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Supporting information for article:

Crystal structure, spectroscopic studies and theoretical studies of thiobarbituric acid derivatives: understanding the hydrogen-bonding pattern

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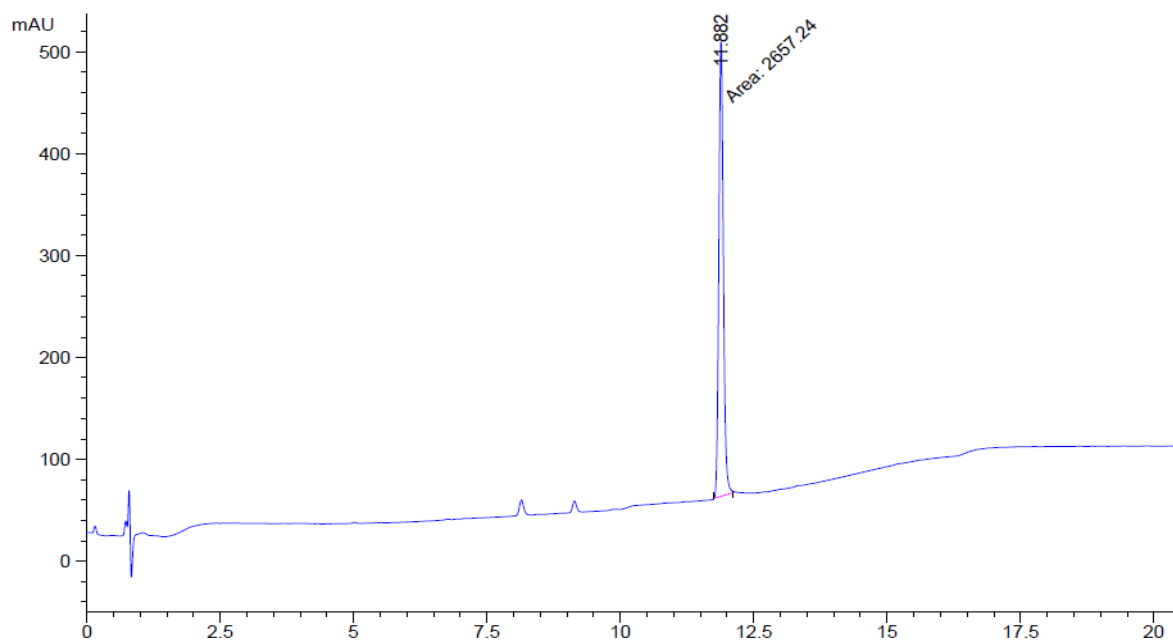


Figure S1 HPLC for compound A01

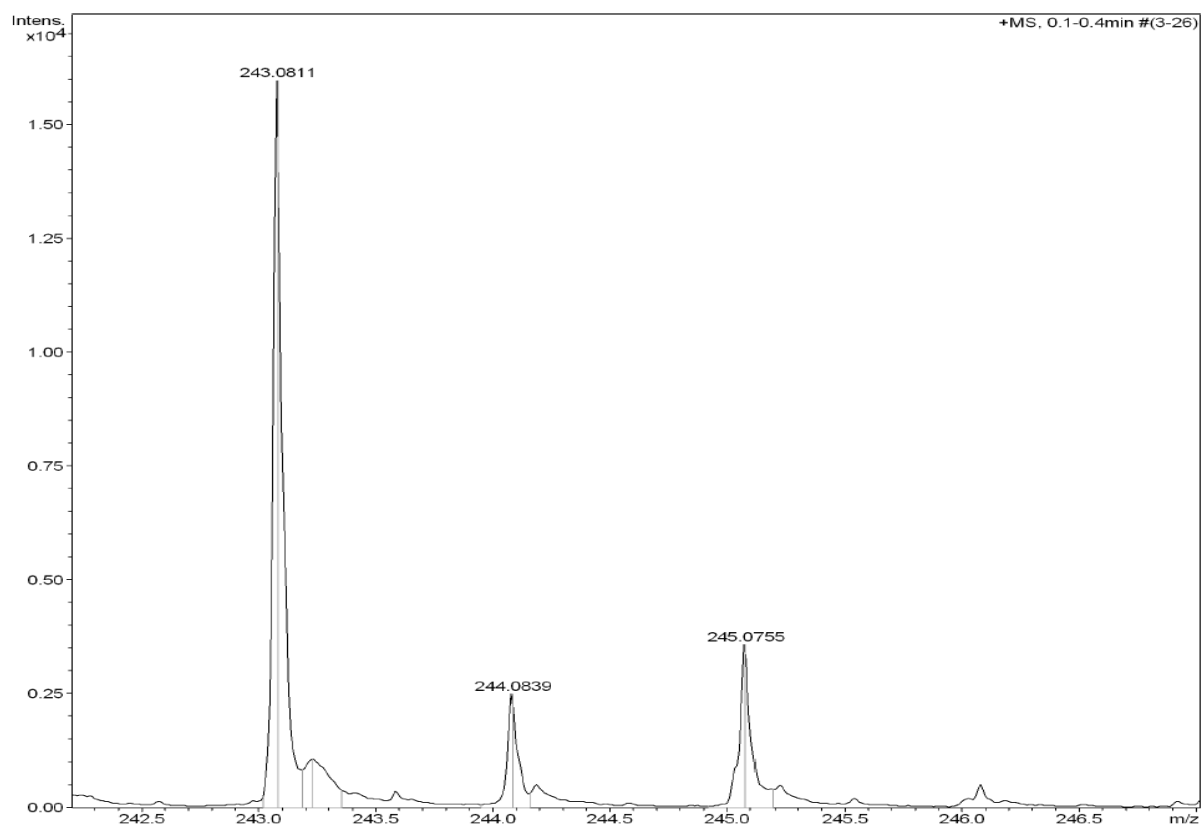
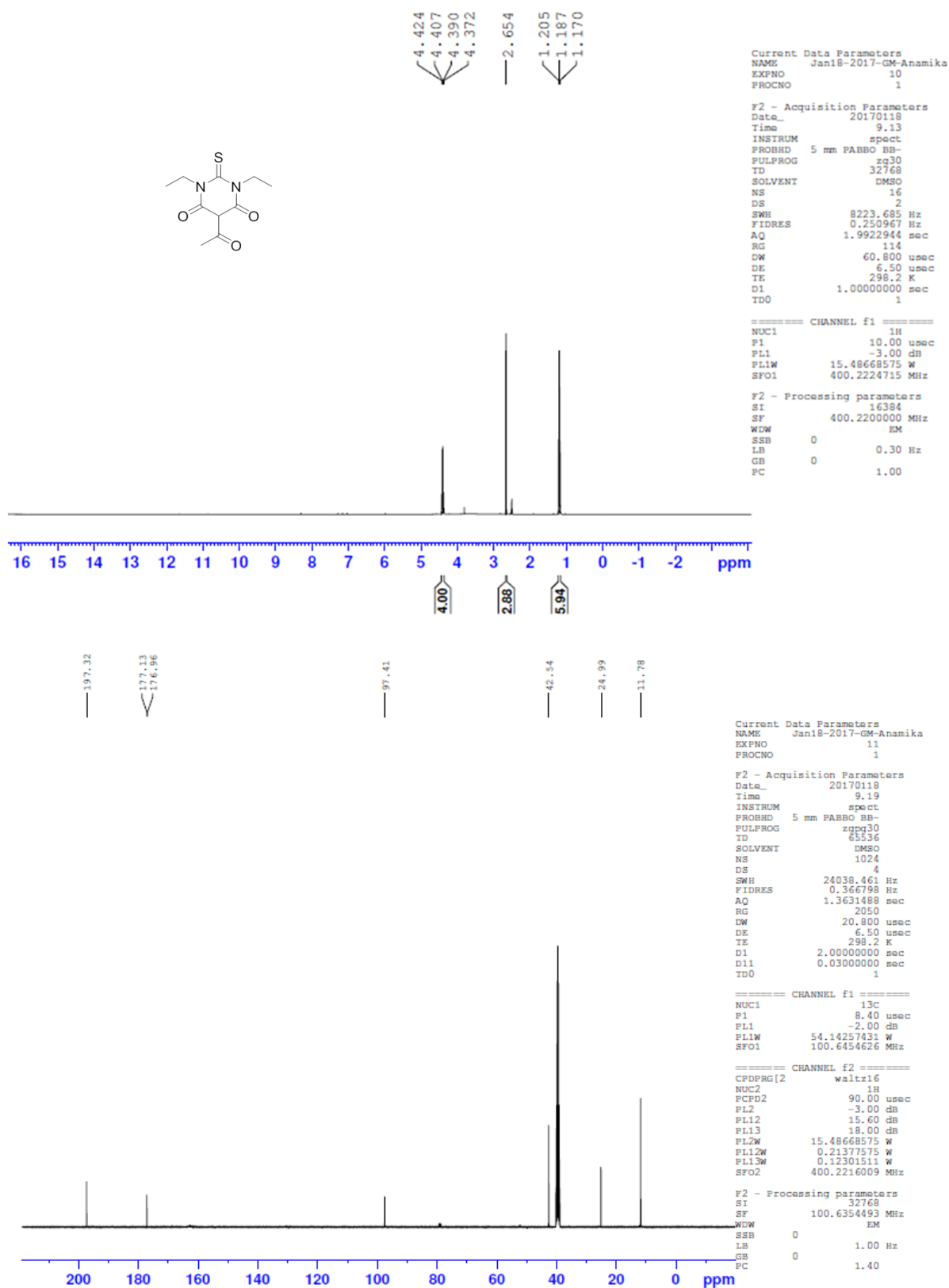
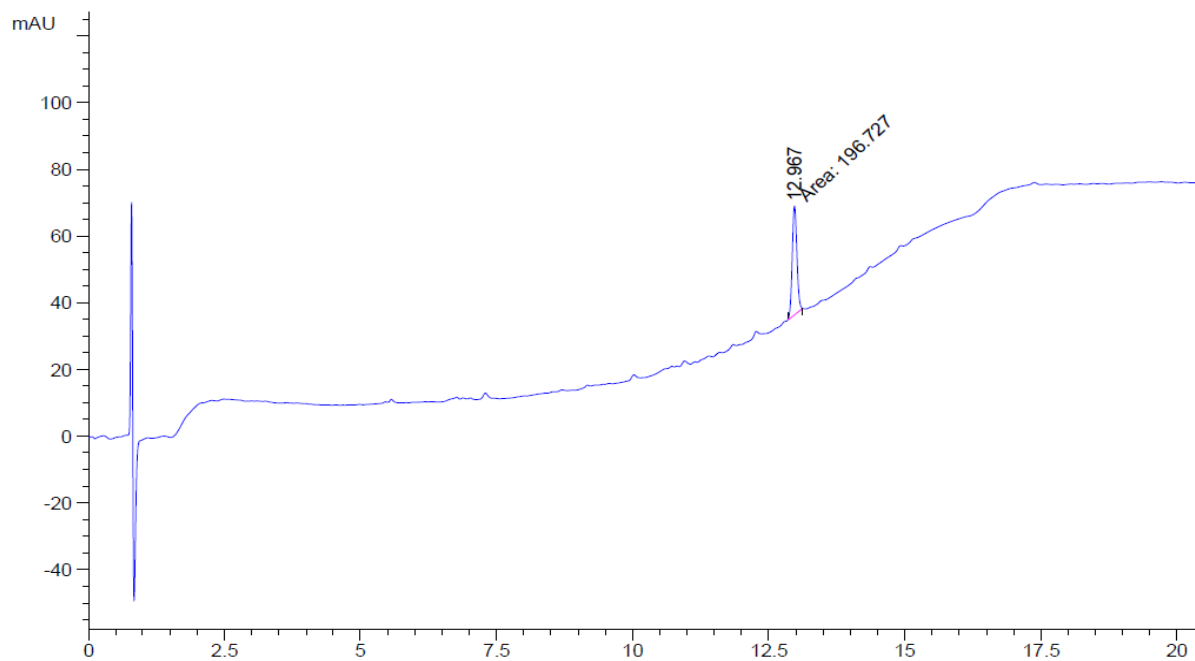
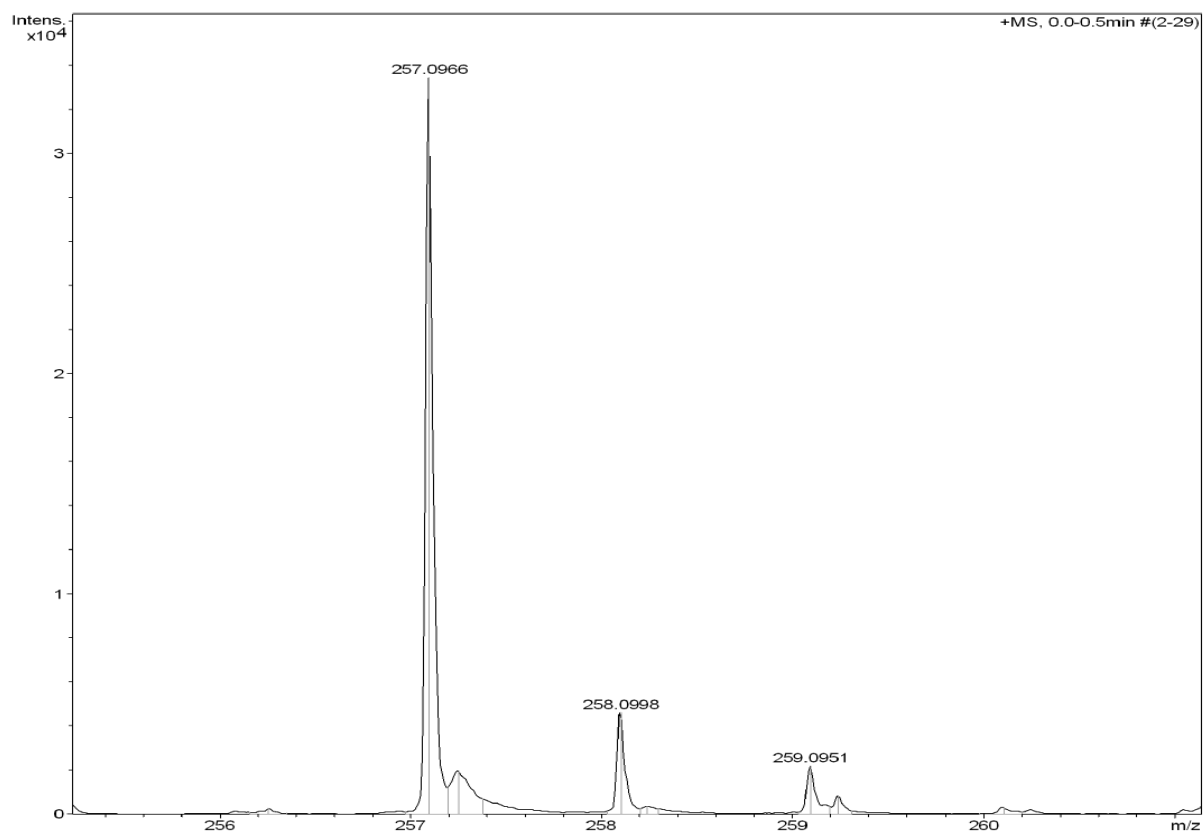
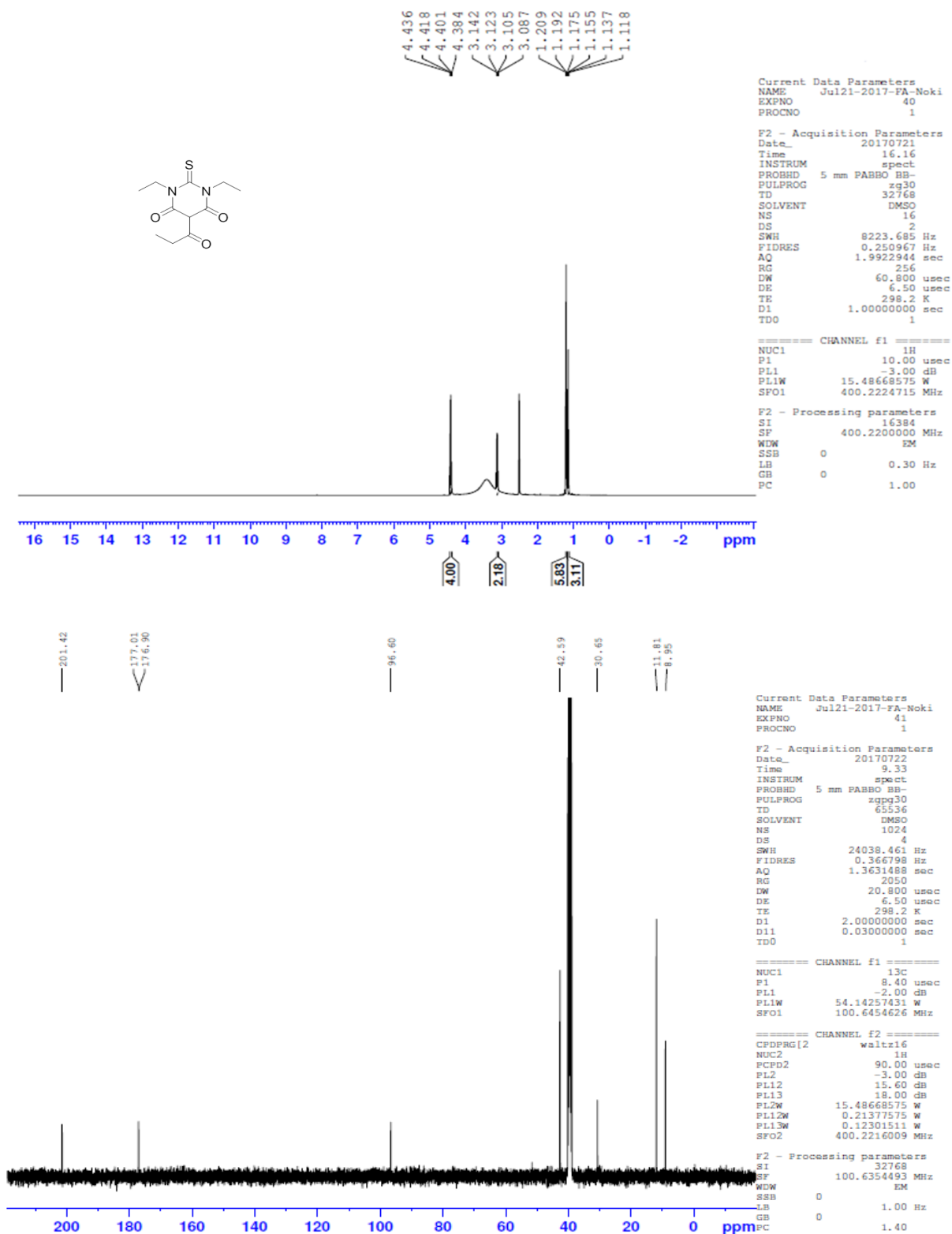
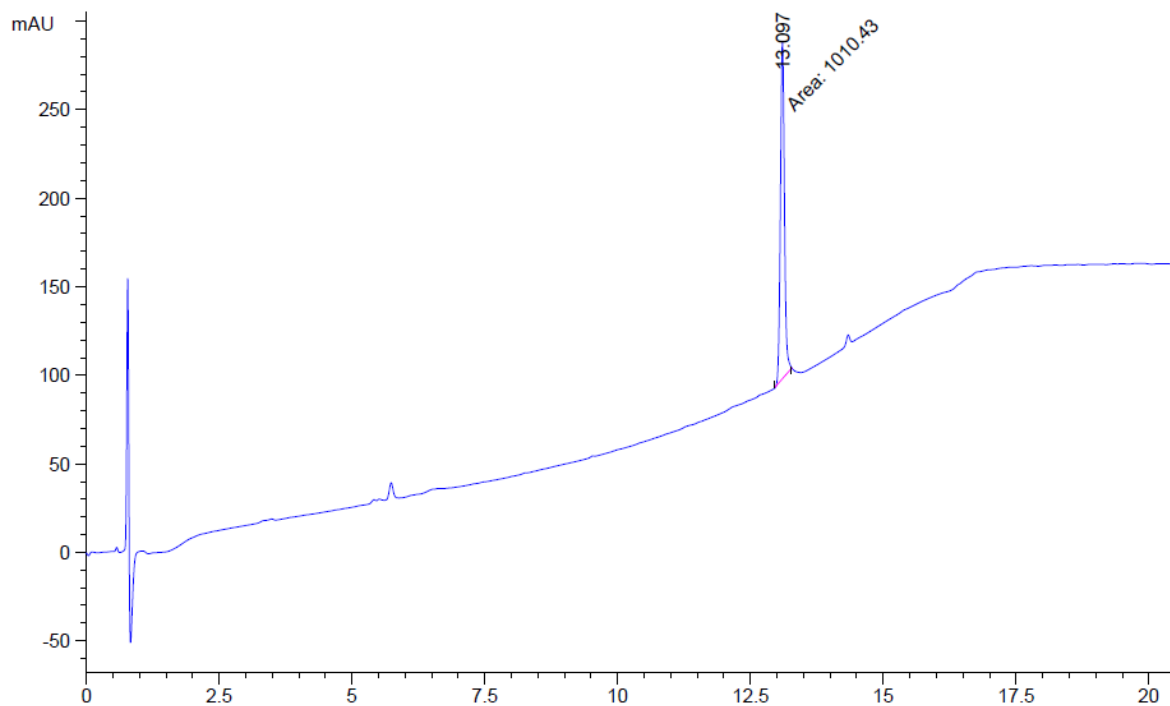
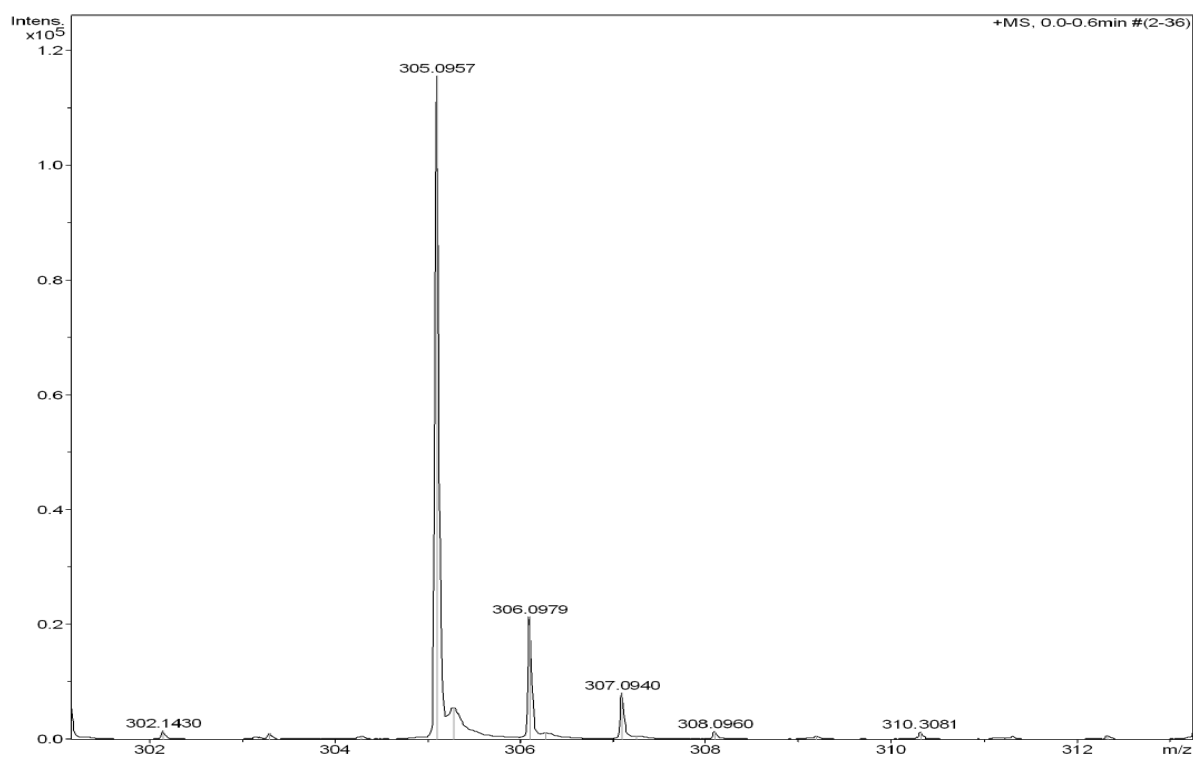


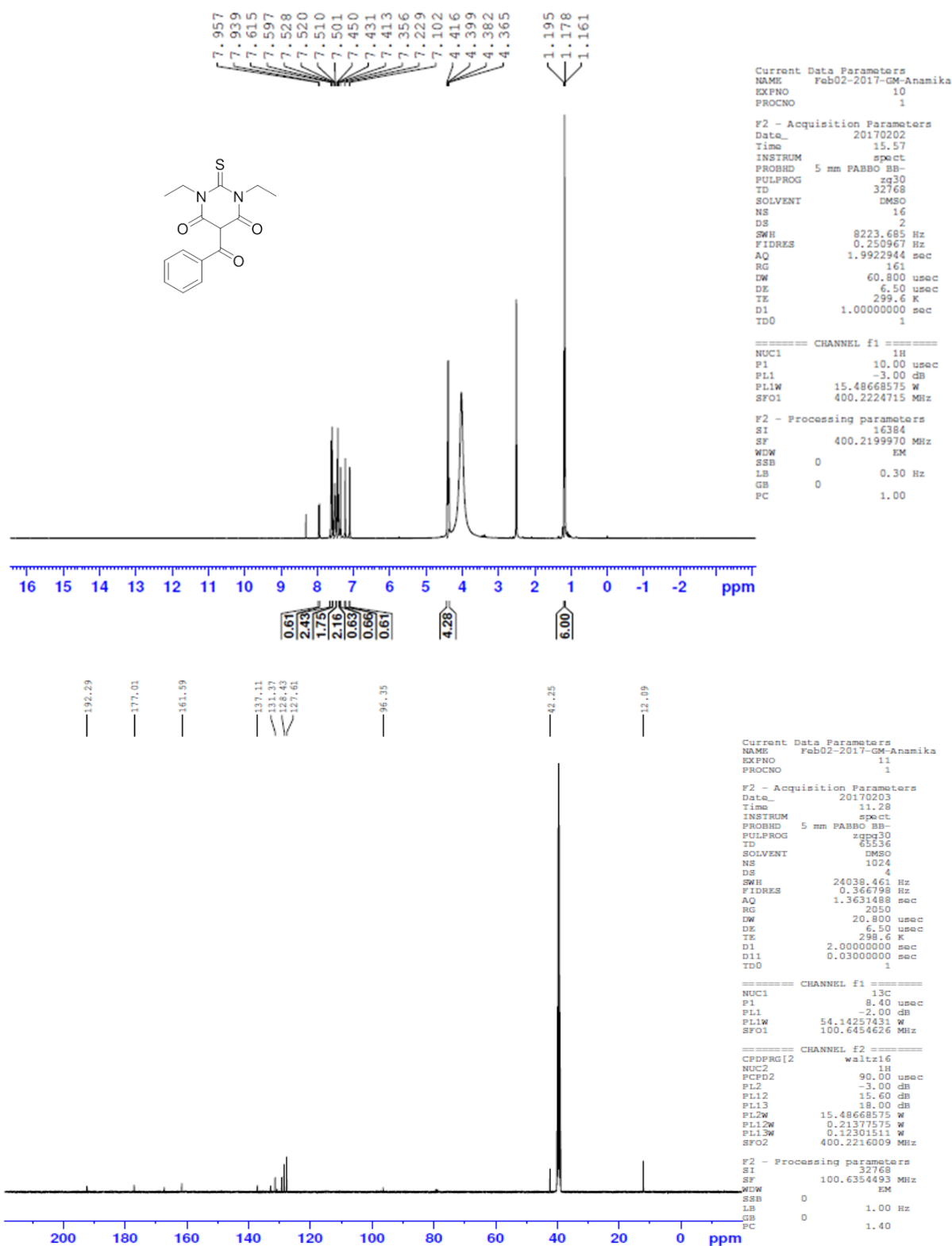
Figure S2 HRMS for compound A01

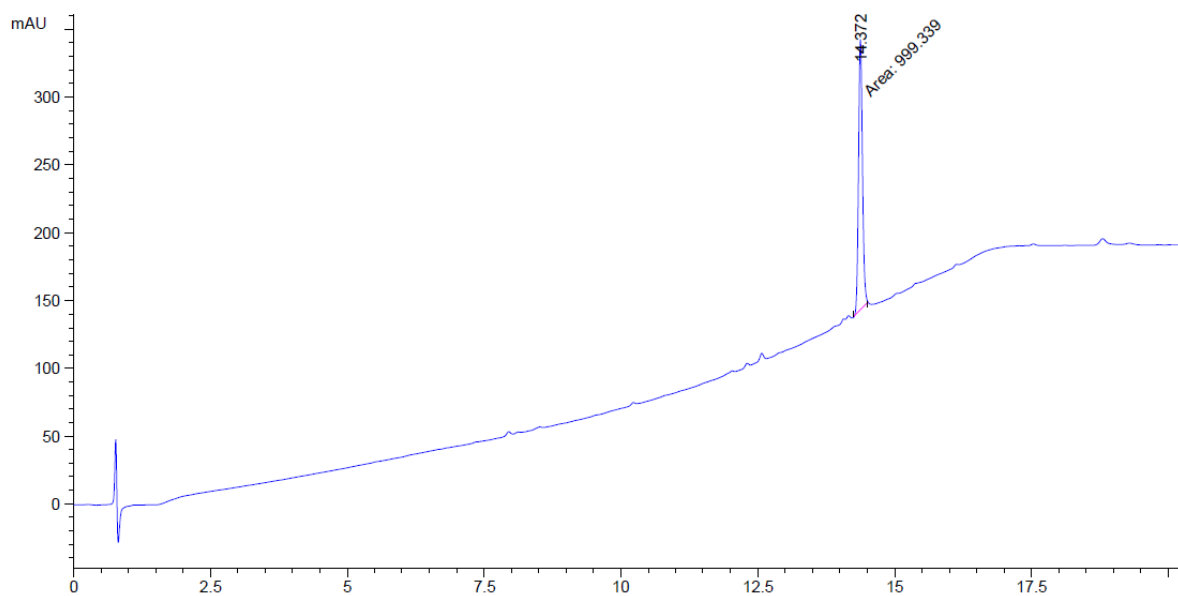
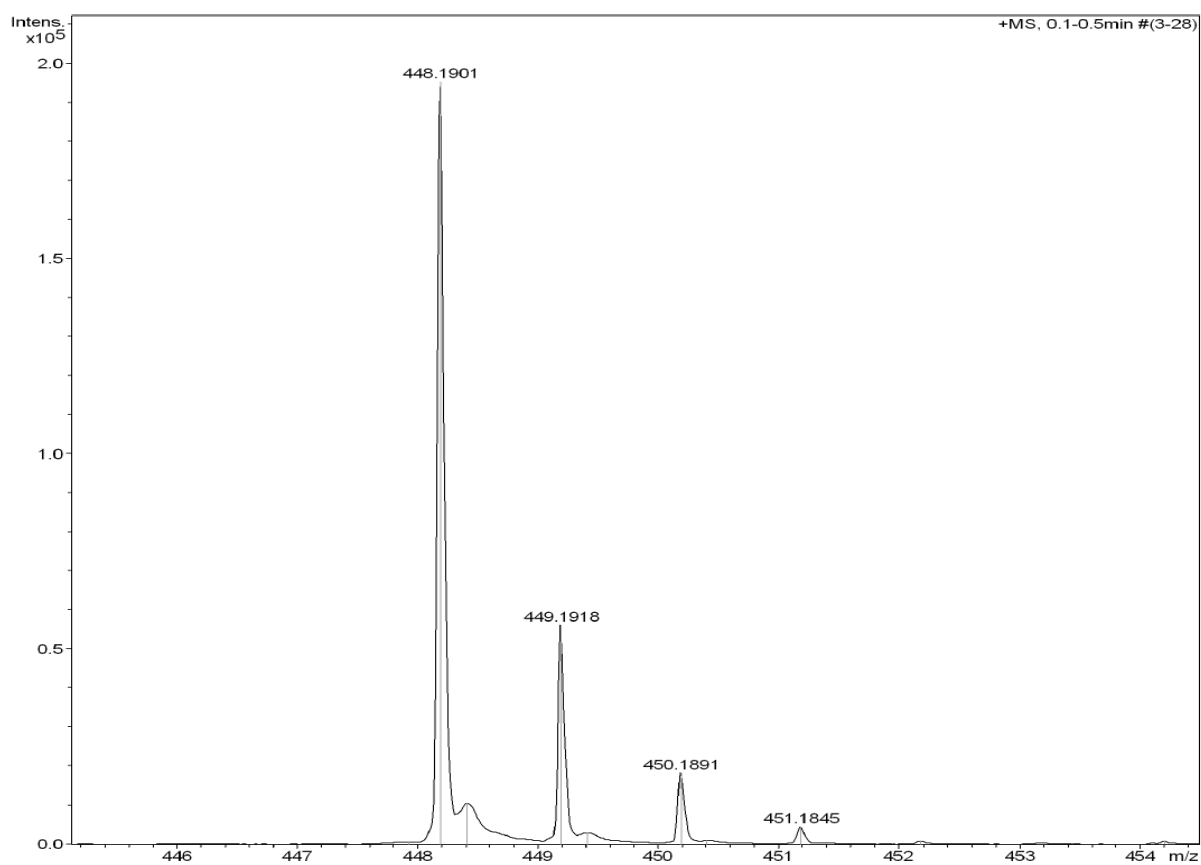
Figure S3 ¹H NMR and ¹³C NMR of compound A01

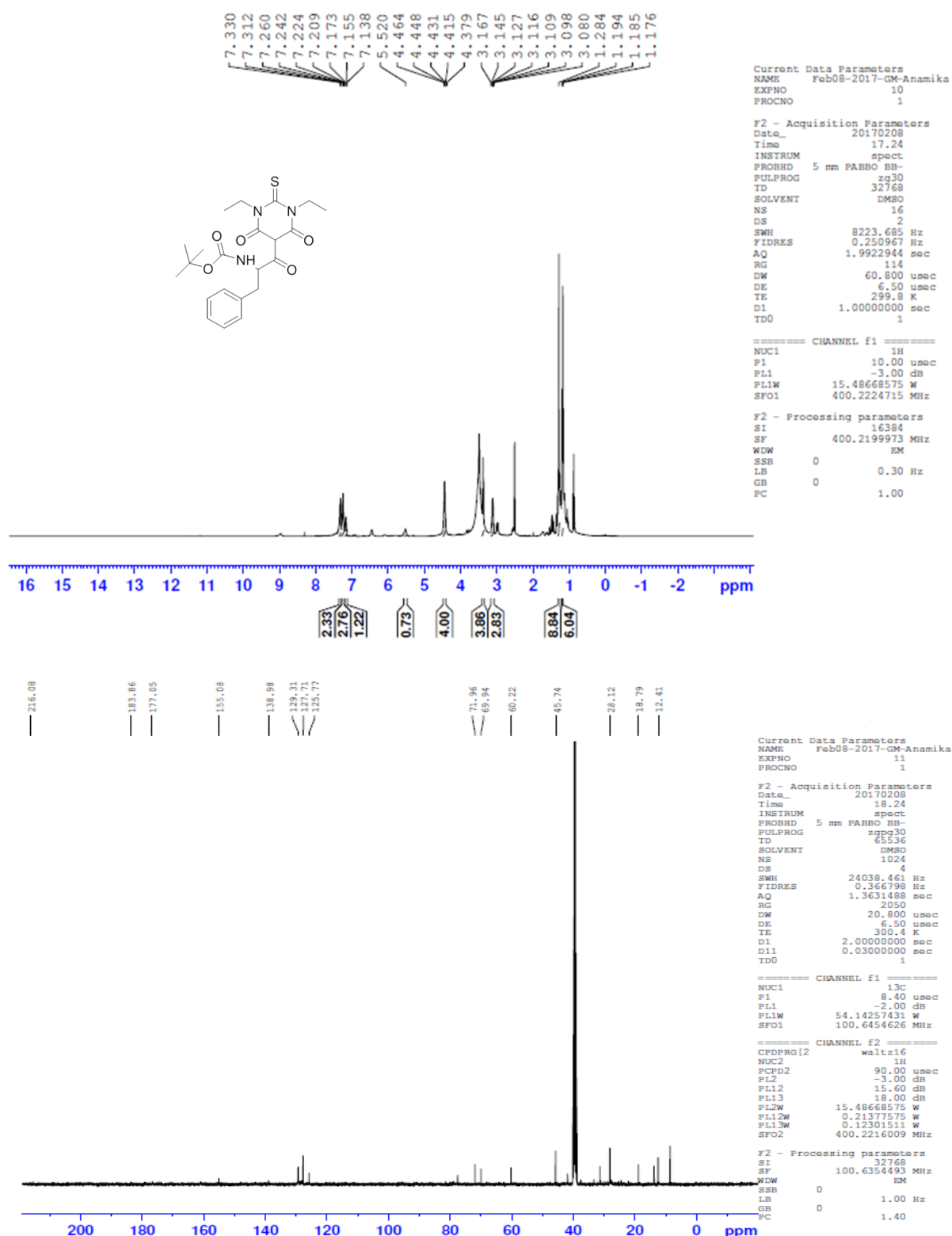
**Figure S4** HPLC for compound A02**Figure S5** HRMS for compound A02

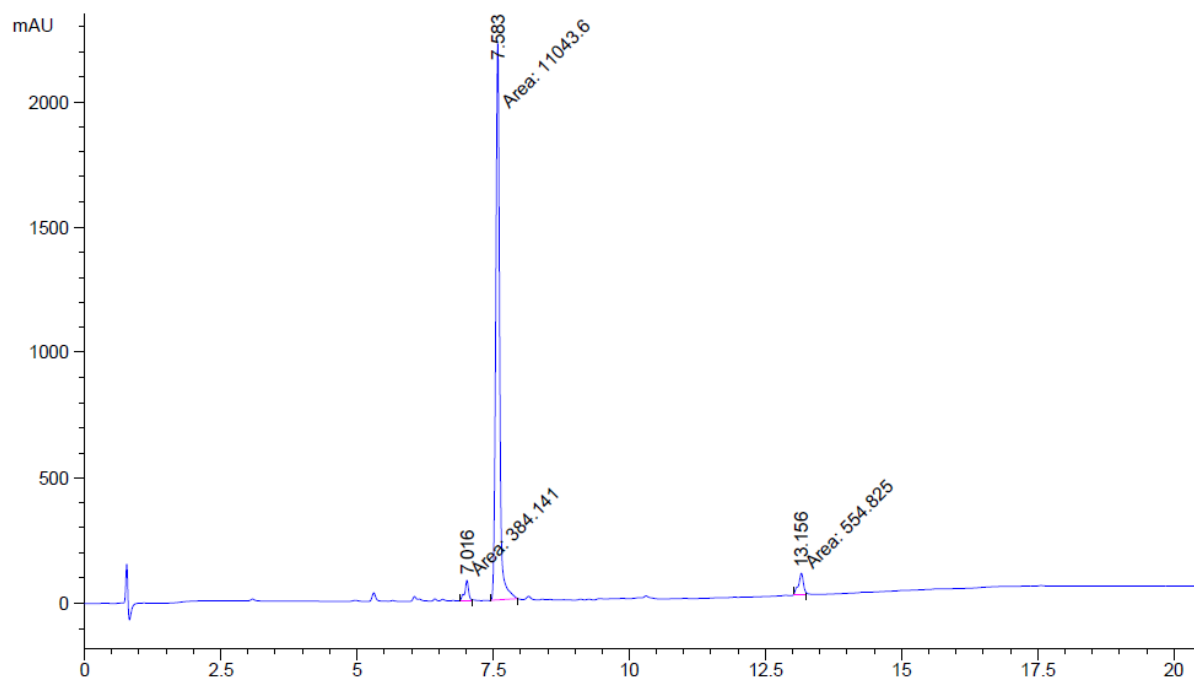
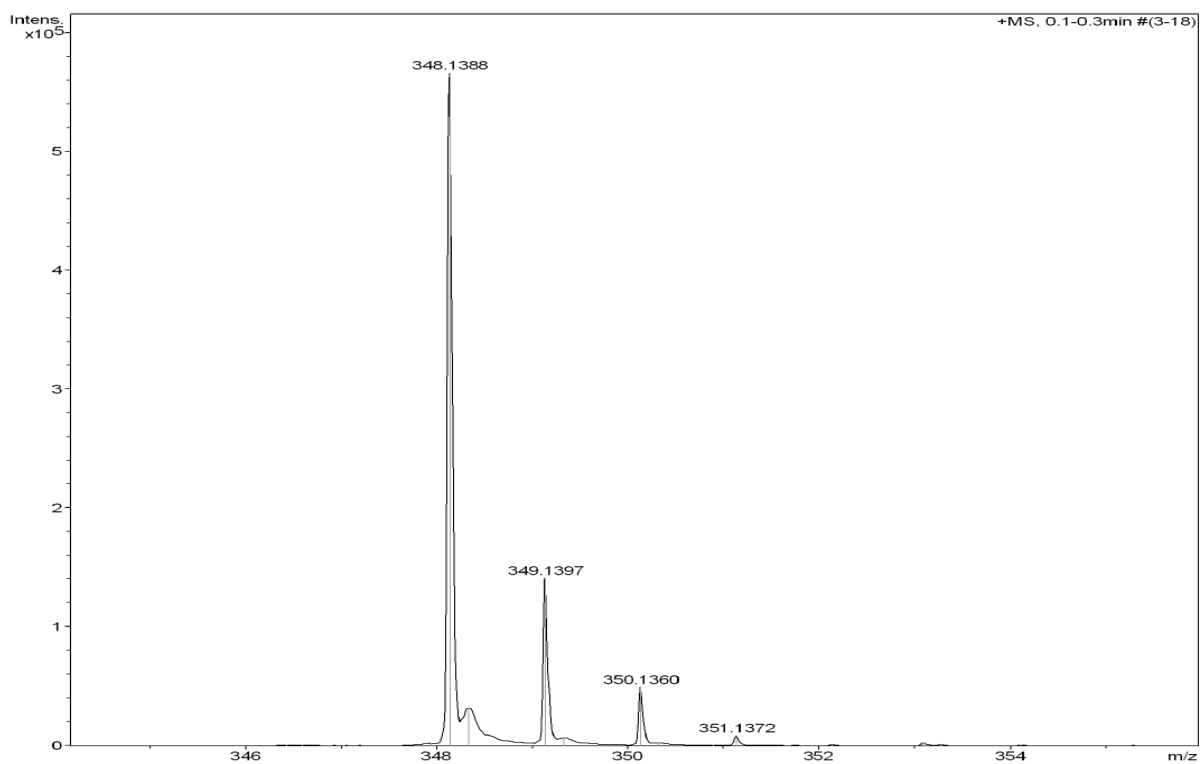
Figure S6 ^1H NMR and ^{13}C NMR of compound A02

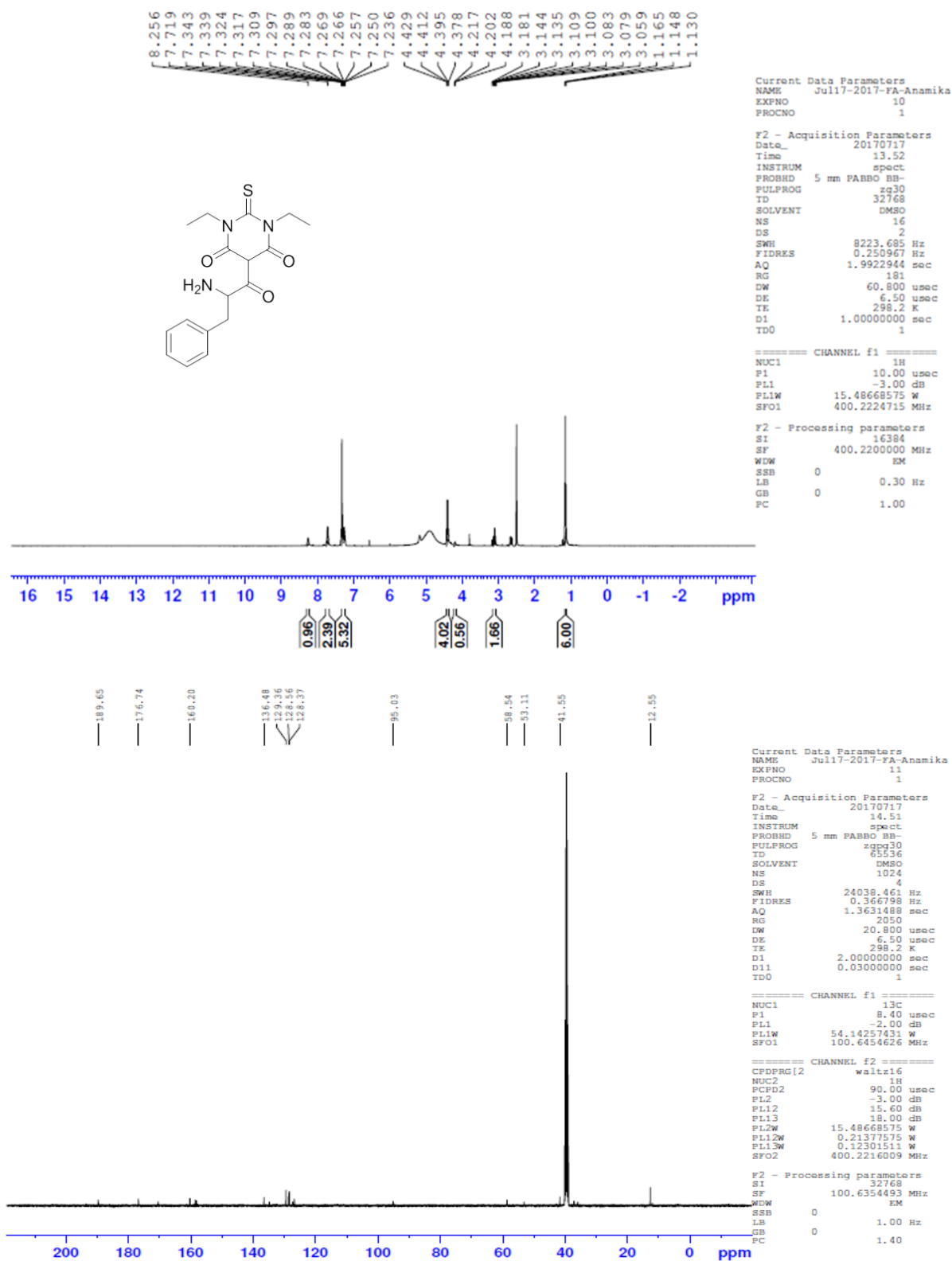
**Figure S7** HPLC for compound A03**Figure S8** HRMS for compound A03

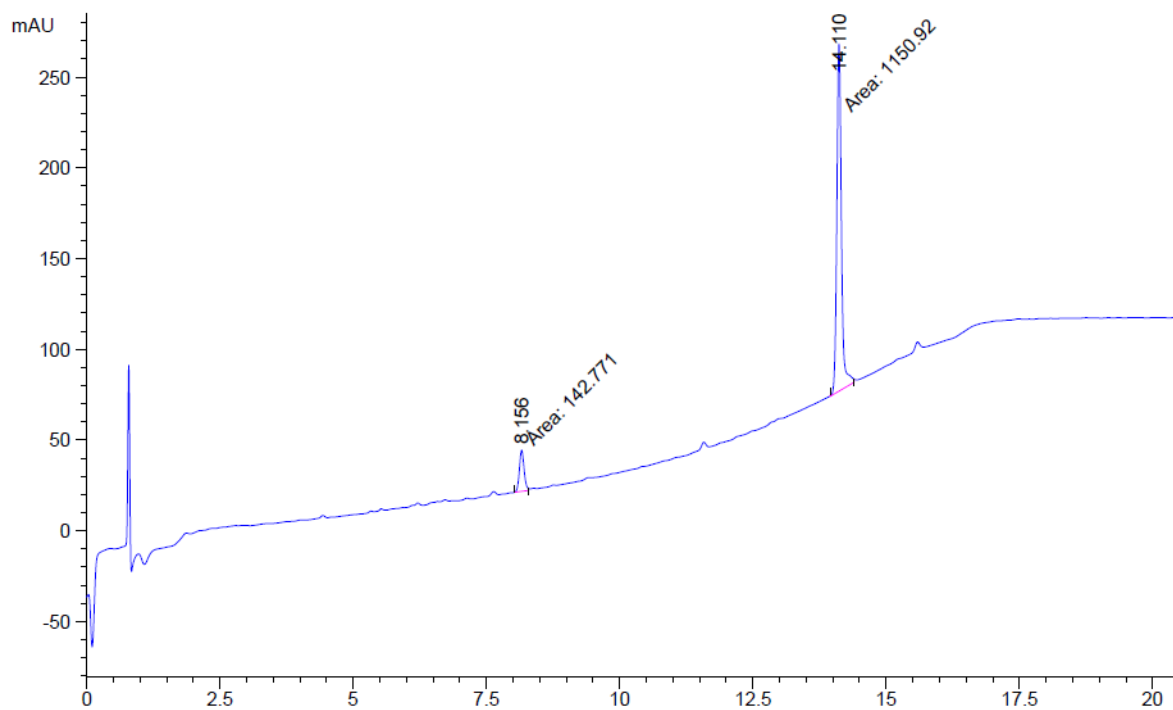
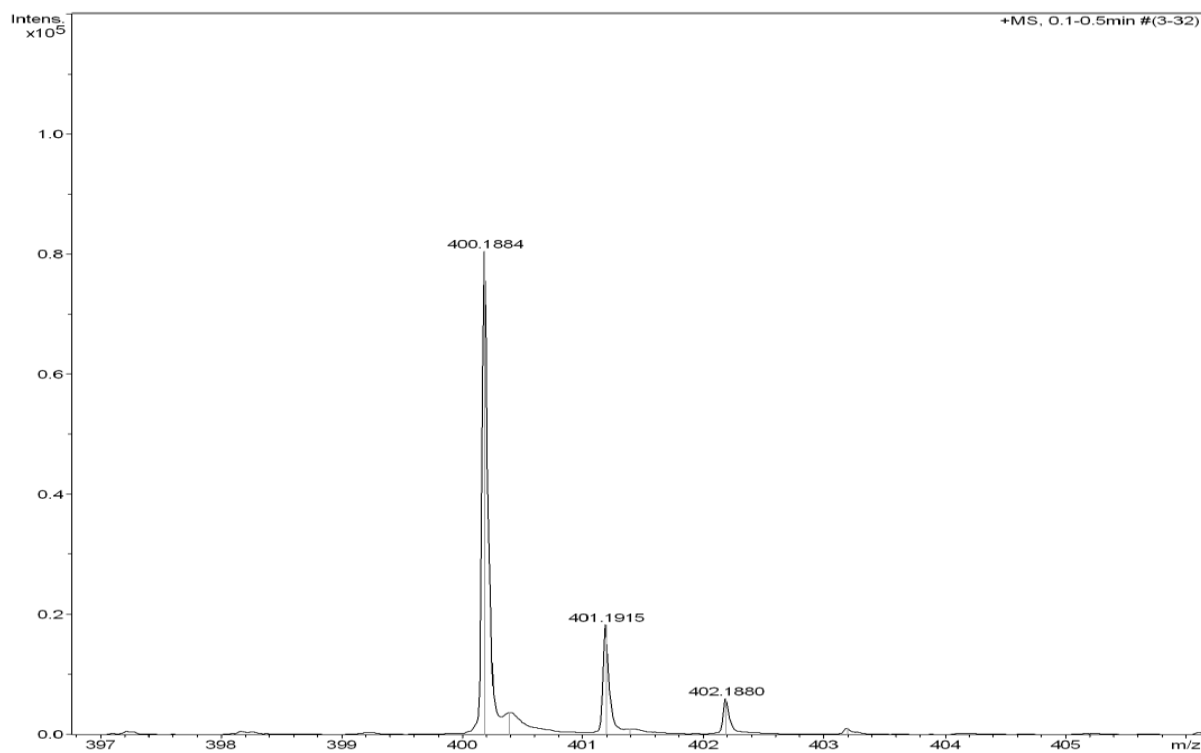
Figure S9 ¹H NMR and ¹³C NMR of compound A03

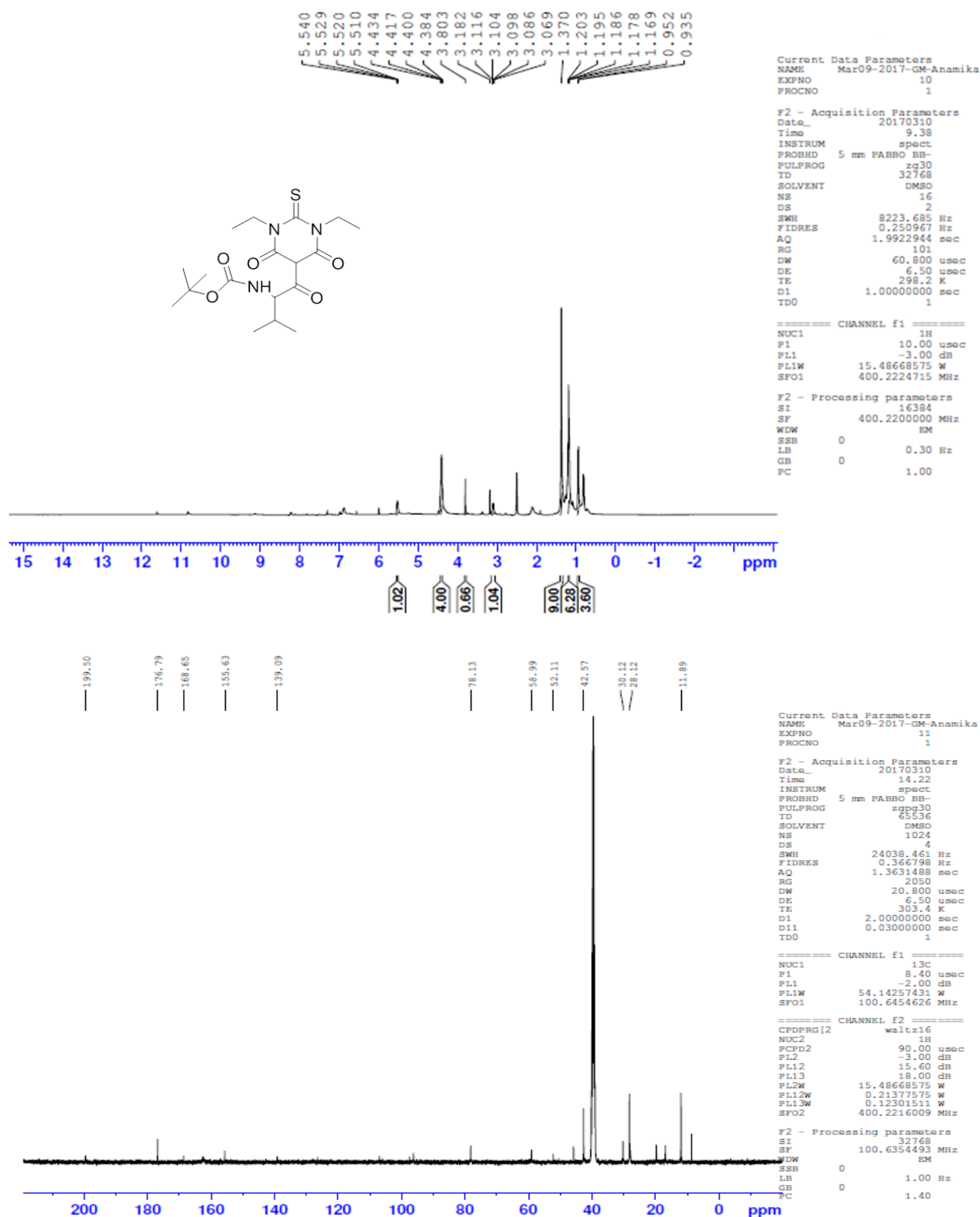
**Figure S10** HPLC for compound A04**Figure S11** HRMS for compound A04

Figure S12 ¹H NMR and ¹³C NMR of compound **A04**

**Figure S13** HPLC for compound A05**Figure S14** HRMS for compound A05

Figure S15 ¹H NMR and ¹³C NMR of compound A05

**Figure S16** HPLC for compound A06**Figure S17** HRMS for compound A06

Figure S18 ^1H NMR and ^{13}C NMR of compound A06

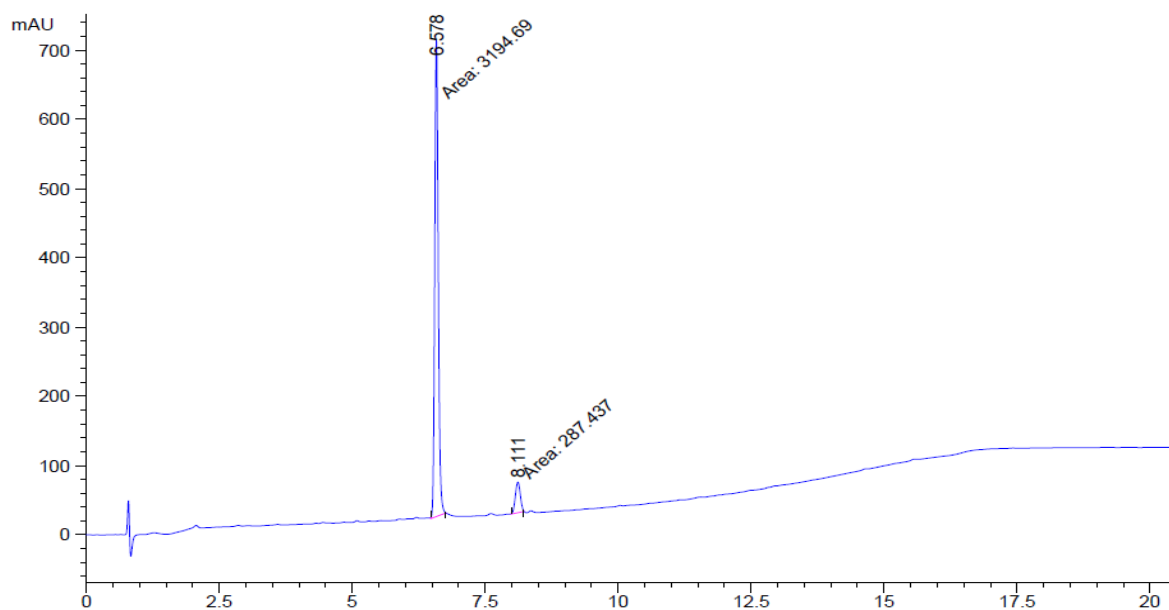


Figure S19 HPLC for compound **A07**

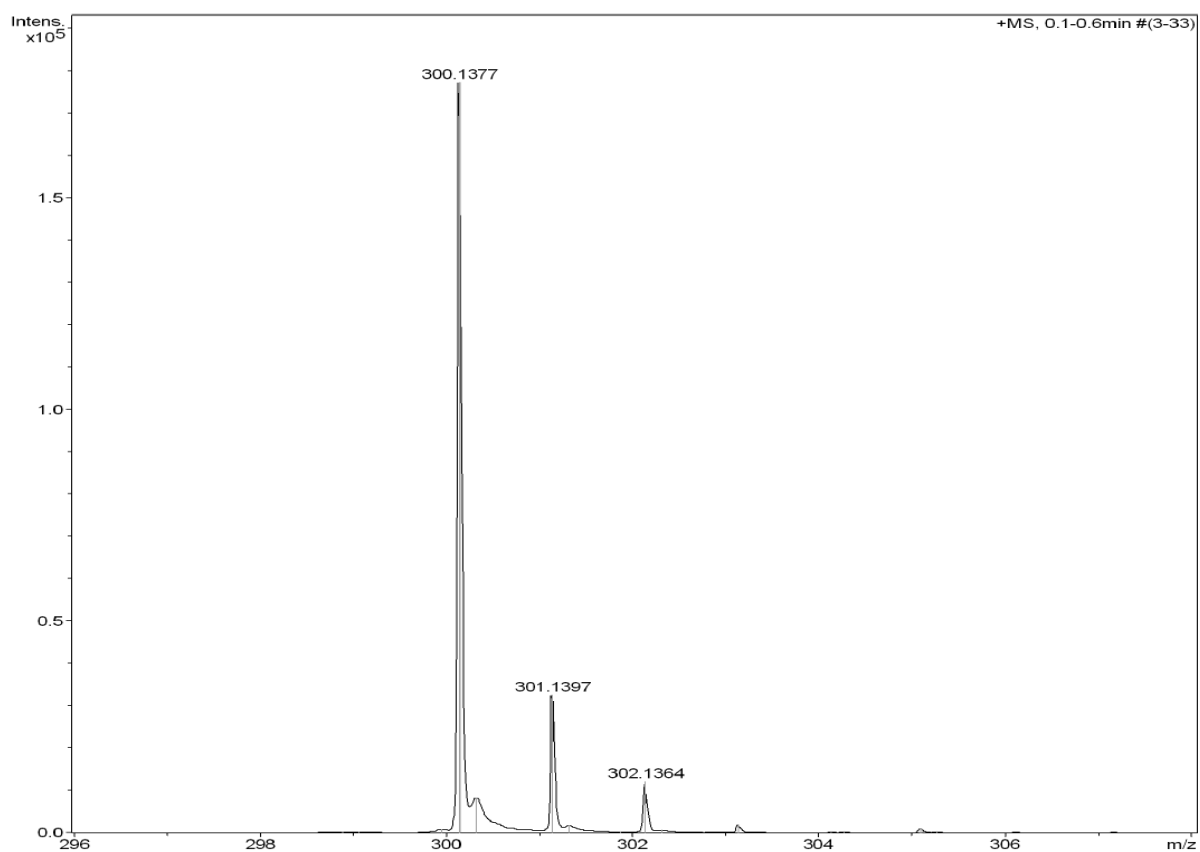
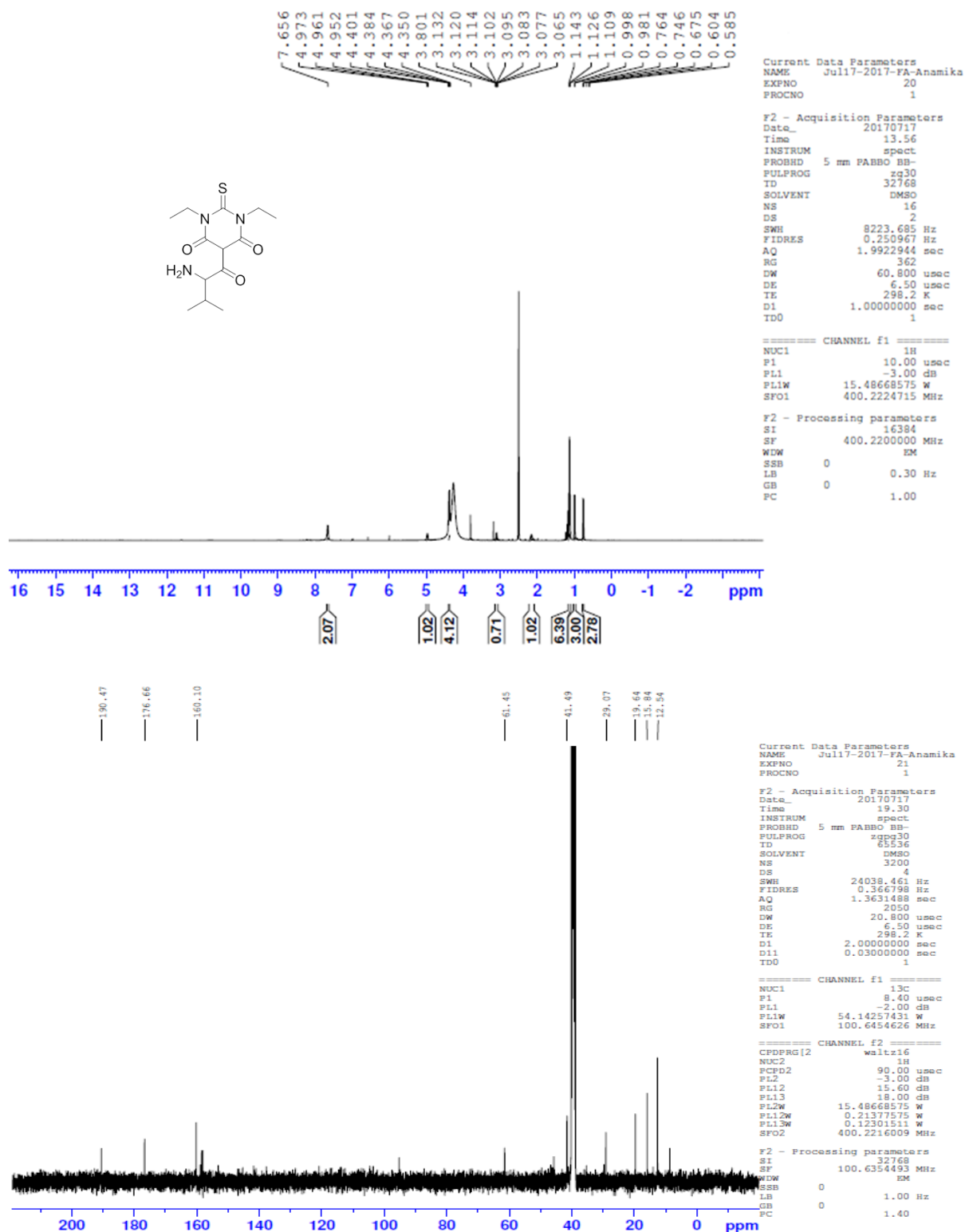


Figure S20 HRMS for compound **A07**

Figure S21 ¹H NMR and ¹³C NMR of compound A07

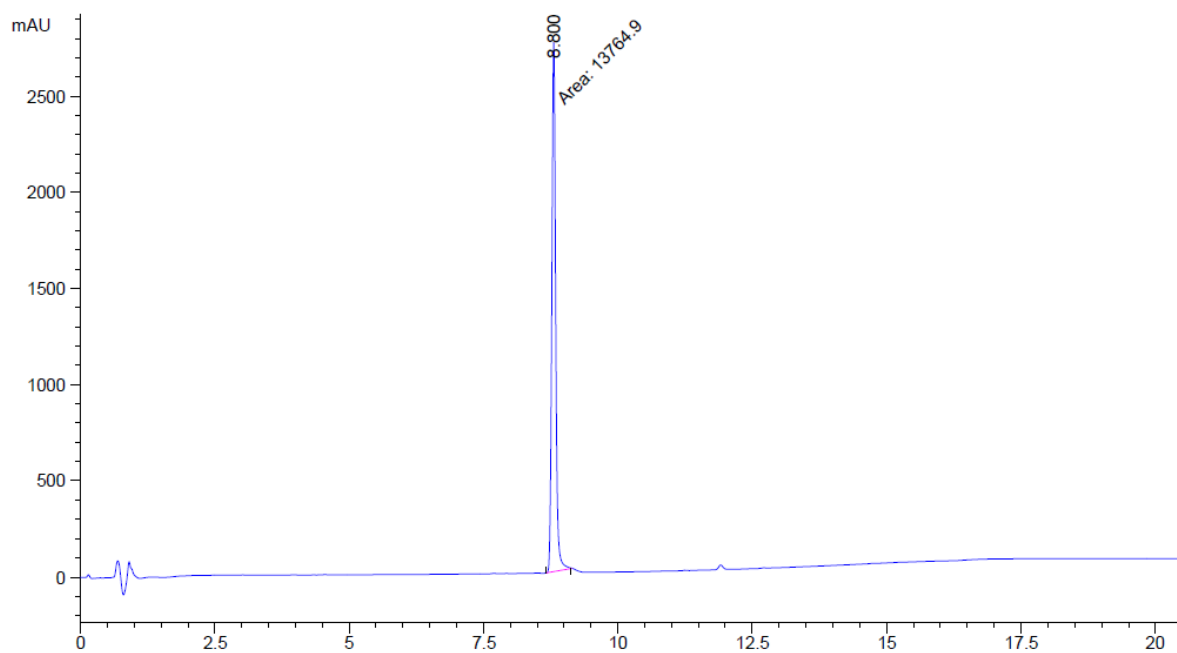


Figure S22 HPLC for compound **A08**

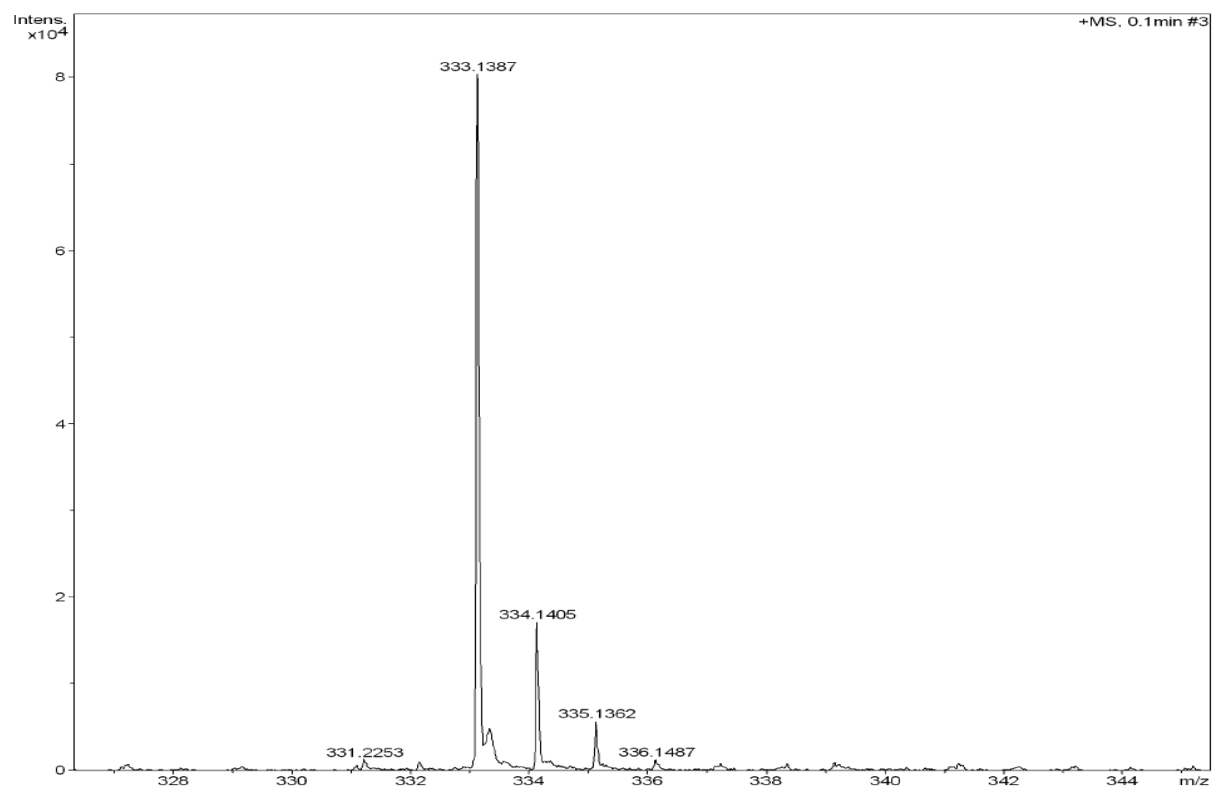
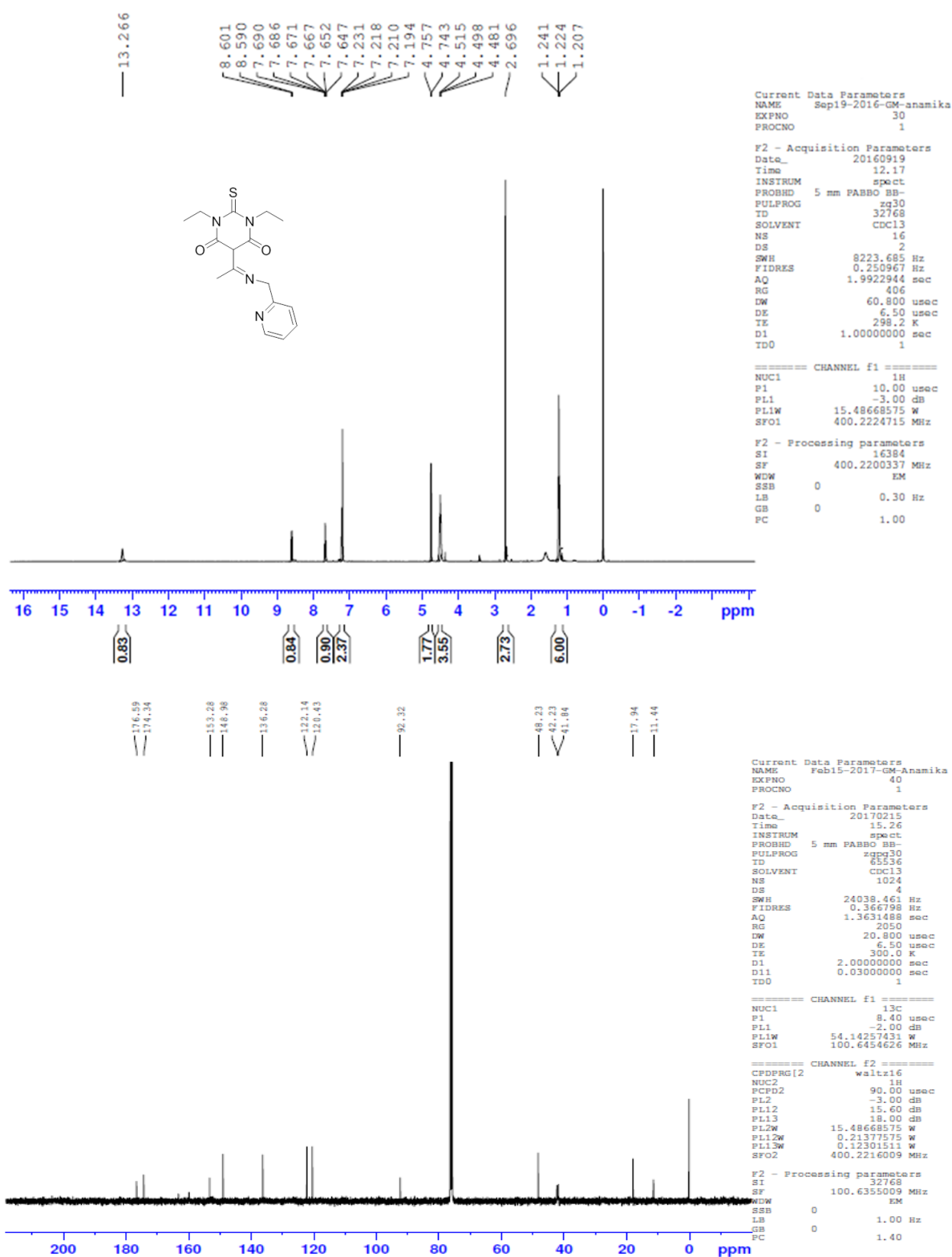


Figure S23 HRMS for compound **A08**

Figure S24 ¹H NMR and ¹³C NMR of compound A08

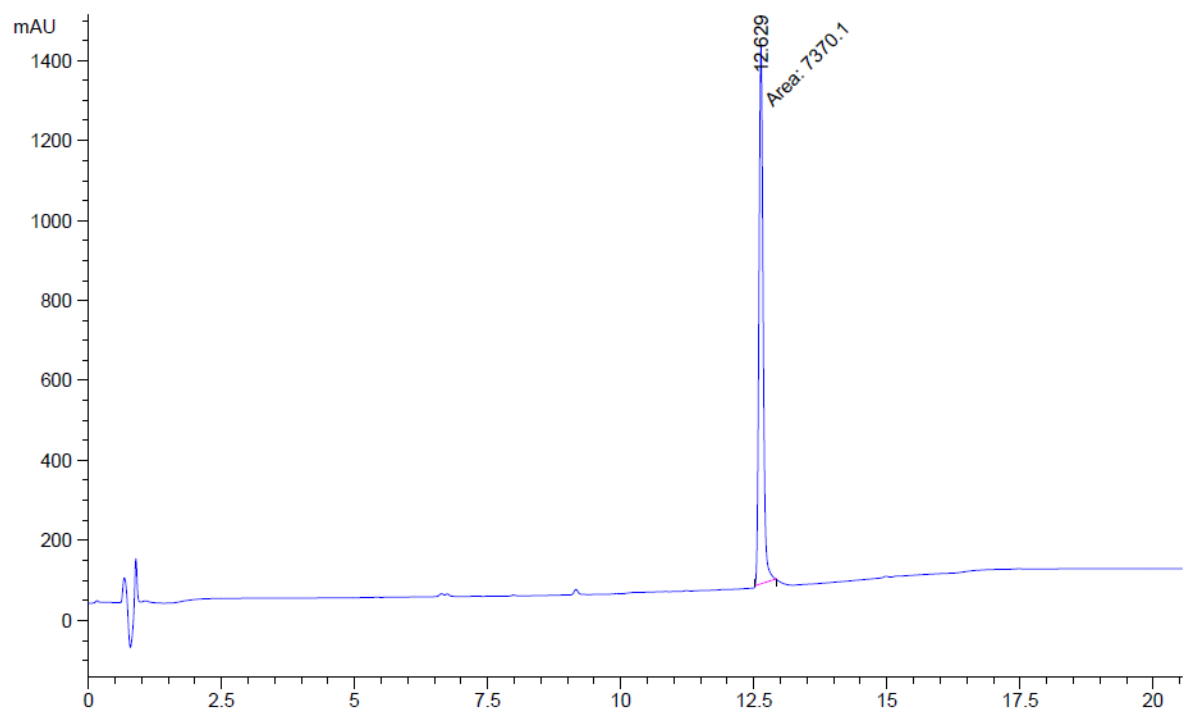


Figure S25 HPLC for compound **A09**

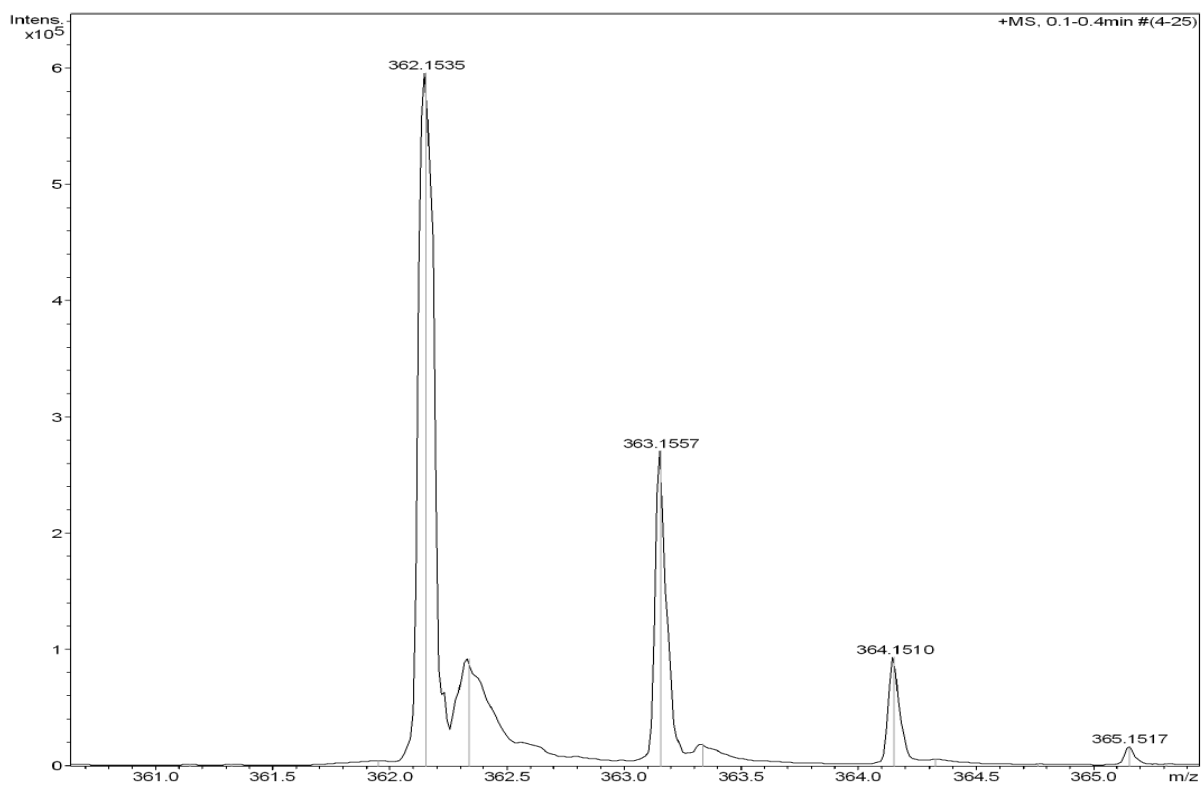
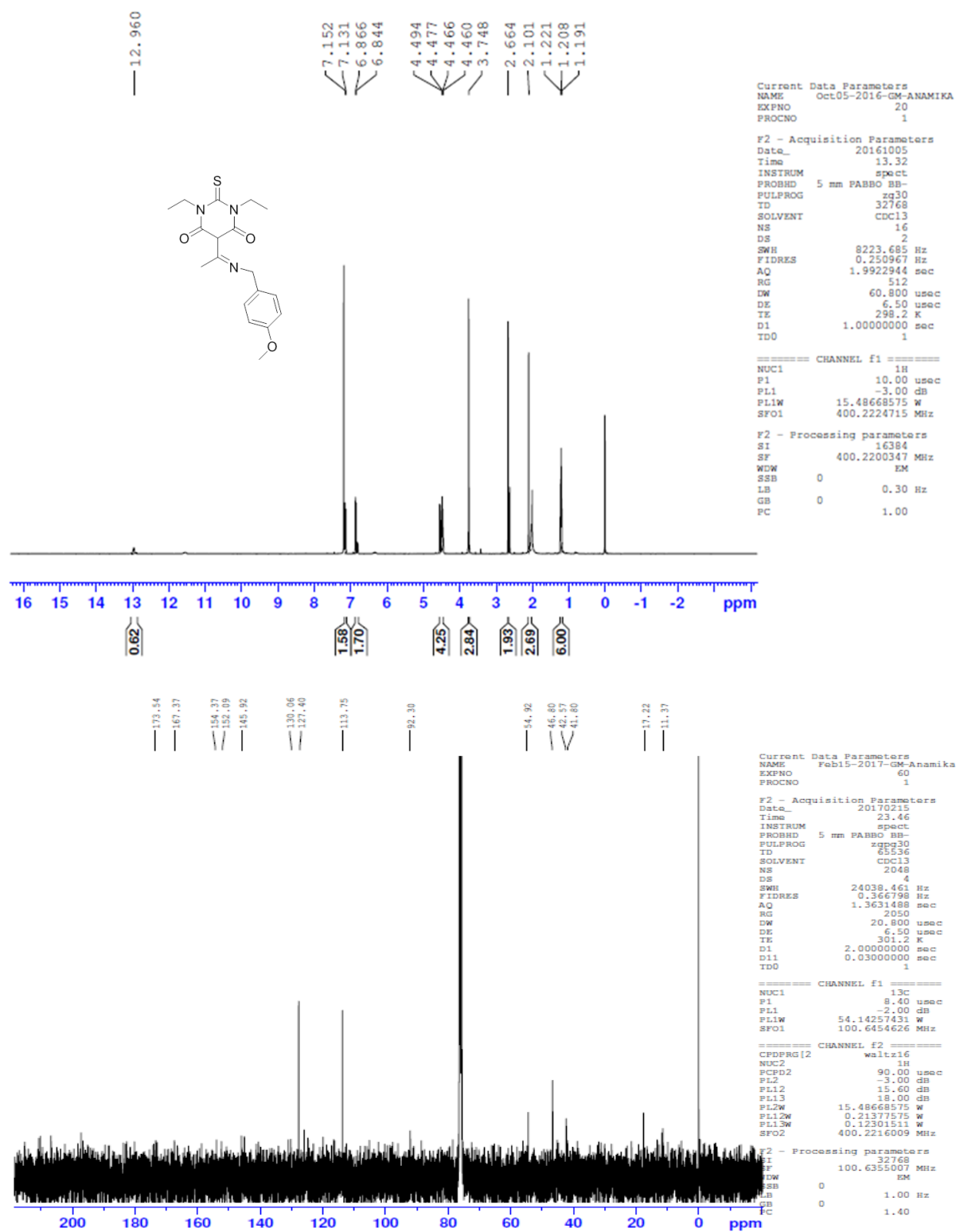
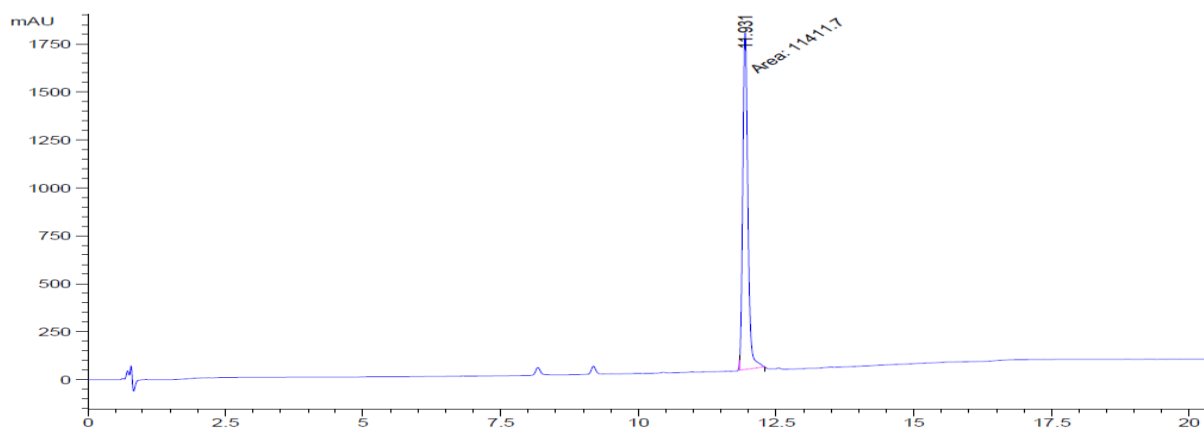
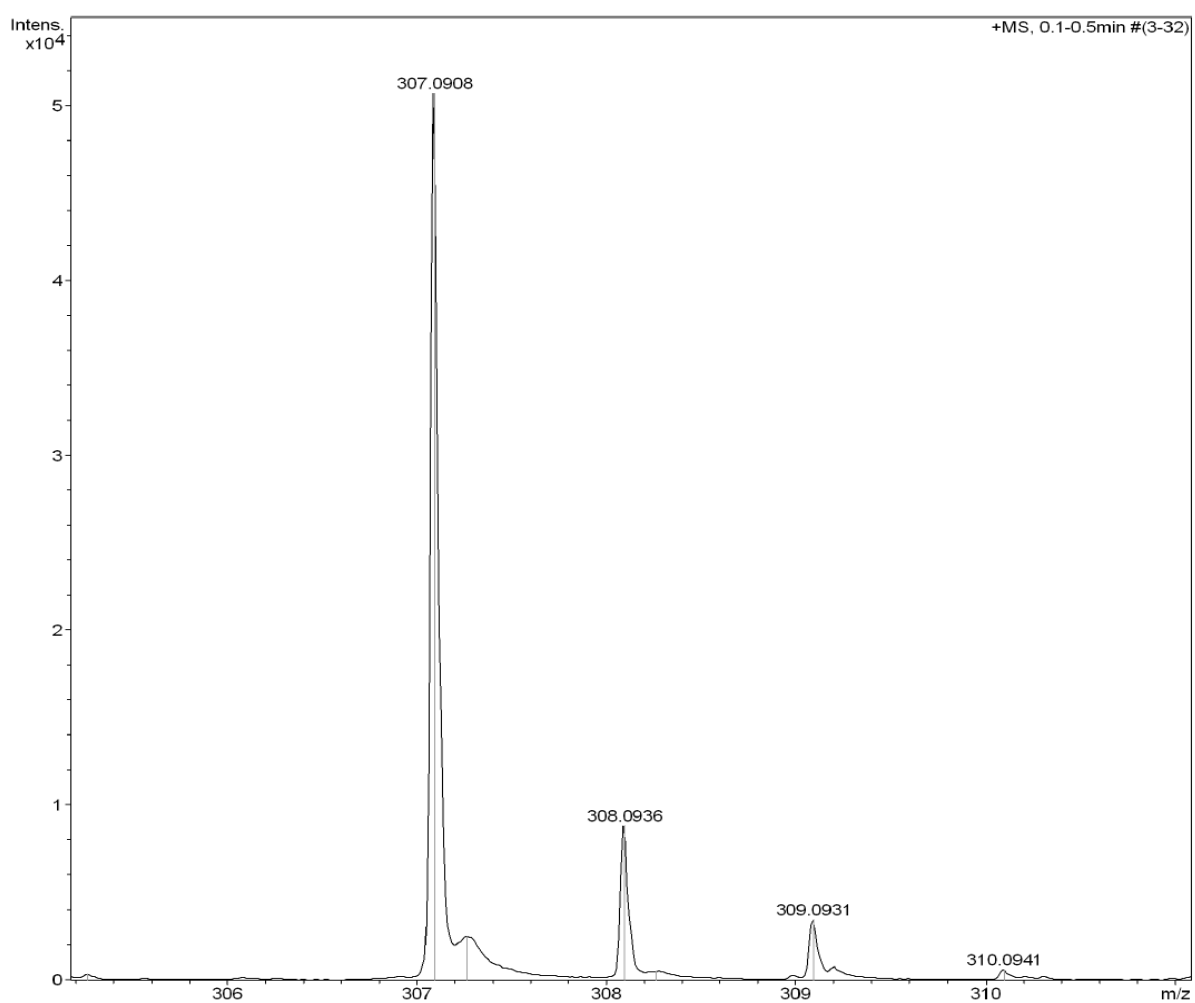
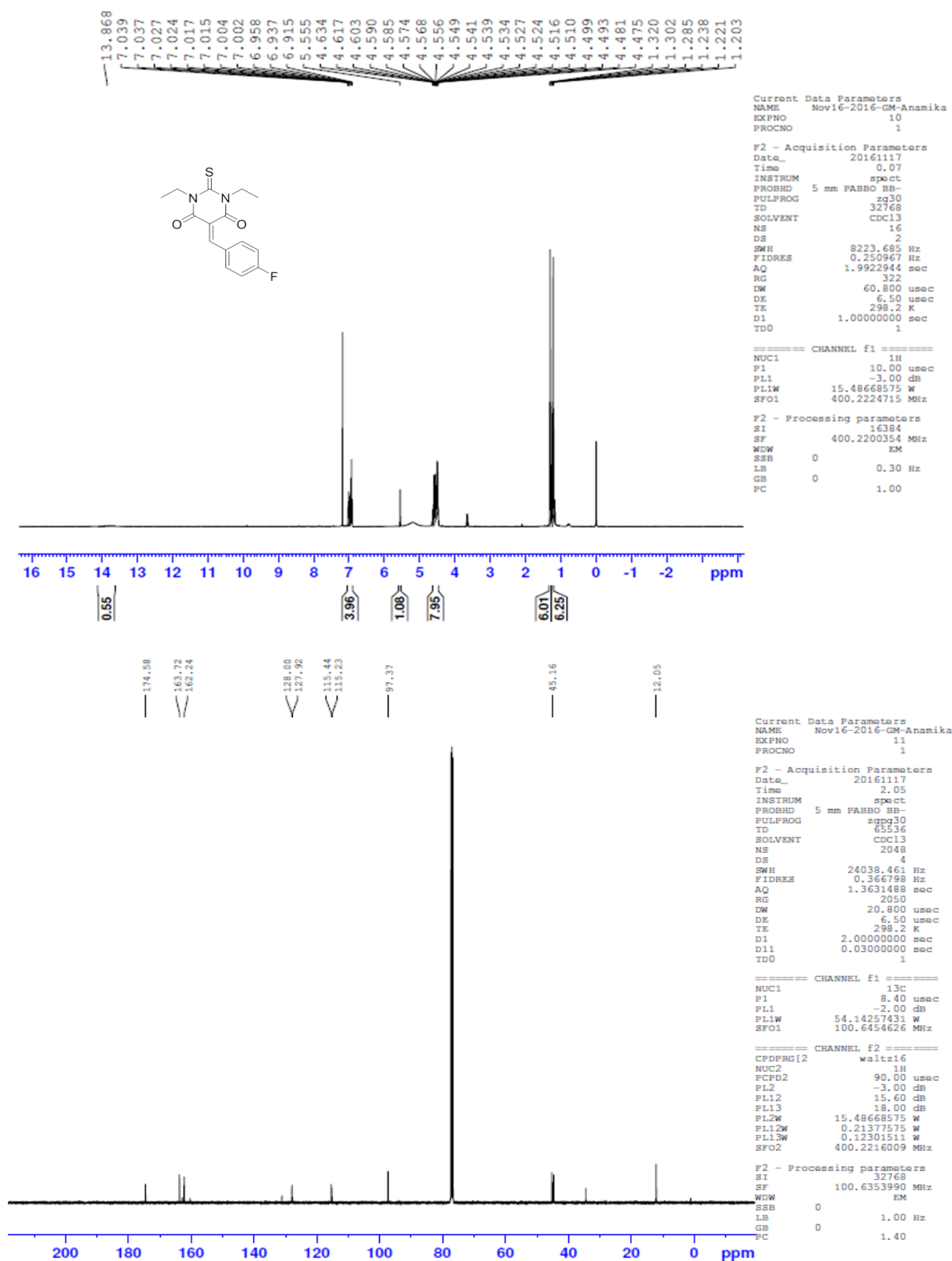


Figure S26 HRMS for compound **A09**

Figure S27 ¹H NMR and ¹³C NMR of compound A09

**Figure S28** HPLC for compound **A10****Figure S29** HRMS for compound **A10**

Figure S30 ¹H NMR and ¹³C NMR of compound A10

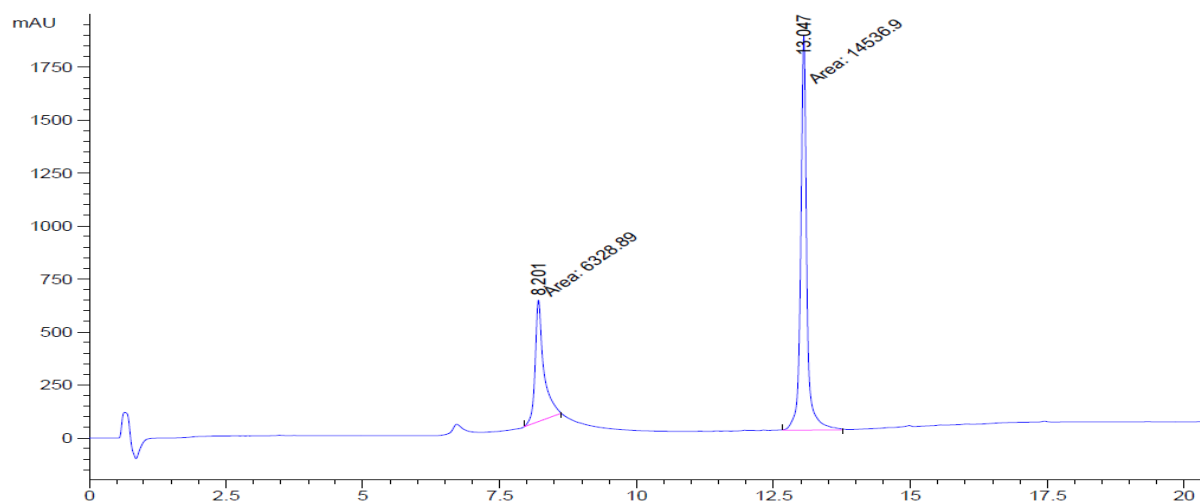


Figure S31 HPLC for compound **A11**

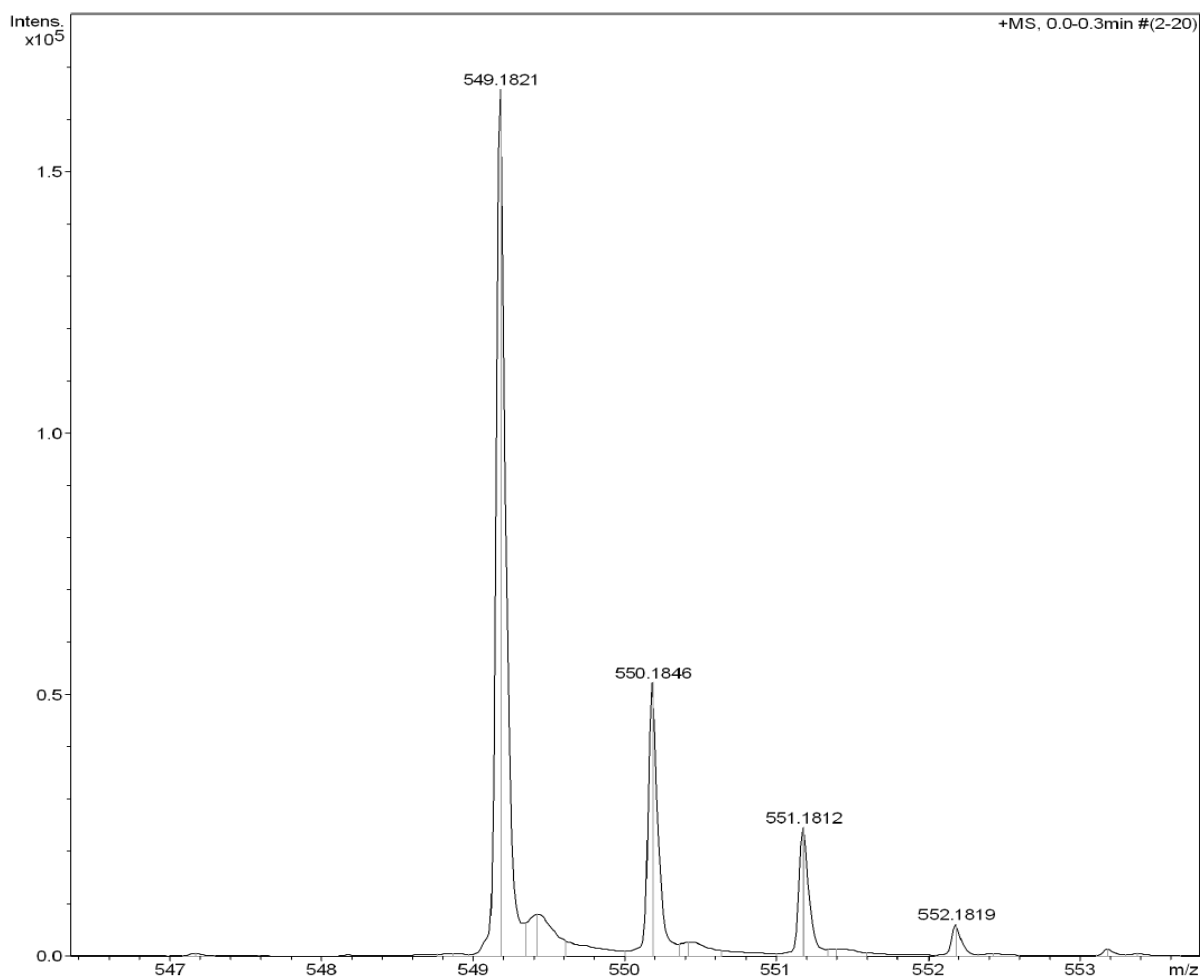


Figure S32 HRMS for compound **A11**

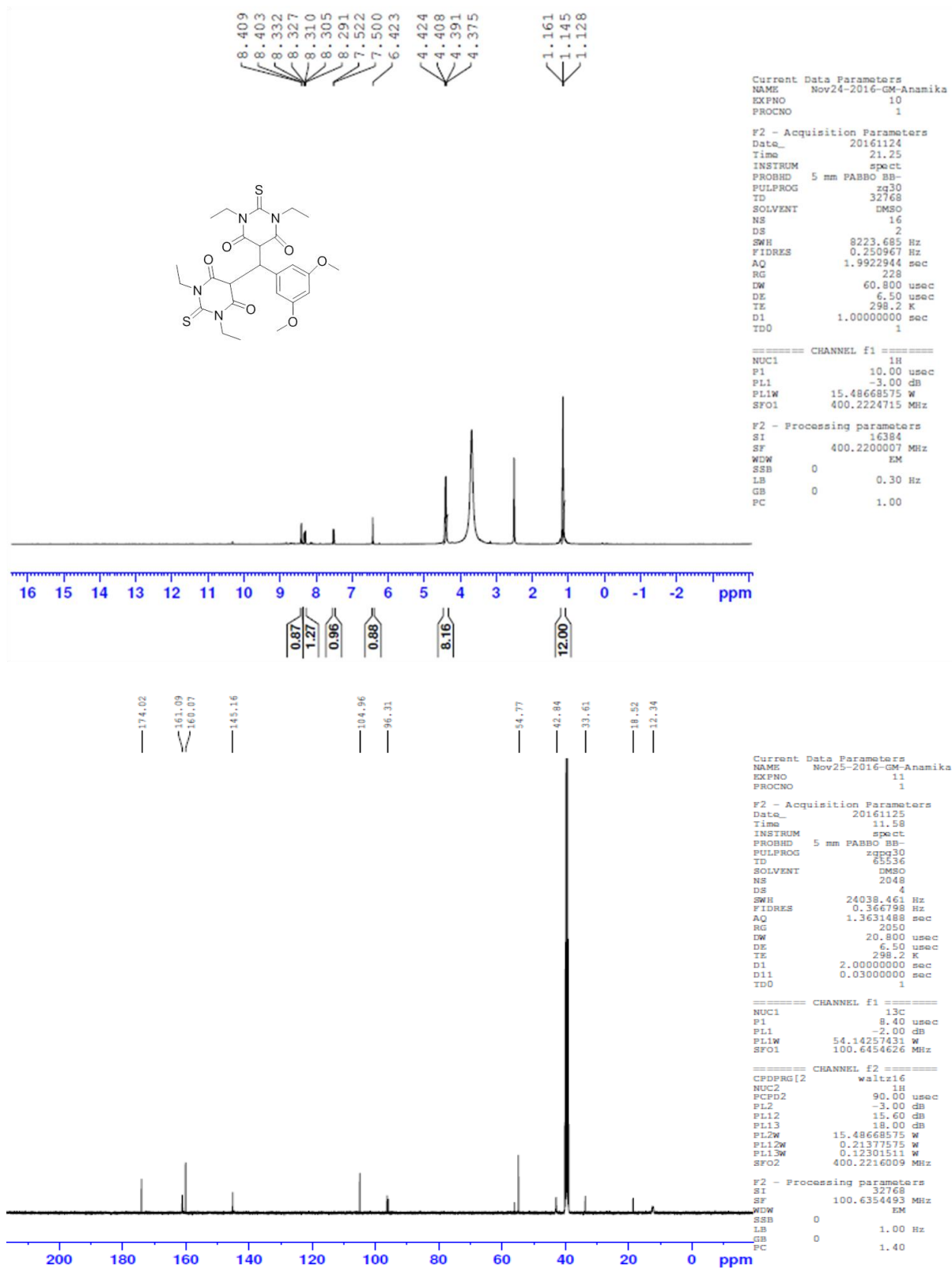
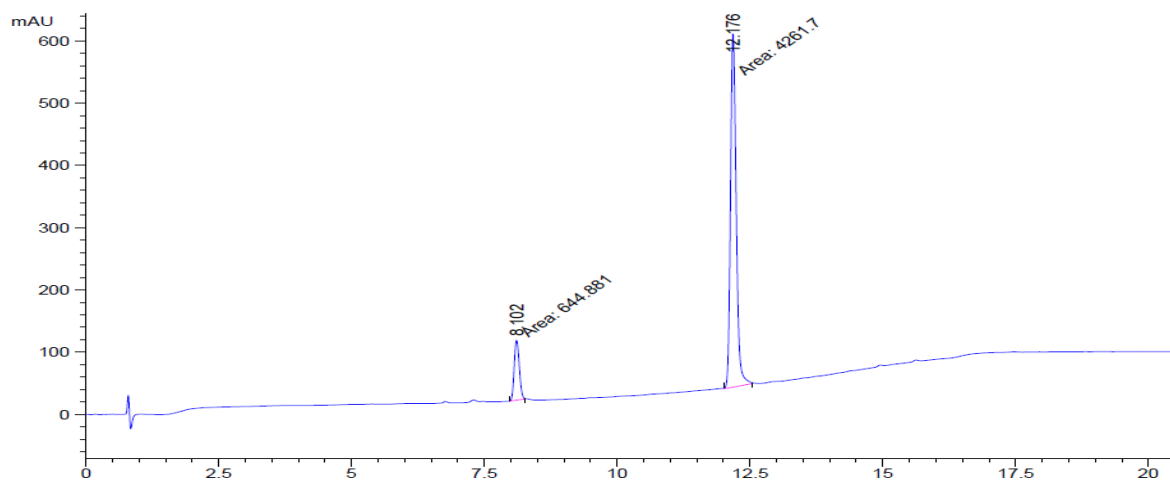
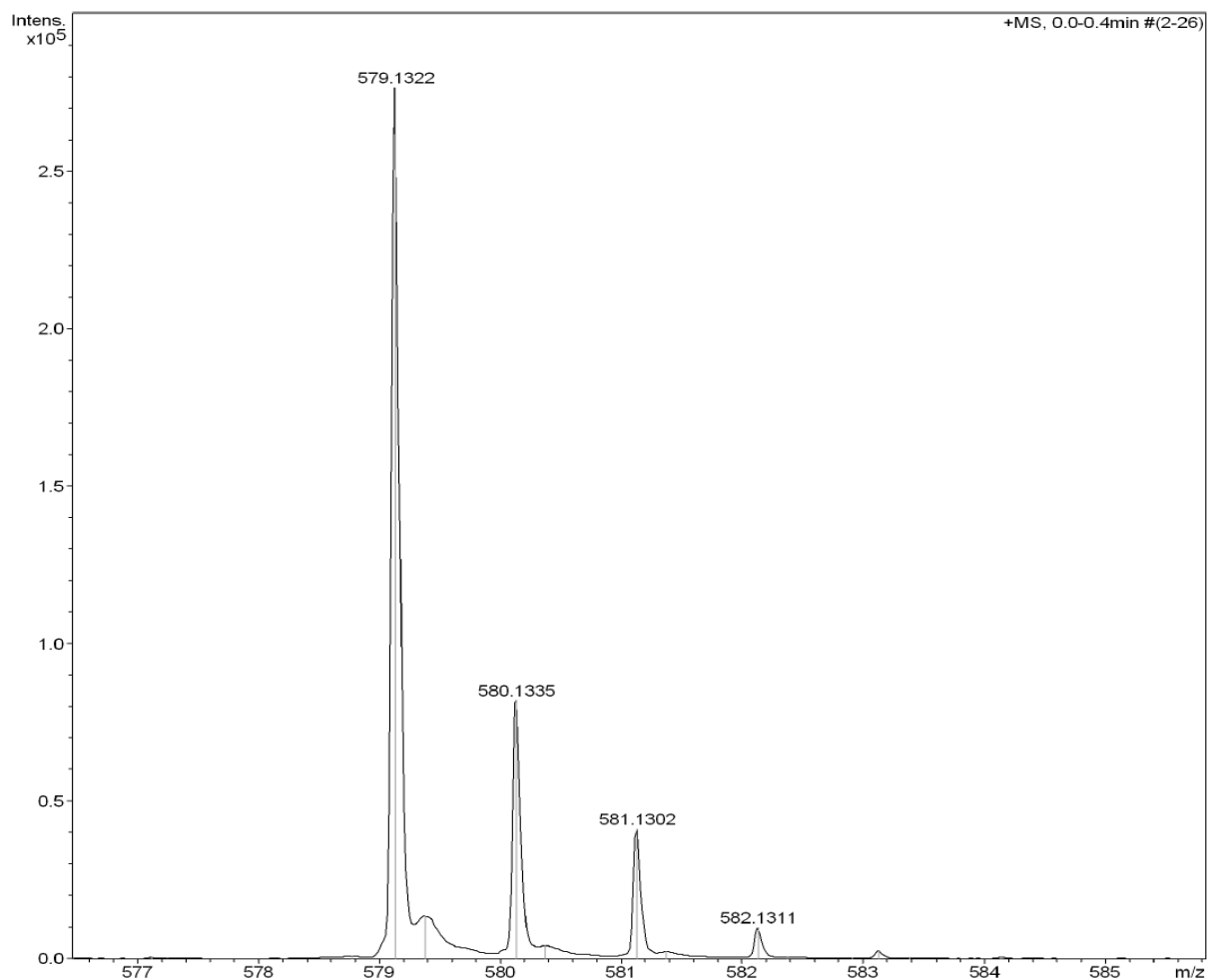
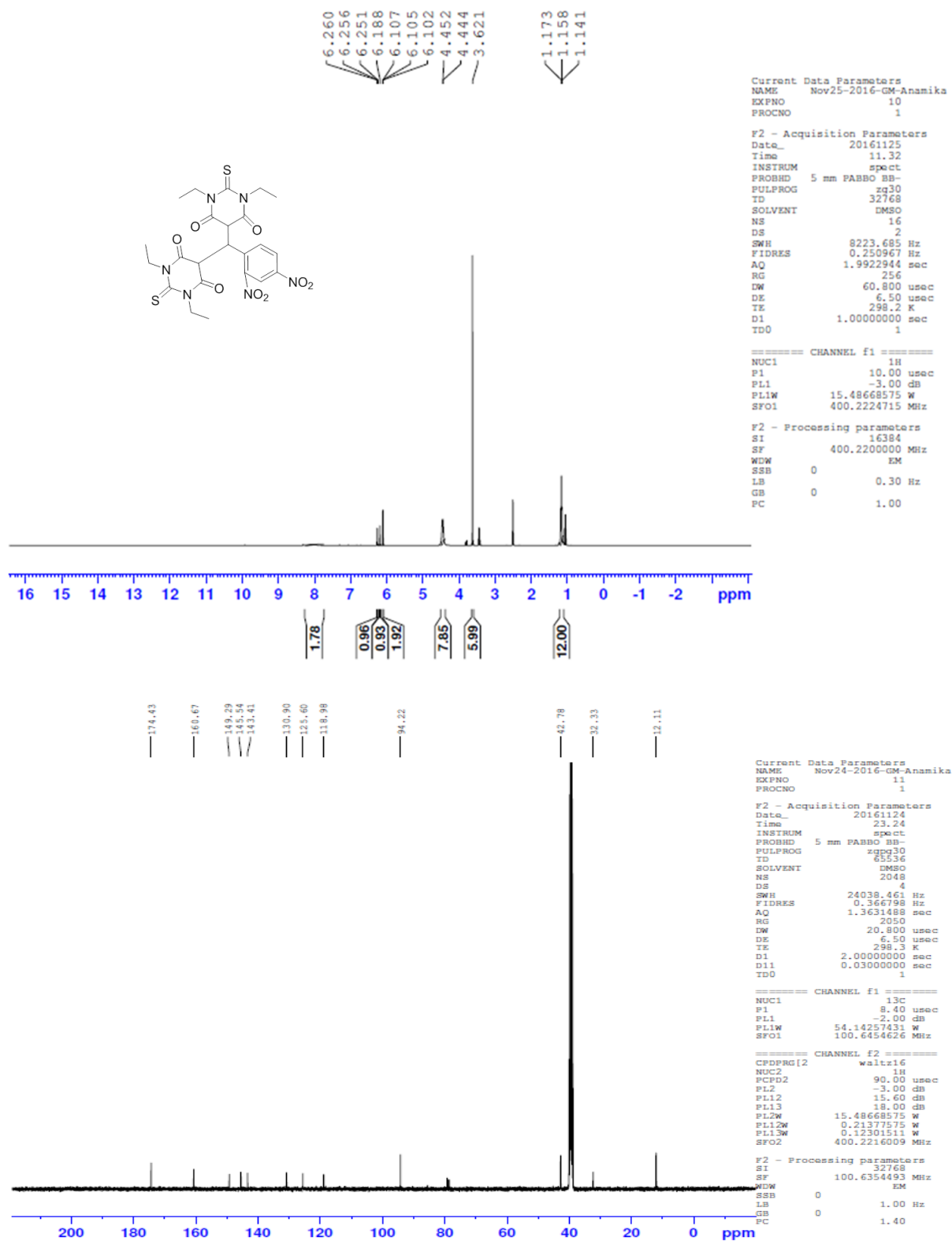


Figure S33 ^1H NMR and ^{13}C NMR of compound A11

**Figure S34** HPLC for compound A12**Figure S35** HRMS for compound A12

Figure S36 ¹H NMR and ¹³C NMR of compound A12

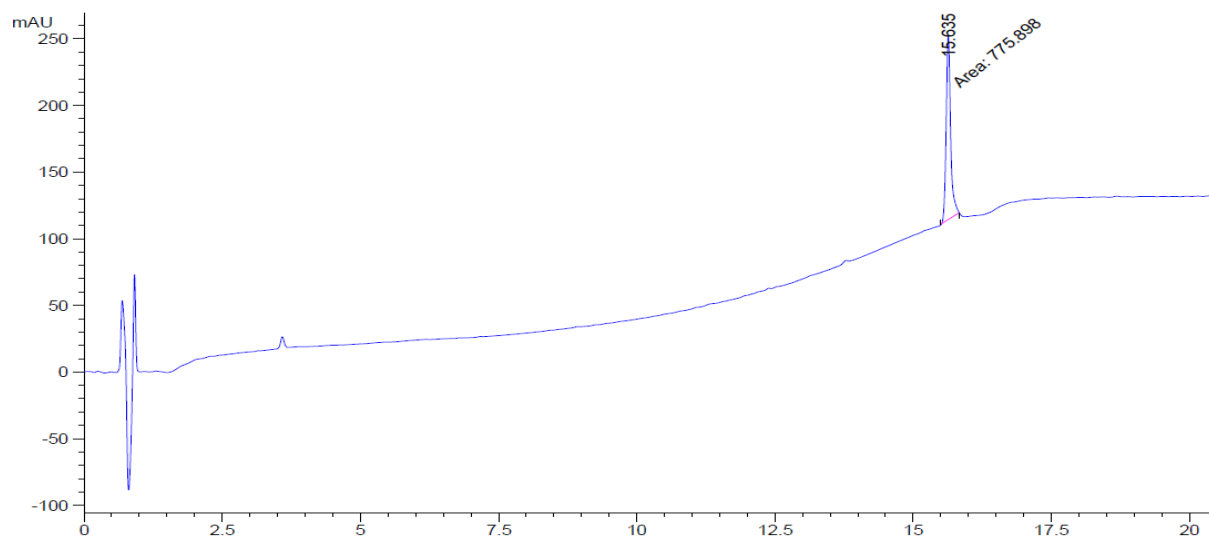


Figure S37 HPLC for compound **A13**

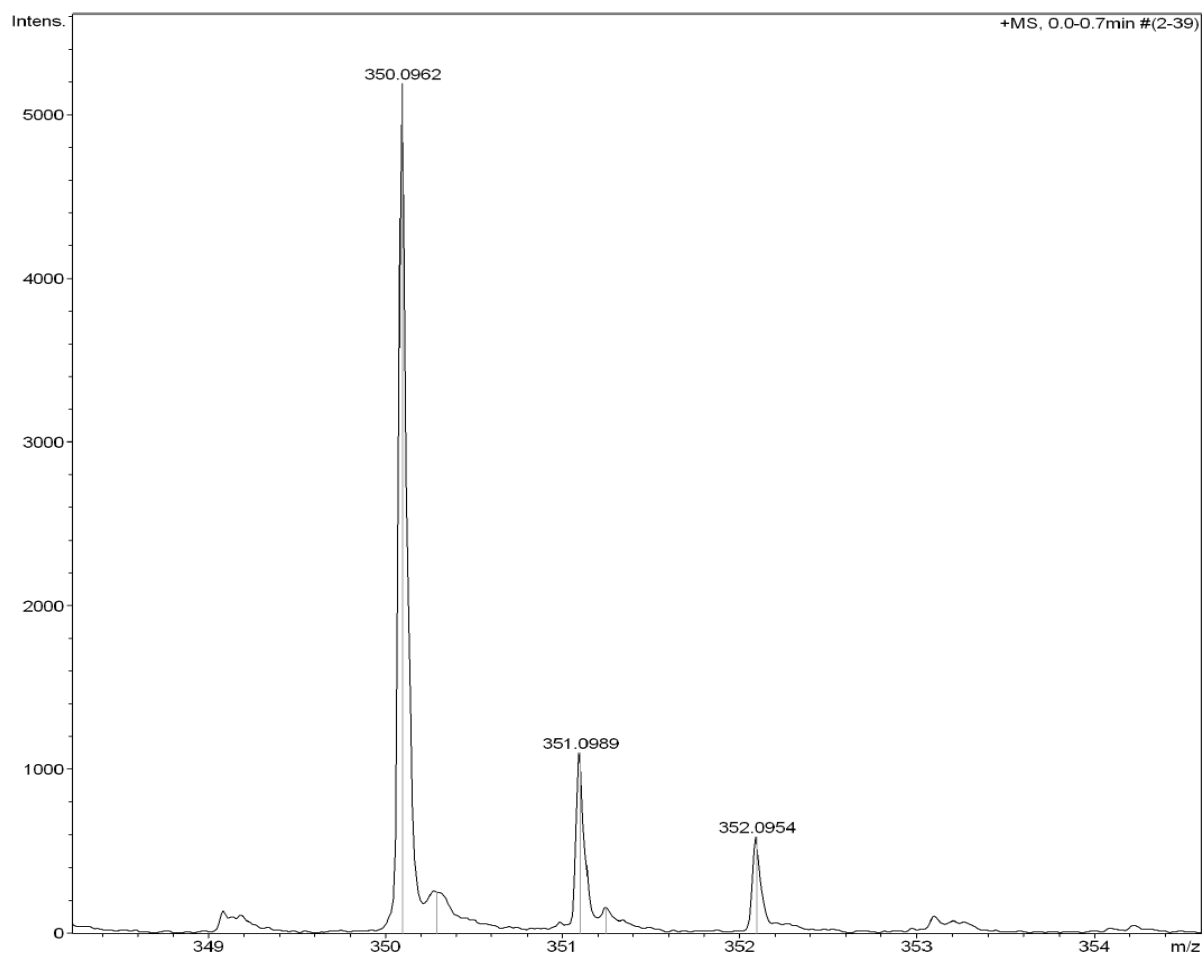
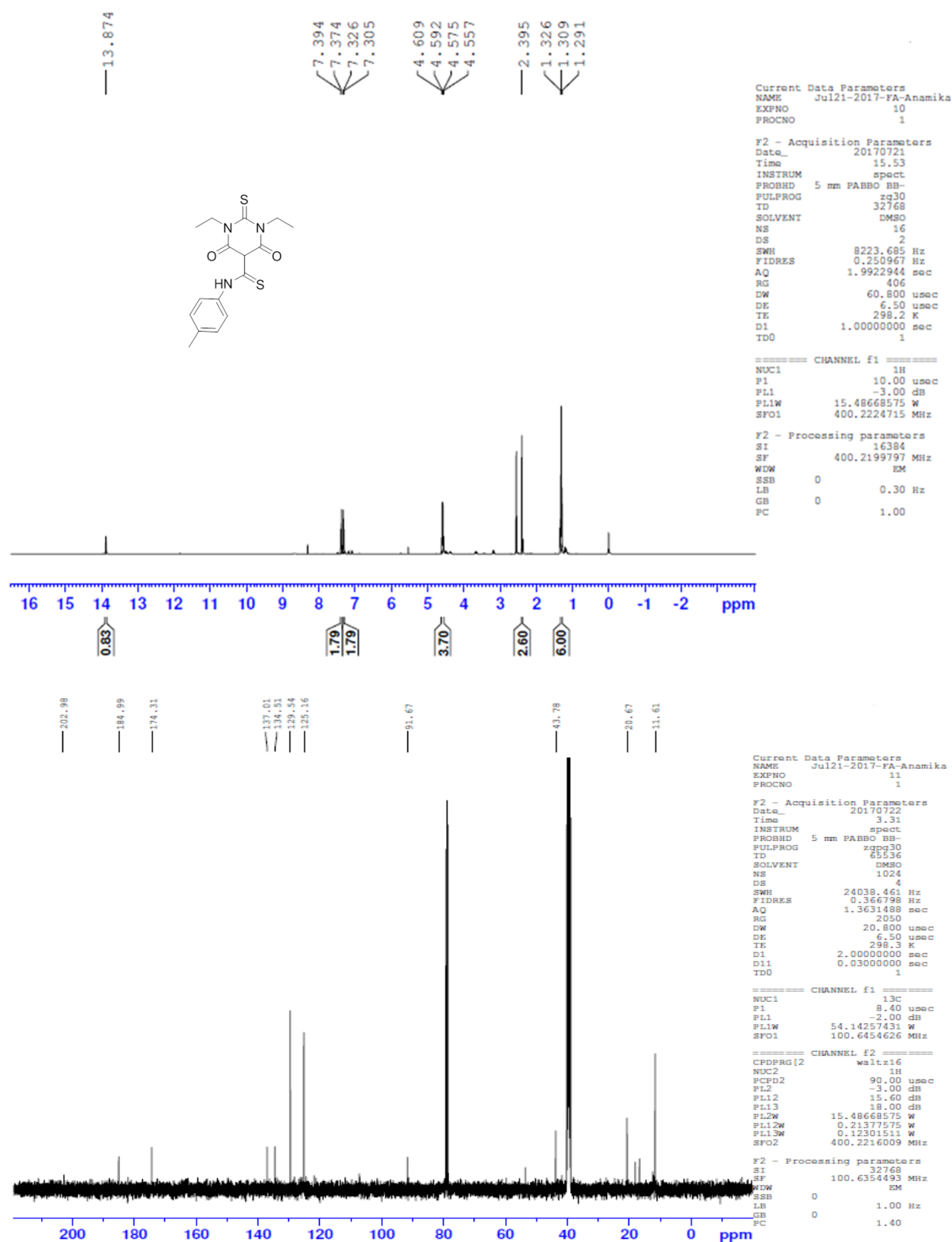


Figure S38 HRMS for compound **A13**

Figure S39 ¹H NMR and ¹³C NMR of compound A13

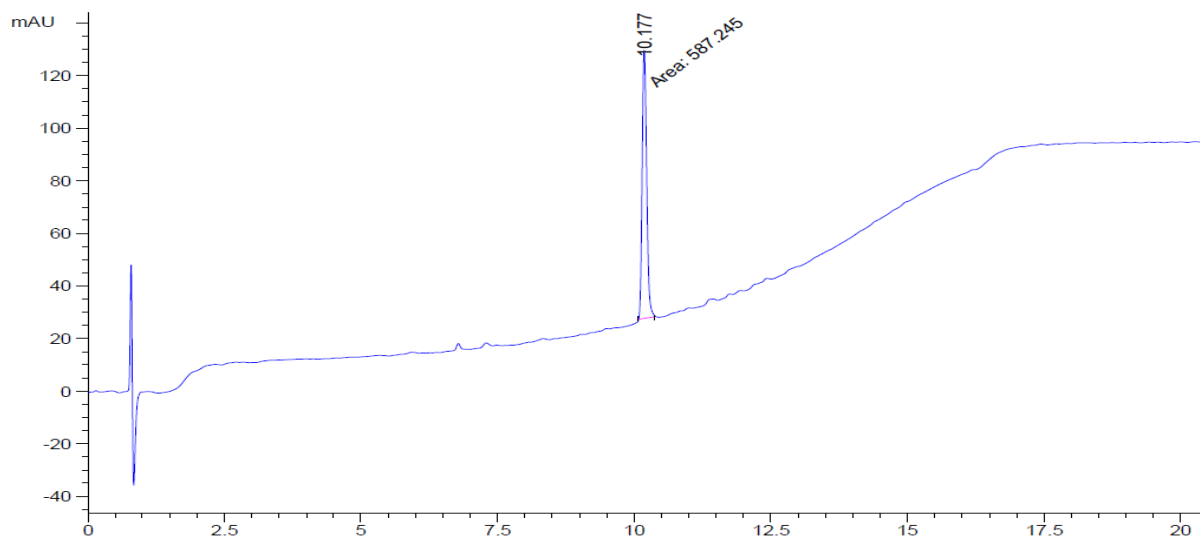


Figure S40 HPLC for compound **A14**

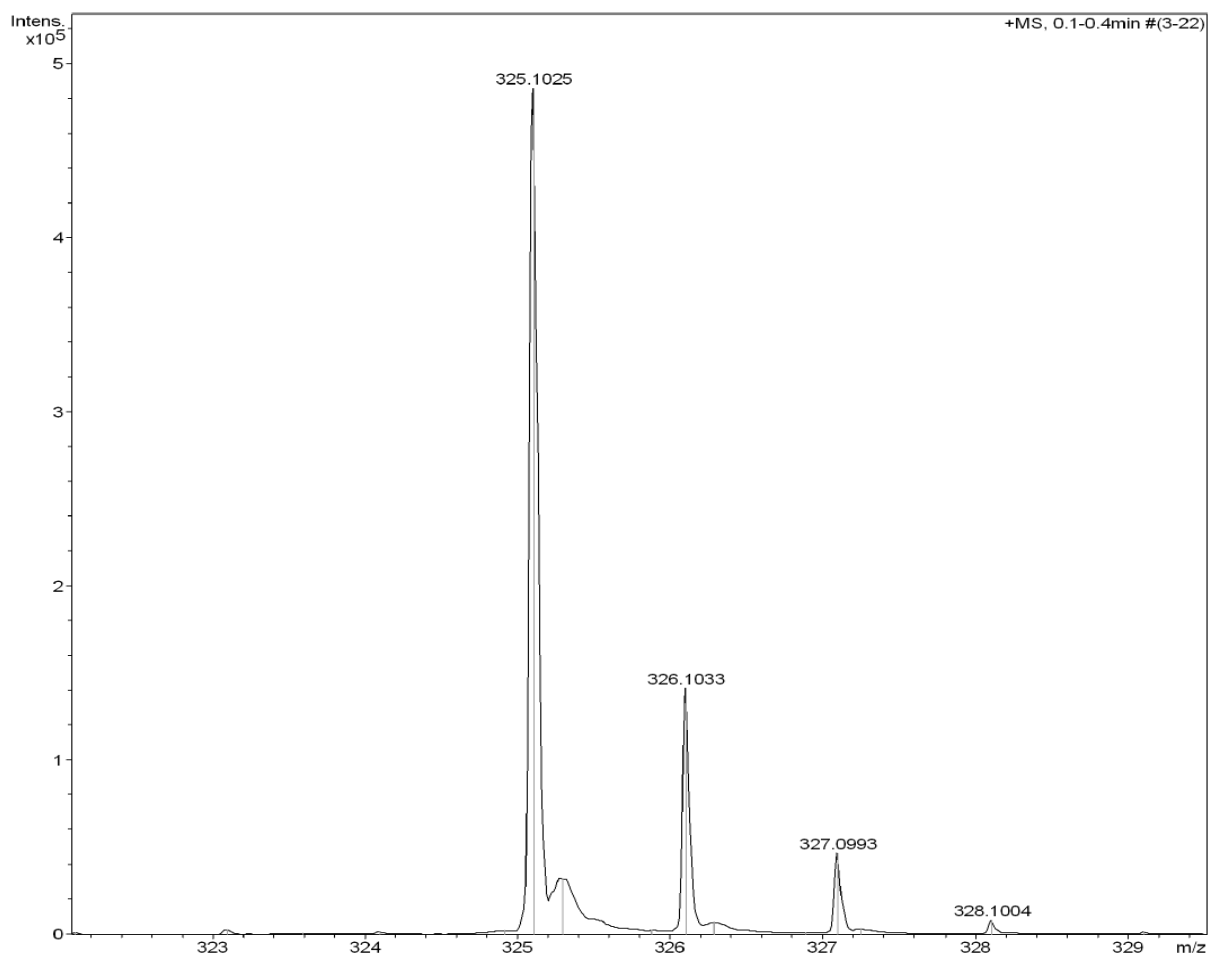
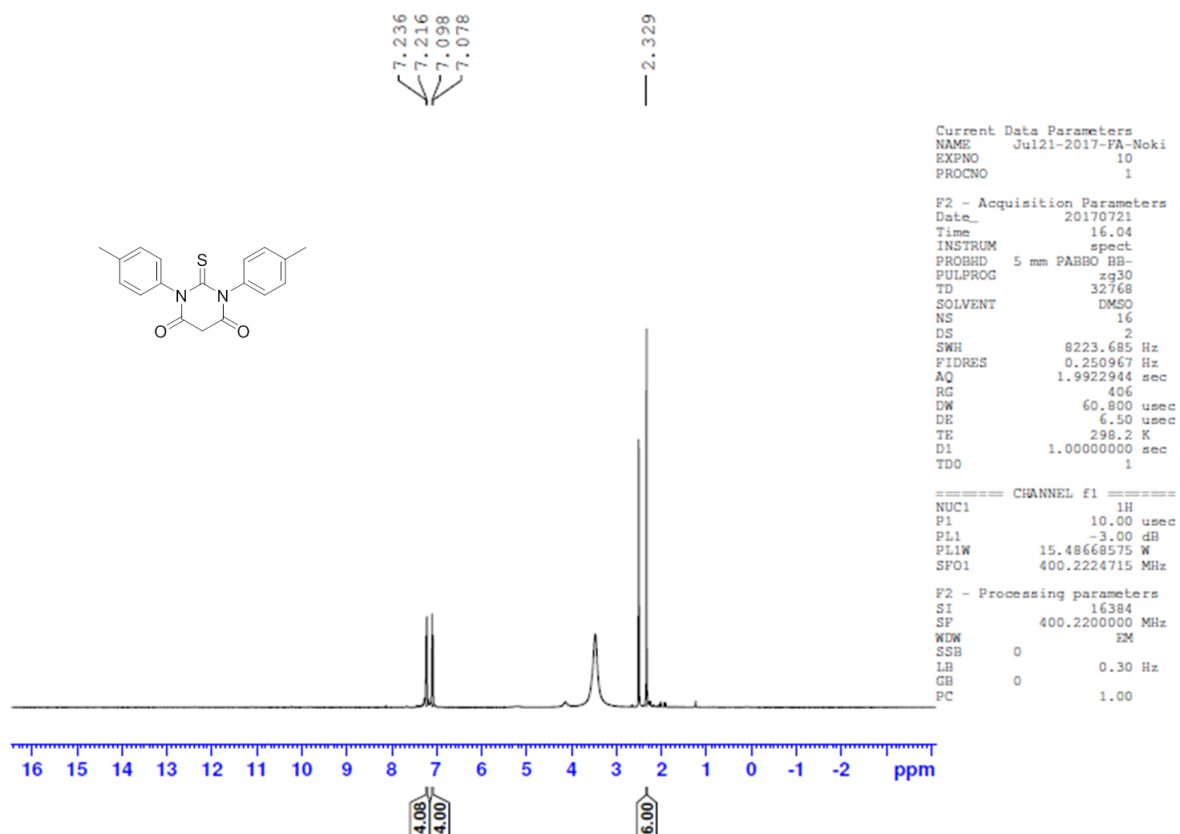
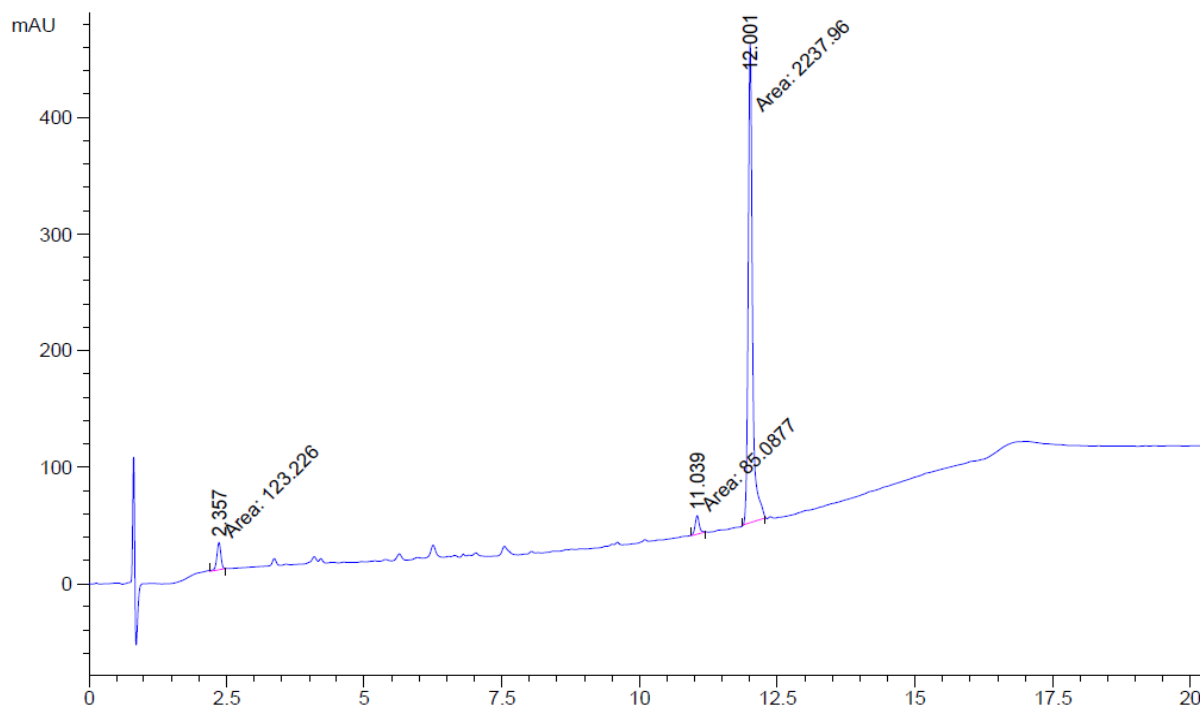


Figure S41 HRMS for compound **A14**

**Figure S42** ^1H NMR of compound A14**Figure S43** HPLC for compound A15

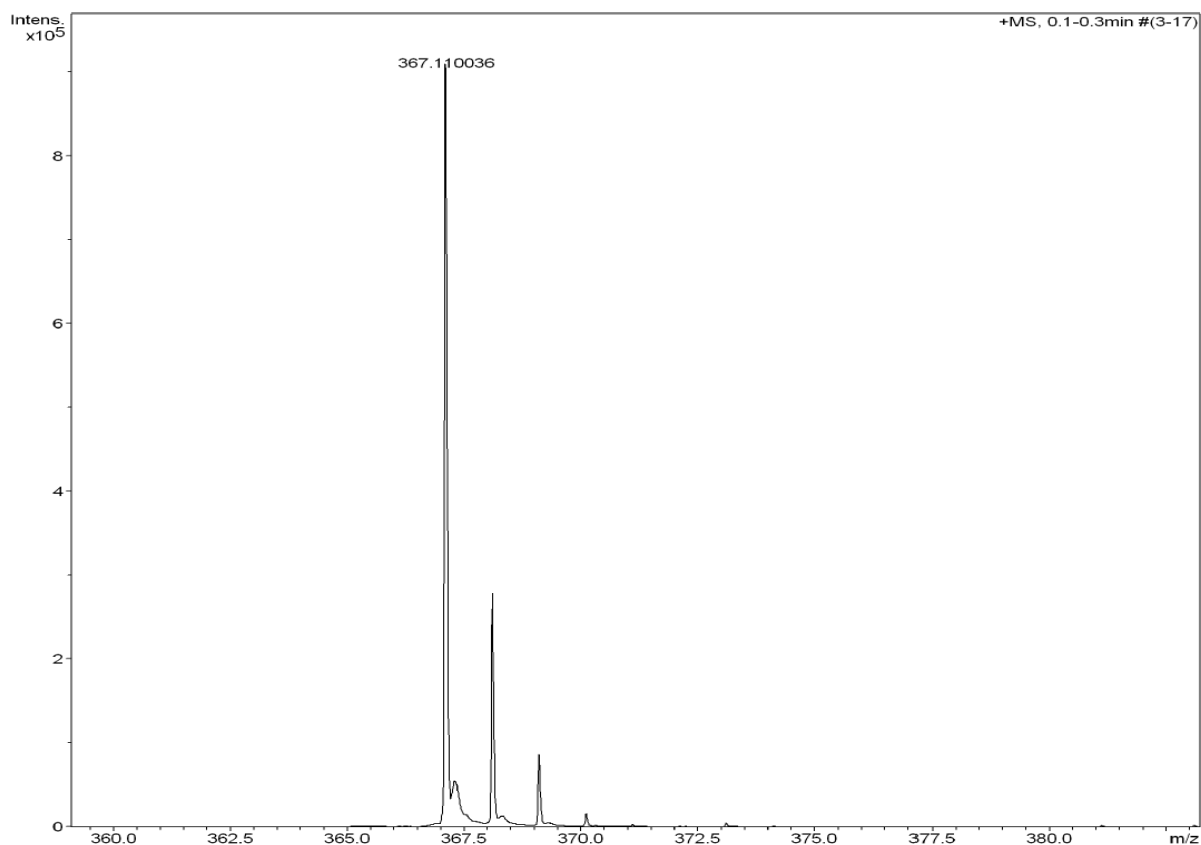
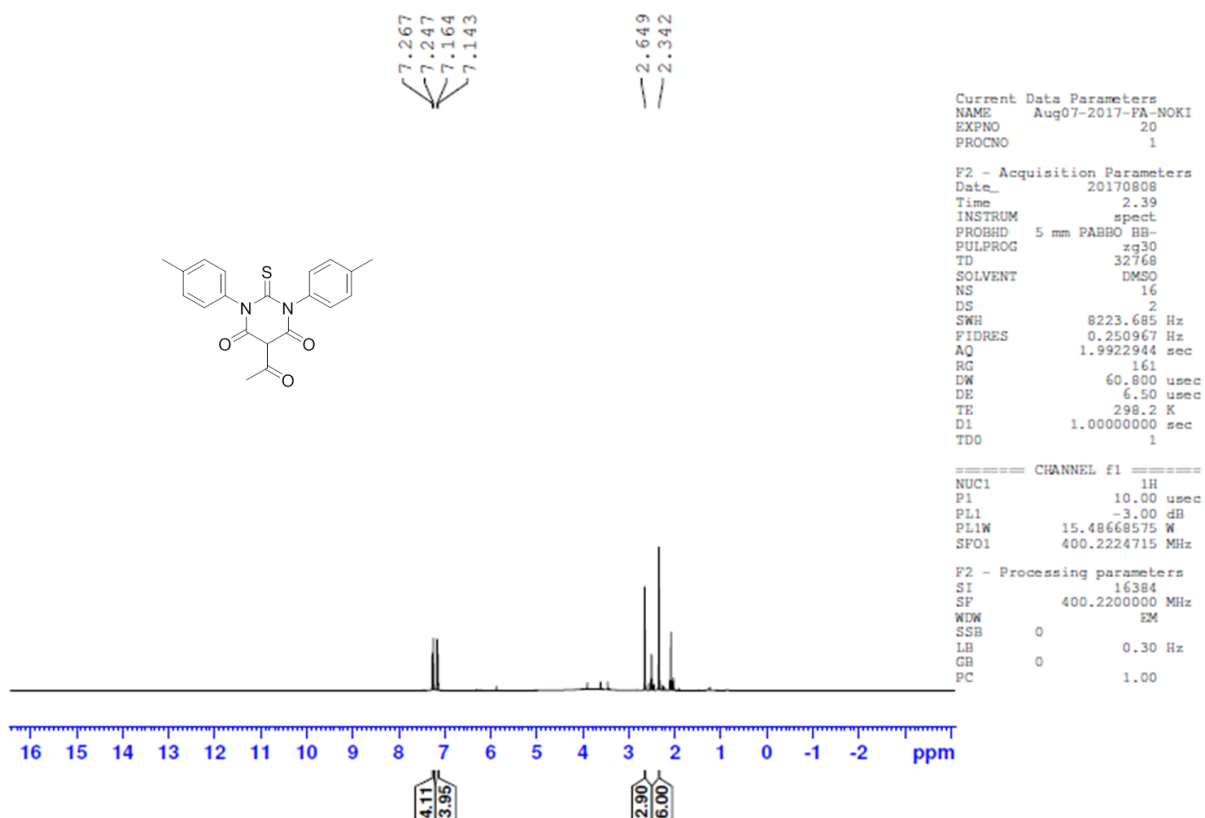
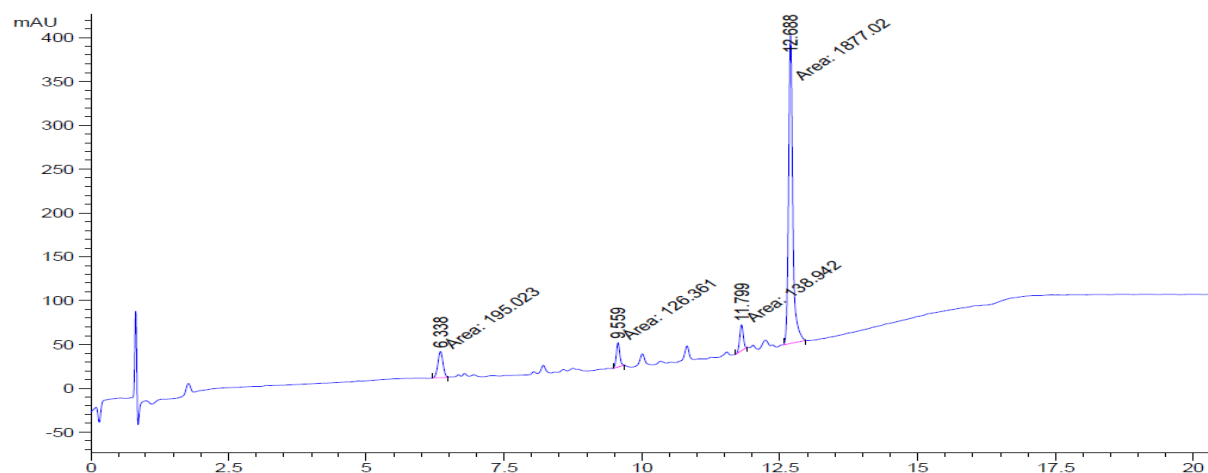
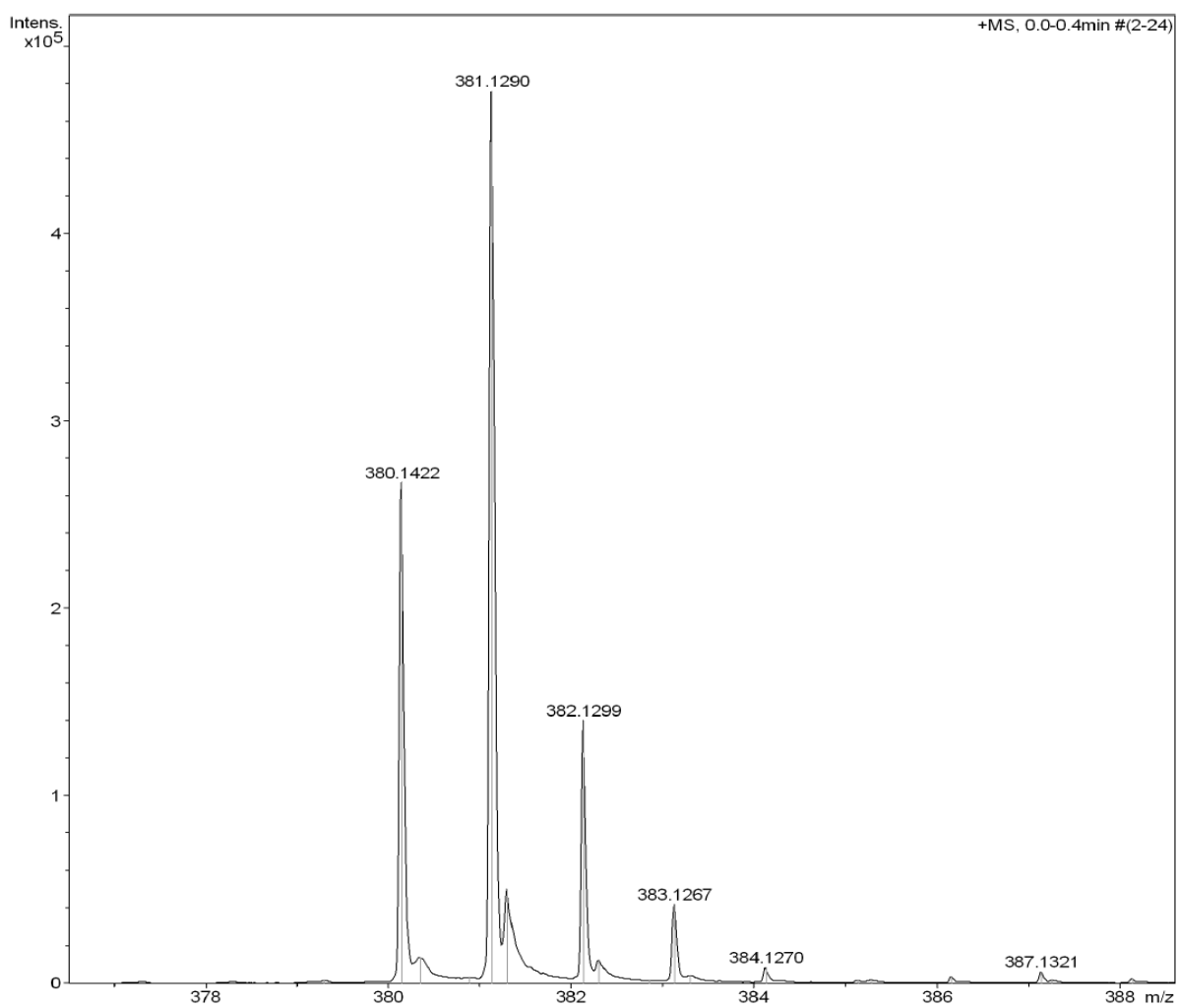
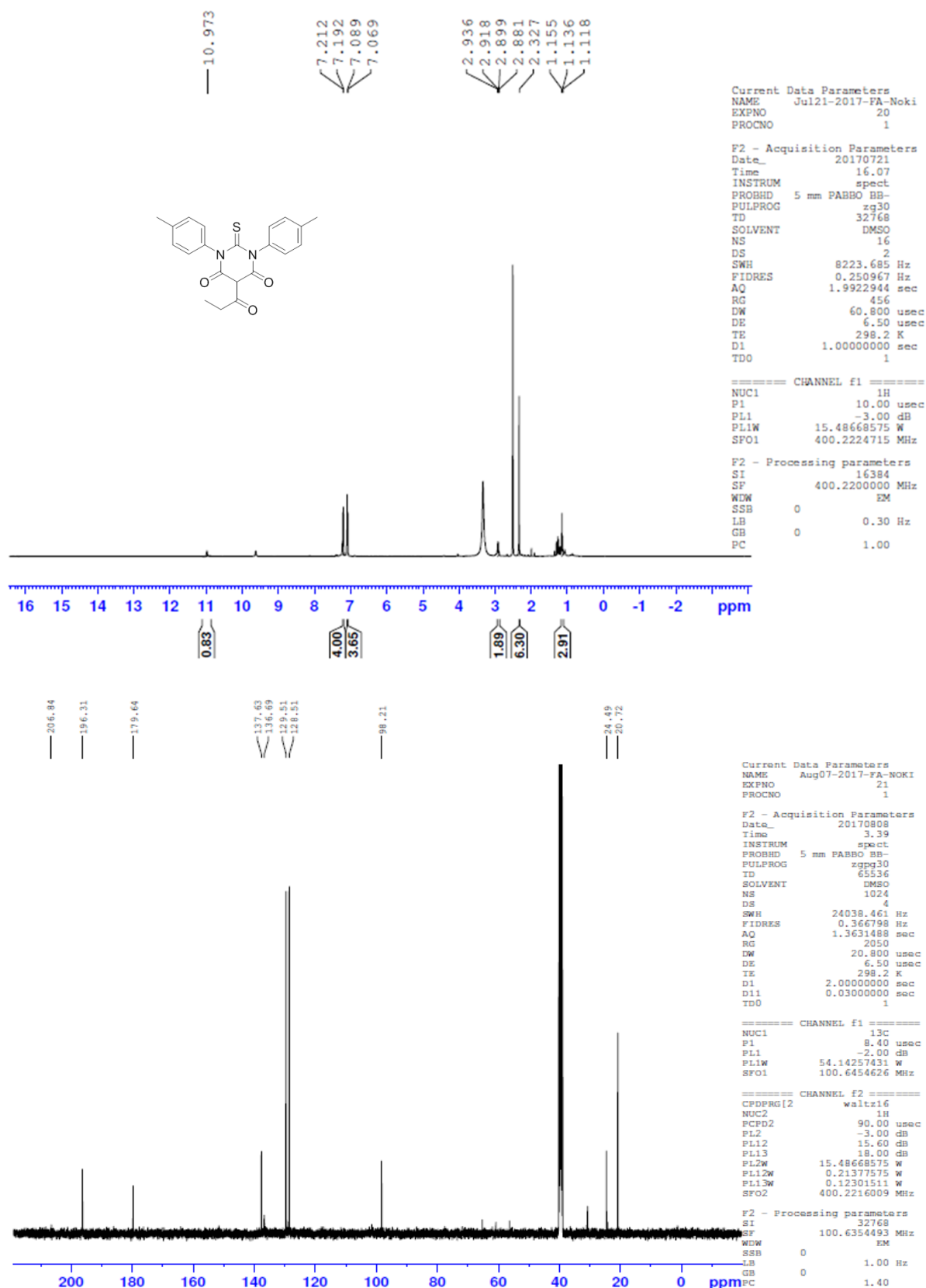


Figure S44 HRMS for compound A15

Figure S45 ¹H NMR of compound A15

**Figure S46** HPLC for compound A16**Figure S47** HRMS for compound A16

Figure S48 ¹H NMR and ¹³C NMR of compound A16

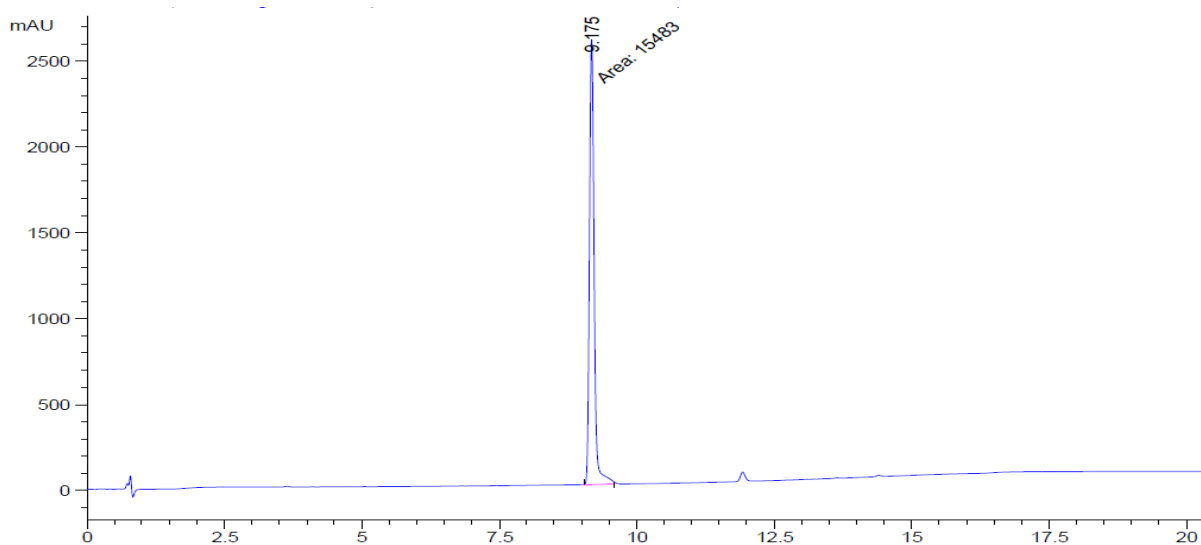


Figure S49 HPLC for compound **A17**

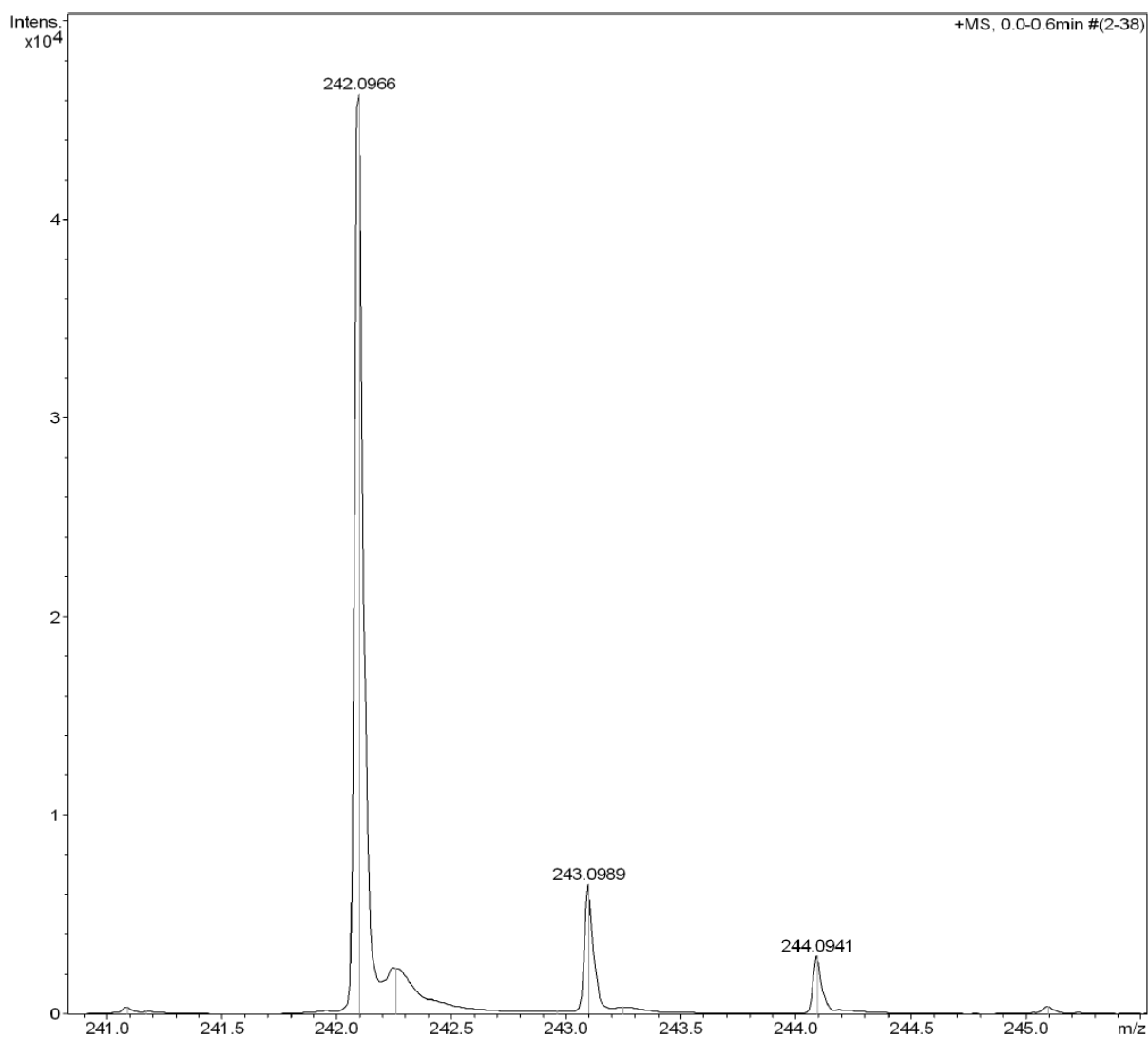
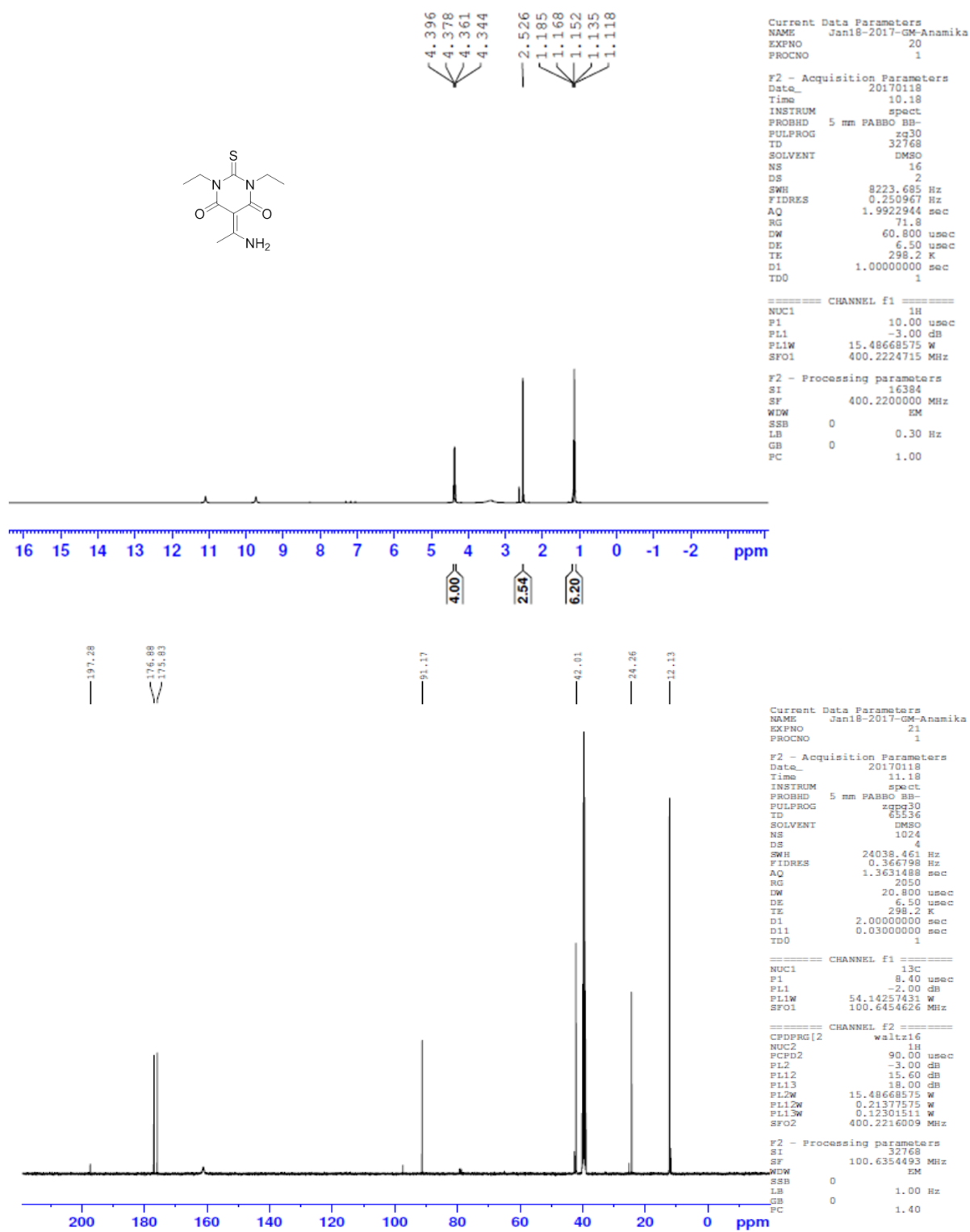


Figure S50 HRMS for compound **A17**

Figure S51 ¹H NMR and ¹³C NMR of compound A17

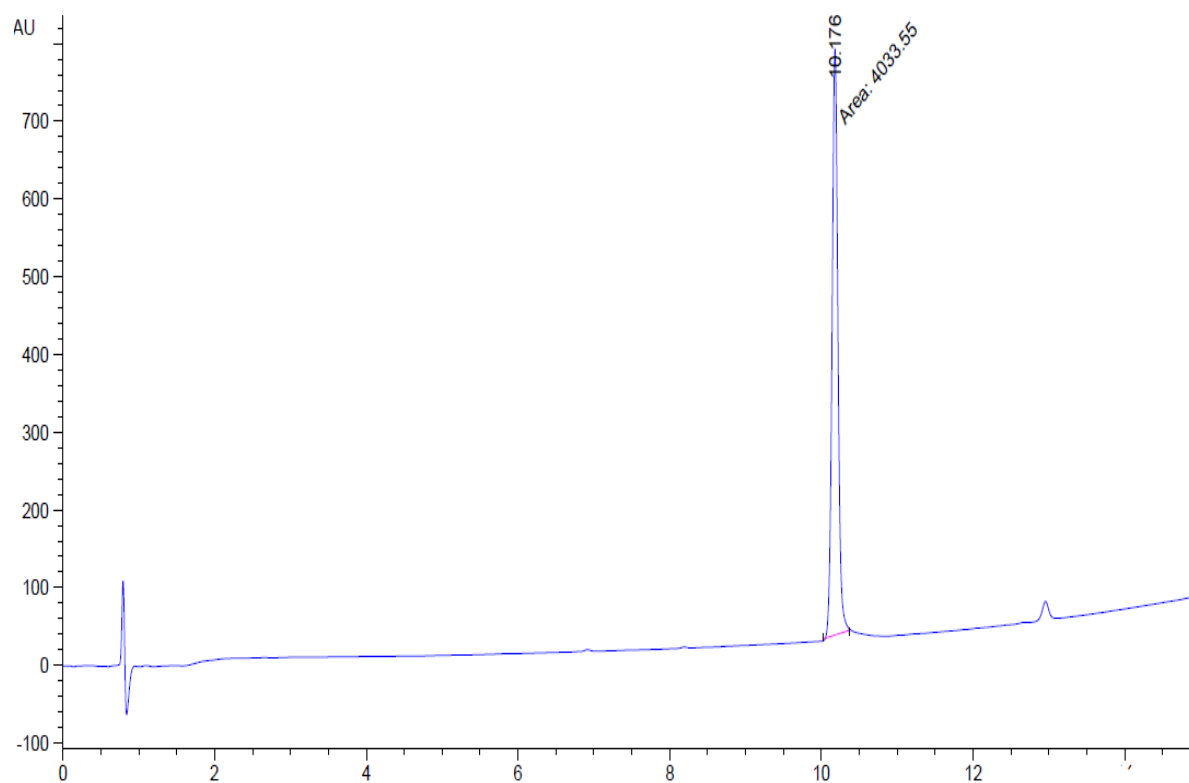


Figure S52 HPLC for compound **A18**

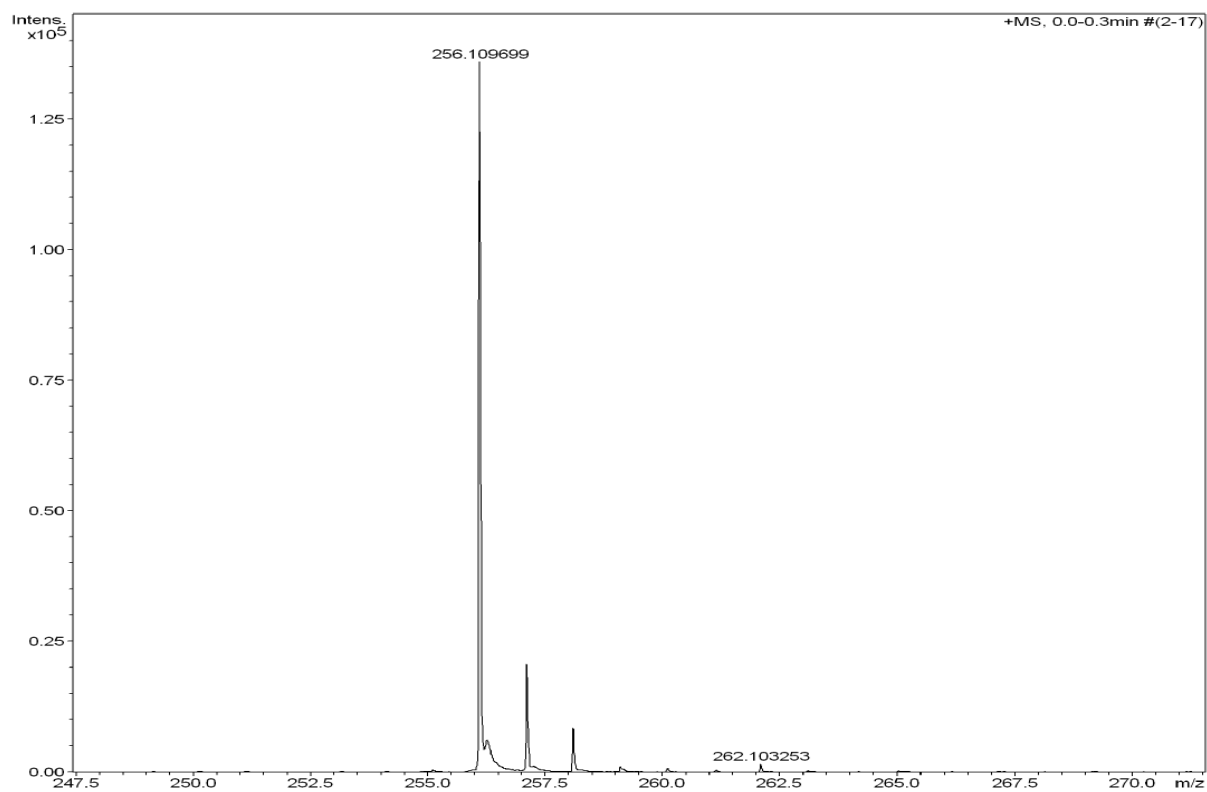
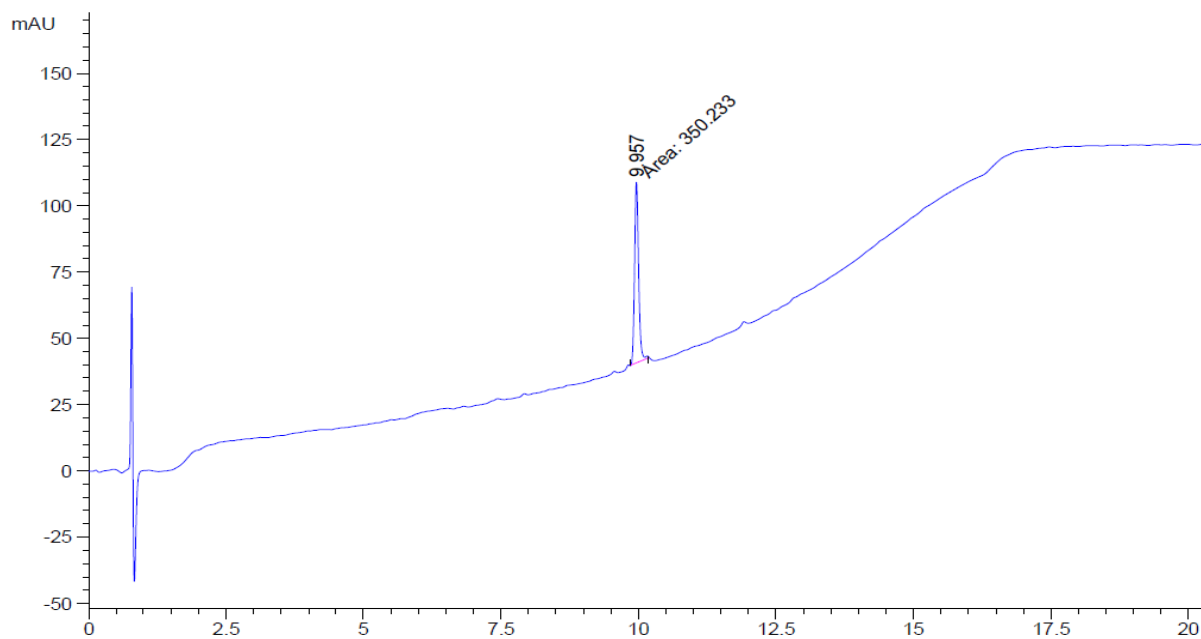
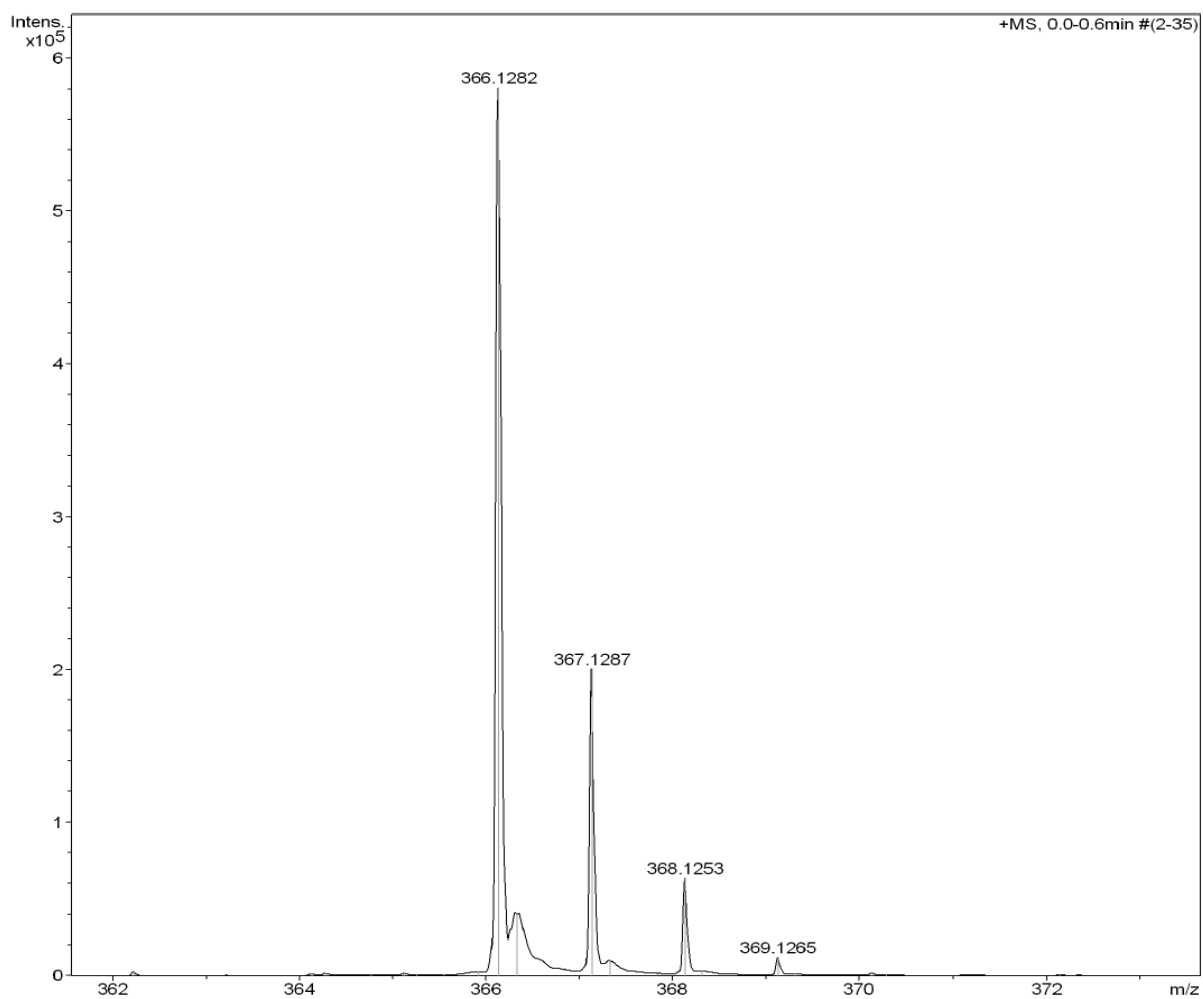
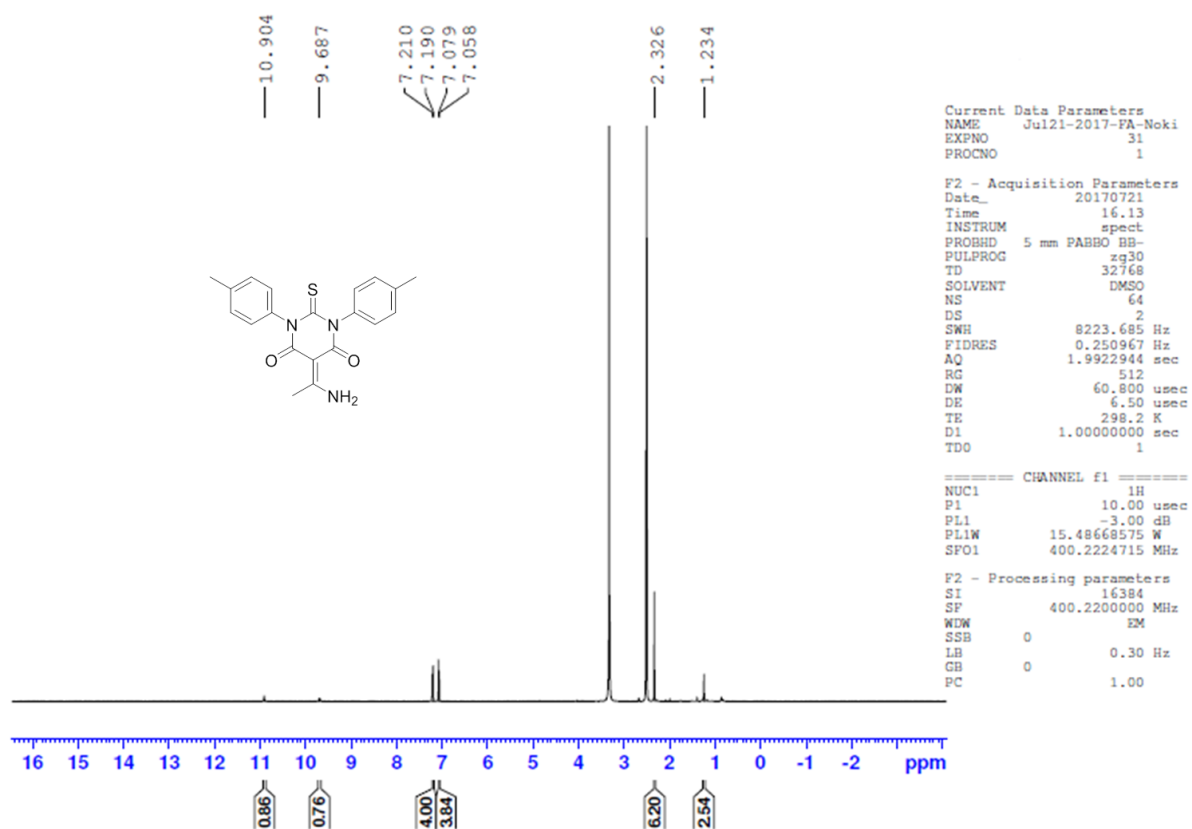
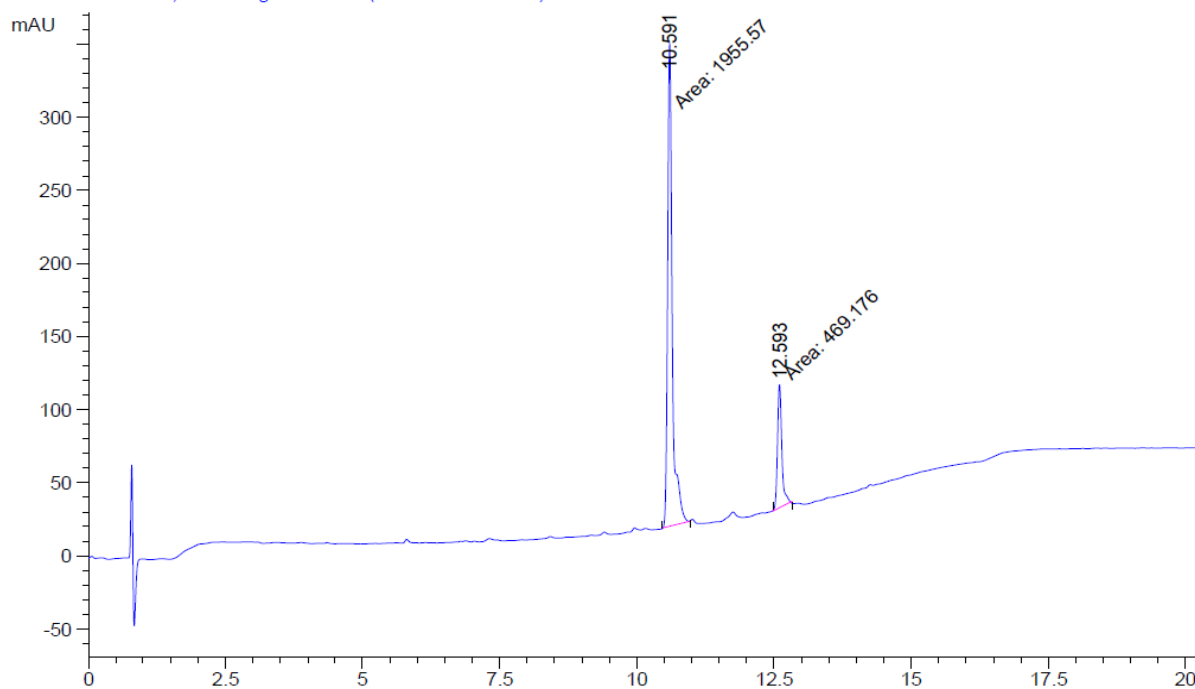


Figure S53 HRMS for compound **A18**

**Figure S54** HPLC for compound **A19****Figure S55** HRMS for compound **A19**

**Figure S56** ^1H NMR of compound A19**Figure S57** HPLC for compound A20

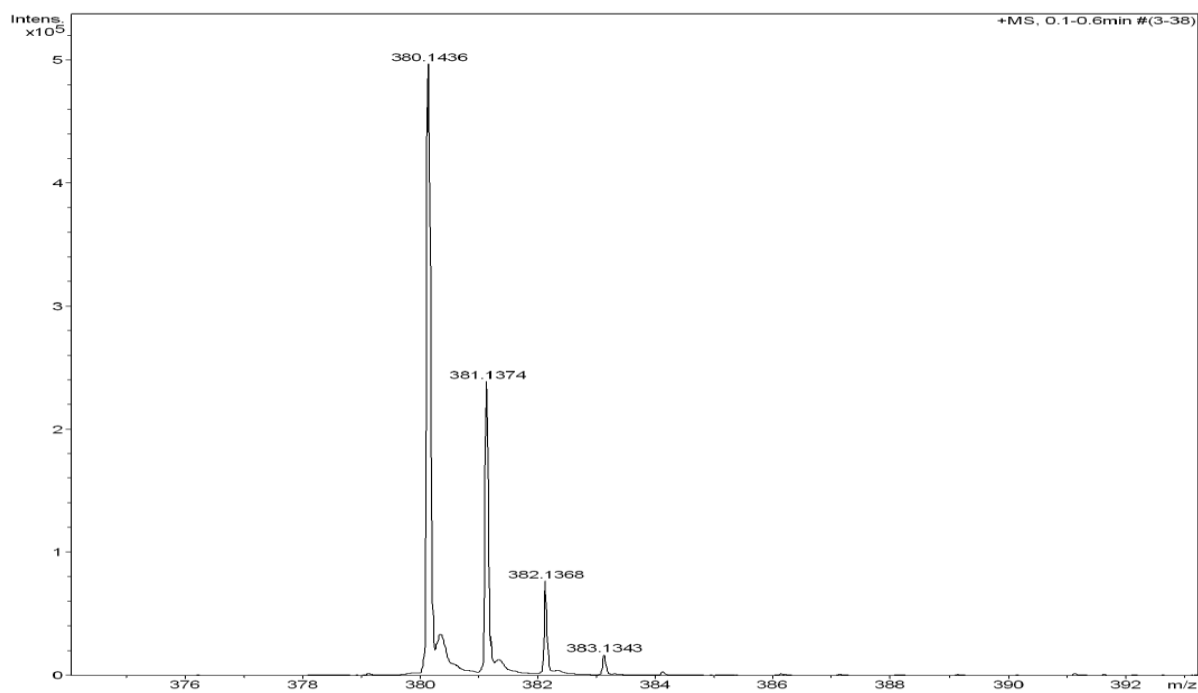
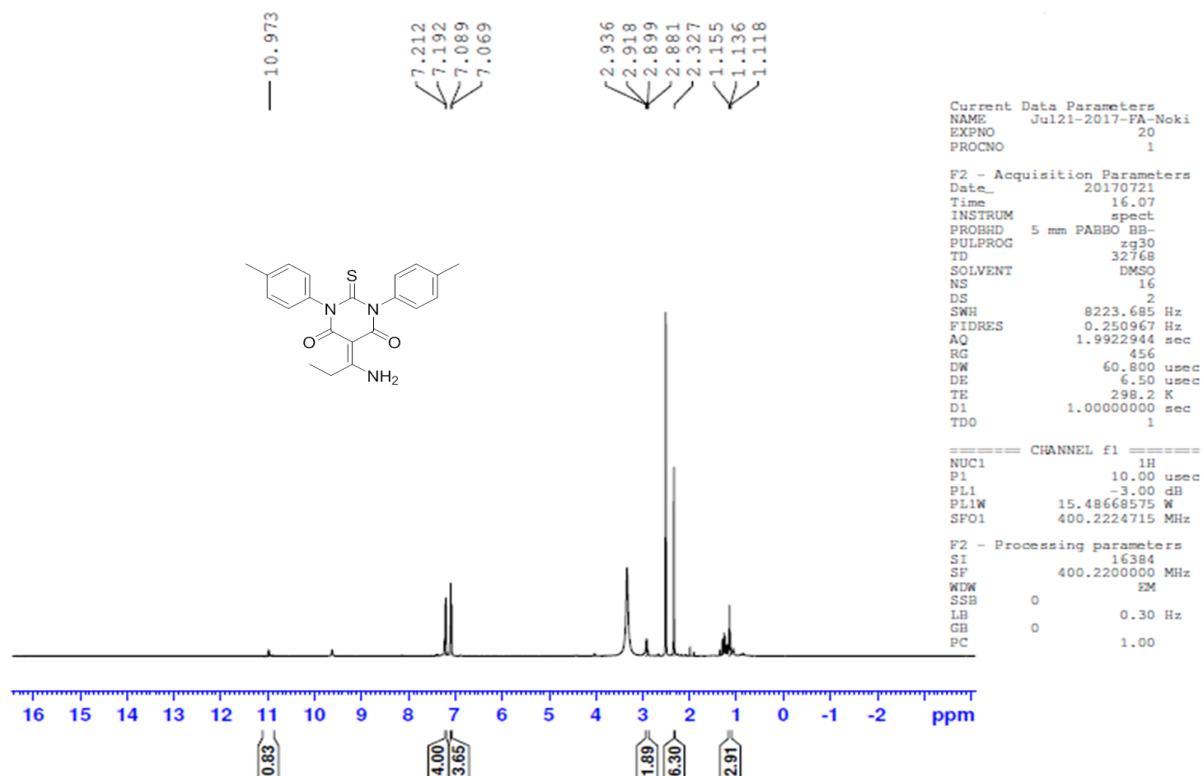


Figure S58 HRMS for compound A20

Figure S59 ^1H NMR of compound A20

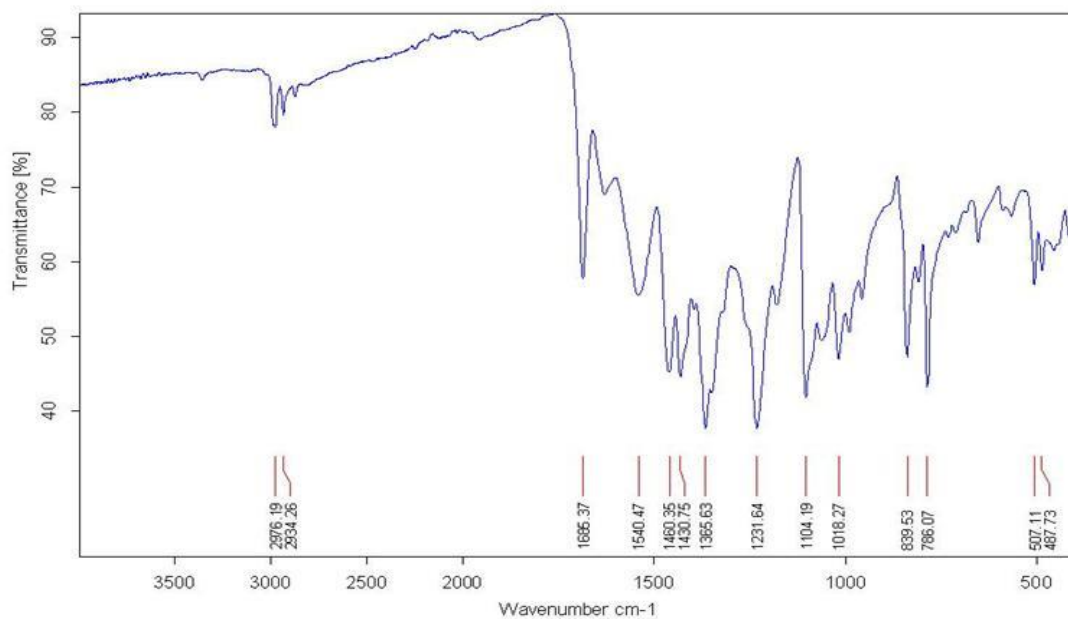


Figure S60 IR for compound A01

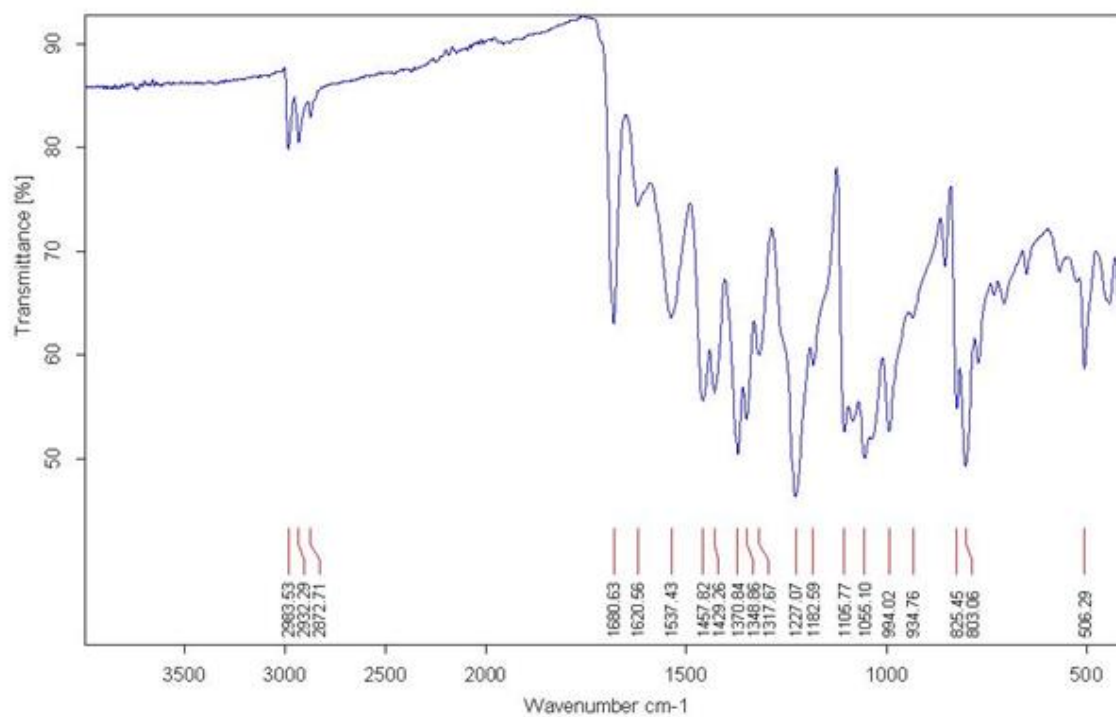


Figure S61 IR for compound A02

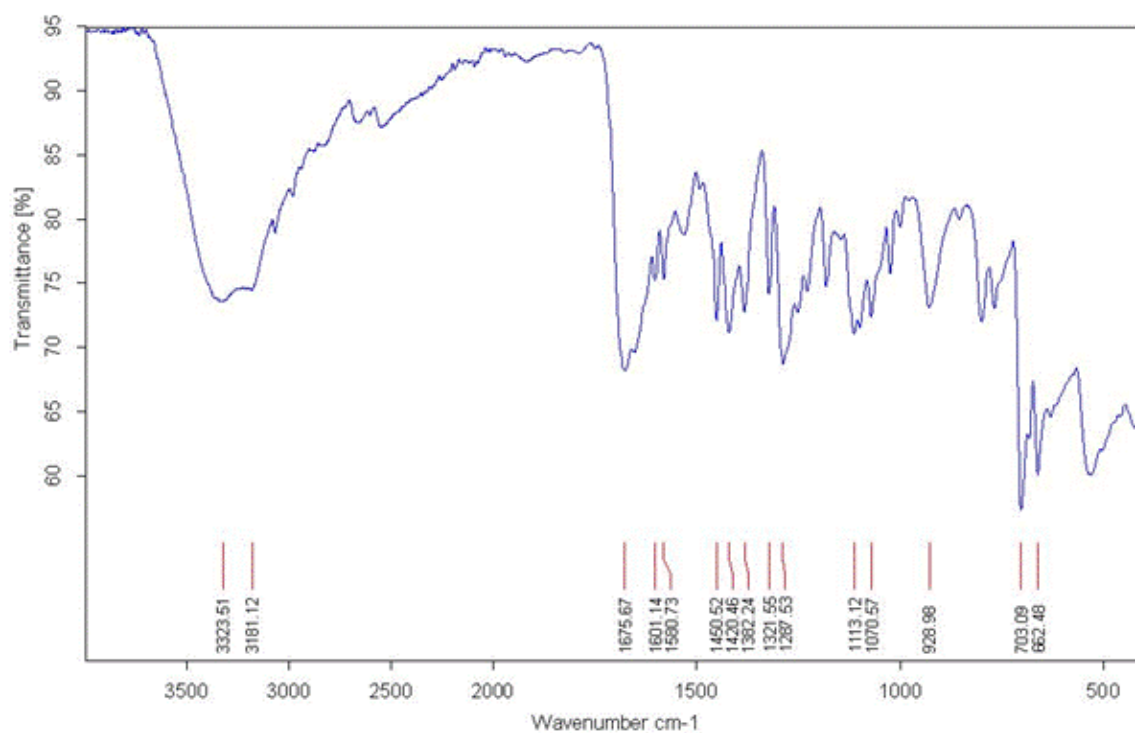


Figure S62 IR for compound A03

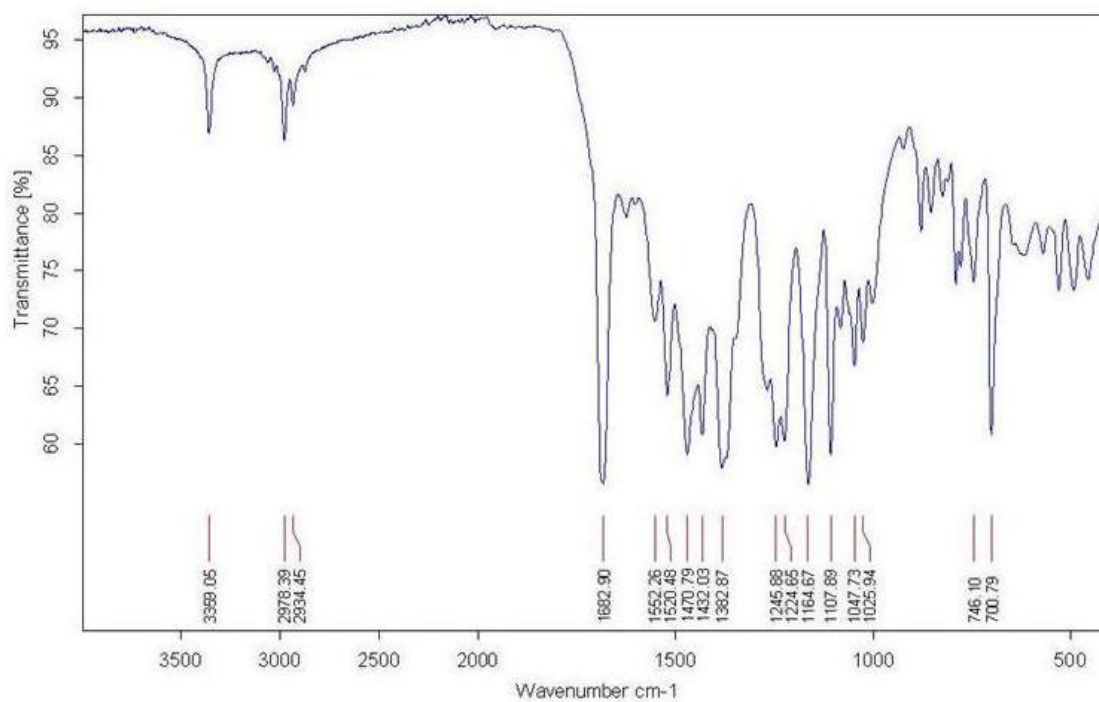


Figure S63 IR for compound A04

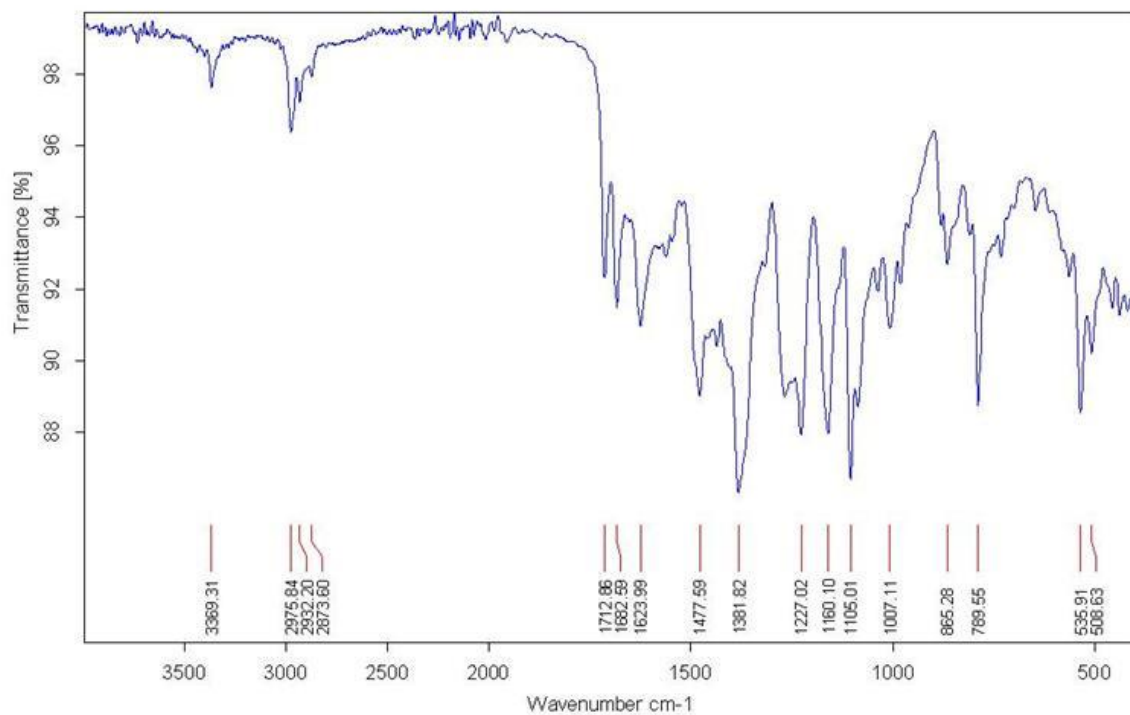


Figure S64 IR for compound A06

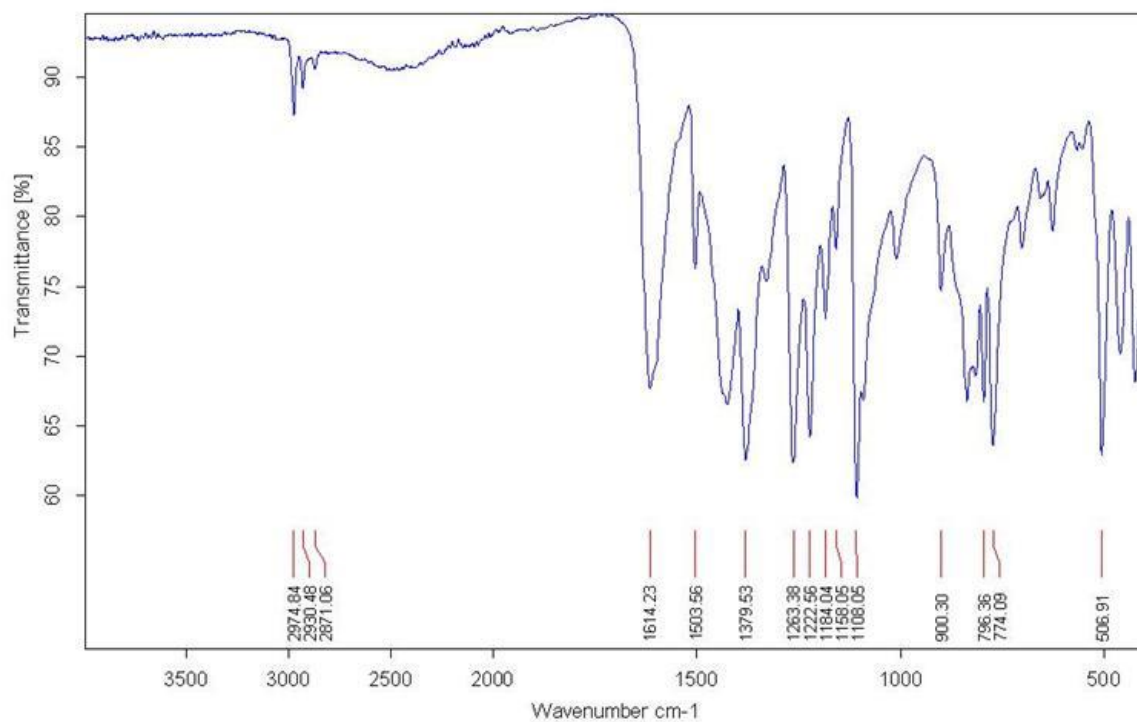


Figure S65 IR for compound A10

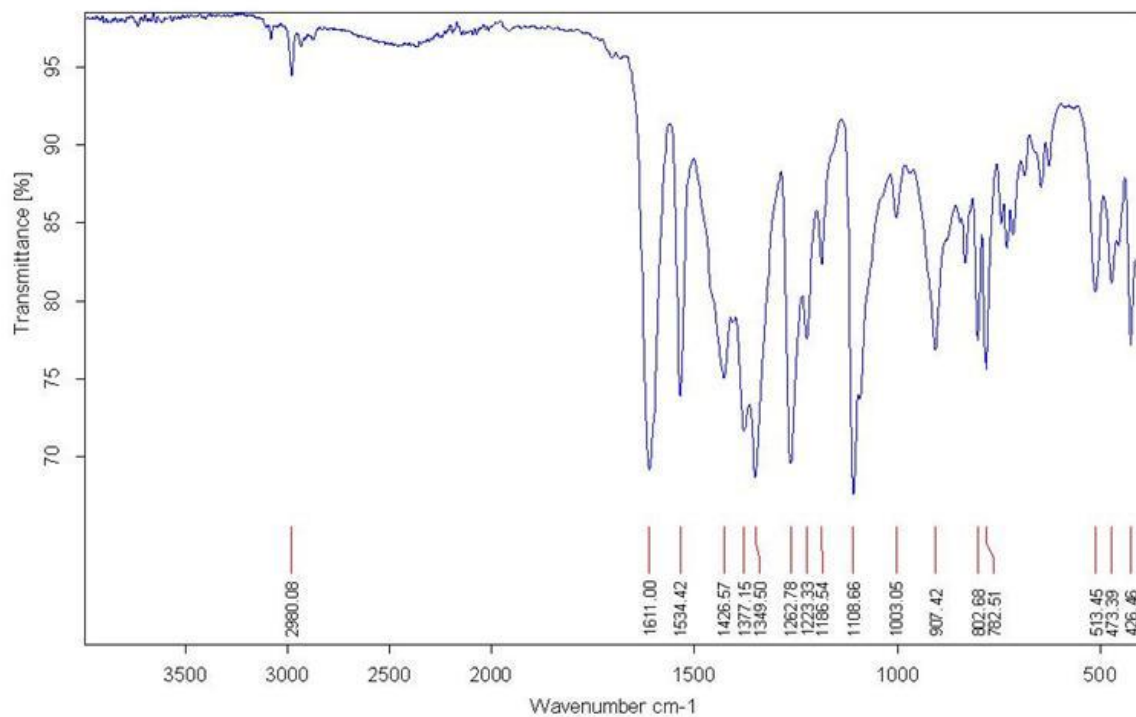


Figure S66 IR for compound A12

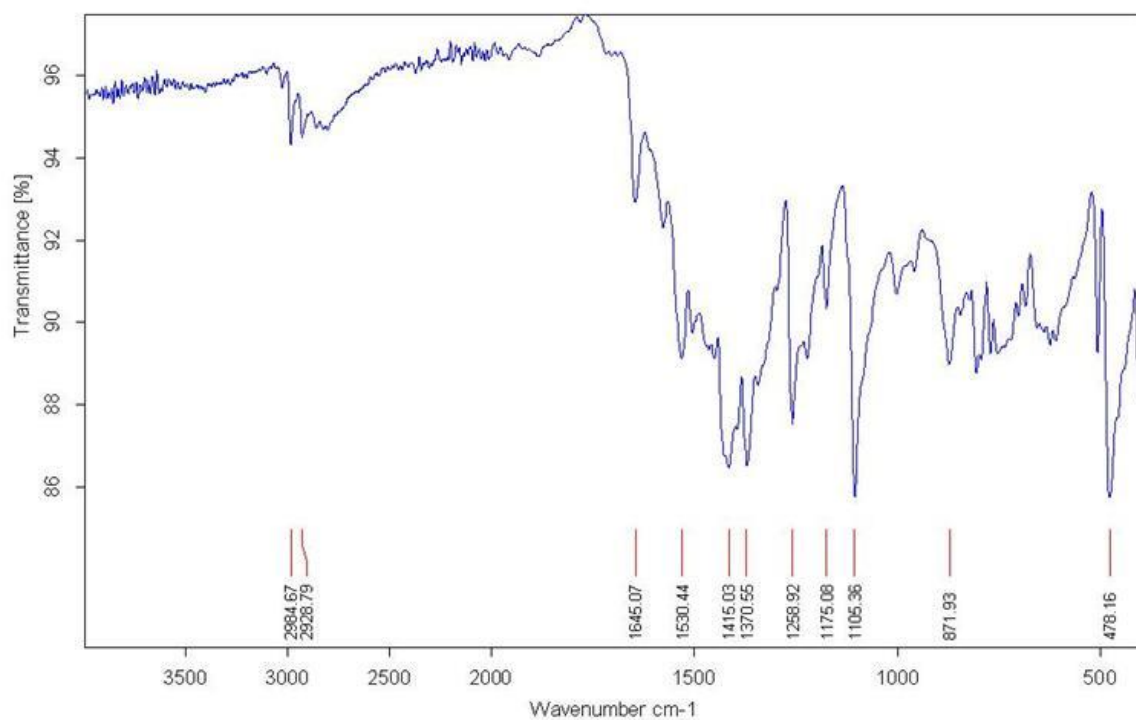
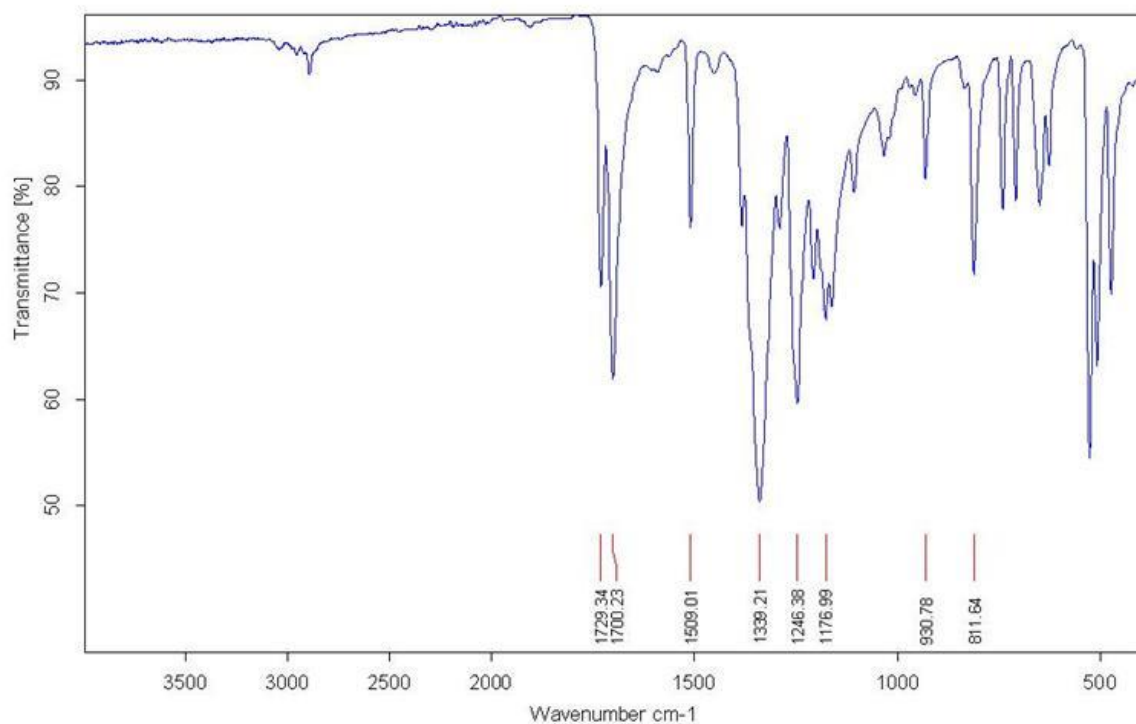
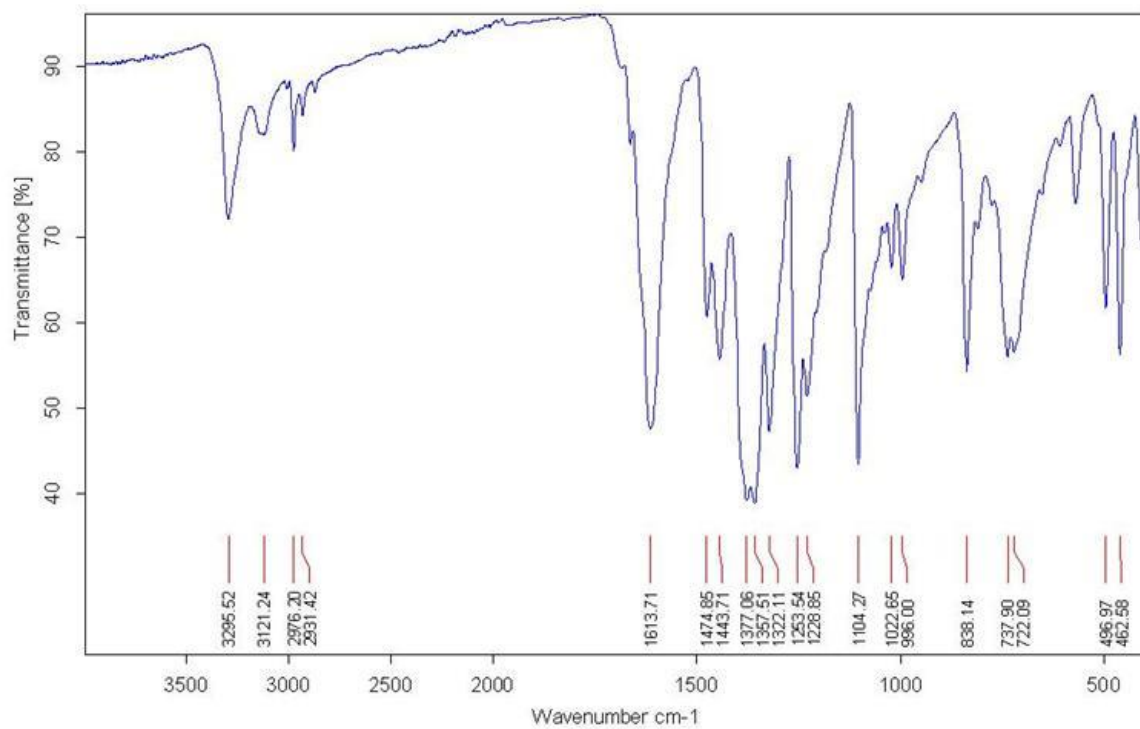


Figure S67 IR for compound A13

**Figure S68** IR for compound A14**Figure S69** IR for compound A17