

Supplementary Materials

The green synthesis of indeno[1,2-b]quinoxalines using β -Cyclodextrin as catalyst

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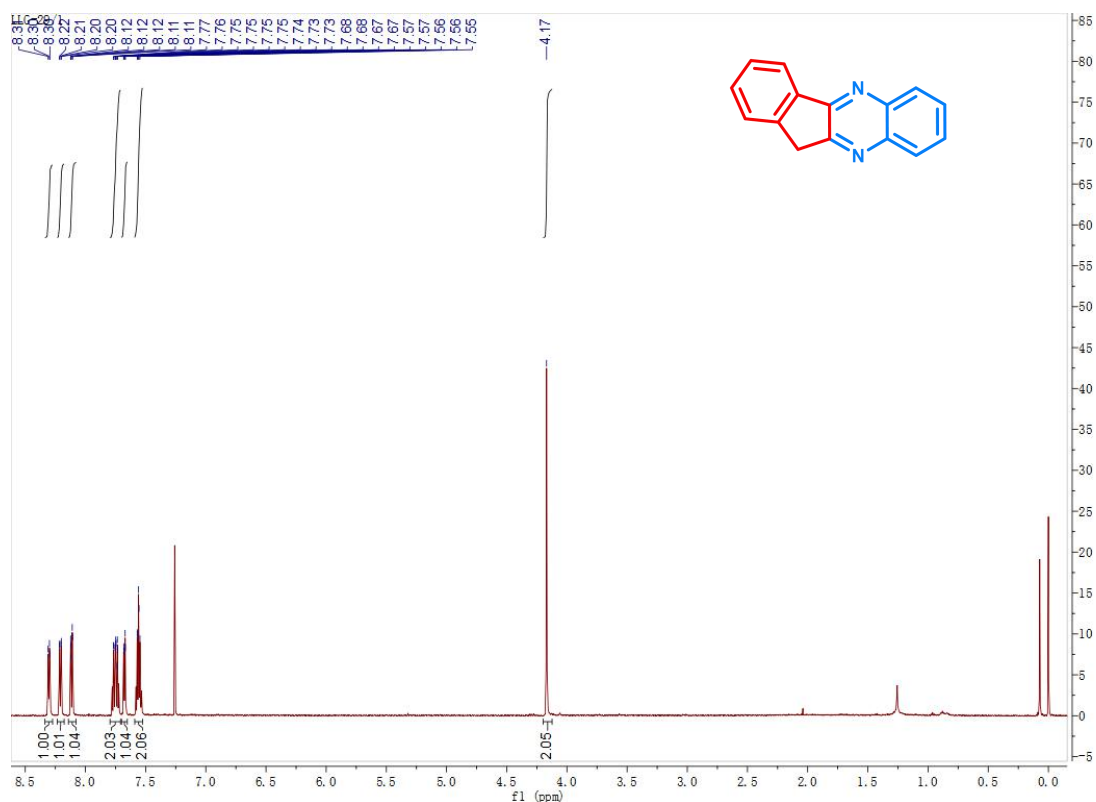


Figure S1. ¹H NMR spectrum of compound **2.3aa**.

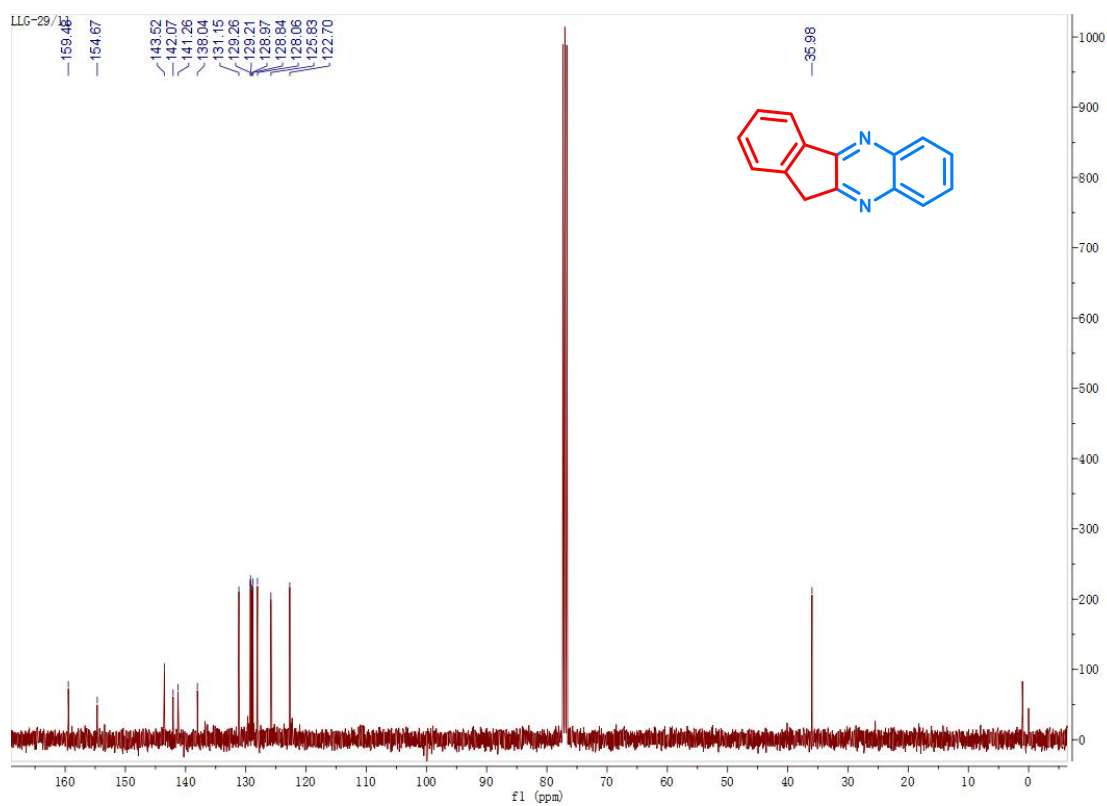


Figure S2. ¹³C NMR spectrum of compound **2.3aa**.

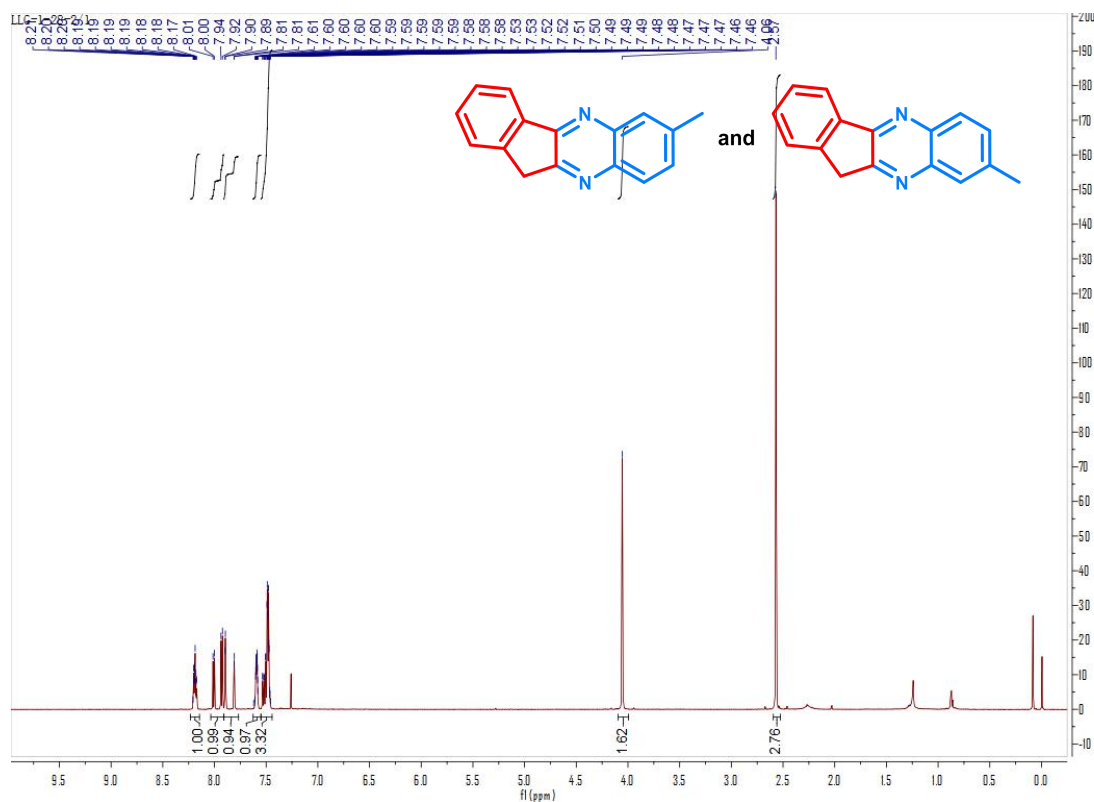


Figure S3. ^1H NMR spectrum of compounds **2.3ab-1** and **2.3ab-2**.

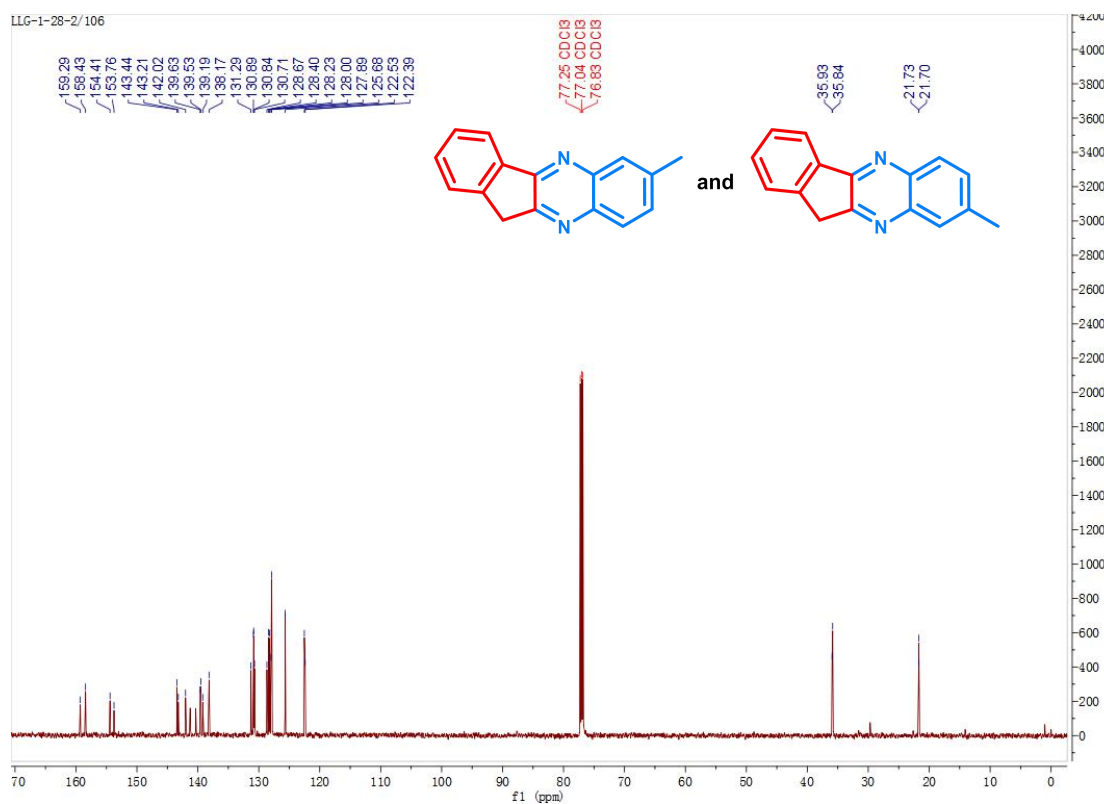


Figure S4. ^{13}C NMR spectrum of compounds **2.3ab-1** and **2.3ab-2**.

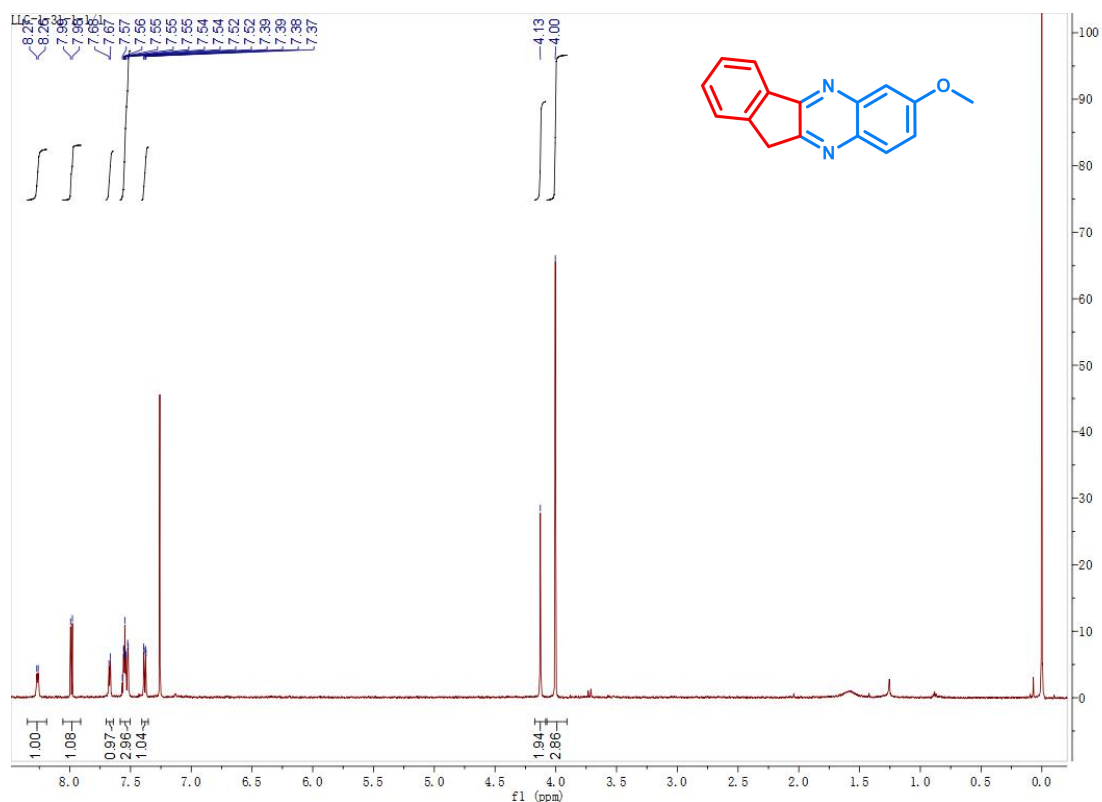


Figure S5. ¹H NMR spectrum of compound 2.3ac-1.

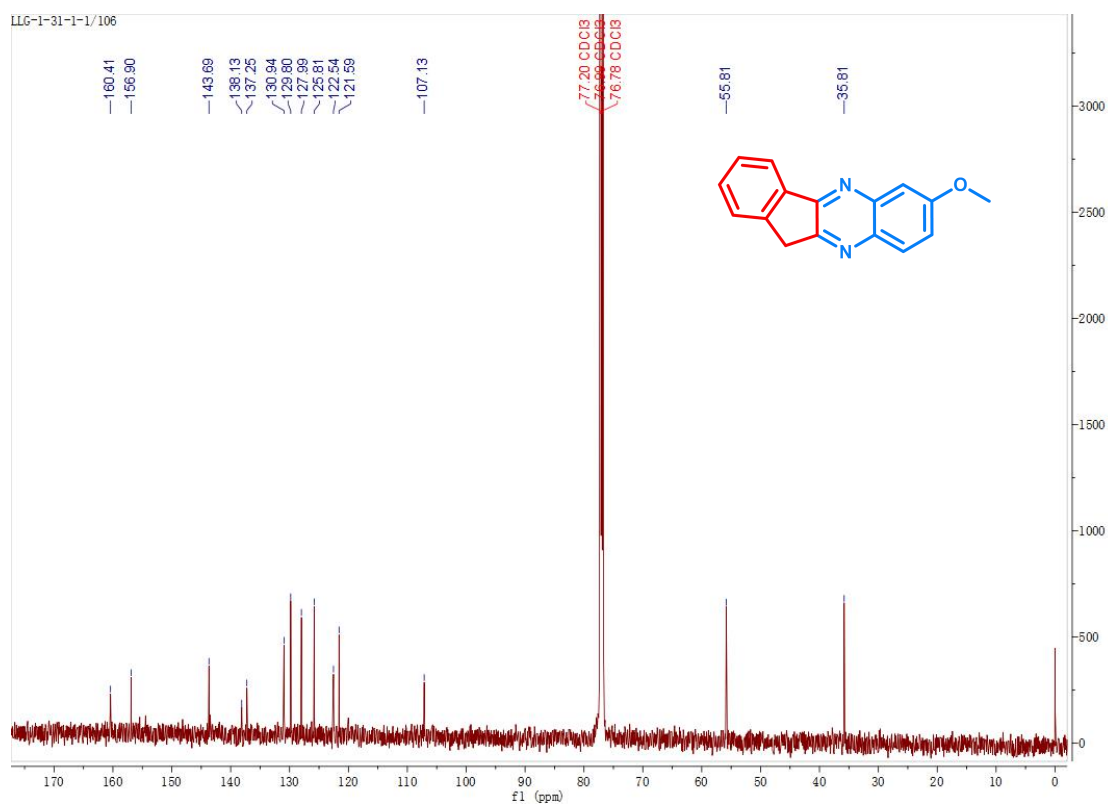


Figure S6. ¹³C NMR spectrum of compound 2.3ac-1.

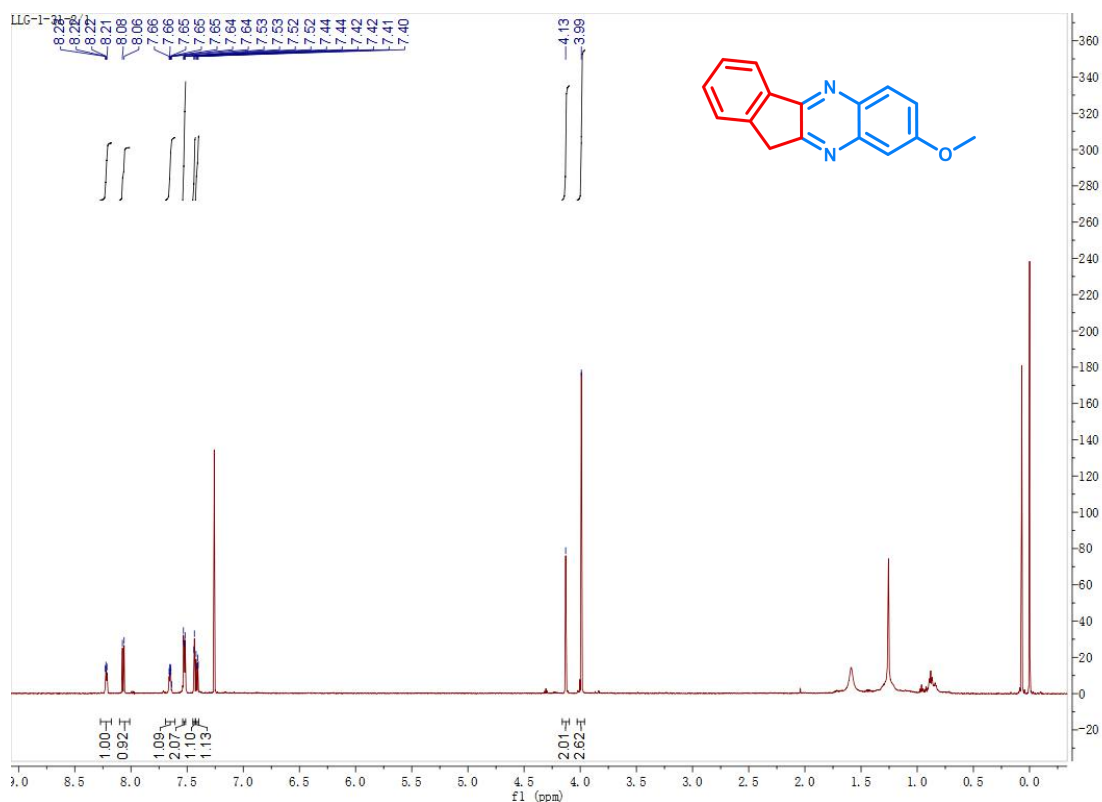


Figure S7. ¹H NMR spectrum of compound 2.3ac-2.

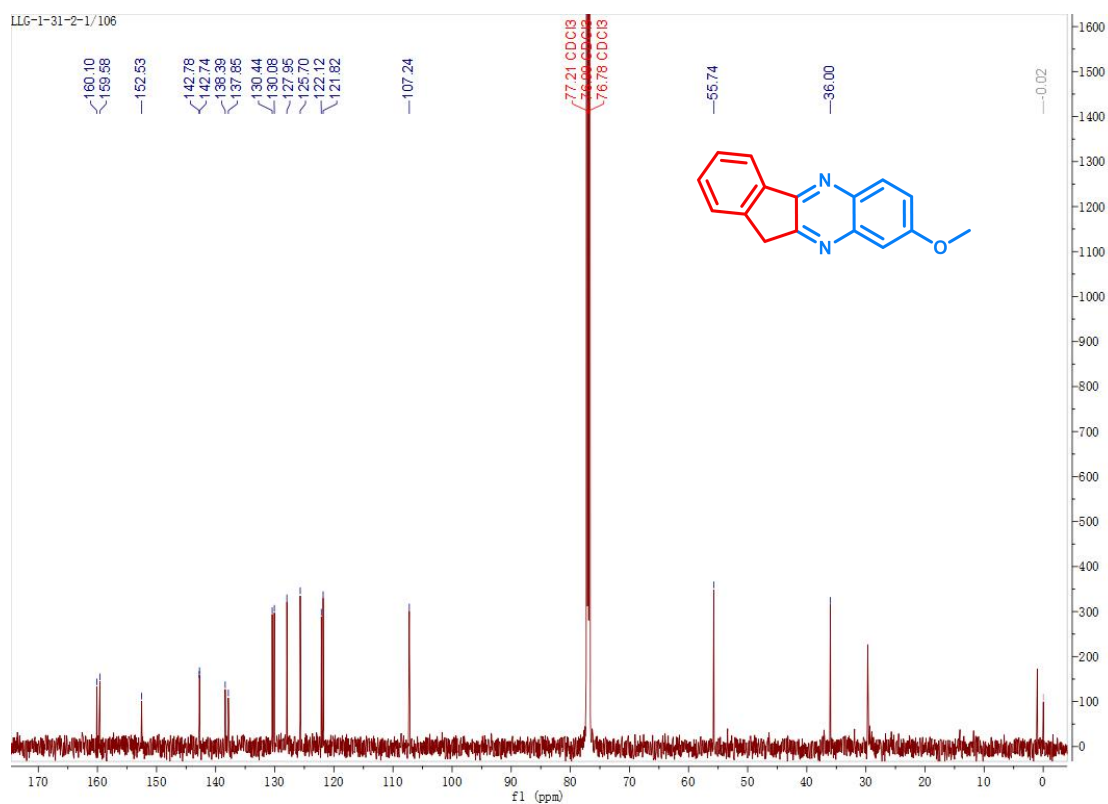


Figure S8. ¹³C NMR spectrum of compound 2.3ac-2.

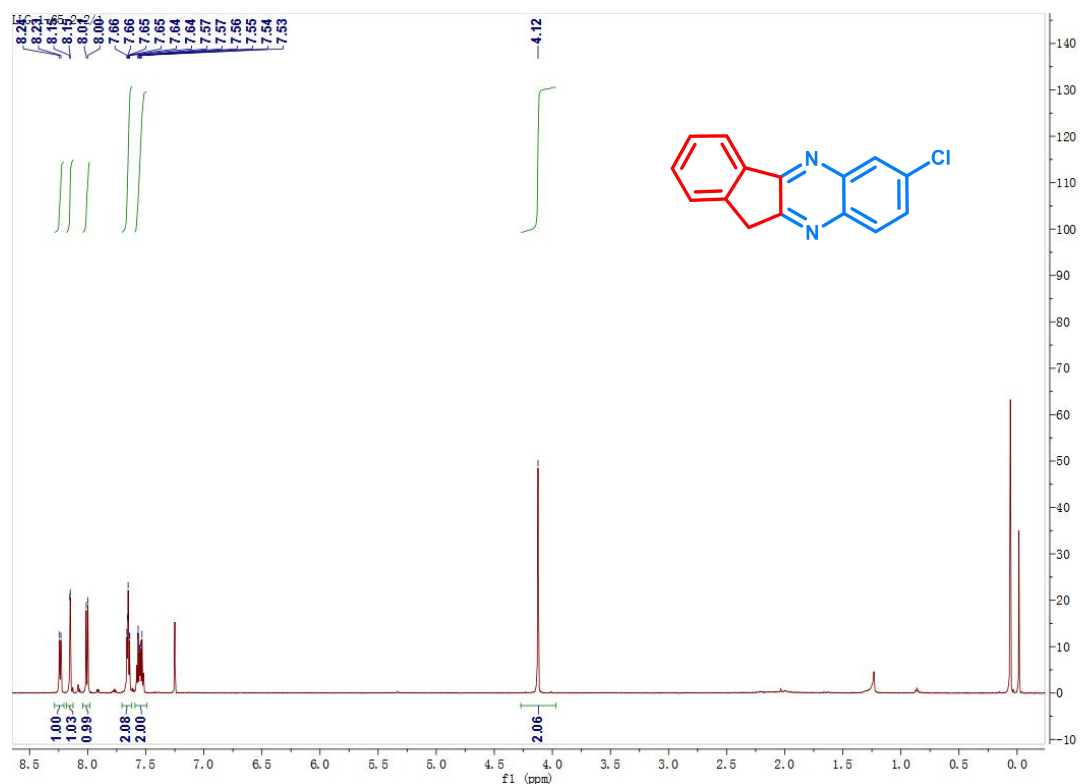


Figure S9. ¹H NMR spectrum of compound 2.3ad-1.

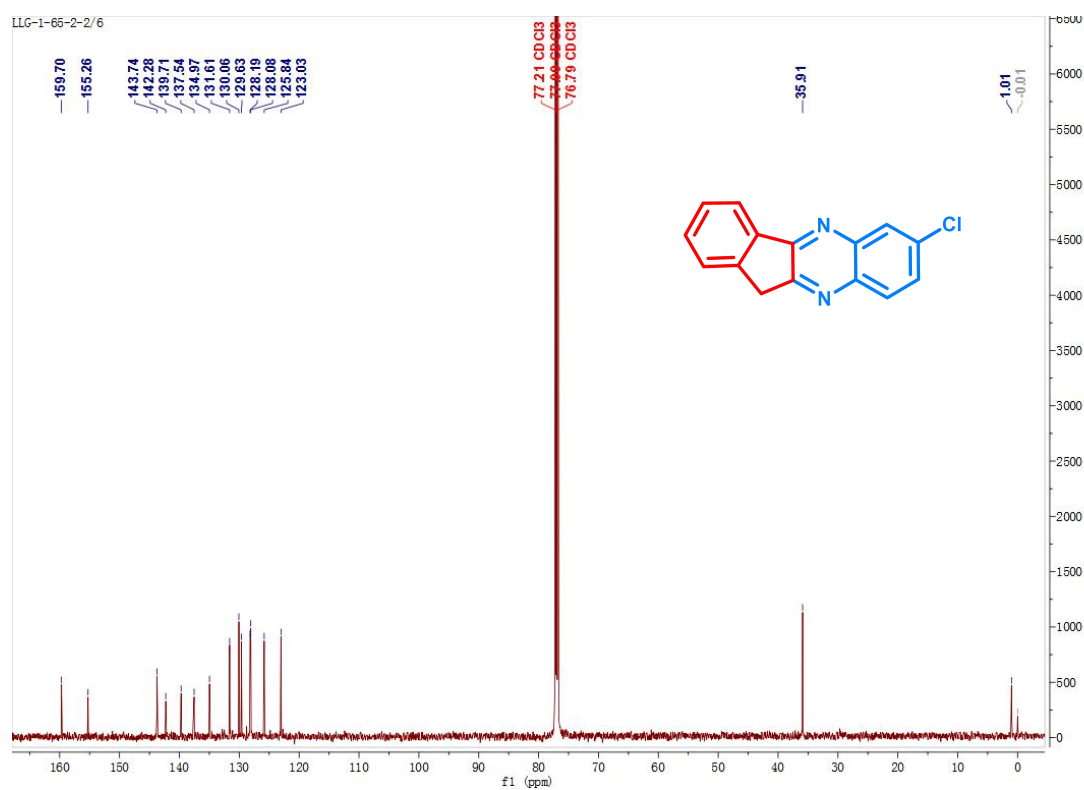


Figure S10. ¹³C NMR spectrum of compound 2.3ad-1.

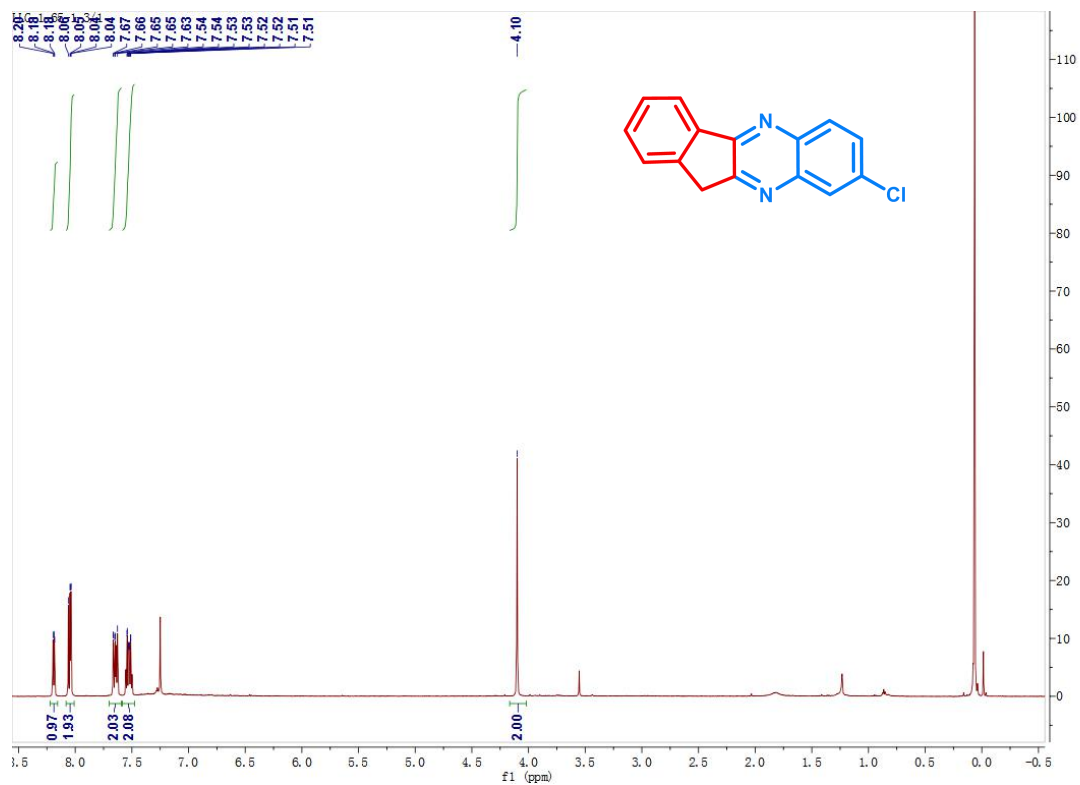


Figure S11. ^1H NMR spectrum of compound 2.3ad-2.

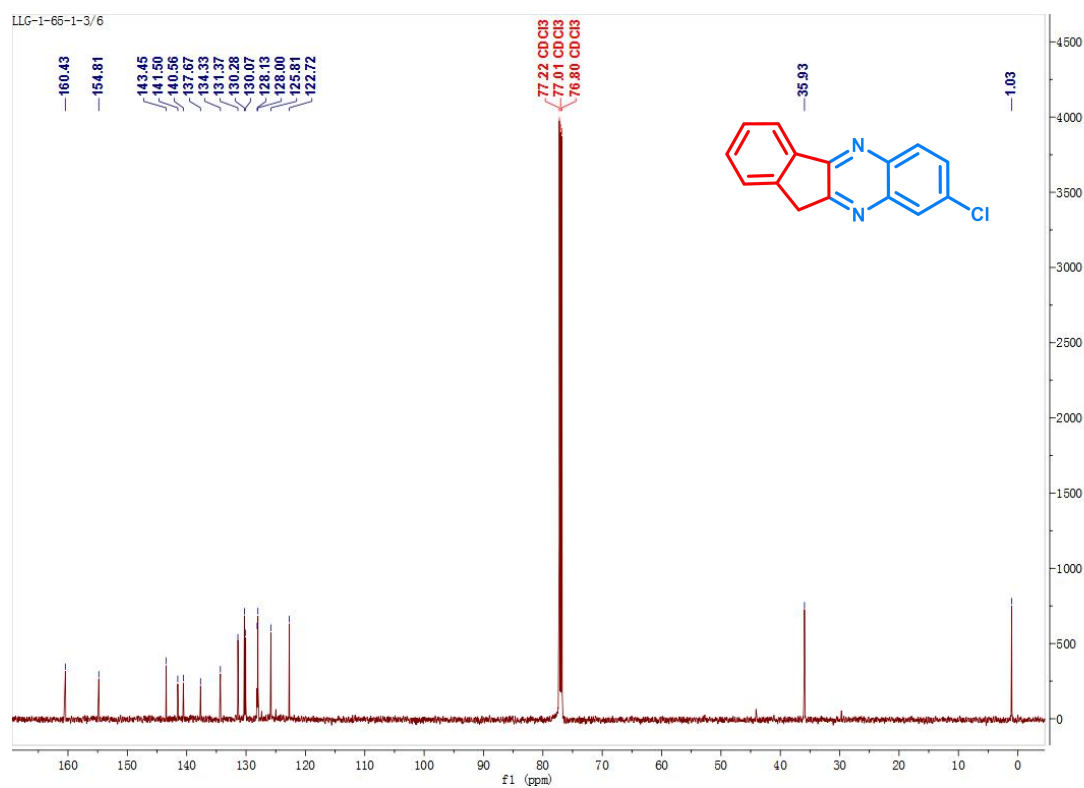


Figure S12. ^{13}C NMR spectrum of compound 2.3ad-2.

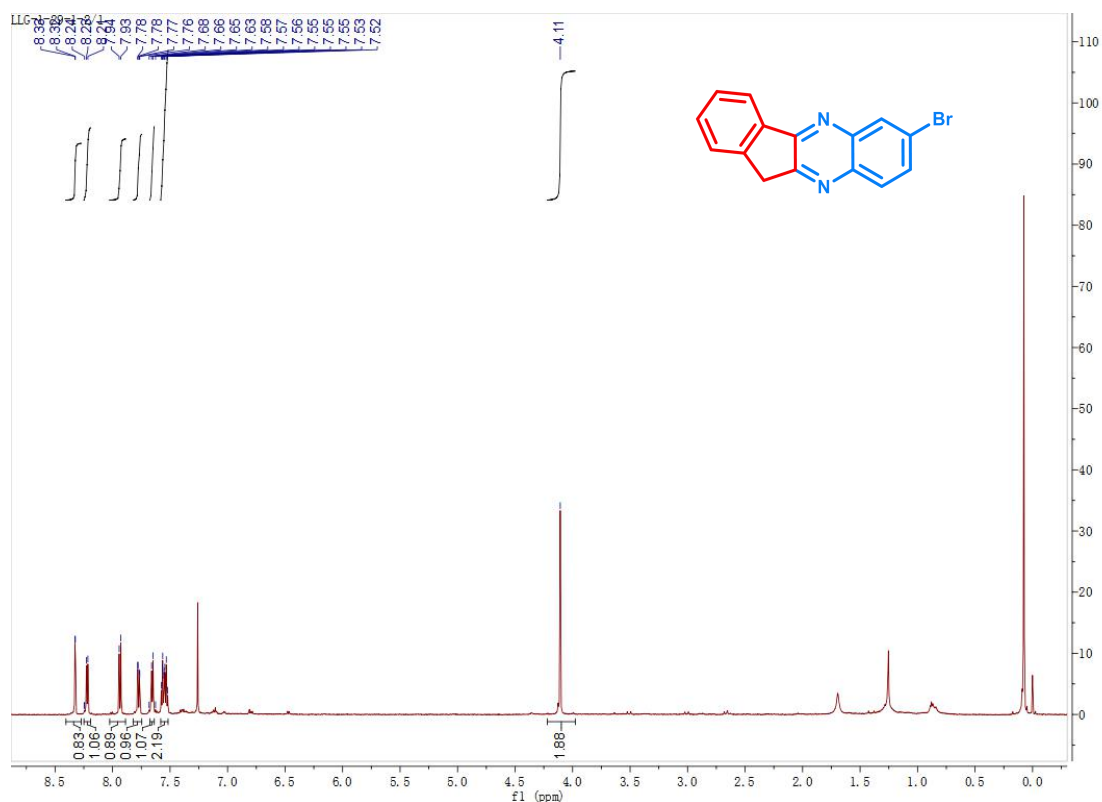


Figure S13. ^1H NMR spectrum of compound 2.3ae-1.

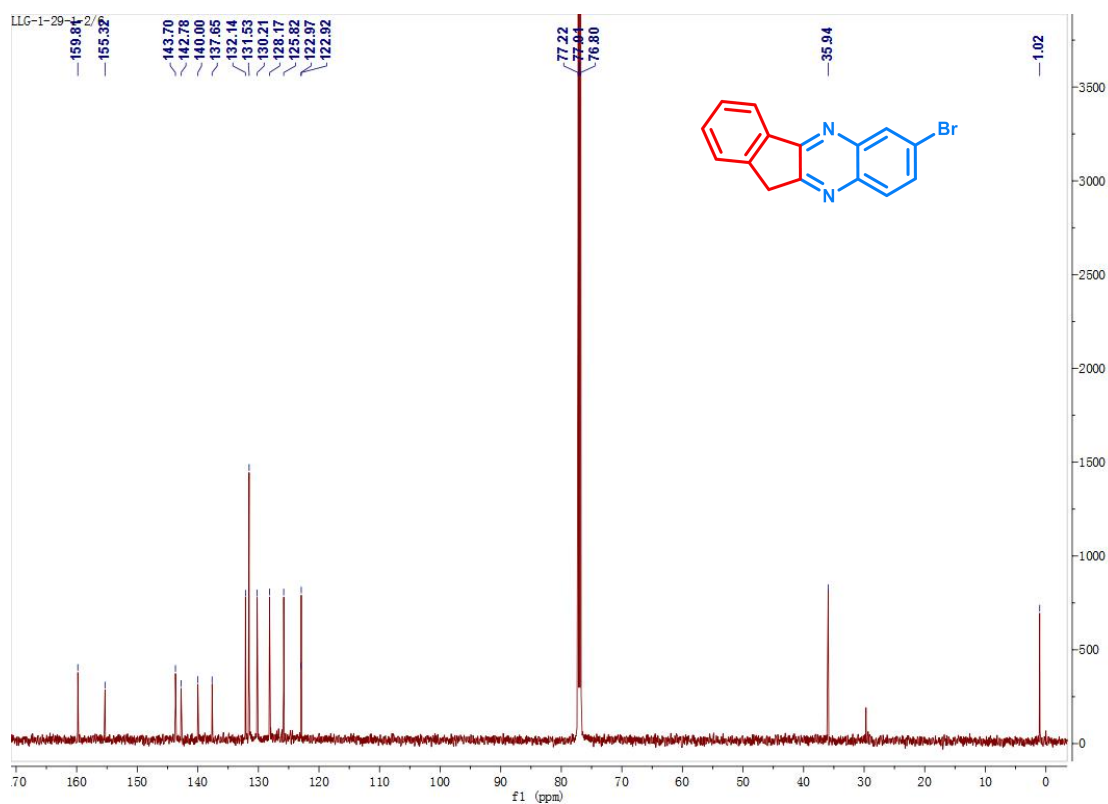


Figure S14. ^{13}C NMR spectrum of compound 2.3ae-1.

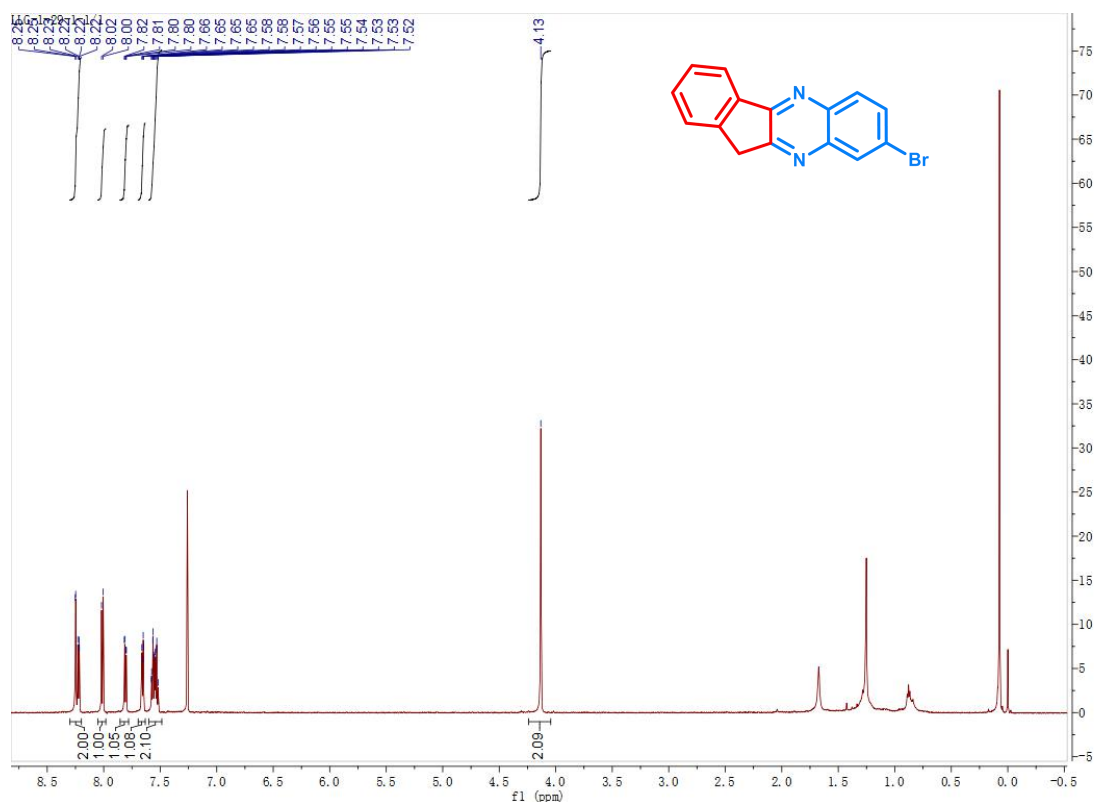


Figure S15. ^1H NMR spectrum of compound 2.3ae-2.

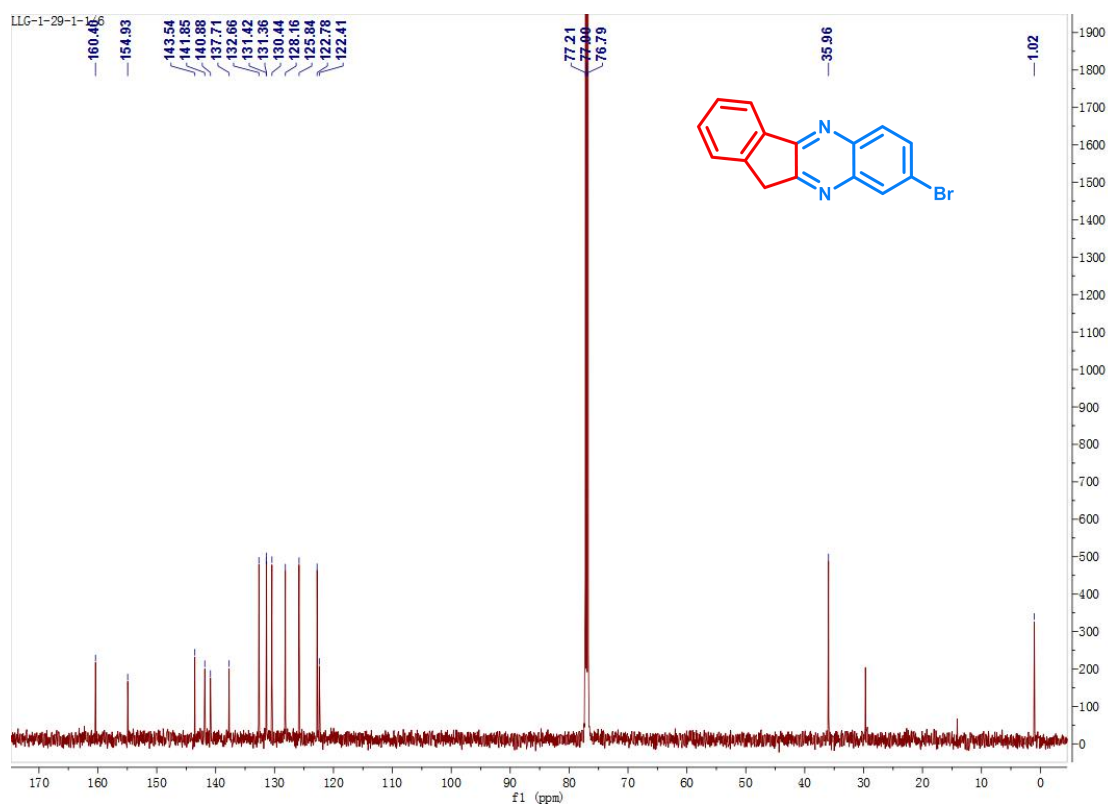


Figure S16. ^{13}C NMR spectrum of compound 2.3ae-2.

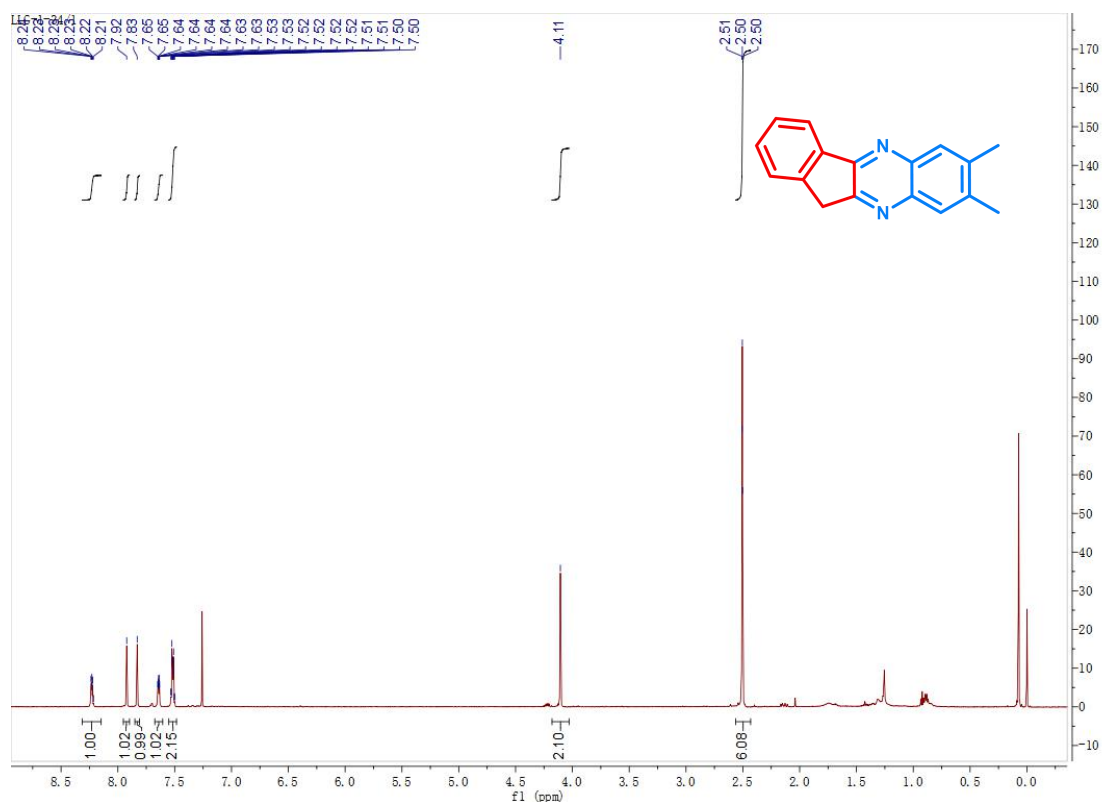


Figure S17. ^1H NMR spectrum of compound **2.3af**.

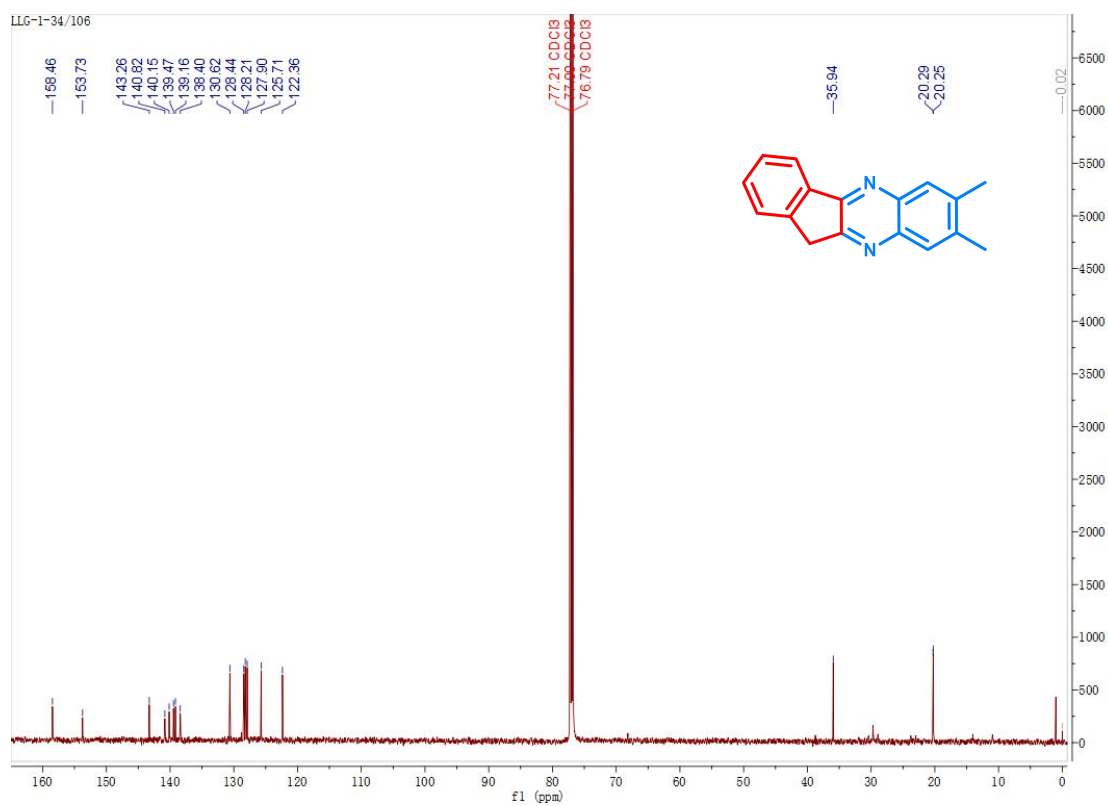


Figure S18. ^{13}C NMR spectrum of compound **2.3af**.

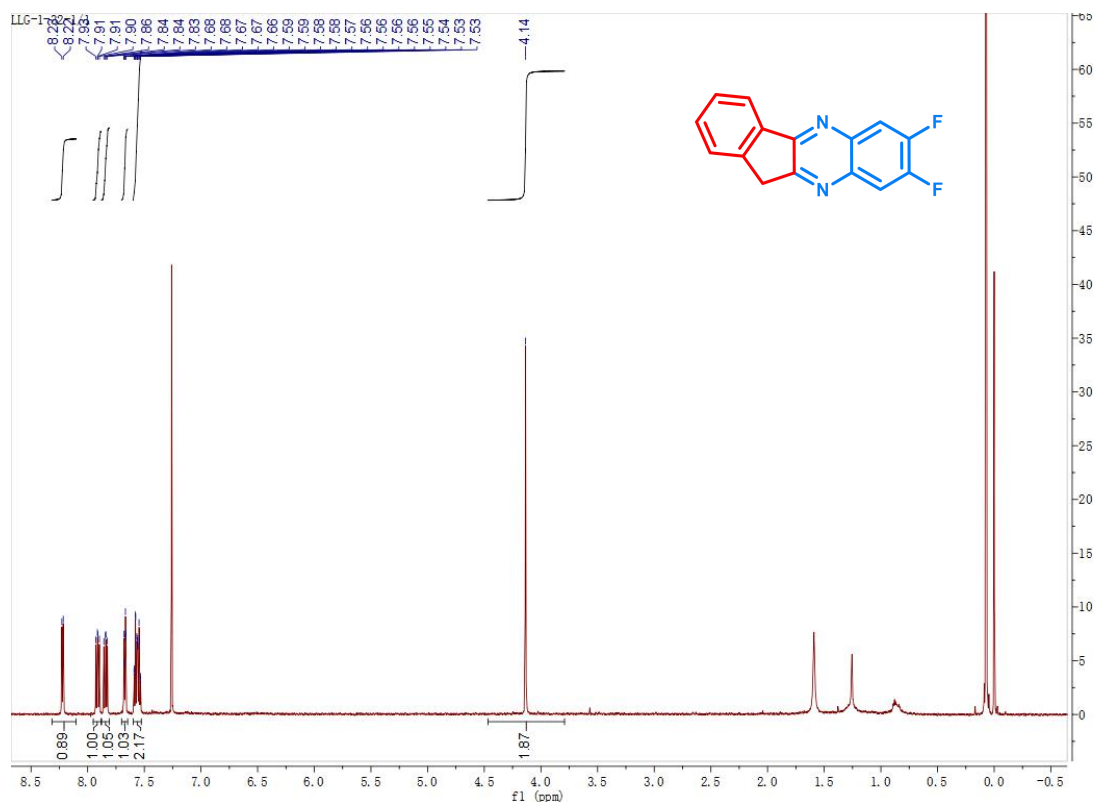


Figure S19. ¹H NMR spectrum of compound 2.3ag.

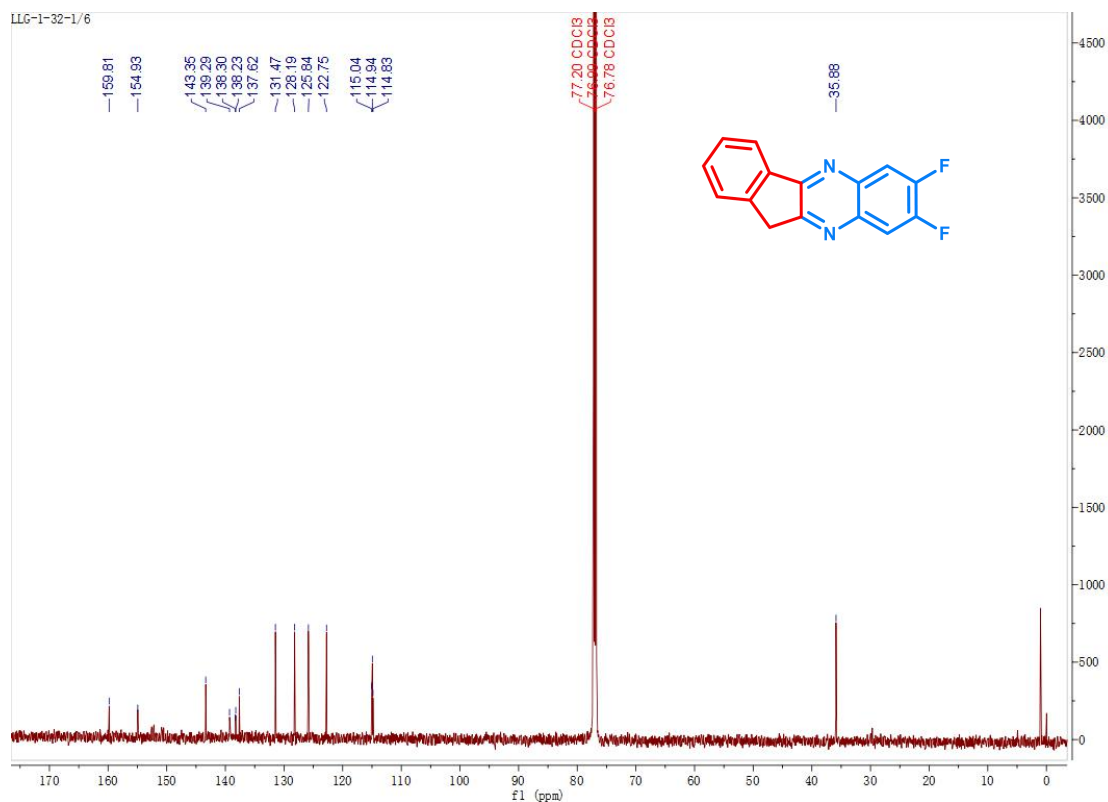


Figure S20. ¹³C NMR spectrum of compound 2.3ag.

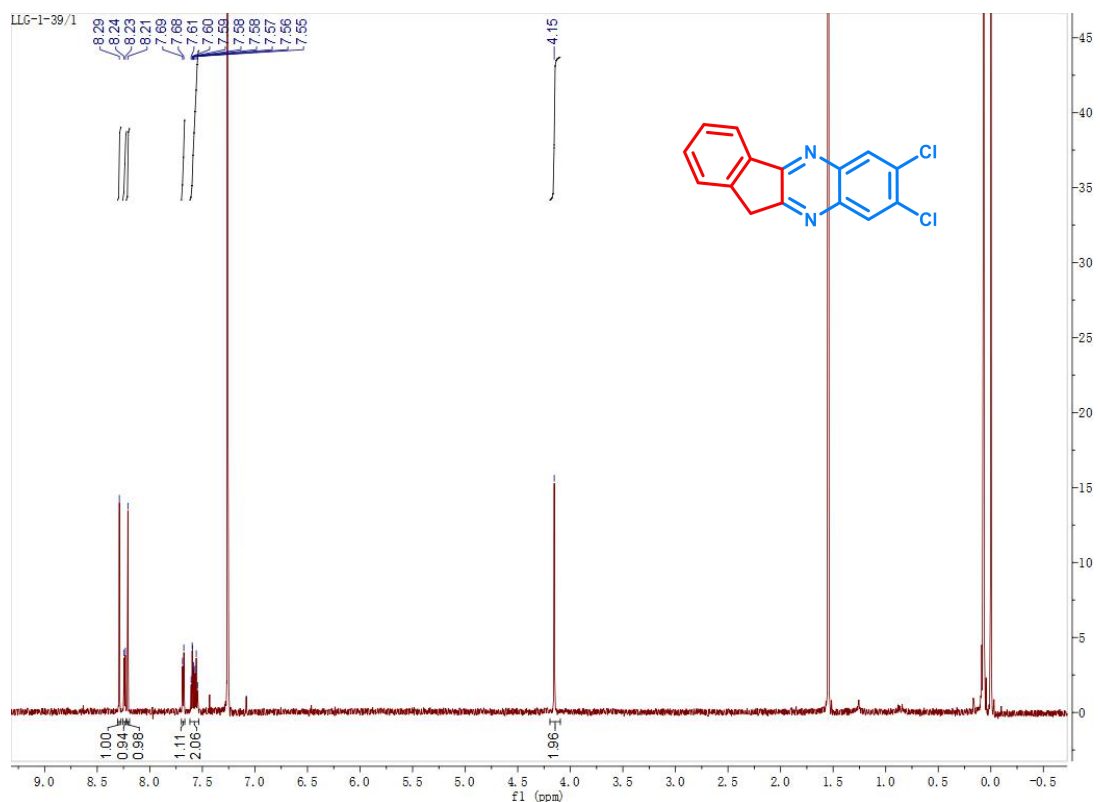


Figure S21. ^1H NMR spectrum of compound 2.3ah.

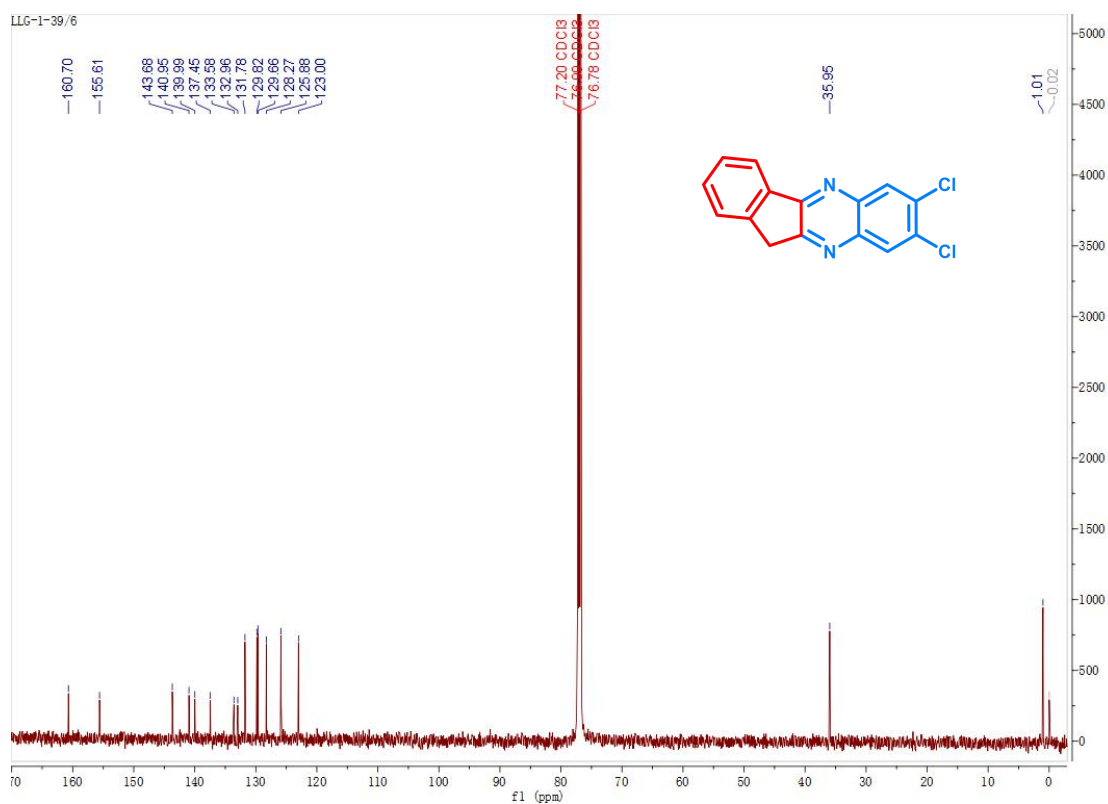


Figure S22. ^{13}C NMR spectrum of compound 2.3ah.

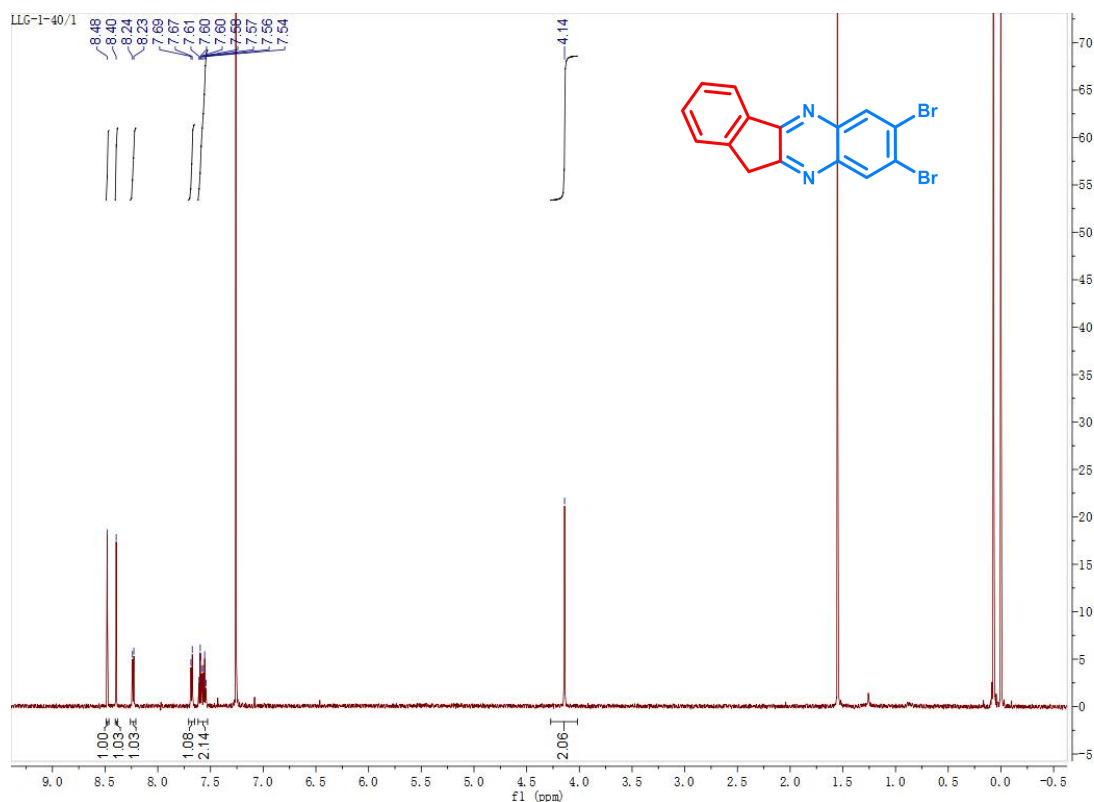


Figure S23. ¹H NMR spectrum of compound **2.3ai**.

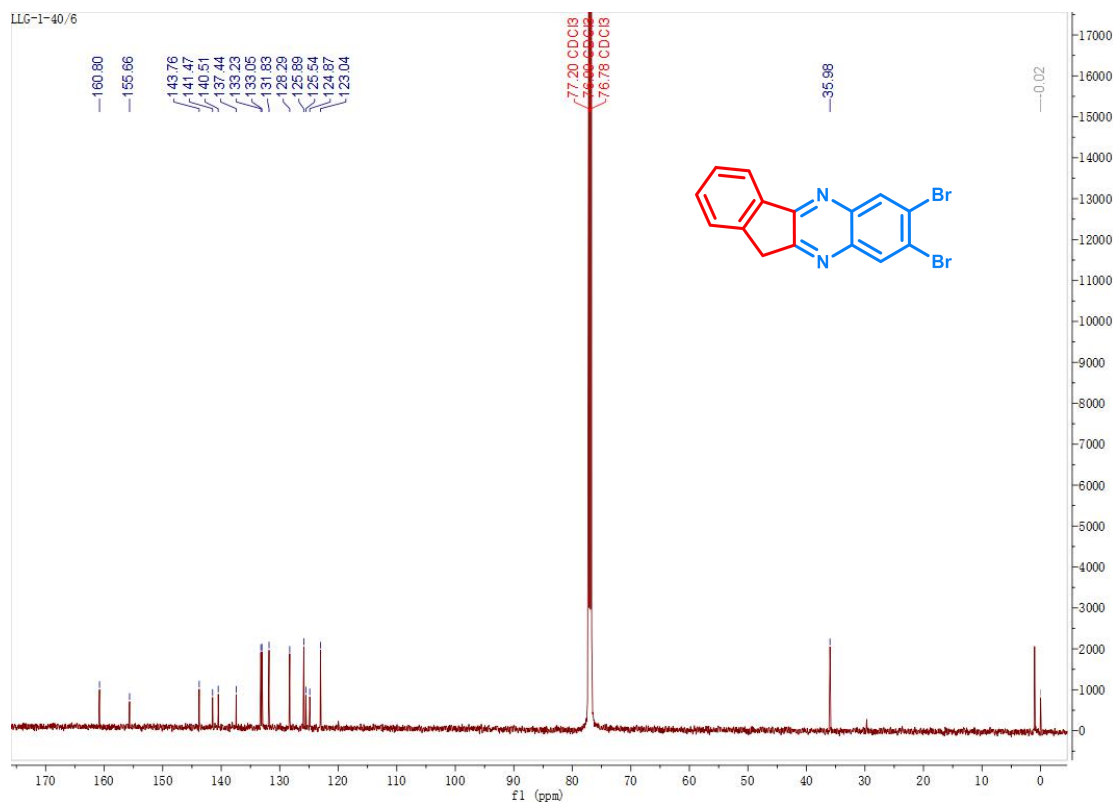


Figure S24. ¹³C NMR spectrum of compound **2.3ai**.

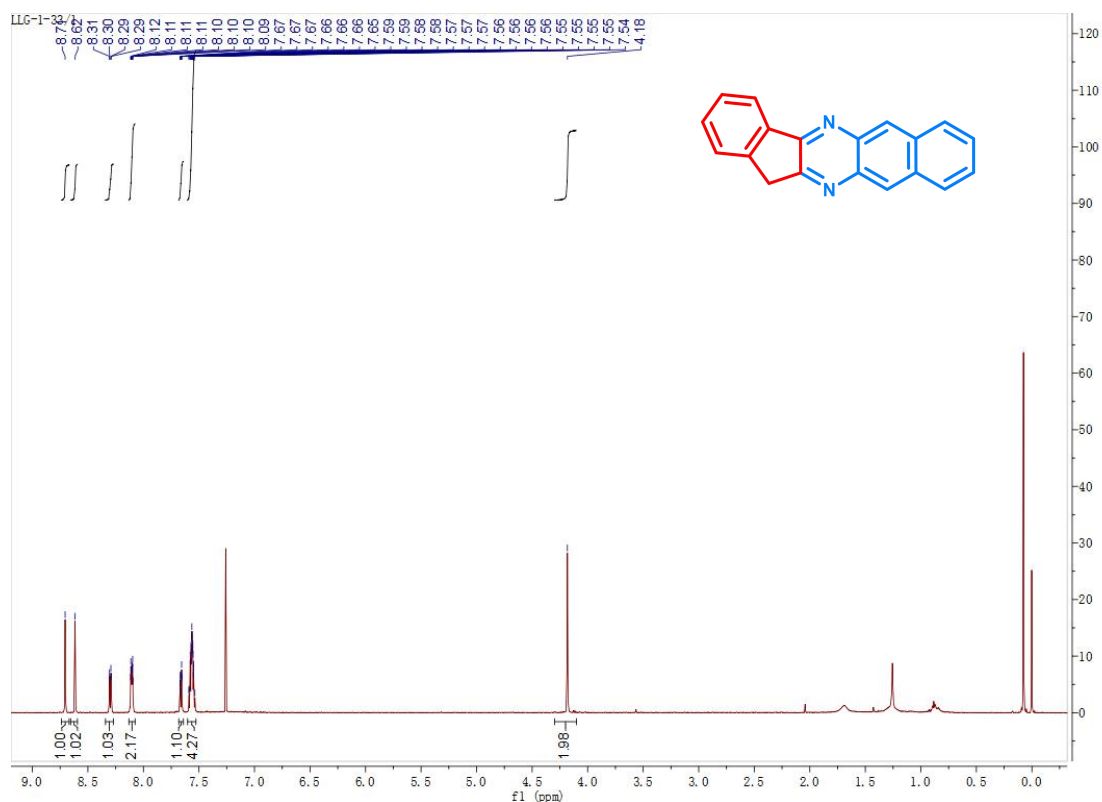


Figure S25. ¹H NMR spectrum of compound 2.3aj.

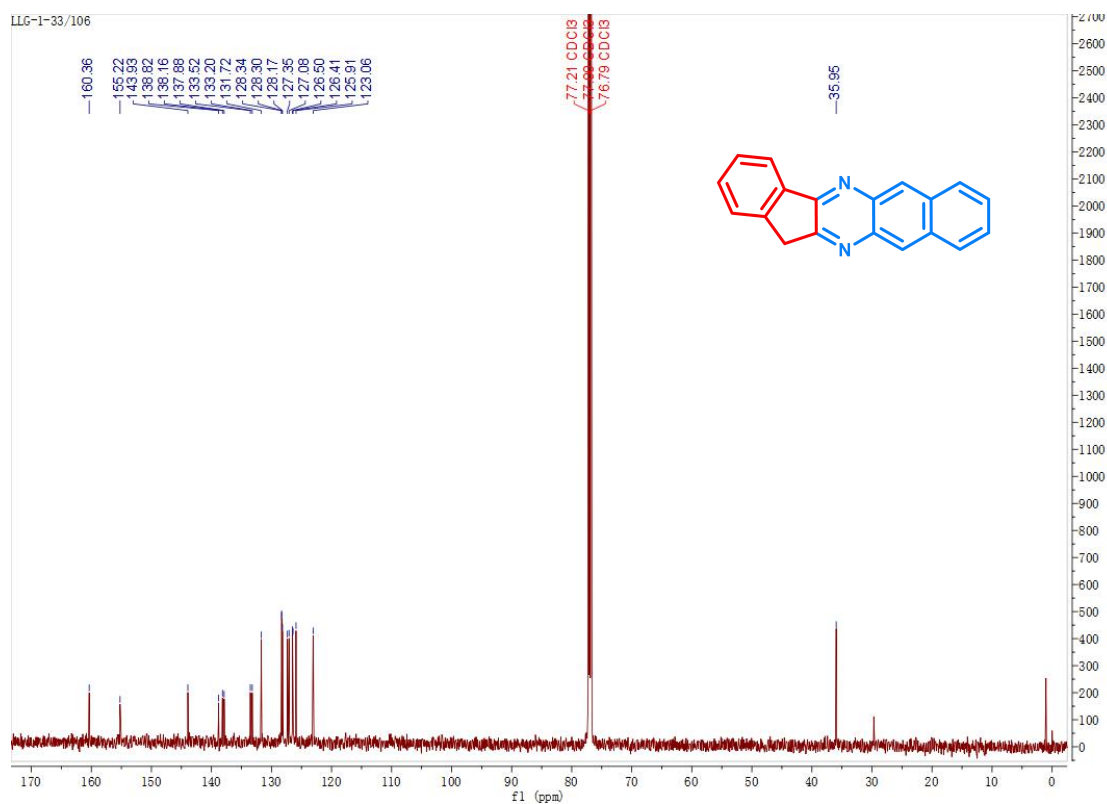


Figure S26. ¹³C NMR spectrum of compound 2.3aj.

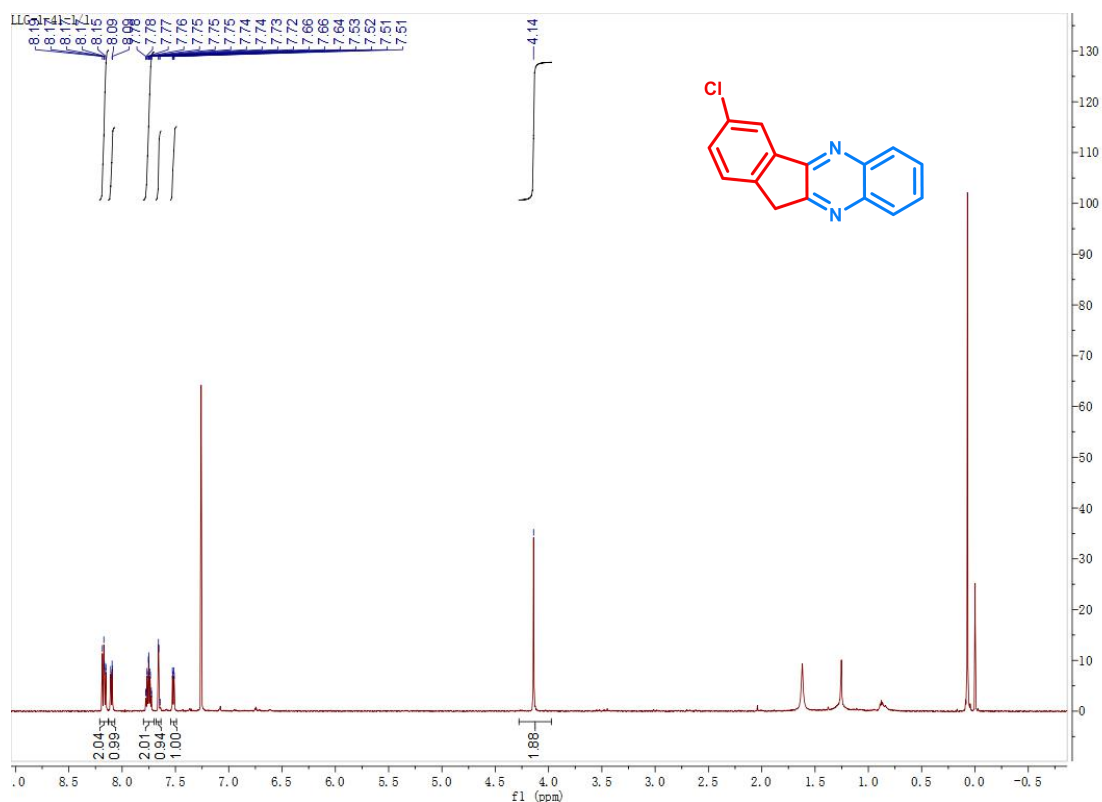


Figure S27. ¹H NMR spectrum of compound 2.3ba-1.

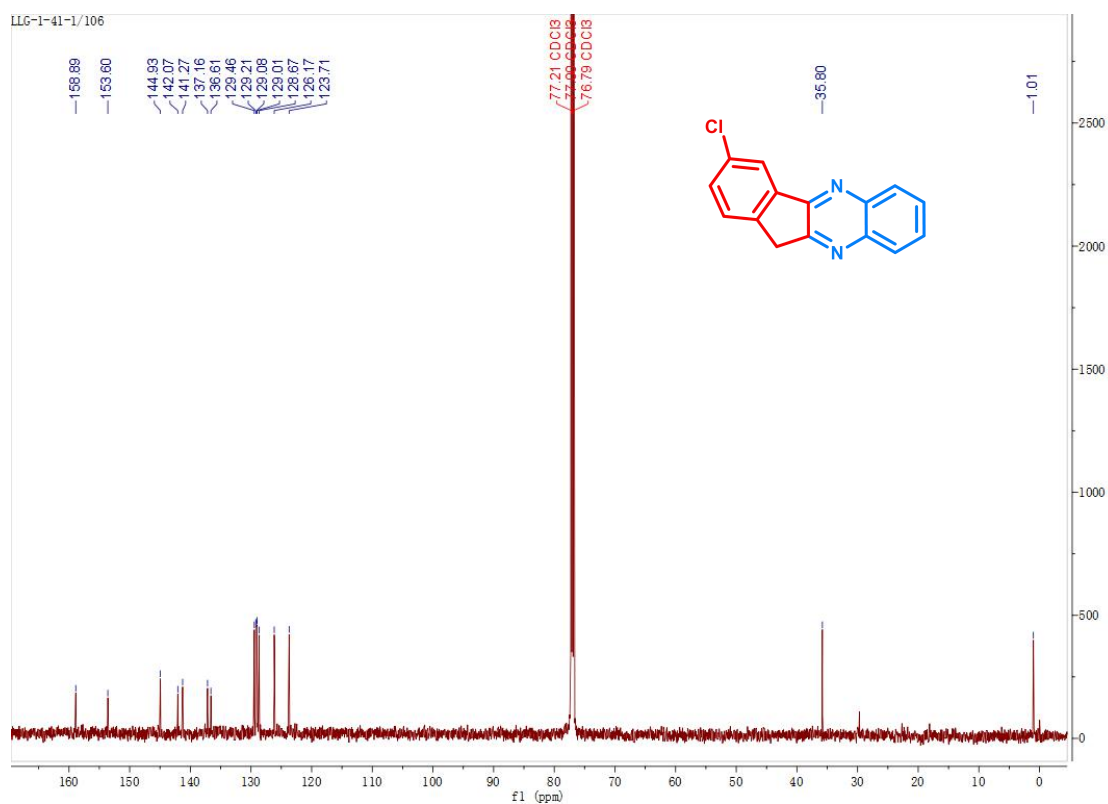


Figure S28. ¹³C NMR spectrum of compound 2.3ba-1.

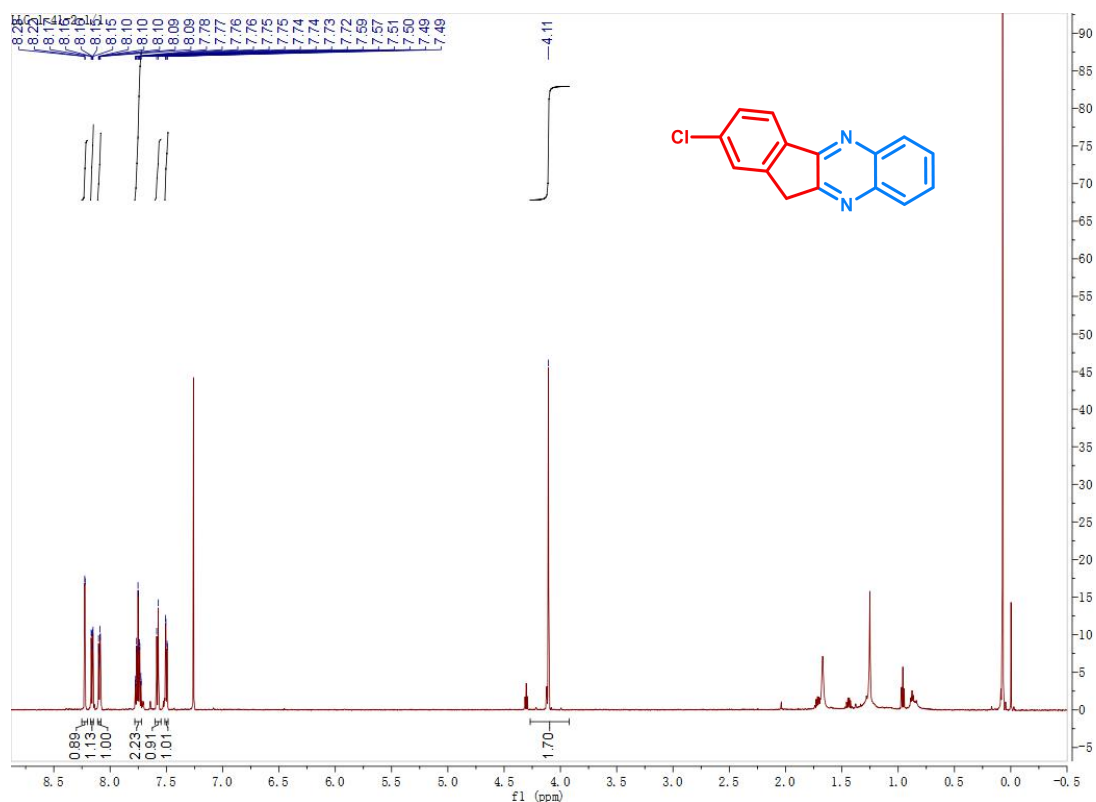


Figure S29. ¹H NMR spectrum of compound 2.3ba-2.

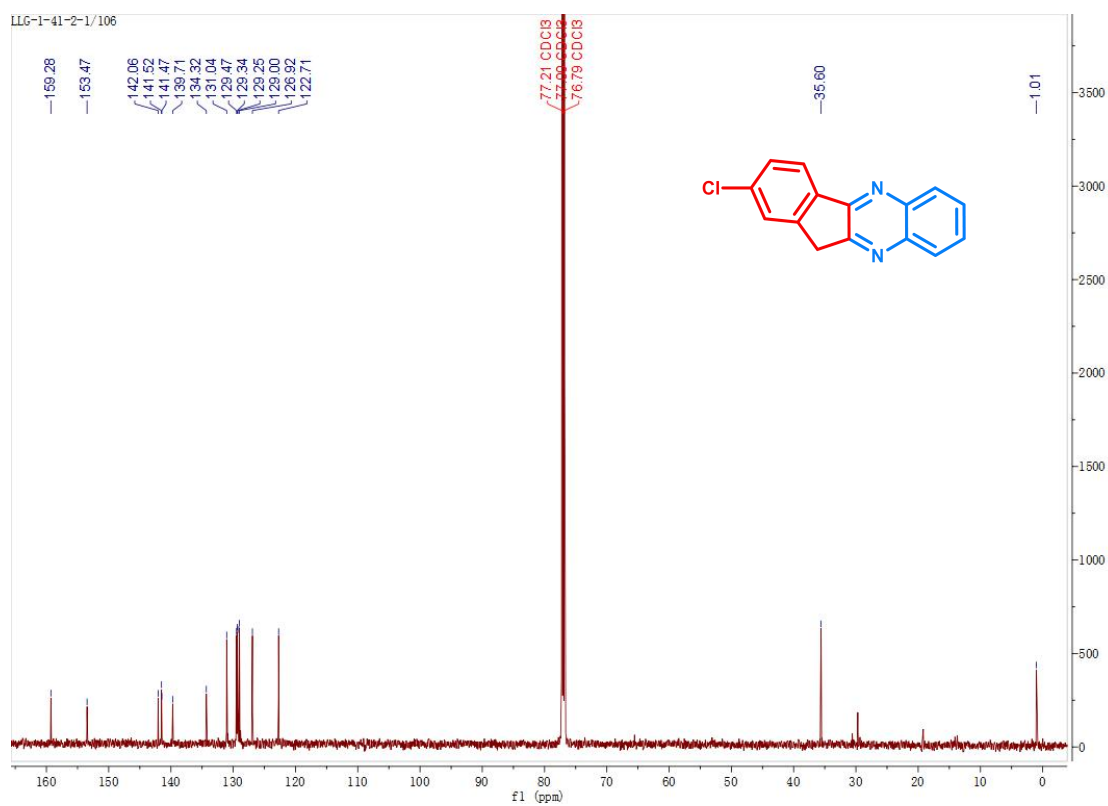


Figure S30. ¹³C NMR spectrum of compound 2.3ba-2.

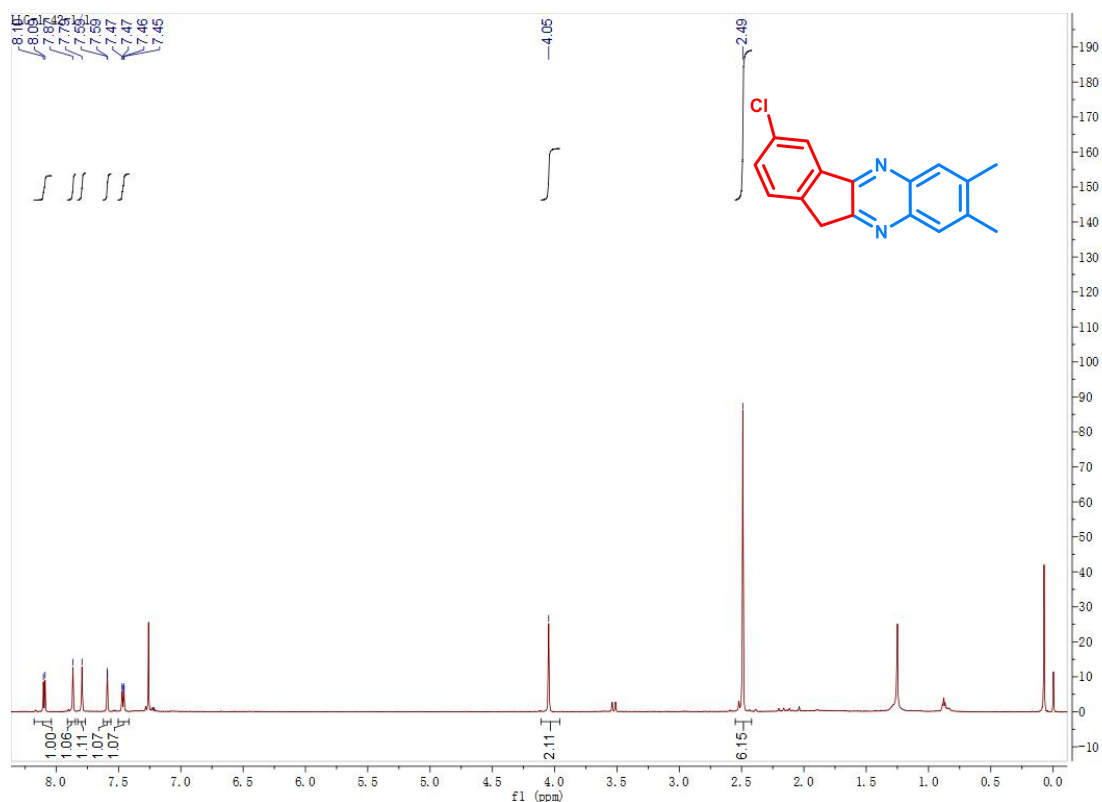


Figure S31. ¹H NMR spectrum of compound 2.3bb-1.

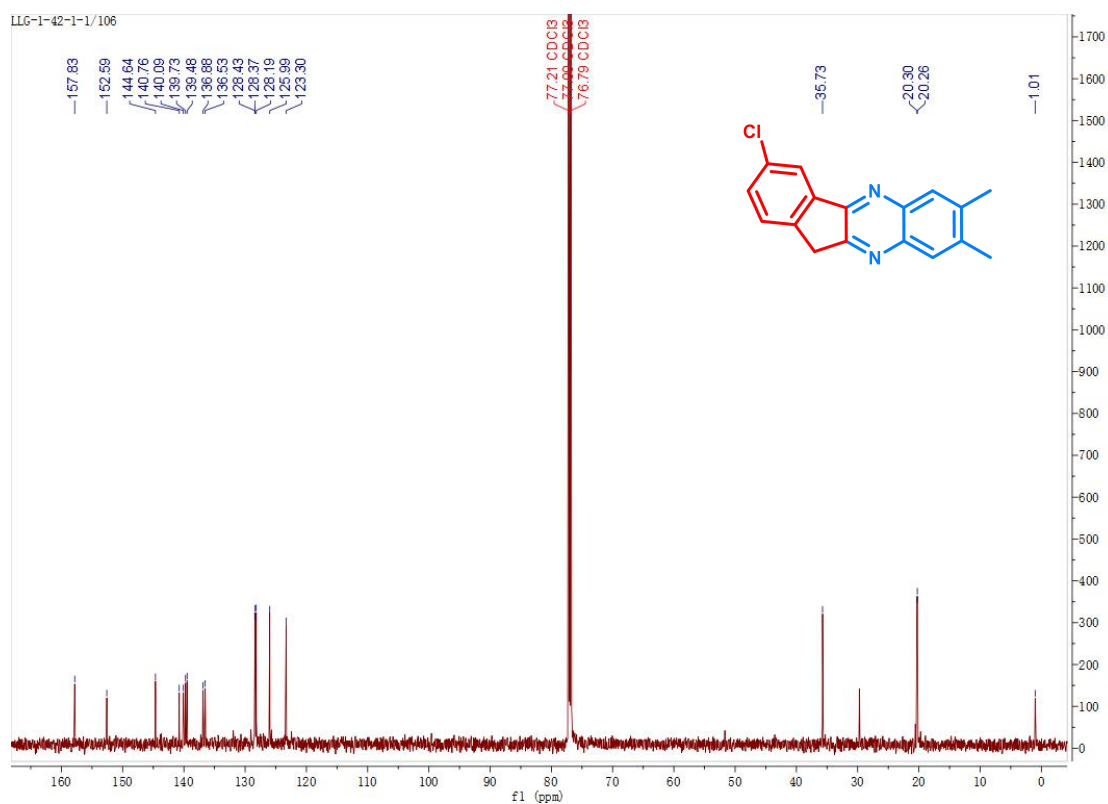
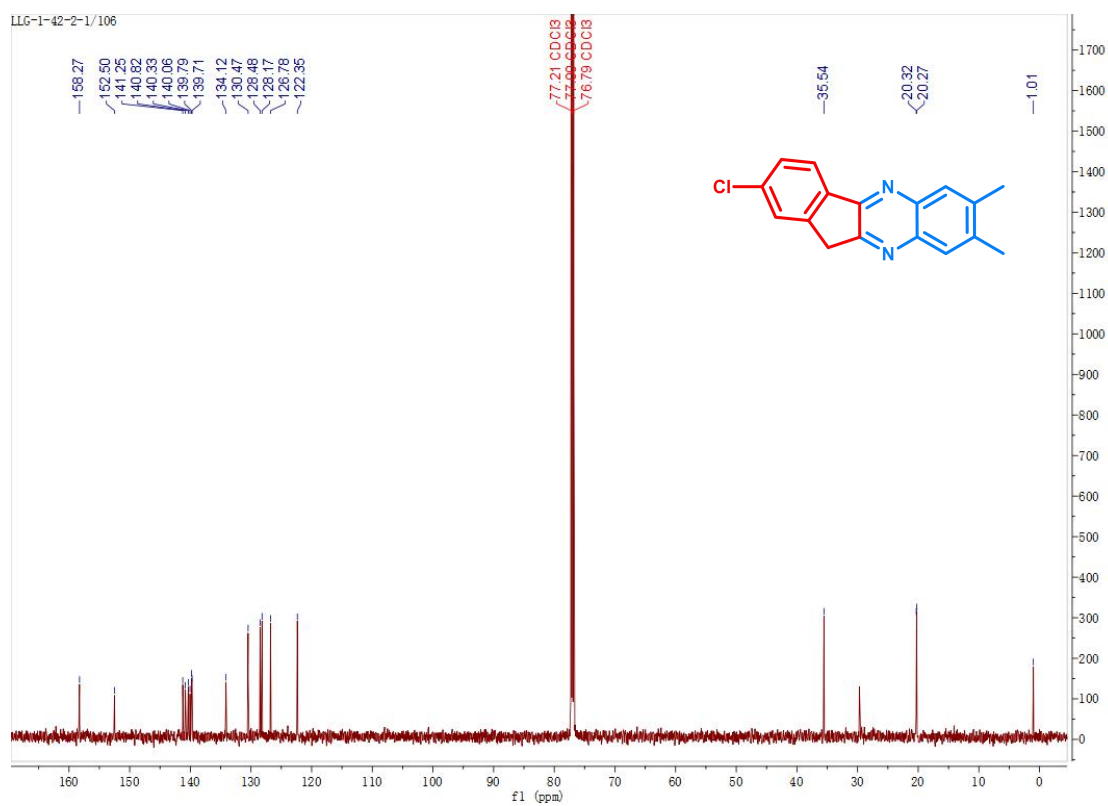
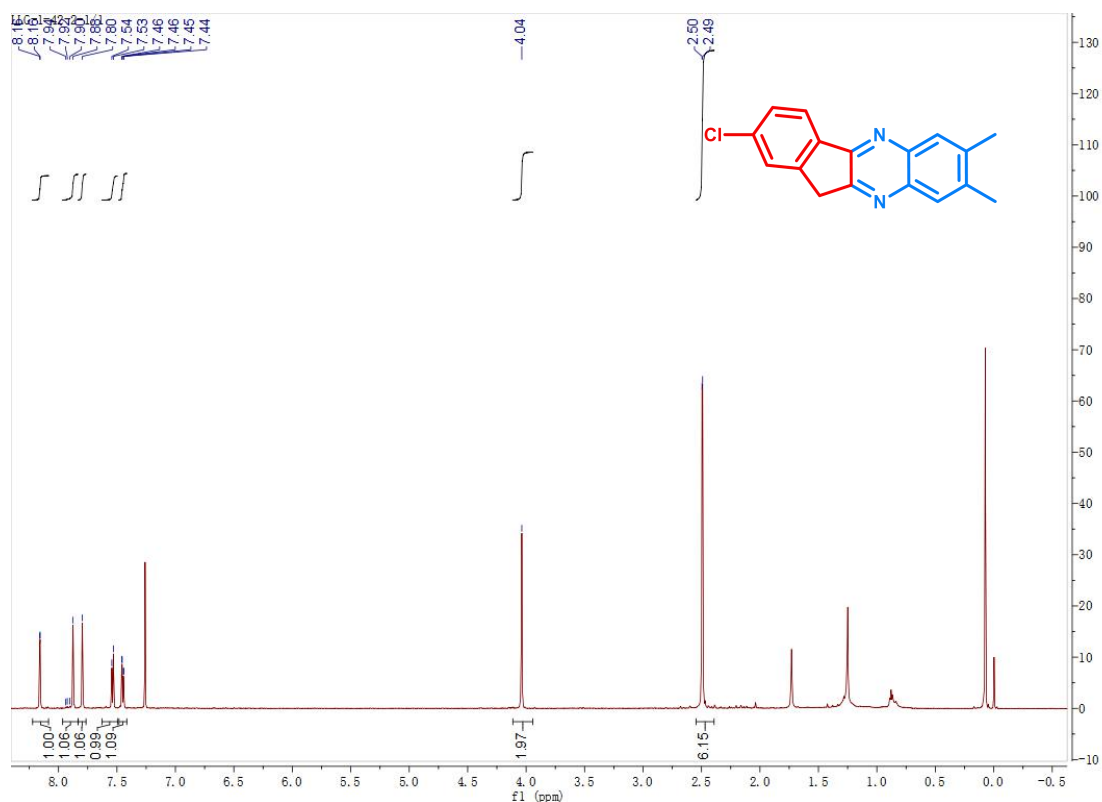


Figure S32. ¹³C NMR spectrum of compound 2.3bb-1.



Mass Spectrum SmartFormula Report

Analysis Info

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 Method tune_low_NEW.m
 Sample Name LLG-1-29
 Comment

Acquisition Date 8/27/2021 2:38:12 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

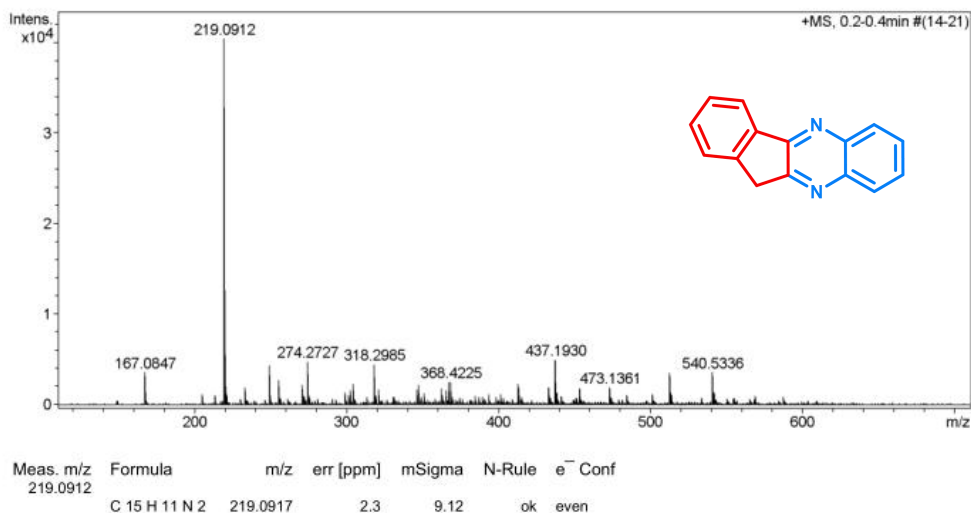


Figure S35. Mass spectrum smartFormula report of compound 2.3aa.

Mass Spectrum SmartFormula Report

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 Sample Name LLG-1-28
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 Instrument / Ser# micrOTOF-Q II 10203

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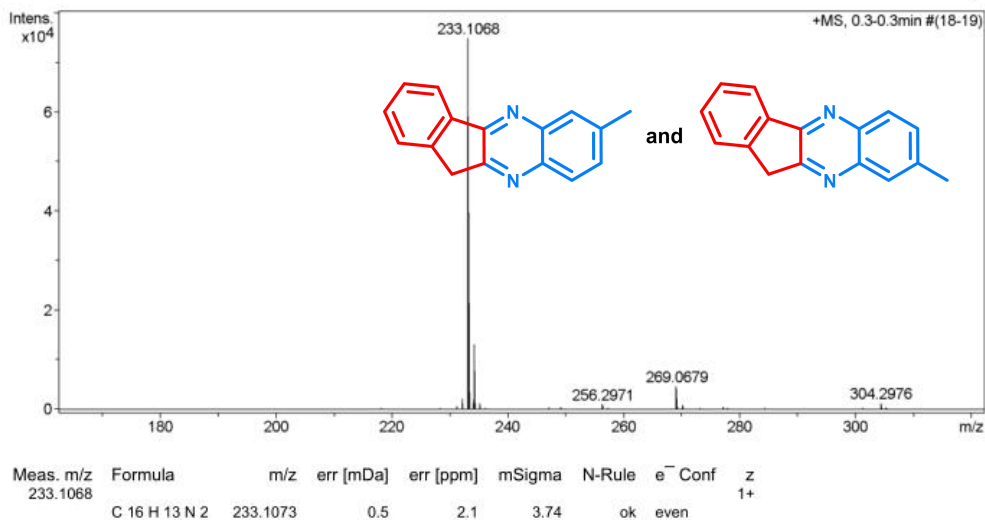


Figure S36. Mass spectrum smartFormula report of compounds 2.3ab-1 and 2.3ab-2.

Mass Spectrum SmartFormula Report

Analysis Info

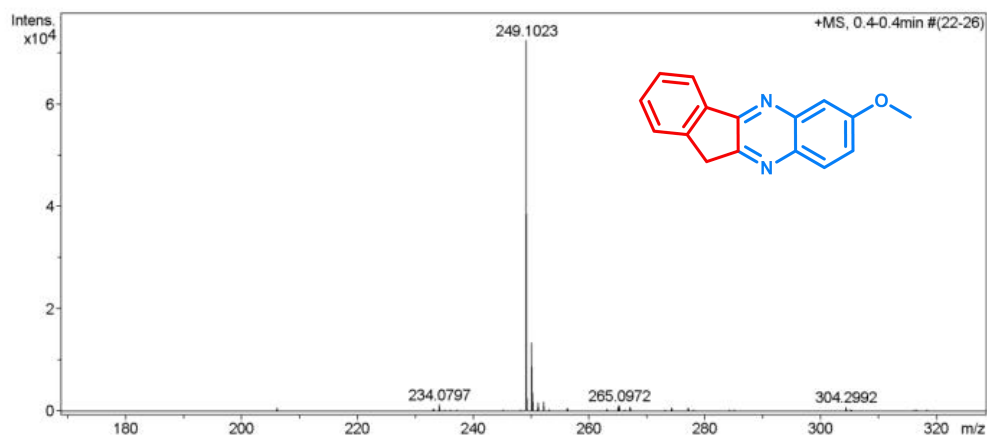
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 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
249.1023	C 16 H 13 N 2 O	249.1022	-0.0	-0.1	6.00	ok	even	1+

Figure S37. Mass spectrum smartFormula report of compound 2.3ac-1.

Mass Spectrum SmartFormula Report

Analysis Info

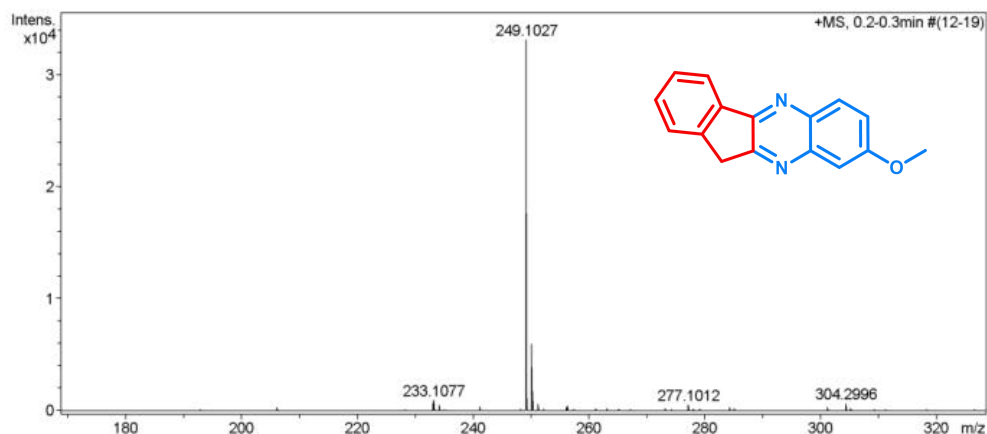
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 Sample Name LLG-1-31-2
 Comment

Acquisition Date 6/25/2021 2:26:59 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
249.1027	C 16 H 13 N 2 O	249.1022	-0.4	-1.8	2.26	ok	even	1+

Figure S38. Mass spectrum smartFormula report of compound 2.3ac-2.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\data\USER-2021\LLG- 1-65-2-2.d
 Method tune_low_NEW.m
 Sample Name LLG- 1-65-2-2
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Acquisition Date 12/3/2021 3:12:23 PM

Operator Ma
 Instrument / Ser# microTOF-Q II 10203

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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

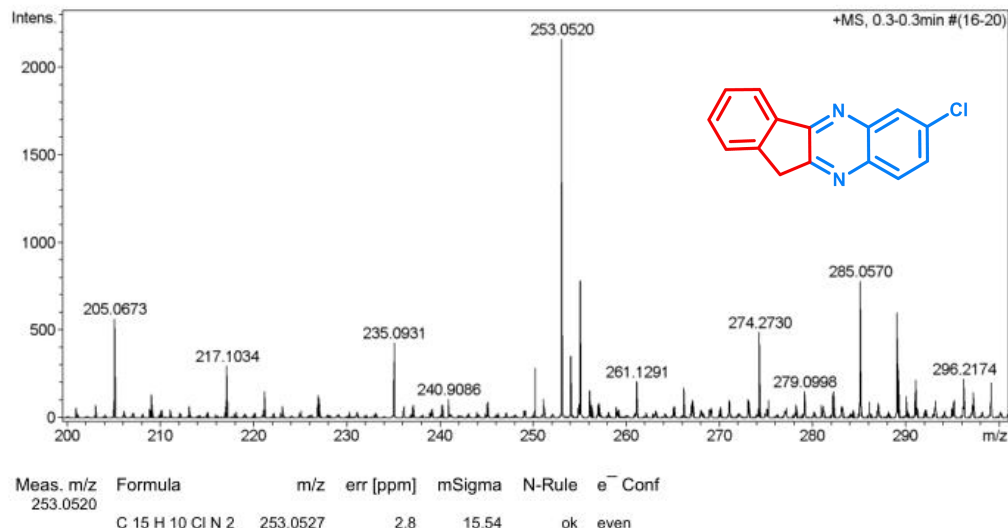


Figure S39. Mass spectrum smartFormula report of compound 2.3ad-1.

Mass Spectrum SmartFormula Report

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Operator Ma
 Instrument / Ser# microTOF-Q II 10203

Acquisition Parameter

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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

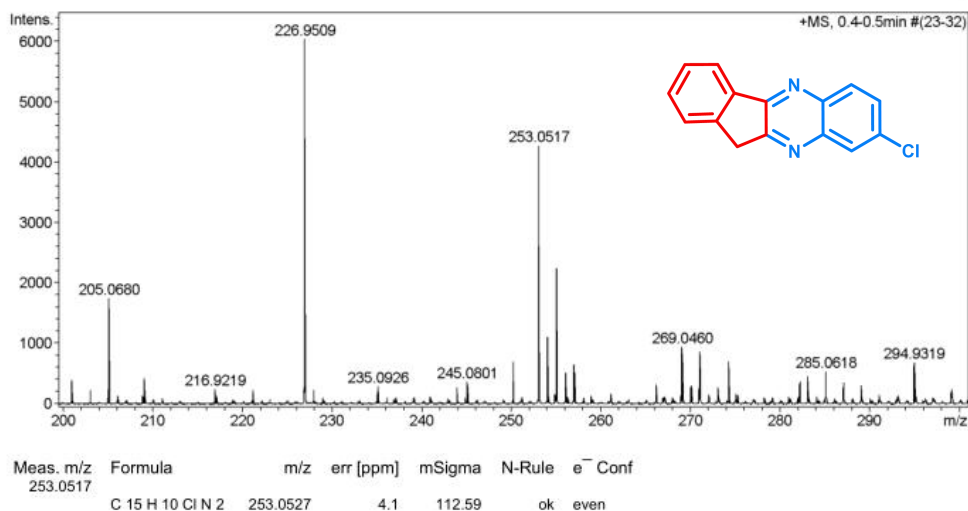


Figure S40. Mass spectrum smartFormula report of compound 2.3ad-2.

Mass Spectrum SmartFormula Report

Analysis Info

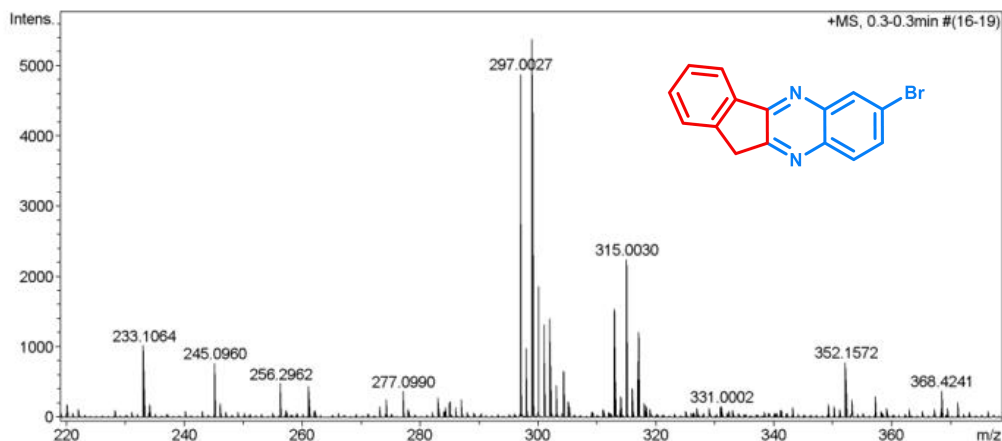
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Sample Name LLG-1-29-2
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Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
297.0027	C 15 H 10 Br N 2	297.0022	-0.5	-1.6	466.27	ok	even	1+

Figure S41. Mass spectrum smartFormula report of compound 2.3ae-1.

Mass Spectrum SmartFormula Report

Analysis Info

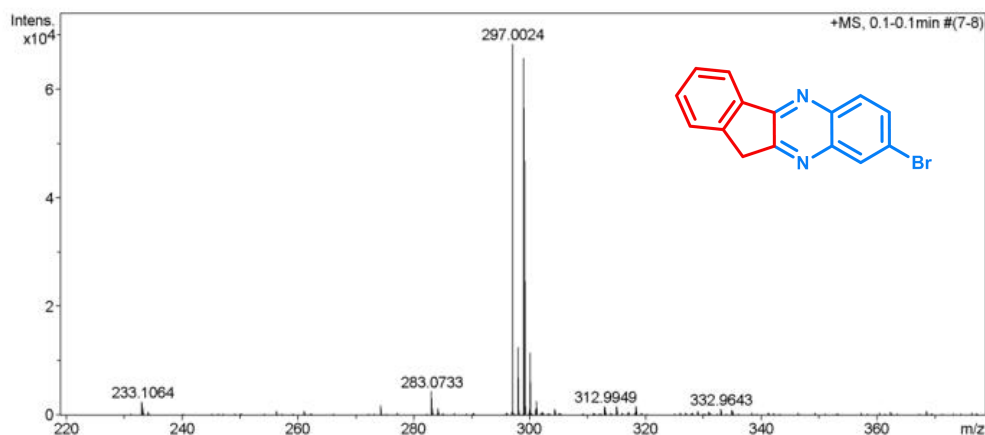
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Sample Name LLG-1-28
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Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
297.0024	C 15 H 10 Br N 2	297.0022	-0.2	-0.8	12.61	ok	even	1+

Figure S42. Mass spectrum smartFormula report of compound 2.3ae-2.

Mass Spectrum SmartFormula Report

Analysis Info

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Method tune_low_NEW.m
Sample Name LLG-1-34
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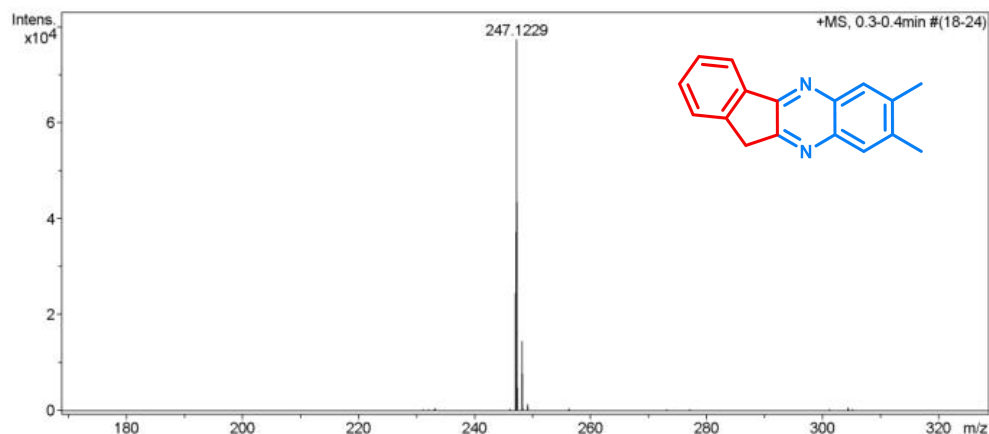
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Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Set Collision Cell RF 150.0 Vpp

Set Nebulizer 0.8 Bar
Set Dry Heater 180 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
247.1229	C 17 H 15 N 2	247.1230	0.1	0.5	2.28	ok	even	1+

Figure S43. Mass spectrum smartFormula report of compound 2.3af.

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name LLG-1-32
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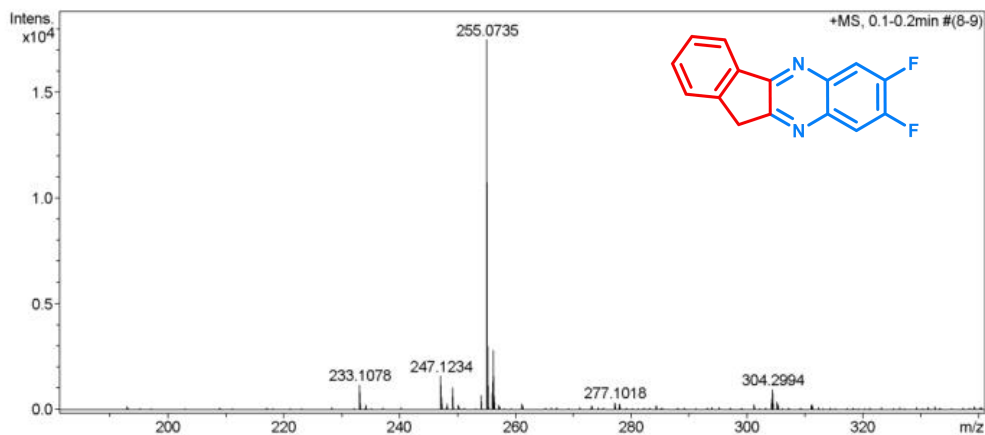
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Operator Ma
Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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Focus Not active
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Scan End 1200 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 150.0 Vpp

Set Nebulizer 0.8 Bar
Set Dry Heater 180 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
255.0735	C 15 H 9 F 2 N 2	255.0728	-0.7	-2.6	5.31	ok	even	1+

Figure S44. Mass spectrum smartFormula report of compound 2.3ag.

Mass Spectrum SmartFormula Report

Analysis Info

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 Sample Name LLG-1-39
 Comment

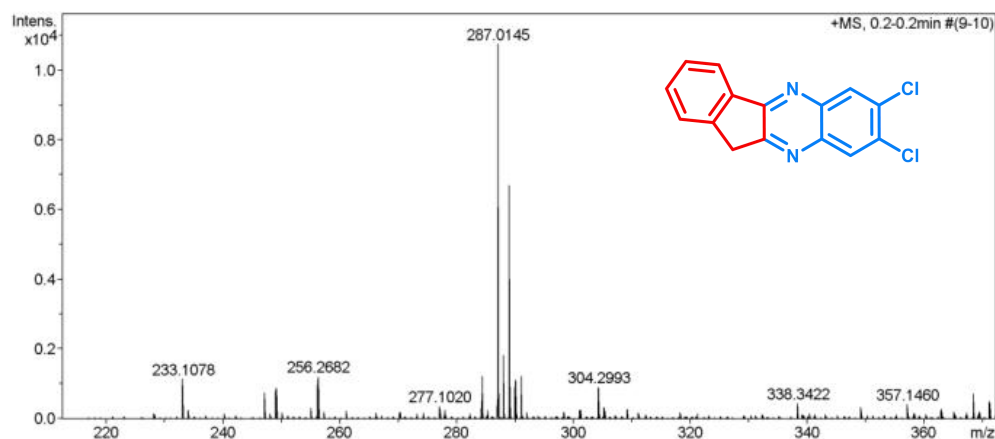
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Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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 Ion Polarity Positive
 Set Capillary 4500 V
 Set End Plate Offset -500 V
 Set Collision Cell RF 150.0 Vpp

Set Nebulizer 0.8 Bar
 Set Dry Heater 180 °C
 Set Dry Gas 6.0 l/min
 Set Divert Valve Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
287.0145	C ₁₅ H ₉ Cl ₂ N ₂	287.0137	-0.7	-2.6	12.40	ok	even	1+

Figure S45. Mass spectrum smartFormula report of compound 2.3ah.

Mass Spectrum SmartFormula Report

Analysis Info

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 Sample Name LLG-1-40
 Comment

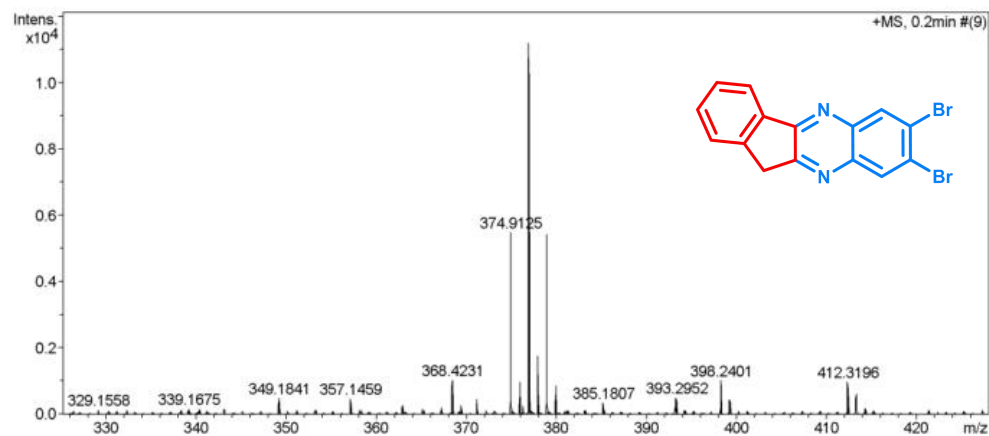
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 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

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 Set End Plate Offset -500 V
 Set Collision Cell RF 150.0 Vpp

Set Nebulizer 0.8 Bar
 Set Dry Heater 180 °C
 Set Dry Gas 6.0 l/min
 Set Divert Valve Source



Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	N-Rule	e ⁻ Conf	z
374.9125	C ₁₅ H ₉ Br ₂ N ₂	374.9127	0.2	0.6	466.03	ok	even	1+

Figure S46. Mass spectrum smartFormula report of compound 2.3ai.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\USER-2021\LLG-1-33.d
 Method tune_low_NEW.m
 Sample Name LLG-1-33
 Comment

Acquisition Date 6/25/2021 2:36:00 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

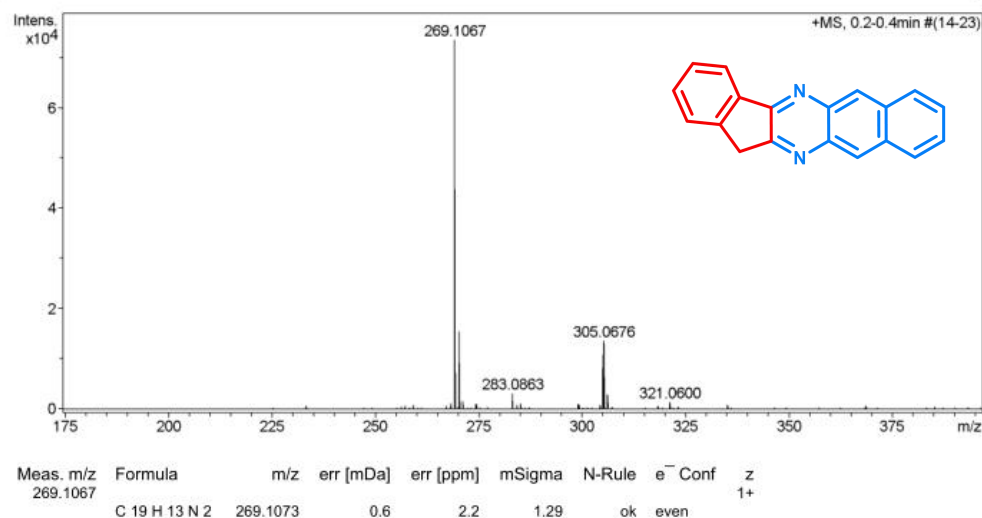


Figure S47. Mass spectrum smartFormula report of compound 2.3aj.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\data\USER-2021\LLG-1-41-1.d
 Method tune_low_NEW.m
 Sample Name LLG-1-41-1
 Comment

Acquisition Date 6/25/2021 2:39:43 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

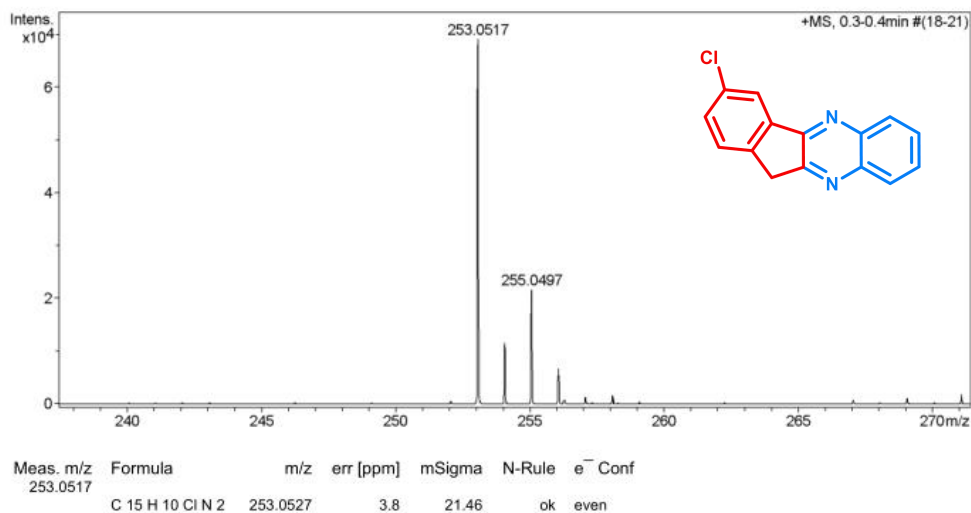


Figure S48. Mass spectrum smartFormula report of compound 2.3ba-1.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\USER-2021\LLG-1-41-2.d
 Method tune_low_NEW.m
 Sample Name LLG-1-41-2
 Comment

Acquisition Date 6/25/2021 2:41:38 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

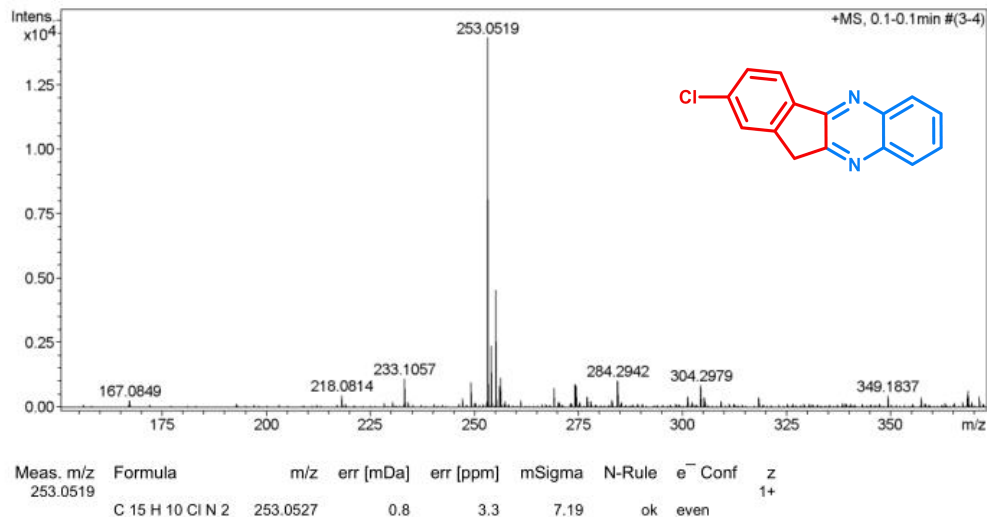


Figure S49. Mass spectrum smartFormula report of compound 2.3ba-2.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\USER-2021\LLG-1-42-2.d
 Method tune_low_NEW.m
 Sample Name LLG-1-42-2
 Comment

Acquisition Date 6/25/2021 2:44:04 PM

Operator Ma
 Instrument / Ser# micrOTOF-Q II 10203

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

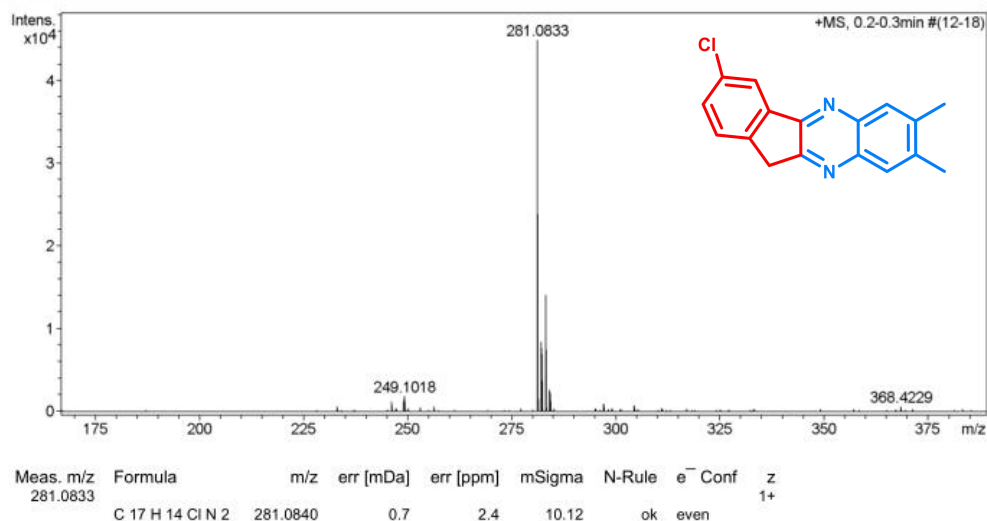


Figure S50. Mass spectrum smartFormula report of compound 2.3bb-1.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\USER-2021\LLG-1-42-1.d
 Method tune_low_NEW.m
 Sample Name LLG-1-42-1
 Comment

Acquisition Date 6/25/2021 2:42:52 PM

Operator Ma
 Instrument / Ser# microTOF-Q II 10203

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

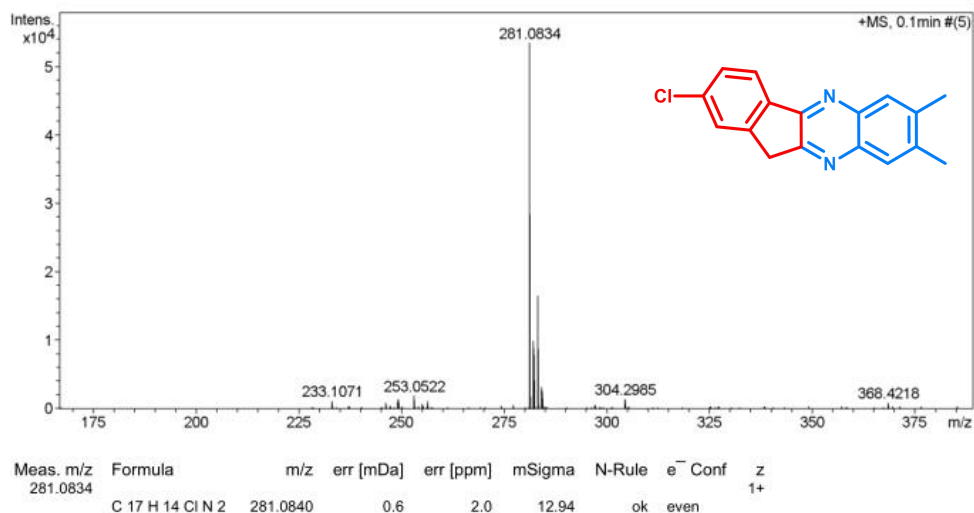


Figure S51. Mass spectrum smartFormula report of compound 2.3bb-2.

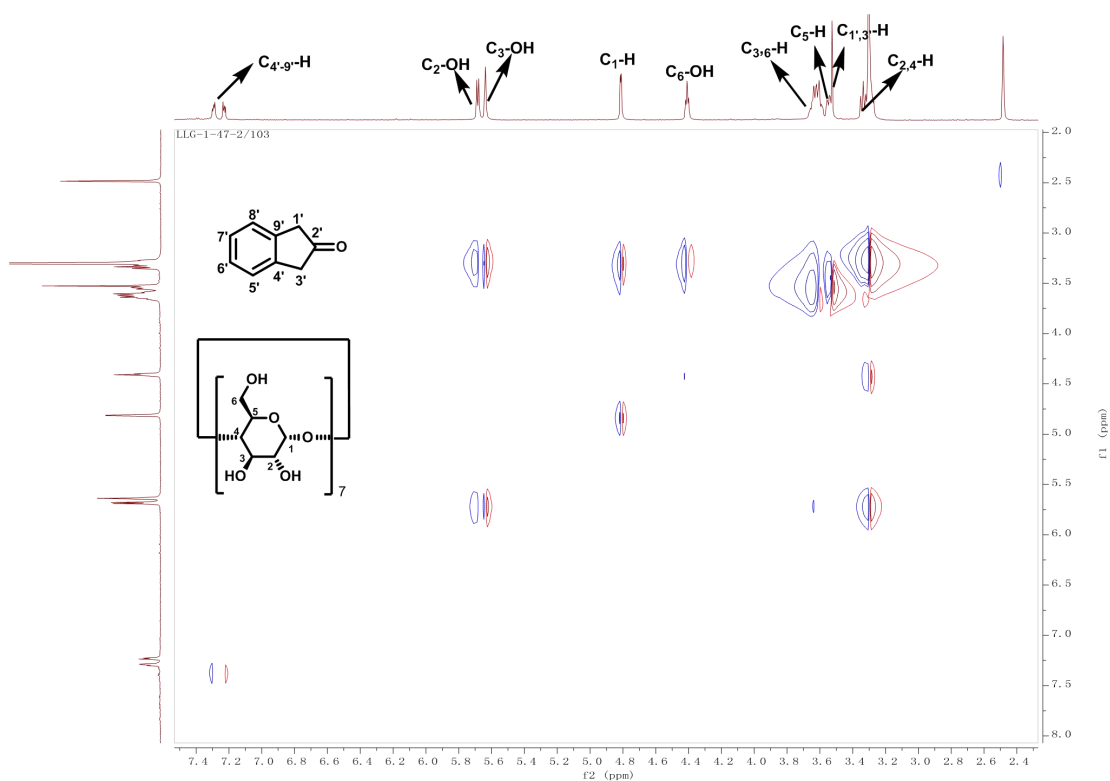


Figure S52. The NOESY spectrum of 2-indenone (1.0 eqv.) and β -CD (15 mol%) mixed after stirring in water for 12h.

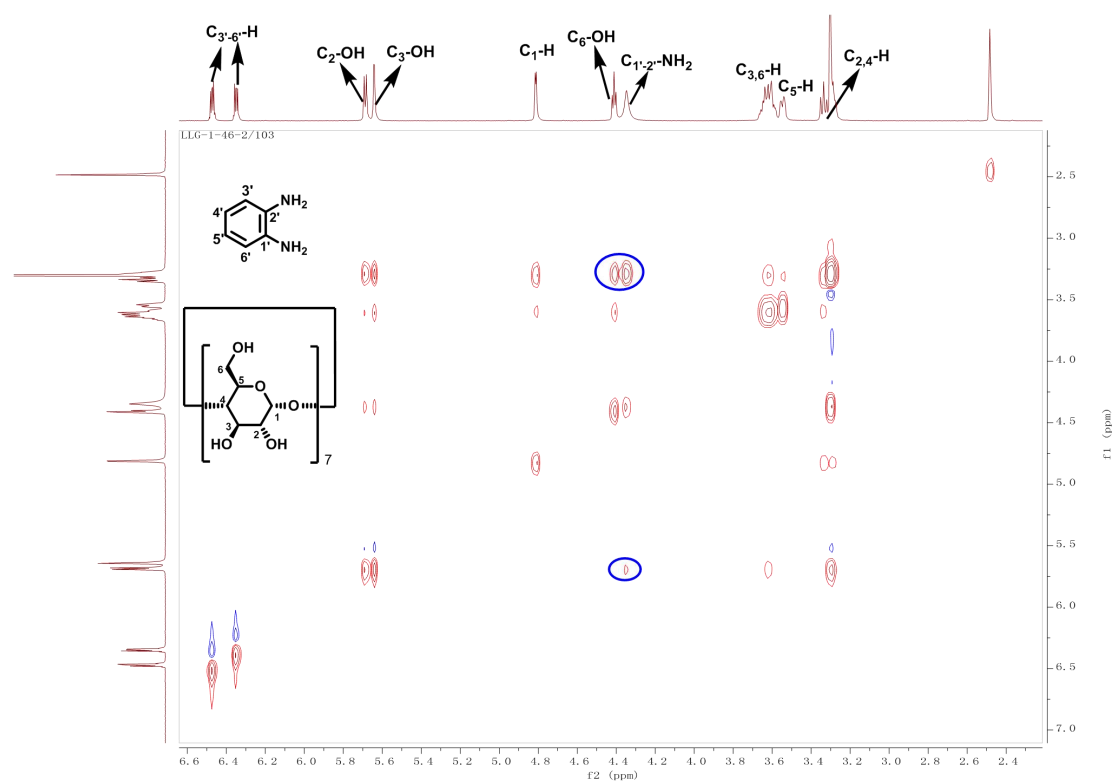


Figure S53. The NOESY spectrum of OPD (1.2 eqv.) and β -CD (15 mol%) mixed after stirring in water for 12h.

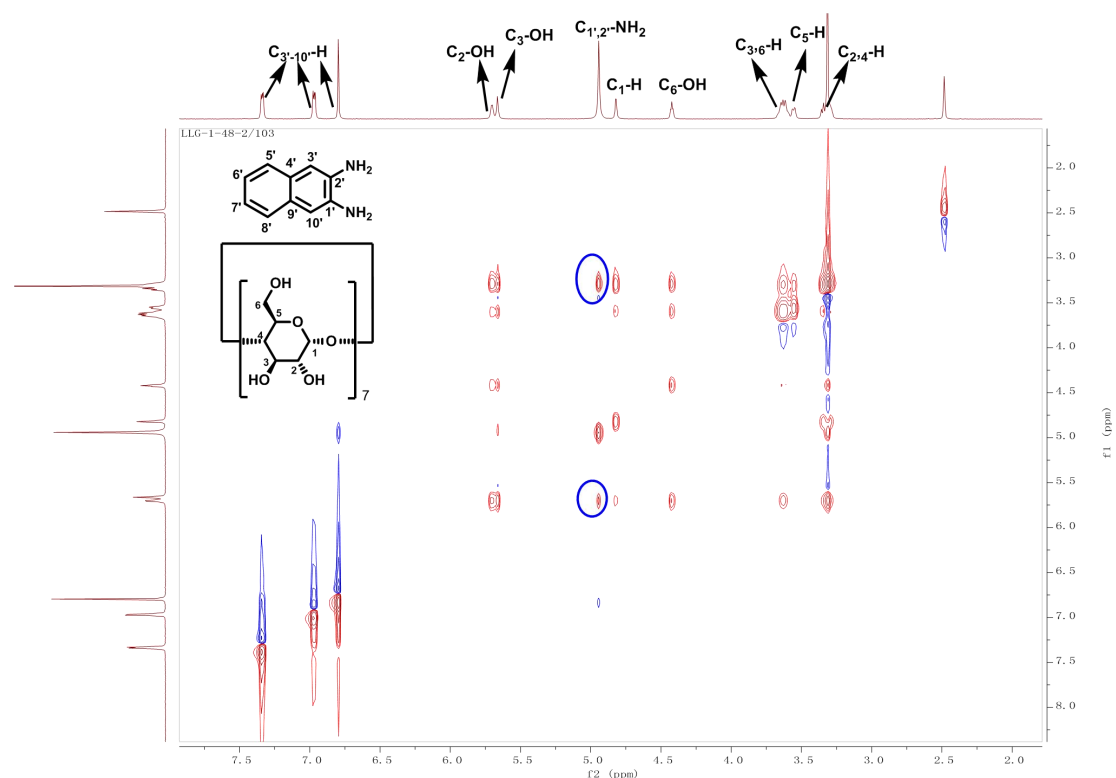


Figure S54. The NOESY spectrum of 2,3-diaminonaphthalene (1.2 eqv.) and β -CD (15 mol%) mixed after stirring in water for 12h.

Analysis Information

Item name:	MS-20220104	Analysis Method Item name:	MS-NOPDA-0916
Version:	3	Analysis Method Version:	2
Modified date:	Jan 04, 2022 14:25:44 China Standard Time	Sample Set Created date:	Jan 04, 2022 11:07:11 China Standard Time
Modified by:	Waters, Waters	Sample Set Instrument system name:	UPLC_QToF_2
Folder:	Company/sample/2022		

MS Instrument Type: Waters Vion® IMS QToF

Experiment Settings:

Experiment type:	ESI+	Scan Mode:	MS
Capillary voltage:	3.0 kV	Low mass:	50 m/z
Source temperature:	120°C	High mass:	2000 m/z
Desolvation temperature:	450°C	Scan time:	0.200 s
Cone gas:	50 L/h		
Desolvation gas:	800 L/h		

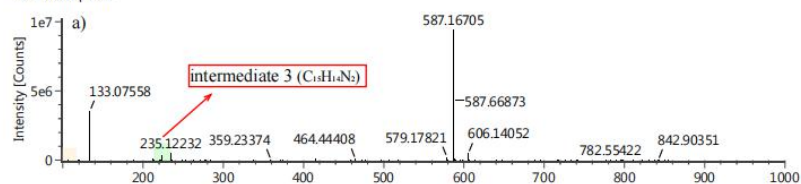
Item name: 20220104-LLG20220103, Sample position: 1:A,8, Replicate number: 1

	Formula	Neutral mass (Da)	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
1	C ₁₅ H ₁₄ N ₂	222.11570	223.12199	-1.0	-4.4	67393	+H	Identified
2	C ₁₅ H ₁₂ N ₂ O	236.09496	237.10165	-0.6	-2.5	3955403	+H, -e	Identified

Item name: 20220104-LLG20220103

Channel name: Time 0.1835 +/- 0.0500 minutes

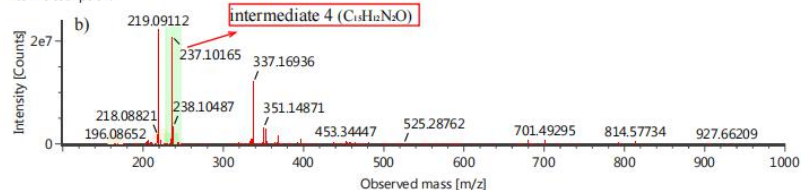
Item description:



Item name: 20220104-LLG20220103

Channel name: Time 0.1233 +/- 0.0500 minutes

Item description:

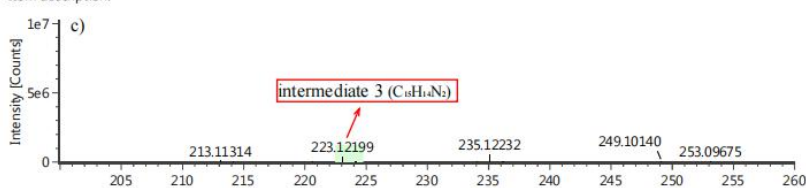


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Item name: 20220104-LLG20220103

Channel name: Time 0.1835 +/- 0.0500 minutes

Item description:



Item name: 20220104-LLG20220103

Channel name: Time 0.1233 +/- 0.0500 minutes

Item description:

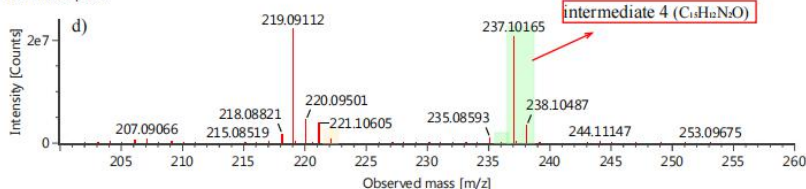


Figure S55. The HRMS of template reaction (**2.1a** (0.2 mmol), **2.2a** (0.24 mmol) and β -CD (15 %) in air) in water after 1h: **a)** the extraction mass spectrometry of intermediate **3**; **b)** the extraction mass spectrometry of intermediate **4**; **c)** the enlarged view of the abscissa of **Figure S55a**; **c)** the enlarged view of the abscissa of **Figure S55b**.