Supporting Information

Discovery of a Novel 2,6-Difunctionalized 2H-Benzopyran Inhibitors Toward Sphingosylphosphorylcholine Synthetic Pathway as New Anti-inflammatory Target

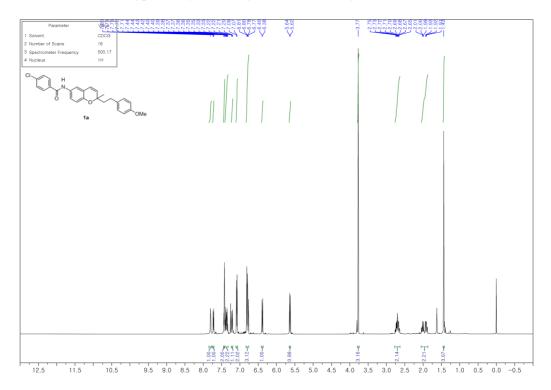
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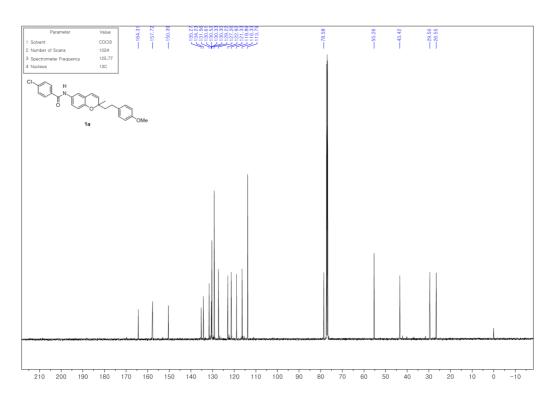
†Pharmacology Research Center, Drug Discovery Division, Korea Research Institute of Chemical Technology, Daejeon 305-343, Korea. *E-mail: hycho@krict.re.kr

[‡]College of Pharmacy, Research Institute of Pharmaceutical Sciences, Kyungpook National University, Daegu 702-701, Korea $^{\S}College$ of Pharmacy, Research Institute of Pharmaceutical Sciences, Keimyung University, Daegu 704-701, Korea Received February 24, 2014, Accepted April 21, 2014

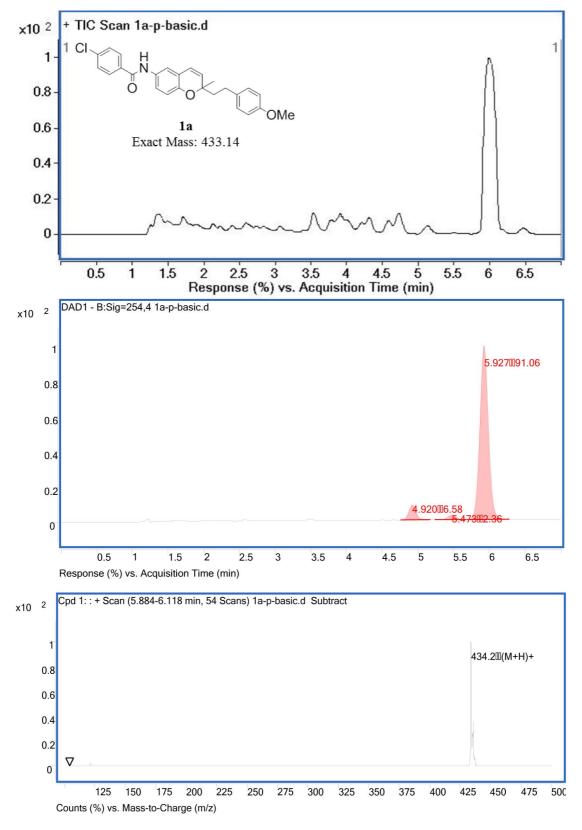
4-Chloro-N-(2-(4-methoxyphenethyl)-2-methyl-2H-chromen-6-yl)benzamide 1a.



1a-1H NMR Spectroscopy

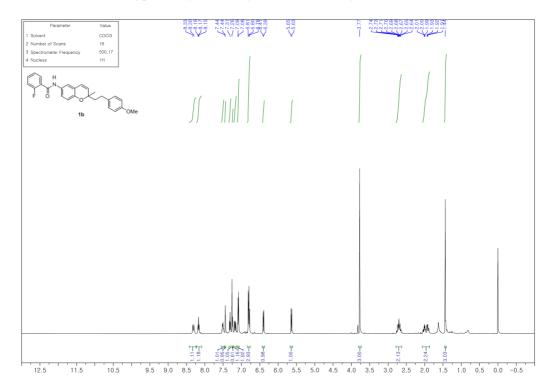


1a-13C NMR Spectroscopy

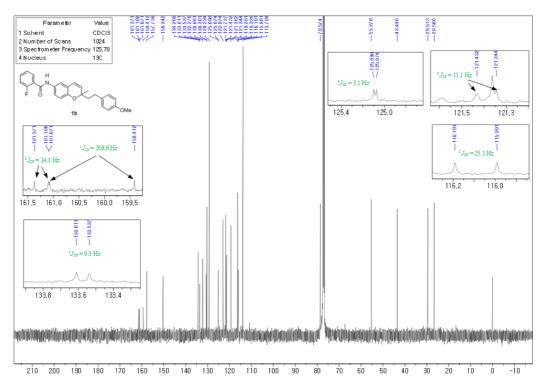


1a-LC/MS/MS Spectroscopy

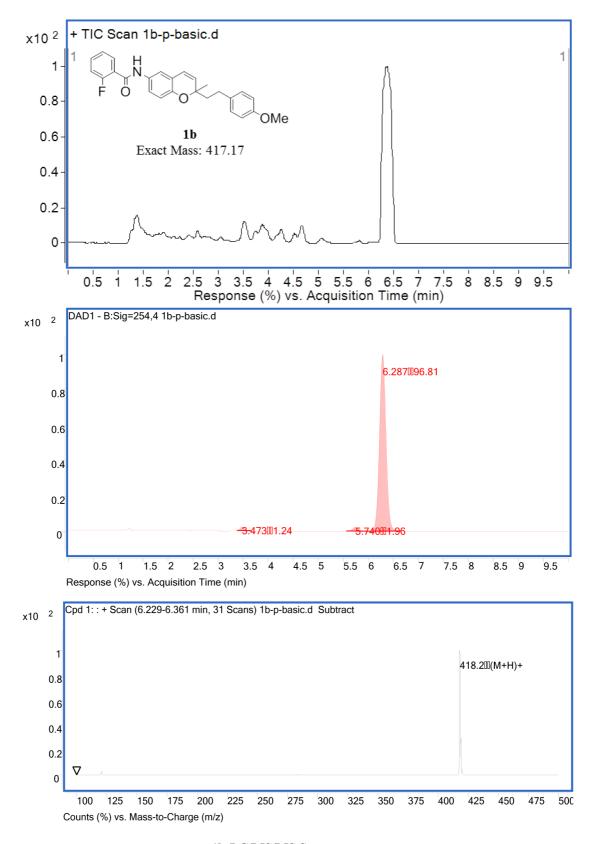
2-Fluoro-N-(2-(4-methoxyphenethyl)-2-methyl-2H-chromen-6-yl)benzamide 1b.



1b-1H NMR Spectroscopy

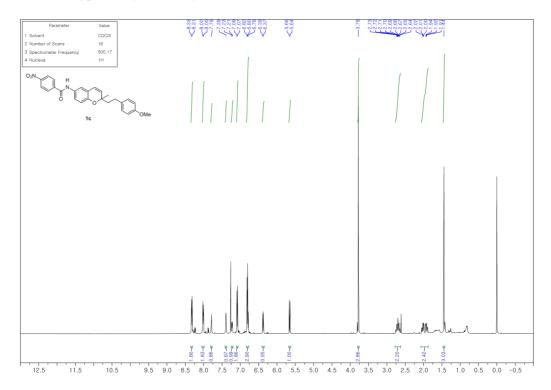


1b-13C NMR Spectroscopy

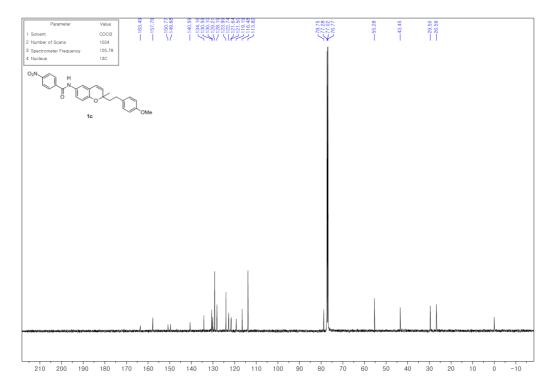


1b-LC/MS/MS Spectroscopy

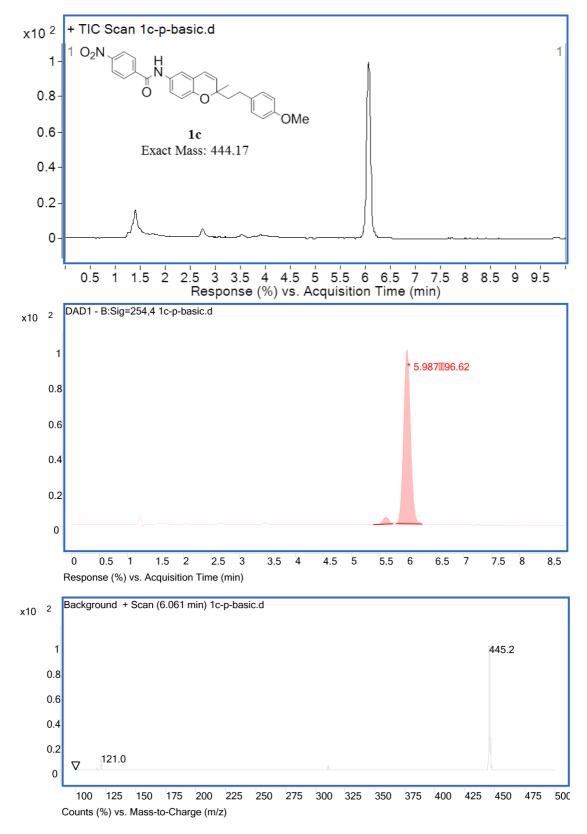
N-(2-(4-methoxyphenethyl)-2-methyl-2H-chromen-6-yl)-4-nitrobenzamide 1c.



1c-1H NMR Spectroscopy

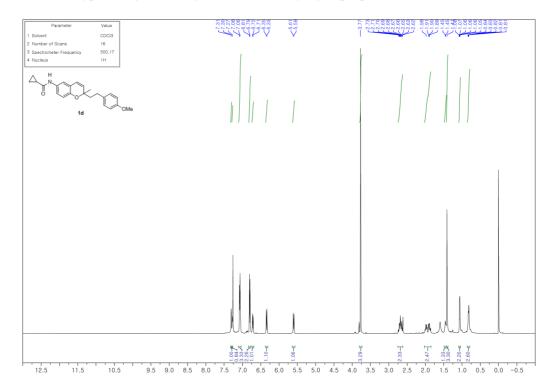


1c-13C NMR Spectroscopy

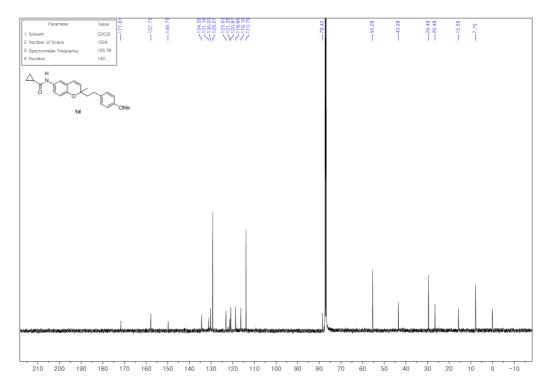


1c-LC/MS/MS Spectroscopy

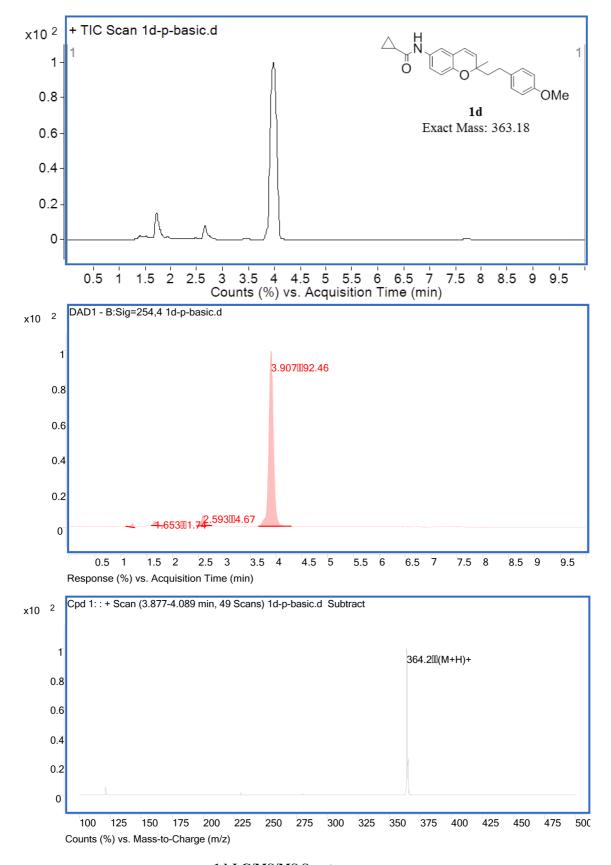
N-(2-(4-methoxyphenethyl)-2-methyl-2H-chromen-6-yl)cyclopropanecarboxamide 1d.



1d-1H NMR Spectroscopy

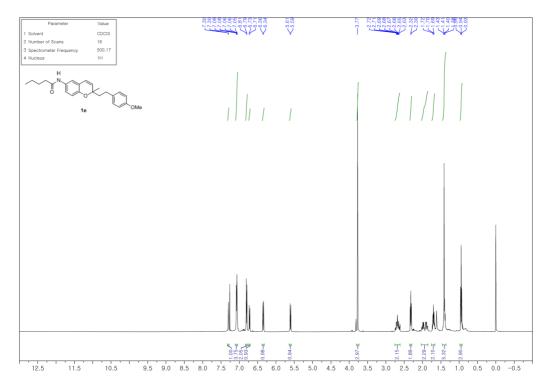


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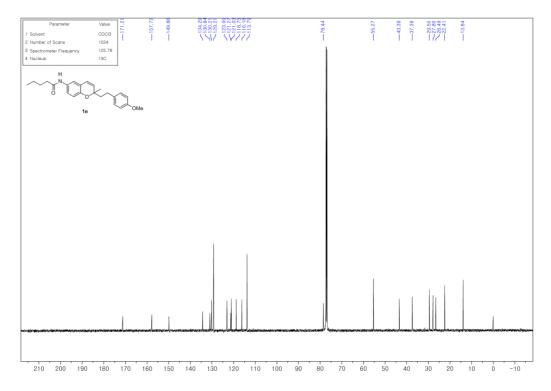


1d-LC/MS/MS Spectroscopy

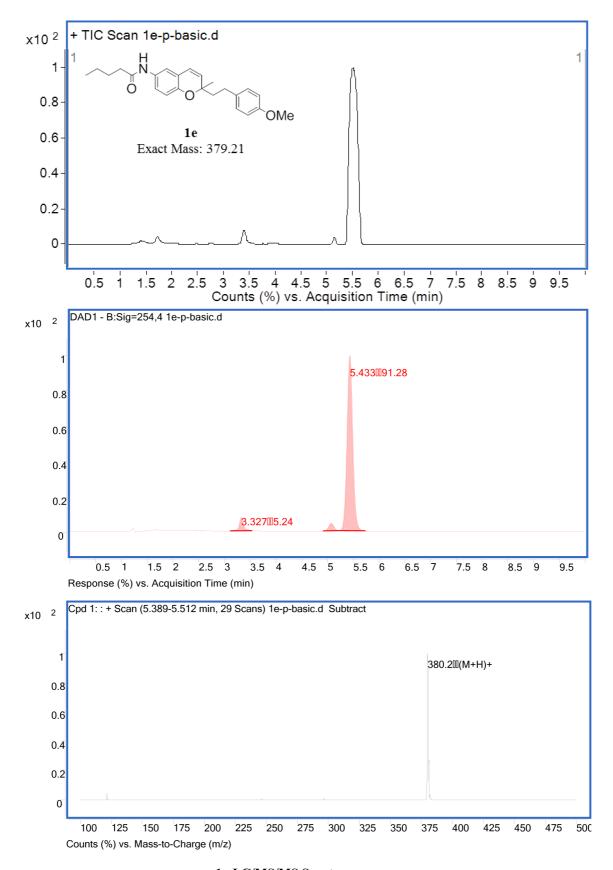
N-(2-(4-methoxyphenethyl)-2-methyl-2H-chromen-6-yl)pentanamide 1e.



1e-1H NMR Spectroscopy

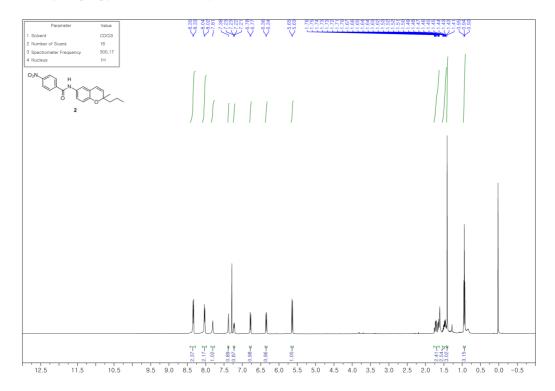


1e-13C NMR Spectroscopy

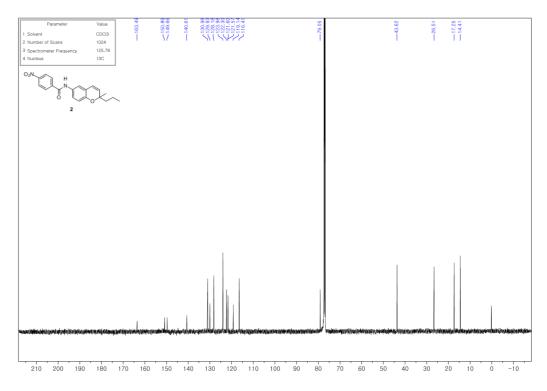


1e-LC/MS/MS Spectroscopy

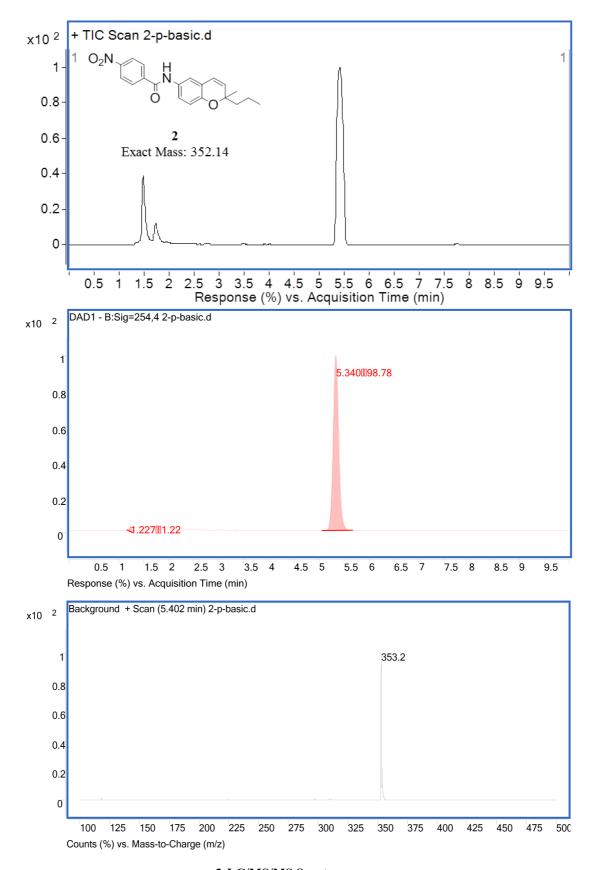
N-(2-methyl-2-propyl-2H-chromen-6-yl)-4-nitrobenzamide 2.



2-1H NMR Spectroscopy

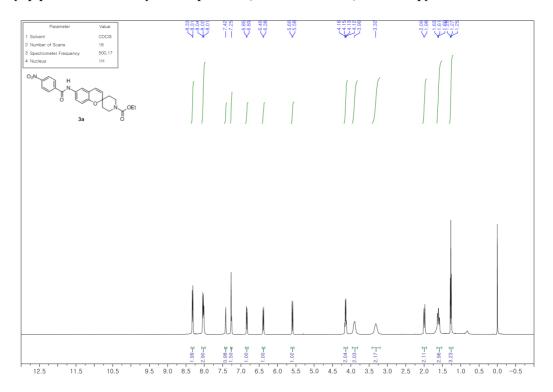


2-13C NMR Spectroscopy

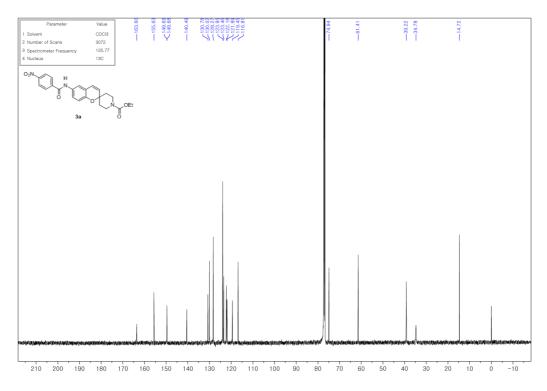


2-LC/MS/MS Spectroscopy

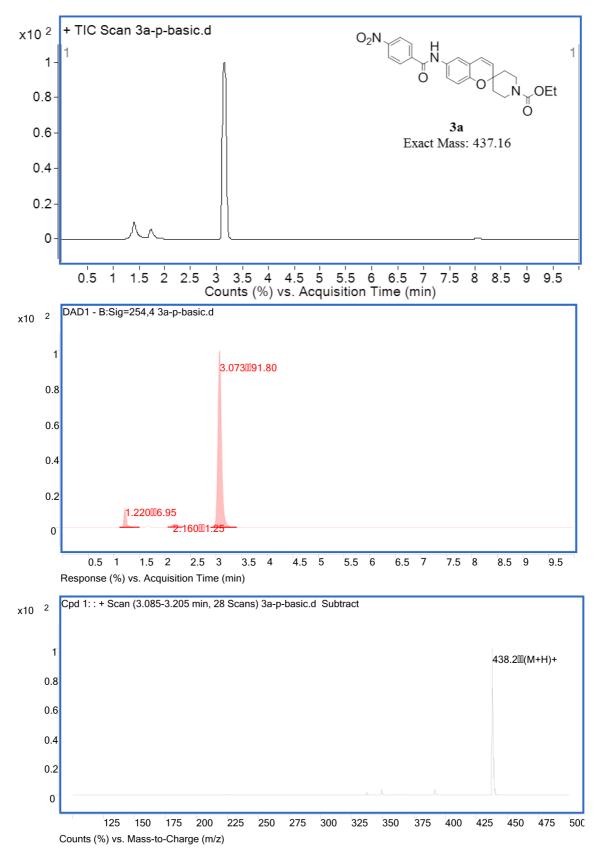
Ethyl piperidine-1'-carboxylate-4'-spiro-2-6-(4-nitrobenzamido)-2*H*-benzopyran 3a.



3a-1H NMR Spectroscopy

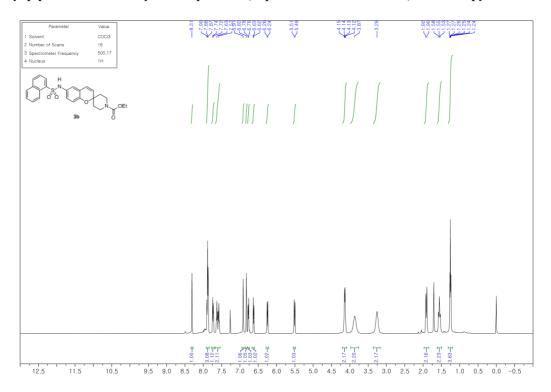


3a-¹³C NMR Spectroscopy

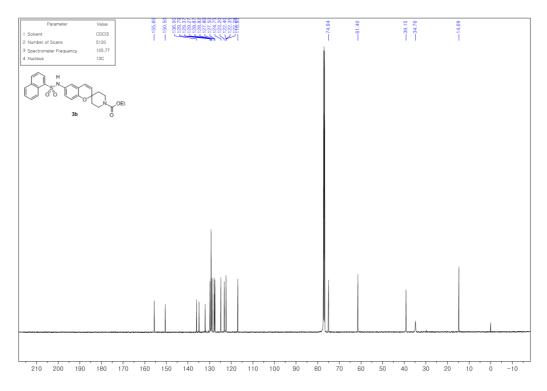


3a-LC/MS/MS Spectroscopy

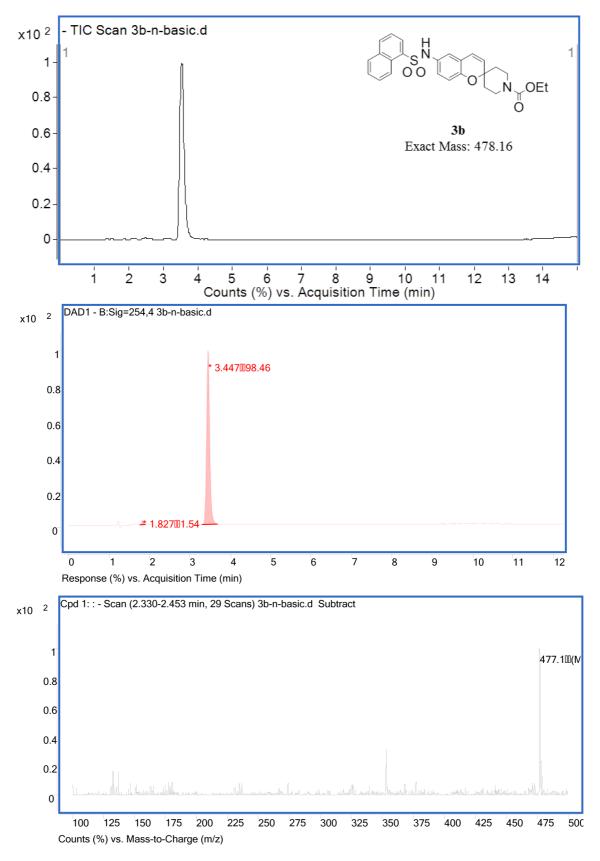
Ethyl piperidine-1'-carboxylate-4'-spiro-2-6-(naphthalene-1-sulfonamido)-2H-benzopyran 3b.



3b-1H NMR Spectroscopy



3b-13C NMR Spectroscopy



3b-LC/MS/MS Spectroscopy