Cationic and betaine-type boronated acridinium dyes: synthesis, characterization and photocatalytic activity

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Supporting Information

Table of contents

1 NMR spectra of compounds 1-10 ................................................................................. S3
2 Optical properties – additional information ............................................................. S12
3 Theoretical calculations ......................................................................................... S18
4 Thermal analysis .................................................................................................. S28
5 HR-MS ................................................................................................................ S32
1 NMR spectra of compounds 1-10

Figure S1. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 1.

Figure S2. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of 1.
Figure S3. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 2.

Figure S4. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 2.
Figure S5. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 4.

Figure S6. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 4.

S5
Figure S7. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 5.

Figure S8. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 5.
Figure S9. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 6.

Figure S10. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 6.
Figure S11. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 7.

Figure S12. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 7.
Figure S13. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 8.

Figure S14. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 8.
Figure S15. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 9.

Figure S16. $^{13}$C NMR spectrum (101 MHz, CDCl$_3$) of compound 9.
Figure S17. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 10.

Figure S18. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 10.
2 Optical properties – additional information

Figure S19. Overlay of UV-VIS absorption spectra of 5-10 in DCM.

Figure S20. Overlay of UV-VIS absorption spectra of 5-10 in MeCN.
Figure S21. Overlay of UV-VIS absorption spectra of 5-10 in PhMe.

Figure S22. Overlay of UV-VIS absorption spectra of 5 and 8 in various solvents.

Figure S23. Overlay of UV-VIS absorption spectra 6 and 9 in various solvents.
Figure S24. Overlay of UV-VIS absorption spectra of 7 and 10 in various solvents.

Table S1. The complete list of UV-VIS absorption bands of compounds 5–10 in various solvents.

| compound | solvent | \( \lambda_{\text{max}} \)/ nm | \( \varepsilon \)/dm\(^3\)mol\(^{-1}\)cm\(^{-1}\) |
|----------|---------|-----------------|------------------|
| 5        | DCM     | 436             | 8780             |
|          |         | 362             | 23600            |
|          | MeCN    | 430             | 8130             |
|          |         | 361             | 20200            |
|          | PhMe    | 432             | 10400            |
|          |         | 375             | 32800            |
| 6        | DCM     | 436             | 11800            |
|          |         | 362             | 31200            |
|          | MeCN    | 430             | 10300            |
|          |         | 361             | 27300            |
|          | PhMe    | 434             | 7790             |
|          |         | 336             | 17500            |
| 7        | DCM     | 431             | 10700            |
|          |         | 360             | 27800            |
|          | MeCN    | 428             | 9880             |
|          |         | 360             | 27500            |
|          | PhMe    | 433             | 10400            |
|          |         | 364             | 25420            |
| 8        | DCM     | 446             | 12700            |
|          |         | 358             | 19500            |
|          | MeCN    | 435             | 9660             |
|          |         | 359             | 17500            |
|          | PhMe    | --              | --               |
| 9        | DCM     | 441             | 10800            |
|          |         | 357             | 18700            |
|          | MeCN    | 431             | 10900            |
|          |         | 359             | 22200            |
|        | PhMe  | DCM  | MeCN | PhMe |
|--------|-------|------|------|------|
| λ / nm |   436 |   430 |   426 |   433 |
|        |   361 |   356 |   356 |   357 |
| ε    |  8470 | 10900 | 10200 |  7630 |
|        | 14000 |  21800 |  19600 |  7630 |

**Figure S25.** Overlay of normalized UV-VIS absorption and emission bands for 5 and 8 in DCM.

**Figure S26.** Overlay of normalized UV-VIS absorption and emission bands for 6 and 9 in DCM.
Figure S27. Overlay of normalized UV-VIS absorption and emission bands for 7 and 10 in DCM.

Figure S28. Overlay of normalized UV-VIS absorption and emission bands for 5 in toluene. For comparison, emission spectrum in DCM was also depicted by thin dotted line.
Figure S29. Overlay normalized UV-VIS absorption and emission bands for 6 and 9 in PhMe. For comparison, emission spectrum in DCM was also depicted by thin dash-dot line.

Figure S30. Overlay of normalized UV-VIS absorption and emission bands for 7 and 10 in PhMe. For comparison, emission spectrum in DCM was also depicted by thin dash-dot line.
3 Theoretical calculations

Figure S31. The disposition of molecular orbitals from HOMO-4 to LUMO in 5. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ⁻³.
Figure S32. The disposition of molecular orbitals from HOMO-4 to LUMO in 6. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ⁻³.
Figure S33. The disposition of molecular orbitals from HOMO-4 to LUMO in 7. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ$^{-3}$. 
Figure S34. The disposition of molecular orbitals from HOMO-4 to LUMO in 8. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ⁻³.

Figure S35. The disposition of molecular orbitals from HOMO-4 to LUMO in 9. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ⁻³.
Figure S36. The disposition of molecular orbitals from HOMO-4 to LUMO in 10. Blue and red areas correspond to negative and positive signs of the function, respectively, depicted with isovalue of 0.2 eÅ⁻³.

Table S2. Selected atomic charges (all values given in e) in 5-10 calculated at PBE0/6-311+G(d,p) level of theory.

|          | 5 \( (p\text{-BOH}_2) \) | 6 \( (m\text{-BOH}_2) \) | 7 \( (o\text{-BOH}_2) \) | 8 \( (p\text{-BF}_3) \) | 9 \( (m\text{-BF}_3) \) | 10 \( (o\text{-BF}_3) \) |
|----------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| N        | 0.967                | 0.918                | 1.103                | 1.204                | 1.205                | 1.184                |
| B        | 0.623                | 0.612                | 0.426                | 0.847                | 0.886                | 0.889                |
| C9       | 1.200                | 1.024                | 1.081                | 0.355                | 0.389                | 0.571                |
| C10      | 0.781                | 0.084                | 0.823                | 1.378                | 1.297                | 1.033                |
Table S3. Group charges (all values given in e) in 5-10 calculated at PBE0/6-311+G(d,p) level of theory.

|       | 5 (p-B(OH)₂) | 6 (m-B(OH)₂) | 7 (o-B(OH)₂) | 8 (p-BF₃) | 9 (m-BF₃) | 10 (o-BF₃) |
|-------|--------------|--------------|--------------|-----------|-----------|-----------|
| NPh   | -0.295       | -0.433       | -0.223       | -0.127    | -0.122    | -0.334    |
| Acr   | 1.454        | 1.206        | 1.174        | 0.822     | 0.853     | 1.077     |
| B     | -0.281       | 0.166        | -0.056       | -0.696    | -0.731    | -0.743    |
| ClO₄⁻ | -0.878       | -0.939       | -0.895       | -         | -         | -         |

Table S4. Cartesian coordinates for optimized structure of 5.

| Atom | x     | y     | z     | Atom | x     | y     | z     |
|------|-------|-------|-------|------|-------|-------|-------|
| C1   | -0.6281 | 3.2935 | -1.9004 | H31  | 5.7809 | 2.2043 | 1.3510 |
| C2   | -1.3111 | 2.4416 | -1.0737 | C32  | -2.7106 | 0.6507 | 0.5351 |
| C3   | -0.6015 | 1.5410 | -0.2520 | C33  | -3.4293 | 1.5462 | 1.3218 |
| C4   | 0.8232  | 1.5309 | -0.2863 | C34  | -3.3564 | -0.2664 | -0.2778 |
| C5   | 1.4860  | 2.4214 | -1.1727 | C35  | -4.8111 | 1.5279 | 1.2852 |
| C6   | 0.7810  | 3.2880 | -1.9568 | H36  | -2.9065 | 2.2539 | 1.9573 |
| C7   | 1.5266  | 0.5985 | 0.4953  | C37  | -4.7467 | -0.2861 | -0.3135 |
| C8   | 0.8166  | -0.2806 | 1.3285 | H38  | -2.7709 | -0.9793 | -0.8535 |
| C9   | -0.6083 | -0.2338 | 1.3476 | H39  | -5.4802 | 0.6124 | 0.4640 |
| C10  | -1.3234 | -1.1172 | 2.1824 | H40  | -5.3978 | 2.2130 | 1.8864 |
| H11  | -2.403 | -1.0953 | 2.1835 | H41  | -5.2398 | -1.0105 | -0.9490 |
| C12  | -0.6447 | -2.0129 | 2.9636 | O42  | -6.8262 | 0.6726 | 0.4959 |
| C13  | 0.7650  | -2.0690 | 2.9627 | C3  | -7.5687 | -0.2330 | -0.3121 |
| C14  | 1.4756  | -1.2221 | 2.1650 | H44  | -7.3200 | -1.2640 | -0.0301 |
| H15  | -1.1871 | 3.9725  | -2.5358 | H45  | -7.2959 | -0.0920 | -1.3657 |
| H16  | -2.3924 | 2.4376  | -1.0619 | C46  | -9.0335 | 0.0493 | -0.0906 |
| H17  | 2.5669  | 2.3829  | -1.2261 | H47  | -9.6380 | -0.6297 | -0.6975 |
| H18  | 1.2979  | 3.9555  | -2.6368 | H48  | -9.3015 | -0.0941 | 0.9586 |
| H19  | -1.2071 | -2.6964 | 3.5910 | H49  | -9.2775 | 1.0757 | -0.3740 |
| H20  | 1.2777  | -2.7901 | 3.5889 | N50  | -1.2665 | 0.6705 | 0.5630 |
| H21  | 2.5575  | -1.2567 | 2.1464 | Cl5  | -0.0921 | -2.2278 | -1.7208 |
| C22  | 3.0038  | 0.5178  | 0.4161 | O52  | 1.1319  | -2.5635 | -0.9566 |
| C23  | 3.5960  | -0.5703 | -0.2308 | O53  | -0.1297 | -0.7554 | -1.9290 |
| C24  | 3.8049  | 1.5148  | 0.9754 | O54  | -0.0997 | -2.9244 | 3.0063 |
| C25  | 4.9801  | -0.6413 | -0.3175 | O55  | -1.2833 | -2.5044 | -0.9187 |
| H26  | 2.9605  | -1.3399 | -0.6634 | B56  | 7.3614  | 0.2181 | 0.1119 |
| C27  | 5.1869  | 1.4186  | 0.8881 | O57  | 7.8722  | -0.9185 | -0.4345 |

S23
Table S5. Cartesian coordinates for optimized structure of \( \text{6} \).

![Diagram of \( \text{6} \)](image)

| Atom | \( x \) | \( y \) | \( z \) | Atom | \( x \) | \( y \) | \( z \) |
|------|--------|--------|--------|------|--------|--------|--------|
| C1   | -0.7695| 3.0794 | -2.5059| H31  | 6.8300 | 0.9098 | 0.0719 |
| C2   | -1.3952| 2.3479 | -1.5305| C32  | -2.6548| 0.7397 | 0.3714 |
| C3   | -0.6402| 1.7884 | -0.4787| C33  | -3.6003| 1.6555 | 0.8239 |
| C4   | 0.7711 | 1.9811 | -0.4474| C34  | -3.0403| -0.4677| -0.1887|
| C5   | 1.3773 | 2.7213 | -1.4963| C35  | -4.9456| 1.3620 | 0.7014 |
| C6   | 0.6266 | 3.2724 | -2.4949| H36  | -3.2814| 2.5930 | 1.2682 |
| C7   | 1.5317 | 1.3497 | 0.5546 | C37  | -4.3933| -0.7644| -0.3111|
| C8   | 0.8714 | 0.6405 | 1.5749 | H38  | -2.2826| -1.1832| -0.5002|
| C9   | -0.5431| 0.4842 | 1.5236 | C39  | -5.3524| 0.1503 | 0.1293 |
| C10  | -1.2017| -0.2434| 2.5357 | H40  | -5.7048| 2.0556 | 1.0443 |
| H11  | -2.2740| -0.3750| 2.4897 | H41  | -4.6807| -1.7123| -0.7476|
| C12  | -0.4769| -0.7918| 3.5605 | O42  | -6.6832| -0.0425| 0.0521 |
| C13  | 0.9232 | -0.6413| 3.6324 | C43  | -7.1658| -1.2548| -0.5163|
| C14  | 1.5794 | 0.0562 | 2.6600 | H44  | -6.7860| -2.1067| 0.0619 |
| H15  | -1.3627| 3.5002 | -3.3111| H45  | -6.7967| -1.3485| -1.5455|
| H16  | -2.4635| 2.1841 | -1.5688| C46  | -8.6727| -1.2085| -0.4845|
| H17  | 2.4553 | 2.8230 | -1.4954| H47  | -9.0809| -2.1267| -0.9146|
| H18  | 1.1022 | 3.8327 | -3.2917| H48  | -9.0362| -1.1167| 0.5416 |
| H19  | -0.9952| -1.3539| 4.3302 | H49  | -9.0469| -0.3605| -1.0626|
| H20  | 1.4736 | -1.0833| 4.4548 | N50  | -3.2462| 1.0347 | 0.4887 |
| H21  | 2.6544 | 0.1810 | 2.6967 | C51  | 0.6638 | -2.2769| -1.0782|
| C22  | 3.0065 | 1.3074 | 0.4770 | O52  | 1.9144 | -2.6441| -0.3510|
| C23  | 3.5614 | 0.0677 | 0.1555 | O53  | 0.7295 | -0.8338| -1.4188|
| C24  | 3.8395 | 2.4104 | 0.6624 | O54  | 0.5287 | -3.0879| -2.2843|
| C25  | 4.9344 | -0.0962| 0.0119 | O55  | -0.4863| -2.4880| -0.1727|
| H26  | 2.8894 | -0.7708| 0.0089 | B56  | 5.5126 | -1.4997| -0.4330|
| C27  | 5.2162 | 2.2547 | 0.5291 | O57  | 6.8752 | -1.6015| -0.5263|
| H28  | 3.4198 | 3.3775 | 0.9237 | H58  | 7.1321 | -2.4859| -0.8000|
| C29  | 5.7562 | 1.0189 | 0.1878 | O59  | 4.7695 | -2.5959| -0.7096|
| H30  | 5.8684 | 3.1075 | 0.6895 | H60  | 3.8013 | -2.5466| -0.6589|

Table S6. Cartesian coordinates for optimized structure of \( \text{7} \).

![Diagram of \( \text{7} \)](image)

| Atom | \( x \) | \( y \) | \( z \) | Atom | \( x \) | \( y \) | \( z \) |
|------|--------|--------|--------|------|--------|--------|--------|
| C1   | 0.2467 | -3.3286| -2.3590| H31  | -7.3112| -1.5336| 0.6431 |
| C2   | 0.9074 | -2.5233| -1.4680| C32  | 2.2594 | -0.9093| 0.3547 |
| C3   | 0.1748 | -1.7729| -0.5232| C33  | 2.9824 | -1.8763| 1.0487 |
| C4   | -1.2451| -1.8600| -0.5082| C34  | 2.9027 | 0.0900 | -0.553 |
| C5   | -1.8855| -2.7009| -1.4548| C35  | 4.3636 | -1.8424| 1.0245 |

S24
Table S7. Cartesian coordinates for optimized structure of 8.

| Atom | x       | y       | z       | Atom | x       | y       | z       |
|------|---------|---------|---------|------|---------|---------|---------|
| C6   | -1.1598 | -3.4243 | -2.3578 | H36  | 2.4626  | -2.6511 | 1.6033  |
| C7   | -1.9783 | -1.0809 | 0.4064  | C37  | 4.2931  | 0.1266  | -0.3779 |
| C8   | -1.2968 | -0.2605 | 1.3160  | H38  | 2.3200  | 0.8609  | -0.8521 |
| C9   | 0.1291  | -0.2018 | 1.2814  | C39  | 5.0300  | -0.8400 | 0.3086  |
| C10  | 0.8144  | 0.6269  | 2.1908  | H40  | 4.9527  | -2.5806 | 1.5566  |
| H11  | 1.8927  | 0.6924  | 2.1483  | H41  | 4.7819  | 0.9204  | -0.9280 |
| C12  | 0.1058  | 1.3720  | 3.0946  | O42  | 6.3758  | -0.8899 | 0.3469  |
| C13  | -1.3052 | 1.3214  | 3.1497  | C43  | 7.1151  | 0.1091  | -0.3463 |
| C14  | -1.9855 | 0.5248  | 2.2799  | H44  | 6.8459  | 1.0993  | 0.0425  |
| H15  | 0.8219  | -3.8937 | -3.0850 | H45  | 6.8588  | 0.0798  | -1.4131 |
| C16  | 1.9862  | -2.4484 | -1.4901 | C46  | 8.5809  | -0.1749 | -0.1345 |
| H17  | -2.9679 | -2.7424 | -1.4523 | H47  | 9.1827  | 0.5749  | -0.6544 |
| H18  | -1.6600 | -4.0578 | -3.0814 | H48  | 8.8321  | -1.1427 | 0.9282  |
| H19  | 0.6432  | 2.0256  | 3.7732  | H49  | 8.8453  | -1.1607 | -0.5240 |
| H20  | -1.8361 | 1.9311  | 3.8694  | N50  | 0.8150  | -0.9587 | 0.3715  |
| H21  | -3.0675 | 0.4813  | 2.2987  | C151 | -0.1130 | 3.2581  | -0.7927 |
| C22  | -3.4640 | -1.1725 | 0.4416  | O52  | -0.9594 | 2.8624  | 0.3515  |
| C23  | -4.2714 | -0.2270 | -0.2174 | O53  | -0.7601 | 2.7842  | -0.2054 |
| C24  | -4.0342 | -2.2196 | 1.1667  | O54  | 0.0538  | 4.7067  | -0.8452 |
| C25  | -5.6576 | -0.3894 | -0.1194 | O55  | 1.2068  | 2.5946  | -0.6649 |
| C26  | -5.4154 | -2.3507 | 1.2444  | B56  | -3.6366 | 0.9619  | -1.0554 |
| H27  | -3.3927 | -2.9330 | 1.6756  | O57  | -2.4263 | 0.7479  | -1.5957 |
| C28  | -6.2317 | -1.4337 | 0.5950  | O58  | -4.3006 | 2.1418  | -1.2359 |
| H29  | -6.3105 | 0.3100  | -0.6363 | H59  | -5.0916 | 2.2309  | -0.7042 |
| H30  | -5.8492 | -3.1686 | 1.8104  | H60  | -1.9238 | 1.5475  | -1.8795 |

![Chemical structure of 8](image-url)
Table S8. Cartesian coordinates for optimized structure of 9.

![Chemical structure of 9]

| Atom | x   | y   | z    | Atom | x   | y   | z    |
|------|-----|-----|------|------|-----|-----|------|
| C2   | -1.1993 | -2.1746 | -0.7377 | C29  | 5.6273  | 0.8573 | -0.6876 |
| C3   | -0.6035 | -0.9126 | -0.5521 | H30  | 5.2735  | 2.3907 | -2.1628 |
| C4   | 0.8098  | -0.7732 | -0.6625 | H31  | 6.7087  | 0.9215 | -0.7674 |
| C5   | 1.5681  | -1.9163 | -1.0327 | C32  | -2.8091 | 0.0311 | -0.1872 |
| C6   | 0.9724  | -3.1351 | -1.2113 | C33  | -3.5975 | 0.1588 | -1.3282 |
| C7   | 1.4175  | 0.4934  | -0.4504 | C34  | -3.3918 | -0.2476 | 1.0382 |
| C8   | 0.5800  | 1.5987  | -0.1411 | C35  | -4.9676 | 0.0074 | -1.2362 |
| C9   | -0.8322 | 1.4317  | -0.0856 | H36  | -3.1327 | 0.3757 | -2.2845 |
| C10  | -1.6572 | 2.5403  | 0.1905  | C37  | -4.7703 | -0.4018 | 1.1387 |
| H11  | -2.7319 | 2.4174  | 0.2097  | H38  | -2.7690 | -0.3467 | 1.9213 |
| C12  | -1.0941 | 3.7664  | 0.4462  | C39  | -5.5668 | -0.2745 | -0.0020 |
| C13  | 0.3016  | 3.9359  | 0.4645  | H40  | -5.6018 | 0.1018 | -2.1102 |
| C14  | 1.1161  | 2.8725  | 0.1843  | H41  | -5.2077 | -0.6203 | 2.1044 |
| C15  | -0.8906 | -4.2282 | -1.1859 | O42  | -6.9044 | -0.4043 | -0.0166 |
| C16  | -2.2710 | -2.2827 | -0.6375 | C43  | -7.5814 | -0.6953 | 1.2022 |
| H17  | 2.6364  | -1.8057 | -1.1677 | H44  | -7.3793 | 0.1007 | 1.9303 |
| C18  | 1.5712  | -3.9965 | -1.4828 | H45  | -7.2037 | -1.6408 | 1.6120 |
| H19  | -1.7422 | 4.6097  | 0.6613  | C46  | -9.0551 | -0.7883 | 0.8979 |
| H20  | 0.7295  | 4.8993  | 0.7167  | H47  | -9.6089 | -1.0113 | 1.8134 |
| H21  | 2.1929  | 2.9766  | 0.2235  | H48  | -9.4271 | 0.1544 | 0.4906 |
| C22  | 2.8639  | 0.6456  | -0.5337 | H49  | -9.2520 | -1.5818 | 0.1737 |
| C23  | 3.6969  | -0.1772 | 0.2421  | N50  | -1.3807 | 0.1885 | -0.2813 |
| C24  | 3.4423  | 1.5989  | -1.3903 | B51  | 5.9941  | -1.0600 | 1.1383 |
| C25  | 5.0839  | -0.0805 | 0.1954  | F52  | 7.2914  | -1.1569 | 0.6044 |
| H26  | 3.2528  | -0.8952 | 0.9269  | F53  | 6.0421  | -0.5334 | 2.4452 |
| C27  | 4.8224  | 1.6852  | -1.4712 | F54  | 5.3798  | -2.3377 | 1.1727 |

Table S9. Cartesian coordinates for optimized structure of 10.

![Chemical structure of 10]

| Atom | x   | y   | z    | Atom | x   | y   | z    |
|------|-----|-----|------|------|-----|-----|------|
| C1   | -0.1573 | -3.2876 | -1.3636 | C28  | 6.1528  | 0.3988 | -0.4615 |
| C2   | -0.8763 | -2.1534 | -1.0730 | H29  | 5.9798  | -0.5604 | 1.4538 |
| C3   | -0.1971 | -0.9489 | -0.8105 | H30  | 6.0140  | 1.3727 | -2.3816 |
| C4   | 1.2252  | -0.9220 | -0.8387 | H31  | 7.2380  | 0.4346 | -0.4331 |
| C5   | 1.9239  | -2.1195 | -1.1386 | C32  | -2.3239 | 0.1374 | -0.4019 |
| C6   | 1.2486  | -3.2779 | -1.4030 | C33  | -3.1345 | 0.3640 | -1.5108 |
| C7   | 1.9102  | 0.2755  | -0.5533 | C34  | -2.8853 | -0.1537 | 0.8305 |
| C8   | 1.1640  | 1.4529  | -0.3290 | C35  | -4.5089 | 0.2994 | -1.3798 |
| C9   | -0.2560 | 1.3966  | -0.3091 | H36  | -2.6845 | 0.5893 | -2.4722 |
| C10  | -0.9963 | 2.5679  | -0.0503 | C37  | -4.2674 | -0.2205 | 0.9692 |
|     |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| H11 | -2.0775 | 2.5292 | -0.0351 | H38 | -2.2404 | -0.3307 | 1.6853 |
| C12 | -0.3402 | 3.7500 | 0.1880 | C39 | -5.0870 | 0.0063 | -0.1388 |
| C13 | 1.0657 | 3.8182 | 0.1968 | H40 | -5.1618 | 0.4714 | -2.2279 |
| C14 | 1.7981 | 2.6898 | -0.0485 | H41 | -4.6887 | -0.4498 | 1.9395 |
| H15 | -0.6924 | -4.2103 | -1.5644 | O42 | -6.4322 | -0.0348 | -0.1139 |
| H16 | -1.9573 | -2.1823 | -1.0435 | C43 | -7.0862 | -0.3326 | 1.1145 |
| H17 | 3.0055 | -2.0910 | -1.1352 | H44 | -6.8091 | 0.4168 | 1.8671 |
| H18 | 1.7921 | -4.1893 | -1.6221 | H45 | -6.7588 | -1.3167 | 1.4737 |
| H19 | -0.9224 | 4.6442 | 0.3863 | C46 | -8.5722 | -0.3178 | 0.8591 |
| H20 | 1.5620 | 4.7570 | 0.4141 | H47 | -9.1096 | -0.5432 | 1.7838 |
| H21 | 2.8806 | 2.7089 | -0.0197 | H48 | -8.8944 | 0.6633 | 0.5029 |
| C22 | 3.3886 | -0.3039 | -0.5104 | H49 | -8.8442 | -1.0656 | 0.1108 |
| C23 | 4.0504 | -0.2453 | 0.6007 | N50 | -0.8909 | 0.2003 | -0.5250 |
| C24 | 4.0840 | 0.8928 | -1.5727 | B51 | 3.2496 | -0.9236 | 1.8551 |
| C25 | 5.4466 | -0.1678 | 0.5929 | F52 | 2.9803 | -2.2854 | 1.5693 |
| C26 | 5.4712 | 0.9289 | -1.5531 | F53 | 4.0047 | -0.8236 | 3.0271 |
| H27 | 3.5398 | 1.3094 | -2.4165 | F54 | 1.9965 | -0.2552 | 2.0272 |
4. Thermal analysis

Figure S37. TGA and DSC curves of 5.
Figure S38. TGA and DSC curves of 6.

Figure S39. TGA and DSC curves of 7.
Figure S40. TGA and DSC curves of 8.

Figure S41. TGA and DSC curves of 9.
Figure S42. TGA and DSC curves of 10.
5. HR-MS

Figure S43. HRMS data for 5.

Figure S44. HRMS data for 6.
Figure S45. HRMS data for 7.

Figure S46. HRMS data for 8.
Figure S47. HRMS data for 9.

Figure S48. HRMS data for 10.