

Supplementary Information

Discovery of novel Isoliquiritigenin analogue ISL-17 as a potential anti-gastric cancer agent

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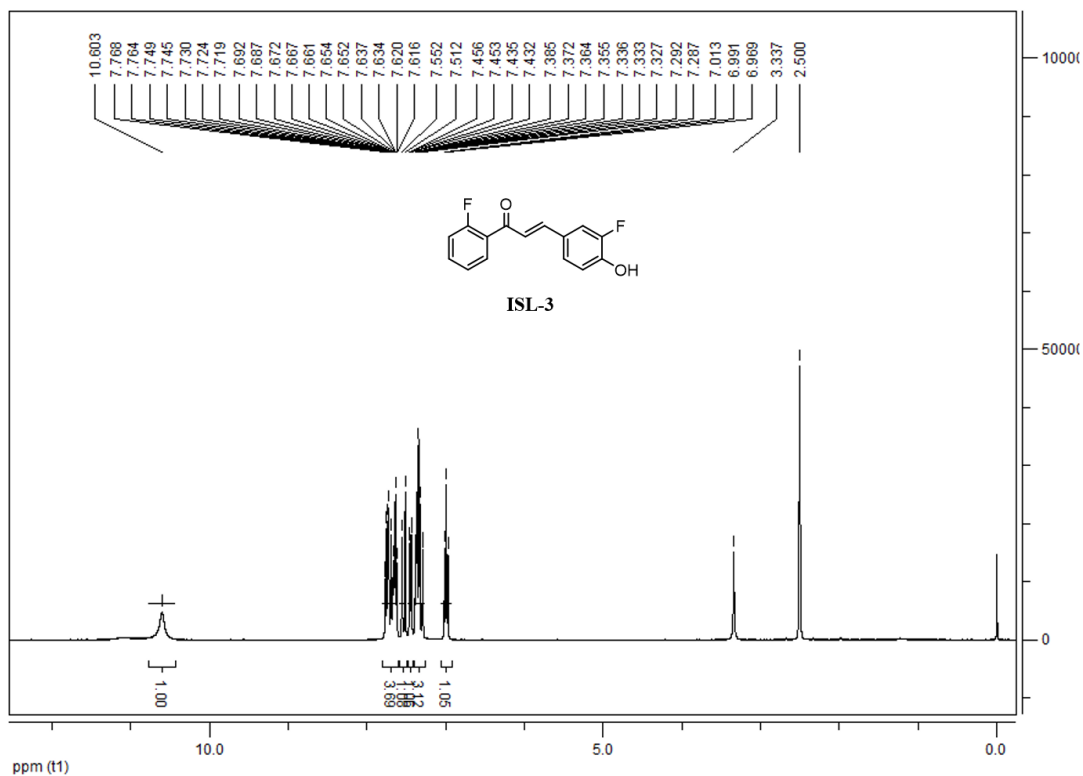


Figure S5. The ^1H NMR spectra of compound **ISL-3** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

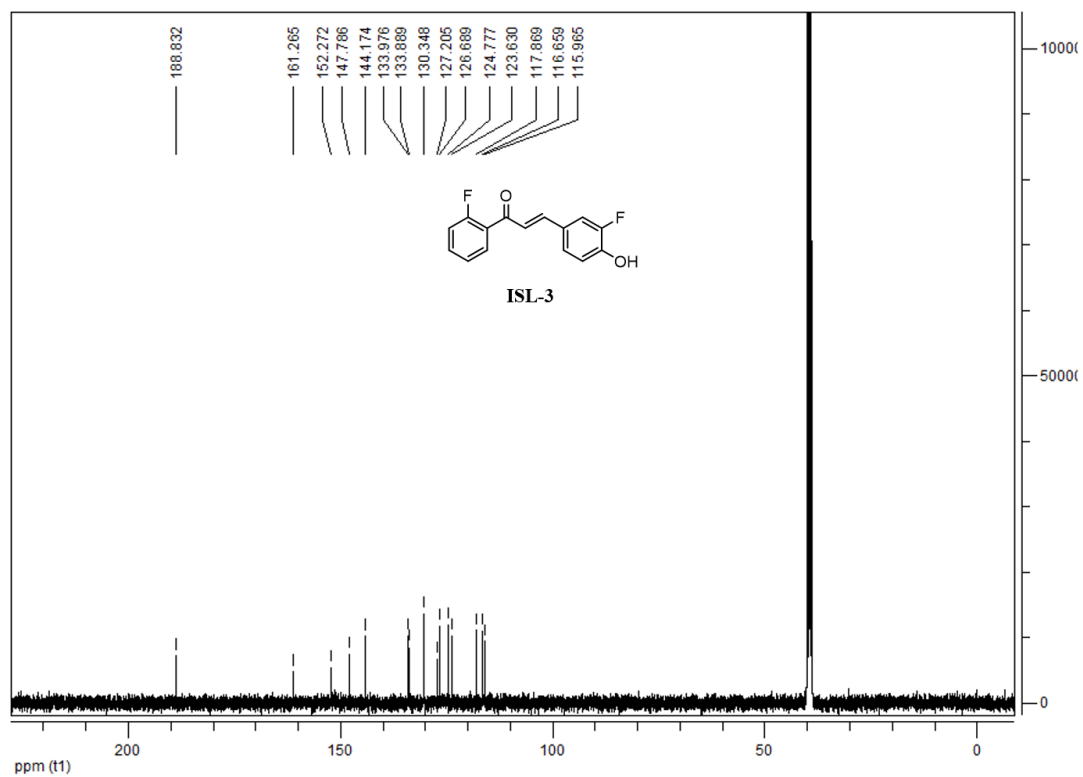


Figure S6. The ^{13}C NMR spectra of compound **ISL-3** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

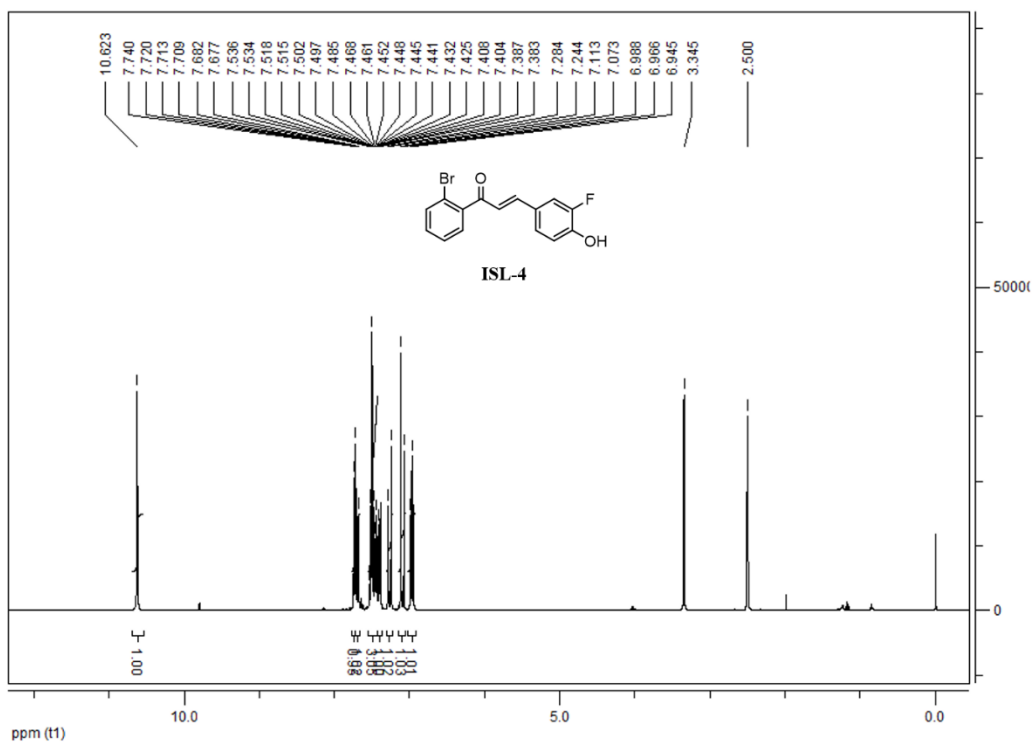


Figure S7. The ^1H NMR spectra of compound **ISL-4** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

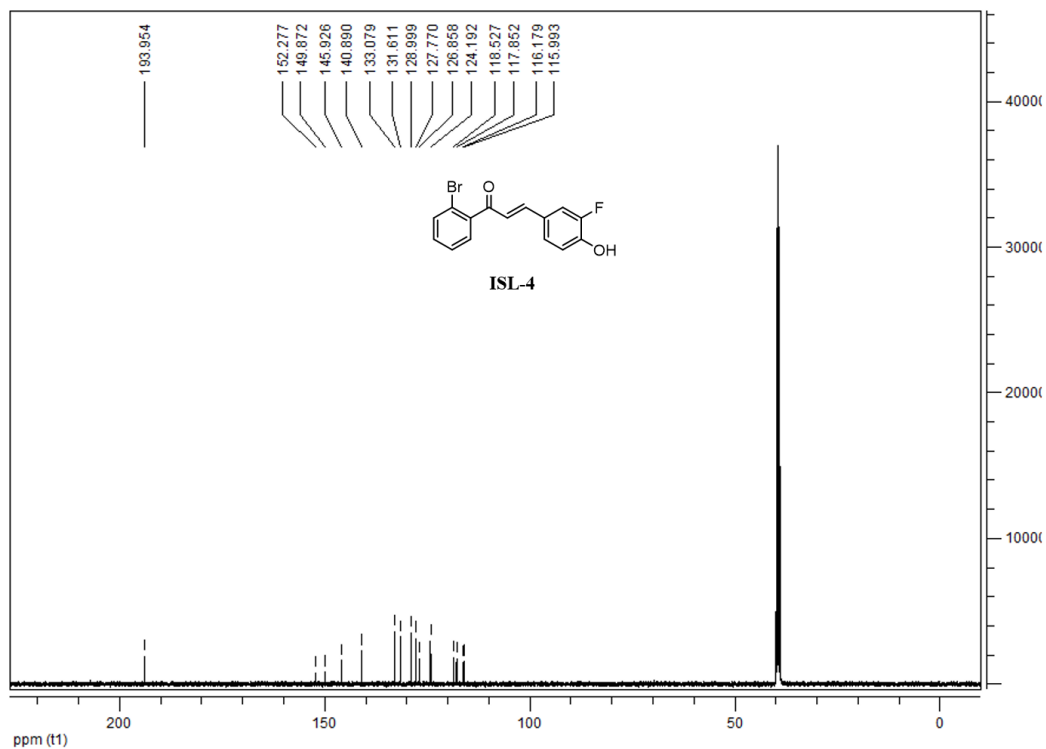


Figure S8. The ^{13}C NMR spectra of compound **ISL-4** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

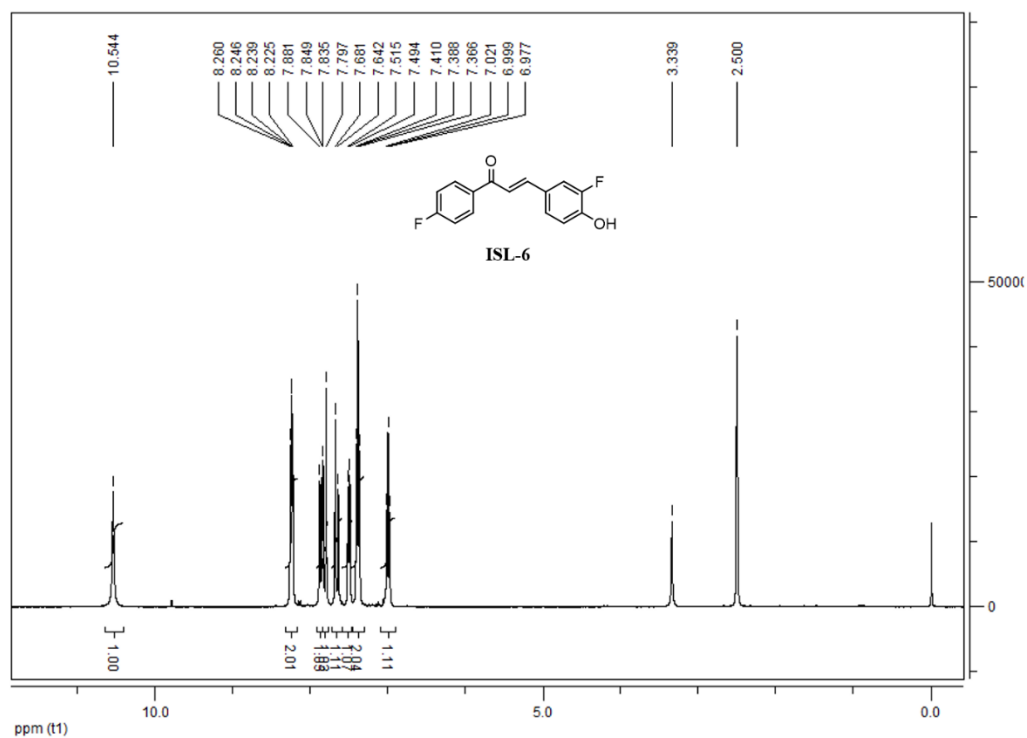


Figure S11. The ^1H NMR spectra of compound **ISL-6** (DMSO- d_6 , Bruker AVANVEIII 400)

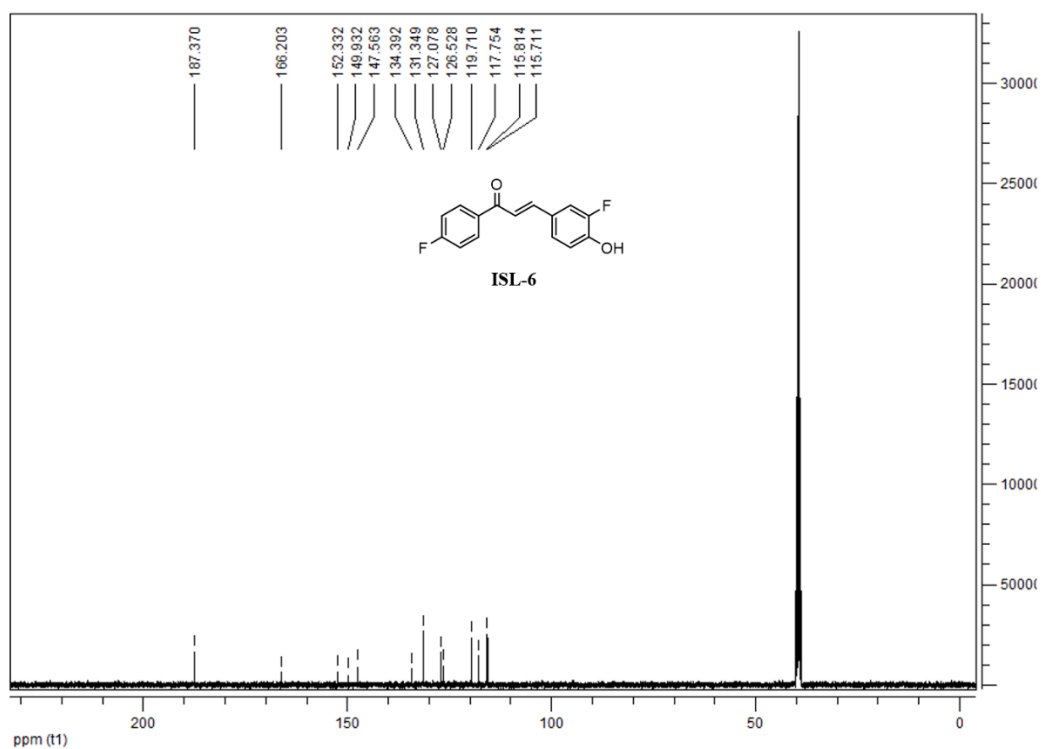


Figure S12. The ^{13}C NMR spectra of compound **ISL-6** (DMSO- d_6 , Bruker AVANVEIII 400)

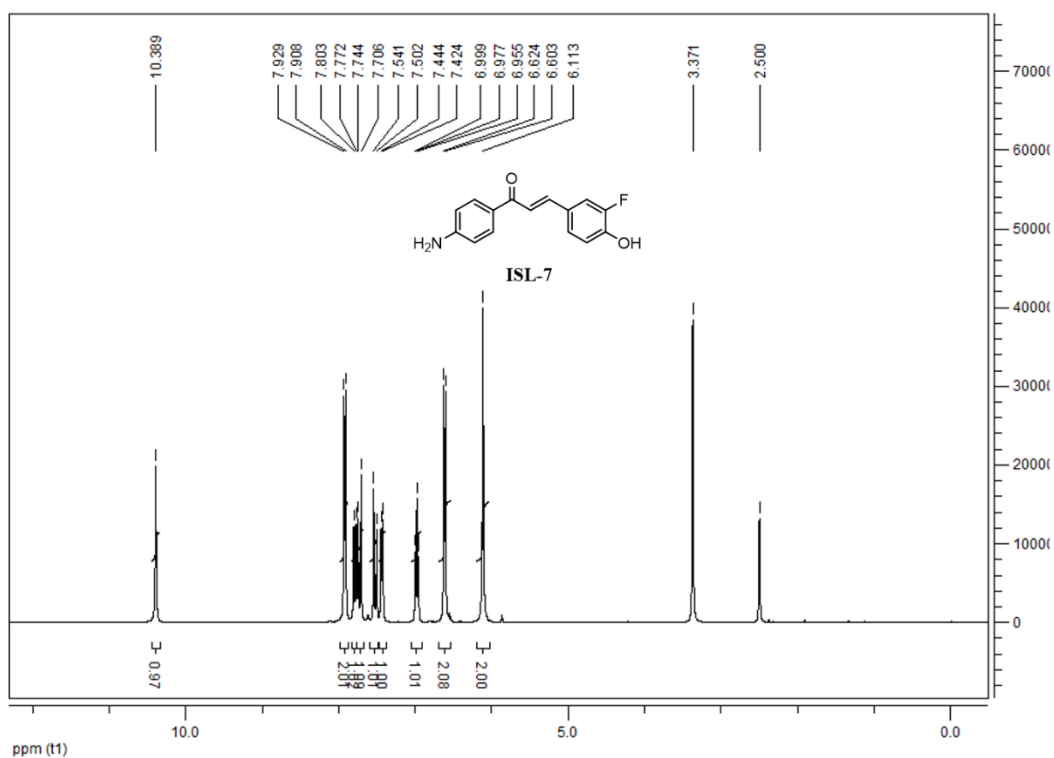


Figure S13. The ^1H NMR spectra of compound **ISL-7** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

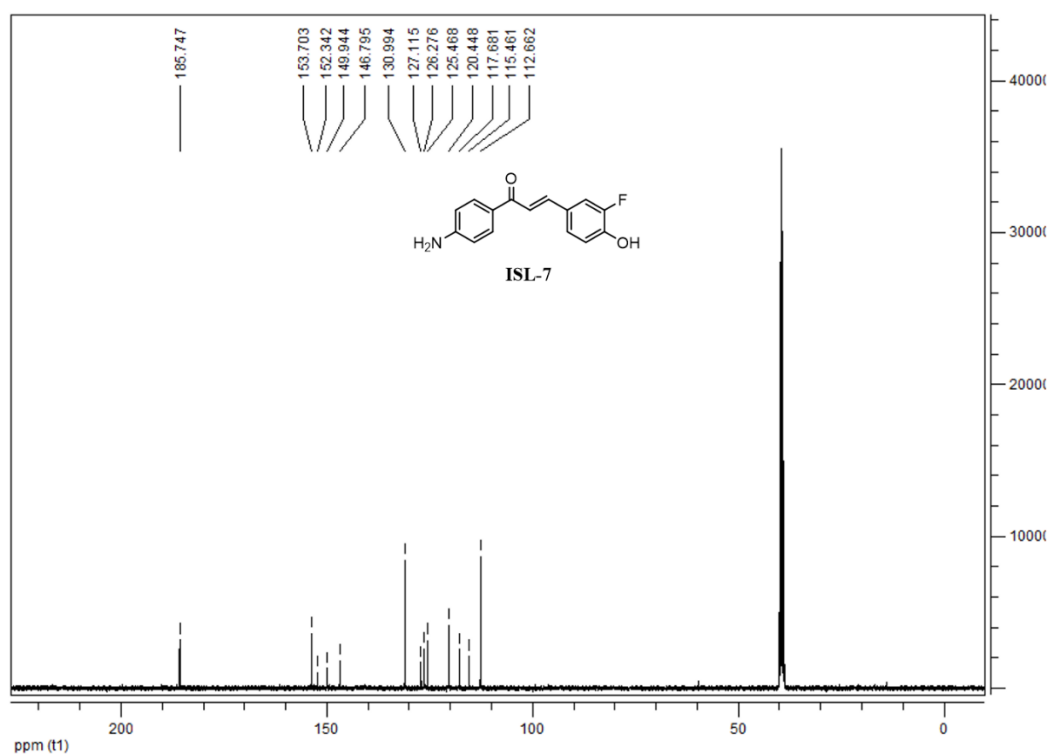
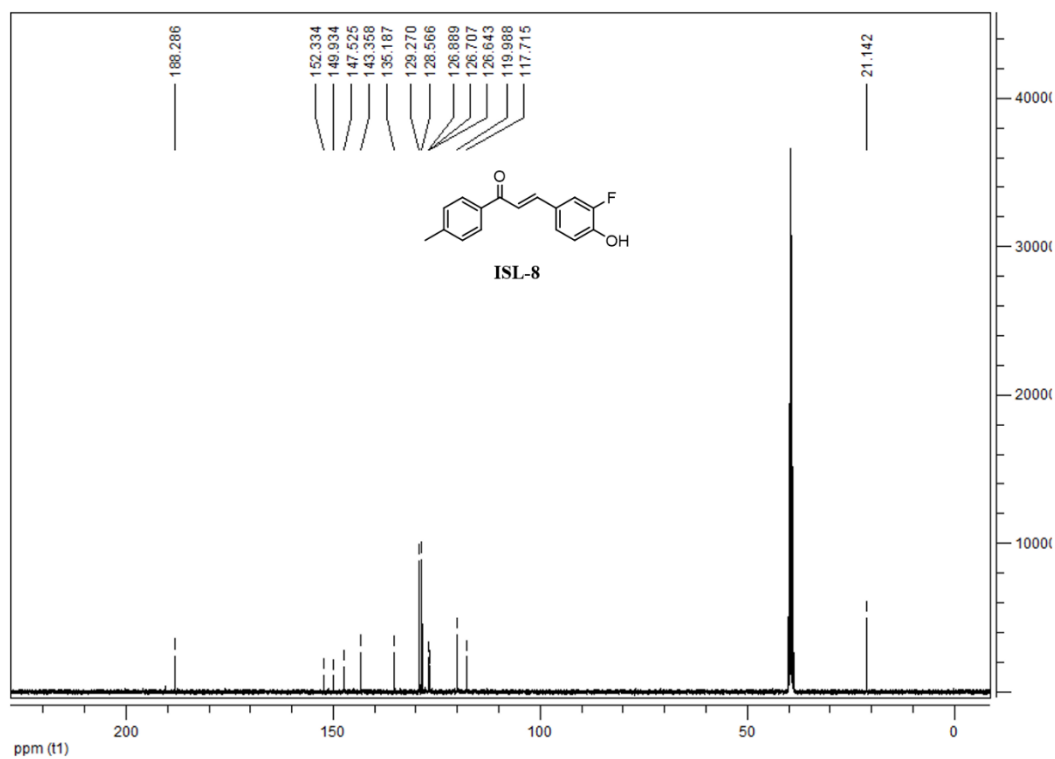
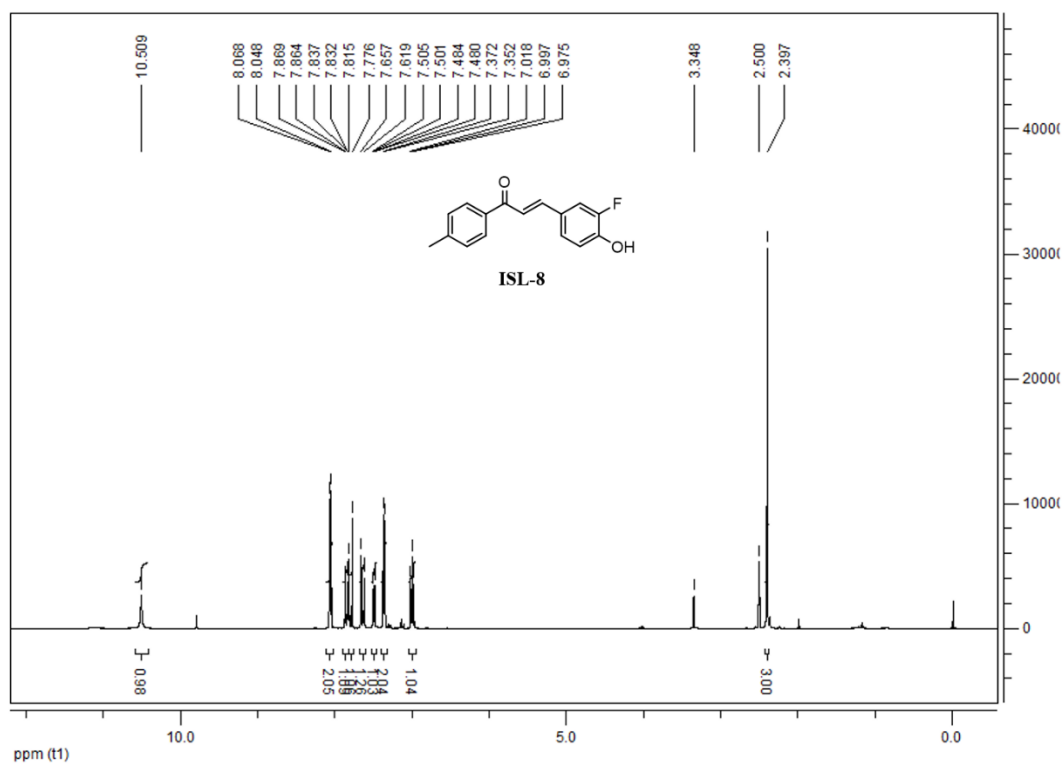
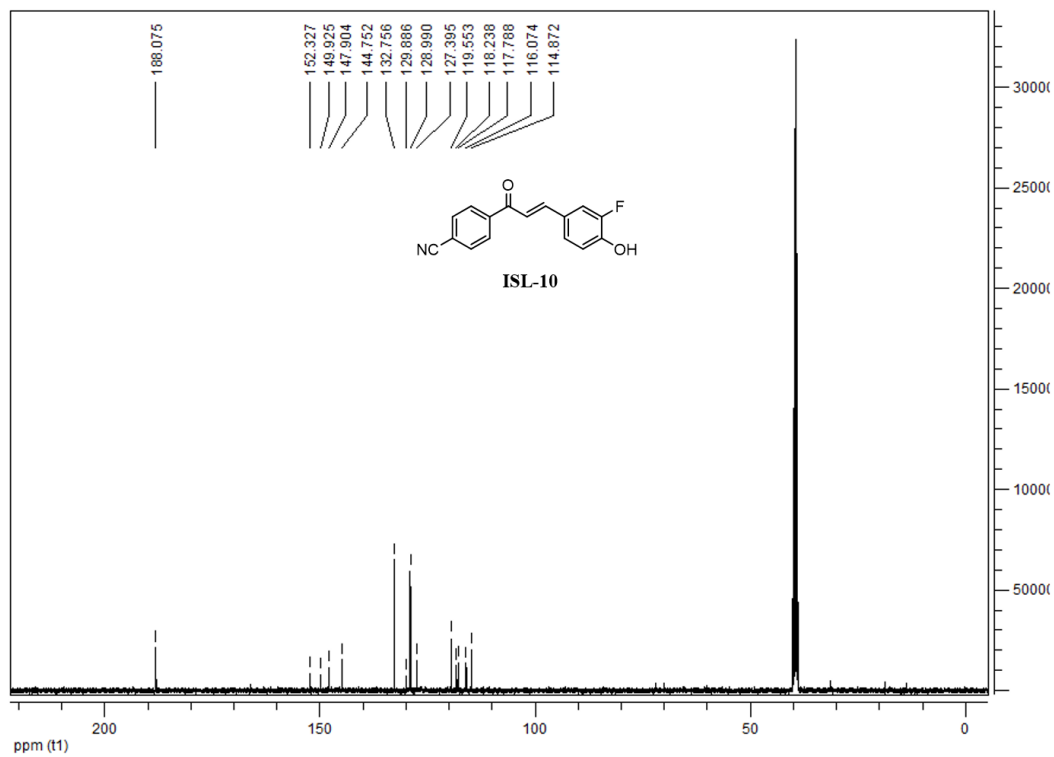
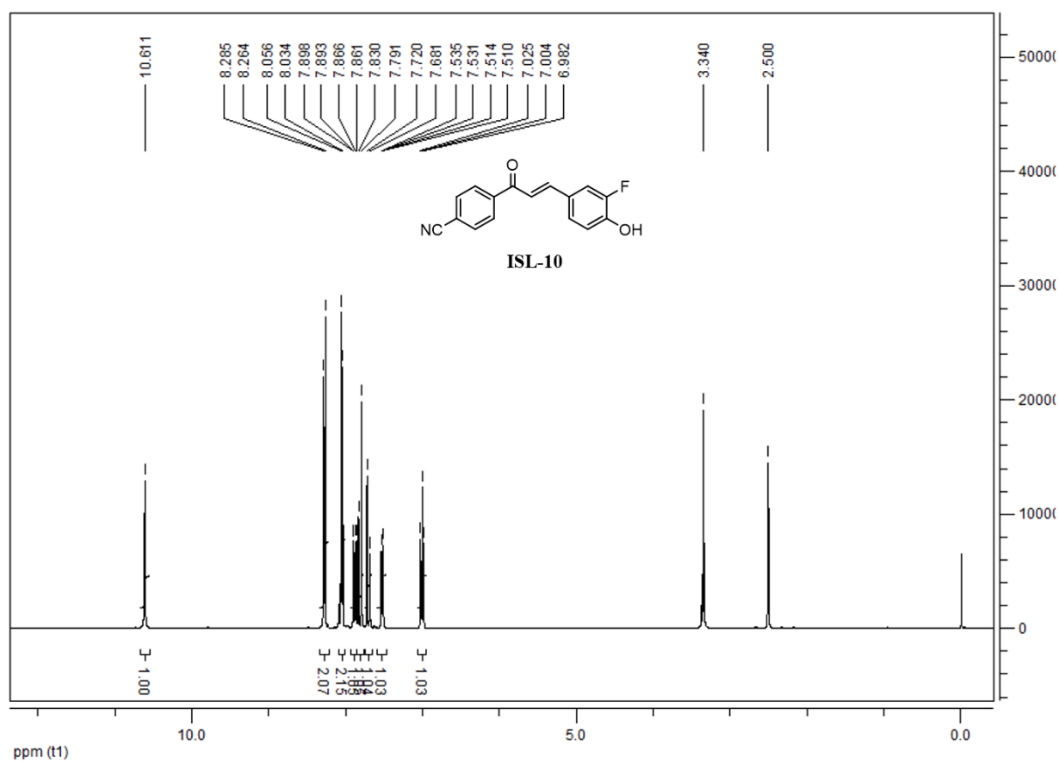


Figure S14. The ^{13}C NMR spectra of compound **ISL-7** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)





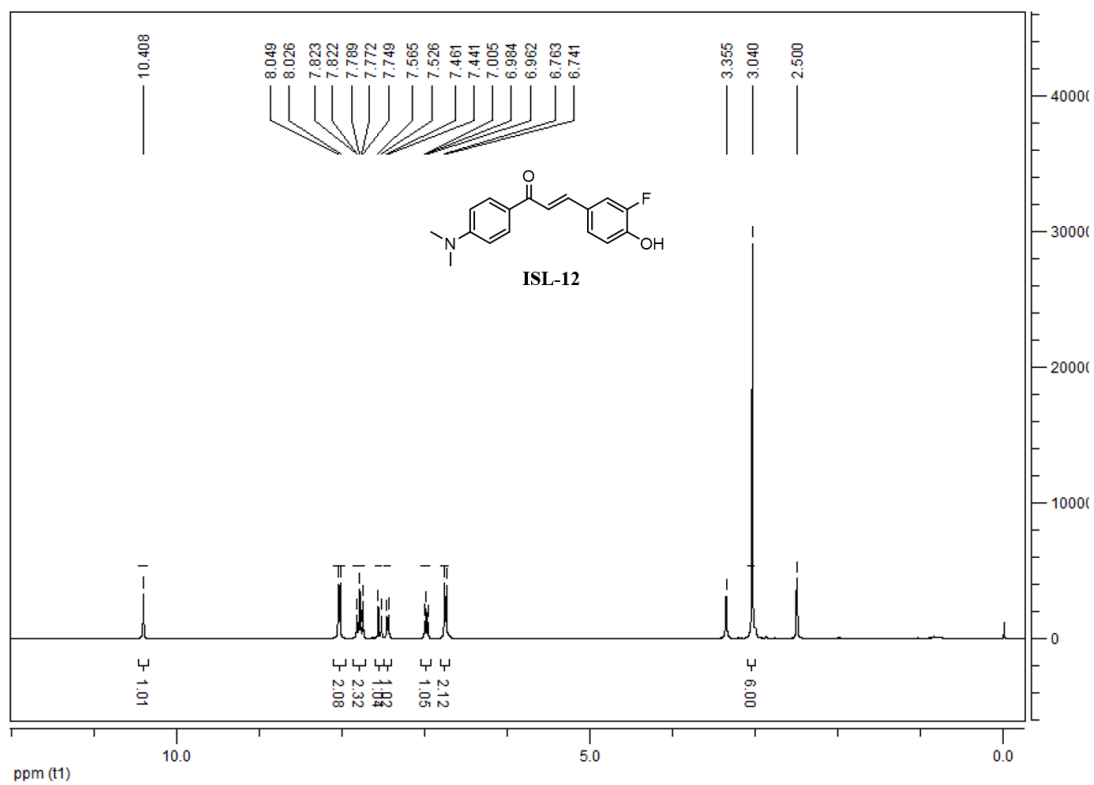


Figure S23. The ^1H NMR spectra of compound ISL-12 (DMSO- d_6 , Bruker AVANVEIII 400)

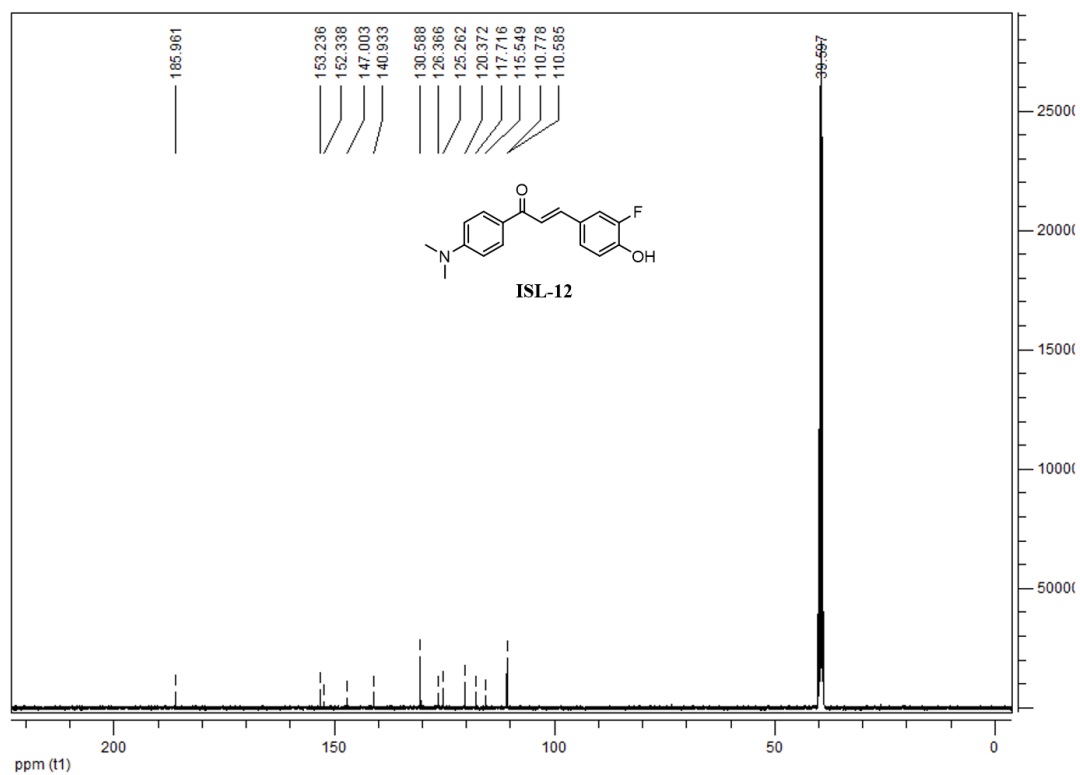


Figure S24. The ^{13}C NMR spectra of compound ISL-12 (DMSO- d_6 , Bruker AVANVEIII 400)

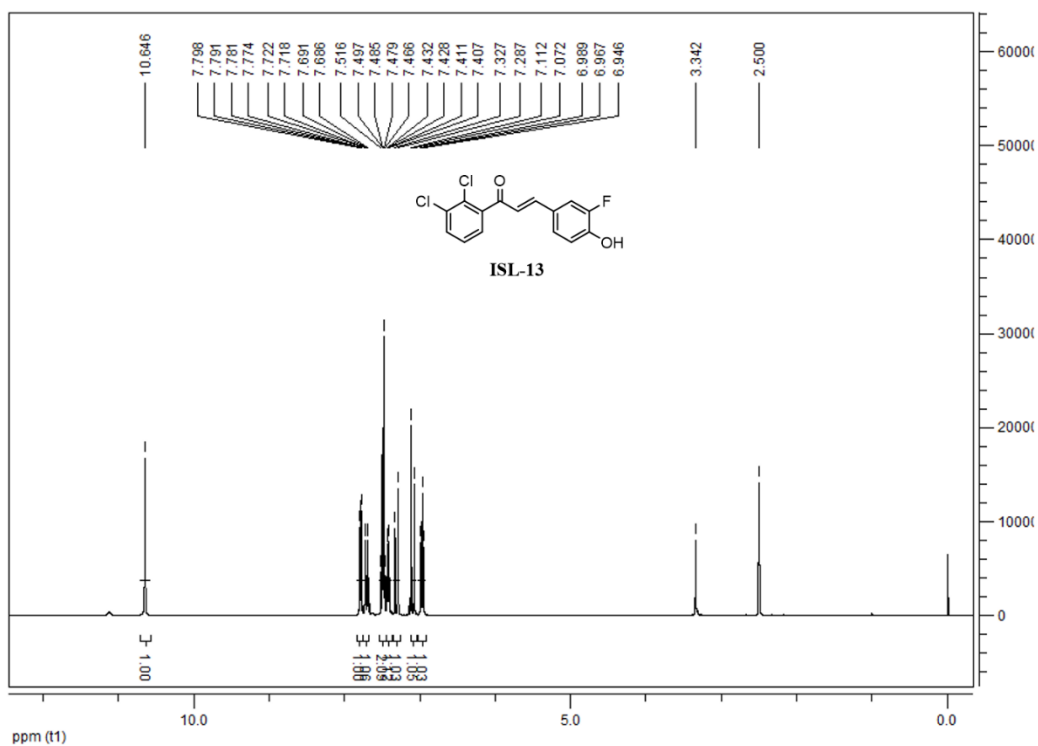


Figure S25. The ^1H NMR spectra of compound ISL-13 (DMSO- d_6 , Bruker AVANVEIII 400)

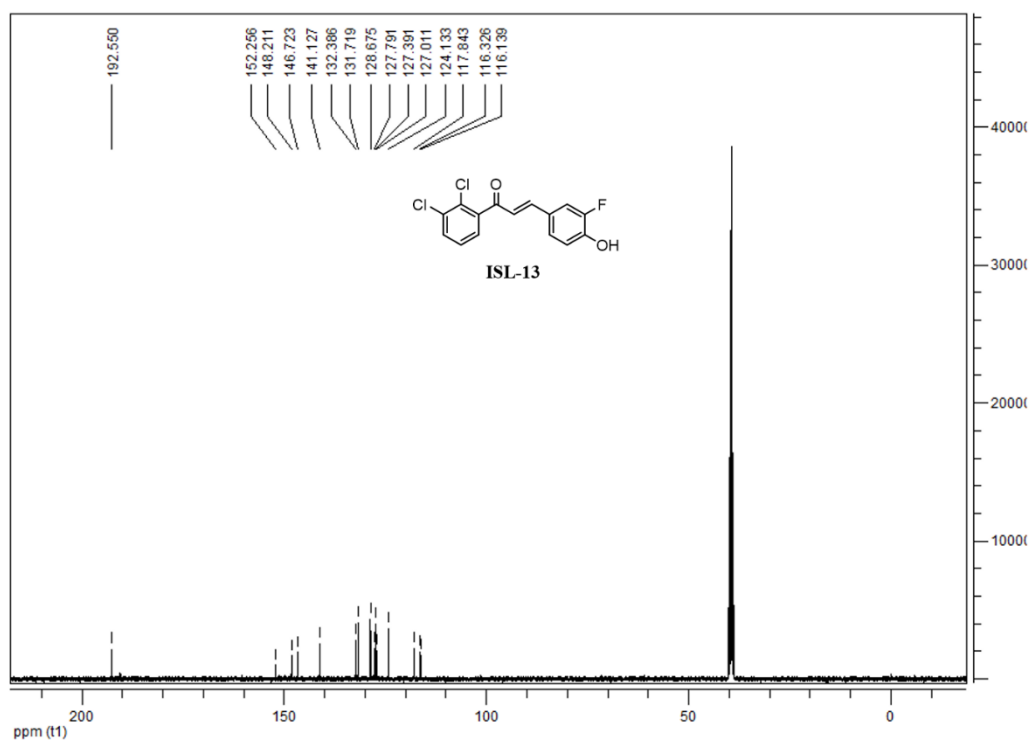


Figure S26. The ^{13}C NMR spectra of compound ISL-13 (DMSO- d_6 , Bruker AVANVEIII 400)

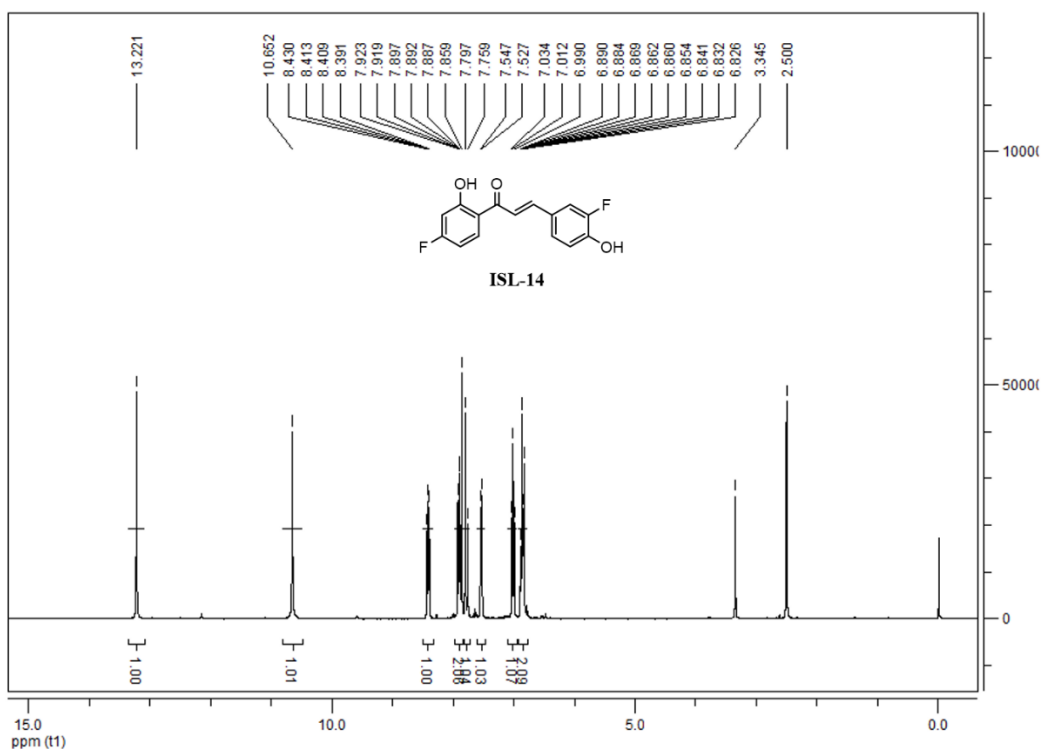


Figure S27. The ^1H NMR spectra of compound **ISL-14** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

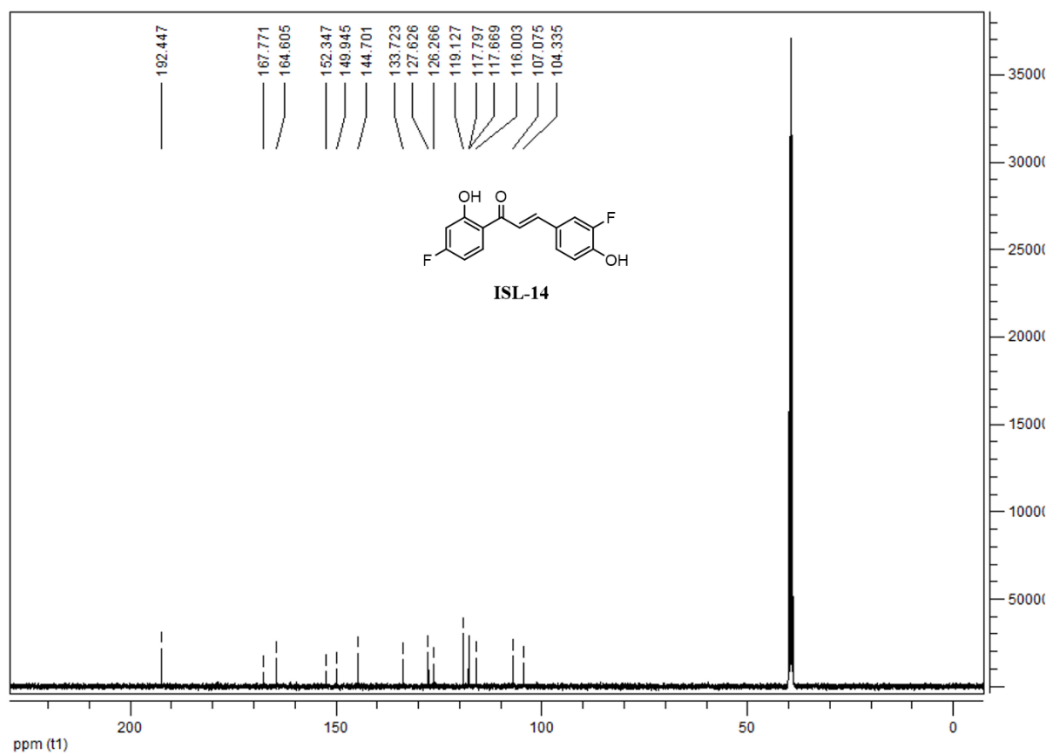
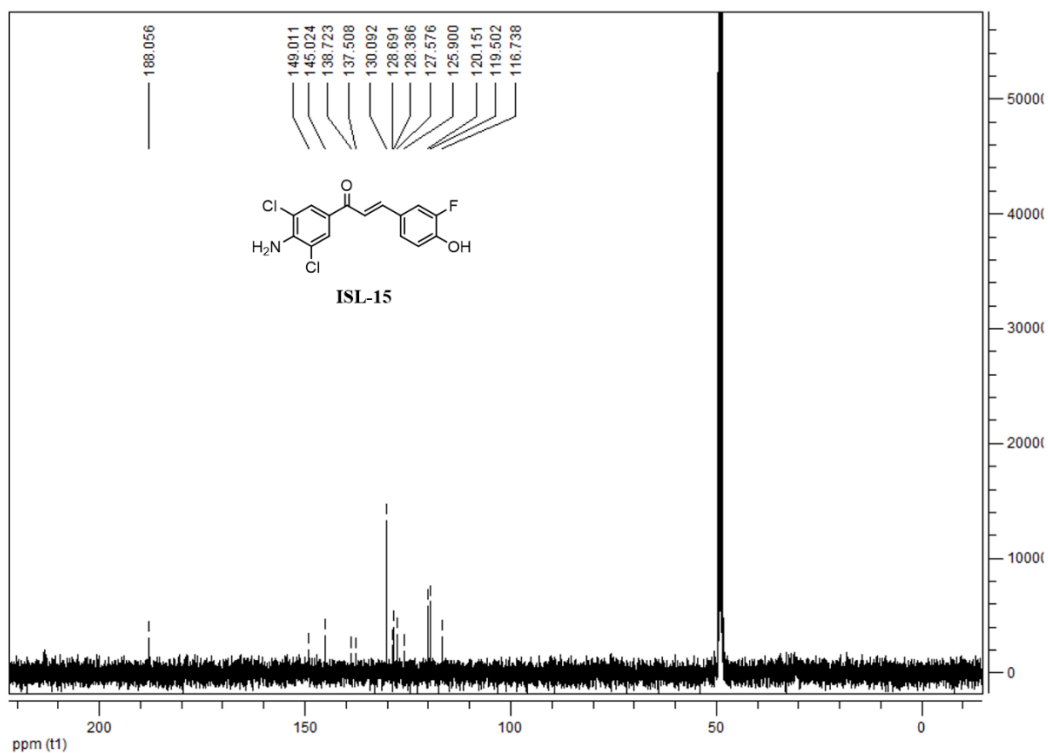
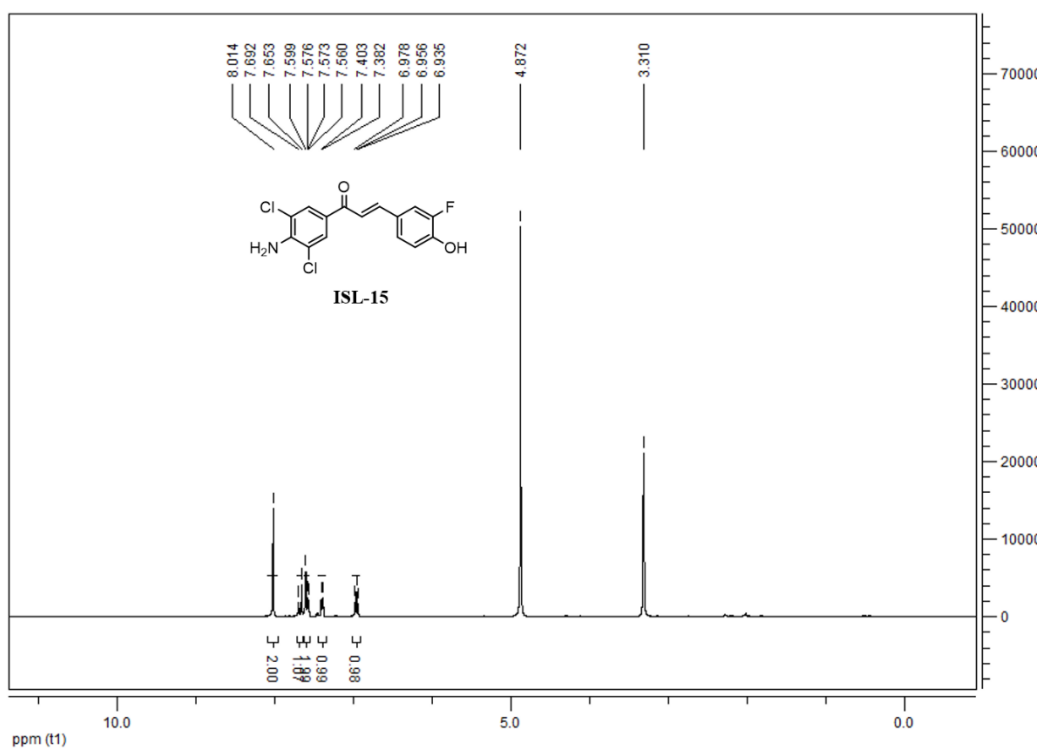
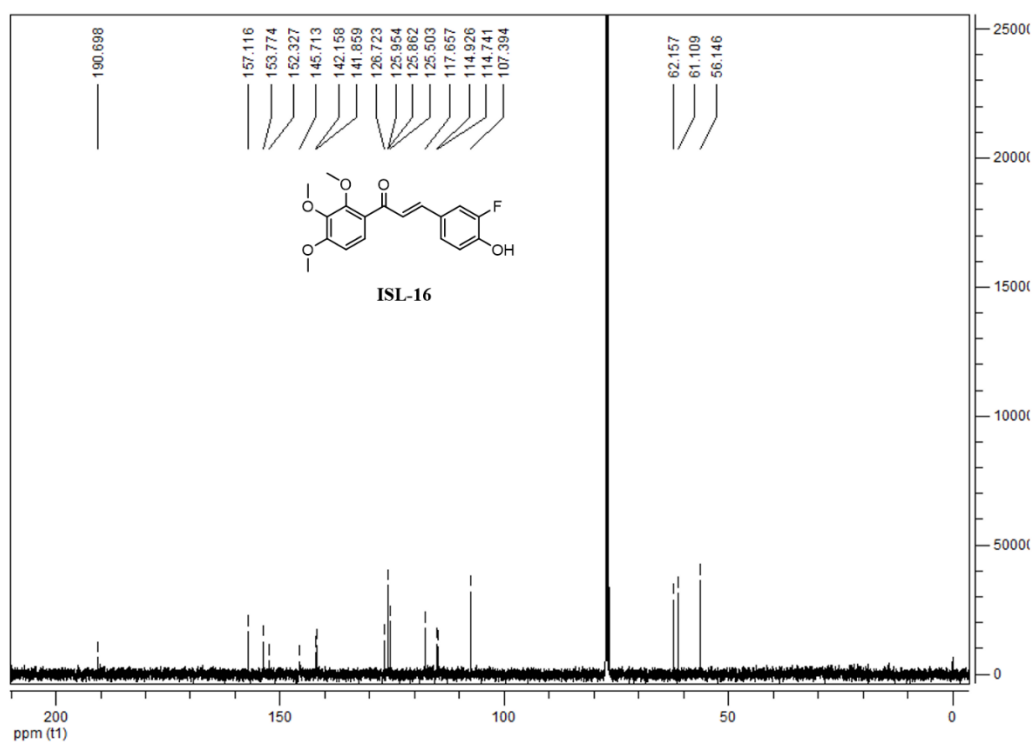
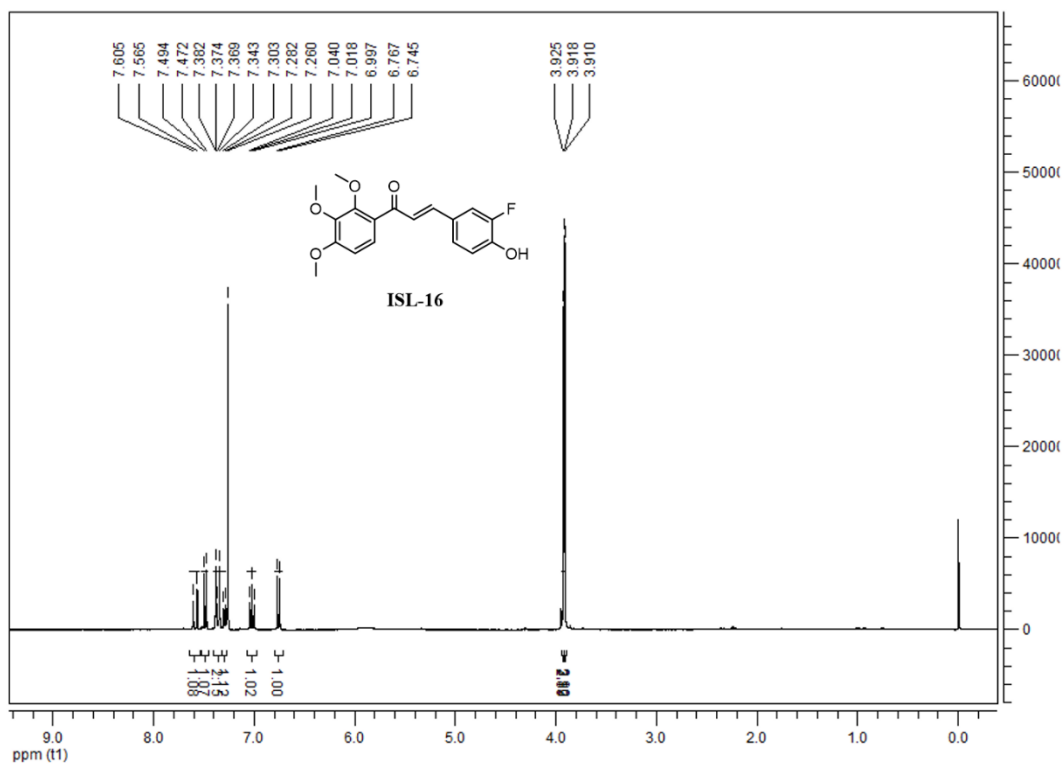


Figure S28. The ^{13}C NMR spectra of compound **ISL-14** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)





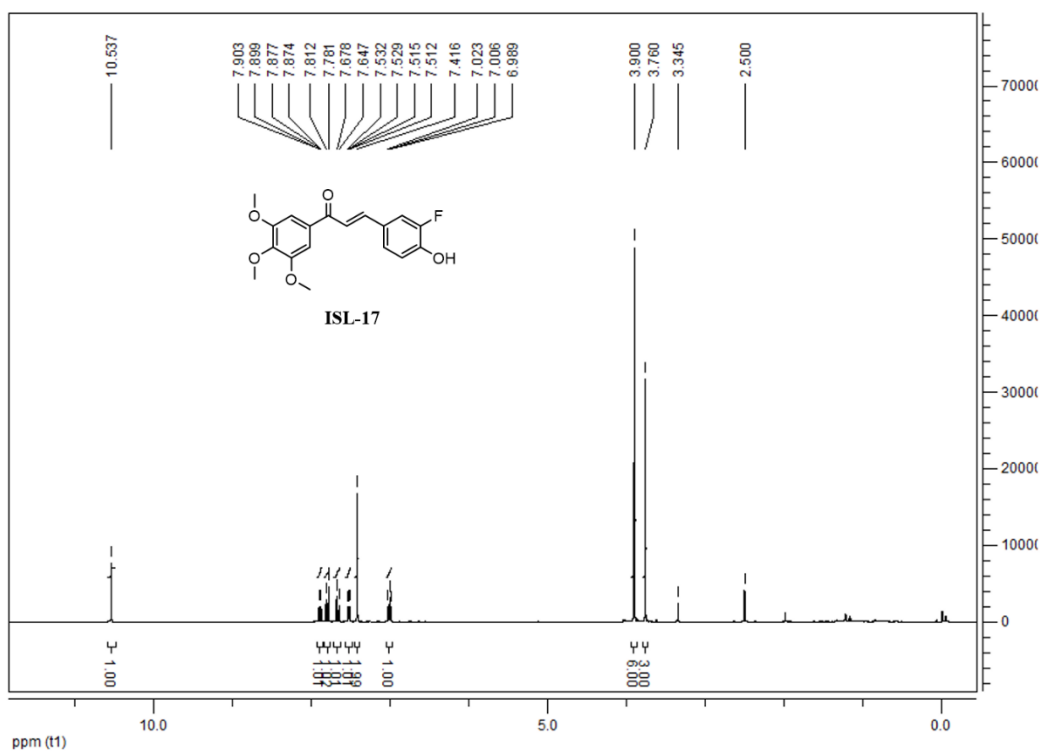


Figure S33. The ^1H NMR spectra of compound **ISL-17** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

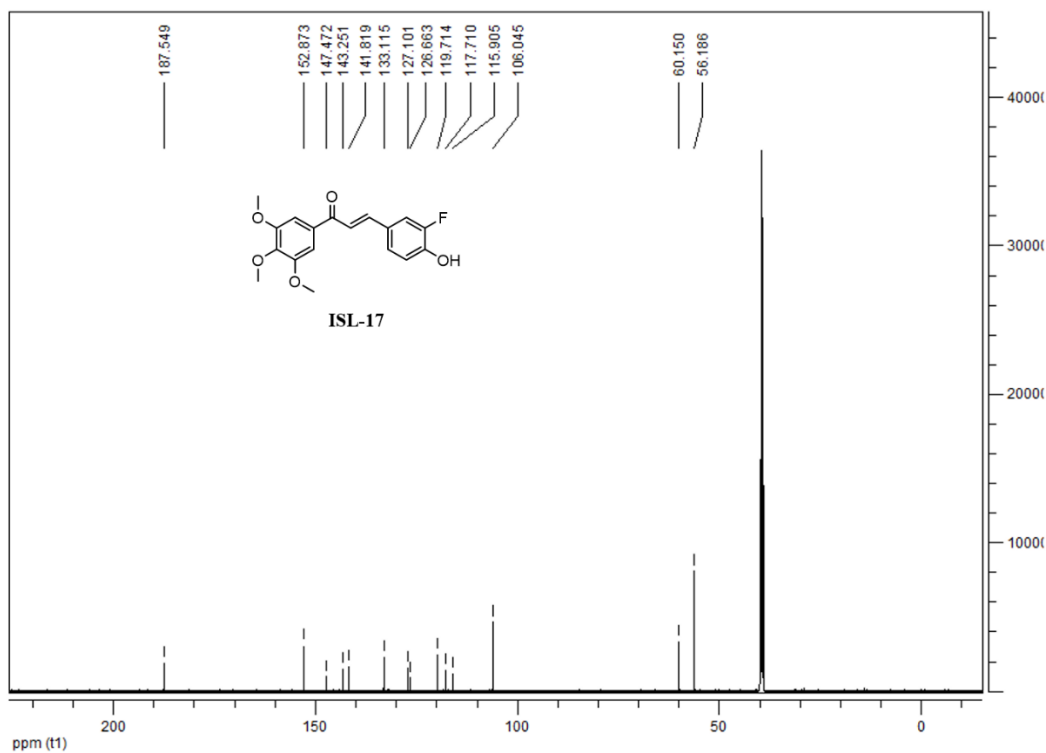


Figure S34. The ^{13}C NMR spectra of compound **ISL-17** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

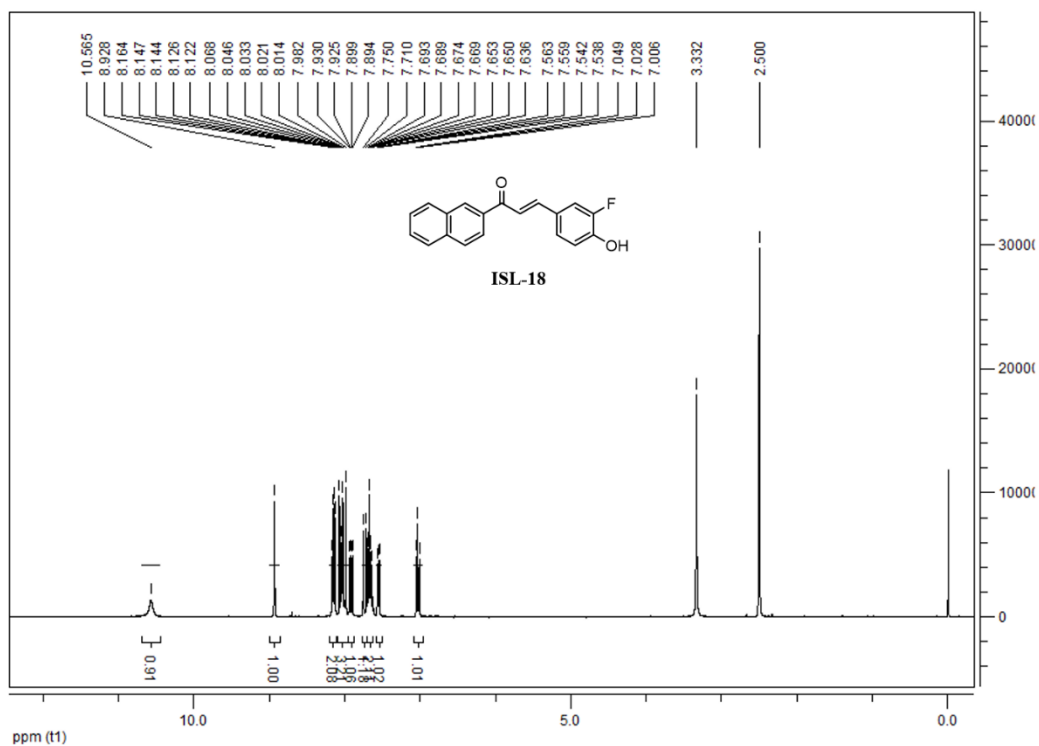


Figure S35. The ^1H NMR spectra of compound **ISL-18** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

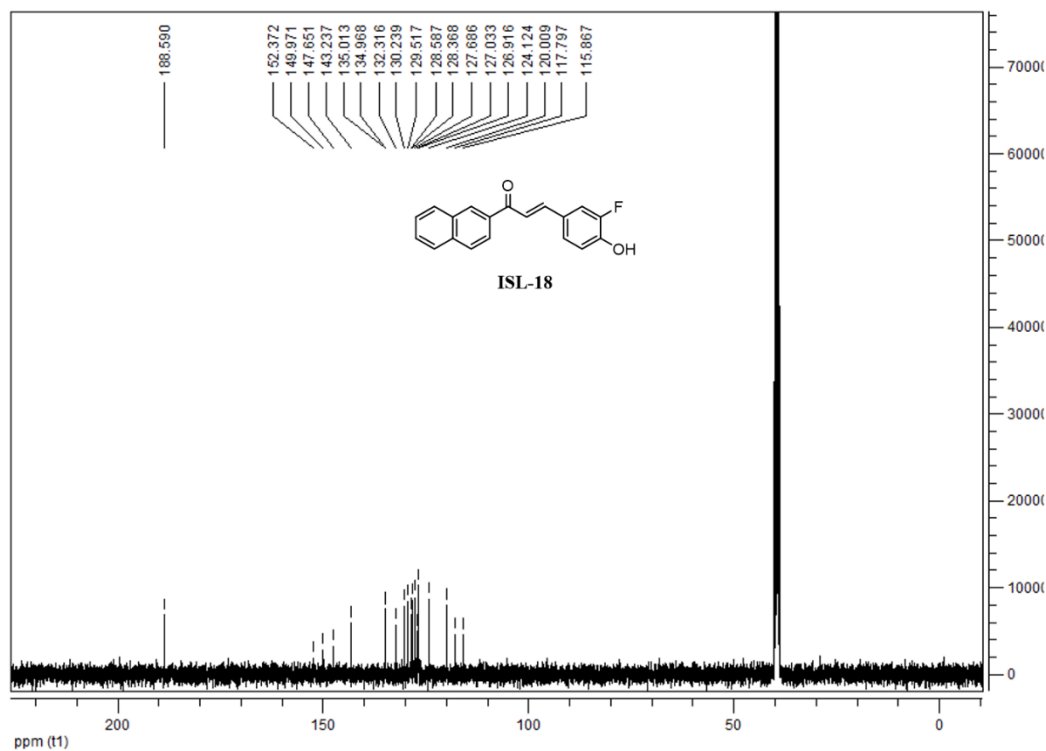


Figure S36. The ^{13}C NMR spectra of compound **ISL-18** ($\text{DMSO-}d_6$, Bruker AVANVEIII 400)

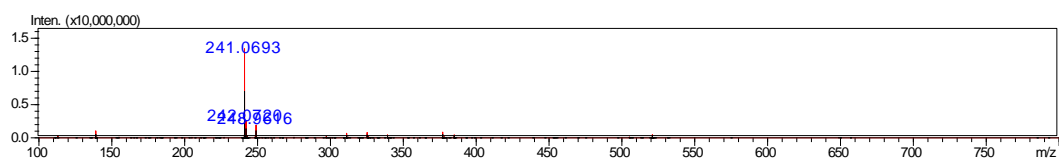


Figure S37. The High Resolution Mass Spectrometry (HRMS) spectra of compound **ISL-1** (HRMS (ESI, m/z) calcd. for $C_{15}H_{11}FO_2$ (M-H) $^-$ 241.0670, found 241.0693).

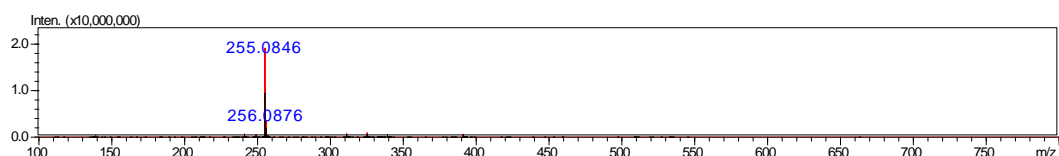


Figure S38. The HRMS spectra of compound **ISL-2** (HRMS (ESI, m/z) calcd. for $C_{16}H_{13}FO_2$ (M-H) $^-$ 255.0827, found 255.0846).

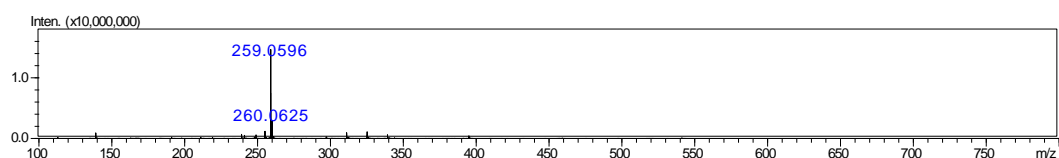


Figure S39. The HRMS spectra of compound **ISL-3** (HRMS (ESI, m/z) calcd. for $C_{15}H_{10}F_2O_2$ (M-H) $^-$ 259.0576, found 259.0596).

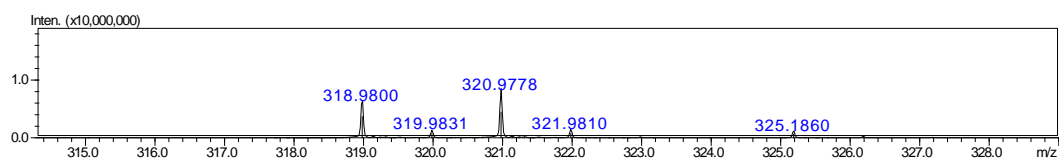


Figure S40. The HRMS spectra of compound **ISL-4** (HRMS (ESI, m/z) calcd. for $C_{15}H_{10}BrFO_2$ (M-H) $^-$ 318.9775, found 318.9800).

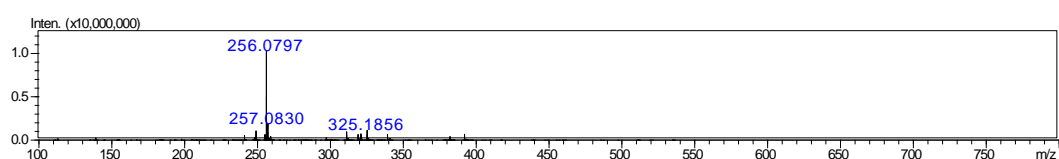


Figure S41. The HRMS spectra of compound **ISL-5** (HRMS (ESI, m/z) calcd. for $C_{15}H_{12}FNO_2$ (M-H) $^-$ 256.0779, found 256.0797).

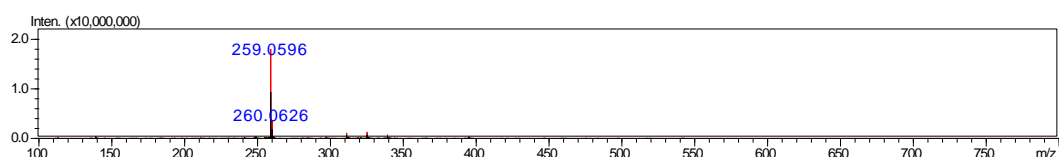


Figure S42. The HRMS spectra of compound **ISL-6** (HRMS (ESI, m/z) calcd. for $C_{15}H_{10}F_2O_2$ (M-H) $^-$ 259.0576, found 259.0596).

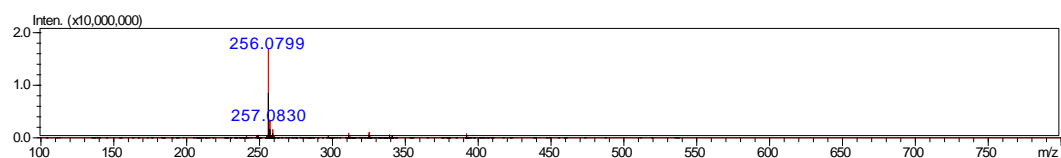


Figure S43. The HRMS spectra of compound **ISL-7** (HRMS (ESI, m/z) calcd. for $C_{15}H_{12}FNO_2$ (M-H)⁻ 256.0779, found 256.0799).

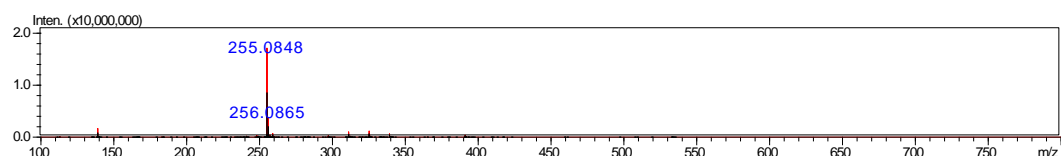


Figure S44. The HRMS spectra of compound **ISL-8** (HRMS (ESI, m/z) calcd. for $C_{16}H_{13}FO_2$ (M-H)⁻ 255.0827, found 255.0848).

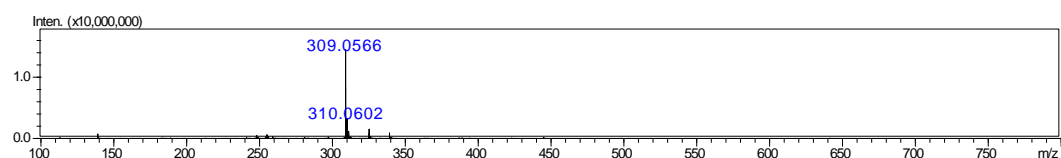


Figure S45. The HRMS spectra of compound **ISL-9** (HRMS (ESI, m/z) calcd. for $C_{16}H_{10}F_4O_2$ (M-H)⁻ 309.0544, found 309.0566).

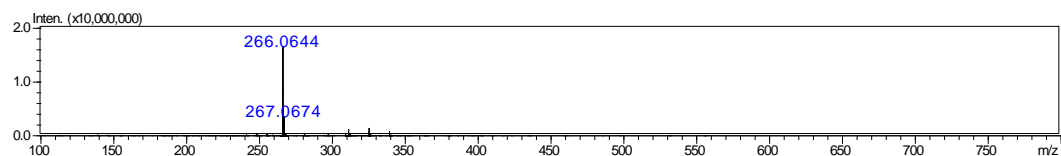


Figure S46. The HRMS spectra of compound **ISL-10** (HRMS (ESI, m/z) calcd. for $C_{16}H_{10}FNO_2$ (M-H)⁻ 266.0623, found 266.0644).

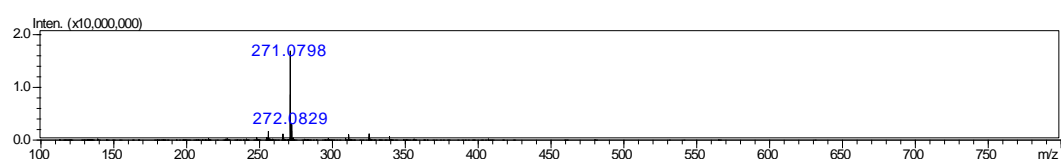


Figure S47. The HRMS spectra of compound **ISL-11** (HRMS (ESI, m/z) calcd. for $C_{16}H_{13}FO_3$ (M-H)⁻ 271.0776, found 271.0798).

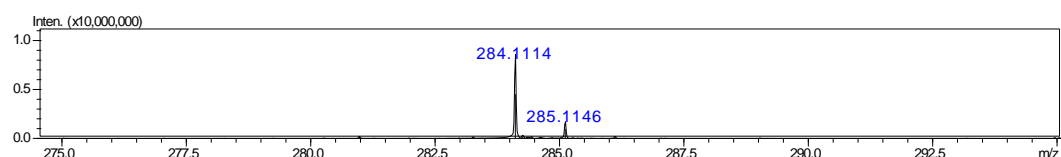


Figure S48. The HRMS spectra of compound **ISL-12** (HRMS (ESI, m/z) calcd. for $C_{17}H_{16}FNO_2$ (M-H)⁻ 284.1092, found 284.1114).

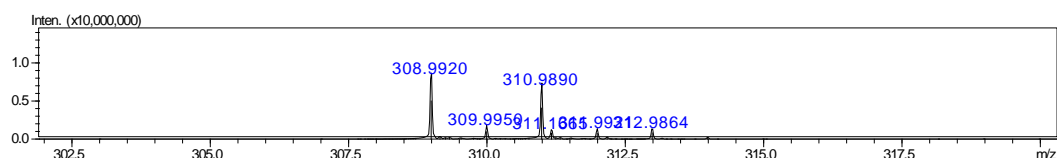


Figure S49. The HRMS spectra of compound **ISL-13** (HRMS (ESI, m/z) calcd. for $C_{15}H_9Cl_2FO_2$ (M-H)⁻ 308.9891, found 308.9920).

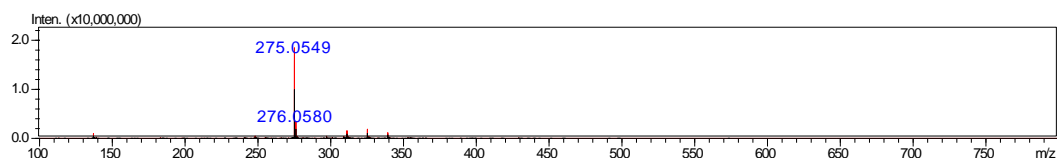


Figure S50. The HRMS spectra of compound **ISL-14** (HRMS (ESI, m/z) calcd. for $C_{15}H_{10}F_2O_3$ (M-H)⁻ 275.0525, found 275.0549).

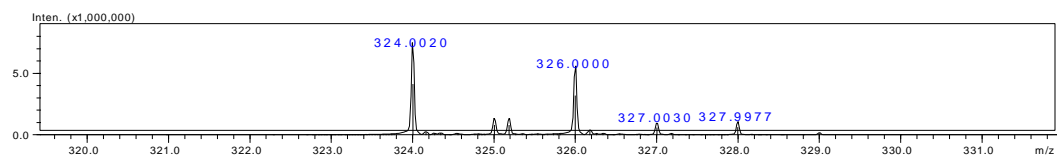


Figure S51. The HRMS spectra of compound **ISL-15** (HRMS (ESI, m/z) calcd. for $C_{15}H_{10}Cl_2FNO_2$ (M-H)⁻ 324.0000, found 324.0020).

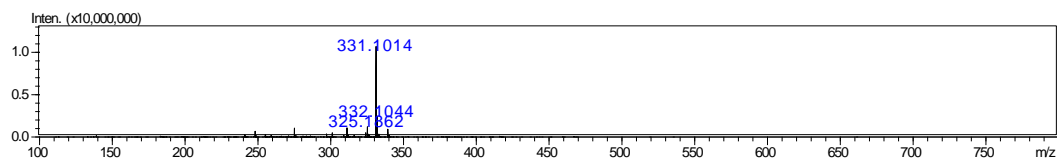


Figure S52. The HRMS spectra of compound **ISL-16** (HRMS (ESI, m/z) calcd. for $C_{18}H_{17}FO_5$ (M-H)⁻ 331.0987, found 331.1014).

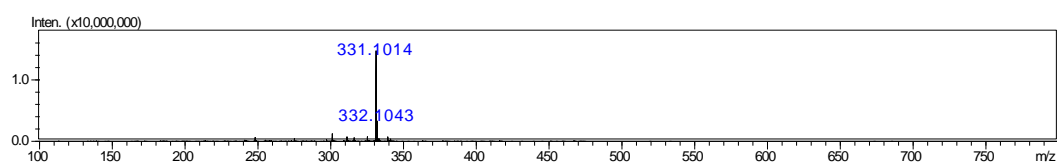


Figure S53. The HRMS spectra of compound **ISL-17** (HRMS (ESI, m/z) calcd. for $C_{18}H_{17}FO_5$ (M-H)⁻ 331.0987, found 331.1014).

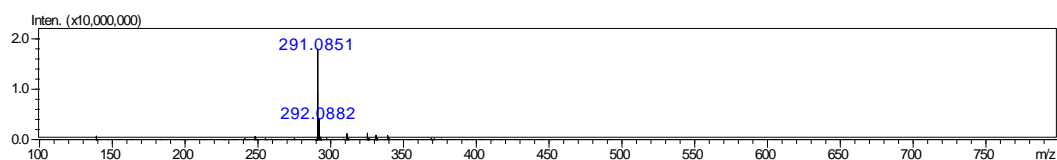


Figure S54. The HRMS spectra of compound **ISL-18** (HRMS (ESI, m/z) calcd. for $C_{19}H_{13}FO_2$ (M-H)⁻ 291.0827, found 291.0851).