Supplementary Information

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Figure S1. $^1$H NMR spectrum of compound 1 in DMSO-$d_6$. 

![NMR Spectrum](image)
Figure S2. $^{13}$C NMR spectrum of compound 1 in DMSO-$d_6$. 
Figure S3. DEPT135 Spectrum of compound 1 in DMSO-d$_6$. 

Figure S3 shows the DEPT135 spectrum of compound 1 in DMSO-d$_6$. The spectrum displays various peaks at different ppm values, indicating the chemical shifts of different protons or carbons in the compound. The molecule structure is shown on the left, with numbers indicating different atoms or groups. The spectrum provides insights into the molecular structure and chemical properties of compound 1.
Figure S4. HSQC spectrum of compound 1 in DMSO-$d_6$. 
Figure S5. HMBC spectrum of compound 1 in DMSO-$d_6$. 
Figure S6. $^1$H-$^1$H COSY spectrum of compound 1 in DMSO-$d_6$. 
**Figure S7.** NOESY spectrum of compound 1 in DMSO-d6.
Figure S8. IR spectrum of compound 1.
Figure S9. HRESIMS of compound 1.

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-20  H: 5-25  N: 1-3  O: 1-2  Na: 1-1

SIPI M.W=307
W014-219H2 15 (0.517) AM (Cen,4, 80.00, Ar,5000.0,335.13,0.70); Sm (SG, 2x3.00); Cm (10:19)

Q-Tof micro

22-Jul-2014,15:21:17
TOF MS ES+
1.02e3

Minimum: 60.00
Maximum: 100.00

Mass RA Calc. Mass mDa PPM DBE i-FIT Formula
330.1220 100.00 330.1219 0.2 0.6 11.5 22.0 C18 H17 N3 O2 Na
Figure S10. UV spectrum of compound 1.
Figure S11. $^1$H NMR spectrum of compound 2 in DMSO-$d_6$. 
Figure S12. $^{13}$C NMR spectrum of compound 2 in DMSO-$d_6$. 
Figure S13. DEPT135 Spectrum of compound 2 in DMSO-$d_6$. 
Figure S14. HSQC spectrum of compound 2 in DMSO-$d_6$. 
Figure S15. HMBC spectrum of compound 2 in DMSO-$d_6$. 
Figure S16. $^1$H-$^1$H COSY spectrum of compound 2 in DMSO-$d_6$. 

The figure shows a COSY spectrum with peaks indicating the connectivity of protons in compound 2. The spectrum is plotted with chemical shifts on the x-axis and y-axis, ranging from 0 to 9 ppm. The compound structure is labeled as 2, with specific atom labels for proton connectivity.
Figure S17. NOESY spectrum of compound 2 in DMSO-$d_6$. 
Figure S18. IR spectrum of compound 2.
Figure S19. HRESIMS of compound 2.

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-20   H: 5-25   N: 1-3   O: 1-2
SIPi

M.W=307

WQ14-220H 27 (0.934) AM (Cen,4, 80.00, Ar,5000.0,313.15,0.70); Sm (SG, 2x3.00); Cm (21:29)
308.1400

Minimum: 50.00
Maximum: 100.00

Mass RA Calc. Mass mDa PPM DBE i-FIT Formula
308.1400 100.00 308.1399 0.1 0.3 11.5 64.9 C18 H16 N3 O2
Figure S20. UV spectrum of compound 2.
Figure S21. $^1$H NMR spectrum of compound 3 in CDCl$_3$. 

[Diagram of compound 3 with labeled peaks for HNMR spectrum.]
Figure S22. $^{13}$C NMR spectrum of compound 3 in CDCl$_3$. 

![NMR spectrum of compound 3]
Figure S23. DEPT135 Spectrum of compound 3 in CDCl₃.
Figure S24. HSQC spectrum of compound 3 in CDCl₃.
Figure S25. HMBC spectrum of compound 3 in CDCl₃.
Figure S26. $^1$H–$^1$H COSY spectrum of compound 3 in CDCl$_3$. 
Figure S27. NOESY spectrum of compound 3 in CDCl3.
Figure S28. IR spectrum of compound 3.
Figure S29. HRESIMS of compound 3.

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-15  H: 10-25  N: 0-4  O: 0-5  Na: 1-1

MW=272
WQ12-149H45 (1.553) AM (Cen,4, 80.00, Ar,5000,0,298.13,0.70); Sm (SG, 2x1,00); Cm (33.45)

| m/z       | 294.3679 | 294.6158 | 294.7555 | 294.9224 | 295.2832 | 295.5149 | 295.62929 | 295.7734 | 295.9349 |
|-----------|----------|----------|----------|----------|----------|----------|-----------|----------|----------|
| Minimum   | 294.20   | 294.40   | 294.60   | 294.80   | 295.00   | 295.20   | 295.40    | 295.60   | 295.80   |
| Maximum   | 294.40   | 294.7555 | 294.9224 | 295.20   | 295.5149 | 295.62929| 295.7734  | 295.9349 | 296.00   |
| RA        | 85.00    | 5.0      | 10.0     | -1.5     | -1.5     | -1.5     | -1.5      | -1.5     | -1.5     |
| Calc. Mass| 295.1058 | 295.1059 | -0.1     | -0.3     | 8.5      | 5546620.0 | C15 H16 N2 O3 Na |

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Figure S30. UV spectrum of compound 3.
Figure S31. $^1$H NMR spectrum of compound 4 in CDCl$_3$. 
**Figure S32.** $^{13}$C NMR spectrum of compound 4 in CDCl$_3$. 
Figure S33. DEPT135 Spectrum of compound 4 in CDCl$_3$. 

![Chemical structure of compound 4 with DEPT135 spectrum]
Figure S34. HSQC spectrum of compound 4 in CDCl₃.
**Figure S35.** HMBC spectrum of compound 4 in CDCl₃.
Figure S36. $^1$H-$^1$H COSY spectrum of compound 4 in CDCl$_3$. 
Figure S37. NOESY spectrum of compound 4 in CDCl₃.
Figure S38. IR spectrum of compound 4.
Figure S39. HRESIMS of compound 4.

Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-20 H: 5-20 N: 1-3 O: 1-3

MW=279
WQ13-259H1 55 (1.894) AM (Cen, 4.00, Ar, 5.000, 0.268.14.0.70); Sm Mn, 2x3.00; Cm (49.66)
280.1452

Minimum: 75.00
Maximum: 100.00
Mass RA Calc. Mass mDa PPM DBE i-FIT Formula
280.1452 100.00 280.1450 0.2 0.7 10.5 366.1 C17 H18 N3 O
Figure S40. UV spectrum of compound 4.
Figure S41. $^1$H NMR spectrum of compound 5 in CDCl$_3$. 

8-CH$_3$

5 2 6 3 7 12 13 14, 15
Figure S42. $^{13}$C NMR spectrum of compound 5 in CDCl$_3$.
Figure S43. DEPT135 Spectrum of compound 5 in CDCl₃.
Figure S44. HSQC spectrum of compound 5 in CDCl$_3$. 
Figure S45. HMBC spectrum of compound 5 in CDCl₃.
Figure S46. $^1$H-$^1$H COSY spectrum of compound 5 in CDCl$_3$. 
Figure S47. NOESY spectrum of compound 5 in CDCl₃.
Figure S48. IR spectrum of compound 5.
Figure S49. HRESIMS of compound 5.

Elemental Composition Report

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-20 H: 5-20 N: 1-3 O: 1-1
SI
M.W. = 279
WQ14-004H23 (0.794) AM (Cen, 4, 80.00, Ar, 5000.0, 268.14, 0.70); Sm (Mn, 2X3.00); Cm (23:38)

% 256.2671 257.2714 265.1267 269.1461 270.1481 275.2903 274.2763 281.1500 282.1532 280.1448
0 260.0 265.0 270.0 275.0 280.0 285.0 290.0 295.0 300.0 305.0 m/z

Minimum: 85.00
Maximum: 100.00

Mass RA Calc. Mass mDa PPM DBE i-FIT Formula
280.1448 100.00 280.1450 -0.2 -0.7 10.5 64.9 C17 H18 N3 O
Figure S50. UV spectrum of compound 5.
Figure S51. $^1$H NMR spectrum of compound 6 in CDCl$_3$. 
Figure S52. $^{13}$C NMR spectrum of compound 6 in CDCl$_3$. 
Figure S53. $^1$H NMR spectrum of compound 7 in CDCl$_3$. 
Figure S54. $^{13}$C NMR spectrum of compound 7 in CDCl$_3$. 
Figure S55. $^1$H NMR spectrum of compound 8 in CDCl$_3$. 
Figure S56. $^{13}$C NMR spectrum of compound 8 in CDCl$_3$. 
Table S1. NMR Spectroscopic Data for Compounds 6–8 in CDCl₃.

| Position | 6<sup>a</sup> | 7<sup>a</sup> | 8<sup>a</sup> |
|----------|--------------|--------------|--------------|
|          | δ<sub>C</sub> | δ<sub>H</sub>, mult. (J in Hz) | δ<sub>C</sub> | δ<sub>H</sub>, mult. (J in Hz) | δ<sub>C</sub> | δ<sub>H</sub>, mult. (J in Hz) |
| 2        | 125.1, CH    | 8.69, d, (6.0) | 129.0, CH | 8.21, s | 129.3, CH | 8.22, s |
| 3        | 116.1, CH    | 7.37, d, (7.2) | 143.4, qC |         | 143.9, qC |         |
| 3a       | 146.9, qC    |            | 135.5, qC |         | 135.8, qC |         |
| 5        | 145.4, CH    | 8.17, d, (7.2) | 150.3, CH | 8.53, d, (4.2) | 150.3, CH | 8.59, d, (4.2) |
| 6        | 116.4, CH    | 7.67, d, (6.0) | 121.4, CH | 7.32, d, (4.2) | 121.5, CH | 7.30, d, (4.2) |
| 6a       | 134.8, qC    |            | 135.5, qC |         | 135.8, qC |         |
| 7        | 96.9, CH     | 7.05, s     | 106.1, CH | 6.43, s | 106.1, CH | 6.47, s |
| 8        | 156.4, qC    |            | 157.2, qC |         | 157.6, qC |         |
| 9        | 126.1, qC    |            | 175.5, qC |         | 175.6, qC |         |
| 9a       | 129.8, qC    |            | 134.1, qC |         | 134.1, qC |         |
| 9b       | 112.9, qC    |            | 117.2, qC |         | 117.6, qC |         |
| 8-OCH₃   | 56.5, CH₃    | 4.23, s     | 55.8, CH₃ | 3.88, s | 55.9, CH₃ | 3.88, s |
| 11       | 152.0, qC    |            |            |         |            |         |
| 12       | 27.6, CH     | 3.64, m     |            |         |            |         |
| 13       | 21.5, CH₃    | 1.62, d, (7.2) |        |         |            |         |
| 14       | 21.5, CH₃    | 1.62, d, (7.2) |        |         |            |         |
| 1'       |               | 6.91, t, (6.0) |        | 6.80, t, (6.0) |        |         |
| 2'       | 43.8, CH₂    | 3.70, q, (13.8, 7.2) | 40.9, CH₂ | 3.45, m |        |         |
| 3'       | 35.0, CH₂    | 3.06, t, (7.2) | 37.8, CH₂ | 1.65, q, (13.0, 7.2) |        |         |
| 4'       | 137.7, qC    |            | 25.8, CH | 1.75, m |        |         |
| 5'       | 128.5, CH    | 7.23, m     | 22.3, CH₃ | 0.96, d, (6.6) |        |         |
| 6'       | 128.6, CH    | 7.30, m     | 22.3, CH₃ | 0.96, d, (6.6) |        |         |
| 7'       | 126.6, CH    | 7.23, m     |            |         |        |         |
| 8'       | 128.6, CH    | 7.30, m     |            |         |        |         |
| 9'       | 128.5, CH    | 7.23, m     |            |         |        |         |

<sup>a</sup> Measured at 600 MHz (¹H) and 150 MHz (¹³C).