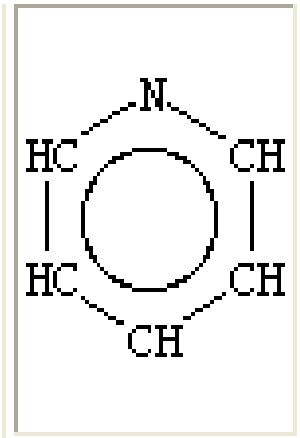
InChIs & SMILES

C1CCCCC1

O=C=O

InChI=1/C12H19Cl3O8/c13-1-4-7(17)10(20)12(3-14,22-4)23-11-9(19)8(18)6(15)5(2-16)21-11/h4-11,16-20H,1-3H2/t4-,5-,6+,7-,8+,9-,10+,11-,12+/m1/s1



n1ccccc1

Pyridine

[235]

N[C@H](C)C(=O)O

InChI=1/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

IUPAC

Kekule

Beilstein number

Molfile

CML

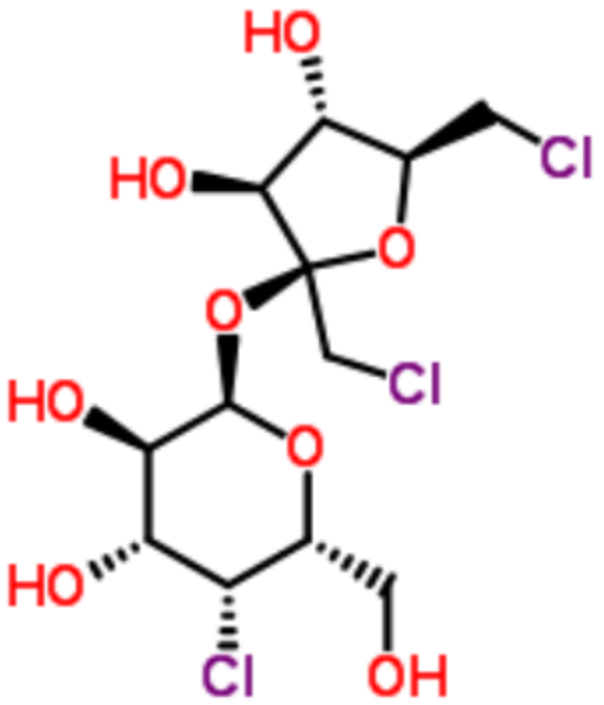
InChi

Cas registry #

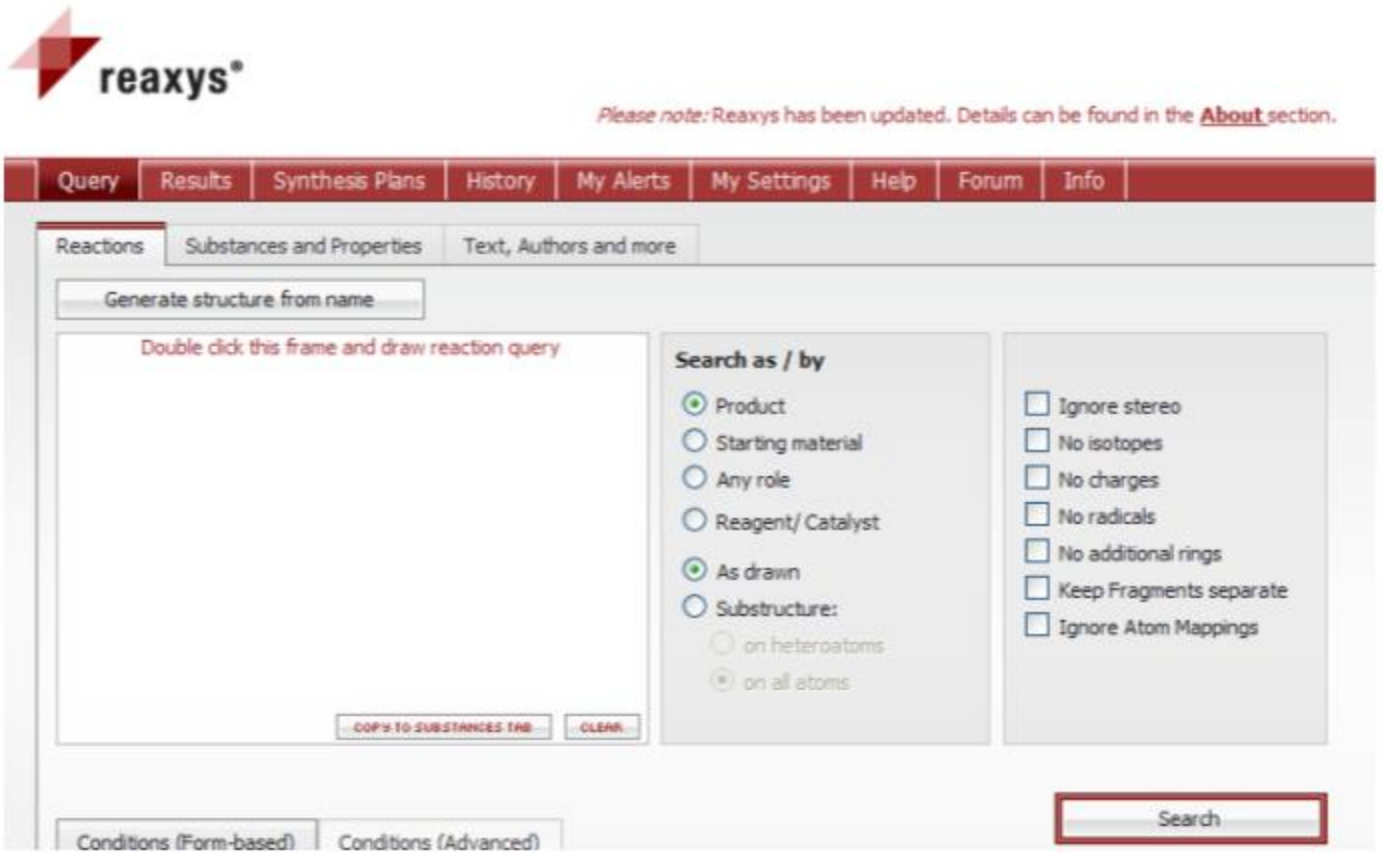
InChiKey

SMILES

Markush



2D 3D Load Save Zoom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Starting material
Any role
Reagent/ Catalyst
As drawn
Substructure:
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on all atoms
Ignore stereo
No isotopes
No charges
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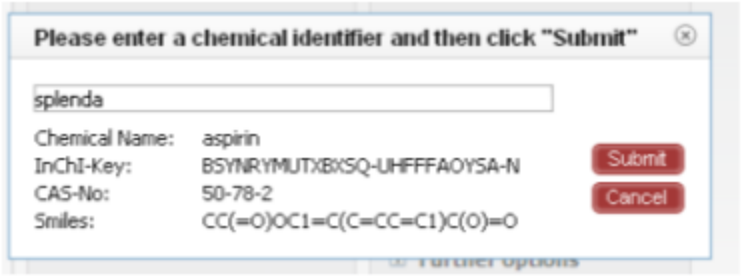
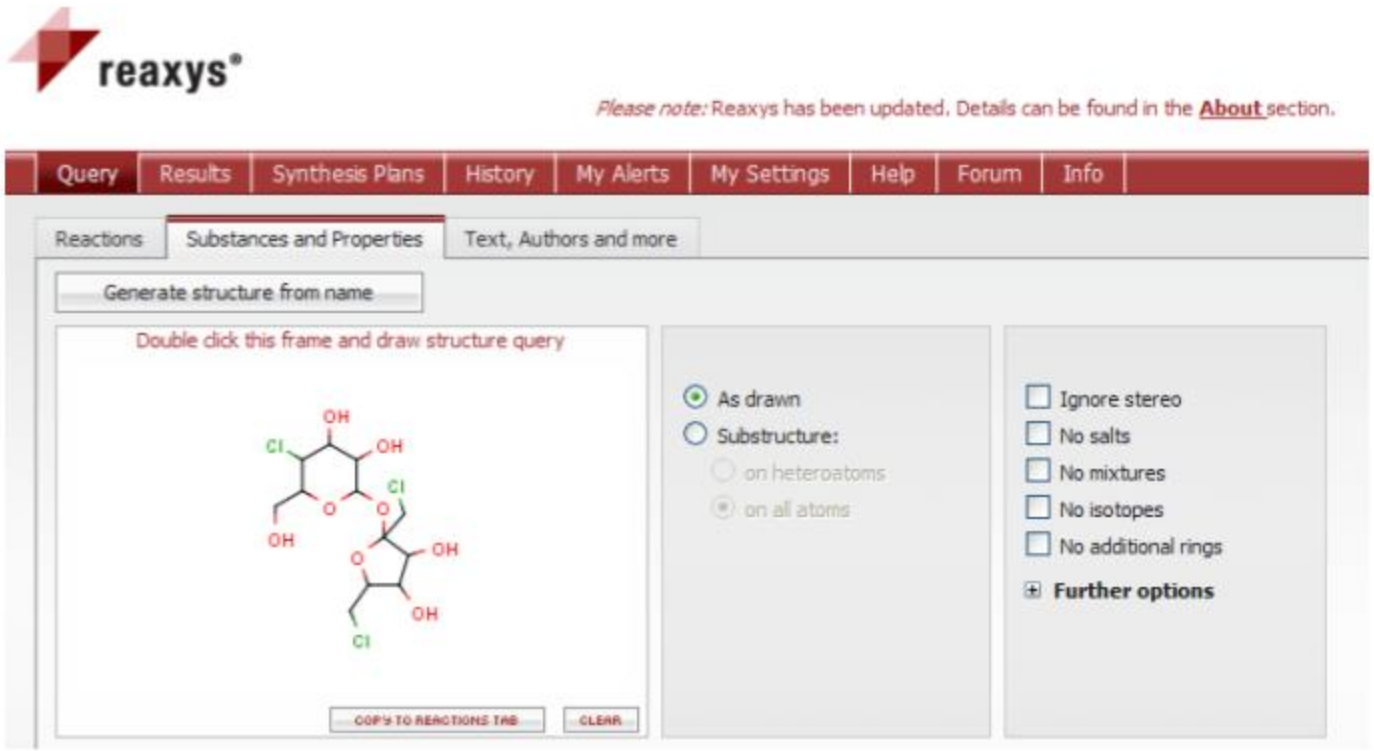

Please enter a chemical identifier and then click "Submit"
splenda
Chemical Name: aspirin
InChI-Key: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
CAS-No: 50-78-2
Smiles: CC(=O)OC1=C(C=CC=C1)C(O)=O
Submit
Cancel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Text, Authors and more
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Double click this frame and draw structure query
OH
Cl
OH
Cl
O
O
OH
O
OH
OH
Cl
COPY TO REACTIONS TAB
CLEAR
As drawn
Substructure:
on heteroatoms
on all atoms
Ignore stereo
No salts
No mixtures
No isotopes
No additional rings
Further options

Structure/Compound Data

Reaxys Registry Number: 3654410

CAS Registry Number: 56038-13-2, 69414-04-6

Chemical Name: sucralose, 1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl 4-chloro-4-deoxy-α-D-galactopyranoside, 1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl-4-chloro-4-deoxy-α-D-galactopyranoside, 4-chloro-4-deoxy-α-D-galactopyranosyl-1,6-dichloro-1,6-dideoxy-β-D-fructofuranoside, 1,6-dichloro-1,6-dideoxy-β-D-fructofuranosyl-4-chloro-α-D-galactopyranoside, 4',1',6'-trichloro-4,1',6'-trideoxy-galacto-sucrose, 4,1',6'-trichloro-4,1',6'-trideoxy-galacto-sucrose

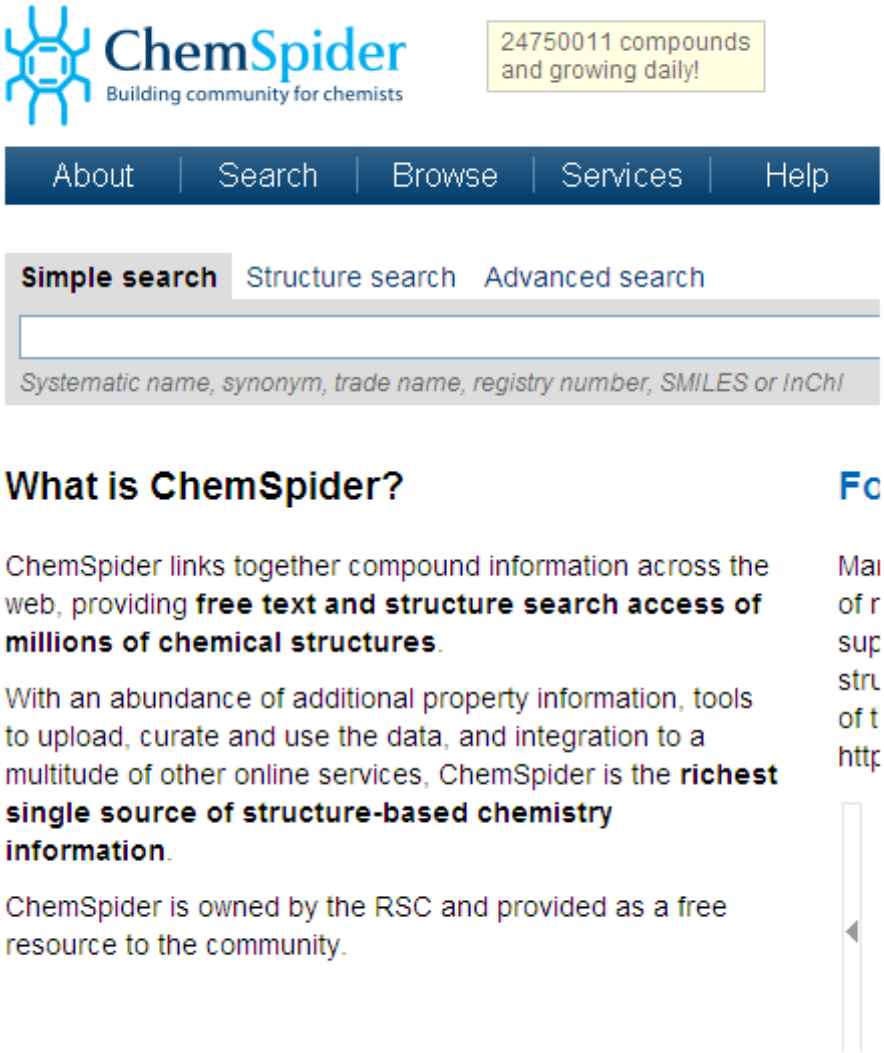
Type of Substance: heterocyclic

Molecular Formula: $C_{12}H_{19}Cl_3O_8$

Linear Structure Formula: $C_{12}H_{19}Cl_3O_8$

Molecular Weight: 397.637

InChi Key: BAQAVOSOZGMPRM-QBMZZYIRSA-N



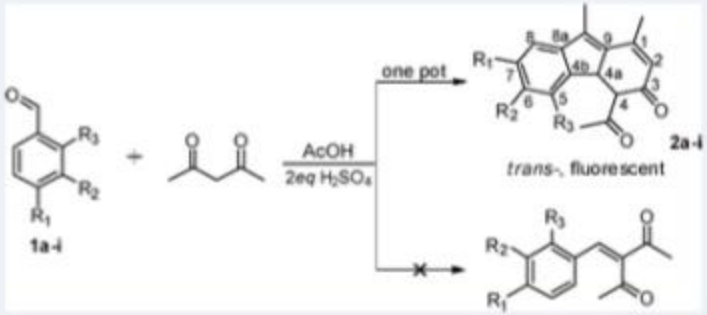
chemspider-splenda

New fluorescent *trans*-dihydrofluoren-3-ones from aldol–Robinson annulation–regioselective addition involved one-pot reaction

Yingpeng Huo, Xu Qiu, Weiyan Shao, Jianing Huang, Yanjun Yu, Yinglin Zuo, Linkun An, Jun Du and Xianzhang Bu

Org. Biomol. Chem., 2010, **8**, 5048-5052
DOI: 10.1039/C0OB00401D

An unexpected discovery of new fluorescent *trans*-dihydrofluoren-3-ones from one pot regioselective reactions of benzaldehydes and acetylacetone is described.



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New fluorescent *trans*-dihydrofluoren-3-ones from aldol–Robinson annulation–regioselective addition involved one-pot reaction†

Yingpeng Huo , Xu Qiu , Weiyan Shao , Jianing Huang , Yanjun Yu , Yinglin Zuo , Linkun An , Jun Du and Xianzhang Bu *

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[RSC Organic & Biomolecular Chemistry article]

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School of Pharmaceutical Sciences, Sun Yat-Sen University, Guangzhou, 510006, China. E-mail: phsbxzh@mail.sysu.edu.cn; Fax: 8620-39943054; Tel: 8620-39943054

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Fluorescent probes have been of great interest to chemists because of their wide usage as biological imaging and chemical sensing reagents[1] for various purposes such as chemical species analysis,[2] cellular process monitoring[3] and tissue visualization.[4] Fluorene derivatives such as 9-fluorenones, which exhibit an extensive aromatic π system, have attracted much attention owning to their antiviral and interferon inducing ability[5] as well as antitumor potency;[6] besides, 9-fluorenones exhibited excellent fluorescence properties[7] and could be used as fluorescent probes for detecting amino acids,[8] hydrogen binding interactions in cyclodextrin[9] and Ca^{2+} ions,[10] *etc*. The skeleton of 9-fluorenones could be formed by intramolecular arylation of biphenyl-2-carbaldehyde[11] or 2-biphenyl carboxylic acid,[12] and other cyclization processes.[13] Despite all the investigations on synthetic methodologies and various properties of 9-fluorenones, the non-extensive aromatic π system derivatives such as dihydrofluorenones, had rarely been investigated especially on their fluorescence. We herein describe an unexpected discovery of a new series of substituted *trans*-4,4a-dihydro-3*H*-fluoren-3-ones as novel fluorophores from one pot reactions of readily available starting materials.

In an exploration to the synthesis of 3-benzylidenepentane-2,4-dione derivatives, which acted as intermediates in our ongoing project on novel curcumin analogues for tumor chemopreventive agents screening, 2 eq concentrated sulfuric acid was adopted as the catalyst in the reaction of 3-ethoxy-4-hydroxybenzaldehyde (**1a**) and excess actylacetone in cold glacial acetic acid. After 3 h stirring, thin-layer chromatography (TLC) revealed a product with apparent green-to-yellow fluorescence. This product was isolated and purified for structural characterization. The MS and elemental analysis of this product indicated a formula of $C_{19}H_{20}O_4$, which differed from the targeted 3-(3-ethoxy-4-hydroxybenzylidene) pentane-2,4-dione ($C_{14}H_{16}O_4$). In the ^{1}H NMR spectrum, two saturated hydrogen atoms were found at δ_H 4.32 ppm (dd, J = 12.79, 1.38 Hz, 1H) and 3.32 ppm (d, J = 12.80 Hz, 1H) respectively, both of which

interferons

A class of glycoproteins (with sugar groups attached at specific locations) important in immune function. They are able to inhibit the multiplication of viruses in cells.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

Fluoren-9-ones

ID: CHEBI:24057

Articles referencing this term

New fluorescent *trans*-dihydrofluoren-3-ones from aldol–Robinson annulation–regioselective addition involved one-pot reaction

Yingpeng Huo, Xu Qiu, Weiyan Shao, Jianing Huang, Yanjun Yu, Yinglin Zuo, Linkun An, Jun Du and Xianzhang Bu, *Org. Biomol. Chem.*, 2010 , **8** , 5048

DOI: 10.1039/c0ob00401d

Cellular process

Definition: Any process that is carried out at the cellular level, but not necessarily restricted to a single cell. For example, cell communication occurs among more than one cell, but occurs at the cellular level.

ID: GO:0009987

Synonyms:

- cell growth and/or maintenance
- cell physiology

InChIs & SMILES

Have a nice afternoon!!

Cn1cnc2c1c(=O)n(c(=O)n2C)C
(caffeine)

InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3 (caffeine)

O[C@@H]1CC(\C(=C)CC1)=C\C=C2/CCC[C@]3([C@H]2CC[C@@H]3[C@H](C)CCCC(C)C)C (Vitamin D)

InChI=1/C27H44O/c1-19(2)8-6-9-21(4)25-15-16-26-22(10-7-17-27(25,26)5)12-13-23-18-24(28)14-11-20(23)3/h12-13,19,21,24-26,28H,3,6-11,14-18H2,1-2,4-5H3/b22-12+,23-13-/t21-,24+,25-,26+,27-/m1/s1 (Vitamin D)