

Supporting Information

Synthesis and anti-hepatocellular carcinoma evaluation of salicylic acid- modified indole trimethoxy flavonoid derivatives

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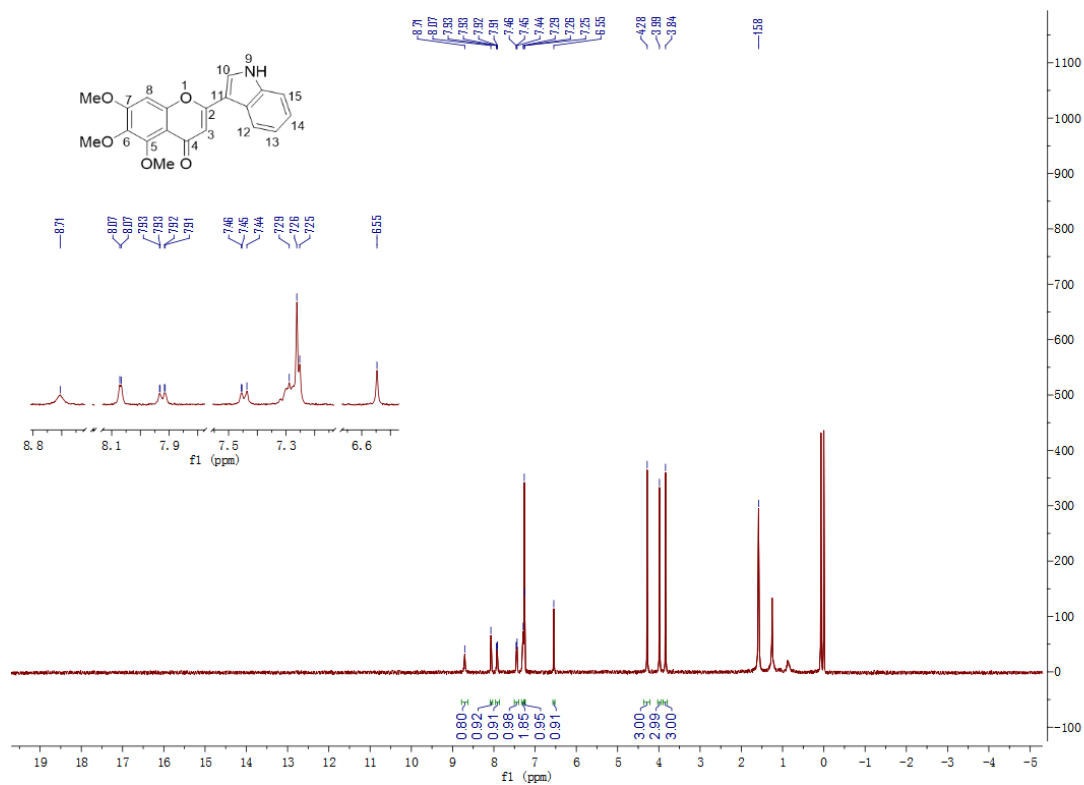


Figure S1. ¹H-NMR (400 MHz) spectrum of compound **6** in CDCl₃.

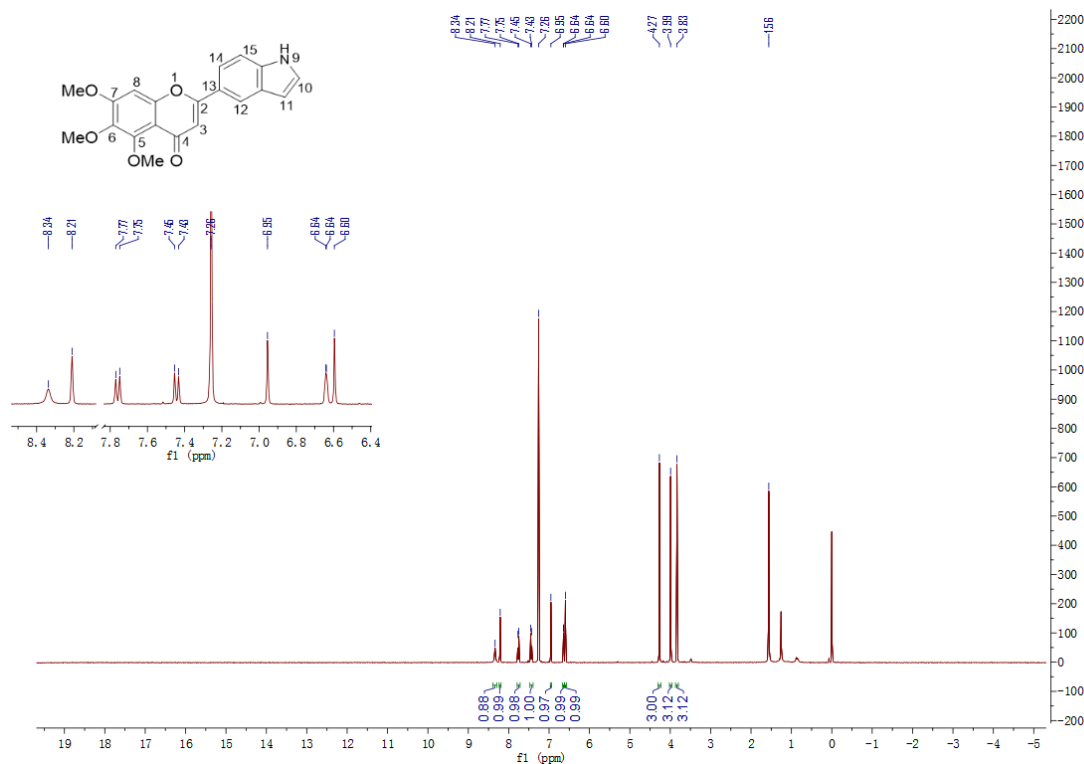


Figure S2. ¹H-NMR (400 MHz) spectrum of compound **7** in CDCl₃.

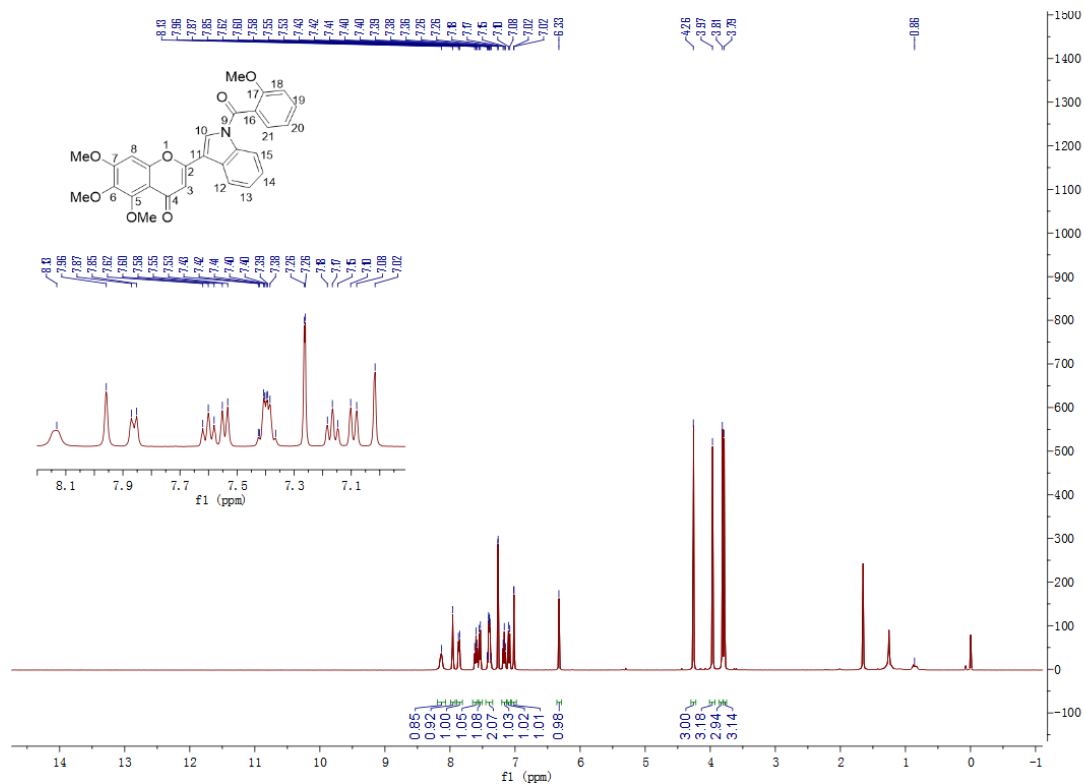


Figure S3. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **8a** in CDCl_3 .

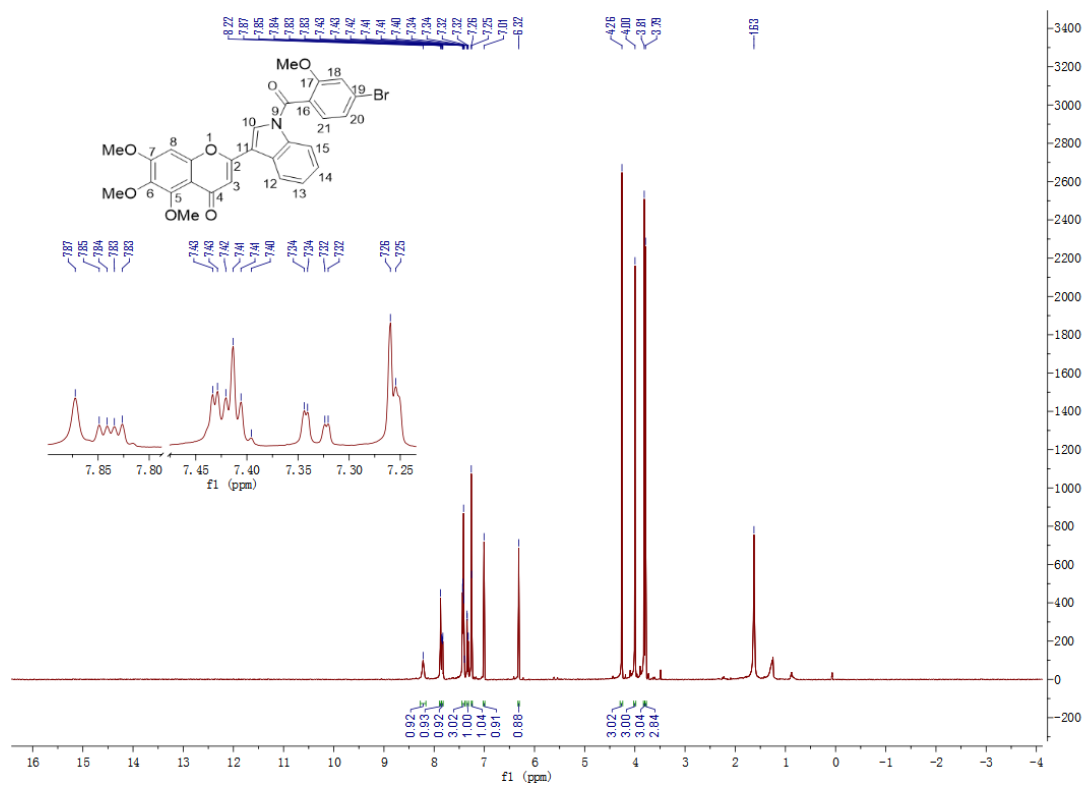


Figure S4. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **8b** in CDCl_3 .

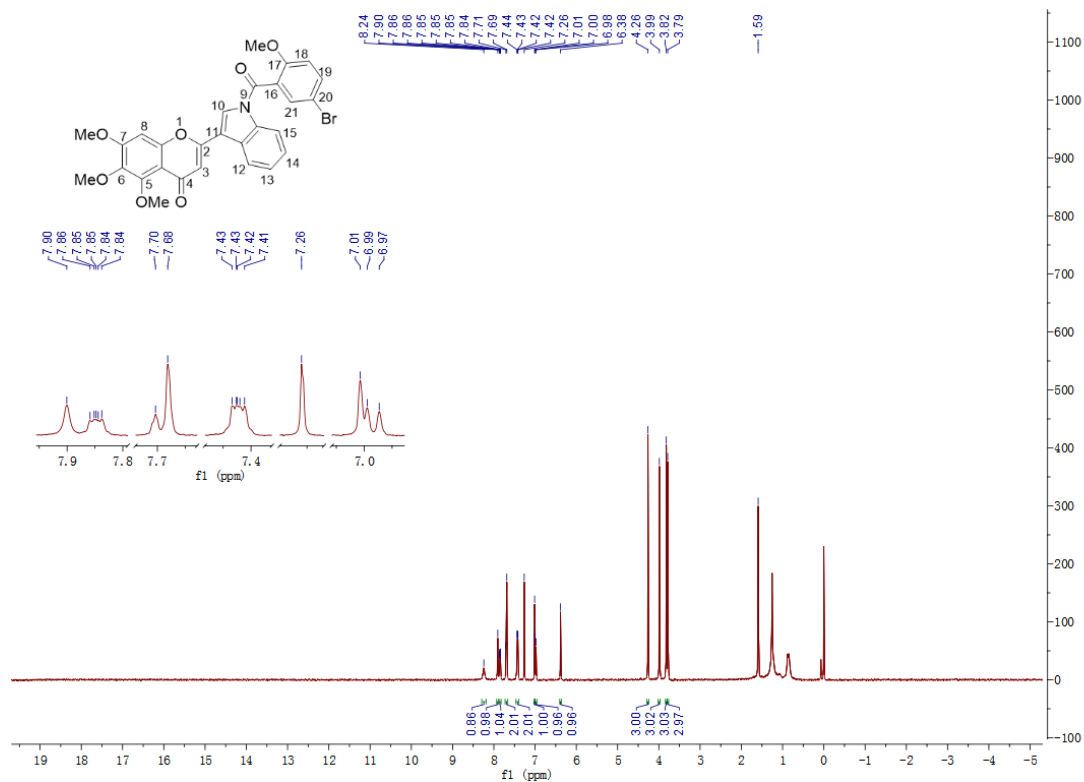


Figure S5. ¹H-NMR (400 MHz) spectrum of compound **8c** in CDCl₃.

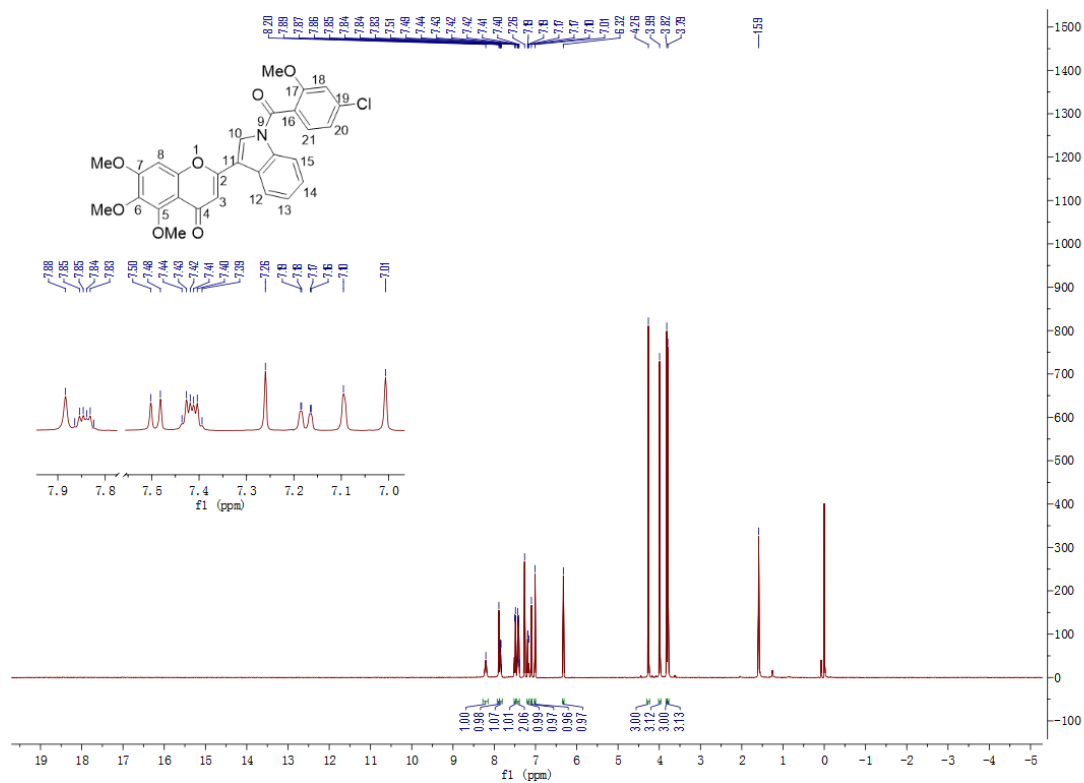


Figure S6. ¹H-NMR (400 MHz) spectrum of compound **8d** in CDCl₃.

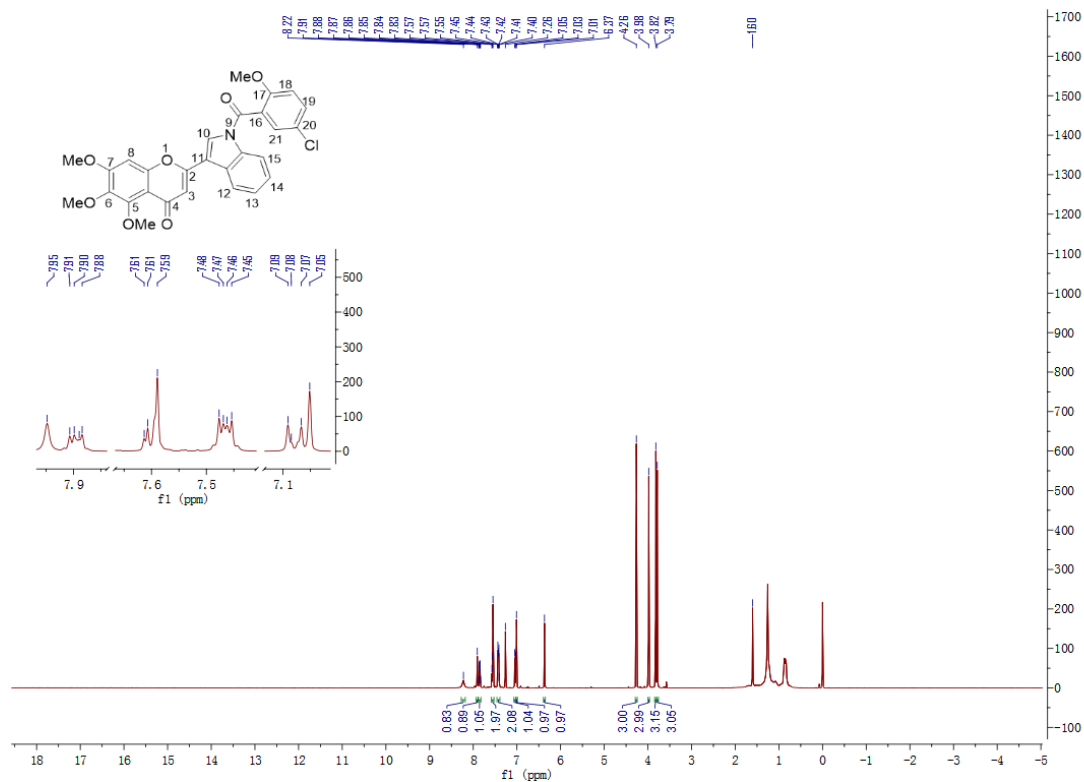


Figure S7. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **8e** in CDCl_3 .

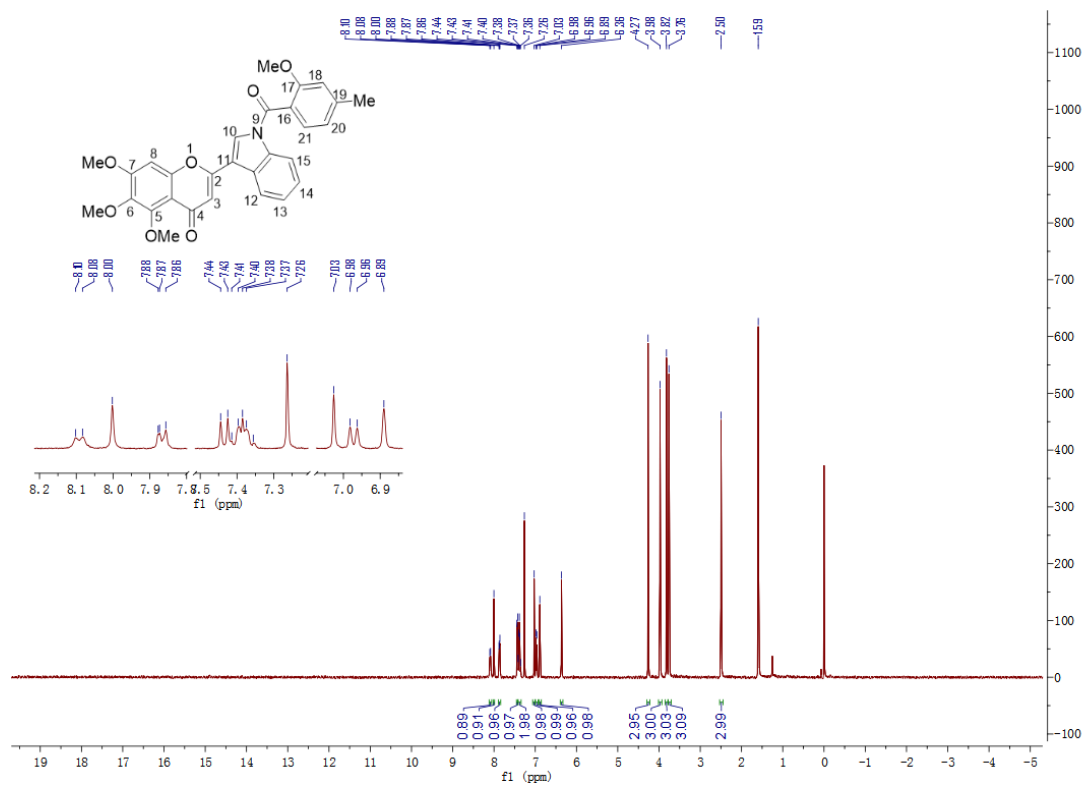


Figure S8. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **8f** in CDCl_3 .

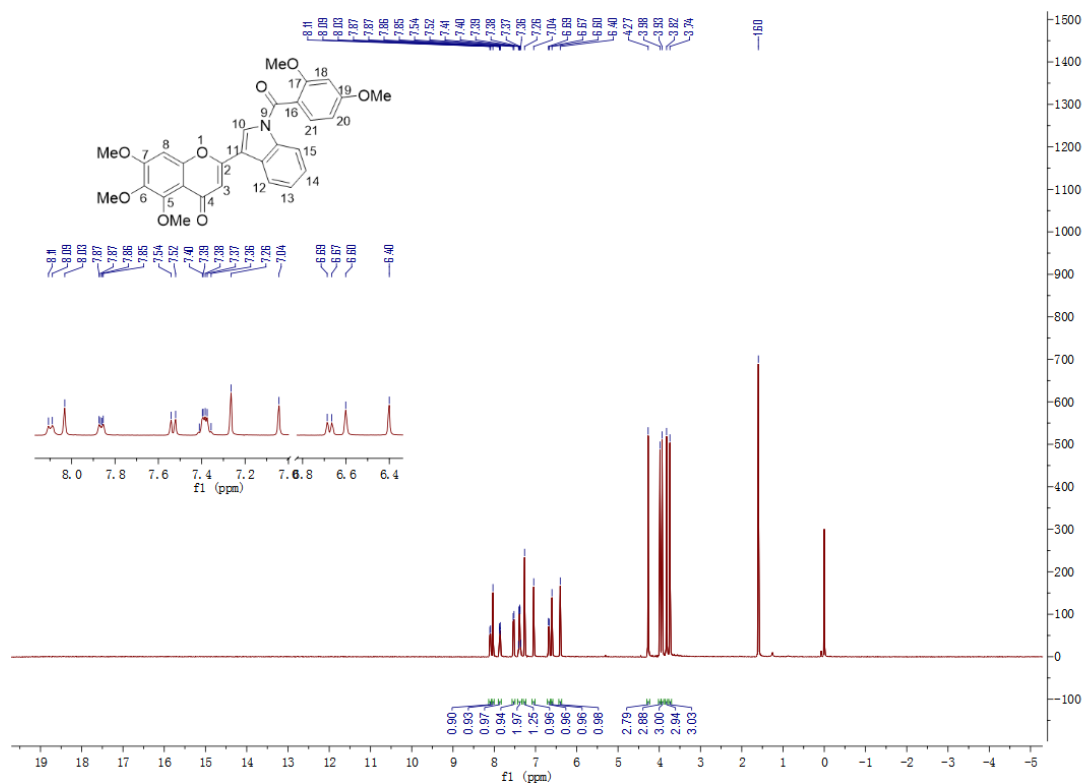


Figure S9. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **8g** in CDCl_3 .

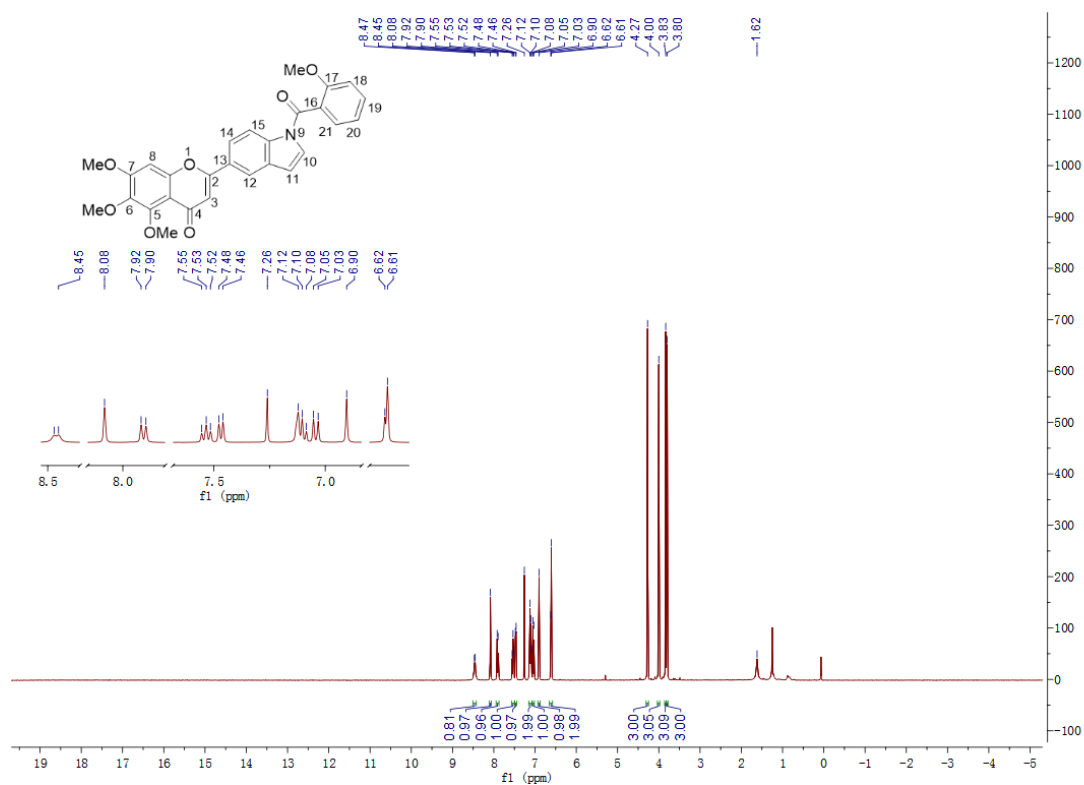


Figure S10. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **9a** in CDCl_3 .

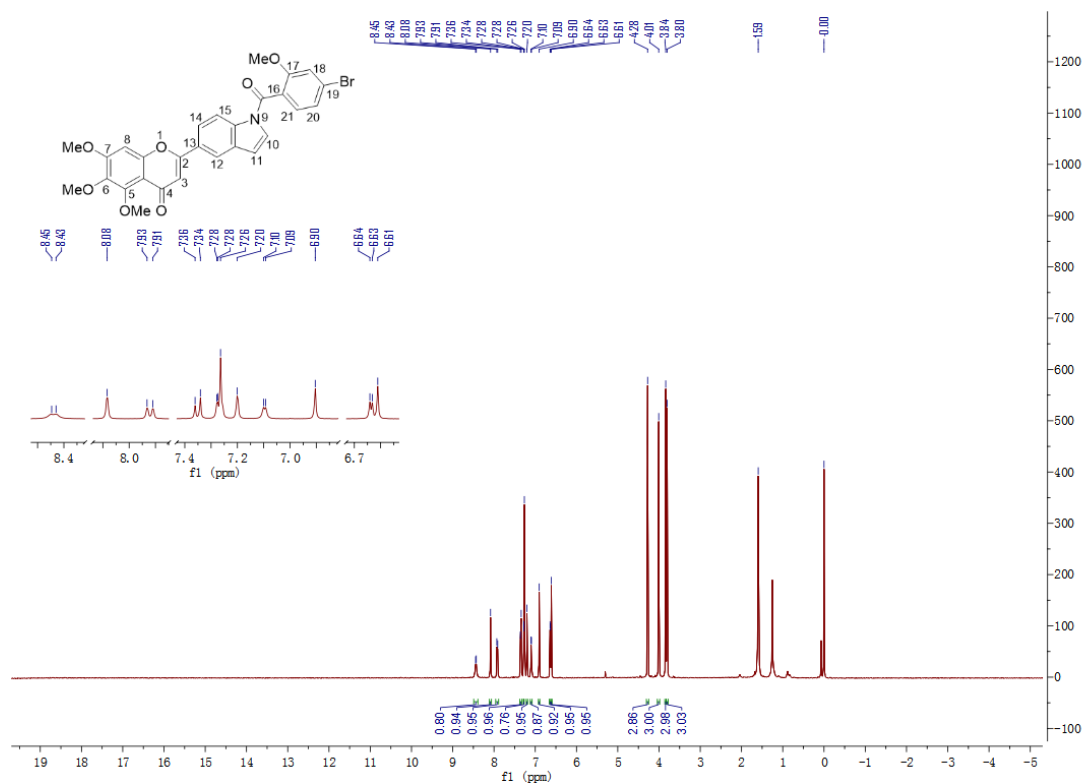


Figure S11. ¹H-NMR (400 MHz) spectrum of compound **9b** in CDCl₃.

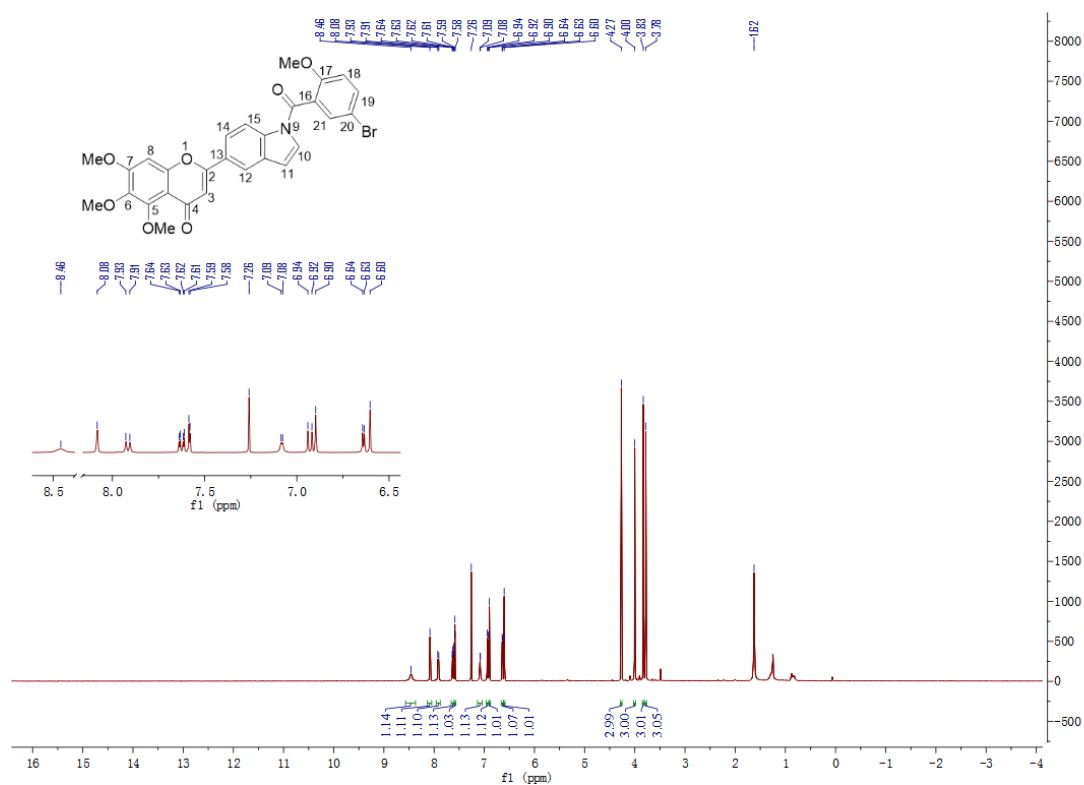


Figure S12. ¹H-NMR (400 MHz) spectrum of compound **9c** in CDCl₃.

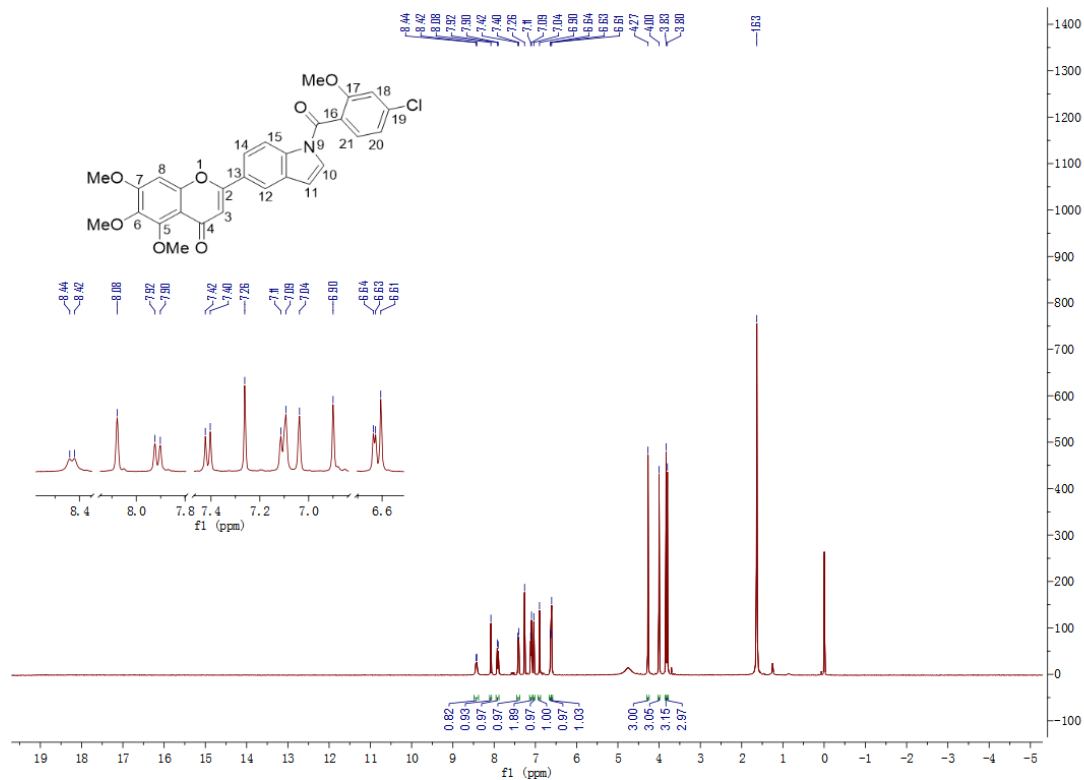


Figure S13. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **9d** in CDCl_3 .

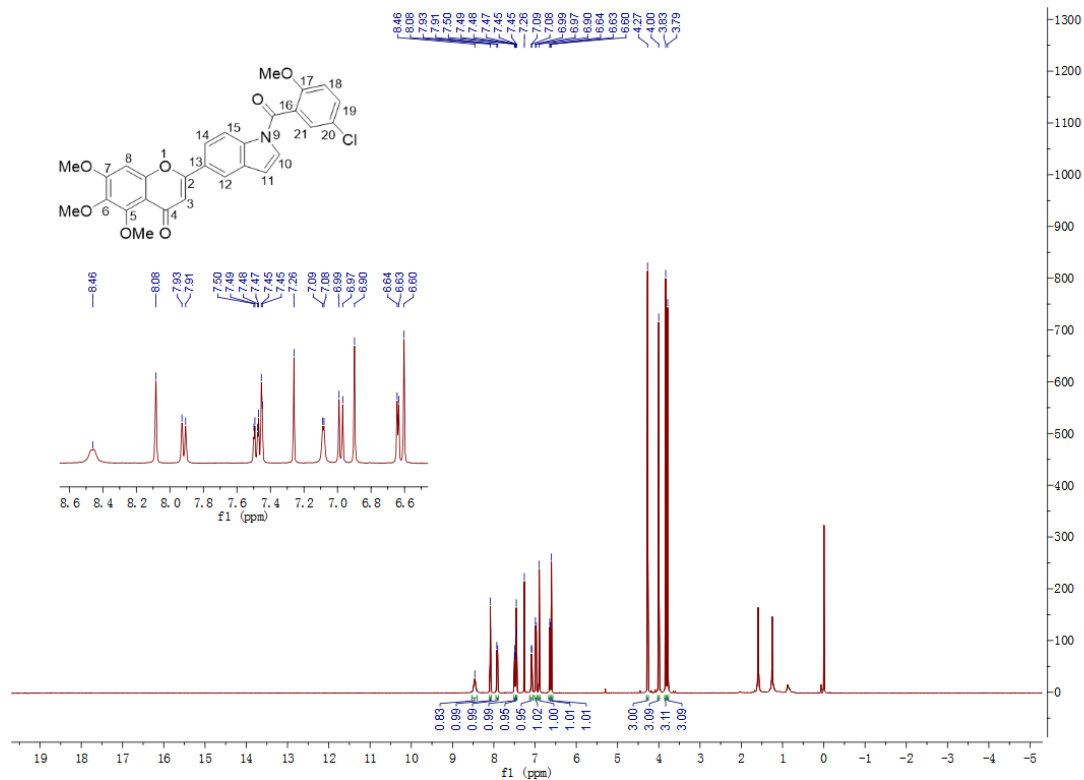


Figure S14. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **9e** in CDCl_3 .

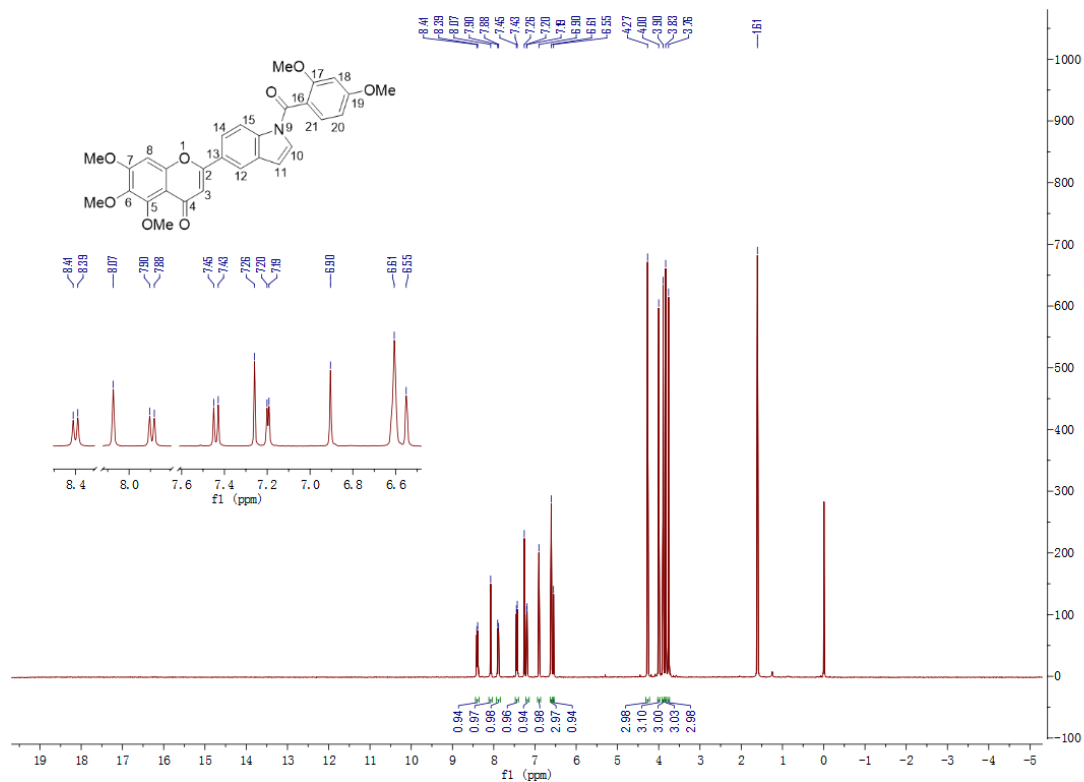


Figure S15. $^1\text{H-NMR}$ (400 MHz) spectrum of compound **9f** in CDCl_3 .

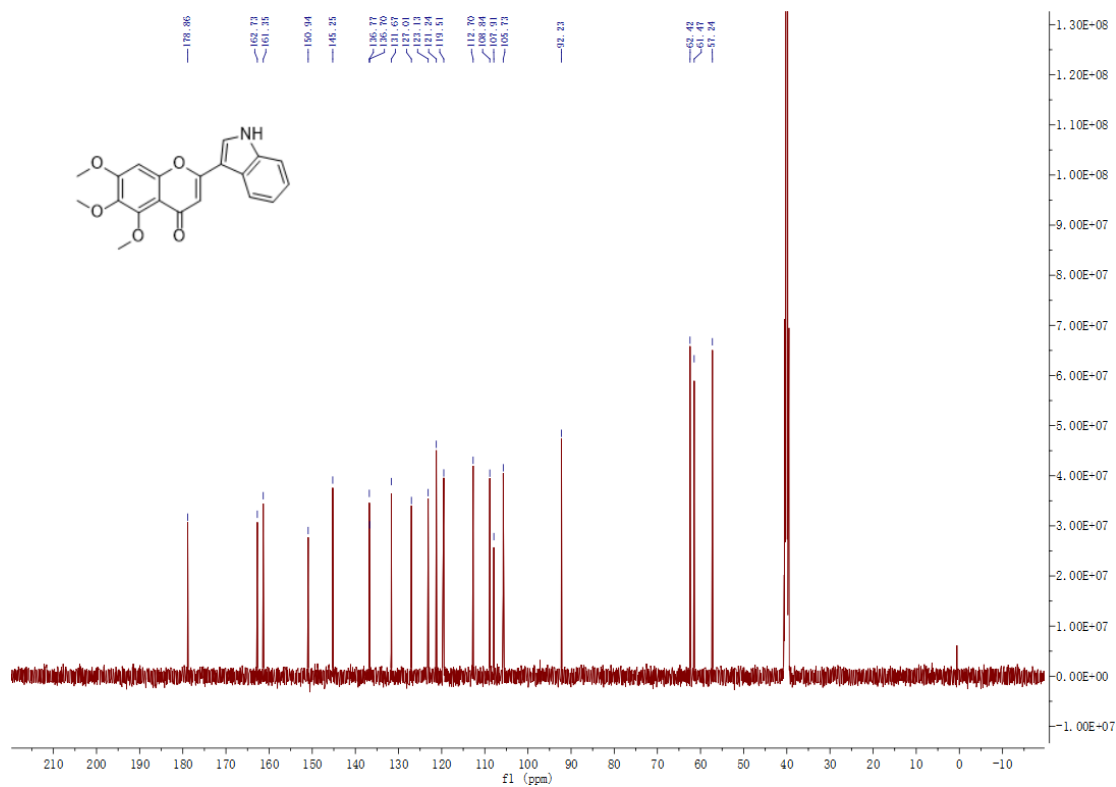


Figure S16. $^{13}\text{C-NMR}$ (125 MHz) spectrum of compound **6** in $\text{DMSO-}d_6$.

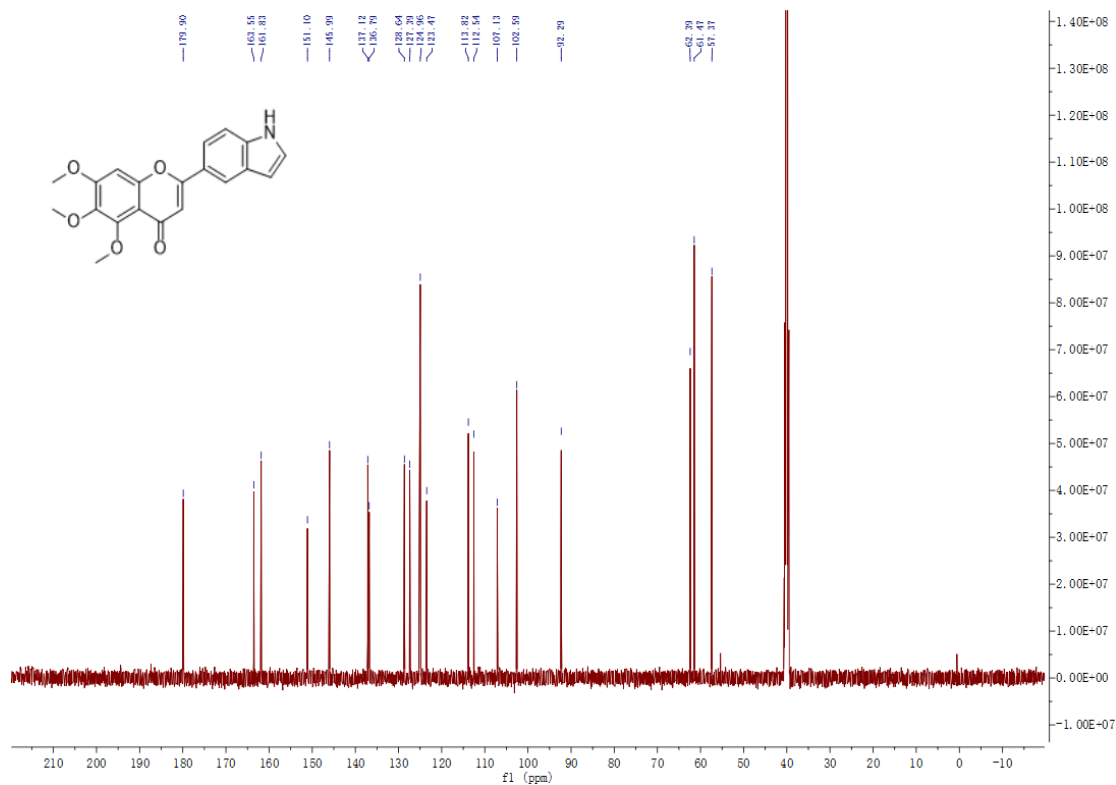


Figure S17. ^{13}C -NMR (125 MHz) spectrum of compound **7** in $\text{DMSO-}d_6$.

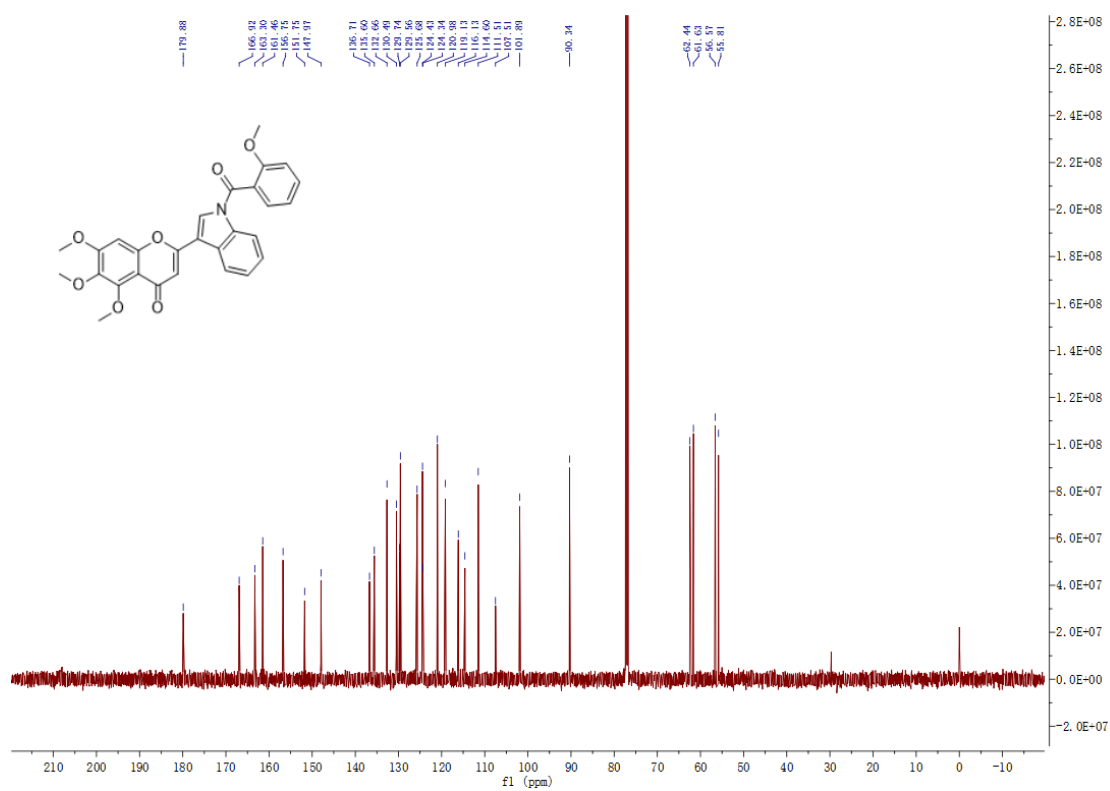


Figure S18. ^{13}C -NMR (125 MHz) spectrum of compound **8a** in CDCl_3 .

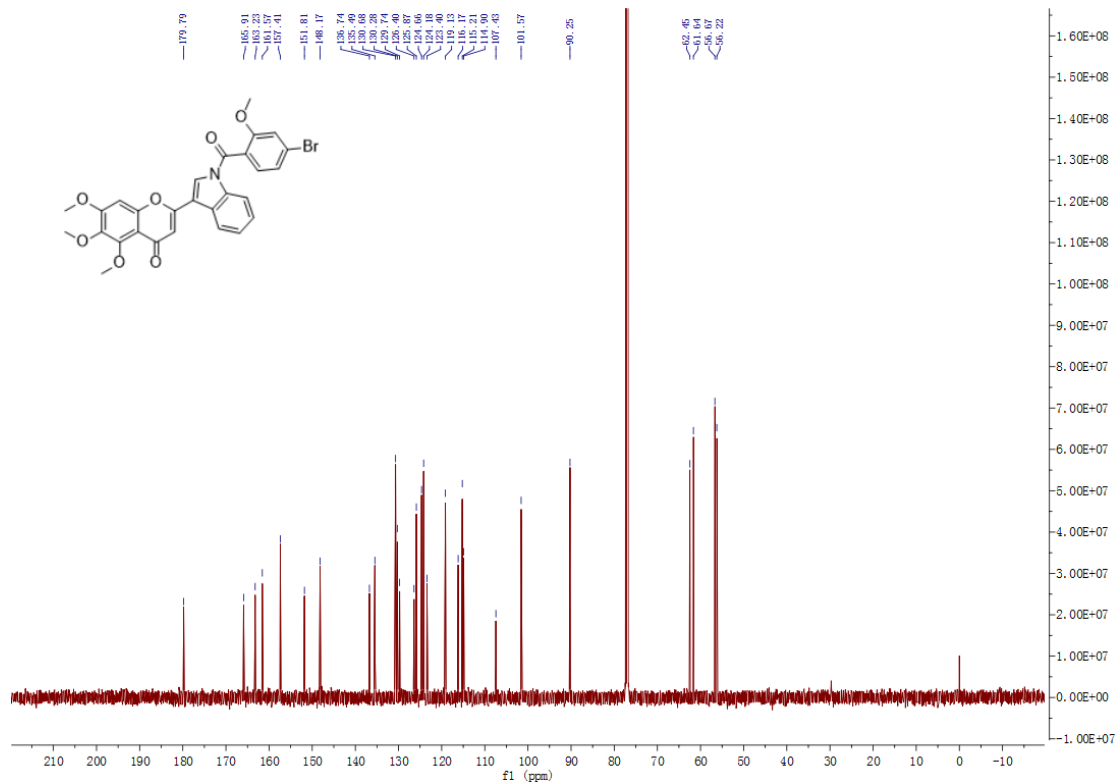


Figure S19. ^{13}C -NMR (125 MHz) spectrum of compound **8b** in CDCl_3 .

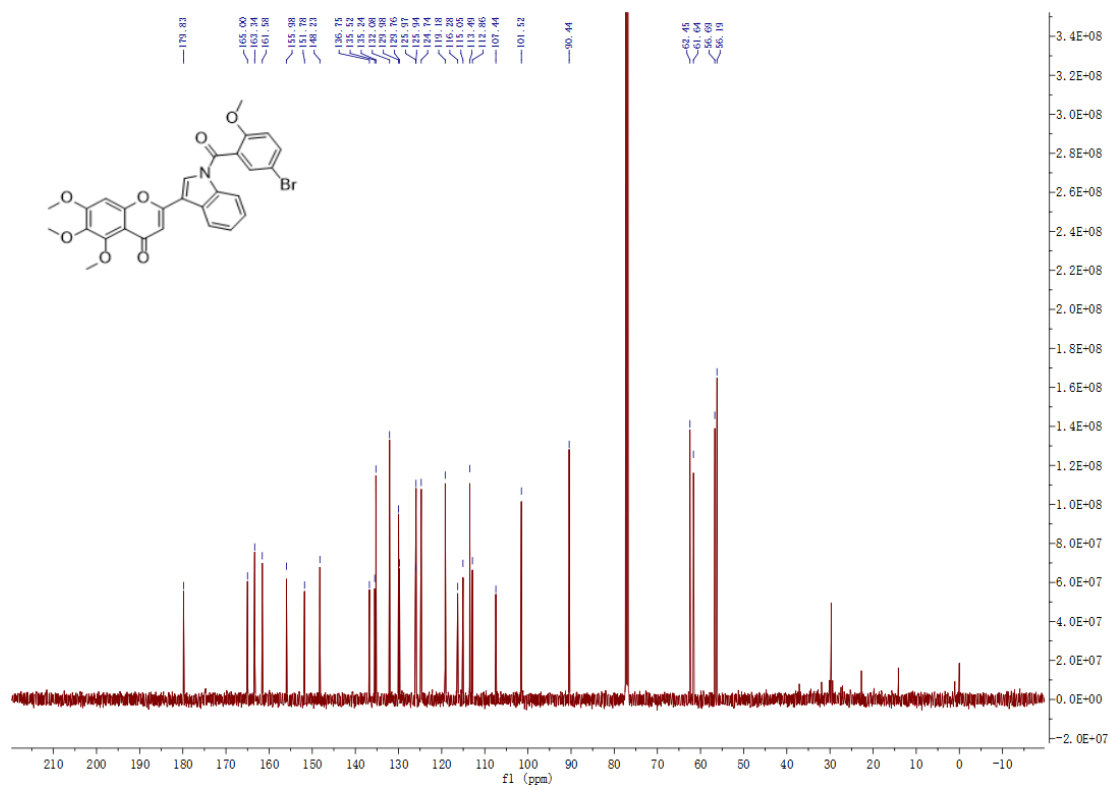


Figure S20. ^{13}C -NMR (125 MHz) spectrum of compound **8c** in CDCl_3 .

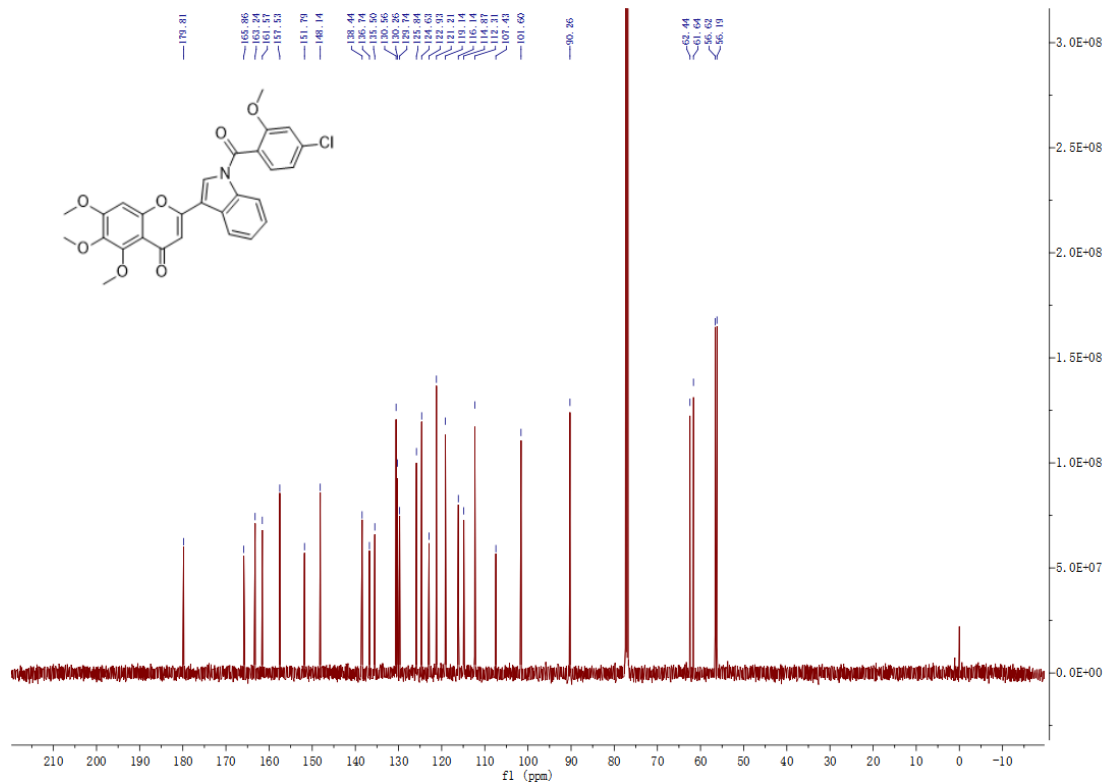


Figure S21. $^{13}\text{C-NMR}$ (125 MHz) spectrum of compound **8d** in CDCl_3 .

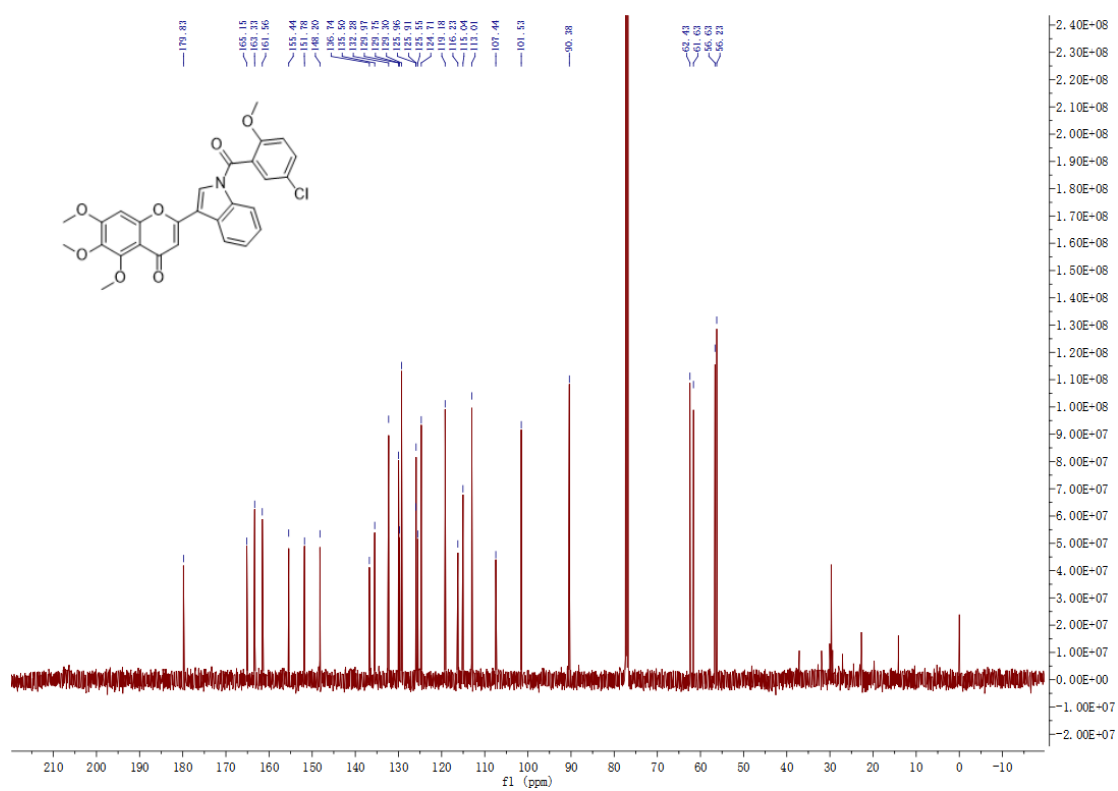


Figure S22. $^{13}\text{C-NMR}$ (125 MHz) spectrum of compound **8e** in CDCl_3 .

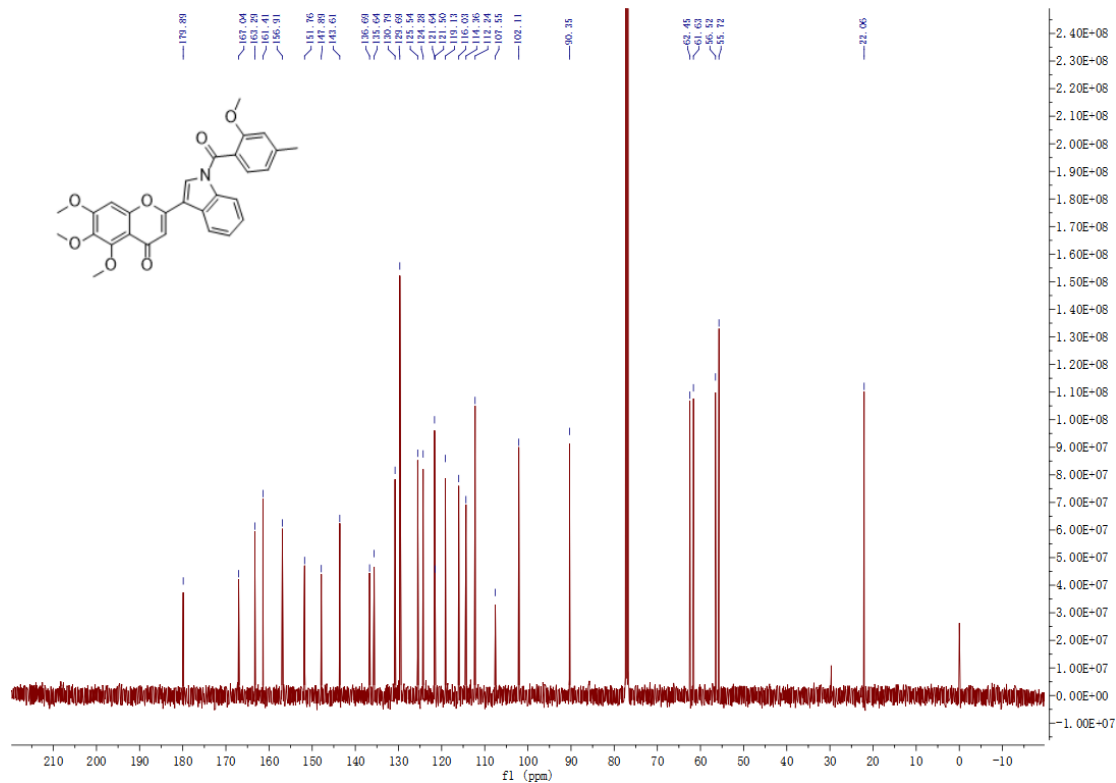


Figure S23. ^{13}C -NMR (125 MHz) spectrum of compound **8f** in CDCl_3 .

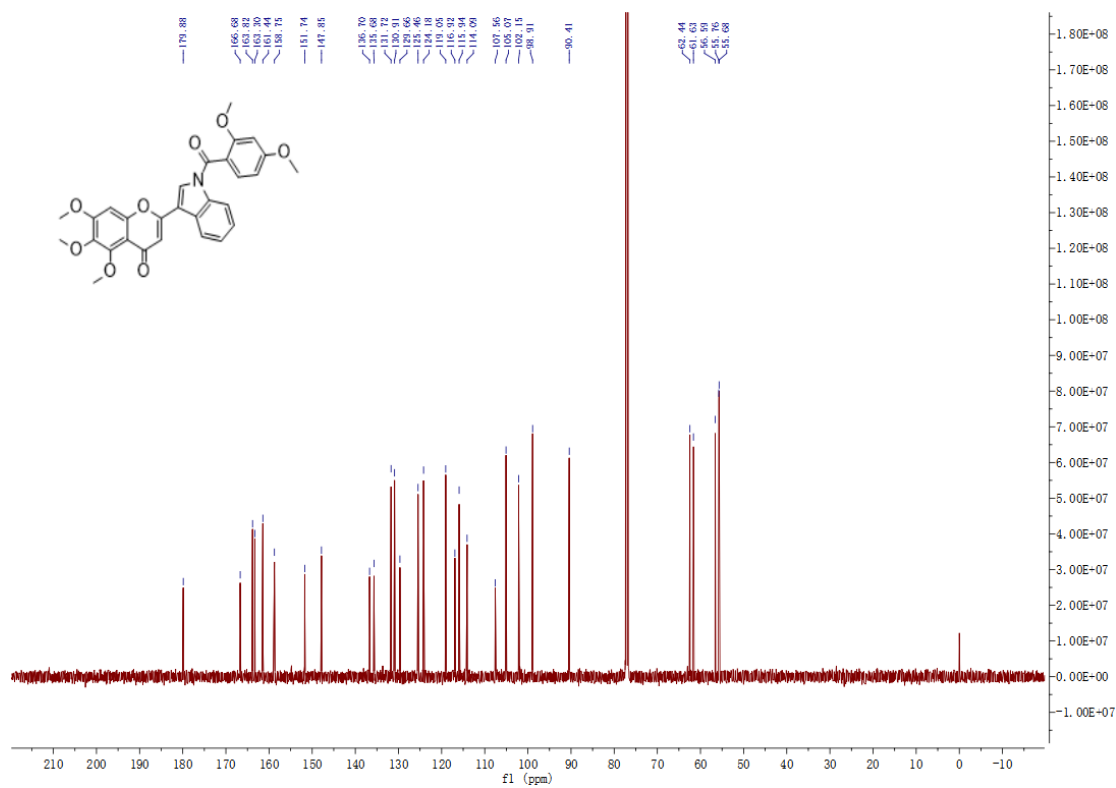


Figure S24. ^{13}C -NMR (125 MHz) spectrum of compound **8g** in CDCl_3 .

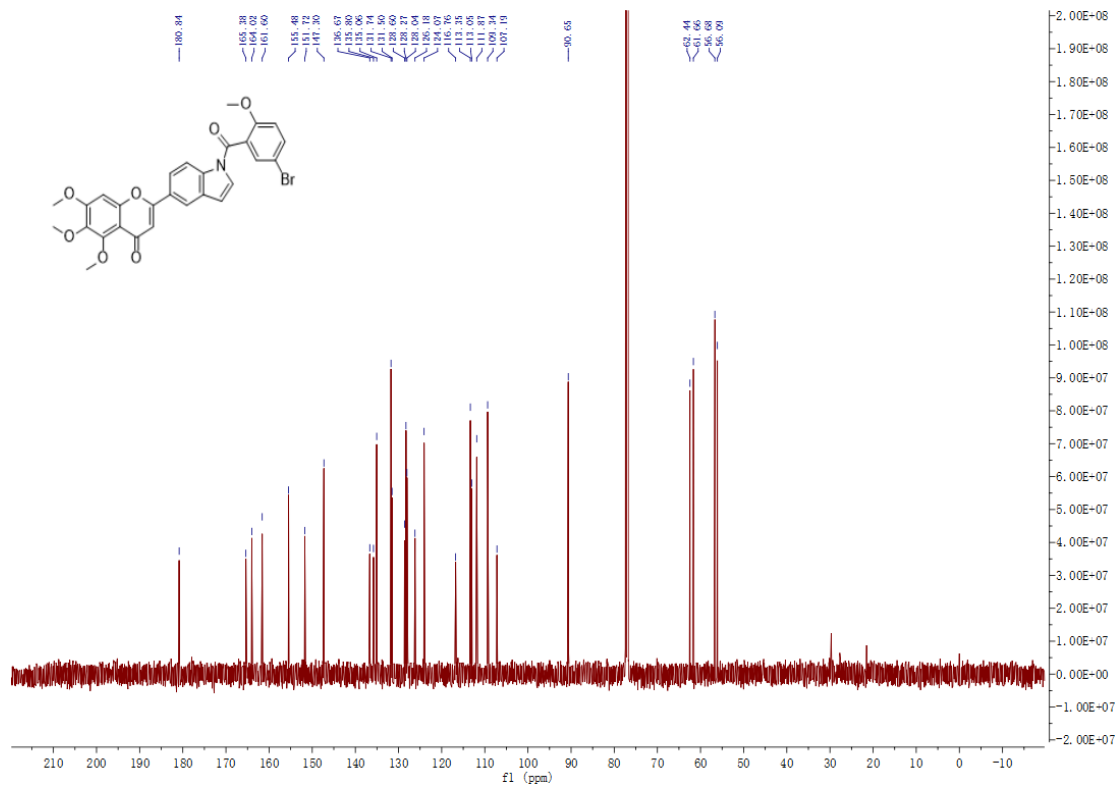


Figure S25. ^{13}C -NMR (125 MHz) spectrum of compound 9c in CDCl_3 .

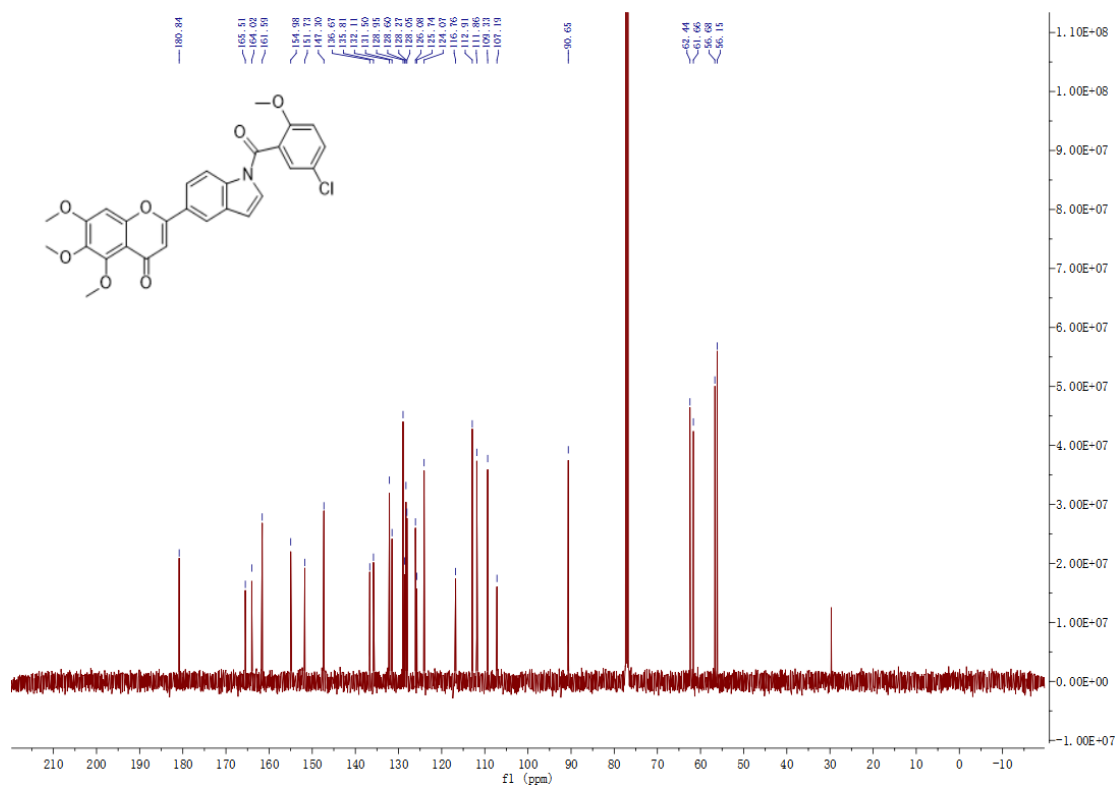


Figure S26. ^{13}C -NMR (125 MHz) spectrum of compound 9e in CDCl_3 .

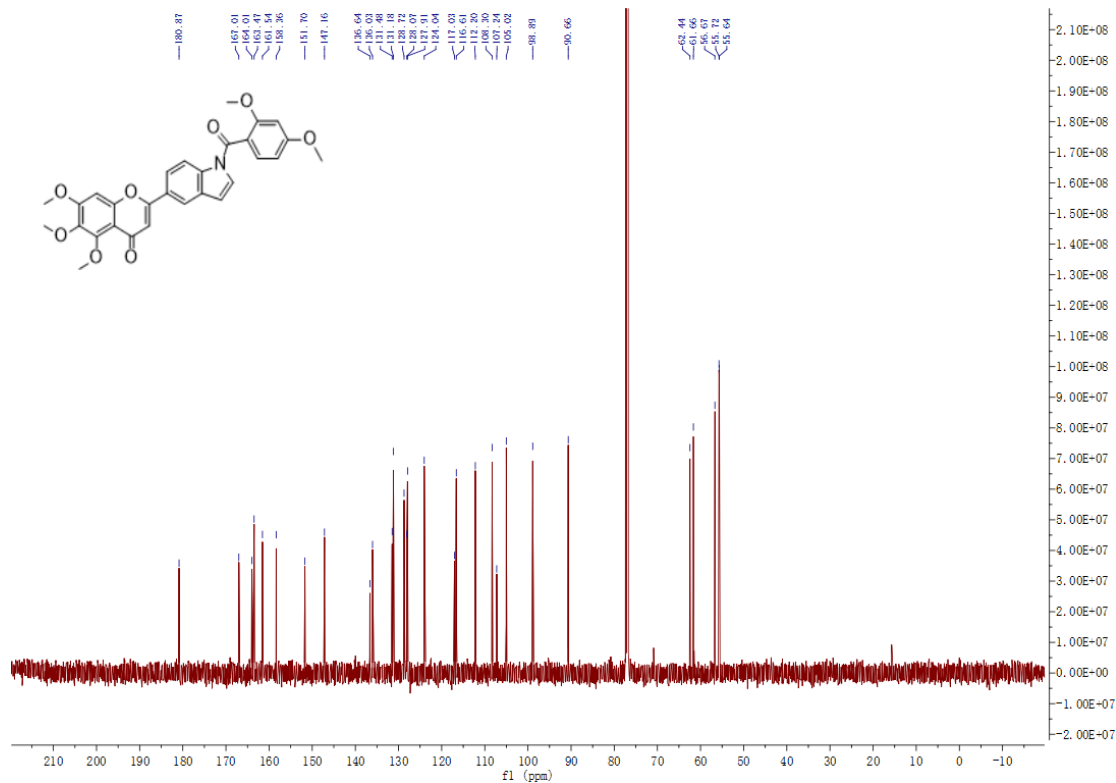


Figure S27. ^{13}C -NMR (125 MHz) spectrum of compound **9f** in CDCl_3 .

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

554 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

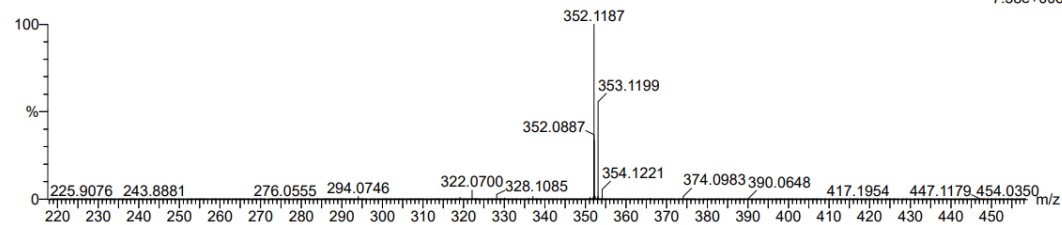
Elements Used:

C: 20-20 H: 18-18 N: 0-5 O: 0-200 S: 0-6

2

0312-2-1a 206 (1.153)

1: TOF MS ES+
7.38e+006



Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
352.1187	352.1185	0.2	0.6	12.5	1309.4	n/a	n/a	C ₂₀ H ₁₈ N O ₅

Figure S28. HRMS spectrum of compound **6**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

99 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

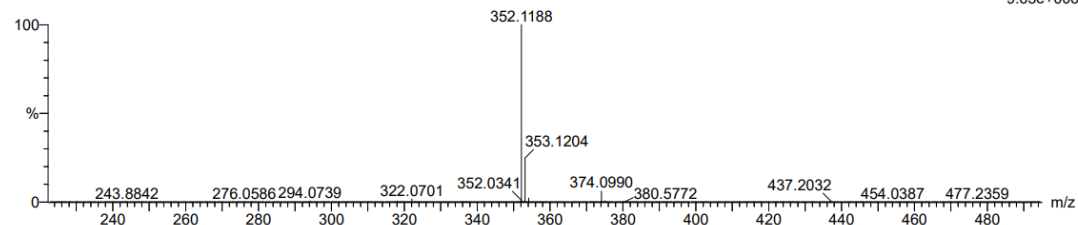
Elements Used:

C: 20-20 H: 18-18 N: 0-5 O: 0-200

2

0312-2-2a 190 (1.069)

1: TOF MS ES+
9.65e+006



Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
352.1188	352.1185	0.3	0.9	12.5	1192.8	n/a	n/a	C20 H18 N 05

Figure S29. HRMS spectrum of compound 7.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

180 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

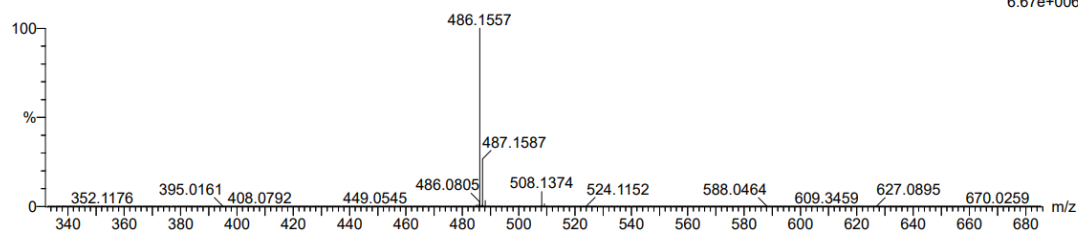
Elements Used:

C: 28-28 H: 24-24 N: 0-7 O: 0-200

2

0312-2-1b 234 (1.308)

1: TOF MS ES+
6.67e+006



Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
486.1557	486.1553	0.4	0.8	17.5	1069.4	n/a	n/a	C28 H24 N 07

Figure S30. HRMS spectrum of compound 8a.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

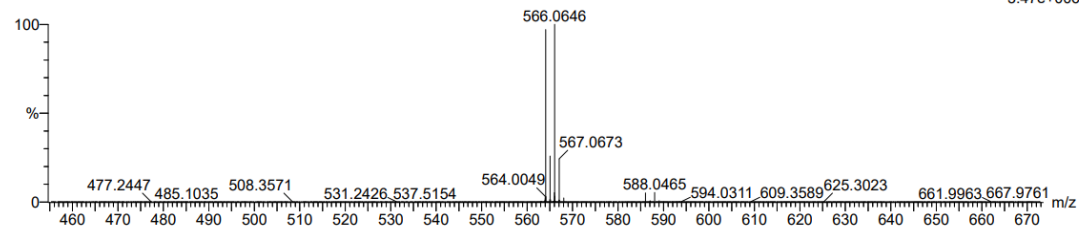
896 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-7 O: 0-200 Br: 0-8

2

0312-2-1c 265 (1.478)

1: TOF MS ES+
3.47e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
564.0662	564.0658	0.4	0.7	17.5	953.0	n/a	n/a	C28 H23 N 07 Br

Figure S31. HRMS spectrum of compound 8b.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

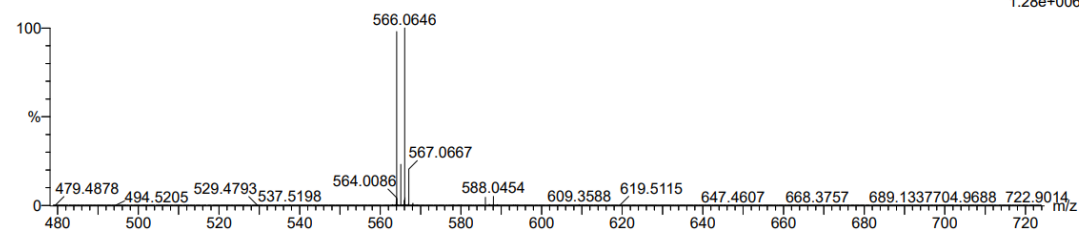
896 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-7 O: 0-200 Br: 0-8

2

0312-2-1d 282 (1.576)

1: TOF MS ES+
1.28e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
564.0662	564.0658	0.4	0.7	17.5	845.0	n/a	n/a	C28 H23 N 07 Br

Figure S32. HRMS spectrum of compound 8c.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

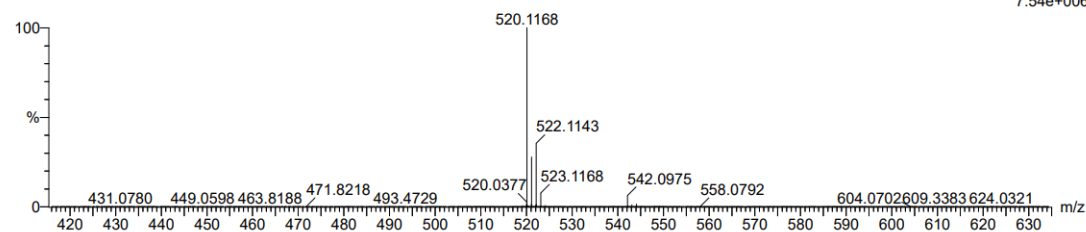
707 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-7 O: 0-200 Cl: 0-3

2

0312-2-1e 244 (1.368)

1: TOF MS ES+
7.54e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
520.1168	520.1163	0.5	1.0	17.5	1034.2	n/a	n/a	C28 H23 N 07 Cl

Figure S33. HRMS spectrum of compound **8d**.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

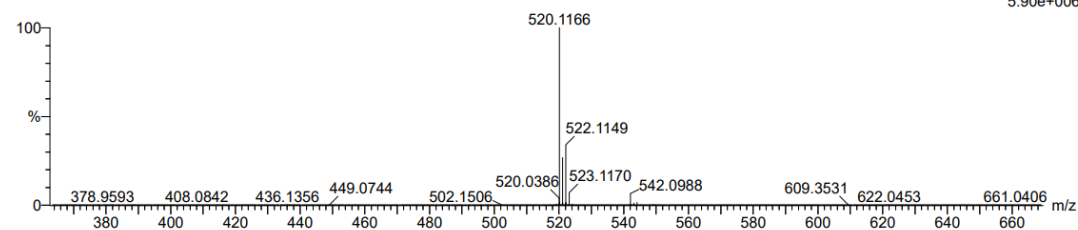
707 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-7 O: 0-200 Cl: 0-3

2

0312-2-1f 248 (1.389)

1: TOF MS ES+
5.90e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
520.1166	520.1163	0.3	0.6	17.5	1034.5	n/a	n/a	C28 H23 N 07 Cl

Figure S34. HRMS spectrum of compound **8e**.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

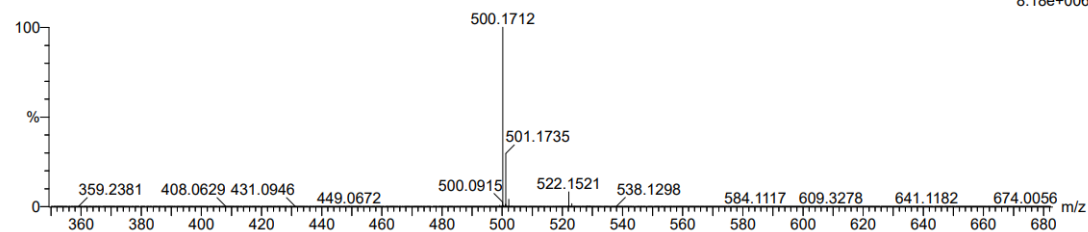
185 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 29-29 H: 26-26 N: 0-7 O: 0-200

2

0312-2-1g 232 (1.297)

1: TOF MS ES+
8.18e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
500.1712	500.1709	0.3	0.6	17.5	1044.0	n/a	n/a	C29 H26 N 07

Figure S35. HRMS spectrum of compound 8f.

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

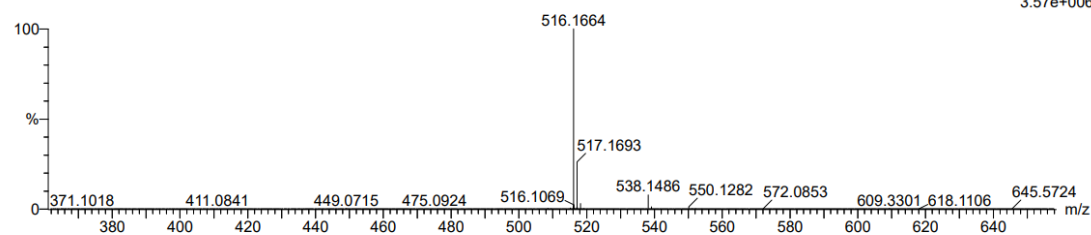
213 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 29-29 H: 26-26 N: 0-8 O: 0-200

2

0312-2-1h 235 (1.313)

1: TOF MS ES+
3.57e+006Minimum: -1.5
Maximum: 5.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
516.1664	516.1658	0.6	1.2	17.5	949.4	n/a	n/a	C29 H26 N 08

Figure S36. HRMS spectrum of compound 8g.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

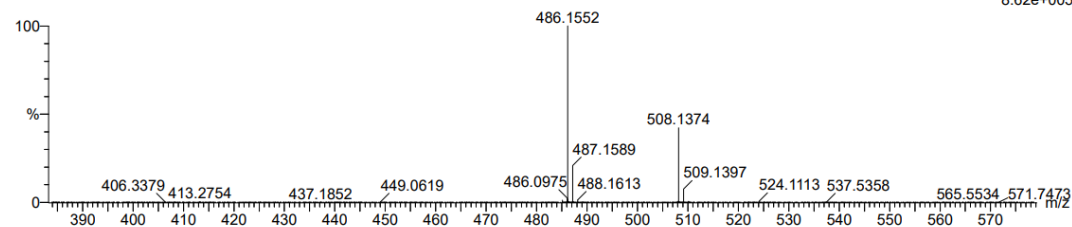
21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 24-24 N: 0-5 O: 0-8

M

0138-3-135-1-2b 291 (1.623)

1: TOF MS ES+
8.62e+005Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
486.1552	486.1553	-0.1	-0.2	17.5	719.9	n/a	n/a	C28 H24 N 07

Figure S37. HRMS spectrum of compound 9a.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

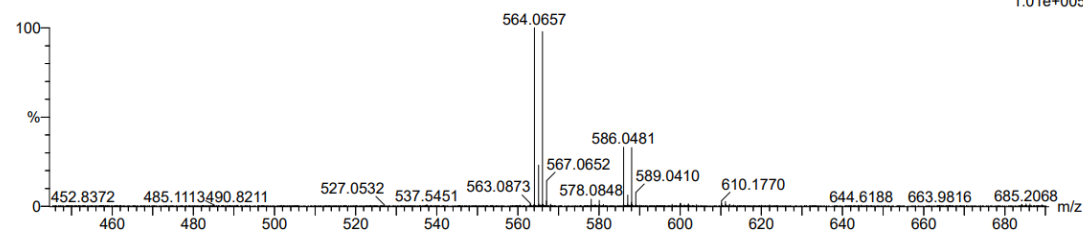
154 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-5 O: 0-8 Br: 0-3

M

0138-3-135-1-2c 312 (1.741)

1: TOF MS ES+
1.01e+005Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
564.0657	564.0658	-0.1	-0.2	17.5	596.1	n/a	n/a	C28 H23 N 07 Br

. Figure S38. HRMS spectrum of compound 9b.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

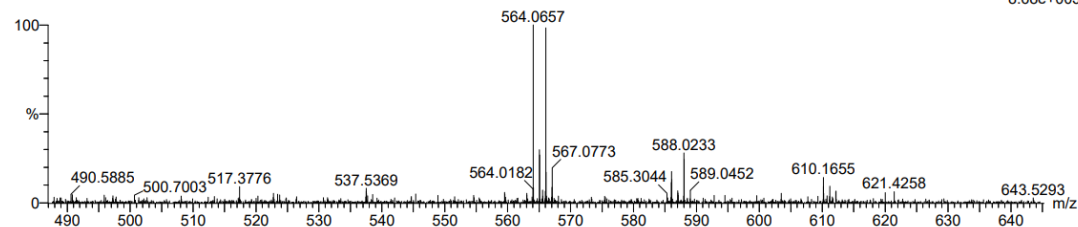
154 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-5 O: 0-8 Br: 0-3

C

0138-3-135-1-2d 330 (1.835)

1: TOF MS ES+
8.68e+003Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
564.0657	564.0658	-0.1	-0.2	17.5	435.9	n/a	n/a	C28 H23 N 07 Br

Figure S39. HRMS spectrum of compound 9c.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

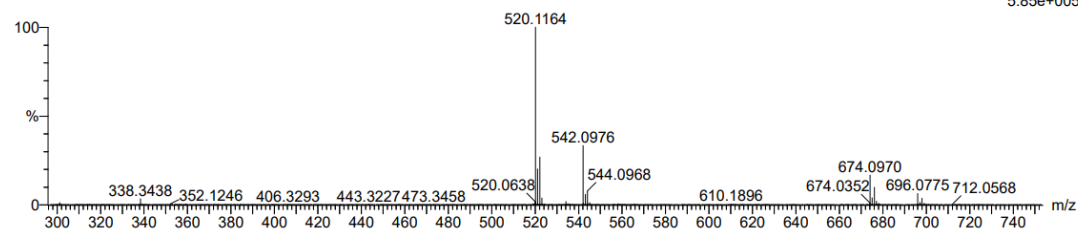
50 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-5 O: 0-8 Cl: 0-1

C

0138-3-135-1-2e 308 (1.720)

1: TOF MS ES+
5.85e+005Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
520.1164	520.1163	0.1	0.2	17.5	611.8	n/a	n/a	C28 H23 N 07 Cl

Figure S40. HRMS spectrum of compound 9d.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

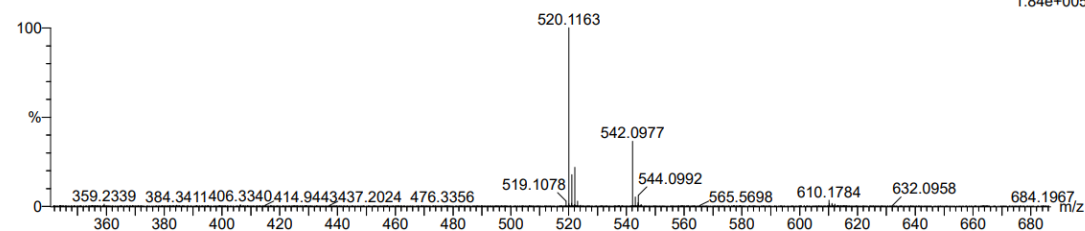
50 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 28-28 H: 23-23 N: 0-5 O: 0-8 Cl: 0-1

C

0138-3-135-1-2f 317 (1.767)

1: TOF MS ES+
1.84e+005Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
520.1163	520.1163	0.0	0.0	17.5	598.6	n/a	n/a	C28 H23 N 07 Cl

Figure S41. HRMS spectrum of compound 9e.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

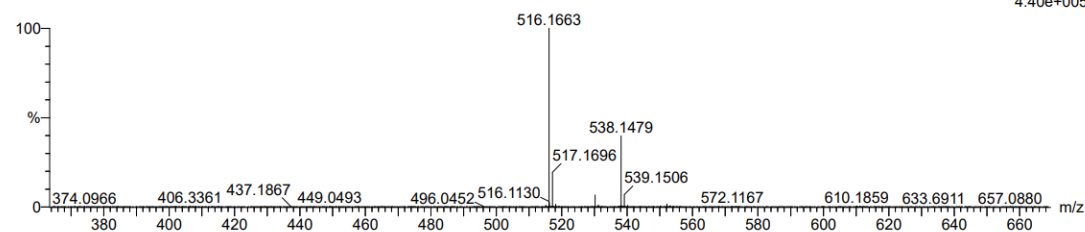
23 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 29-29 H: 26-26 N: 0-5 O: 0-8

C

0138-3-135-1-2h 303 (1.694)

1: TOF MS ES+
4.40e+005Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
516.1663	516.1658	0.5	1.0	17.5	630.1	n/a	n/a	C29 H26 N 08

Figure S42. HRMS spectrum of compound 9f.