Cationic Perylene Antivirals with Aqueous Solubility for Studies in vivo

Supplementary materials

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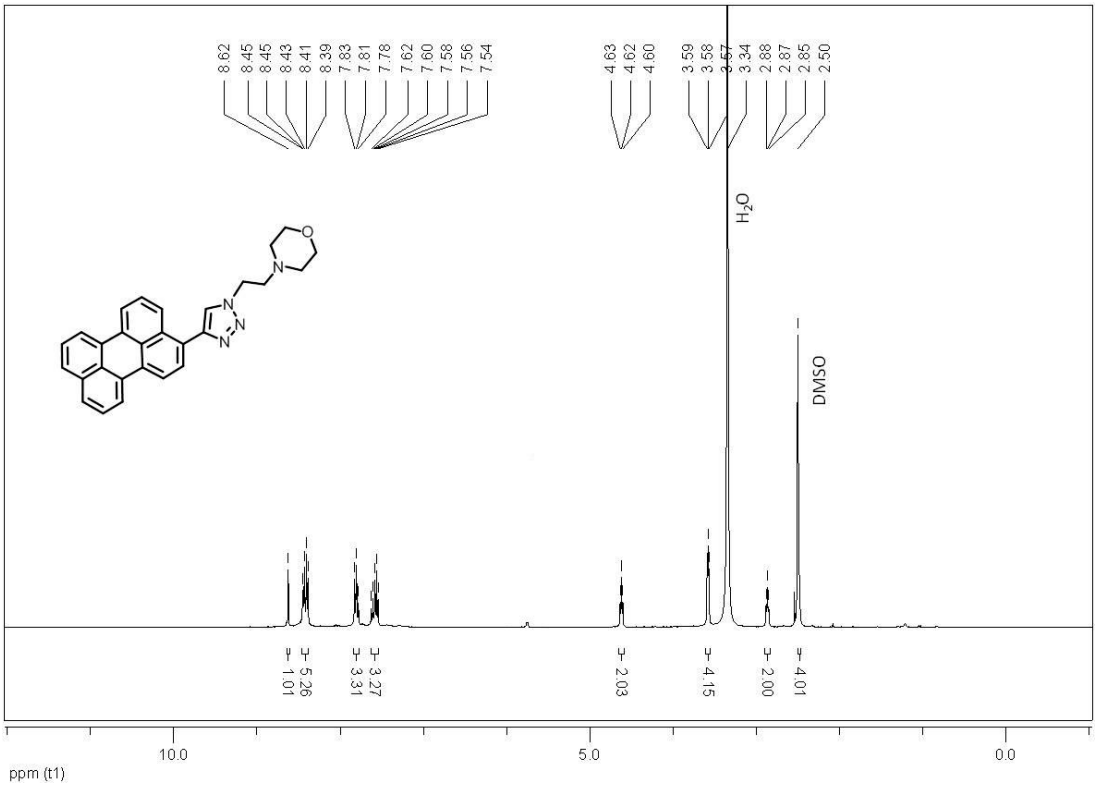
Figure S1. ^{1}H and ^{13}C NMR spectra of the compound **2a**.



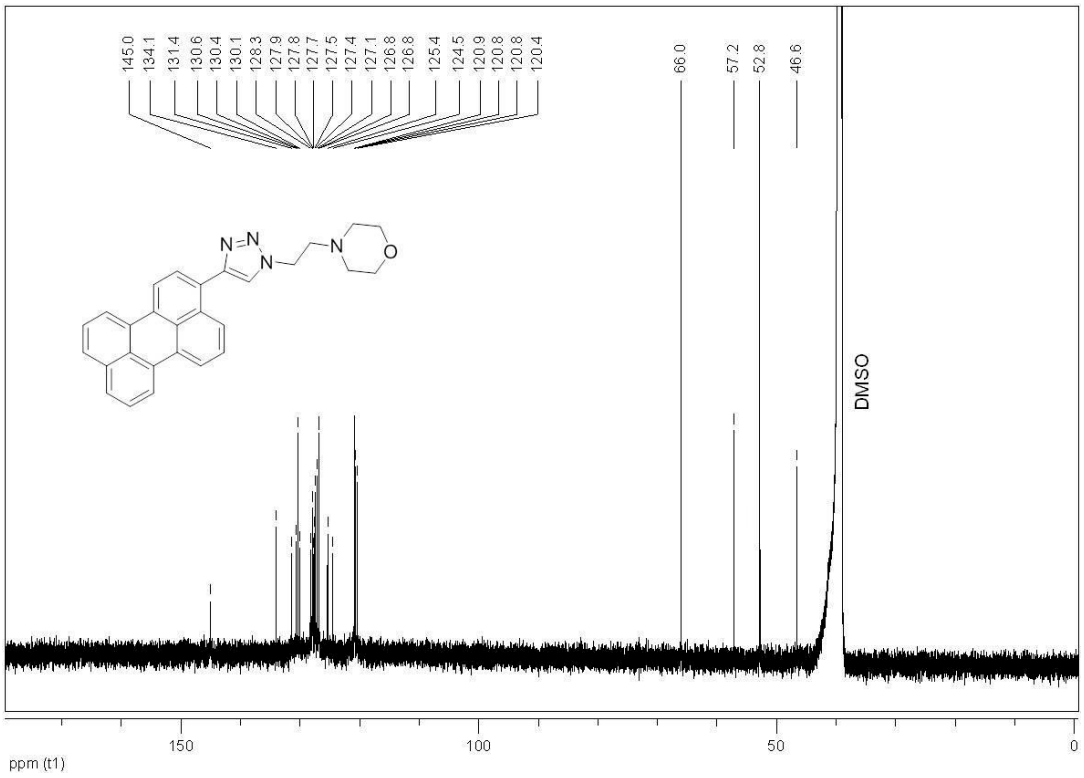


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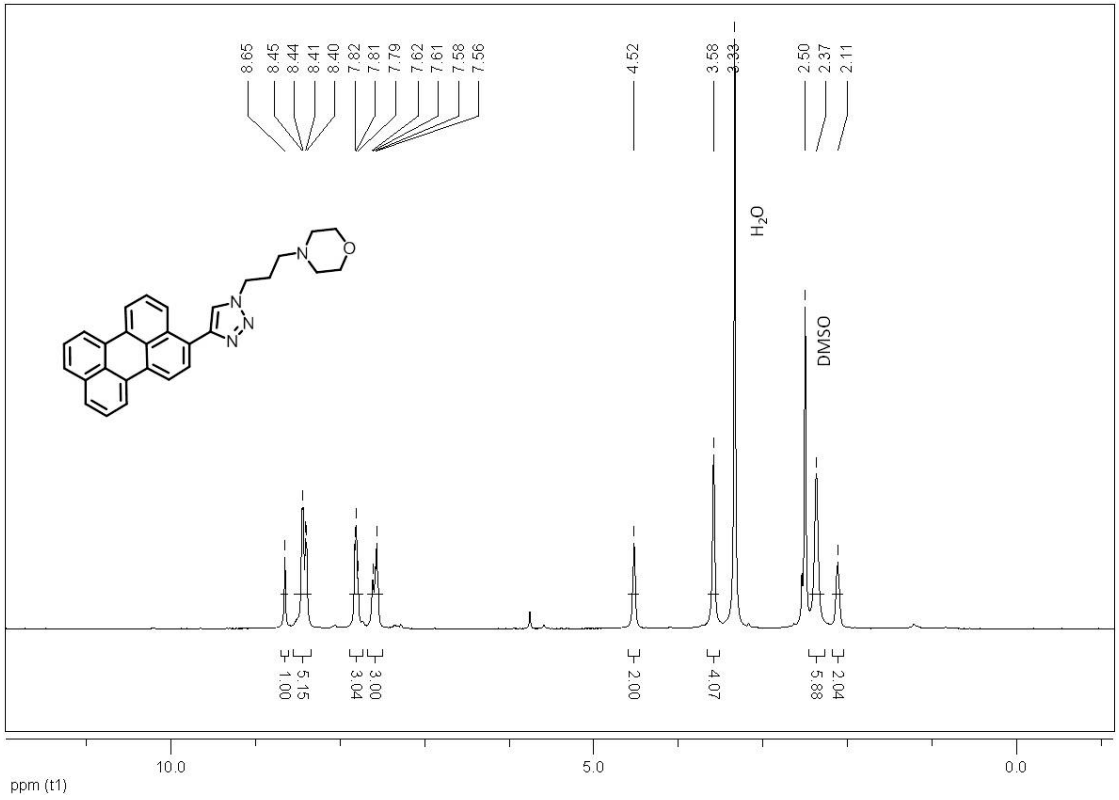
Figure S2. ^{1}H and ^{13}C NMR spectra of the compound **2b**.



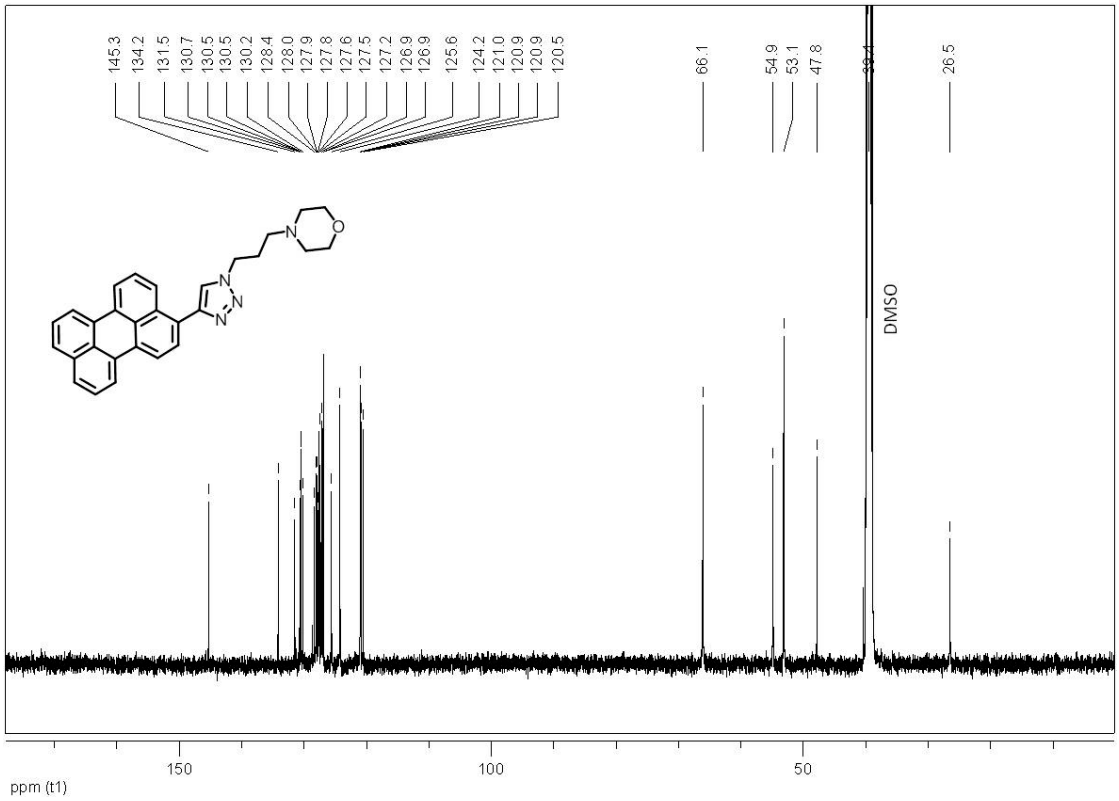


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Figure S3. ^{1}H and ^{13}C NMR spectra of the compound **3a**.

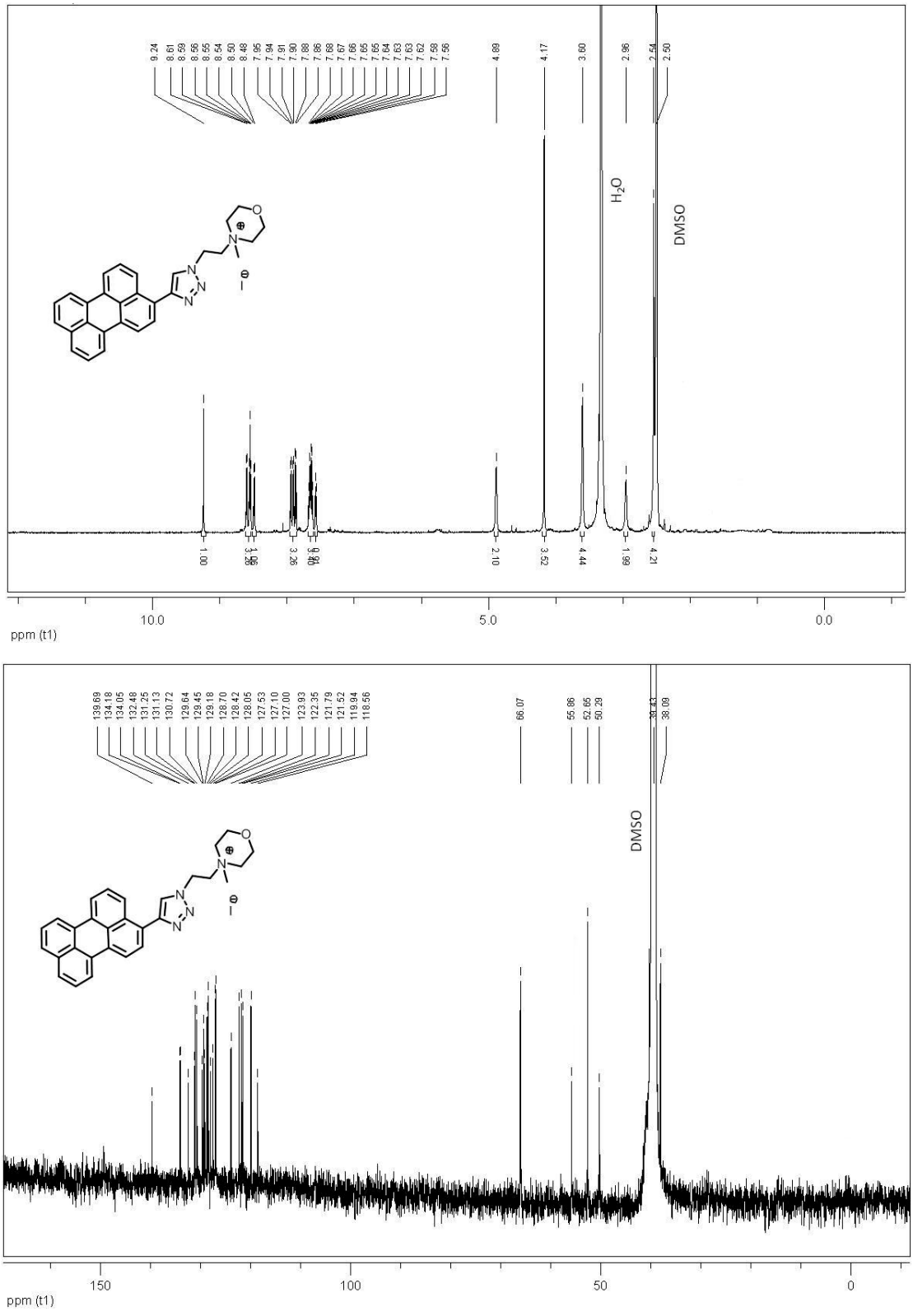

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Figure S4. ^{1}H and ^{13}C NMR spectra of the compound **3b**.

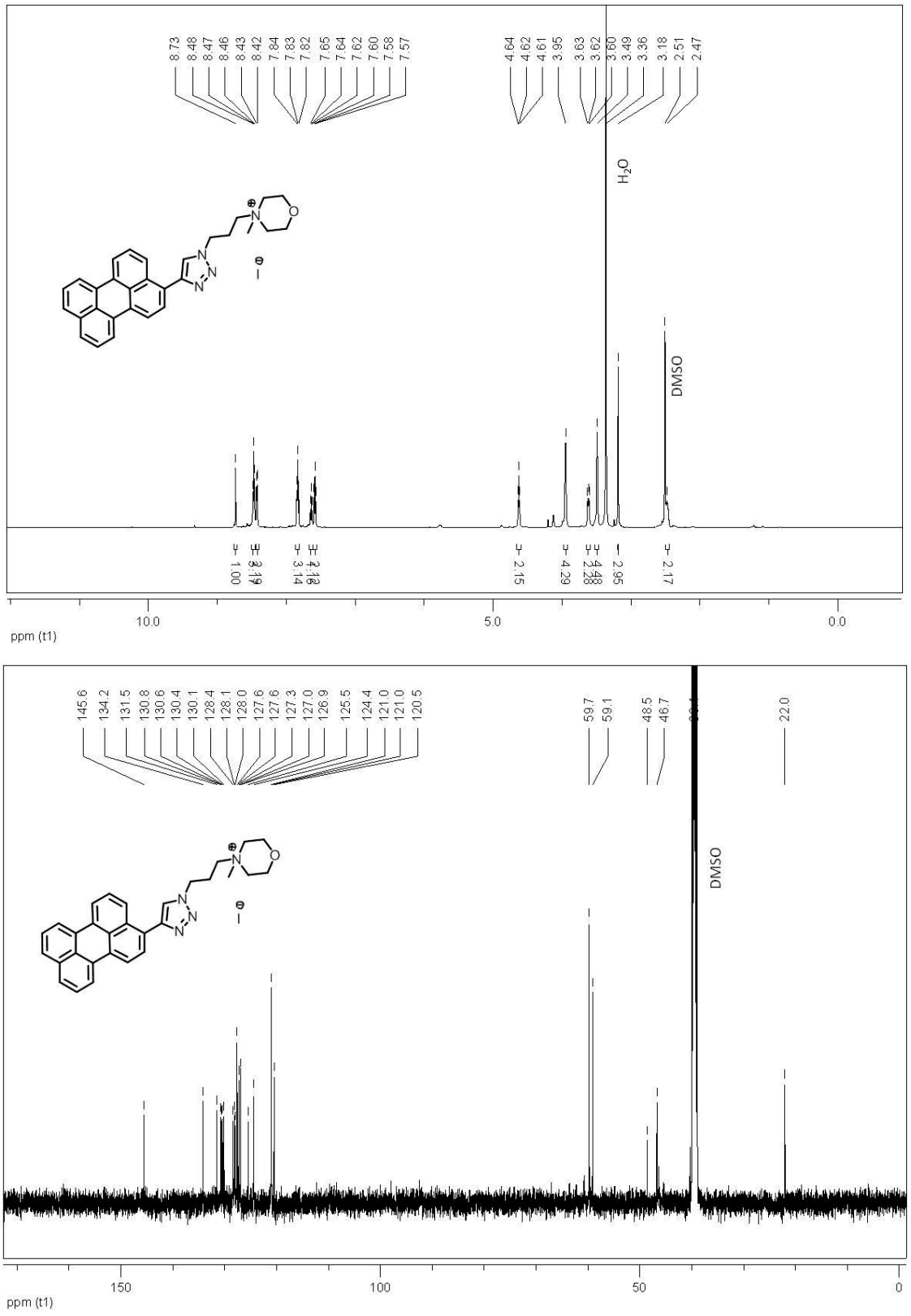

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Figure S5. ^{1}H and ^{13}C NMR spectra of the compound **5**.

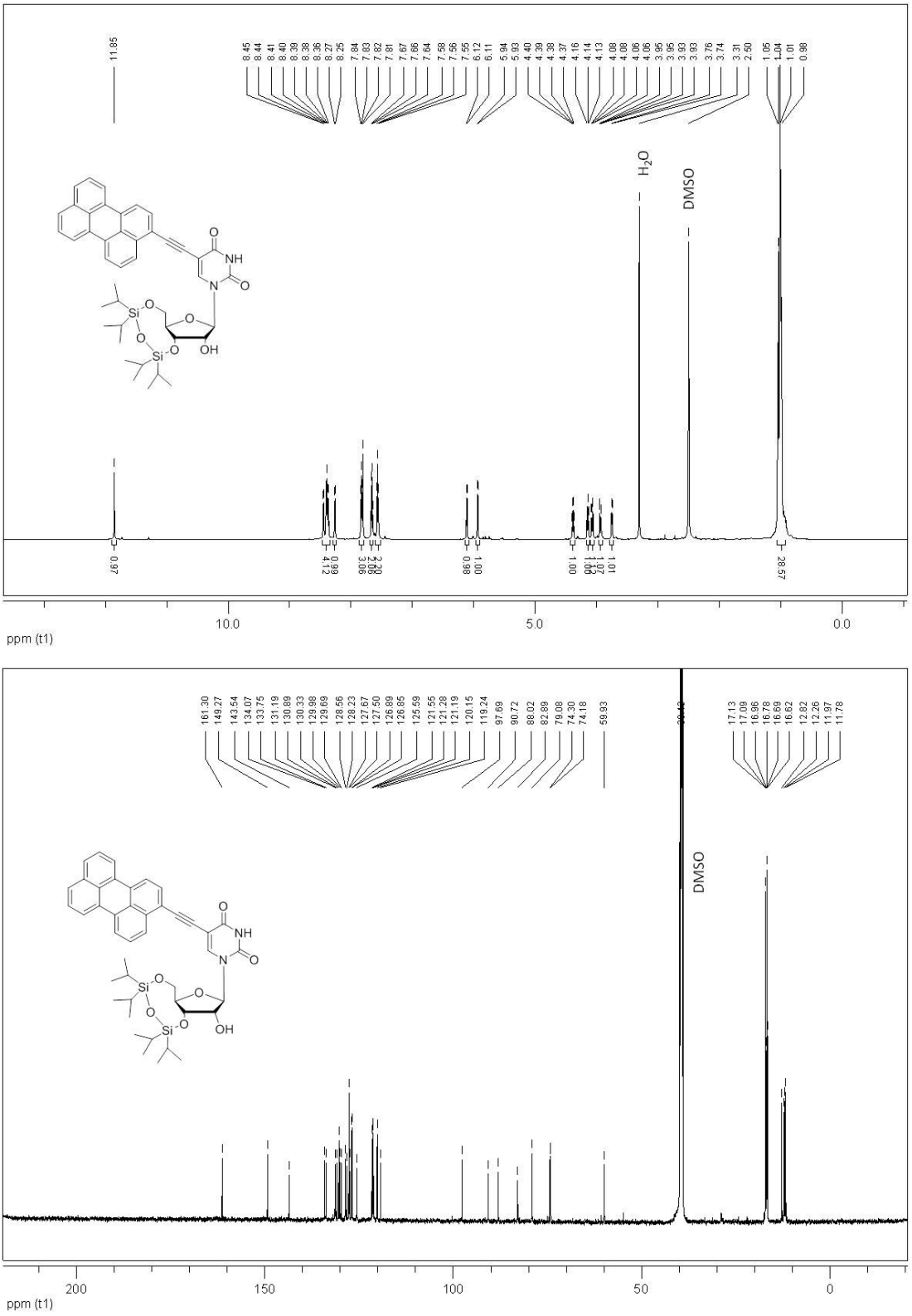

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Figure S6. ^{1}H and ^{13}C NMR spectra of the compound **6**.

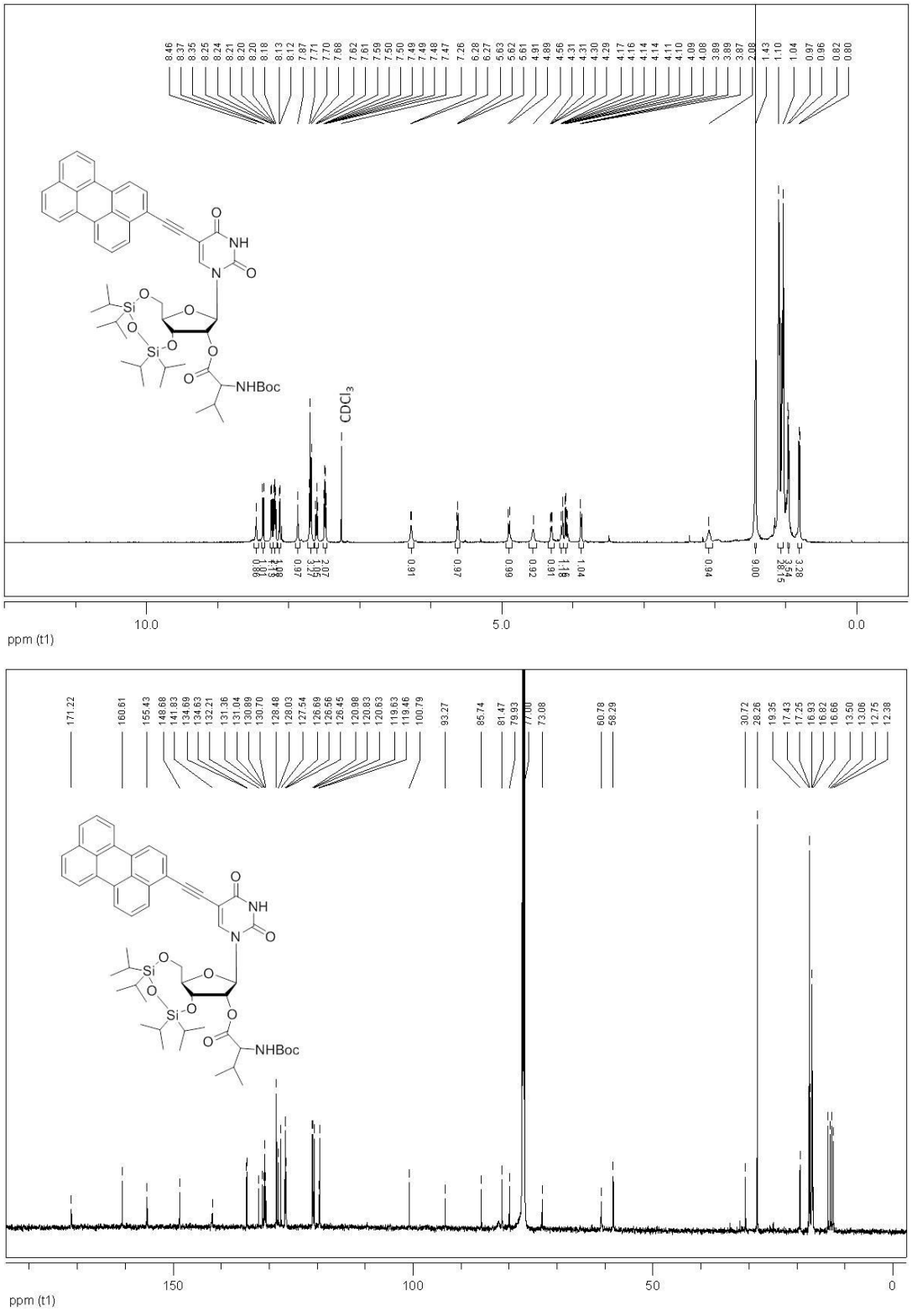

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Figure S7. ^{1}H and ^{13}C NMR spectra of the compound **7**.

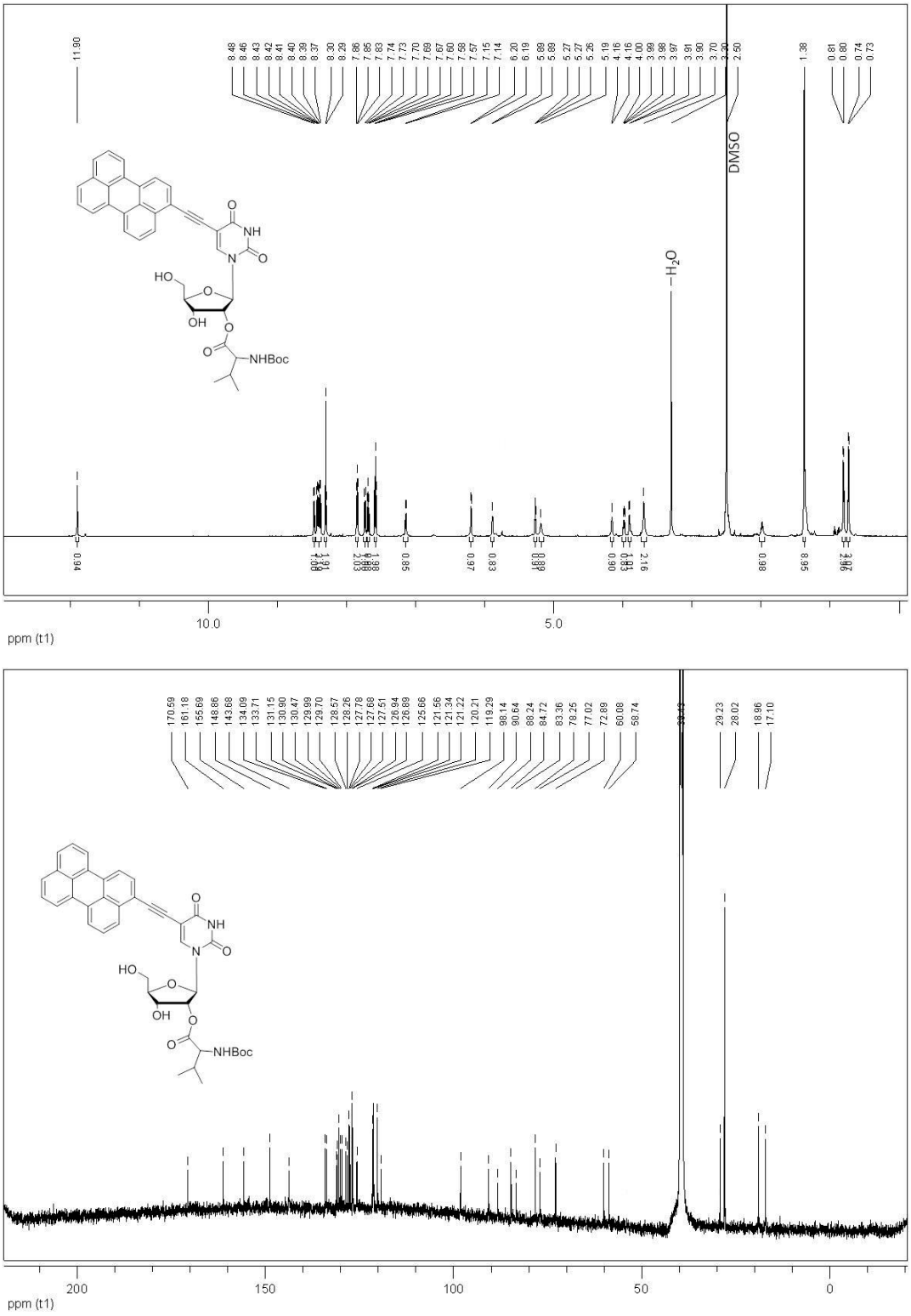

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Figure S8. ^{1}H and ^{13}C NMR spectra of the compound **8**.

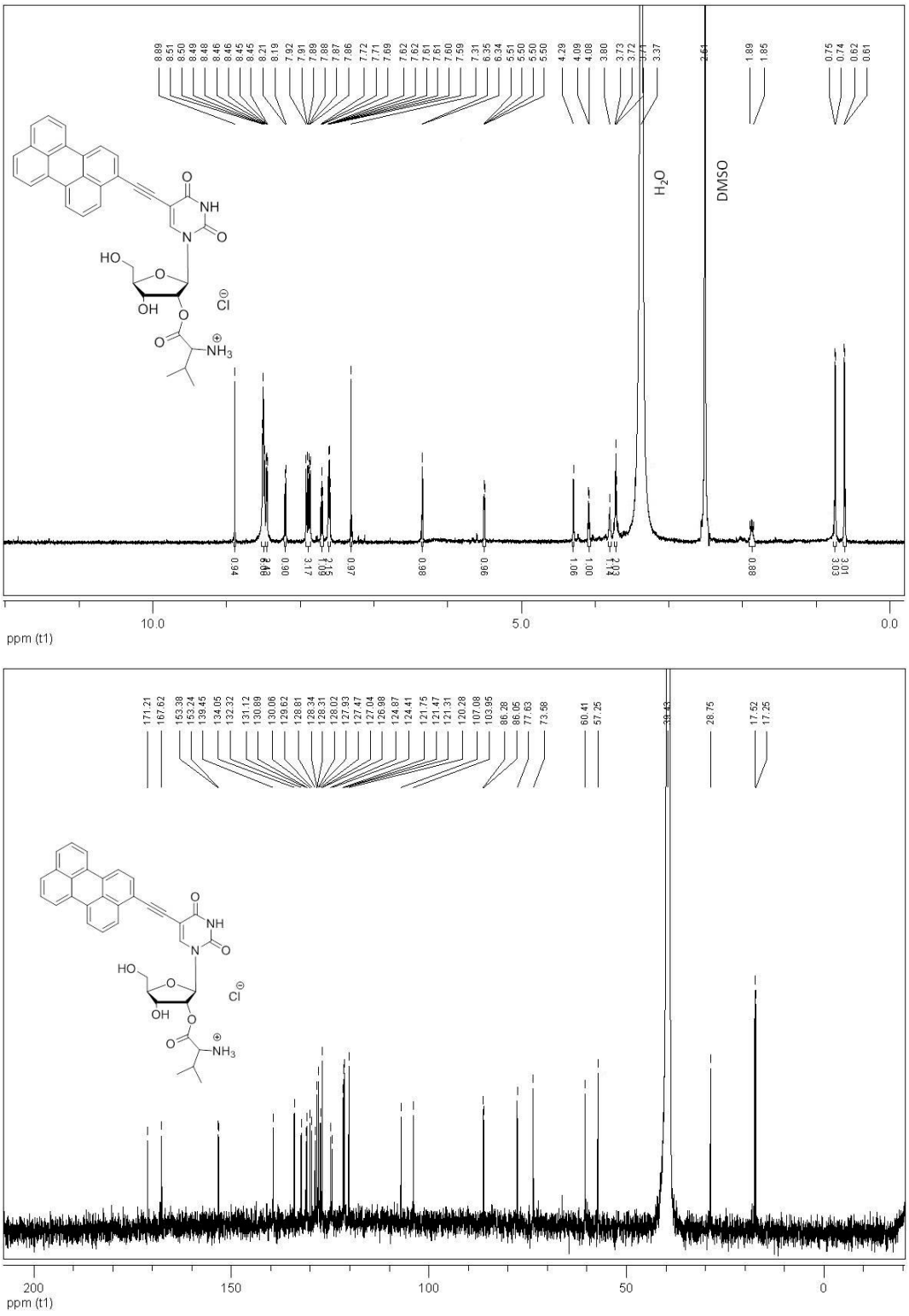

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Figure S9. ^{1}H and ^{13}C NMR spectra of the compound **10**.

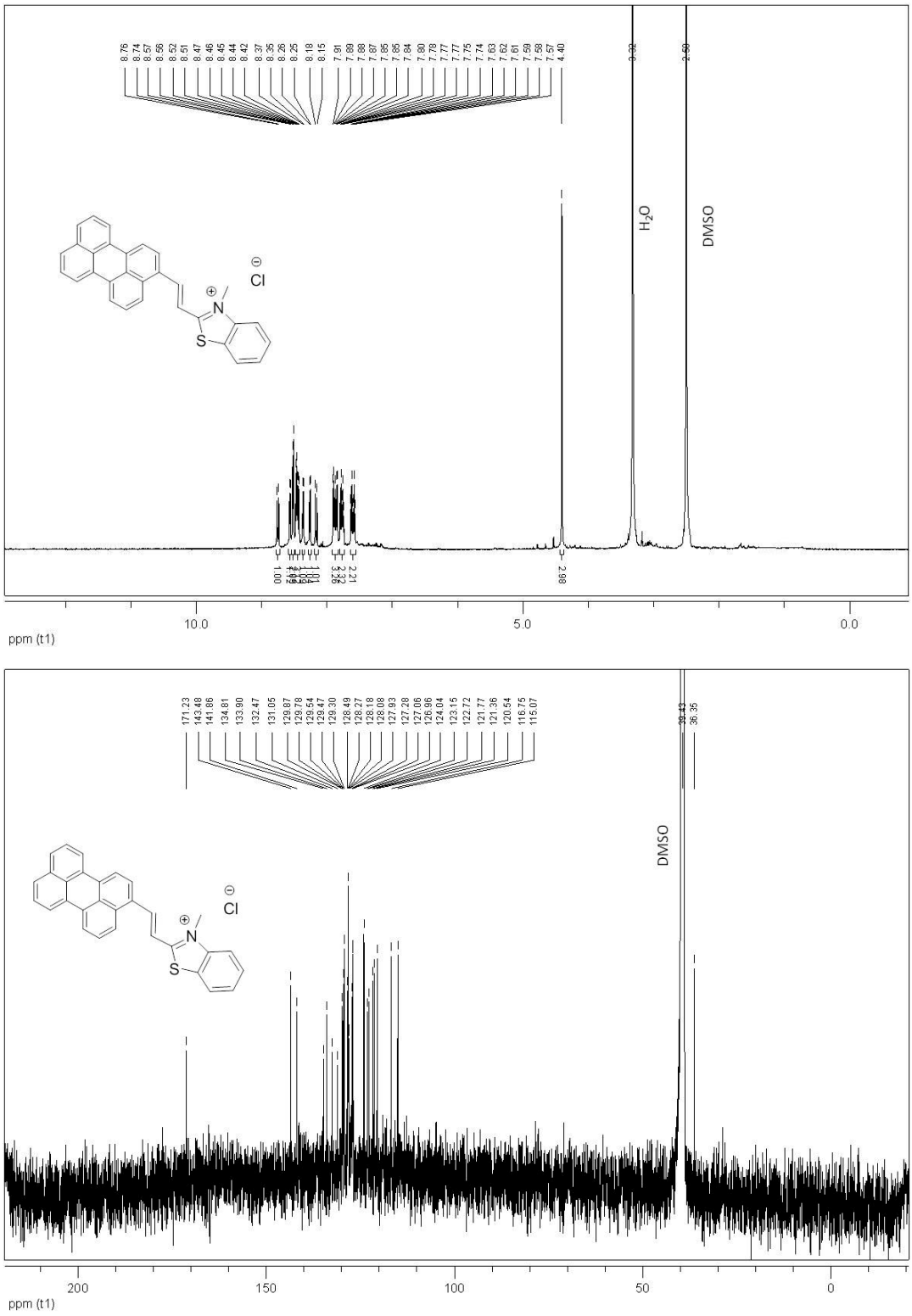

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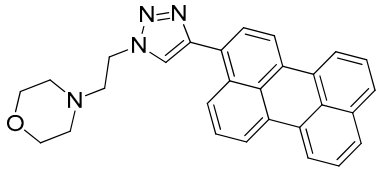
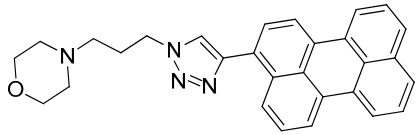
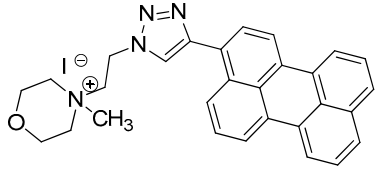
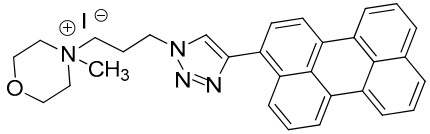
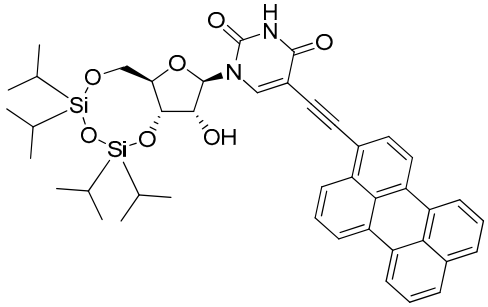
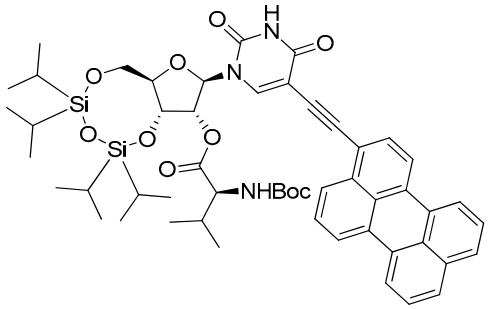
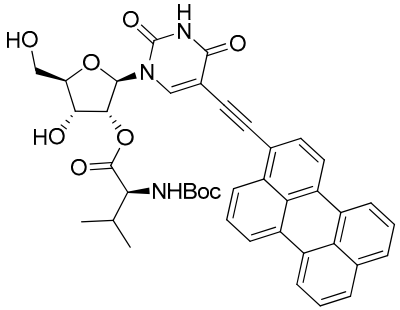
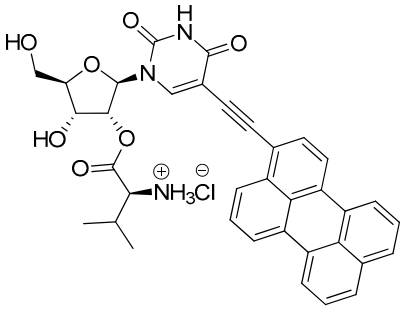
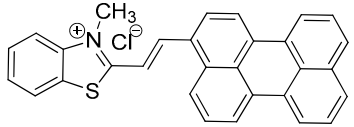
Table S1. Predicted ADMET profiles of the synthesized compounds

compound	Structure	cHIA[a]	clogBB[b]
2a		85.4	0.17
2b		99.97	0.25
3a		10.06	0.04
3b		10.06	0.13
5		83.25	-0.67

6		73.26	0.03
7		42.53	0.53
8		42.53	-0.6
10		97.22	0.01

[a] HIA – human intestinal absorption [%],

[b] LogBB – blood-brain barrier permeability.

Figure S10. Serum stability evaluation

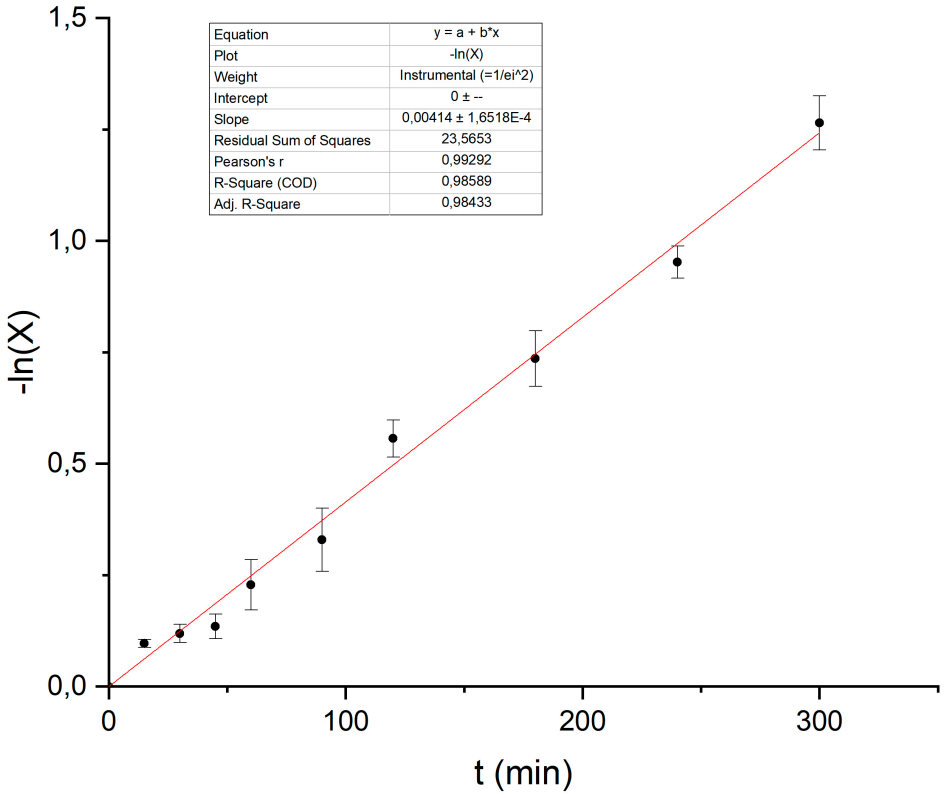


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Figure S11. HPLC trace for compound **3a**

Data File C:\Users\P...cuments\ChemStation\1\Data\Seq1 2022-09-09 22-13-29\005-P2-A8-545.D
Sample Name: 545

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Acq. Operator   : SYSTEM                        Seq. Line :   5
Sample Operator : SYSTEM
Acq. Instrument : LCMS                          Location :   P2-A-08
Injection Date  : 9/9/2022 11:38:16 PM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-09 22-13-29
                  \Purity_test450_SEQ.M
Last changed    : 9/9/2022 10:13:26 PM by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-09 22-13-29
                  \Purity_test450_SEQ.M (Sequence Method)
Last changed    : 9/13/2022 3:37:42 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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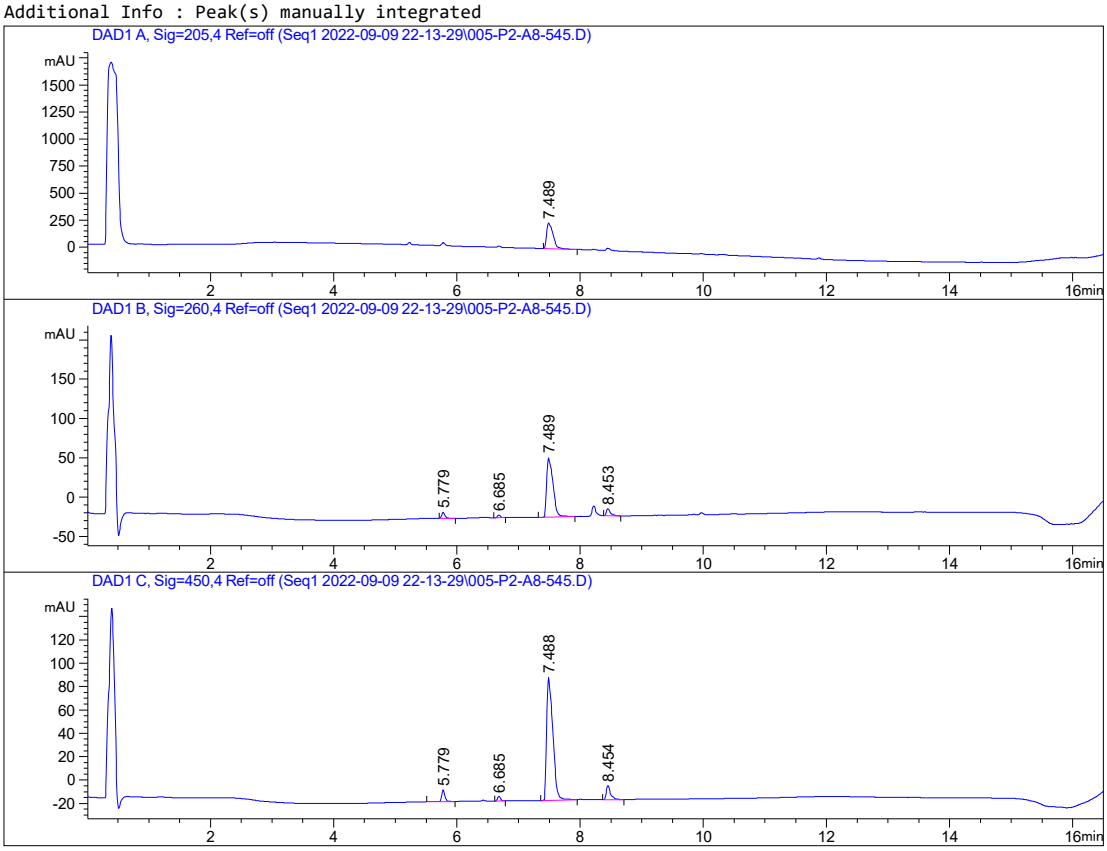

LCMS 9/13/2022 3:55:57 PM SYSTEM Page 1 of 1

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Figure S12. HPLC trace for compound **3b**

```
Data File C:\Users\P...\ChemStation\1\Data\Seq1 2022-09-13 16-06-50\007-P1-A3-ARVI-20-16.D
Sample Name: ARVI-20-16

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Acq. Operator   : SYSTEM                        Seq. Line :   7
Sample Operator : SYSTEM
Acq. Instrument : LCMS                          Location :   P1-A-03
Injection Date  : 9/13/2022 5:59:42 PM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 20.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-13 16-06-50
                  \Purity_test450_SEQ.M
Last changed    : 9/9/2022 10:13:26 PM by SYSTEM
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                  (modified after loading)
Additional Info : Peak(s) manually integrated
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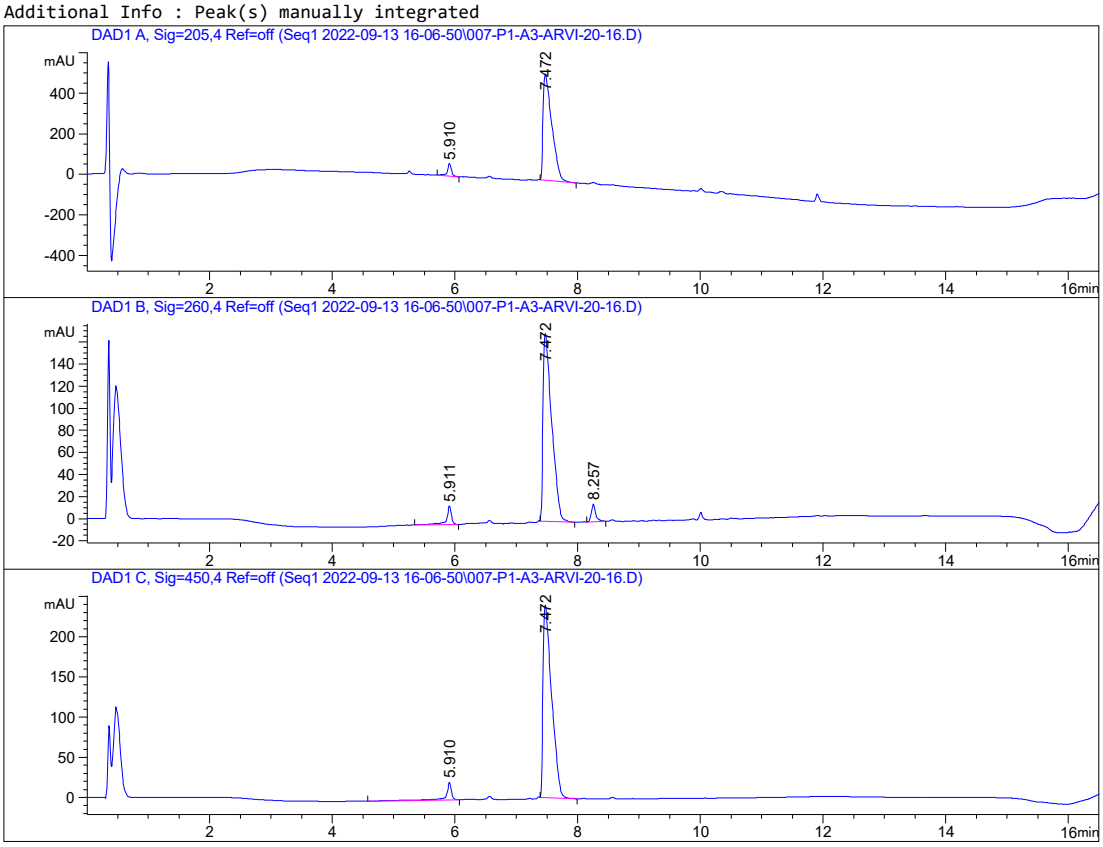

Figure S13. HPLC trace for compound **8**

```
Data File C:\Users\P...ments\ChemStation\1\Data\Seq1 2022-09-13 16-06-50\009-P1-A4-AR554.D
Sample Name: AR554

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Acq. Operator   : SYSTEM                        Seq. Line :   9
Sample Operator : SYSTEM
Acq. Instrument : LCMS                          Location :   P1-A-04
Injection Date  : 9/13/2022 6:35:09 PM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-13 16-06-50
                  \Purity_test450_SEQ.M
Last changed    : 9/9/2022 10:13:26 PM by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-13 16-06-50
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Additional Info : Peak(s) manually integrated
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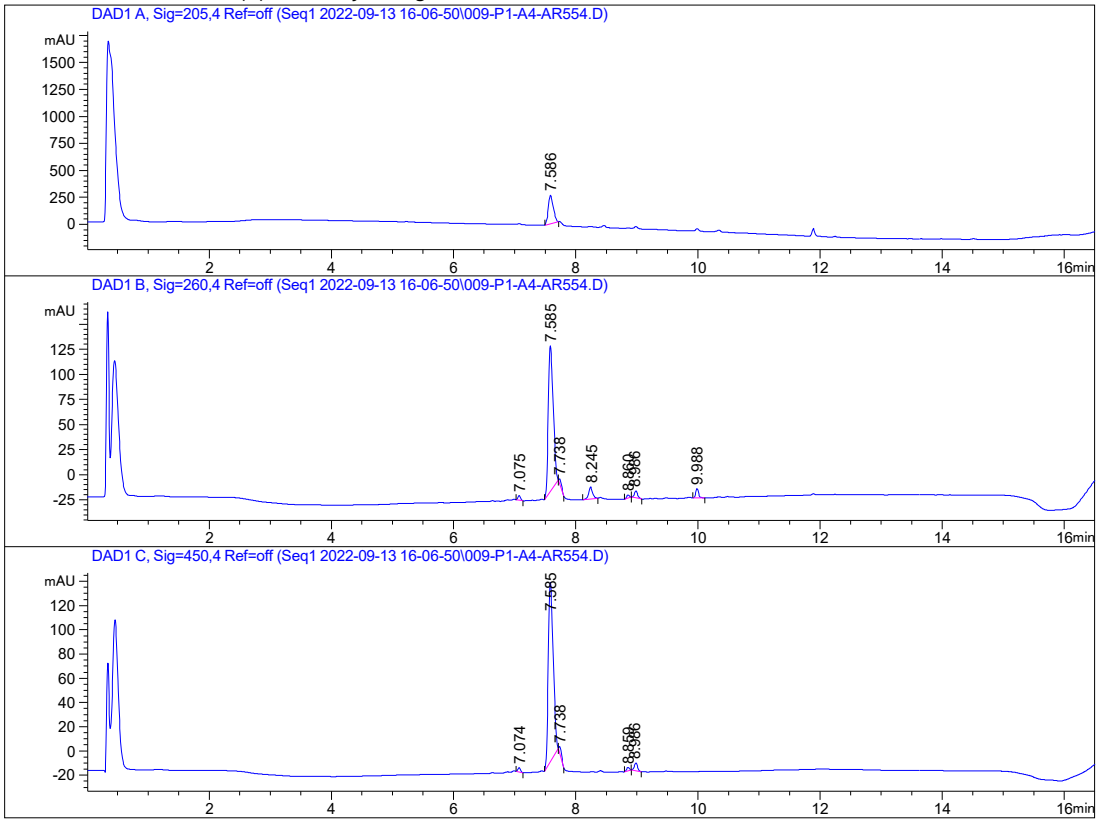

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Figure S14. HPLC trace for compound **10**

Data File C:\Users\P...ments\ChemStation\1\Data\Seq1 2022-09-13 16-06-50\005-P2-A5-AR542.D
Sample Name: AR542

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Sample Operator : SYSTEM
Acq. Instrument : LCMS                          Location :   P2-A-05
Injection Date  : 9/13/2022 5:22:10 PM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\Seq1 2022-09-13 16-06-50
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Last changed    : 9/9/2022 10:05:11 PM by SYSTEM
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Additional Info : Peak(s) manually integrated
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