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

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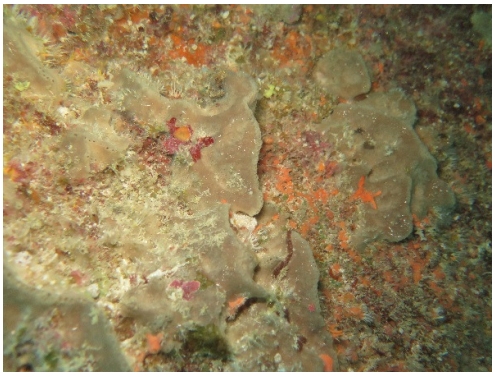
Biological material.



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 uncored, 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.

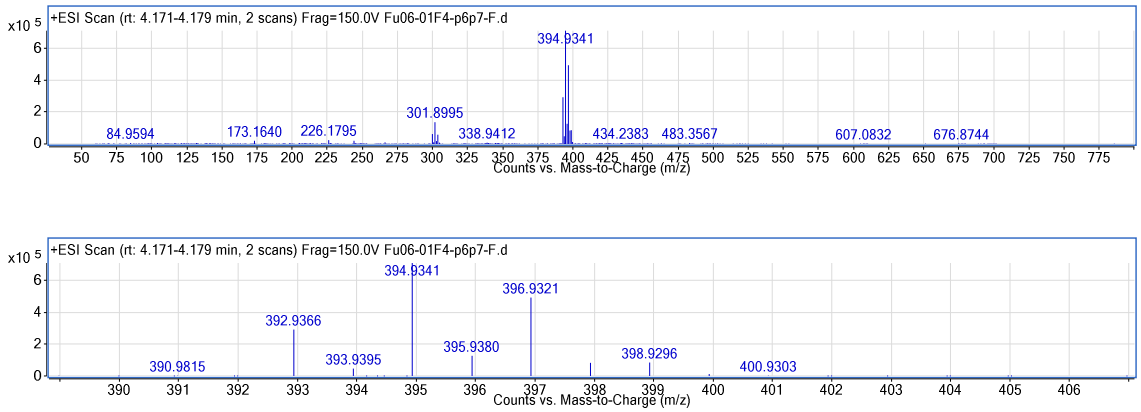
S2. ^{1}H NMR data, δ_H in ppm, mult. (*J* in Hz), in MeOH-d_4 for bromotryptamines

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			

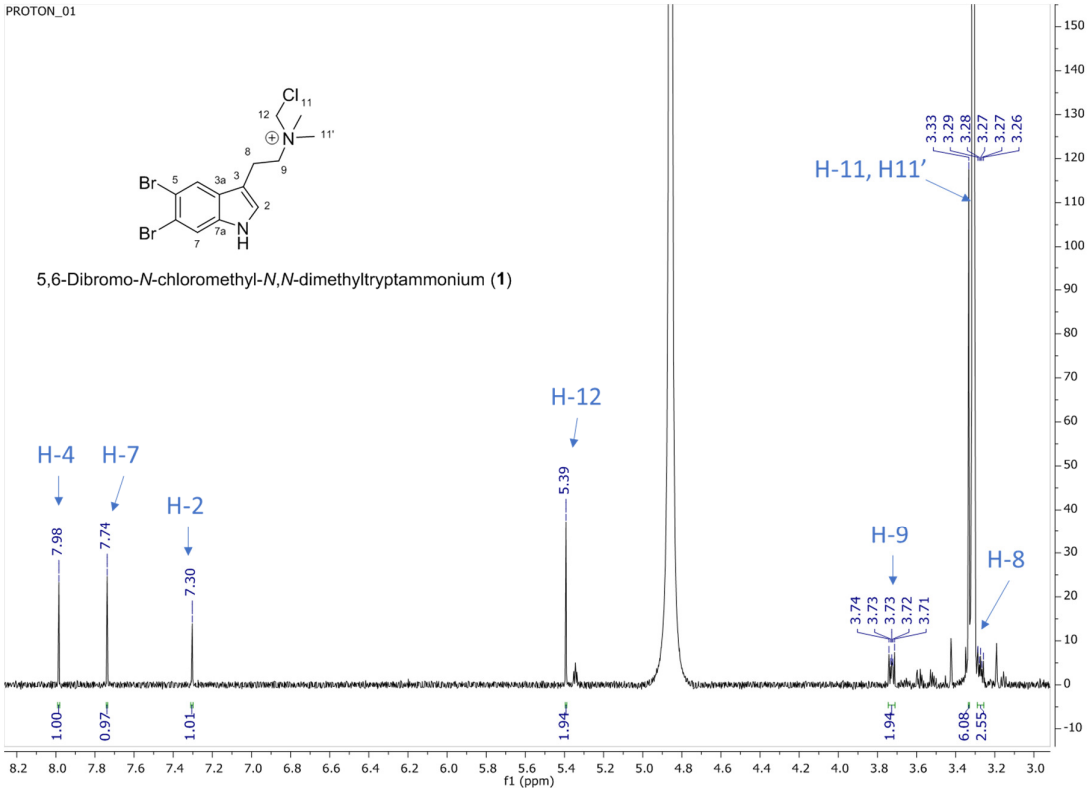
[a] 500MHz [b] 600MHz [c] Overlap with solvent signal

S3. ^{1}H NMR data, δ_H in ppm, mult. (*J* in Hz), in MeOH-d_4 for bromotyramines

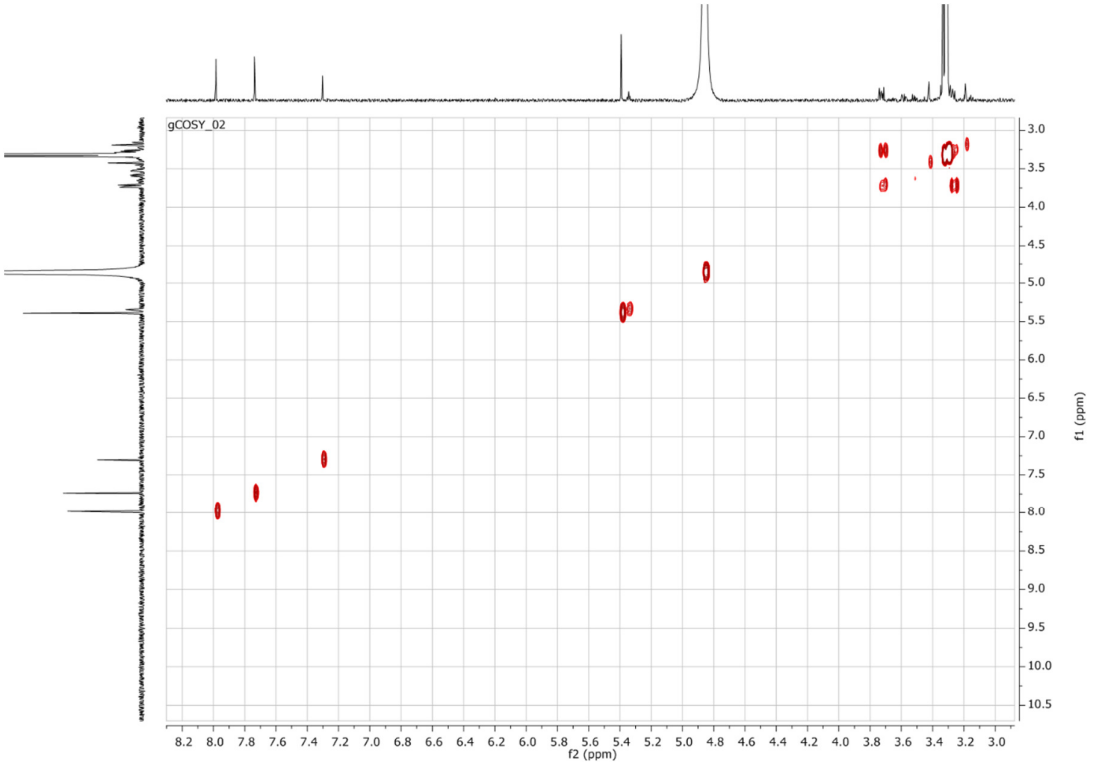
No.	16[a]	17[a]	18[a]
2	7.53, s	7.48, d (1.5)	7.51, d (1.5)
3	-	-	-
4	-	-	-
5	-	7.01, d (8.5)	6.98, d (8.5)
6	7.53, s	7.22, dd (8.5, 1.5)	7.26, dd (8.5, 1.5)
7	2.90, t (7.5)	2.87, d (7.5)	3.96, d (12.0)
8	3.16, t (7.5)	3.13, d (7.5)	3.13, t (12.0)
10			3.29, s
O-C$\underline{H}_3$	3.84, s	3.86, s	3.85, s



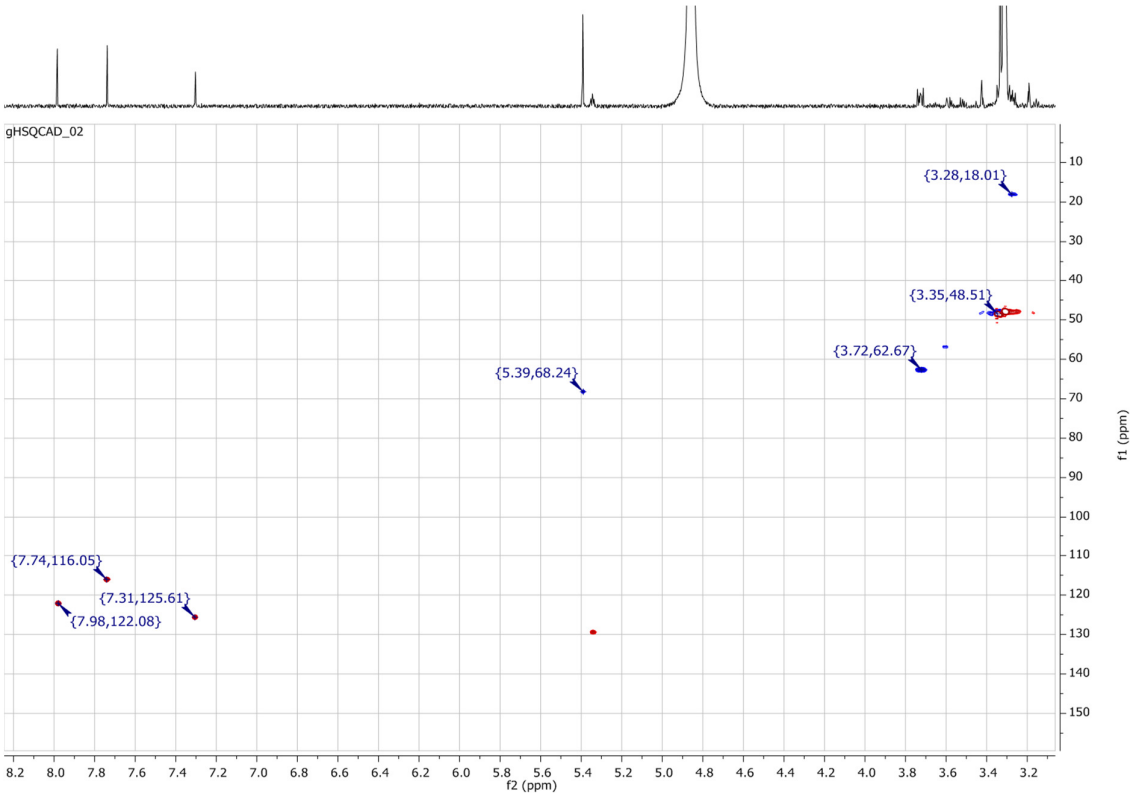
S4. ESI(+)-HRMS analysis of **1** and crop of the molecular ion.



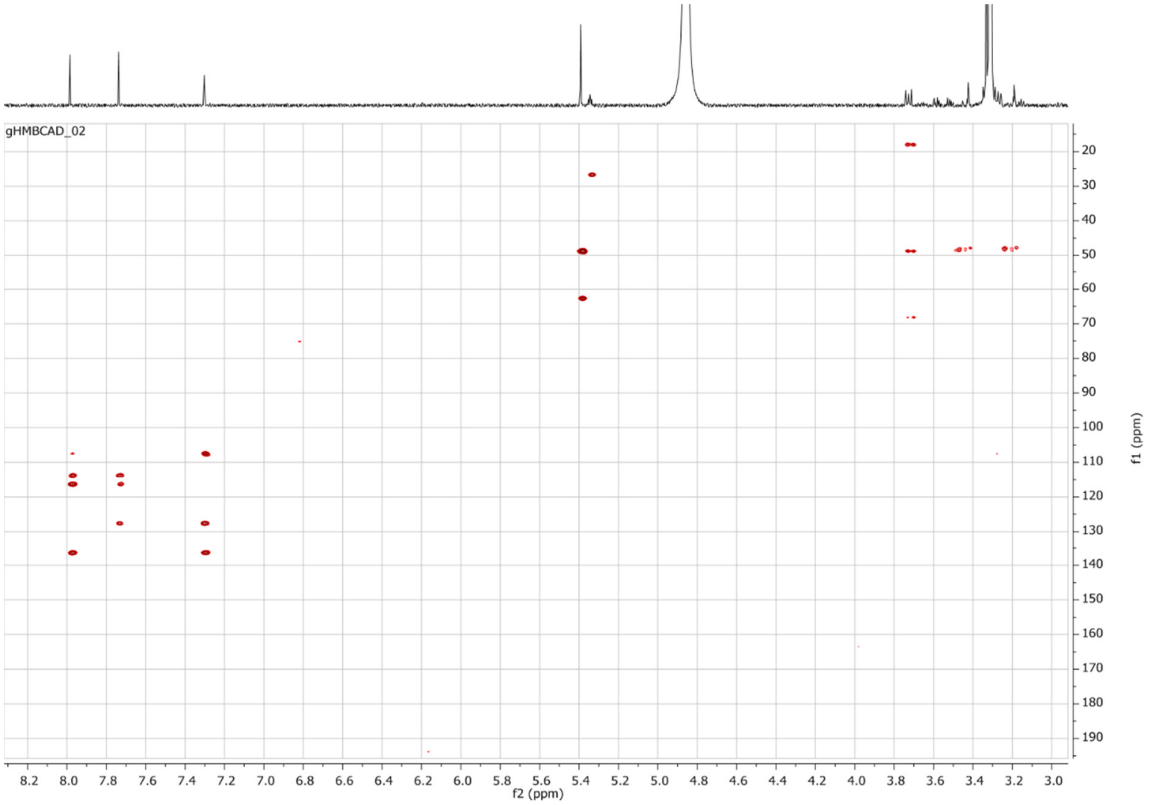
S5. ^{1}H NMR spectrum of **1** (600 MHz, MeOH-d_4).



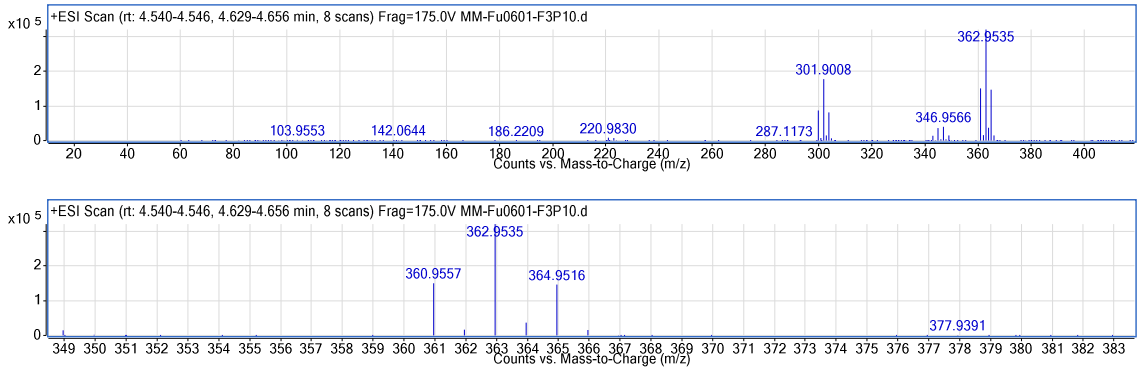
S6. COSY NMR spectrum of **1** (600 MHz, MeOH-d_4).



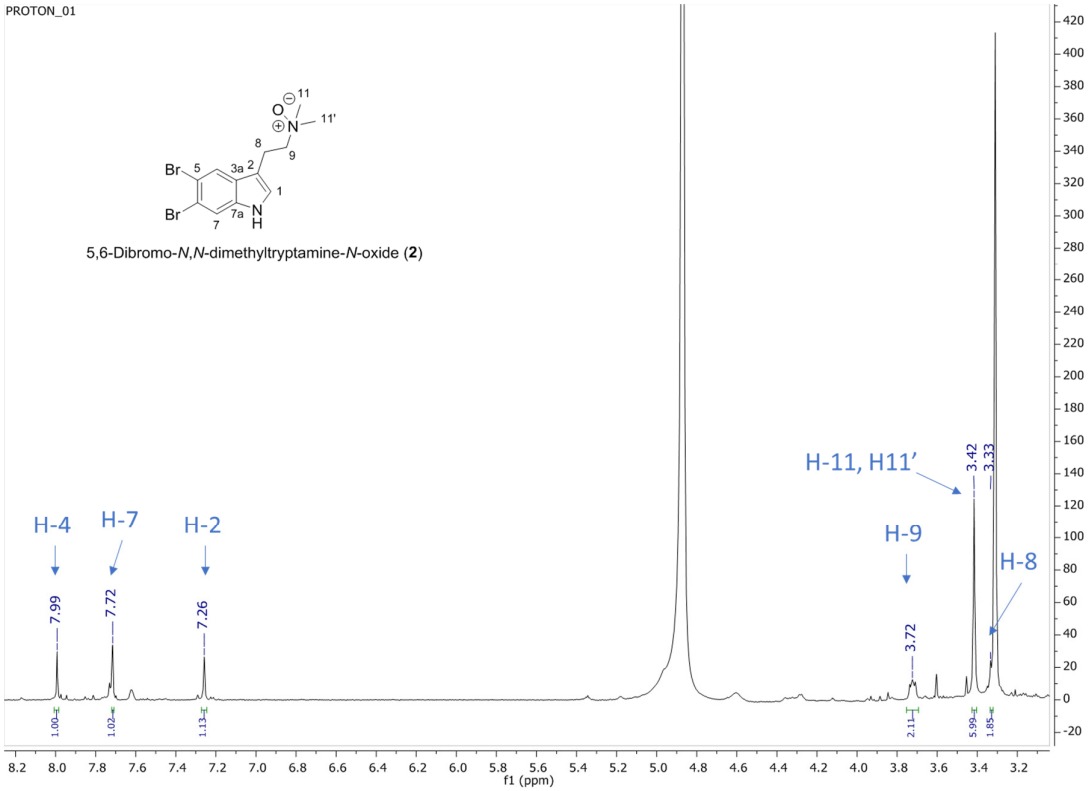
S7. HSQC NMR spectrum of **1** (600 MHz, MeOH-d_4).



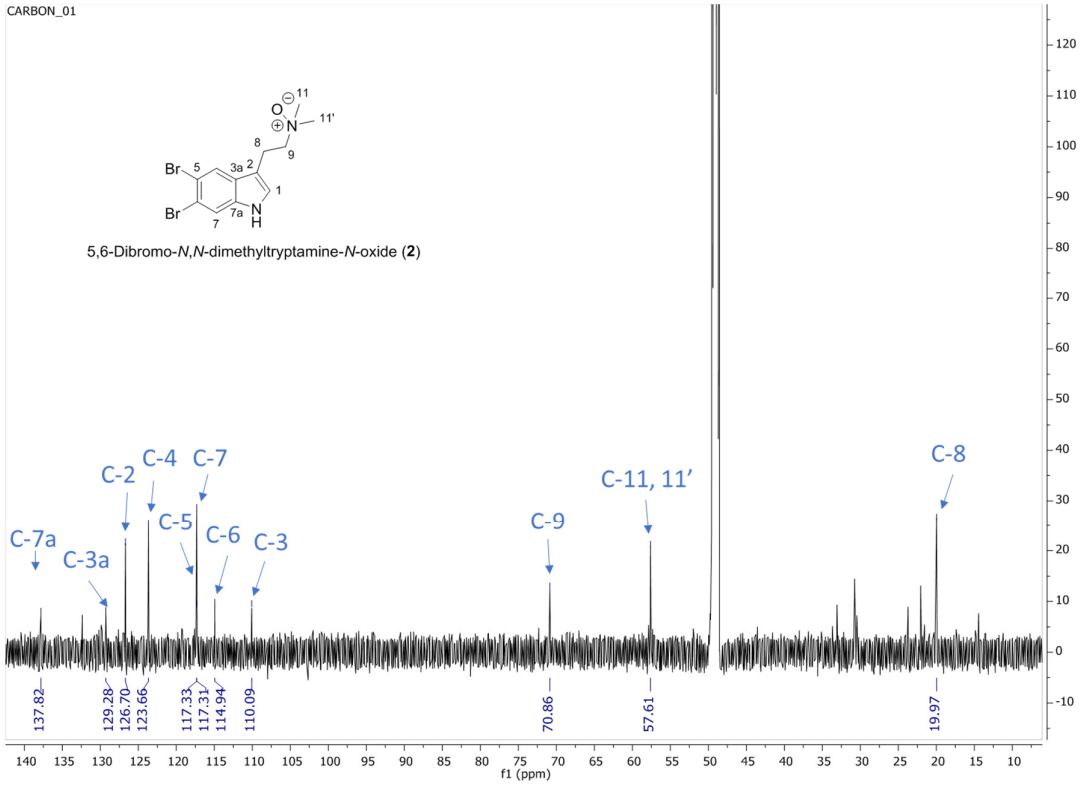
S8. HMBC NMR spectrum of **1** (600 MHz, MeOH-d_4).



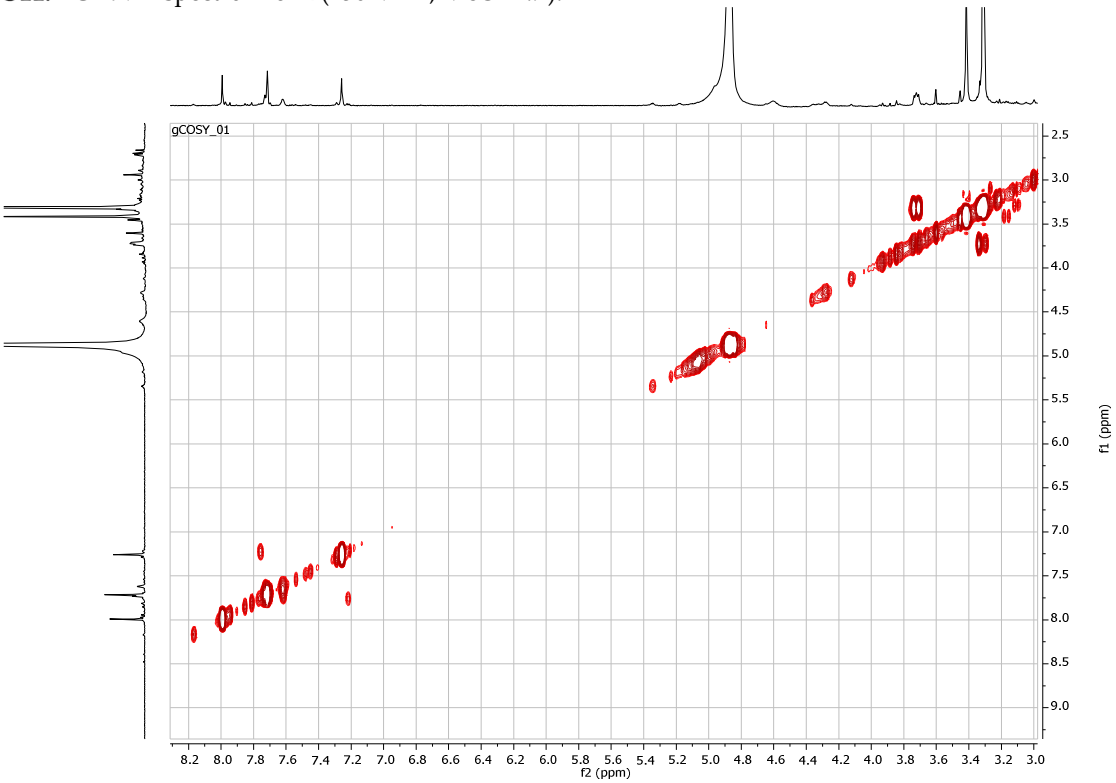
S9. ESI(+)-HRMS analysis of **2** and crop of the molecular ion.



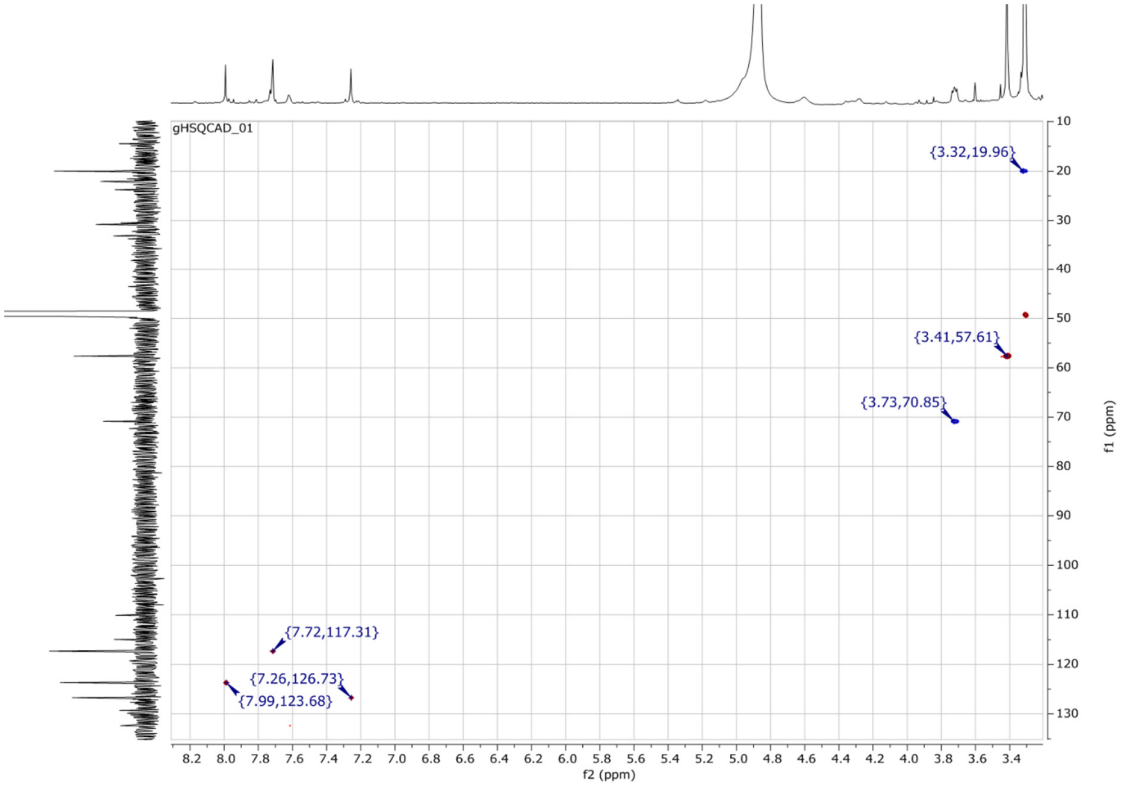
S10. ^{1}H NMR spectrum of **2** (600 MHz, MeOH-d_4).



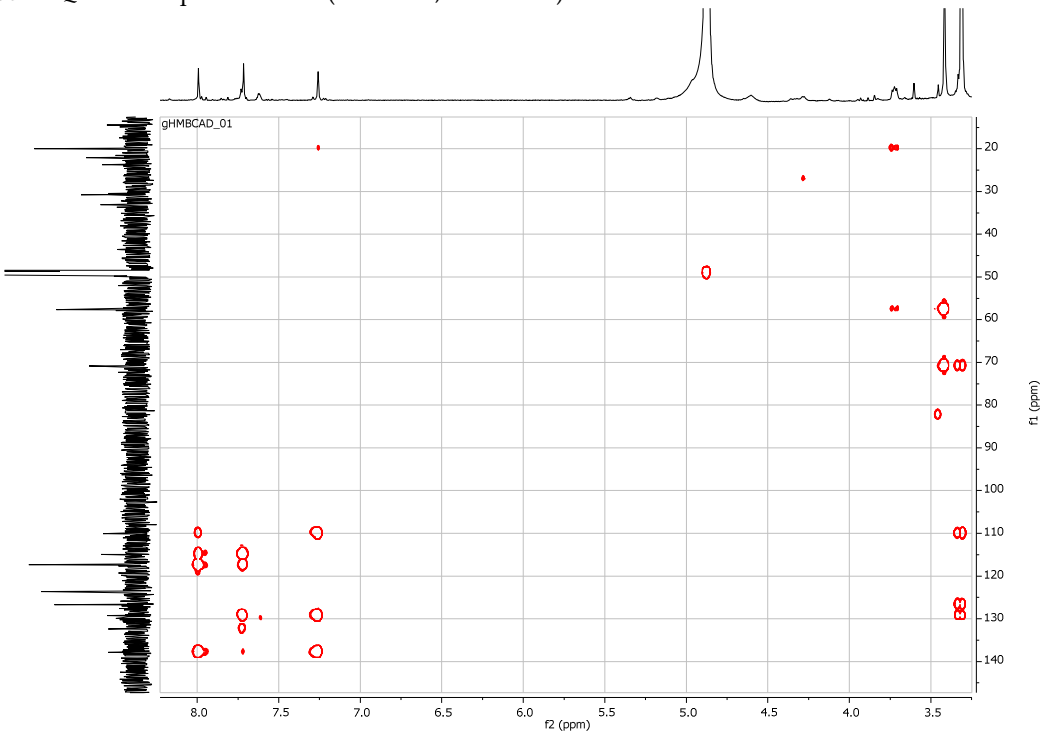
S11. ^{13}C NMR spectrum of **2** (150 MHz, MeOH-d_4).



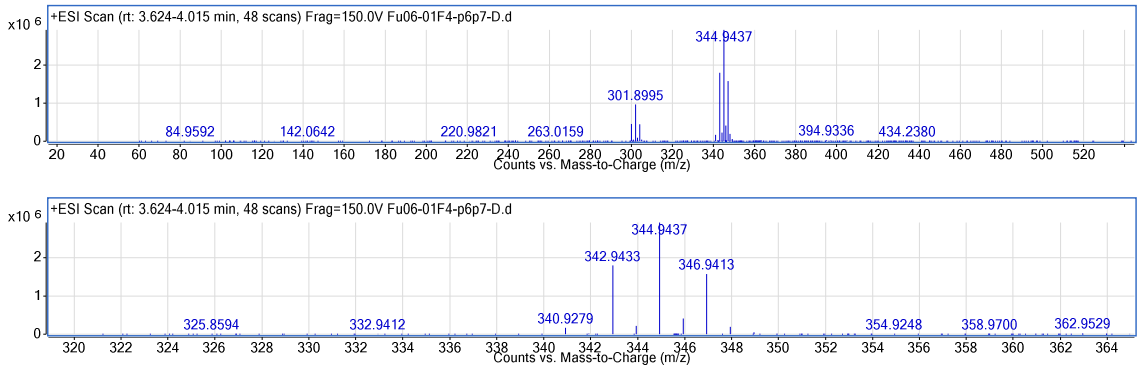
S12. COSY NMR spectrum of **2** (600 MHz, MeOH-d_4).



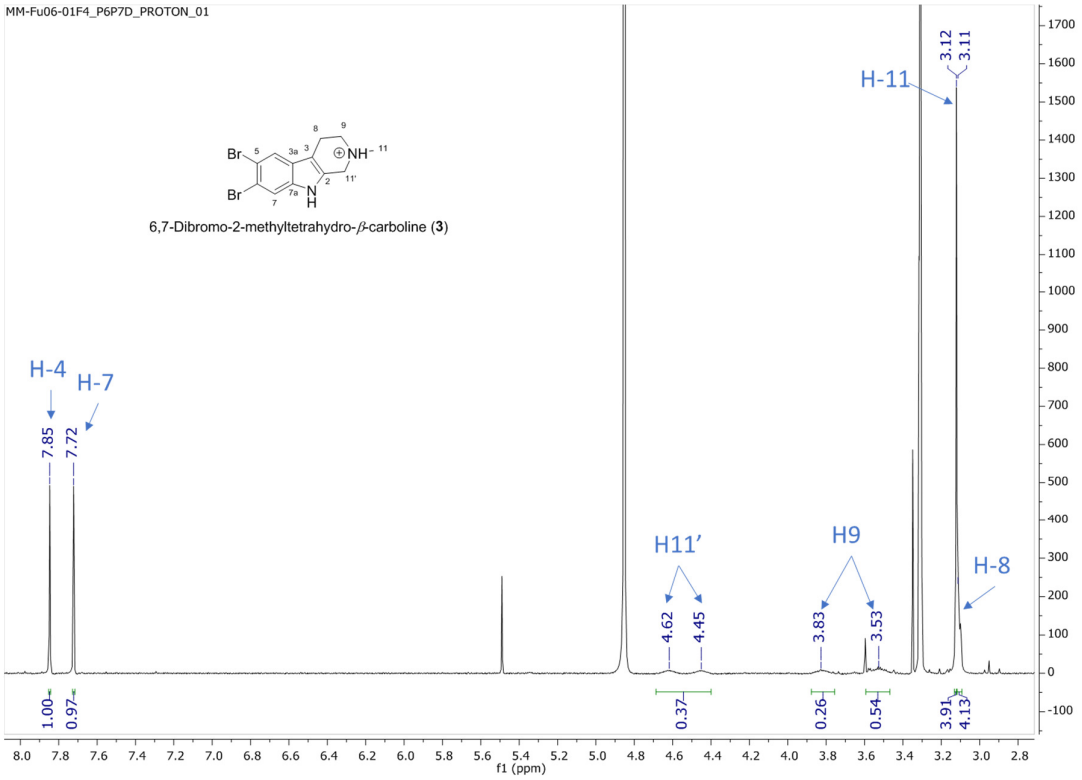
S13. HSQC NMR spectrum of **2** (600 MHz, MeOH-d_4).



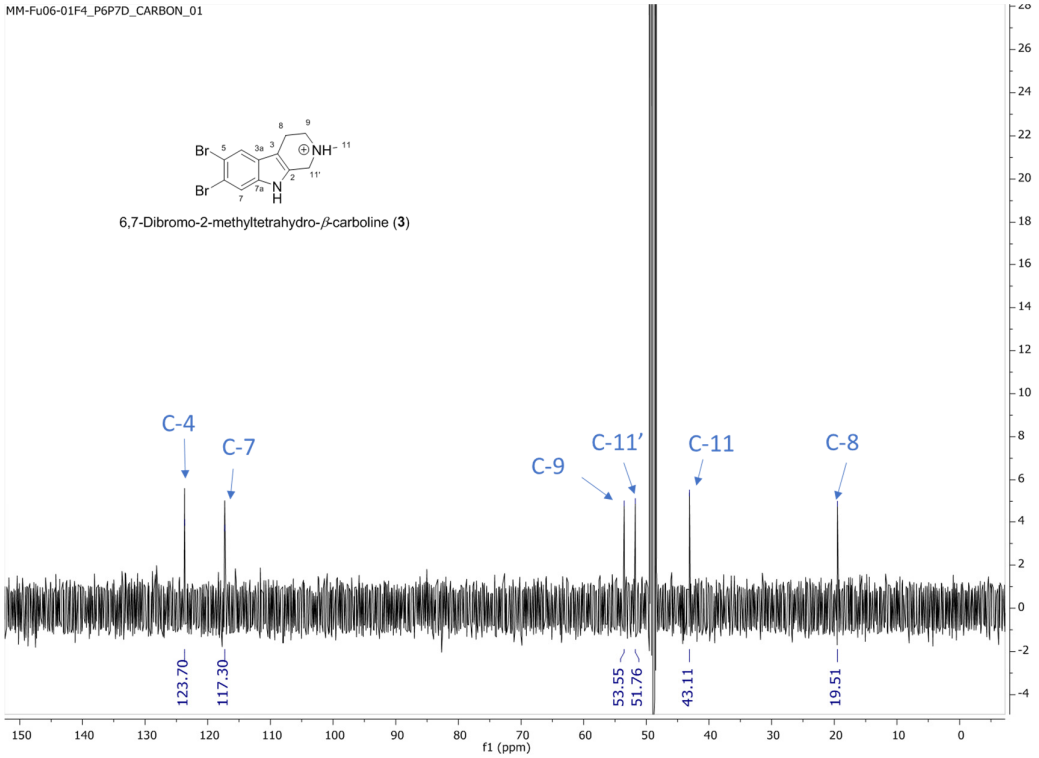
S14. HMBC NMR spectrum of **2** (600 MHz, MeOH-d_4).



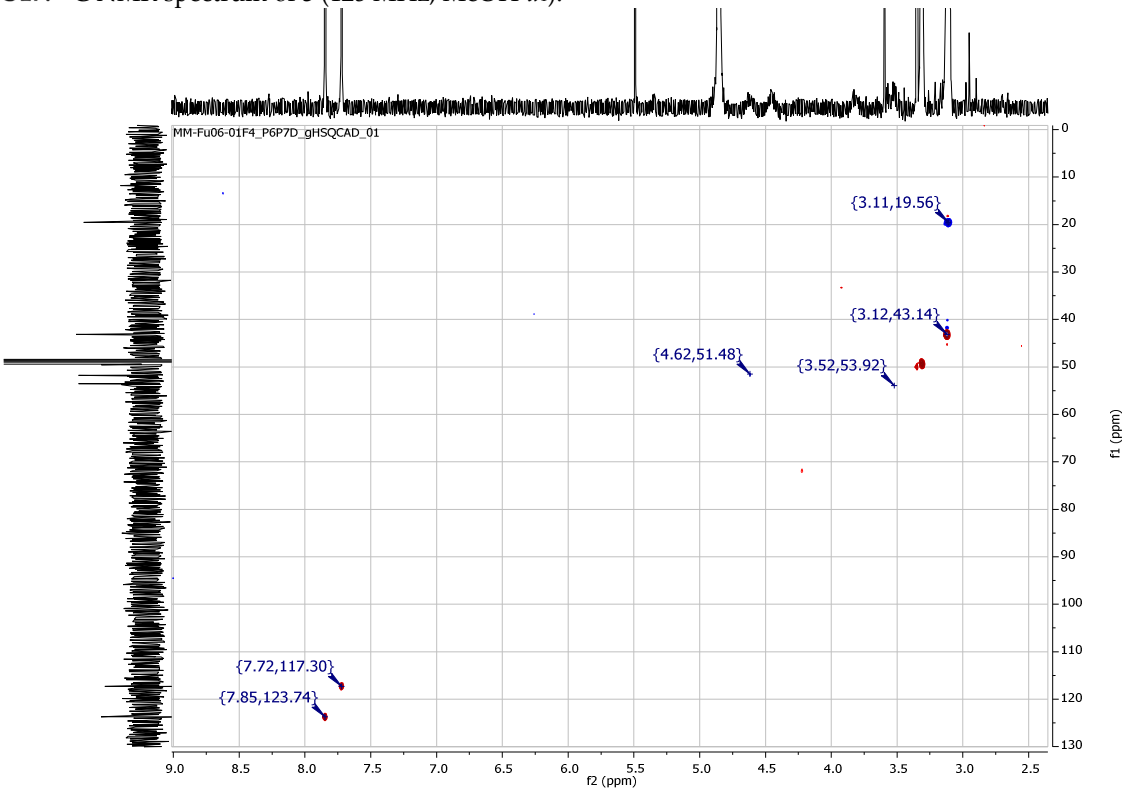
S15. ESI(+)-HRMS analysis of **3** and crop of the molecular ion.



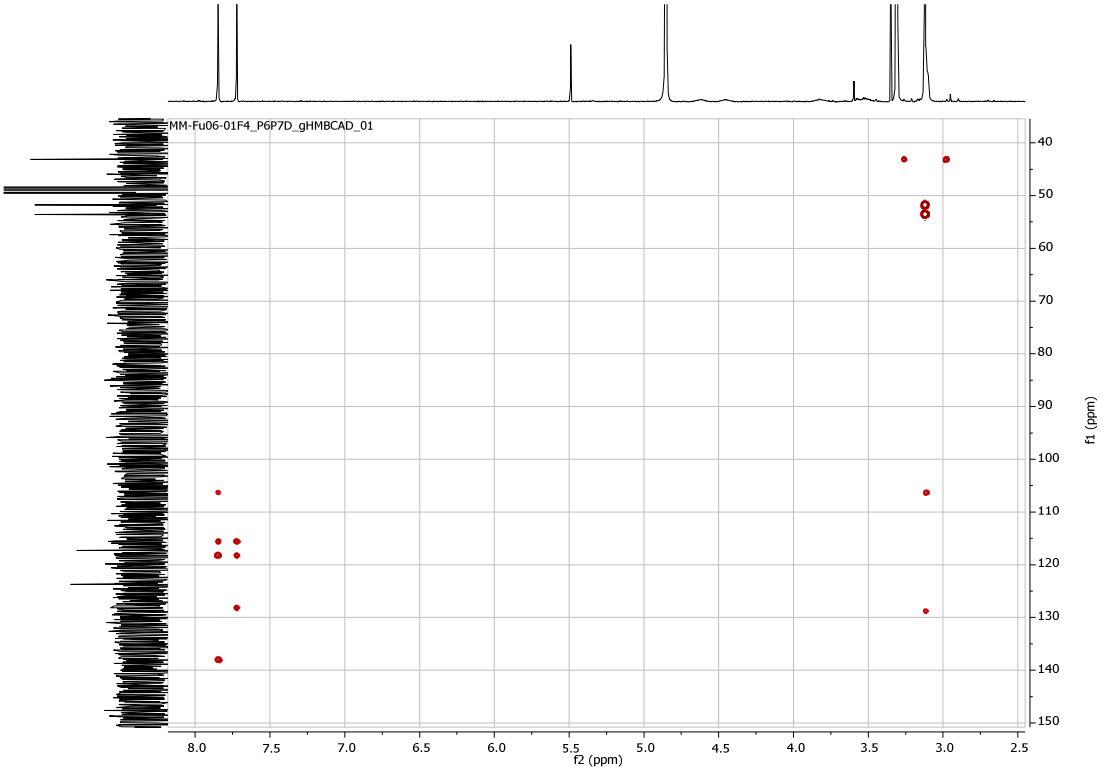
S16. ^{1}H NMR spectrum of **3** (500 MHz, MeOH-d_4).



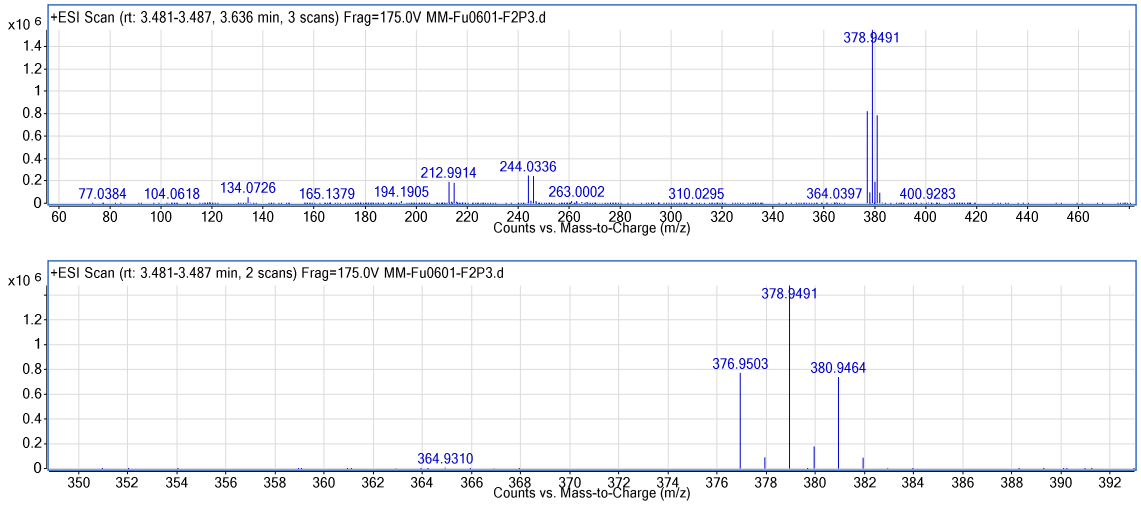
S17. ^{13}C NMR spectrum of **3** (125 MHz, MeOH-d_4).



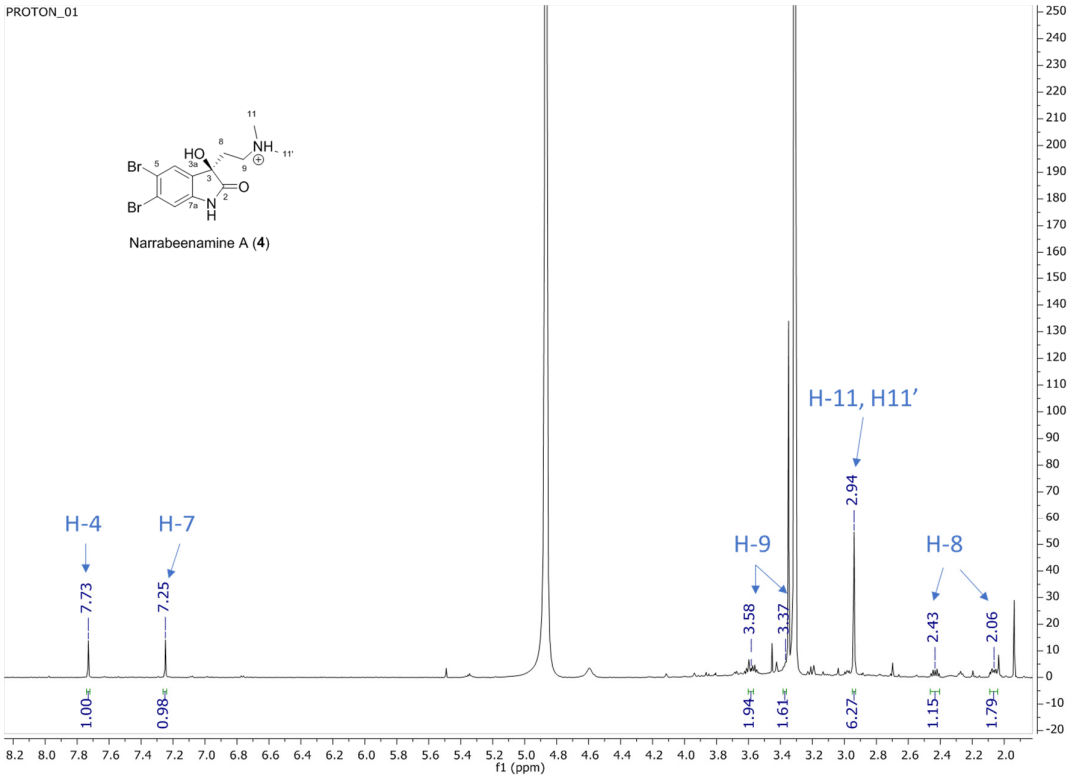
S18. HSQC NMR spectrum of **3** (500 MHz, MeOH-d_4).



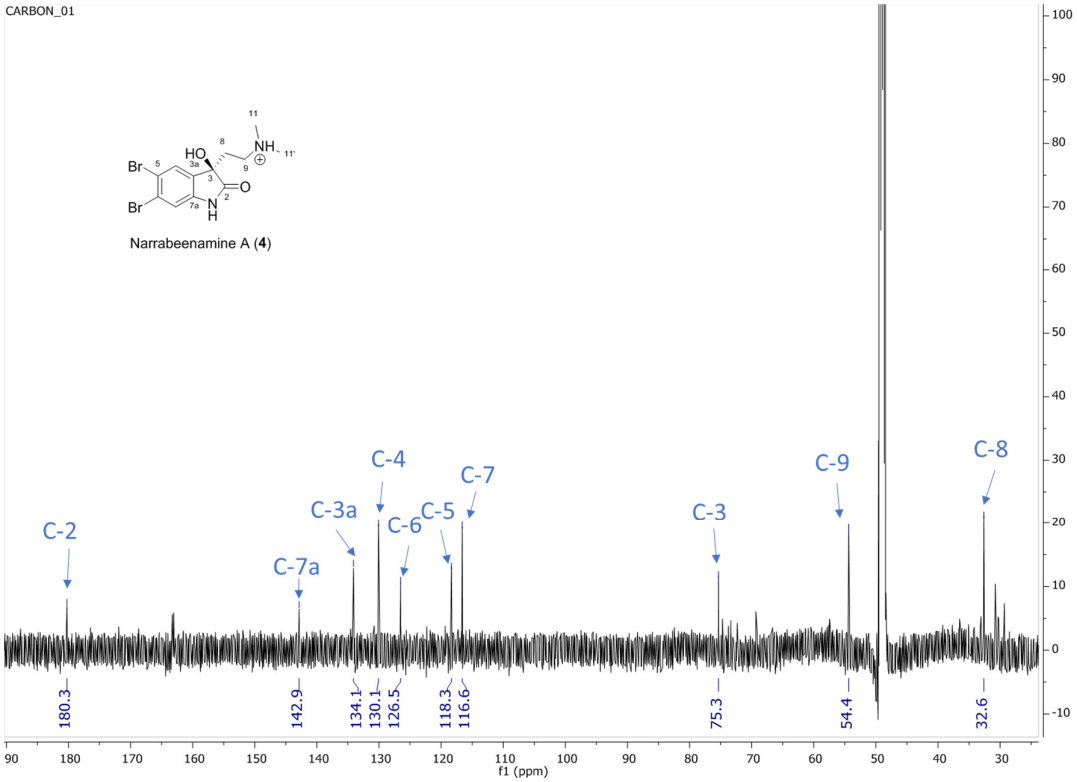
S19. HMBC NMR spectrum of **3** (500 MHz, MeOH-d_4).



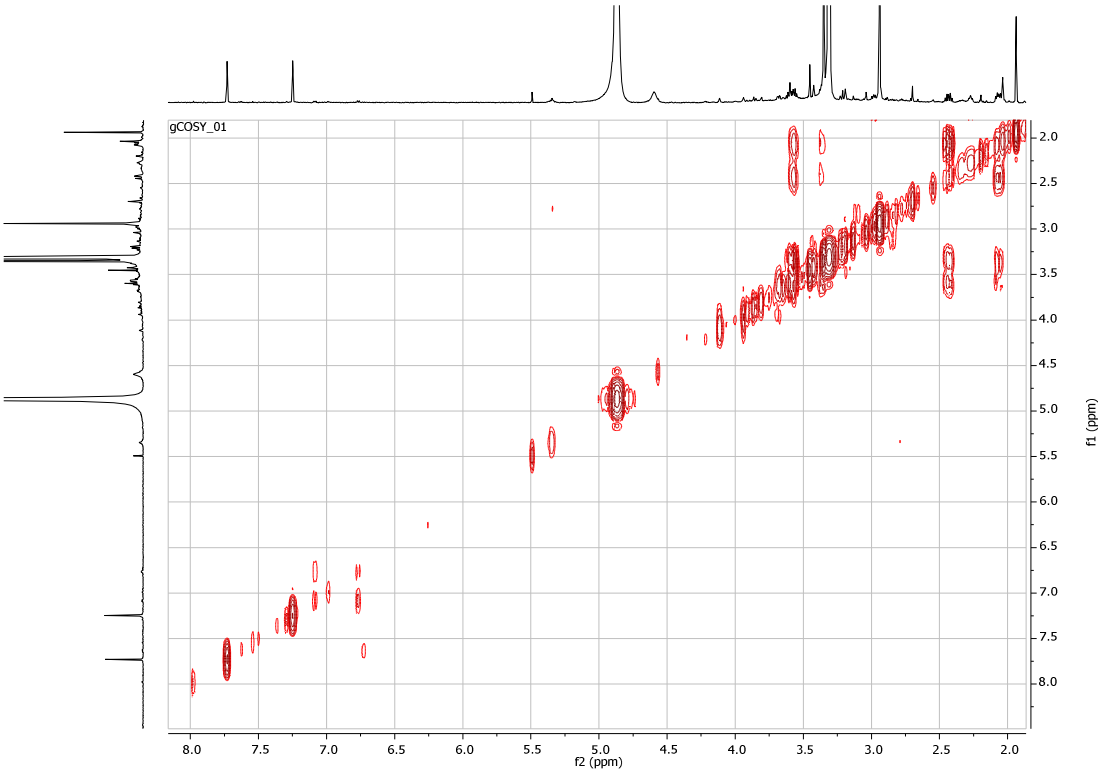
S20. ESI(+)-HRMS analysis of **4** and crop of the molecular ion.



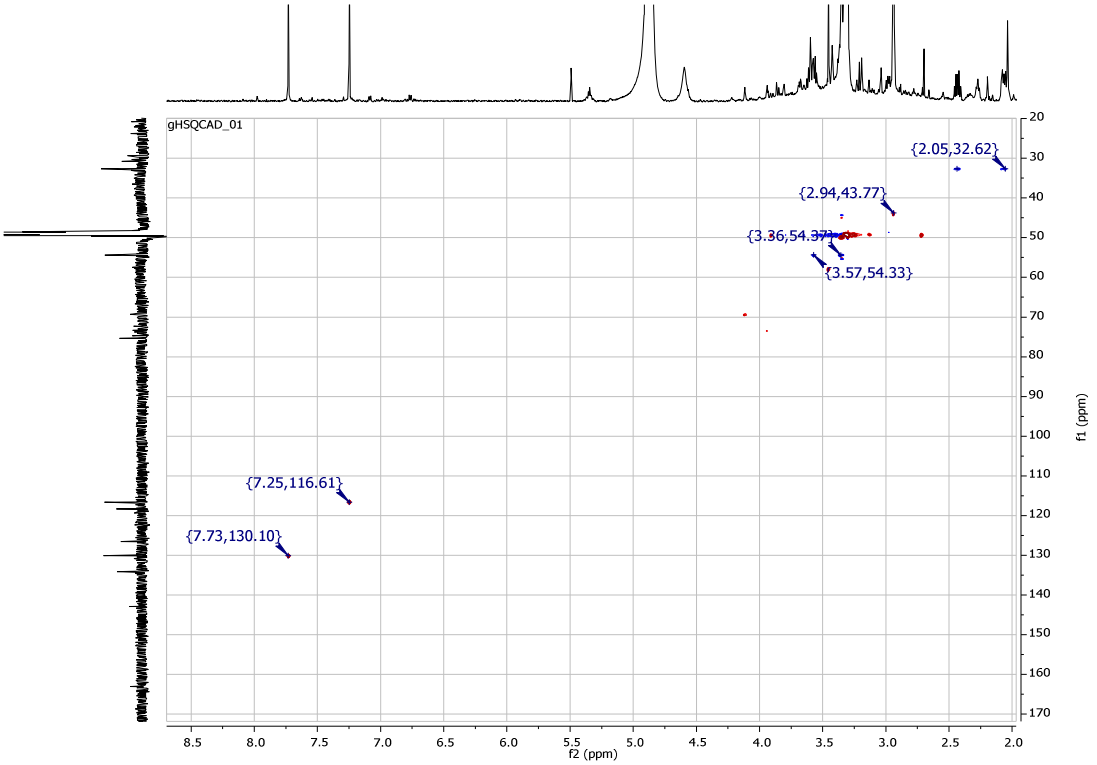
S21. ^{1}H NMR spectrum of **4** (600 MHz, MeOH-d_4).



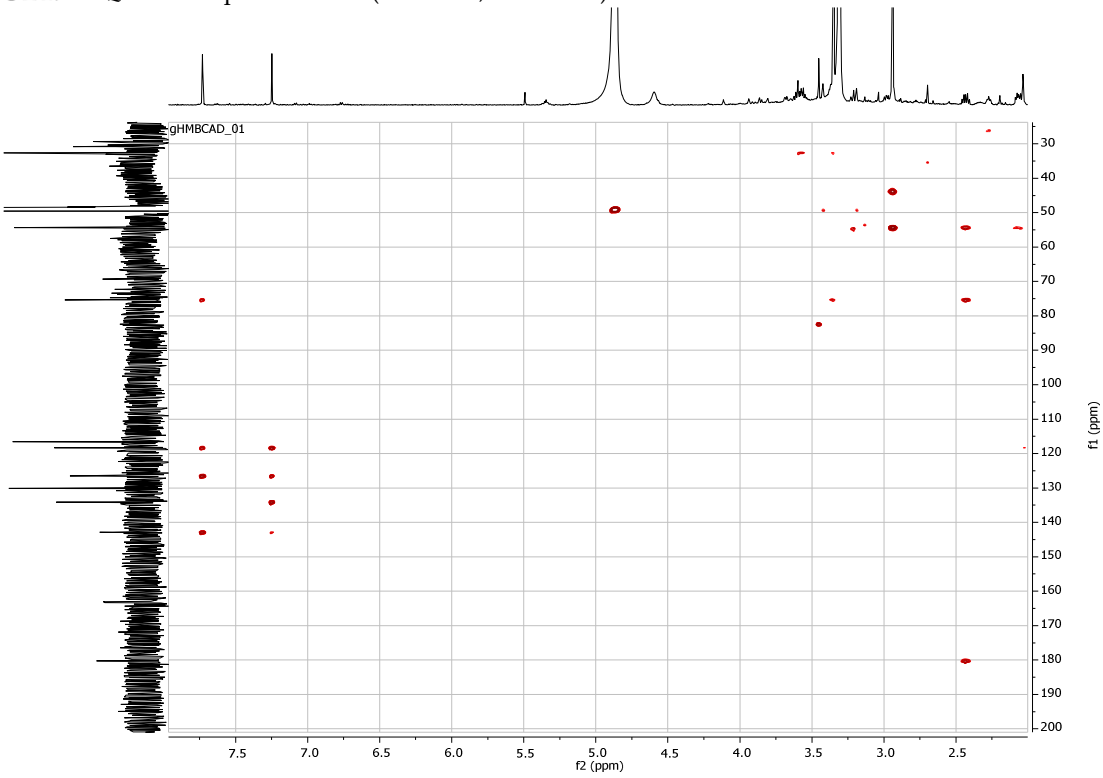
S22. ^{13}C NMR spectrum of **4** (150 MHz, MeOH-d_4).



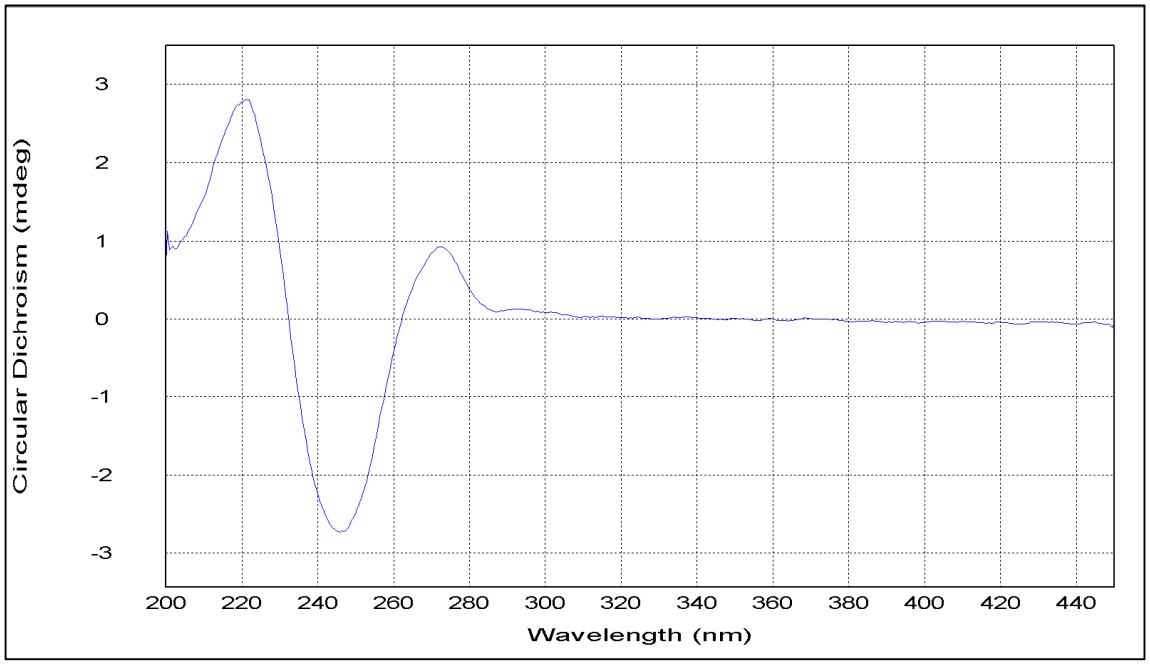
S23. COSY NMR spectrum of **4** (600 MHz, MeOH-d_4).



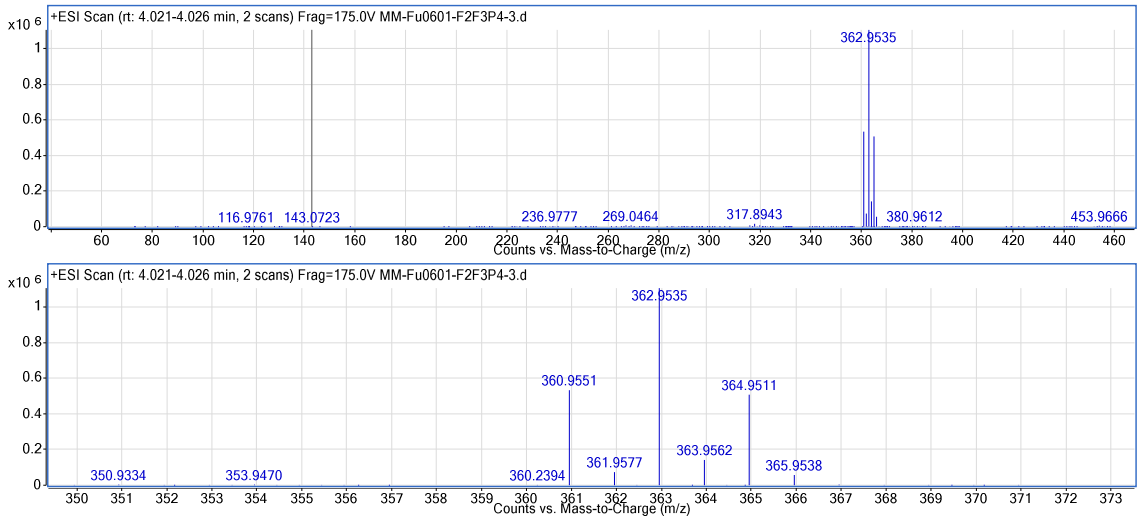
S24. HSQC NMR spectrum of **4** (600 MHz, MeOH-d_4).



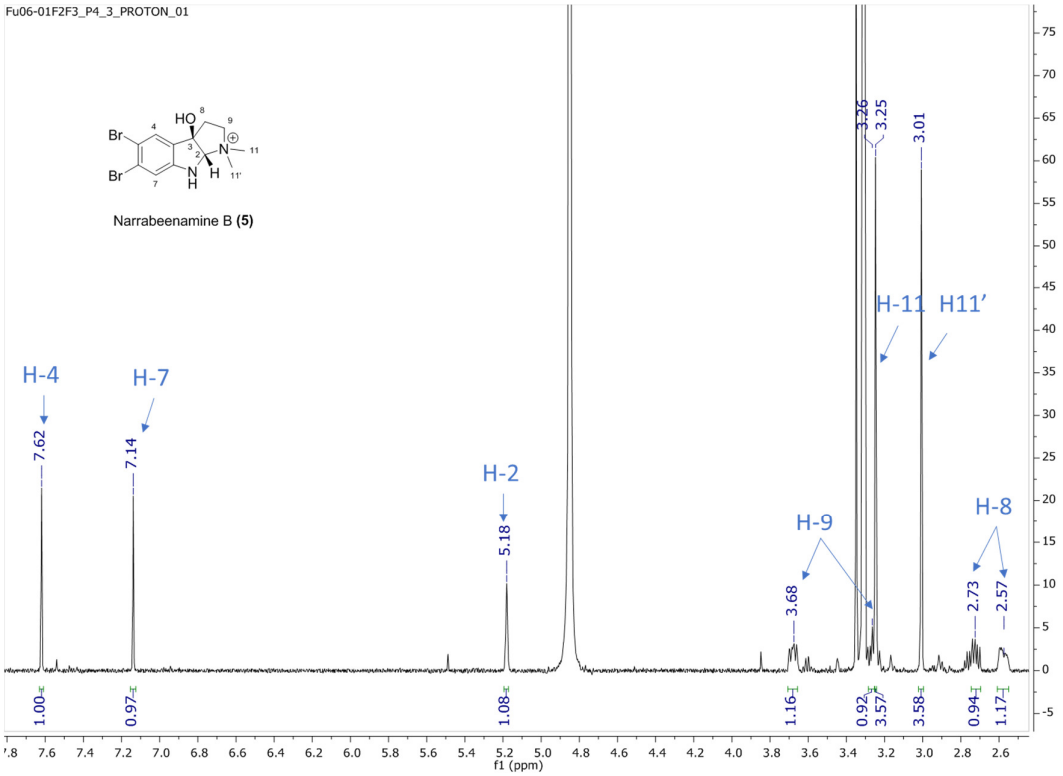
S25. HMBC NMR spectrum of **4** (600 MHz, MeOH-d_4).



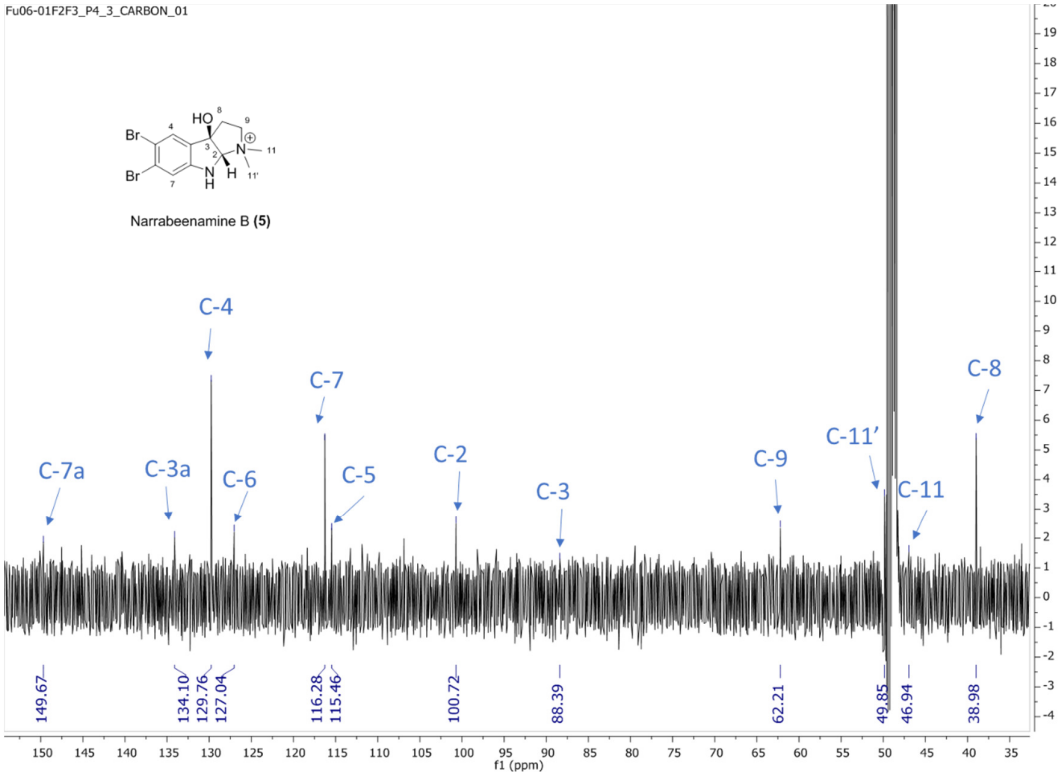
S26. ECD spectrum of compound **4** in CH_3CN at 0.1 mg/mL



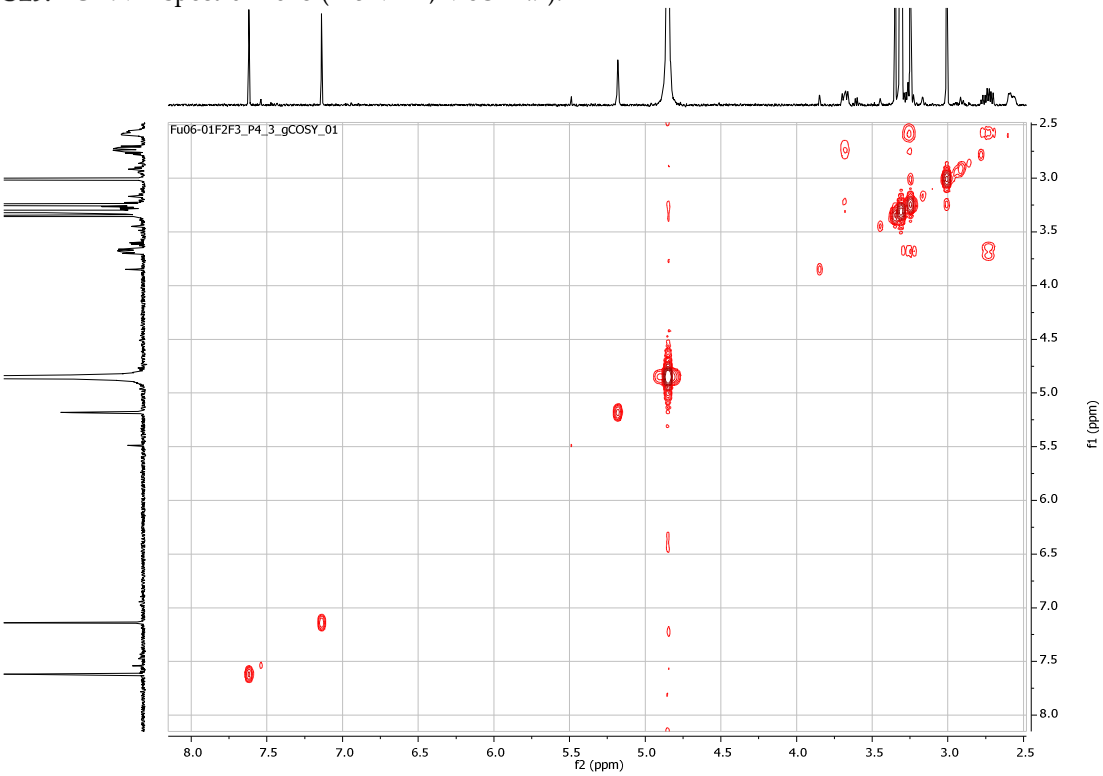
S27. ESI(+)-HRMS analysis of **5** and crop of the molecular ion.



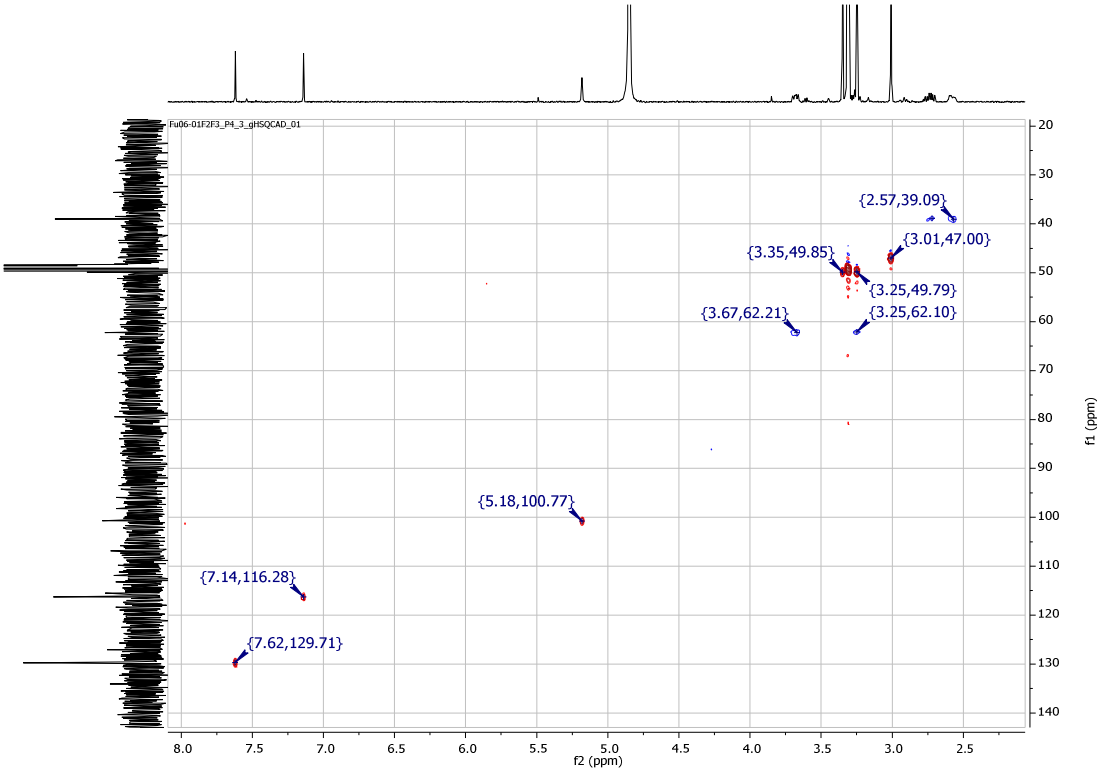
S28. ^{1}H NMR spectrum of **5** (500 MHz, MeOH-d_4).



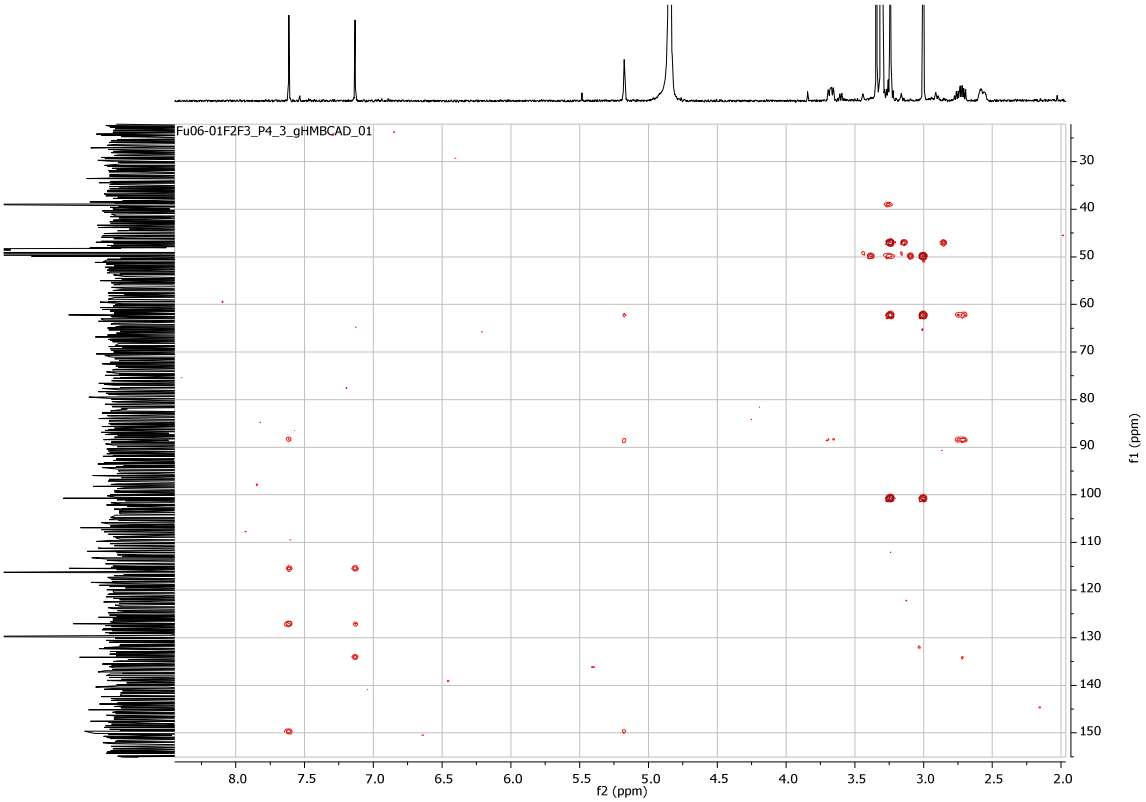
S29. ^{13}C NMR spectrum of **5** (125 MHz, MeOH-d_4).



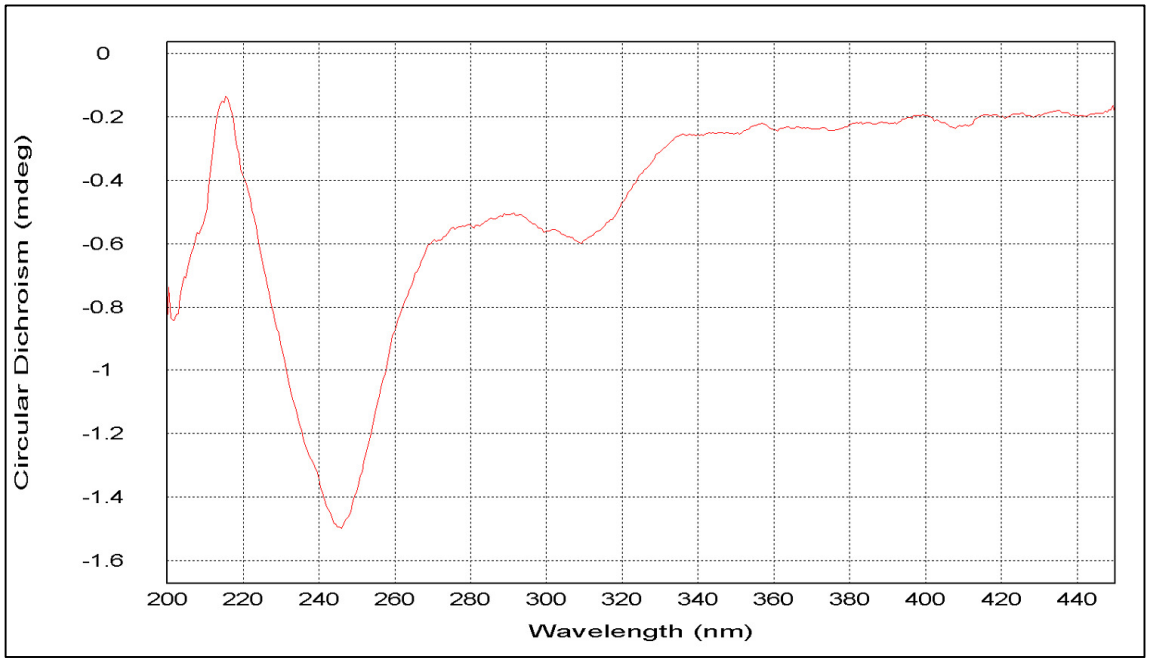
S30. COSY NMR spectrum of **5** (500 MHz, MeOH-d_4).



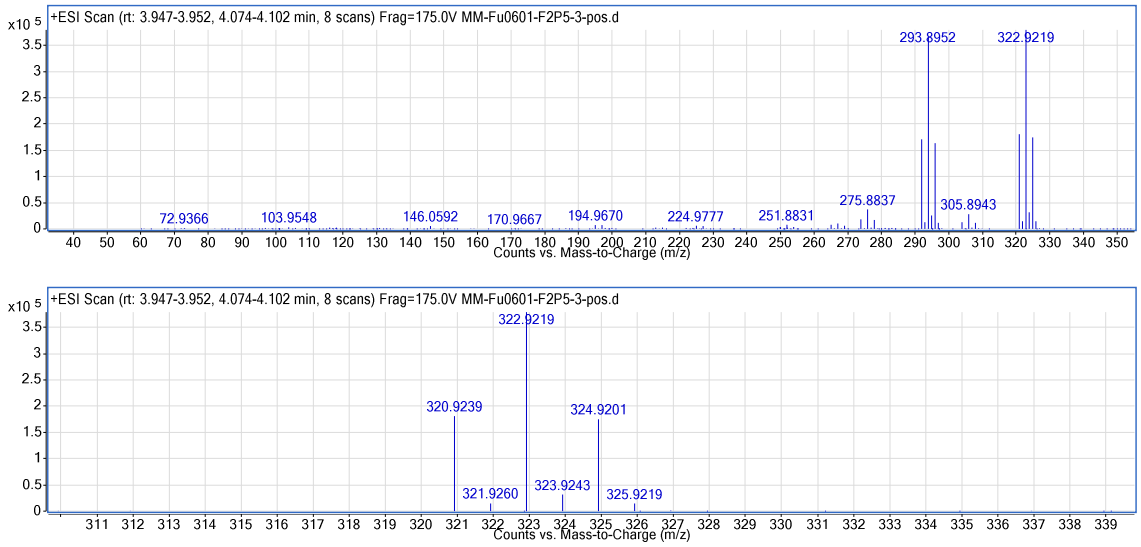
S31. HSQC NMR spectrum of **5** (500 MHz, MeOH-d_4).



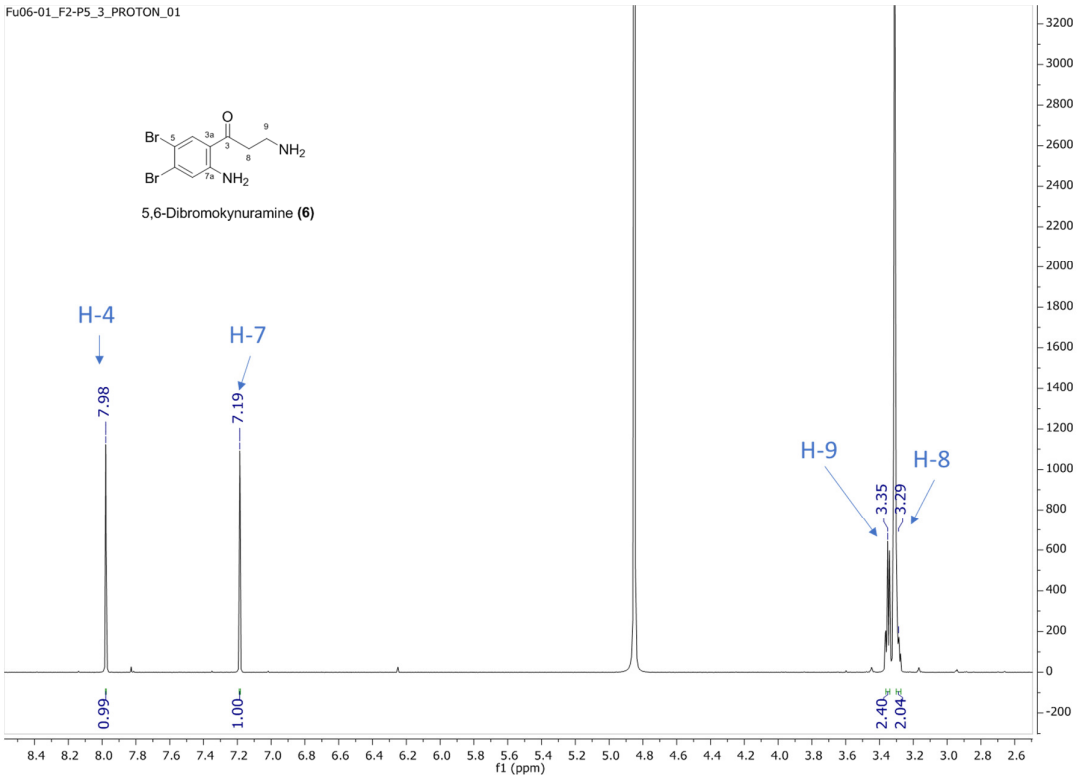
S32. HMBC NMR spectrum of **5** (500 MHz, MeOH-d_4).



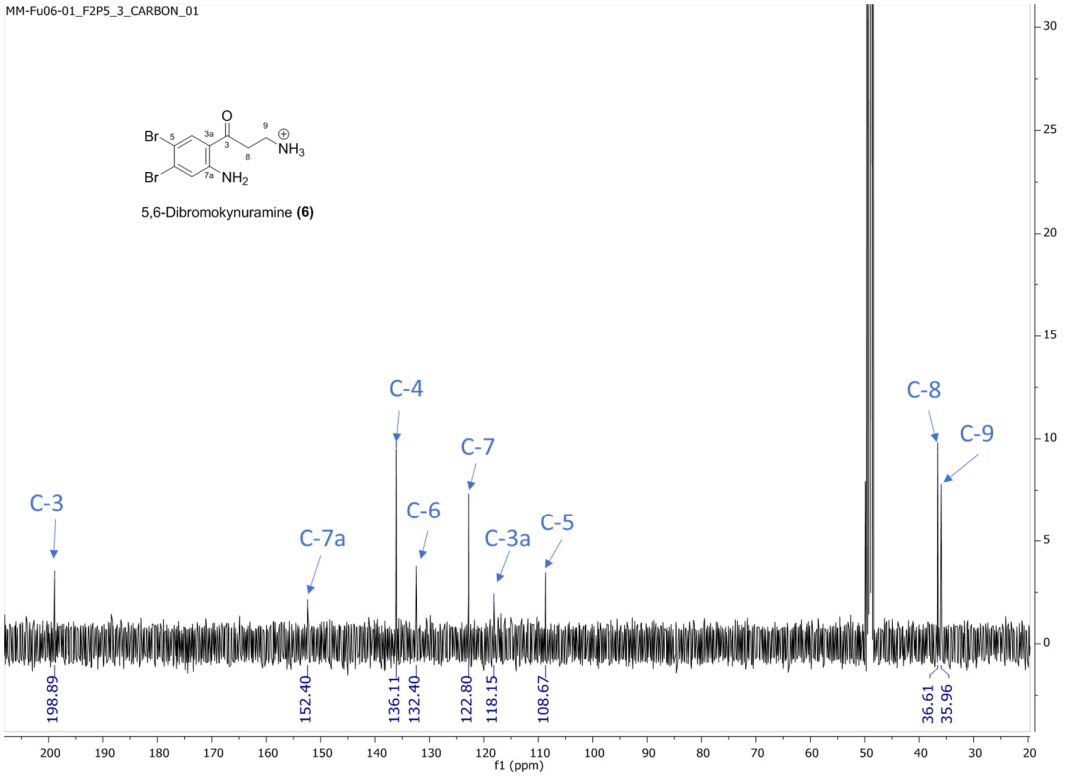
S33. ECD spectrum of compound **5** in CH_3CN at 0.2 mg/mL



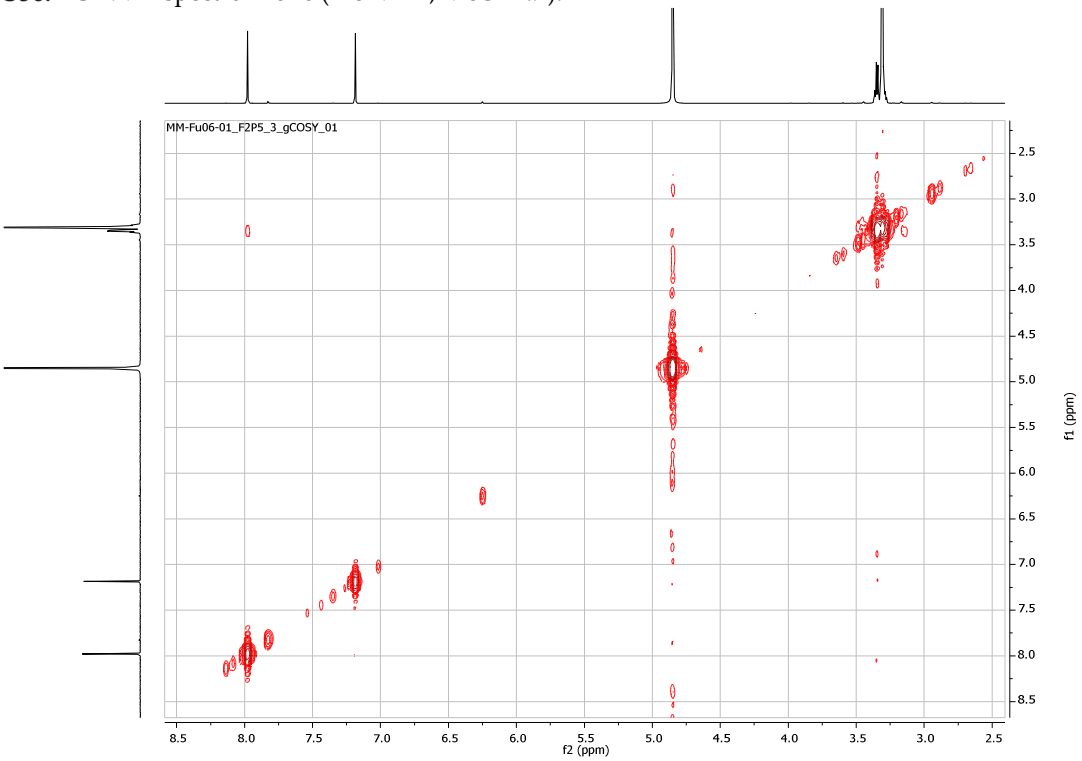
S34. ESI(+)-HRMS analysis of **6** and crop of the molecular ion.



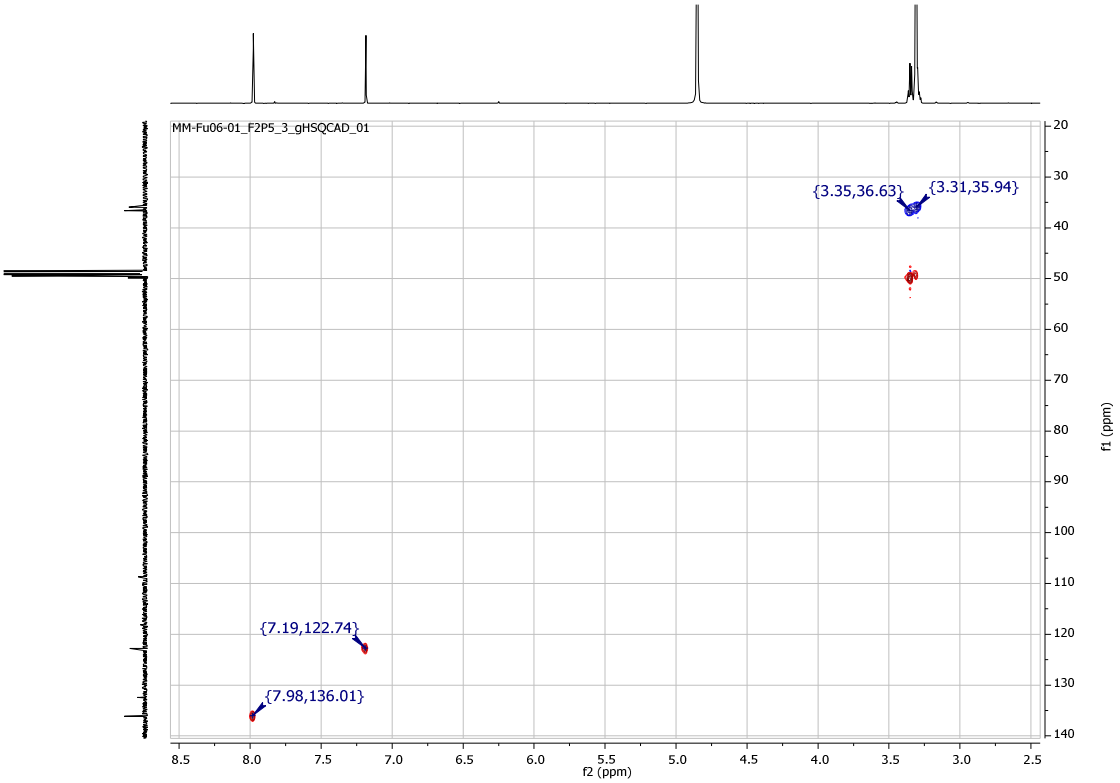
S35. ^{1}H NMR spectrum of **6** (500 MHz, MeOH-d_4).



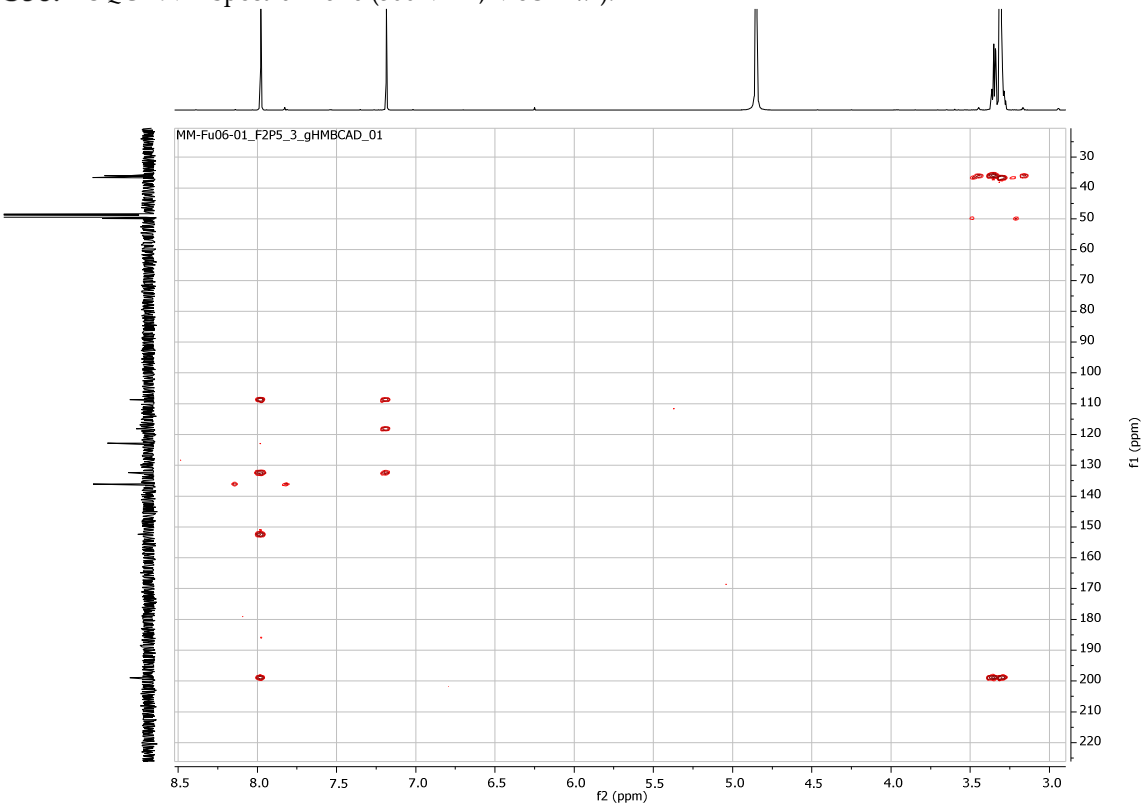
S36. ^{13}C NMR spectrum of **6** (125 MHz, MeOH-d_4).



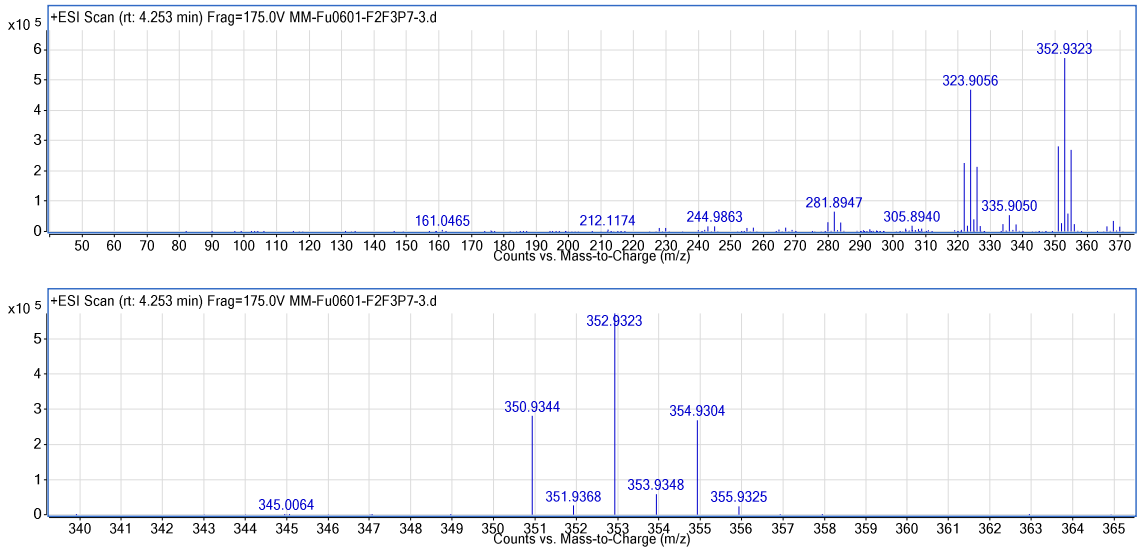
S37. COSY NMR spectrum of **6** (500 MHz, MeOH-d_4).



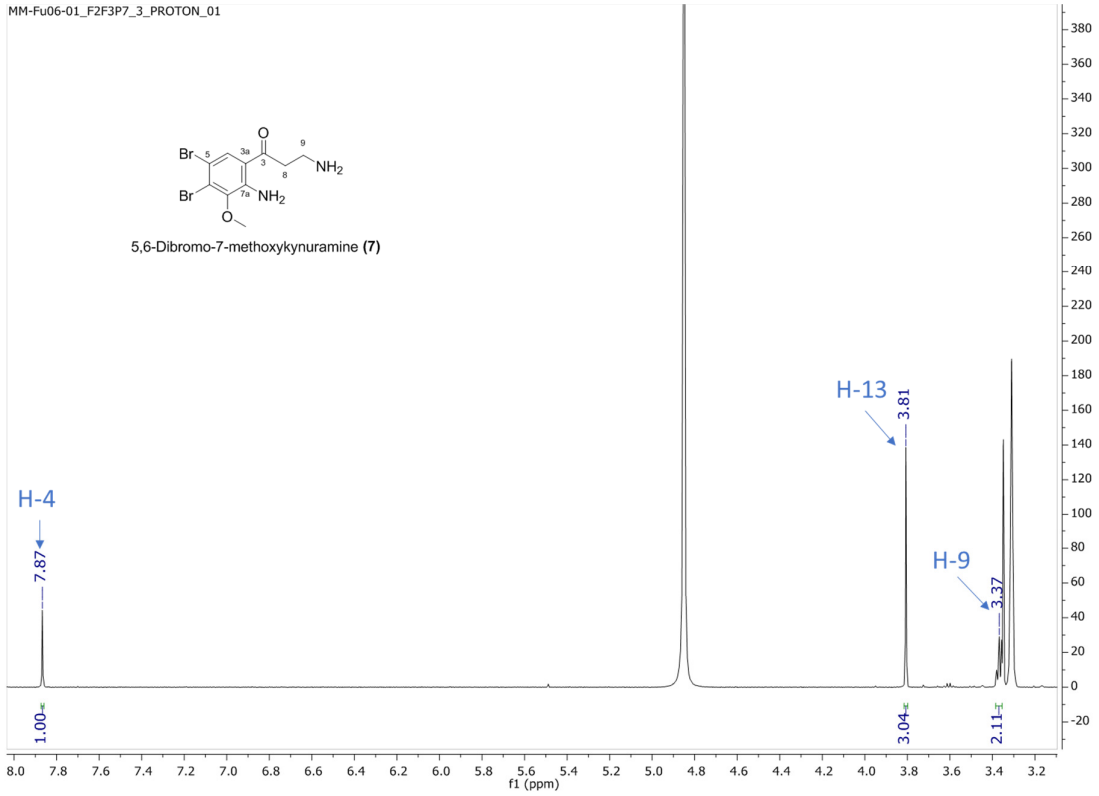
S38. HSQC NMR spectrum of **6** (500 MHz, MeOH-d_4).



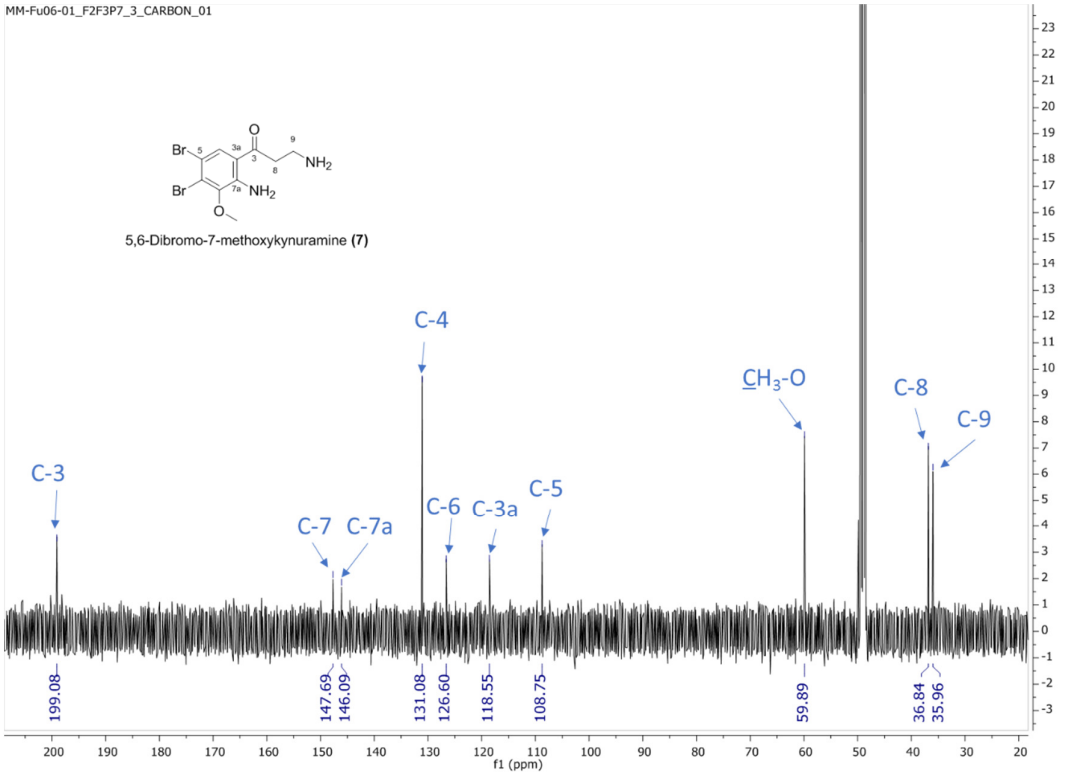
S39. HMBC NMR spectrum of **6** (500 MHz, MeOH-d_4).



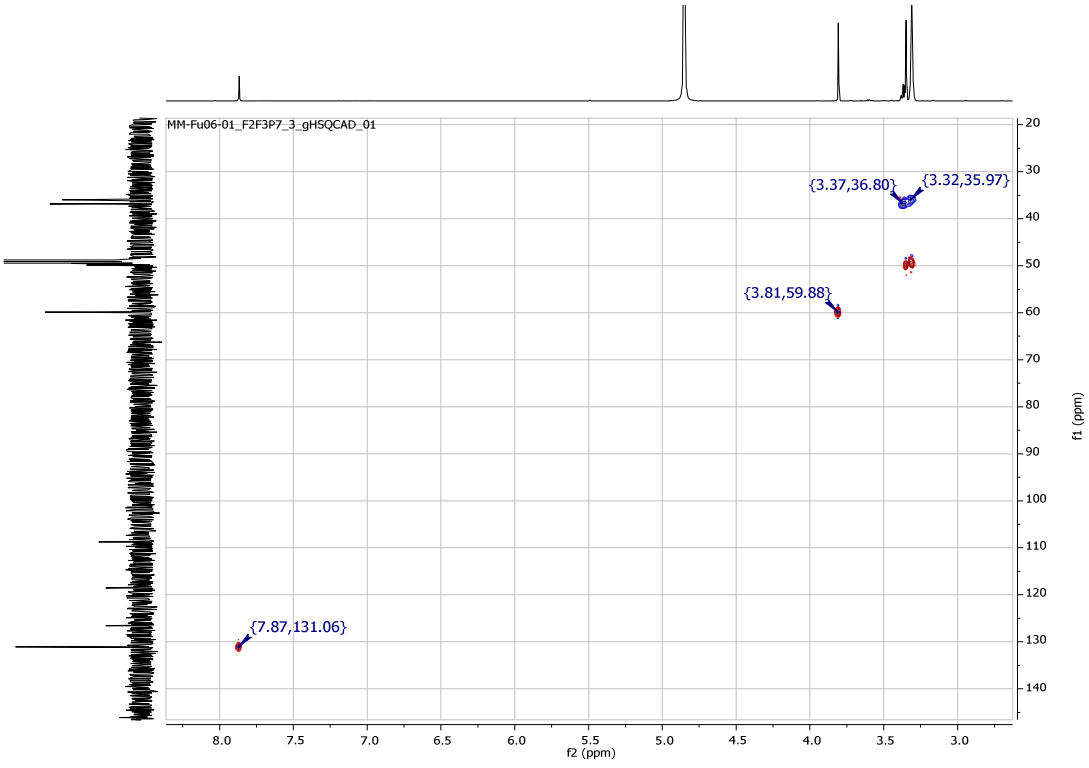
S40. ESI(+)-HRMS analysis of **7** and crop of the molecular ion.



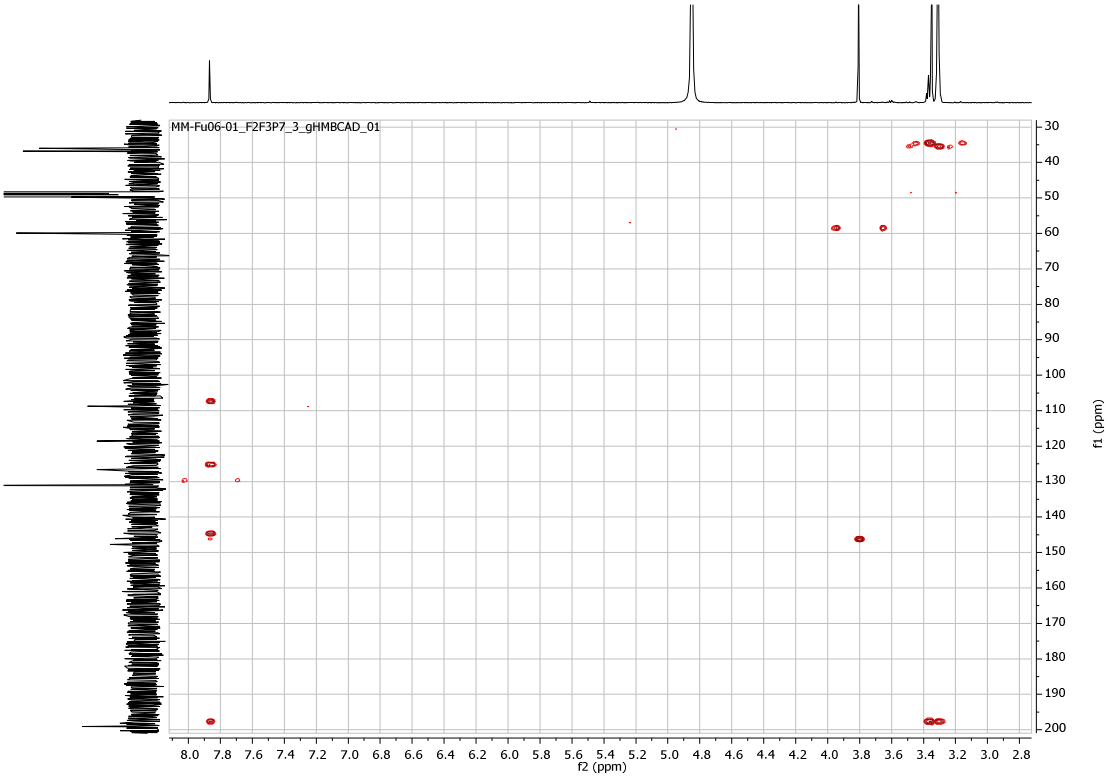
S41. ^{1}H NMR spectrum of **7** (500 MHz, MeOH-d_4).



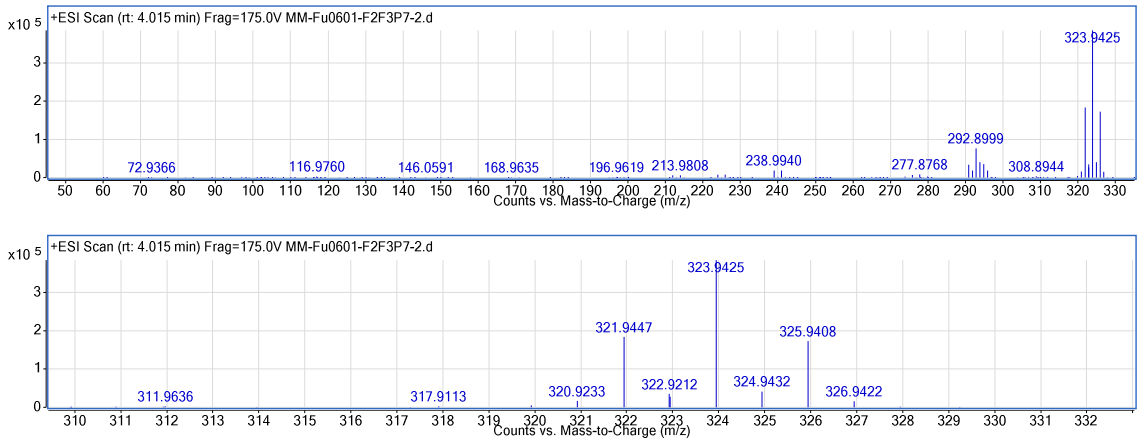
S42. ^{13}C NMR spectrum of **7** (125 MHz, MeOH-d_4).



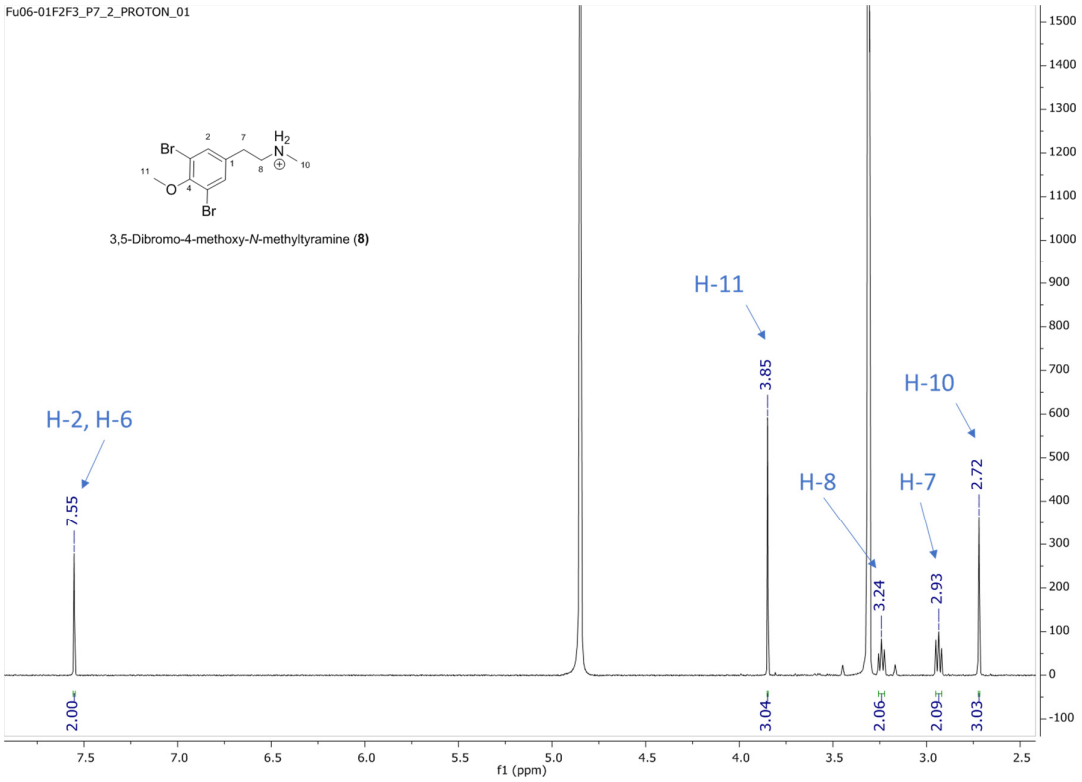
S43. HSQC NMR spectrum of **7** (500 MHz, MeOH-d_4).



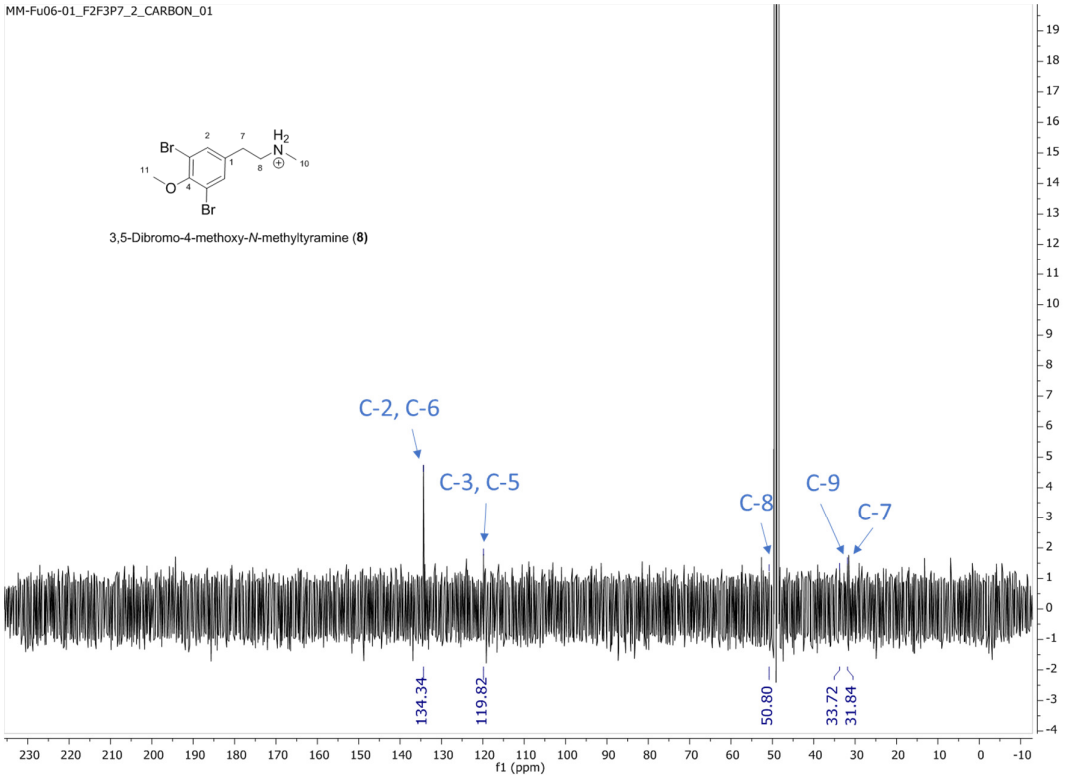
S44. HMBC NMR spectrum of **7** (500 MHz, MeOH-d_4).



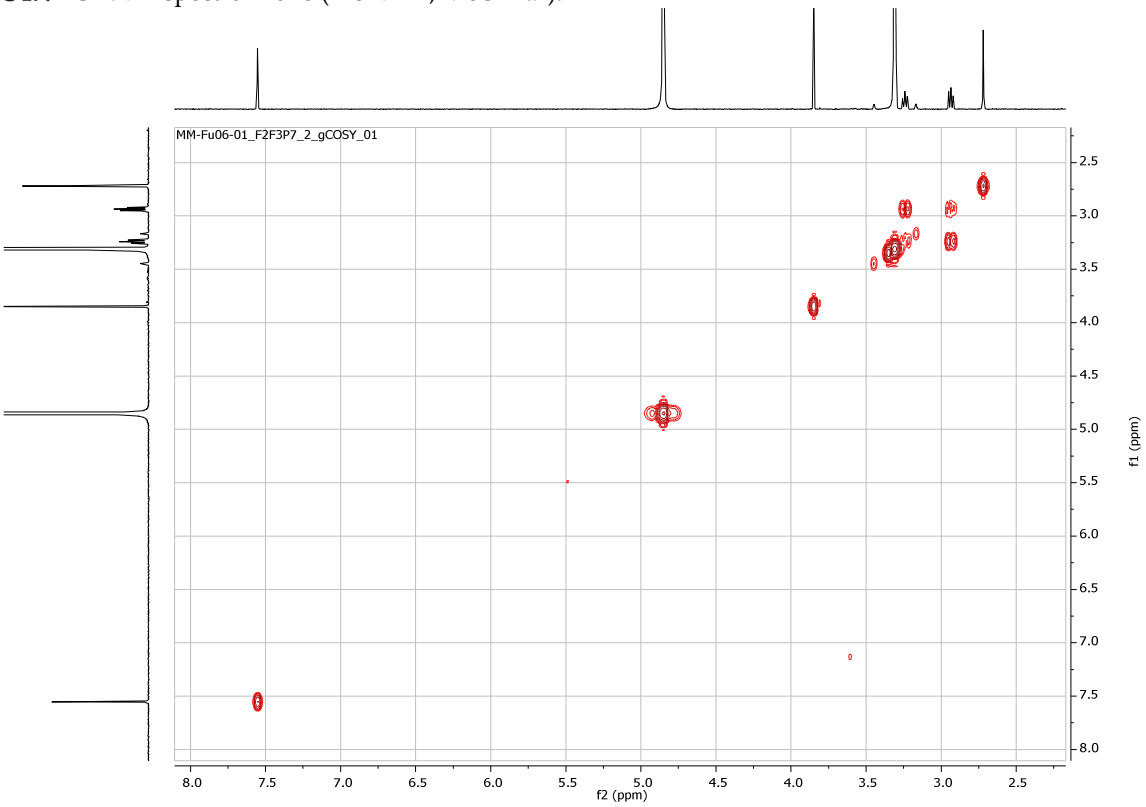
S45. ESI(+)-HRMS analysis of **8** and crop of the molecular ion.



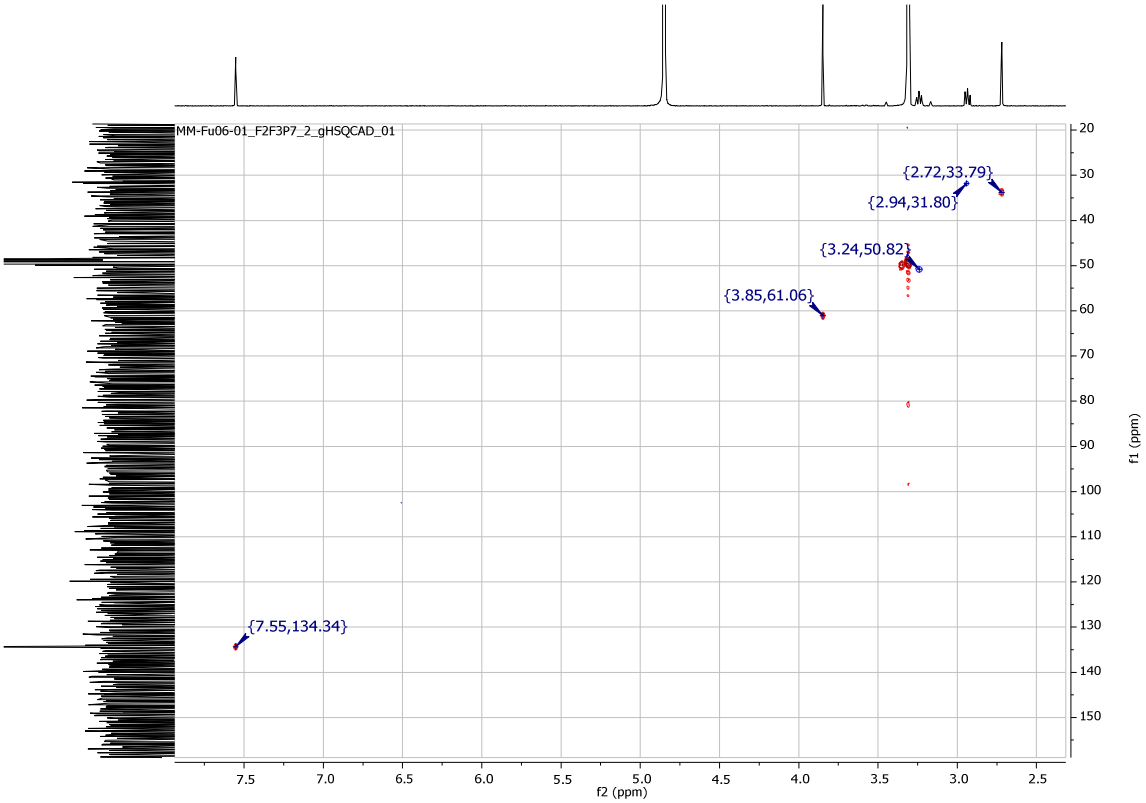
S46. ^{1}H NMR spectrum of **8** (500 MHz, MeOH-d_4).



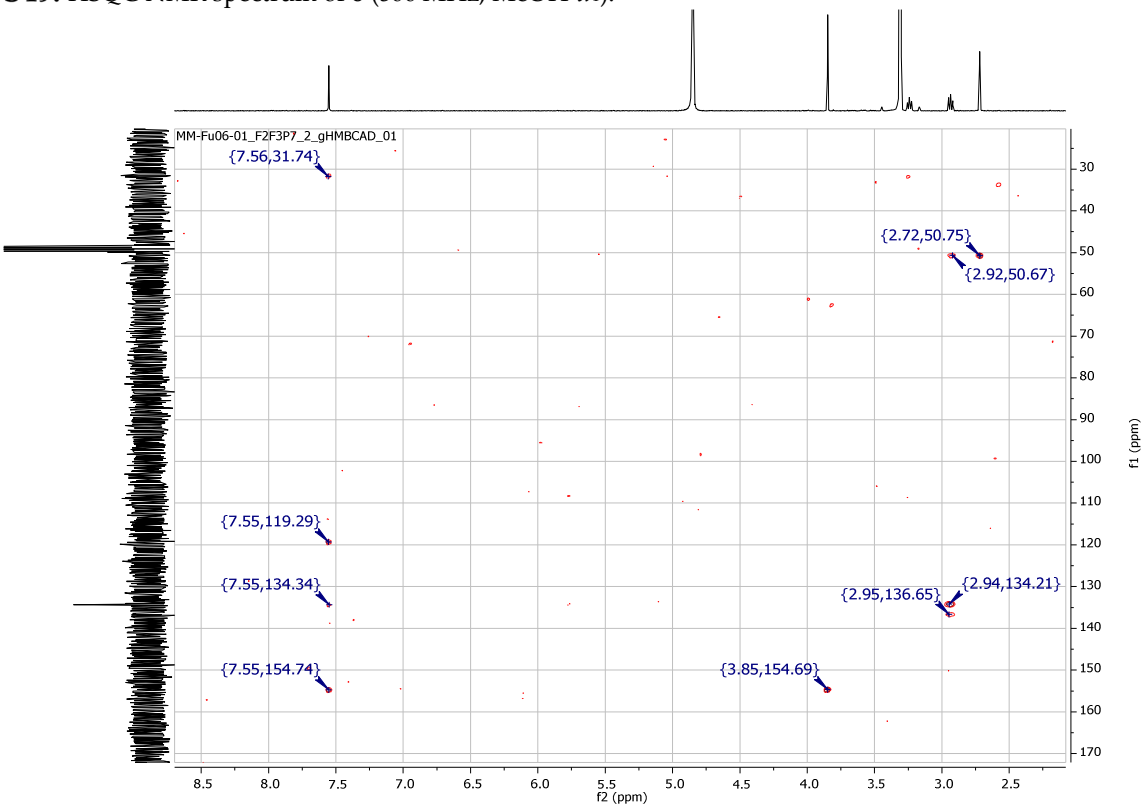
S47. ^{13}C NMR spectrum of **8** (125 MHz, MeOH-d_4).



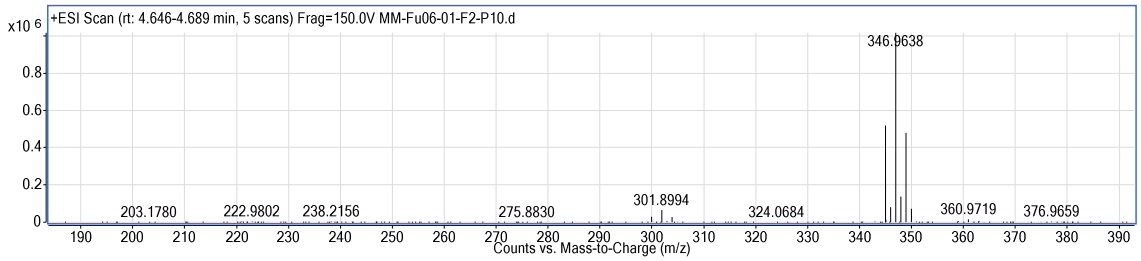
S48. COSY NMR spectrum of **8** (500 MHz, MeOH-d_4).



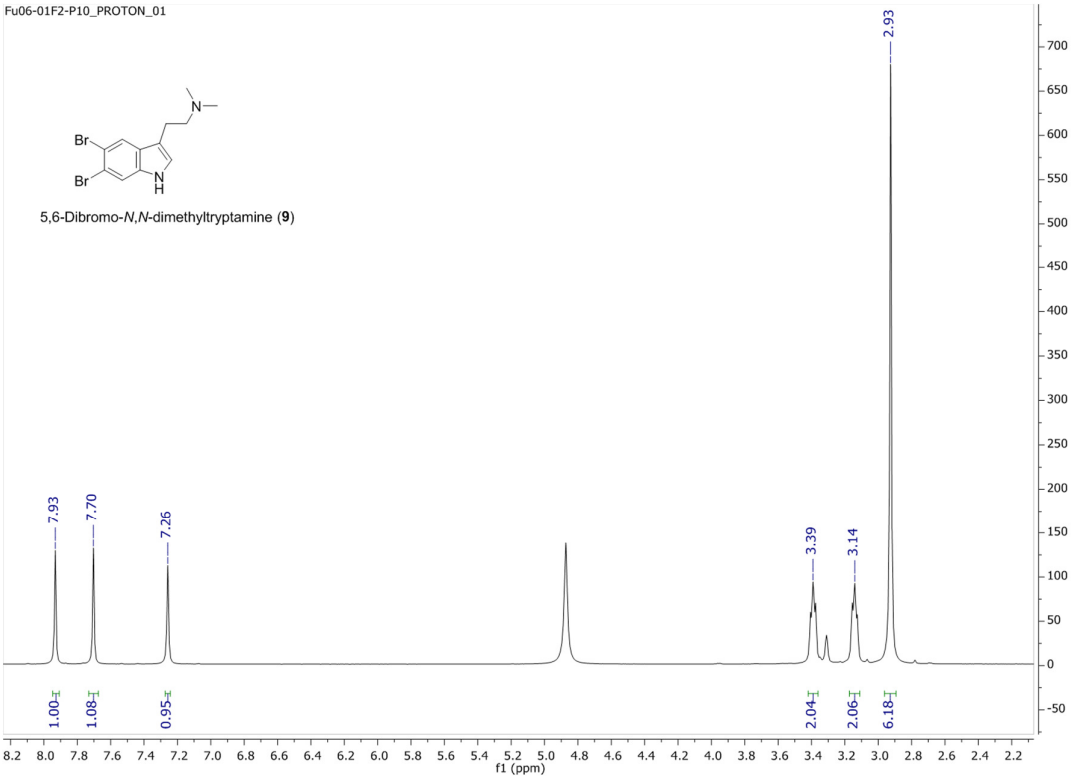
S49. HSQC NMR spectrum of **8** (500 MHz, MeOH-d_4).



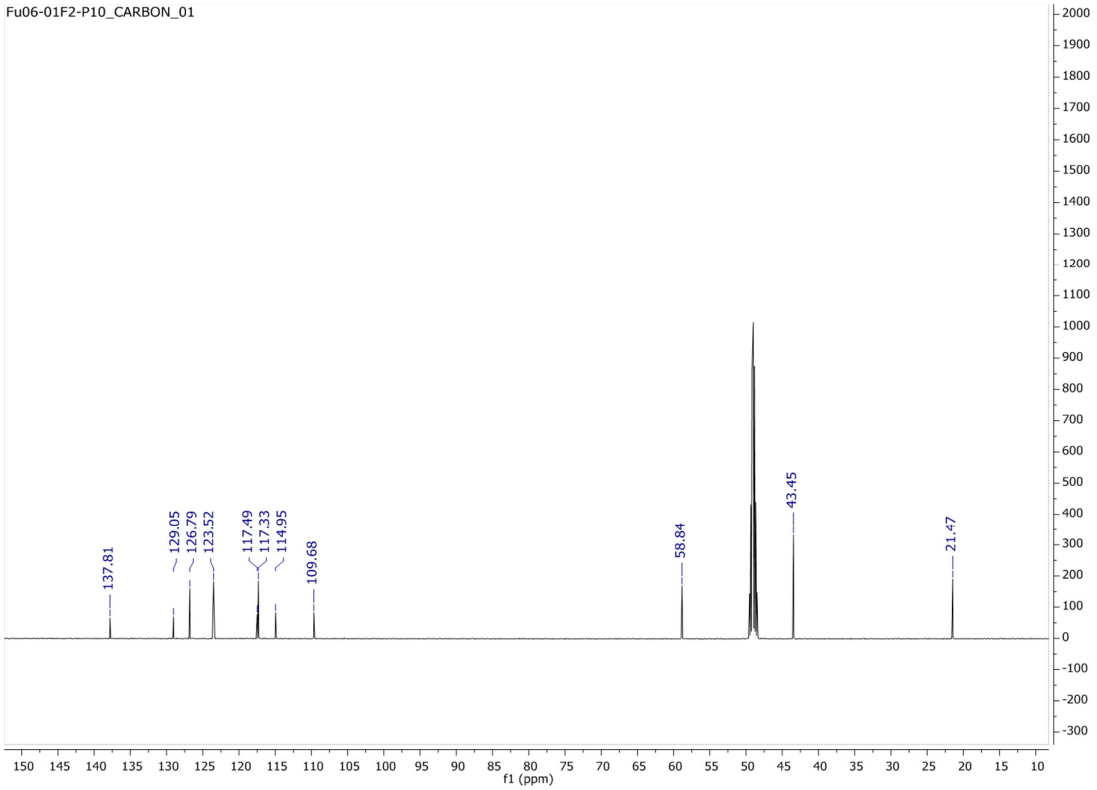
S50. HMBC NMR spectrum of **8** (500 MHz, MeOH-d_4).



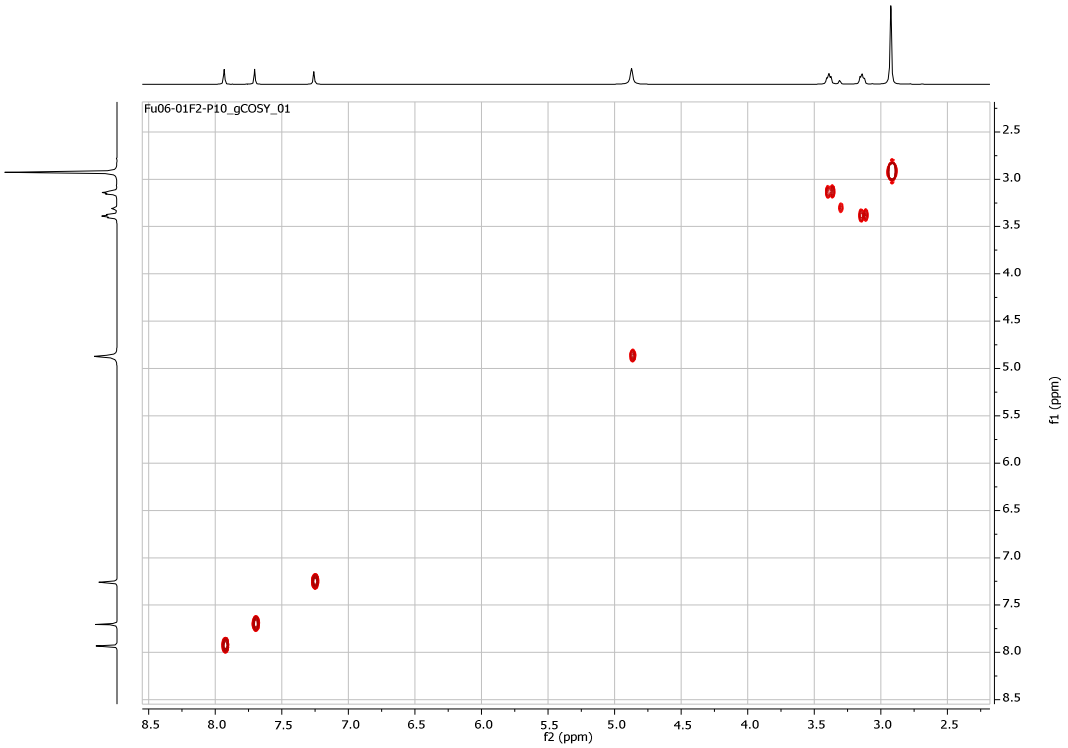
S51. ESI(+)-HRMS analysis of **9**



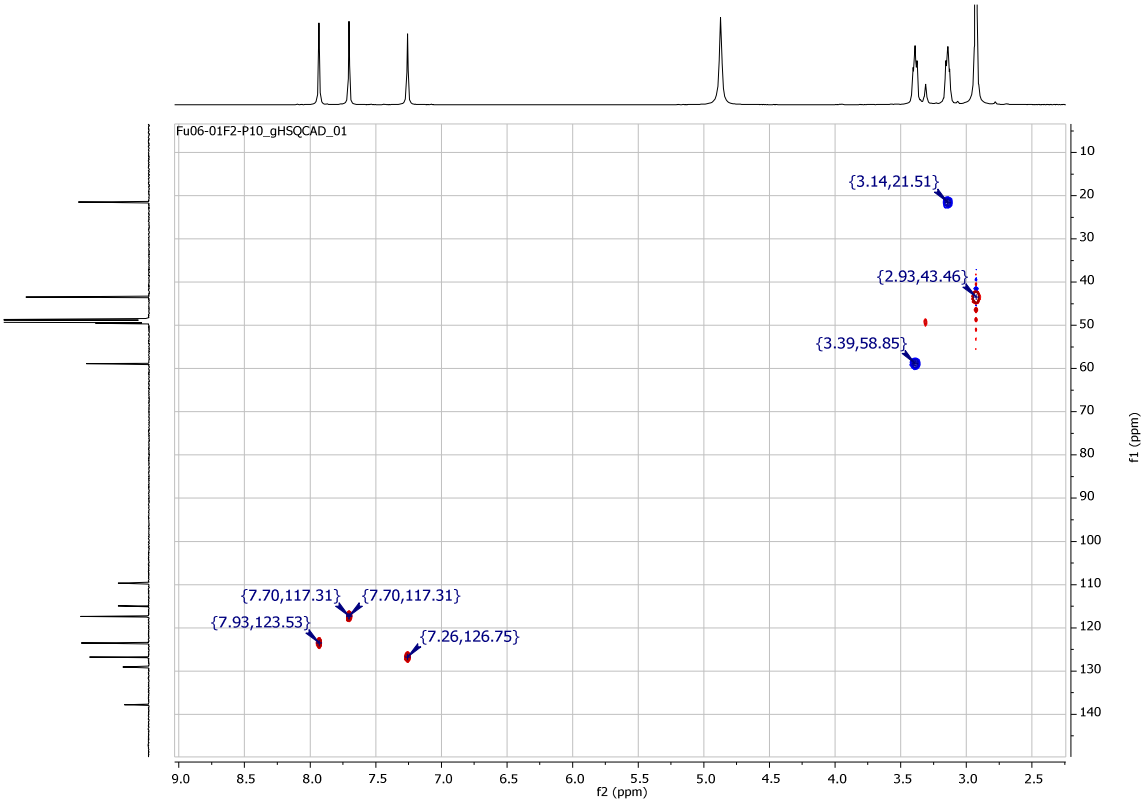
S52. ^{1}H NMR spectrum of **9** (500 MHz, MeOH-d_4).



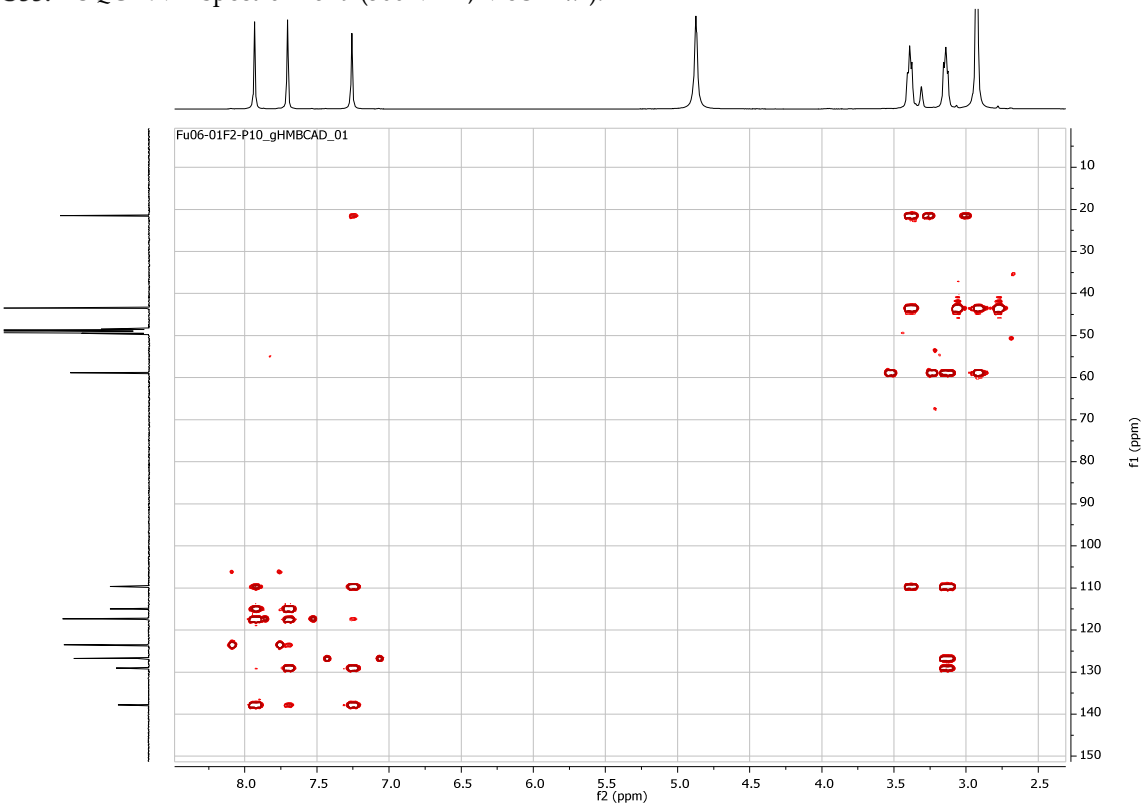
S53. ^{13}C NMR spectrum of **9** (125 MHz, MeOH-d_4).



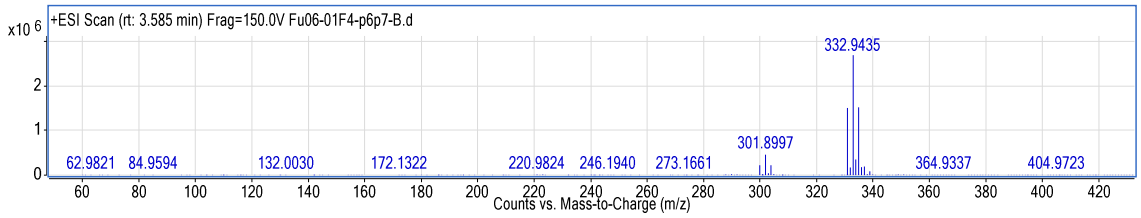
S54. COSY NMR spectrum of **9** (500 MHz, MeOH-d_4).



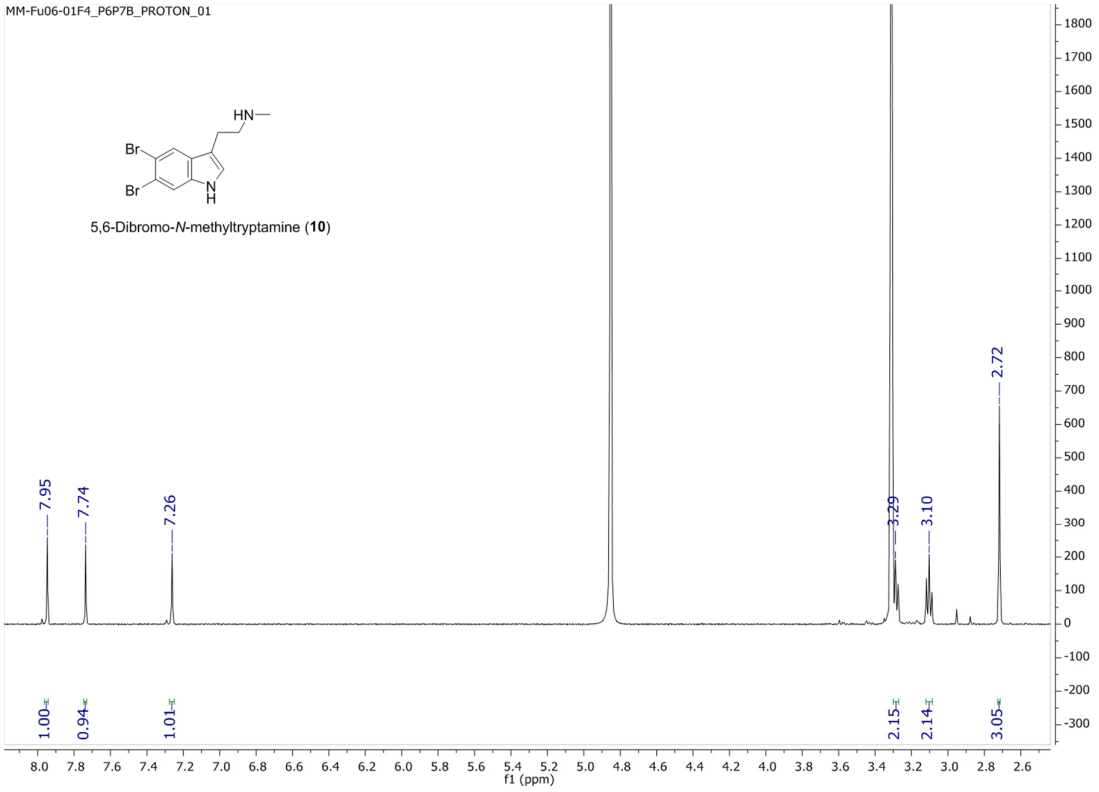
S55. HSQC NMR spectrum of **9** (500 MHz, MeOH-d_4).



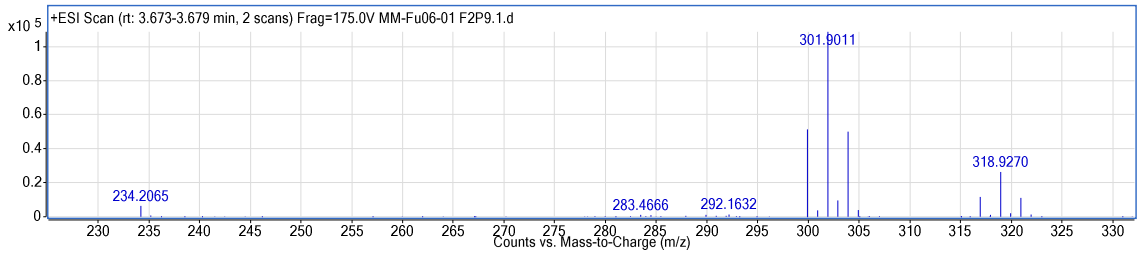
S56. HSQC NMR spectrum of **9** (500 MHz, MeOH-d_4).



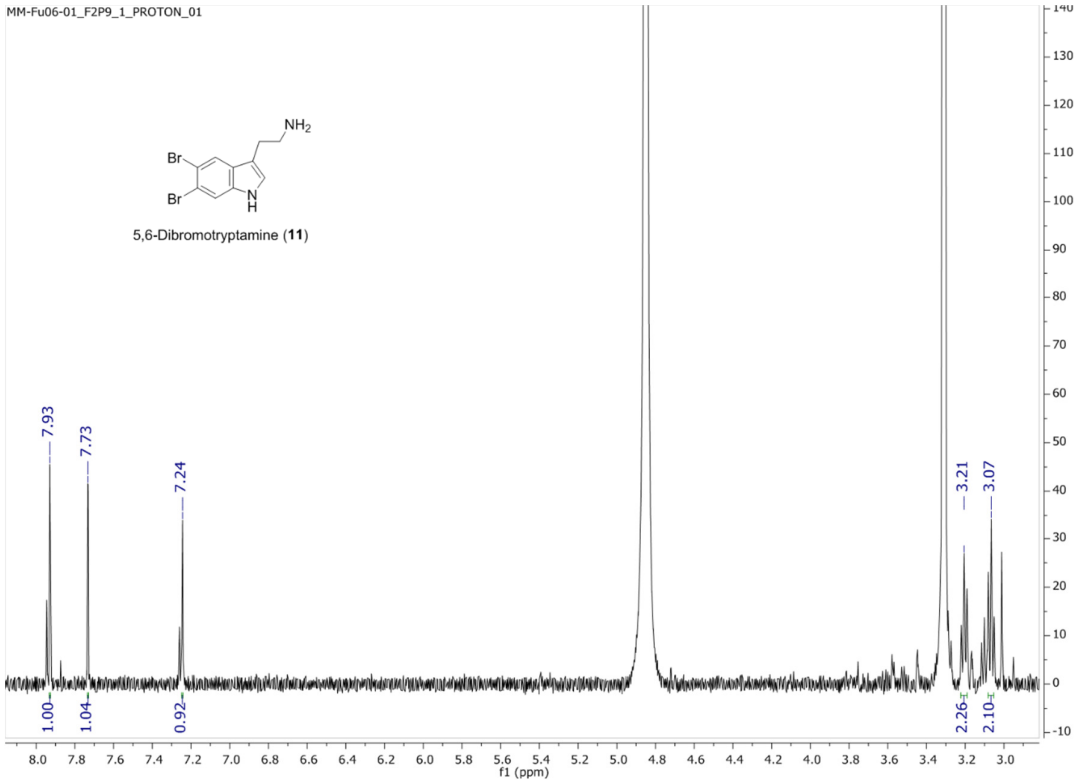
S57. ESI(+)-HRMS analysis of **10**



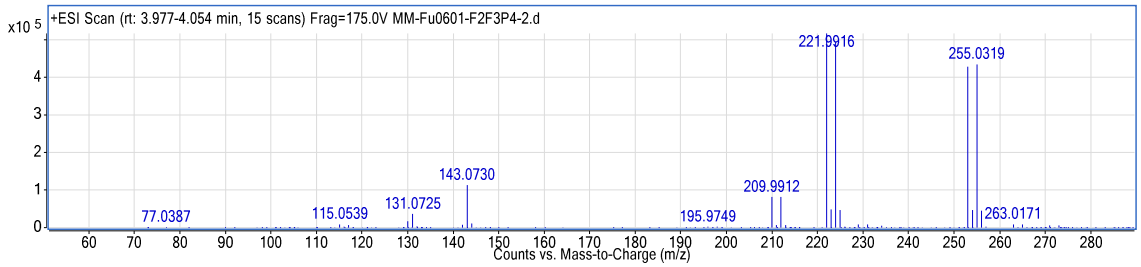
S58. ^{1}H NMR spectrum of **10** (500 MHz, MeOH-d_4).



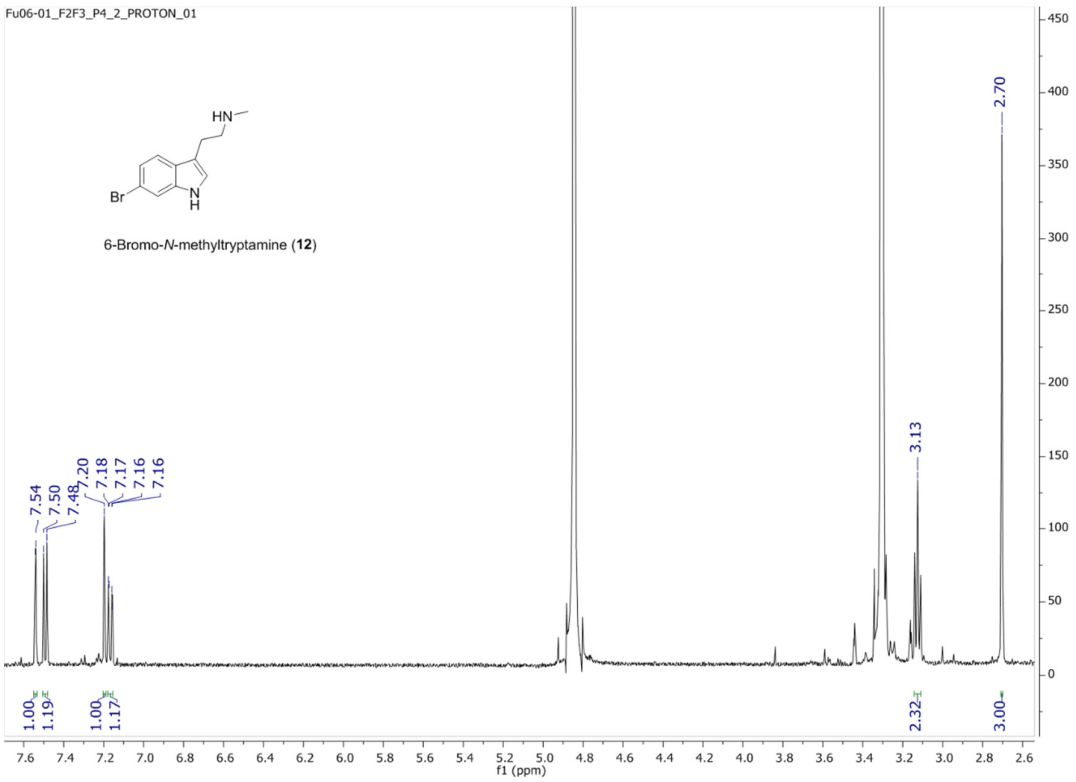
S59. ESI(+)-HRMS analysis of **11**



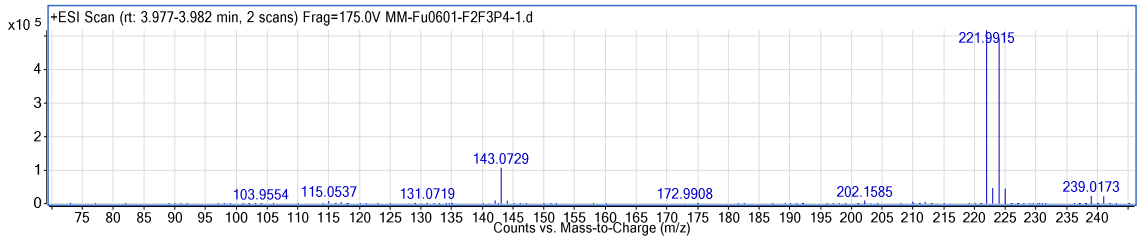
S60. ^{1}H NMR spectrum of **11** (500 MHz, MeOH-d_4).



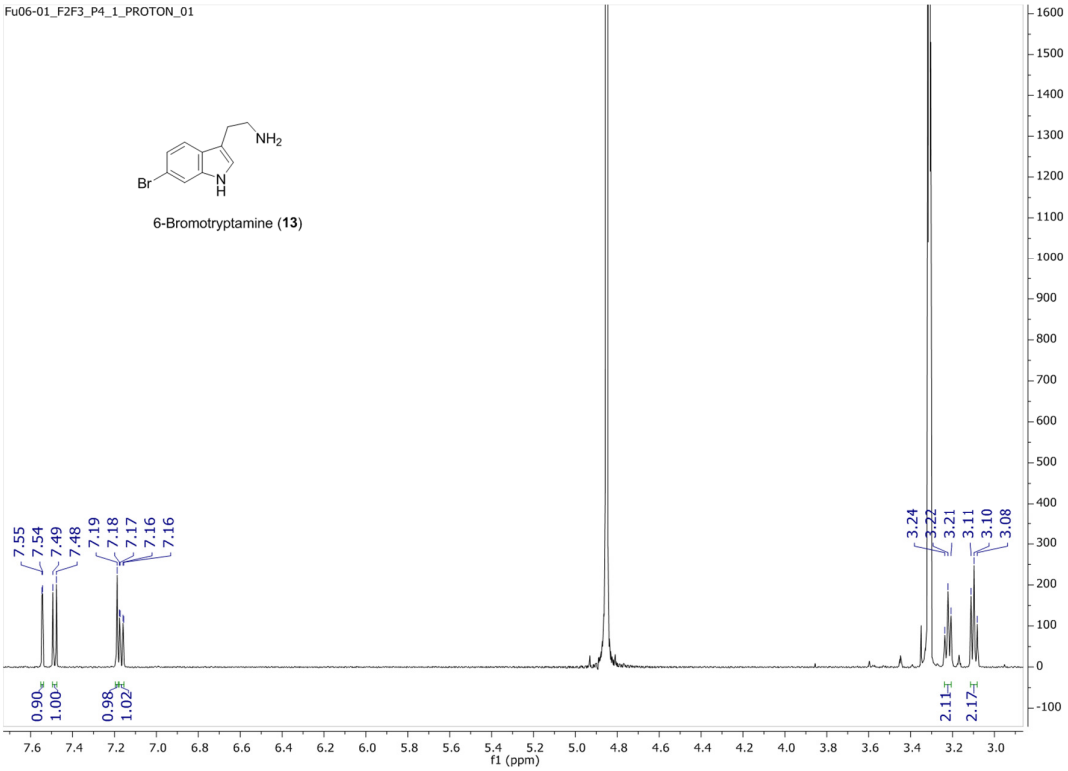
S61. ESI(+)-HRMS analysis of **12**



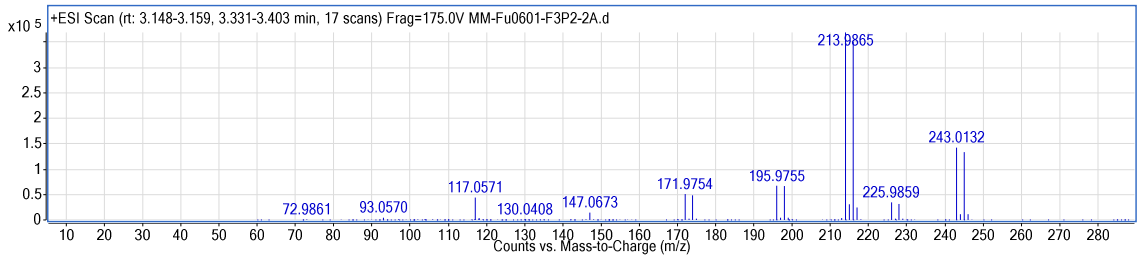
S62. ^{1}H NMR spectrum of **12** (500 MHz, MeOH-d_4).



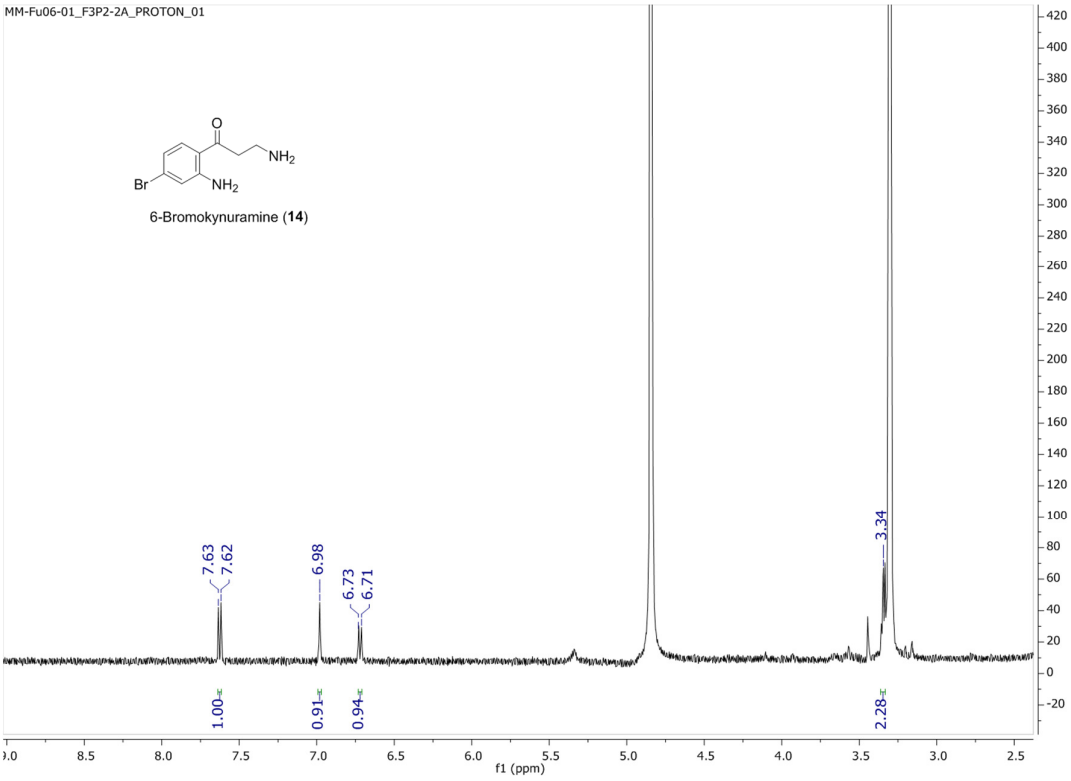
S63. ESI(+)-HRMS analysis of **13**



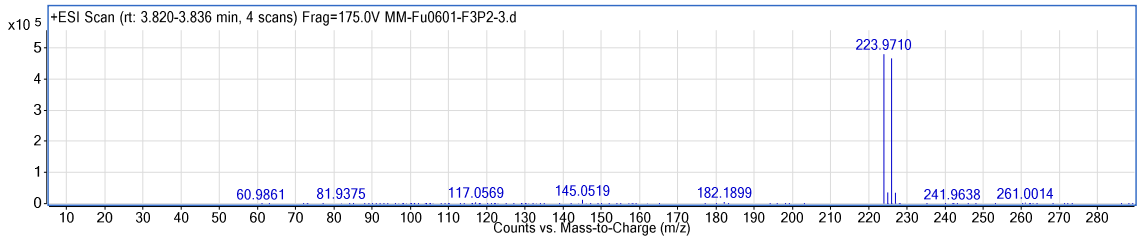
S64. ^{1}H NMR spectrum of **13** (500 MHz, MeOH-d_4).



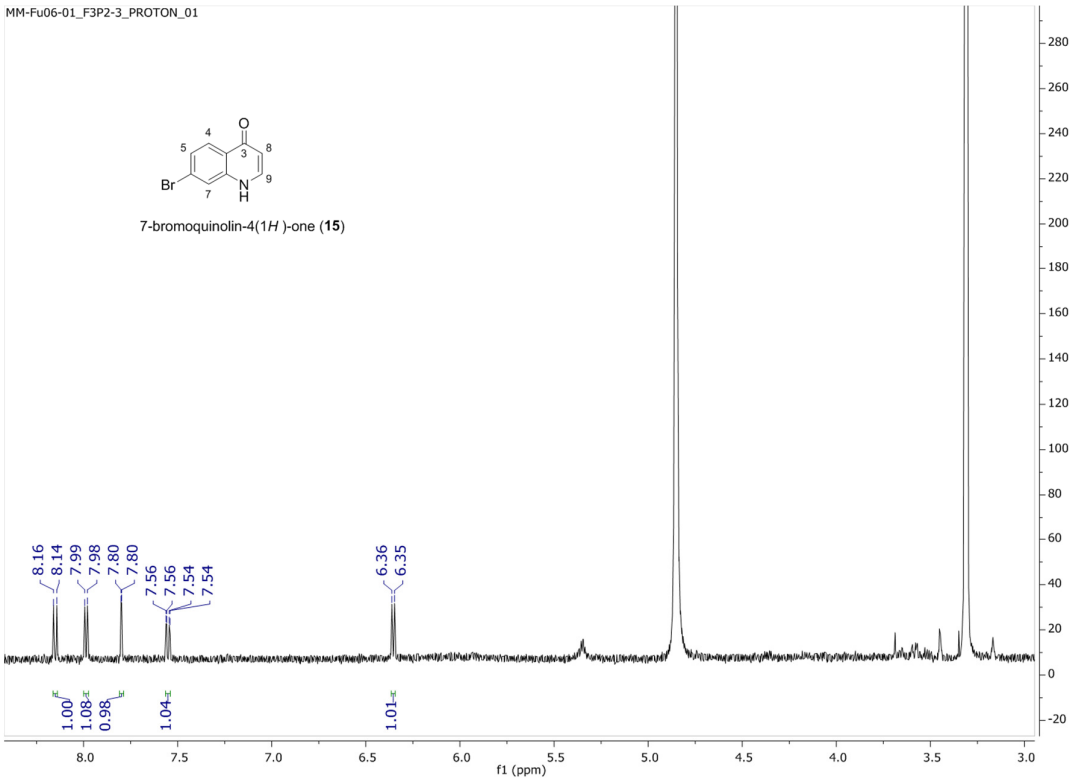
S65. ESI(+)-HRMS analysis of **14**



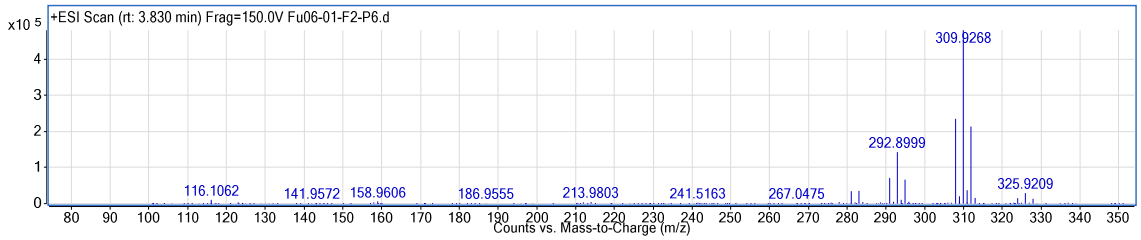
S66. ^{1}H NMR spectrum of **14** (500 MHz, MeOH-d_4).



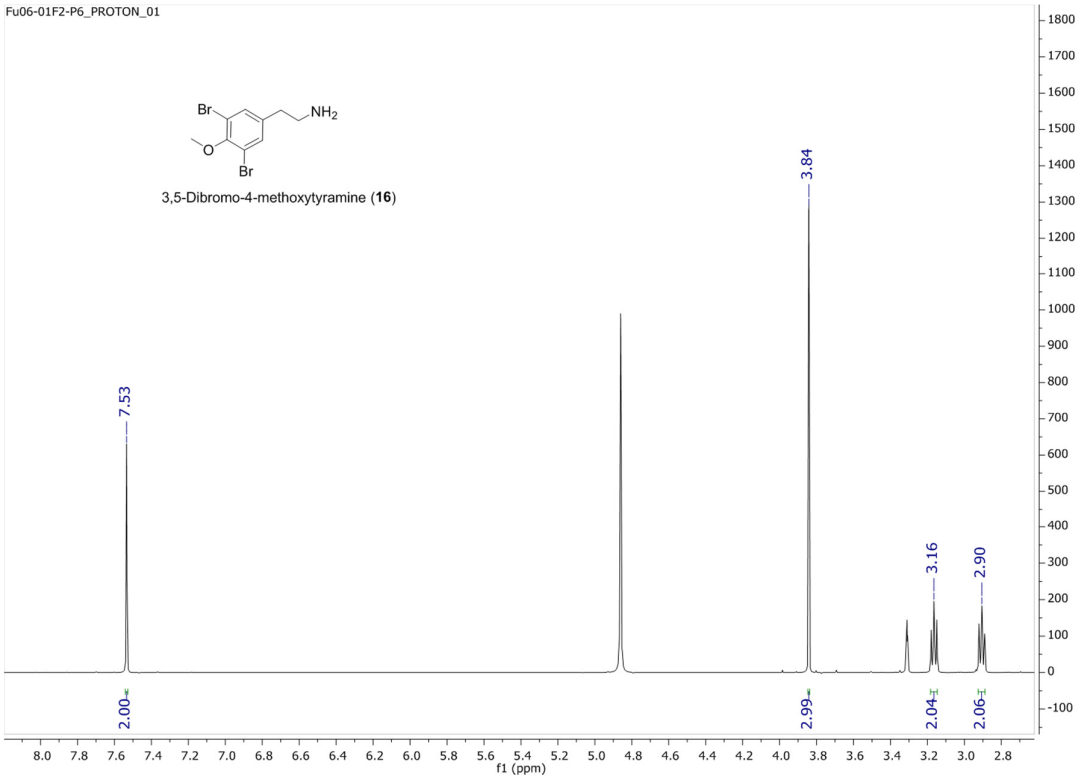
S67. ESI(+)-HRMS analysis of **15**



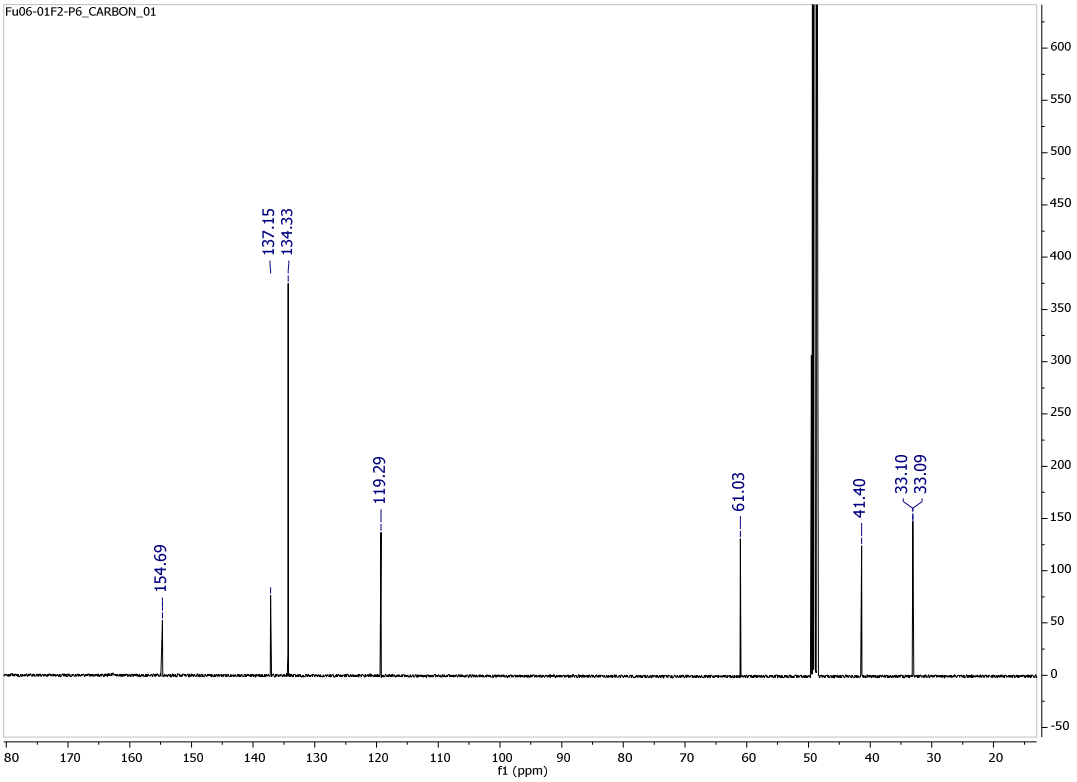
S68. ^{1}H NMR spectrum of **15** (500 MHz, MeOH-d_4).



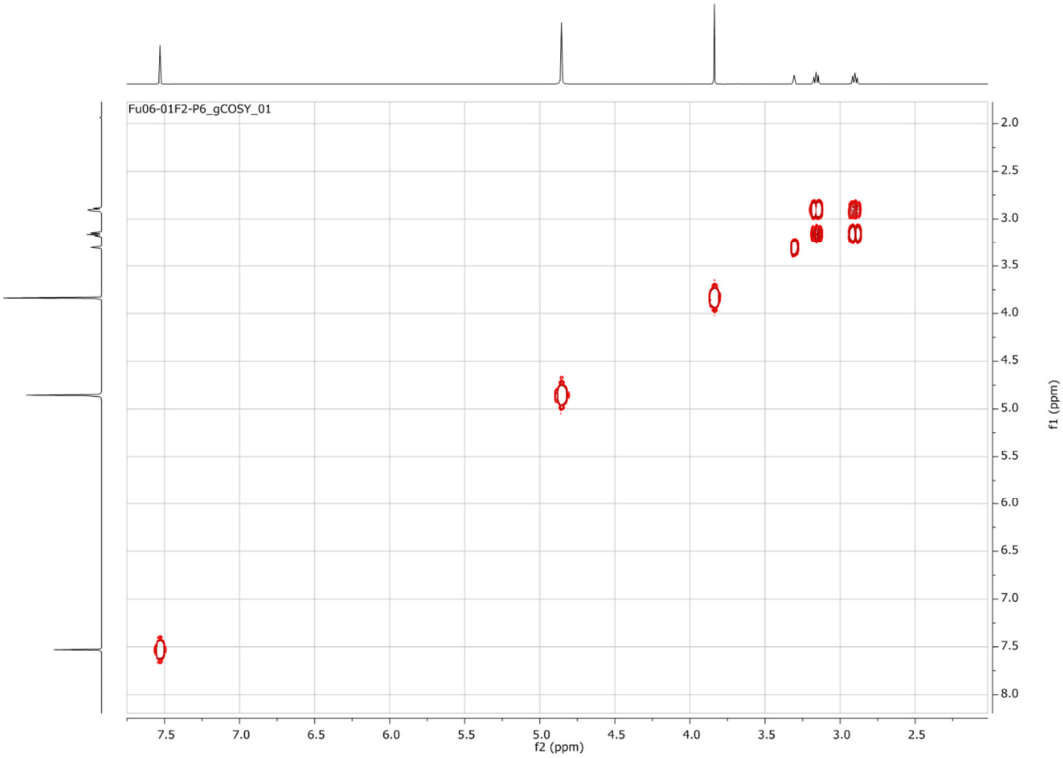
S69. ESI(+)-HRMS analysis of **16**



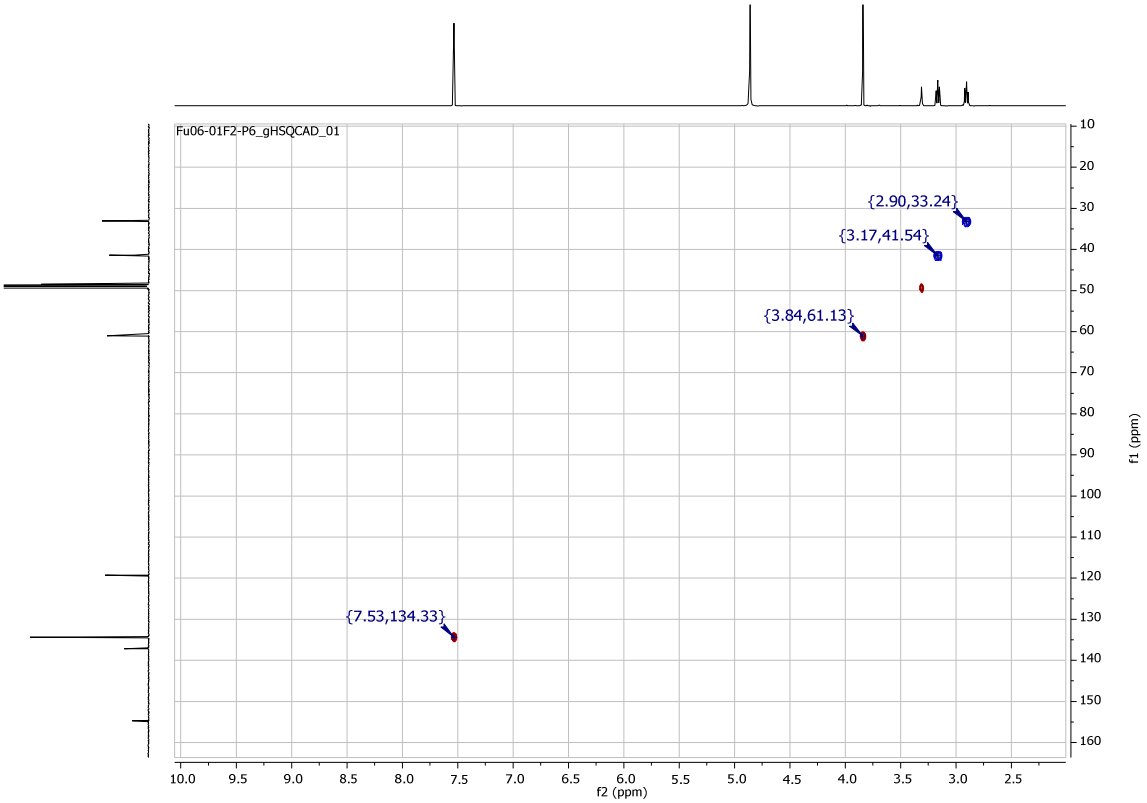
S70. ^{1}H NMR spectrum of **16** (500 MHz, MeOH-d_4).



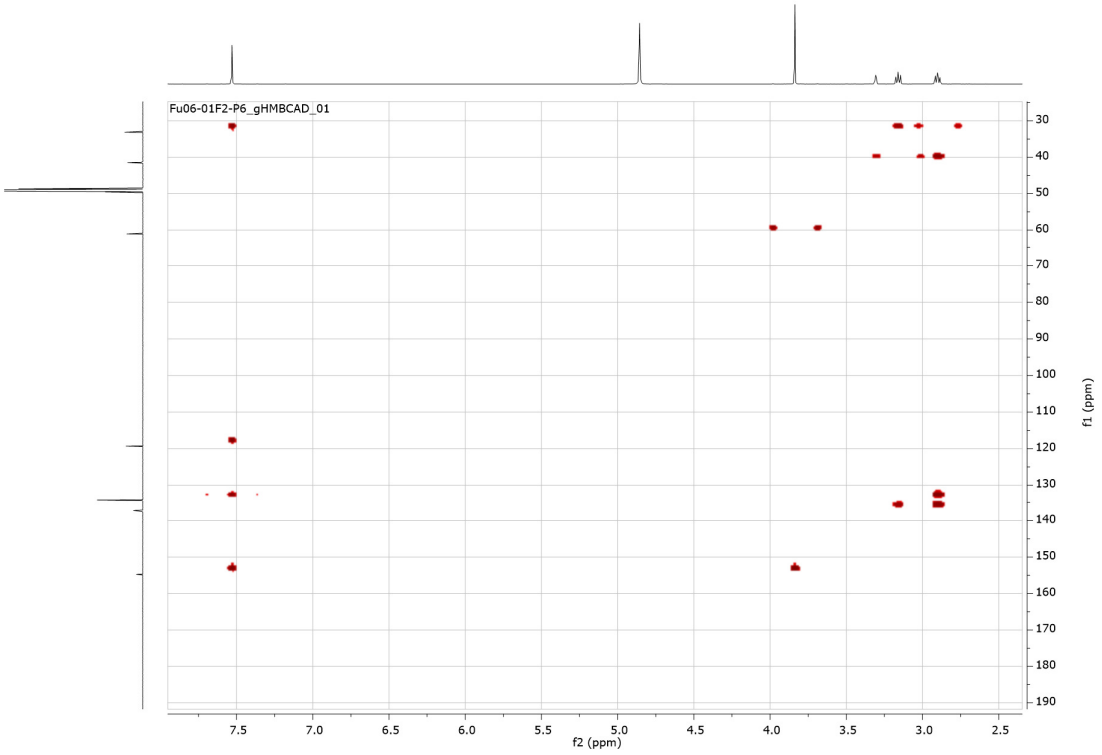
S71. ^{13}C NMR spectrum of **16** (125 MHz, MeOH-d_4).



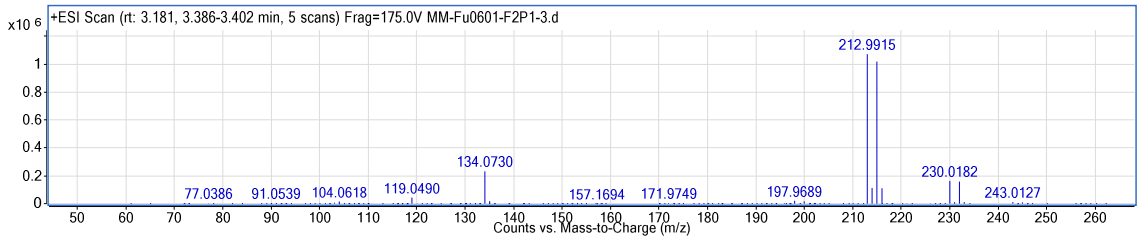
S72. COSY NMR spectrum of **16** (500 MHz, MeOH-d_4).



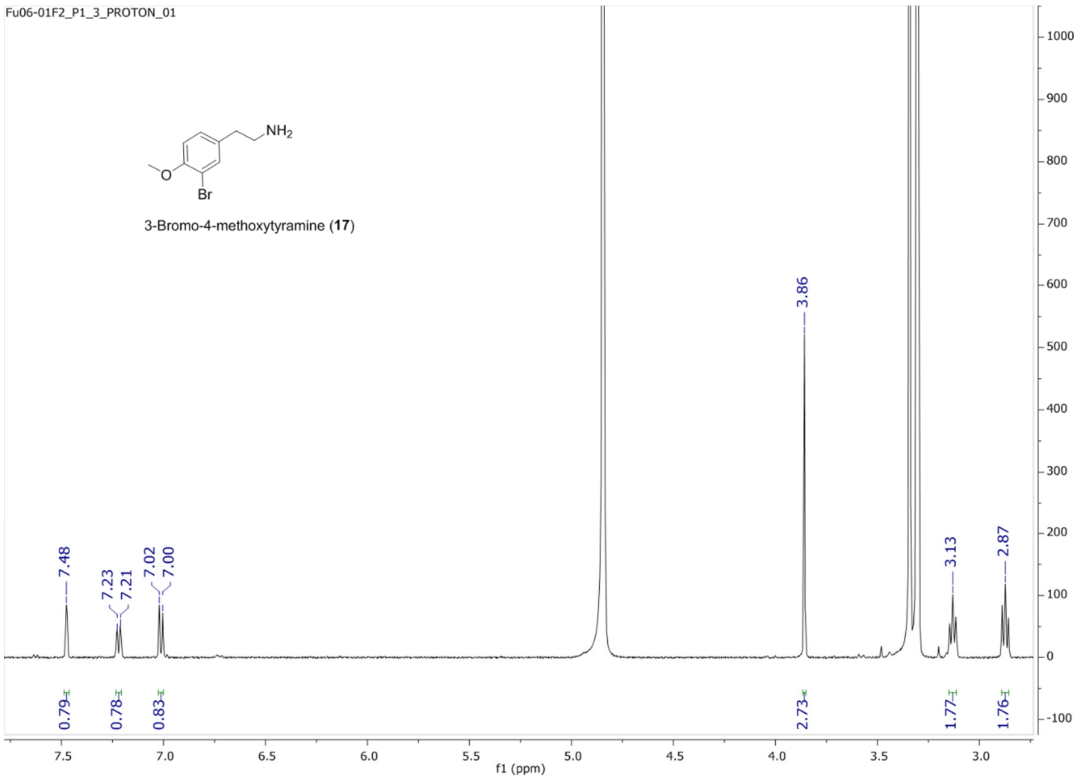
S73. HSQC NMR spectrum of **16** (500 MHz, MeOH-d_4).



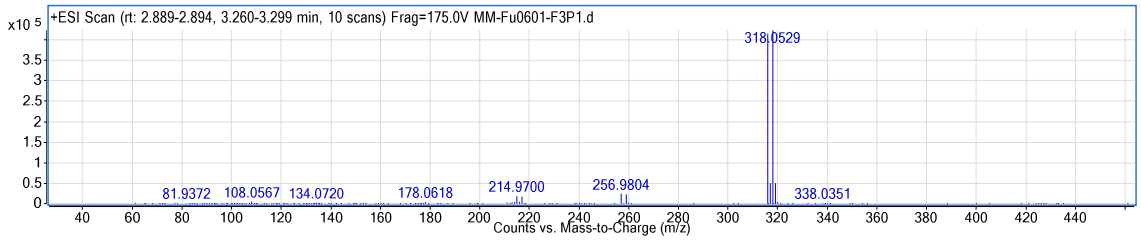
S74. HMBC NMR spectrum of **16** (500 MHz, MeOH-d_4).



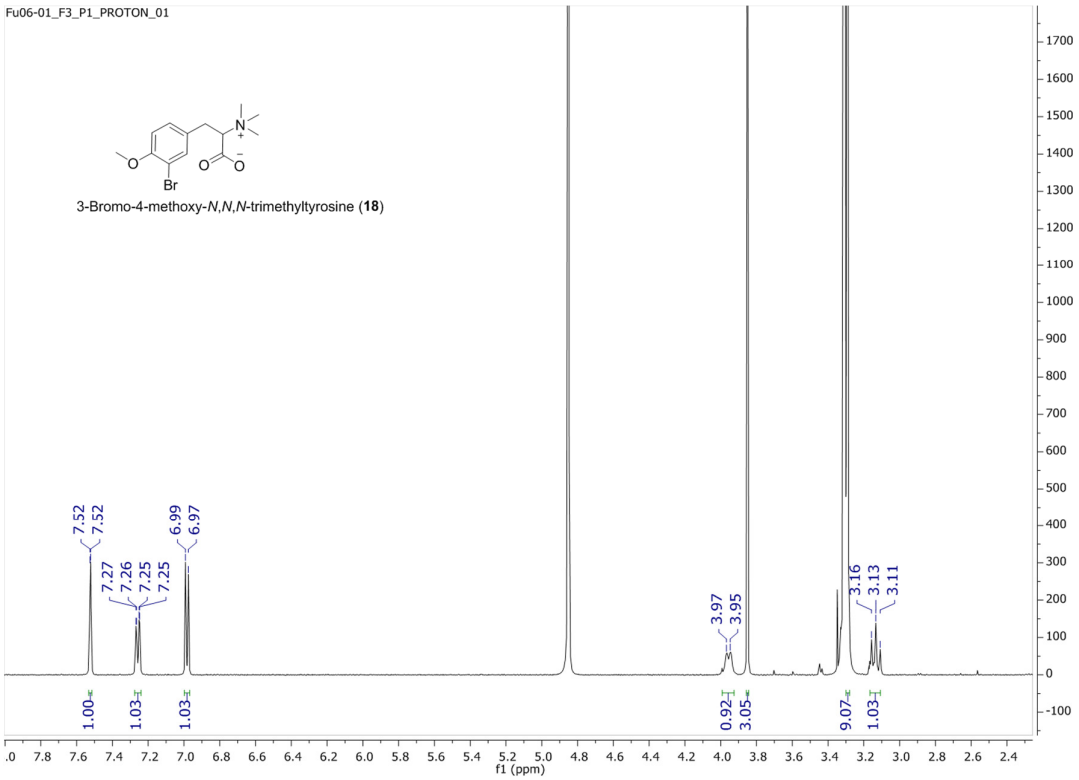
S75. ESI(+)-HRMS analysis of **17**



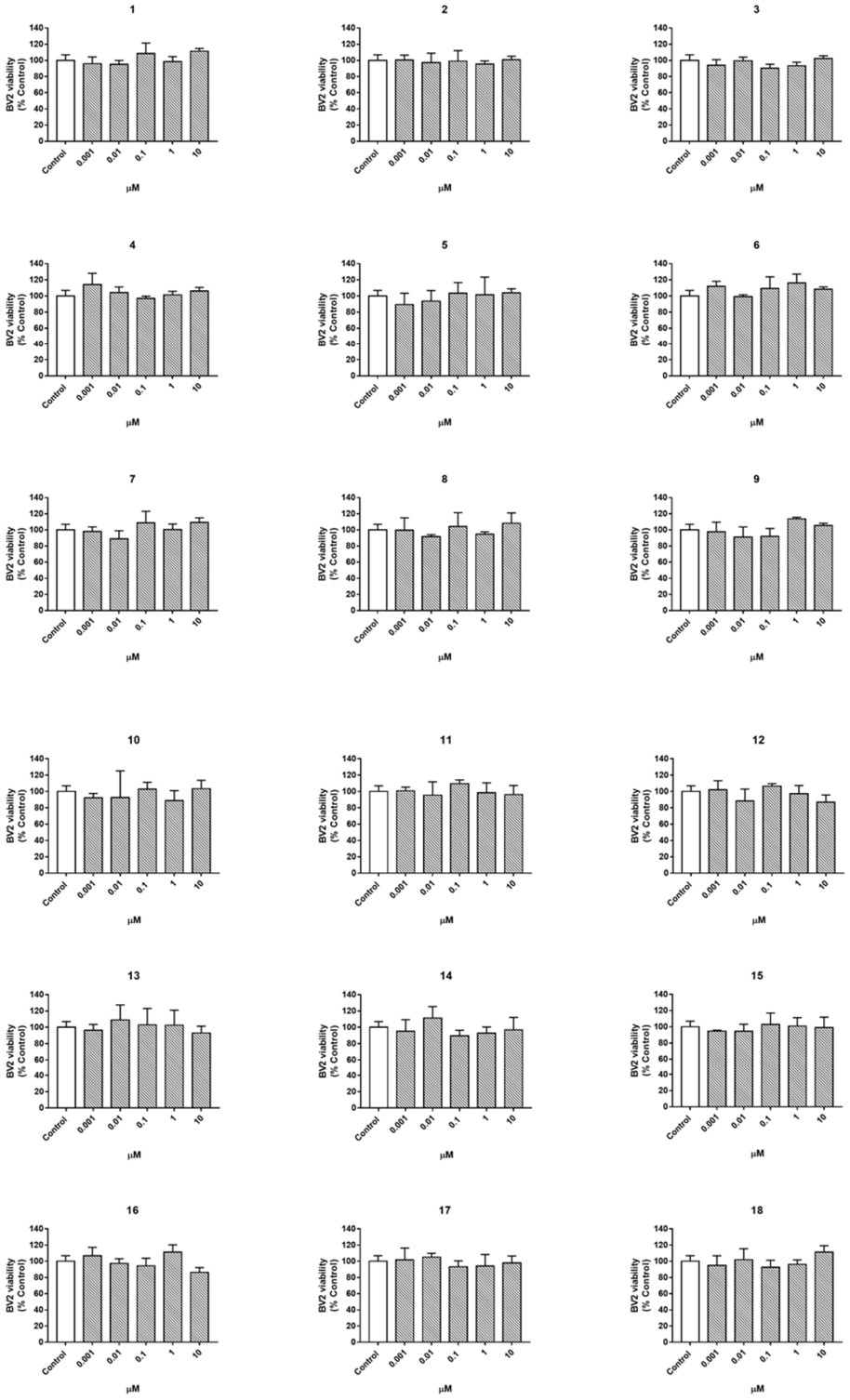
S76. ^{1}H NMR spectrum of **17** (500 MHz, MeOH-d_4).



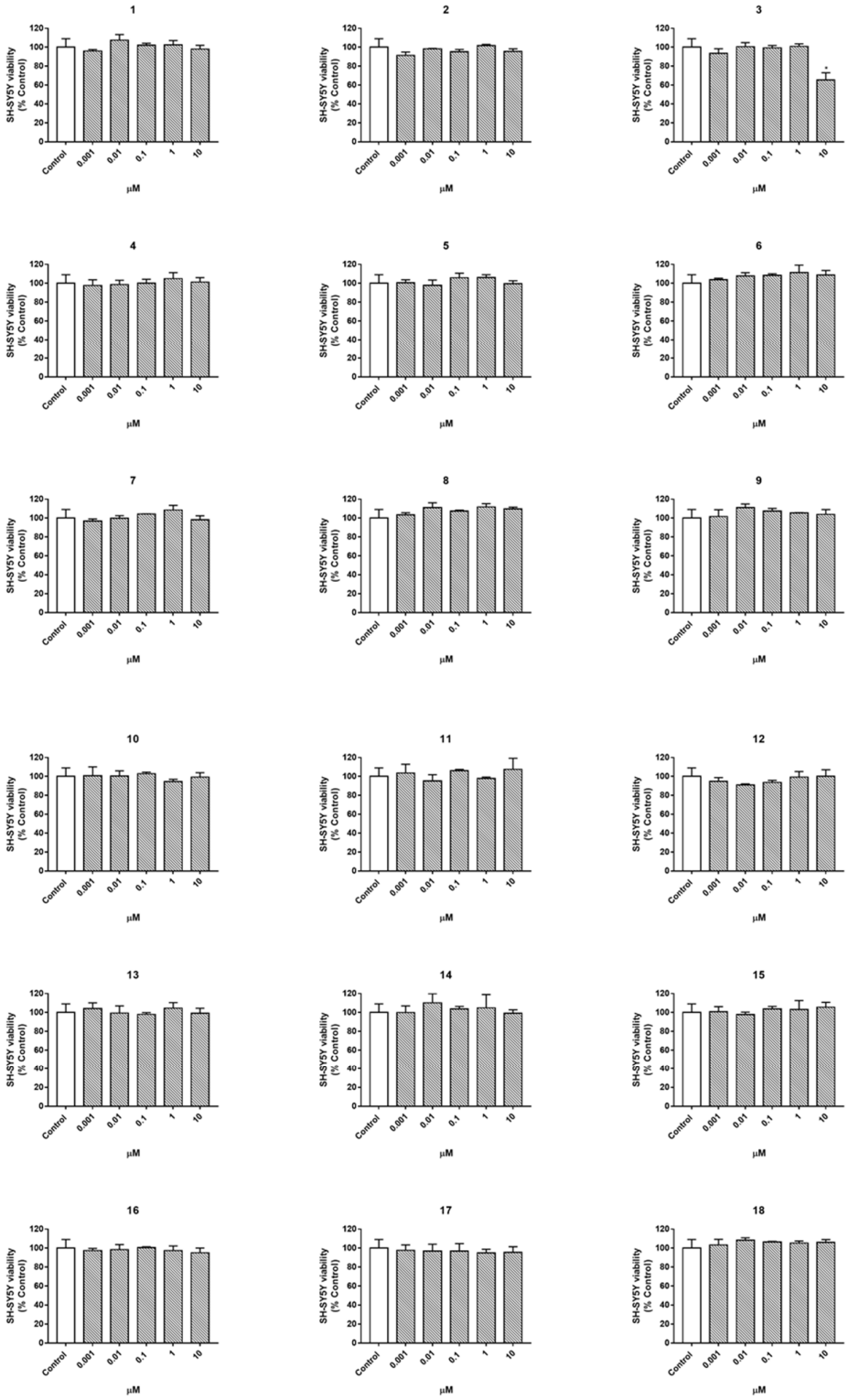
S77. ESI(+)-HRMS analysis of **18**



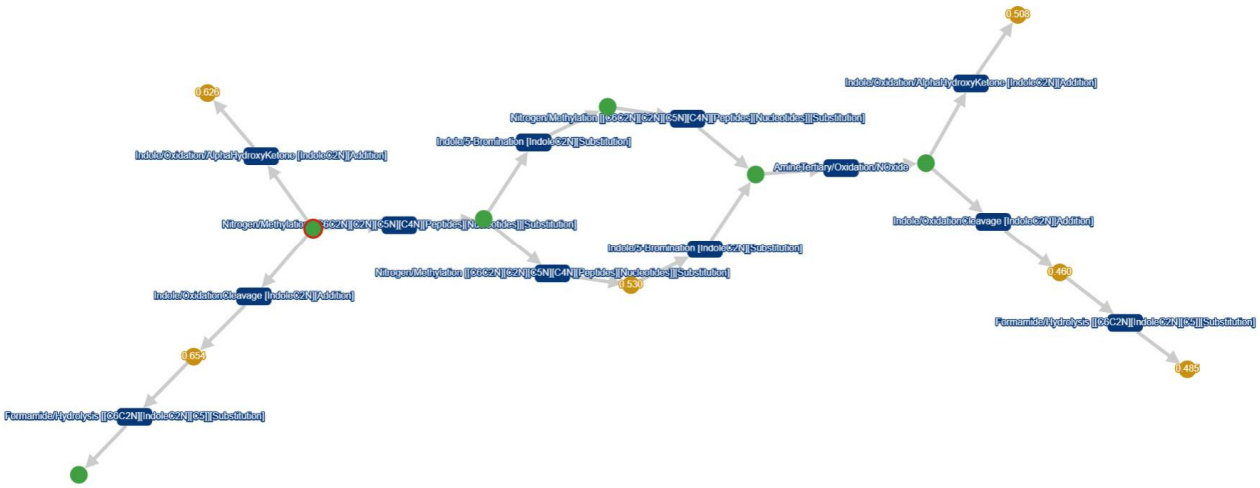
S78. ^{1}H NMR spectrum of **18** (500 MHz, MeOH-d_4).



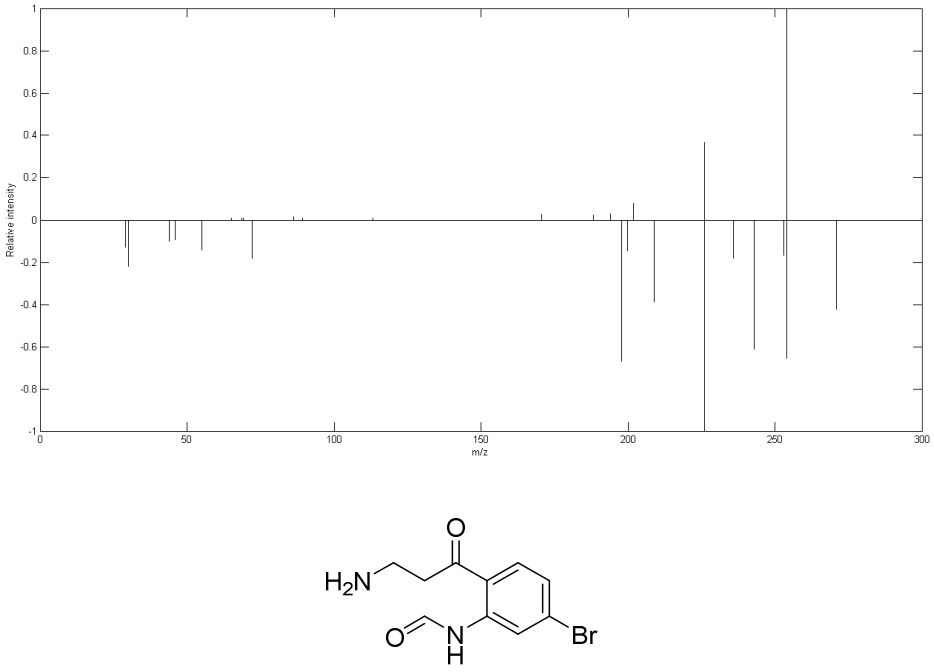
S79. Cell viability of brominated alkaloids over microglia BV2 cell line.
Cells were treated with compounds (0.001, 0.01, 0.1, 1 and 10 μM) for 24 hours. Cell viability was determined using MTT test. Dates are represented in percentage of cells control, being the result of mean absorbance ± SEM of three 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 ± 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.