | Ir/Ni screen base and ligand kit 2 | 2 sets of reaction conditions with iridium catalyst , 4 Ni ligands and 4 bases. |
| | .,, | 32 reaction vials total |
| HCK1009-01-004 | Ir/Ni screen base and ligand kit 3 | 2 sets of reaction conditions with iridium catalyst, 4 Ni ligands, and 8 bases. |
| | · | 32 reaction vials total |
| HCK1009-01-005 | Ir/Ni screen base and Ir cat kit 4 | 2 sets of reaction conditions with 6 iridium catalysts, Ni dtbbpy , and 3 bases. |
| | | 36 reaction vials total |
| HCK1009-01-006 | Ir/Ni base and solvent screen kit | 2 sets of reaction conditions with iridium catalyst $Ir(dF-CF_3-ppy)_2(dtbbpy)PF_6$, $Ni/$ |
| | (C-O coupling) | dtbbpy, Quinuclidine in 8 conditions with Cs ₂ CO ₃ , K ₃ PO ₄ , K ₂ CO ₃ |
| | | (with 3 concentrations of Ni), DABCO, just |





Legal information

| Catalog number | Kit | Description |
|----------------|---|---|
| HCK1009-01-007 | Ir/Ni HAT screening kit | 3 sets of reaction conditions with iridium catalysts $Ir(dF-CF_3-ppy)_2(dtbbpy)PF_6$ and $Ir(ppy)(dtbbpy)_2PF_6$, $NiBr_2*3H_2O$, two ligands 4,7-dOMe-phen and 4,4'-dOMe-bpy and two bases Quinuclidine and 3-Acetoxy-quinuclidine. 15 reaction vials total. |
| HCK1011-01-001 | Ullmann array kit | 2 sets of Ullmann reaction conditions with CuI, 5 different ligands and 3 bases. 36 reaction vials total |
| HCK1013-01-001 | Sulfinate Alkylation Diversification Kit | This kit allows to produce analogues of the lead compound using 6 different sulfinate alkylation reagents. Each vial contains 100 µmol of sulfinate alkylation reagent and a stirring bar to react with 50µmol of substrate. |
| HCK1013-01-002 | Sulfinate Alkylation Screen Kit | This kit allows to screen 6 different sulfinate alkylation reagents. Each vial contains 10µmol of sulfinate alkylation reagent and a stirring bar to react with 5µmol of substrate. |
| HCK1016-01-001 | Photo-catalytic Alkylation Diversification Kit | Photo-catalytic alkylation production kit using 8 different BF3K reagents in 50µmol scale reaction condition. |
| HCK1016-01-002 | Photo-catalytic Alkylation Screen Kit | Photo-catalytic alkylation screen kit using 4 photocatalysts and 8 different alkylation reagents in 5µmol scale reaction condition. |



HOW TO REQUEST MORE INFORMATION, A QUOTATION OR TO PLACE AN ORDER

Please see from the list below:



HOW TO PLACE AN ORDER

Europe, Israël: orders.EU@advion-interchim.com - Phone: +33 4 70 03 88 55 **North America:** orders.NAM@advion-interchim.com - Phone: +1 607 266 9162

NEED TO RECEIVE A QUOTATION?

Europe, **Israël**: quotes.EU@advion-interchim.com **North America**: quotes.NAM@advion-interchim.com

NEED TECHNICAL ASSISTANCE?

Our scientific experts are here to help.

Instrumentation: instrumentation@advion-interchim.com
Consumable: consumables@advion-interchim.com

NEED A GENERAL INFORMATION?

Europe, Israël: info.EU@advion-interchim.com **North America:** info.NAM@advion-interchim.com

Online

www.interchim.com

All your orders will be recorded & processed as quickly as possible.

Live Demo

Our team will be pleased to give you a live demonstration of our products.

Let's arrange a personal appointment!