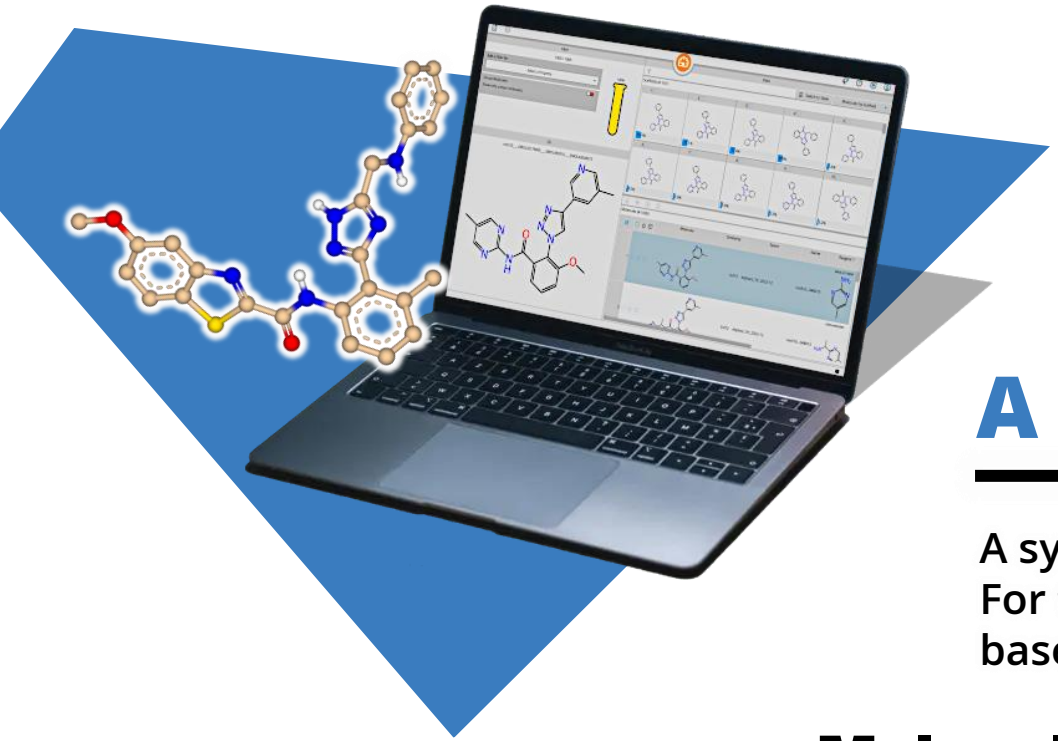
BioSolveIT
expect actives!



A + B → Cookbook

A synthetic guide
For the eXplore space
based on robust chemical reactions

eMolecules

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Introduction

What is this Cookbook?

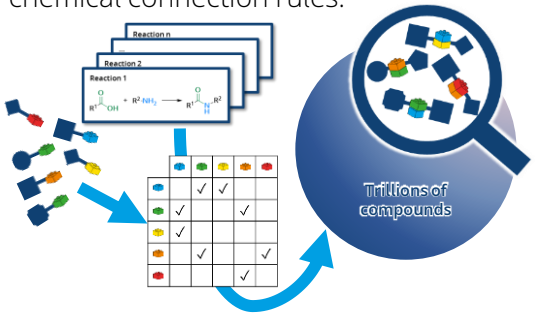
This cookbook shall provide users of infiniSee with information and insights into the reactions used in the generation of the eXplore Chemical Space.

Compounds retrieved from searches in eXplore are based on eMolecules building blocks and robust chemical reactions that can be performed in most synthesis labs with high success. Trillions of compounds can therefore be realized in-house by users, without relying on third party syntheses.

This collection can be considered as a starting point for the planning of the compound synthesis or simply as a compilation for everybody involved and interested in chemistry.

What is a Chemical Space?

A Chemical Space is a vast collection of compounds resulting from building blocks that are combined by applying chemical connection rules.



The beauty of this approach is that the results are generated during the search. Therefore, only interesting compounds will be enumerated and presented to you, without the need to store the data of trillions of other compounds — yet any contained molecule can be found.

"Do it yourself"

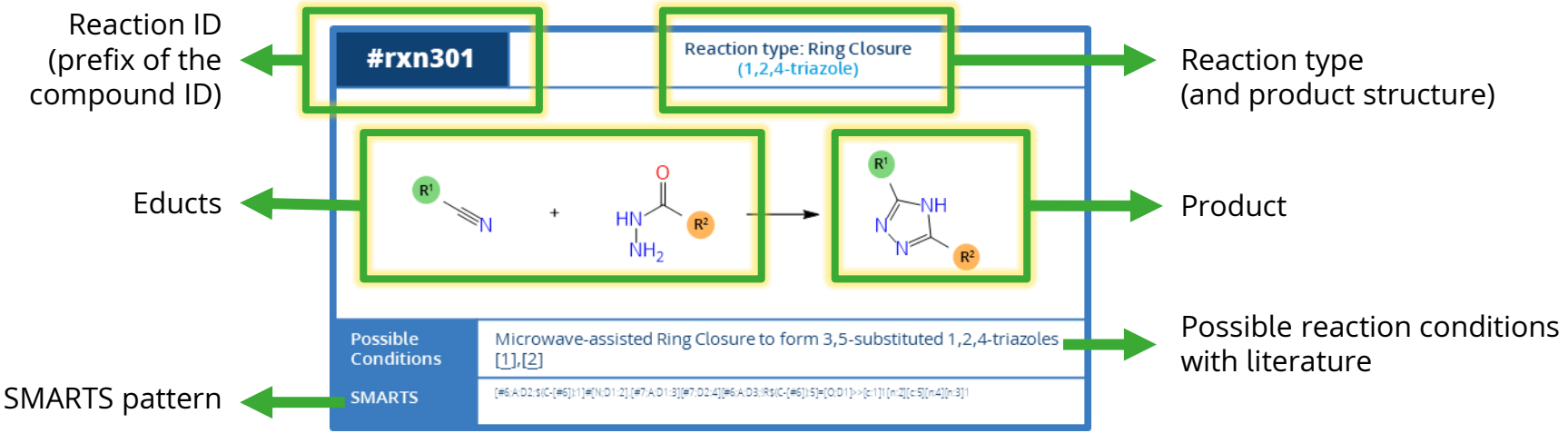
The underlying concept of eXplore is that the users may realize the compounds themselves in a "do it yourself" style:

After ordering the required building blocks for the compounds, bench chemists can make the desired molecules within only a few steps.

Alternatively, eMolecules can help you source on-demand synthesis services from trusted eMolecules suppliers upon request. Visit the eMolecules website for further information.

- Learn more about BioSolveIT's Chemical Space navigation platform infiniSee here.

Reaction summary: How to read it

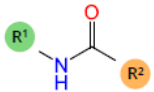
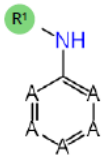
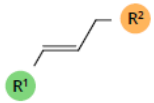
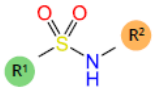
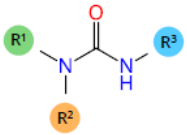


Every compound of eXplore has a unique ID:

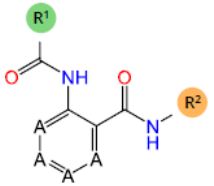
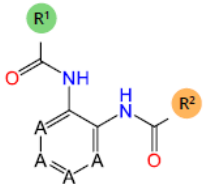
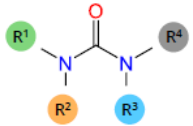
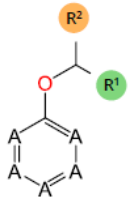
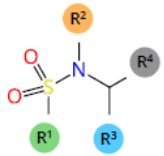
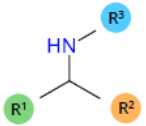
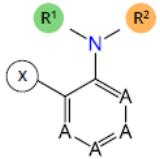
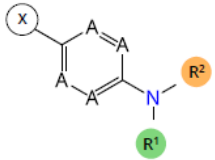
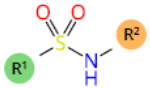
rxn101_bb1_bb2_bb3

- "rxn" prefixes the reaction that is used to create this compound
- "bb1", "bb2", "bb3" stand for building blocks 1, 2, and 3, respectively

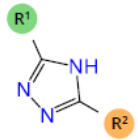
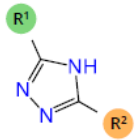
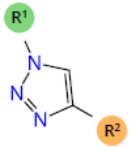
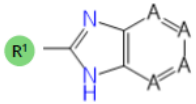
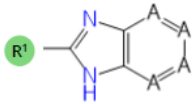
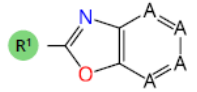
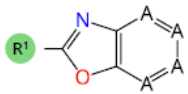
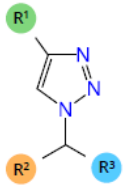
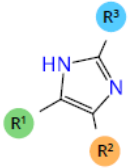
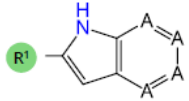
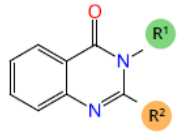
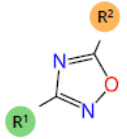
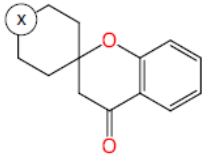
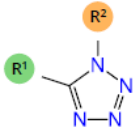
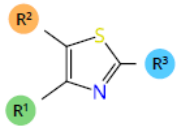
Coupling Reactions

 rxn101 s.10	 rxn102a/b s.10	 rxn108a/b s.10	 rxn110a/b s.10	 rxn111a/b s.11	 rxn113 s.11
 rxn114a/b s.11					

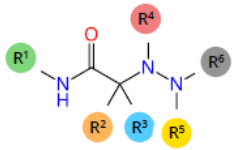
Substitution Reactions

 rxn201 s.12	 rxn202 s.12	 rxn203 s.12	 rxn205 s.12	 rxn206 s.13	 rxn207 s.13
 X = COOH, NO_2, SO_2H rxn208 s.13	 X = COOH, NO_2, SO_2H rxn209 s.13	 rxn210 s.14			

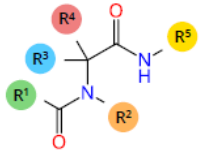
Ring Closures

 rxn301 s.15	 rxn302 s.15	 rxn303 s.15	 rxn304 s.15	 rxn305 s.16	 rxn309 s.16
 rxn310 s.16	 rxn313 s.16	 rxn316 s.17	 rxn317 s.17	 rxn318 s.17	 rxn319 s.17
 X = C, NH rxn320 s.18	 rxn321 s.18	 rxn322 s.18			

Multicomponent Reactions

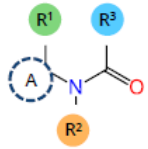
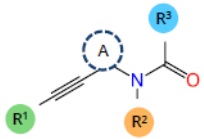
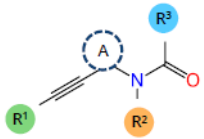
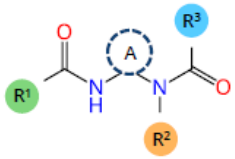
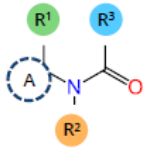
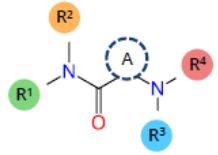
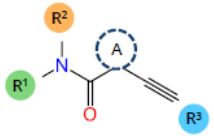
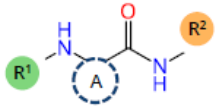
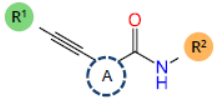
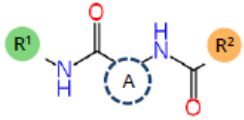
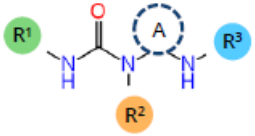
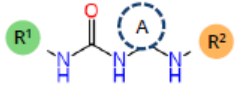


rxn401
s.19



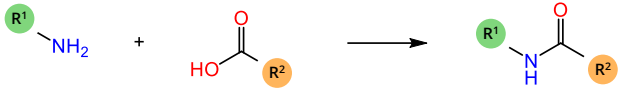
rxn402
s.19

Core Reactions

 rxn501a/b s.20	 rxn503a/b s.20	 rxn505a/b s.20	 rxn506a/b s.20	 rxn511a/b s.21	 rxn512a/b s.21
 rxn513a/b s.21	 rxn514a/b s.21	 rxn515a/b s.22	 rxn516 s.22	 rxn531a/b s.22	 rxn532a/b s.22

#rxn101

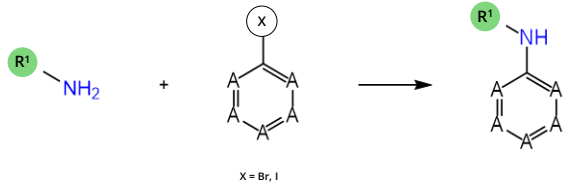
Reaction type: Coupling
(amide)



Possible Conditions	Various coupling reagents; review: [1]
SMARTS	[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]);1].[C;D1,$(C[#6]);2](=[OD1:3])[OD1,Cl]>>[N:1][C:2](=[O:3])

#rxn102a/b

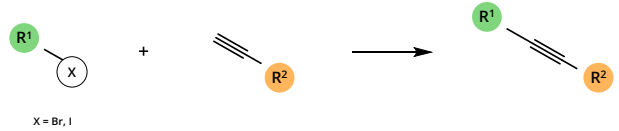
Reaction type: Coupling
(arom. amine)



Possible Conditions	Buchwald Hartwig cross-coupling reaction [1],[2]
SMARTS	A: [#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:[c,n]:1);1][#35;A;D1].[#7;A;$(N([#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]);2]>>[#6:1].[#7:2] B: [#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:[c,n]:1);1][#53;A;D1].[#7;A;$(N([#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]);2]>>[#6:1]-[#7:2]

#rxn108a/b

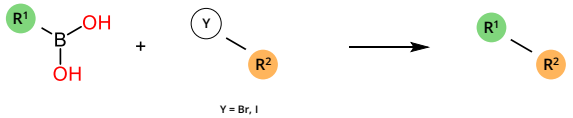
Reaction type: Coupling
(alkynyl)



Possible Conditions	Sonogashira cross-coupling reaction [1],[2]
SMARTS	A: [#6;$(C=C-[#6]),$(c:c):1][#53;A;D1].[#6;A;D1;$(C#C[#6,#14]);2]>>[#6:1]-[#6:2] B: [#6;$(C=C-[#6]),$(c:c):1][#35;A;D1].[#6;A;D1;$(C#C[#6,#14]);2]>>[#6:1]-[#6:2]

#rxn110a/b

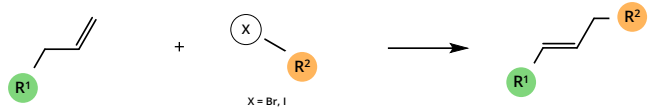
Reaction type: Coupling
(biaryl)



Possible Conditions	Suzuki cross-coupling reaction [1],[2]
SMARTS	A: [#6;a;D3;$([#6][#6])[#6]):1]-[#5][#8;A;D1)][#8;A;D1].[#6;a;D3;$([#6]~[#6])~[#6]):2][#53;A;D1]>>[#6:2]-[#6:1] B: [#6;a;D3;$([#6][#6])[#6]):1]-[#5][#8;A;D1)][#8;A;D1].[#6;a;D3;$([#6]~[#6])~[#6]):2][#35;A;D1]>>[#6:2]-[#6:1]

#rxn111a/b

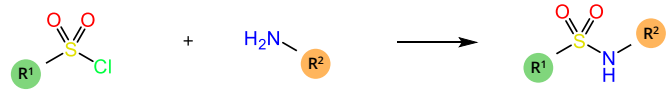
Reaction type: Coupling
(alkylene)



Possible Conditions	Heck cross-coupling reaction [1],[2]
SMARTS	A: [#6;c,$(C(=O)O),$(C#N):3]-,[#6;A;D2:2]=[#6;A;D1:1].[#6,$([#6]=[#6]),$(c:c):4][#53;A;D1]>>[#6:4]\[#6:1]=[#6:2]\[#6:3] B: [#6;c,$(C(=O)O),$(C#N):3]-,[#6;A;D2:2]=[#6;A;D1:1].[#6,$([#6]=[#6]),$(c:c):4][#35;A;D1]>>[#6:4]\[#6:1]=[#6:2]\[#6:3]

#rxn113

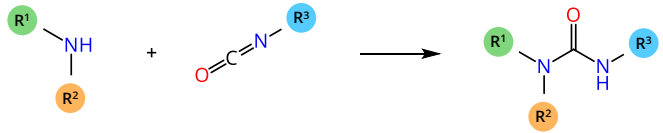
Reaction type: Substitution
(sulfonamide)



Possible Conditions	Green chemistry approach: in water at pH 8 and rt, isolation of product by filtration after acidification [1]
SMARTS	[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]),$(N-C=[O,N,S])]:1].[c:2][S:3](=[O:4])(=[O:5])Cl>>[N:1][S:3](=[O:4])(=[O:5])[c:2]

#rxn114a/b

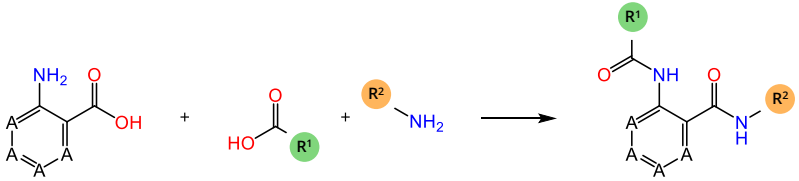
Reaction type: Coupling
(urea)



Possible Conditions	[1],[2]
SMARTS	A: [N;D1$(N[#6]),D2$(N([#6])[#6]),$(N-[#6])]!$(N[C,S]=[O,N,S]):1].[N;D2;$(N[#6]):4]=[C;D2:2]=[O,S;D1:3]>>[N:1][C:2](=[*:3])[N:4] B: [N;D1$(N[#6]),D2$(N([#6])[#6]),$(N-[#6])]!$(N[C,S]=[O,N,S]):1].[N;D1$(N[#6]),D2$(N([#6])[#6]),$(N-[#6])]!$(N[C,S]=[O,N,S]):4]>>[N:1][C](=S)[N:4]

#rxn201

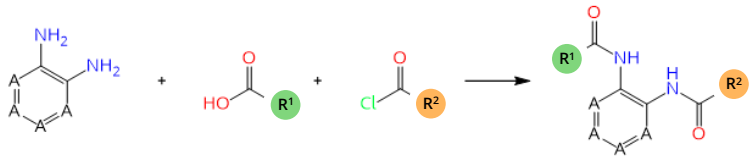
Reaction type: Substitution
(anthranilic acid amides)



Possible Conditions	Coupling of anthranilic acid with amine [1], subsequent coupling of free amine with activated acid to get isatoic anhydride from anthranilic acid [2]
SMARTS	[#7:7]-[c:5]1[c:4][c:3][c:2][c:1][c:6]1-[#6:9]([#8;A;D1])=[O:8].[#7;A;D1$(N(-[#6])),D2$(N(-[#6])-[#6]);!$(N-C=[O,N,S]):10].[#6:13]-[#6:12]([#8;A;D1,Cl])=[O:11]>>[#6:13]-[#6:12](=[O:11])-[#7:7]-[c:5]1[c:4][c:3][c:2][c:1][c:6]1-[#6:9](-[#7:10])=[O:8]

#rxn202

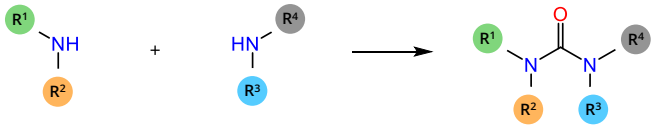
Reaction type: Substitution
(phenylenediamide)



Possible Conditions	2 step synthesis of anthranilic diamide [1]
SMARTS	[#7;D1;$(N-[#6])!$(N-C=[O,N,S]):3]-[c;r6:1]:[c;r6:2]-[#7;D1;$(N-[#6])!$(N-C=[O,N,S]):4].[#6;a:5]-[#6:6](Cl)=[O:7].[#6;a:9]-[#6:10]([#8;A;D1])=[O:8]>>[#6:5]-[#6:6](=[O:7])-[#7:3]-[#6:1]-[#6:2]-[#7:4]-[#6:10](-[#6:9])=[O:8]

#rxn203

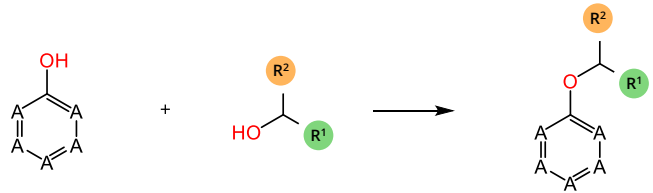
Reaction type: Substitution
(urea)



Possible Conditions	Solid-phase synthesis [1]
SMARTS	[#7;A;$([N;D1][#6])!$(N[C,S]=[O,N,S]),$([N;D2]([#6])[#6])!$(N[C,S]=[O,N,S]):1].[#7;A;$([N;D1][#6])!$(N[C,S]=[O,N,S]),$([N;D2]([#6])[#6])!$(N[C,S]=[O,N,S]):2]>>[*:1]-[#6](-[*:2])=O

#rxn205

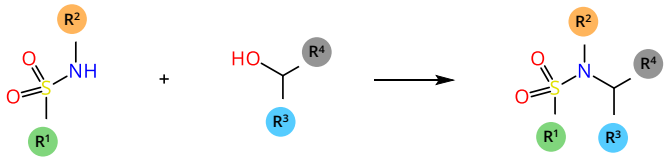
Reaction type: Substitution
(phenyl ether)



Possible Conditions	Mitsunobu reaction [1],[2],[3]
SMARTS	[#6;A;D3$(C([#6])([#6]),D2$(C[#6]):1][#8;A;D1].[#8;A;D1;$(Oc1ccccc1):2]>>[#6:1]-[#8:2]

#rxn206

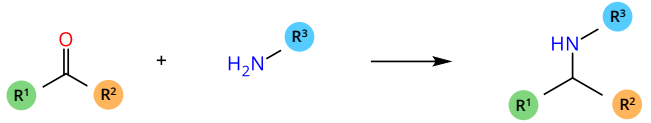
Reaction type: Substitution
(sulfonamide)



Possible Conditions	Mitsunobu reaction [1],[2]
SMARTS	[#6;A;D3$(C([#6])([#6]),D2$(C([#6]):1)[#8;A;D1].[#7;A;D2;$(N([#6])S(=O)=O);2]>>[#6:1]-[#7:2]

#rxn207

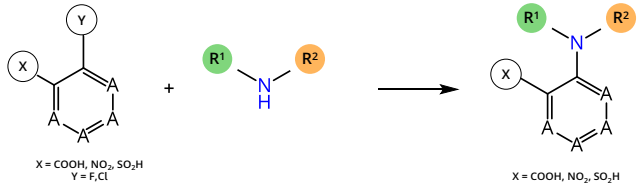
Reaction type: Substitution
(amine)



Possible Conditions	Reductive amination with $BH_3N(C_2H_5)_3$ or other reductants [1],[2]
SMARTS	[#6:4][#6;A;D2,$([C;D3;A](-[#6])[#6]):1]=[O;D1].[#6:5]-[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6]);!$(N-C=[O,N,S]):3]>>[#6:4]-[#6:1]-[#7:3]-[#6:5]

#rxn208

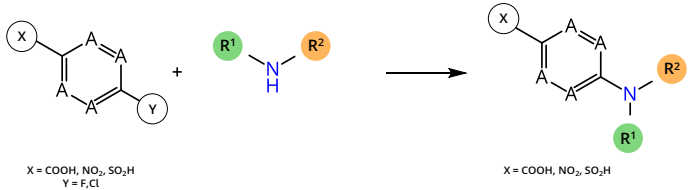
Reaction type: Substitution
(arom. amine)



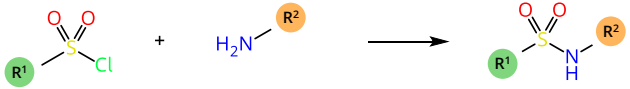
Possible Conditions	Solvent-controlled regioselectivity (S_NAr) [1],[2]
SMARTS	[#9,#17;A;D1][c:1]1[c;D2:6][c:5][c:4][c:3][c:2]1-{N$(N(=O)O),S$(S(=O)O),C$(C(=O)O),C$(C#N):7].[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):8]>>[#7:8]-[c:1]1[c:6][c:5][c:4][c:3][c:2][*:7]

#rxn209

Reaction type: Substitution
(amide)

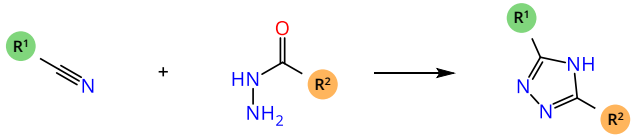


Possible Conditions	Solvent-controlled regioselectivity (S_NAr) [1],[2]
SMARTS	[#9,#17;A;D1][c:1]1[c:2][c:3][c:4](-{N$(N(=O)O),S$(S(=O)O),C$(C(=O)O),C$(C#N):7])[c:5][c;D2:6]1.[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):8]>>[#7:8]-[c:1]1[c:6][c:5][c:4](-[*:7])[c:3][c:2]1

#rxn210	Reaction type: Substitution (sulfonamide)
	
Possible Conditions	Several conditions to synthesize sulfonamides: [1],[2]
SMARTS	[#16;A;$(S(=O)(=O)[C,N,c,n]);1]Cl.[N;D1$(N-[#6]);$(N-[#6])!$(N-C=[O,N,S]):2]>>[#7:2]-[#16:1]

#rxn301

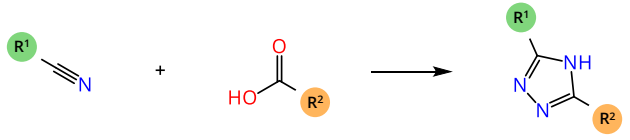
Reaction type: Ring Closure
(1,2,4-triazole)



Possible Conditions	Microwave-assisted Ring Closure to form 3,5-substituted 1,2,4-triazoles [1],[2]
SMARTS	[#6;A;D2;$(C-[#6]):1]#[N;D1:2].[#7;A;D1:3][#7;D2:4][#6;A;D3;!R$(C-[#6]):5]=[O;D1]>>[c:1]1[n:2][c:5][n:4][n:3]1

#rxn302

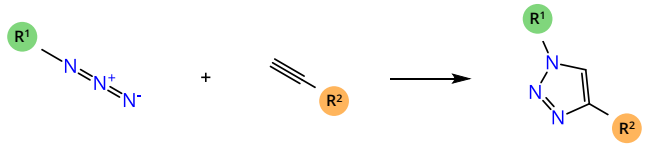
Reaction type: Ring Closure
(1,2,4-triazole)



Possible Conditions	With carbonyldiimidazole (CDI) and hydrazine in THF [1],[2]
SMARTS	[#6;A;D2;$(C-[#6]):1]#[#7;A;D1:2].[#8;A;D1,D2;$(O-[CD1])][#6;A;D3;$([#6;D3;!R][#6]):5]=[O;D1]>>[c:1]1[n:2][c:5]nn1

#rxn303

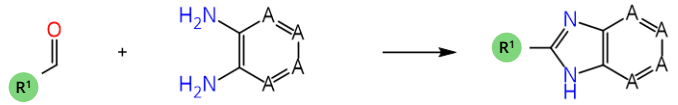
Reaction type: Ring Closure
(1,2,3-triazole)



Possible Conditions	Copper-catalyzed azide-alkyne cycloaddition [1]
SMARTS	[#6:1][N:2]=[N+:3]=[N-:4].[#6;A;D1:5]#[#6;A;D2$(C[#6]),D1:6]>>[#6:1][N:2]1[N:3]=[N:4][C:6]=[C:5]1

#rxn304

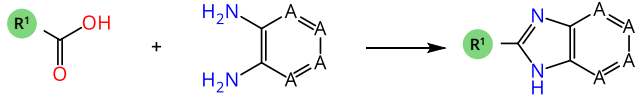
Reaction type: Ring Closure
(benzoimidazole)



Possible Conditions	Cu/Zn/Fe-based nanocatalyst to form Benzimidazoles [1],[2],[3]
SMARTS	[#7;D1;$(N-[#6])!$(N-[C,S]=[O,N,S]):4]-[#6;a;D3r6:3]:[#6;a;D3r6:1][#7;A;NH2,NH1$(N-[#6])!$(N-[C,S]=[O,N,S]):2].[#6:6][#6;A;D2;!R:5]=[O;D1]>>[#6:6]-[c:5]1[n:4][c:3][c:1][n:2]1

#rxn305

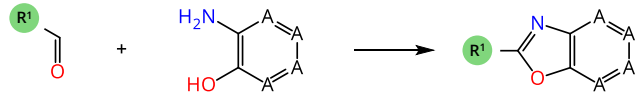
Reaction type: Ring Closure
(benzoimidazole)



Possible Conditions	*p*-TsOH as catalyst [1],[2]
SMARTS	[#7;D1;$(N-[#6])!$(N-[C,S]=[O,N,S]):4]-[#6;a;D3r6:3]:[#6;a;D3r6:1][#7;A;NH2,NH1$(N-[#6])!$(N-[C,S]=[O,N,S]):2].[#6:6]-[#6:5]([#8;A;D1,D2;$(O-[CD1])])=O>>[#6:6]-[c:5]1[n:4][c:3][c:1][n:2]1

#rxn309

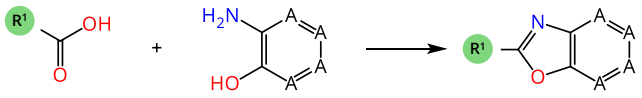
Reaction type: Ring Closure
(benzoxazole)



Possible Conditions	Sulfur promoted oxidative condensation [1],[2],[3]
SMARTS	[#7;A;D1;$(N-!@[#6])!$(N-C=[O,N,S]):4][#6;a;D3r6:3]:[#6;a;D3r6:1][#8;A;D1;$(O-c):2].[#6;a:6][#6;A;D2;!R:5]=[O;D1]>>[#6:6]-[c:5]1[n:4][c:3][c:1][o:2]1

#rxn310

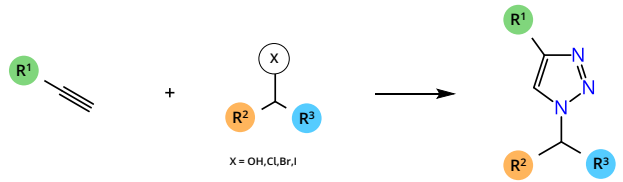
Reaction type: Ring Closure
(benzoxazole)



Possible Conditions	Microwave assisted one step synthesis [1],[2]
SMARTS	[#7;A;D1;$(N-!@[#6])!$(N-C=[O,N,S]):4][#6;a;D3r6:3]:[#6;a;D3r6:1][#8;A;D1;$(O-c):2].[#6:6][#6;A;D3;!R:5]([#8;A;D1])=[O;D1]>>[#6:6]-[c:5]1[n:4][c:3][c:1][o:2]1

#rxn313

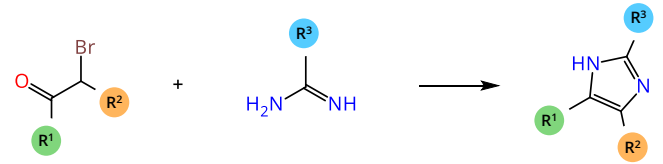
Reaction type: Ring Closure
(1,2,3-triazole)



Possible Conditions	Huisgen-Cu; Several conditions reported; starting from alkylhalide/sec. alcohol to azide [1],[2],[3],[4]
SMARTS	[#6;A;D2;$(C-[#6,#14]):1]#[#6;A;D1:2].[#6;A;D3,D2;!$(C=O):3][#17,#35,#53,#8;A;D1]>>[#6:3]-n1[c:2][c:1]nn1

#rxn316

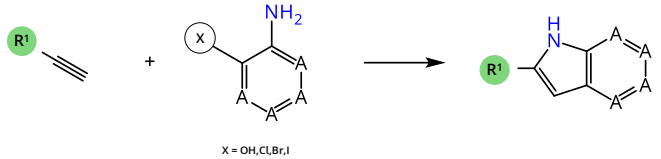
Reaction type: Ring Closure
(imidazole)



Possible Conditions	Amidine can be further substituted [1],[2],[3]
SMARTS	[Br;D1][#6;AH1;$(C([#6])([#6])):5][#6;A;$(C([#6])([#6;!$([#6]Br)]):4]=[O;D1].[#7;A;D1,D2:3][#6;A;$(C(=N)(N)[c,#7]):2]=[#7;A;D1:1]>>[c:4]1[c:5][n:3][c:2][n:1]1

#rxn317

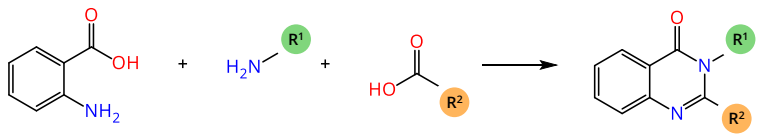
Reaction type: Ring Closure
(indole)



Possible Conditions	Alkyne and amine can be substituted; Larock Indole synthesis [1],[2],[3],[4]
SMARTS	[#7;A;D1:3][c:2]:[c:1]-[#35,#53;D1;$(*c1ccccc1)].[#6;A;D1:5]#[#6;A;$(C-[#6,#14]):4]>>[c:1]1[c:5][c:4][n:3][c:2]1

#rxn318

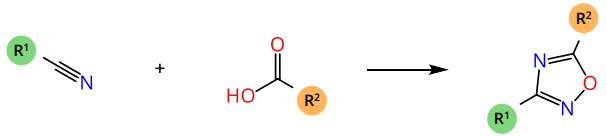
Reaction type: Ring Closure
(quinazolin-4(3*H*)-one)



Possible Conditions	Amide formation in the first step, Microwave-assisted Niementowski reaction as second step [1],[2]
SMARTS	[N;D1;$(N-[#6D2!R])!$(N-C=[O,N,S]):1].[C;D1,$(C[#6]):2]=[OD1])[OD1,Cl].[#7;A;D1;$(N-[#6])!$(N-C=[O,N,S]):8][c:7]:[c:4][#6;A;$(C-c1ccccc1):5][#8;A;D1])=[O;D1:6]>>[O:6]=[#6:5]-1-[#6:4]-[#6:7]-[#7:8]=[#6:2]-[#7:1]-1

#rxn319

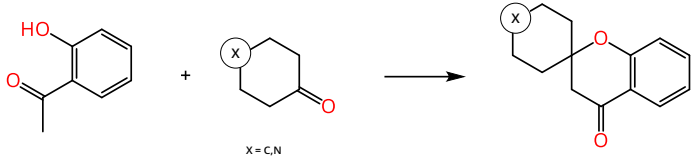
Reaction type: Ring Closure
(1,2,4-oxadiazole)



Possible Conditions	Mild one-pot reaction using Vilsmeier reagent [1],[2]
SMARTS	[#6;A;!R:6][C:5]#[N;D1:4].[#6:1][#6;A;!R:2]([#8;A;D1])=[O;D1:3]>>[#6:6]-[c:5]1n[o:3][c:2](-[#6:1])[n:4]1

#rxn320

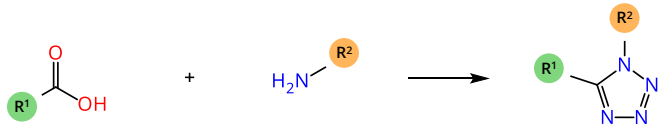
Reaction type: Ring Closure
(spirochromanone)



Possible Conditions	In presence of pyrrolidine in toluol or methanol, or LDA [1],[2],[3],[4]
SMARTS	[#6;A;D1:4][#6;A;$(C-c1ccccc1):2](=[O;D1:3])[c:1]-[c:5][#8;A;D1:6].[#6;A;$(C1-[C;D2]-[C;D2]-[N,C]-[C;D2]-[C;D2]-1):7]=[O;D1]>>[O:3]=[#6:2]-1-[#6:4]-[#6:7]-[#8:6]-[#6:5]=[#6:1]-1

#rxn321

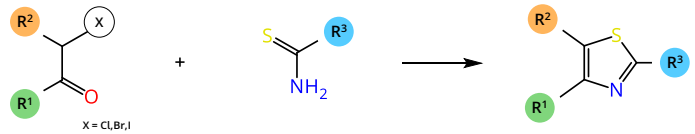
Reaction type: Ring closing
(tetrazole)



Possible Conditions	Other functional groups at R^1 reported [1],[2]
SMARTS	[N;D1$(N-[#6]),$(N-[#6])!$(N-C=[O,N,S]):1].[C:2](=[OD1])[OD1,Cl]>>[#7]=1[#7:1][#6:2]=[#7][#7]1

#rxn322

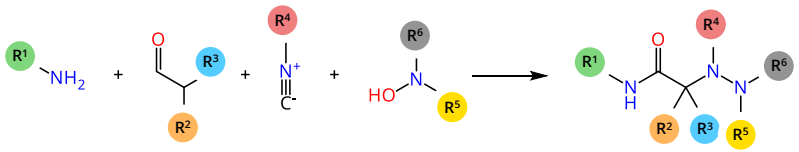
Reaction type: Ring Closure
(thiazole)



Possible Conditions	Hantzsch thiazole synthesis [1],[2],[3]
SMARTS	[#17,#35,#53;A;D1][#6;A;D1,D2;!$(C=A);5][#6;A;R0;!$(C-[O,N]):1]=[O;D1].[#7;D1:2]-[#6:3]=[S;D1:4]>>[c:1]1[c:5][s:4][c:3][n:2]1

#rxn401

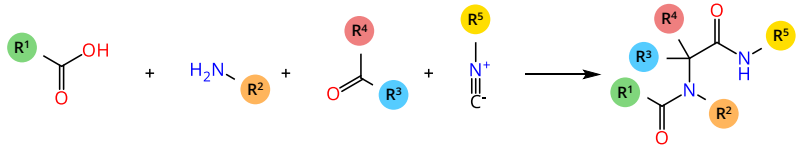
Reaction type: Multicomponent
(α-hydrazino amide)



Possible Conditions	Ugi four-component reaction (U-4CR) [1]
SMARTS	[C;D2$(C[#6]),D3$(C([#6])[#6]):2](=[OD1]).[#6:4][#7;A;D1,!$(N-C=[O,N,S]):5].[#6:7][N+:6]#[C-].[N;D3;$(N(C=O)C=O):9][OD1]>>[#6:7]-[#7:6]-[#6](=[O])-[#6:2]-[#7:5](-[#6:4])-[#7:9]

#rxn402

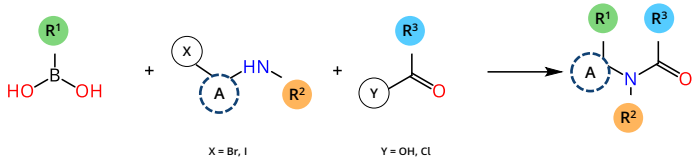
Reaction type: Multicomponent
(diamide)



Possible Conditions	Ugi four-component reaction [1],[2],[3],[4]
SMARTS	[#6:3][#6;A;!R;D2$([#6][#6]),D3$([#6]([#6])[#6]):2]=O.[N;D1$(N-[#6]),$(N-[#6])!$(N-C=[O,N,S]):5].[#6:7][N+:8]#[C-:9].[#6:11]-[#6:12]([#8;A;D1])=[OD1:10]>>[#6:7]-[#7:8]-[#6:9](=O)[C:2]([#6:3])[#7:5]-[#6:12](-[#6:11])=[O:10]

#rxn501a/b

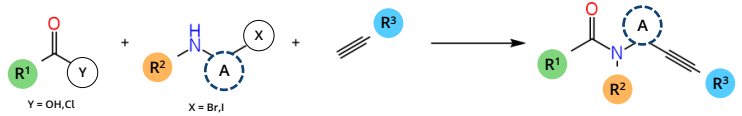
Reaction type: Amide and Suzuki coupling
(Core amide)



Possible Conditions	-
SMARTS	A: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;aD3$([#6][#6])([#6]),AD2$([#6][#6]):4][#53;A;D1]).[#6,a;D3,$([#6][#6])[#6]):5]-[#5][#8;A;D1])[#8;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;aD3$([#6][#6])([#6]),AD2$([#6][#6]):4][#35;A;D1]).[#6,a;D3,$([#6][#6])[#6]):5]-[#5][#8;A;D1])[#8;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn503a/b

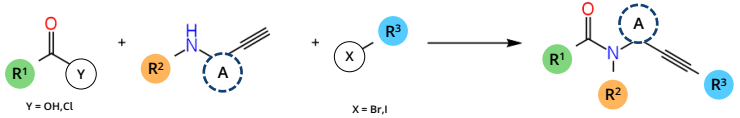
Reaction type: Amide and Sonogashira coupling
(Core amide and alkynyl)



Possible Conditions	-
SMARTS	A: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;aD3$([#6][#6])([#6]),AD2$([#6][#6]):4][#53;A;D1]).[#6,A;D1;$(C#C[#6,#14]):5]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;aD3$([#6][#6])([#6]),AD2$([#6][#6]):4][#35;A;D1]).[#6,A;D1;$(C#C[#6,#14]):5]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn505a/b

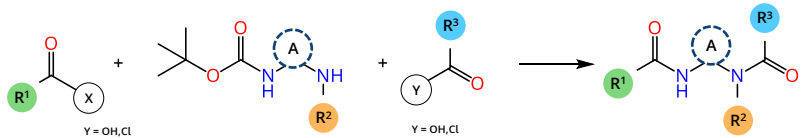
Reaction type: Amide and Sonogashira coupling
(Core amide and alkynyl)



Possible Conditions	-
SMARTS	A: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;A;D1;$(C#C[#6,#14]):4]).[#6;$(C=C-[#6]),$(c:c):5][#53;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].[#6;A;D1;$(C#C[#6,#14]):4]).[#6;$(C=C-[#6]),$(c:c):5][#35;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn506

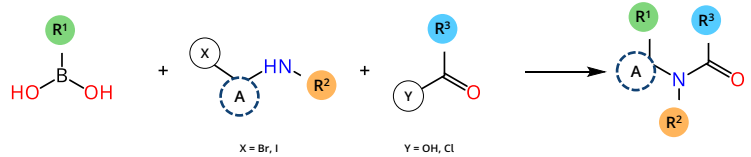
Reaction type: 2x Amide coupling and deprotection
(Diamide core)



Possible Conditions	-
SMARTS	[C;D2,$(C[#6]):1](=[OD1:2])[OD1,Cl].([N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):3].[N;D2;$(N(-[#6])-[#6]):4]C(=[OD1])[OD2]C([CD1])([CD1])([CD1]),[C;D2,$(C[#6]):5](=[OD1:6])[OD1,Cl]>>([N:3][C:1](=[O:2]),[N:4][C:5](=[O:6]))

#rxn511a/b

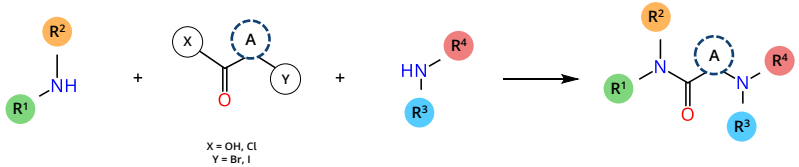
Reaction type: Amide and Suzuki coupling
(Core amide)



Possible Conditions	-
SMARTS	A: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#53;A;D1]).[#6;a;D3;$([#6][#6])[#6]):5]-[#5].[#8;A;D1])[#8;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#35;A;D1]).[#6;a;D3;$([#6][#6])[#6]):5]-[#5].[#8;A;D1])[#8;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn512a/b

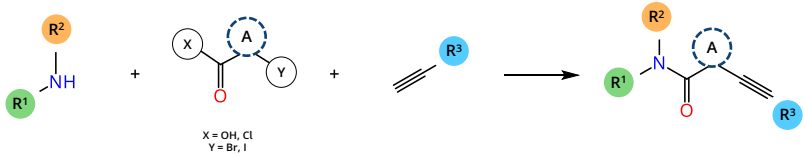
Reaction type: Amide and Buchwald Hartwig coupling
(Core amide and amine)



Possible Conditions	-
SMARTS	A: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]),$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#53;A;D1]).[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):5]>>([N:1][C:2](=[O:3]).[#7:5]-[#6:4]) B: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]),$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#35;A;D1]).[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):5]>>([N:1][C:2](=[O:3]).[#7:5]-[#6:4])

#rxn513a/b

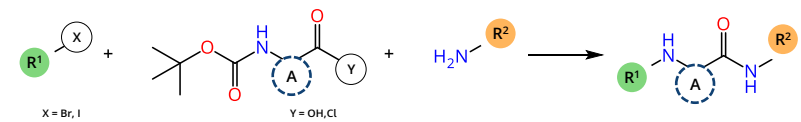
Reaction type: Amide and Sonogashira coupling
(Core amide and alkynyl)



Possible Conditions	-
SMARTS	A: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#53;A;D1]).[#6;A;D1;$(C#C[#6,#1 4]):5]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[#6;aD3$([#6][#6])[#6]),AD2$([#6][#6]):4][#35;A;D1]).[#6;A;D1;$(C#C[#6,#1 4]):5]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn514a/b

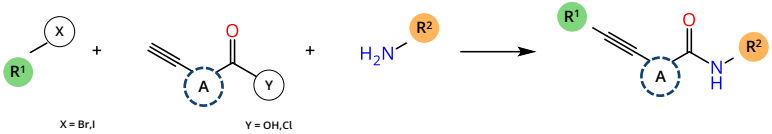
Reaction type: Amide and Buchwald Hartwig coupling
(Core amide and amine)



Possible Conditions	-
SMARTS	A: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]),$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[N;D2;$(N(-[#6])-[#6]):4]C(=[OD1])[OD2]C([CD1])([CD1])[CD1].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#53;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#7:4]) B: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]),$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]):2](=[OD1:3])[OD1,Cl].[N;D2;$(N(-[#6])-[#6]):4]C(=[OD1])[OD2]C([CD1])([CD1])[CD1].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#35;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#7:4])

#rxn515a/b

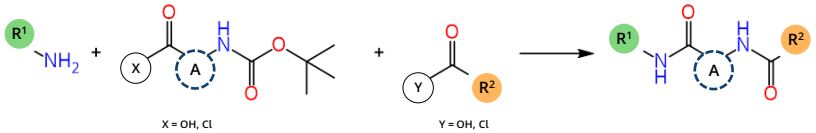
Reaction type: Amide and Sonogashira coupling
(Core amide and alkynyl)



Possible Conditions	-
SMARTS	A: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]);2](=[OD1:3])[OD1,Cl].[#6;A;D1;$(C#C[#6,#14]);4]).[#6;$(C=C-[#6]),$(c:c);5][#53;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4]) B: [N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]);2](=[OD1:3])[OD1,Cl].[#6;A;D1;$(C#C[#6,#14]);4]).[#6;$(C=C-[#6]),$(c:c):5][#35;A;D1]>>([N:1][C:2](=[O:3]).[#6:5]-[#6:4])

#rxn516

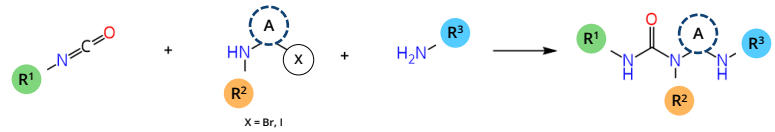
Reaction type: 2x Amide coupling and deprotection
(Diamide core)



Possible Conditions	-
SMARTS	[N;D1$(N-[#6]),D2$(N(-[#6])-[#6]);$(N-[#6])!$(N-C=[O,N,S]):1].([C;D2,$(C[#6]);2](=[OD1:3])[OD1,Cl].[N;D2;$(N(-[#6])-[#6]):4]C(=[OD1])[OD2]C([CD1])([CD1])[CD1]).[C;D2,$(C[#6]):5](=[OD1:6])[OD1,Cl]>>([N:1][C:2](=[O:3]).[N:4][C:5](=[O:6]))

#rxn531a/b

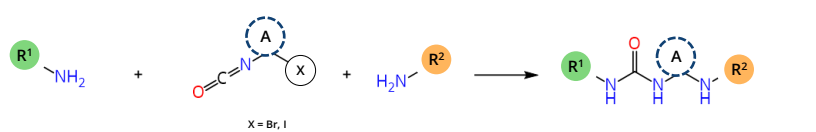
Reaction type: Amide and ring closure
(Core urea and aromatic amine)



Possible Conditions	-
SMARTS	A: [N;D2;$(N[#6]);4]=[C;D2:2]=[O,S;D1:3].([N;D1$(N[#6]),D2$(N([#6])[#6]);$(N-[#6])!$(N[C,S]=[O,N,S]):1].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#53;A;D1]).[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):6]>>([N:1][C:2](=[*:3])[N:4].[#6:5]-[#7:6]) B: [N;D2;$(N[#6]);4]=[C;D2:2]=[O,S;D1:3].([N;D1$(N[#6]),D2$(N([#6])[#6]);$(N-[#6])!$(N[C,S]=[O,N,S]):1].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#35;A;D1]).[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):6]>>([N:1][C:2](=[*:3])[N:4].[#6:5]-[#7:6])

#rxn532a/b

Reaction type: Amide and ring closure
(Core urea and aromatic amine)



Possible Conditions	-
SMARTS	A: [N;D1$(N[#6]),D2$(N([#6])[#6]);$(N-[#6])!$(N[C,S]=[O,N,S]):1].([N;D2;$(N[#6]);4]=[C;D2:2]=[O,S;D1:3].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#53;A;D1]).[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):6]>>([N:1][C:2](=[*:3])[N:4].[#6:5]-[#7:6]) B: [N;D1$(N[#6]),D2$(N([#6])[#6]);$(N-[#6])!$(N[C,S]=[O,N,S]):1].([N;D2;$(N[#6]);4]=[C;D2:2]=[O,S;D1:3].[#6;a;$(c1:[c,n]:[c,n]:[c,n]:[c,n]:1):5][#35;A;D1]).[#7;A;$(N[#6])!$(N=*)!$([N-])!$(N#*)!$([ND3])!$([ND4])!$(N[O,N])!$(N[C,S]=[S,O,N]):6]>>([N:1][C:2](=[*:3])[N:4].[#6:5]-[#7:6])

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