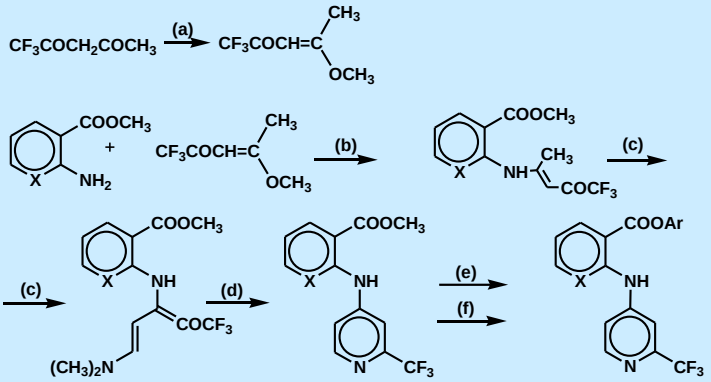
P&M-Invest Ltd.
Contact to: http://www.fluorine1.ru
Tel: +7 (499)135-64-94, Fax: +7 (499)135-65 -09
E-mail: igumnov@fluorine1.ru

1,1,1-Trifluoroacetylacetone(abb.TFAcAc)
$CF_3COCH_2COCH_3$

Purity	99%
CAS Number	367-57-7
Molecular Formula	C5H5F3O2
Molecular Weight	154.09
Application	Developed a method for synthesizing various derivatives with a 2-trifluoromethyl-pyridine skeleton similar to flufenamic acid from TFAcAc. In vitro screening of NCI full cancer cell line for growth inhibitory effects on various cancer cells, and in vivo effects of xenotransplantation of human cancer cells into mice were confirmed. A growth inhibitory effect of 67% was observed. No biotoxicity of flufenamic acid was observed.



(a) CH(OCH3)3,MeOH,p-TsOH,55C, (b) 120C, (c) DMF-DMA 3eq,Toluene,reflux, (d) CH3COONH4 2eq,DMF,reflux, (e) 10% aq-NaOH,reflux,acidify, (f) ArOH,DCC,CHCl3

Table 1; Inhibitory effect on cancer cell growth(in vitro) NCI Full Cancer Cell Lines (pGI_{50})

No.	leukemia K562	Non-small cell lung NCI-H23	Colon SW-620	Central nerv. Systm. SF628	Melanoma UACC62	renal SN12C	breast MFC7
1	7.37	7.44	7.39	6.48	6.54	7.15	7.34
2nd	7.29	6.59	6.44	5.65	6.51	6.48	6.55

No.1; Ar=pyridin-3-yl, X=CH, No.2; Ar=2-chlorophenyl, X=CH

Table 2; Antitumor activity and biotoxicity of the No. 1 compound in xenografts

No.	dose	OPT T/C% (24days)	% growth delay	weight loss Max%	Drug deaths
3	100	27%	67%	No wt loss	0
4	67	75%	15%	No wt loss	0

注；(1) Number of mice=10, (2) ip, (3)dose；mg/kg/day, (4) 24days, tumor weight % to body weight

(a) ARKIVOC 2011(1) P246-328, (b) CHEMIC nr-4, tom-65, 2011, p278-283, (c) Chem. Pharm. Bull. 49(6), 2001, p703-706, (d) Bioorganic & Med. Chem. 14, 2004, p5787-5791, (e) J.Med. Chem. 2005, 48, p8245-8252

Properties:	
Appearance	Liquid
Boiling point, °C	107
Capacity:	150kg/month
Packing:	-
UN, PG:	-