

Bromotryptamine and bromotyramine derivatives from the Tropical Southwestern Pacific sponge *Narrabeena nigra*.

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Biological material.**S1.** *Narrabeena nigra* specimen collected at Alofi Island.

Irregularly lamellar or thickly encrusting sponge, beige gray in life, surface becoming dark grey in alcohol. Skeleton of uncured, laminated fibers, 15-100 μm in diameter, arranged in an irregular reticulation with meshes 150-500 μm in size. Primary fibers 50-100 μm in diameter, with a small central pith, ending free on 350-500 μm at the surface. Secondary fibers 15-50 μm in diameter, without pith.

S2. ^1H NMR data, δ_{H} in ppm, mult. (J in Hz), in $\text{MeOH}-d_4$ for bromotryptamines

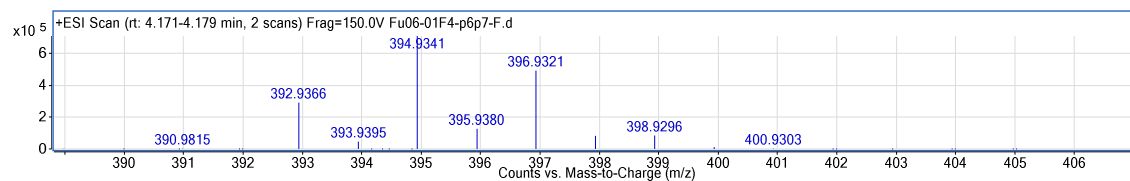
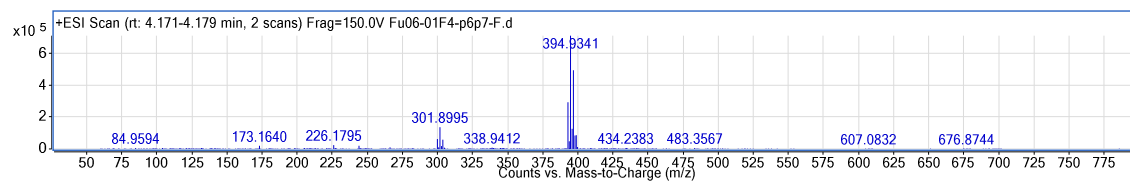
No.	9 ^b	10 ^a	11 ^a	12 ^a	13 ^a	14 ^a	15 ^a
2	7.26, s	7.26, s	7.24, s	7.20, s	7.19, s		
4	7.93, s	7.95, s	7.93, s	7.49, d (8.5)	7.49, d (8.5)	7.63, d (8.5)	8.15, d (8.5)
5	-	-	-	7.17, dd (8.5, 1.5)	7.17, dd (8.5, 1.5)	6.72, dd (8.5, 1.5)	7.55, dd (8.5, 1.5)
6	-	-	-	-	-	-	-
7	7.70, s	7.74, s	7.73, s	7.54, d (1.5)	7.54, d (1.5)	6.98, d (1.5)	7.80, d (1.5)
7a	-	-	-	-	-	-	-
8	3.14, t (7.5)	3.10, t (7.5)	3.07, t (7.5)	3.13, t (7.5)	3.10, t (7.5)	^c	6.35, d (7.5)
9	3.39, t (7.5)	3.29, t (7.5)	3.21, t (7.5)	3.30 ^c	3.22, t (7.5)	3.34, t (5.5)	7.99, d (7.5)
11	2.93, s			2.70, s			

^a 500MHz ^b 600MHz ^c Overlap with solvent signal

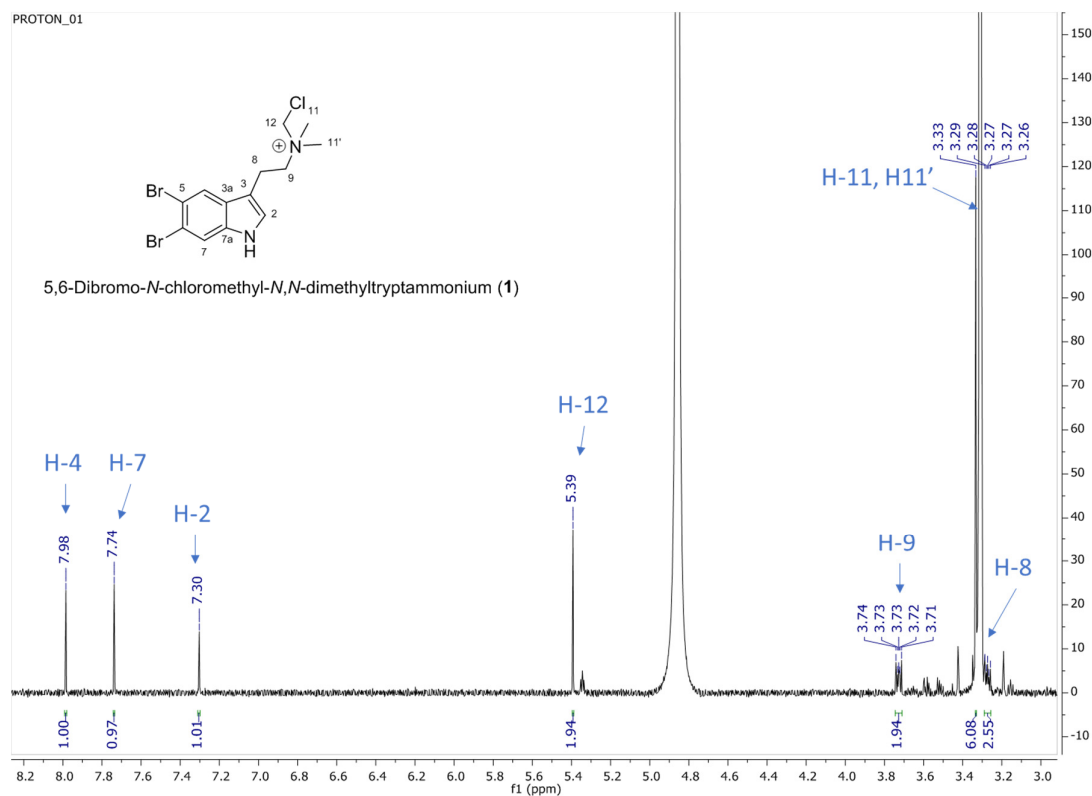
S3. ^1H NMR data, δ_{H} in ppm, mult. (J in Hz), in $\text{MeOH}-d_4$ for bromotyramines

No.	16 ^a	17 ^a	18 ^a
2	7.53, s	7.48, d (1.5)	7.51, d (1.5)
3	-	-	-
4	-	-	-
5	-	7.01, d (8.5)	6.98, d (8.5)
6	7.53, s	7.22, dd (8.5, 1.5)	7.26, dd (8.5, 1.5)
7	2.90, t (7.5)	2.87, d (7.5)	3.96, d (12.0)
8	3.16, t (7.5)	3.13, d (7.5)	3.13, t (12.0)
10			3.29, s
O-CH ₃	3.84, s	3.86, s	3.85, s

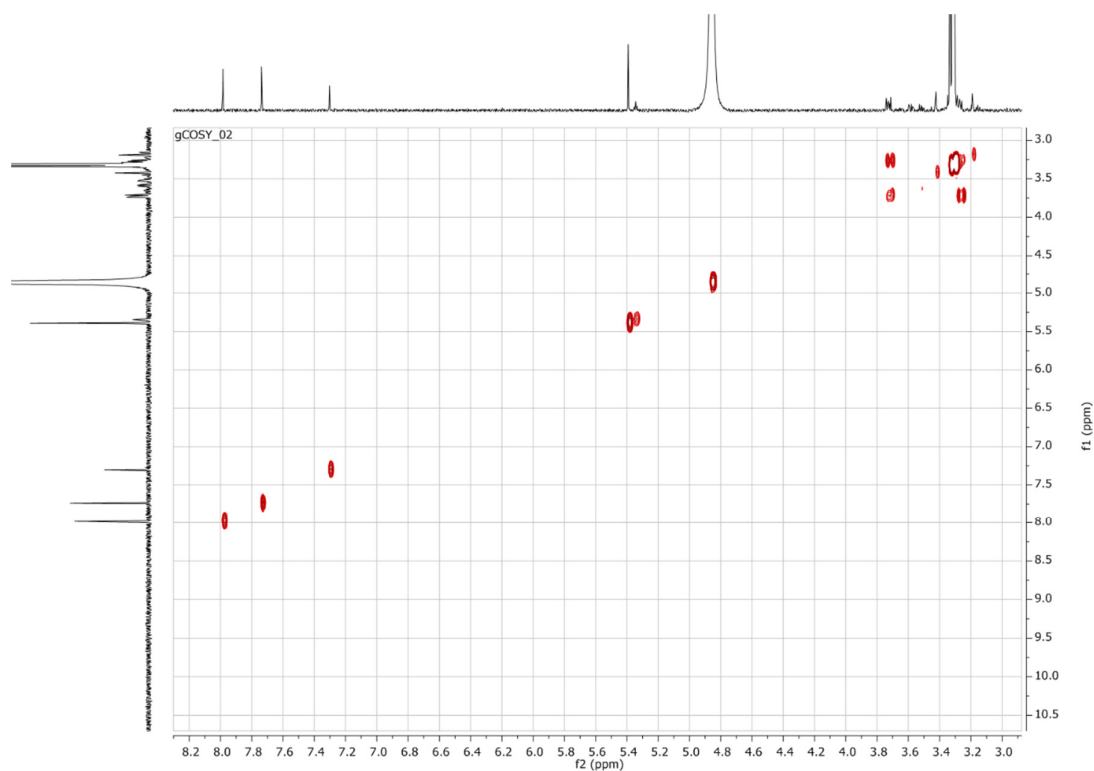
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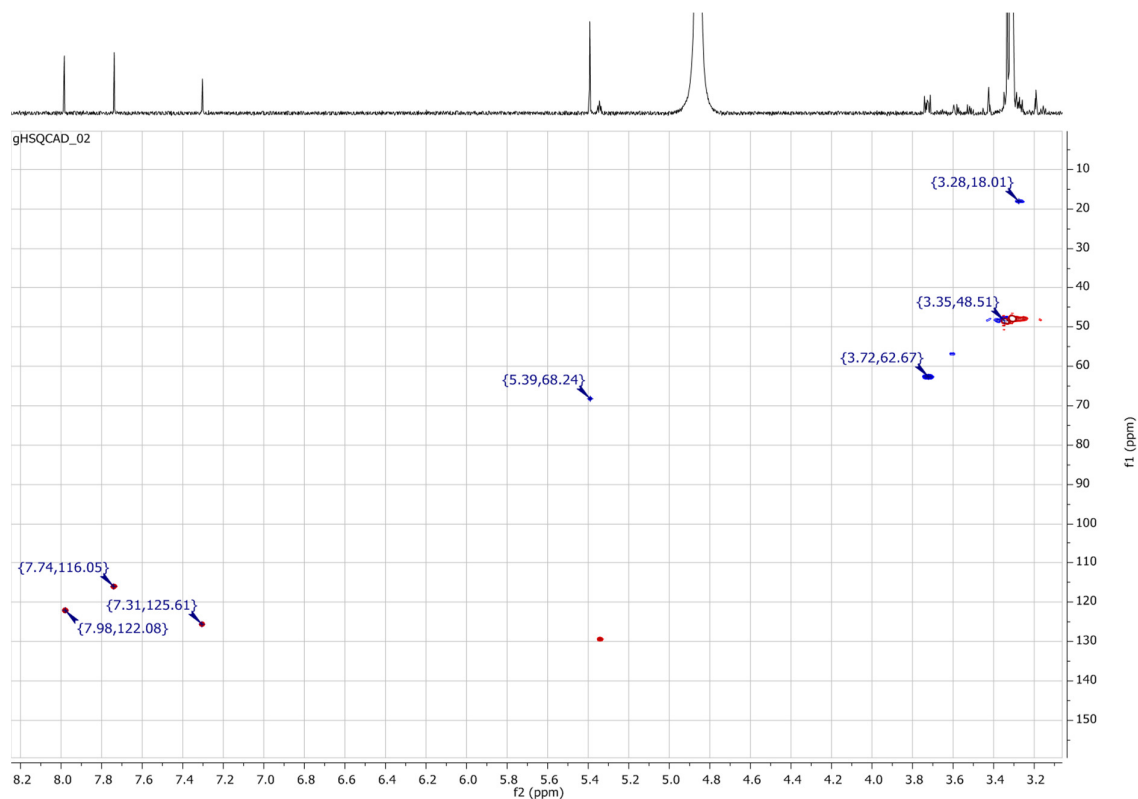
S4. ESI(+)-HRMS analysis of **1** and crop of the molecular ion.



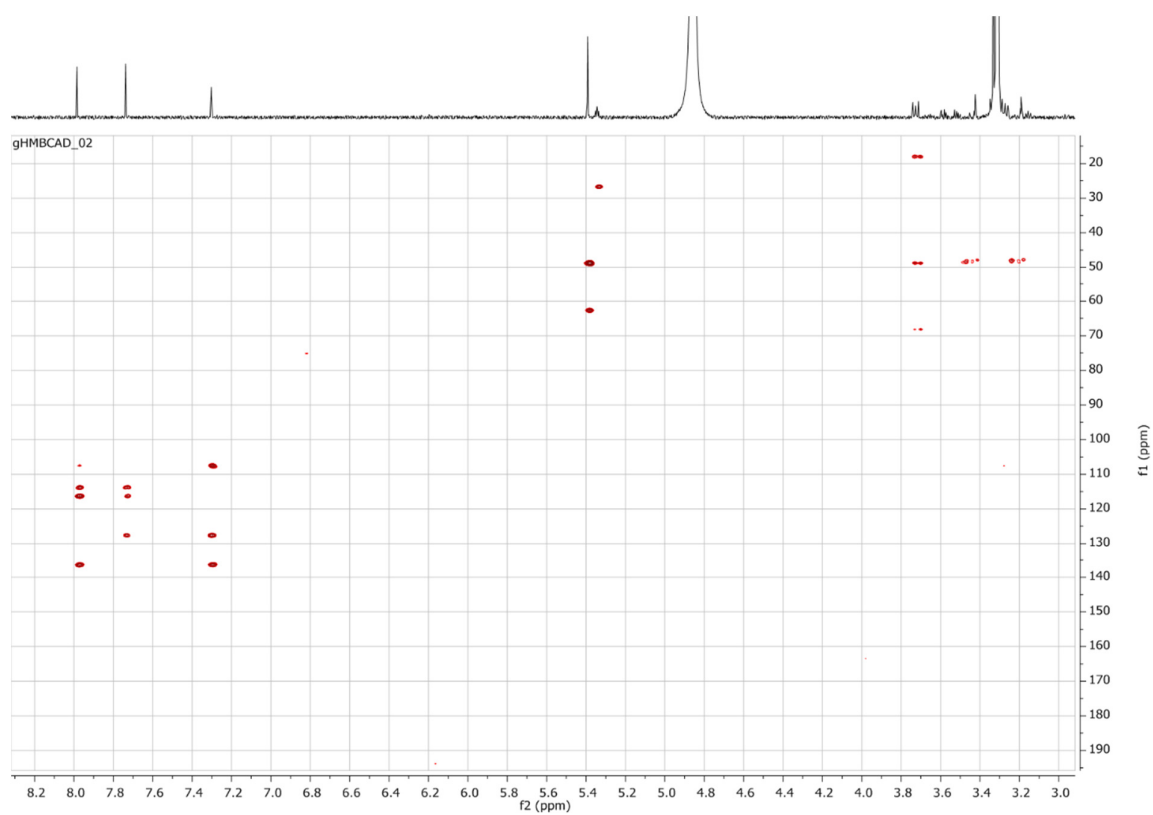
S5. ¹H NMR spectrum of **1** (600 MHz, MeOH-*d*₄).



S6. COSY NMR spectrum of **1** (600 MHz, MeOH-*d*₄).

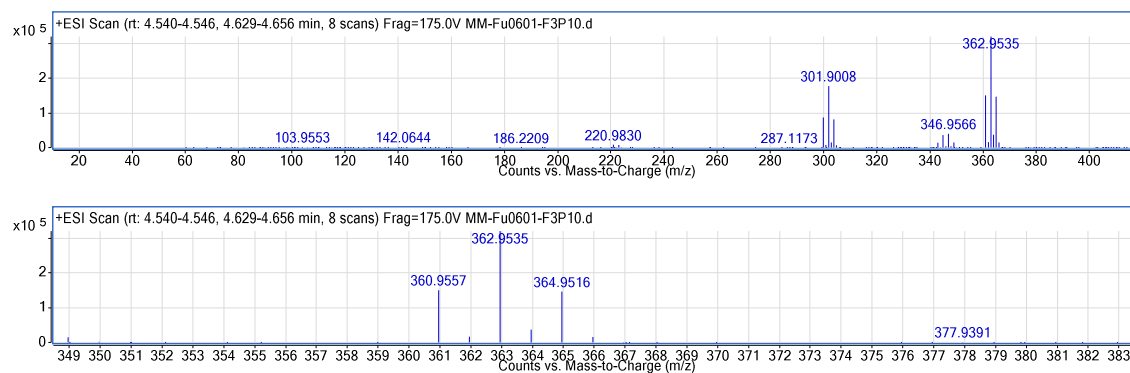


S7. HSQC NMR spectrum of **1** (600 MHz, MeOH-*d*₄).

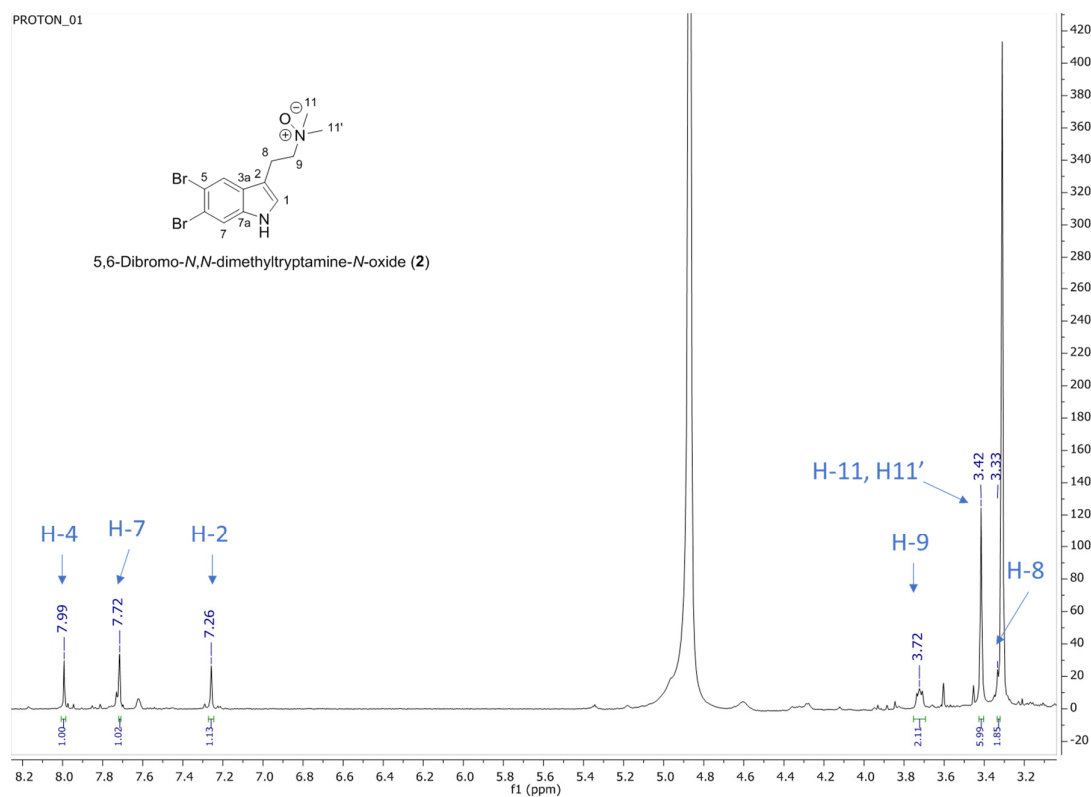


S8. HMBC NMR spectrum of **1** (600 MHz, $\text{MeOH-}d_4$).

Supporting information

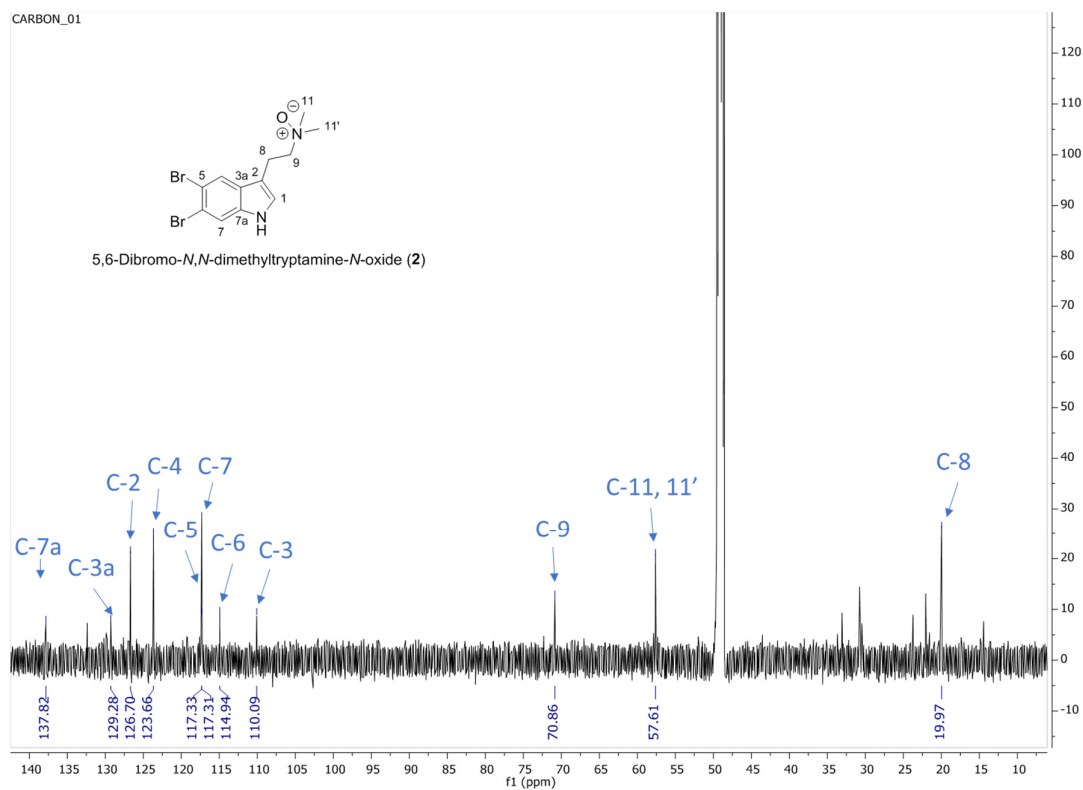


S9. ESI(+)-HRMS analysis of **2** and crop of the molecular ion.

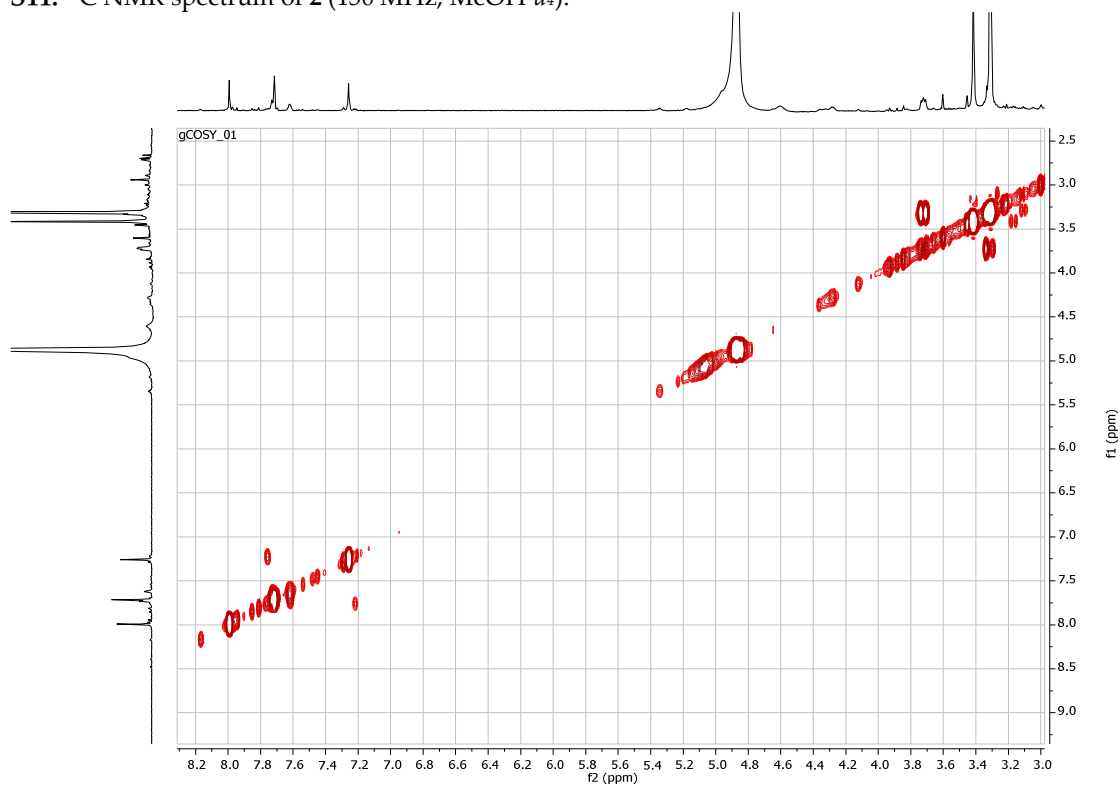


S10. ^1H NMR spectrum of **2** (600 MHz, $\text{MeOH-}d_4$).

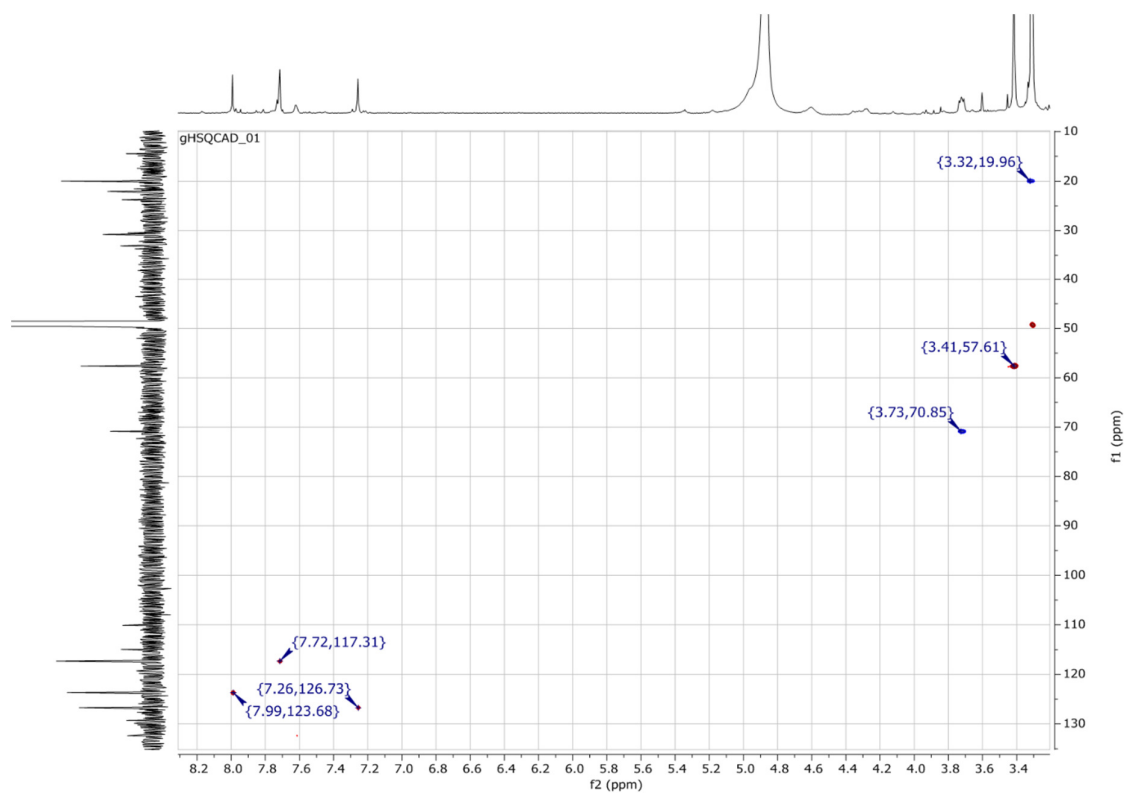
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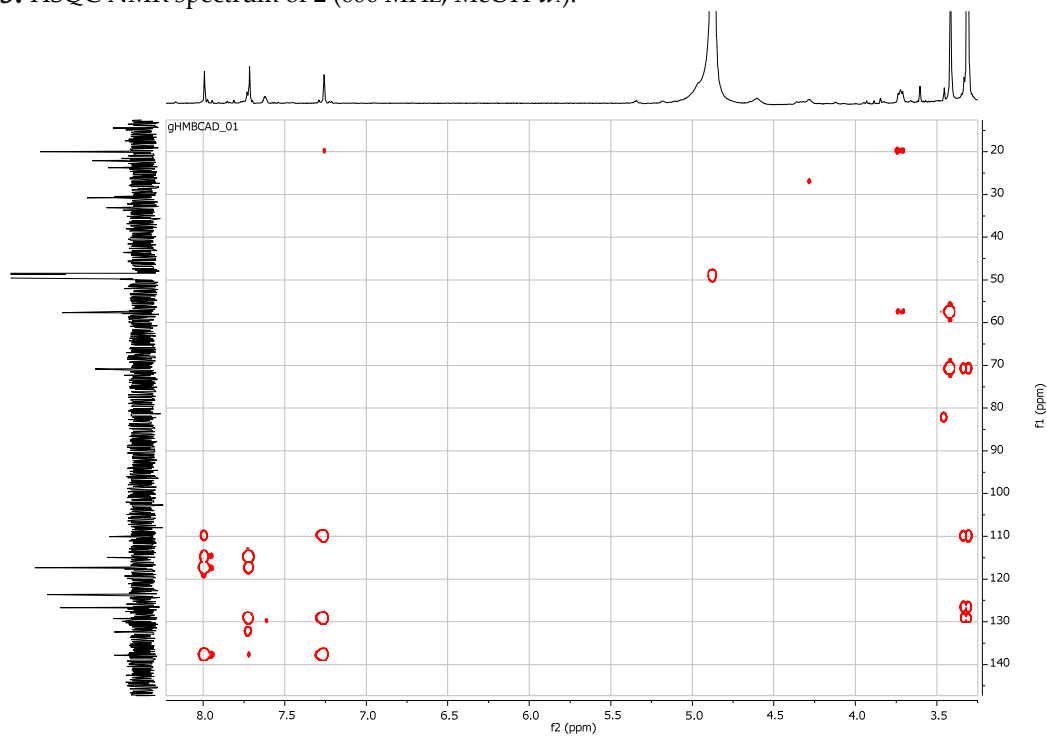
S11. ^{13}C NMR spectrum of **2** (150 MHz, $\text{MeOH-}d_4$).



S12. COSY NMR spectrum of **2** (600 MHz, $\text{MeOH-}d_4$).

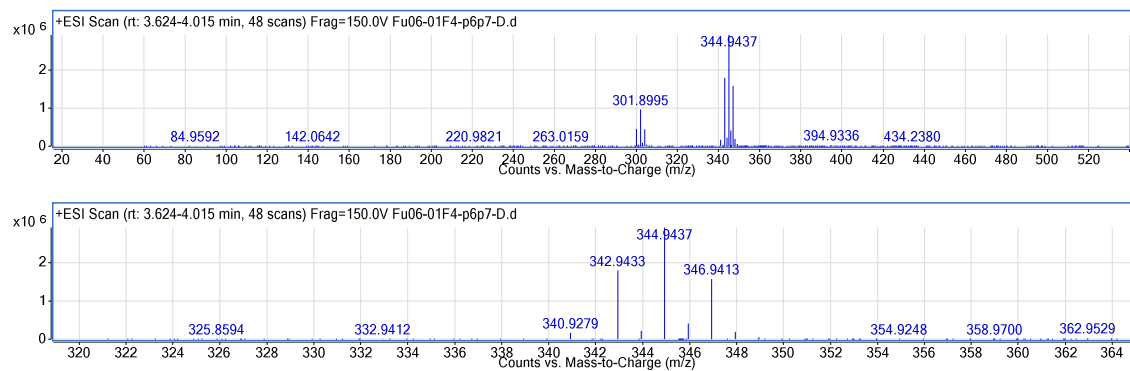


S13. HSQC NMR spectrum of **2** (600 MHz, MeOH- d_4).

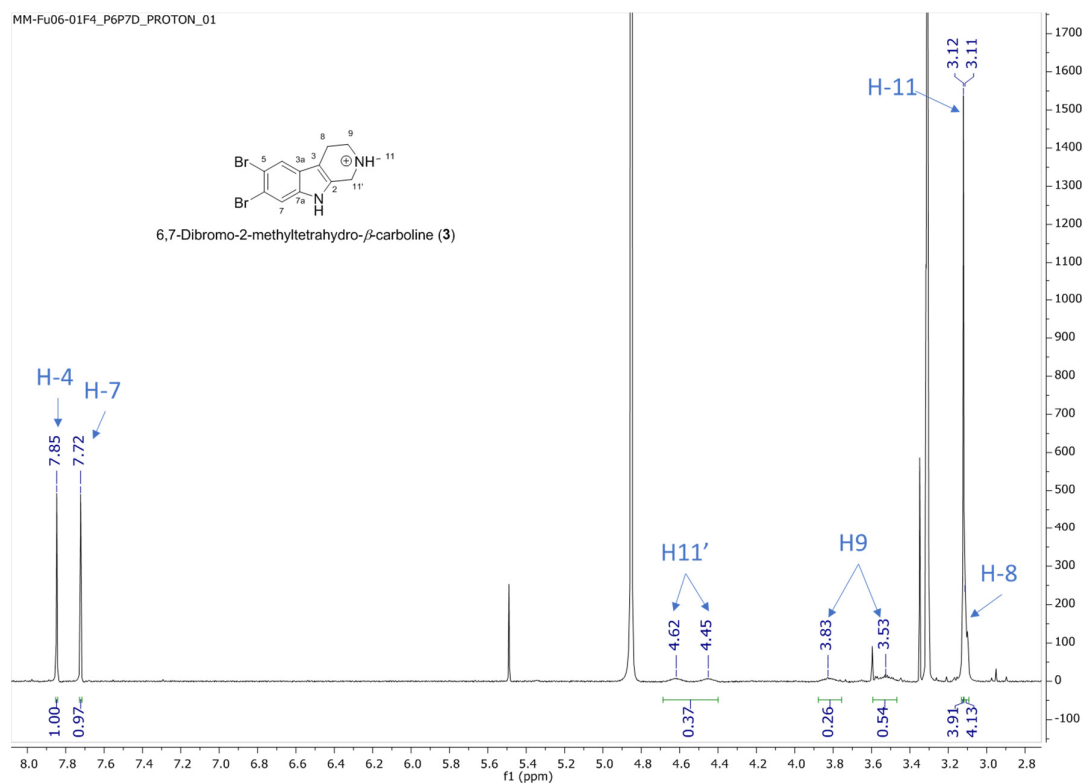


S14. HMBC NMR spectrum of **2** (600 MHz, MeOH- d_4).

Supporting information

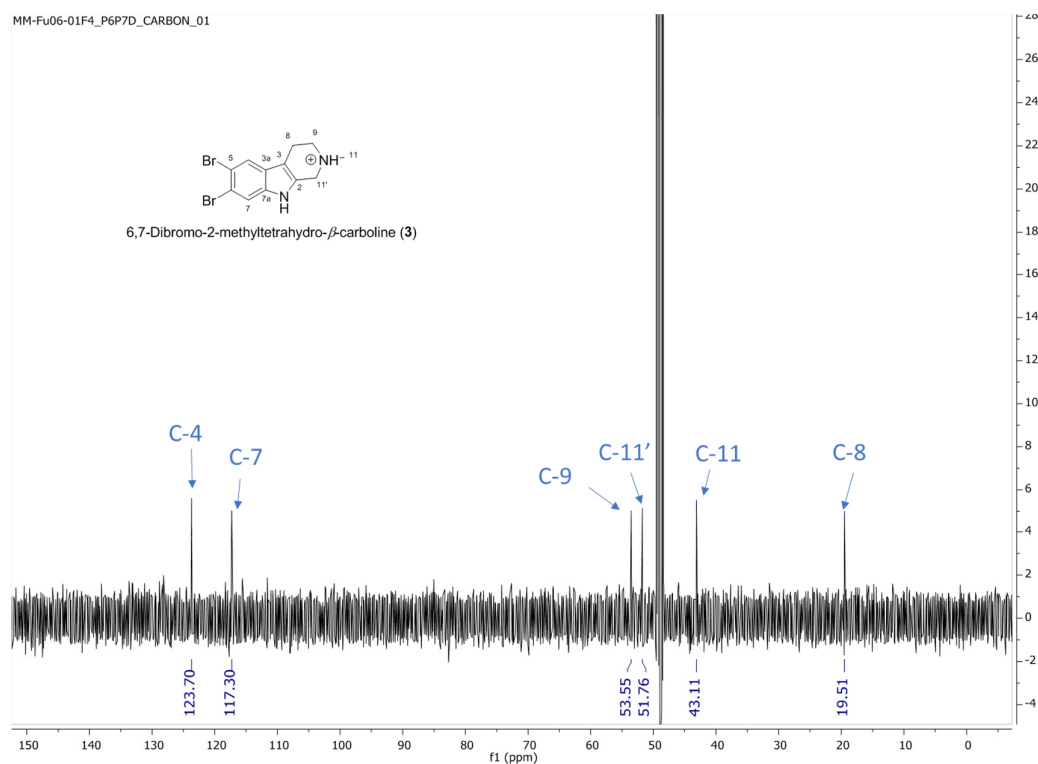


S15. ESI(+)-HRMS analysis of **3** and crop of the molecular ion.

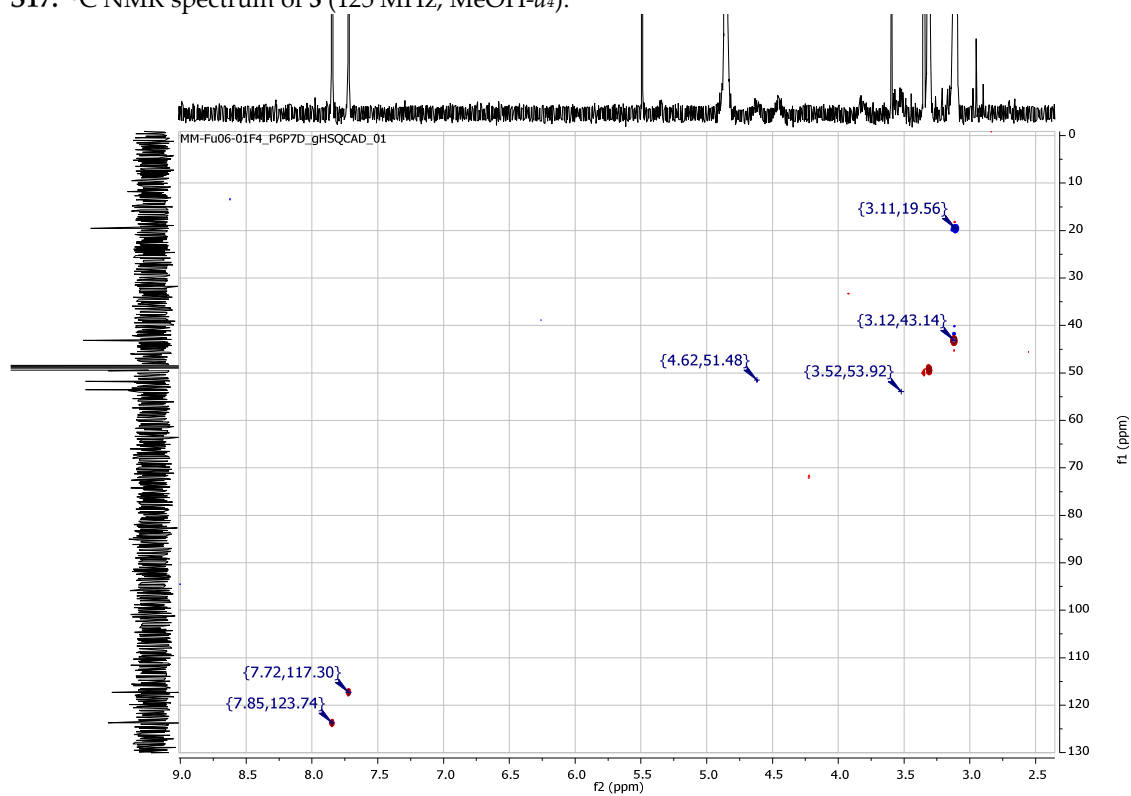


S16. ^1H NMR spectrum of **3** (500 MHz, $\text{MeOH-}d_4$).

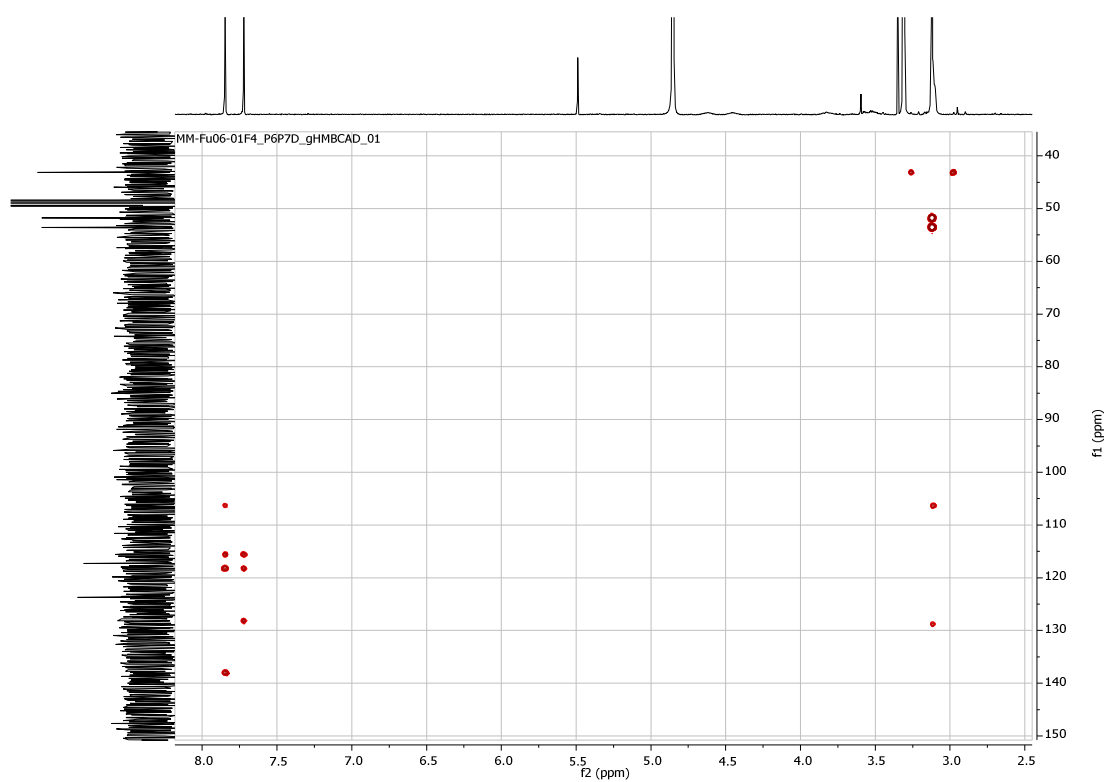
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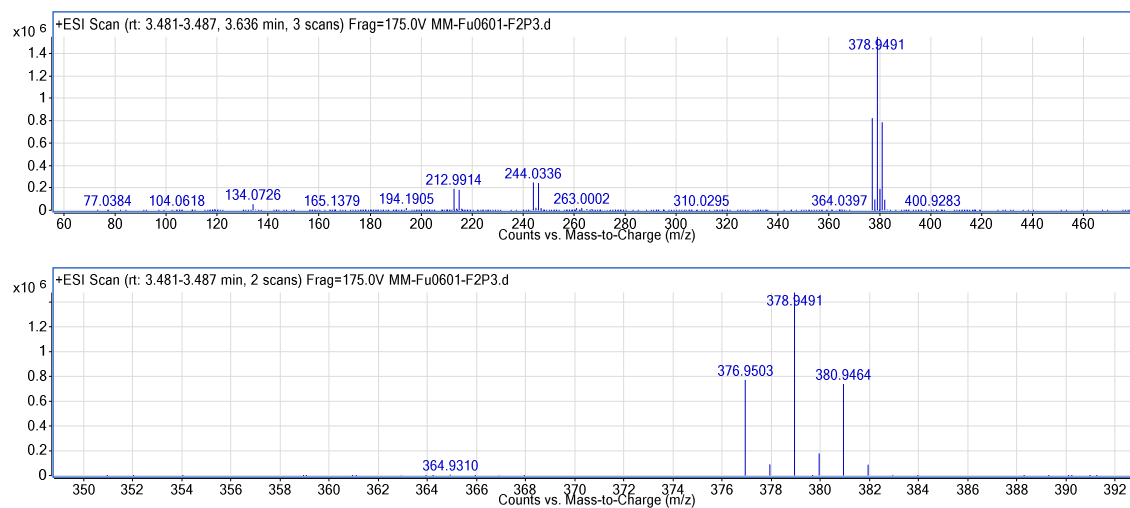
S17. ^{13}C NMR spectrum of **3** (125 MHz, $\text{MeOH-}d_4$).



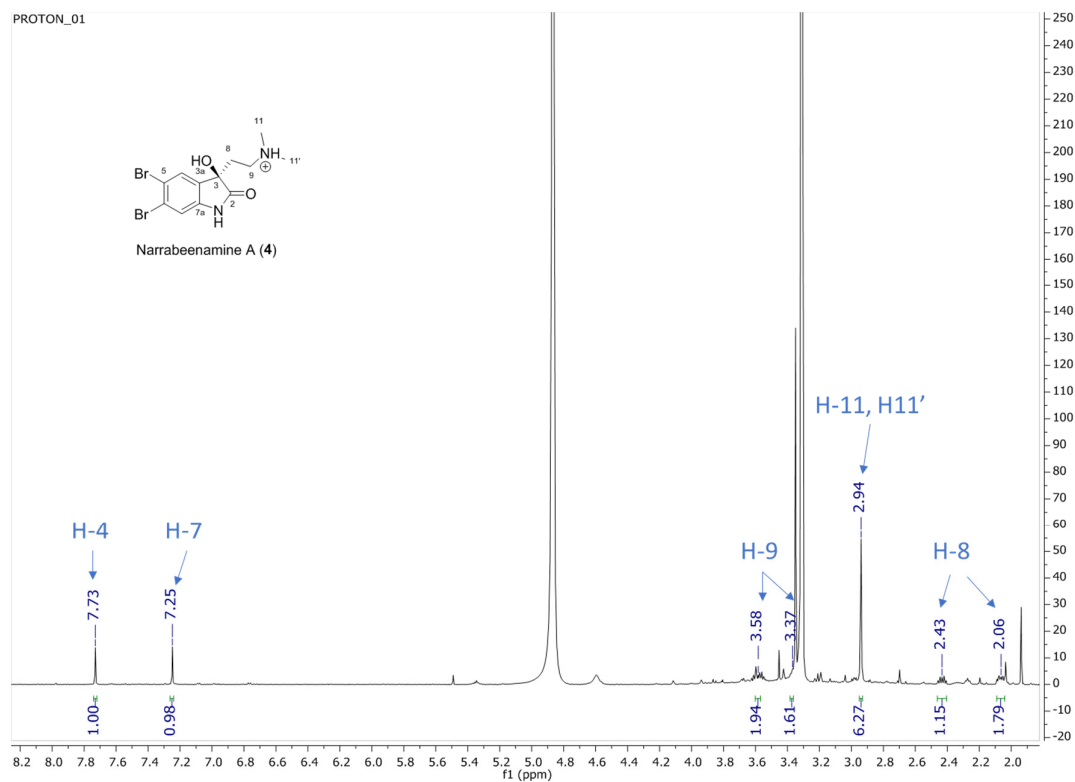
S18. HSQC NMR spectrum of **3** (500 MHz, $\text{MeOH-}d_4$).



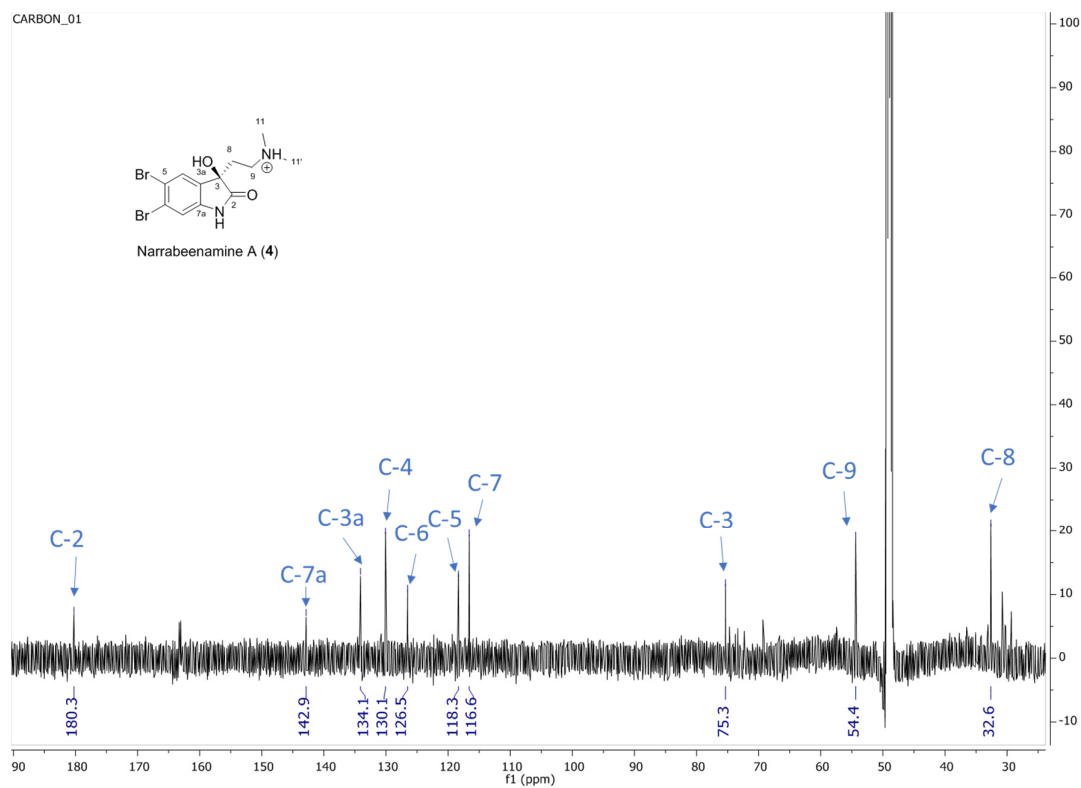
S19. HMBC NMR spectrum of **3** (500 MHz, $\text{MeOH-}d_4$).



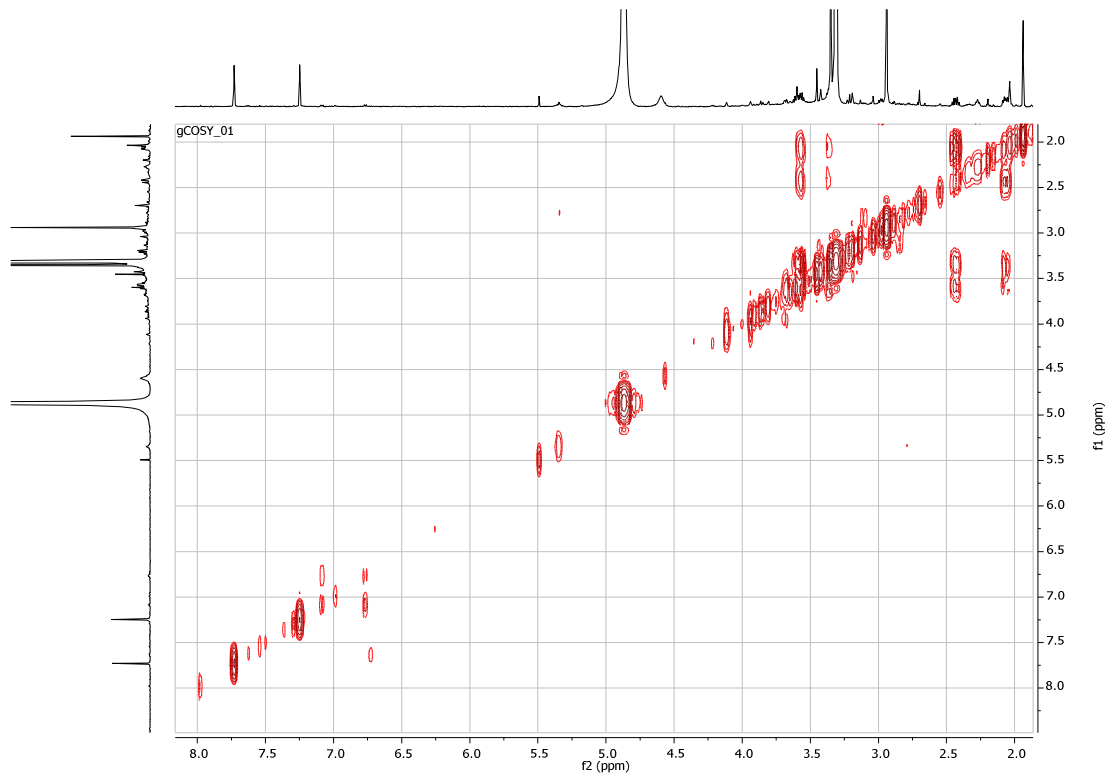
S20. ESI(+)-HRMS analysis of **4** and crop of the molecular ion.



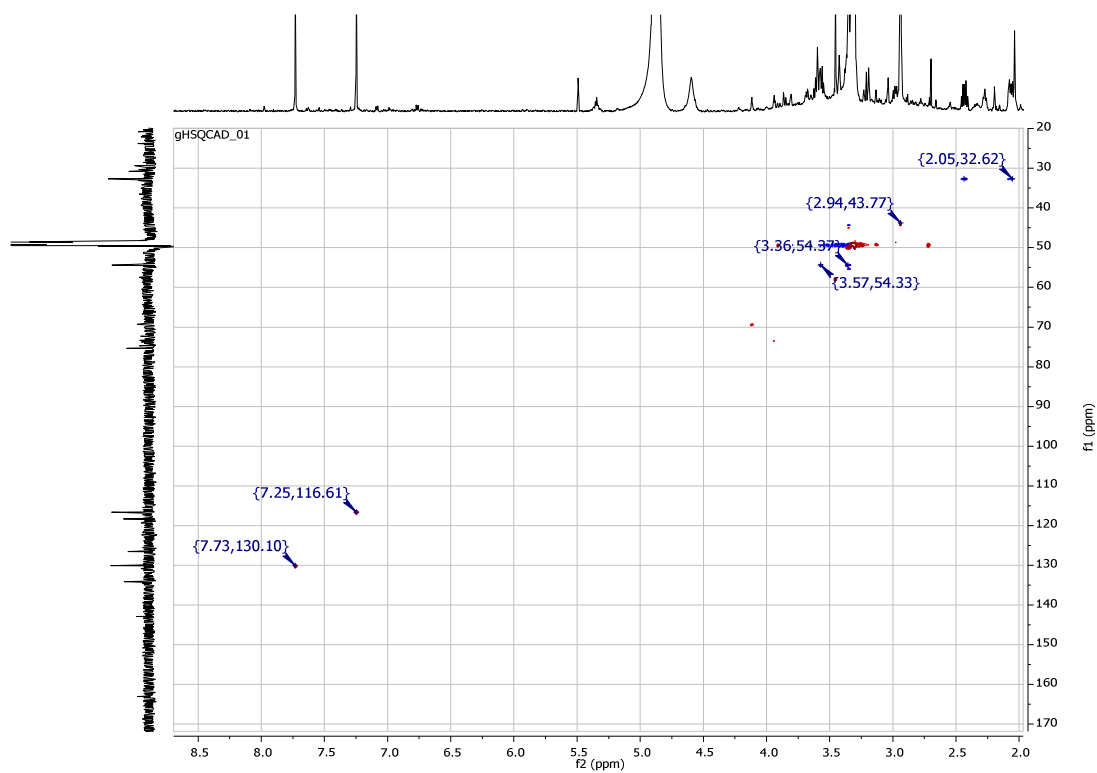
S21. ^1H NMR spectrum of **4** (600 MHz, $\text{MeOH-}d_4$).



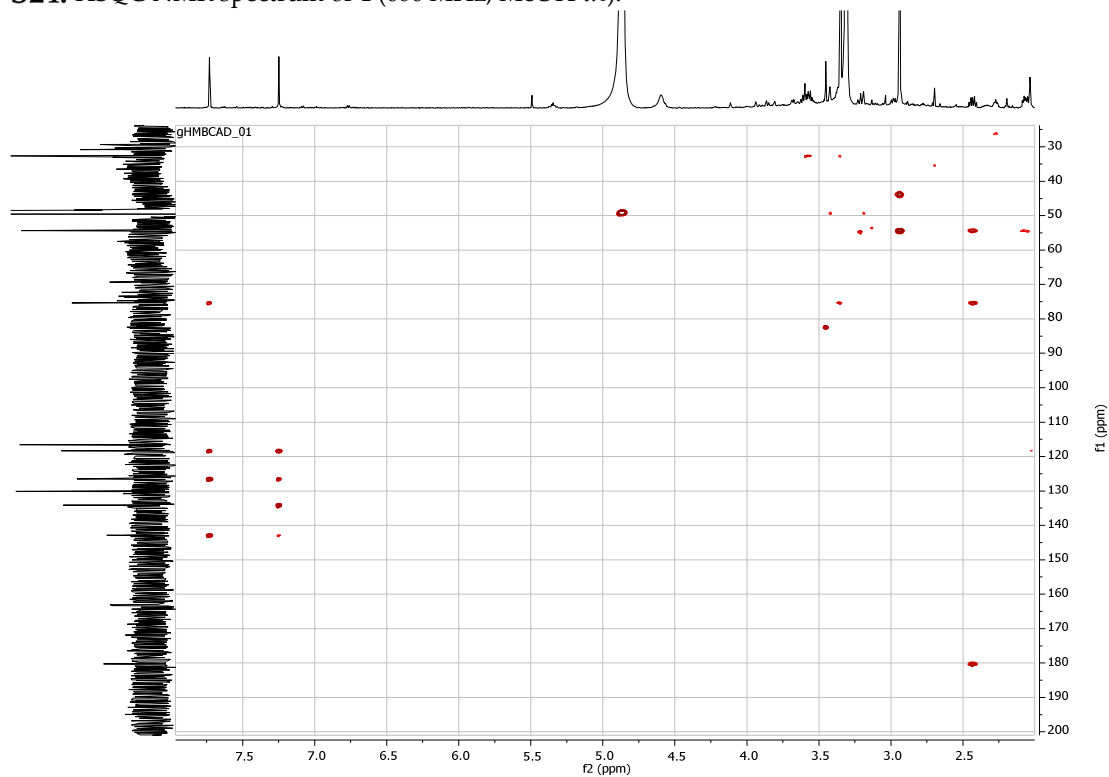
S22. ¹³C NMR spectrum of **4** (150 MHz, MeOH-*d*₄).



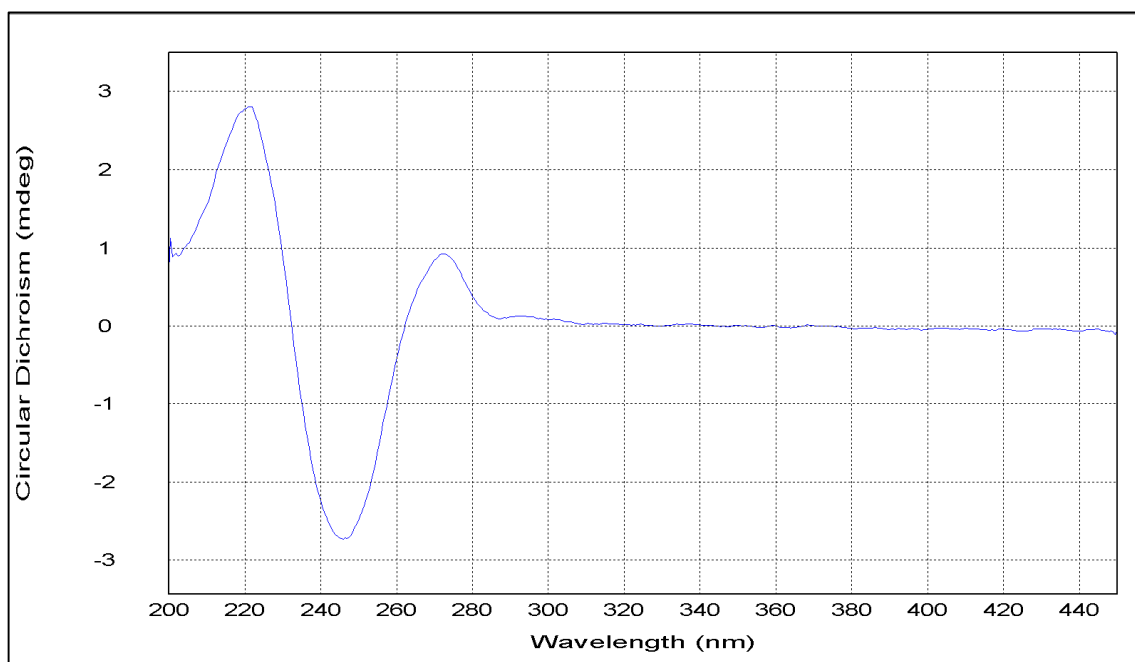
S23. COSY NMR spectrum of **4** (600 MHz, MeOH-*d*₄).



S24. HSQC NMR spectrum of **4** (600 MHz, MeOH- d_4).

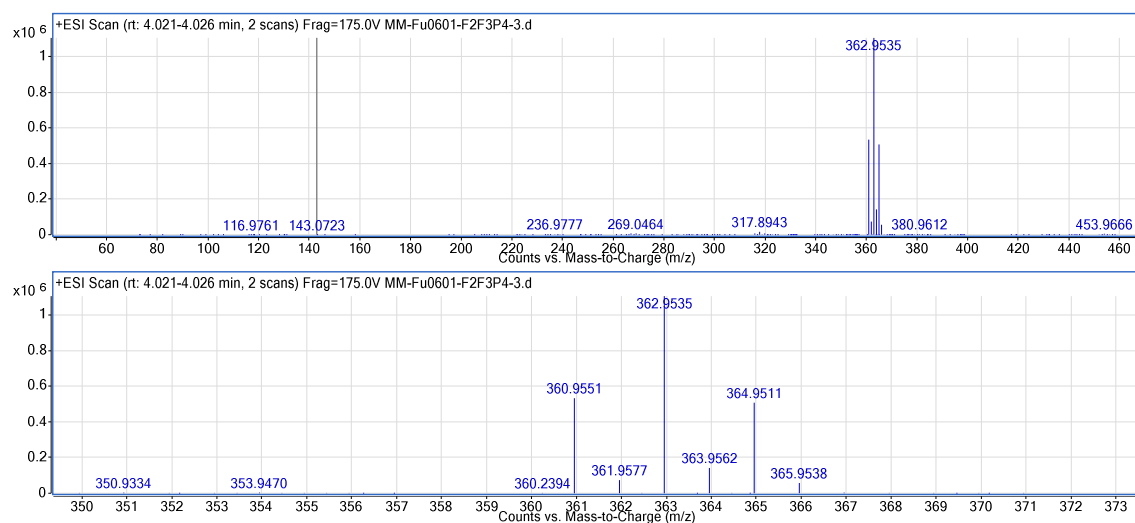


S25. HMBC NMR spectrum of **4** (600 MHz, MeOH- d_4).

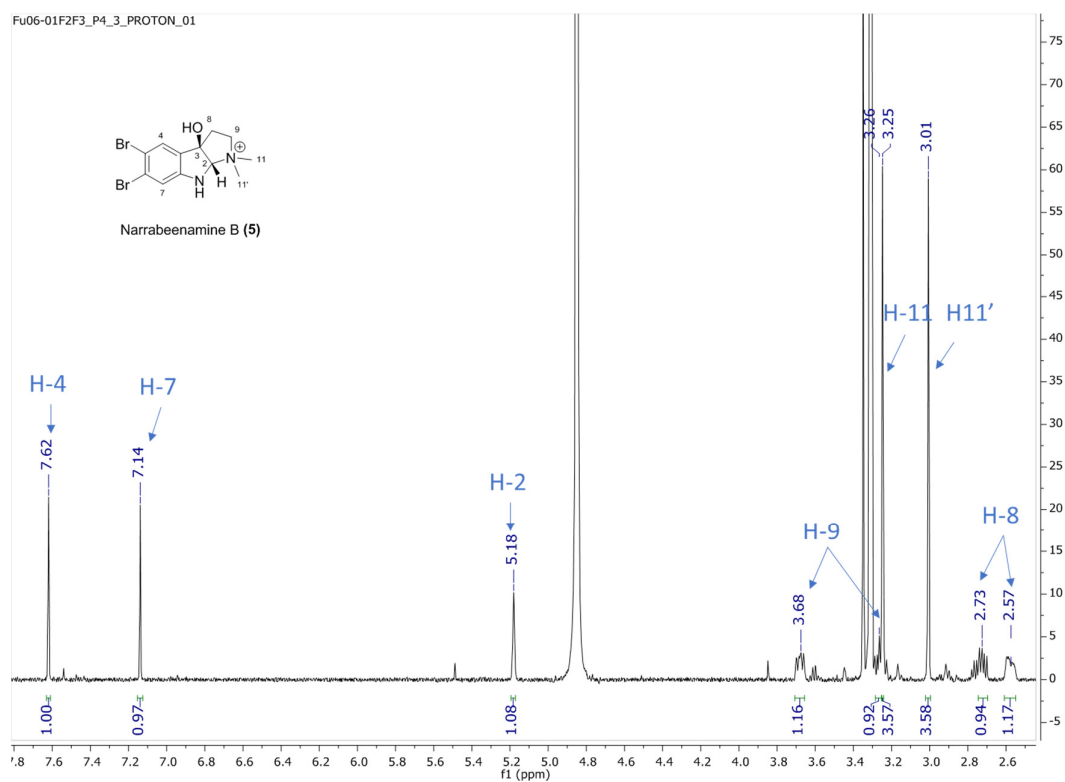


S26. ECD spectrum of compound **4** in CH₃CN at 0.1 mg/mL

Supporting information

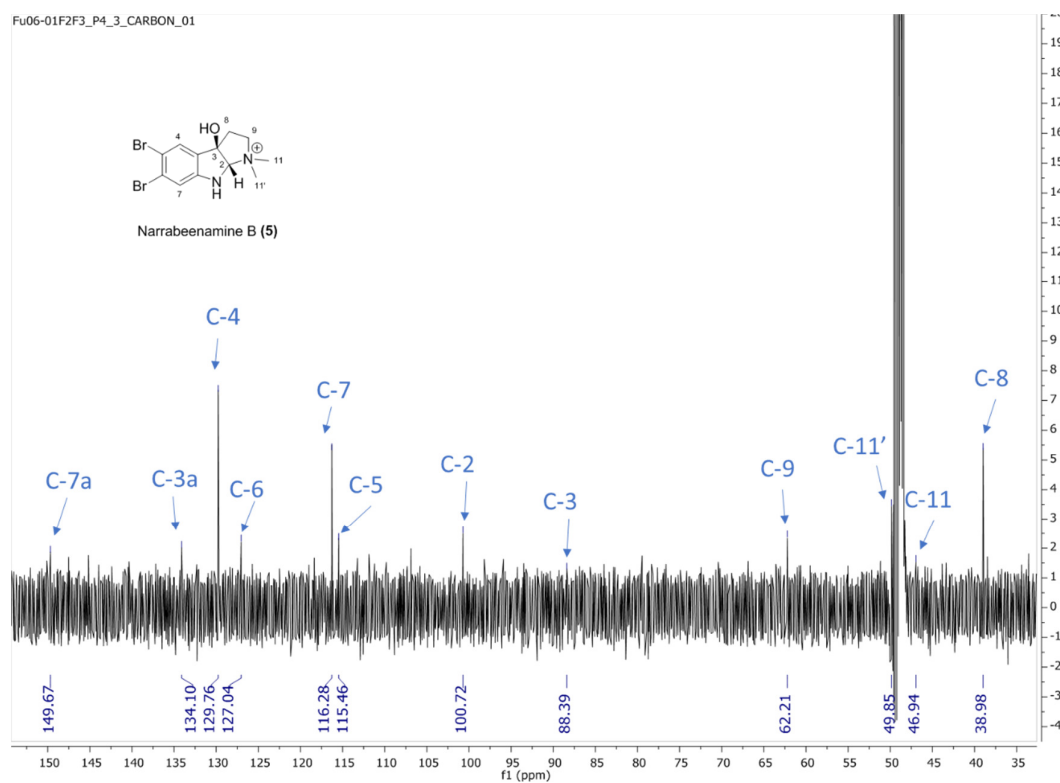
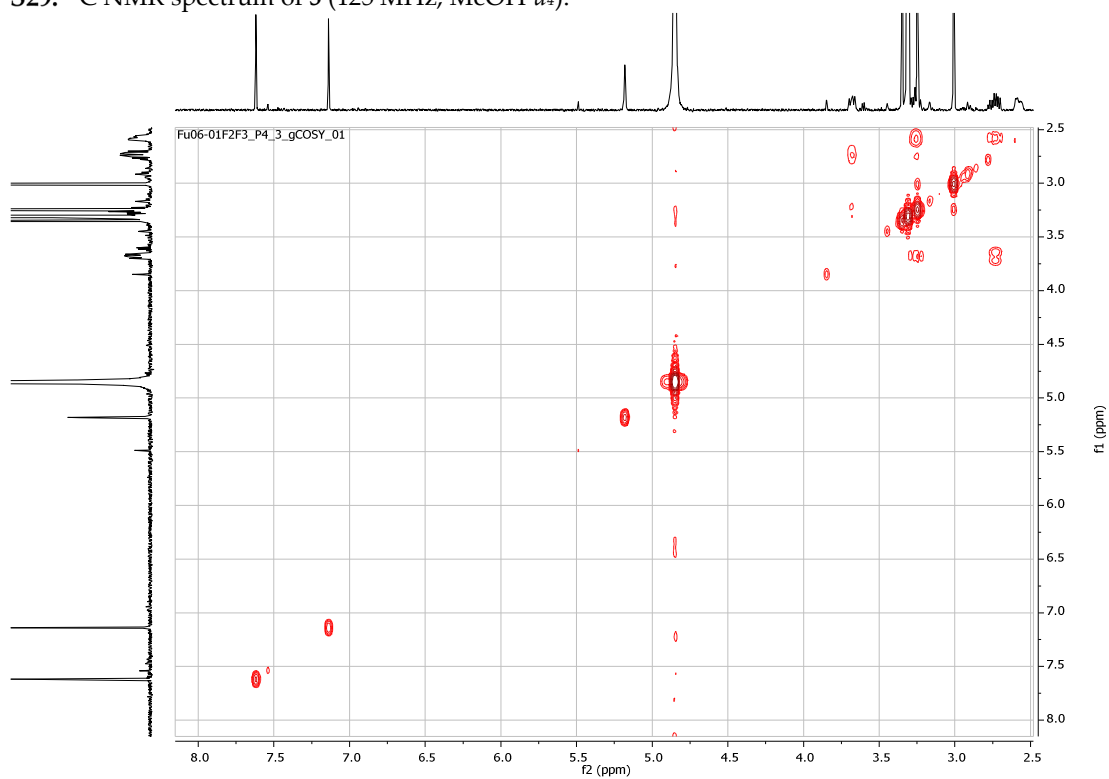


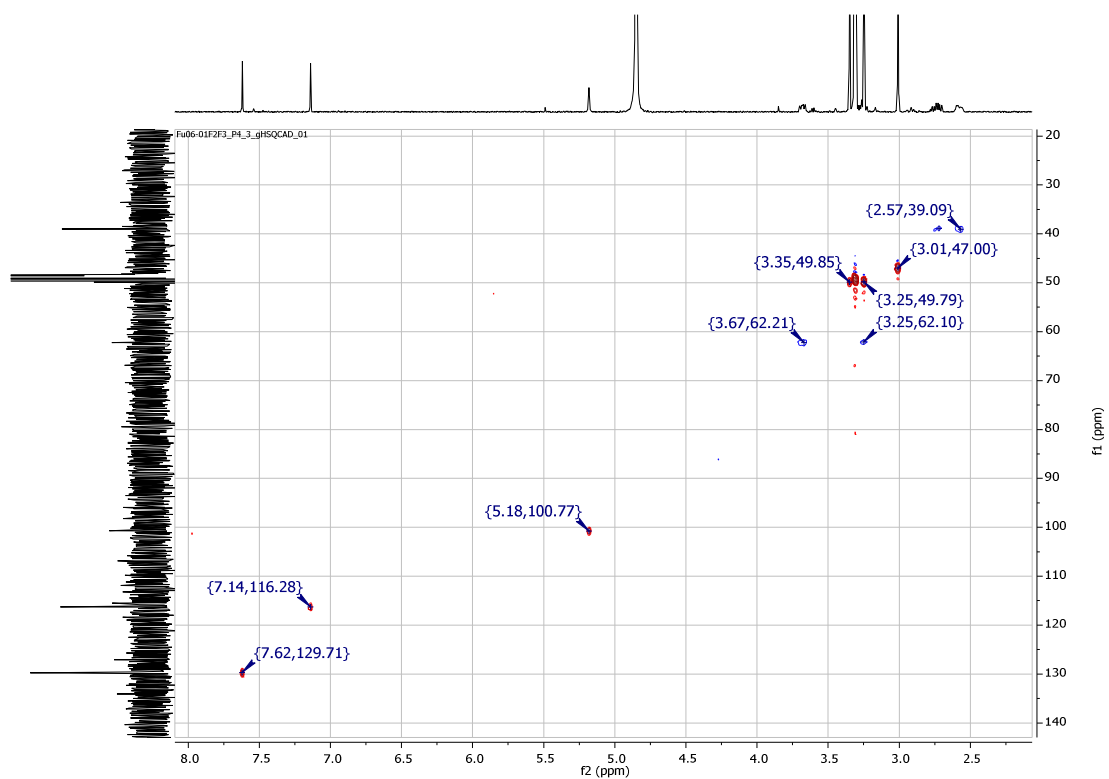
S27. ESI(+)-HRMS analysis of **5** and crop of the molecular ion.



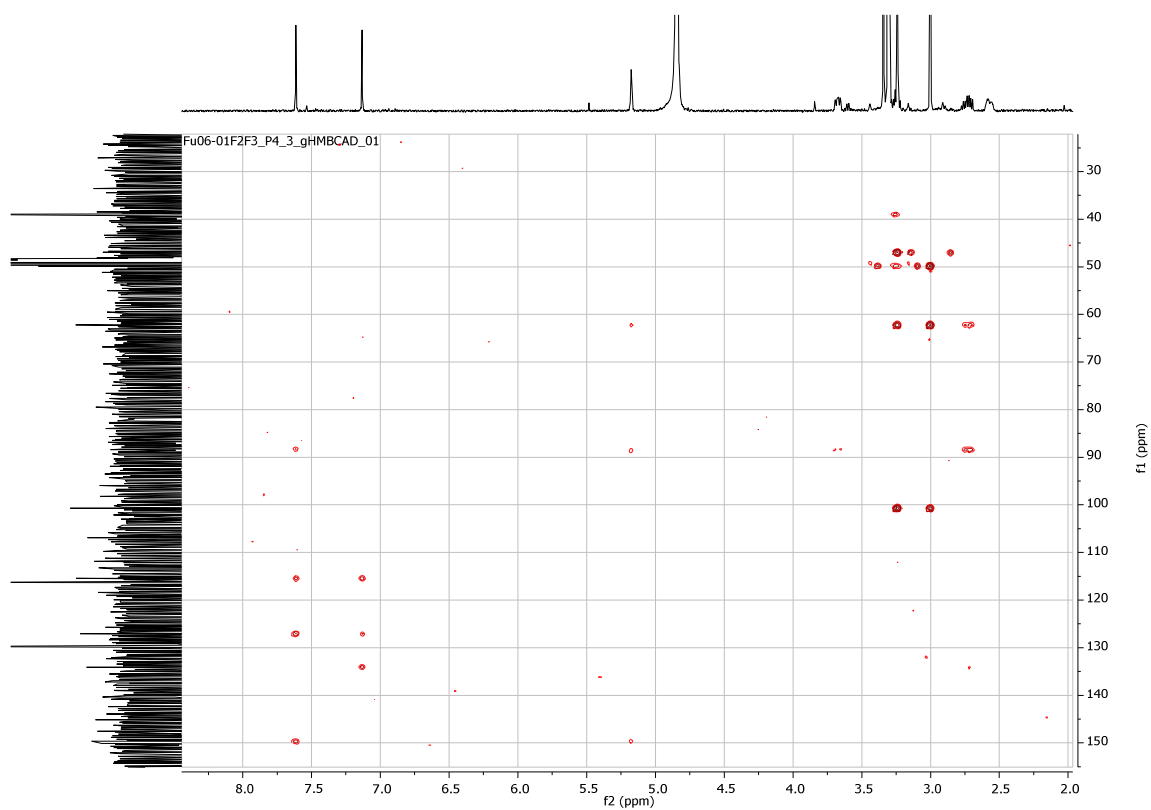
S28. ^1H NMR spectrum of **5** (500 MHz, $\text{MeOH-}d_4$).

Fu06-01F2F3_P4_3_CARBON_01

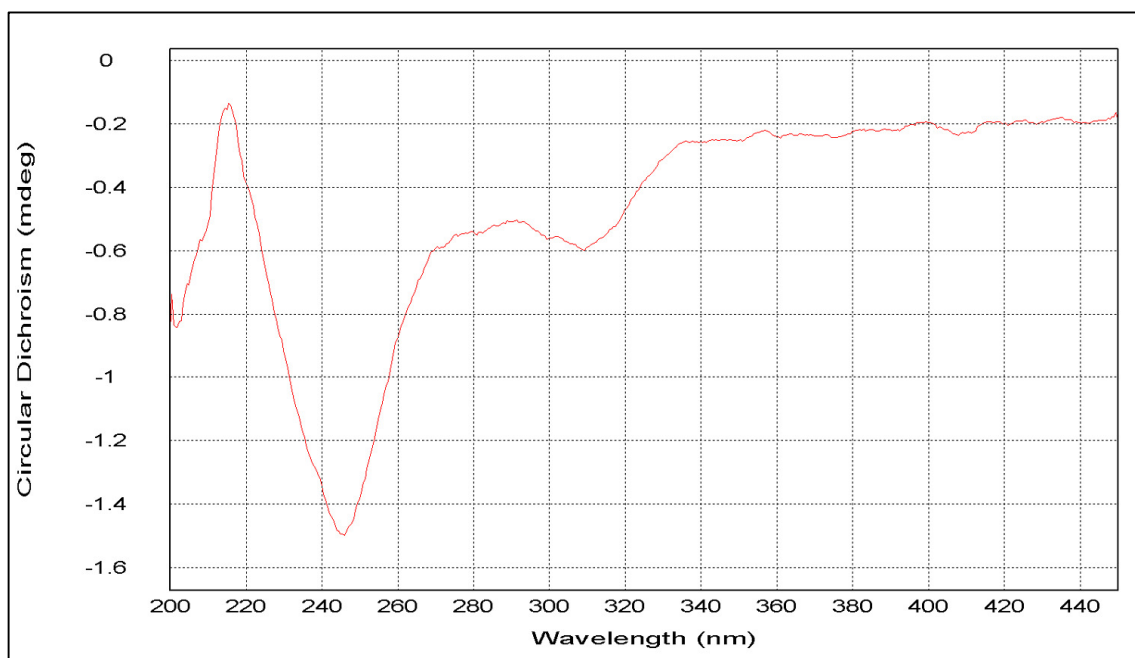
S29. ¹³C NMR spectrum of 5 (125 MHz, MeOH-*d*₄).S30. COSY NMR spectrum of 5 (500 MHz, MeOH-*d*₄).



S31. HSQC NMR spectrum of **5** (500 MHz, MeOH- d_4).

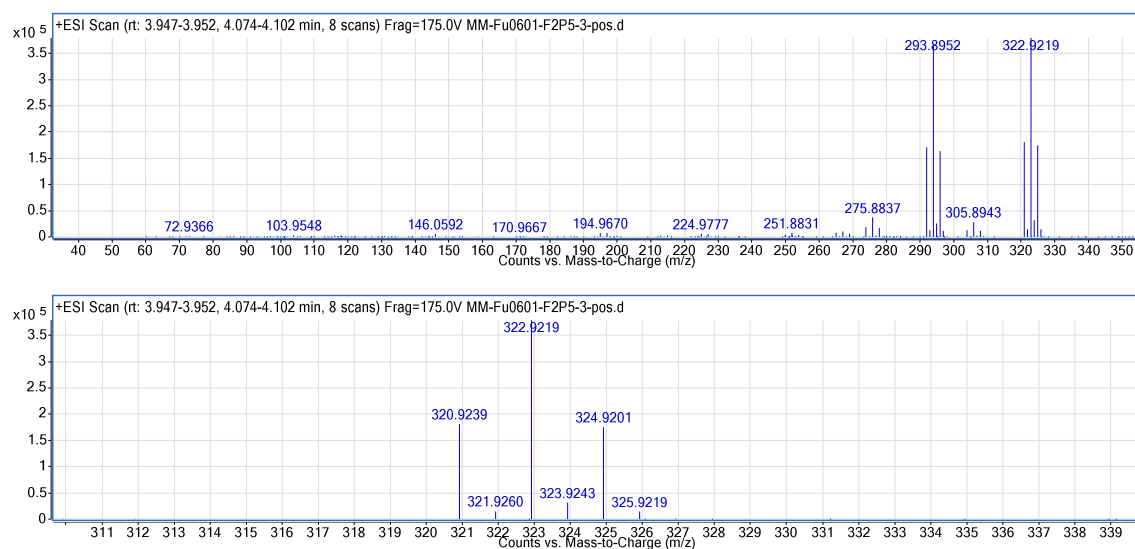


S32. HMBC NMR spectrum of **5** (500 MHz, MeOH- d_4).

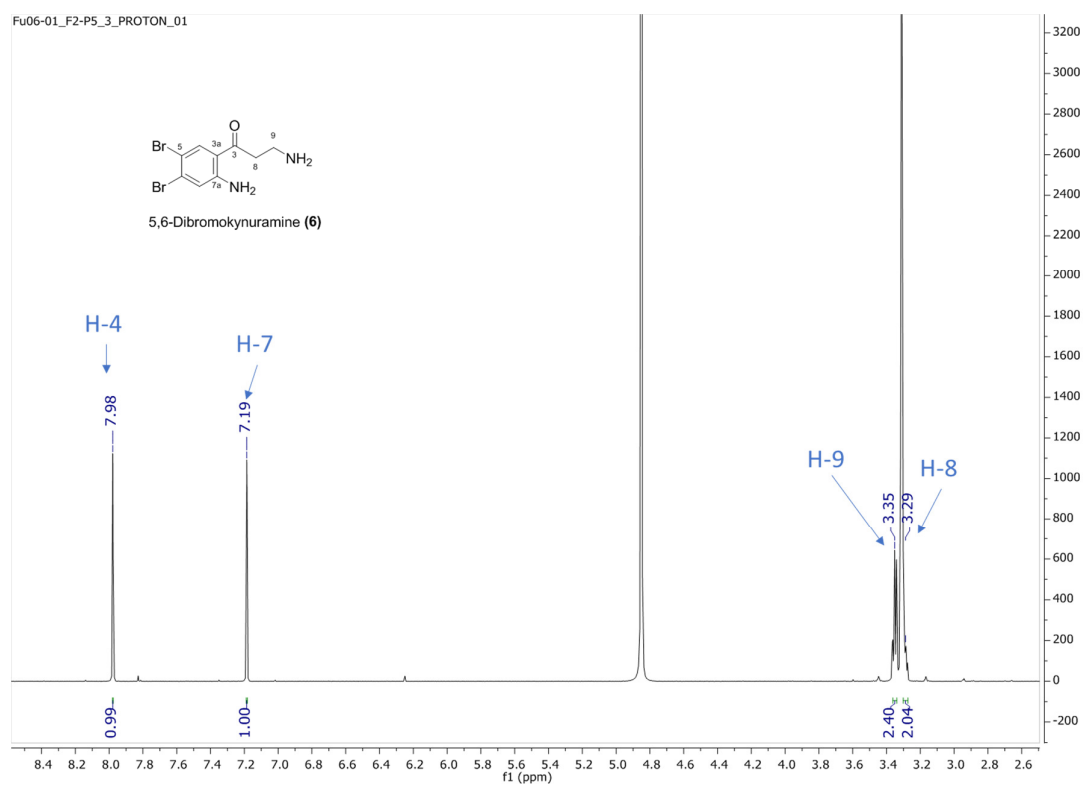


S33. ECD spectrum of compound **5** in CH₃CN at 0.2 mg/mL

Supporting information

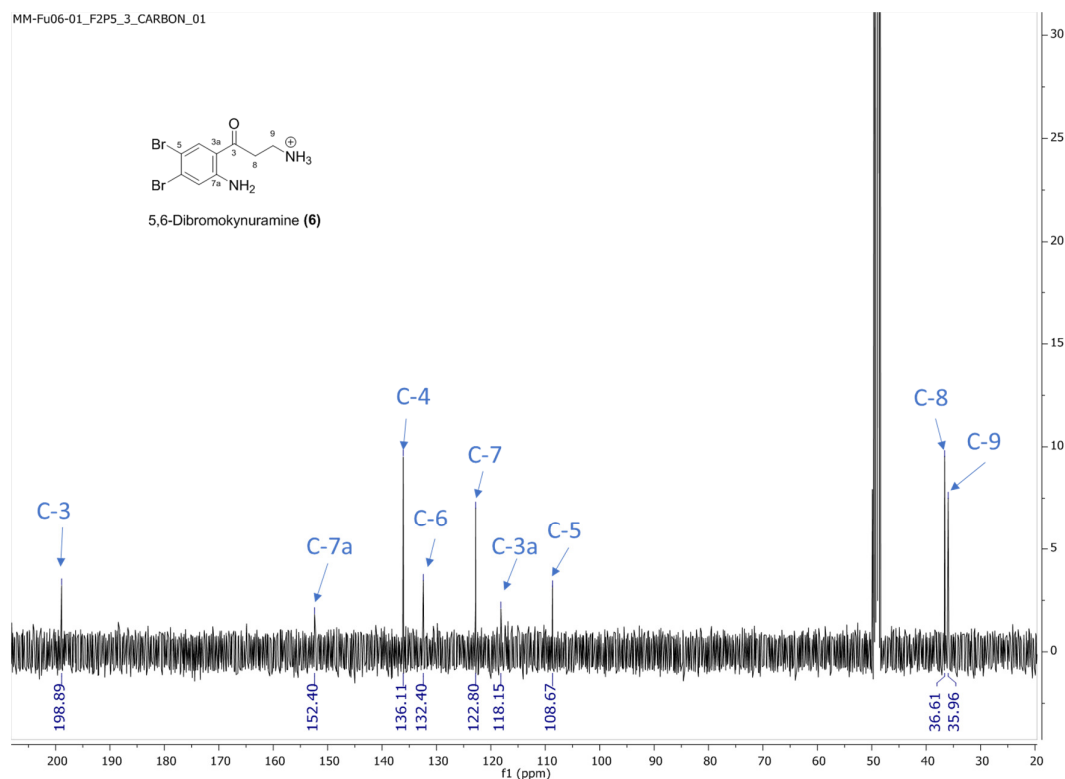


S34. ESI(+)-HRMS analysis of **6** and crop of the molecular ion.

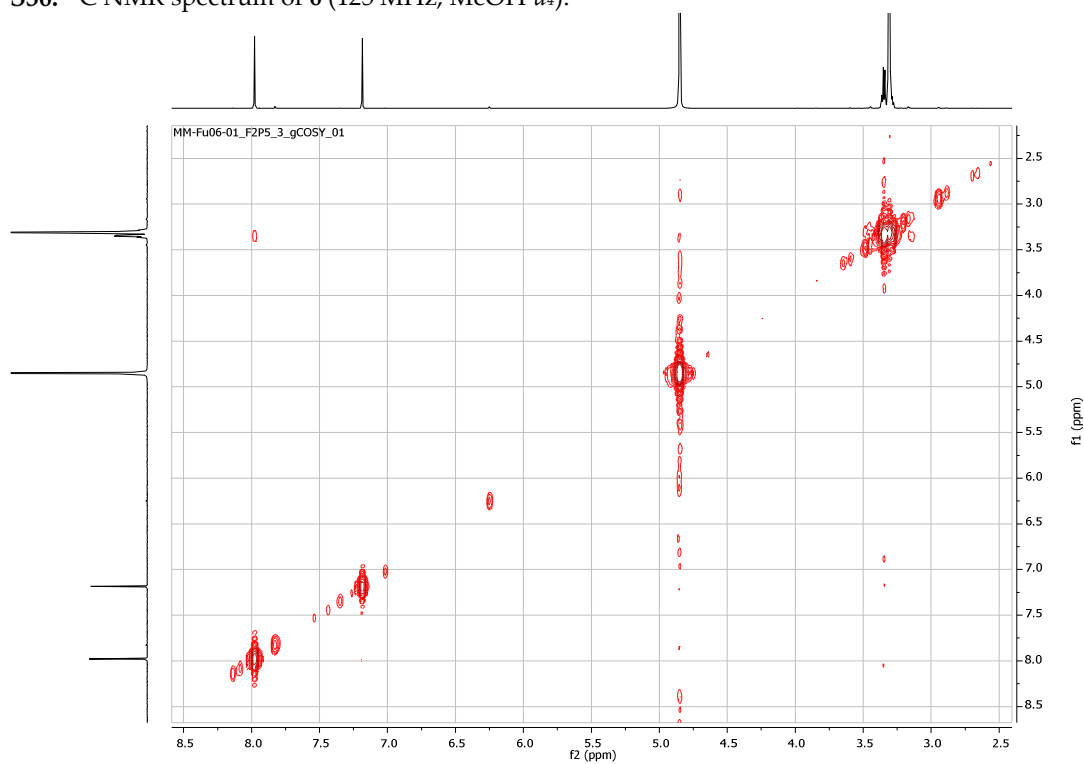


S35. ^1H NMR spectrum of **6** (500 MHz, $\text{MeOH-}d_4$).

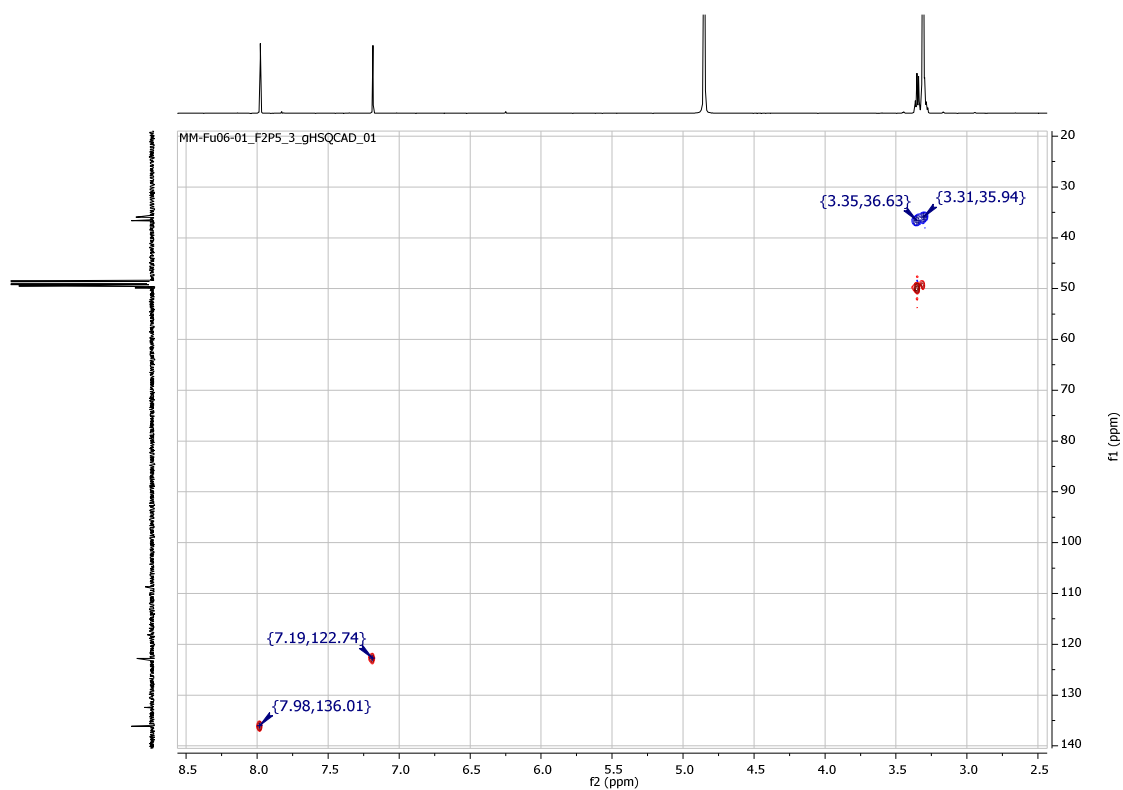
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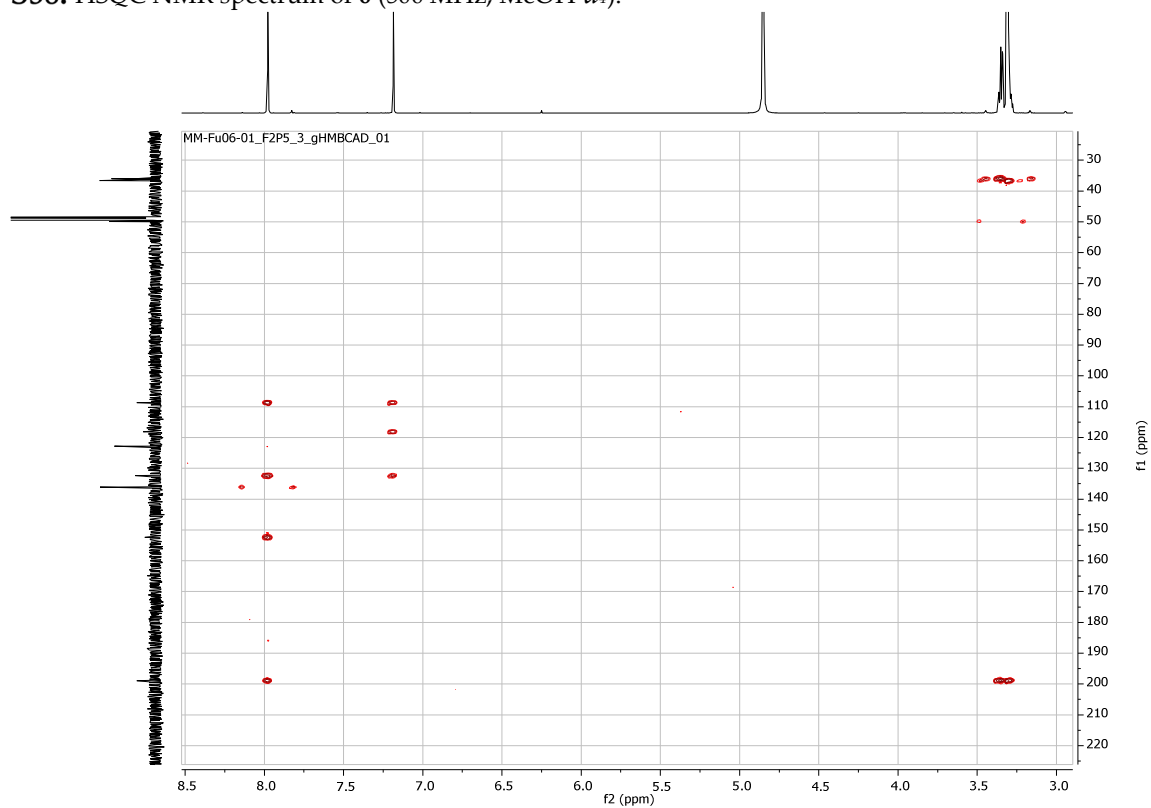
S36. ^{13}C NMR spectrum of **6** (125 MHz, $\text{MeOH-}d_4$).



S37. COSY NMR spectrum of **6** (500 MHz, $\text{MeOH-}d_4$).

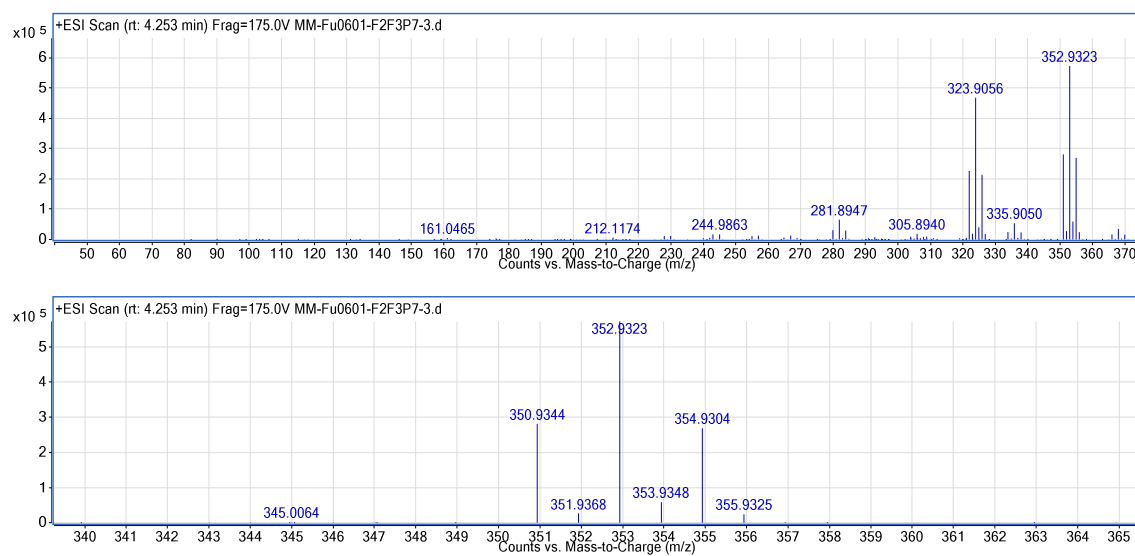


S38. HSQC NMR spectrum of **6** (500 MHz, MeOH- d_4).

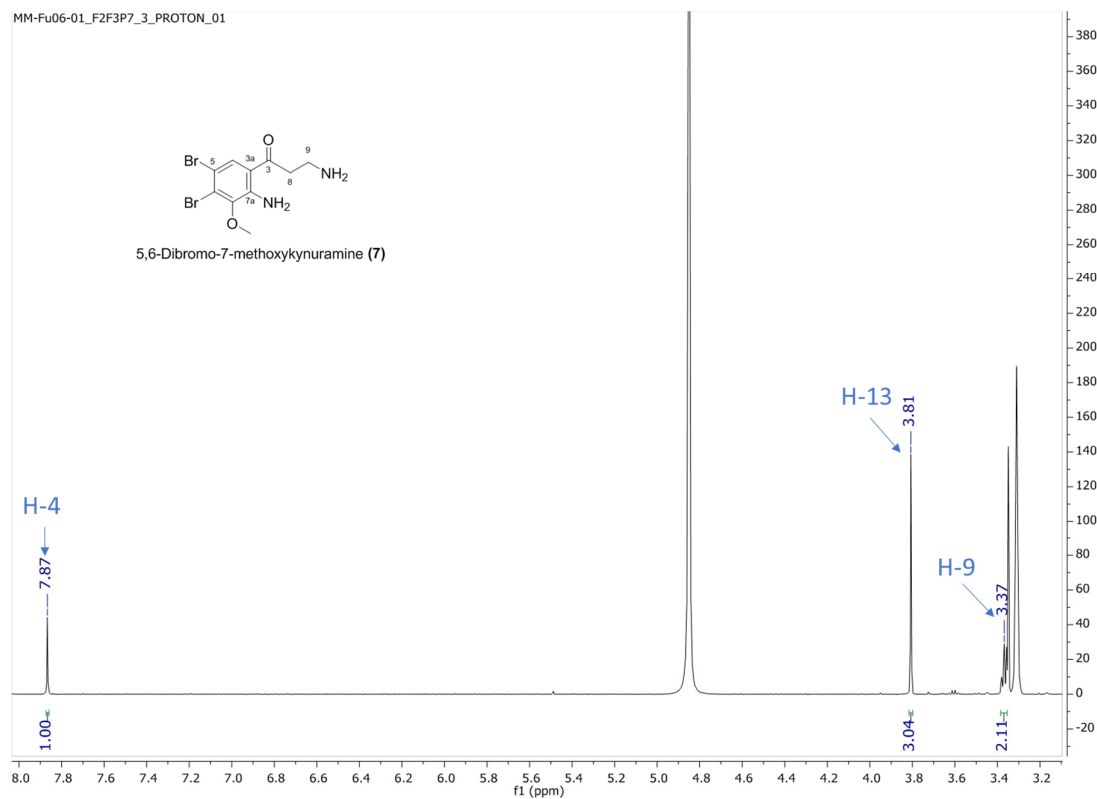


S39. HMBC NMR spectrum of **6** (500 MHz, MeOH- d_4).

Supporting information

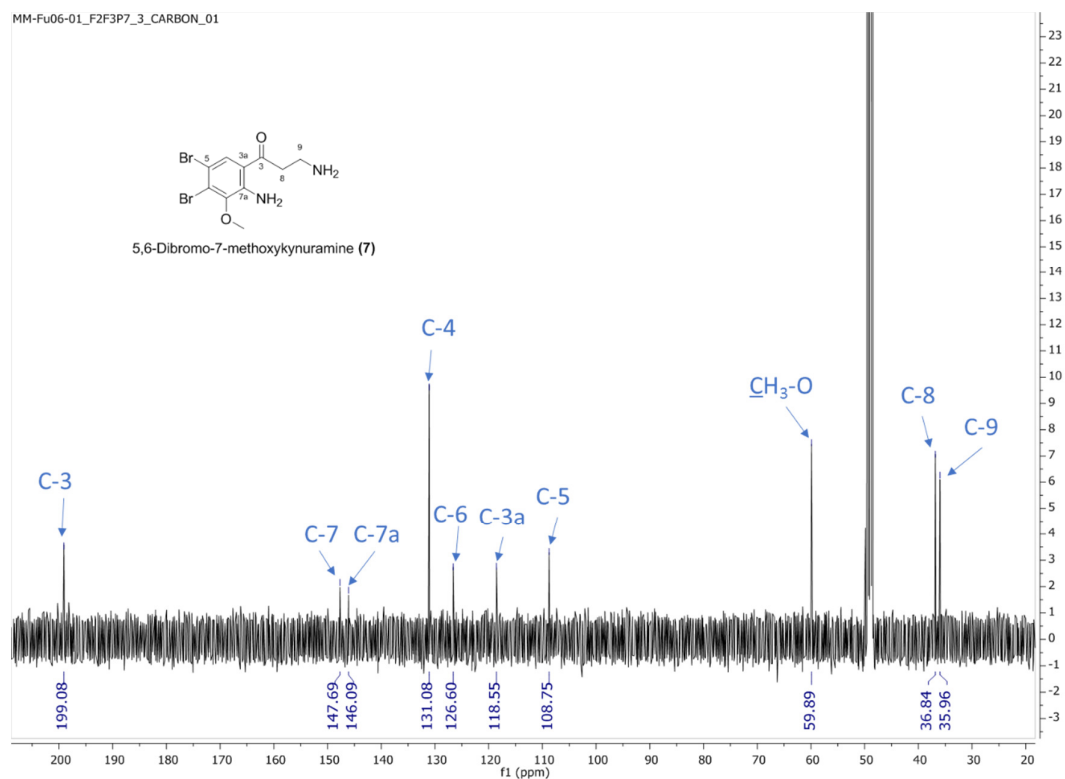


S40. ESI(+)-HRMS analysis of **7** and crop of the molecular ion.

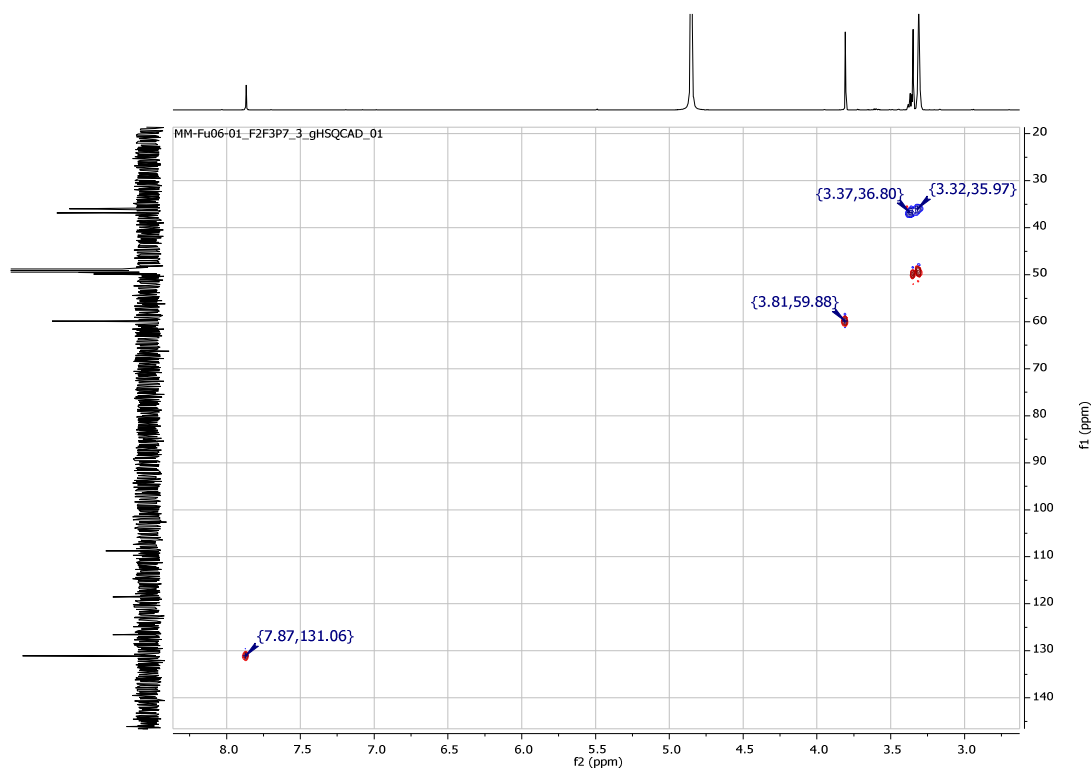


S41. ¹H NMR spectrum of **7** (500 MHz, MeOH-*d*₄).

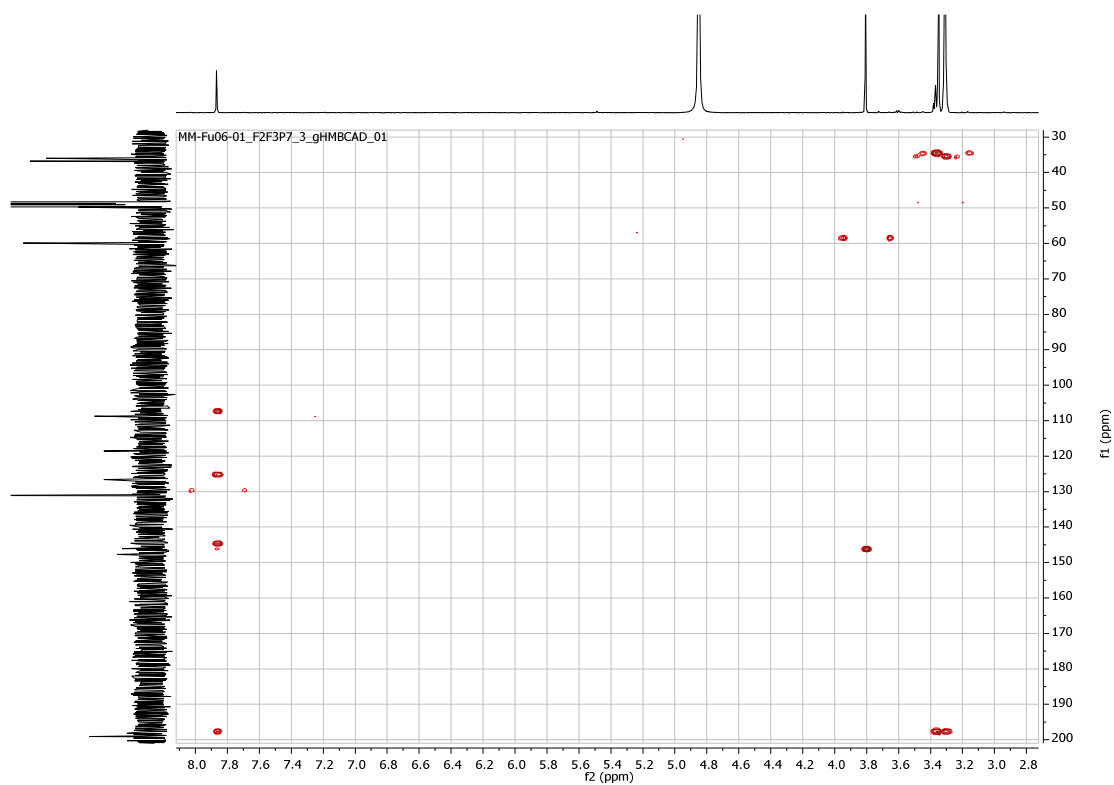
Supporting information



S42. ¹³C NMR spectrum of 7 (125 MHz, MeOH-*d*₄).

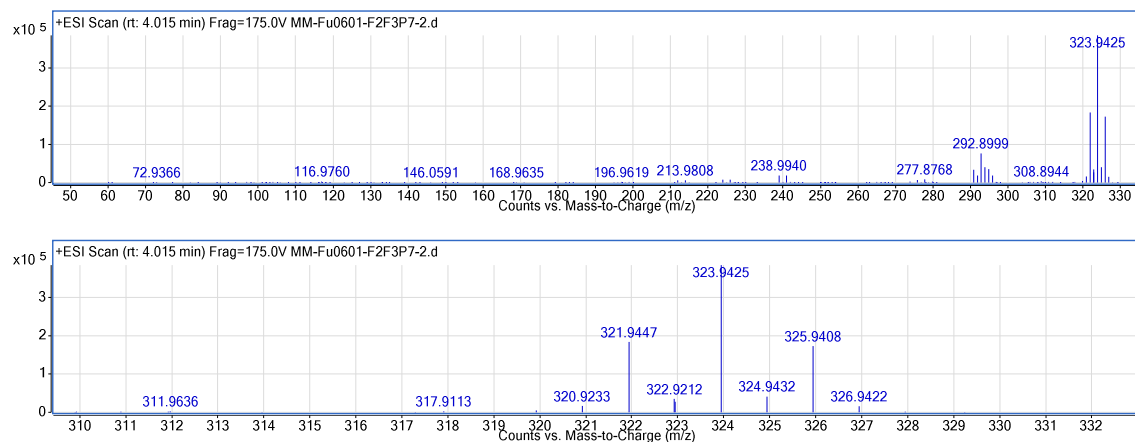


S43. HSQC NMR spectrum of 7 (500 MHz, MeOH-*d*₄).

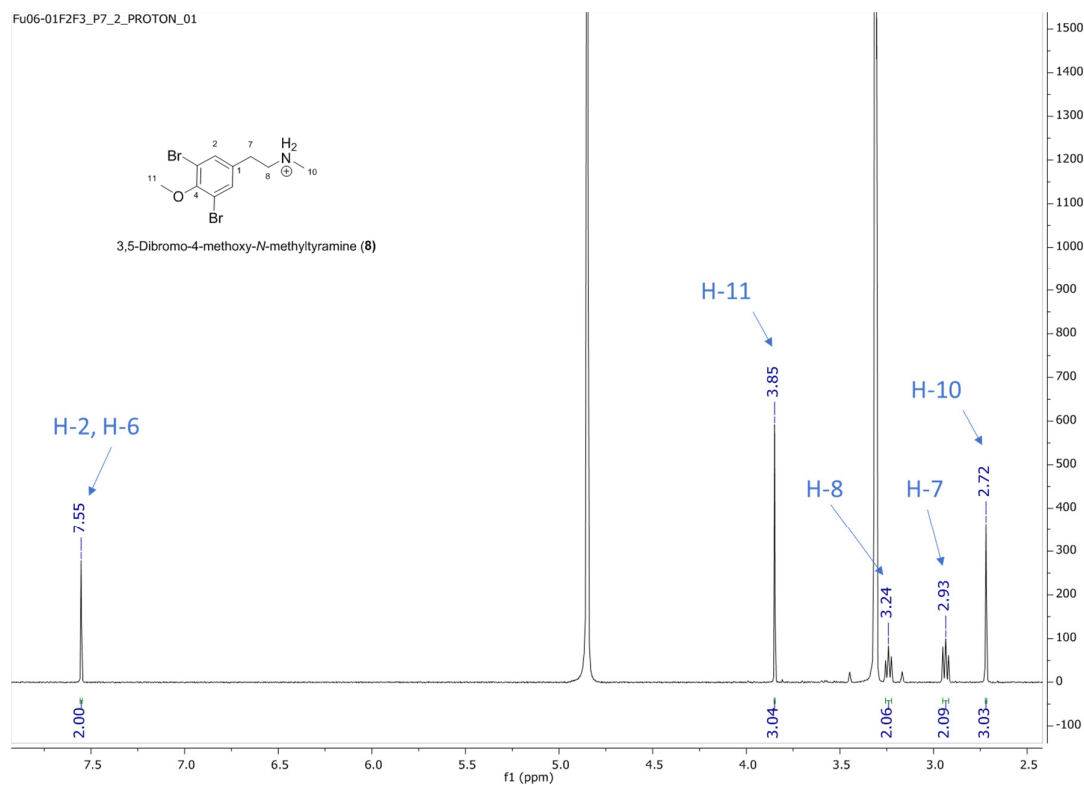


S44. HMBC NMR spectrum of **7** (500 MHz, MeOH- d_4).

Supporting information



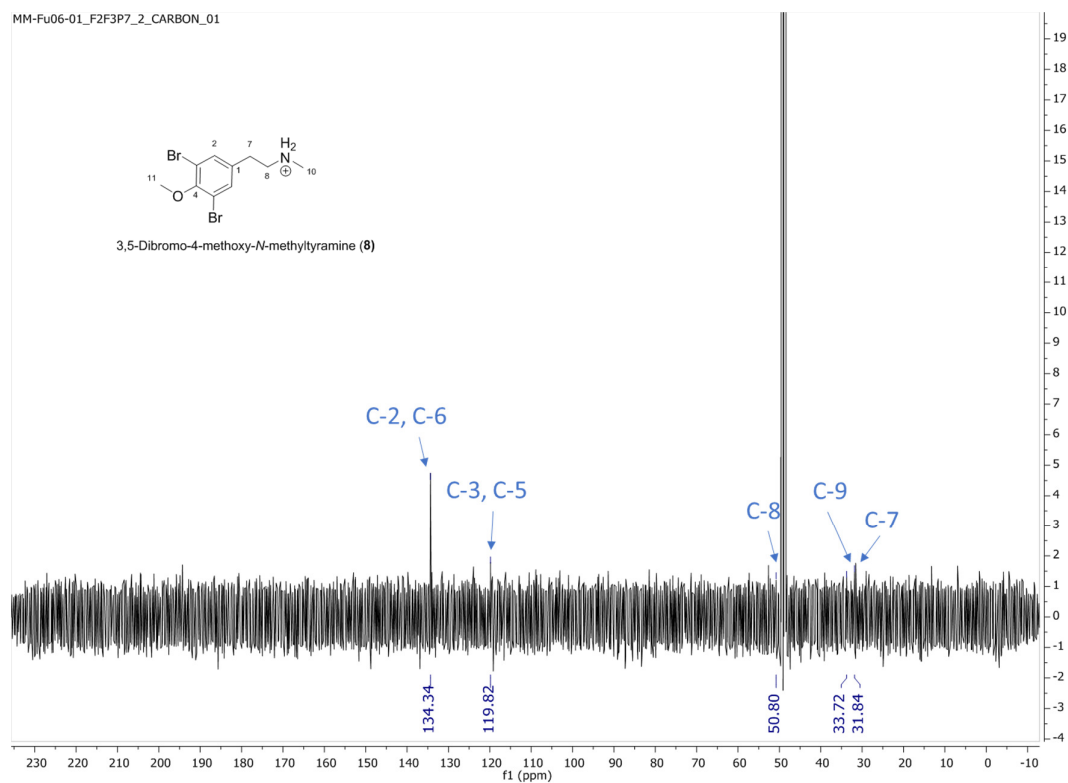
S45. ESI(+)-HRMS analysis of **8** and crop of the molecular ion.



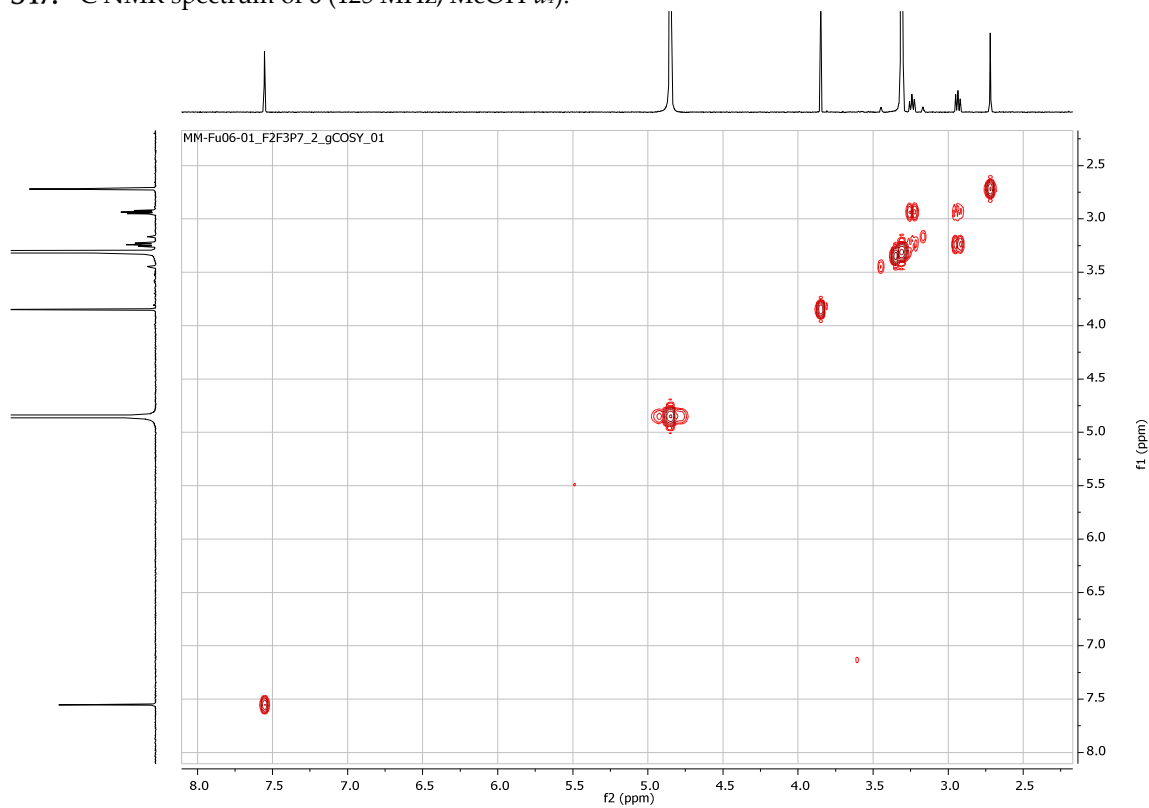
S46. ¹H NMR spectrum of **8** (500 MHz, MeOH-*d*₄).

Supporting information

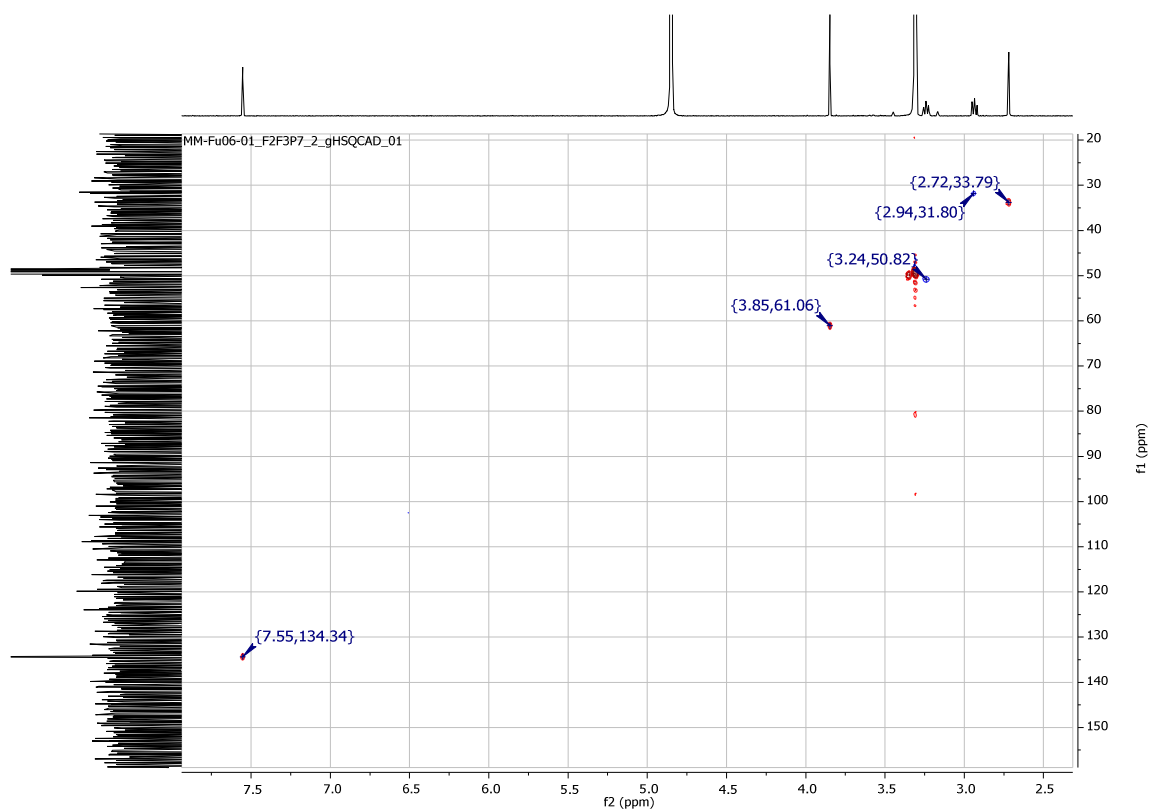
MM-Fu06-01_F2F3P7_2_CARBON_01



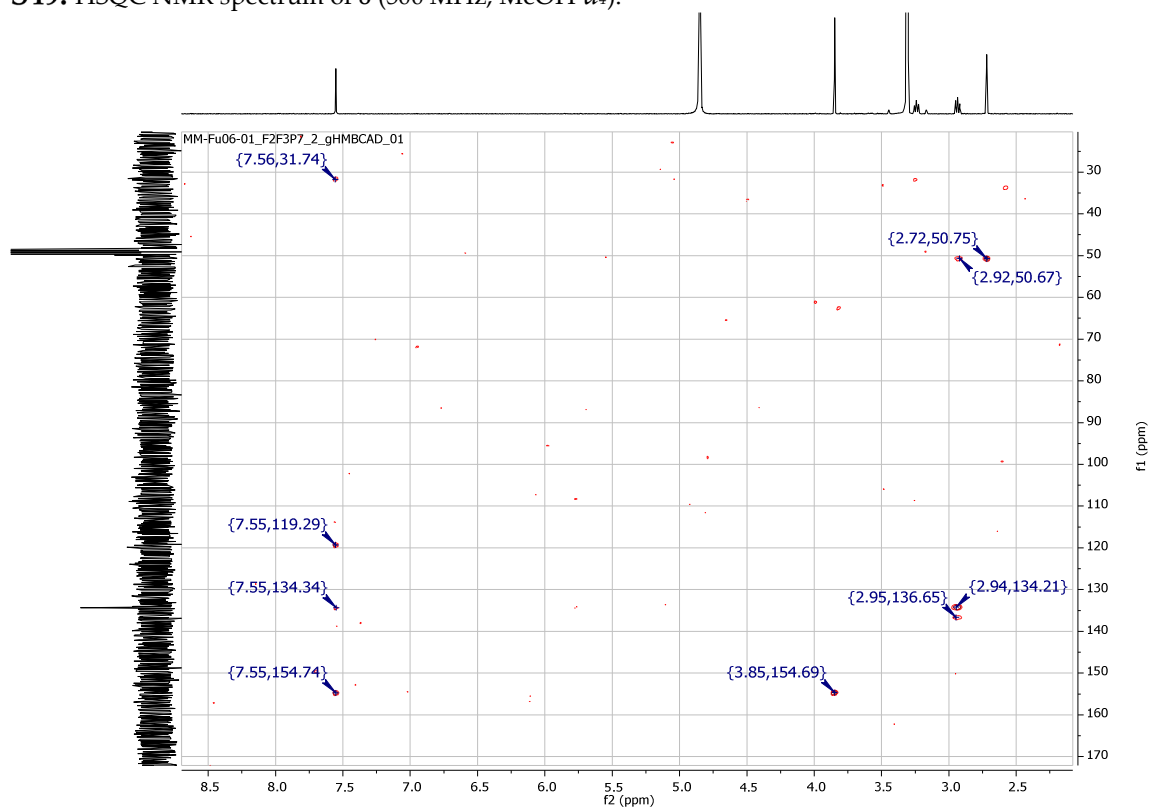
S47. ^{13}C NMR spectrum of 8 (125 MHz, $\text{MeOH-}d_4$).



S48. COSY NMR spectrum of 8 (500 MHz, $\text{MeOH-}d_4$).

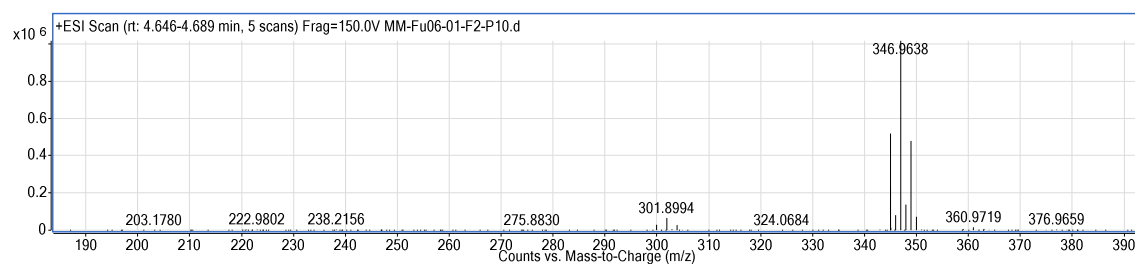


S49. HSQC NMR spectrum of **8** (500 MHz, $\text{MeOH-}d_4$).

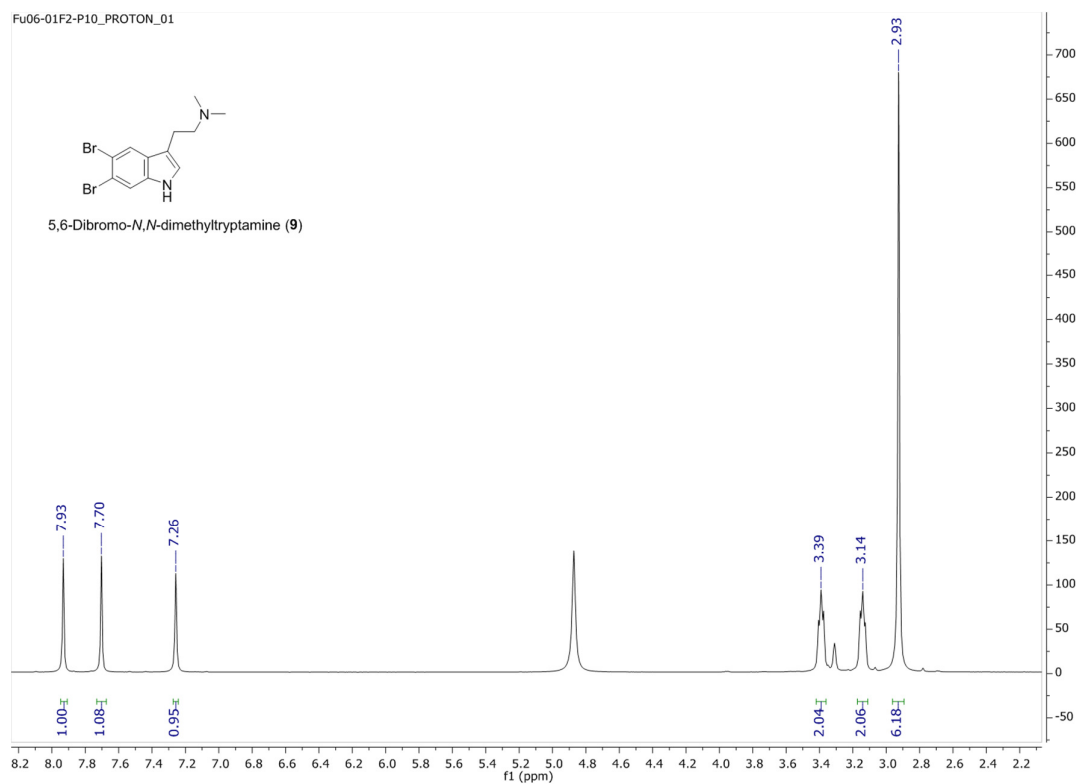


S50. HMBC NMR spectrum of **8** (500 MHz, $\text{MeOH-}d_4$).

Supporting information

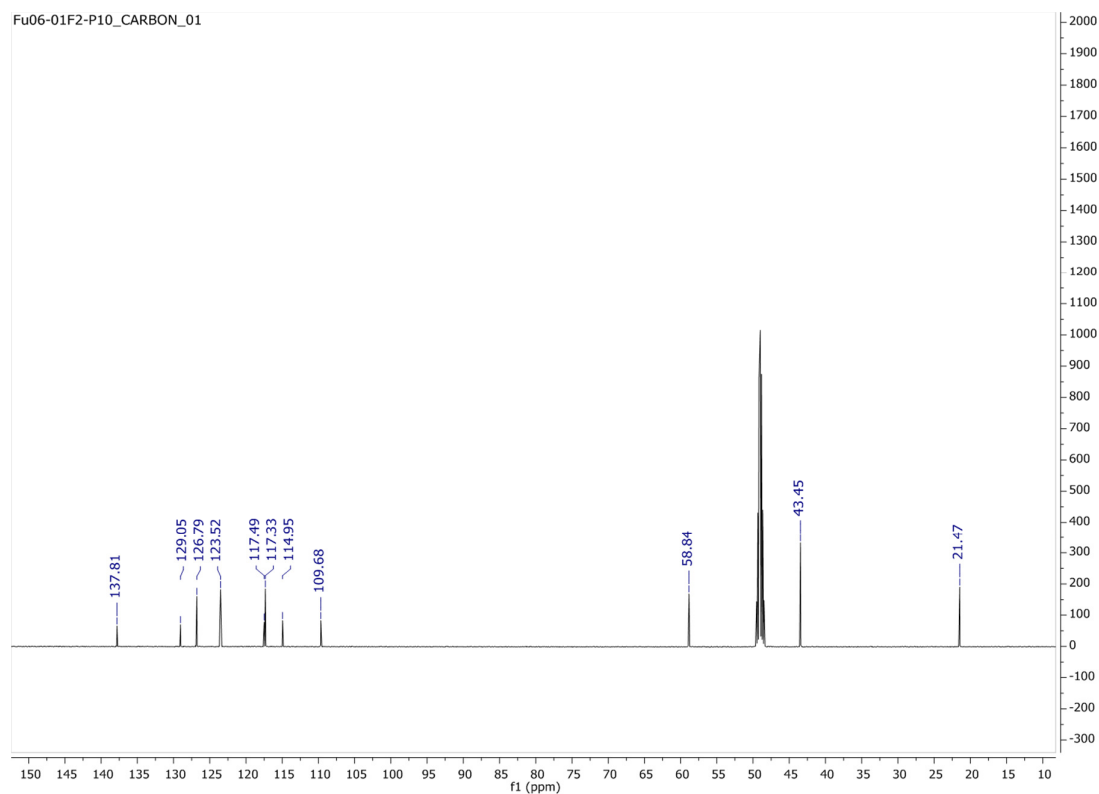


S51. ESI(+)-HRMS analysis of **9**

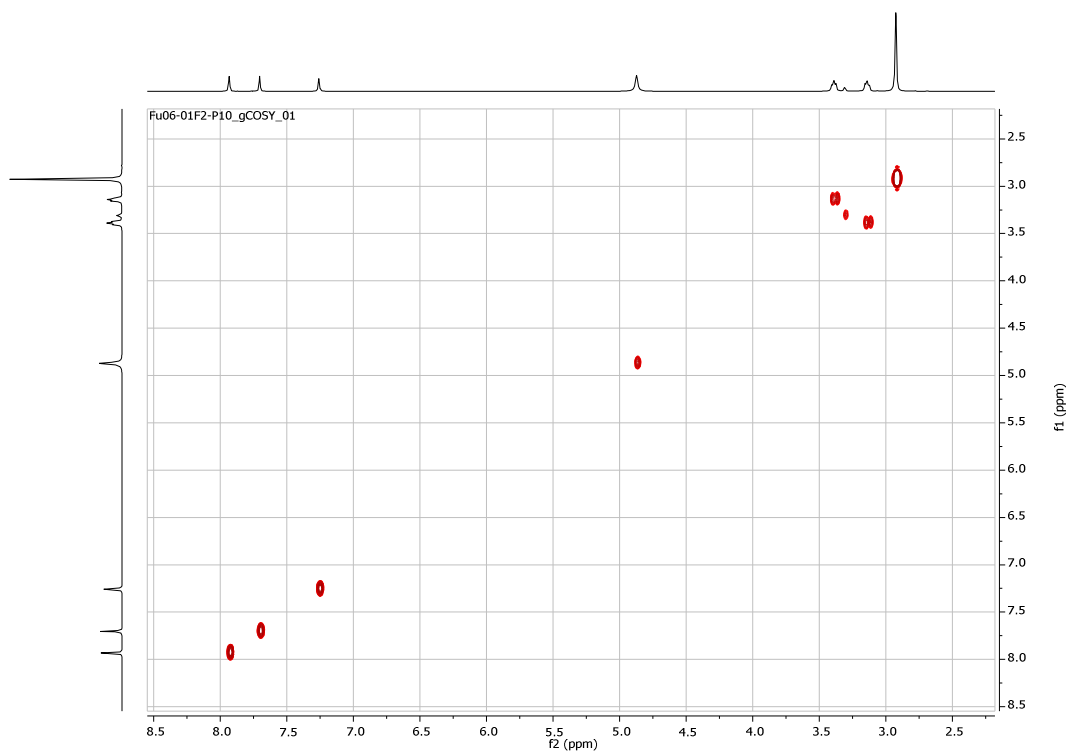


S52. ^1H NMR spectrum of **9** (500 MHz, $\text{MeOH-}d_4$).

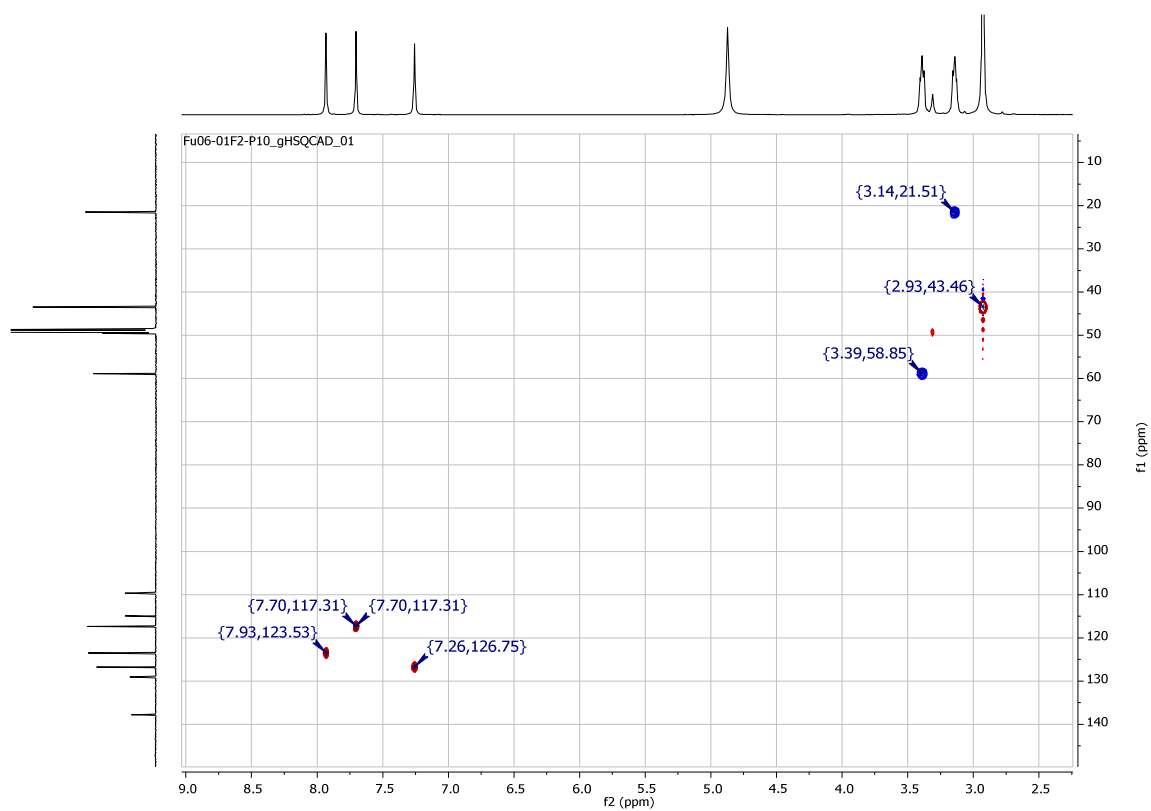
Supporting information



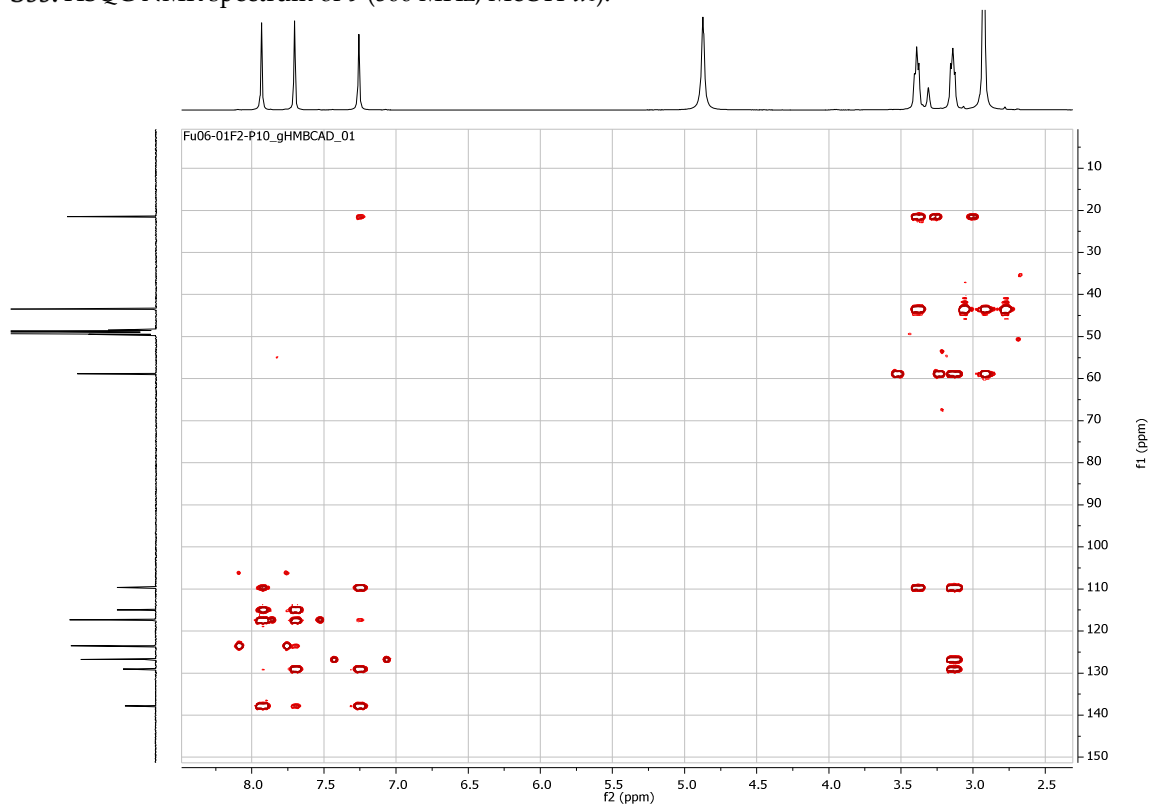
S53. ^{13}C NMR spectrum of **9** (125 MHz, $\text{MeOH-}d_4$).



S54. COSY NMR spectrum of **9** (500 MHz, $\text{MeOH-}d_4$).

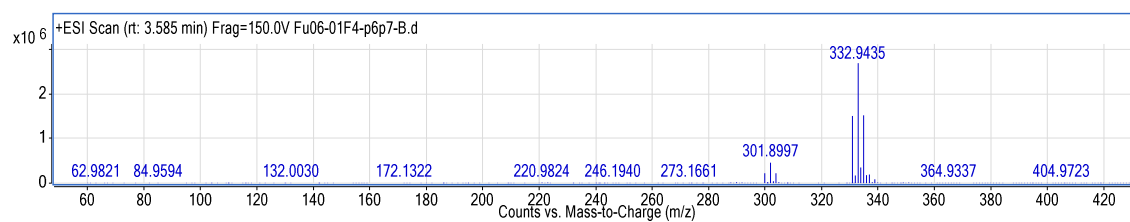


S55. HSQC NMR spectrum of **9** (500 MHz, $\text{MeOH-}d_4$).

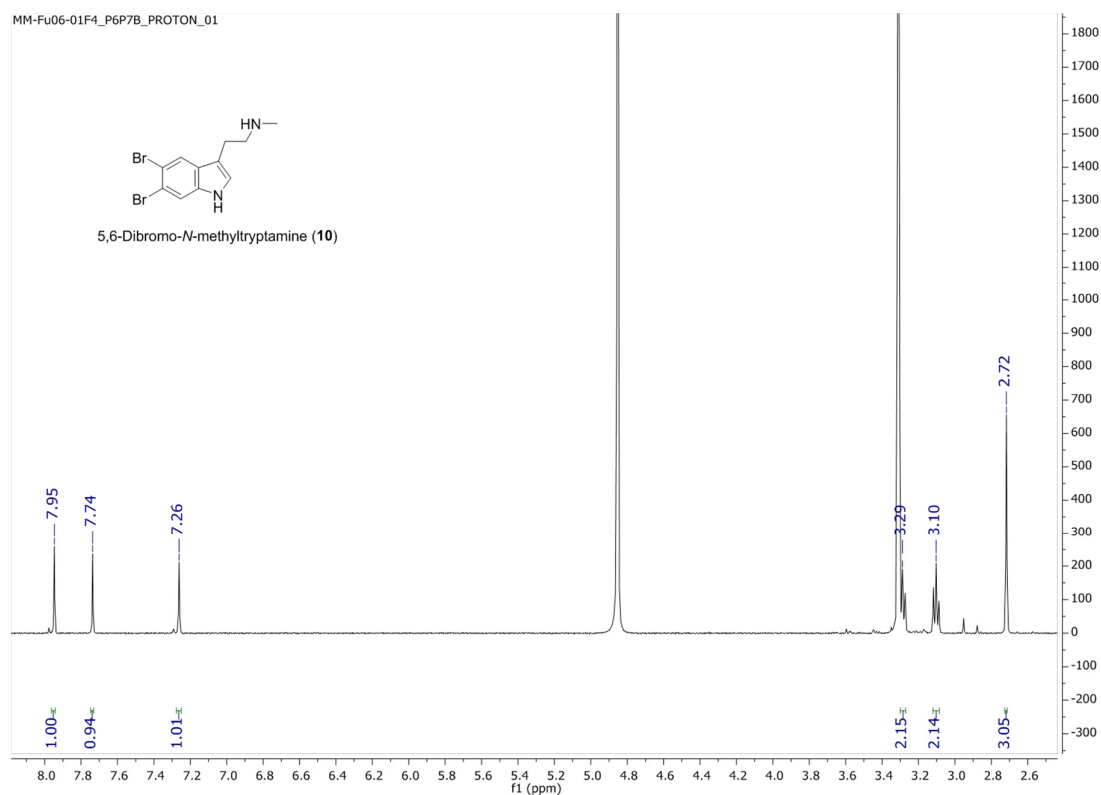


S56. HSQC NMR spectrum of **9** (500 MHz, $\text{MeOH-}d_4$).

Supporting information

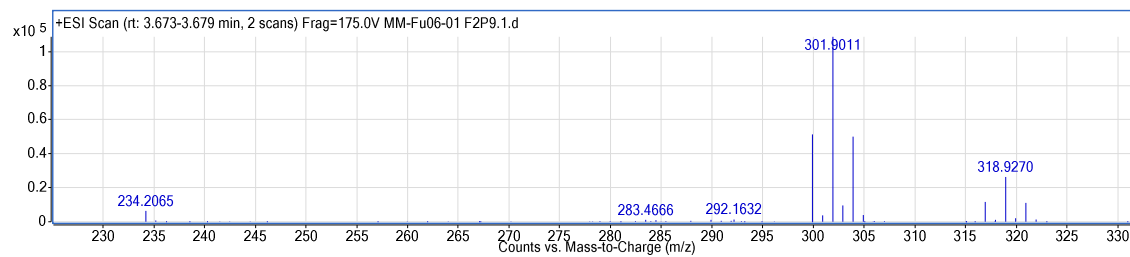


S57. ESI(+)-HRMS analysis of **10**

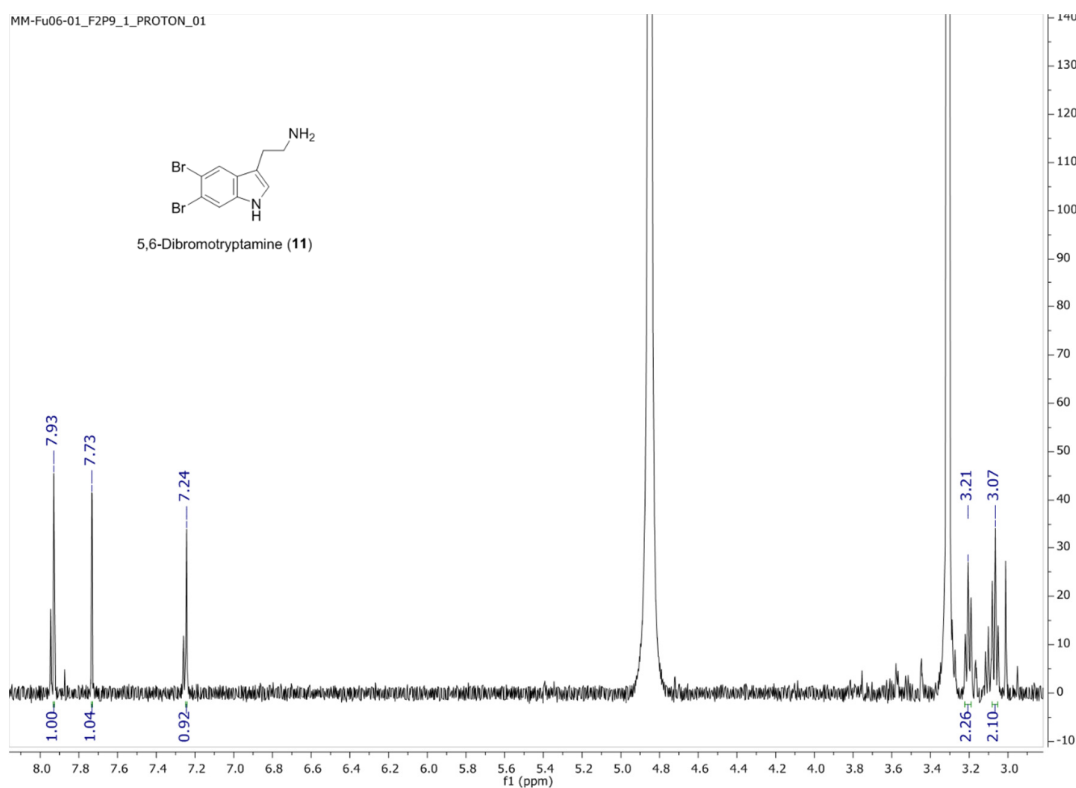


S58. ¹H NMR spectrum of **10** (500 MHz, MeOH-*d*₄).

Supporting information

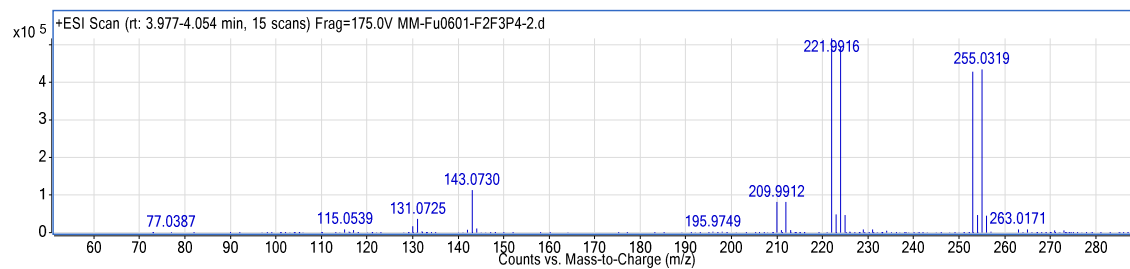


S59. ESI(+)-HRMS analysis of **11**

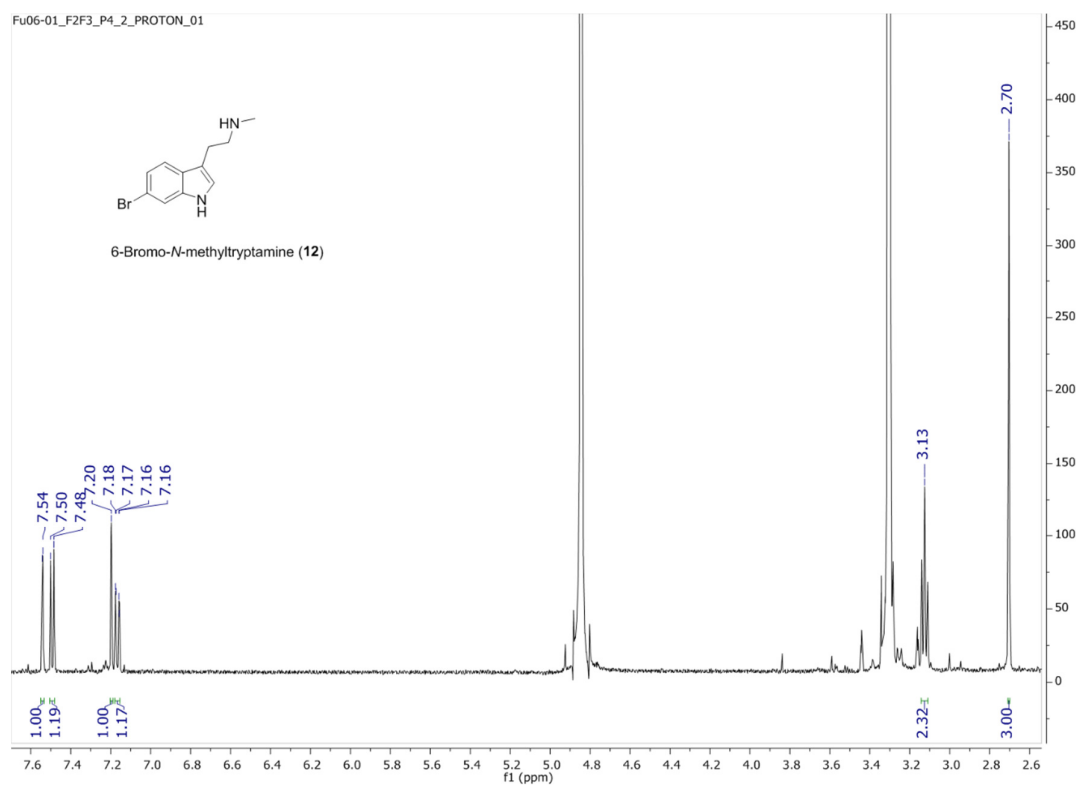


S60. ^1H NMR spectrum of **11** (500 MHz, $\text{MeOH-}d_4$).

Supporting information

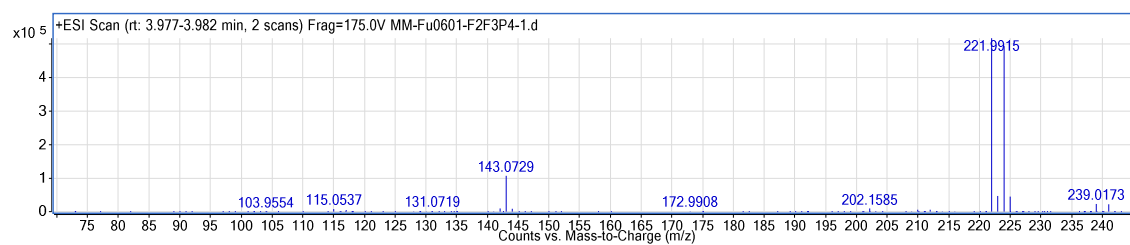


S61. ESI(+)-HRMS analysis of **12**

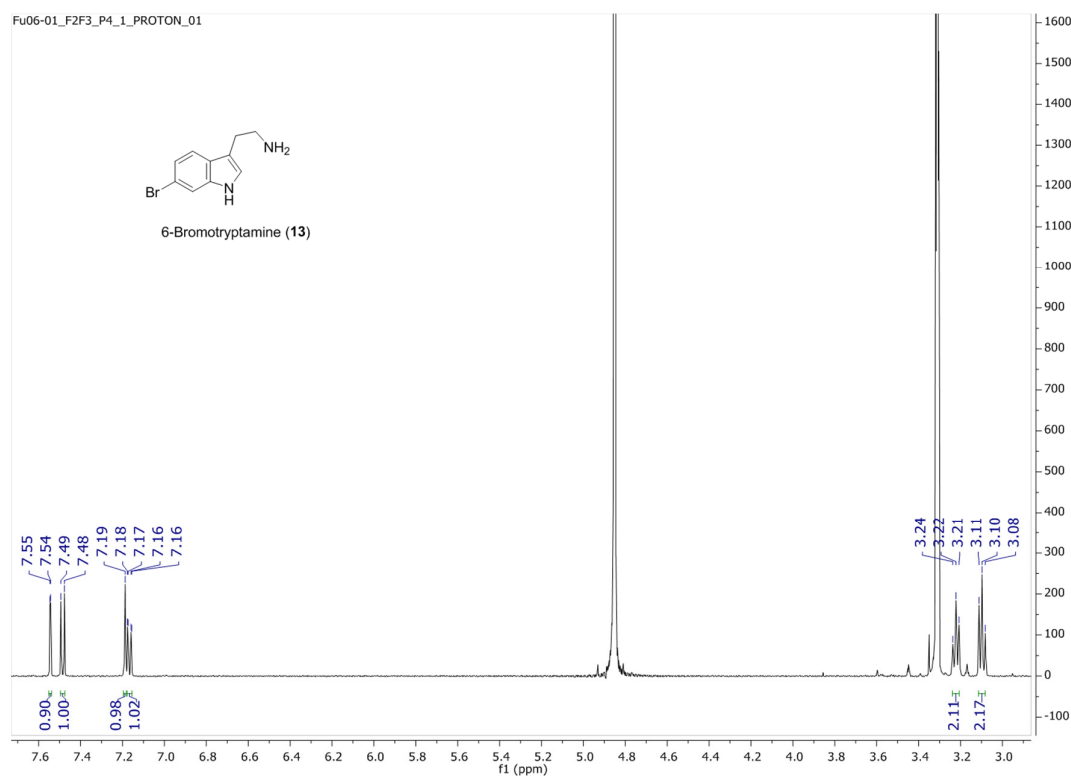


S62. ¹H NMR spectrum of **12** (500 MHz, MeOH-*d*₄).

Supporting information

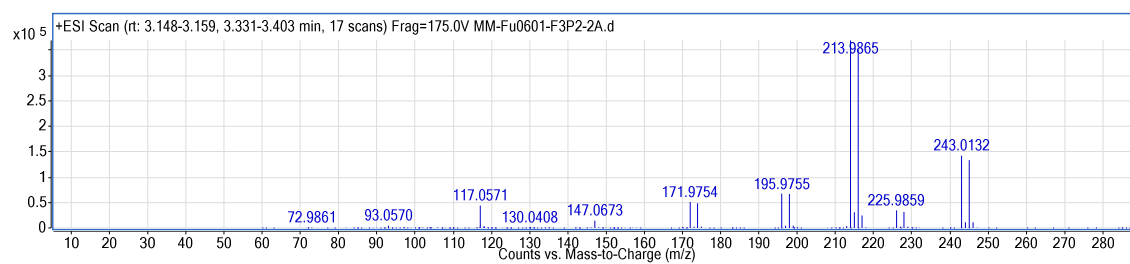


S63. ESI(+)-HRMS analysis of **13**

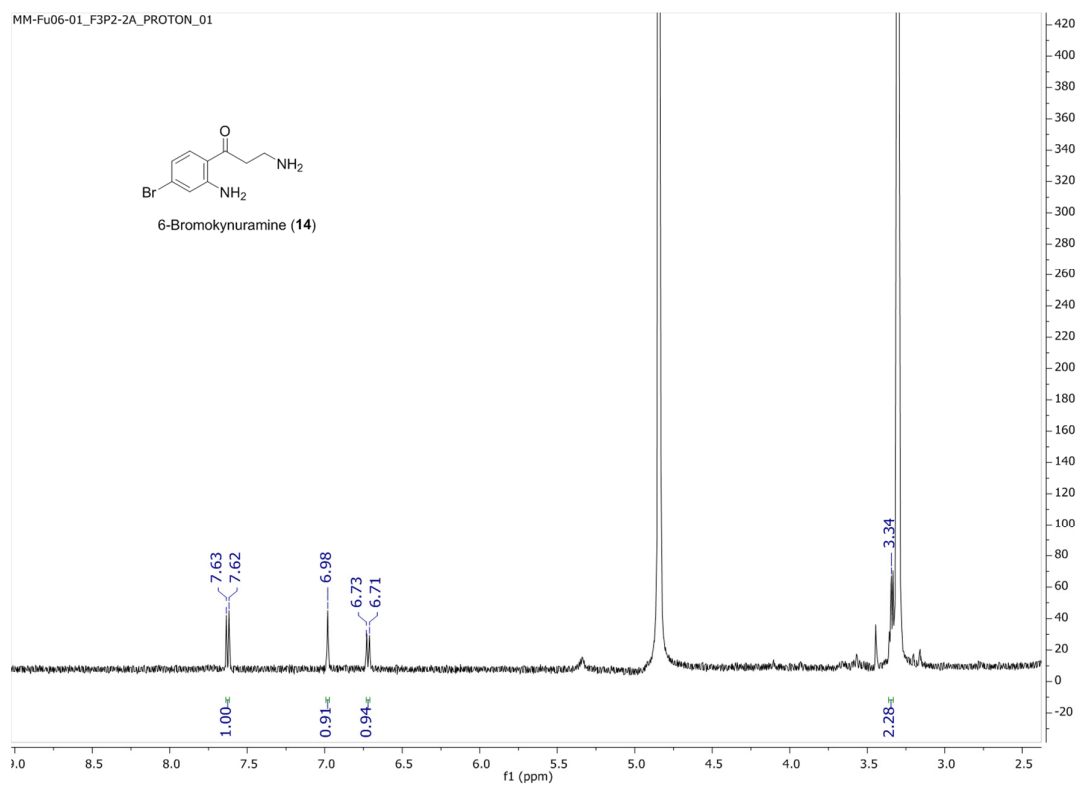


S64. ¹H NMR spectrum of **13** (500 MHz, MeOH-*d*₄).

Supporting information

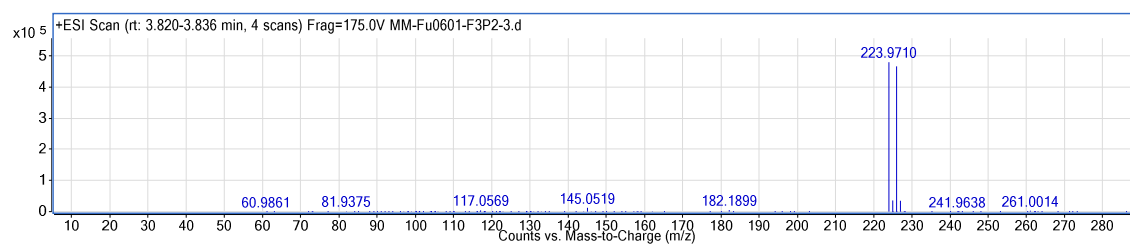


S65. ESI(+)-HRMS analysis of **14**

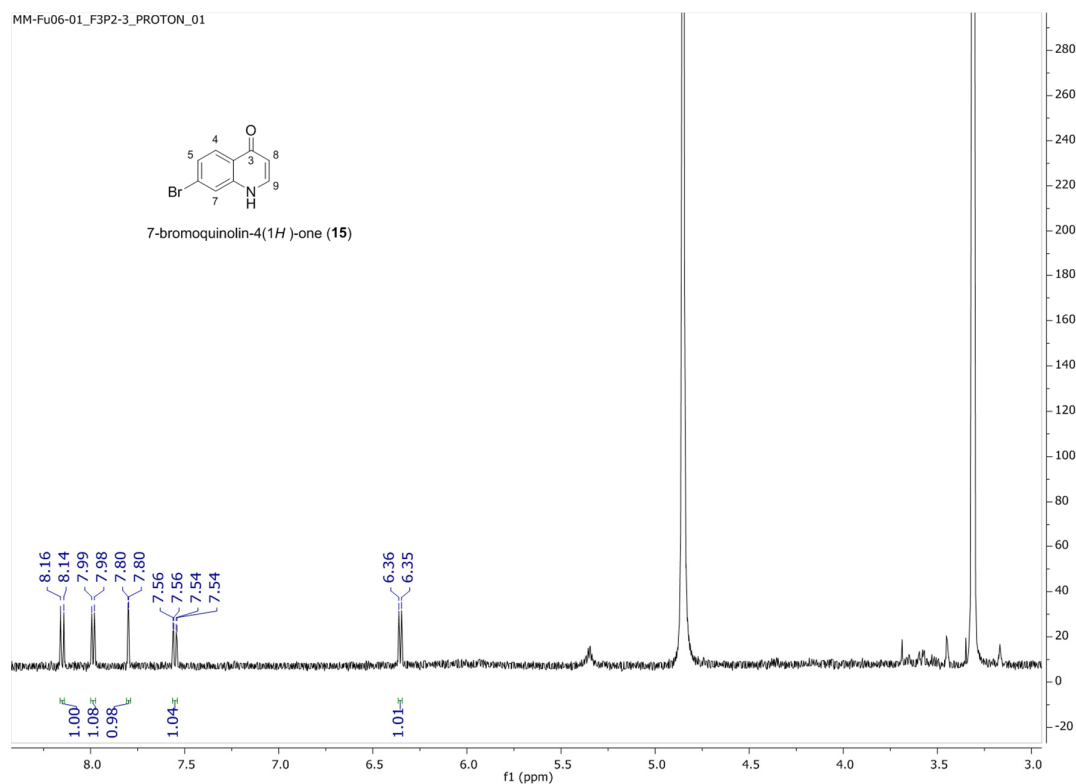


S66. ¹H NMR spectrum of **14** (500 MHz, MeOH-*d*₄).

Supporting information

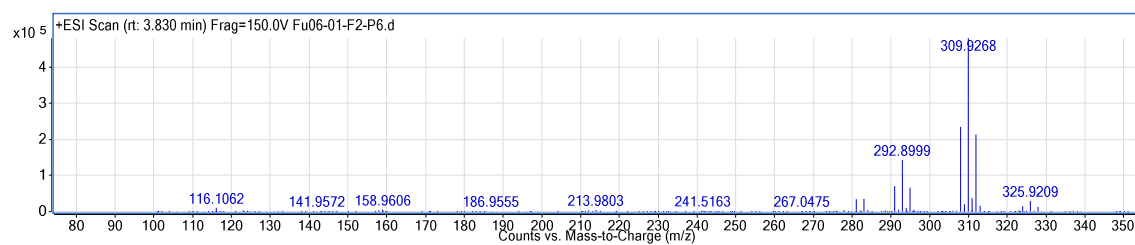


S67. ESI(+)-HRMS analysis of **15**

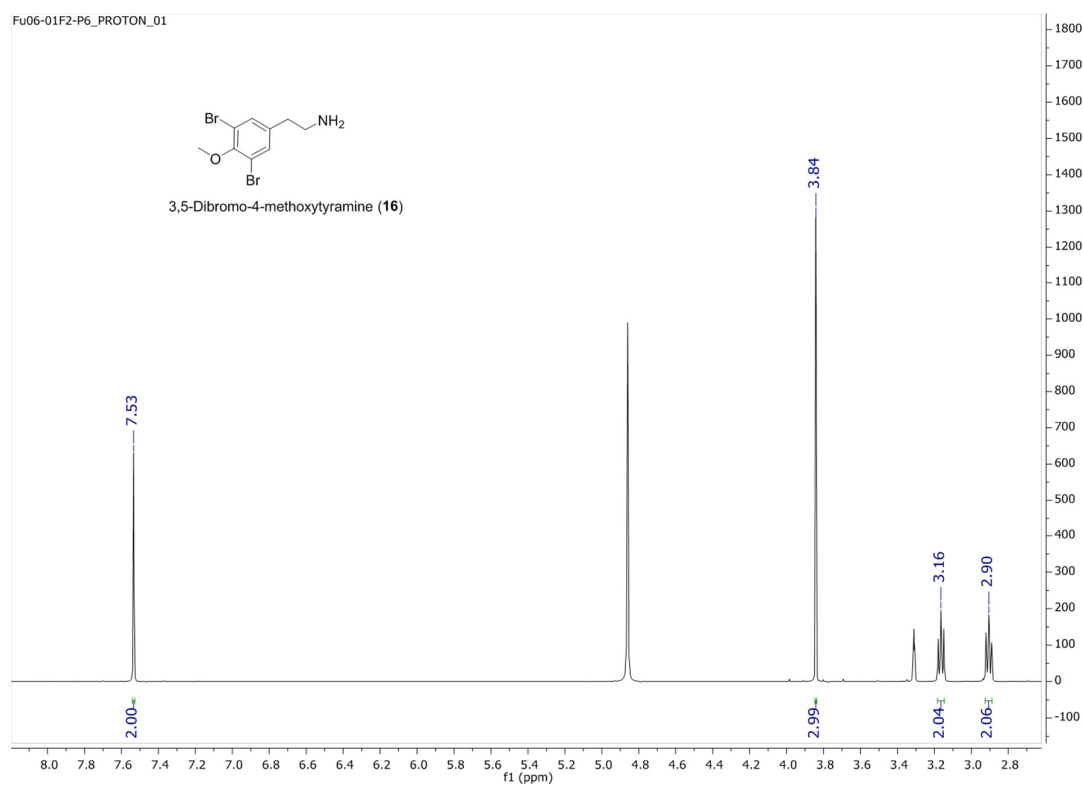


S68. ¹H NMR spectrum of **15** (500 MHz, MeOH-*d*₄).

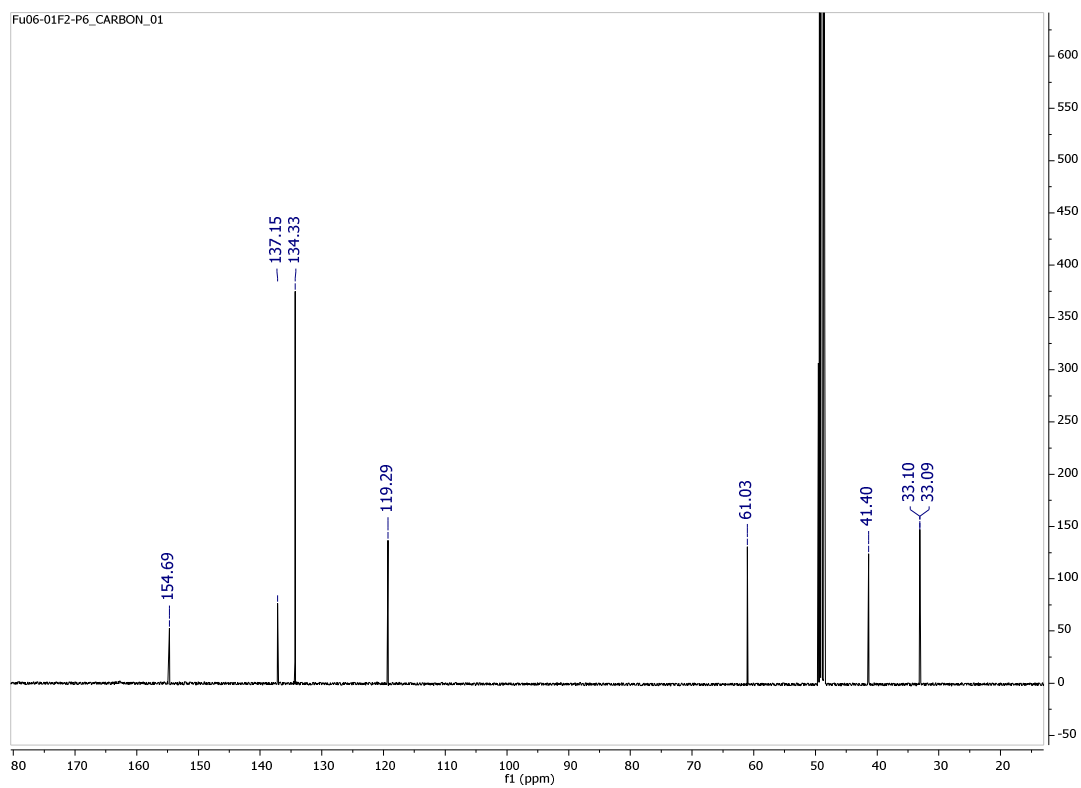
Supporting information



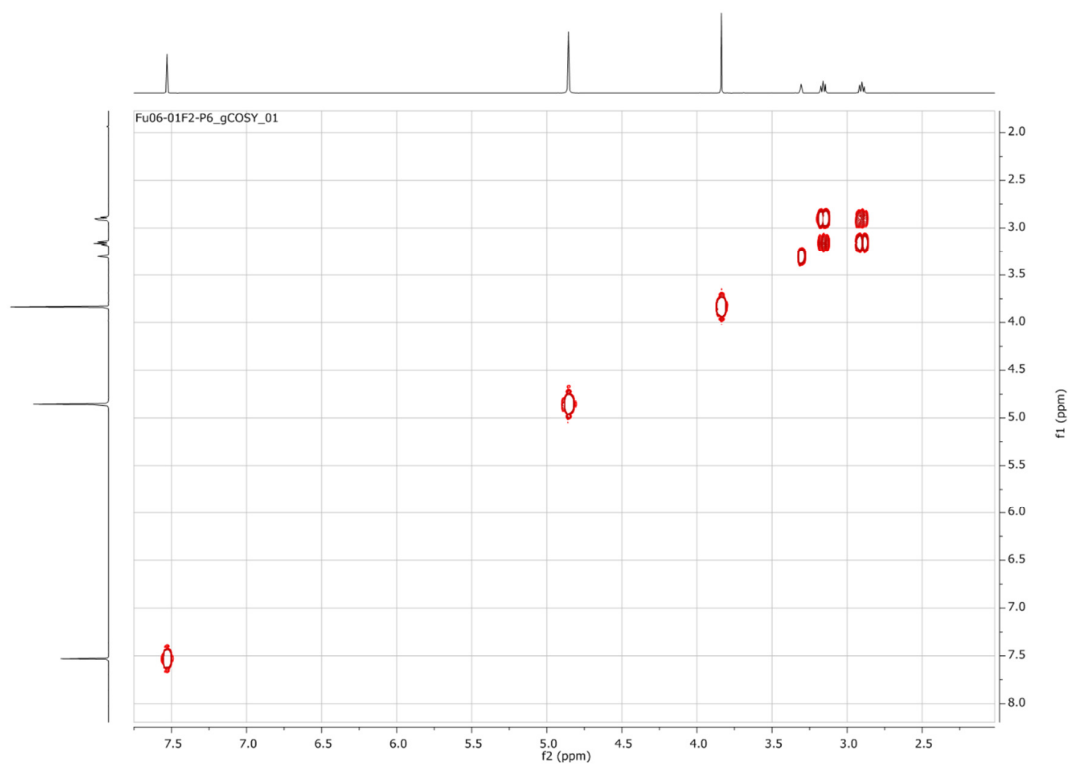
S69. ESI(+)-HRMS analysis of **16**



S70. ¹H NMR spectrum of **16** (500 MHz, MeOH-*d*₄).



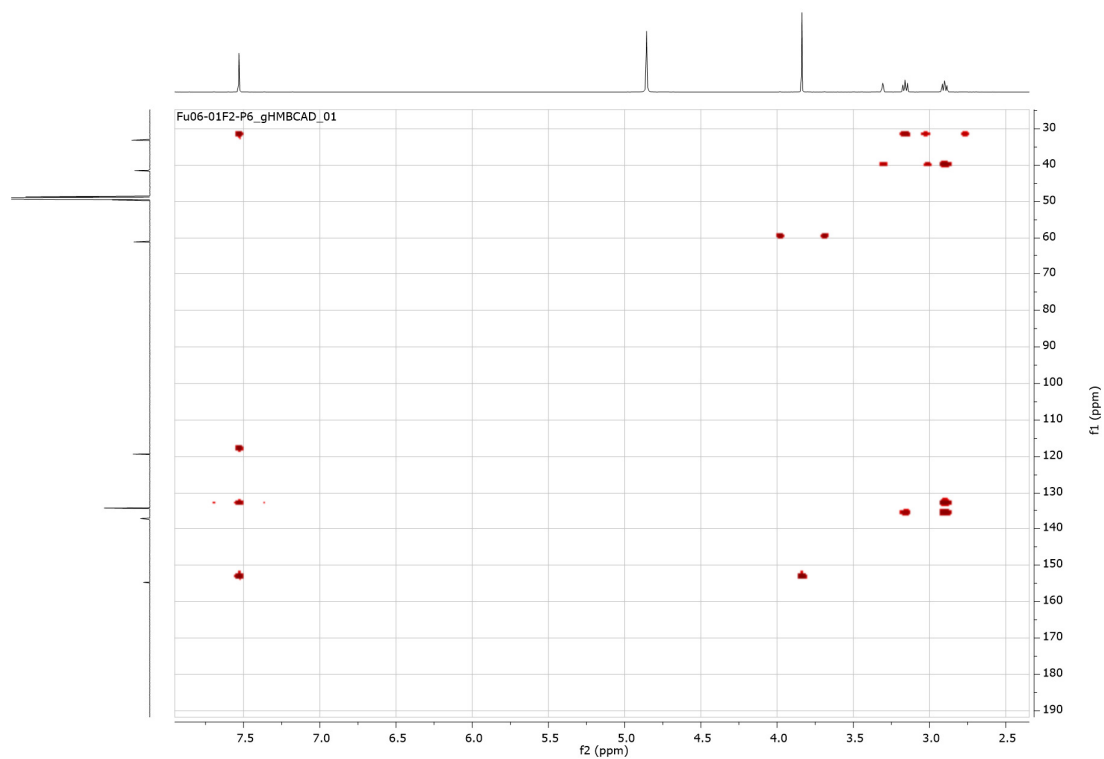
S71. ^{13}C NMR spectrum of **16** (125 MHz, $\text{MeOH-}d_4$).



S72. COSY NMR spectrum of **16** (500 MHz, $\text{MeOH-}d_4$).

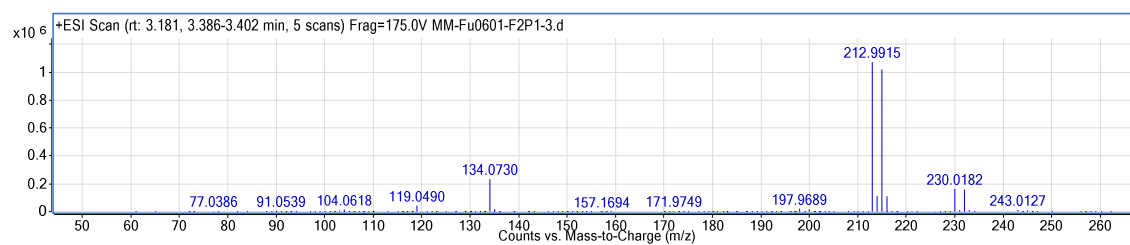


S73. HSQC NMR spectrum of **16** (500 MHz, MeOH- d_4).

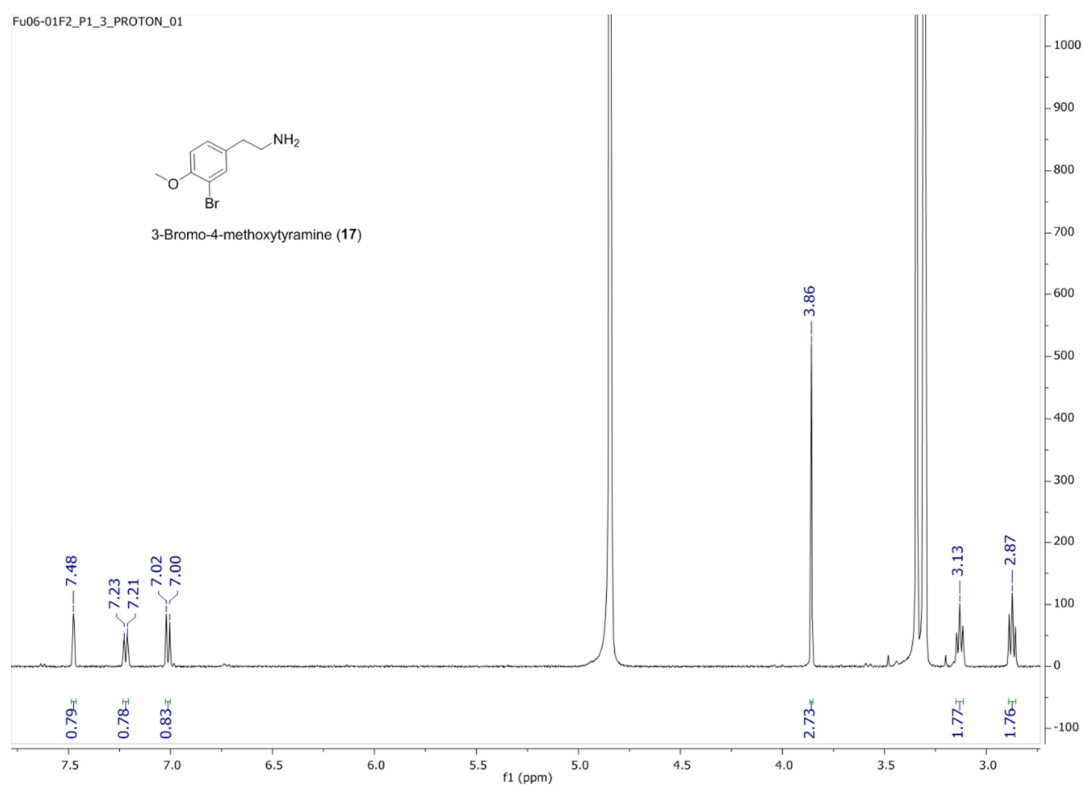


S74. HMBC NMR spectrum of **16** (500 MHz, MeOH- d_4).

Supporting information

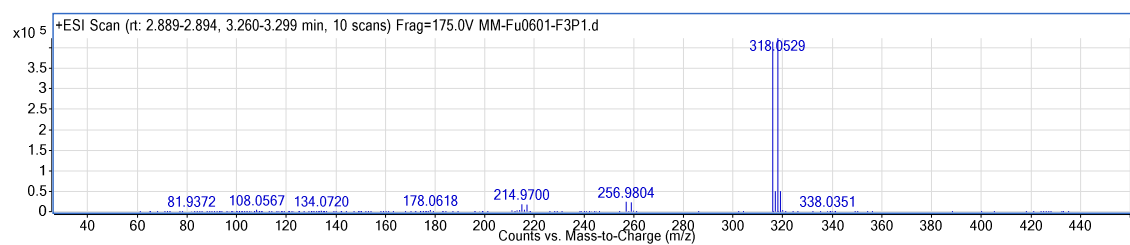


S75. ESI(+)-HRMS analysis of **17**

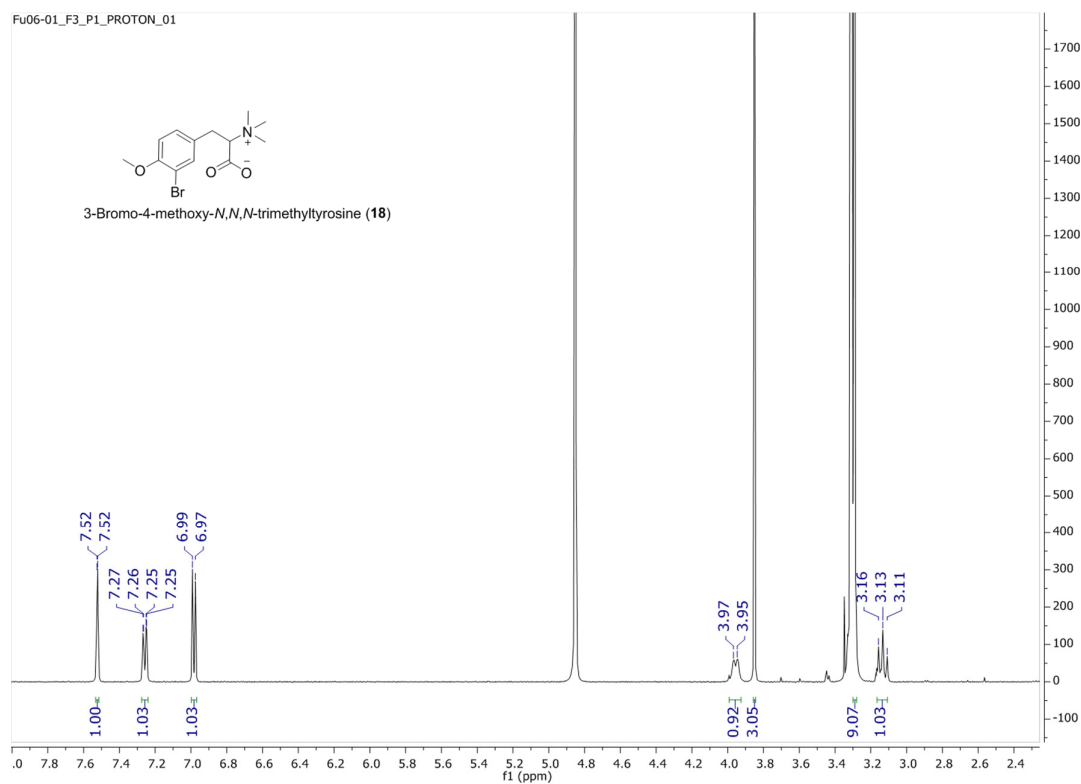


S76. ^1H NMR spectrum of **17** (500 MHz, $\text{MeOH-}d_4$).

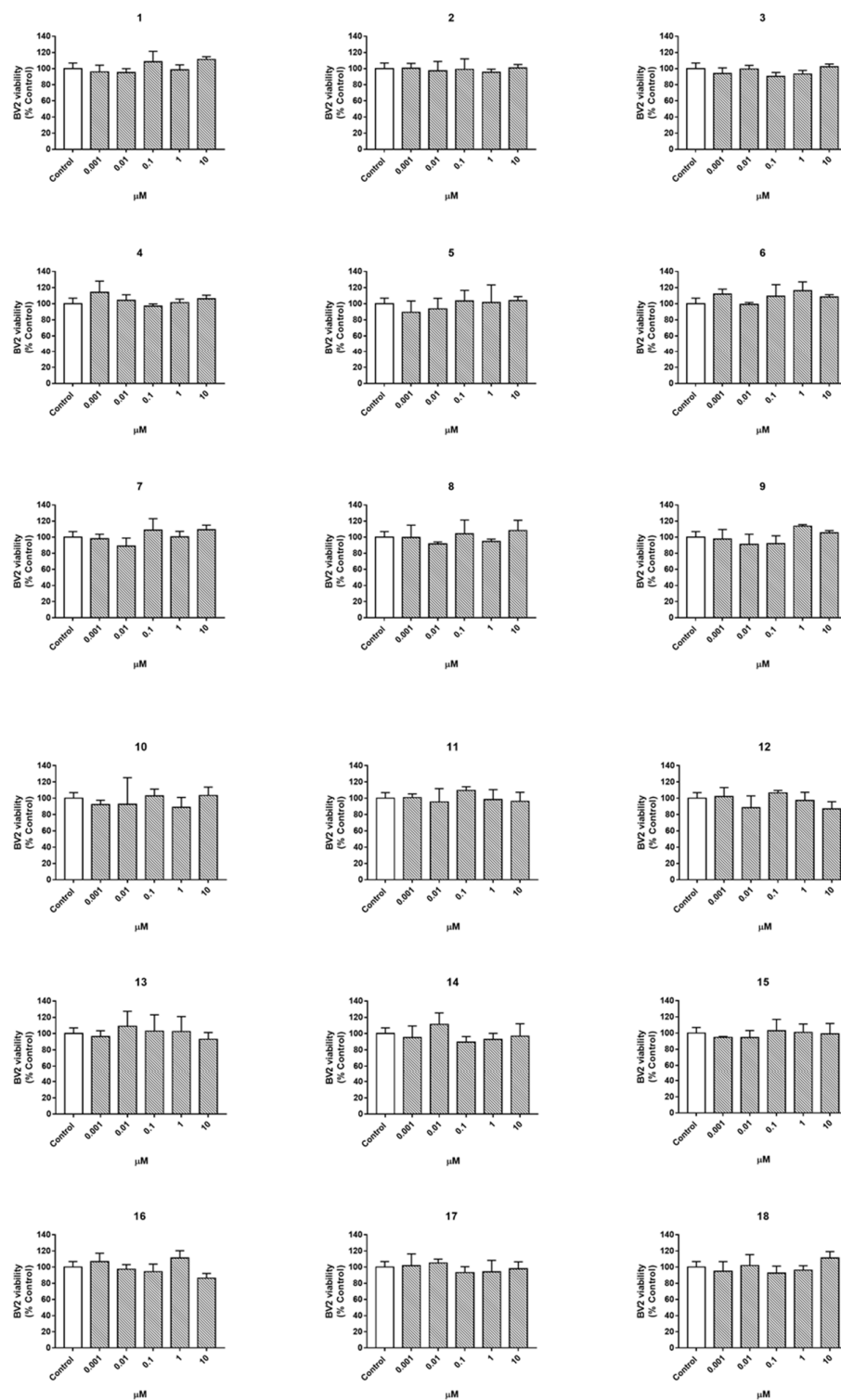
Supporting information



S77. ESI(+)-HRMS analysis of **18**

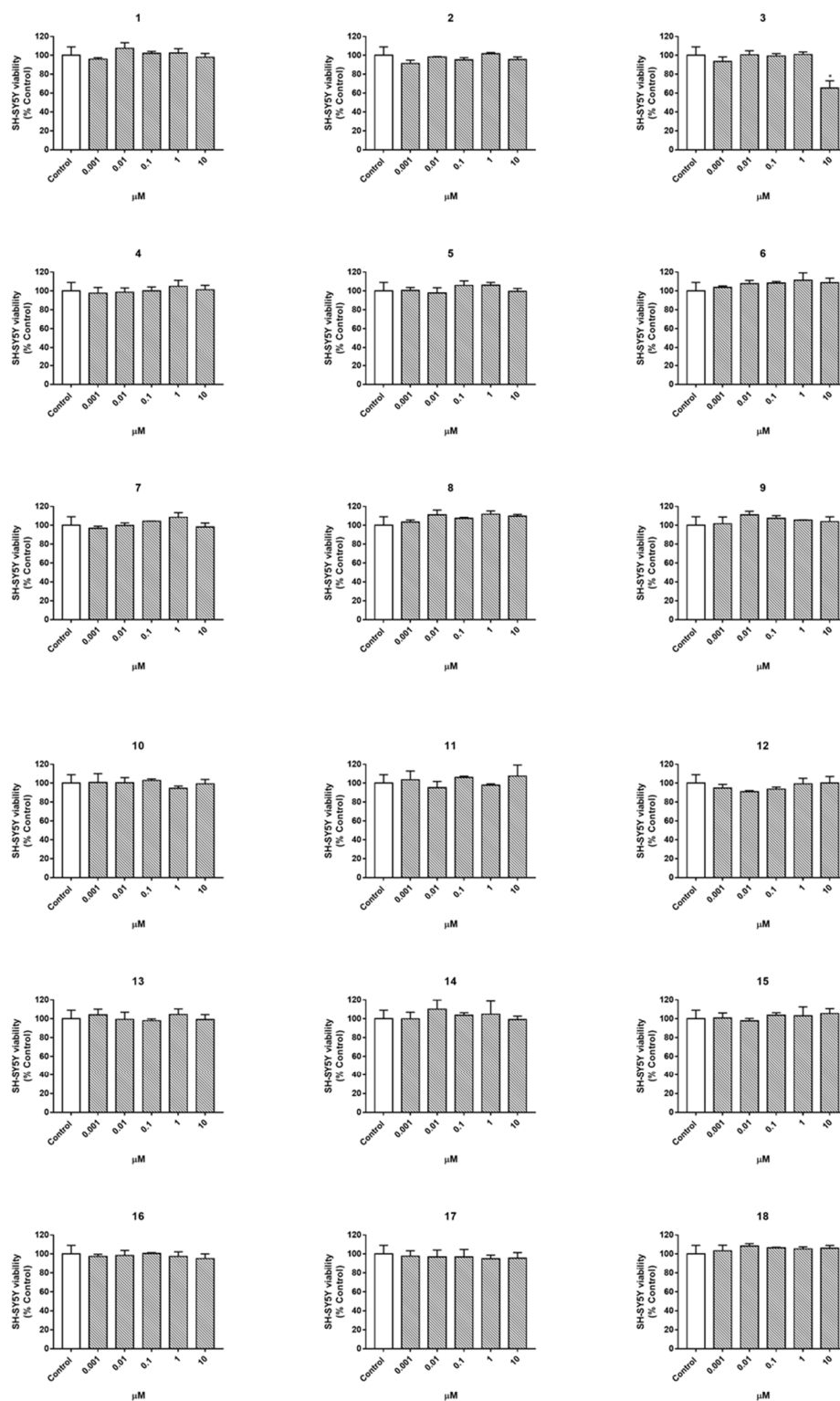


S78. ¹H NMR spectrum of **18** (500 MHz, MeOH-*d*₄).



S79. Cell viability of brominated alkaloids over microglia BV2 cell line.

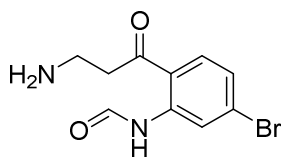
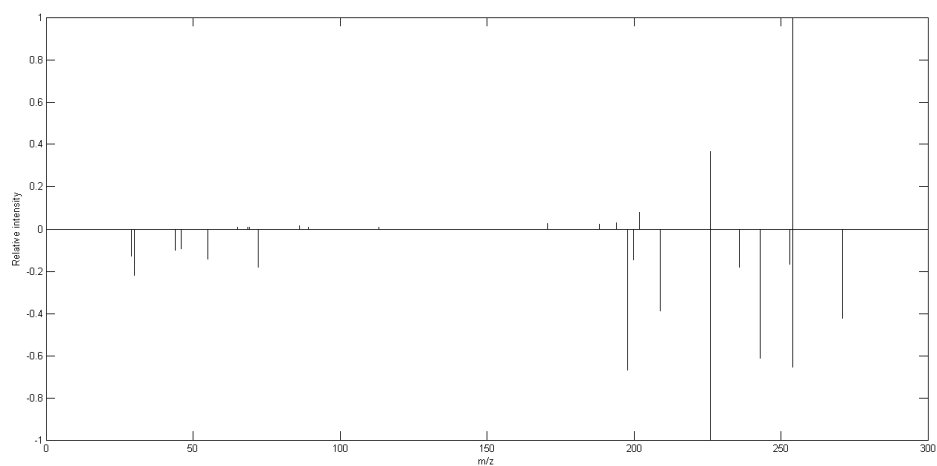
Cells were treated with compounds (0.001, 0.01, 0.1, 1 and 10 μM) for 24 hours. Cell viability was determined using MTT test. Dates are represented in percentage of cells control, being the result of mean absorbance $\pm$ SEM of three independent experiments done in triplicate.



S80. Cell viability of brominated alkaloids over neuroblastoma SH-SY5Y cell line.

Cells were treated with compounds (0.001, 0.01, 0.1, 1 and 10 μM) for 24 hours. Cell viability was determined using MTT test. Dates are represented in percentage of cells control, being the result of mean absorbance $\pm$ SEM of three independent experiments done in triplicate.

S81. Cosine values of all newly identified compounds in orange in the MetWork software.



S82. Comparison between the experimental and calculated MS/MS spectrum of the minor compound below.