

Supplementary material

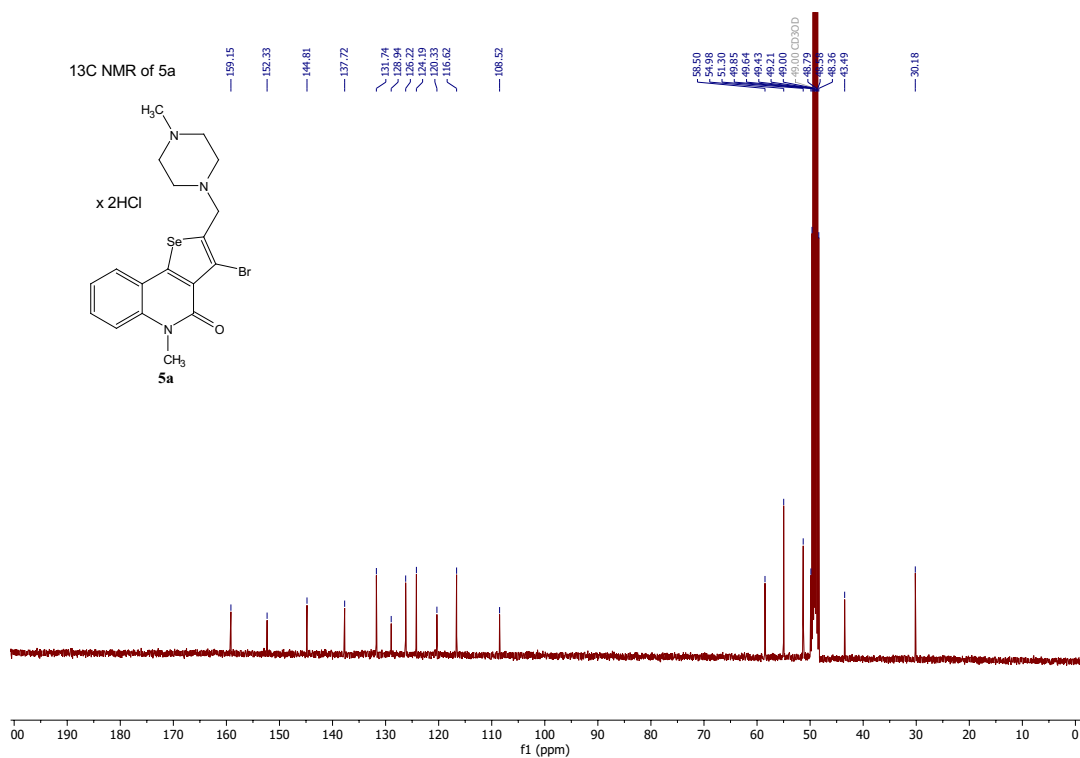
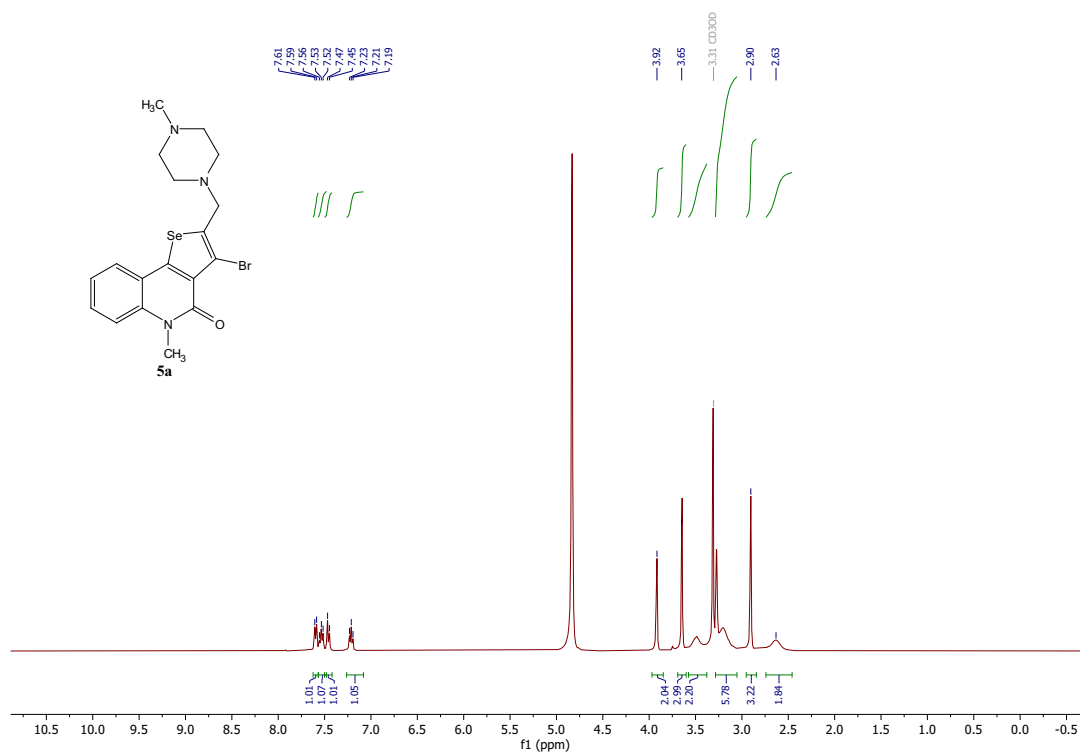
Development of prospective non-toxic inhibitors of ABCB1 activity and expression in series of selenophenoquinolinones

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Dimitrijevs, Pavel Arsenyan*

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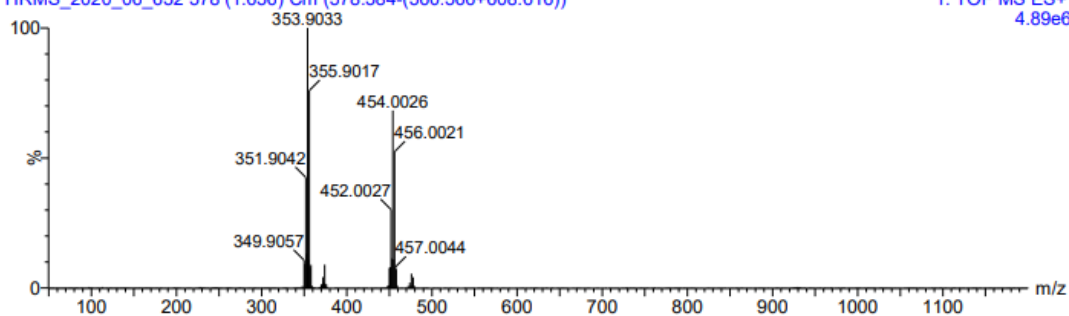
pavel@osi.lv

Compound 5a



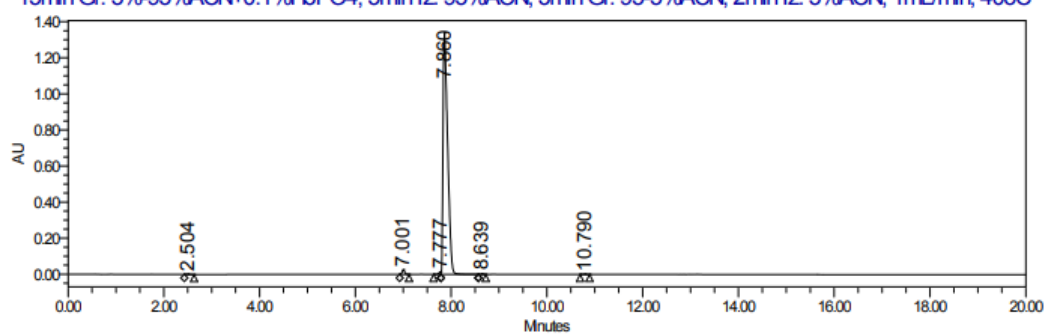
HRMS_2020_06_652 578 (1.656) Cm (578:584-(560:566+608:616))

1: TOF MS ES+
4.89e6

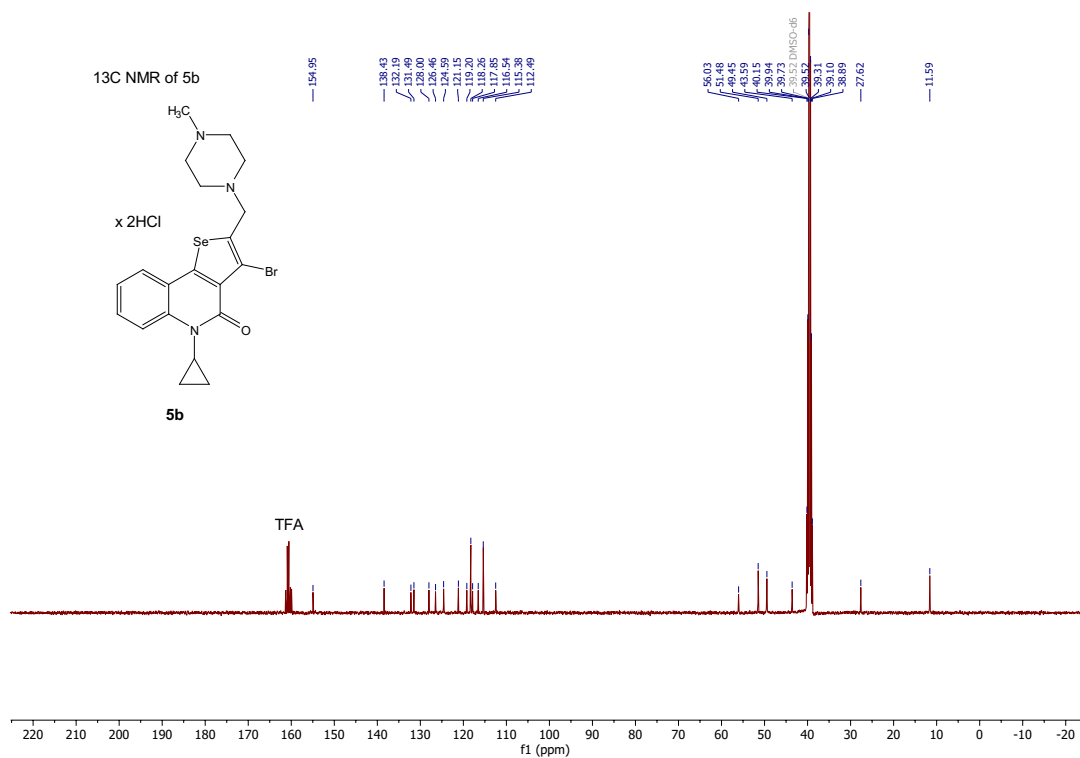
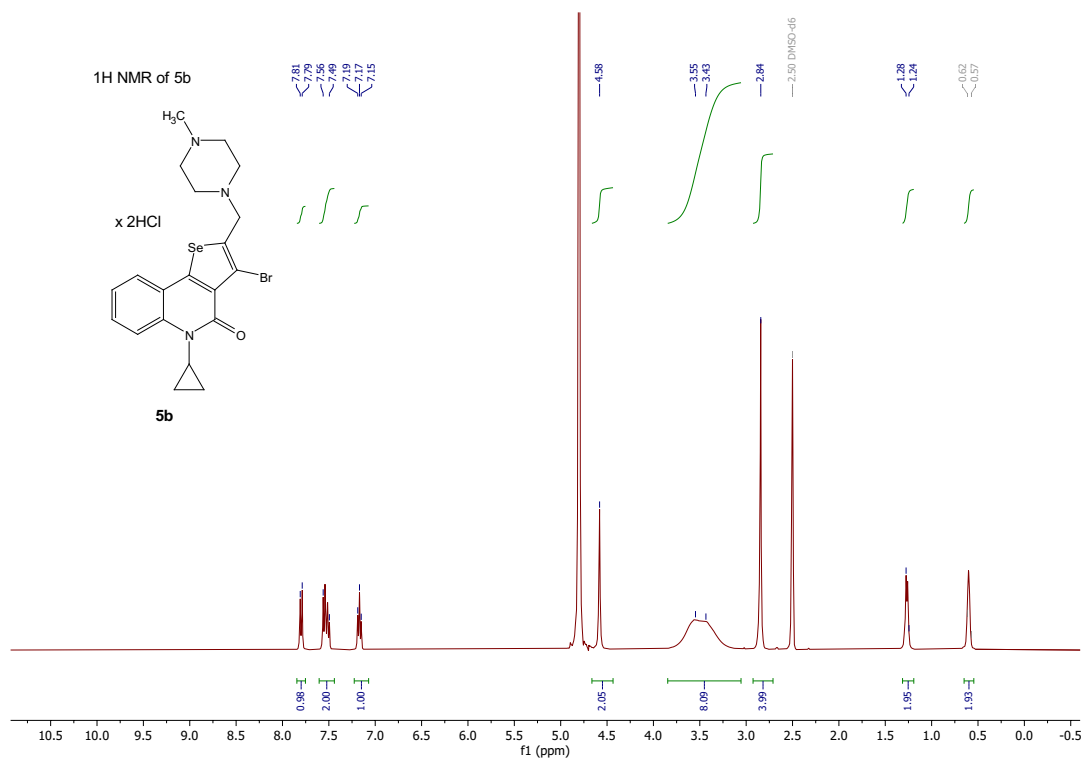


Apollo C18-9 (4,6x150 mm)

15min Gr. 5%-95%ACN+0.1% H_3PO_4 ; 5min Iz. 95%ACN; 3min Gr. 95-5%ACN, 2min Iz. 5%ACN; 1mL/min; 40°C

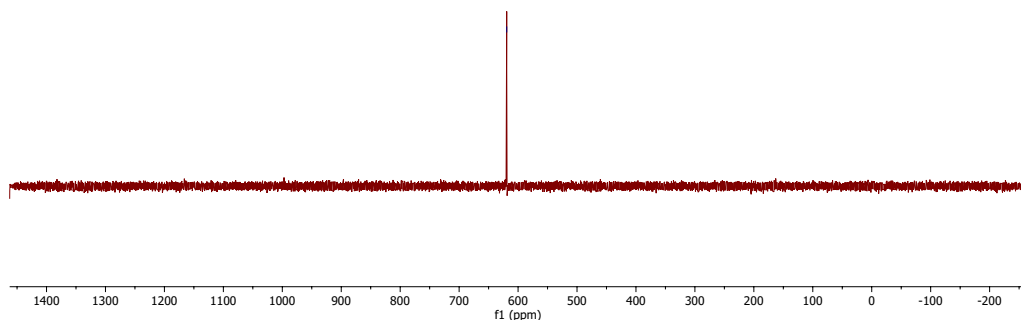
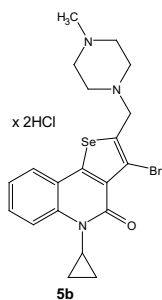


Compound **5b**



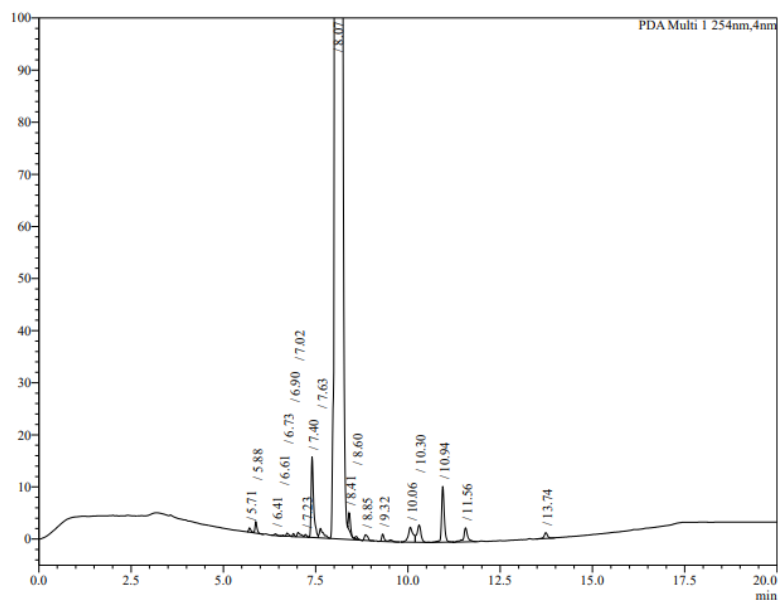
⁷⁷Se NMR for 5b

619.28



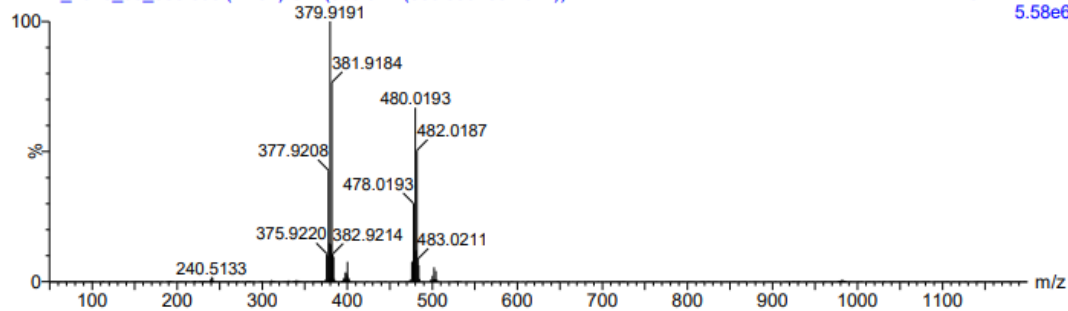
Apollo C18-11 (4.6 x 150mm); F - 1mL/min; t = 40°C
 15min Gr. 5-95%ACN + 0.1% H3PO4;
 5min Iz. 95%ACN;
 2min Gr. 95-5%ACN;
 3min Iz. 5%ACN;

mAU

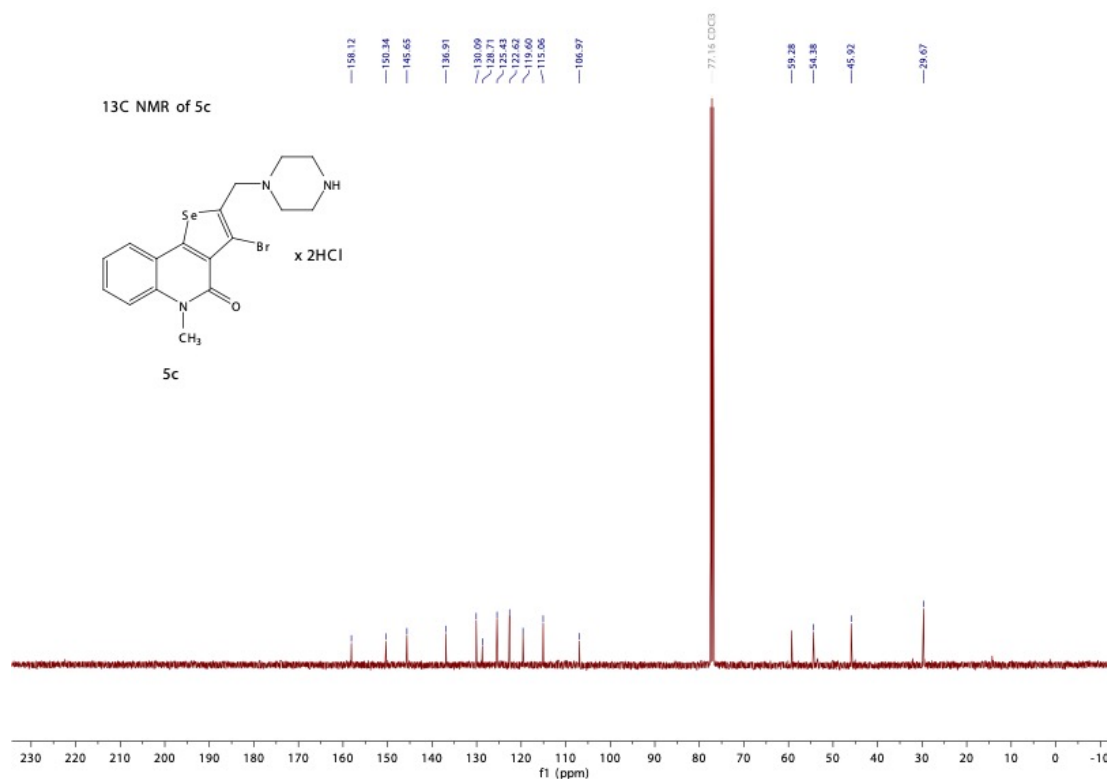
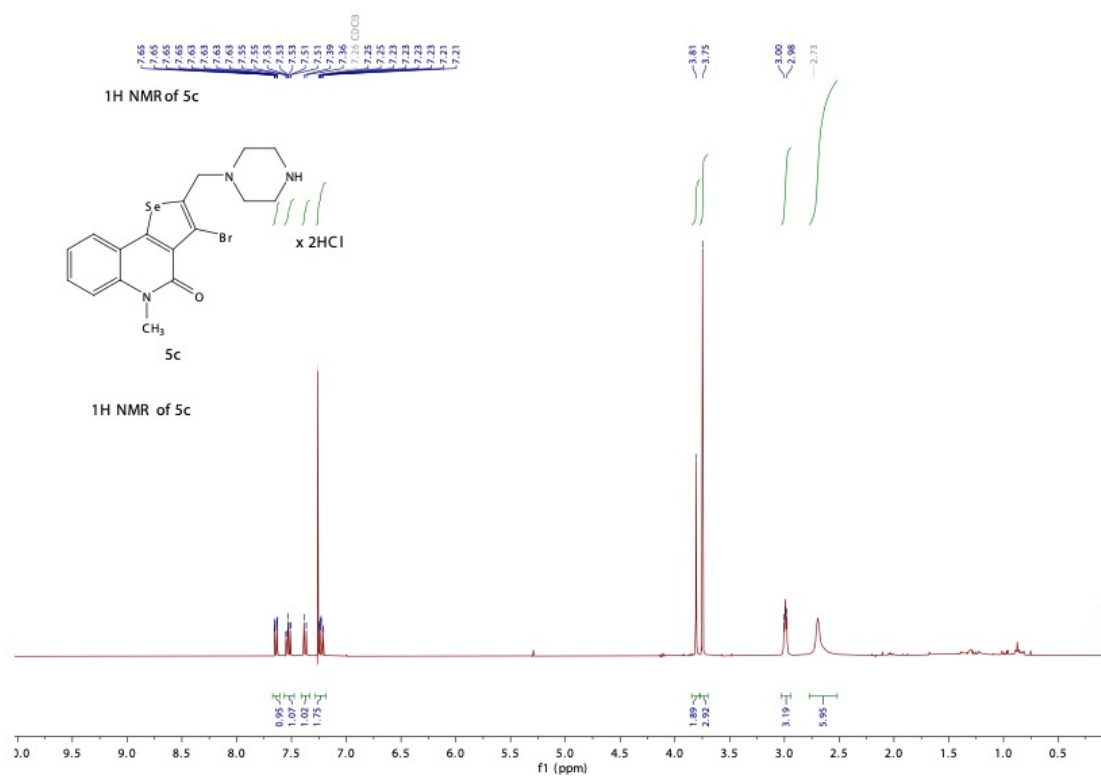


HRMS_2020_06_656 606 (1.737) Cm (606:612-(580:586+637:642))

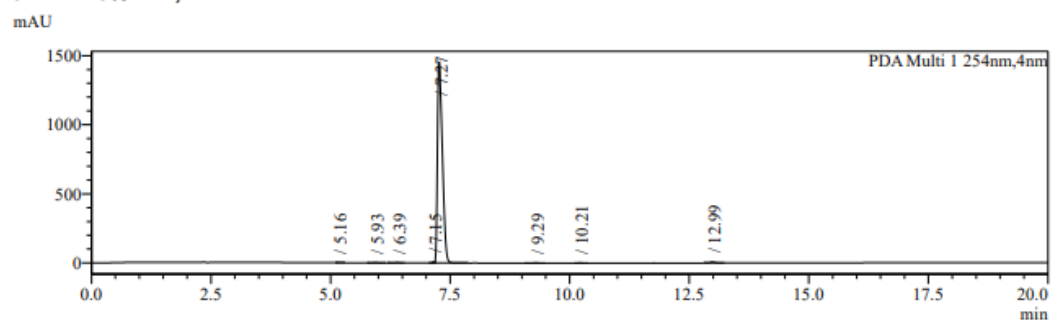
1: TOF MS ES+
 5.58e6



Compound 5c



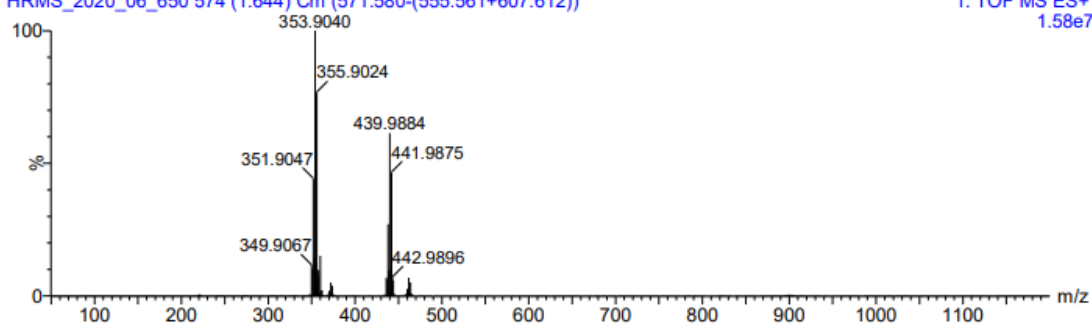
Apollo C18-13 (4.6 x 150mm); F - 1mL/min; t = 40°C
 15min Gr. 5-95%ACN + 0.1% H3PO4;
 5min Iz. 95%ACN;
 2min Gr. 95-5%ACN;
 3min Iz. 5%ACN;



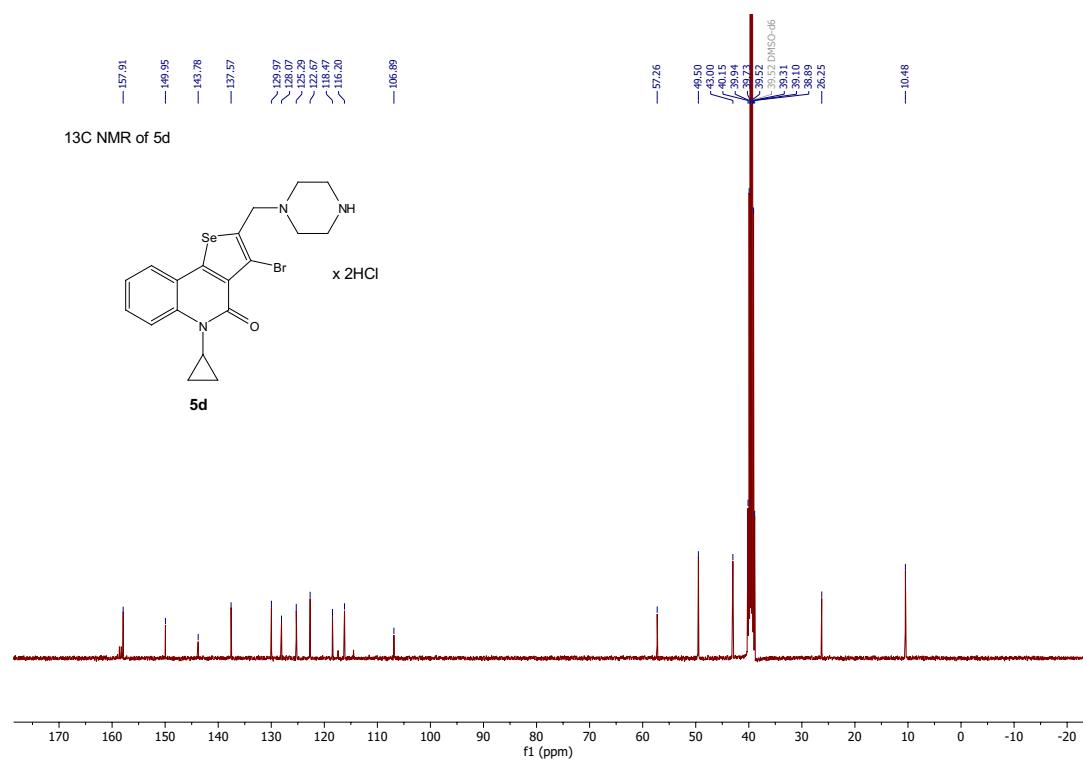
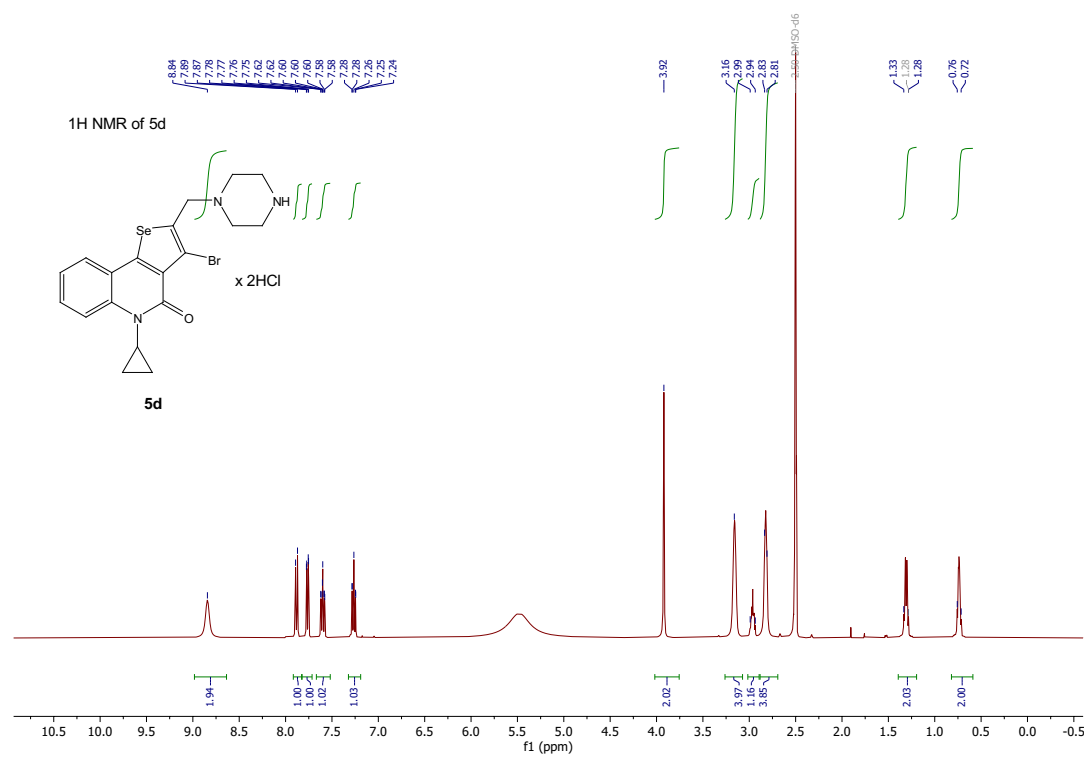
C ~ 0,45 mg/ml; diluent -15%ACN in 0.1%PA

HRMS_2020_06_650 574 (1.644) Cm (571:580-(555:561+607:612))

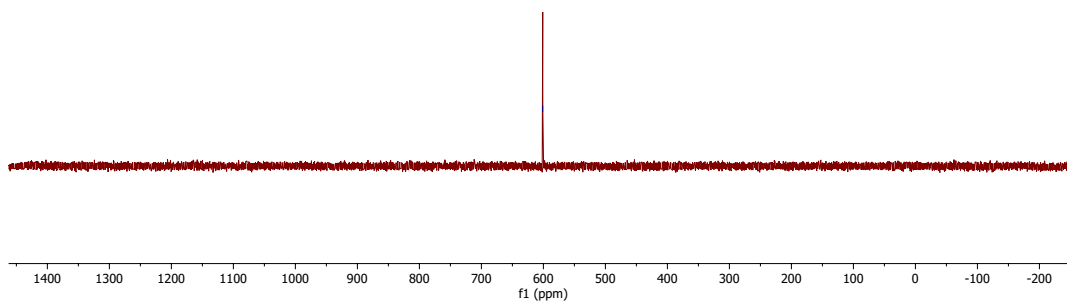
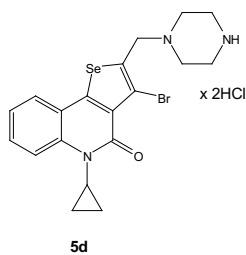
1: TOF MS ES+
 1.58e7



Compound 5d

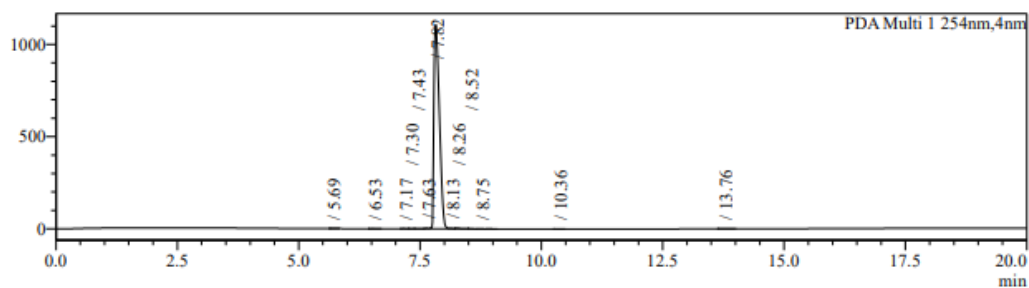


⁷⁷Se NMR of 5d



Apollo C18-11 (4.6 x 150mm); F - 1mL/min; t = 40°C
 15min Gr. 5-95%ACN + 0.1% H₃PO₄;
 5min Iz. 95%ACN;
 2min Gr. 95-5%ACN;
 3min Iz. 5%ACN;

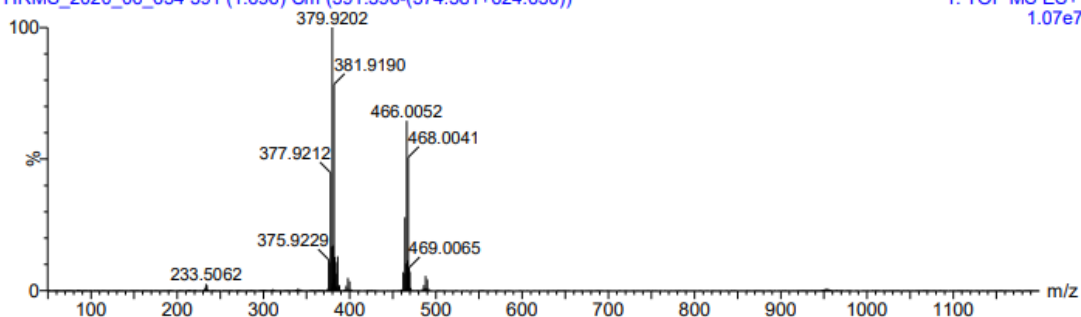
mAU



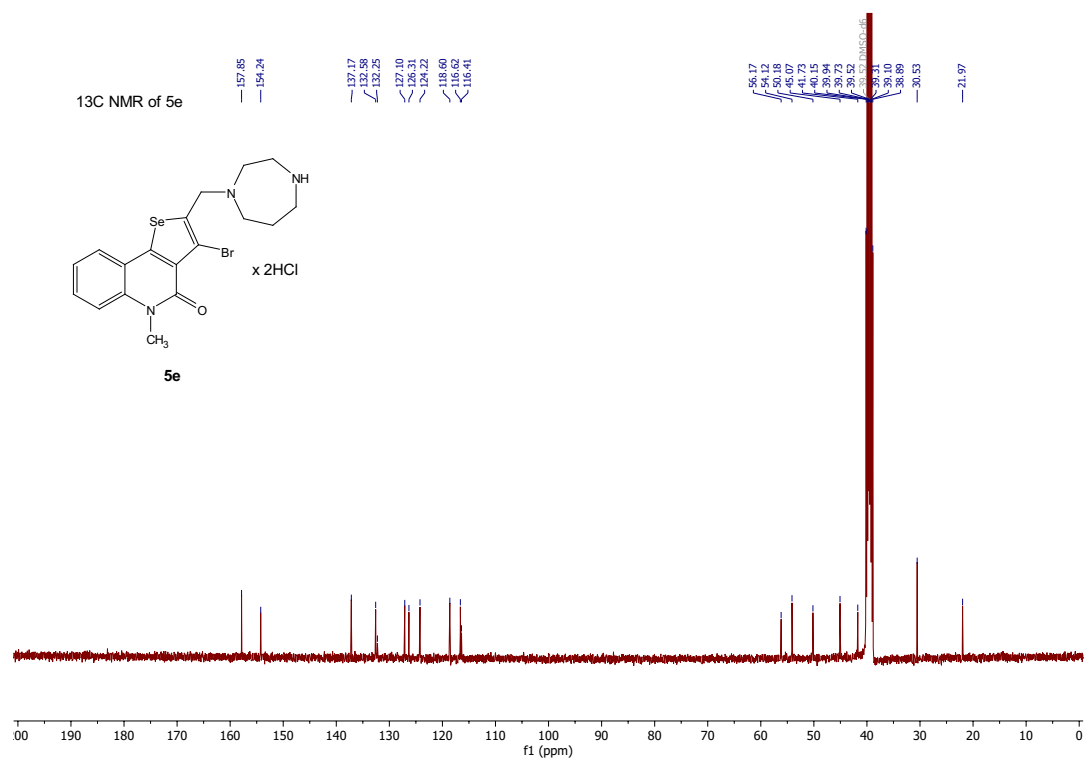
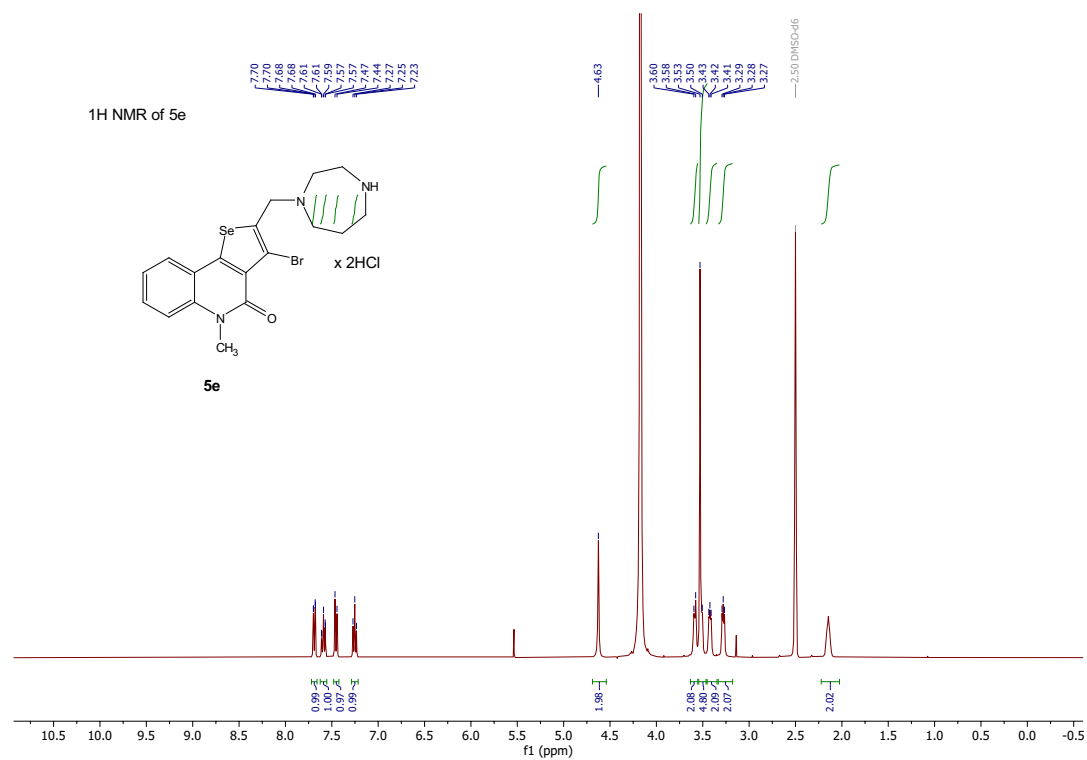
C ~ 0,5 mg/ml; diluent - 5%ACN in 0.1%PA

HRMS_2020_06_654 591 (1.696) Cm (591:596-(574:581+624:630))

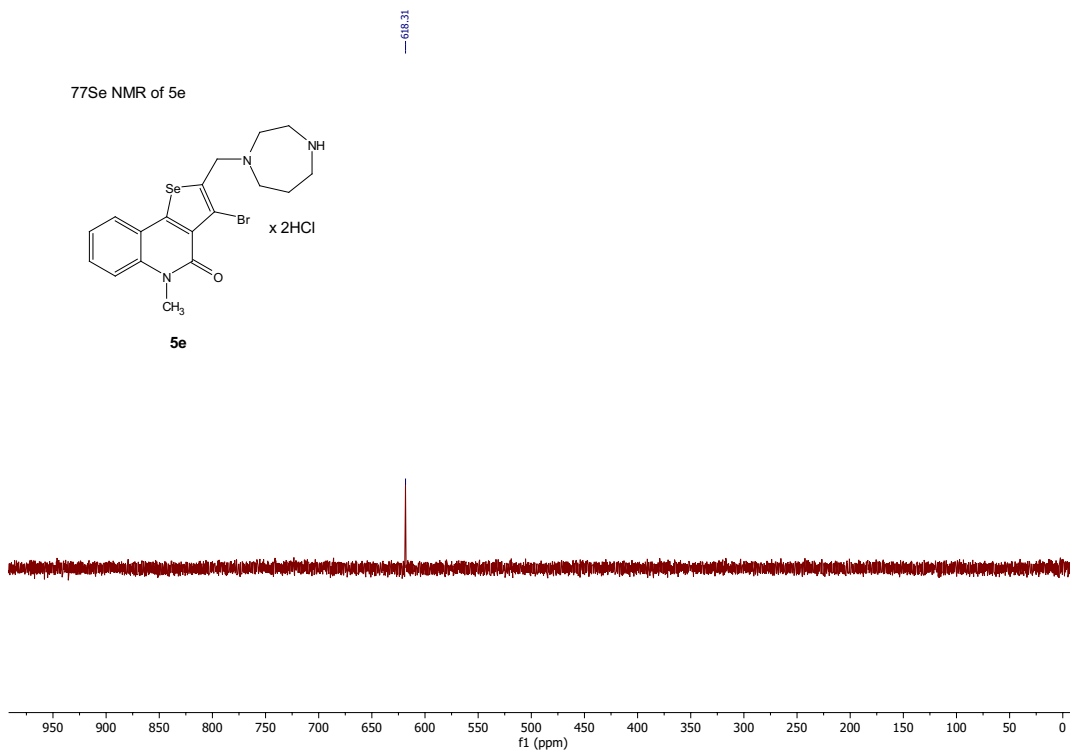
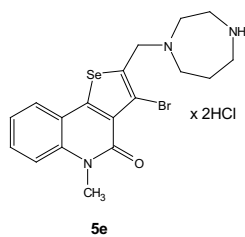
1: TOF MS ES+
 1.07e7



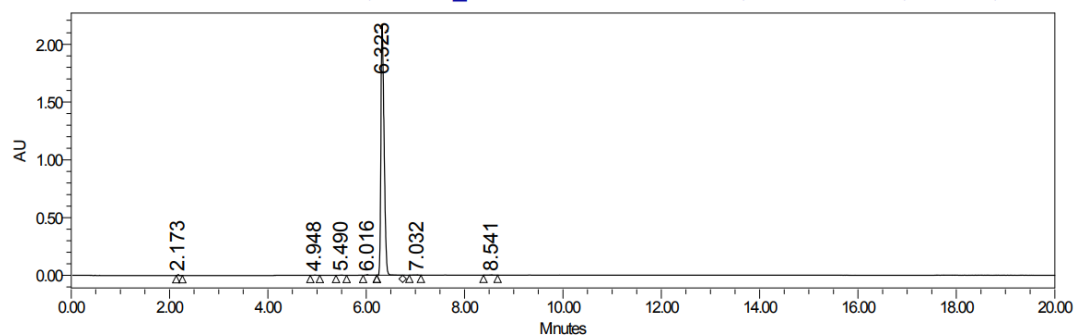
Compound 5e



⁷⁷Se NMR of 5e

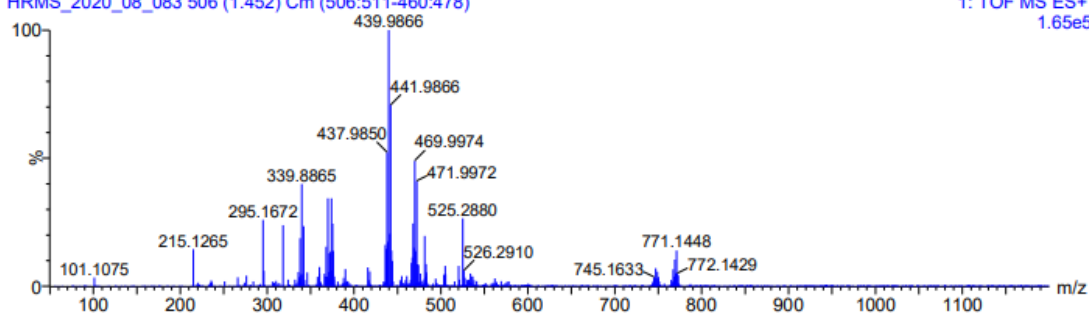


Adamas C18-Classic (4,6x150 mm)
15min Gr 5%-95%ACN+0.1% H_3PO_4 ; 5 min IZ 95%ACN 3min Gr 95-5%ACN, 2min IZ 5%ACN; 1mL/min; 40°C

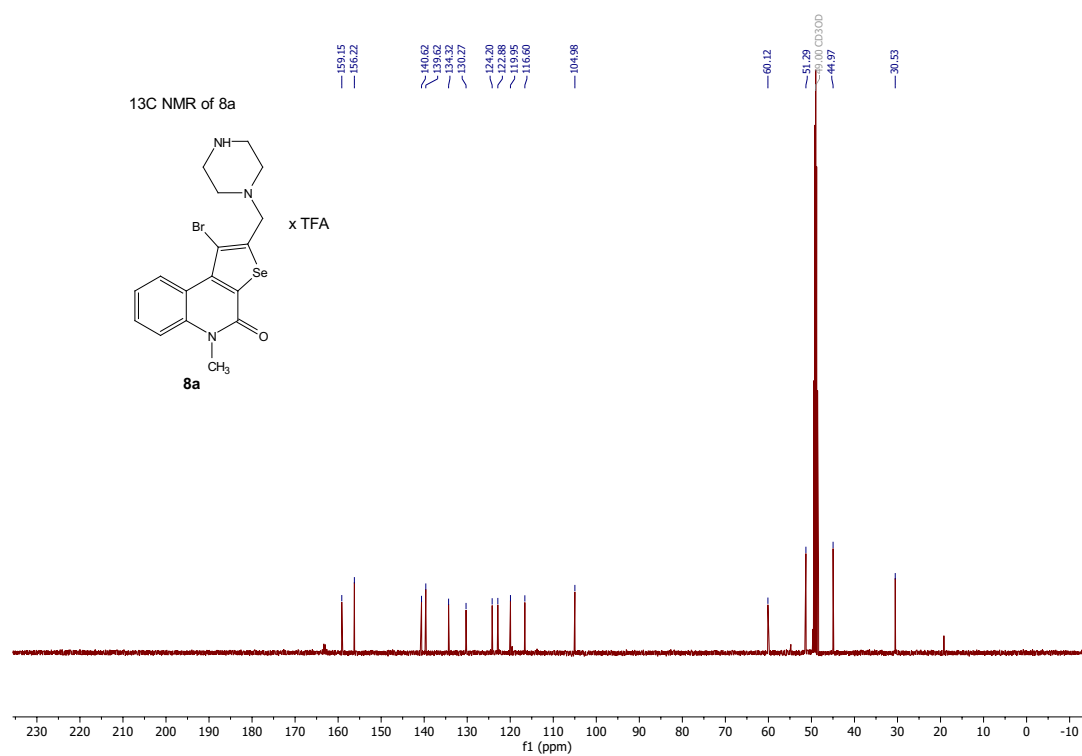
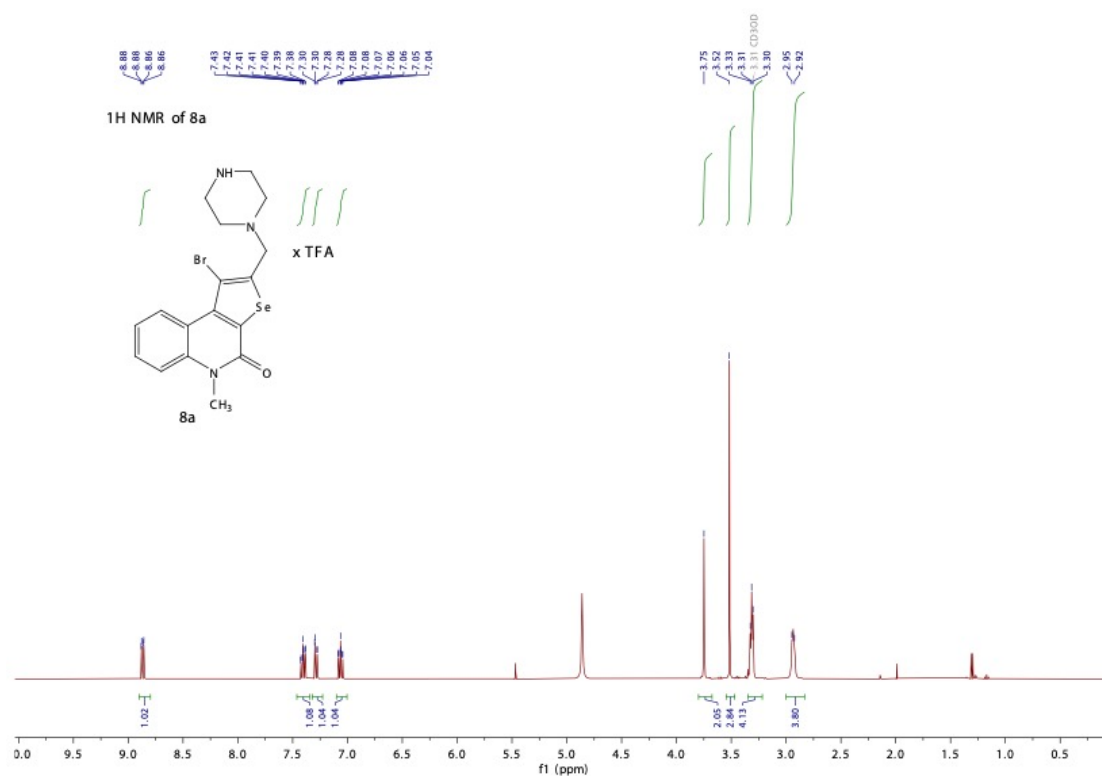


HRMS_2020_08_083 506 (1.452) Cm (506:511-460:478)

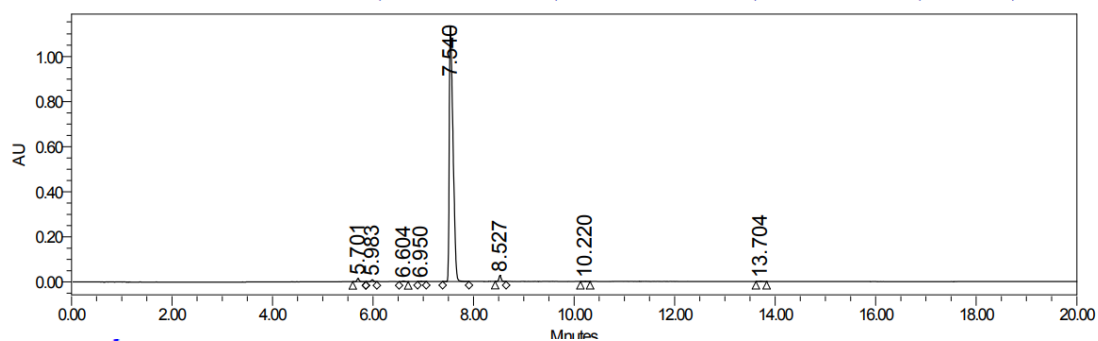
1: TOF MS ES+
1.65e5



Compound **8a**

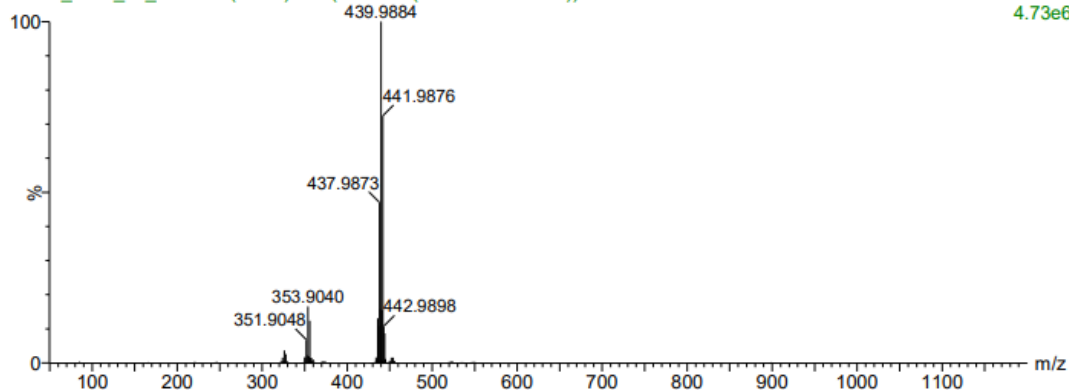


Adamas C18-Classic (4,6x150 mm)
15min Gr 5%-95%ACN+0.1% H_3PO_4 ; 5min IZ 95%ACN; 3min Gr 95-5%ACN, 2min IZ 5%ACN; 1mL/min; 40oC

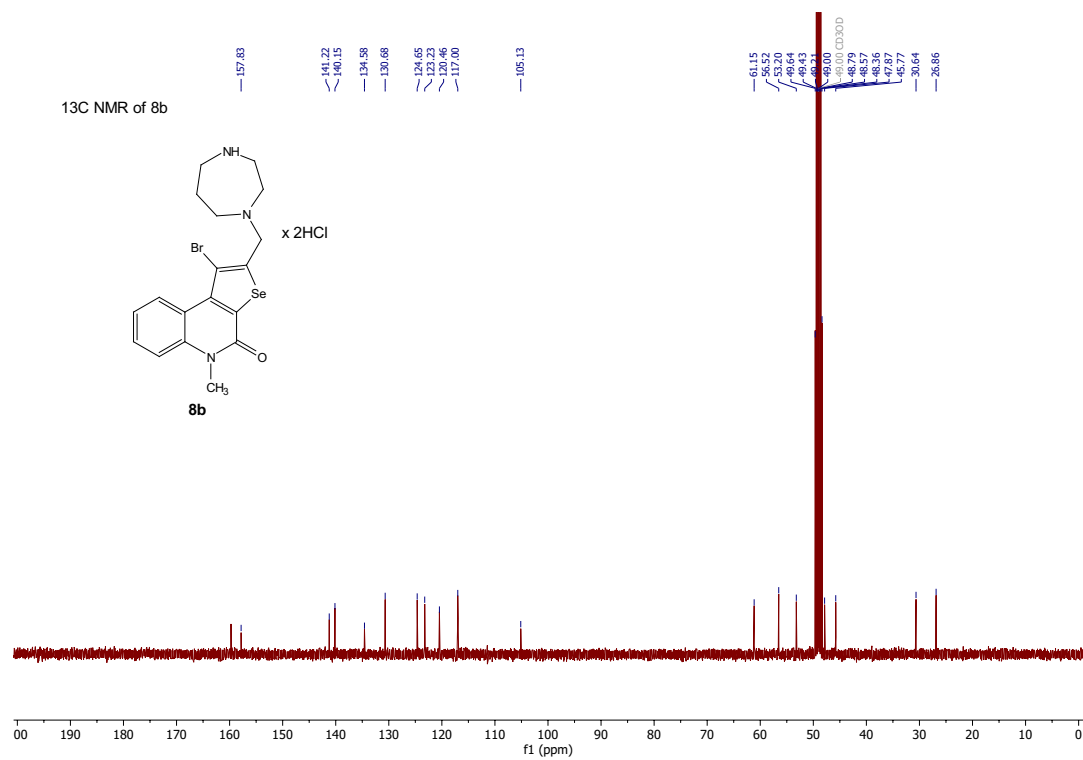
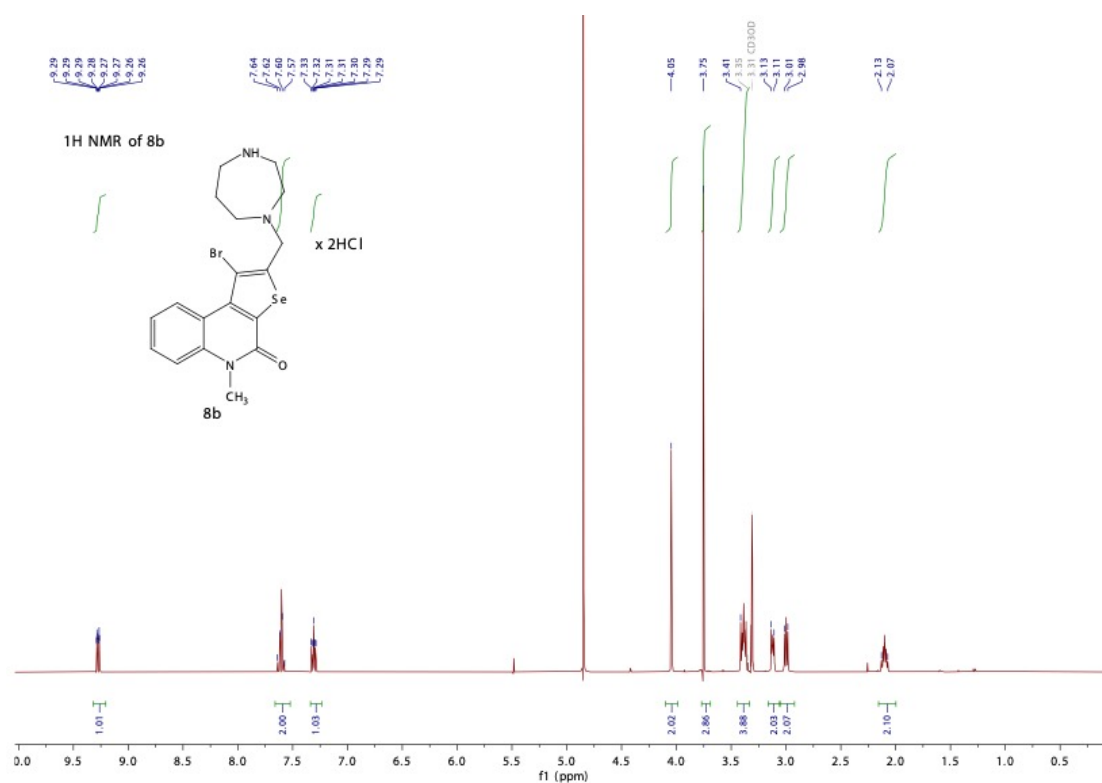


HRMS_2020_06_545 608 (1.743) Cm (608:615-(559:566+661:668))

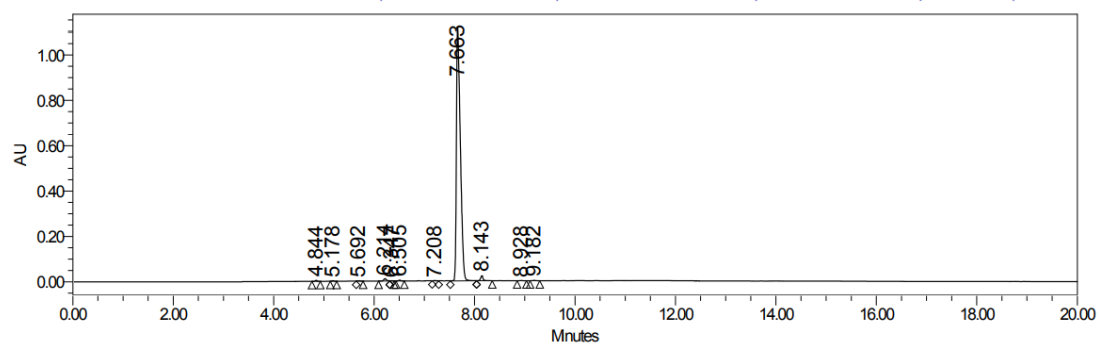
1: TOF MS ES+
4.73e6



Compound **8b**

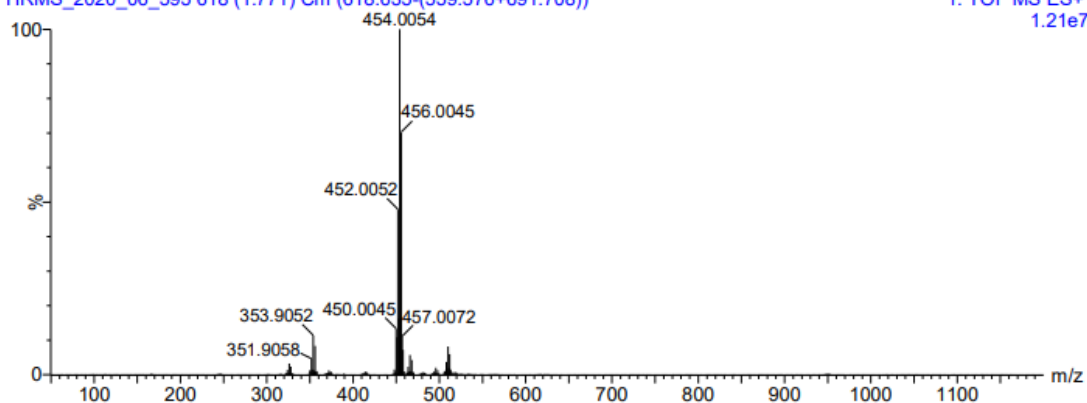


Adamas C18-Classic (4,6x150 mm)
15min Gr 5%-95%ACN+0.1%H3PO4; 5min IZ 95%ACN; 3min Gr 95-5%ACN, 2min IZ 5%ACN; 1mL/min; 40oC

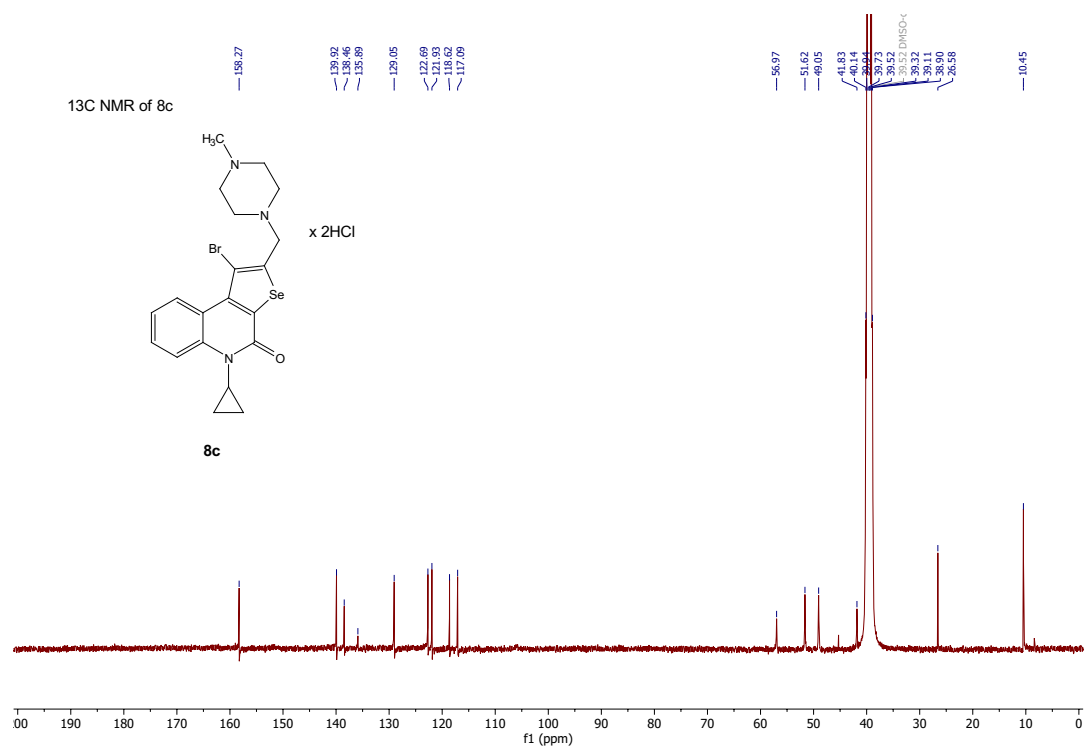
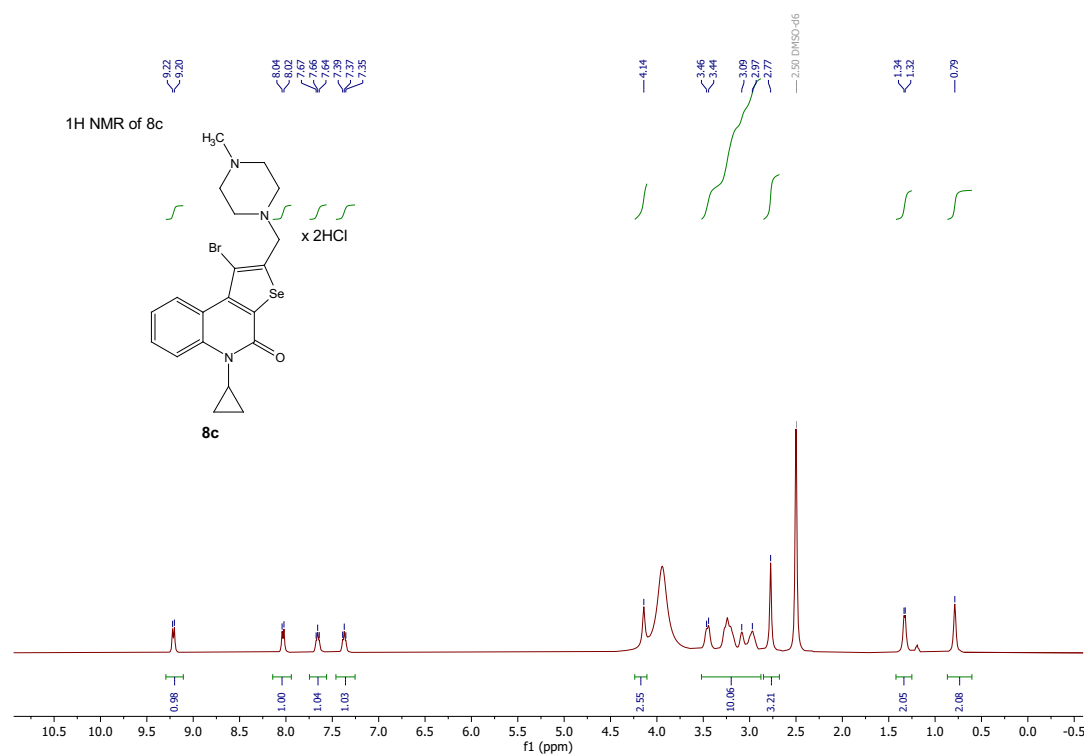


HRMS_2020_06_595 618 (1.771) Cm (618:635-(559:576+691:708))

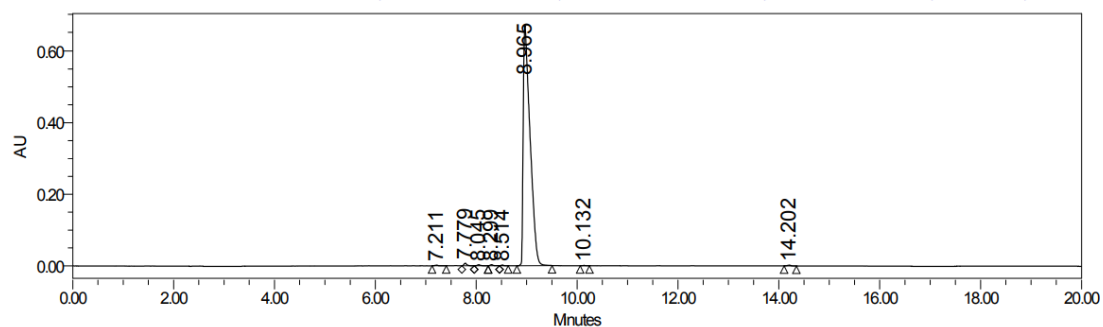
1: TOF MS ES+
1.21e7



Compound **8c**

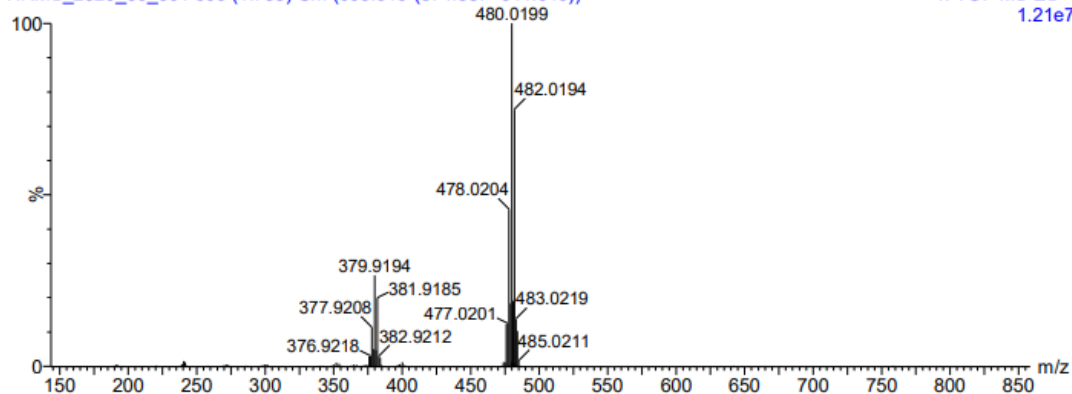


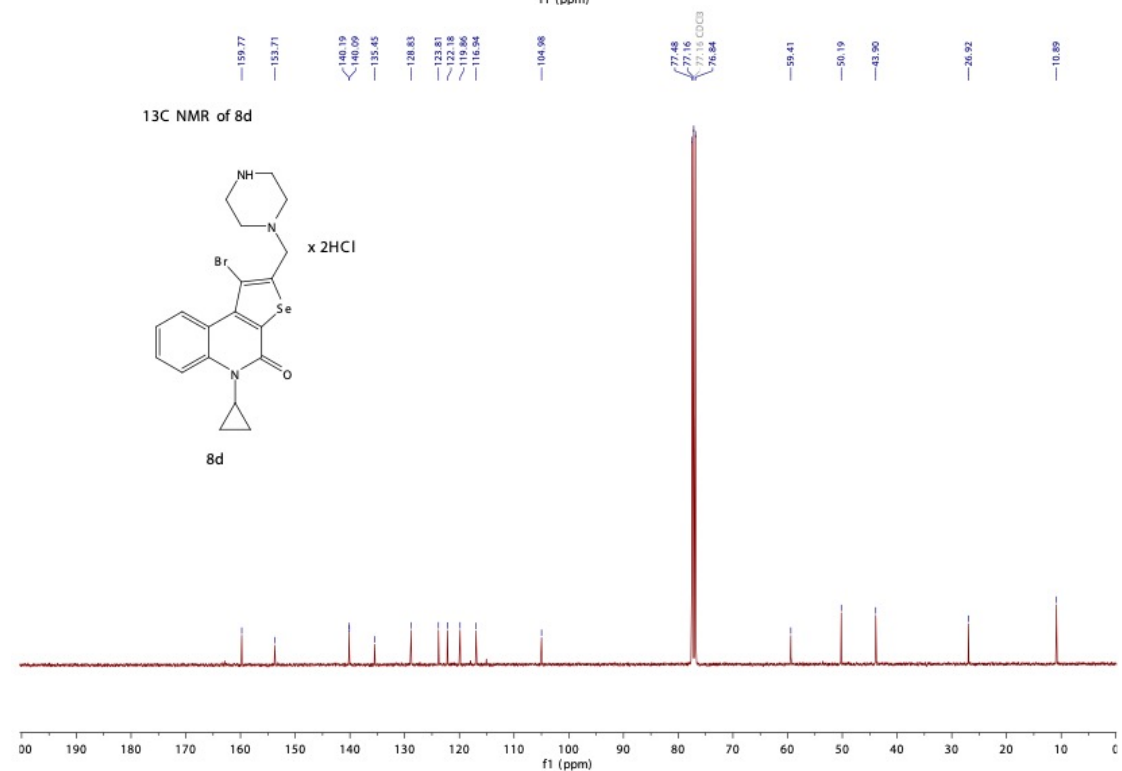
Apollo C18-9 (4,6x150 mm)
 15min Gr. 5%-95%ACN+0.1%H₃PO₄; 5min Iz. 95%ACN; 3min Gr. 95-5%ACN, 2min Iz. 5%ACN; 1mL/min; 40°C



HRMS_2020_06_561 606 (1.738) Cm (605:616-(574:587+641:649))

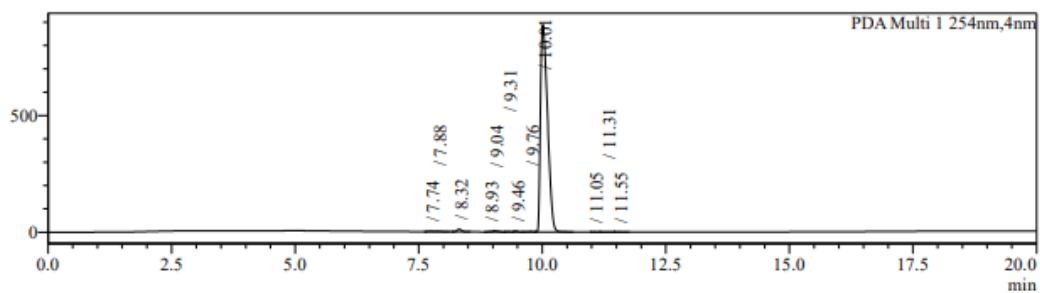
1: TOF MS ES+
 1.21e7



[illegible]

Apollo C18-11 (4.6 x 150mm); F - 1mL/min; t = 40°C
 15min Gr. 5-95%ACN + 0.1% H3PO4;
 5min Iz. 95%ACN;
 2min Gr. 95-5%ACN;
 3min Iz. 5%ACN;

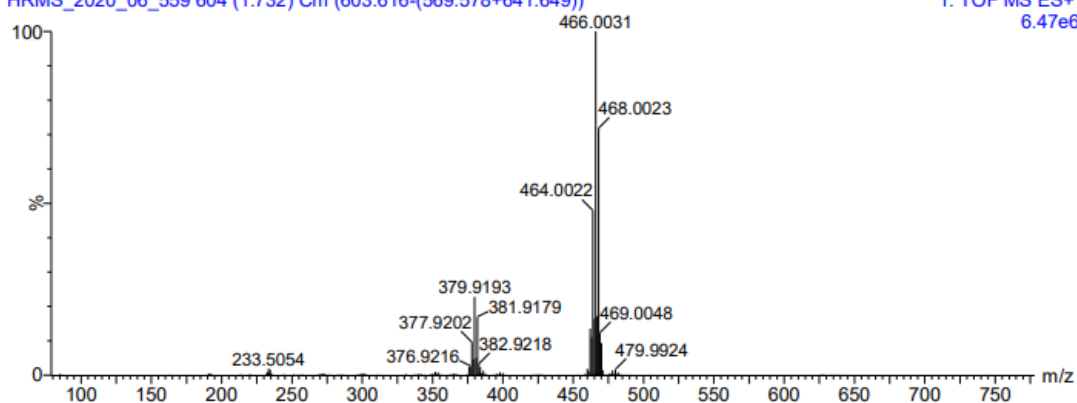
mAU



C ~ 0,5 mg/ml; diluent - 5%ACN in 0.1%PA

HRMS_2020_06_559 604 (1.732) Cm (603:616-(569:578+641:649))

1: TOF MS ES+
 6.47e6



¹H NMR of 8e

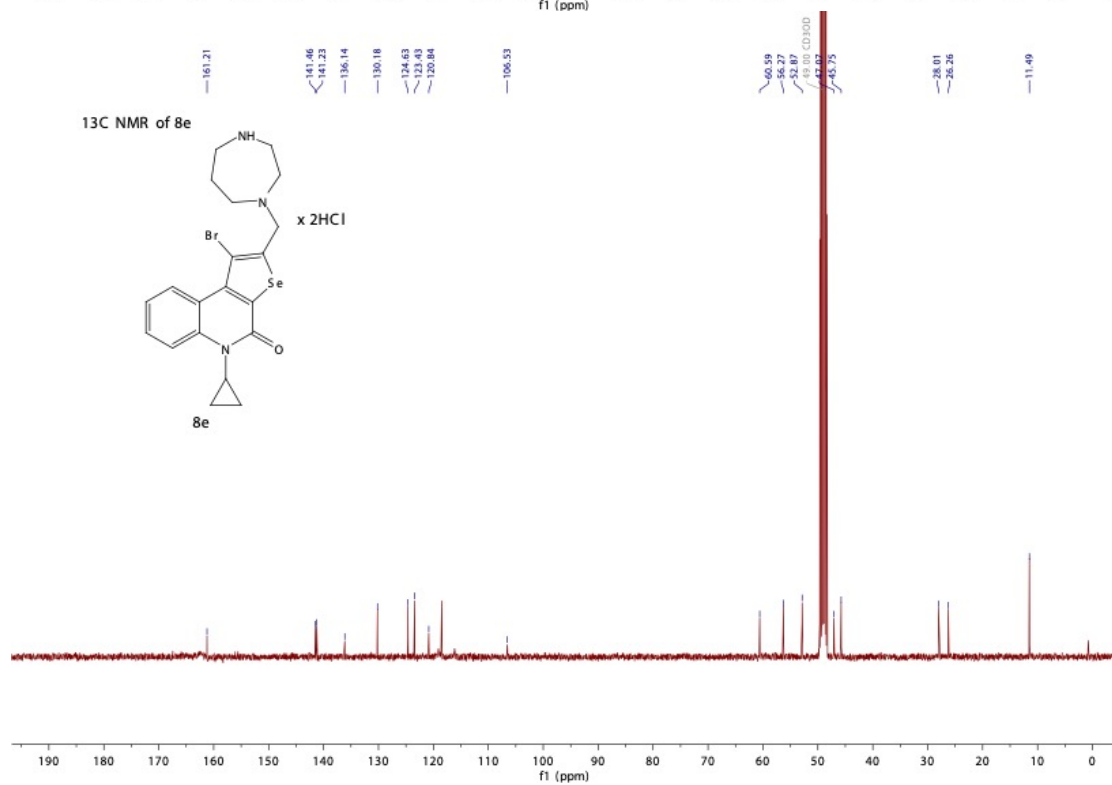
Chemical structure of 8e is shown, which is a 1-(cyclopropyl)-2-(2-(2-bromo-1-(8-azabicyclo[3.2.1]oct-2-yl)vinyl)sephen-3-yl)isoquinolin-3(1H)-one. The structure is labeled **8e** and **x 2HCl**.

¹H NMR of 8e

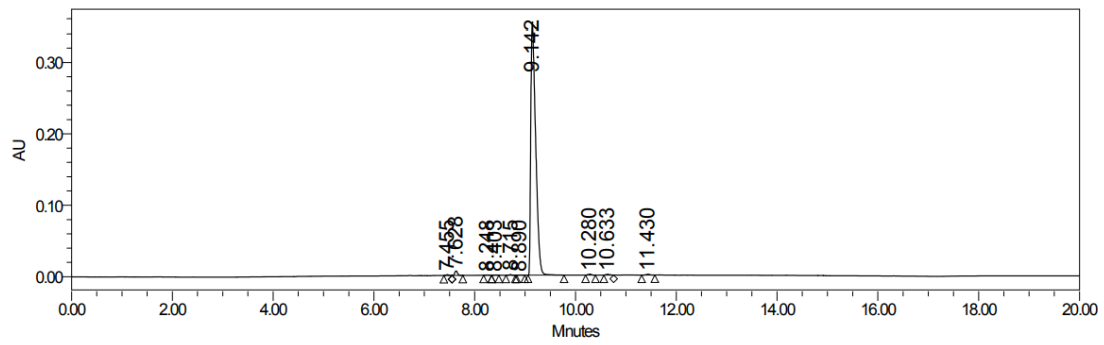
Chemical structure of 8e is shown, which is a 1-(cyclopropyl)-2-(2-(2-bromo-1-(8-azabicyclo[3.2.1]oct-2-yl)vinyl)sephen-3-yl)isoquinolin-3(1H)-one. The structure is labeled **8e** and **x 2HCl**.

¹H NMR of 8e

Chemical structure of 8e is shown, which is a 1-(cyclopropyl)-2-(2-(2-bromo-1-(8-azabicyclo[3.2.1]oct-2-yl)vinyl)sephen-3-yl)isoquinolin-3(1H)-one. The structure is labeled **8e** and **x 2HCl**.

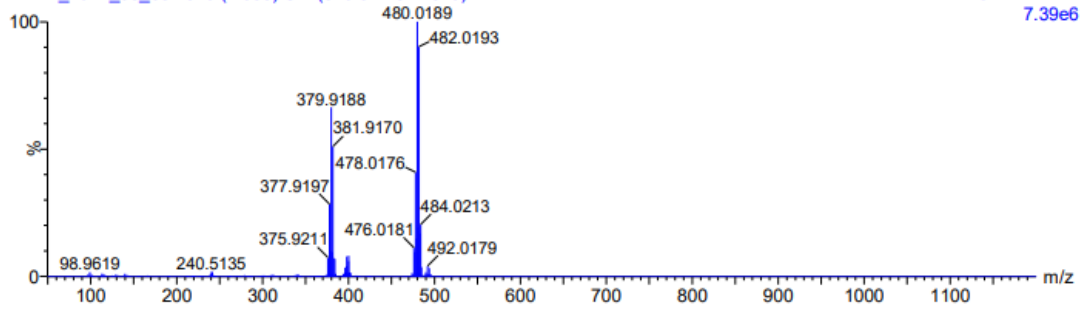


Apollo C18-9 (4,6x150 mm)
15min Gr. 5%-95%ACN+0.1% H_3PO_4 ; 5min Iz. 95%ACN; 3min Gr. 95-5%ACN, 2min Iz. 5%ACN; 1mL/min; 40°C

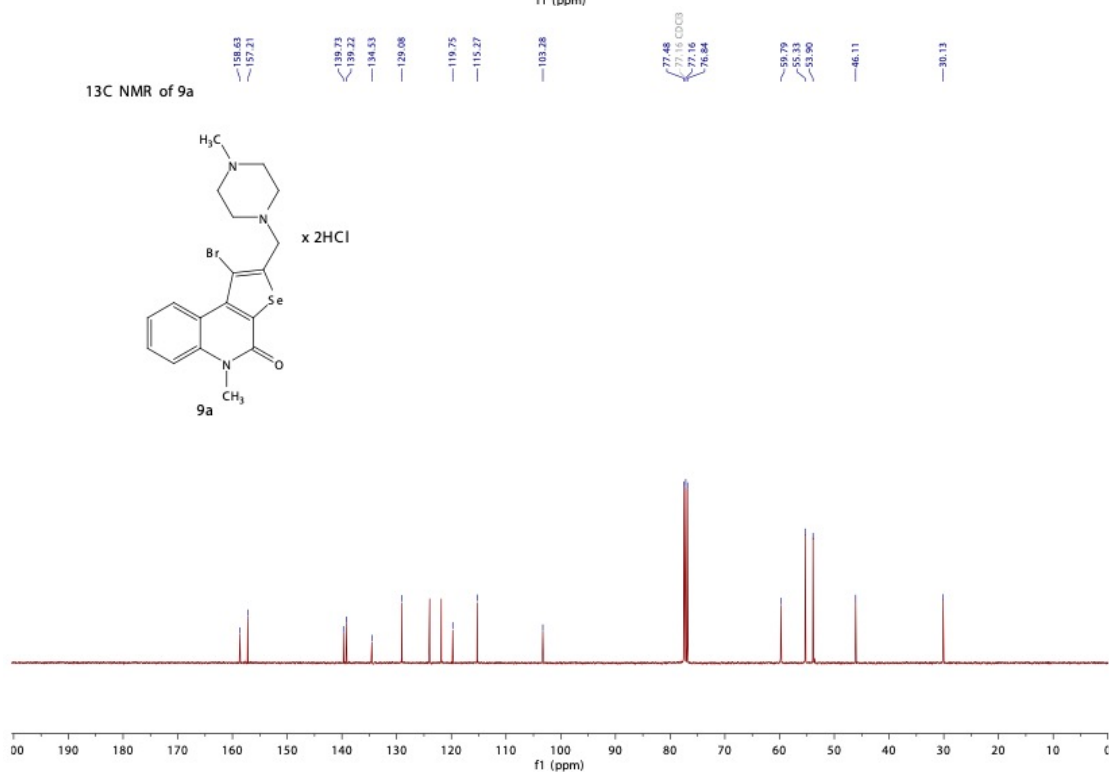
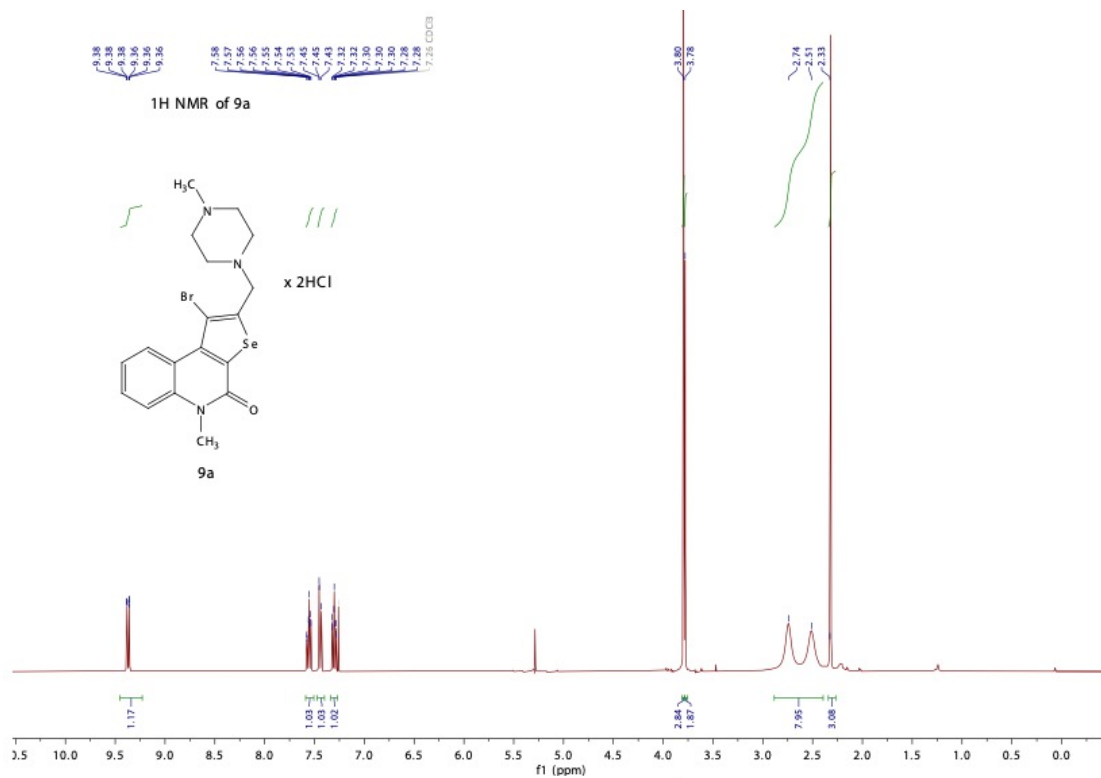


HRMS_2021_05_681 570 (1.633) Cm (570:577-544:549)

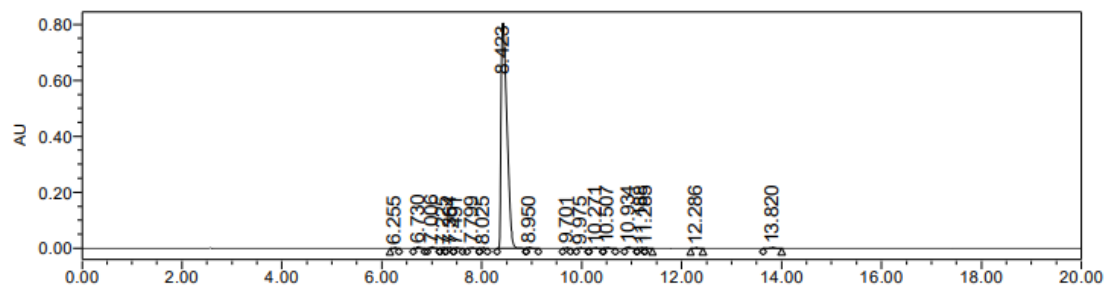
1: TOF MS ES+
7.39e6



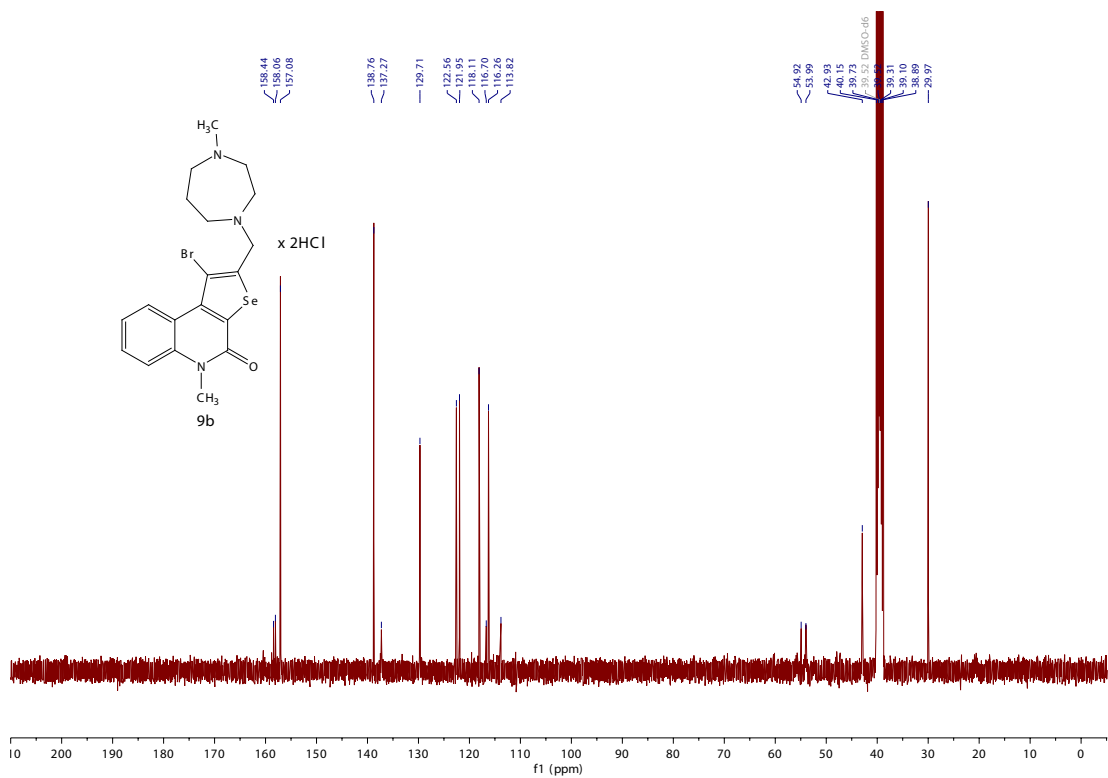
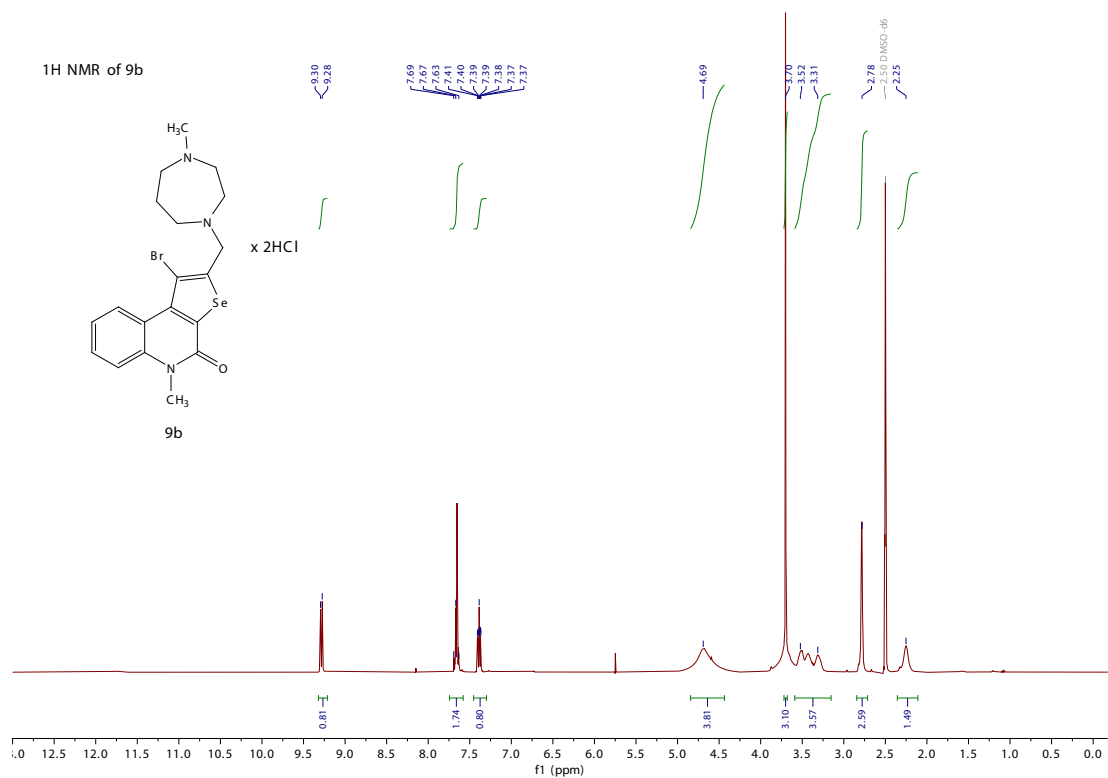
Compound 9a



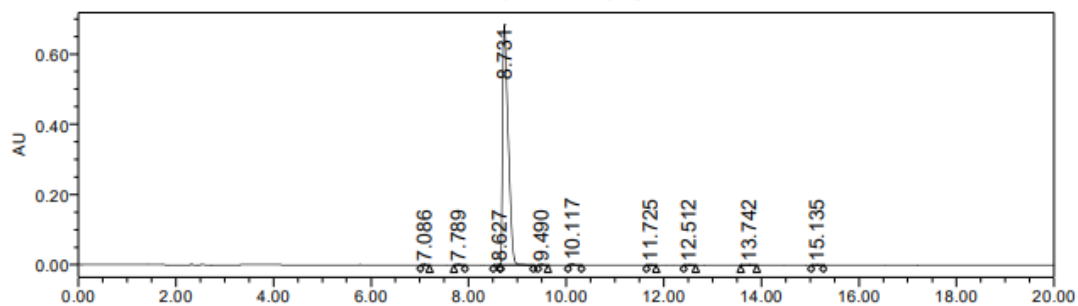
Apollo C18-12 5um (4.6x150 mm)
 15 min Gr. 5-95%ACN + 0.1% H3PO4; 5 min Iz. 95%ACN; 2 min Gr. 95-5% ACN; 3 min Iz. 5% ACN.
 F=1mL/min. T=40oC.



Compound 9b



Apollo C18-12 5um (4.6x150 mm)
 15 min Gr. 5-95%ACN + 0.1% H3PO4; 5 min Iz. 95%ACN; 2 min Gr. 95-5% ACN; 3 min Iz. 5% ACN.
 F=1mL/min. T=40oC.



HRMS_2020_06_597 616 (1.765) Cm (616:623-(568:573+667:673))

1: TOF MS ES+
 8.13e6

