Electronic Supplementary Material (ESI) for RSC Advances.

Effect of branching in remote substituents on light emission and stability of chemiluminescent acridinium esters

Supplementary Material

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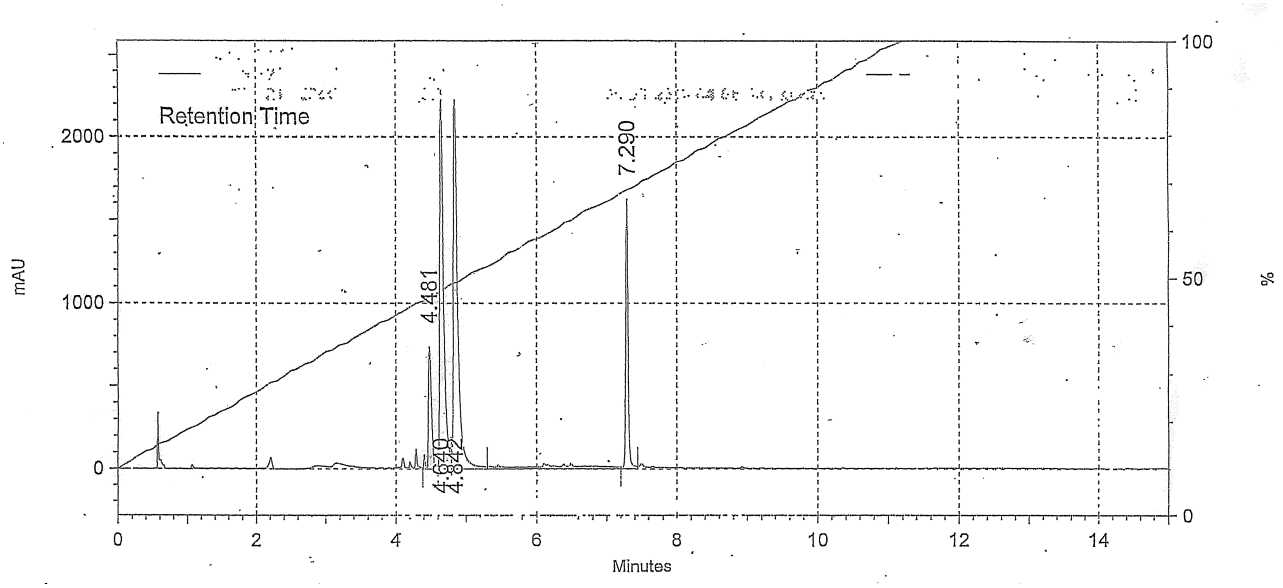
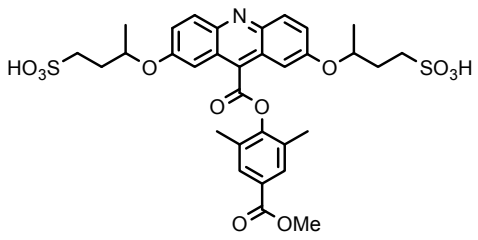


Figure S1a. HPLC trace of the crude reaction mixture showing a pair of diastereomers for compound **3** eluting at 4.6 and 4.8 minutes. Peak eluting at 4.4 minutes is related to the ionic liquid and peak eluting at 7.3 min is dibenzo-18-crown-6. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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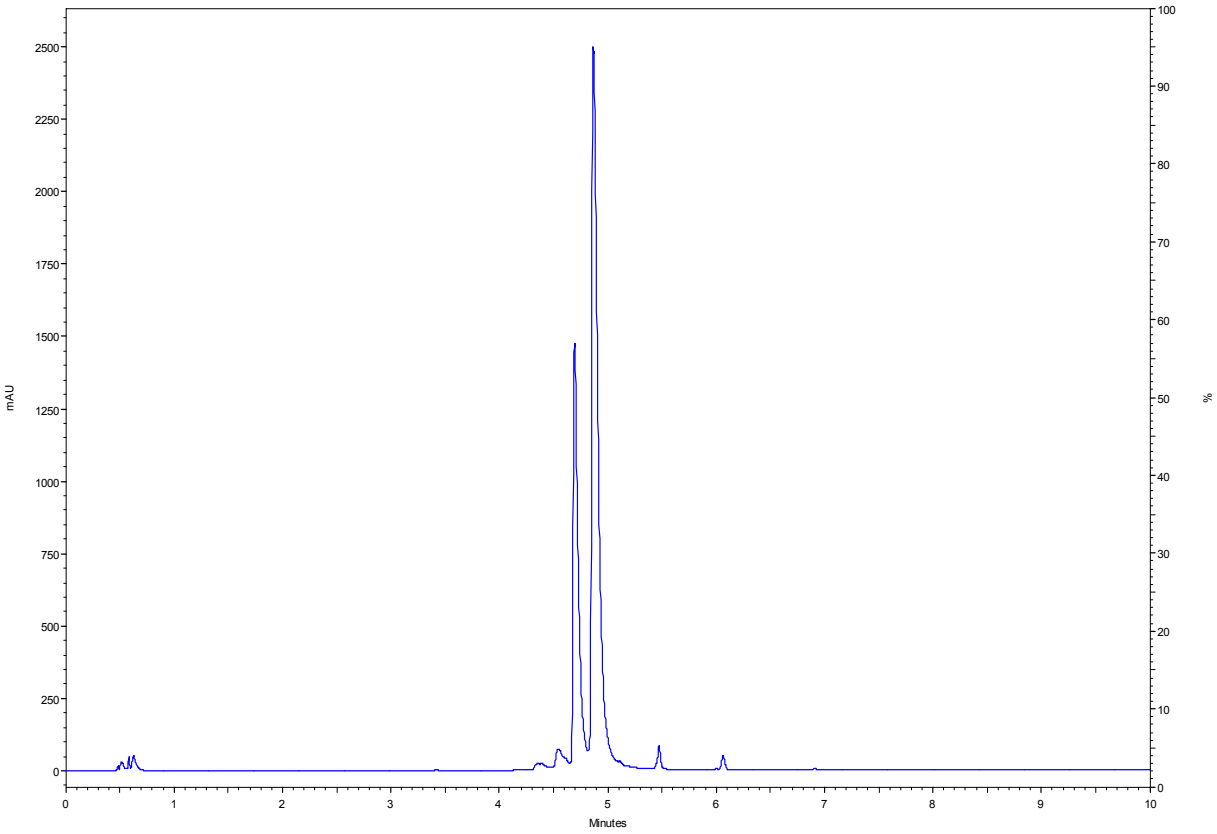
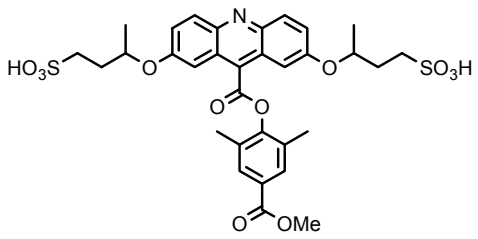


Figure S1b. HPLC trace of compound **3** showing a pair of diastereomers after purification of the mixture. During purification, some loss of the earlier eluting diastereomer was observed. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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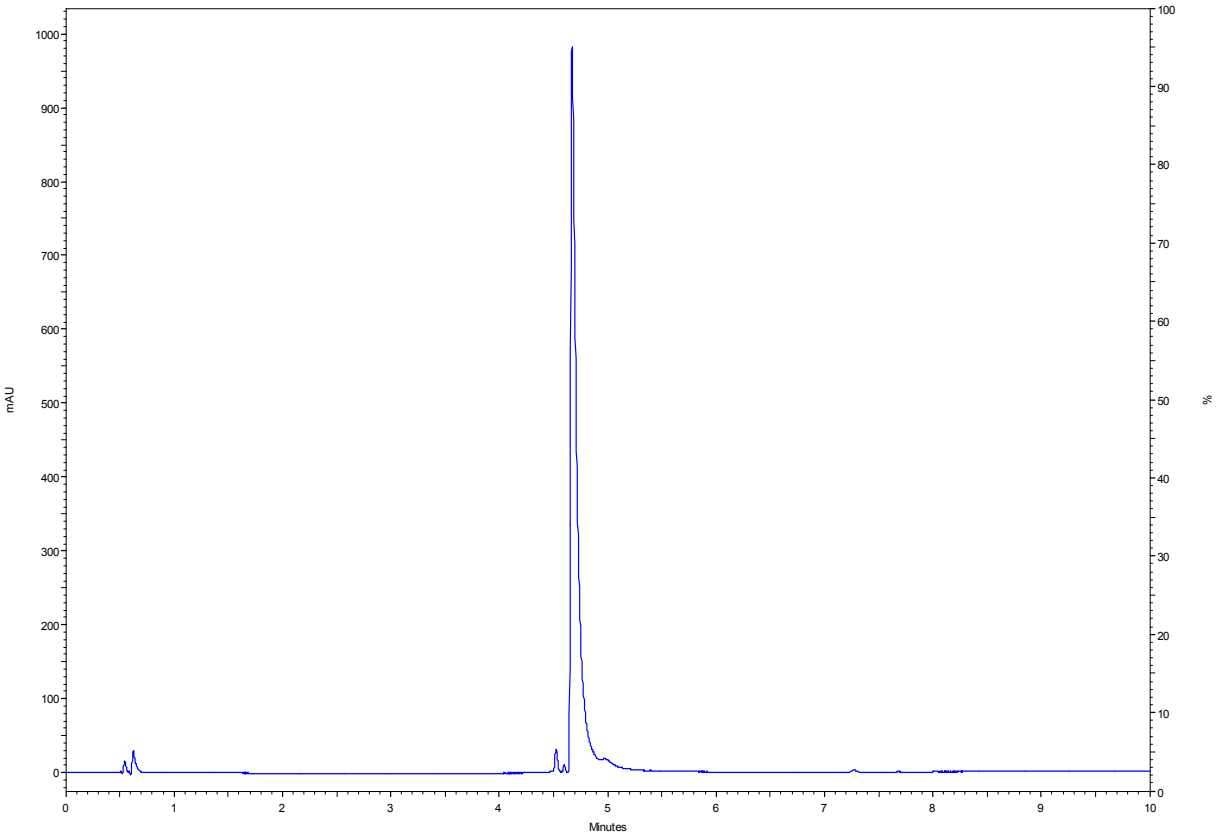
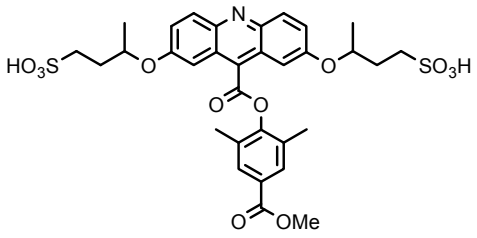


Figure S1c. HPLC trace of compound **3** after purification showing the early eluting diastereomer. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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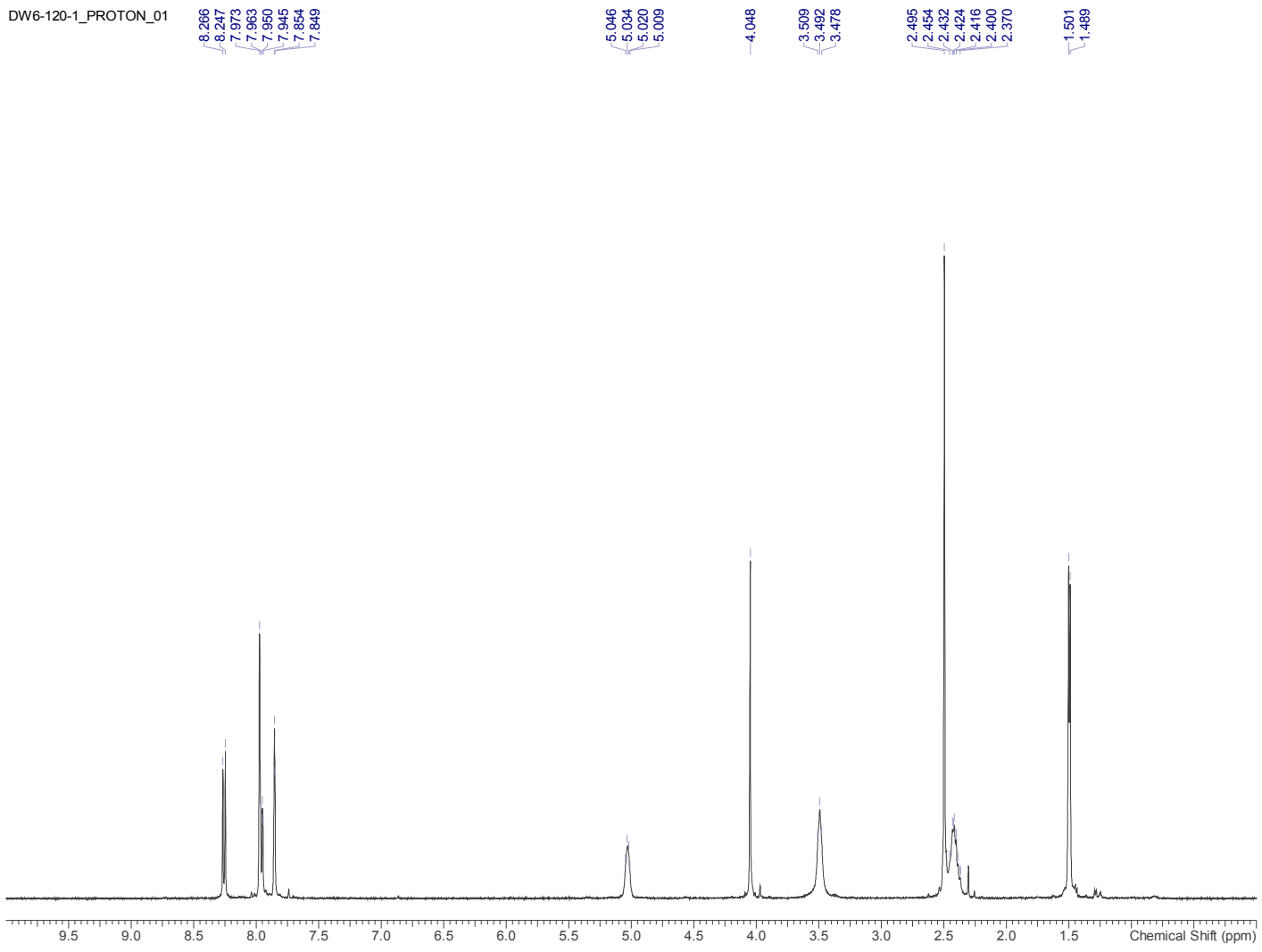


Figure S1d. ^{1}H NMR of compound **3** in CF_3COOD (earlier eluting diastereomer, refer to Figure S1c).

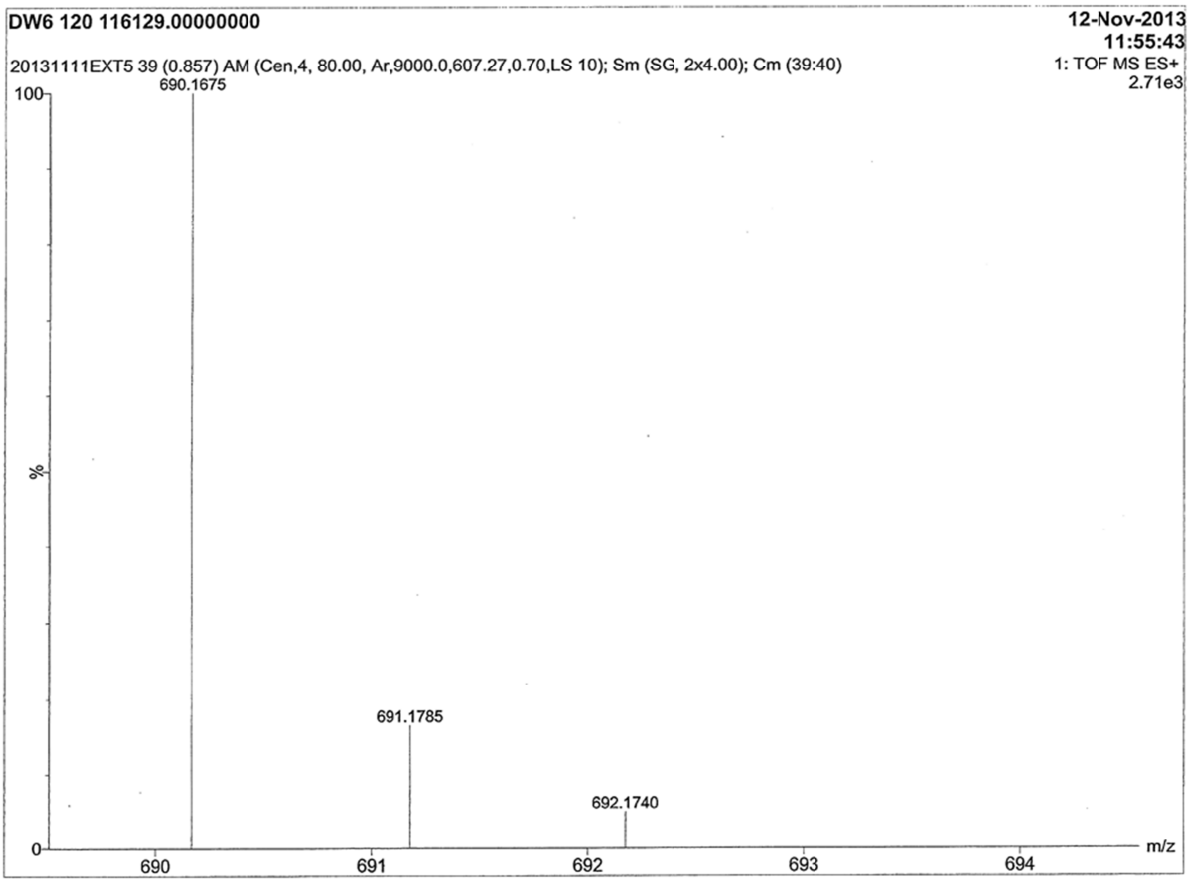


Figure S1e. HRMS of compound **3** (earlier eluting diastereomer, refer to Figure S1c).

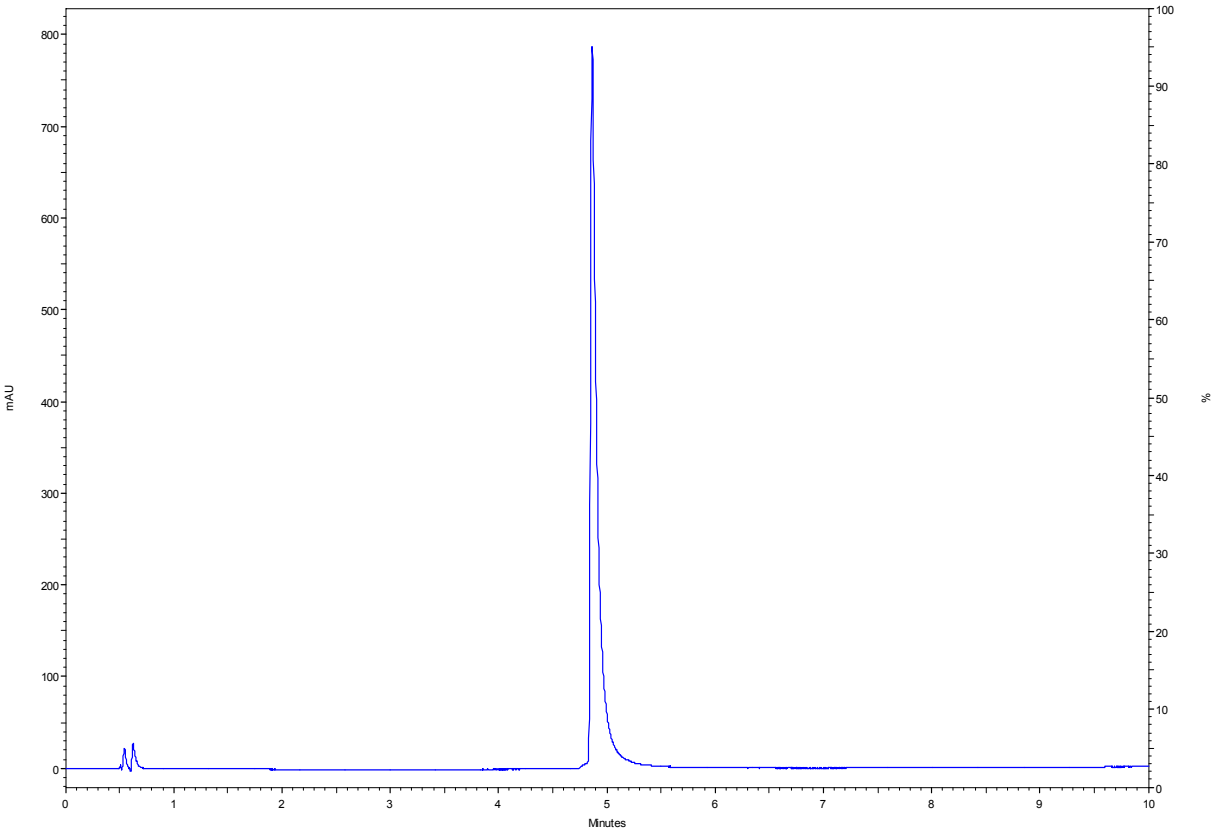
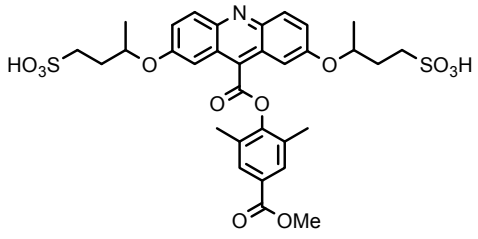


Figure S1f. HPLC trace of compound **3** after purification showing the later eluting diastereomer. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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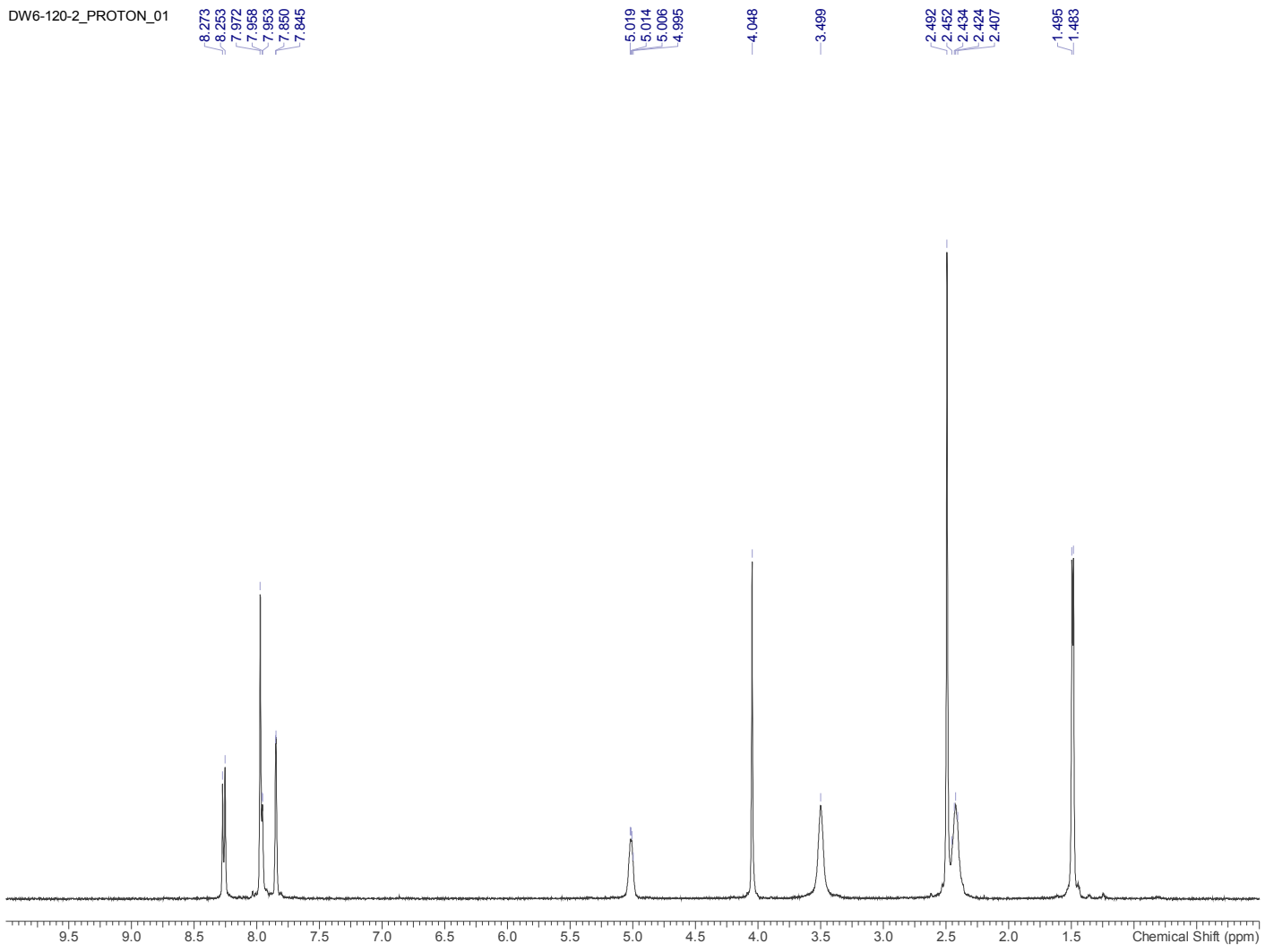


Figure S1g. ^{1}H NMR of compound **3** in CF_3COOD (later eluting diastereomer, refer to Figure S1f).

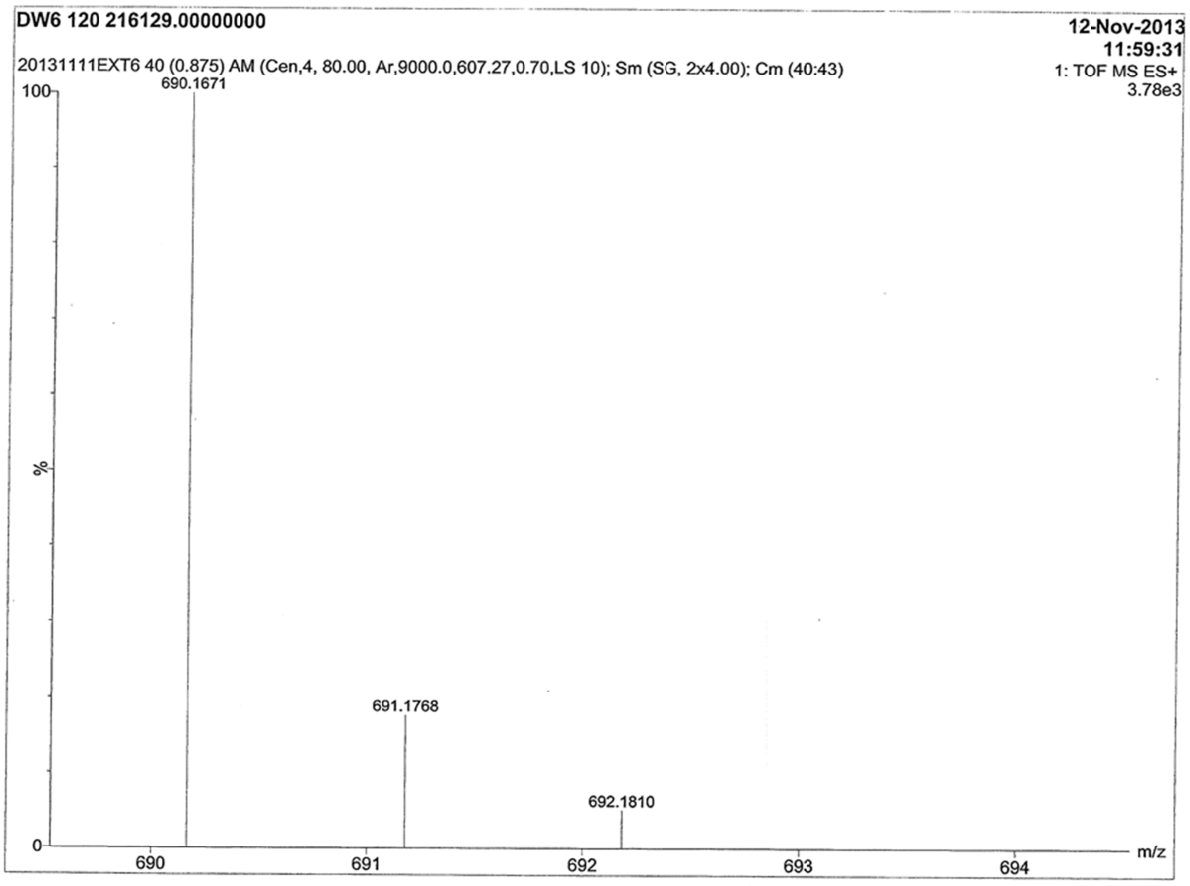


Figure S1h. HRMS of compound **3** (later eluting diastereomer, refer to Figure S1f).

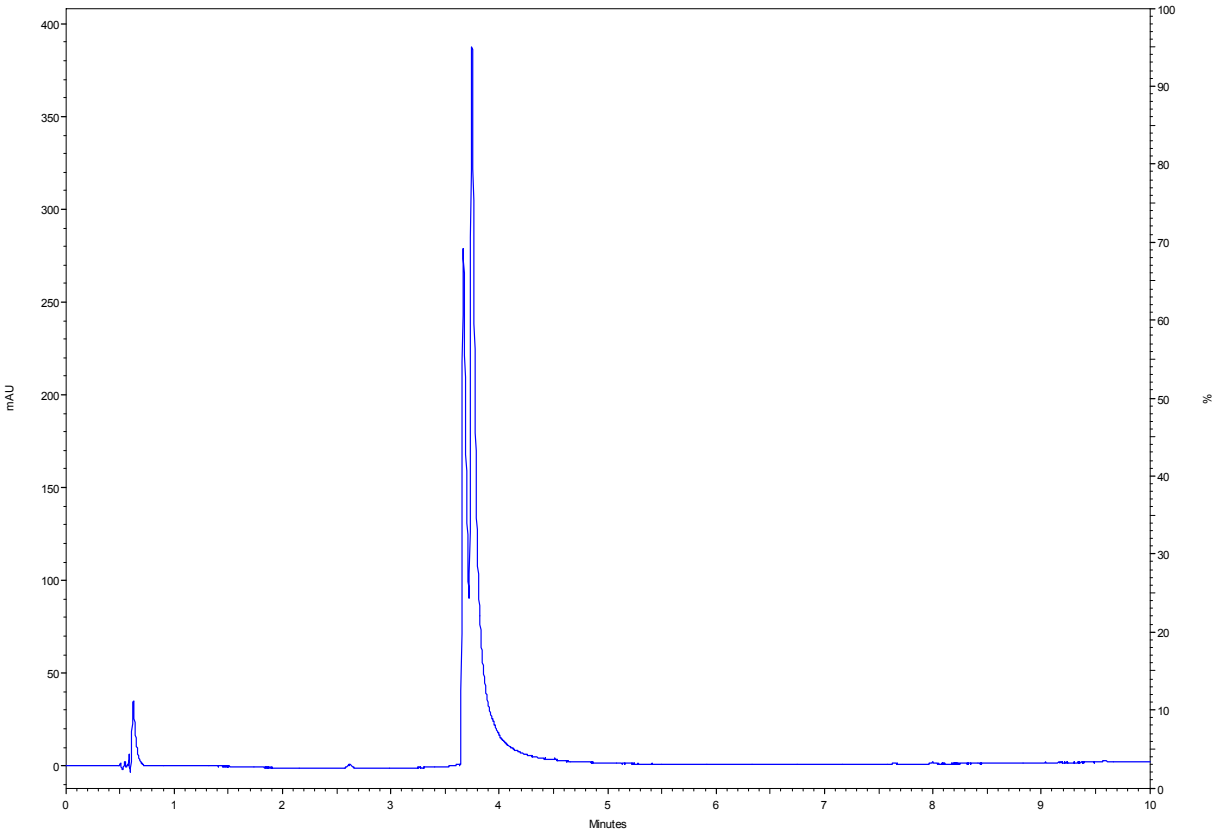
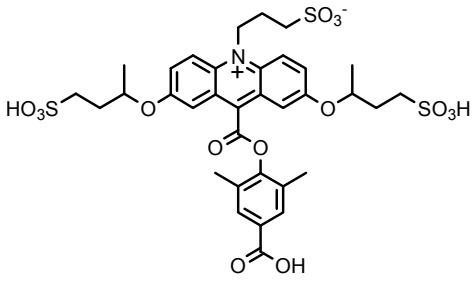


Figure S2a. HPLC trace of compound **4** showing a pair of diastereomers. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm. As observed previously during purification of compound **3**, purification of **4** resulted in some loss of the earlier eluting diastereomer due to closely eluting impurities.



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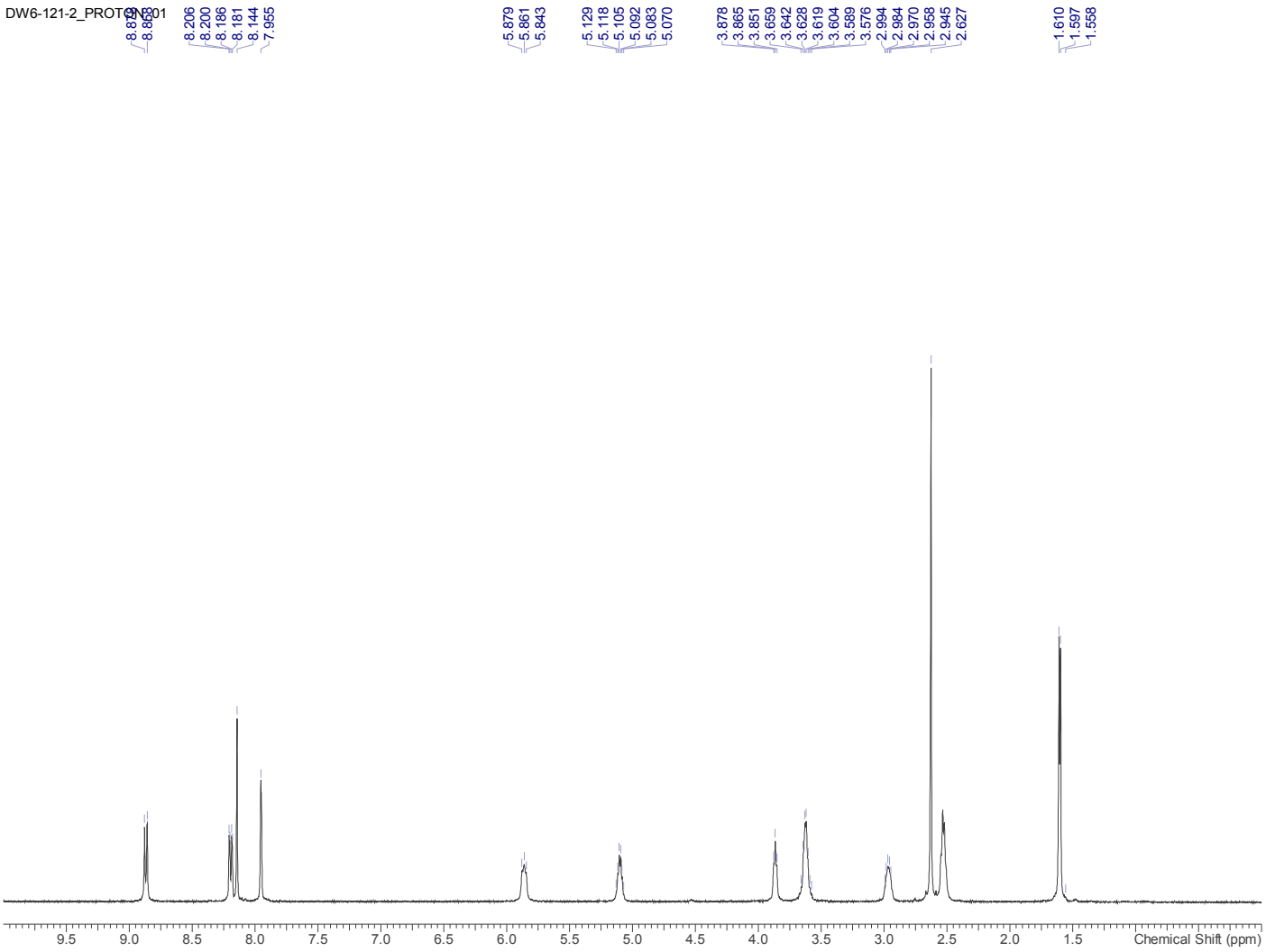


Figure S2b. ^{1}H NMR of compound **4** in CF_3COOD.

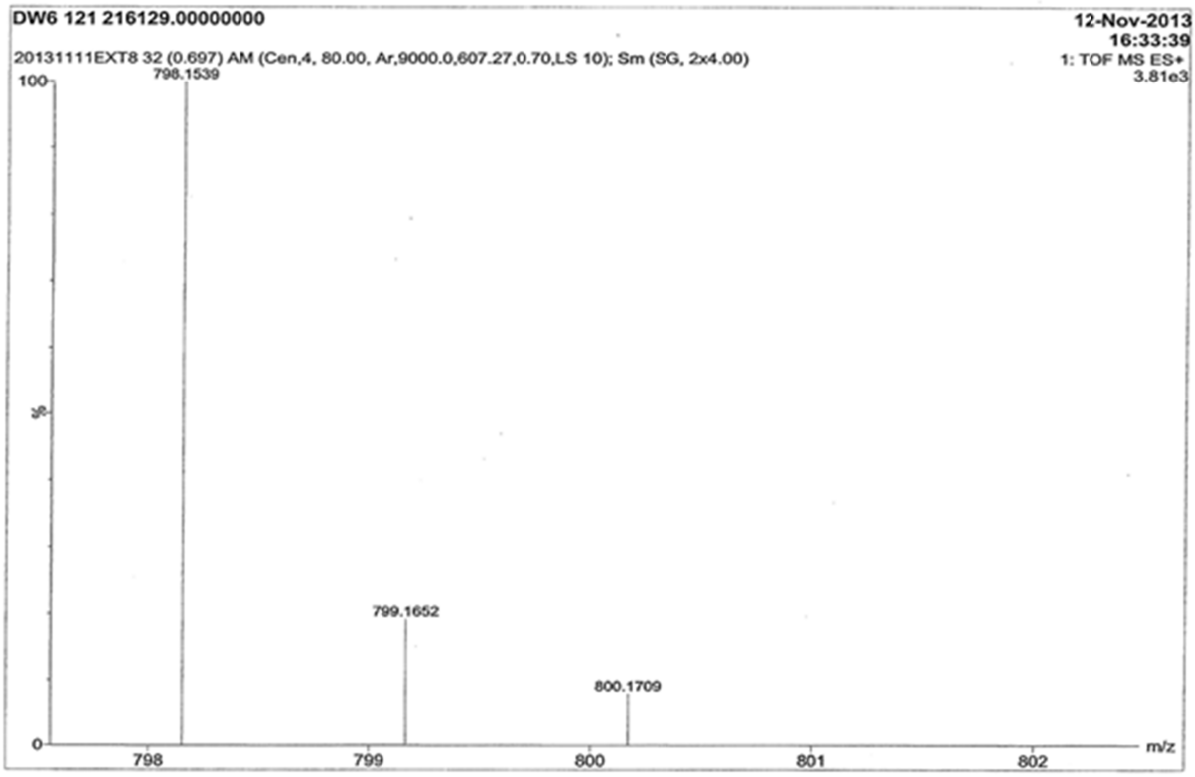


Figure S2c. HRMS of compound **4.**

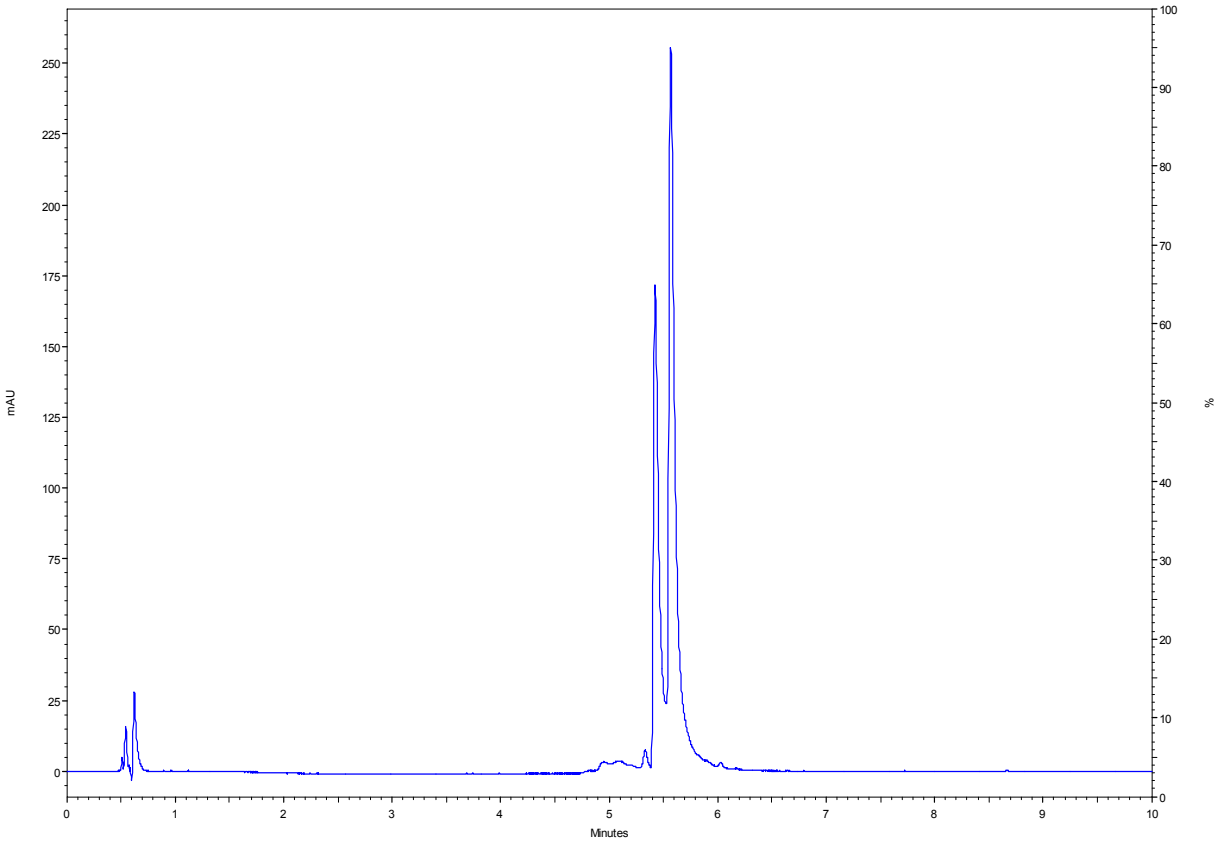
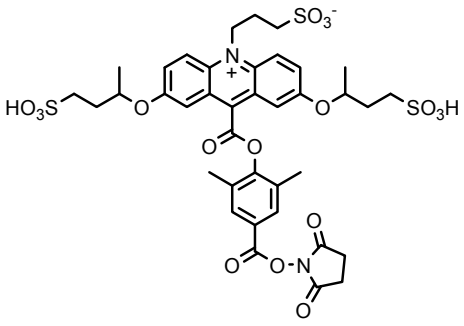


Figure S3a. HPLC trace of compound **5** showing a pair of diastereomers. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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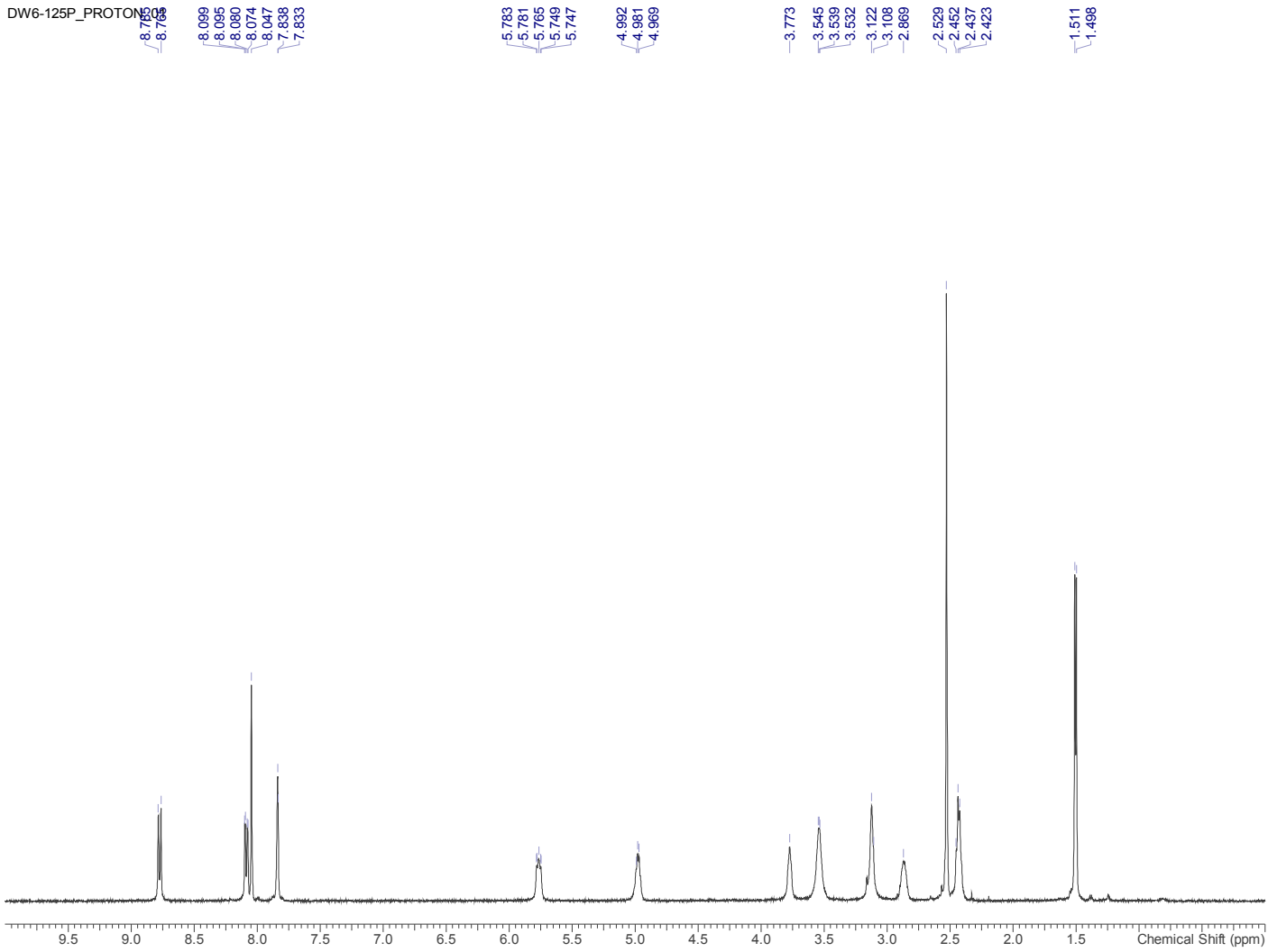


Figure S3b. ^{1}H NMR of compound **5** in CF_3COOD.

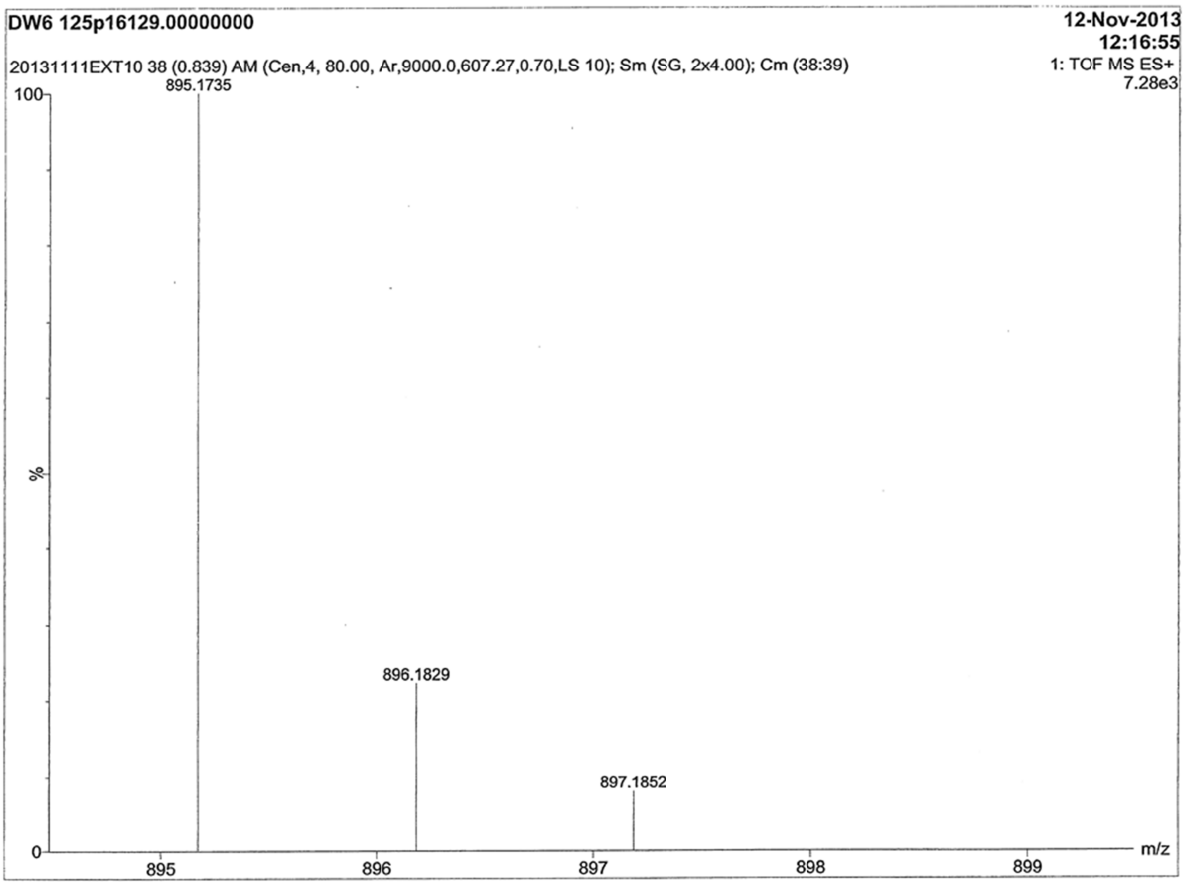


Figure S3c. HRMS of compound **5**.

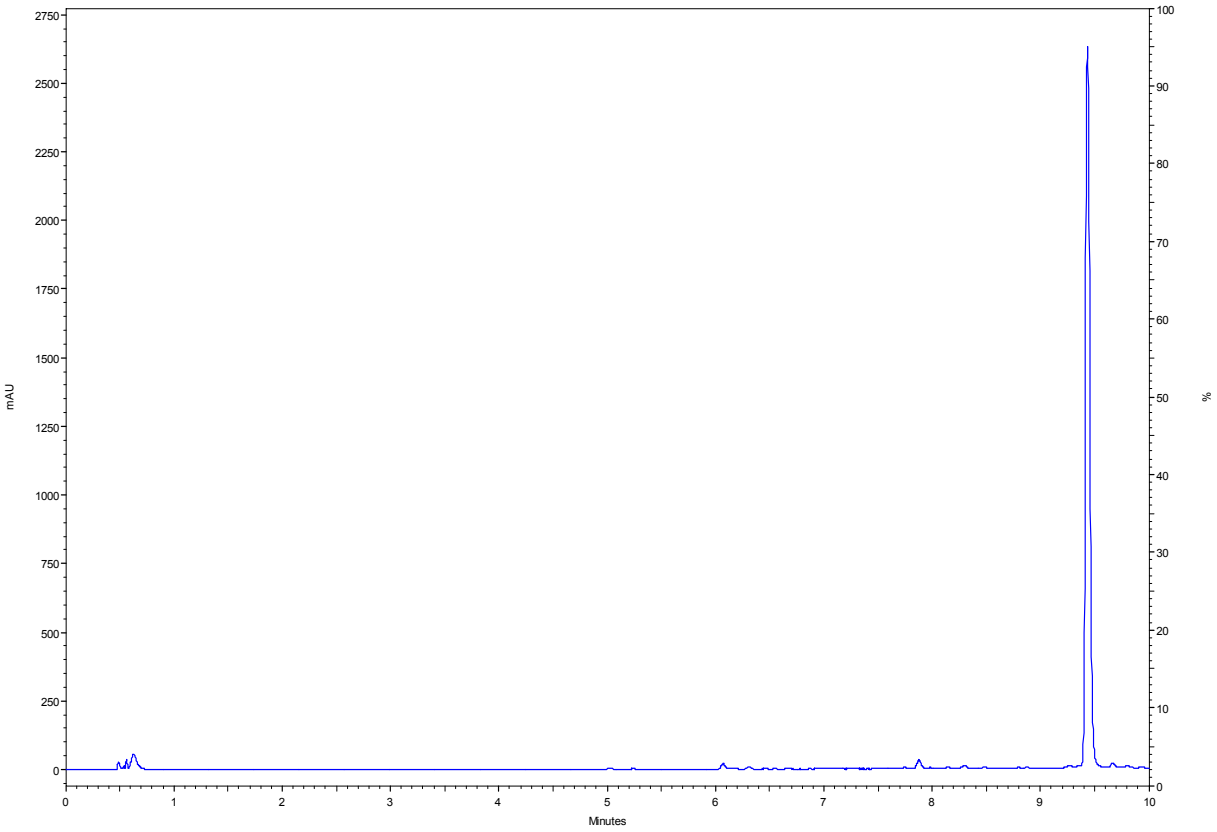
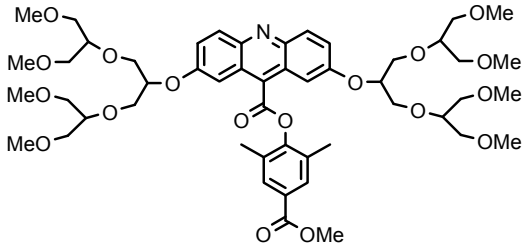


Figure S4a. HPLC trace of compound **7**. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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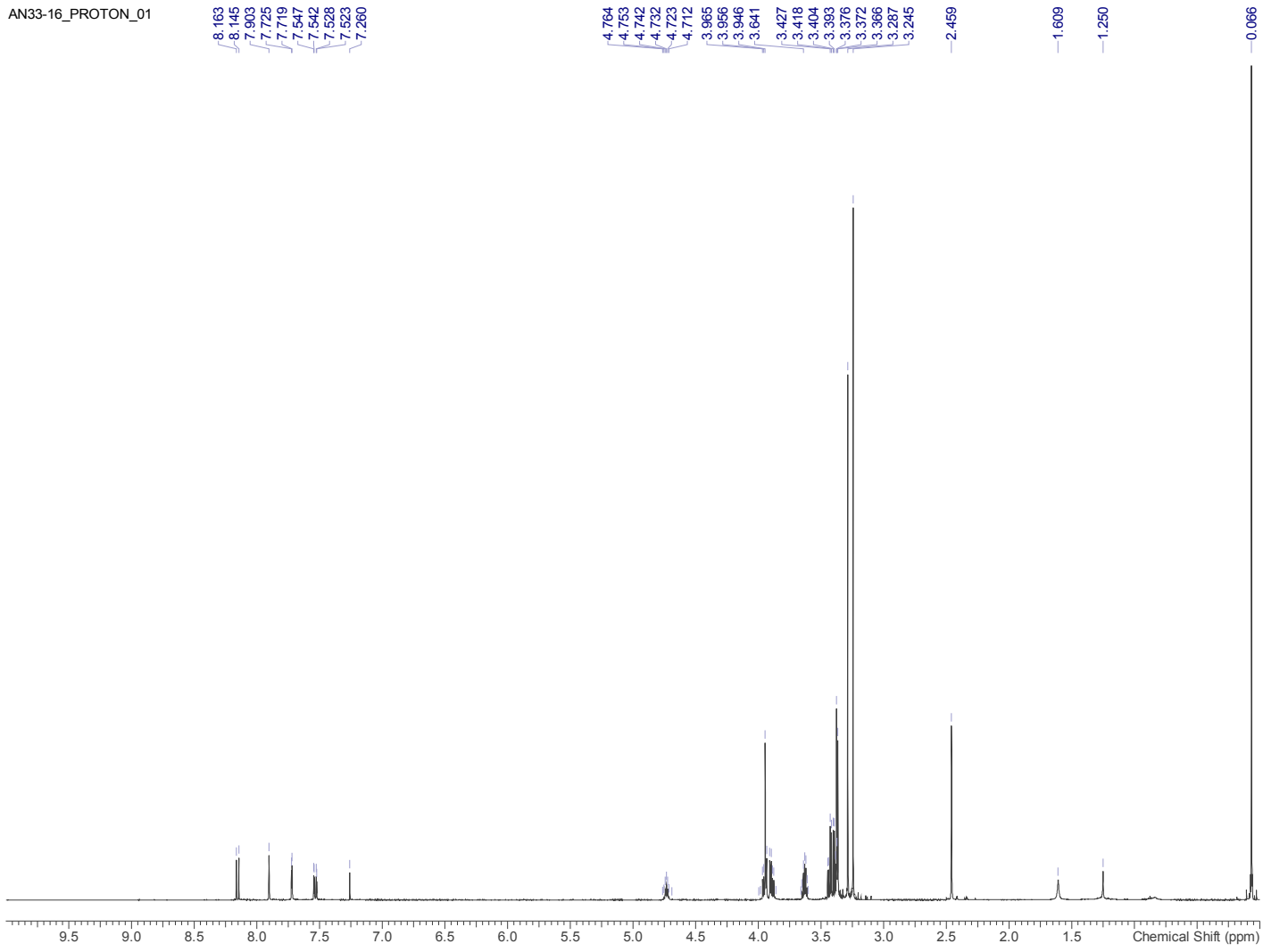


Figure S4b. ^{1}H NMR of compound **7** in $CDCl_3$

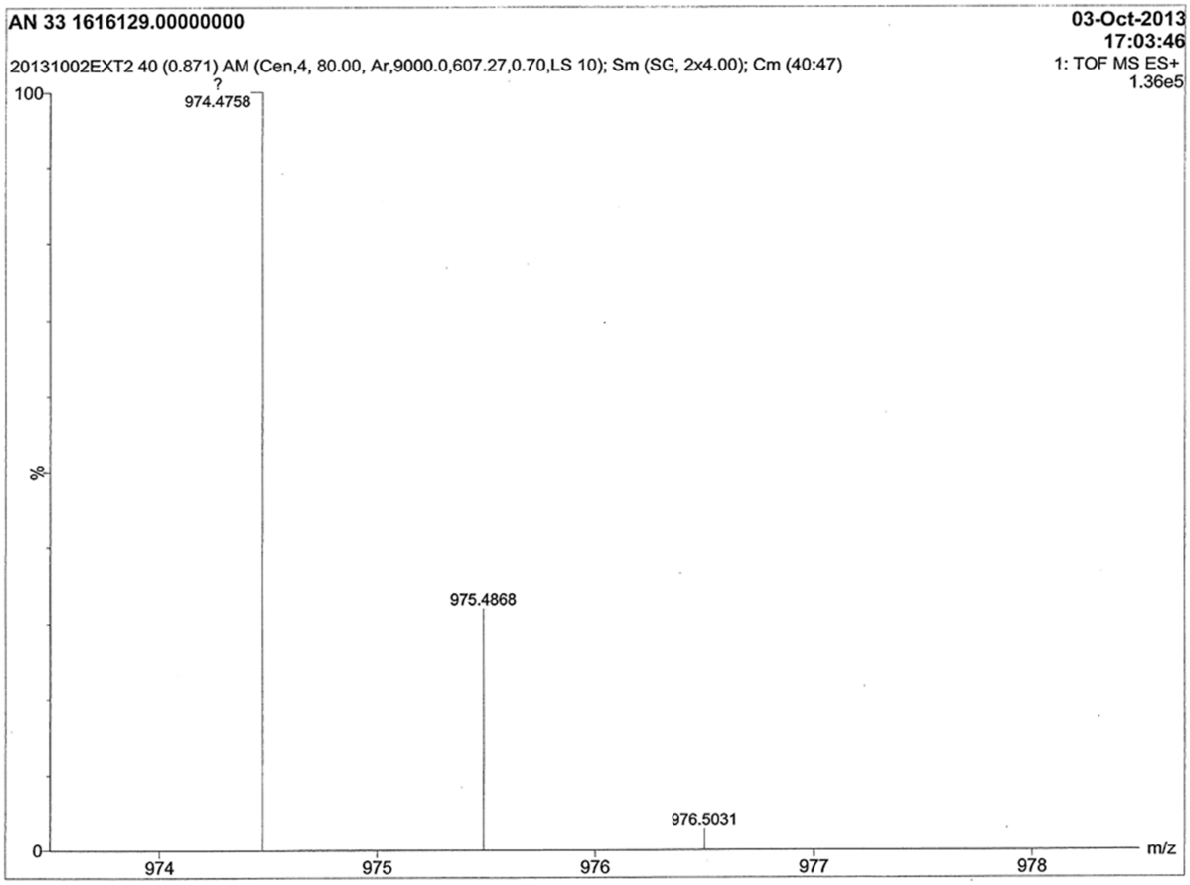


Figure S4c. HRMS of compound **7**

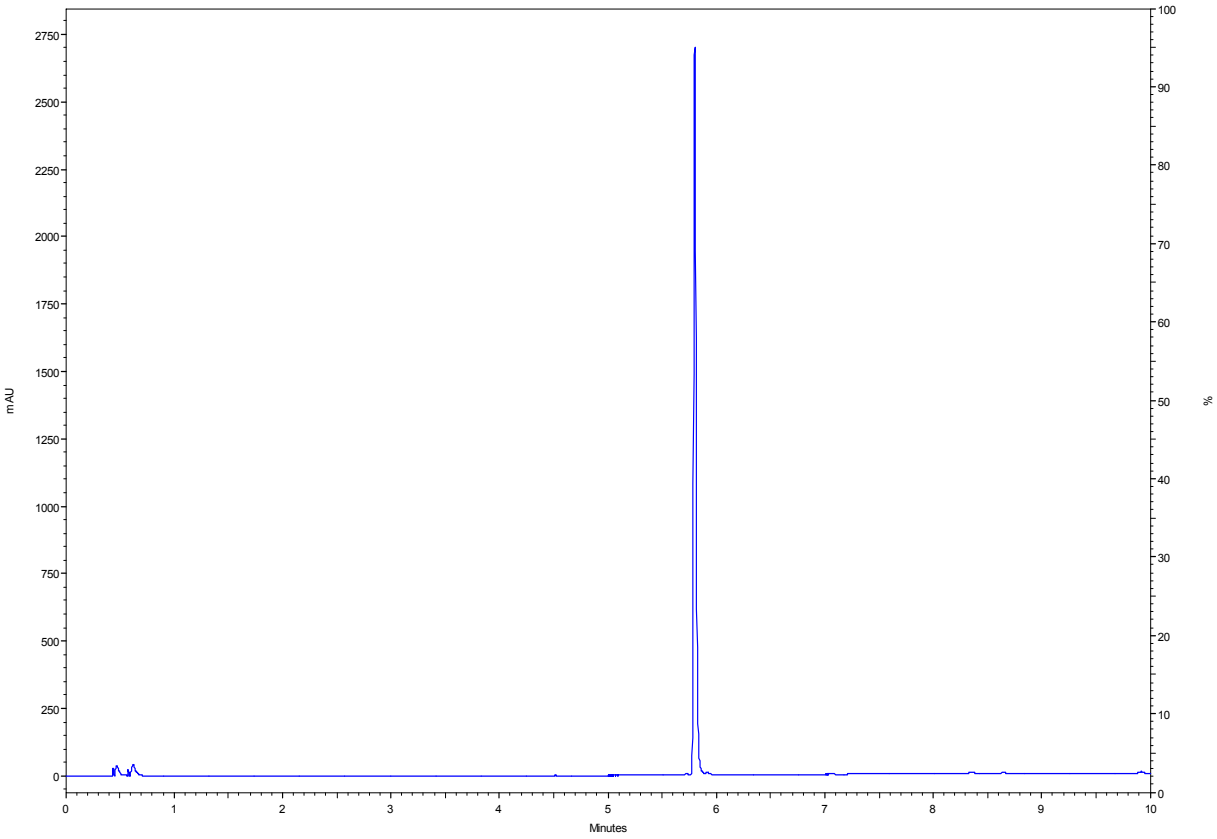
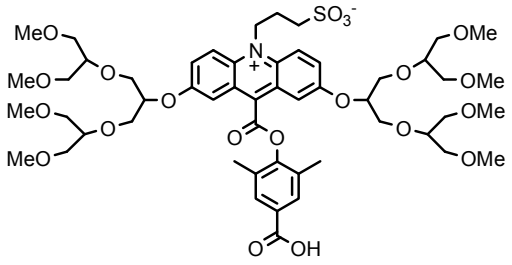


Figure S5a. HPLC trace of compound **8**. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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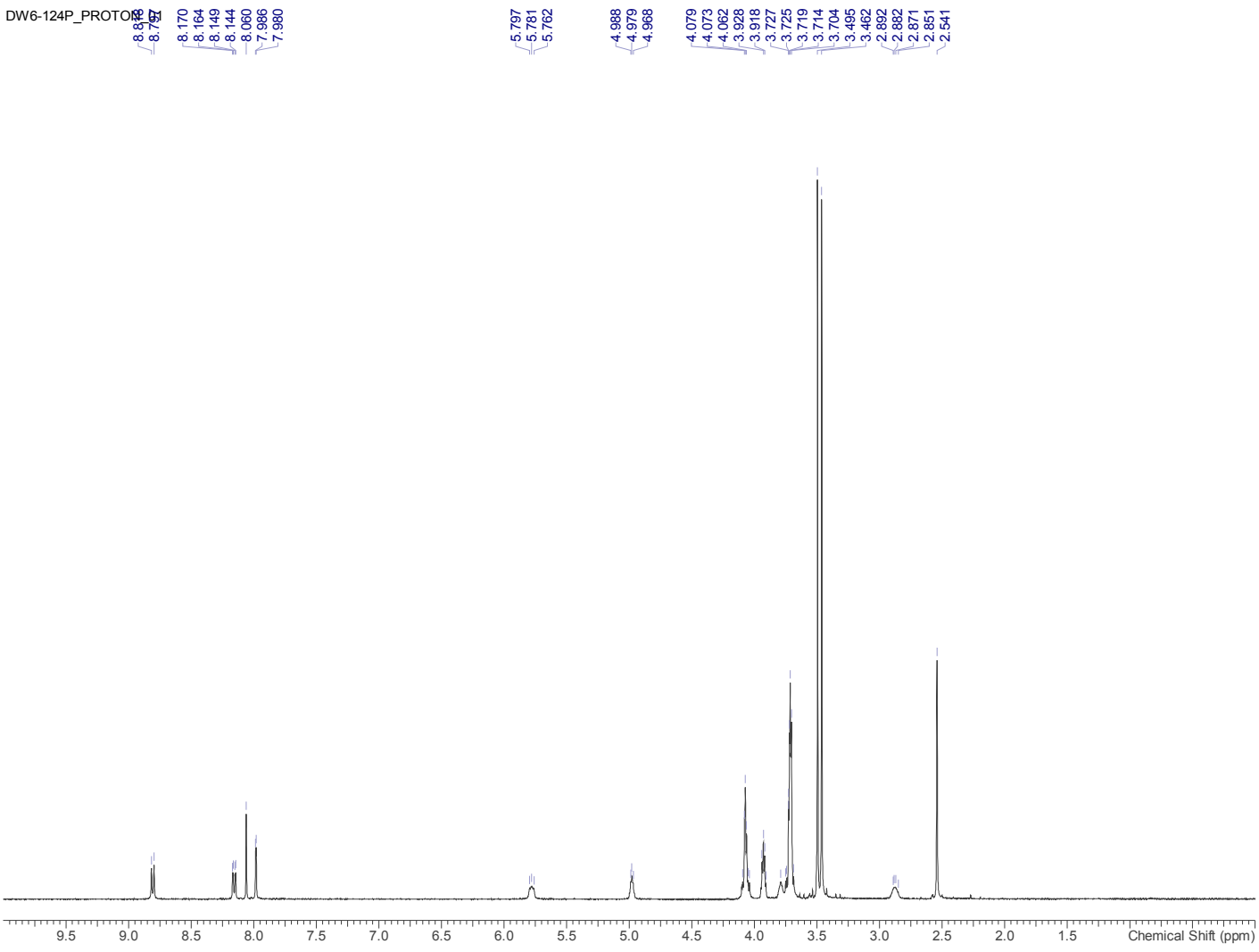


Figure S5b. ^{1}H NMR of compound **8** in CF_3COOD.

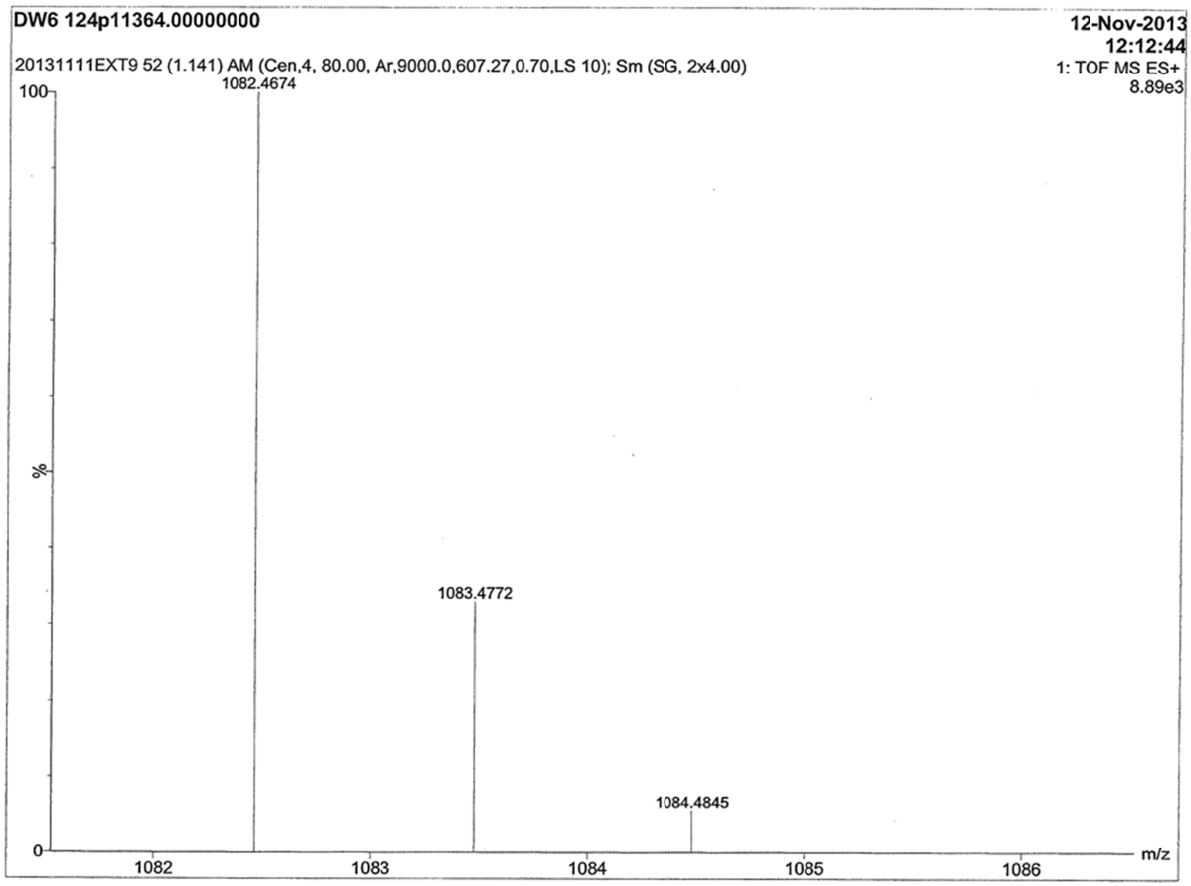


Figure S5c. HRMS of compound **8**.

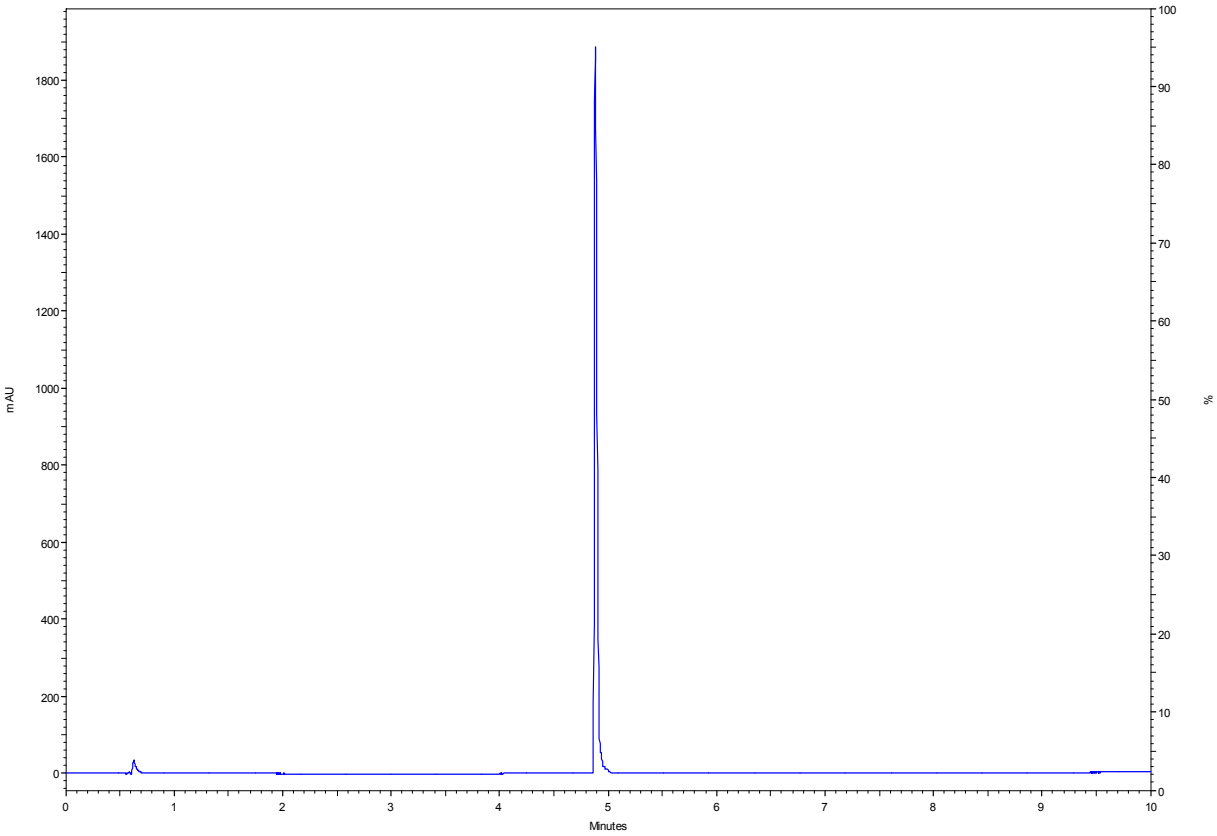
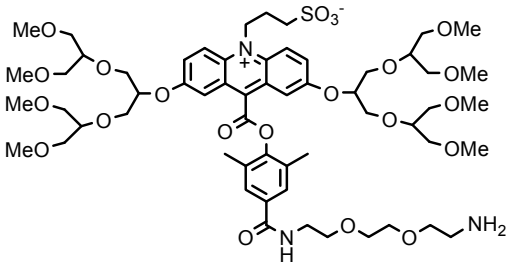


Figure S6a. HPLC trace of compound **9**. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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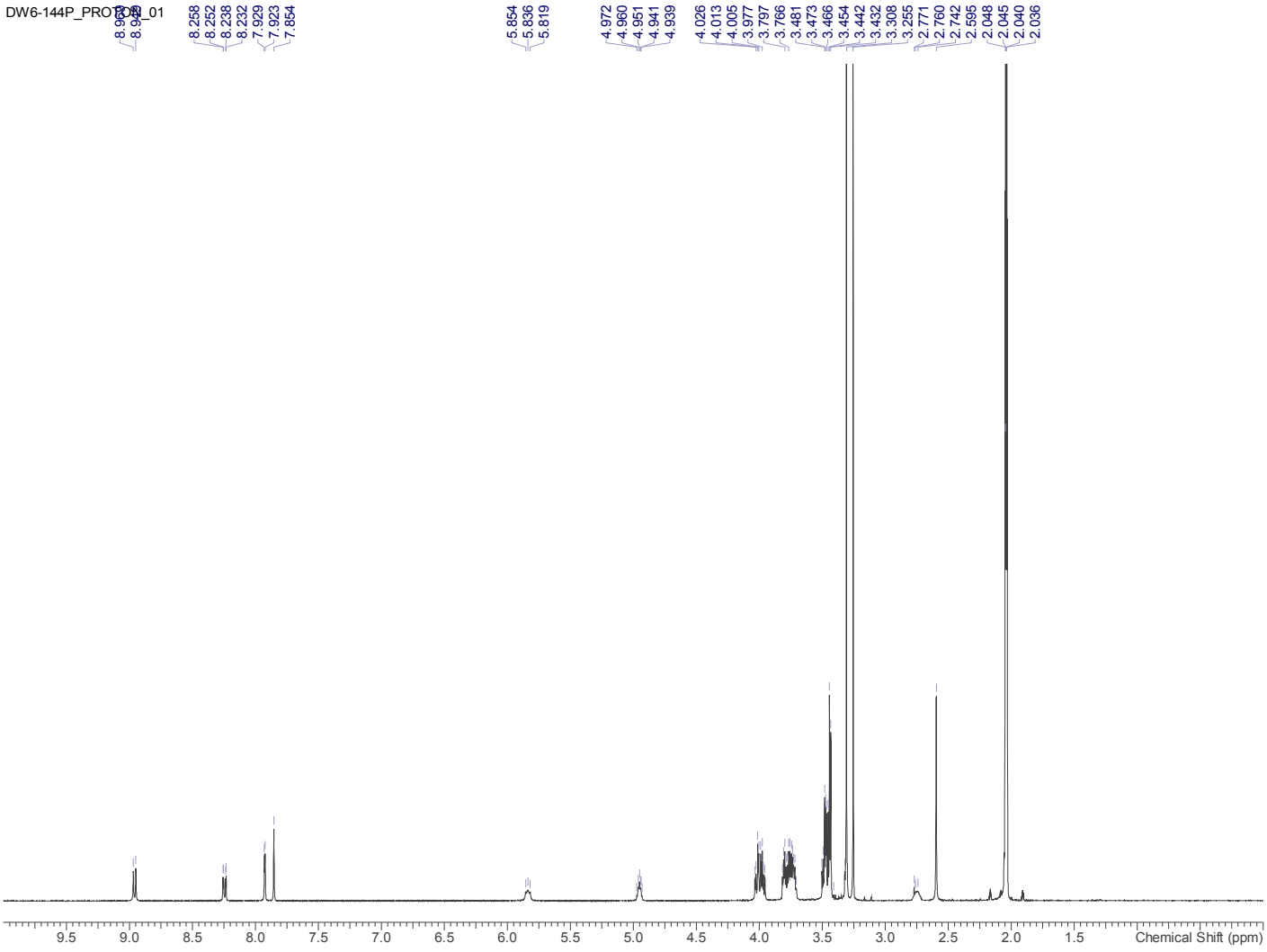


Figure S6b. ^{1}H NMR of compound **9** in CD_3COOD.

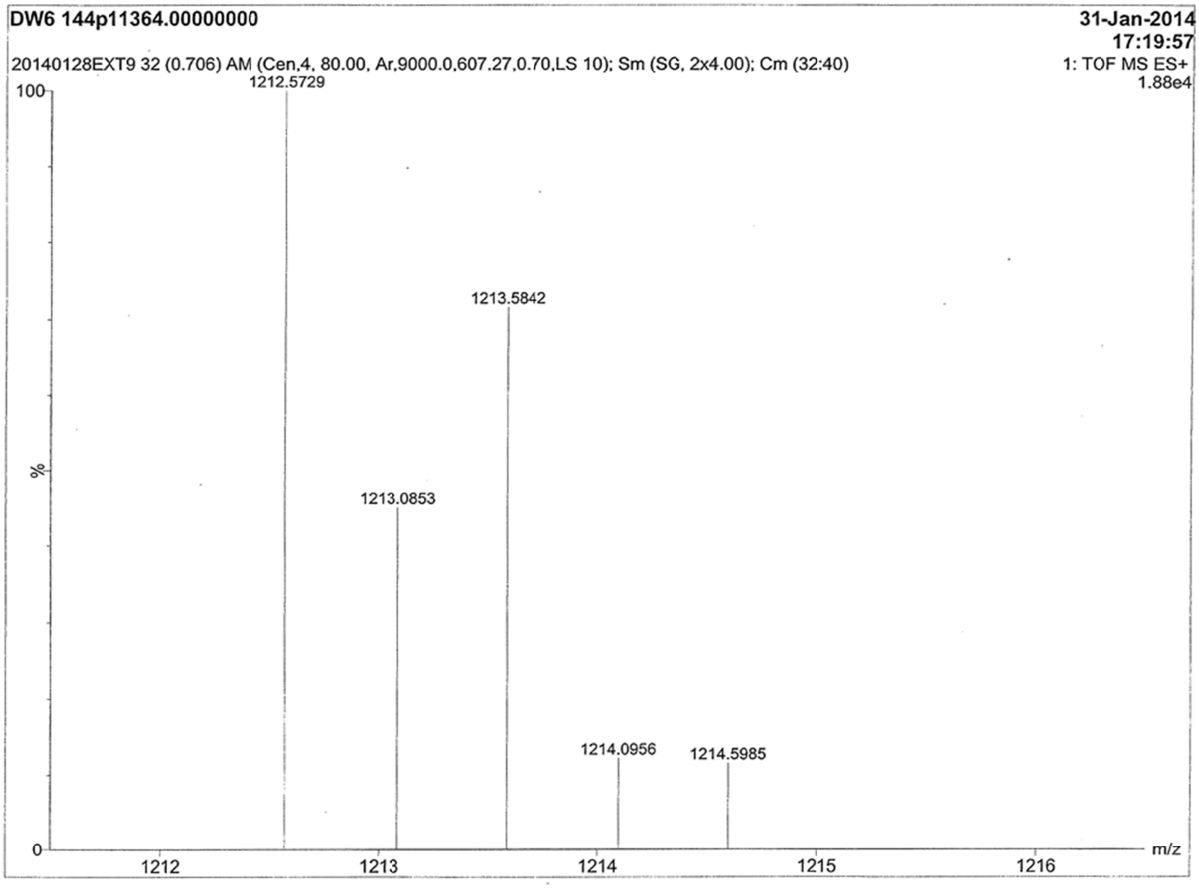


Figure S6c. HRMS of compound **9**.

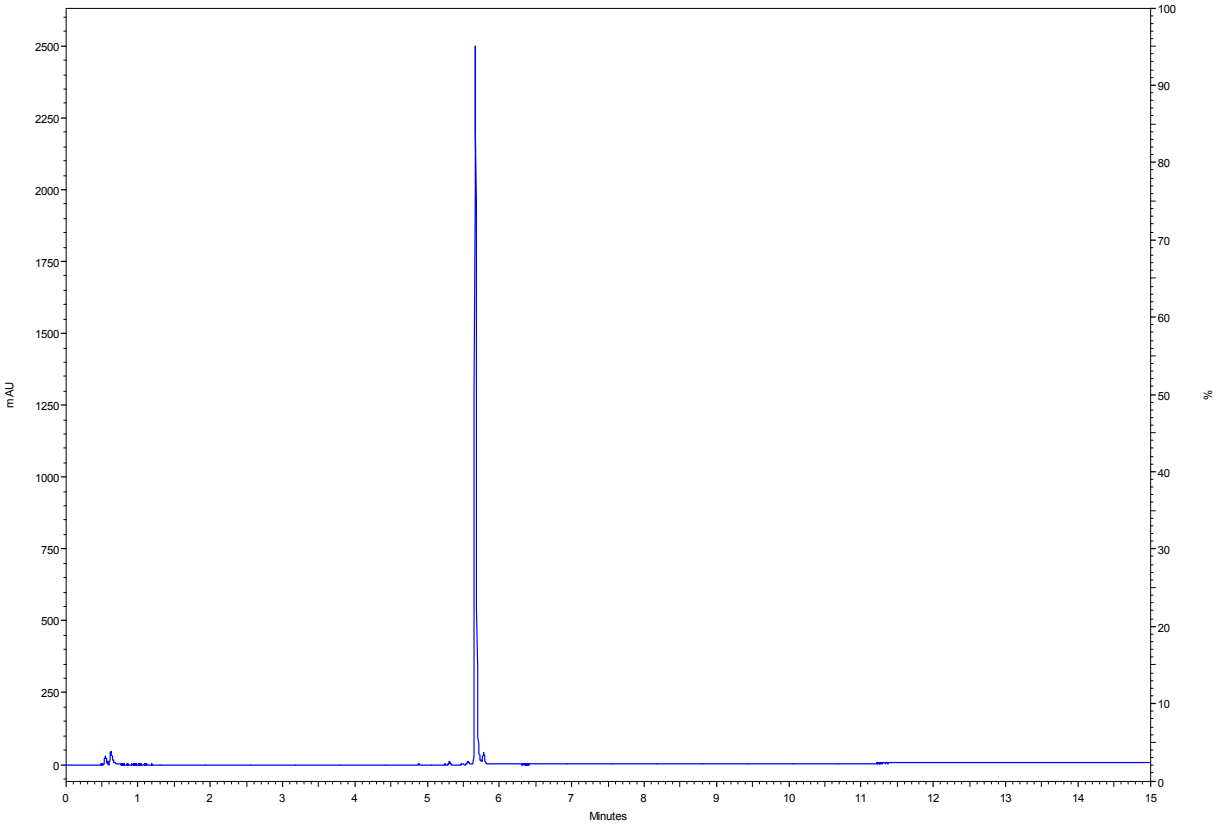
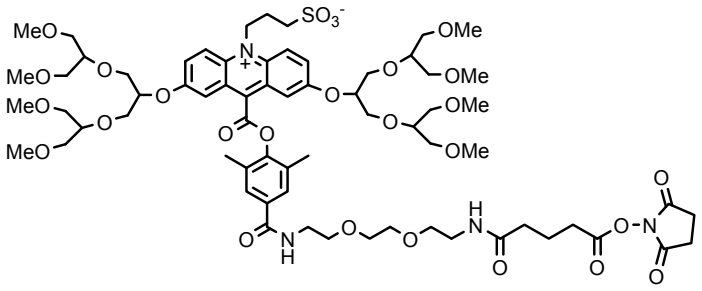


Figure S7a. HPLC trace of compound **10**. HPLC conditions: Phenomenex, Kinetex, C_{18}, 2.6 micron, 50 x 4.6 mm column, 10 minute gradient of 10→90% MeCN/water (each with 0.05% TFA), flow = 1 ml/minute, UV detection at 260 nm.



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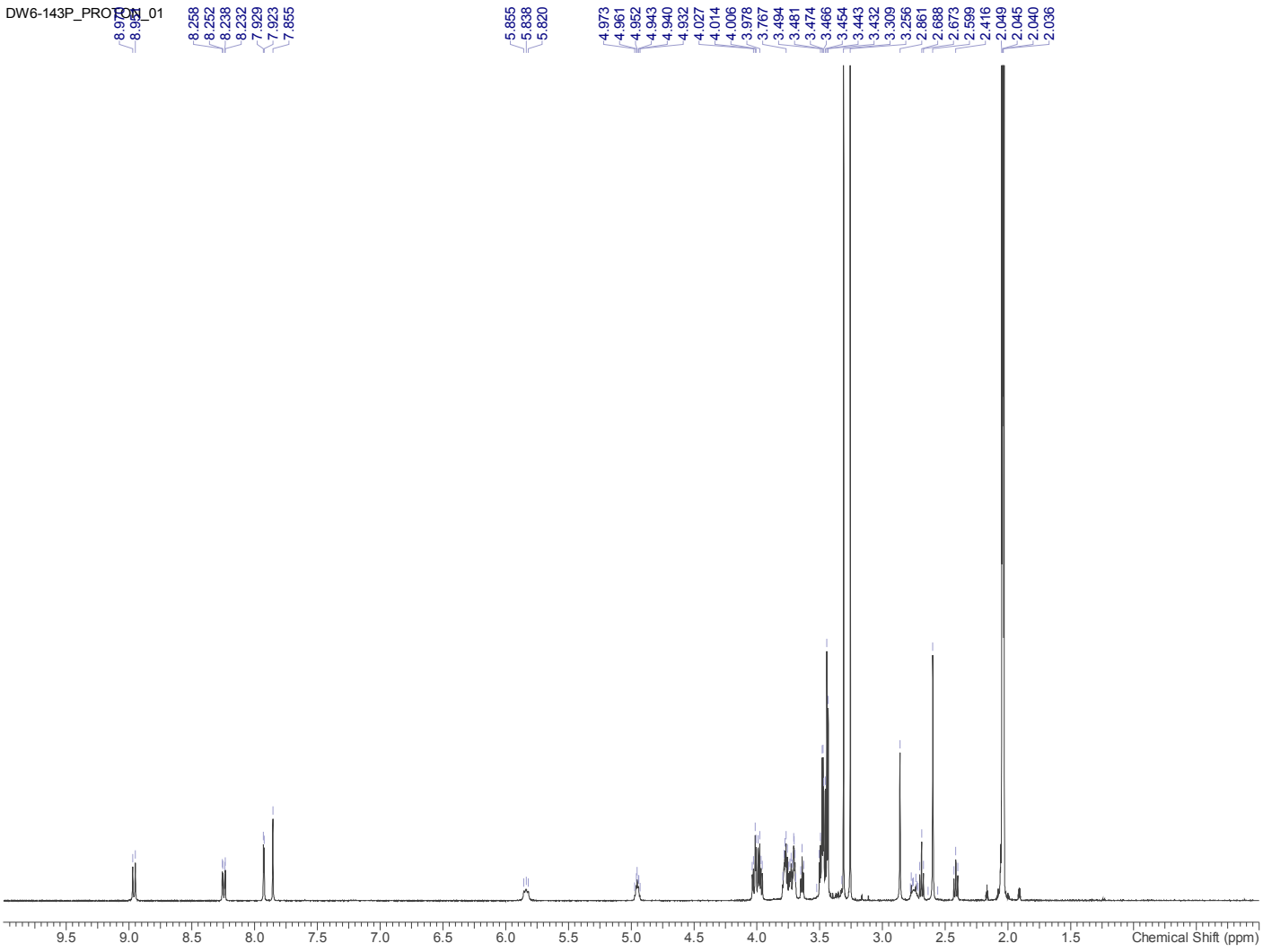

Figure S7b. ^{1}H NMR of compound **10** in CD_3COOD.

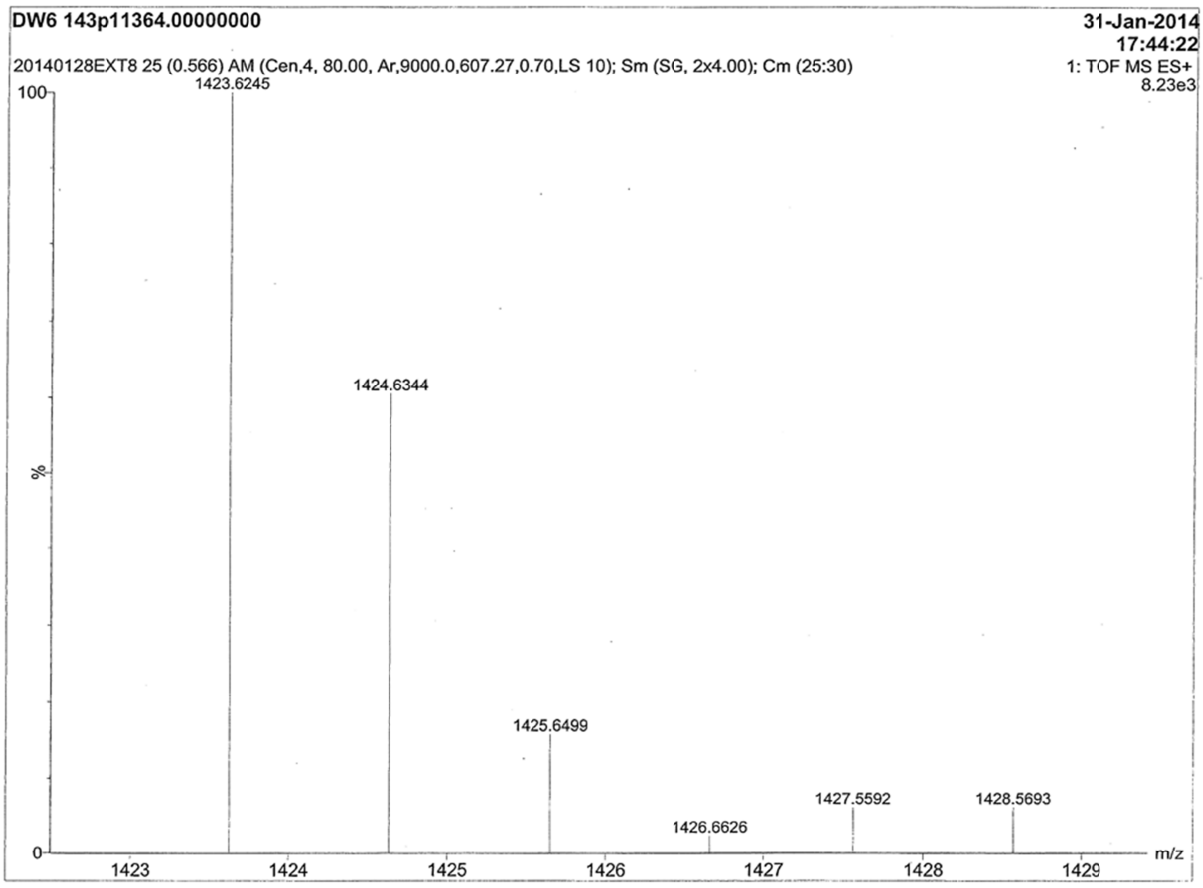

Figure S7c. HRMS of compound **10**