

Science of Synthesis

Your expert guide to making molecules

Science of Synthesis provides critical reviews on synthetic methodology in organic and organometallic chemistry. It is organized systematically and logically based on the product, specifically the main functional group being made. Its insightful, didactic reviews include knowledge that you can't find anywhere else.

What can I get from SoS?

Science of Synthesis answers questions such as:

- What is the best method to use? Are there alternatives?
- What is the background to the field of research I am interested in?
- What is the context of a transformation in relation to other methods?
- Which experimental procedures should I use?
- Am I going to need specialist equipment?
- What should I avoid based on the experience of experts working in the field?

What can I use SoS for?

SoS helps if you are:

- Starting out in a new area of chemistry
- Writing a paper
- Preparing for a talk
- Writing a thesis
- Looking for a new way of teaching advanced synthesis

Why choose Science of Synthesis?

Save time and resources by finding the most important information fast!

A community of experts provides reliable knowledge that is readily applicable in the lab:

- Unique insights to help you choose the best approach
- Tips and tricks to solve your synthetic problems
- All necessary information in one place
- Inclusion of procedures for immediate consideration

The screenshot shows the Science of Synthesis interface. At the top, there are navigation tabs: Query, Results, Full Text, Explore Contents, and Training & Support. The main content area displays a search result for '6.1.4.2 Fragmentation of Quaternary Center Alcohols with Halogen Trapping'. The result includes the DOI: 10.1055/sos-SD-229-00118 and a citation: Thullen, S. M.; Ashley, M. A.; Rovis, T., *Science of Synthesis: Photocatalysis in Organic Synthesis*, (2018) 1, 228. Below the citation is a short text summary: 'This strategy can also be employed in the presence of other radical trapping reagents, such as halogenation reagents to generate the corresponding alkyl halides 15 after β -oxidation and subsequent trapping with an electrophilic halide reagent (Scheme 4).^[14] Fluorination, chlorination, and bromination have all been effectively demonstrated to proceed in good to excellent yields.' A chemical reaction scheme (Scheme 4) shows the conversion of a quaternary alcohol (14) to a ketone (15) with a halogen (X) at the end of the side chain. The reaction conditions are: $(\text{Ir}(\text{ICl}_2)_2)(\text{D}_2\text{O})_2/\text{P}(\text{Ph})_3$, halide source, collidine, in CH_2Cl_2 , 23 °C. Below the scheme is a table with experimental conditions:

X	Halide Source (Equiv)	Catalyst (mol%)	Collidine (Equiv)	Solvent	Time (h)	Yield (%)	Ref
F	Selectfluor (4)	2	1	$\text{d}_2\text{-MeCN}/\text{D}_2\text{O}$ (1:1)	3	52	[14]
Cl	CCl_4 (20)	5	3	PhCF_3	18	98	[14]
Br	CBrCl_3 (3)	3	3	CH_2Cl_2	24	95	[14]

Below the table is a 'Typical Procedure' section for the synthesis of 5-Fluoro-1-(4-methoxyphenyl)pentan-1-one (15, X = F). The procedure describes a screw-cap culture tube fitted with a PTFE/silicone septum, charged with 1-(4-methoxyphenyl)cyclopentan-1-ol (14) (96 mg, 0.5 mmol), redistilled collidine (55 μL , 0.5 mmol), $[\text{Ir}(\text{ICl}_2)_2](\text{D}_2\text{O})_2(\text{S}-\text{d}_2\text{-Ph}_3\text{P})_3$ (1.1 mg, 0.02 mmol, 2 mol%), and Selectfluor (708 mg, 2 mmol). The vial is then evacuated and backfilled with N_2 (3 \times). Degassed $\text{d}_2\text{-MeCN}$ (5 mL) and D_2O (5 mL) were added to form a suspension. The mixture was sparged with H_2 for 20 min. The mixture was irradiated with blue LEDs strips set inside a beaker, and stirred at rt with a fan to cool the reaction setup. After 3 h, the mixture was concentrated, washed with H_2O , extracted with EtOAc , and then purified by column chromatography (silica gel); yield: 55 mg (52%).

References: [14] Yajla, H. G.; Wang, H.; Tarantino, K. T.; Orbe, H. S.; Knowles, R. R., *J. Am. Chem. Soc.*, (2016) 138, 10794.

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