

Revised. II

**Computer-aided design and synthesis of (functionalized quinazoline)–
(α -substituted coumarin)–arylsulfonate conjugates
against chikungunya virus**

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² Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University, Hsinchu 300044, Taiwan

³ Department of Chemical Engineering, National Tsing Hua University, Hsinchu 300044, Taiwan

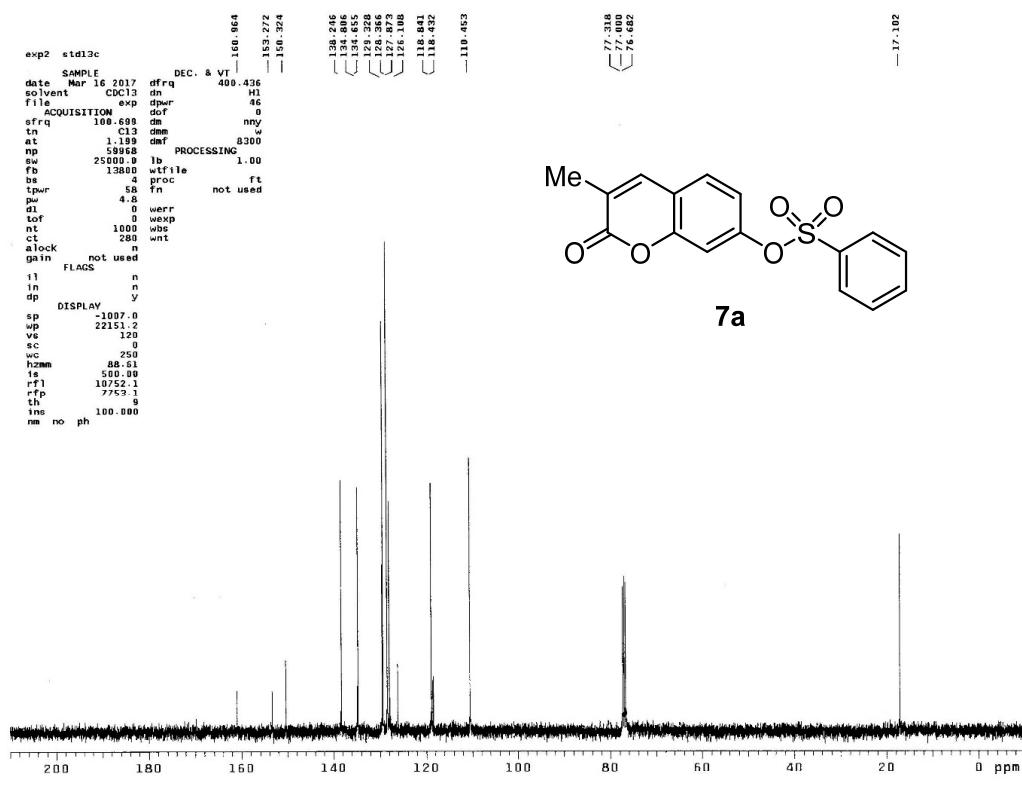
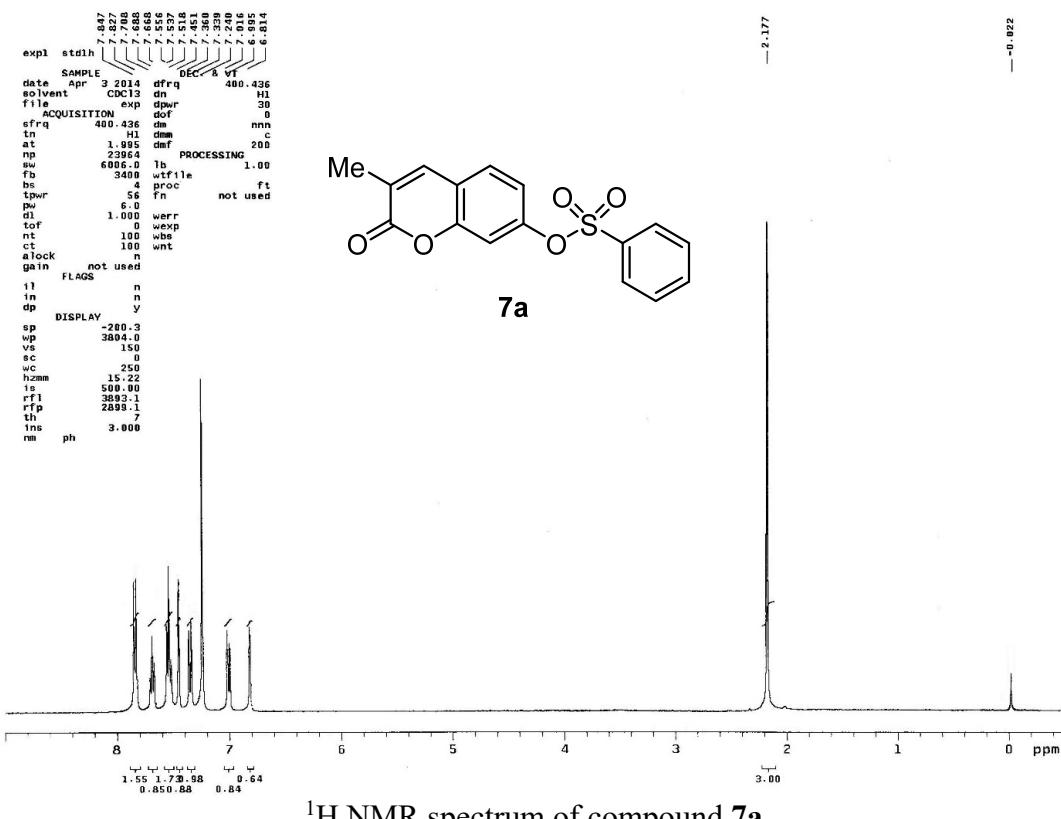
⁴ Department of Chemistry, National Central University, Jhongli City 320317, Taiwan

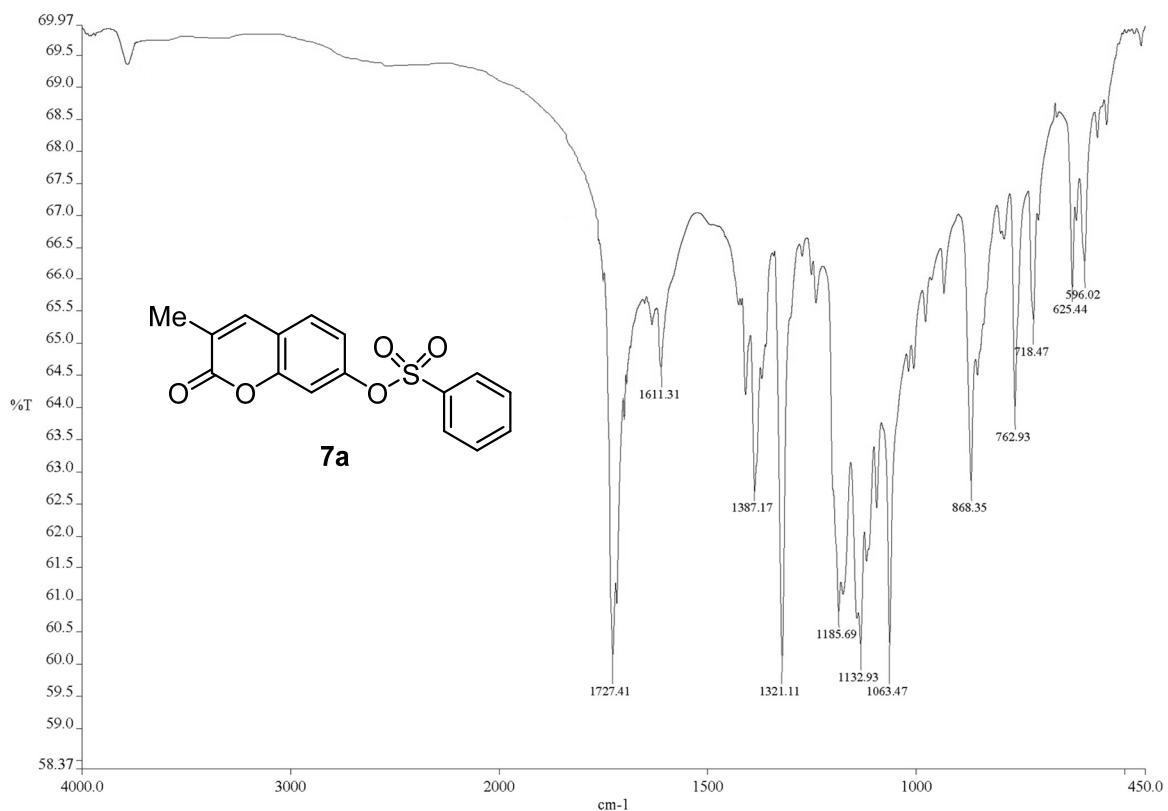
⁵ Rega Institute for Medical Research, Katholieke Universiteit Leuven, Minderbroedersstraat 10, B-3000 Leuven, Belgium

*Corresponding Author

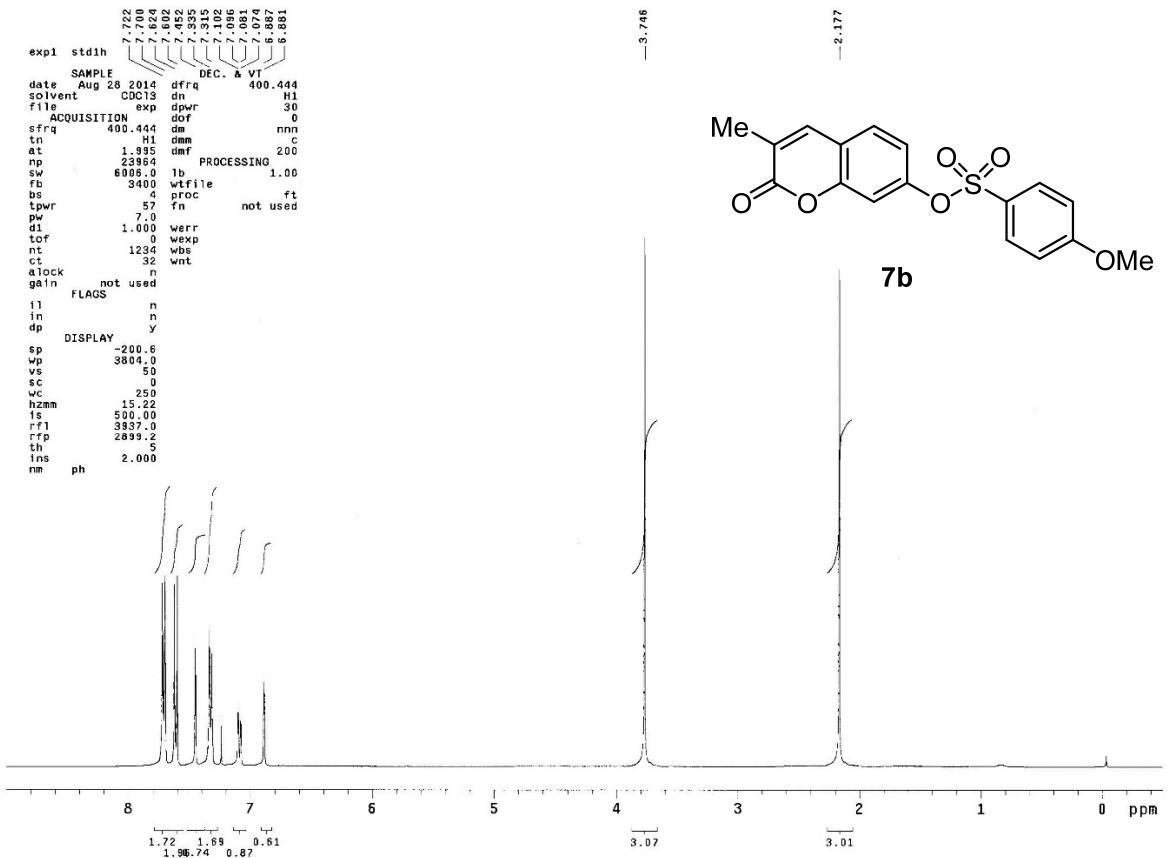
E-mail addresses: jrhwu@mx.nthu.edu.tw (J.R. Hwu)

¹H NMR, ¹³C NMR, and IR Spectra of New Compounds

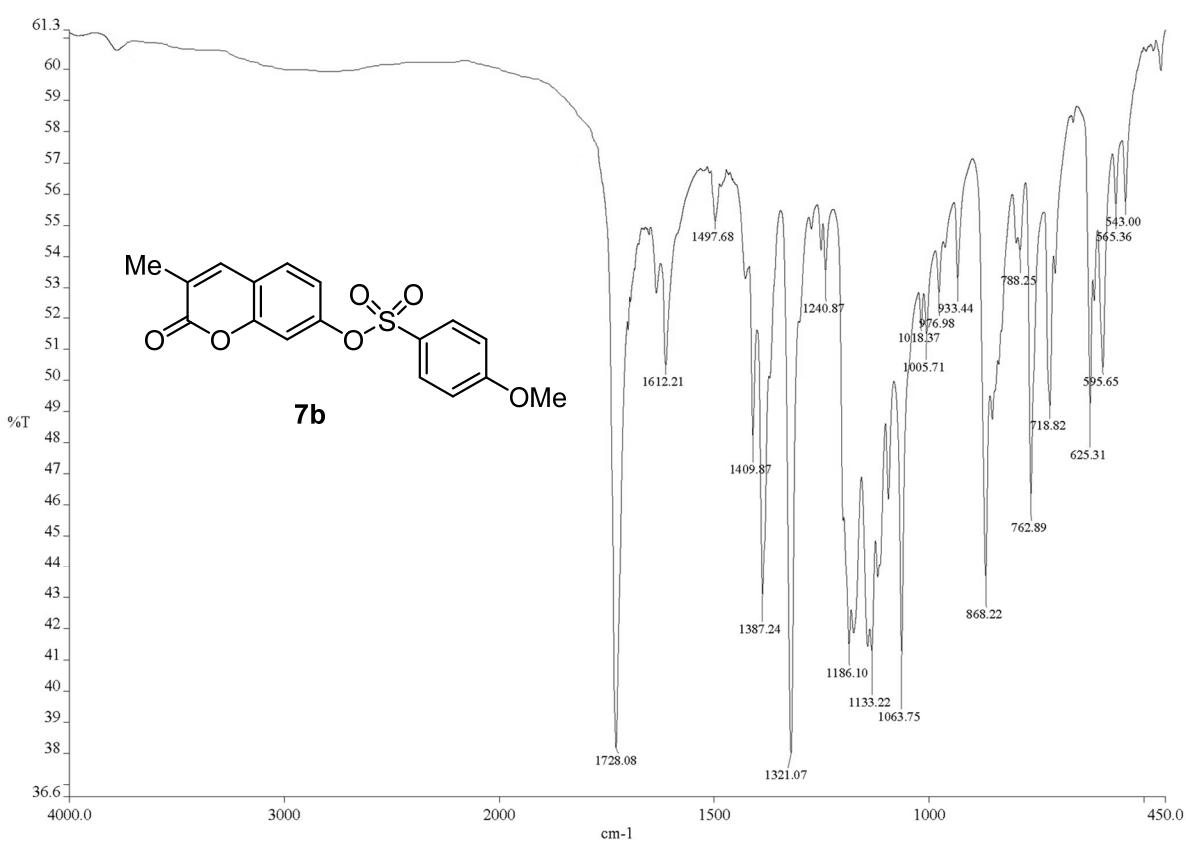
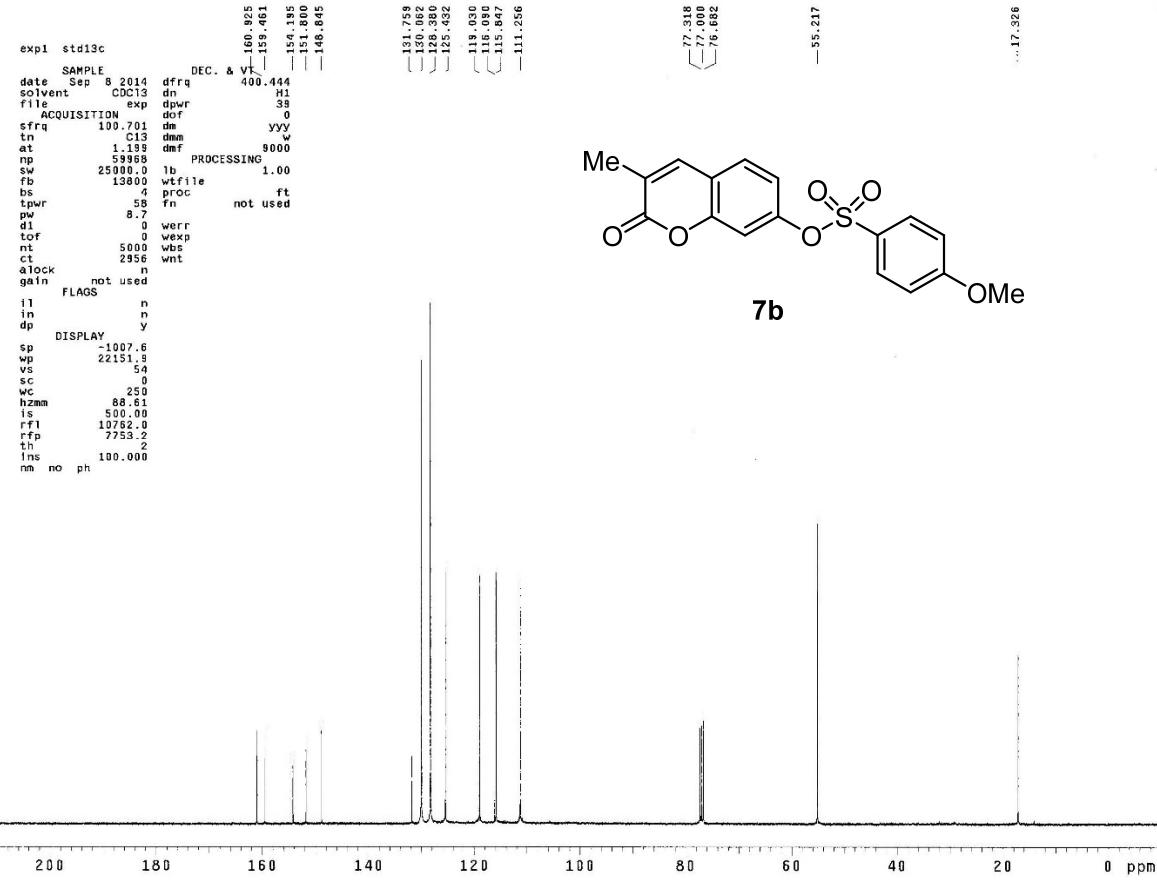


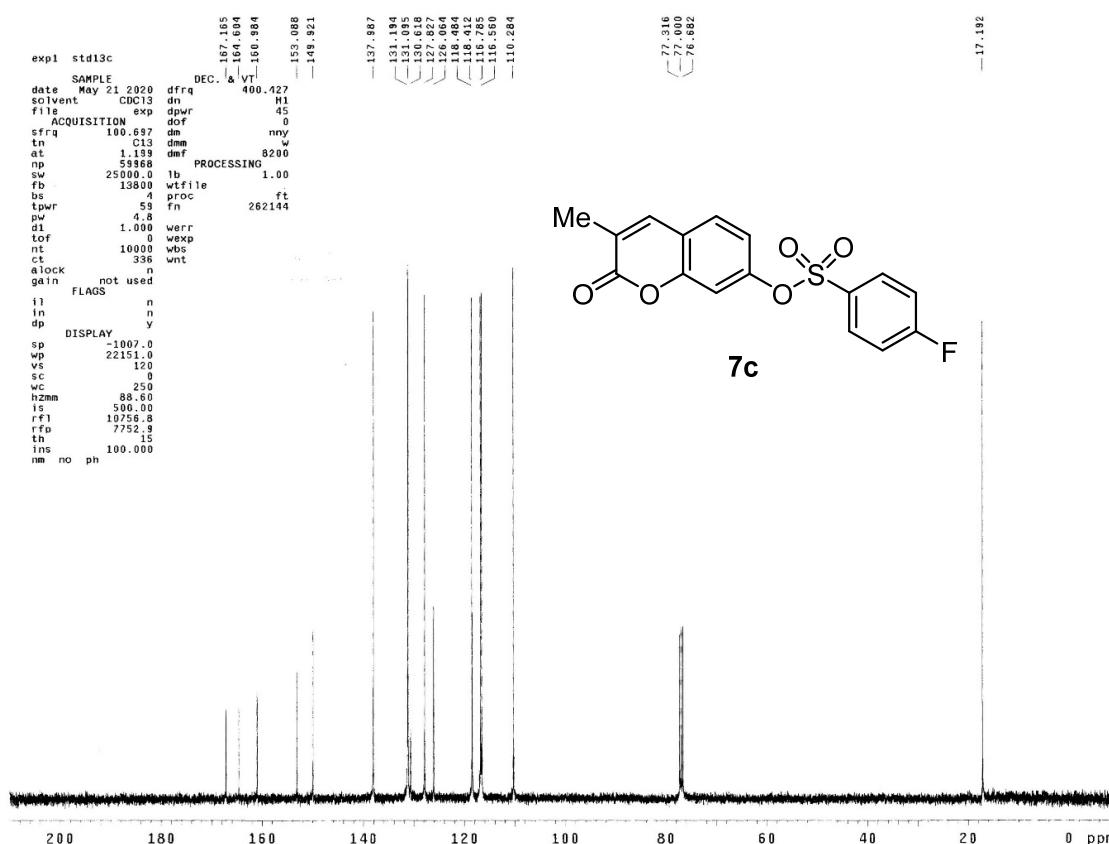
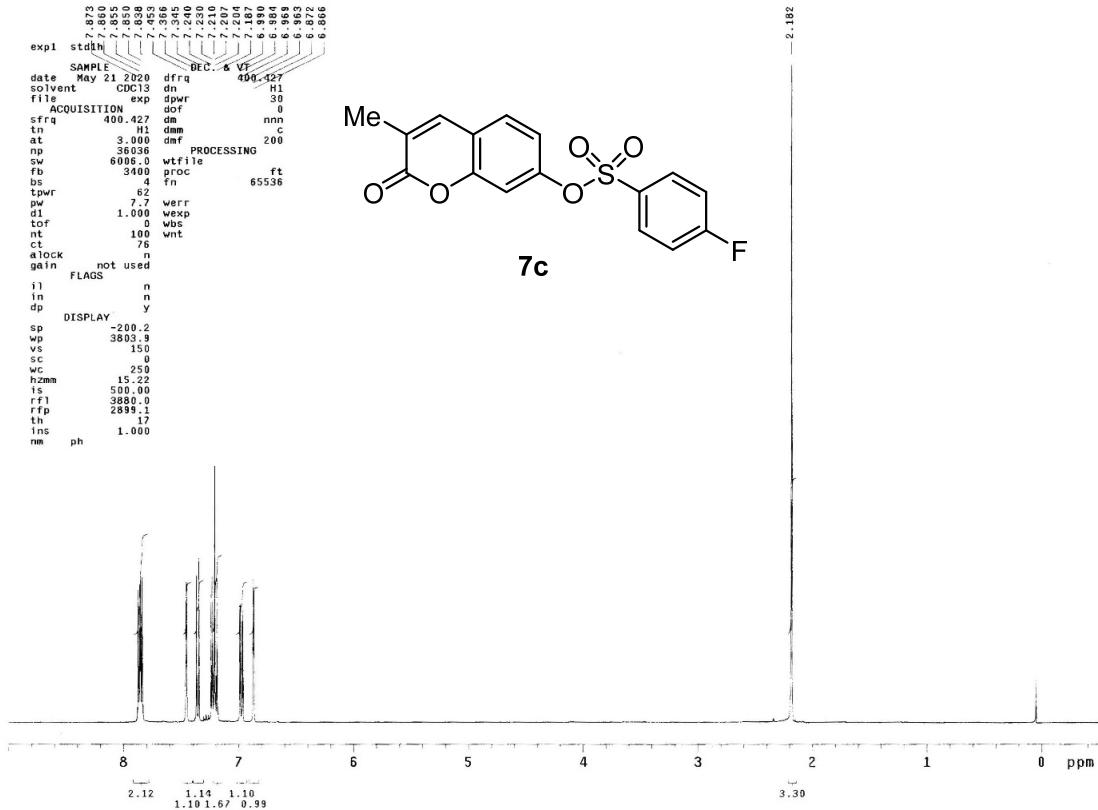


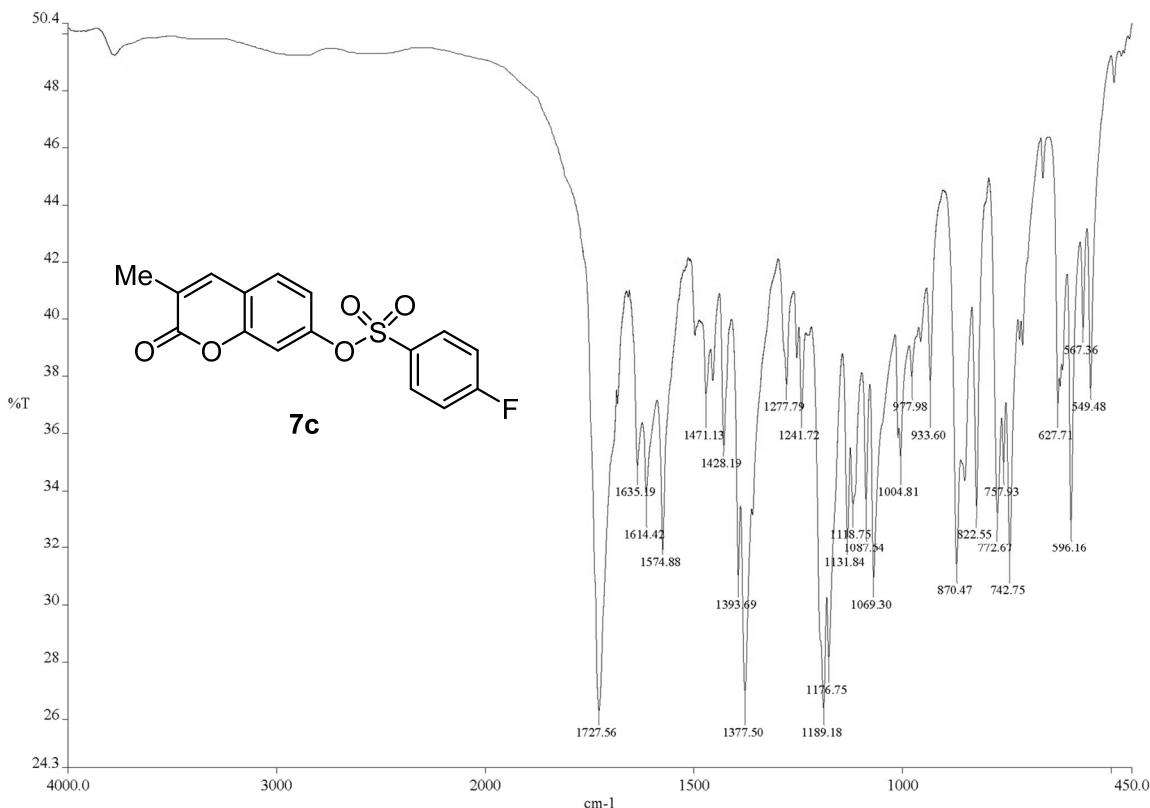
IR spectrum of compound 7a



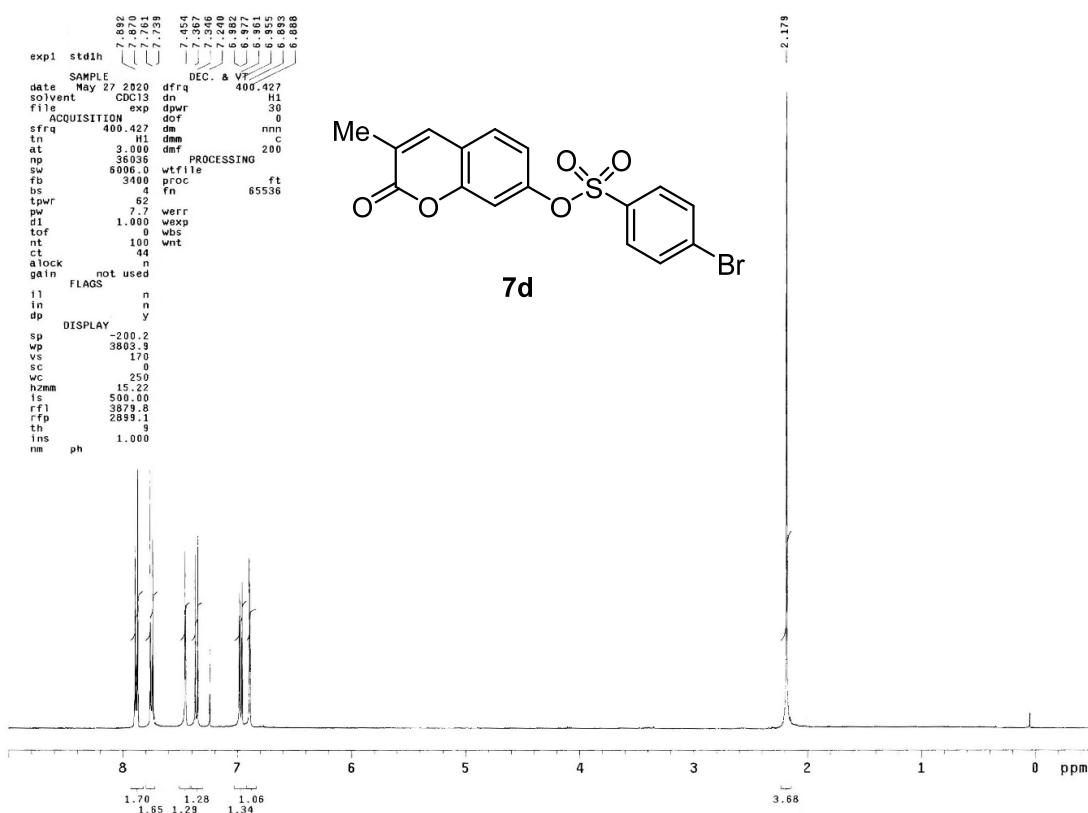
¹H NMR spectrum of compound 7b







IR spectrum of compound **7c**

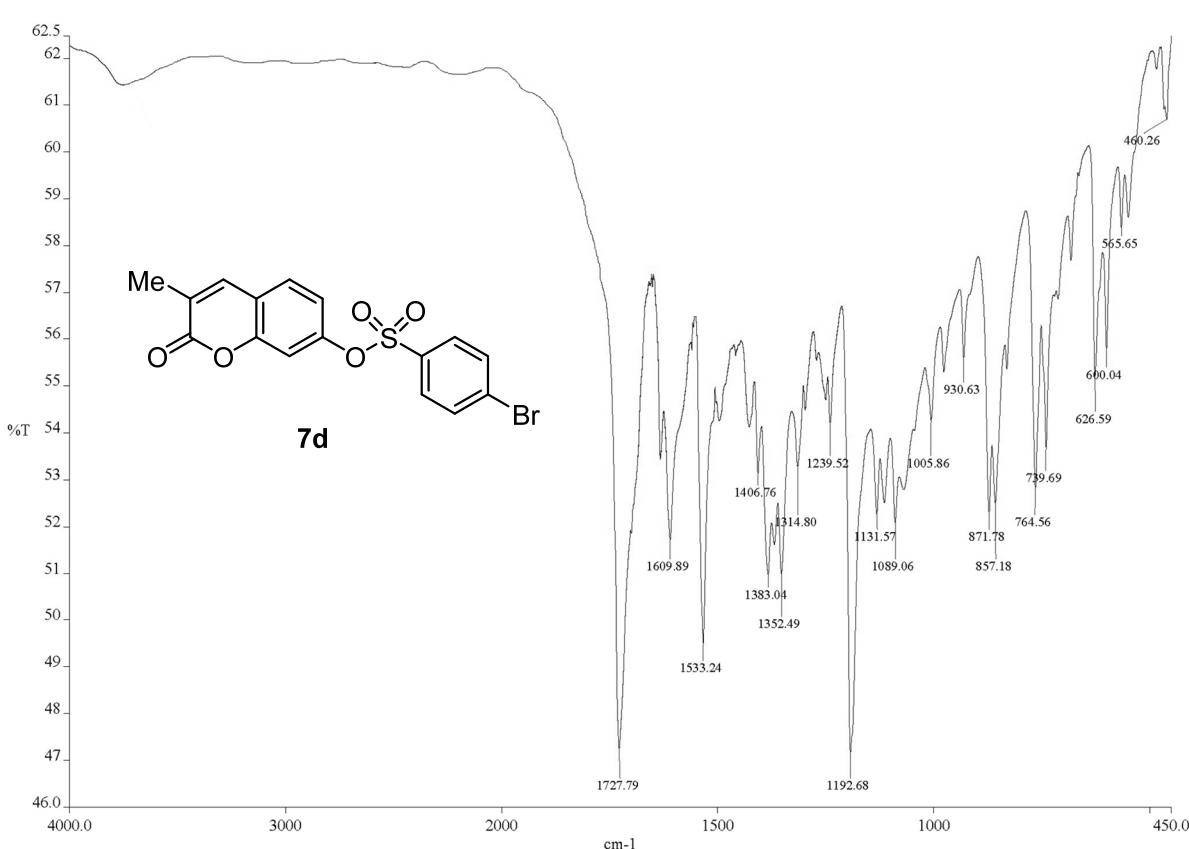
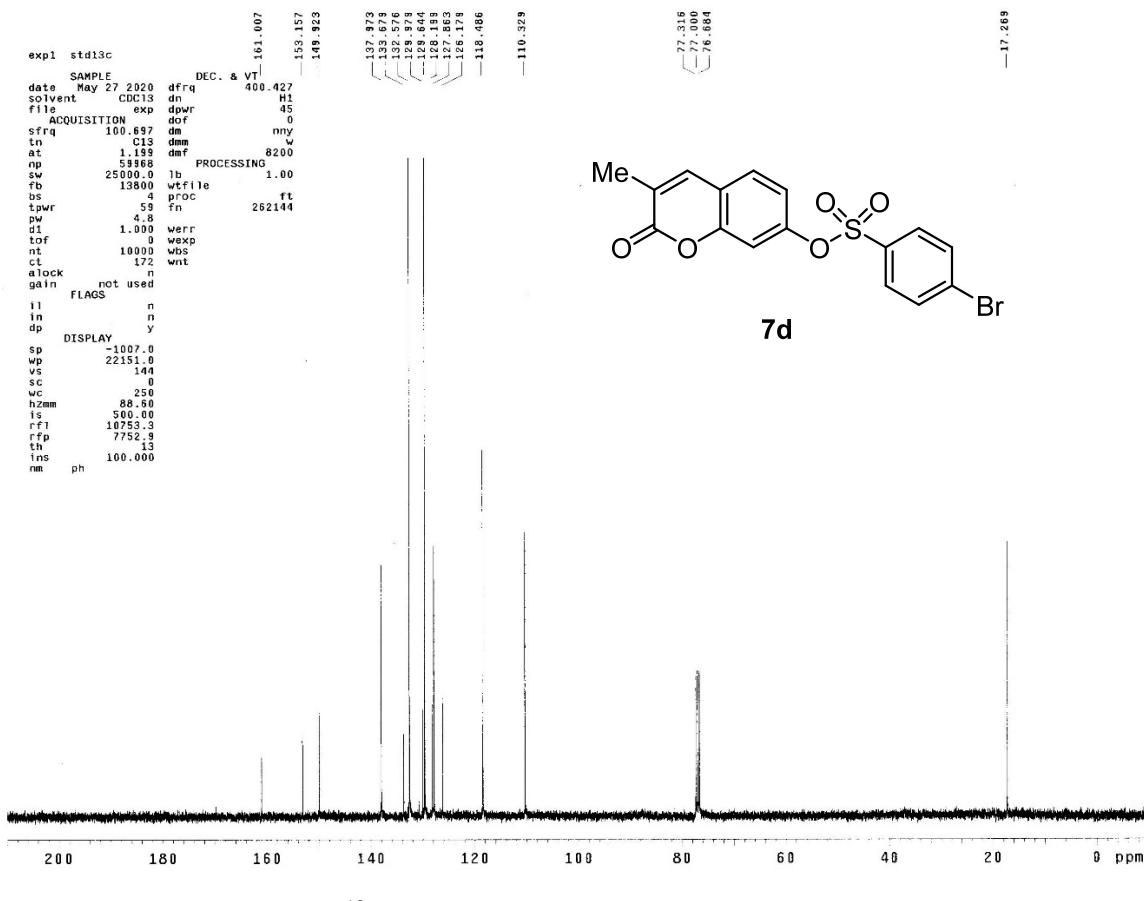
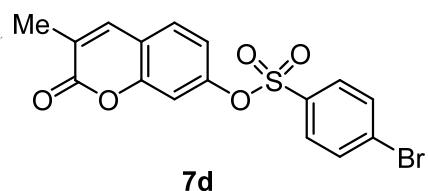


¹H NMR spectrum of compound **7d**

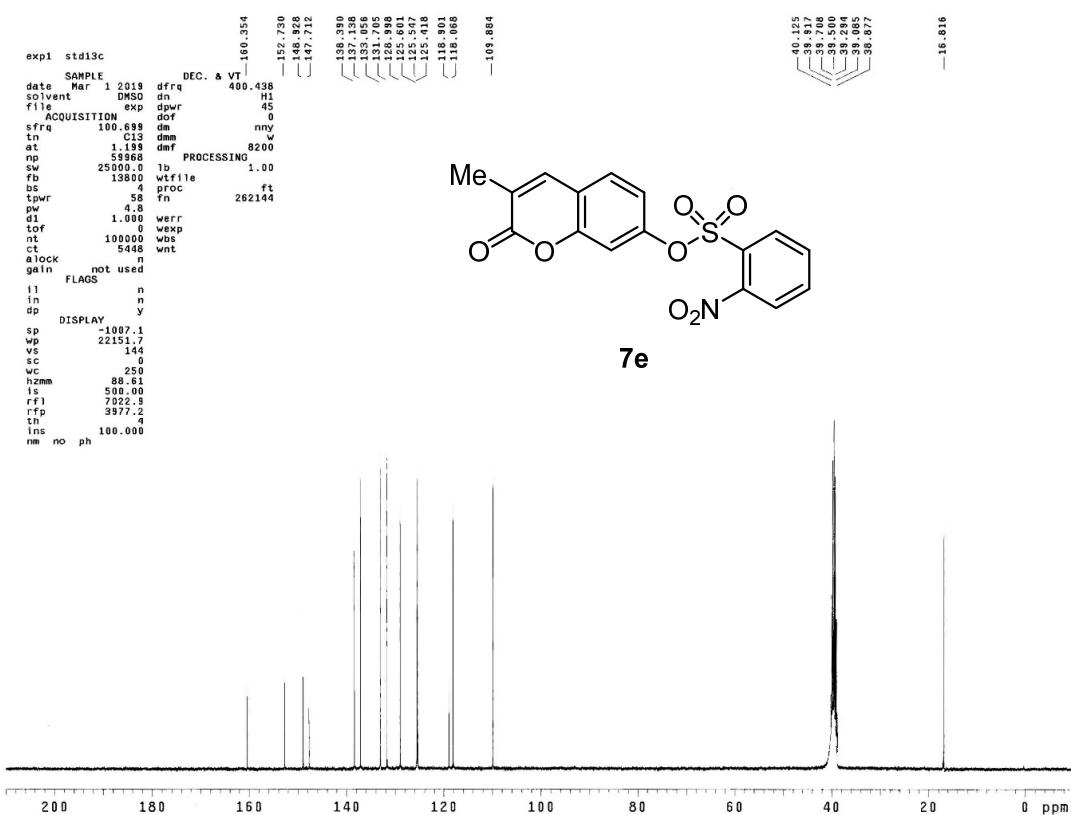
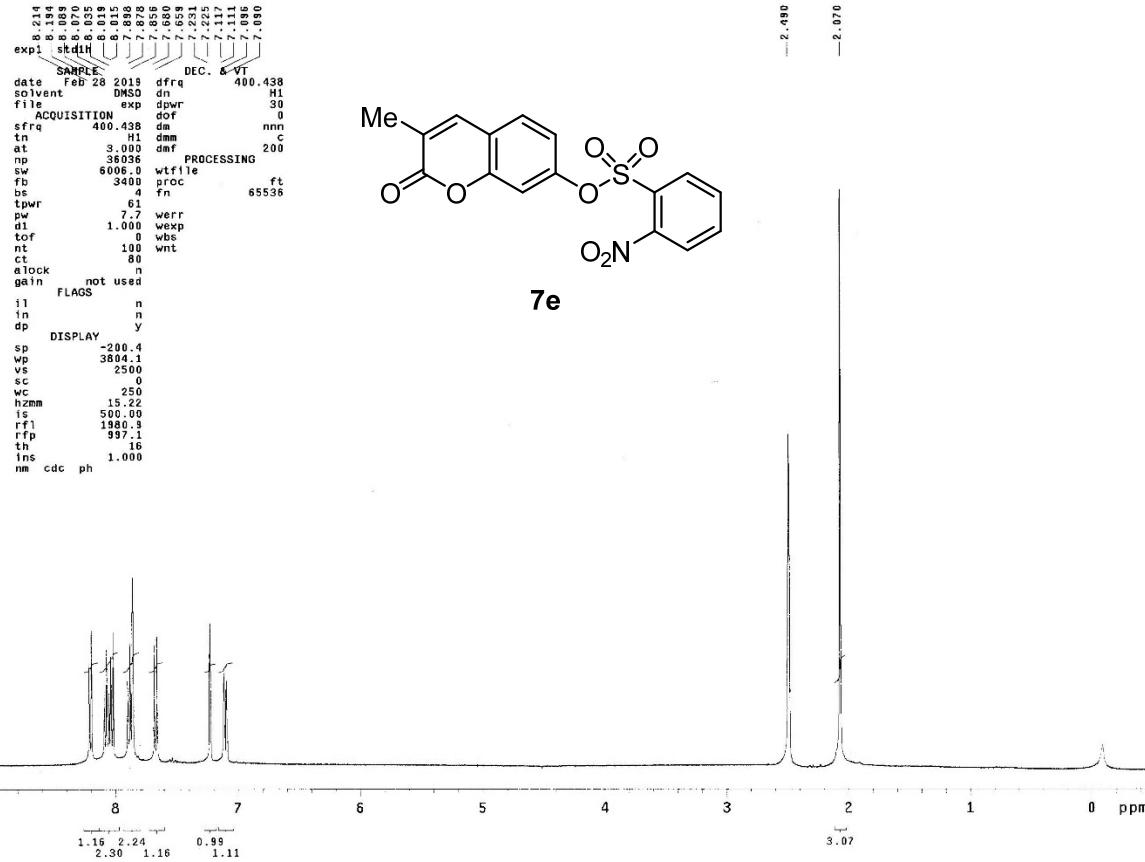
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tn     C13 dmm   200
at     1.000 dmt   2000
np     53668 lb   PROCESSING 1.00
sw     25000.0 fb   13800 wfile ft
bs     13800 proc
tppr   59 fn   262144
pw     4.8
d1     1.000 werr
tof     0 wexp
nt     100000 abs
ct     172 whi
alock   not used
gain   not used
FLAGS
il     n
in     n
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DISPLAY
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nm   ph

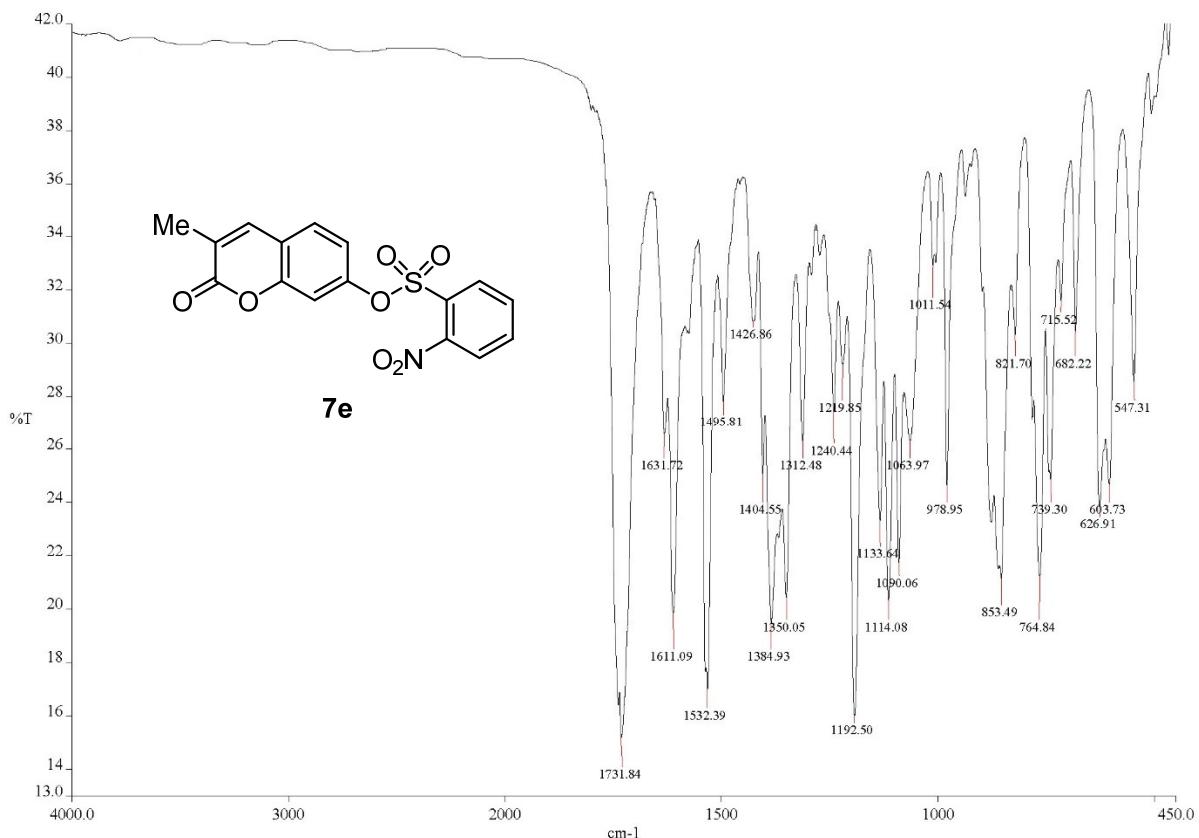
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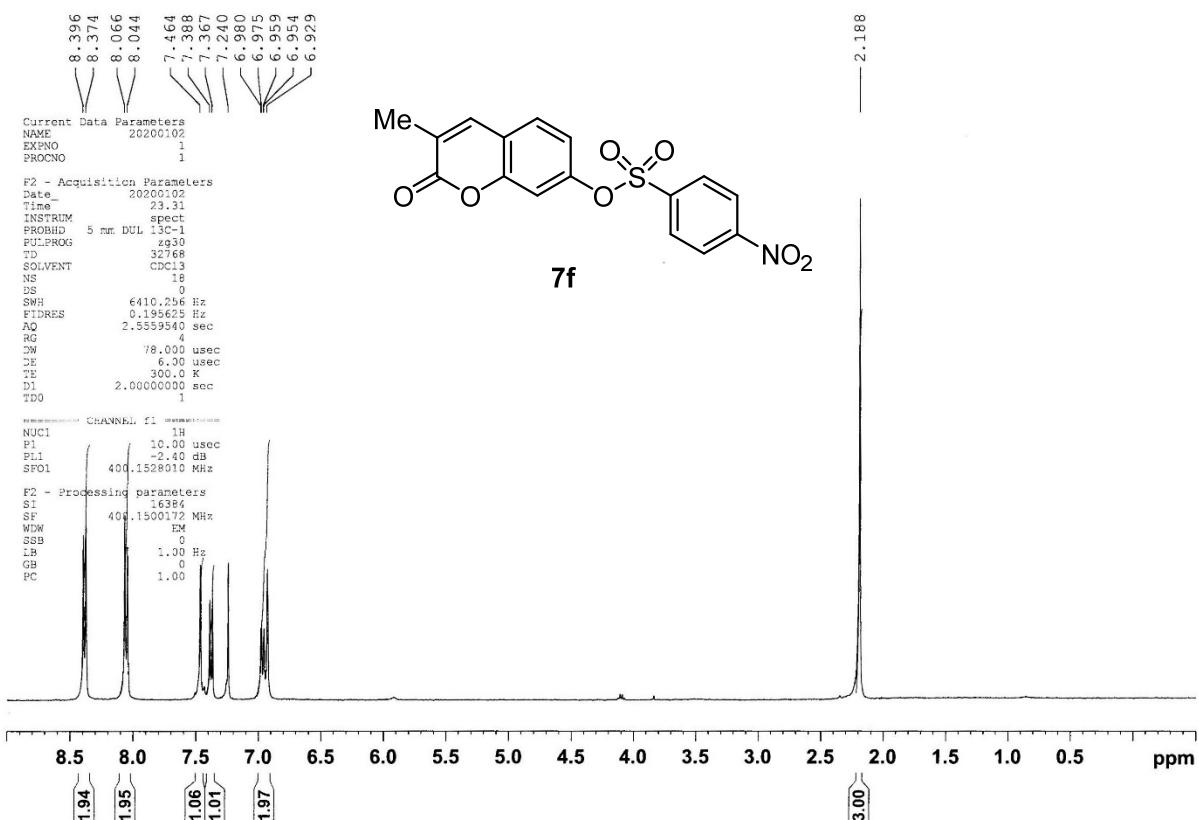
IR spectrum of compound **7d**



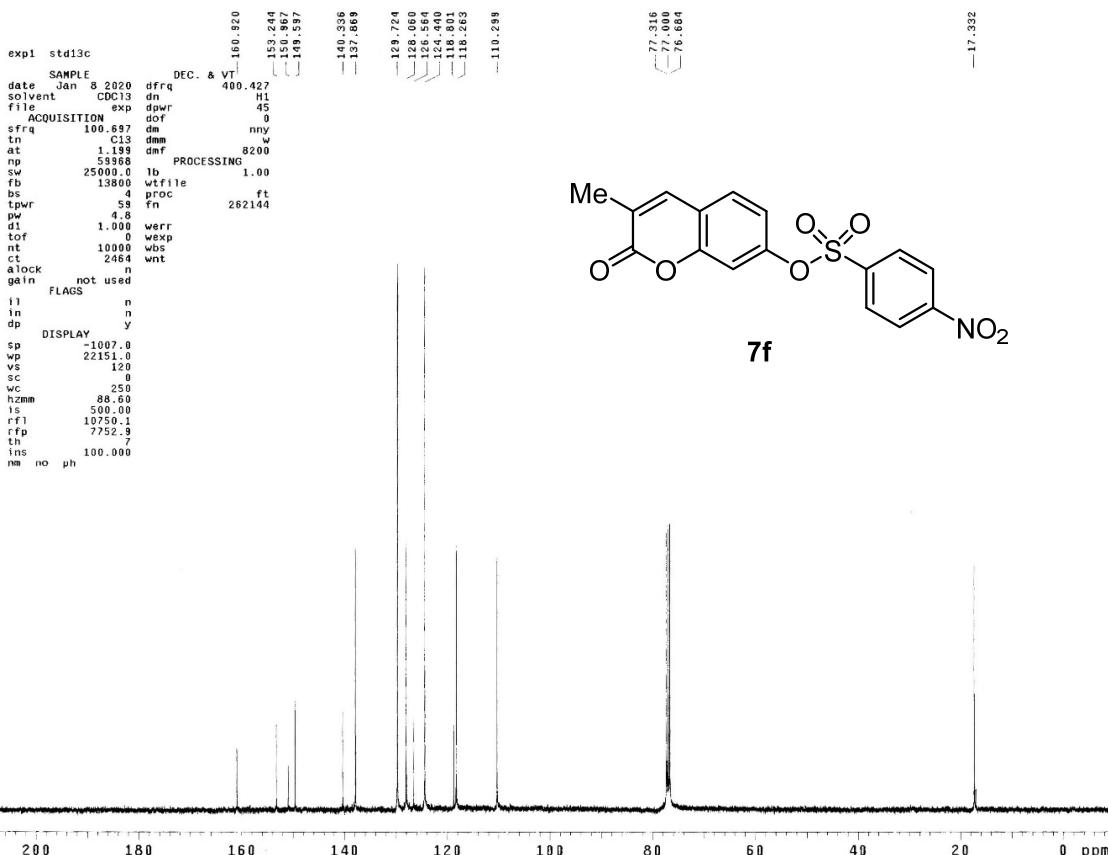
¹³C NMR spectrum of compound 7e



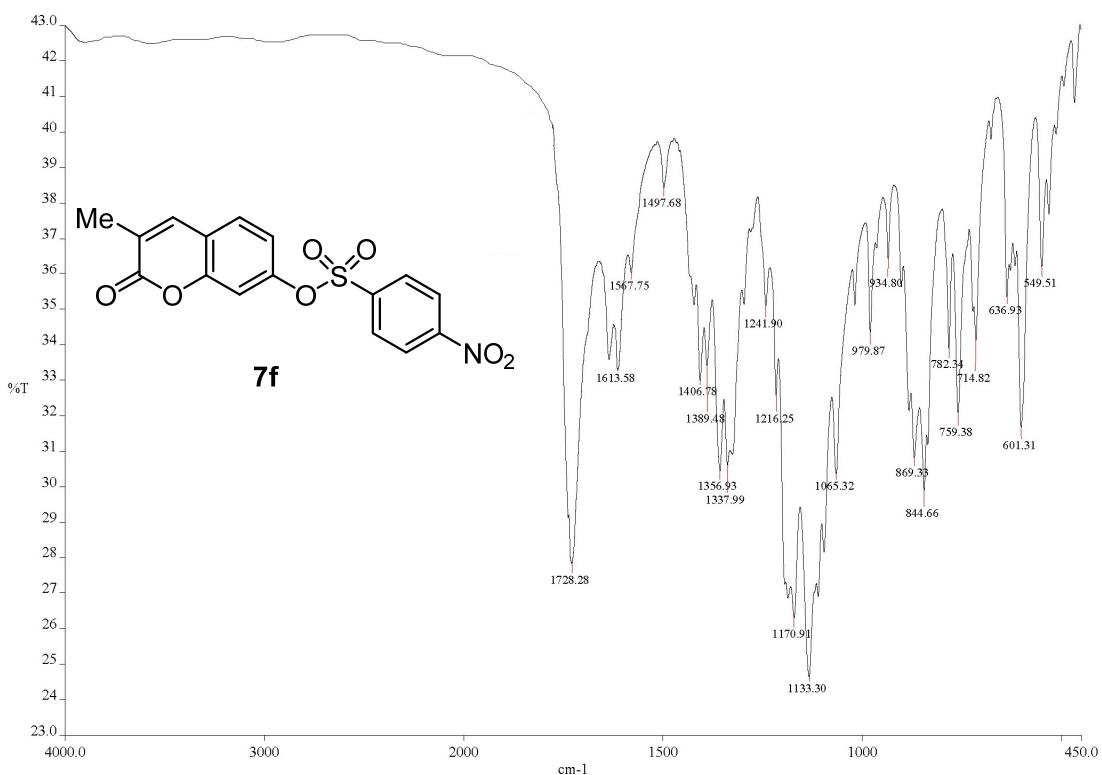
IR spectrum of compound **7e**



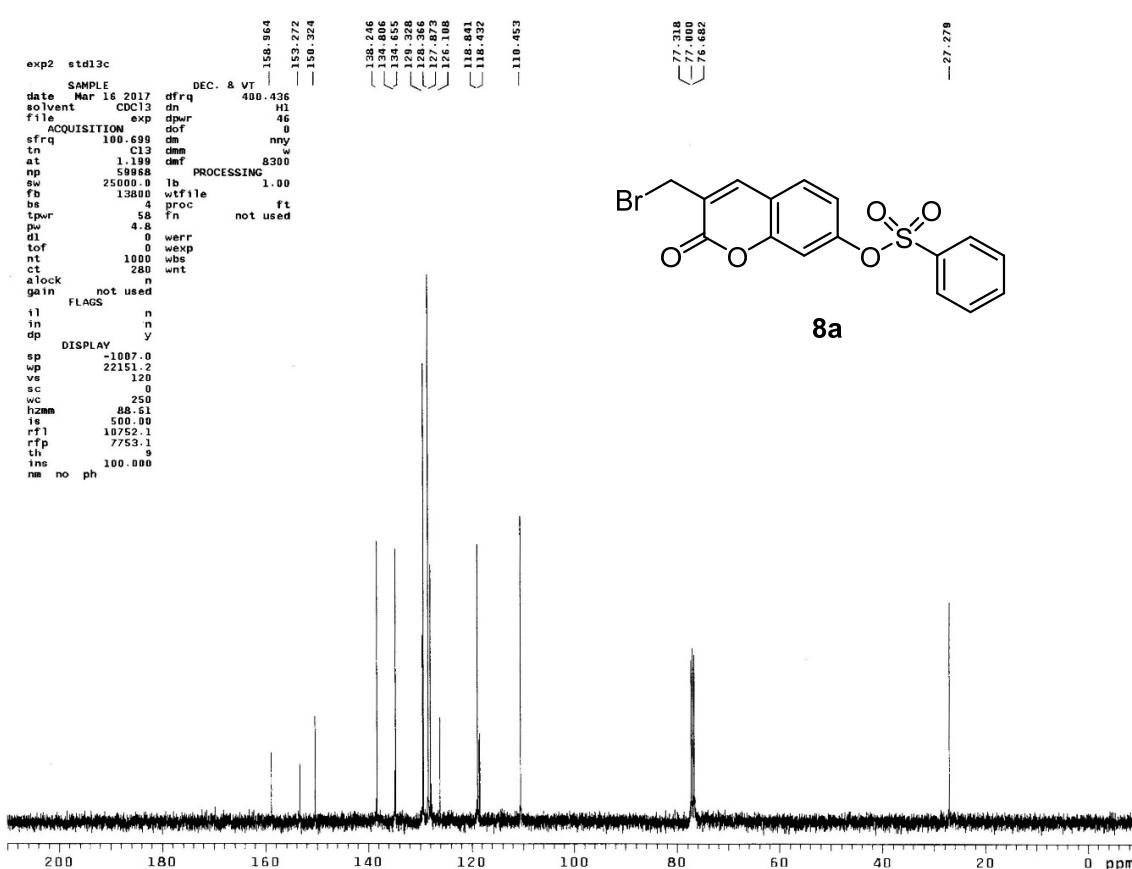
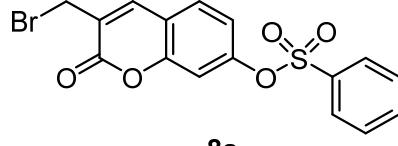
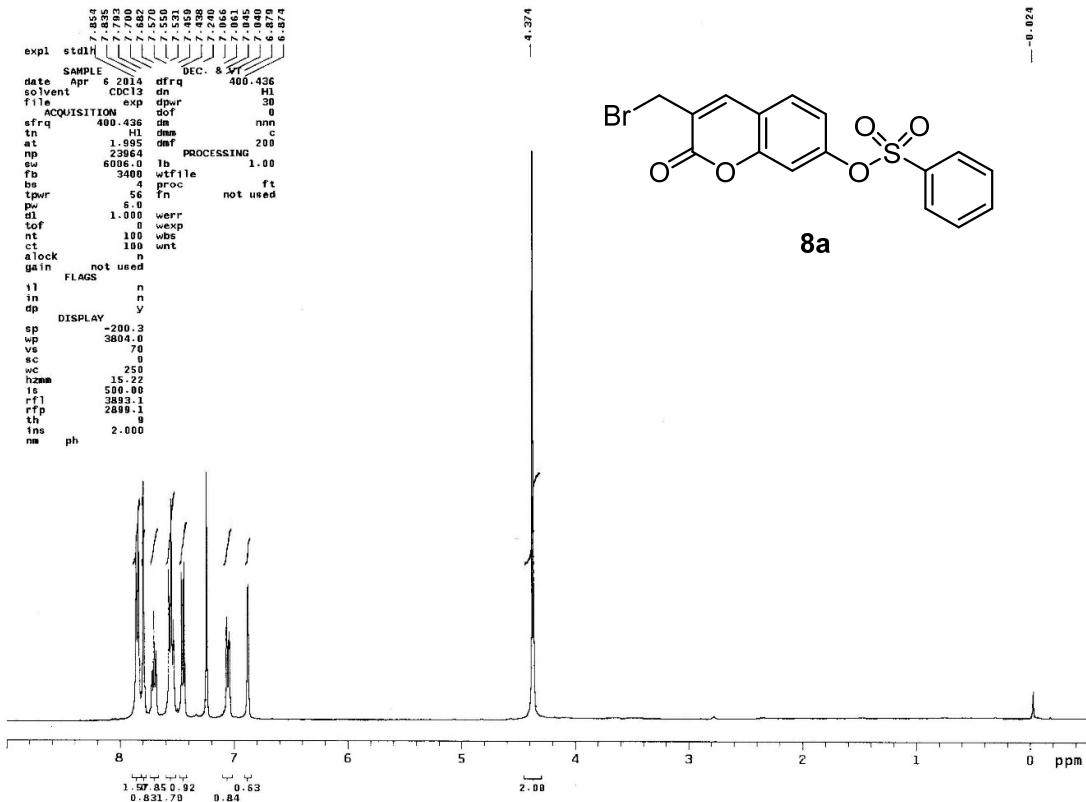
¹H NMR spectrum of compound **7f**

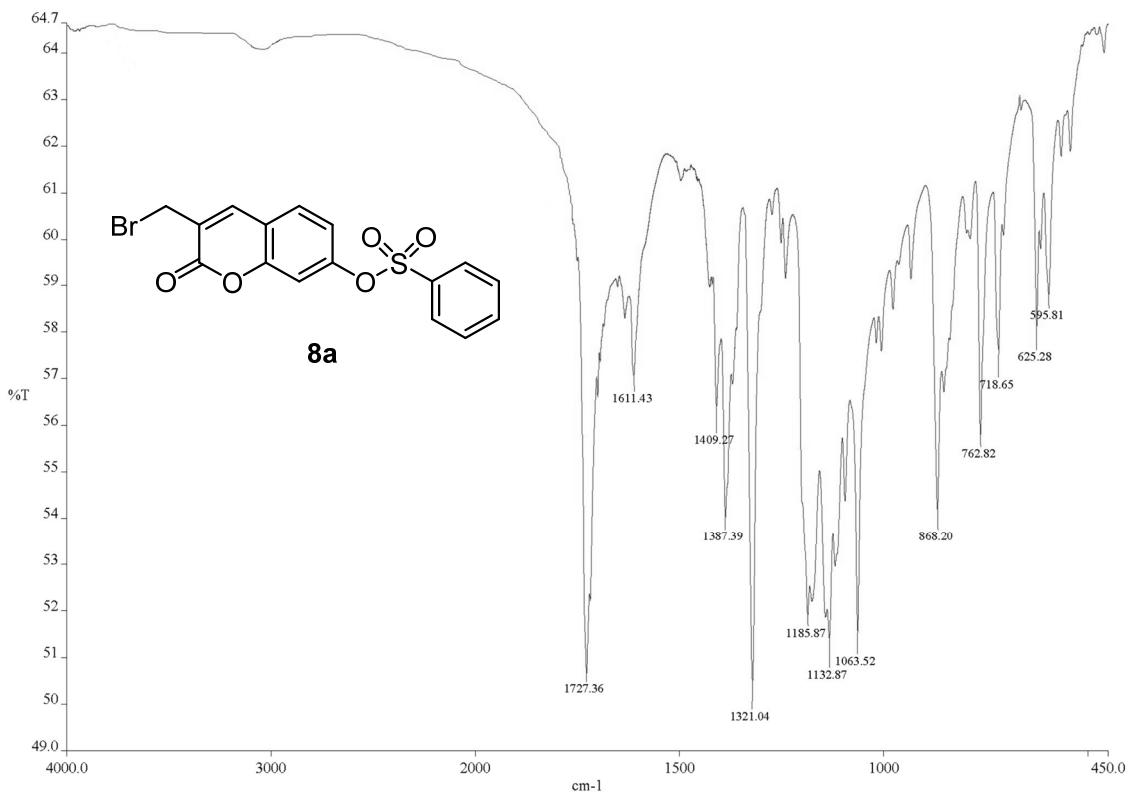


¹³C NMR spectrum of compound 7f

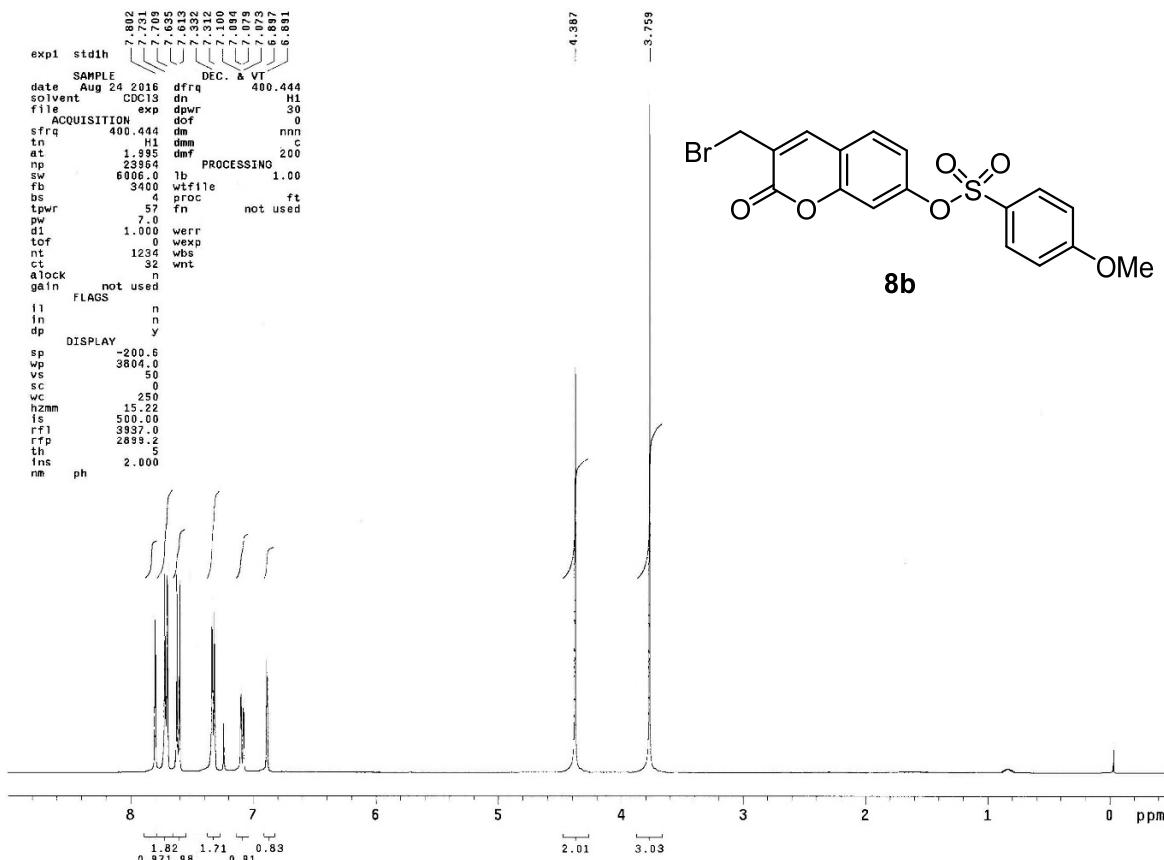


IR spectrum of compound 7f





IR spectrum of compound **8a**

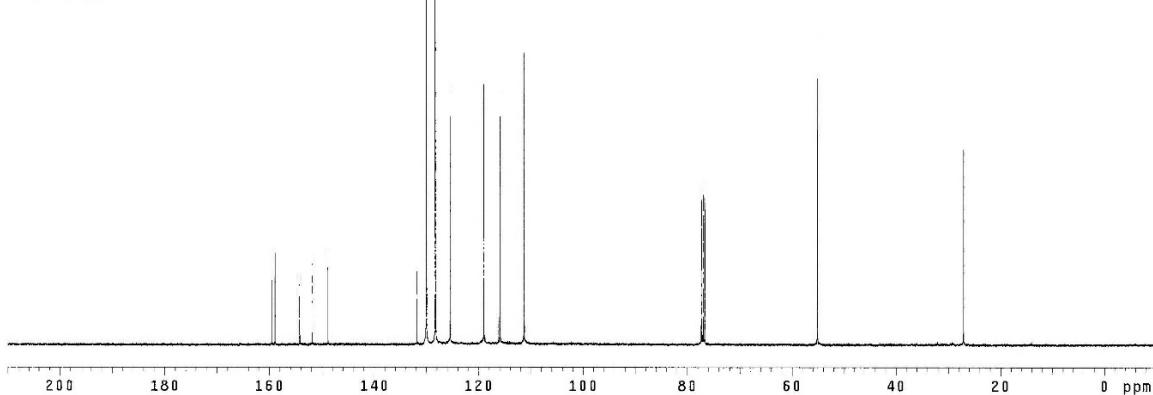
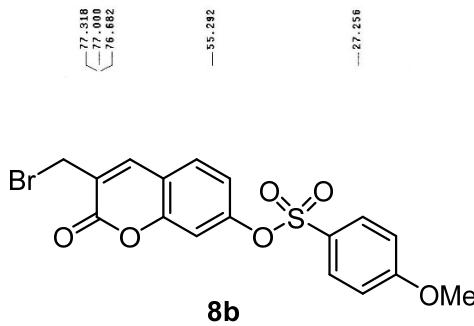


¹H NMR spectrum of compound **8b**

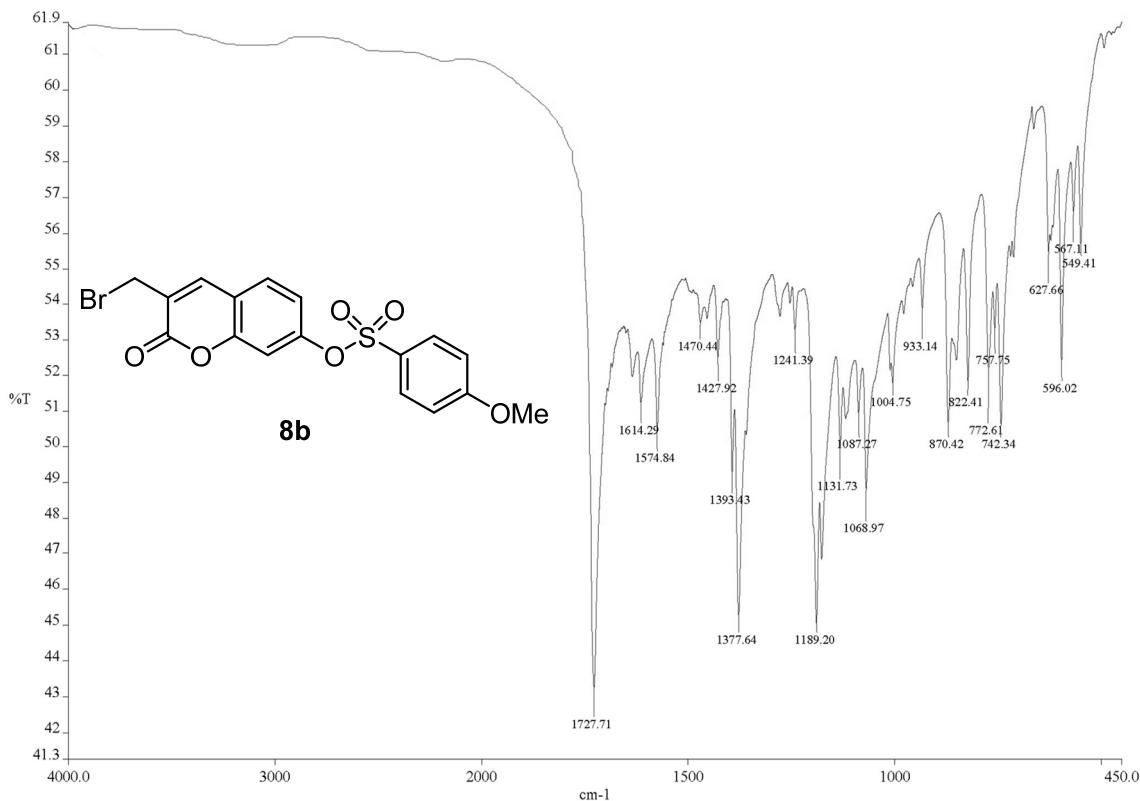
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tn C13 dmm VVY
at 1.000 dm 8000
np 53998 PROCESSING
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fb 13800 wfile ft
bs proc ft
tpur 58 fn not used
pw 8.7
d1 0 werr
t1 0 wexp
nt 5000 nse
ct 2356 wnt
a1ock 2356 nse
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1007.6
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nm no ph

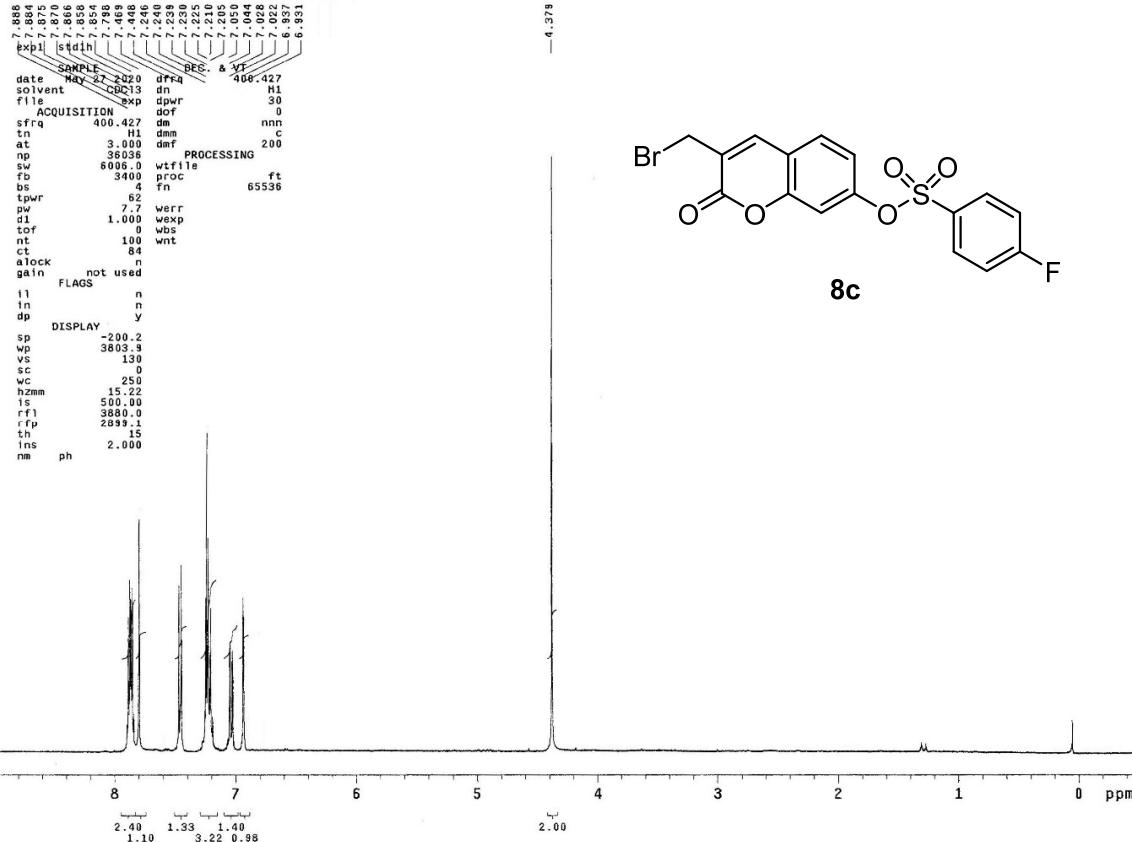
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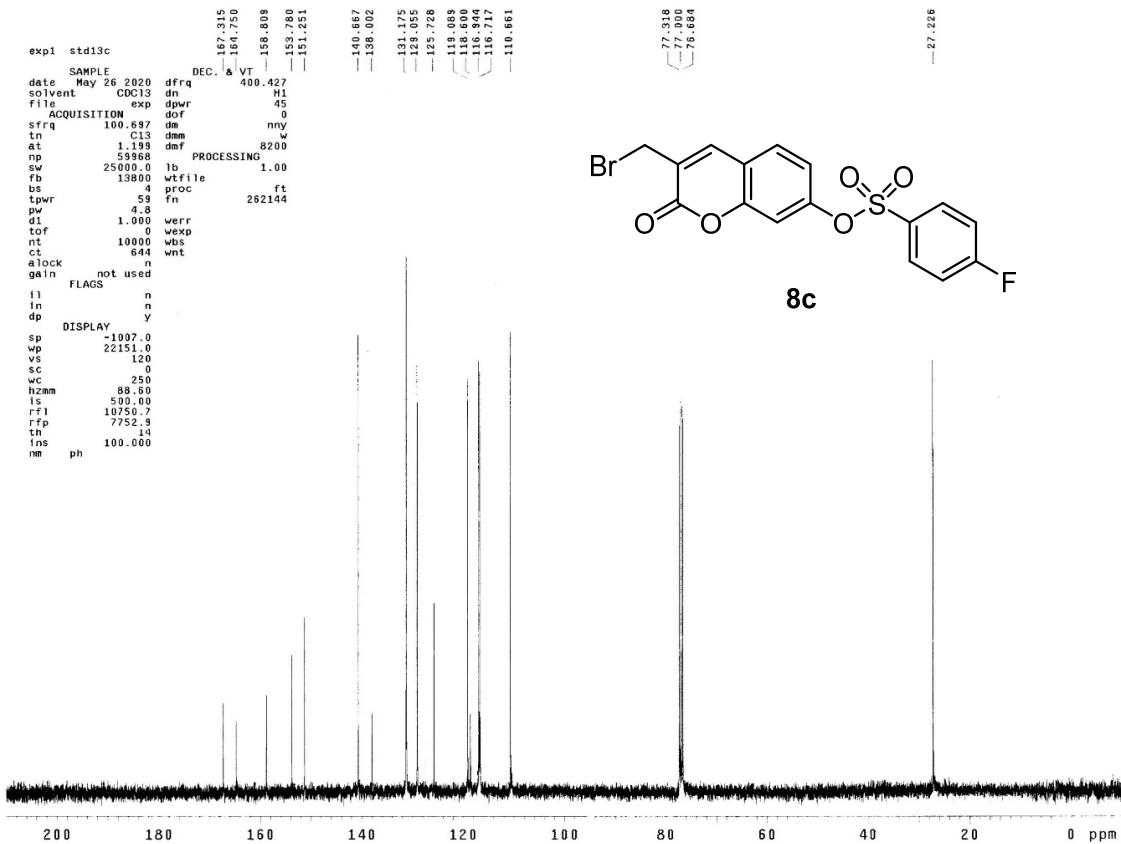
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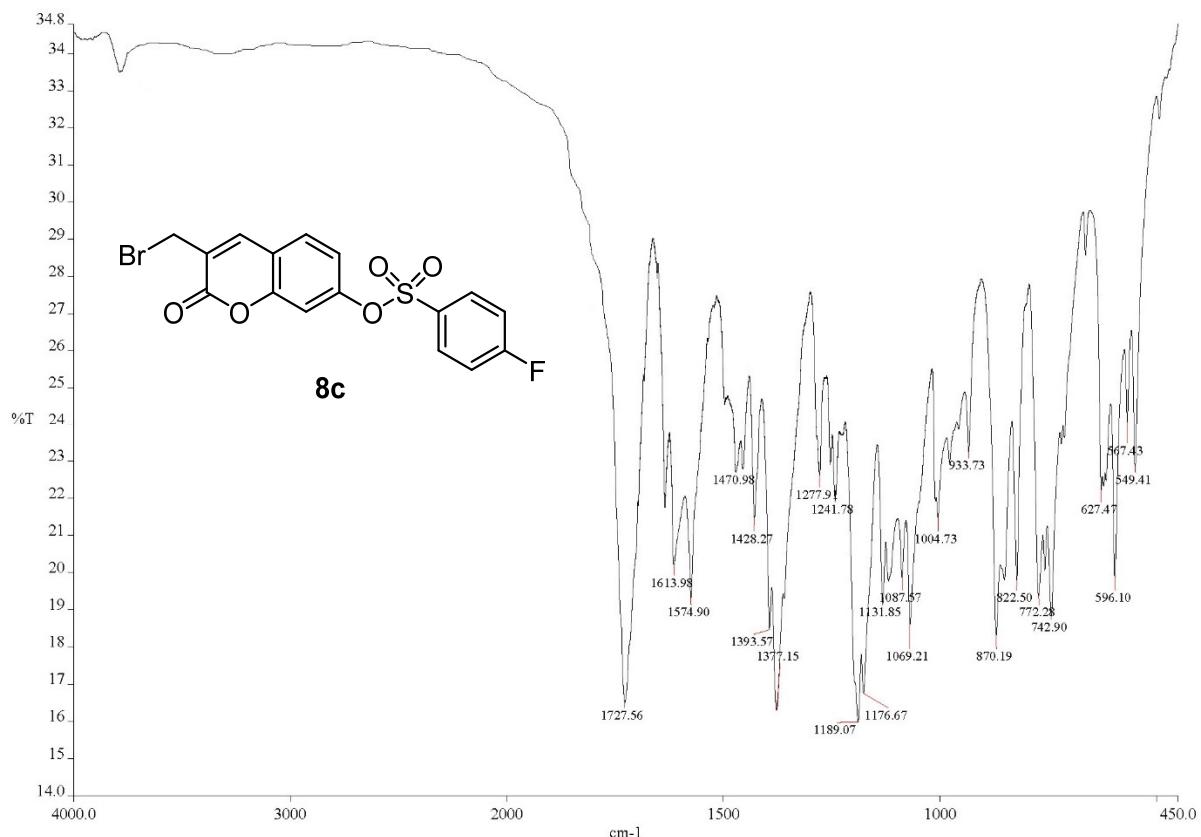
IR spectrum of compound **8b**



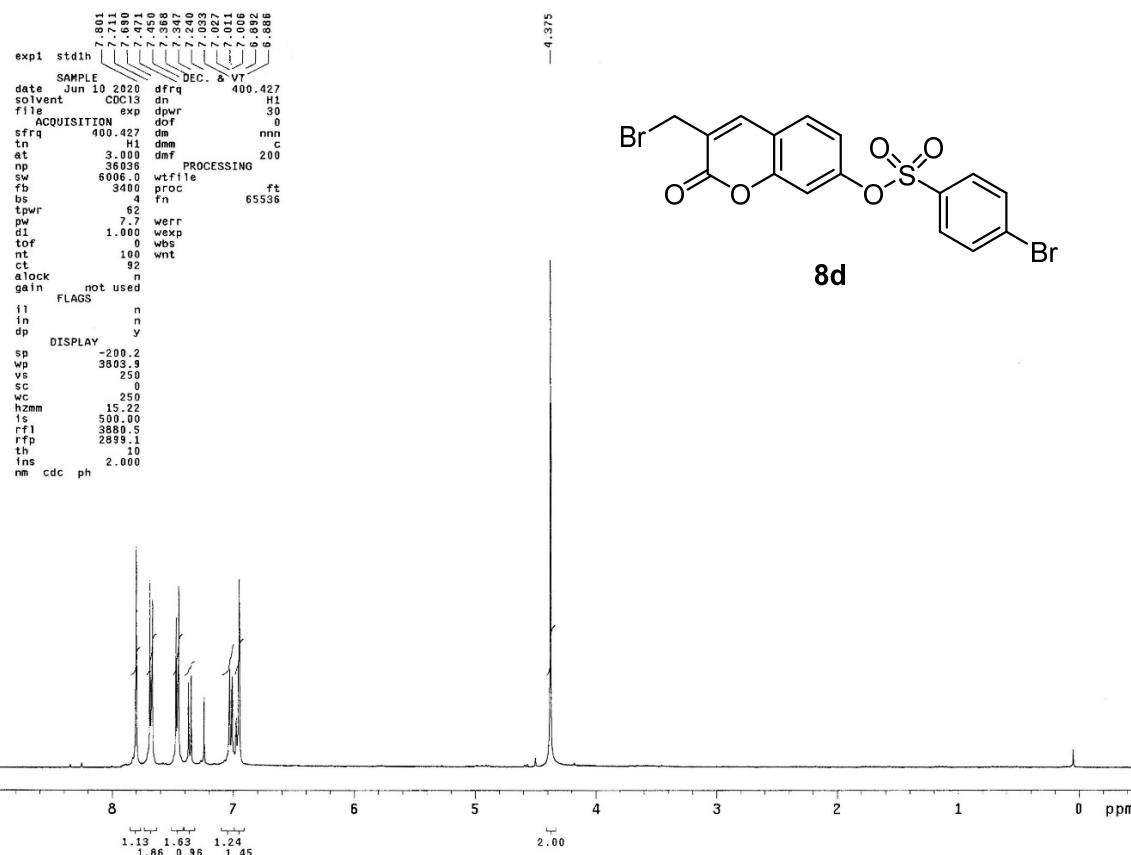
¹H NMR spectrum of compound **8c**



¹³C NMR spectrum of compound **8c**



IR spectrum of compound **8c**

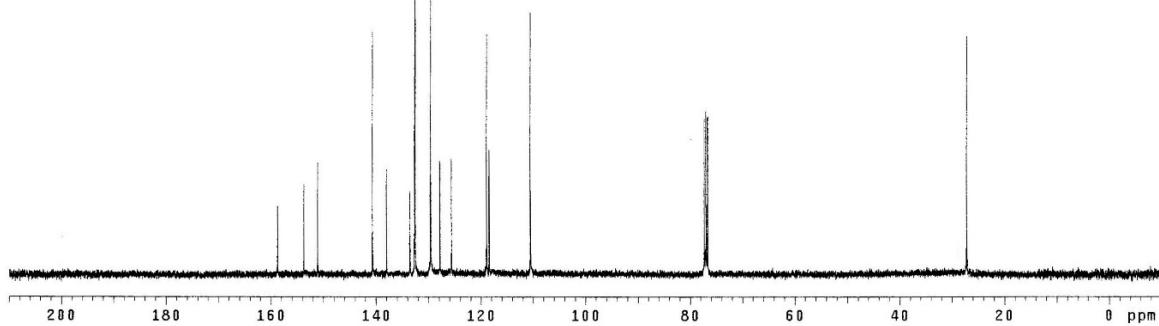
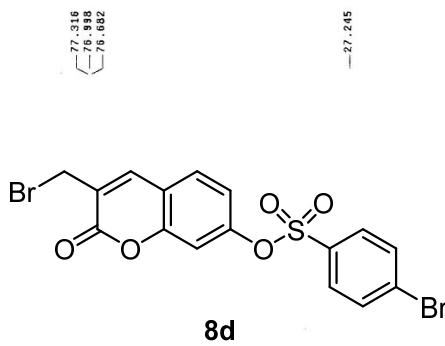


¹H NMR spectrum of compound **8d**

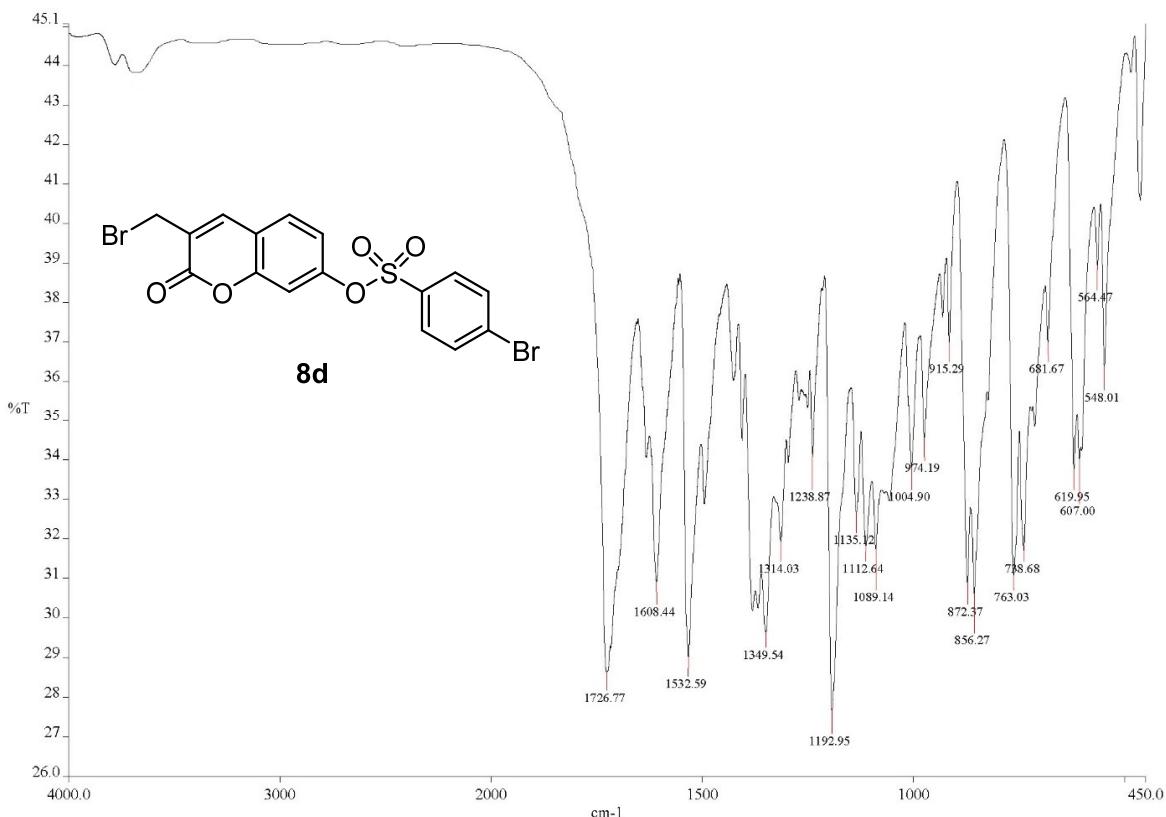
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tn      C13      dmm      137.973
at      1        dmt      138.508
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at      1        dmt      129.696
at      1        dmt      127.861
at      1        dmt      125.666
at      1        dmt      118.943
at      1        dmt      118.452
at      1        dmt      110.568
np      53368    PROCESSING
sw      25000.0   lb        262144
fb      13800    wfile      1.00
bs      58       proc      77.316
tpwr   4.8      fn        76.938
pw      1.000   werr      76.682
d1      1.000   wexp
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gain   not used
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nm no ph

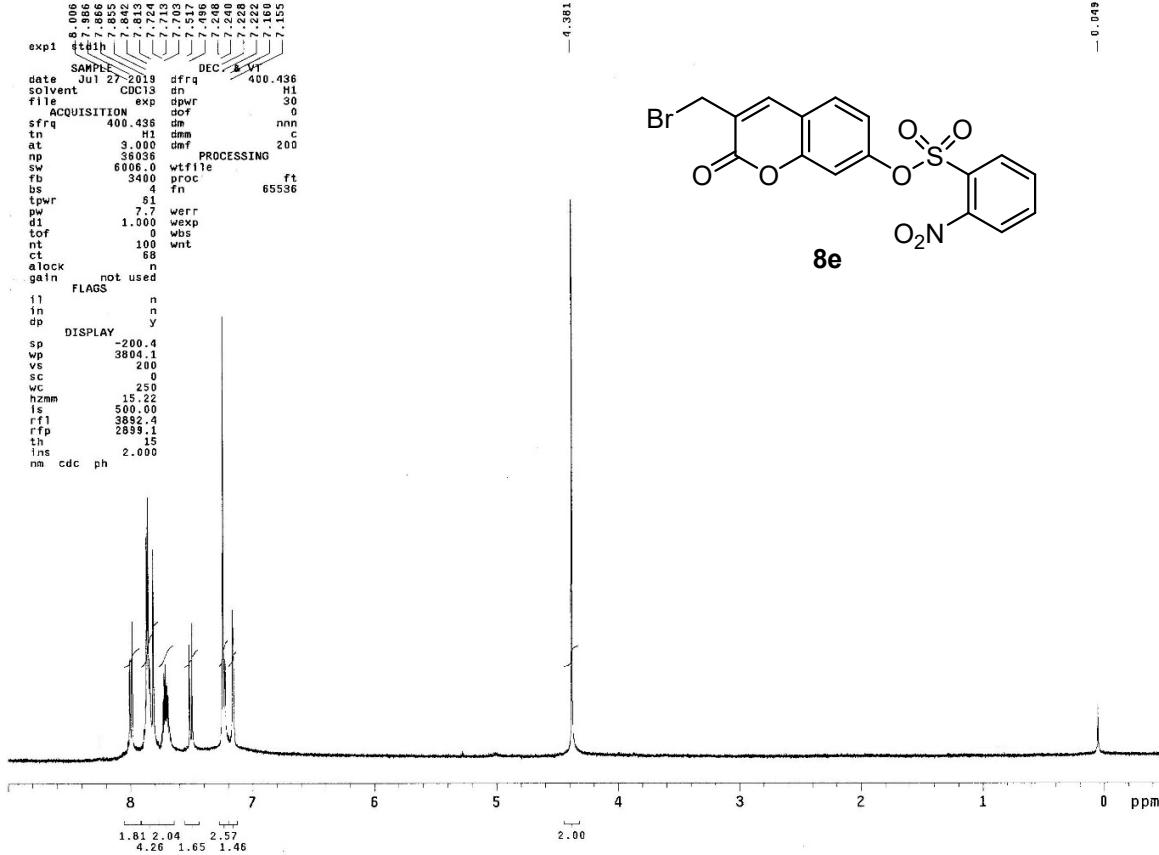
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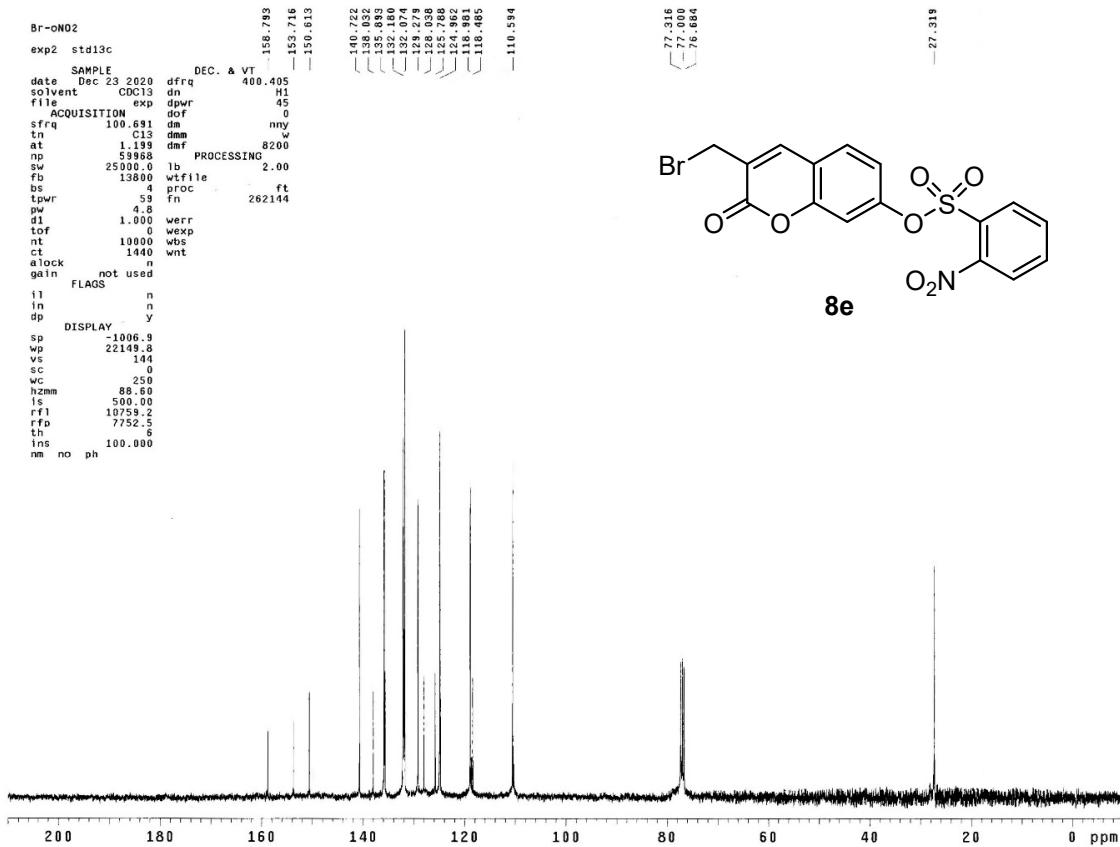
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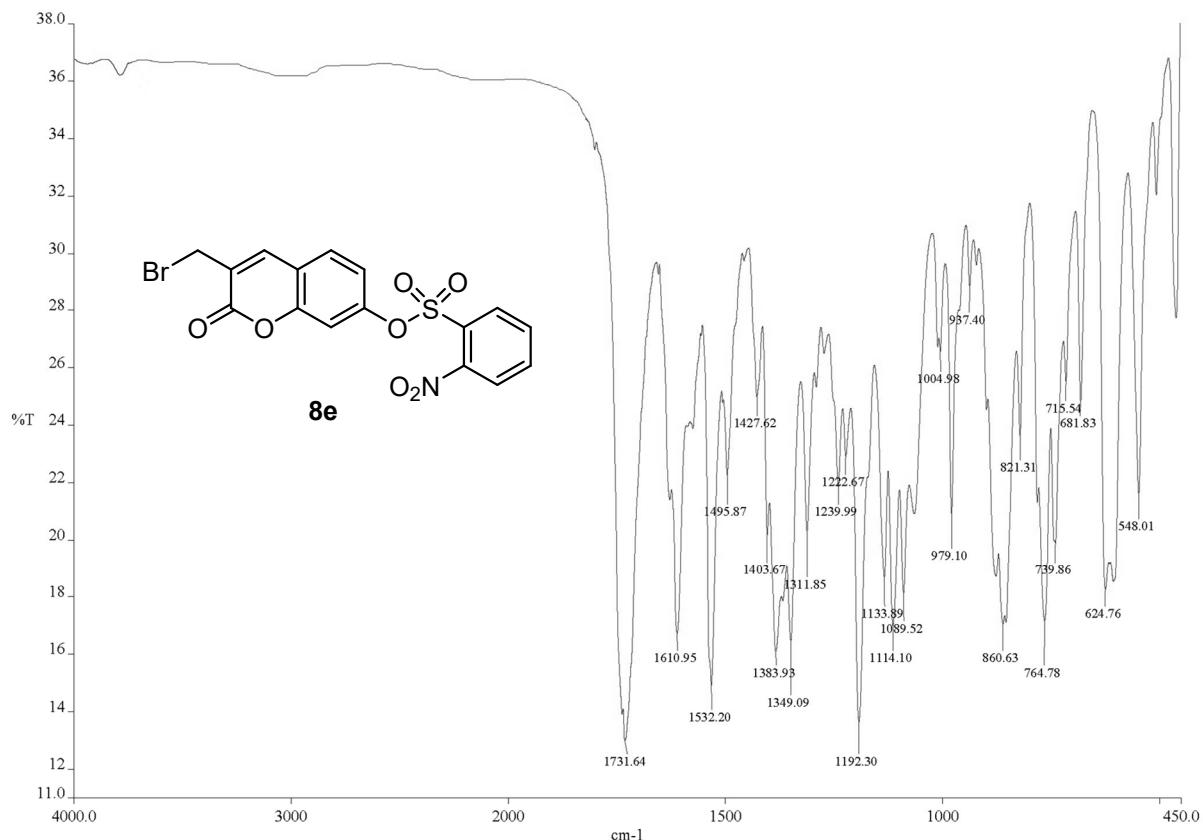
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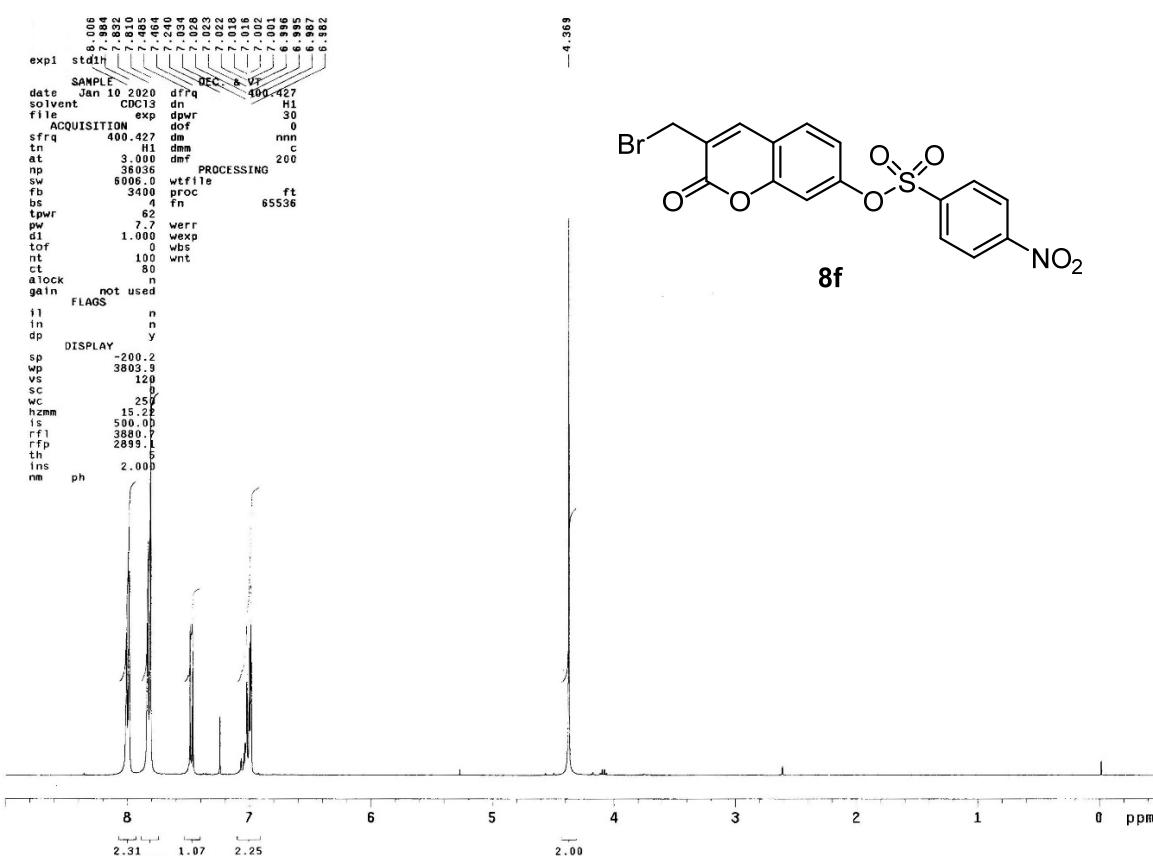
¹H NMR spectrum of compound **8e**



¹³C NMR spectrum of compound **8e**



IR spectrum of compound **8e**

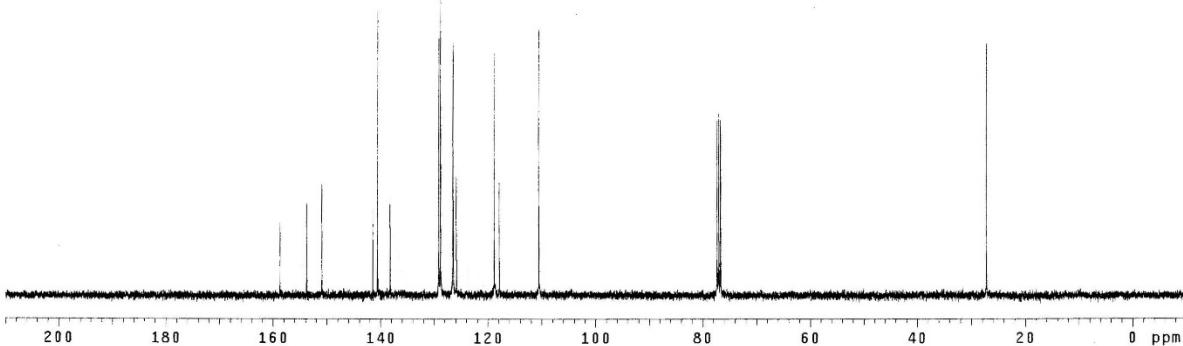
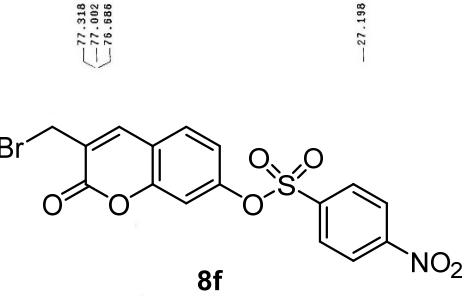


¹H NMR spectrum of compound **8f**

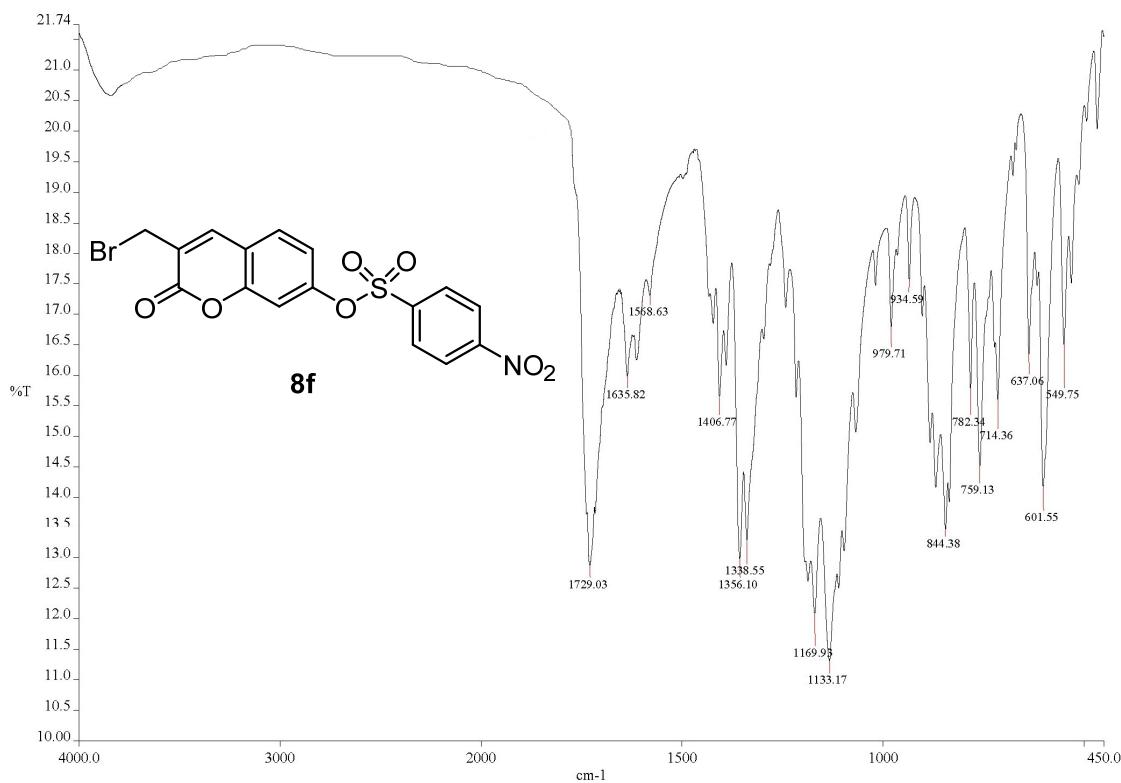
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sw      25000.0 wfile
fb      138000 wtfle
bs      4 proc
tppr    5 fn        262144
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dl      1.000 werr
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gain
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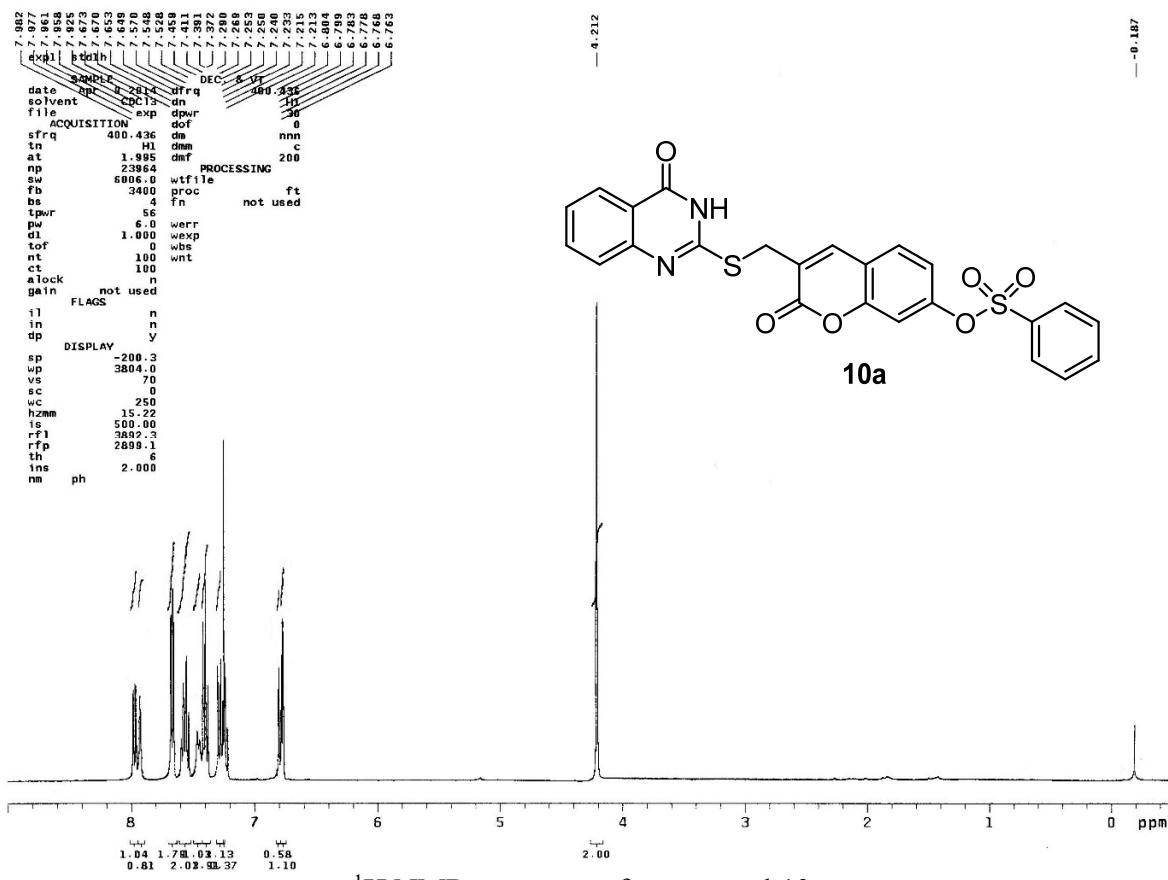
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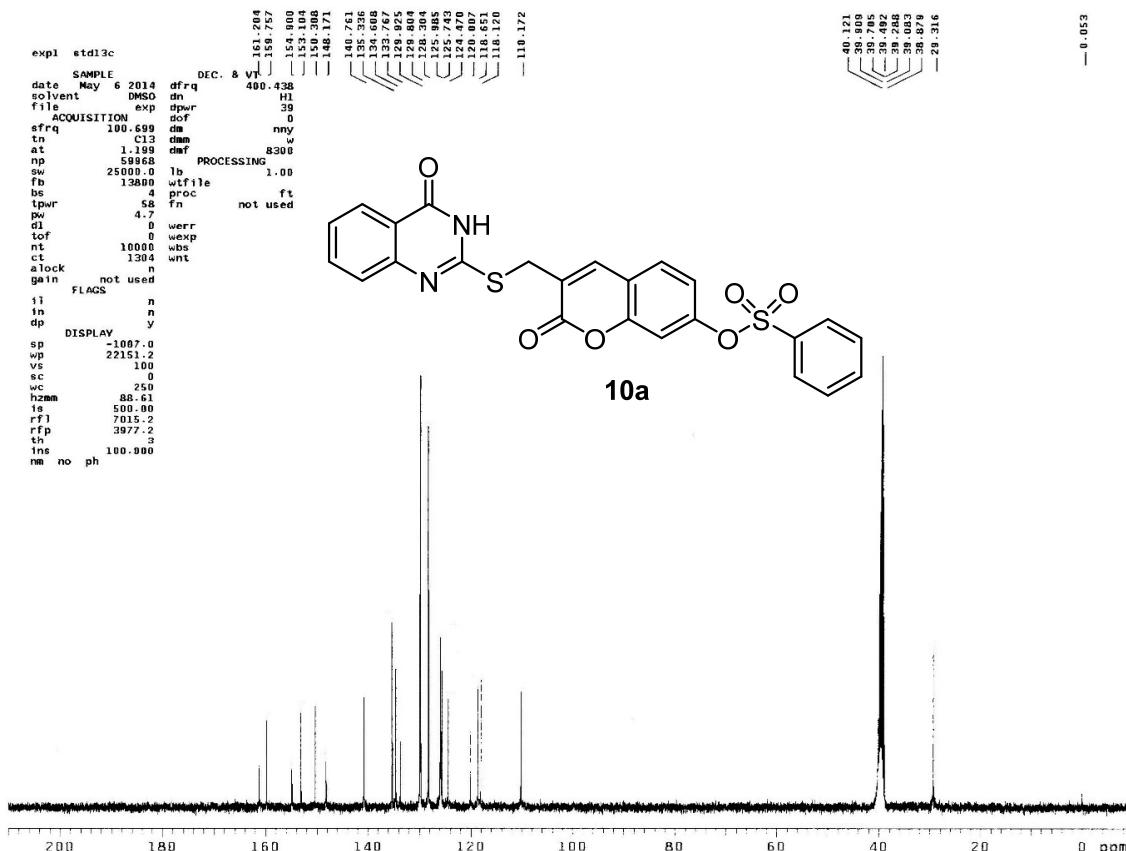
^{13}C NMR spectrum of compound **8f**



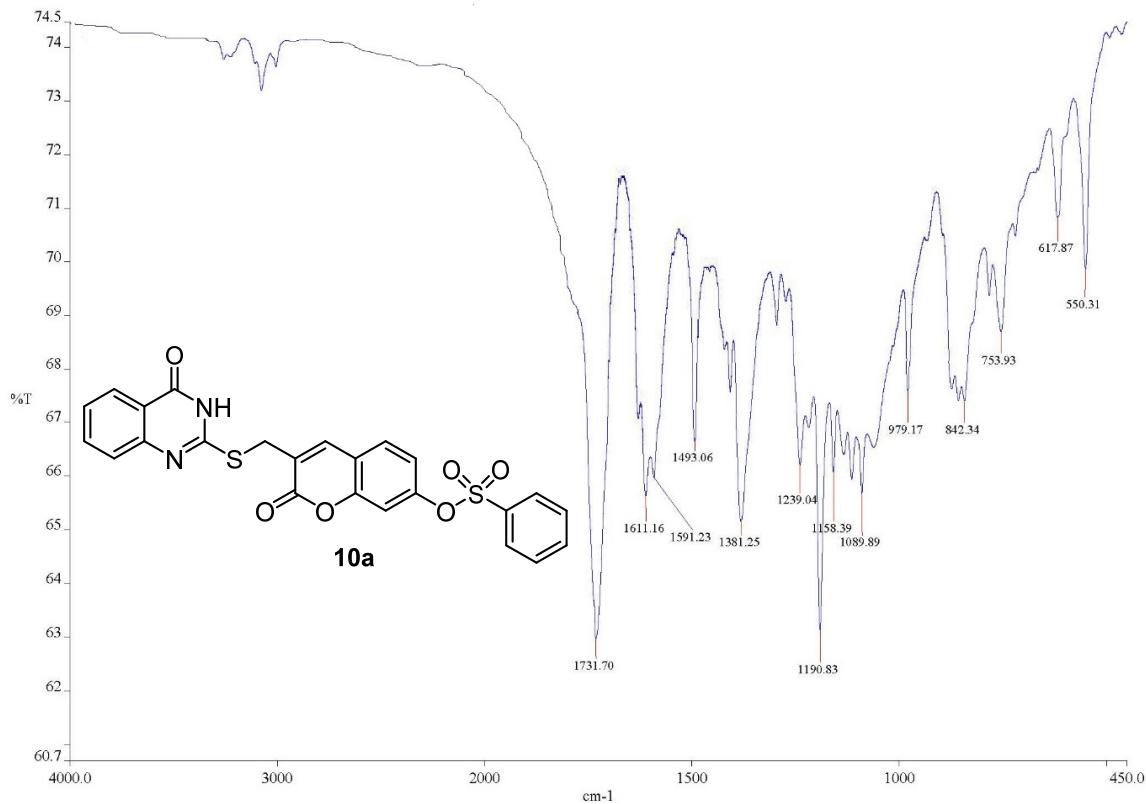
IR spectrum of compound **8f**



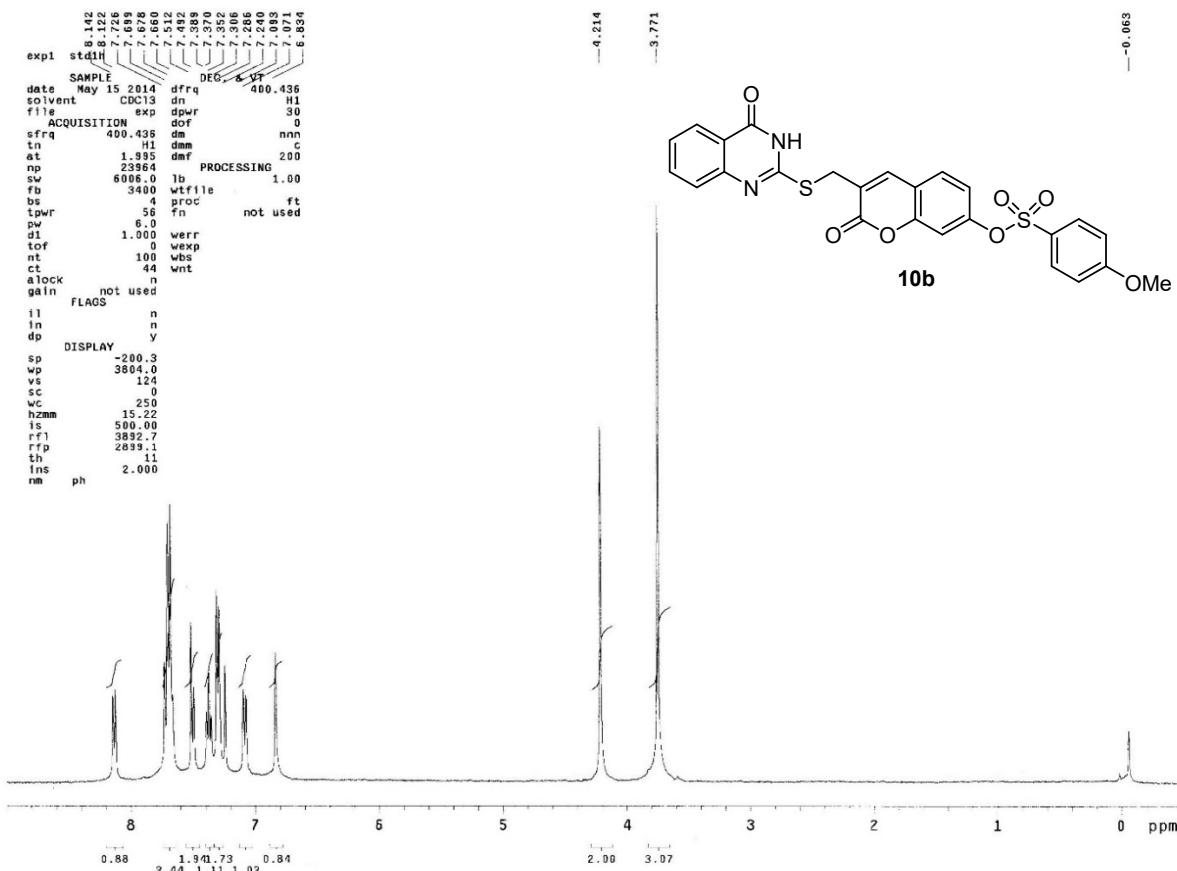
¹H NMR spectrum of compound **10a**



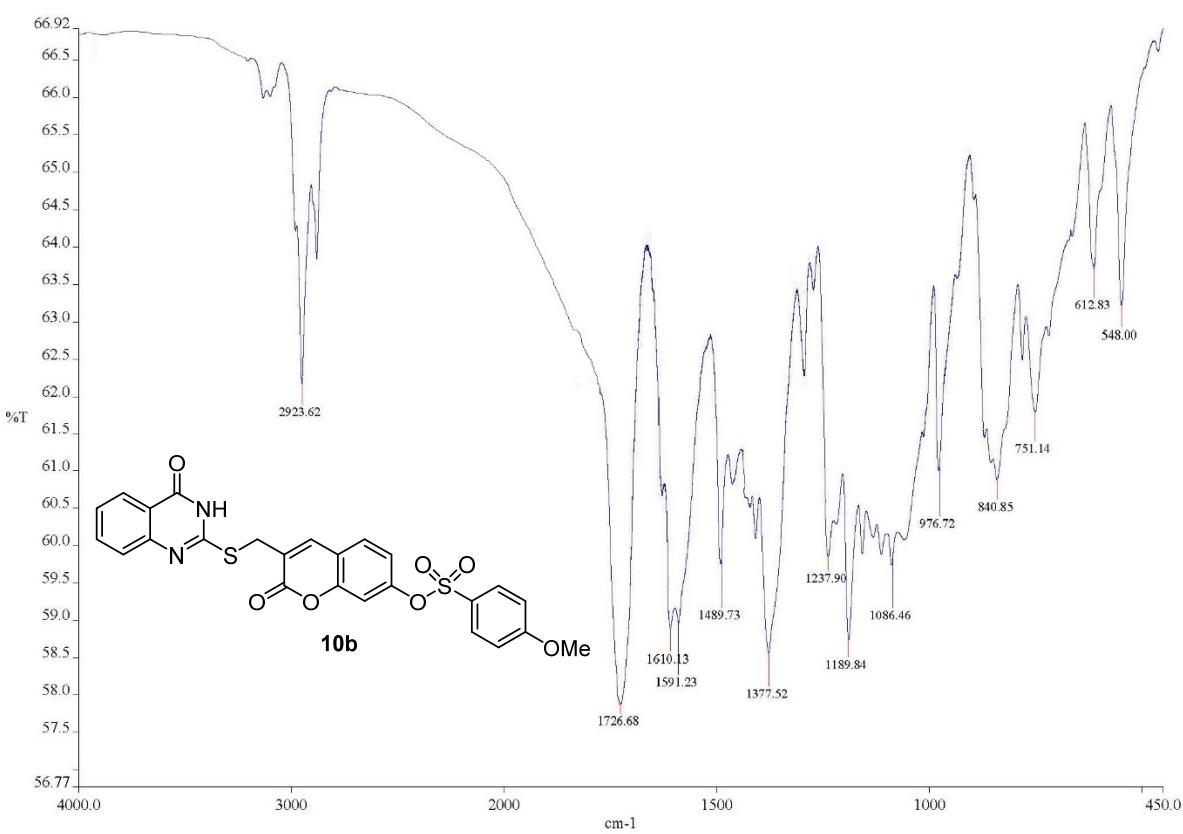
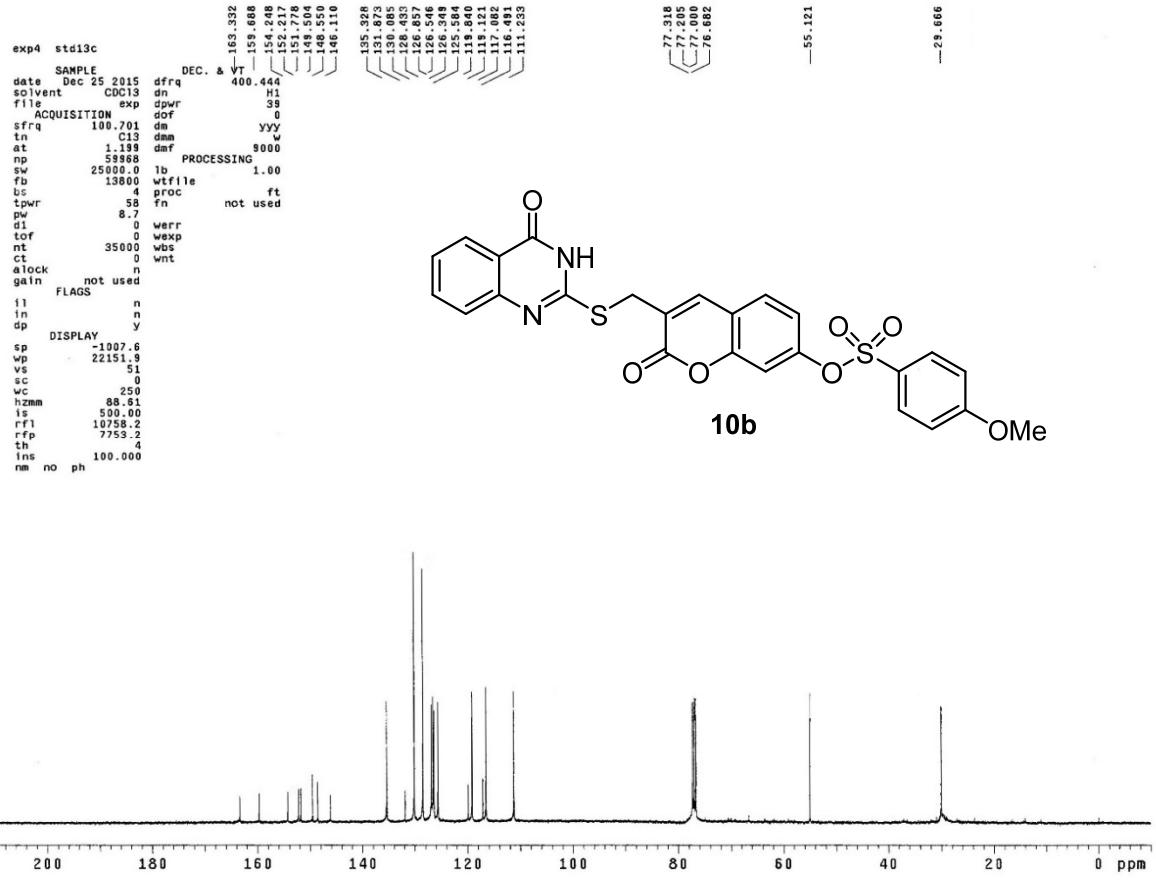
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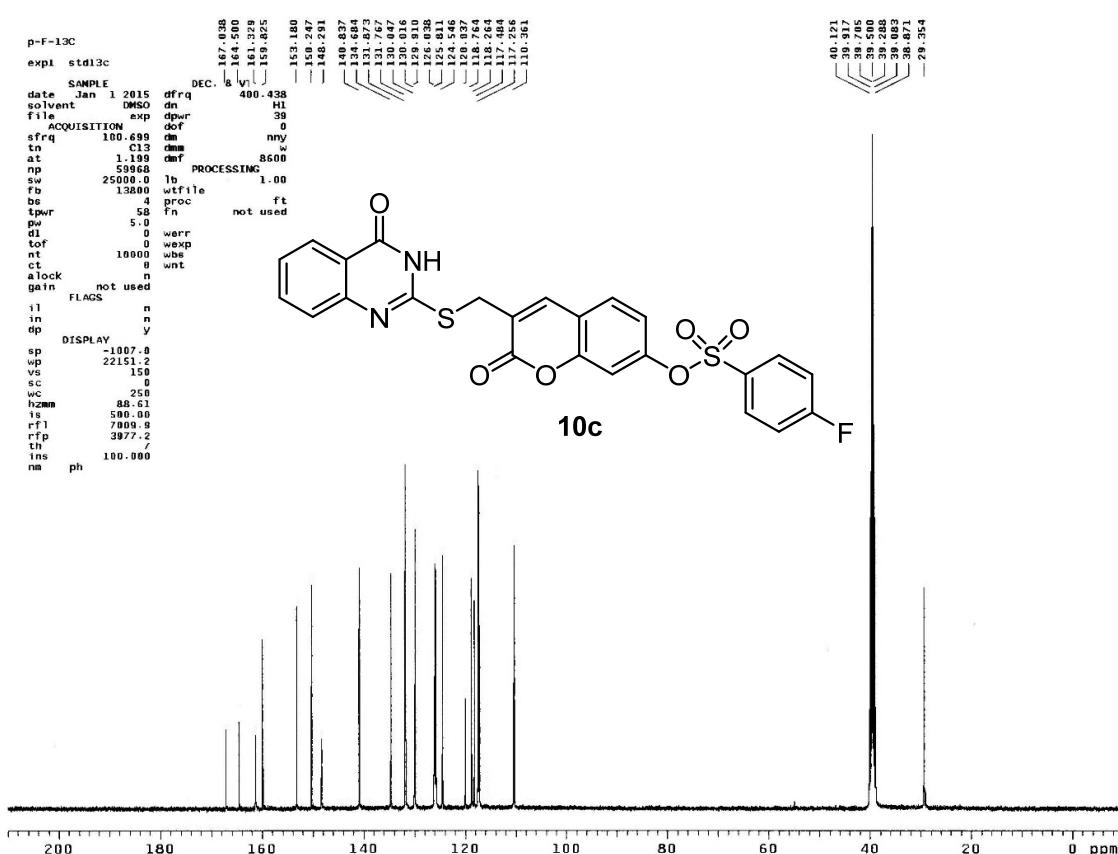
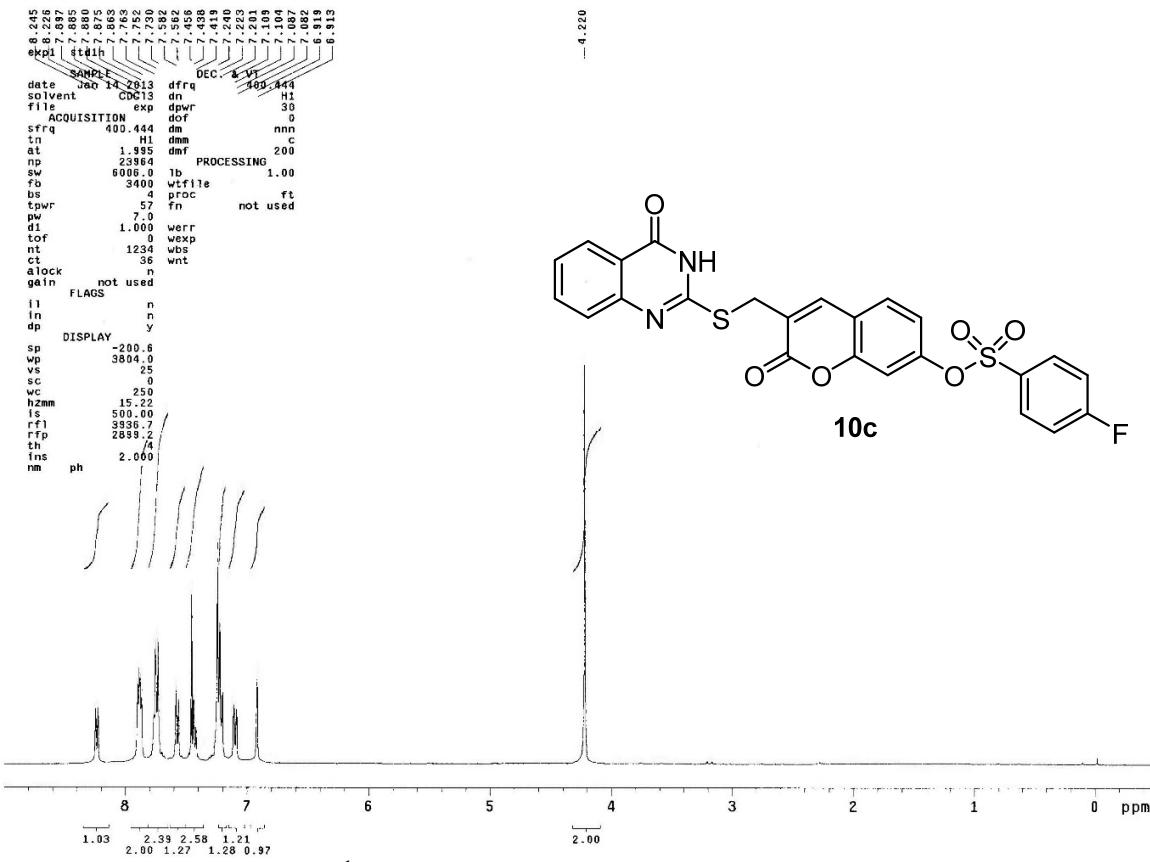


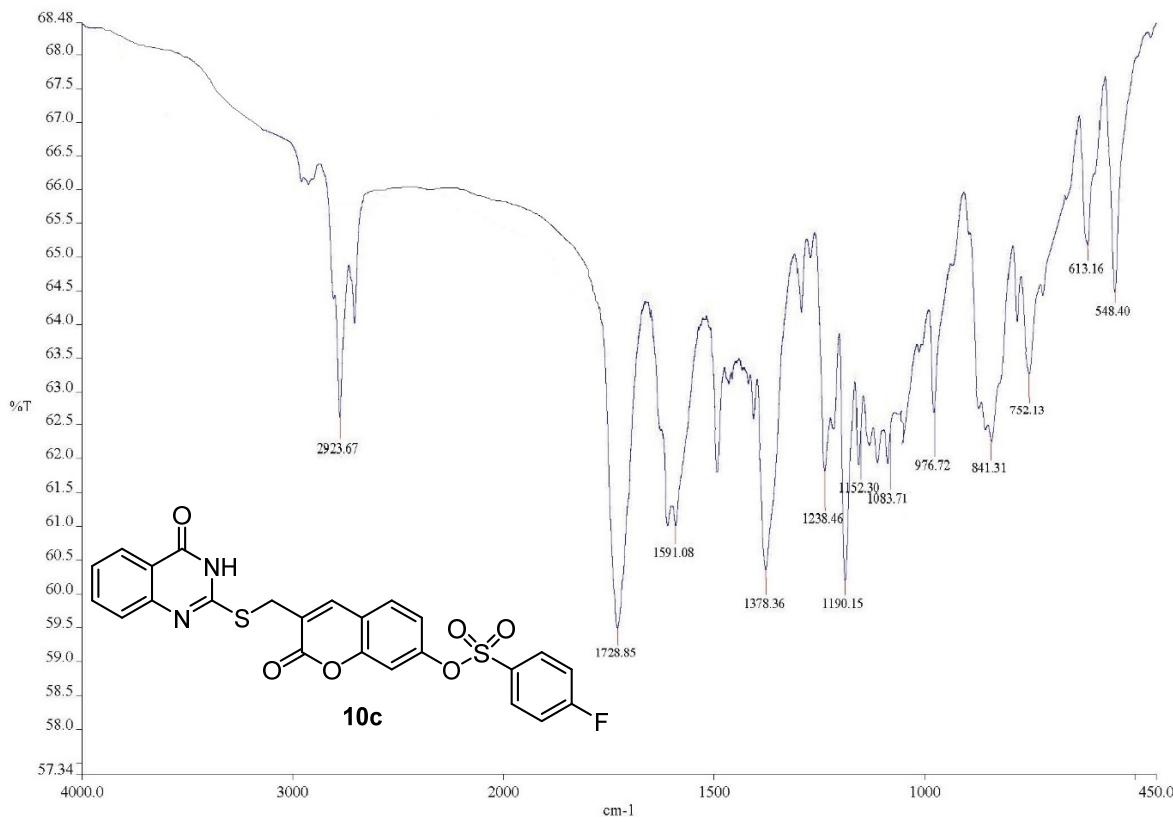
IR spectrum of compound **10a**



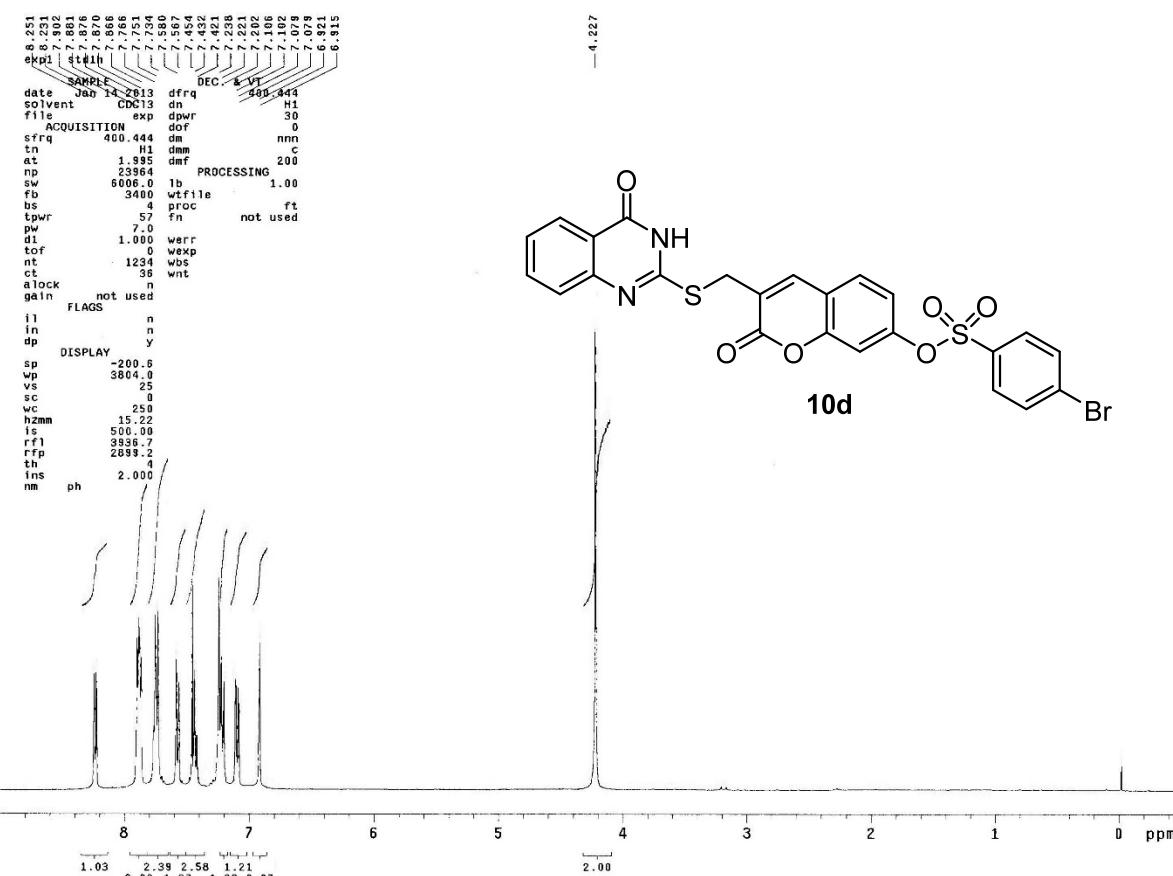
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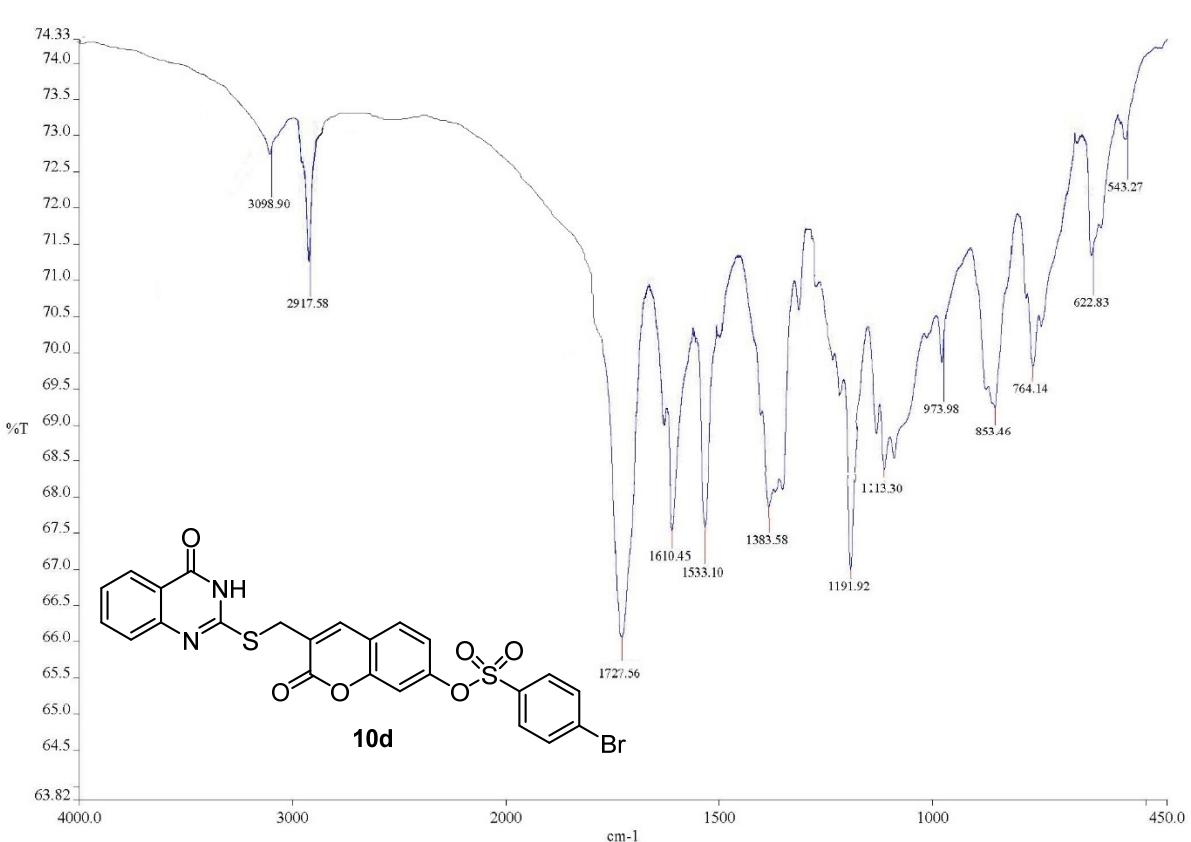
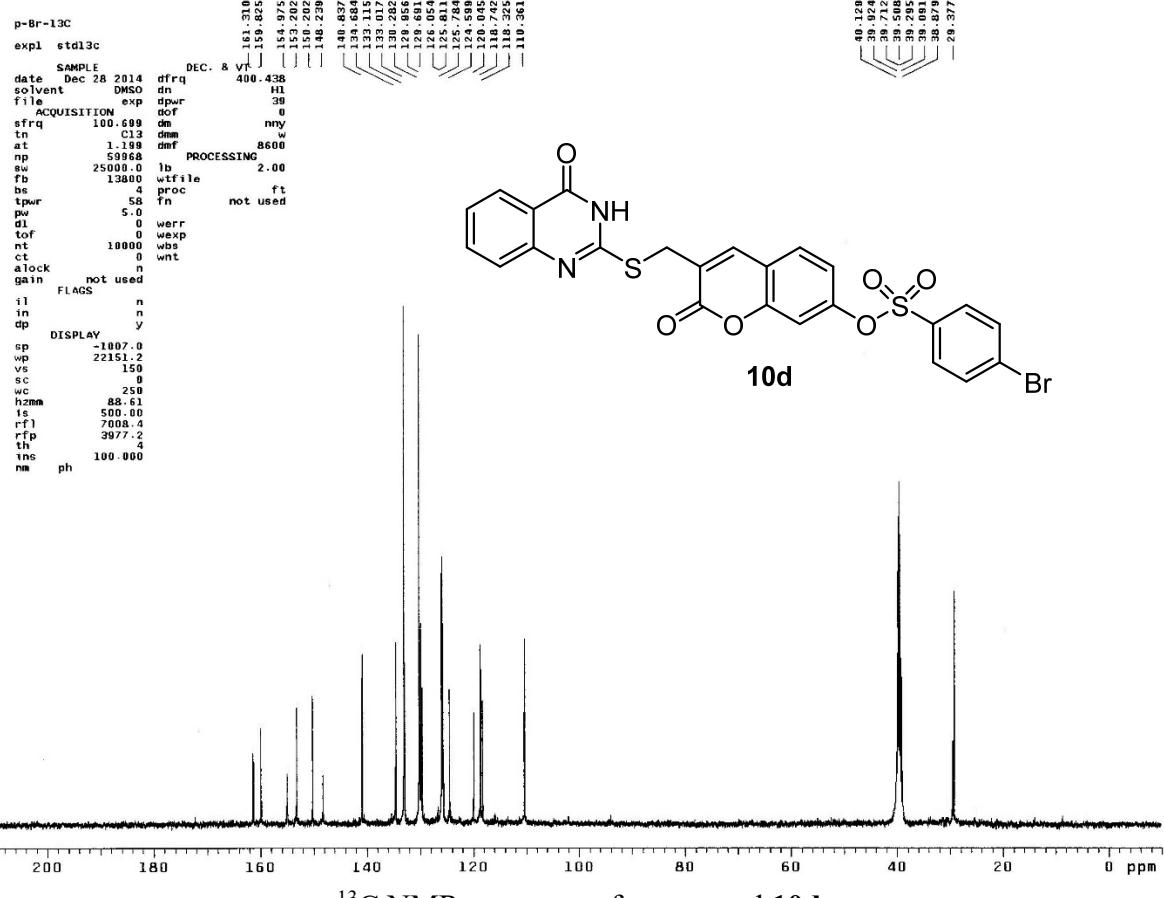


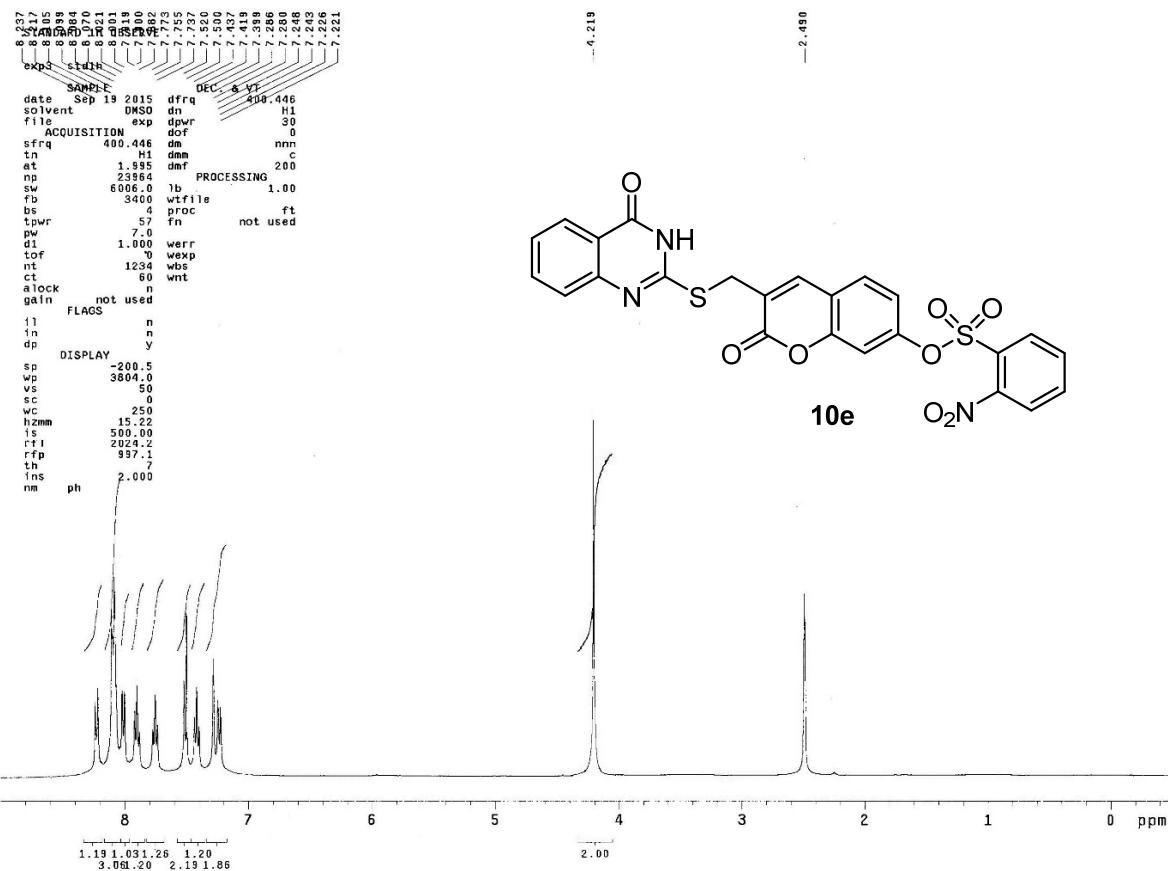


IR spectrum of compound **10c**

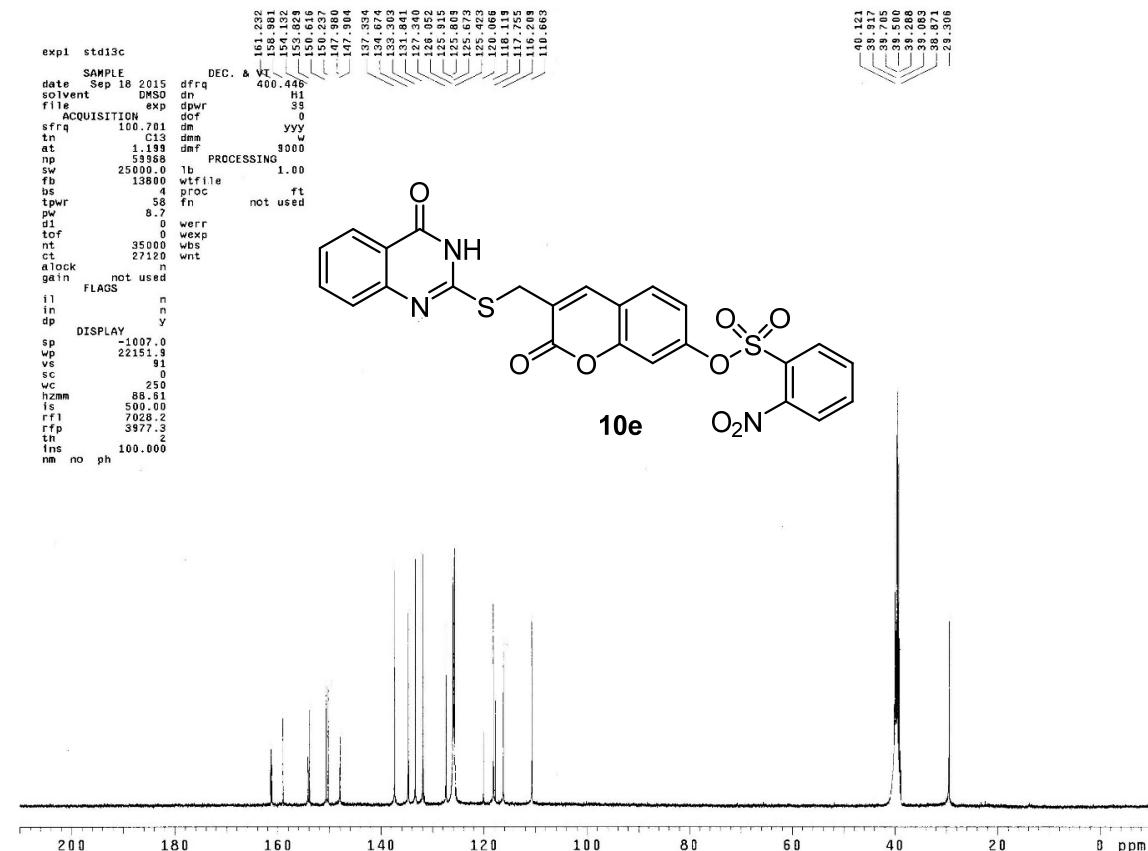


¹H NMR spectrum of compound **10d**

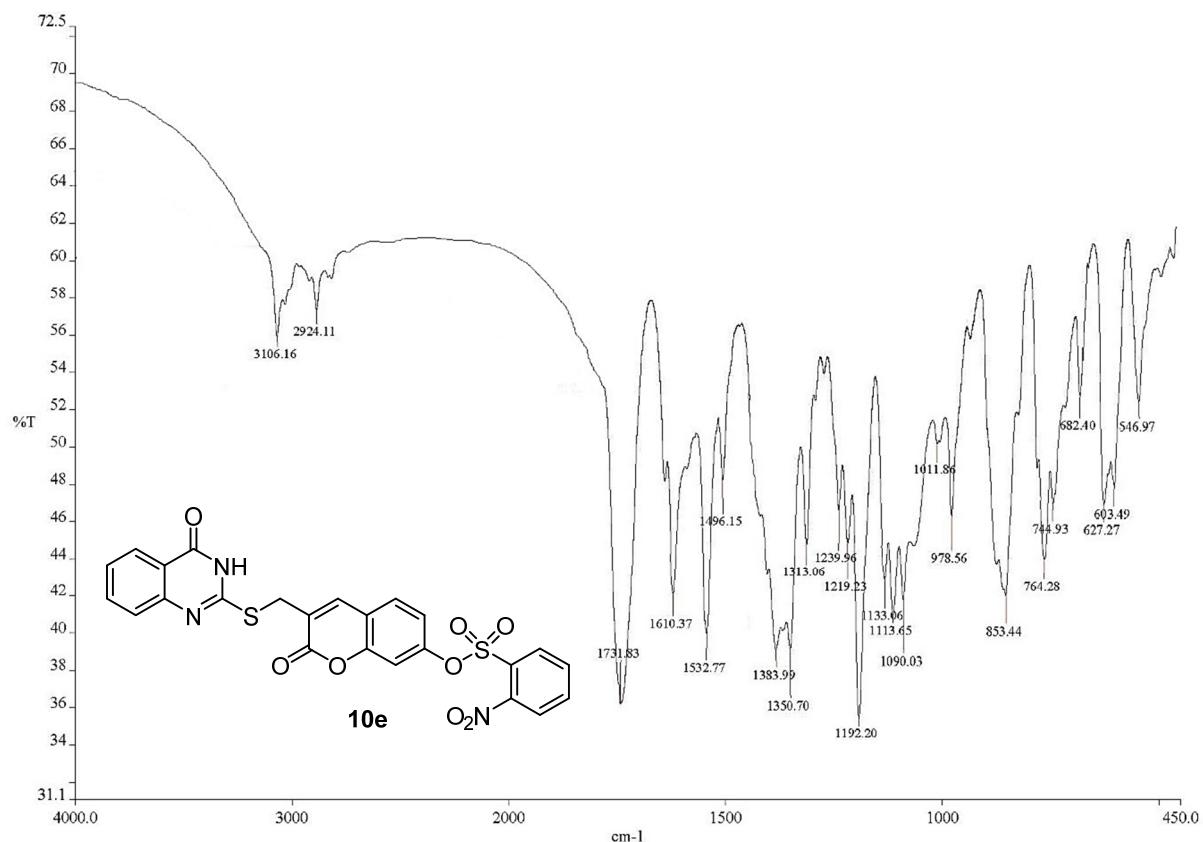




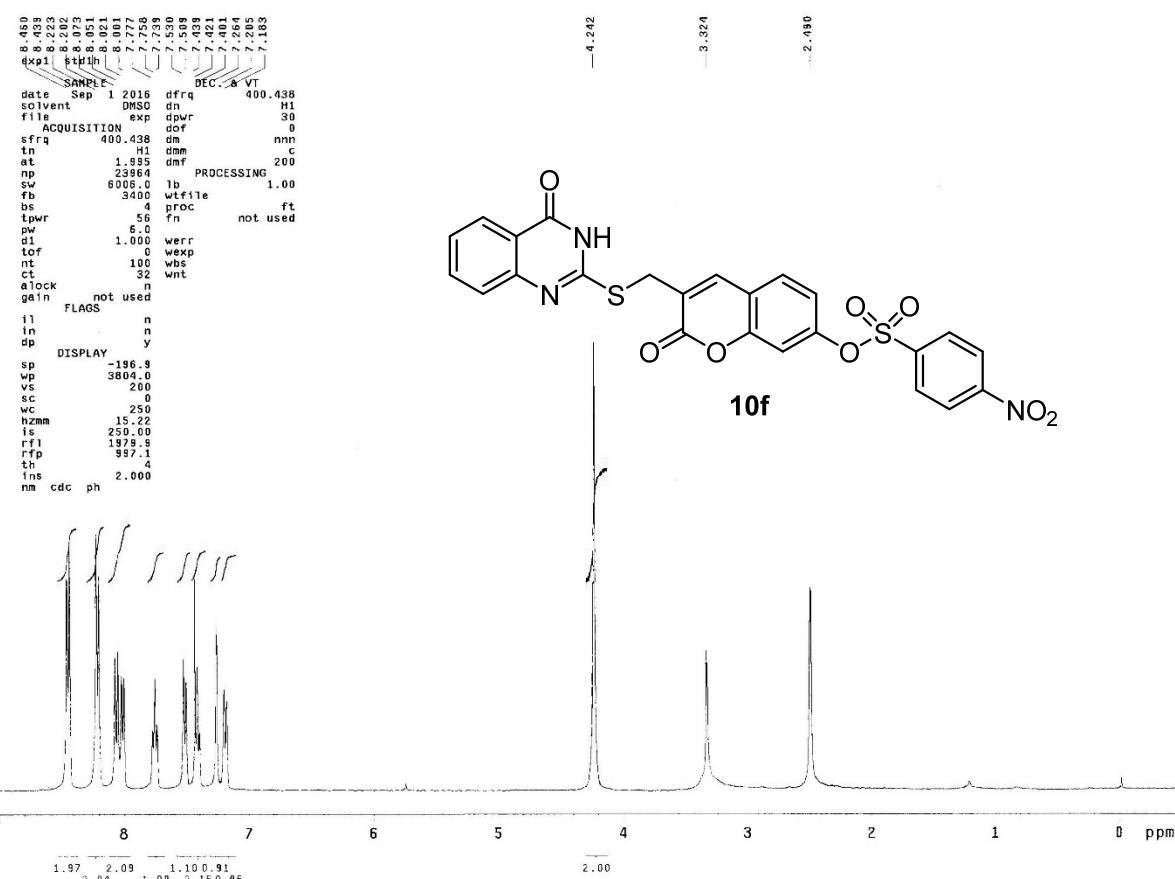
¹H NMR spectrum of compound 10e



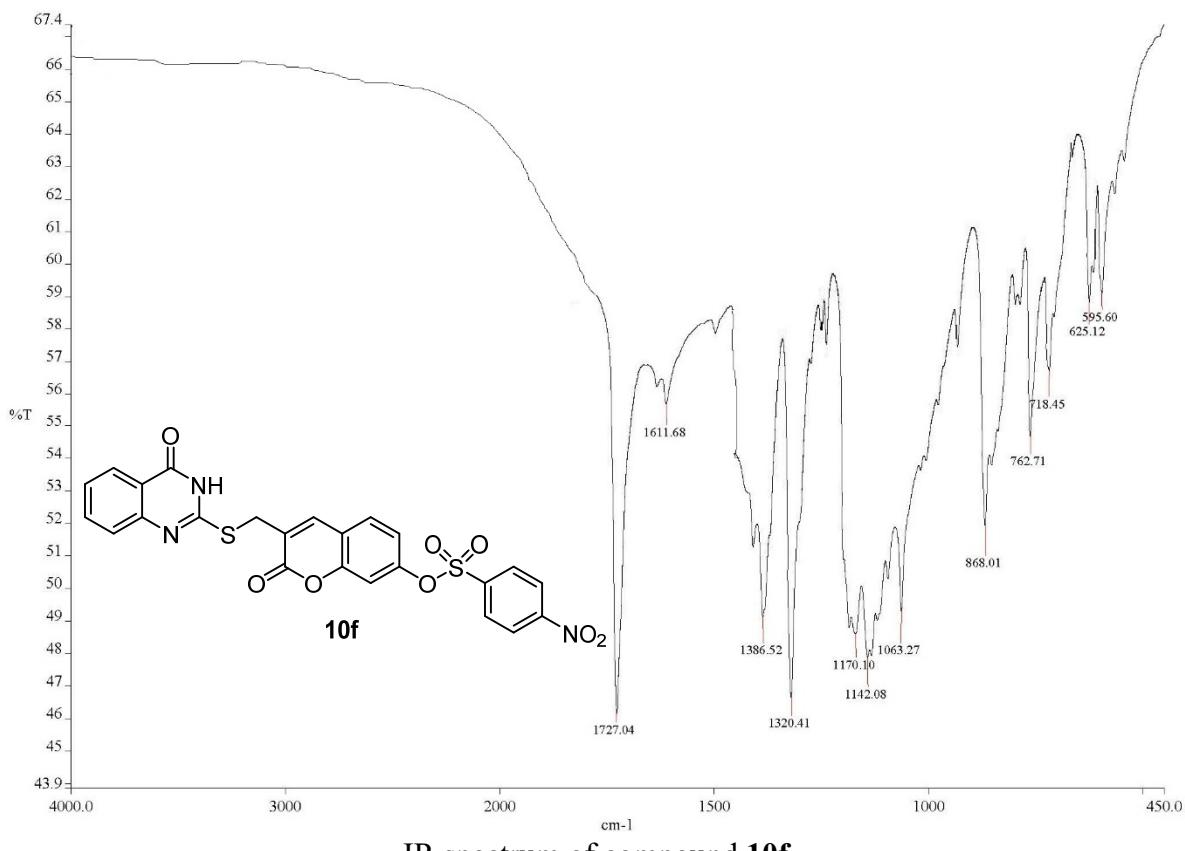
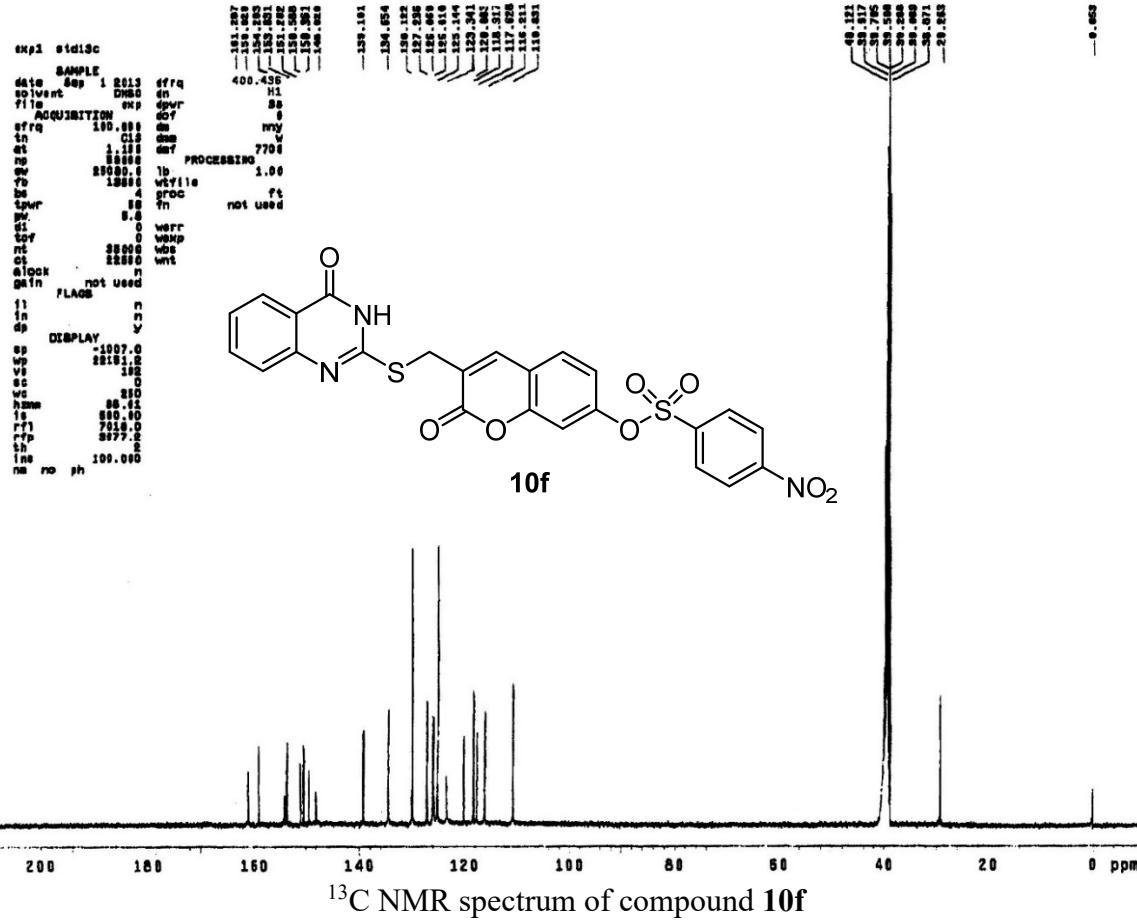
¹³C NMR spectrum of compound 10e

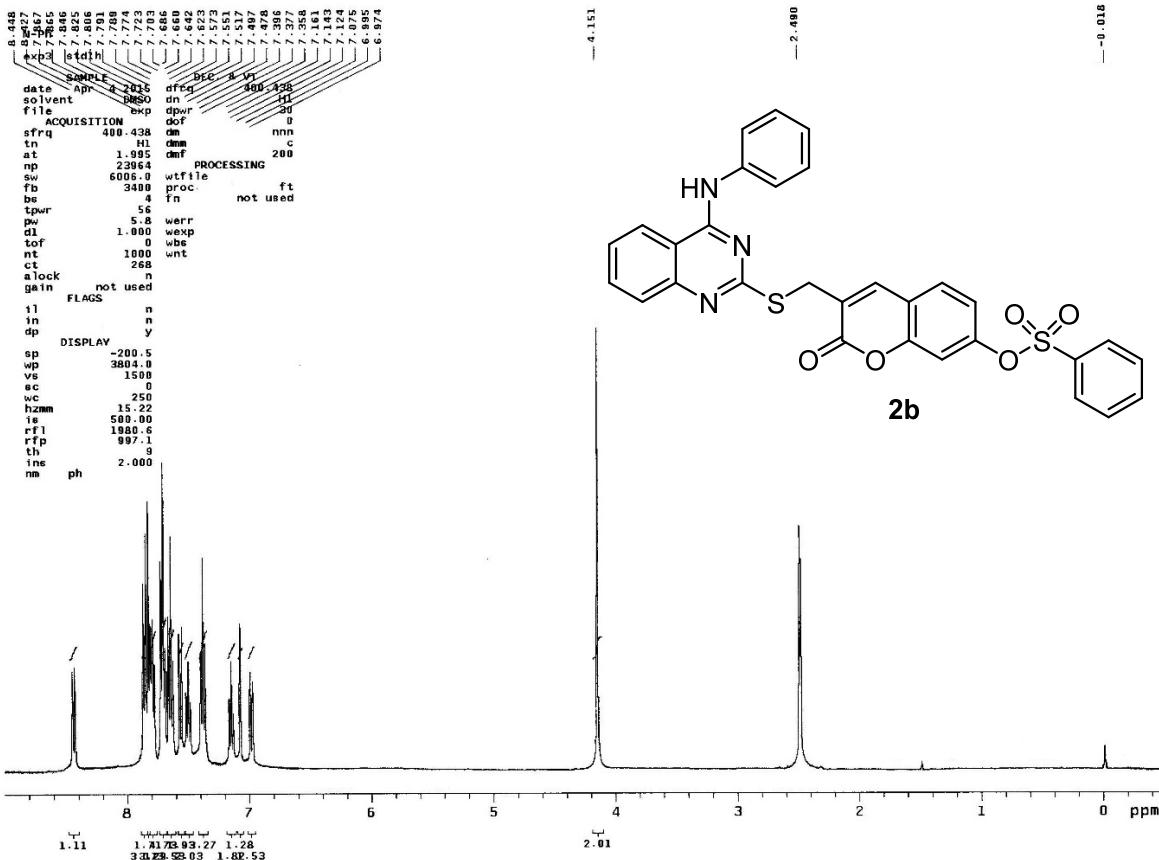


IR spectrum of compound **10e**

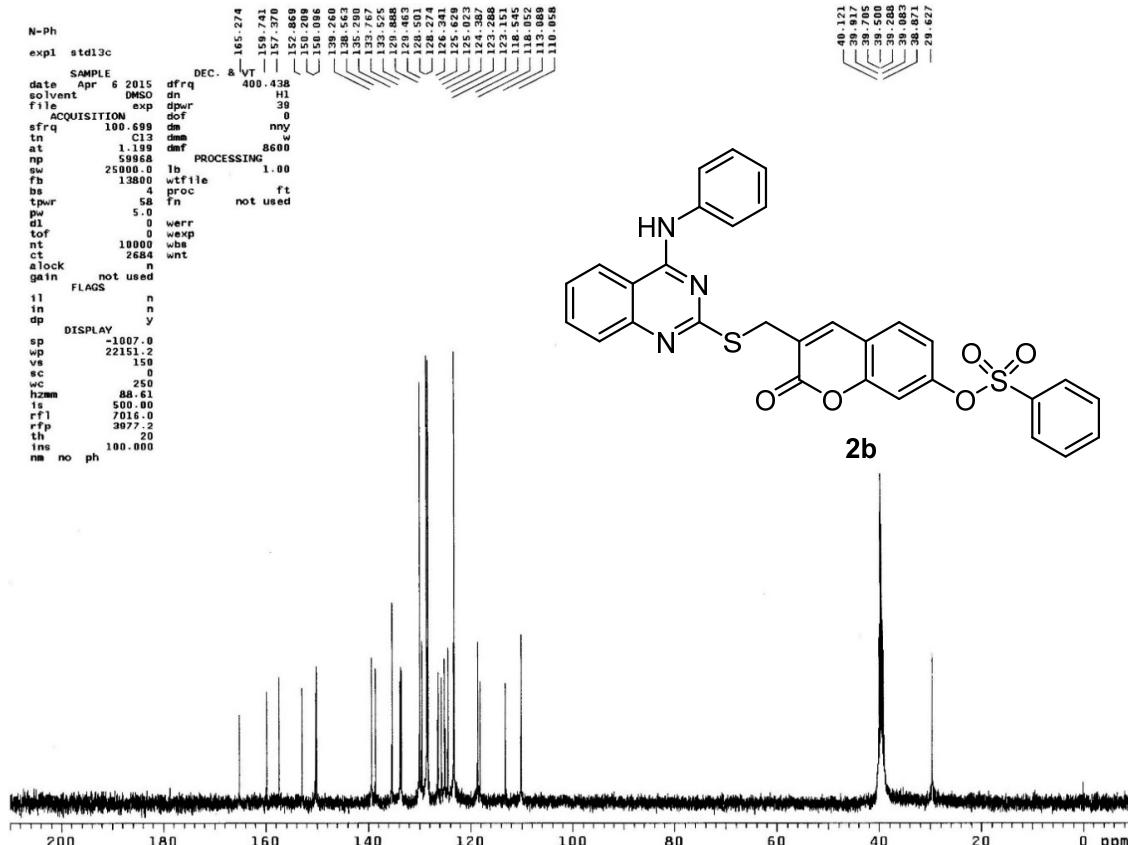


¹H NMR spectrum of compound **10f**

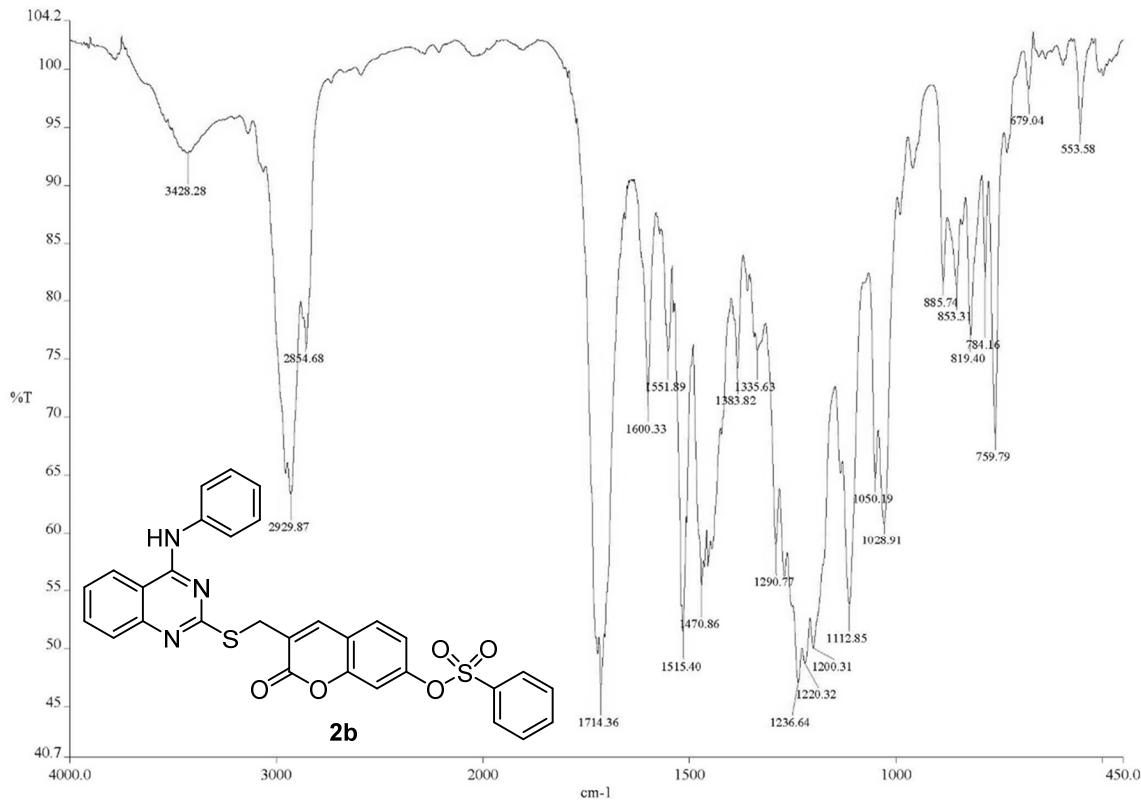




¹H NMR spectrum of compound **2b**

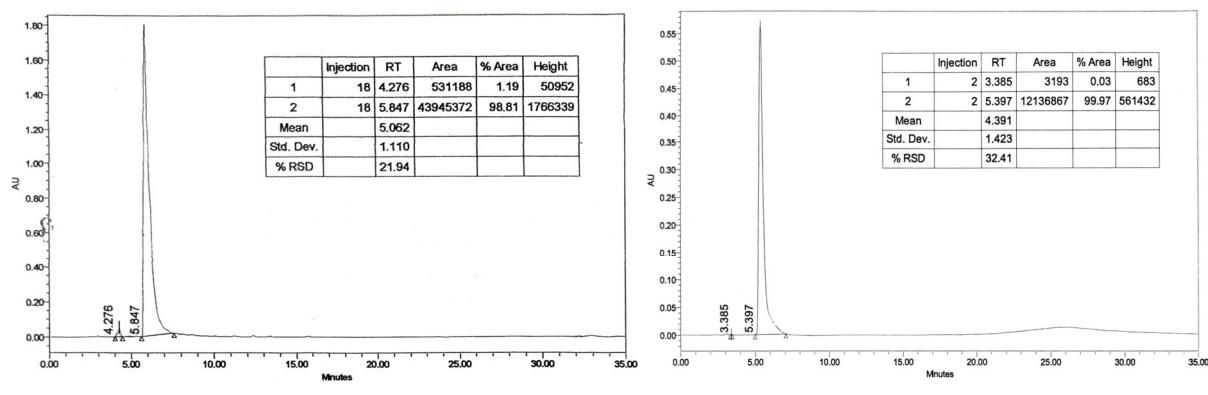


¹³C NMR spectrum of compound **2b**



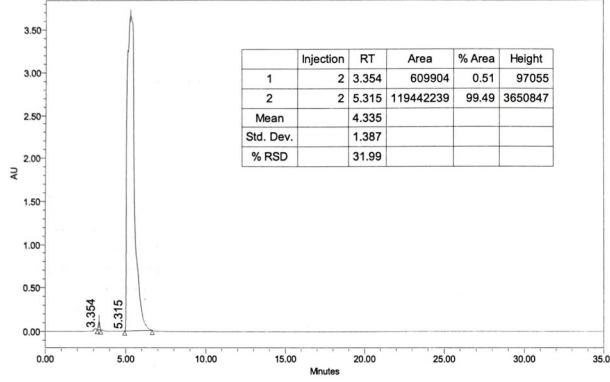
IR spectrum of compound **2b**

HPLC chromatograms for traces of final compounds

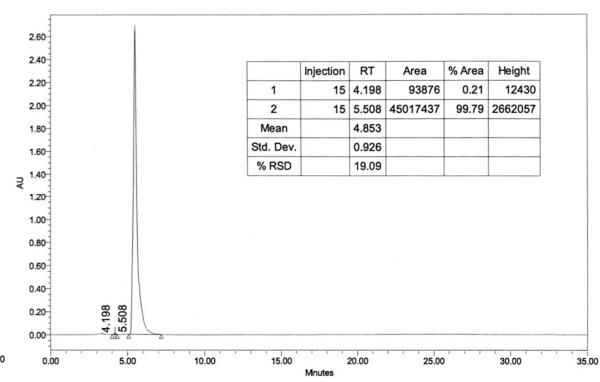


10a

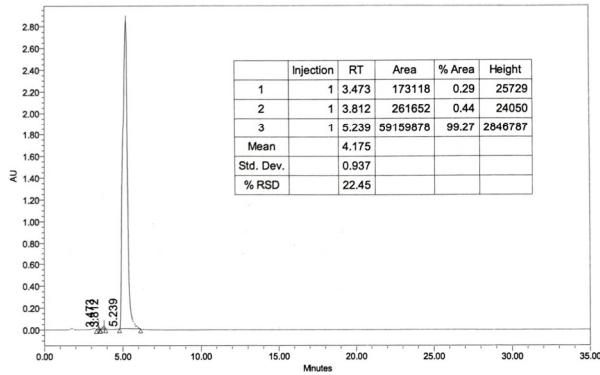
10b



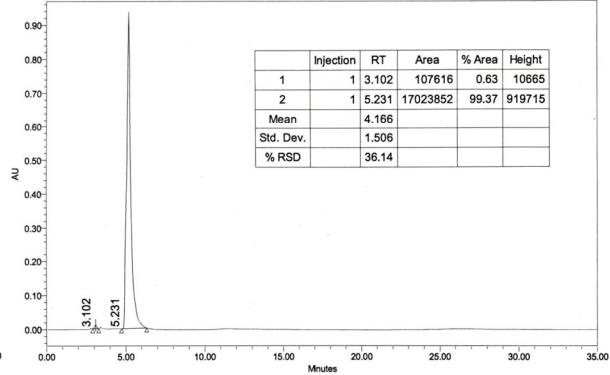
10c



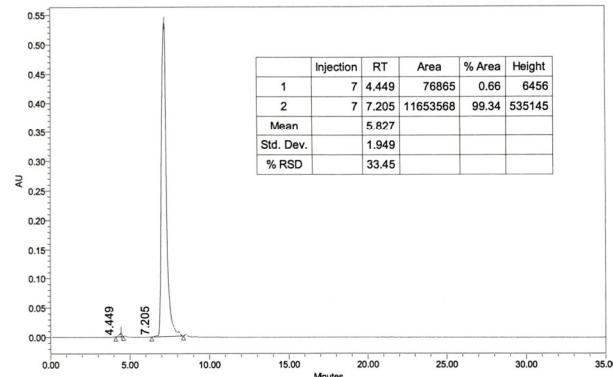
10d



10e



10f



2b