Supporting Information

Development of anthraquinone derivatives with selectivity for ectonucleoside triphosphate diphosphohydrolases (NTPDases) 2 and 3

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Table S1. Calculated LogD of all anthraquinone derivatives (5, 6& 11–58) using Instant JChem version 5.3.4

| Compound | Structure | ClogD at pH 7.4 |
|----------|-----------|-----------------|
| 5        | ![Structure 5](image) | -1.12           |
| 6        | ![Structure 6](image) | 2.80            |
| 11       | ![Structure 11](image) | 0.55            |
| 12       | ![Structure 12](image) | 1.39            |
| 13       | ![Structure 13](image) | 1.68            |
| 14       | ![Structure 14](image) | 2.28            |
|   | Chemical Structure | Value |
|---|--------------------|-------|
| 15 | ![Structure 15](image) | 3.27  |
| 16 | ![Structure 16](image) | 3.79  |
| 17 | ![Structure 17](image) | 0.08  |
| 18 | ![Structure 18](image) | 3.27  |
| 19 | ![Structure 19](image) | -0.23 |
| 20 | ![Structure 20](image) | 4.26  |
| No. | Image | Value |
|-----|-------|-------|
| 21  | ![Image](Image1.png) | 2.43  |
| 22  | ![Image](Image2.png) | 3.05  |
| 23  | ![Image](Image3.png) | 3.21  |
| 24  | ![Image](Image4.png) | 2.22  |
| 25  | ![Image](Image5.png) | 1.45  |
| 26  | ![Image](Image6.png) | -0.66 |
| 27  | ![Image](Image7.png) | 1.52  |
|   | Structure   |   |  
|---|-------------|---|---  
| 28 | ![Structure 28](image) |   | 1.52  
| 29 | ![Structure 29](image) |   | 1.52  
| 30 | ![Structure 30](image) |   | -1.61  
| 31 | ![Structure 31](image) |   | -1.74  
| 32 | ![Structure 32](image) |   | -1.74  
| 33 | ![Structure 33](image) |   | -1.24  
| 34 | ![Structure 34](image) |   | 3.49  

|   | Chemical Structure | Value |
|---|--------------------|-------|
| 35 | ![Chemical Structure](image1.png) | -1.44 |
| 36 | ![Chemical Structure](image2.png) | -0.98 |
| 37 | ![Chemical Structure](image3.png) | 2.10  |
| 38 | ![Chemical Structure](image4.png) | 3.40  |
| 39 | ![Chemical Structure](image5.png) | 4.38  |
| 40 | ![Chemical Structure](image6.png) | 3.78  |
| 41 | ![Chemical Structure](image7.png) | 4.47  |
|     | Chemical Structure | Value   |
|-----|-------------------|---------|
| 42  | ![Chemical 42](image) | 0.77    |
| 43  | ![Chemical 43](image) | 4.38    |
| 44  | ![Chemical 44](image) | 4.47    |
| 45  | ![Chemical 45](image) | 5.08    |
| 46  | ![Chemical 46](image) | 4.55    |
| 47  | ![Chemical 47](image) | 4.32    |
|   | Chemical Structure | pKa   |
|---|--------------------|-------|
| 48 | ![Chemical Structure](image1) | 5.08  |
| 49 | ![Chemical Structure](image2) | 5.50  |
| 50 | ![Chemical Structure](image3) | 5.50  |
| 51 | ![Chemical Structure](image4) | 5.50  |
| 52 | ![Chemical Structure](image5) | 3.31  |
| 53 | ![Chemical Structure](image6) | 7.21  |
| 54 | ![Chemical Structure](image7) | 6.14  |
| 55 | ![Chemical Structure](image) | 5.84 |
|----|----------------------------|------|
| 56 | ![Chemical Structure](image) | 6.95 |
| 57 | ![Chemical Structure](image) | 2.61 |
| 58 | ![Chemical Structure](image) | -1.72 |
Figure S1. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra of sodium 1-amino-4-(3-iodophenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (23) in DMSO-$d_6$
Figure S2. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(2-(hydroxymethyl)phenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (27) in DMSO-$d_6$
Figure S3. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(3-(hydroxymethyl)phenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (28) in DMSO-$d_6$
Figure S4. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(4-(hydroxymethylphenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (29) in DMSO-$d_6$.
Figure S5. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(3-(carboxymethyl)phenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (30) in DMSO-$d_6$
Figure S6. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(2,3-dichlorophenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (34) in DMSO-$d_6$
Figure S7. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(2-carboxy-3-fluorophenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (35) in DMSO-$d_6$
Figure S8. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(2-fluoro-4-hydroxyphenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (37) in DMSO-$d_6$
Figure S9. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(3-phenylsulfanylphenylamino)-9,10-dioxo-9,10-dihydro-anthracene-2-sulfonate (41) in DMSO-$d_6$.
Figure S10. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-Amino-4-[4-(4-chlorophenylthio)phenylamino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (45) in DMSO-$d_6$. 
Figure S11. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-[4-(4-methoxyphenylthio)phenylamino]-9,10-dioxo-9,10-dihydroanthracene-2-sulfonate (47) in DMSO-$d_6$.
Figure S12. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra sodium 1-amino-4-(3-chloro-4-phenylsulfanyl)phenylamino-9,10-dioxo-9,10-dihydro-anthracene-2-sulfonate (48) in DMSO-$d_6$
Figure S13. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra of 1-amo}$^1$-bromo-4-(3-ethylphenylamino)anthracene-9,10-dione (53) in DMSO-$d_6$
Figure S14. $^1$H (500 MHz) and $^{13}$C (126 MHz) spectra of 4-(3-Fluorophenylamino)-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (57) in DMSO-$d_6$. 
Figure S15. LC-MS spectrum of compound 23*

* The purity of compound 23 is 100% (retention time: 18.97 belongs to the desired compound 23).
Figure S16. LC-MS spectrum of compound 27*

* The purity of compound 27 is 100% (retention time: 20.83 belongs to the desired compound 27).
Figure S17. LC-MS spectrum of compound 28*

* The purity of compound 28 is 100% (retention time: 21.60 belongs to the desired compound 28).
Figure S18. LC-MS spectrum of compound 29*

* The purity of compound 29 is 98% (retention time: 21.60 belongs to the desired compound 29).
Figure S19. LC-MS spectrum of compound 30*

* The purity of compound 30 is 100% (retention time: 10.60 belongs to the desired compound 30).
Figure S20. LC-MS spectrum of compound 34*

* The purity of compound 34 is 100% (retention time: 17.29 belongs to the desired compound 34).
Figure S21. LC-MS spectrum of compound 35*

* The purity of compound 35 is 98% (retention time: 14.44 belongs to the desired compound 35).
Figure S22. LC-MS spectrum of compound 37*

* The purity of compound 37 is 97% (retention time: 18.06 belongs to the desired compound 37).
Figure S23. LC-MS spectrum of compound 41*

* The purity of compound 41 is 99.4% (retention time: 11.59 belongs to the desired compound 41).
Figure S24. LC-MS spectrum of compound 45*

*The purity of compound 45 is 99% (retention time: 12.02 belongs to the desired compound 45).
Figure S25. LC-MS spectrum of compound 47*

* The purity of compound 47 is 98.9% (retention time: 11.74 belongs to the desired compound 47).
Figure S26. LC-MS spectrum of compound 48*

* The purity of compound 48 is 97.7% (retention time: 12.06 belongs to the desired compound 48).
The purity of compound 53 is 95% (retention time: 14.83 belongs to the desired compound 53).
Figure S28. LC-MS spectrum of compound 57*

* The purity of compound 57 is 99% (retention time: 10.36 belongs to the desired compound 57).