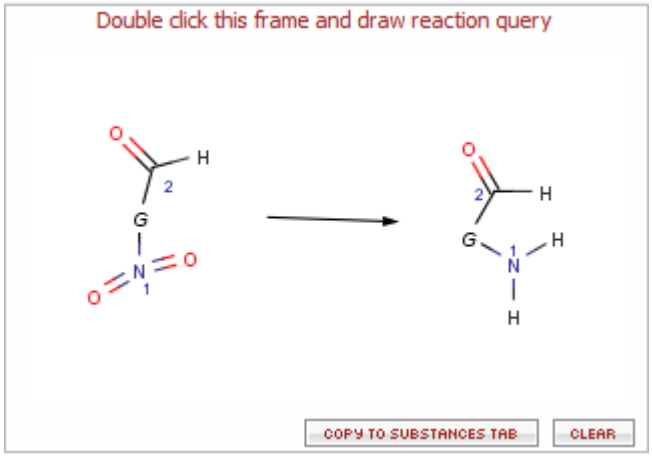
Reaxys Fragment Based Reaction Search with Generic Groups

Did you know that the Reaxys generic groups can be used in fragment based reaction search? Imagine that you need to search for any reaction where a nitro function is reduced into the corresponding amino group in the presence of an aldehyde, this one being unchanged. A nice solution to this problem is given by the use of the G Generic group. As you can see below this proposal allows you to directly access the required reactions, without any additional research and combining of reactions hitsets.

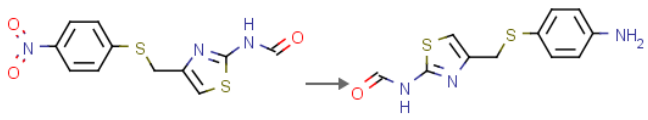
G and G* are used to replace any arbitrary structure, or any arbitrary cyclic structure, and can have more than one attachment point.

Draw your reaction with the generic group G linked to the aldehyde and to the nitro fragments and remember to map the nitrogen and the carbon atoms of the two functional groups.

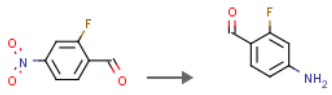


If needed, you can add data constraints using the form-based or advanced search tabs.
When you analyze the 347 retrieved reactions, you will find nice examples of such fragment transformation, on any type of chemical structure.

Some examples:

Yield	Conditions	References
 Synthesize Synthesize Rx-ID: 24436517	**With** anhydrous ammonium chloride **in** tetrahydrofuran; ethanol; water Hide Experimental Procedure	**Fujisawa Pharmaceutical Co., Ltd.** **Patent:** US5256675 A1, **1993** ; Title/Abstract Full Text Show Details

EXAMPLE 46
To a mixture of 2-formylamino-4-(4-nitrophenylthiomethyl)thiazole (2.2 g) and ammonium chloride (0.5 g) in a mixture of tetrahydrofuran (30 ml), ethanol (50 ml) and water (10 ml) was added portionwise the iron powder at 80.deg. C. with stirring.
The mixture was refluxed for 2 hours with stirring.
The reaction mixture was filtered by suction and the residue was triturated with water.
The precipitates were collected by filtration, washed with water and dried in vacuo to give 2-formylamino-4-(4-aminophenylthiomethyl)thiazole (1.6 g, yield: 81percent).
mp: 180.deg.-182.deg. C.
IR (Nujol): 3350, 3300, 1680, 1625, 1600, 1325, 1290 cm^{-1}
NMR (DMSO-d_6, 60 MHZ, ppm): 4.00 (2H, s), 5.23 (2H, s), 6.57 (2H, d, J=8Hz), 6.83 (1H, s), 7 10 (2H, d, J=8Hz), 8.50 (1H, s) Mass: M^{+1} 266, M 265, m/e 237, 205, 141, 124

Yield	Conditions	References
 Synthesize Synthesize Rx-ID: 23316295	**With** iron; threo-amine hydrochloride **in** ethanol; water T=80°C; 2 h; Hide Experimental Procedure	**PHARMACIA and UPJOHN COMPANY** **Patent:** WO2004/89943 A1, **2004** ; Title/Abstract Full Text Show Details

Ammonium chloride (38 g, 0.71 mol) was added to a solution of 2-fluoro-4- nitrobenzaldehyde (12 g, 0.071 mol, prepared as described by Gordeev, et. al. , U. S. Patent No. 6,239, 152, which is incorporated herein by reference in its entirety) in 2: 1 ethanol-H20 (300 mL). The mixture was heated to 80 .deg.C and treated with iron metal in 6 portions over 1 hour (11.9 g total, 0.212 mmol). After the addition was complete the reaction mixture was stirred another hour and the warm solution filtered with the aid of more water and ethanol. The filtrate was then concentrated to remove ethanol and the resulting aqueous solution extracted thrice with ethyl acetate. The combined organic phases were washed with water, brine, and dried (MGS04), filtered, and concentrated to provide 9.6 g of the crude amine.The crude amine (9.6 g, 0.069 mol) was dissolved in dichloromethane (230 mL) and pyridine (11.1 mL, 0.138 mol) and the solution cooled to 0 .deg.C. The solution was then treated with benzyl CHLOROFORMATE (11.8 mL, 0.083 mol) dropwise and the solution stirred at room temperature for 18 h. The reaction mixture was then diluted with more dichloromethane and the organic solution washed thrice with water, once with brine, and dried (MGS04), filtered, and concentrated. Trituration with hexane provided the title compound as a yellow solid. Yield 15 G (77percent). 'H NMR (300 MHz, CDC13) : 5.23 (s, 2H), 6.99 (bs, 1H), 7.03 (dd, J= 9,2 Hz, 1H), 7.37-7. 42 (m, SH), 7.57 (dd, J= 13, 2 Hz, 1H), 7.81 (t, J= 9 Hz, 1H), 10.23 (s, 1H).

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