Supporting Information

For

Design, synthesis, and antioxidant and anti-tyrosinase activities of (*Z*)-5-benzylidene-2-(naphthalen-1-ylamino)thiazol-4(5*H*)-one analogs: In vitro and in vivo insights

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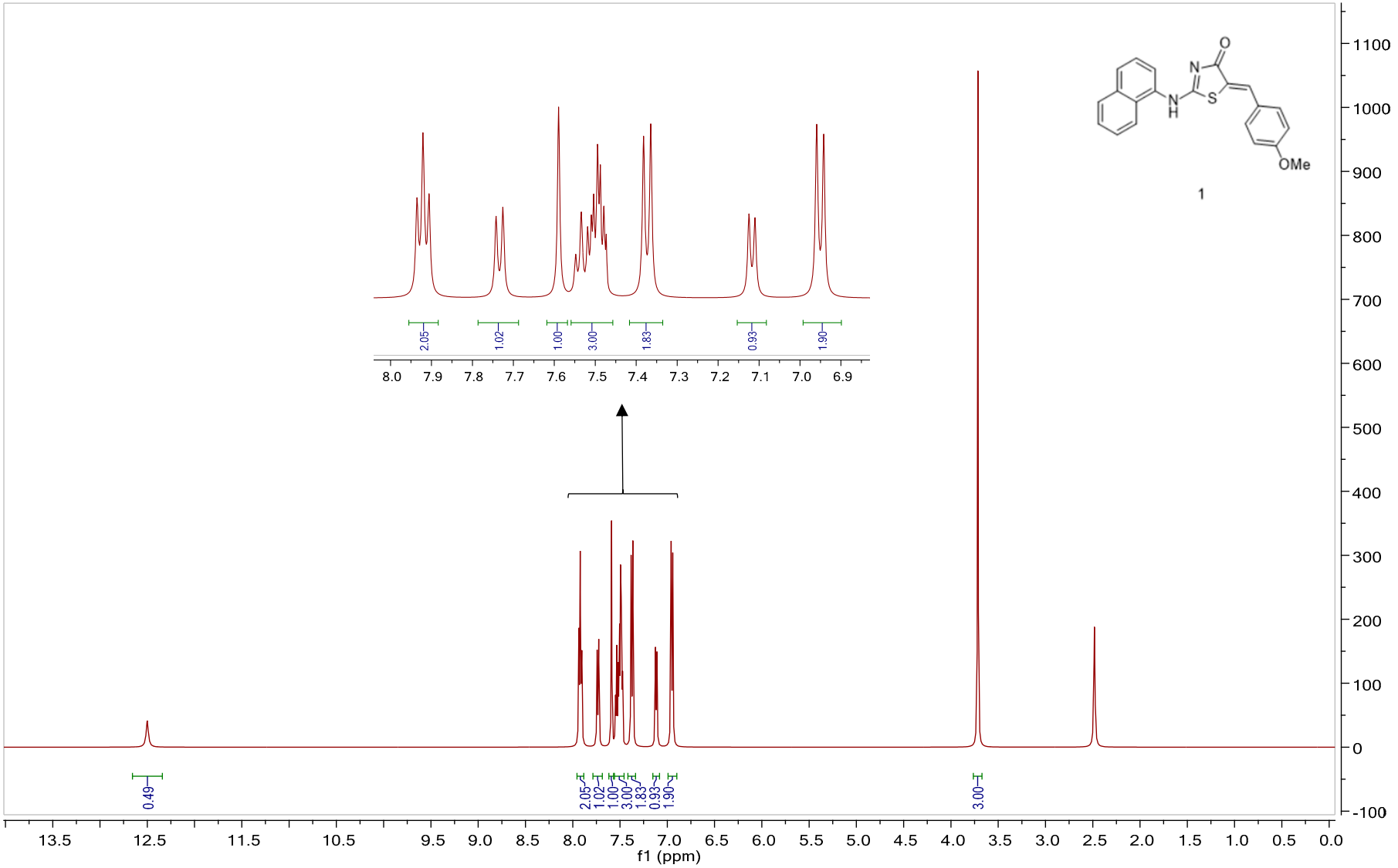
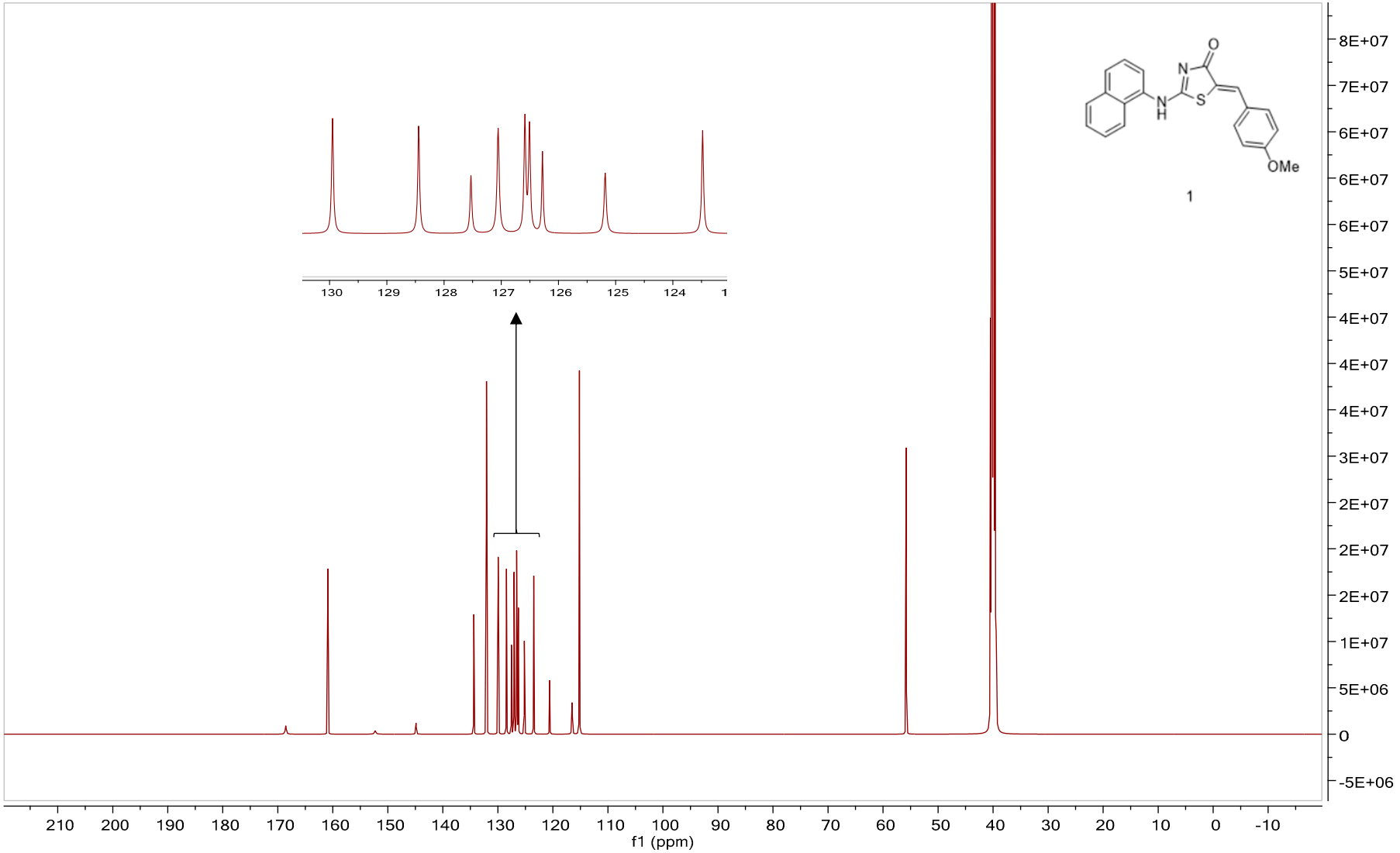


Figure S1. ^{1}H NMR spectrum of analog **1**



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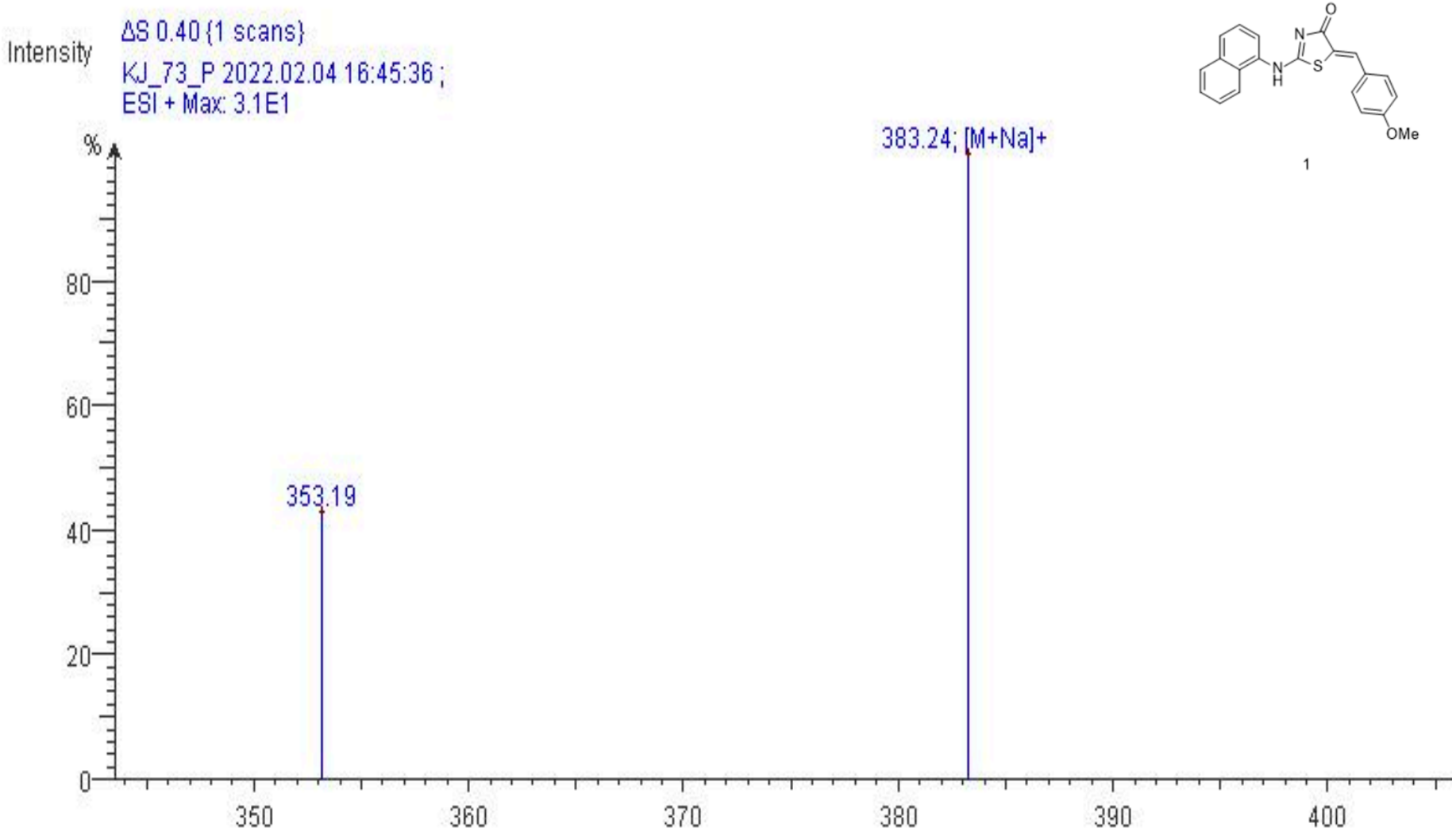

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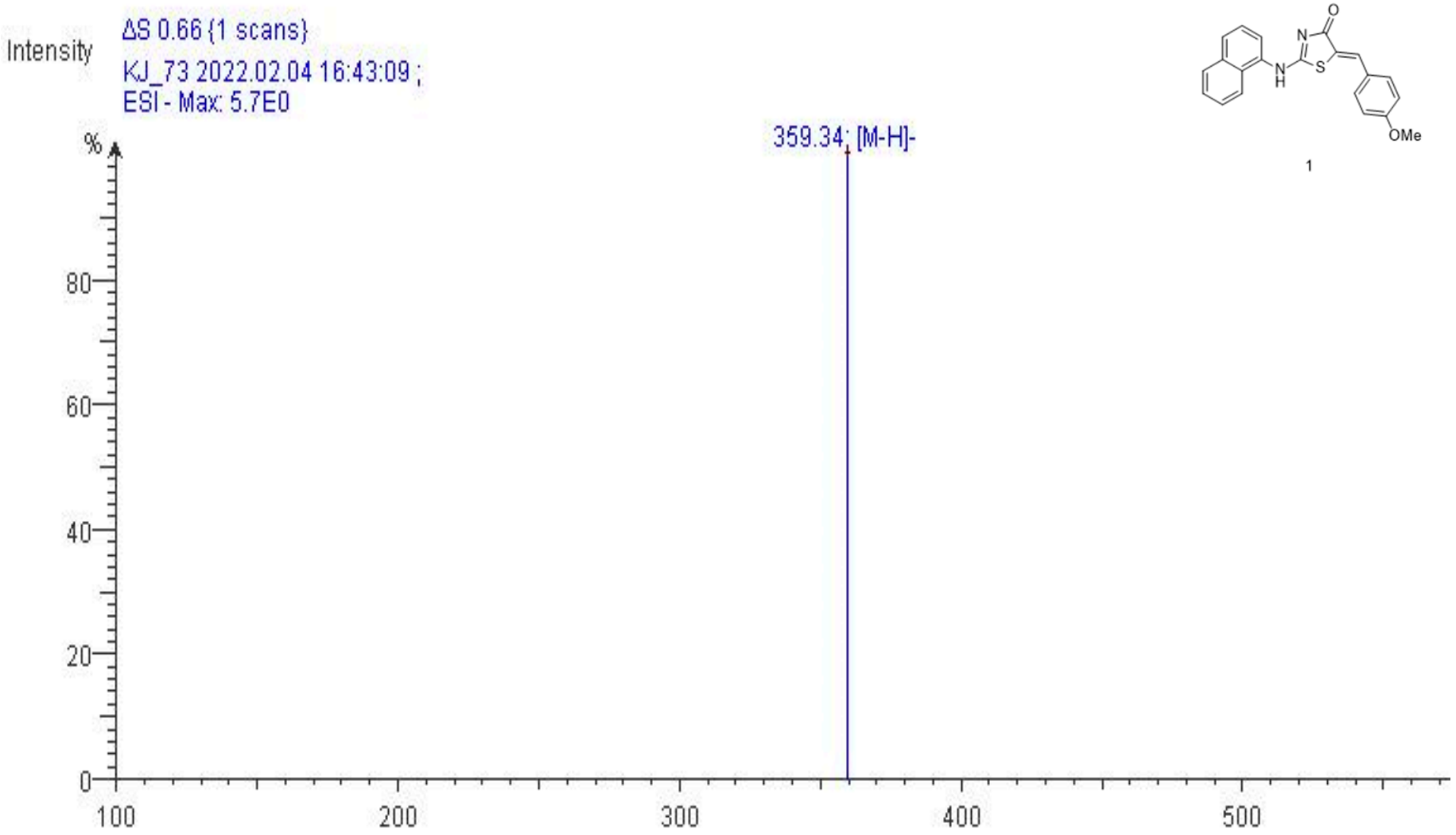

Figure S4. LRMS (ESI–) spectrum of analog **1**

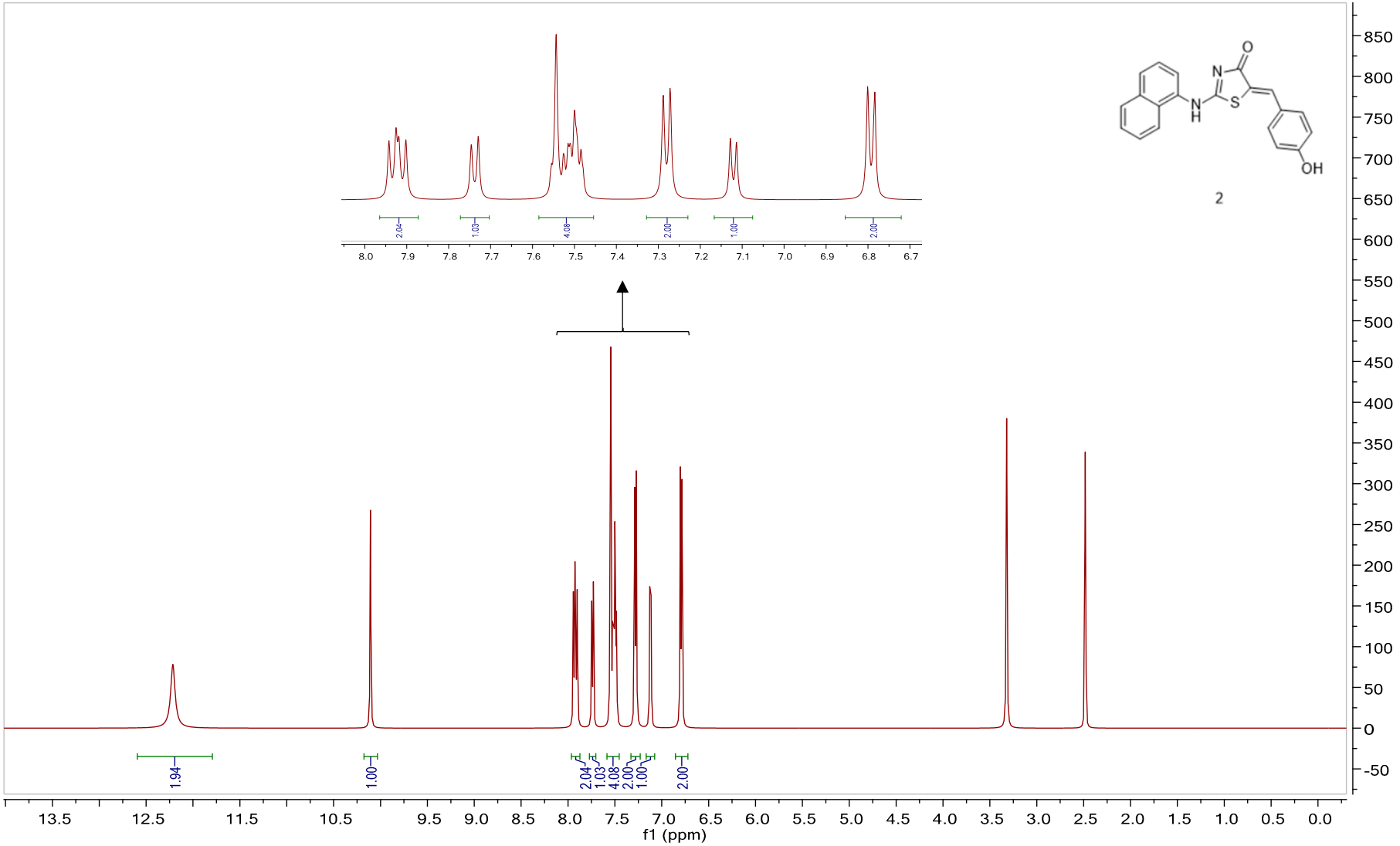

Figure S5. ^{1}H NMR spectrum of analog **2**

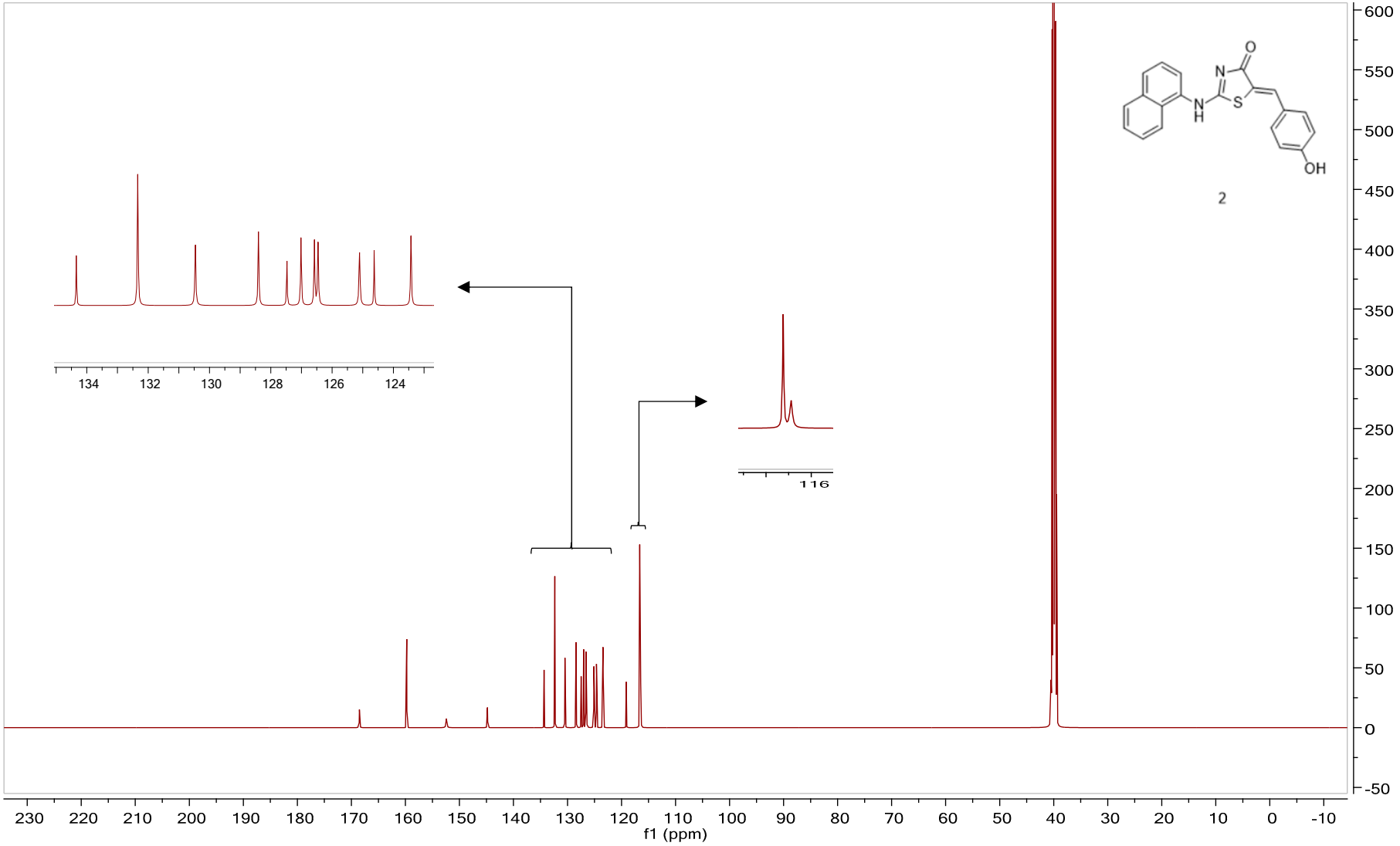

Figure S6. ^{13}C NMR spectrum of analog **2**

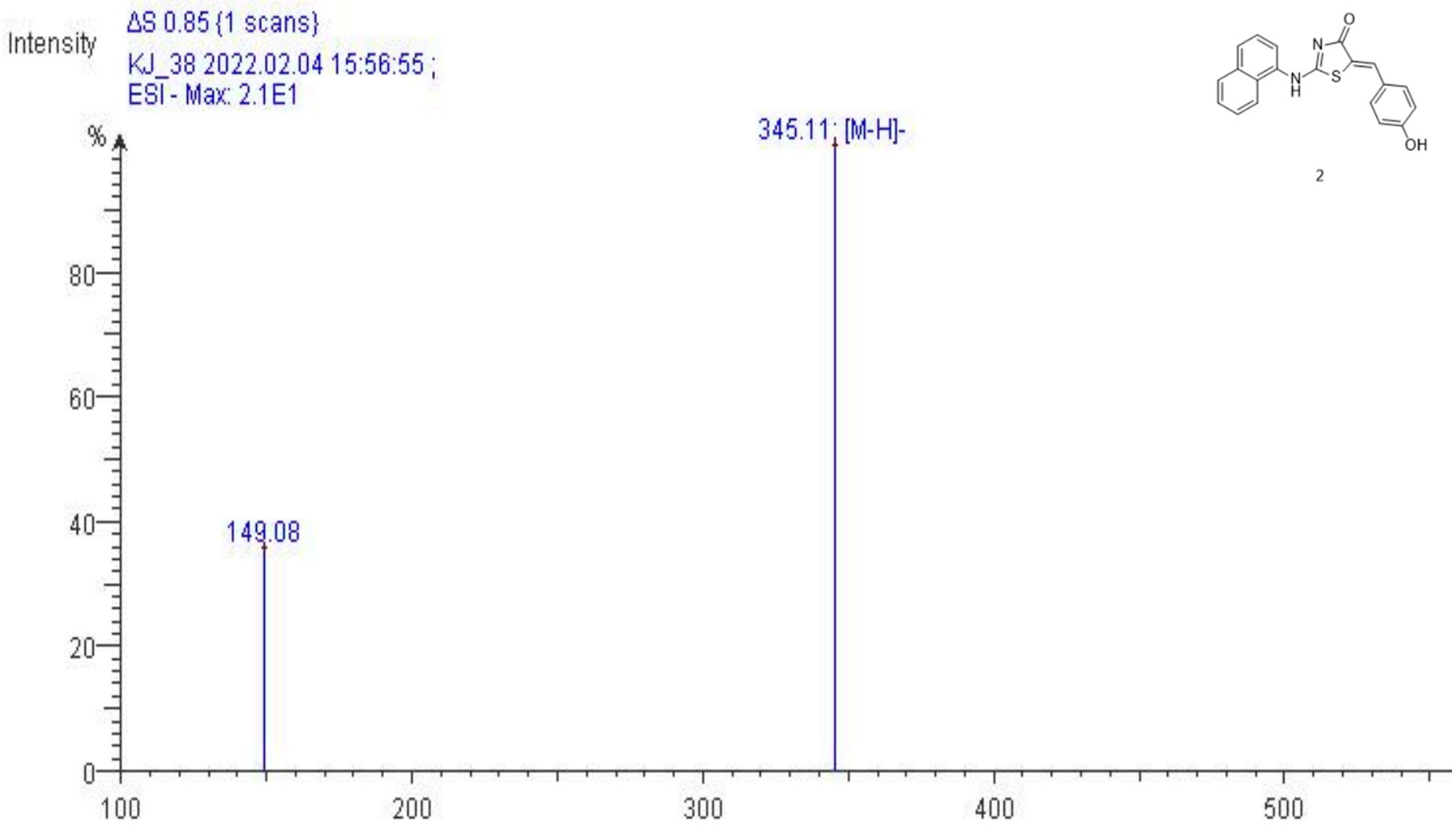

Figure S7. LRMS (ESI–) spectrum of analog **2**

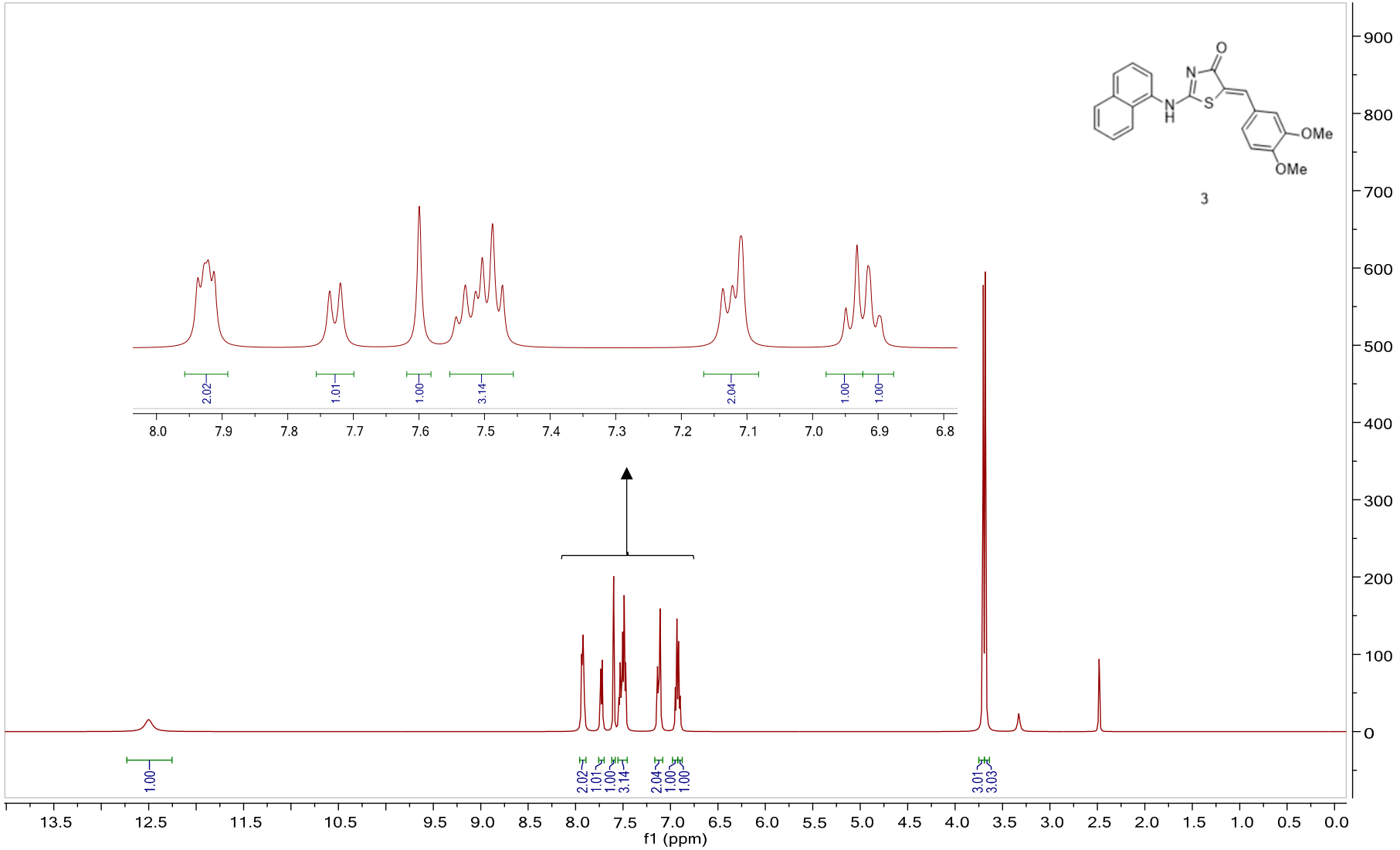

Figure S8. ^{1}H NMR spectrum of analog **3**

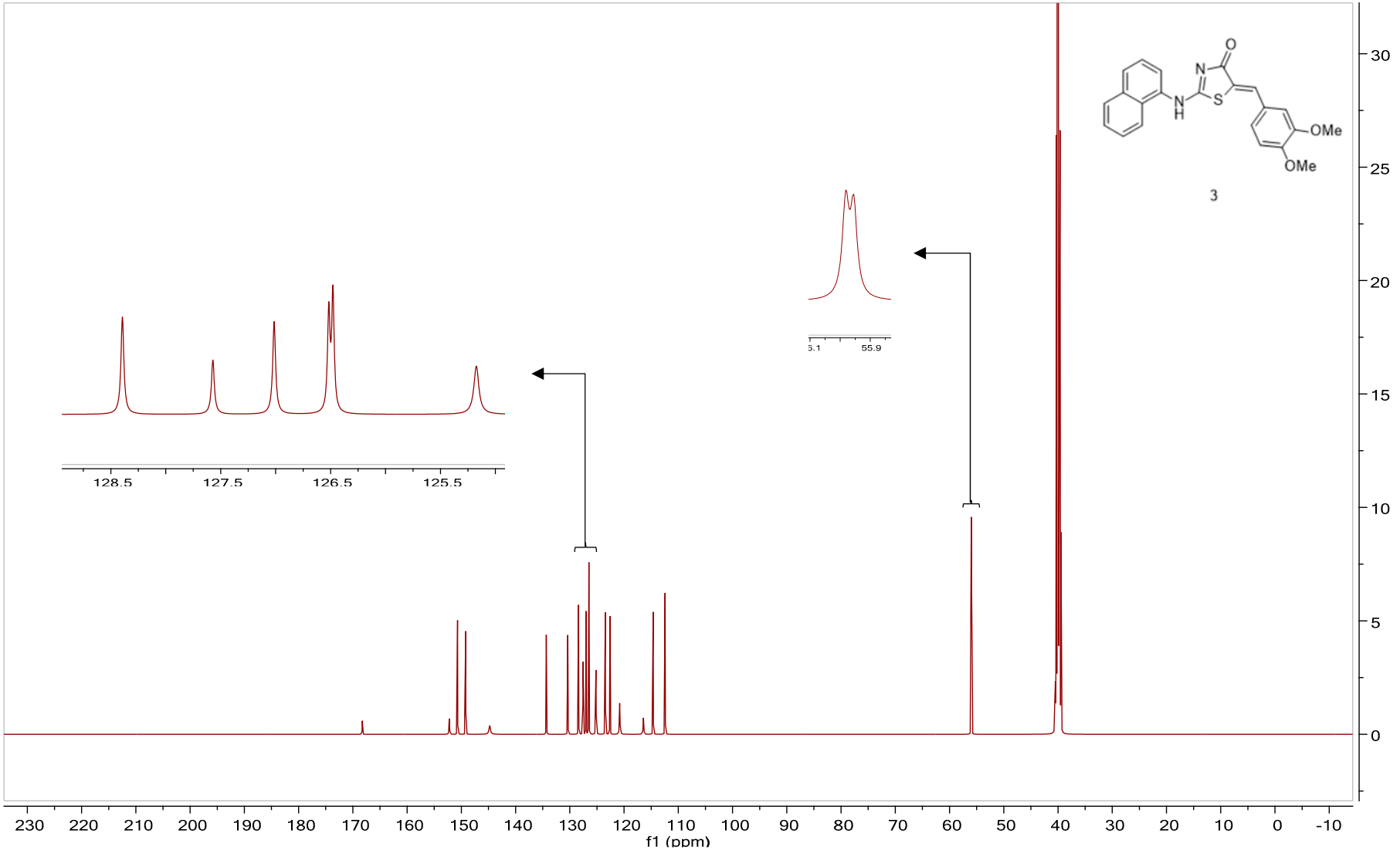

Figure S9. ^{13}C NMR spectrum of analog **3**

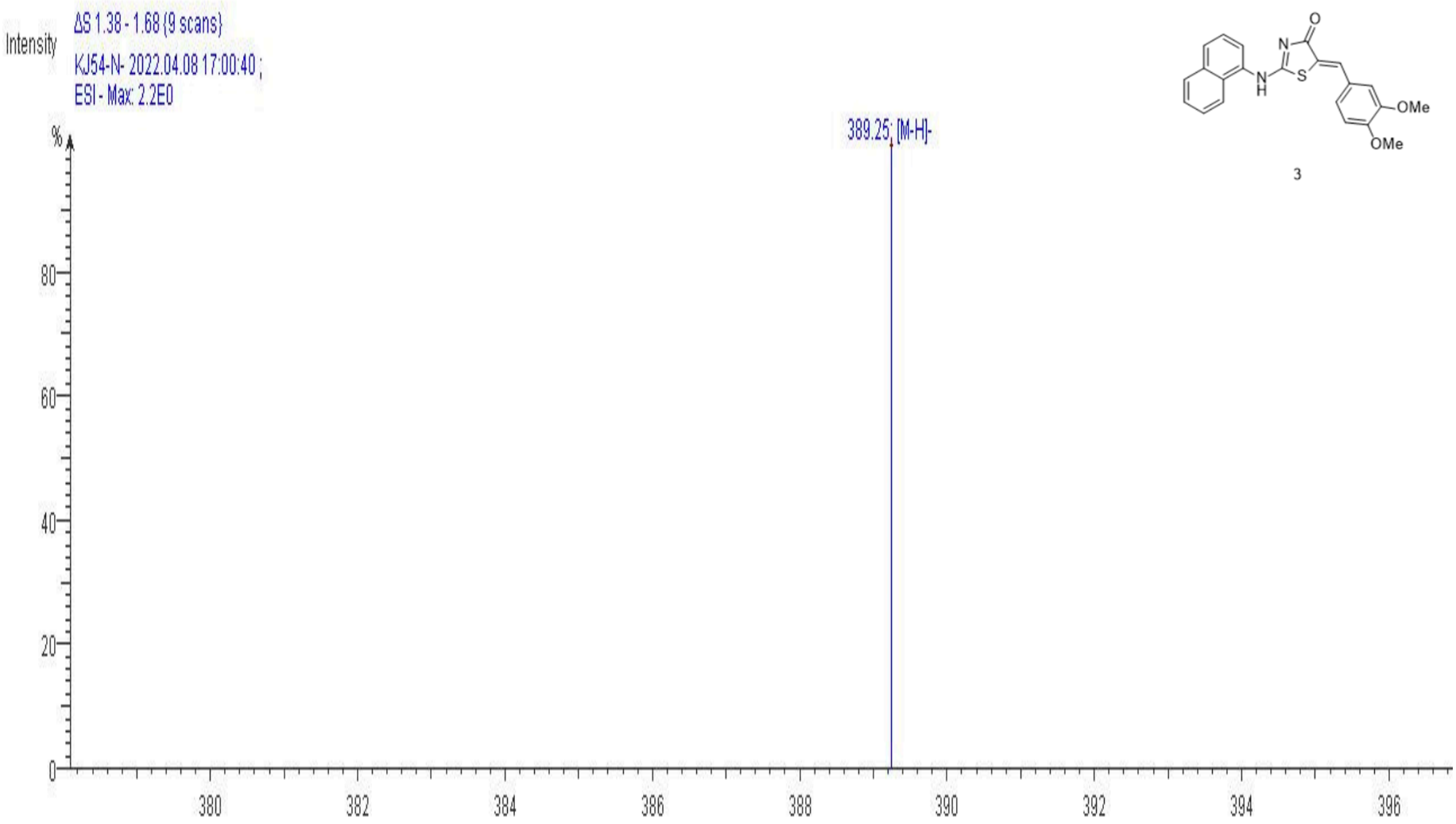

Figure S10. LRMS (ESI–) spectrum of analog **3**

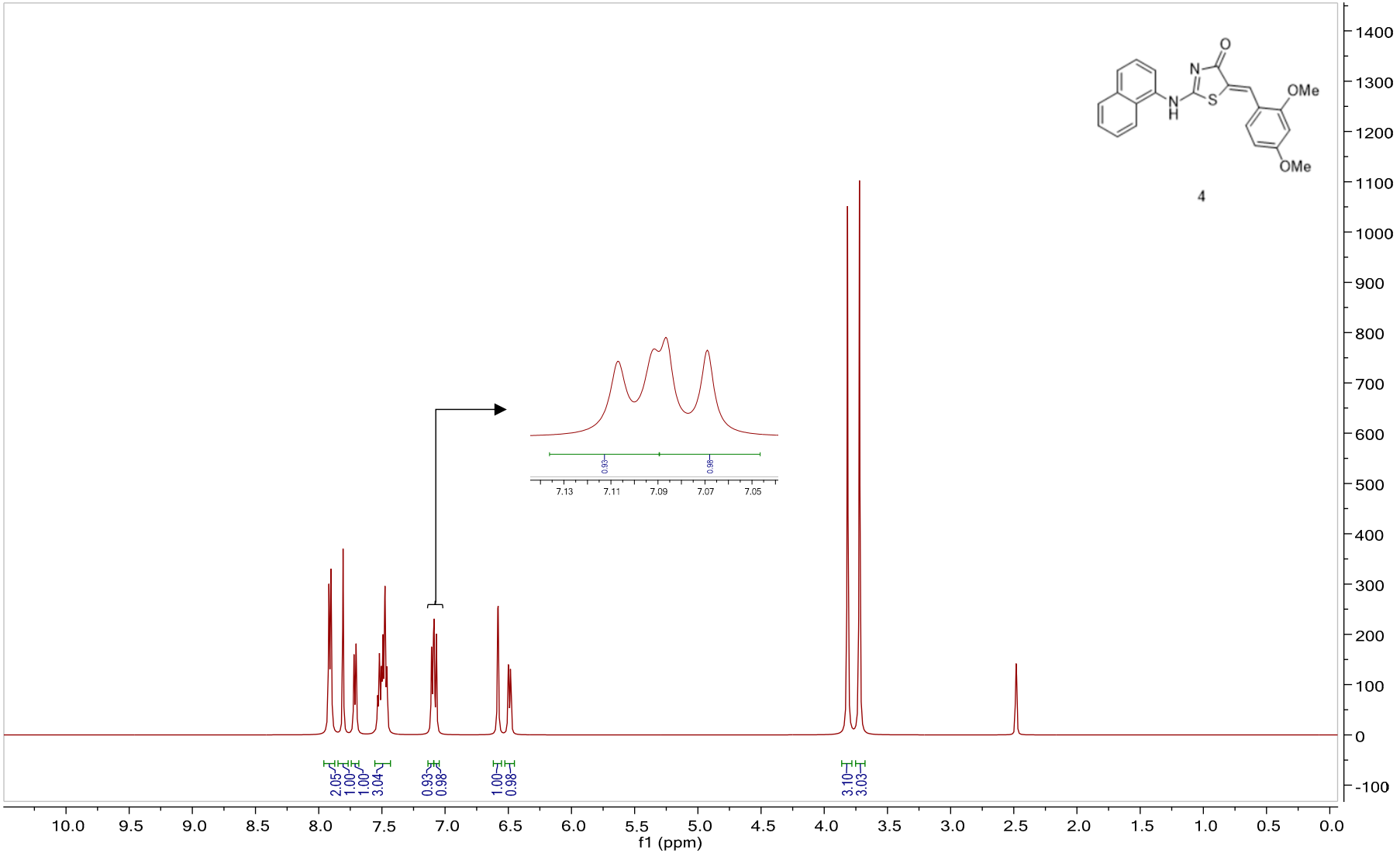

Figure S11. ^{1}H NMR spectrum of analog **4**

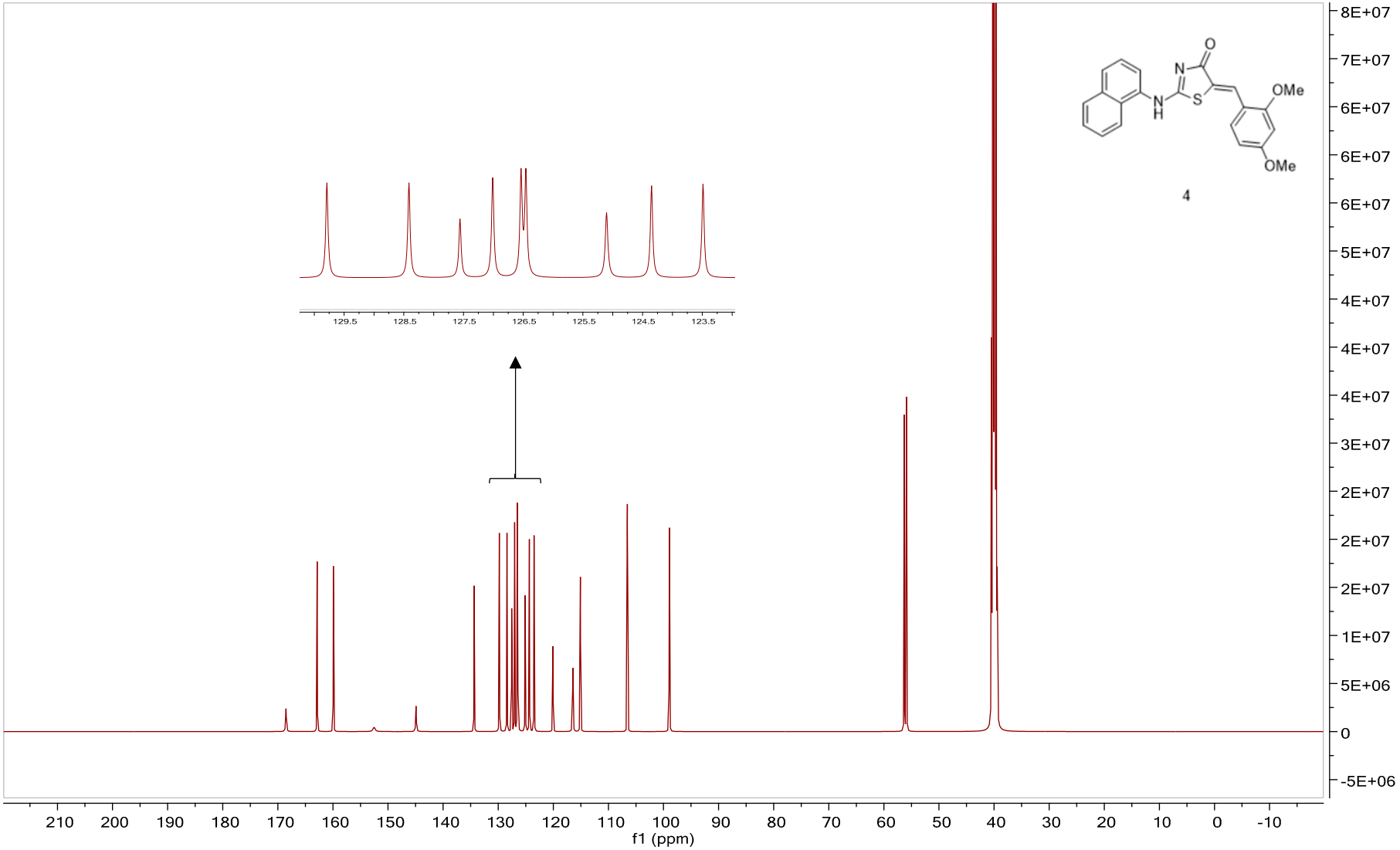

Figure S12. ^{13}C NMR spectrum of analog **4**

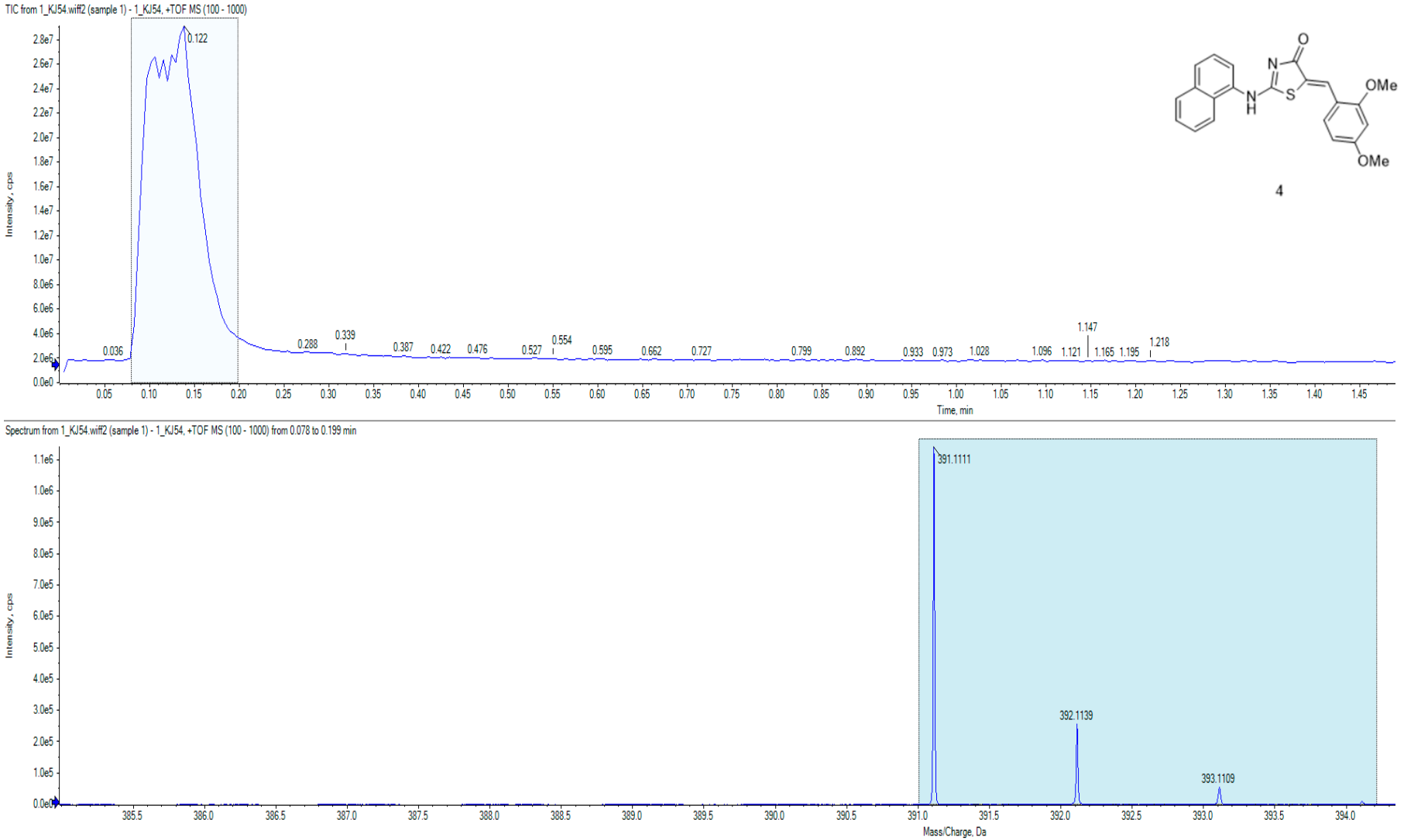

Figure S13-1. HRMS (ESI+) spectrum of analog **4**

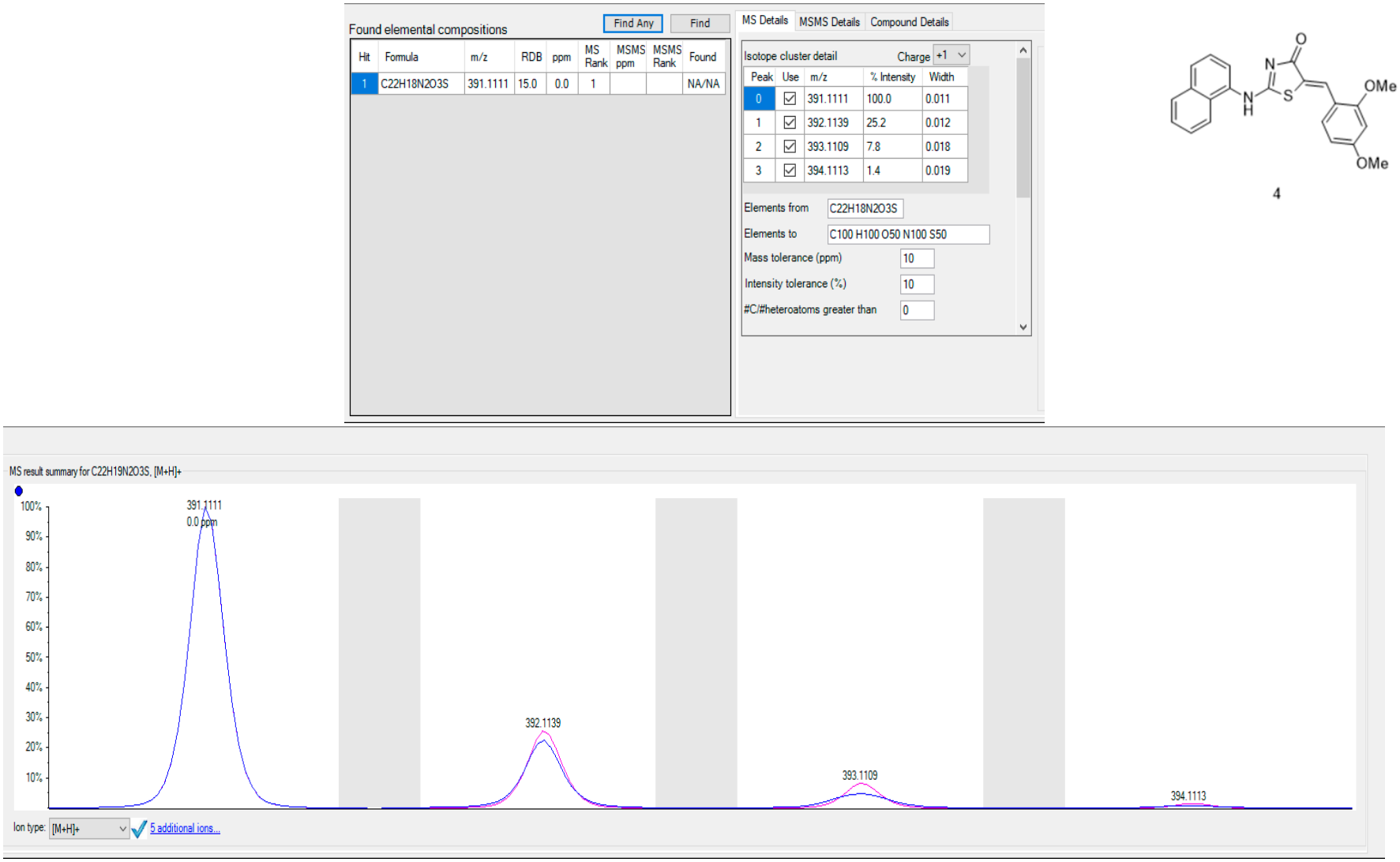

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Figure S13-2. HRMS (ESI+) spectrum of analog **4**

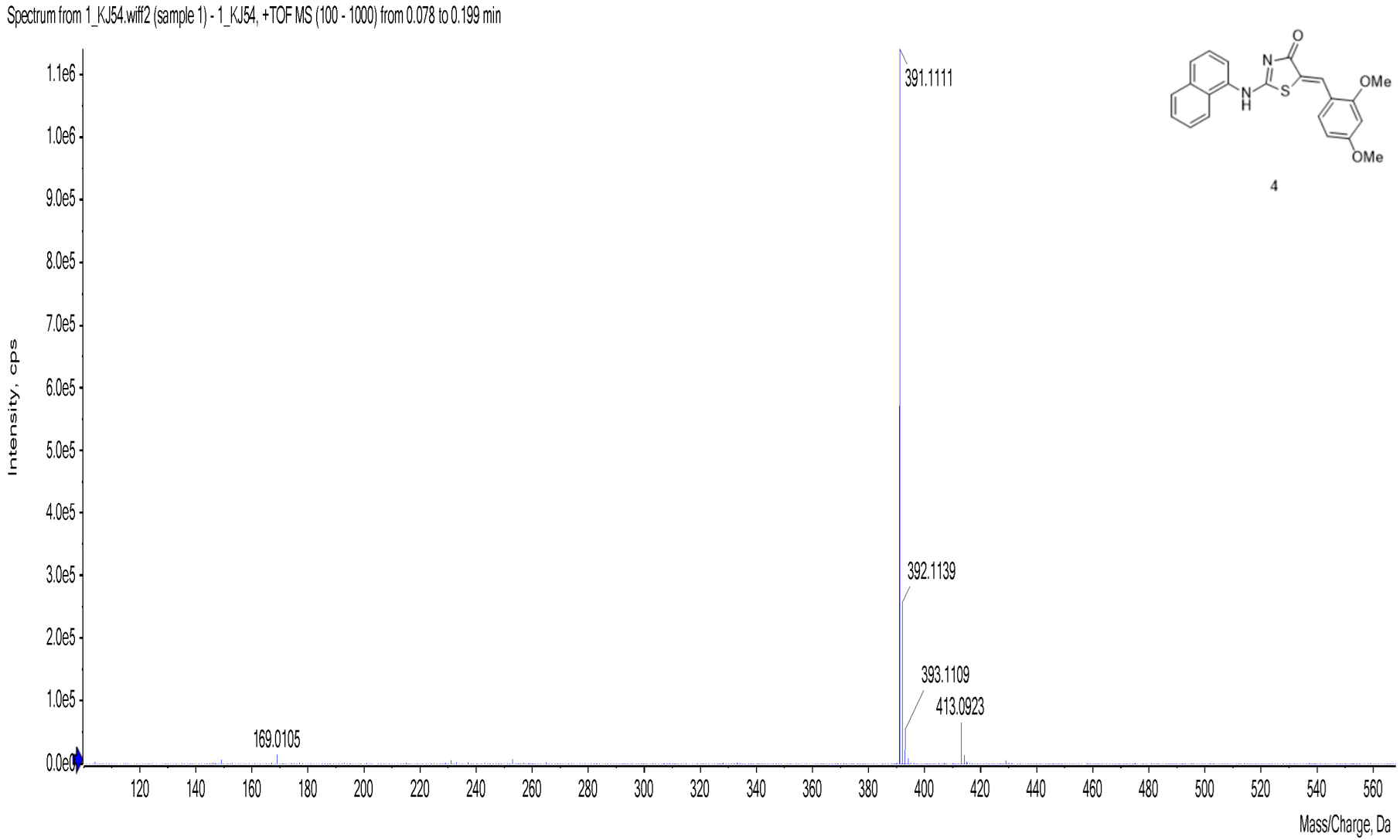


Figure S13-3. HRMS (ESI+) spectrum of analog **4**

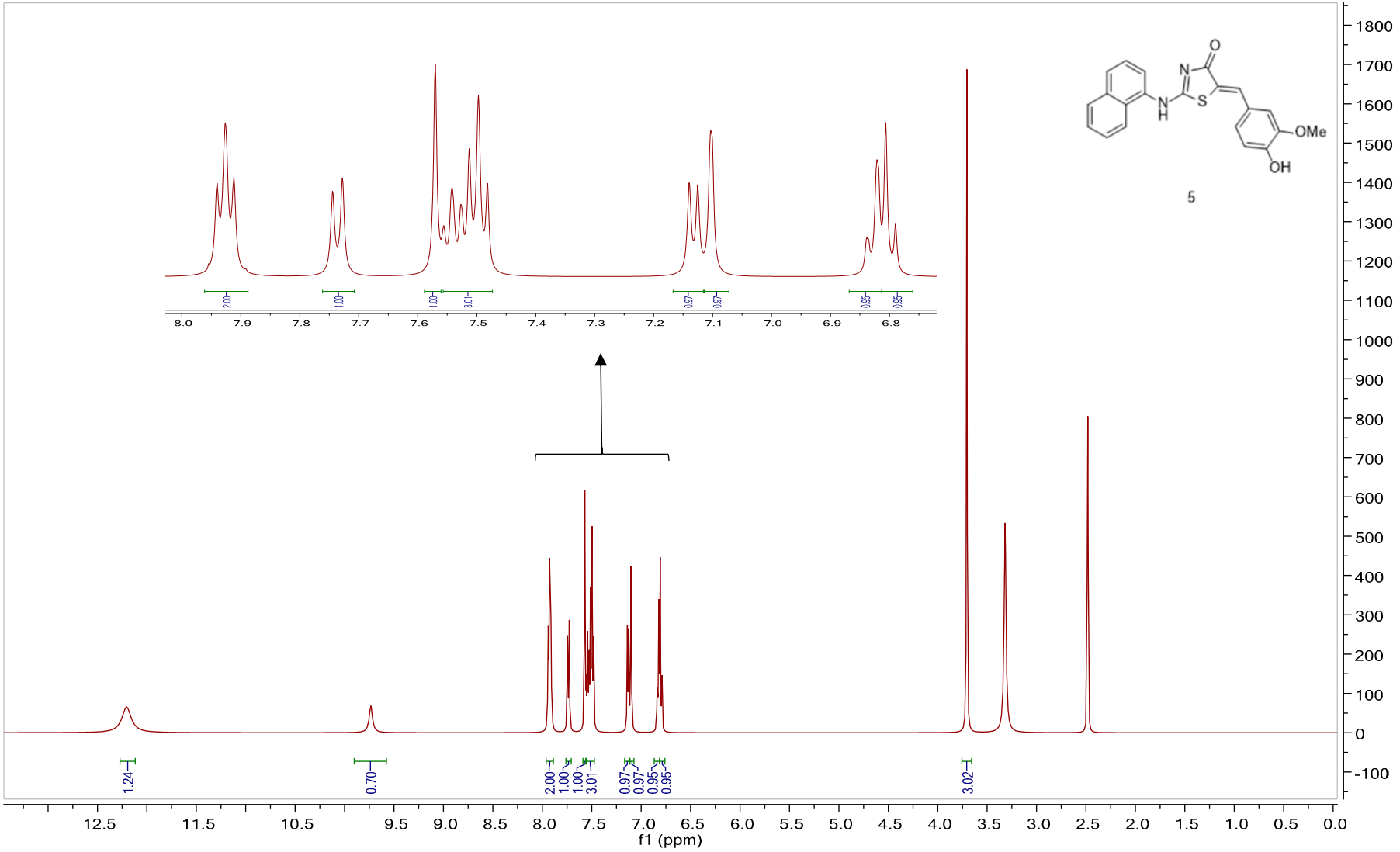


Figure S14. ^{1}H NMR spectrum of analog **5**

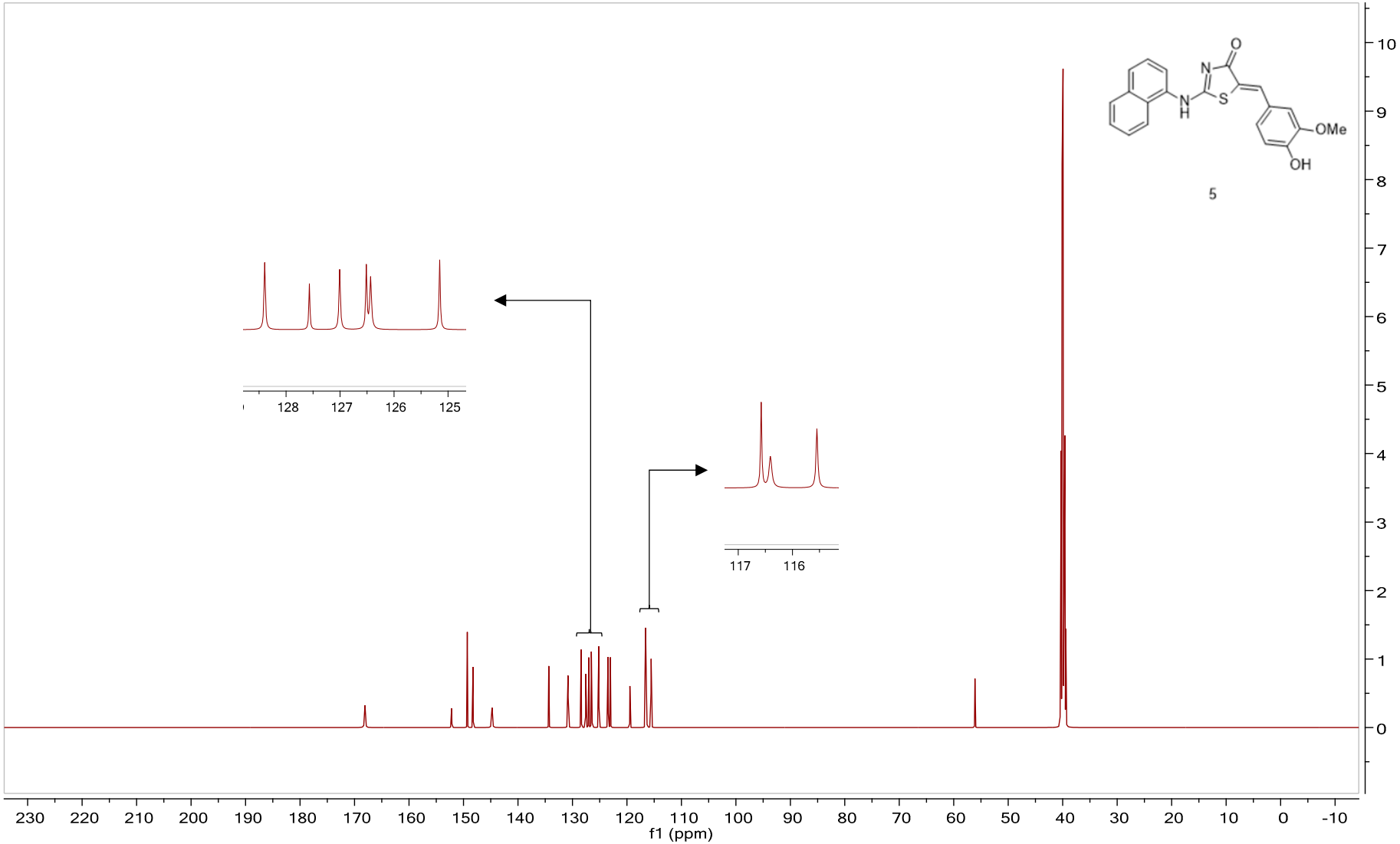


Figure S15. ^{13}C NMR spectrum of analog **5**

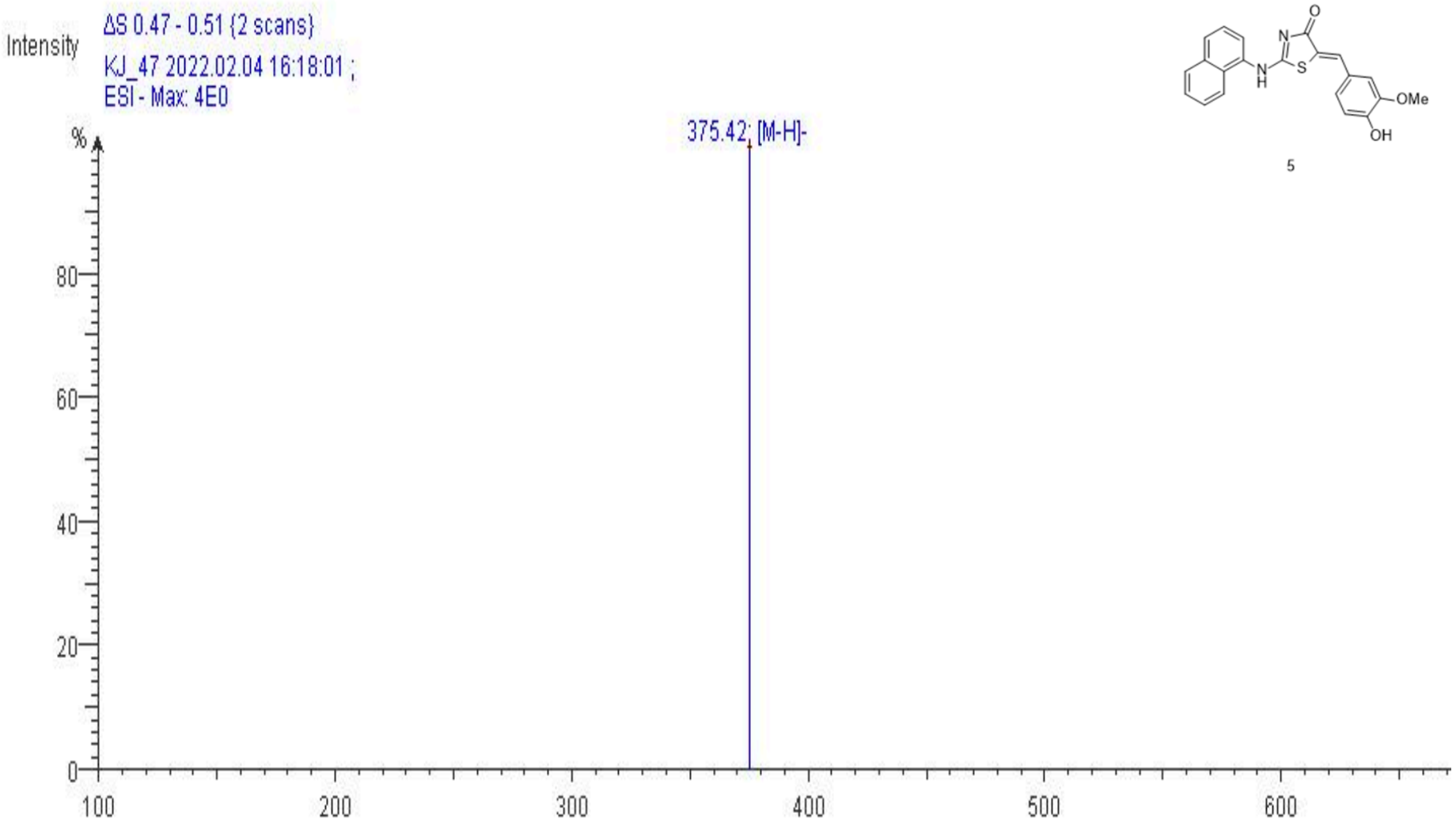


Figure S16. LRMS (ESI–) spectrum of analog **5**

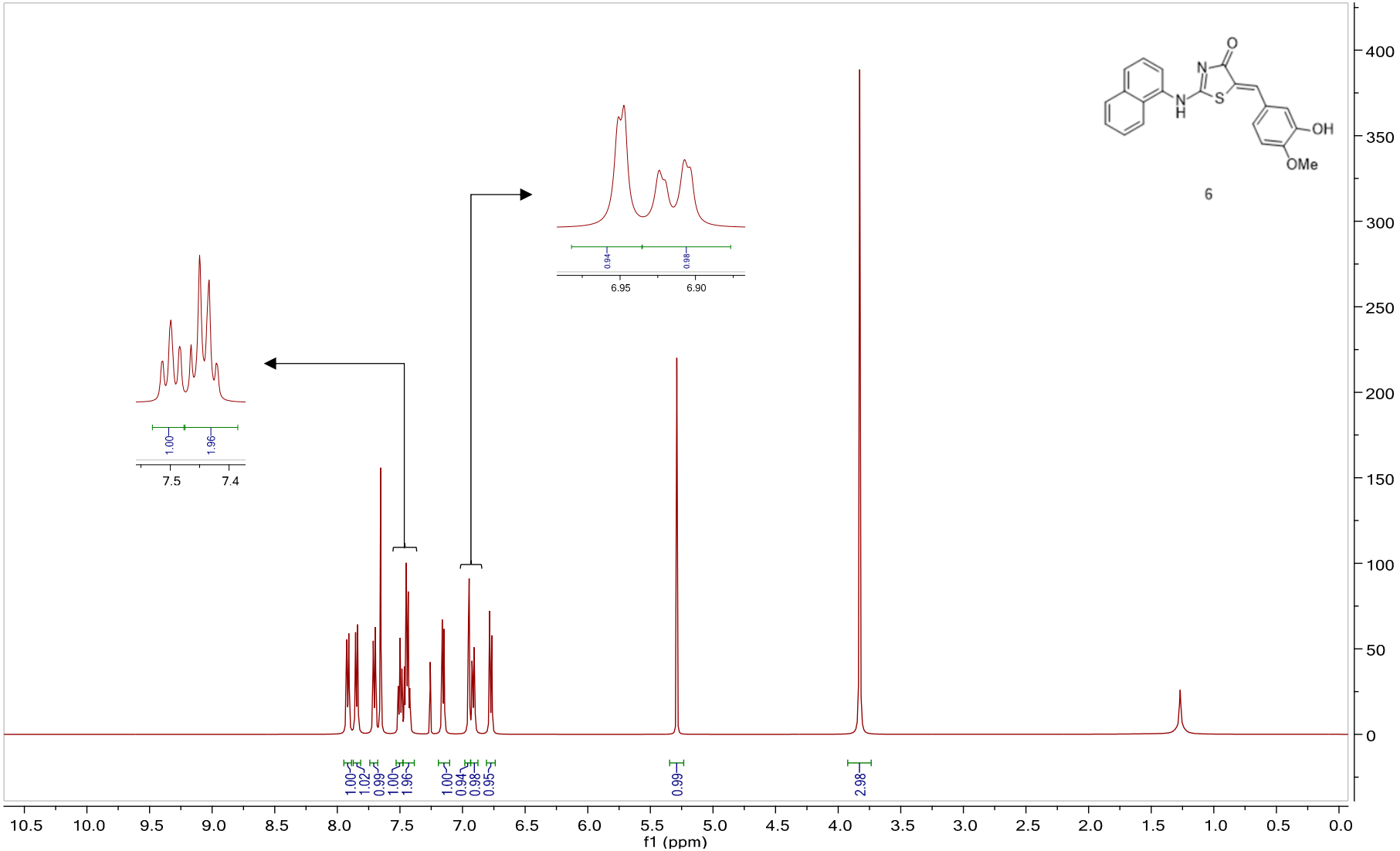


Figure S17. ^{1}H NMR spectrum of analog **6**

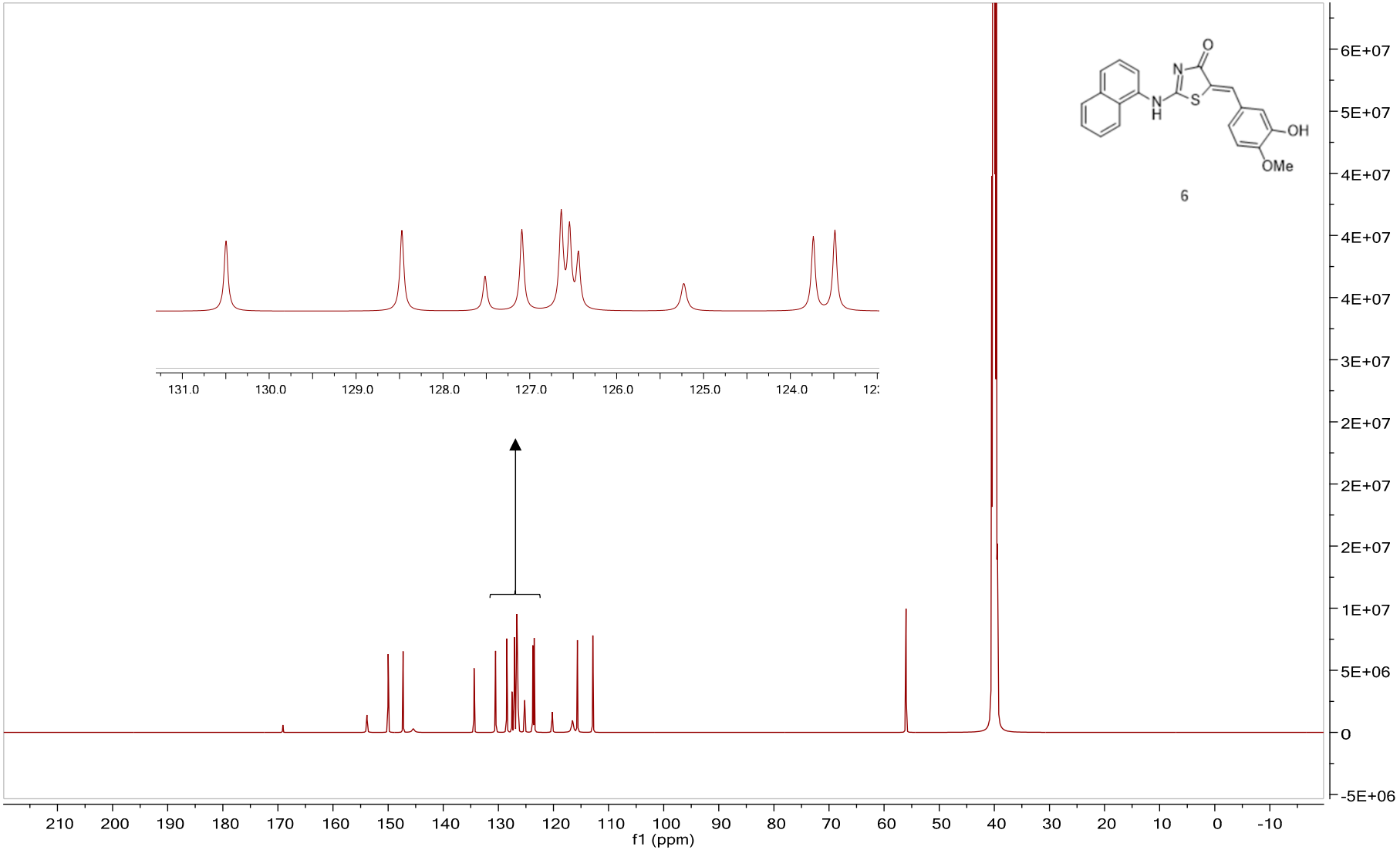


Figure S18. ^{13}C NMR spectrum of analog **6**

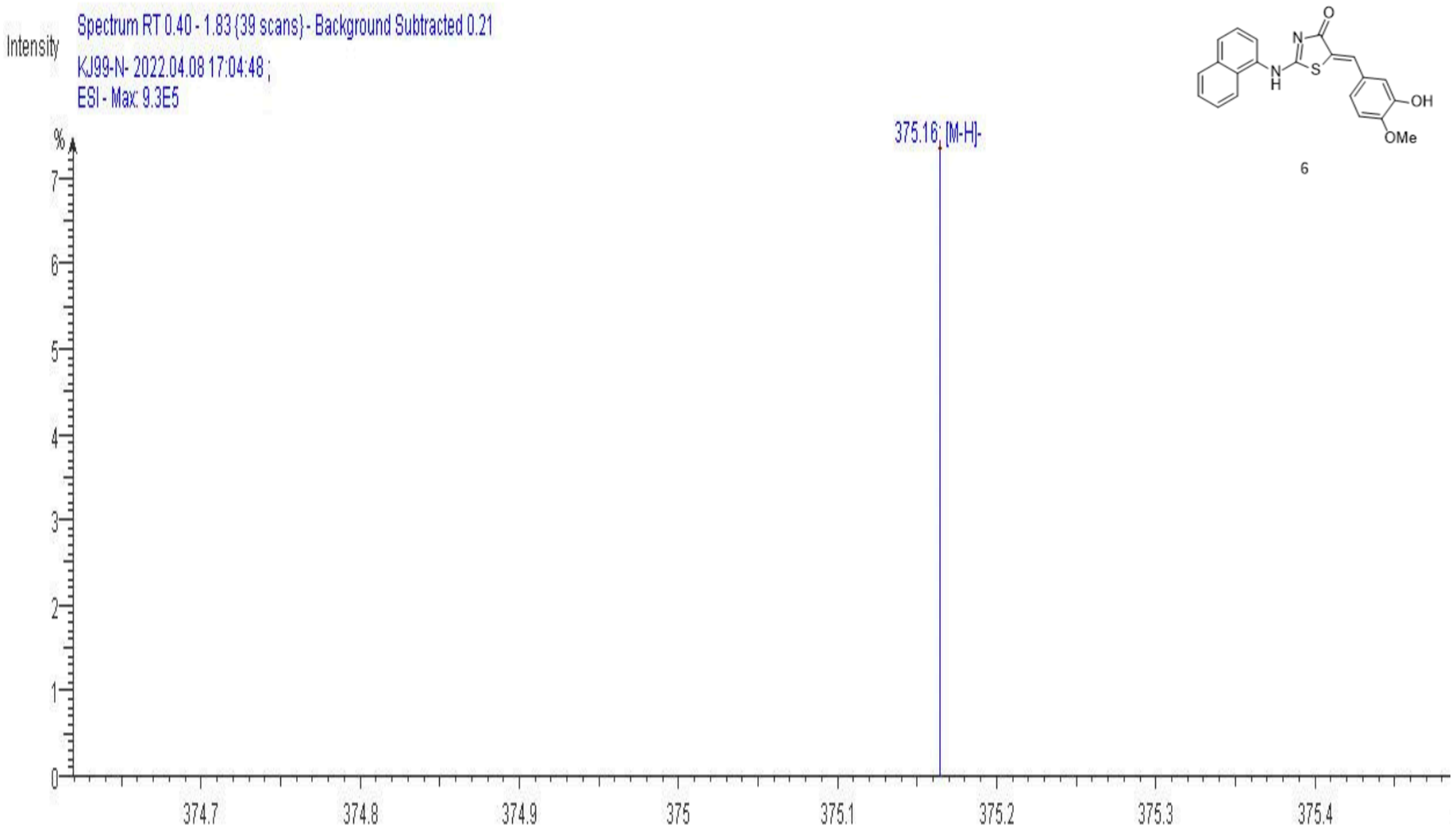


Figure S19. LRMS (ESI–) spectrum of analog **6**

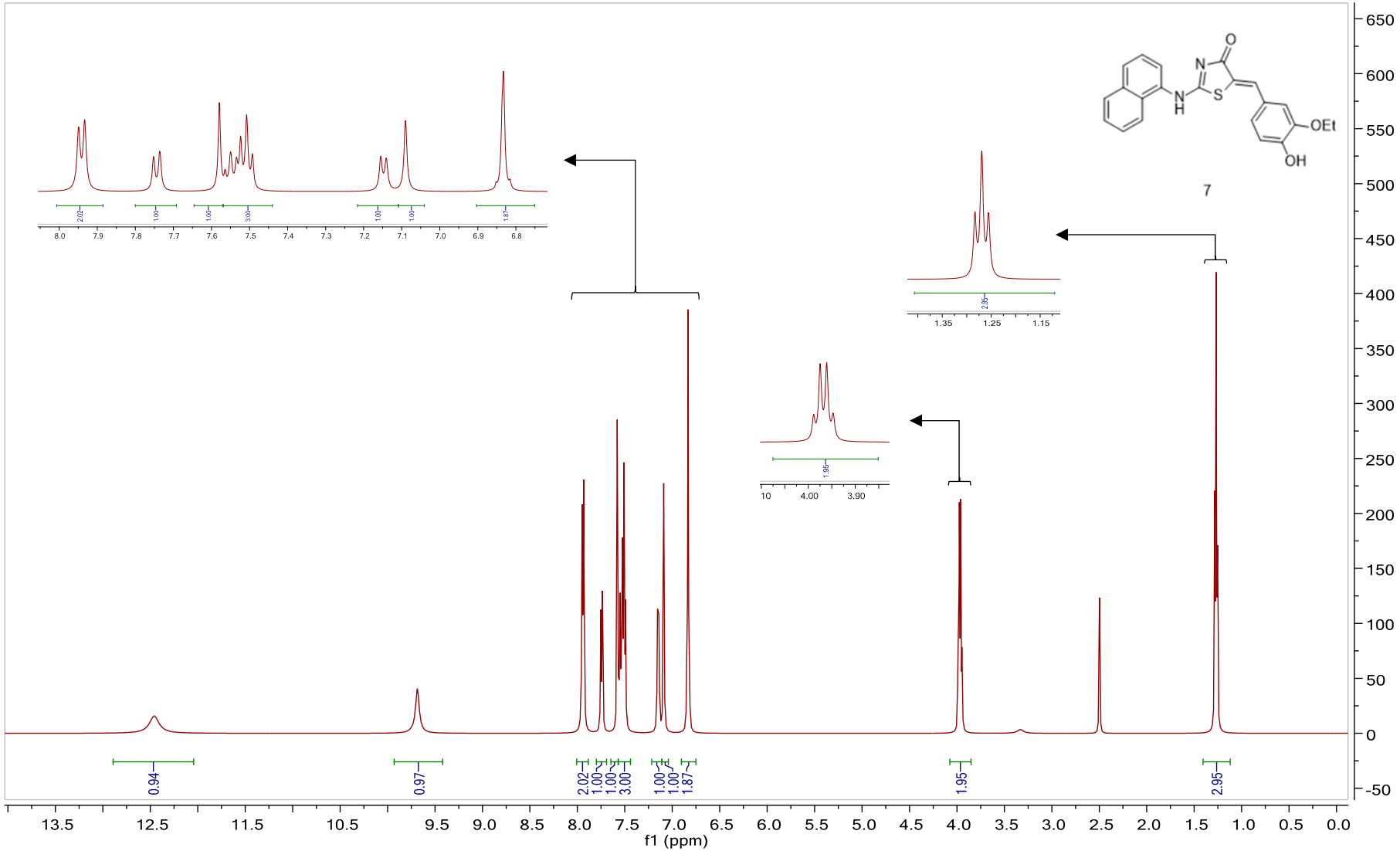


Figure S20. ^{1}H NMR spectrum of analog **7**

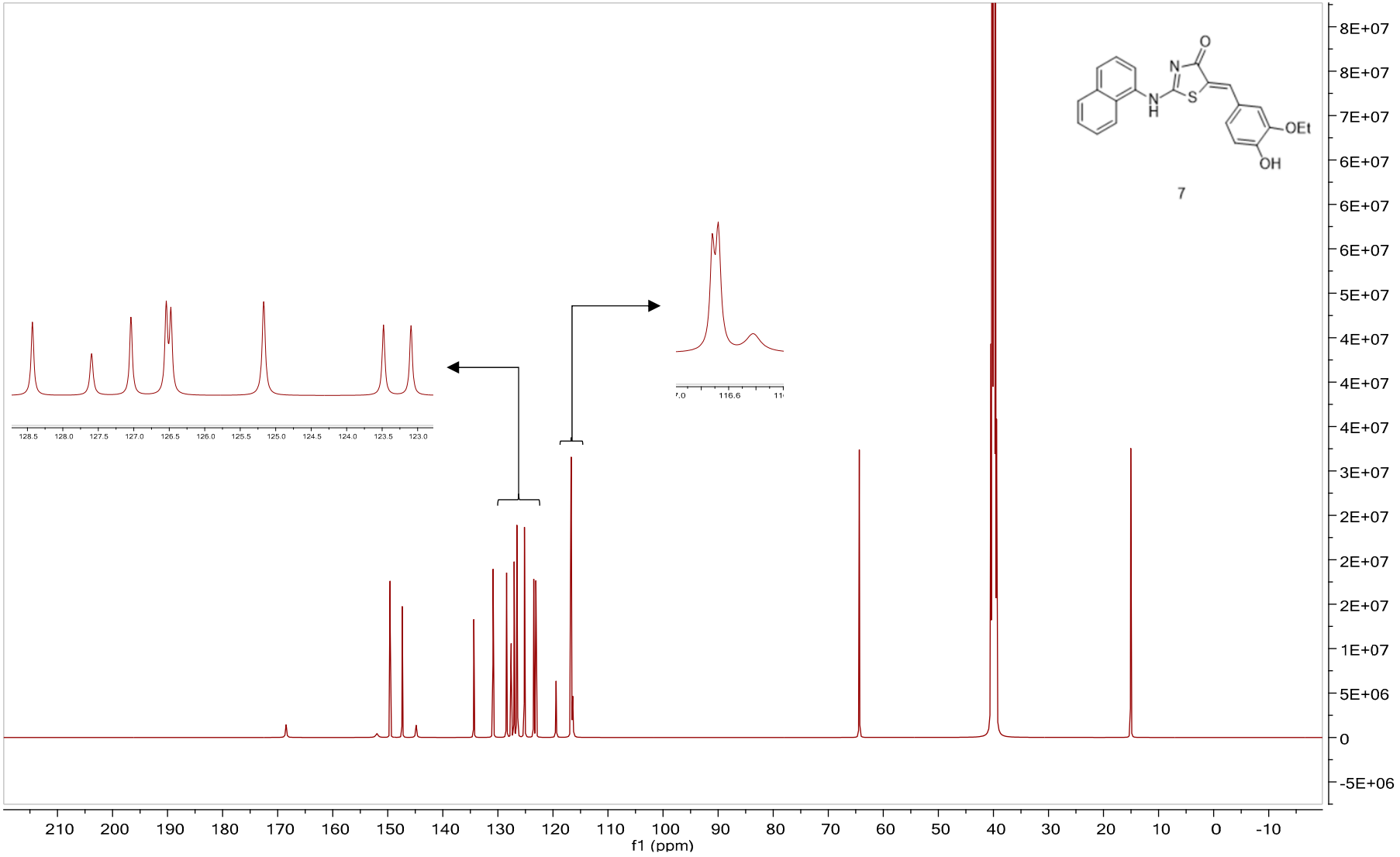


Figure S21. ^{13}C NMR spectrum of analog **7**

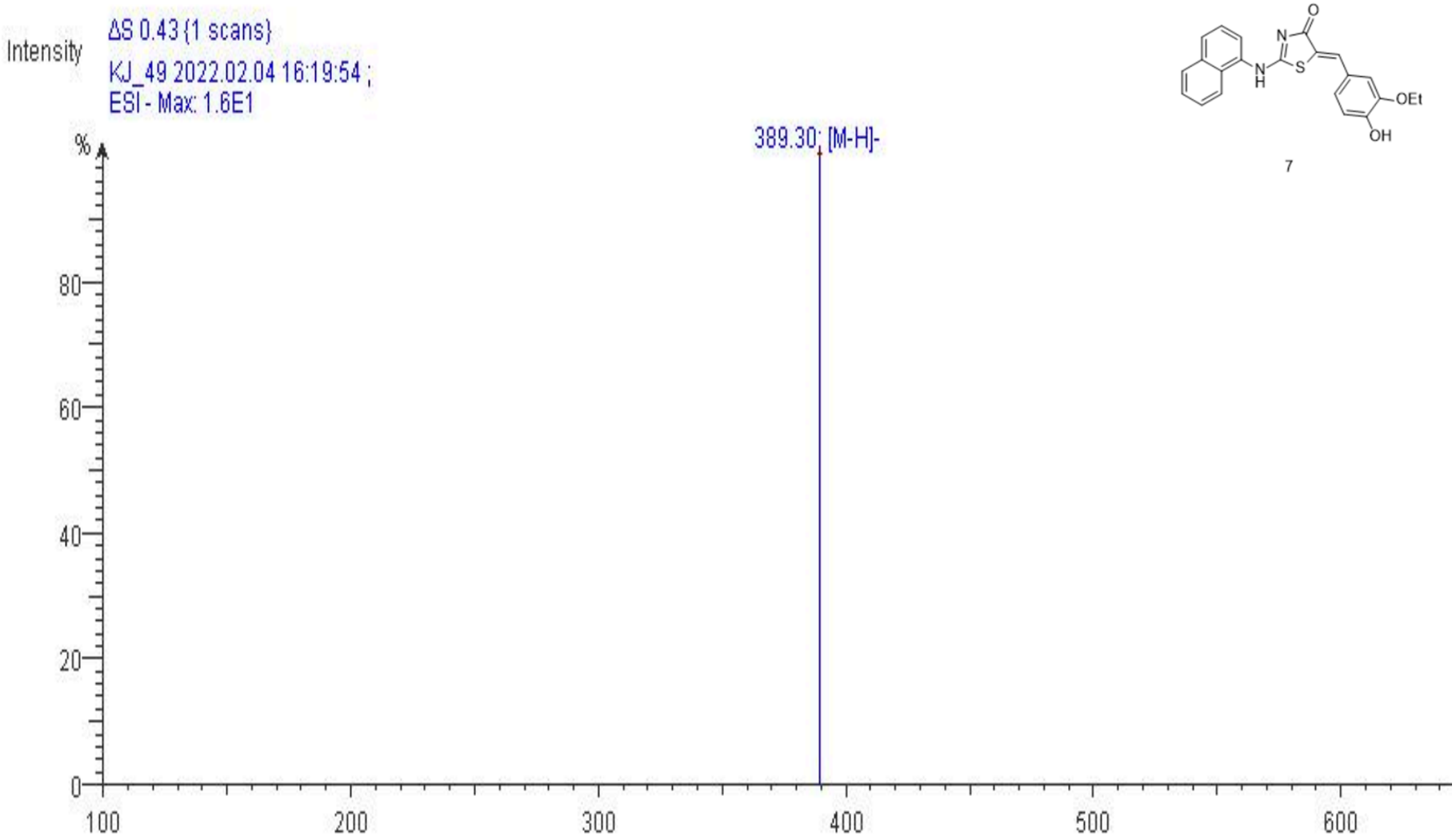


Figure S22. LRMS (ESI–) spectrum of analog **7**

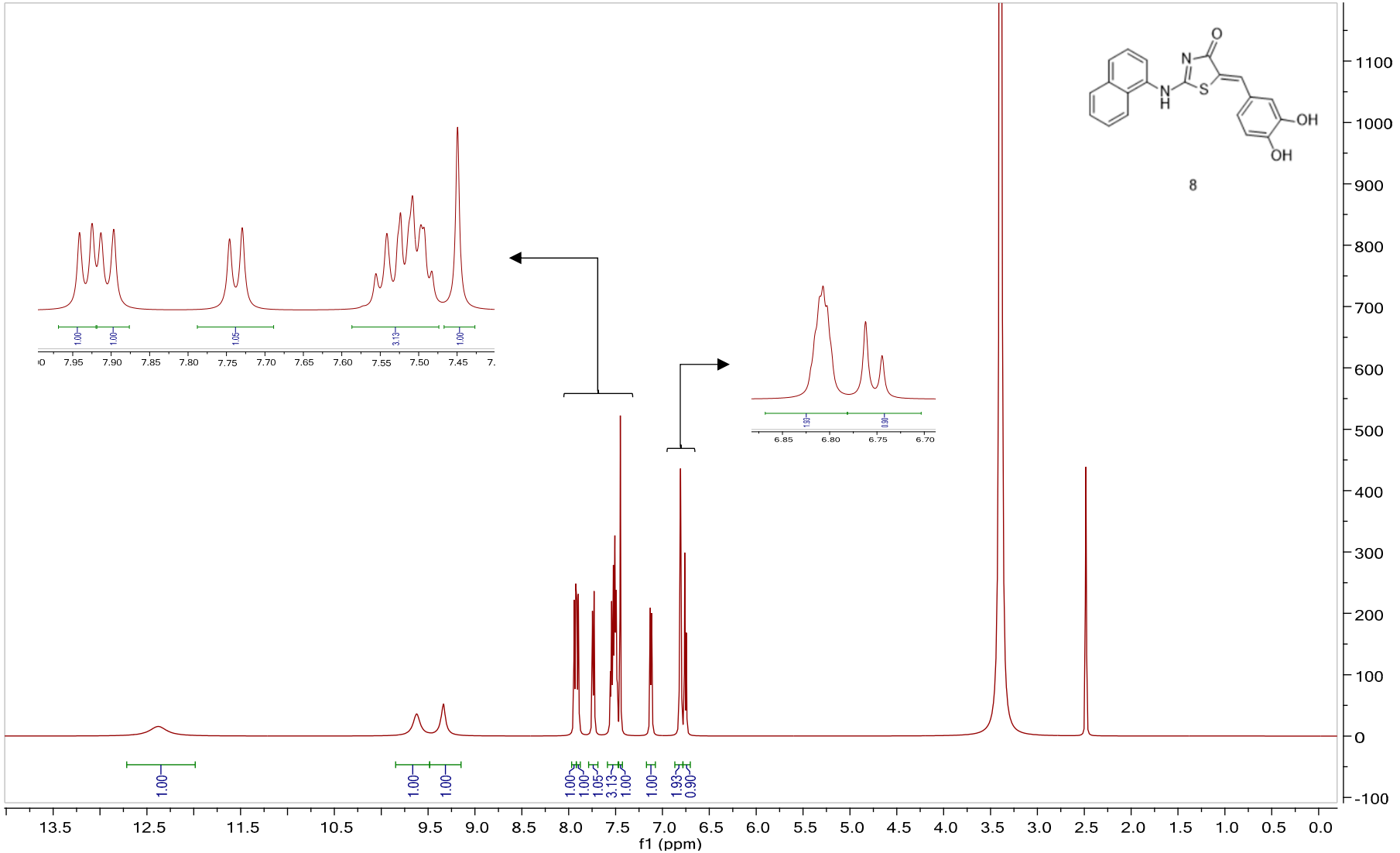


Figure S23. ^{1}H NMR spectrum of analog **8**

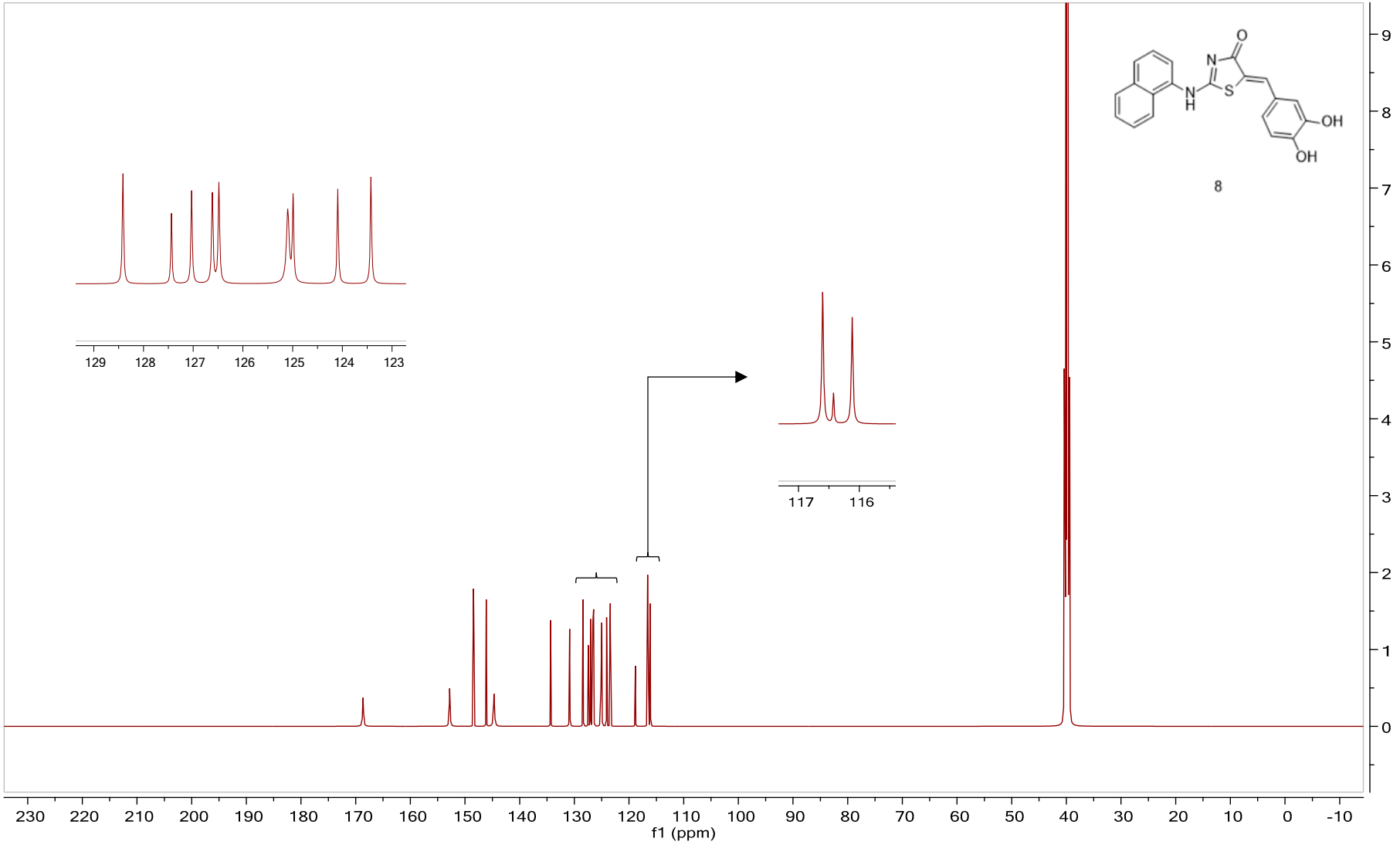


Figure S24. ^{13}C NMR spectrum of analog **8**

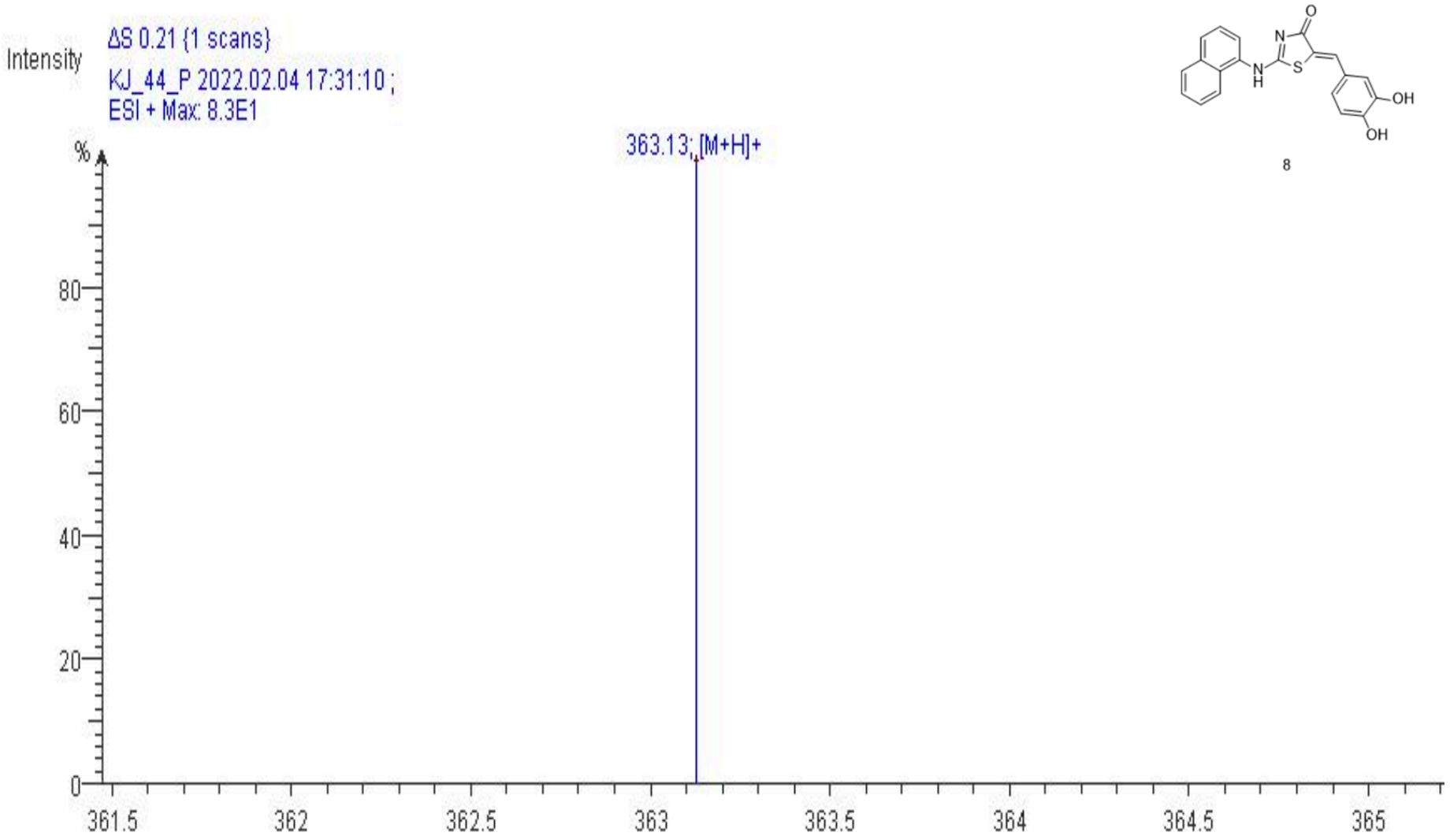


Figure S25. LRMS (ESI+) spectrum of analog **8**

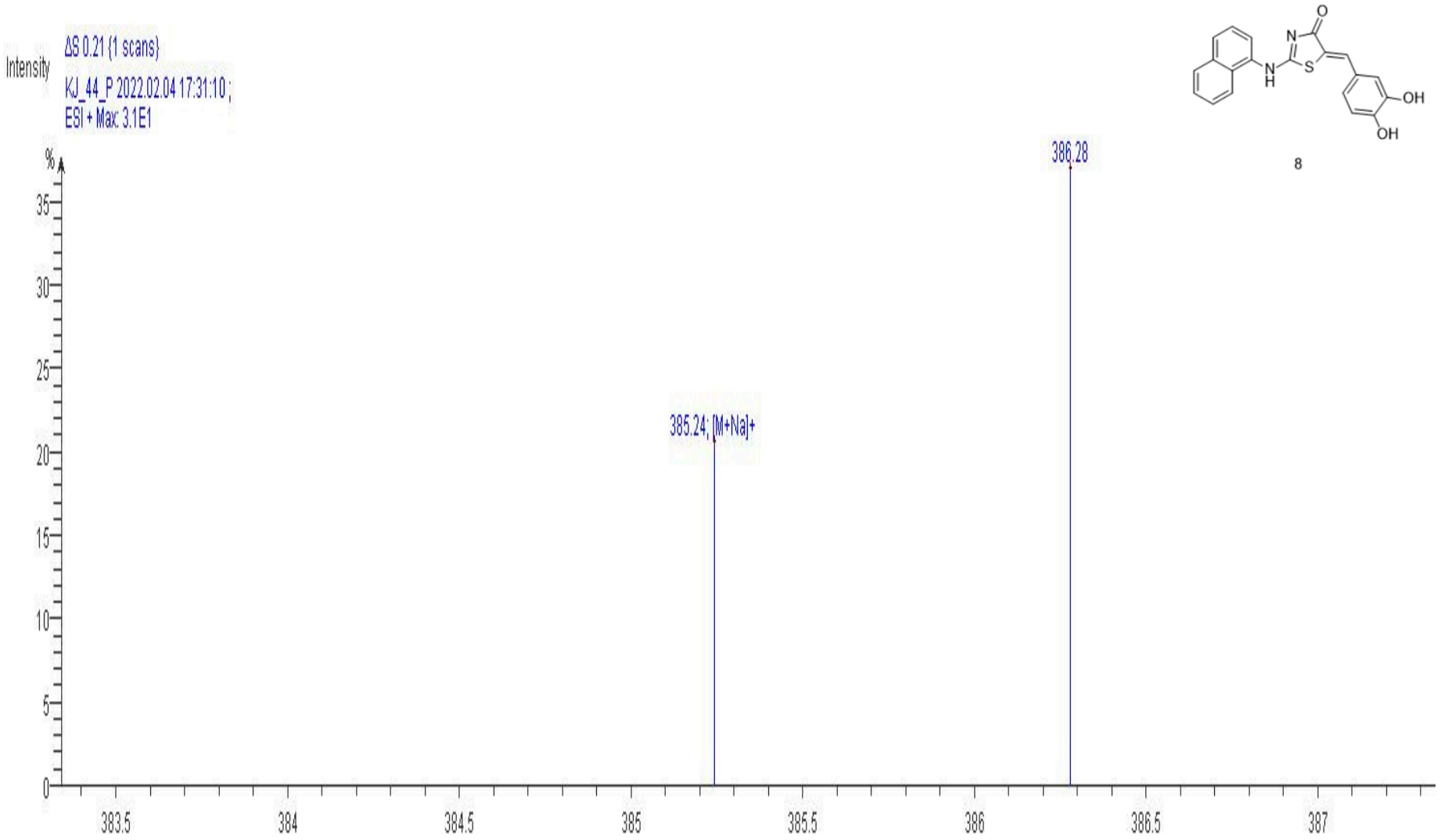


Figure S26. LRMS (ESI+) spectrum of analog **8**

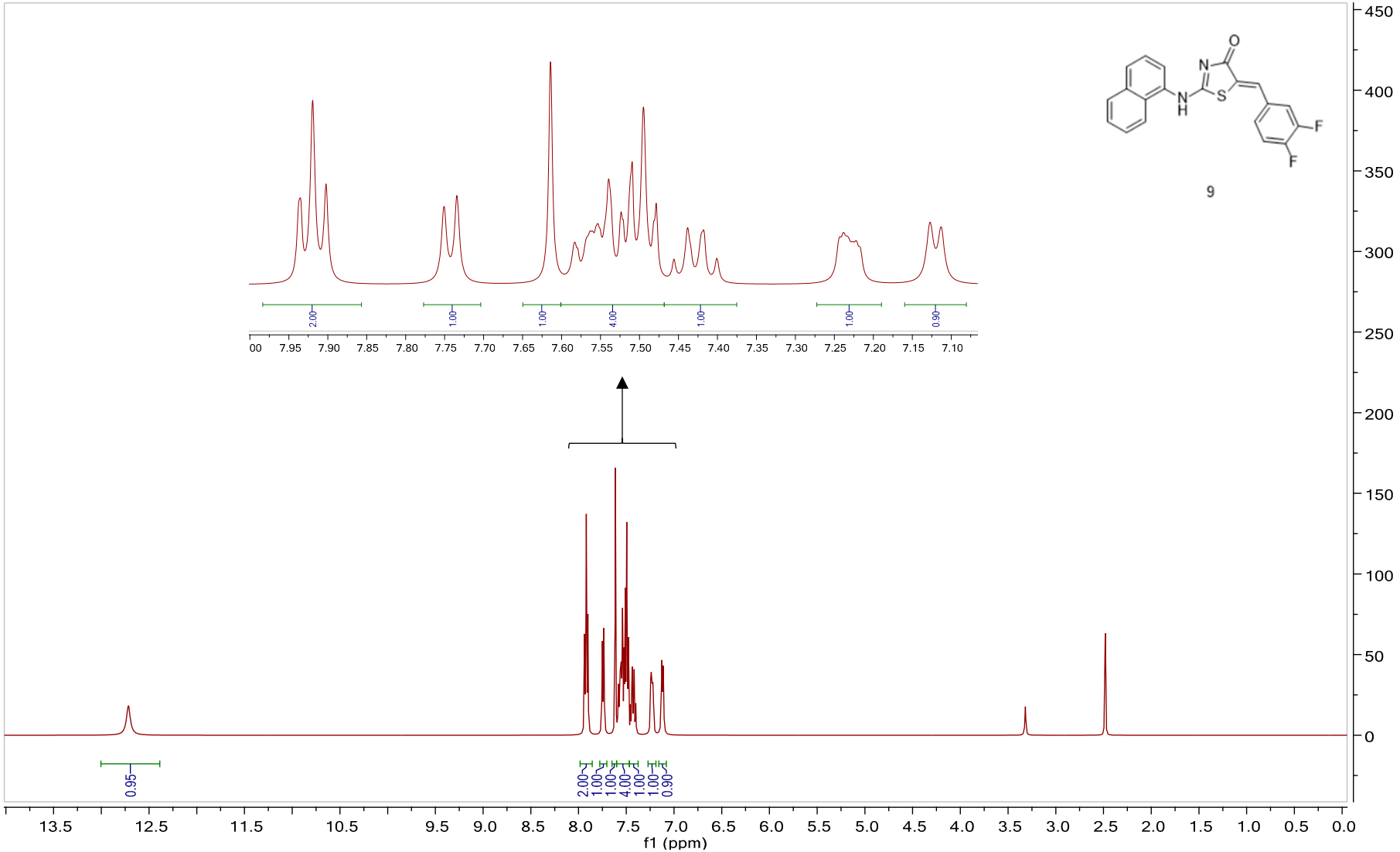


Figure S27. ^{1}H NMR spectrum of analog **9**

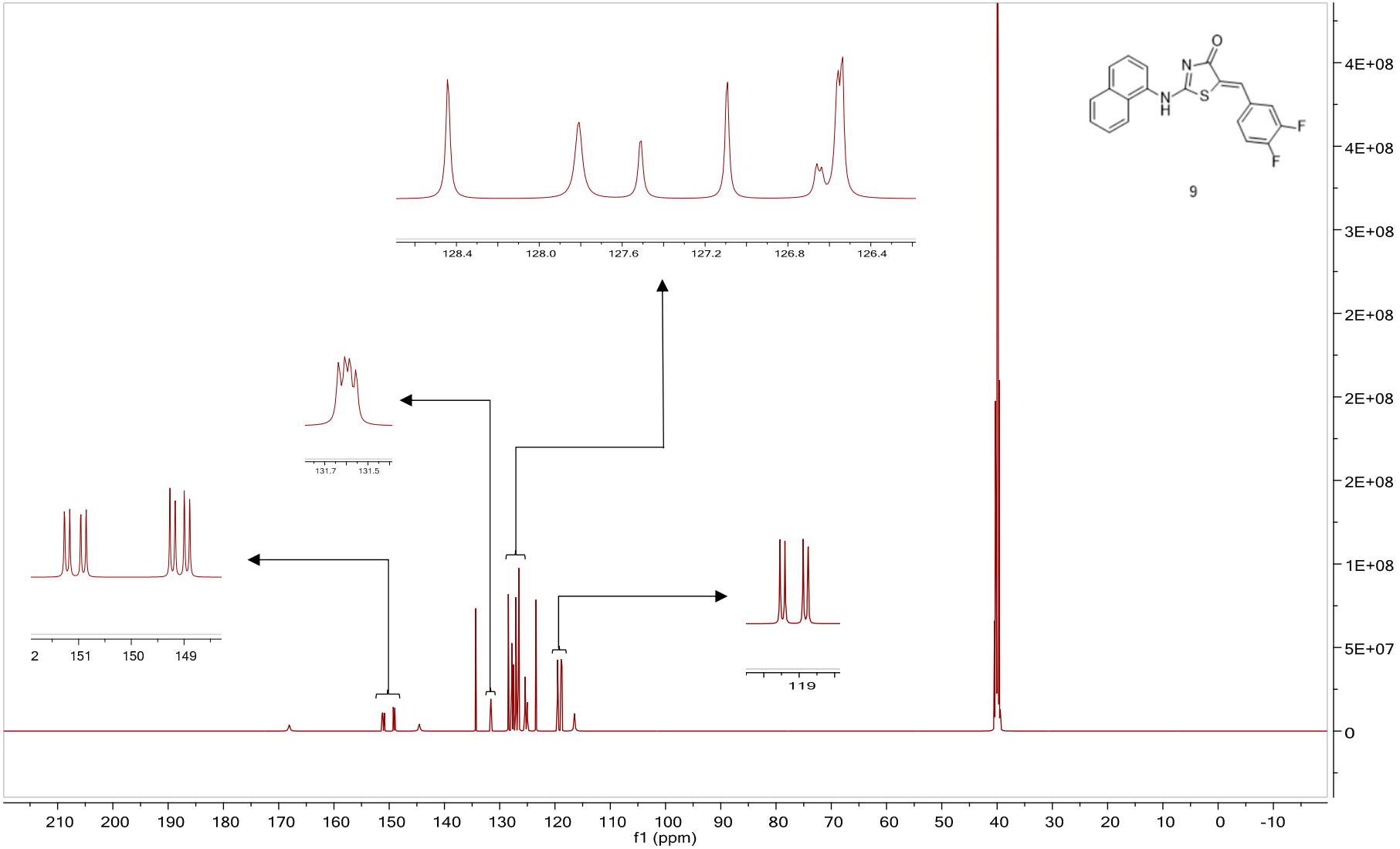


Figure S28. ^{13}C NMR spectrum of analog **9**

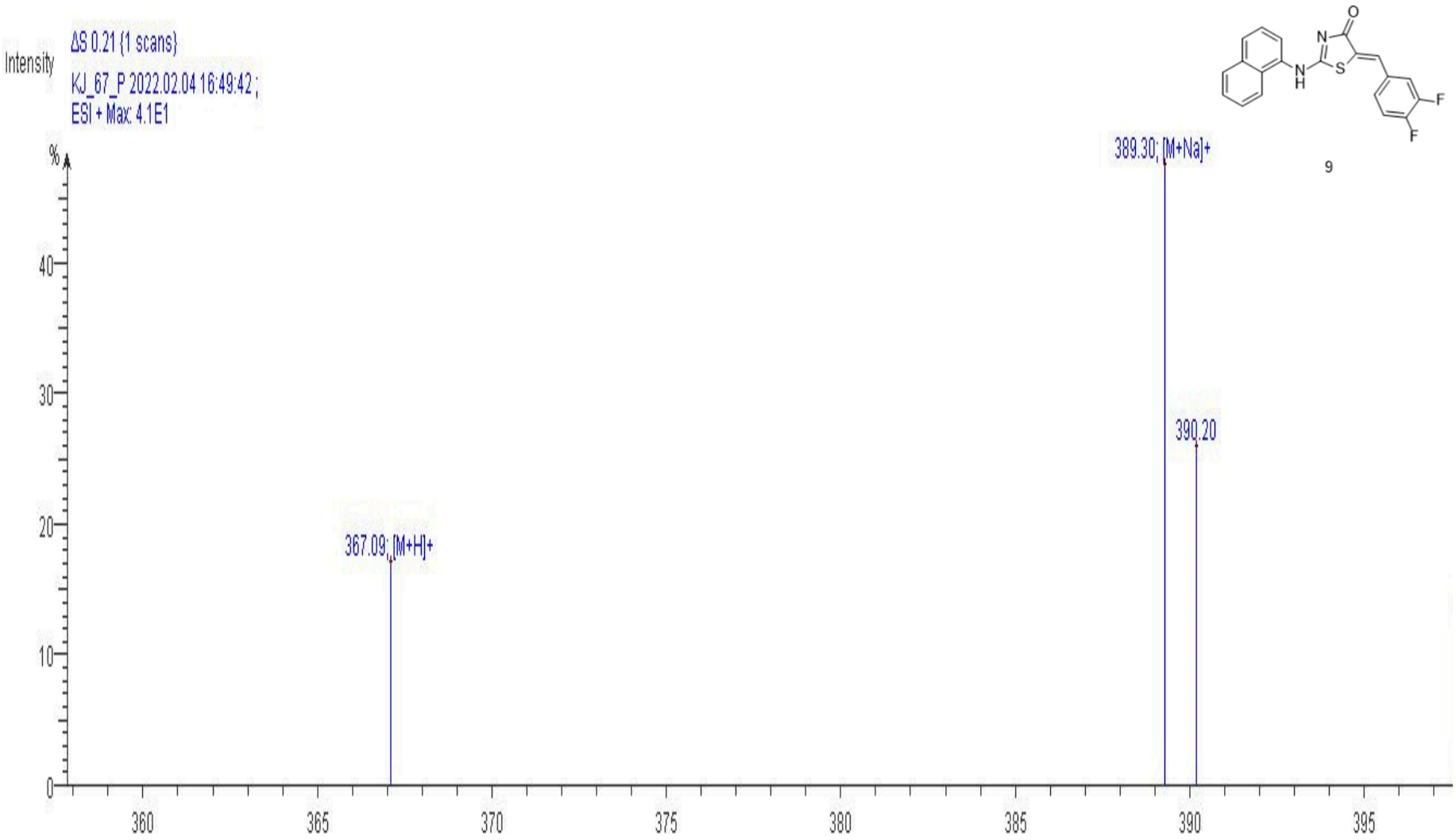


Figure S29. LRMS (ESI+) spectrum of analog **9**

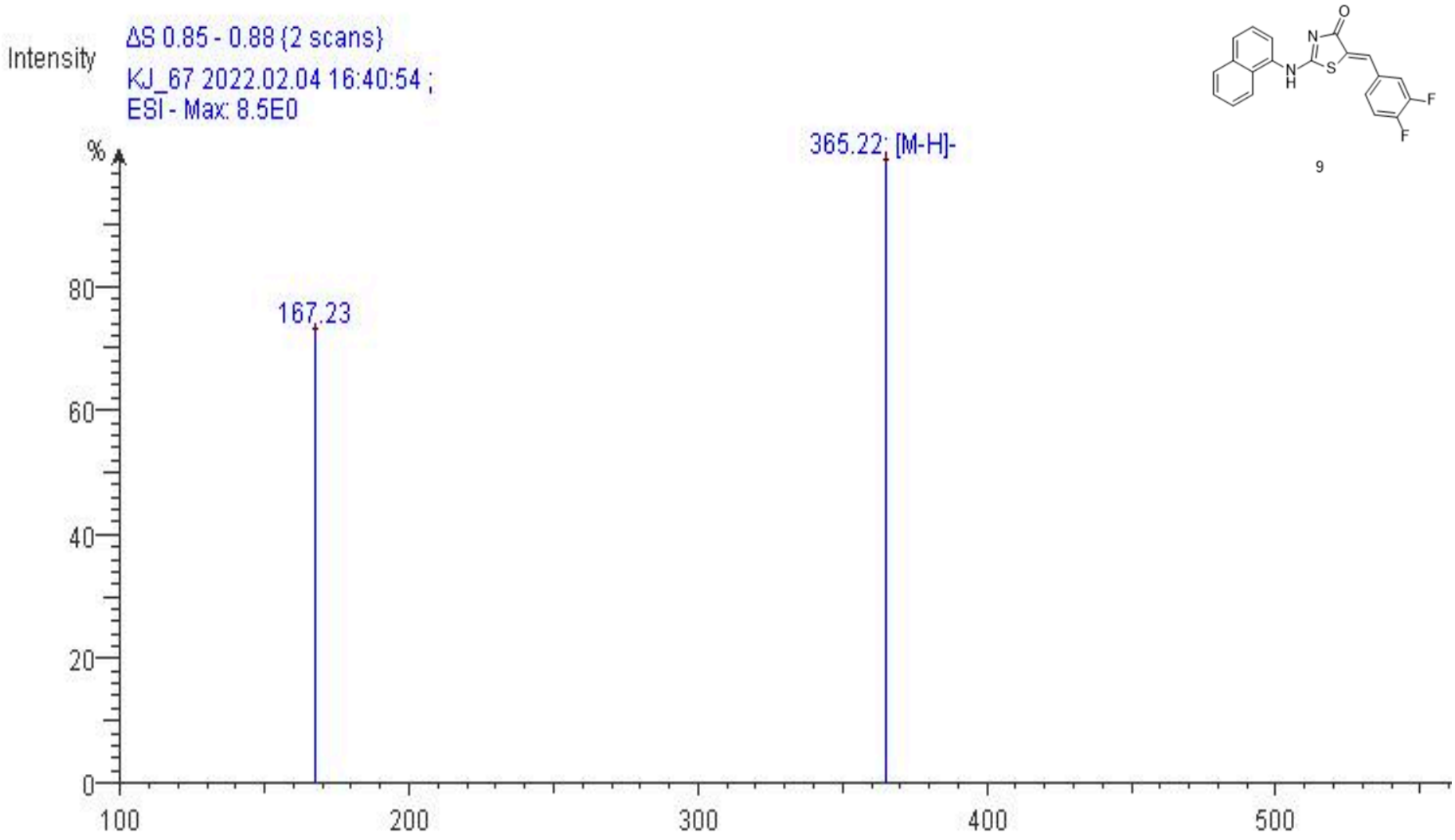


Figure S30. LRMS (ESI–) spectrum of analog **9**

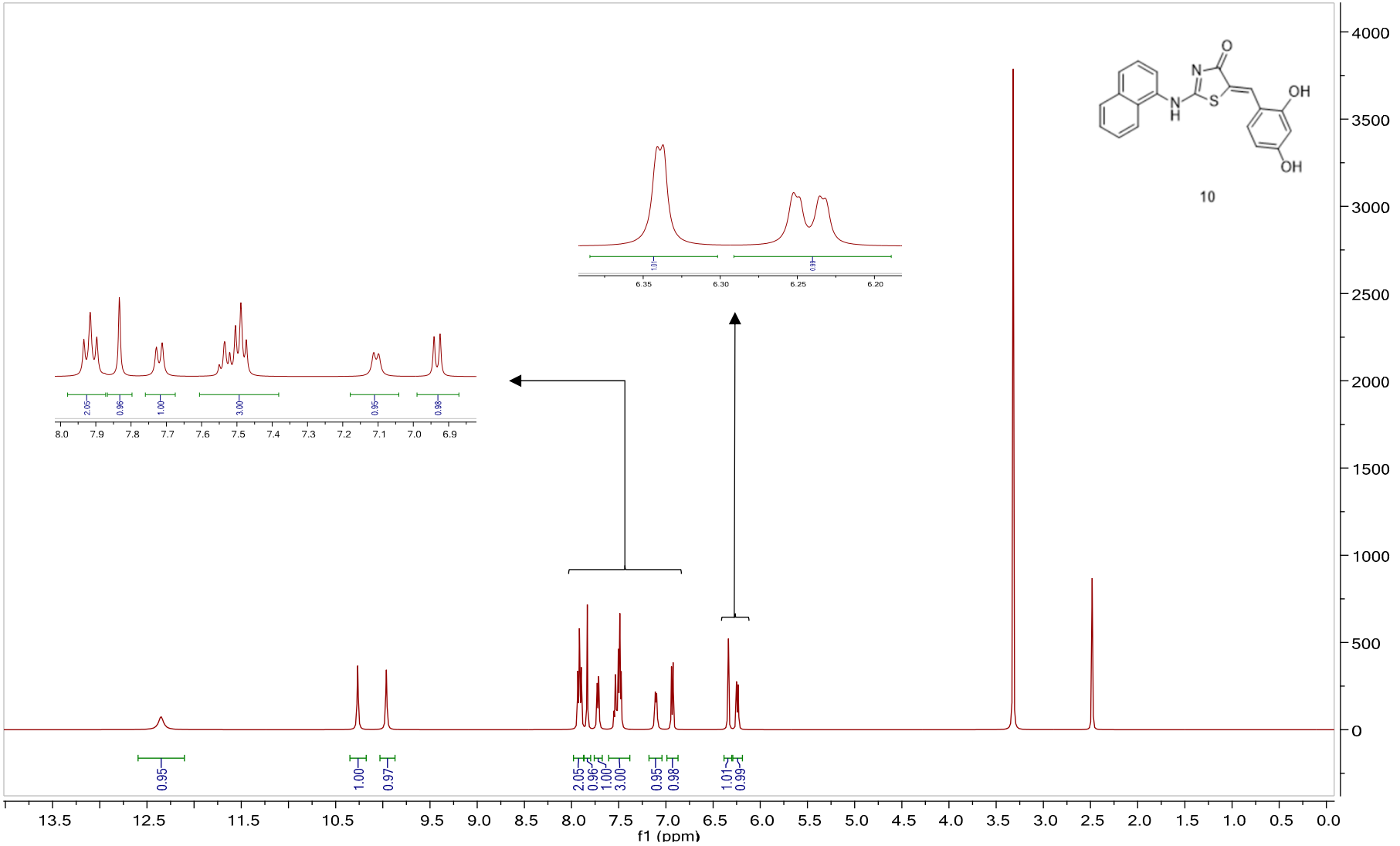


Figure S31. ^{1}H NMR spectrum of analog **10**

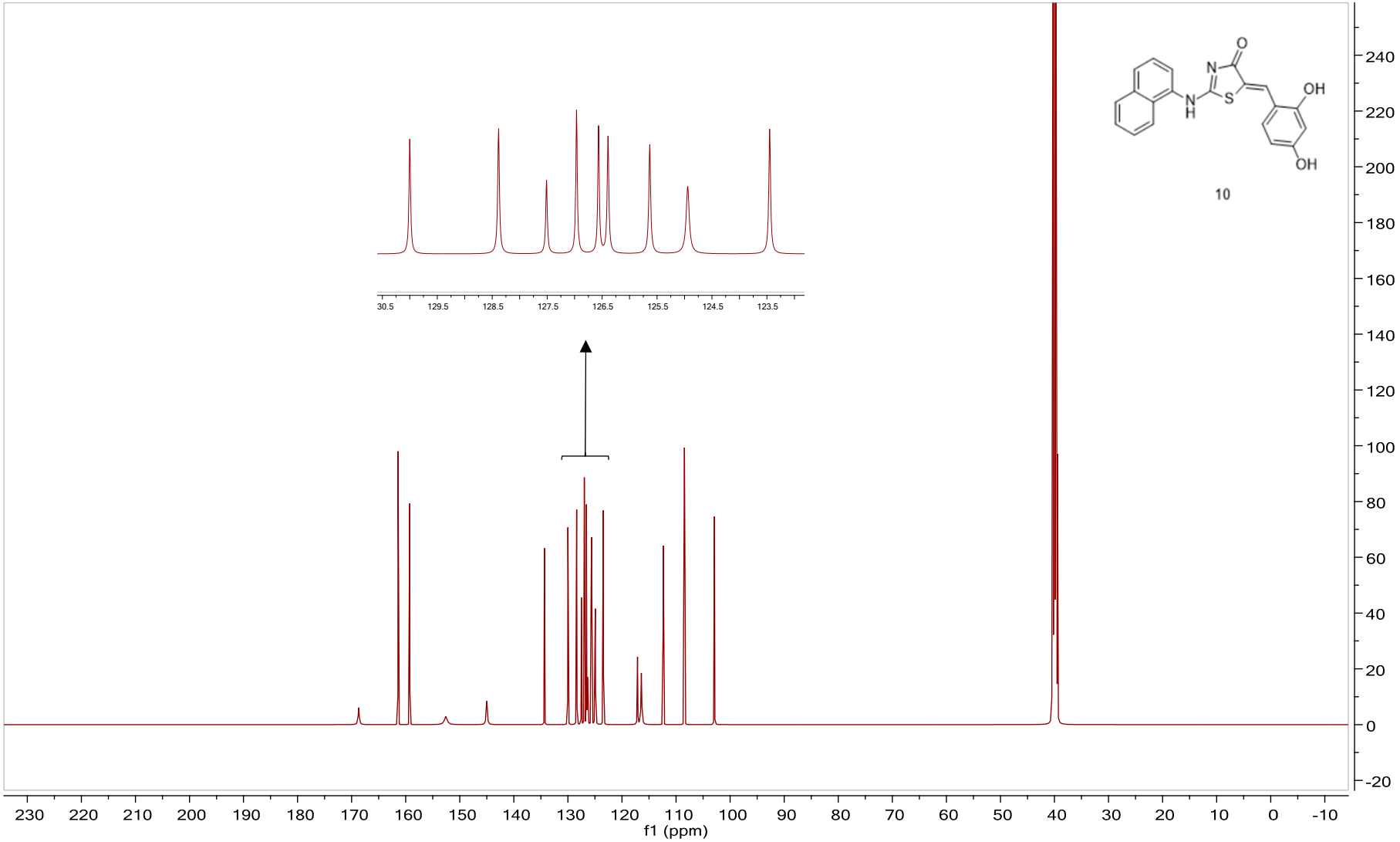


Figure S32. ^{13}C NMR spectrum of analog **10**

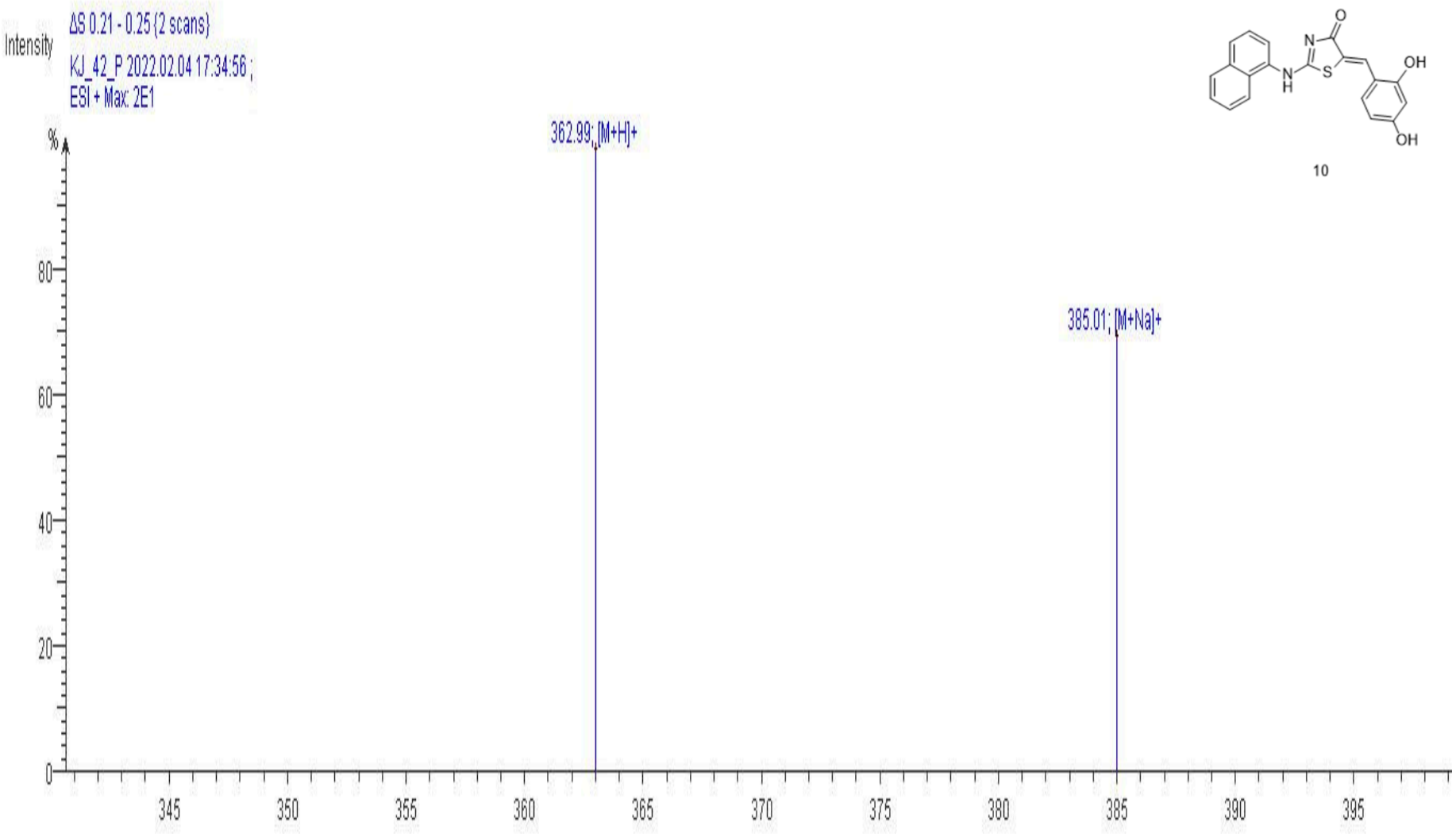


Figure S33. LRMS (ESI+) spectrum of analog **10**

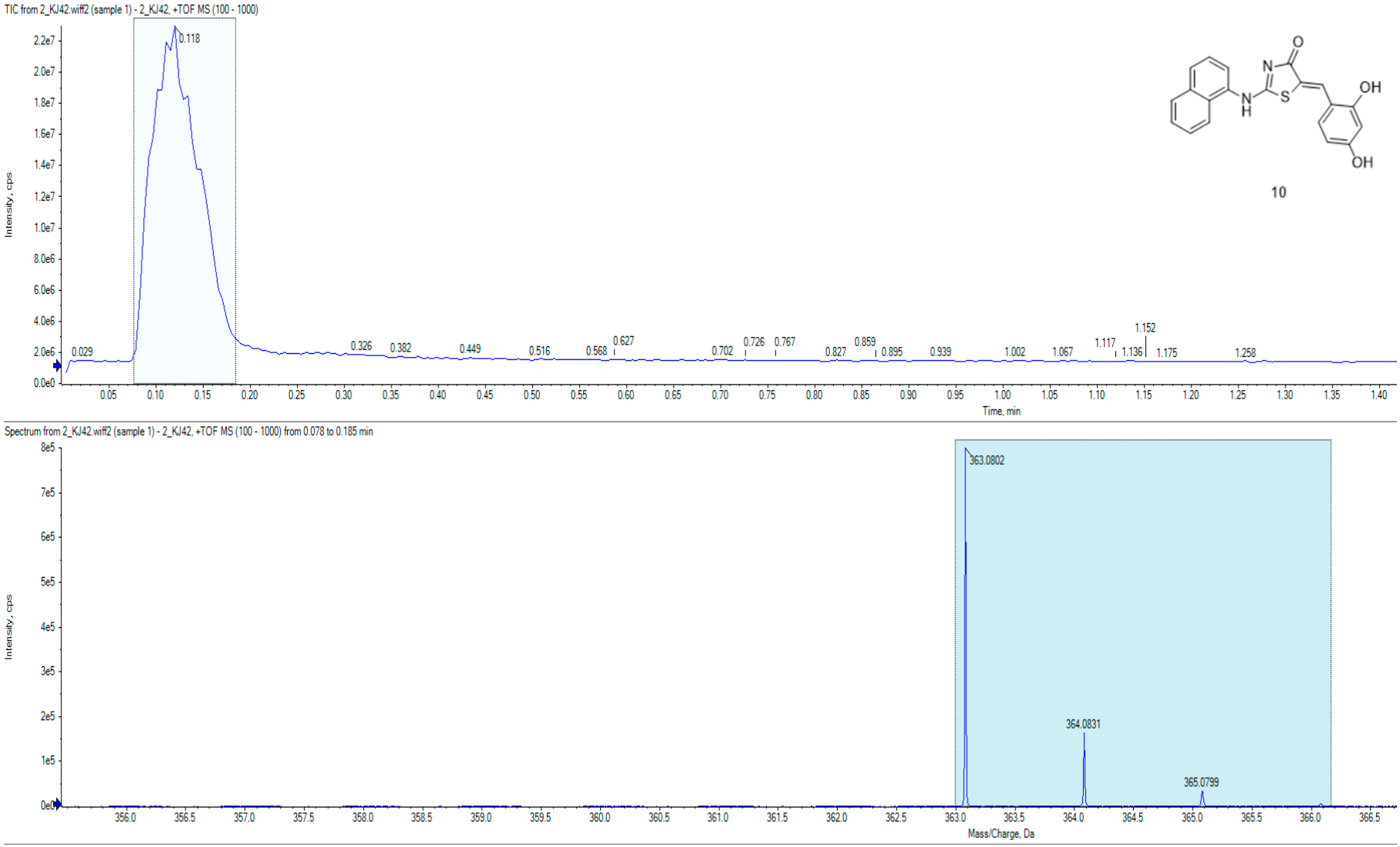
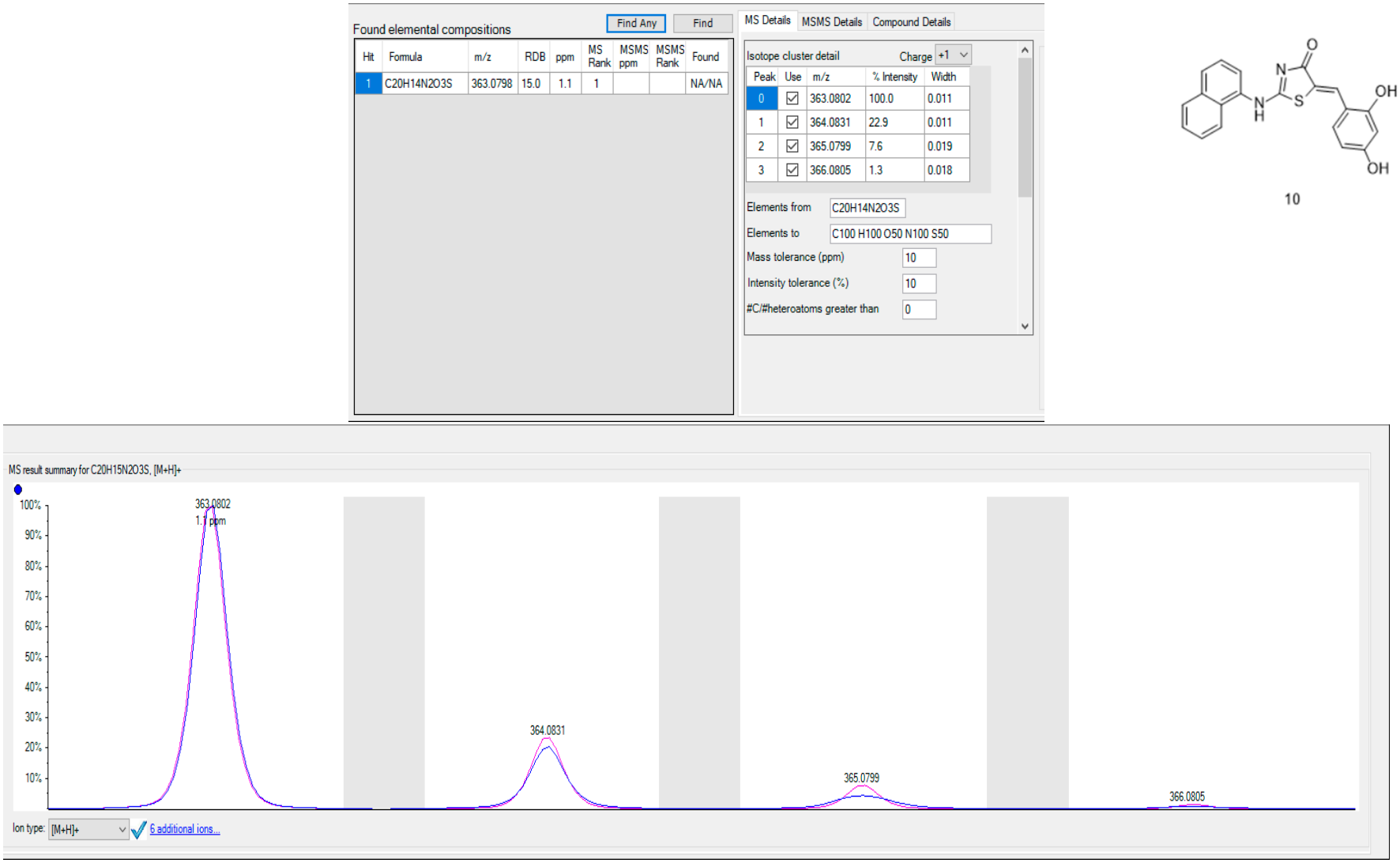


Figure S34-1. HRMS (ESI+) spectrum of analog **10**



10

Figure S34-2. HRMS (ESI+) spectrum of analog **10**

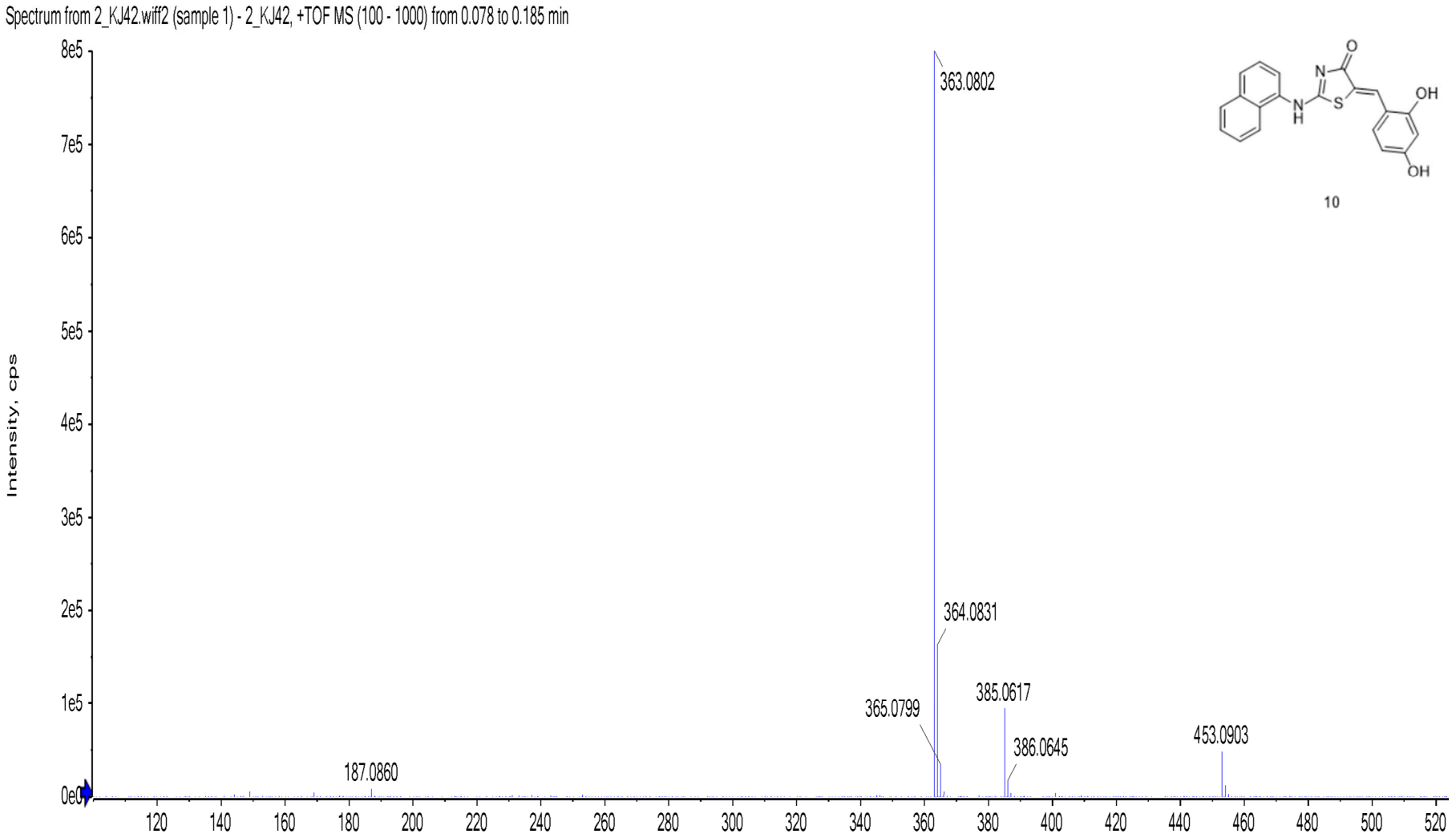


Figure S34-3. HRMS (ESI+) spectrum of analog **10**

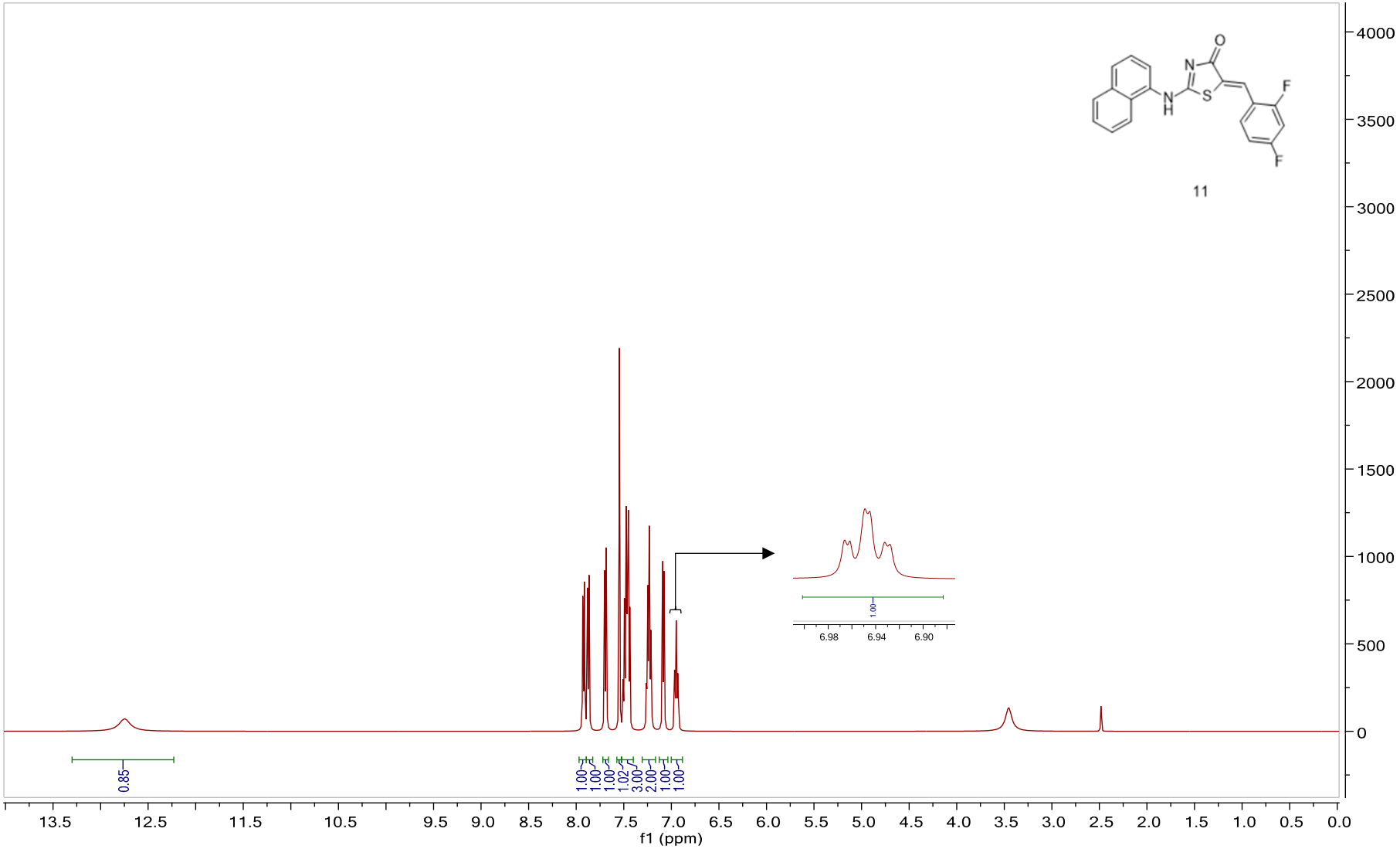


Figure S35. ^{1}H NMR spectrum of analog **11**

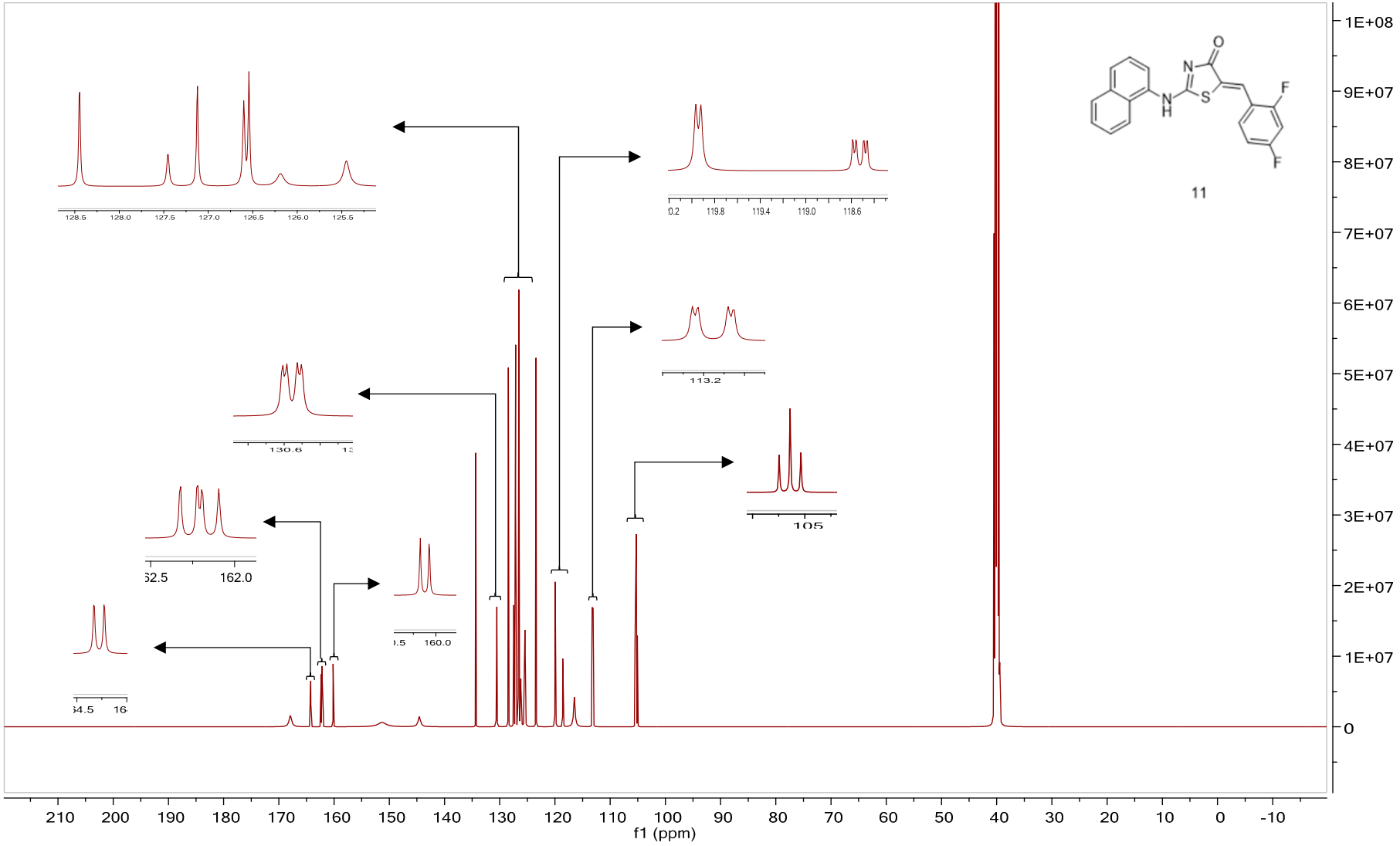


Figure S36. ^{13}C NMR spectrum of analog **11**

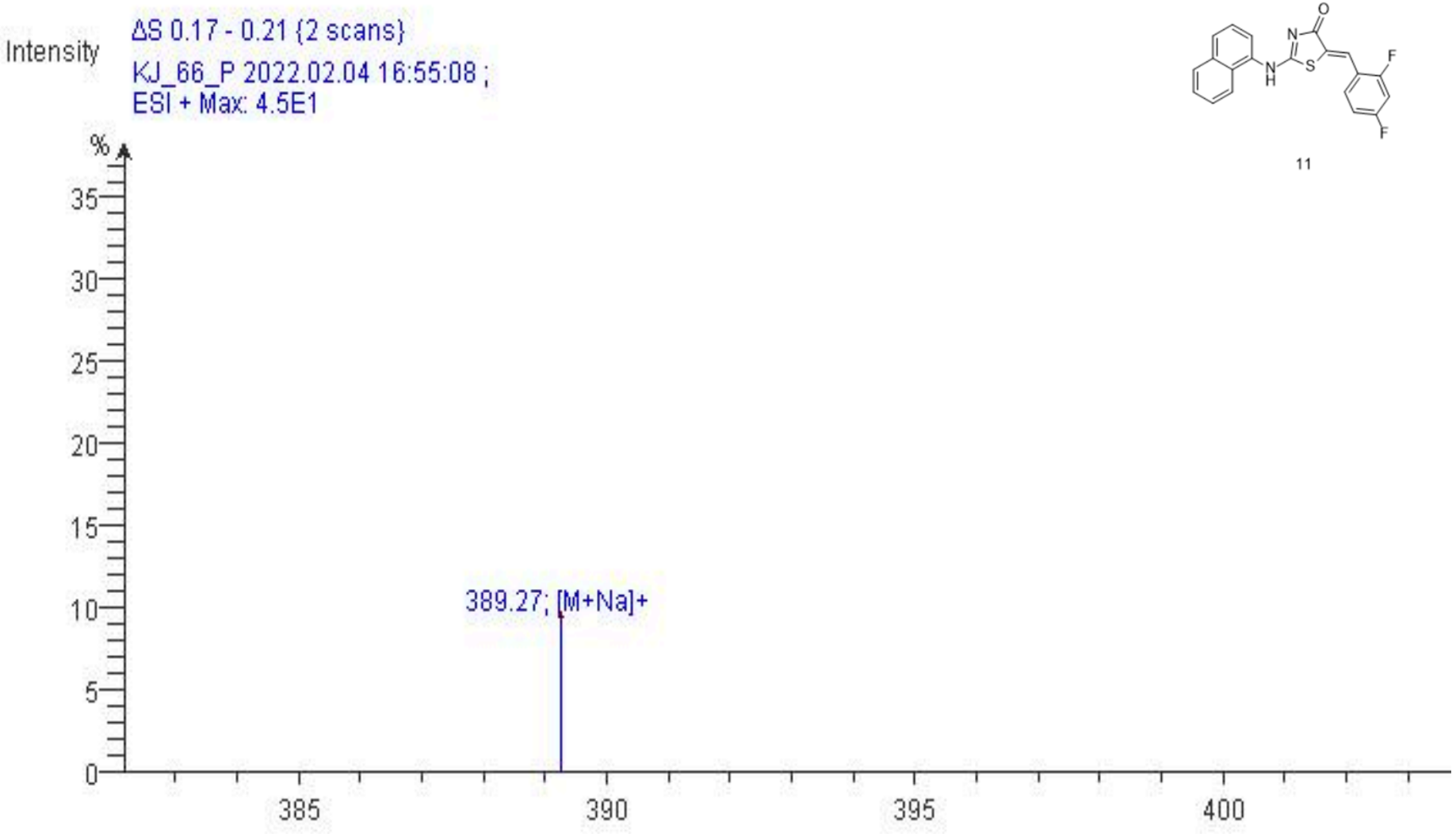


Figure S37. LRMS (ESI+) spectrum of analog **11**

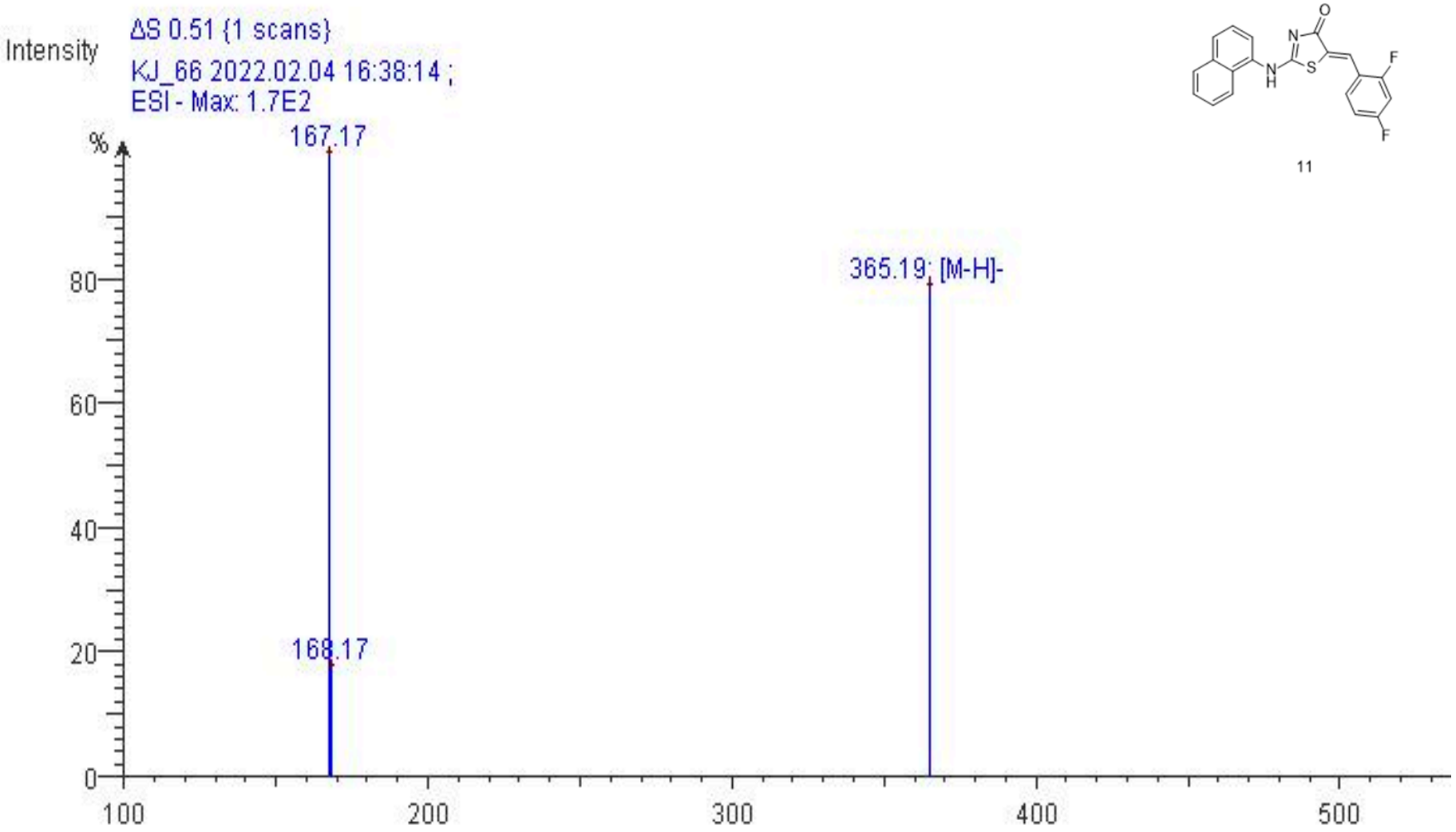


Figure S38. LRMS (ESI–) spectrum of analog **11**

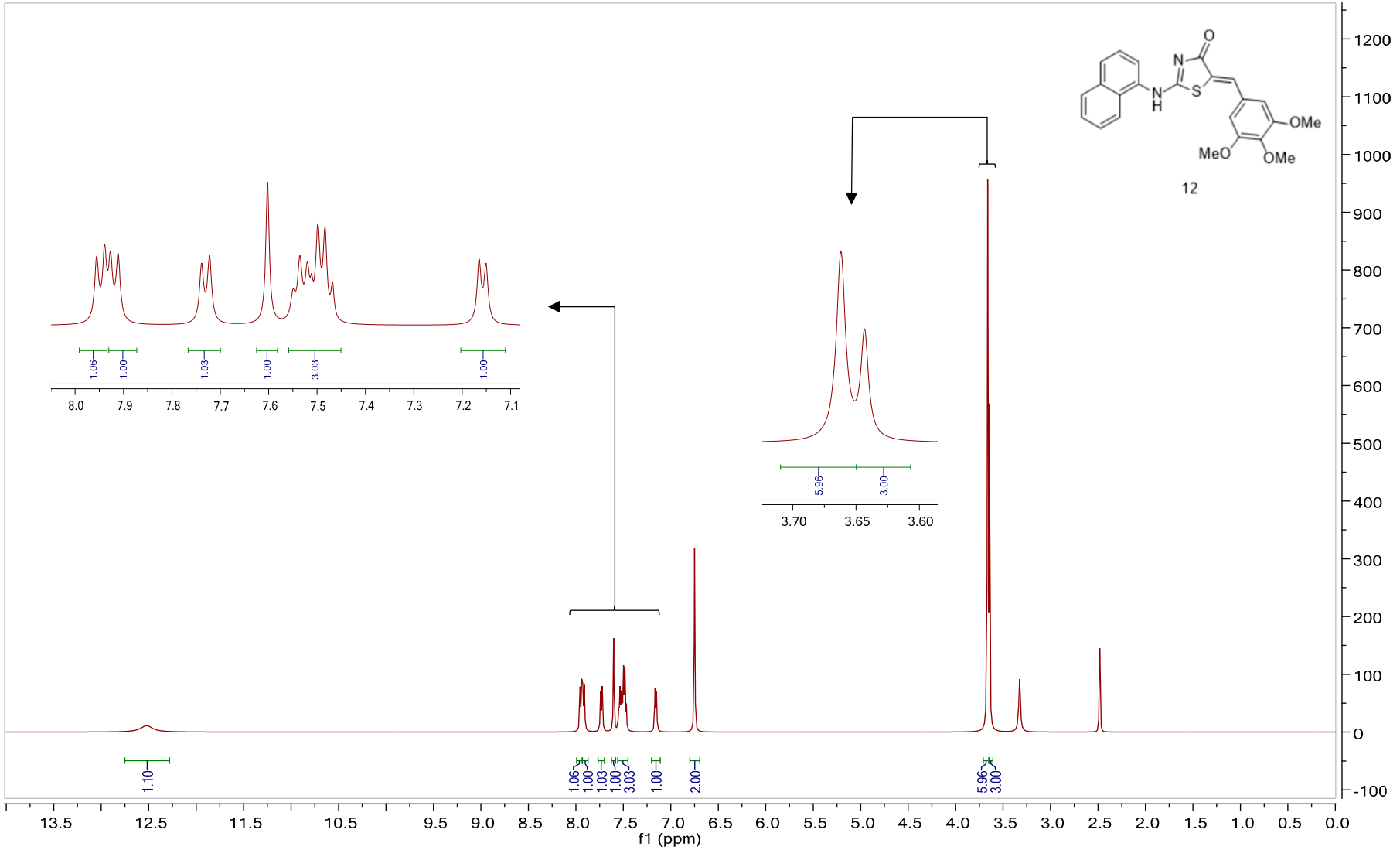


Figure S39. ^{1}H NMR spectrum of analog **12**

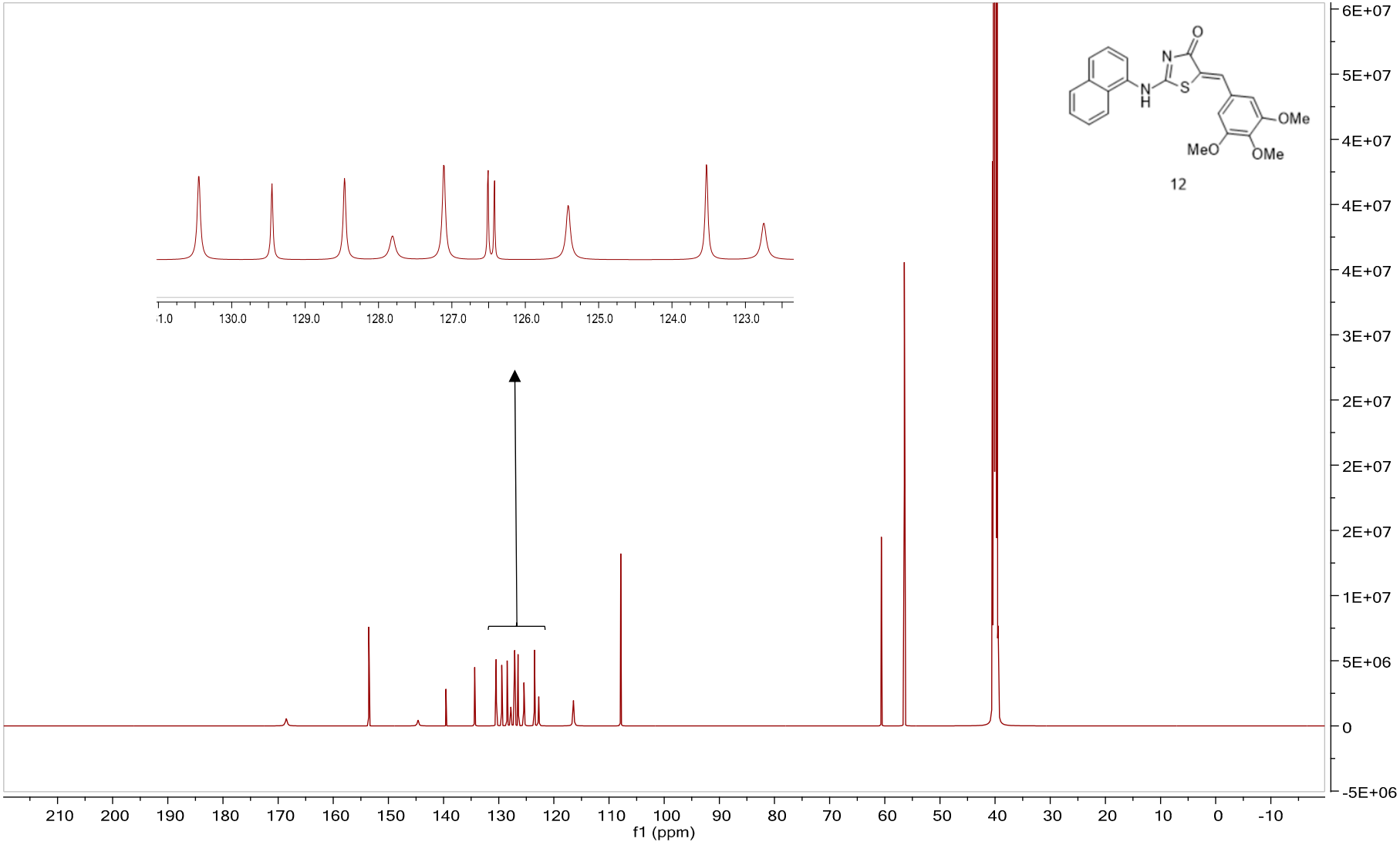


Figure S40. ^{13}C NMR spectrum of analog **12**

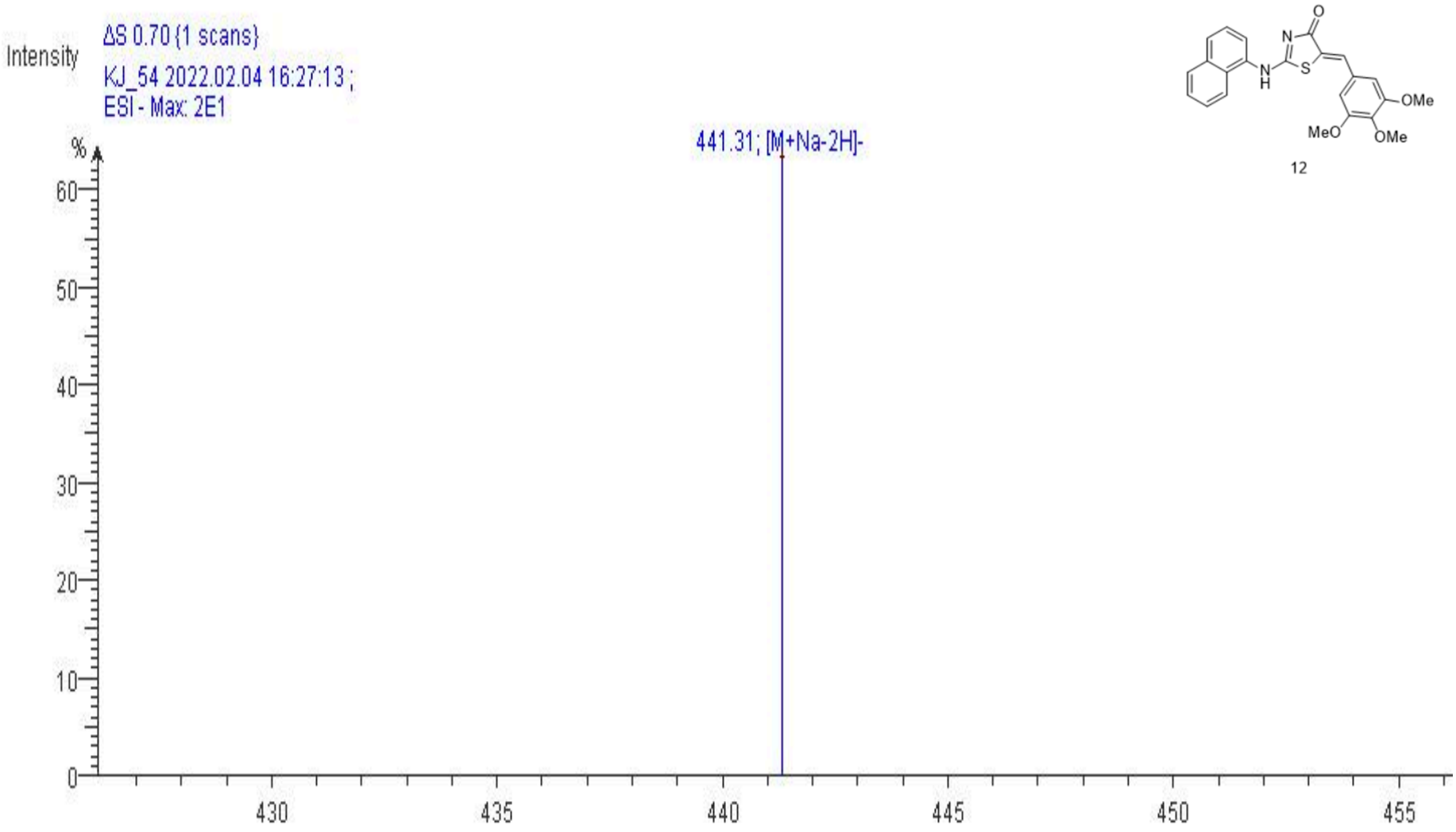


Figure S41. LRMS (ESI–) spectrum of analog **12**

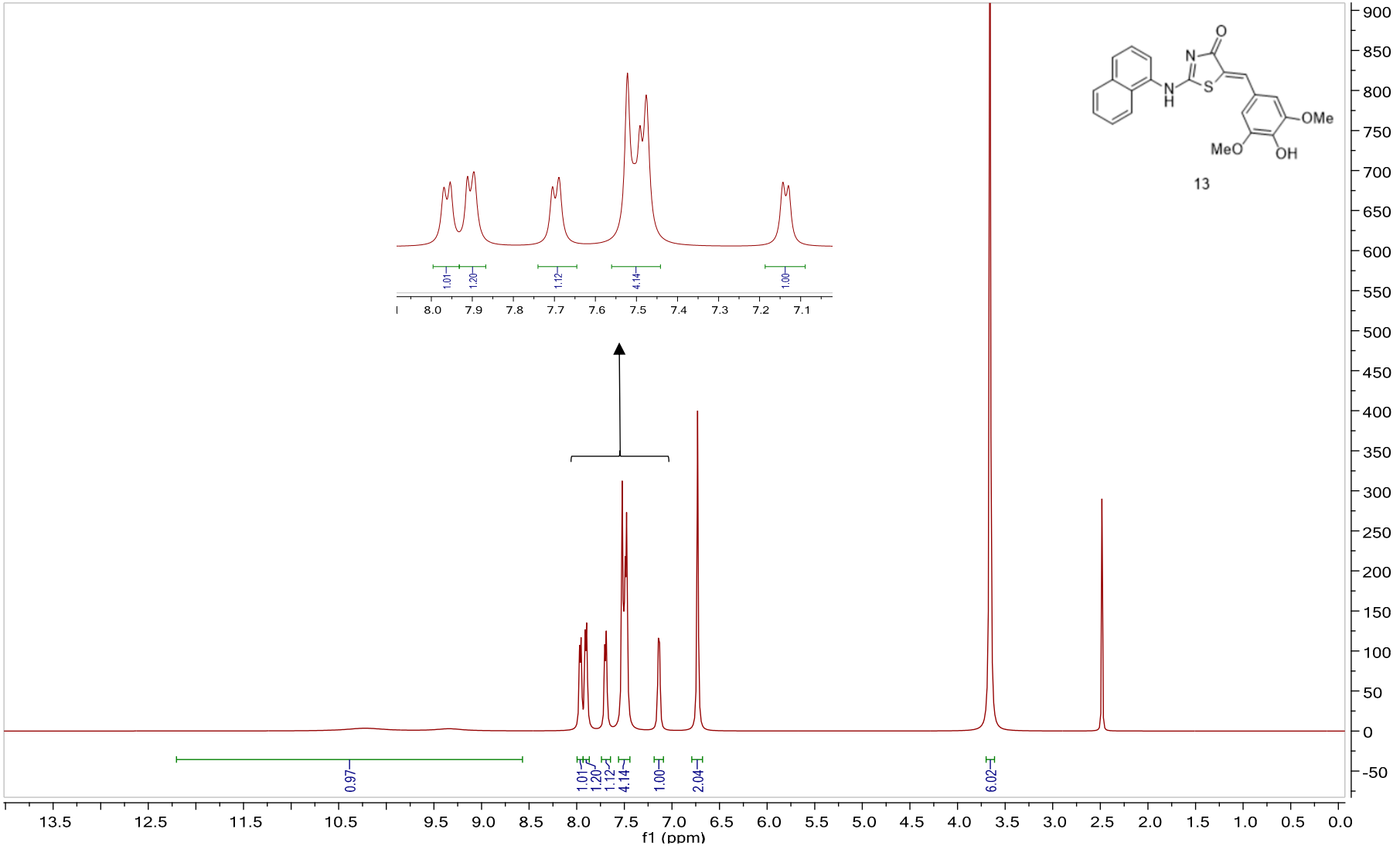


Figure S42. ^{1}H NMR spectrum of analog **13**

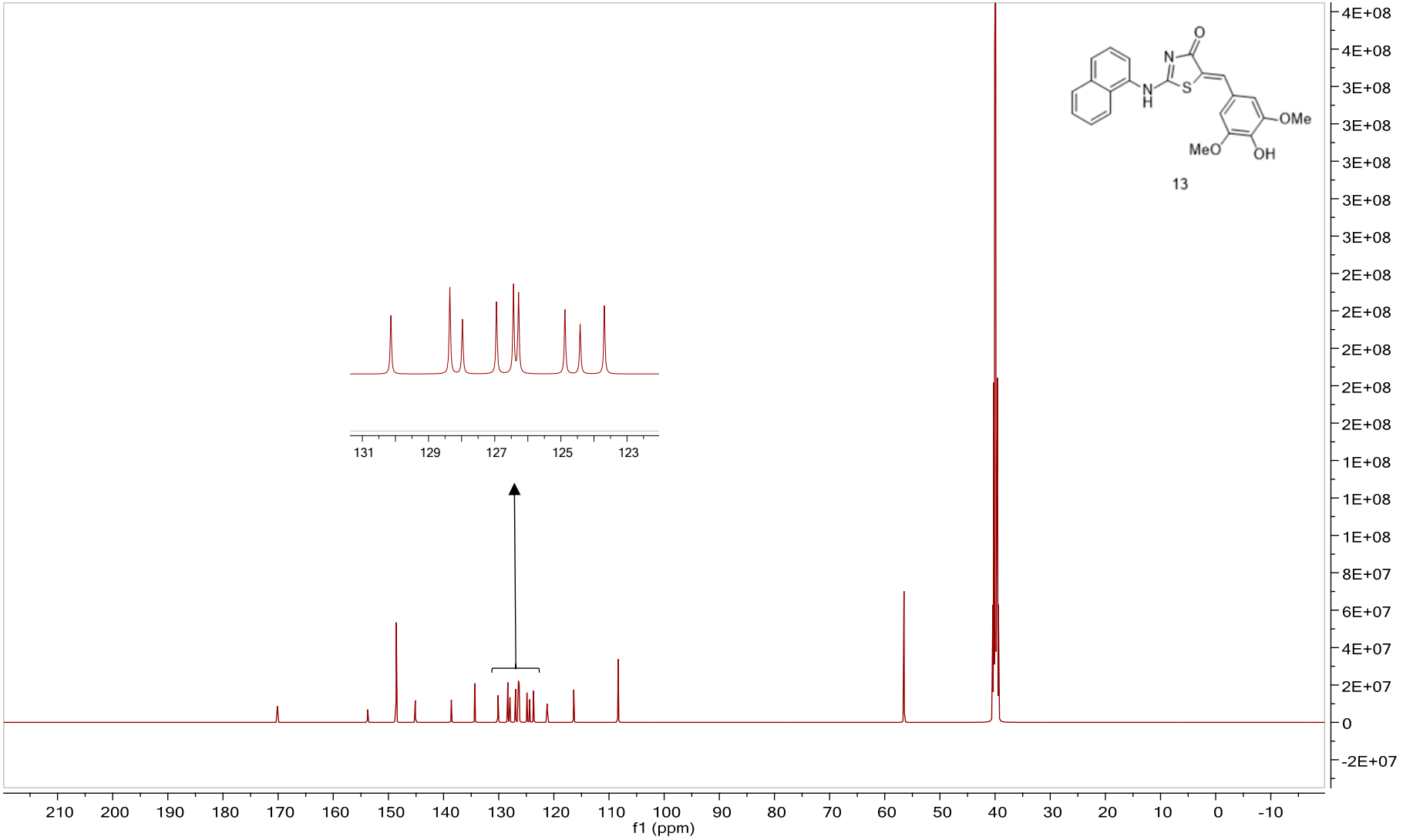


Figure S43. ^{13}C NMR spectrum of analog **13**

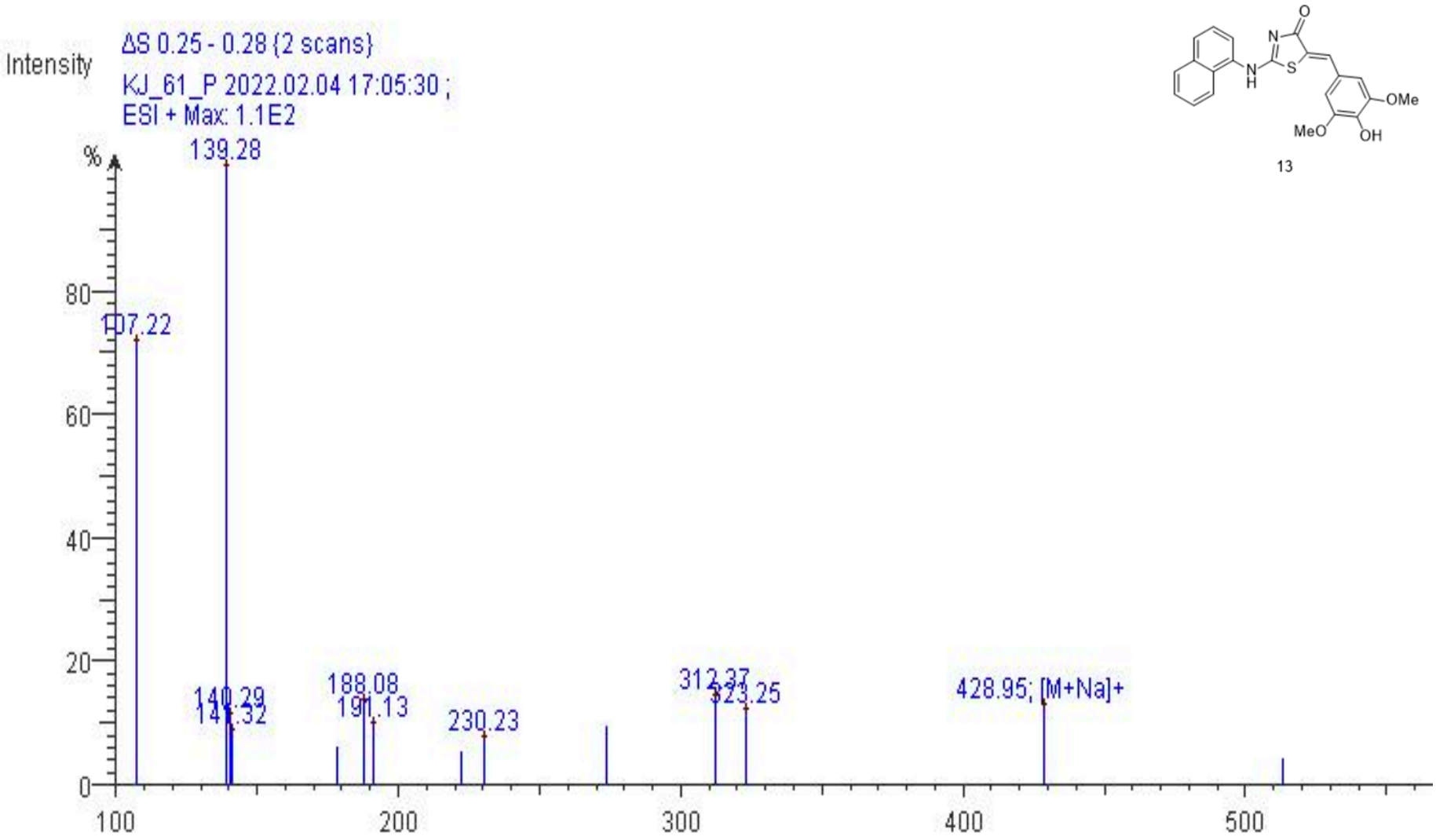


Figure S44. LRMS (ESI+) spectrum of analog **13**

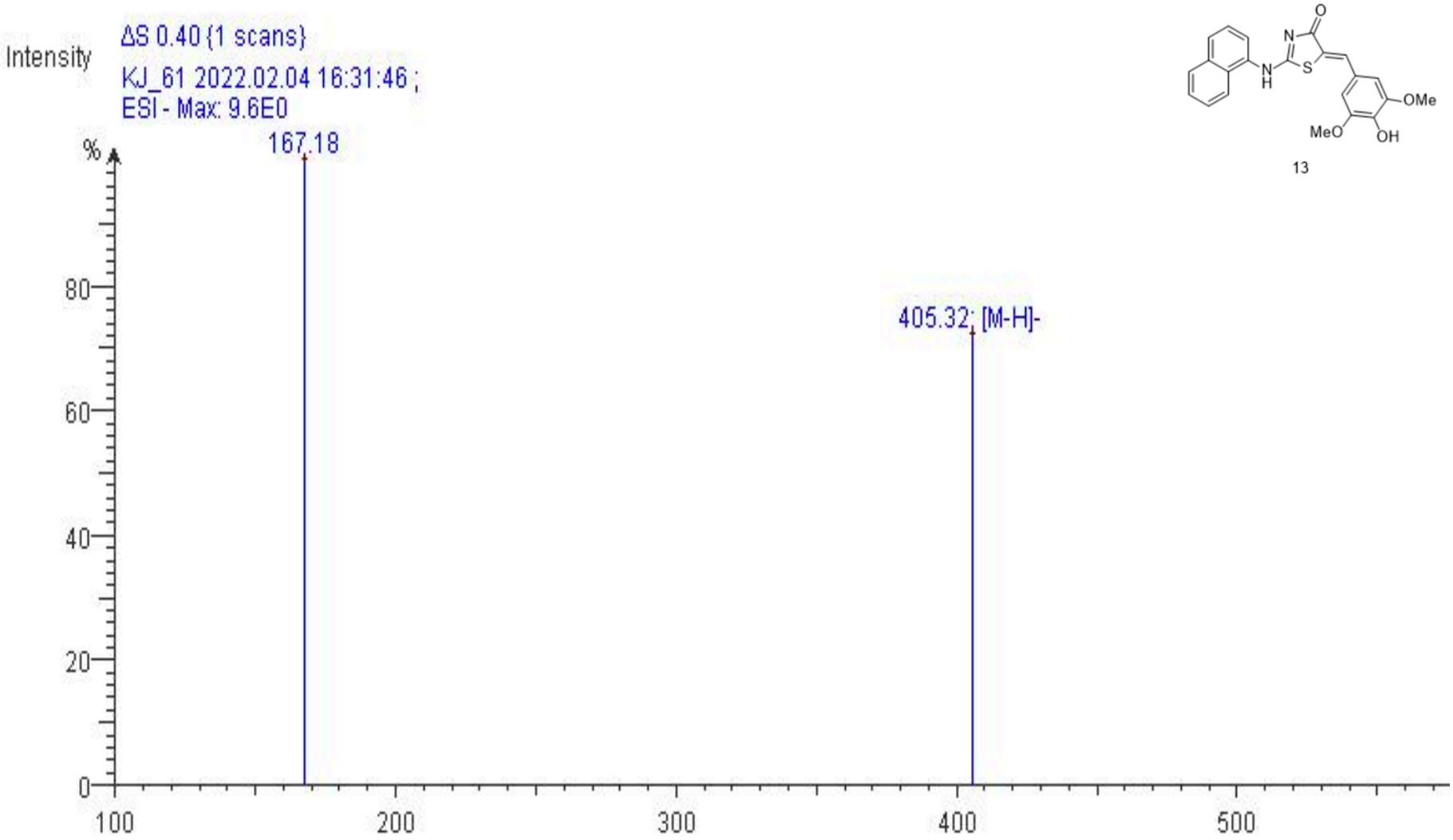


Figure S45. LRMS (ESI–) spectrum of analog **13**

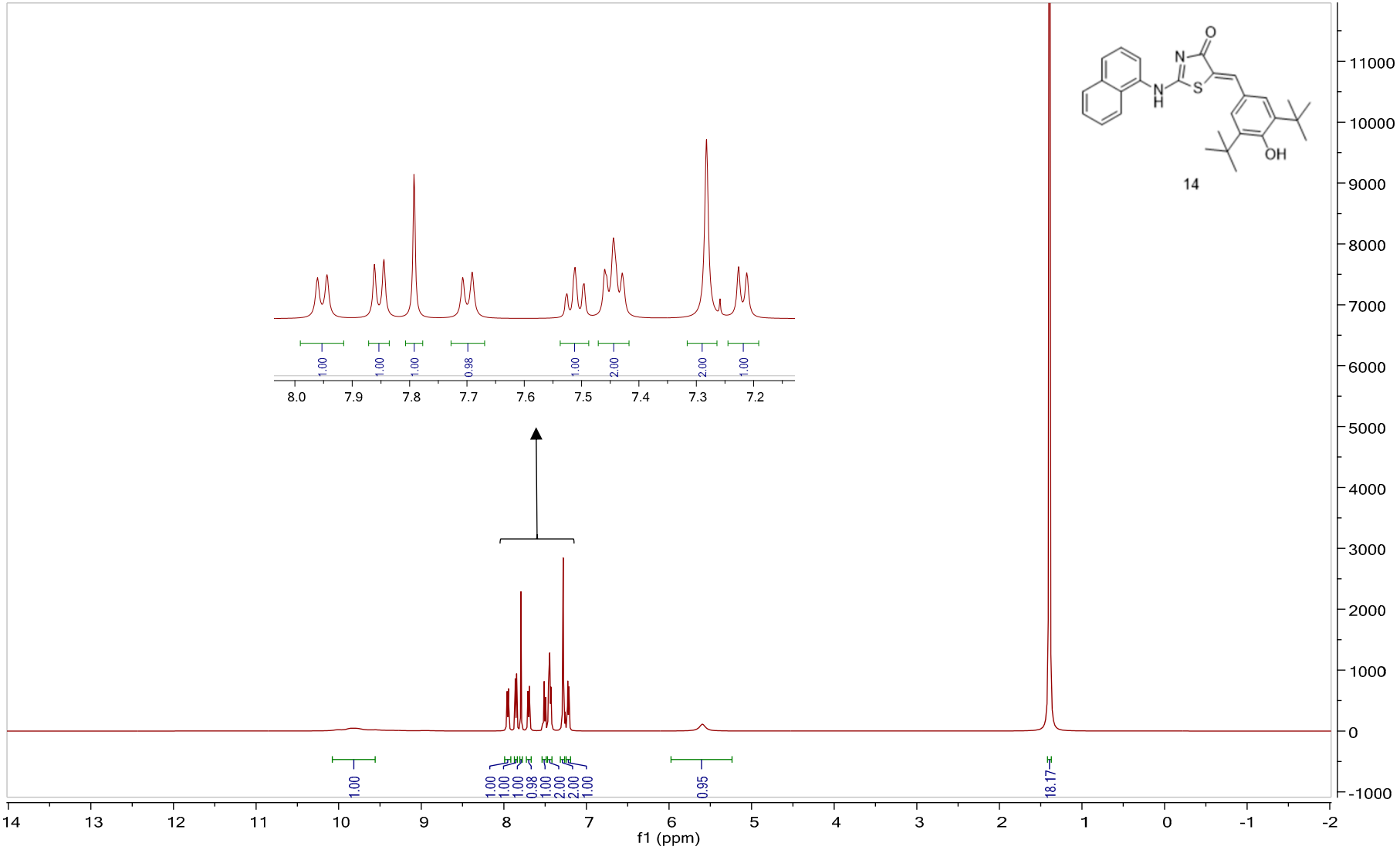


Figure S46. ^{1}H NMR spectrum of analog **14**

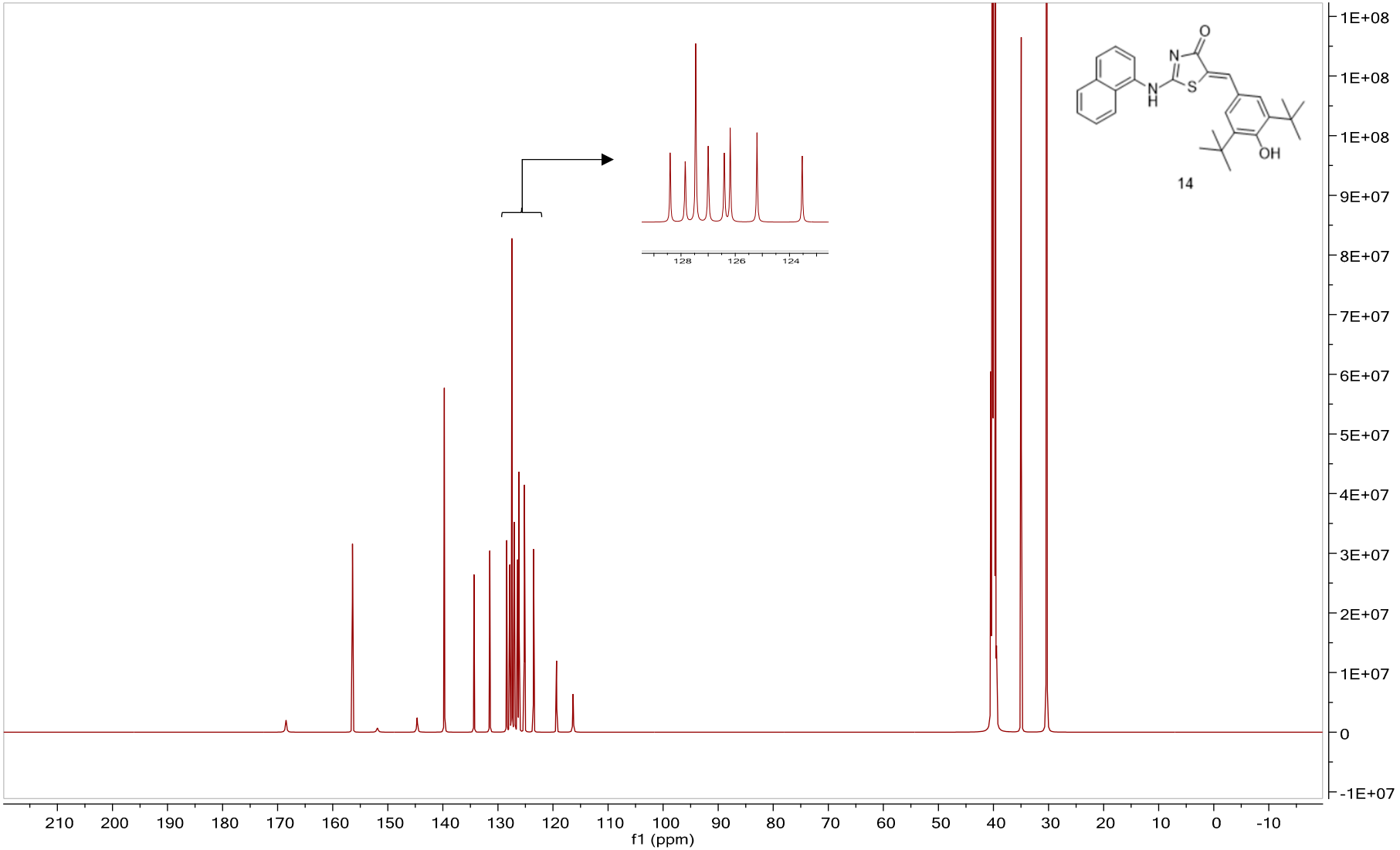


Figure S47. ^{13}C NMR spectrum of analog **14**

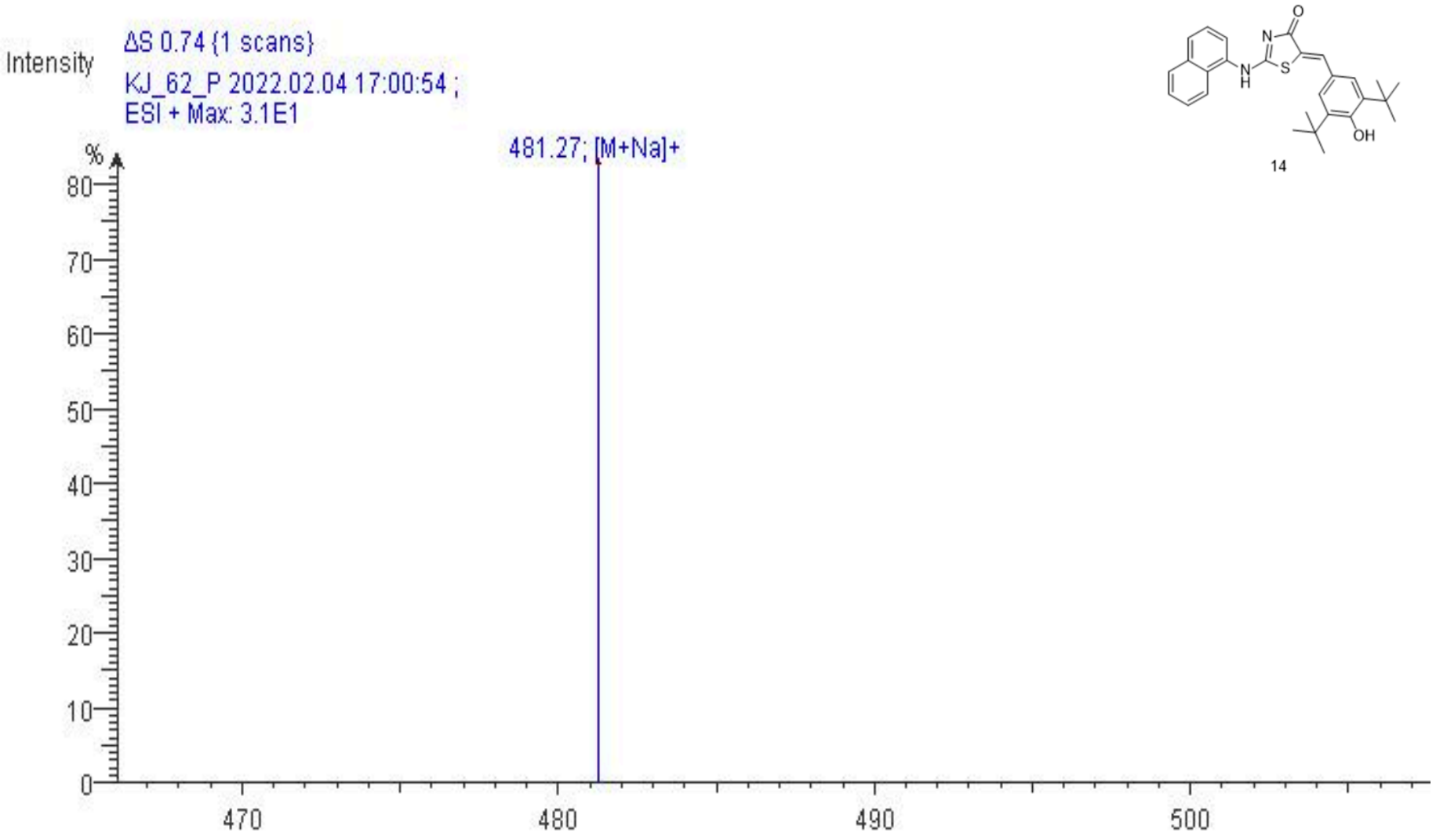


Figure S48. LRMS (ESI+) spectrum of analog **14**

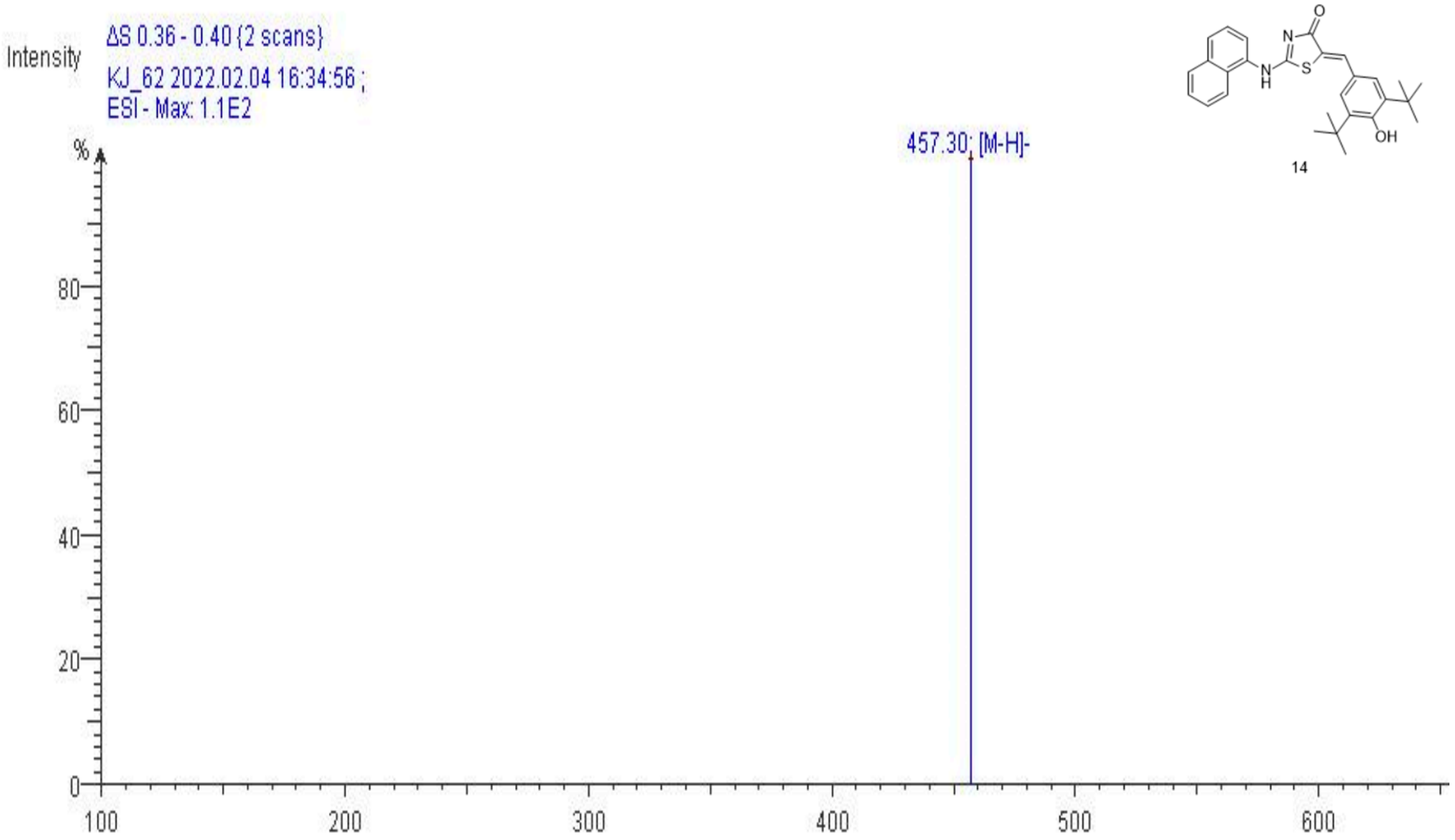


Figure S49. LRMS (ESI–) spectrum of analog **14**

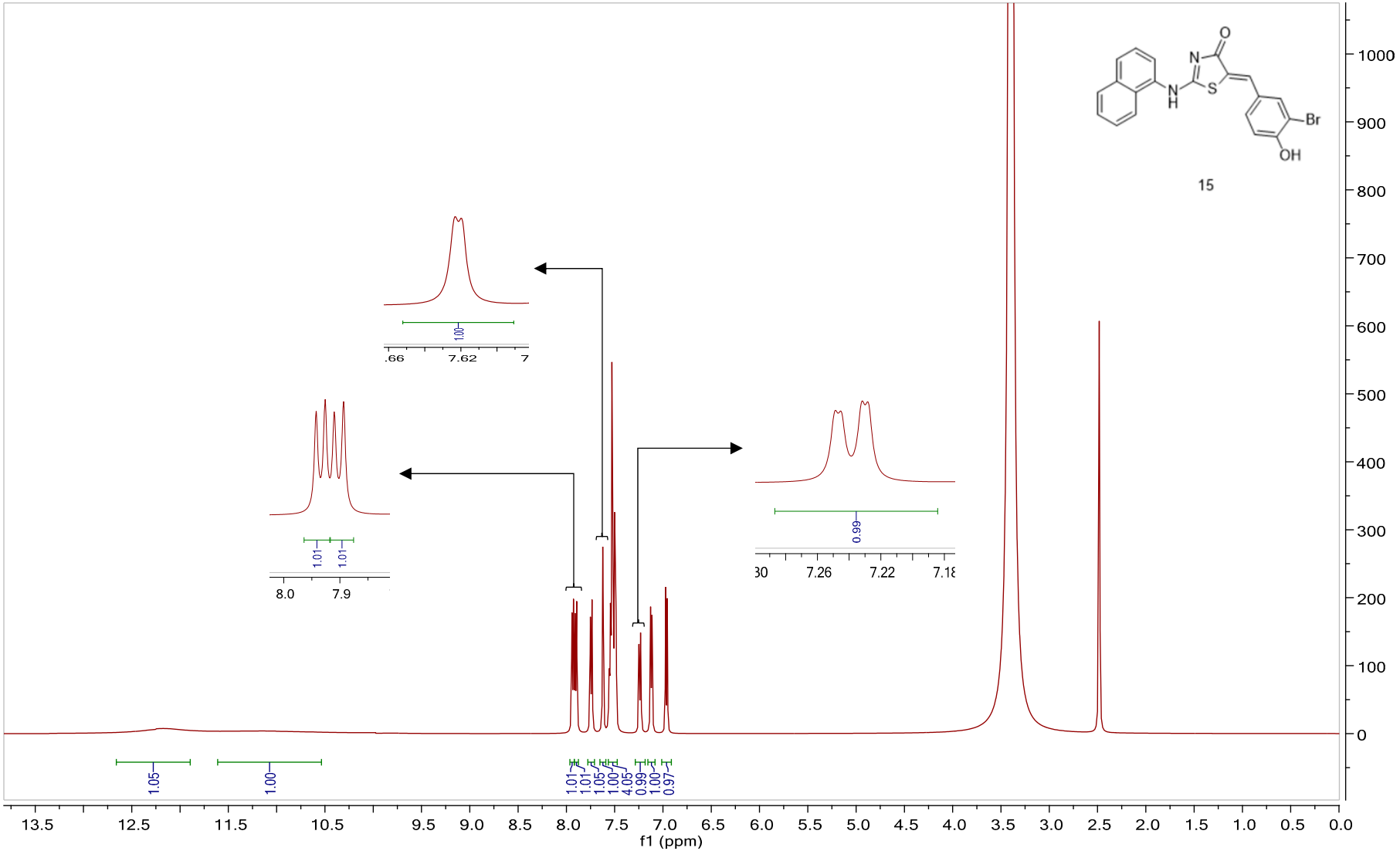


Figure S50. ^{1}H NMR spectrum of analog **15**

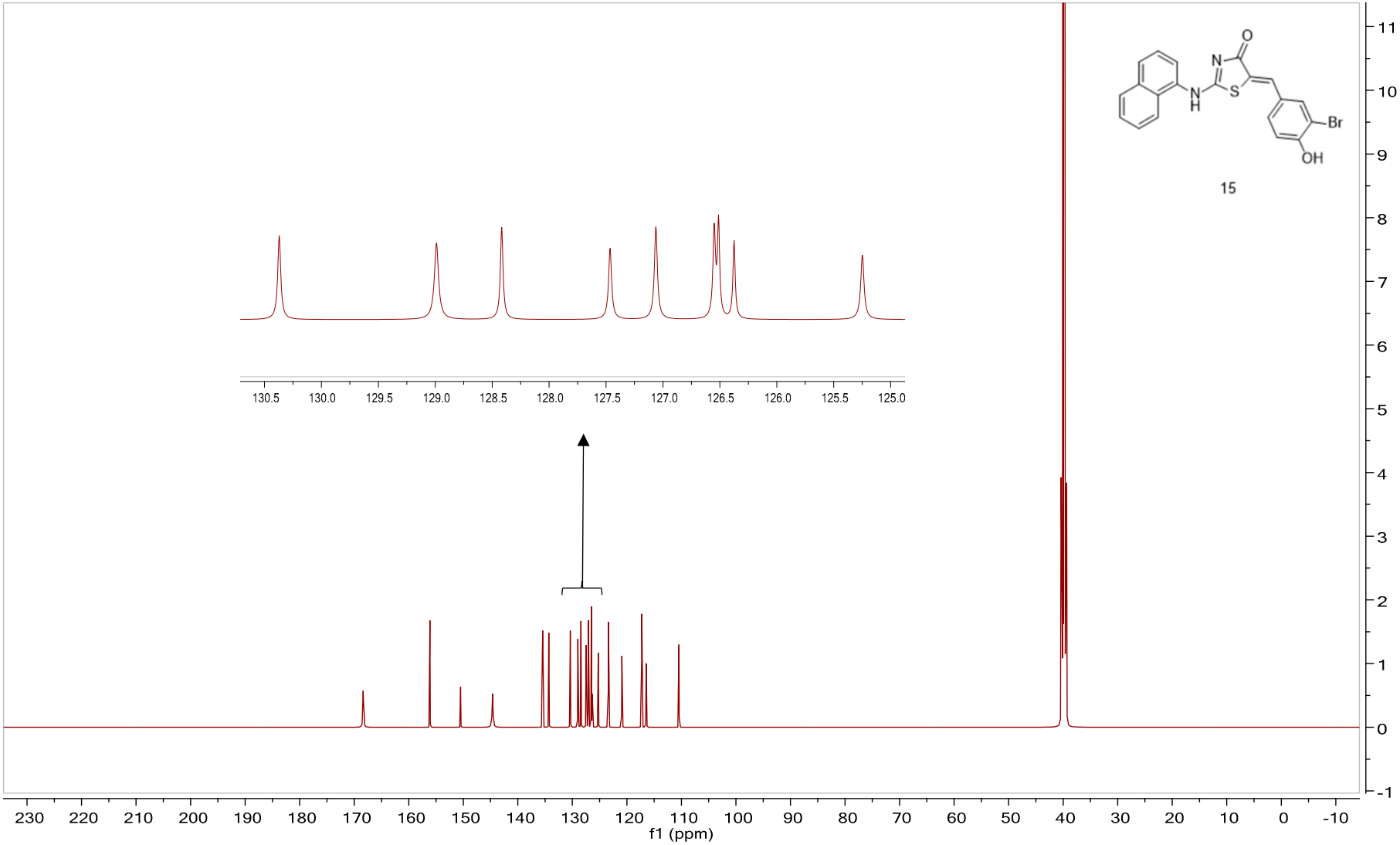


Figure S51. ^{13}C NMR spectrum of analog **15**

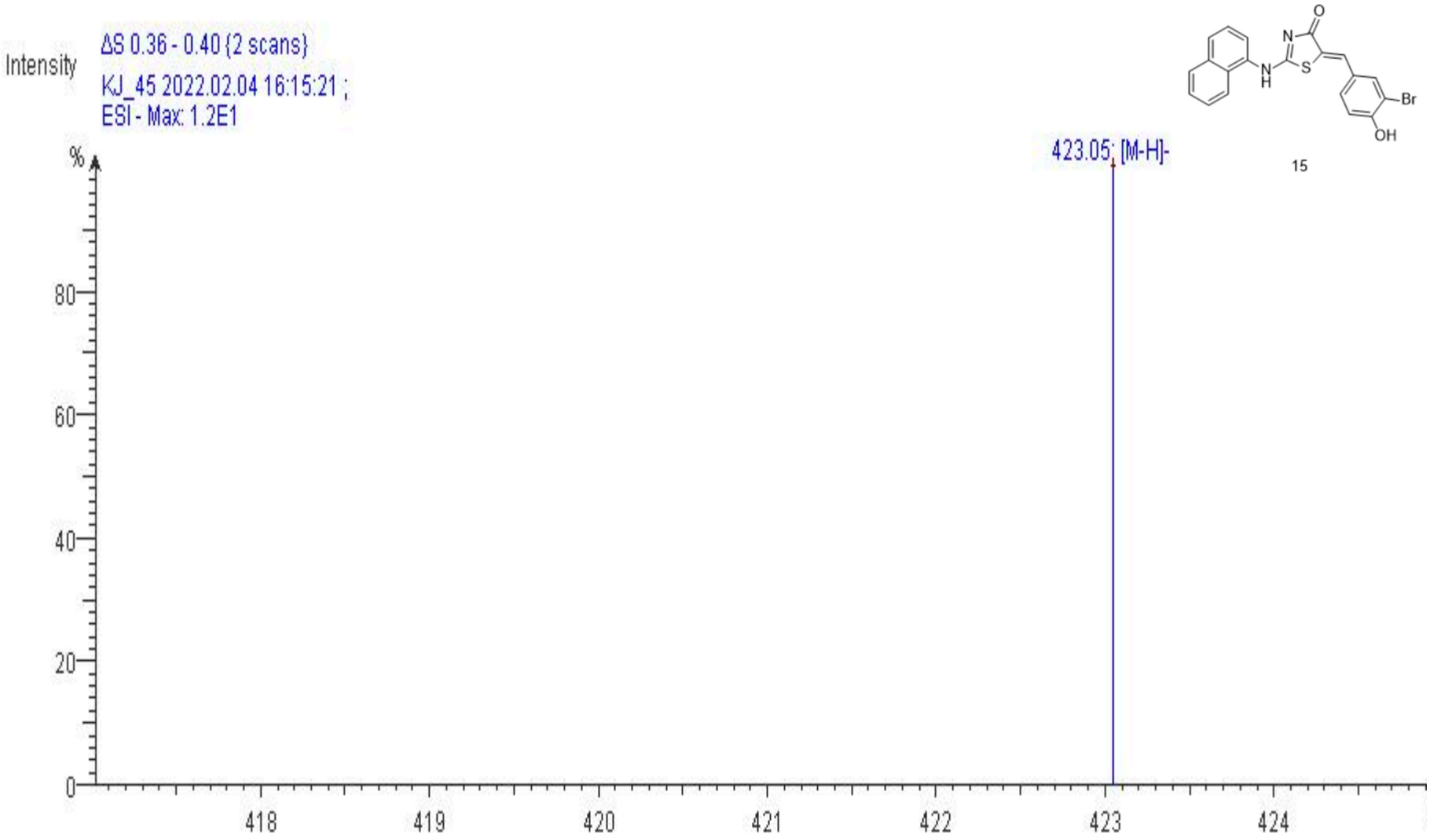


Figure S52. LRMS (ESI–) spectrum of analog **15**

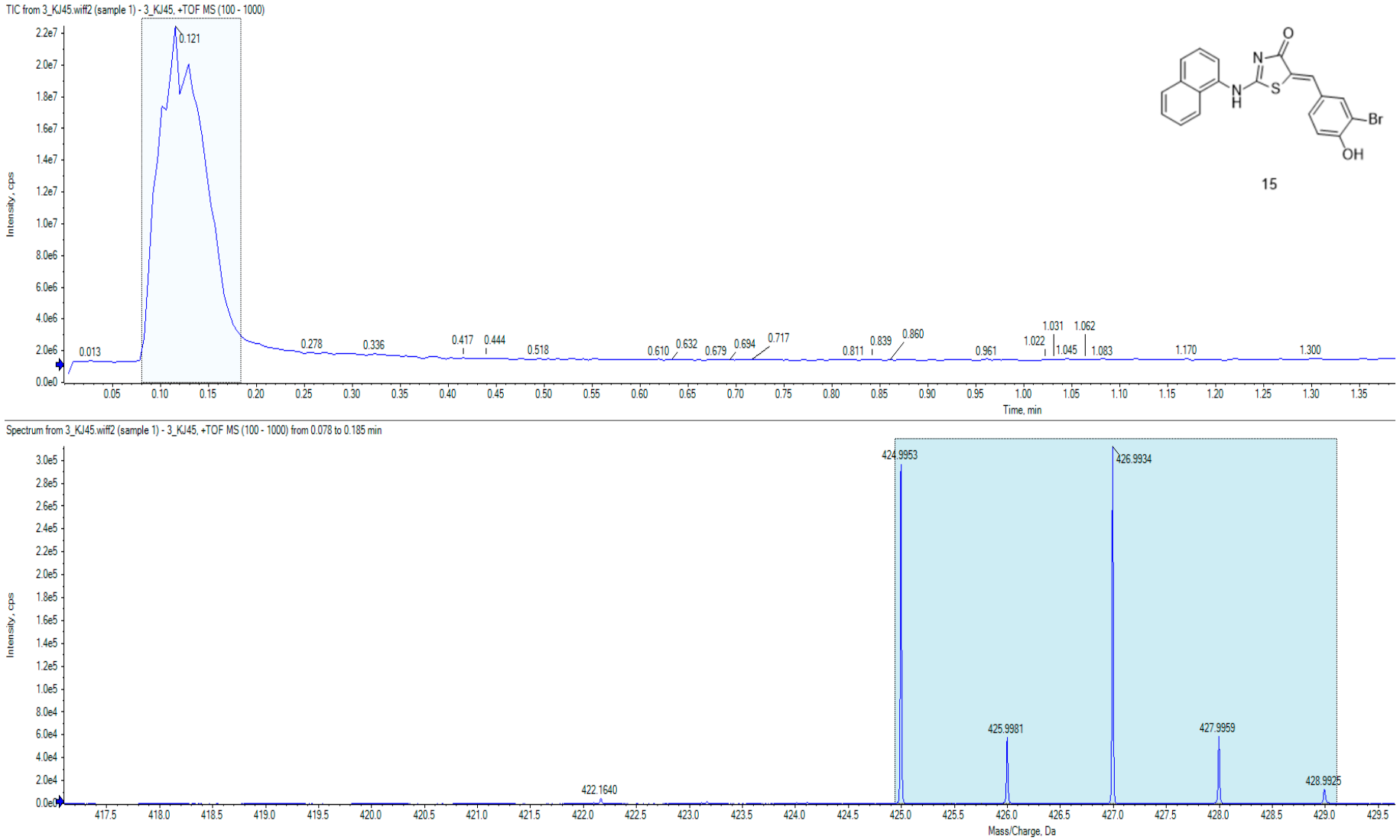
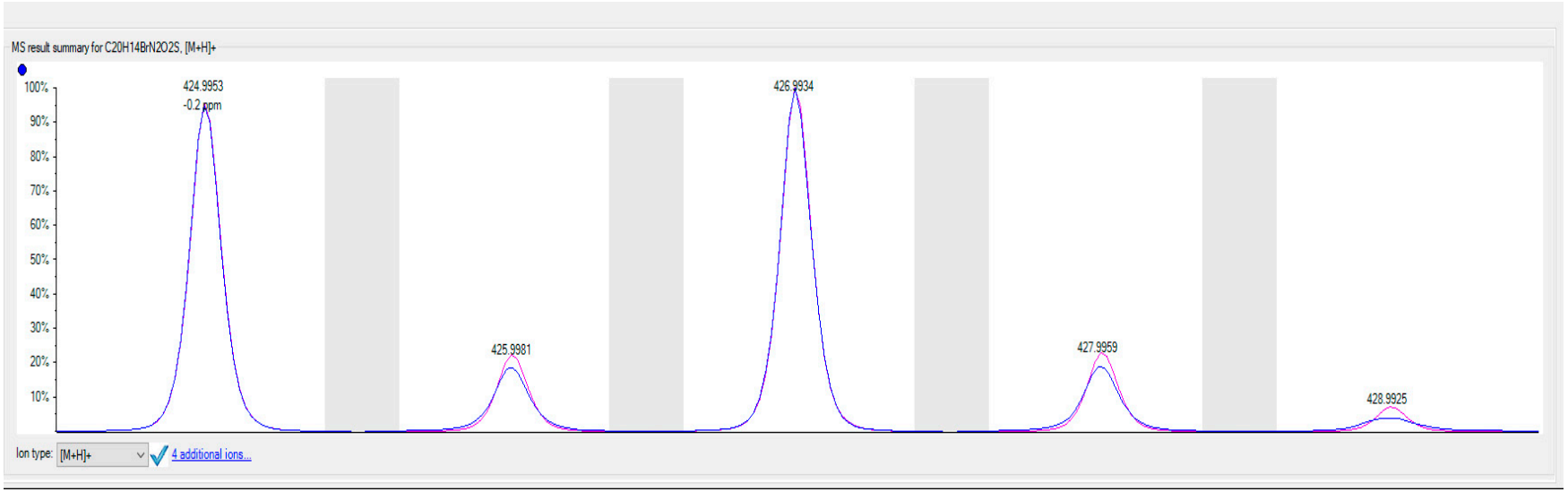
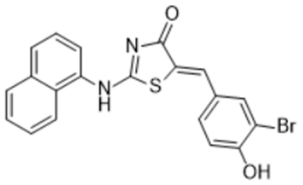


Figure S53-1. HRMS (ESI+) spectrum of analog **15**





15

Figure S53-2. HRMS (ESI+) spectrum of analog **15**

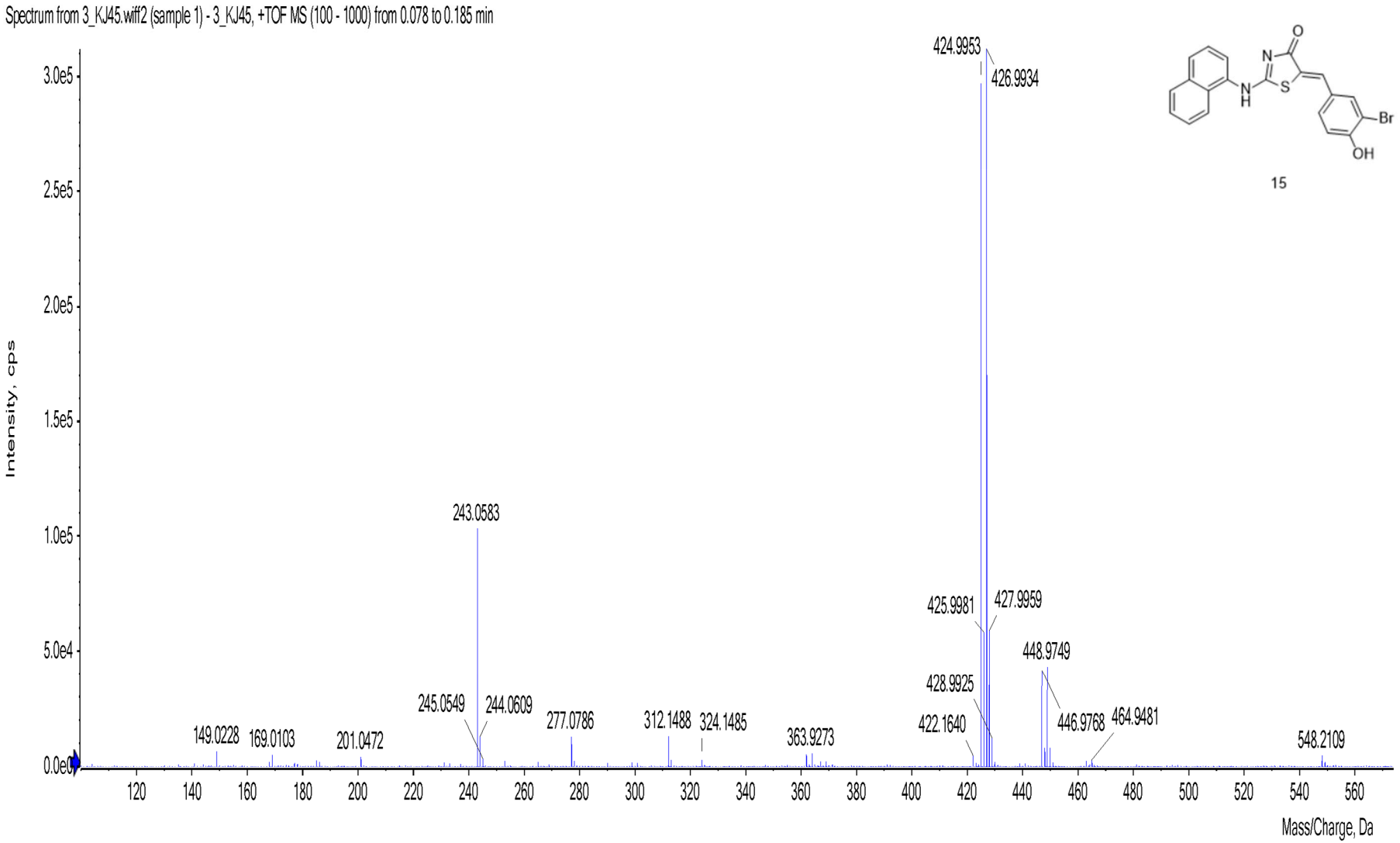


Figure S53-3. HRMS (ESI+) spectrum of analog **15**

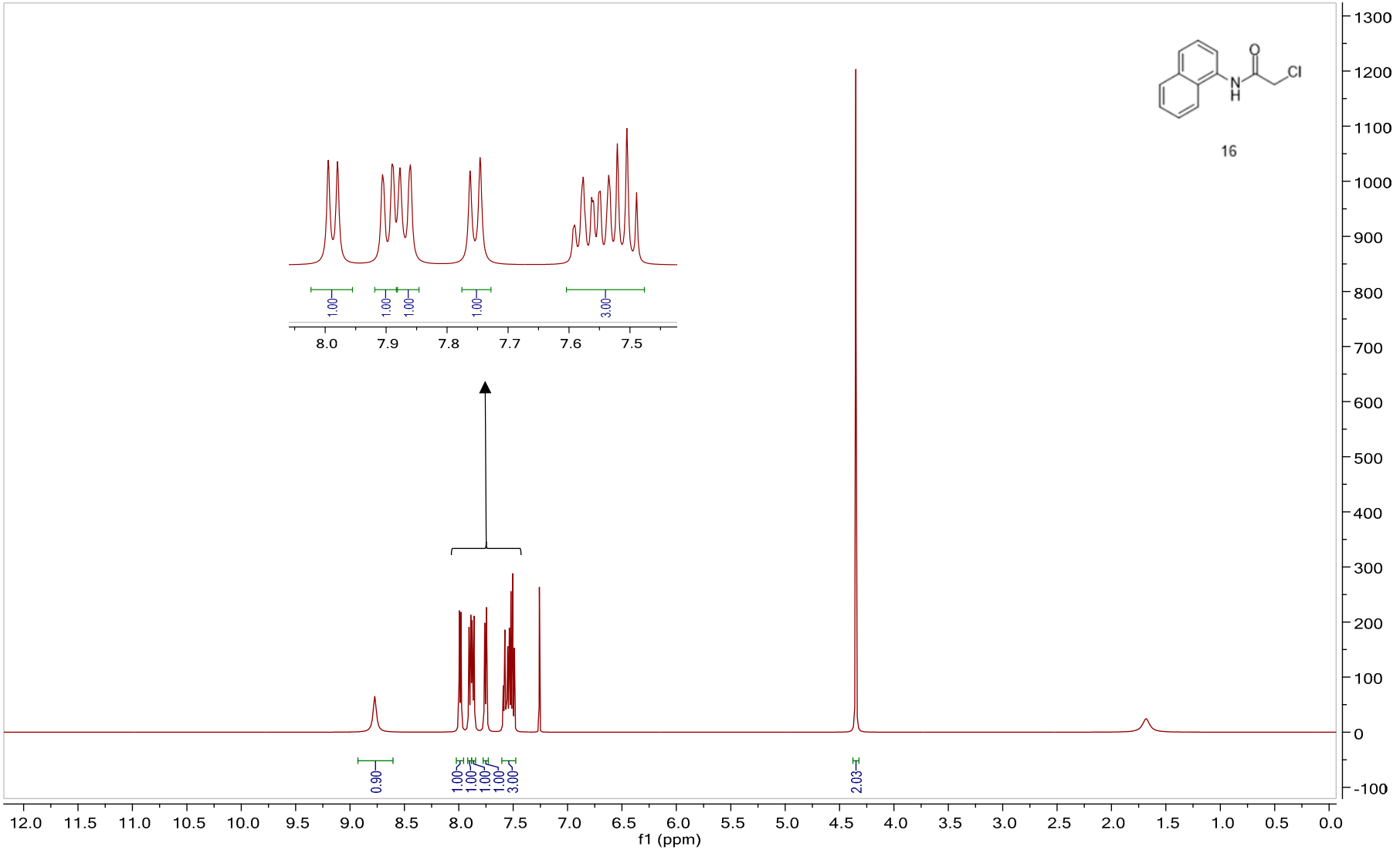


Figure S54. ^{1}H NMR spectrum of analog **16**

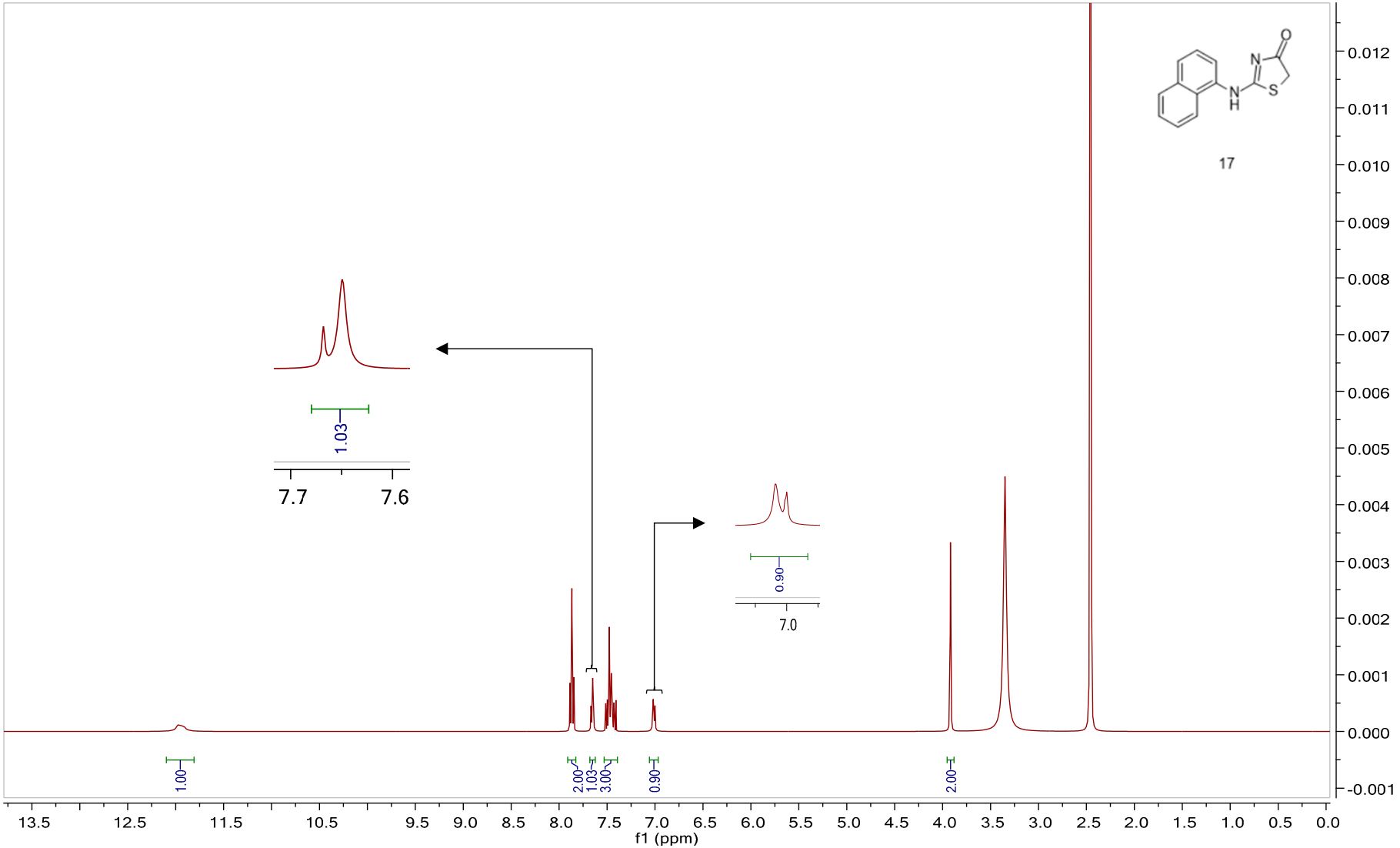


Figure S55. ^{1}H NMR spectrum of analog **17**

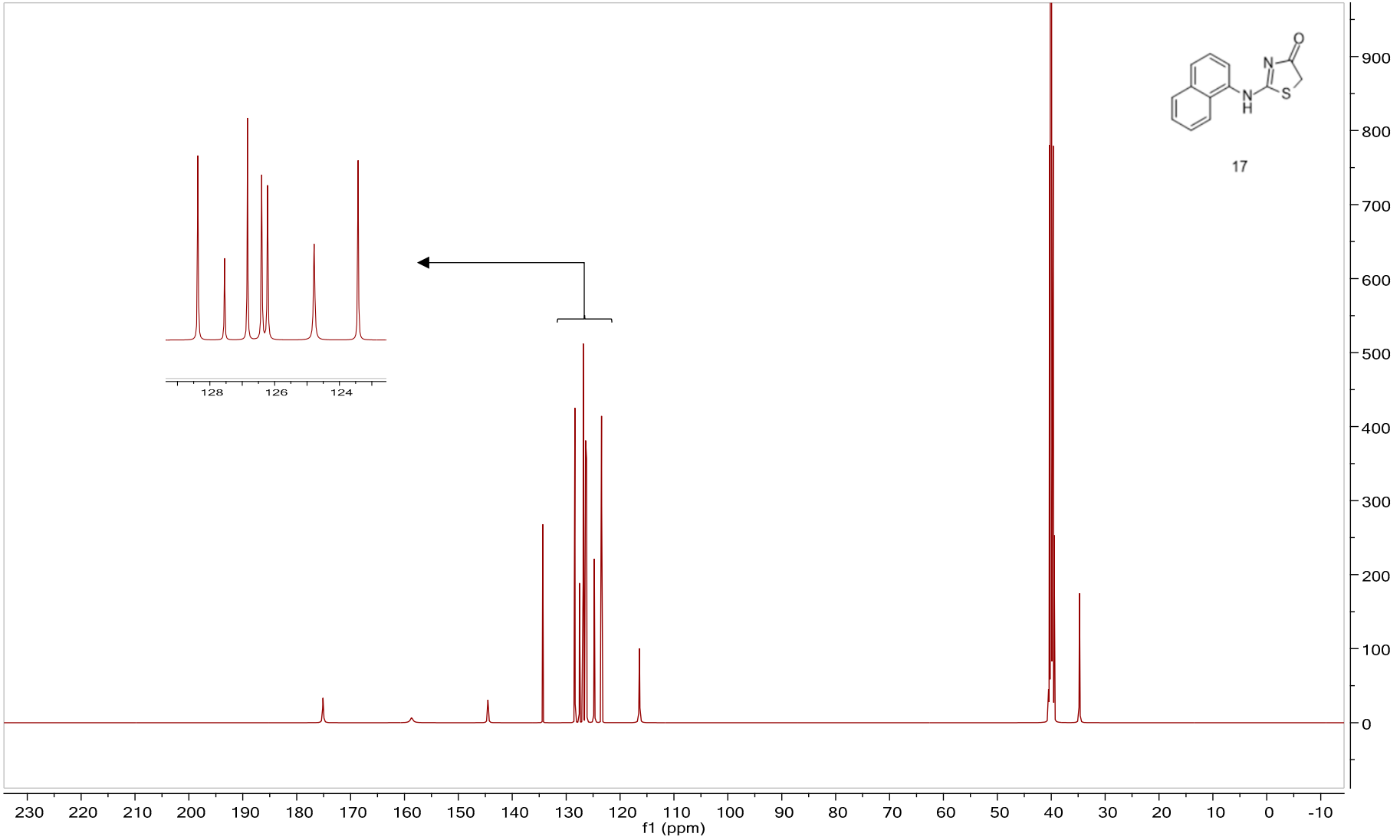


Figure S56. ^{13}C NMR spectrum of analog **17**

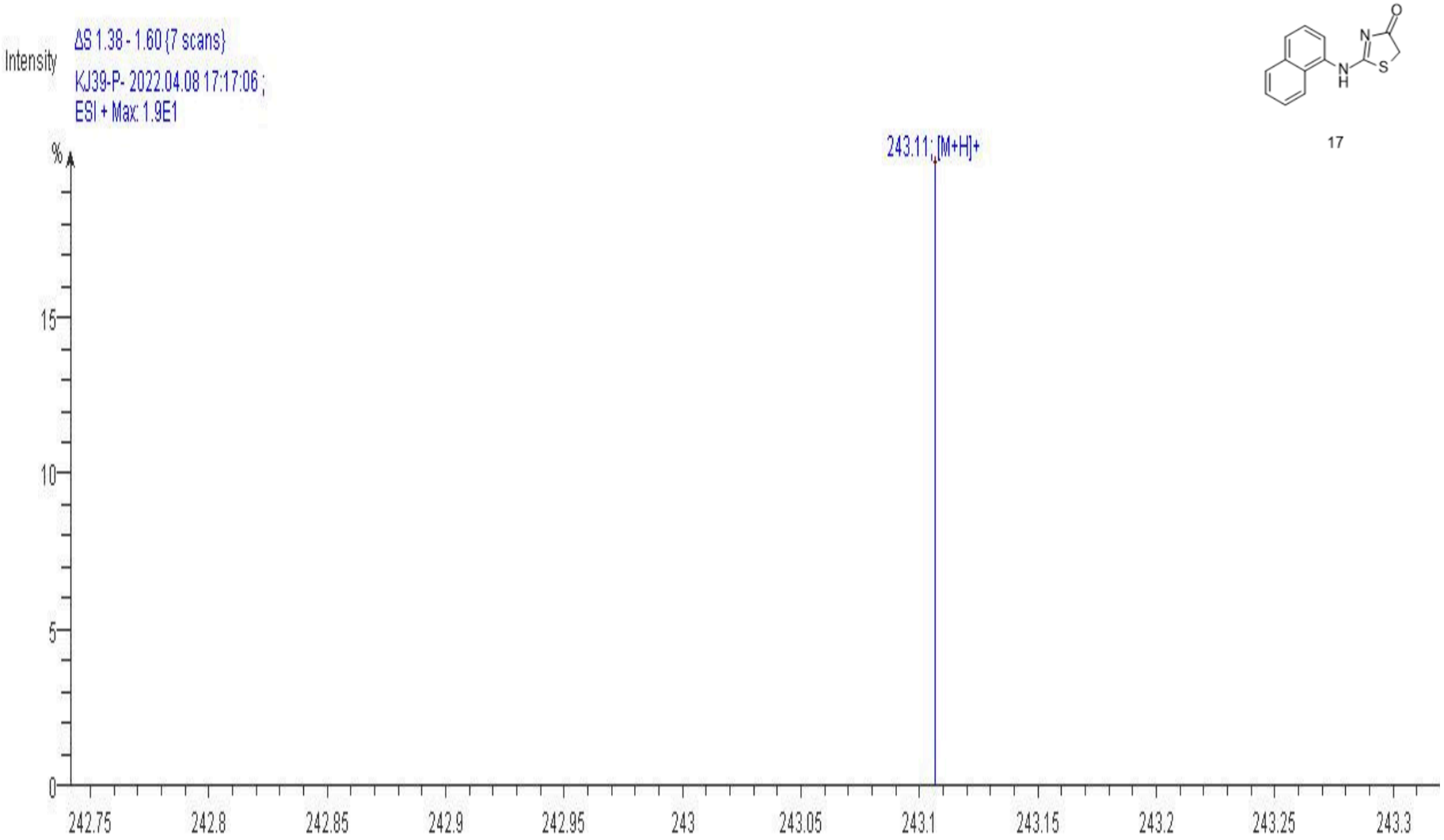


Figure S57. LRMS (ESI+) spectrum of analog **17**

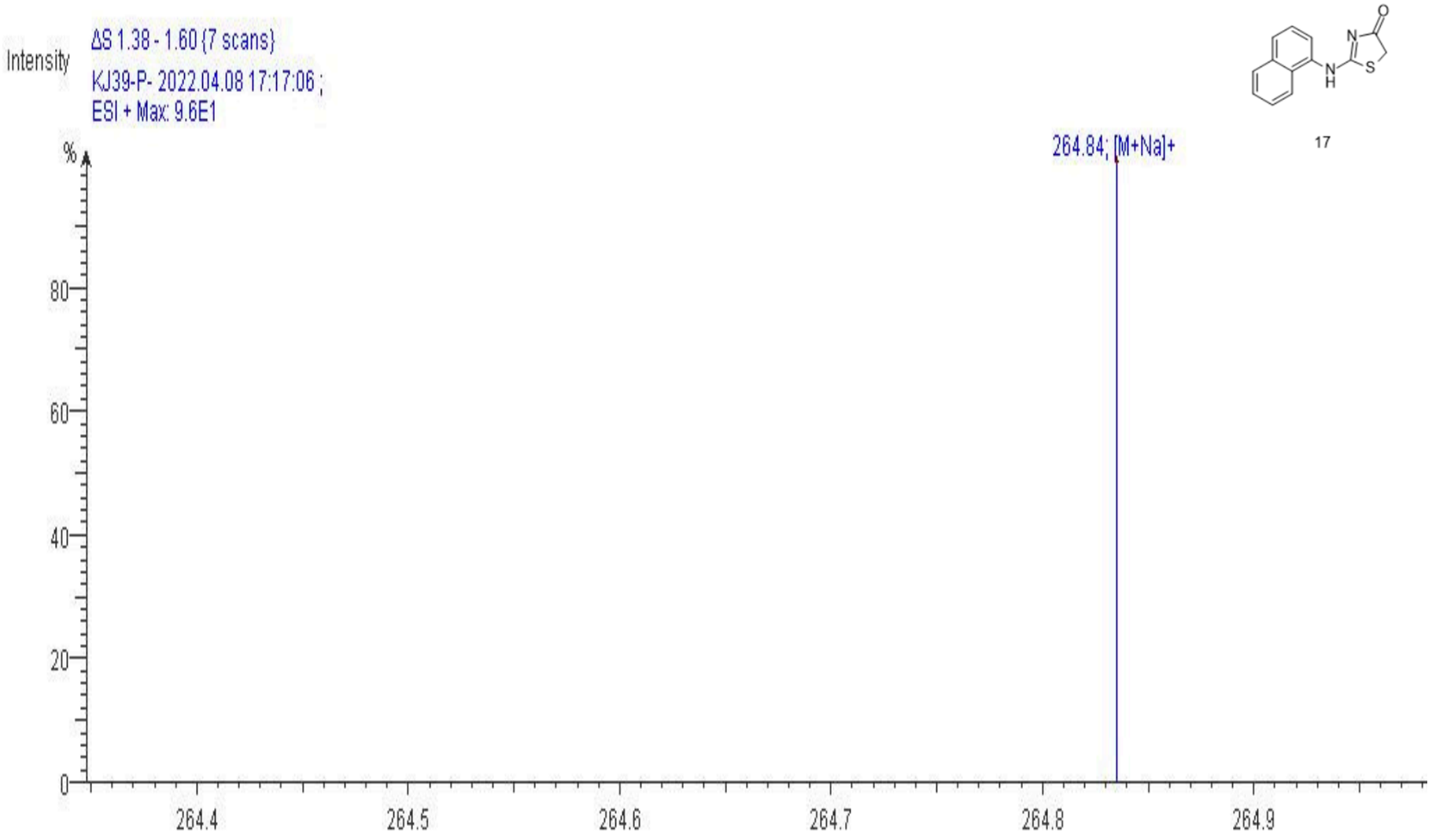
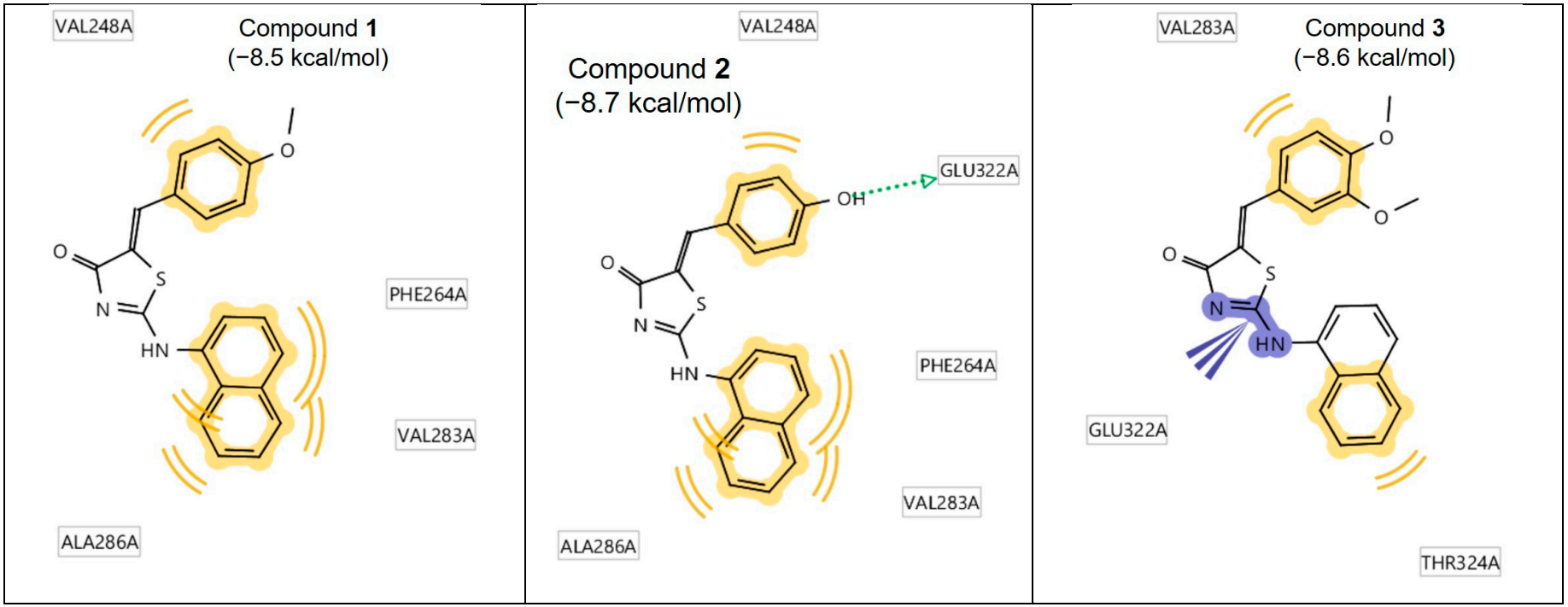
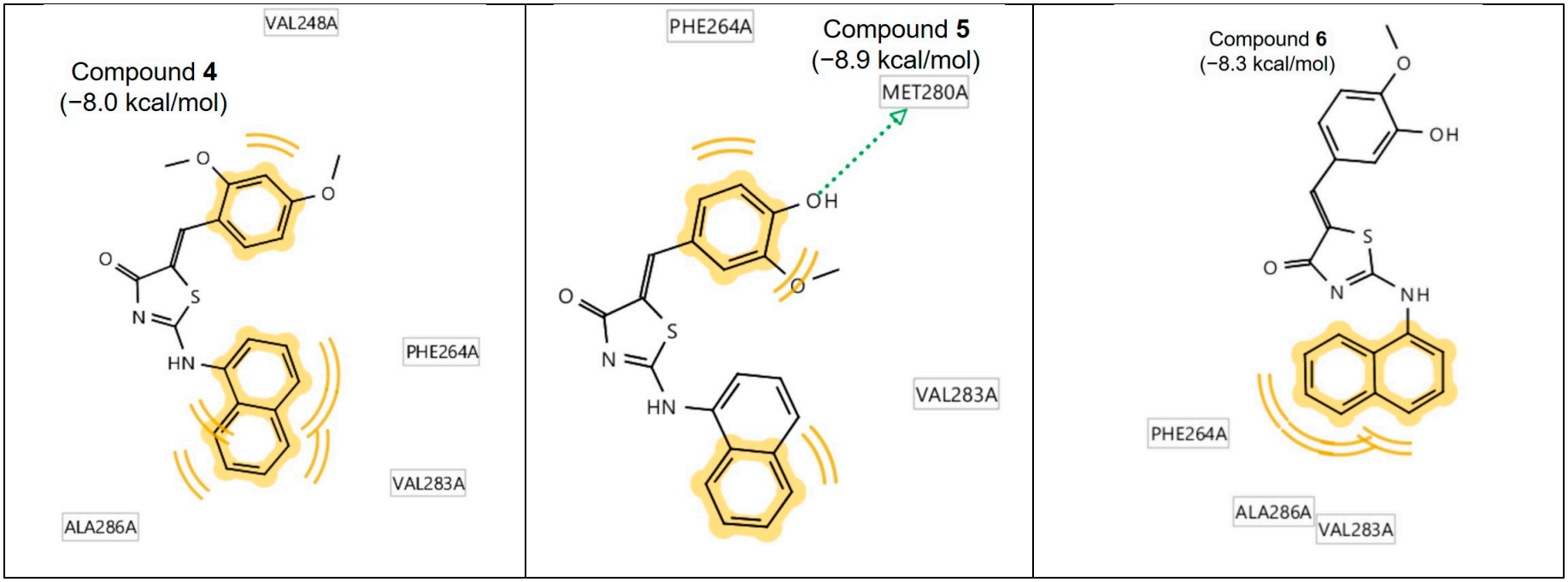
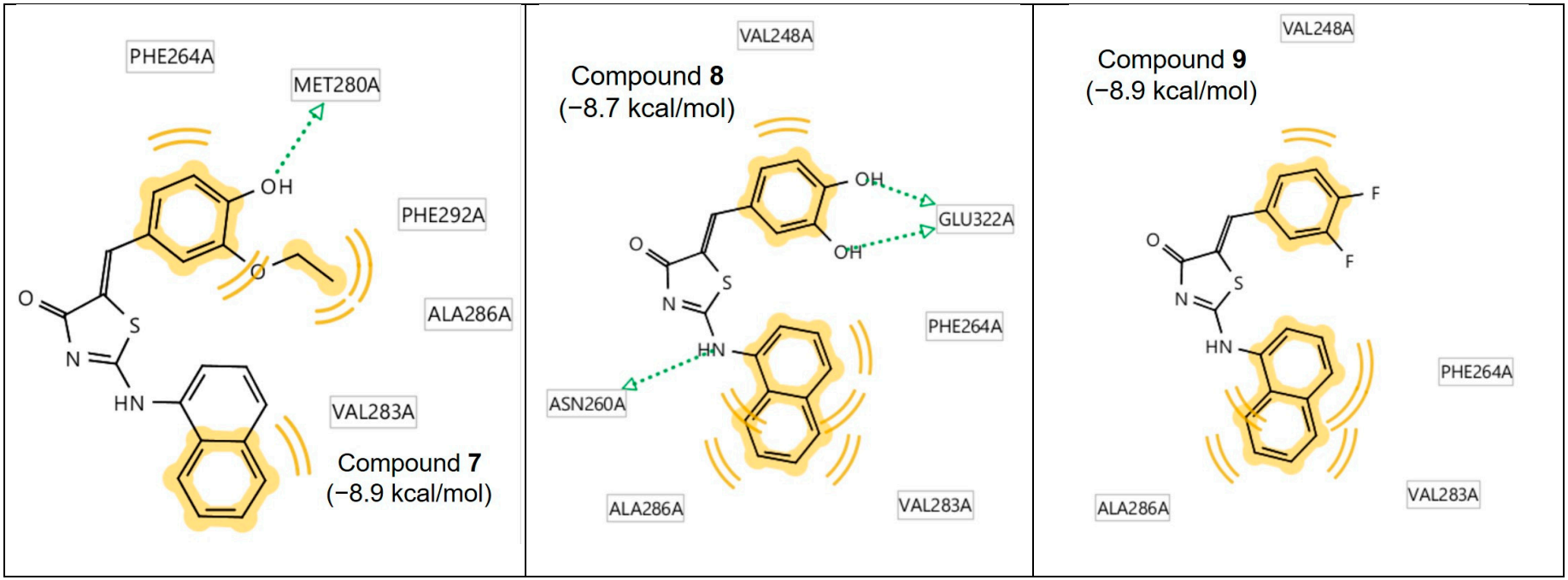


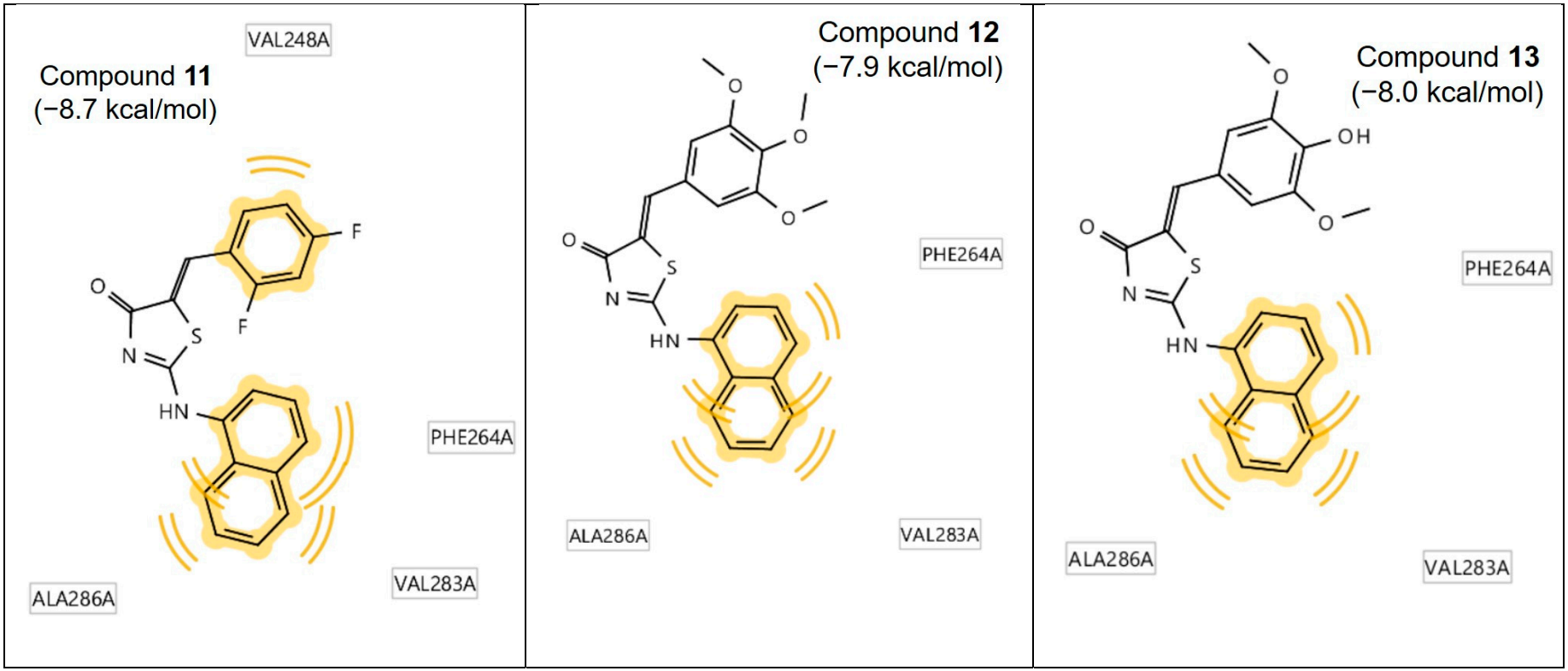
Figure S58. LRMS (ESI+) spectrum of analog **17**

Figure S59. In silico 2D results obtained from docking simulation of ligands (1–9 and 11–15) with mushroom tyrosinase (PDB ID: 2Y9X)




VAL248A
Compound 4
(−8.0 kcal/mol)
PHE264A
VAL283A
ALA286A
PHE264A
Compound 5
(−8.9 kcal/mol)
MET280A
VAL283A
Compound 6
(−8.3 kcal/mol)
PHE264A
ALA286A
VAL283A


PHE264A
MET280A
OH
PHE292A
O
O
S
N
HN
ALA286A
VAL283A
Compound 7
(−8.9 kcal/mol)
VAL248A
Compound 8
(−8.7 kcal/mol)
OH
GLU322A
OH
O
S
N
HN
PHE264A
ASN260A
ALA286A
VAL283A
VAL248A
Compound 9
(−8.9 kcal/mol)
F
F
O
S
N
HN
PHE264A
ALA286A
VAL283A


VAL248A
Compound 11
(−8.7 kcal/mol)
F
F
O
S
N
HN
PHE264A
ALA286A
VAL283A
Compound 12
(−7.9 kcal/mol)
O
O
O
O
S
N
HN
PHE264A
ALA286A
VAL283A
Compound 13
(−8.0 kcal/mol)
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O
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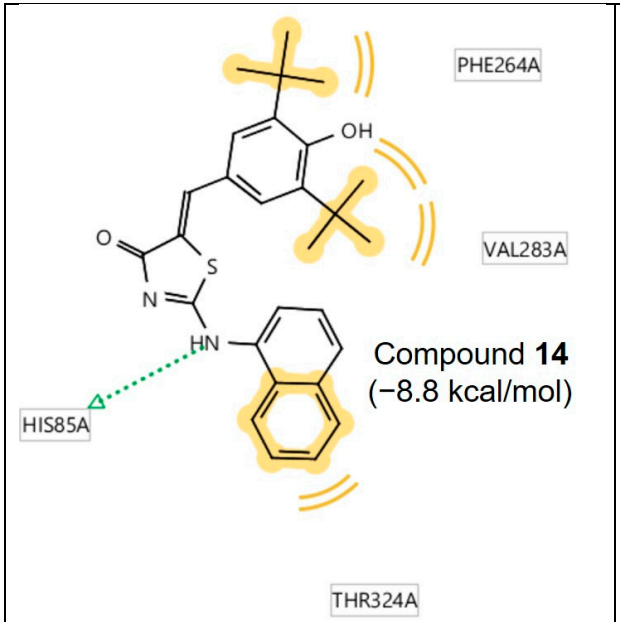
S
N
HN
PHE264A
ALA286A
VAL283A

PHE264A OH VAL283A O S N HN Compound **14** (−8.8 kcal/mol) HIS85A THR324A		