Supplementary Information

Synthesis and anion recognition studies of new oligomethylene bis(nitrophenylureyl)benzamide receptors

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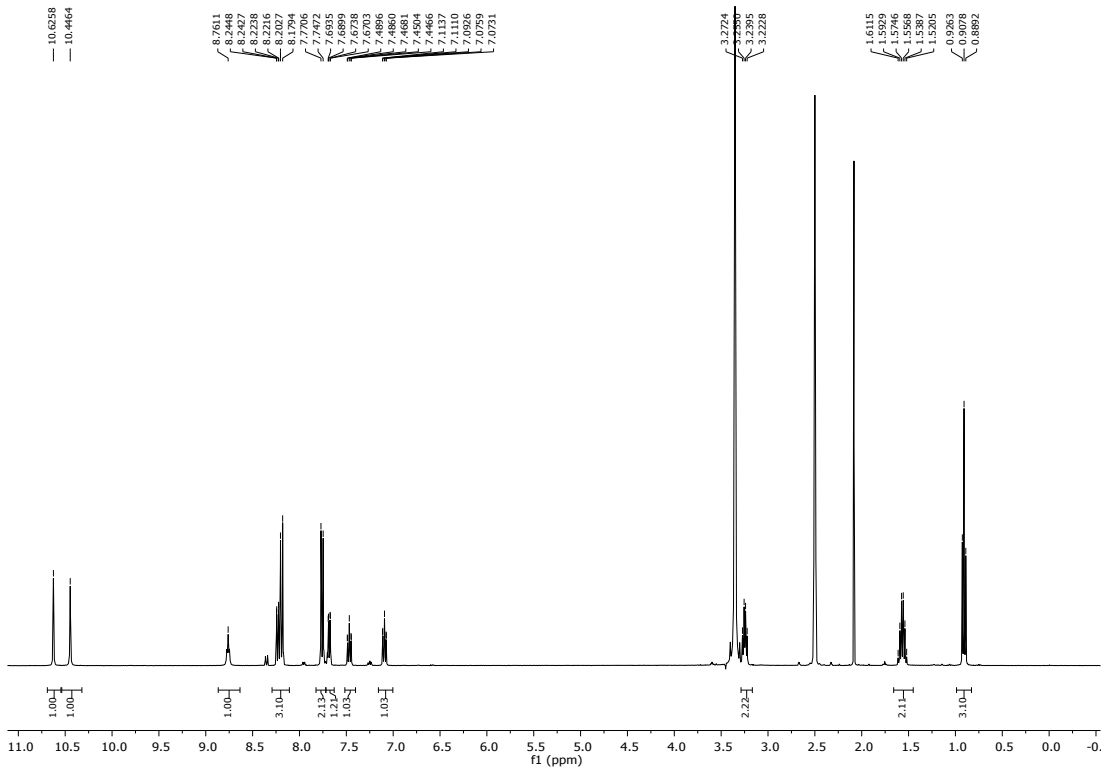


Figure S1. [1]H NMR spectra of *ortho* mono-ureabenzamide in DMSO-d_6.

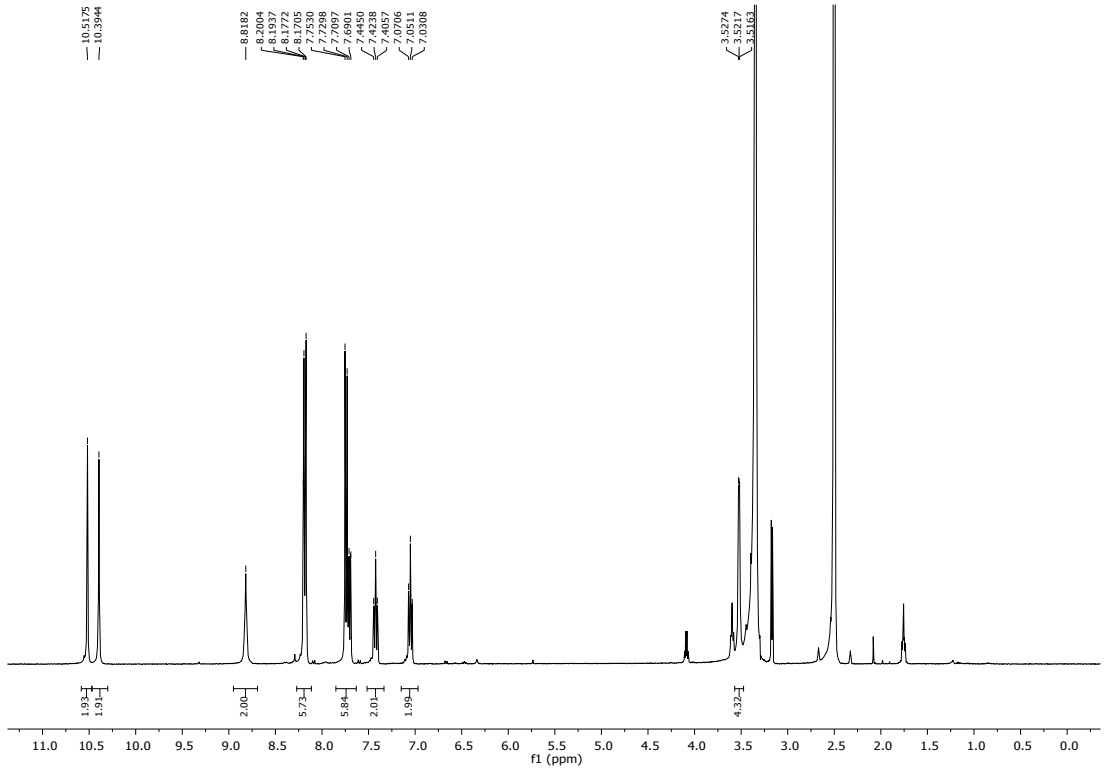


Figure S2. [1]H NMR spectra of **4a** in DMSO-d_6.

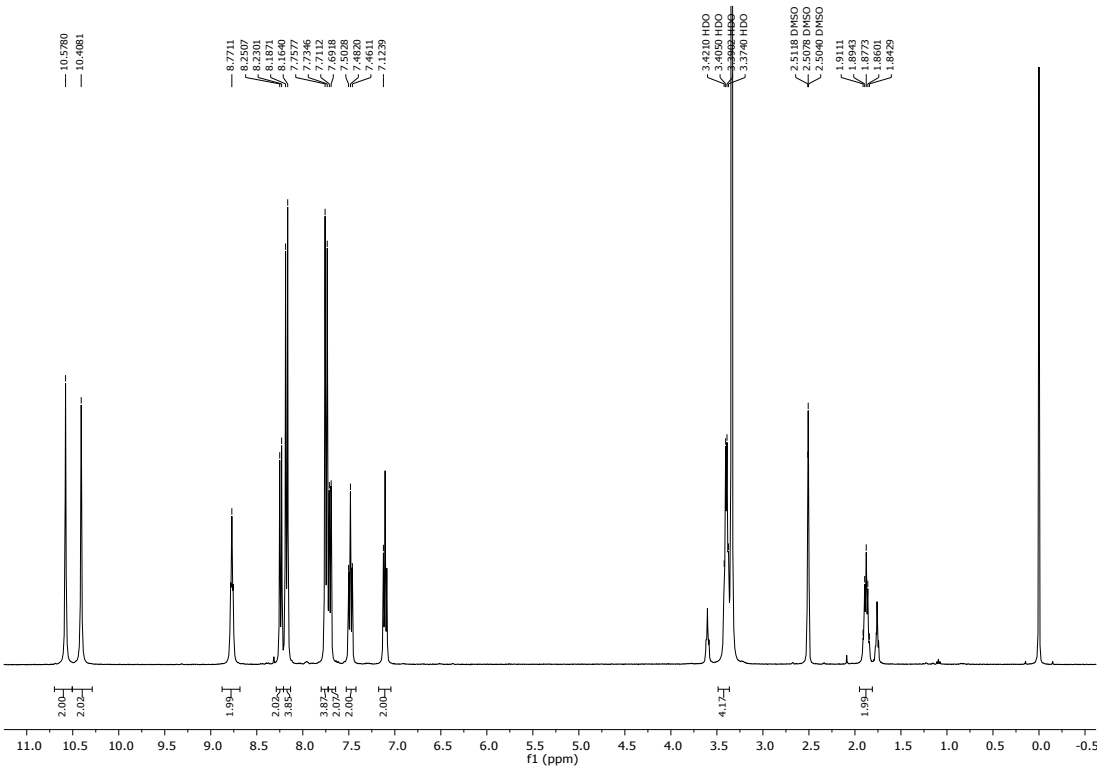


Figure S3. [1]H NMR spectra of **4b** in DMSO-d_6.

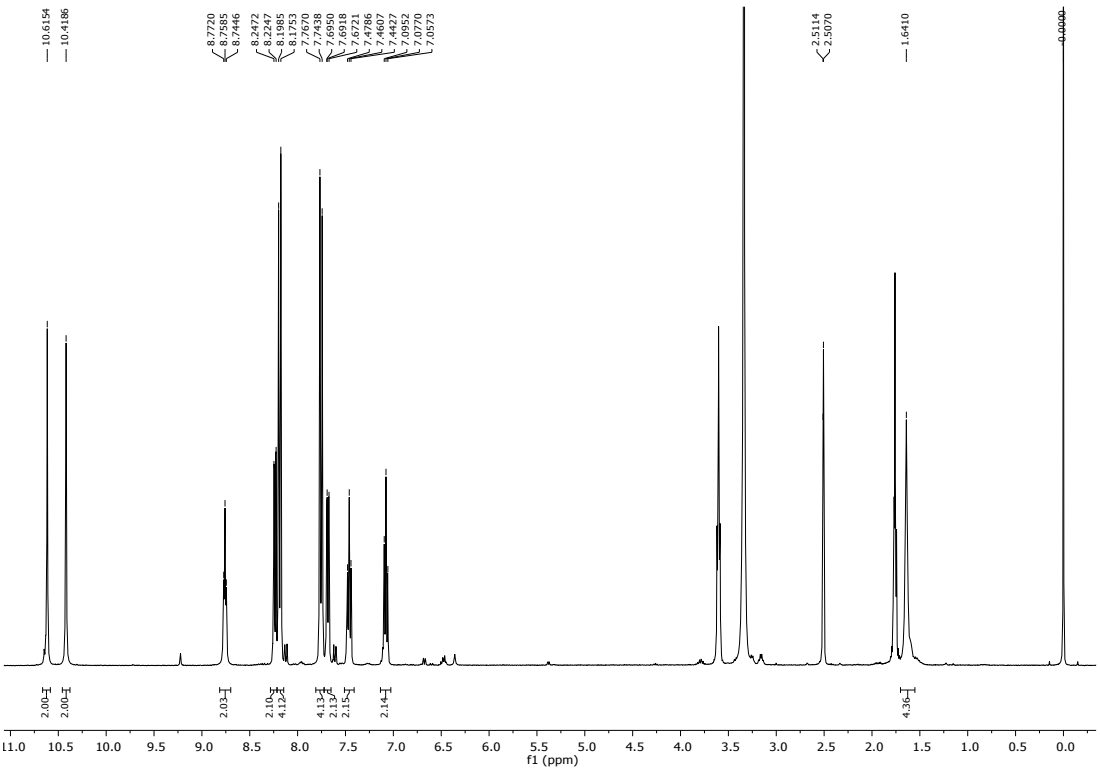


Figure S4. [1]H NMR spectra of **4c** in DMSO-d_6.

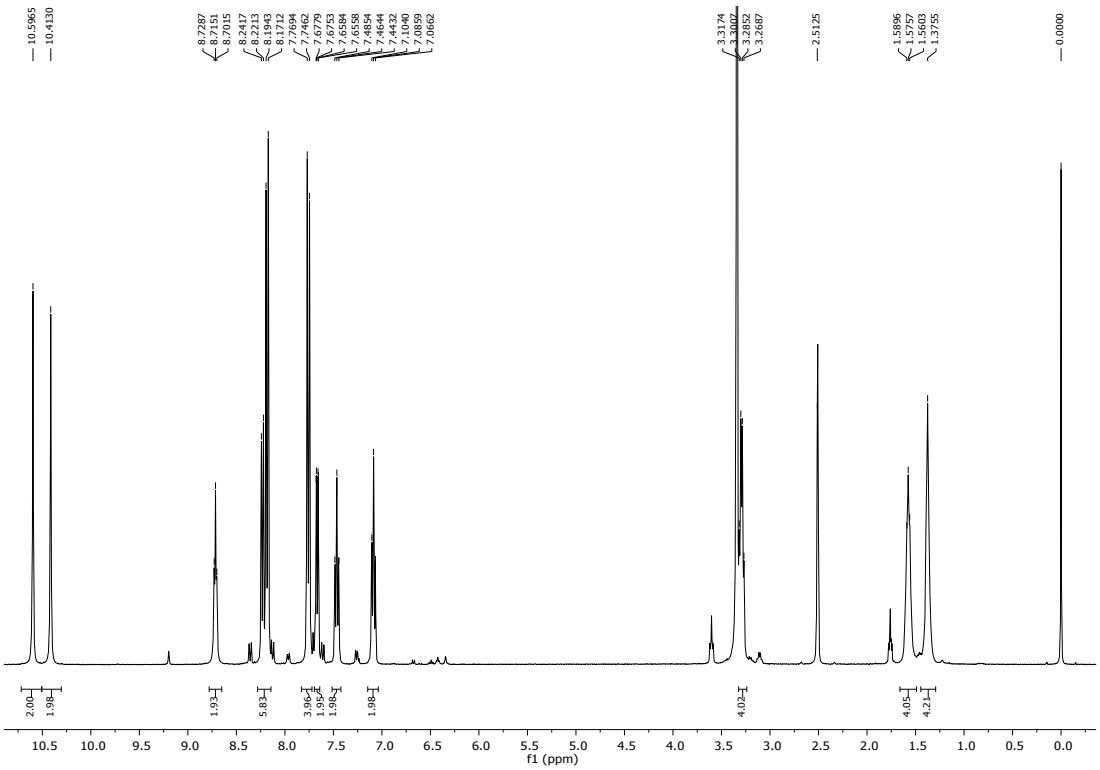


Figure S5. ^{1}H NMR spectra of **4d** in DMSO-d_6.

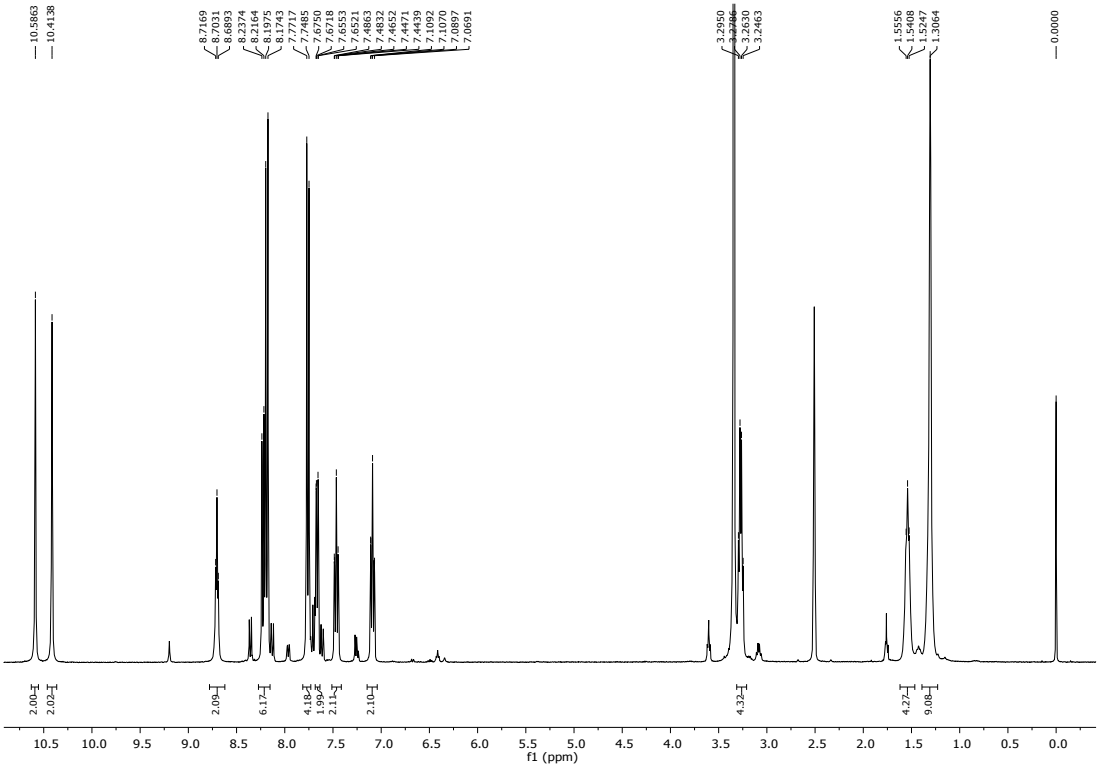


Figure S6. ^{1}H NMR spectra of **4e** in DMSO-d_6.

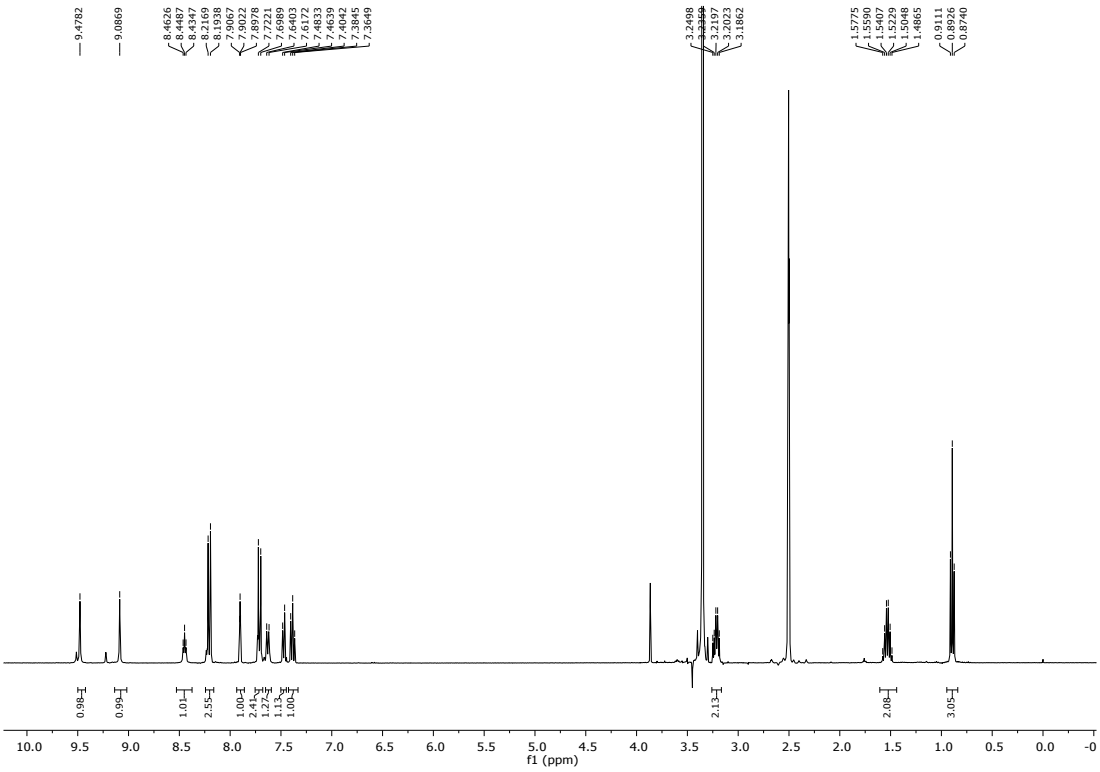


Figure S7. [1]H NMR spectra of *meta* mono-ureabenzamide in DMSO-d_6.

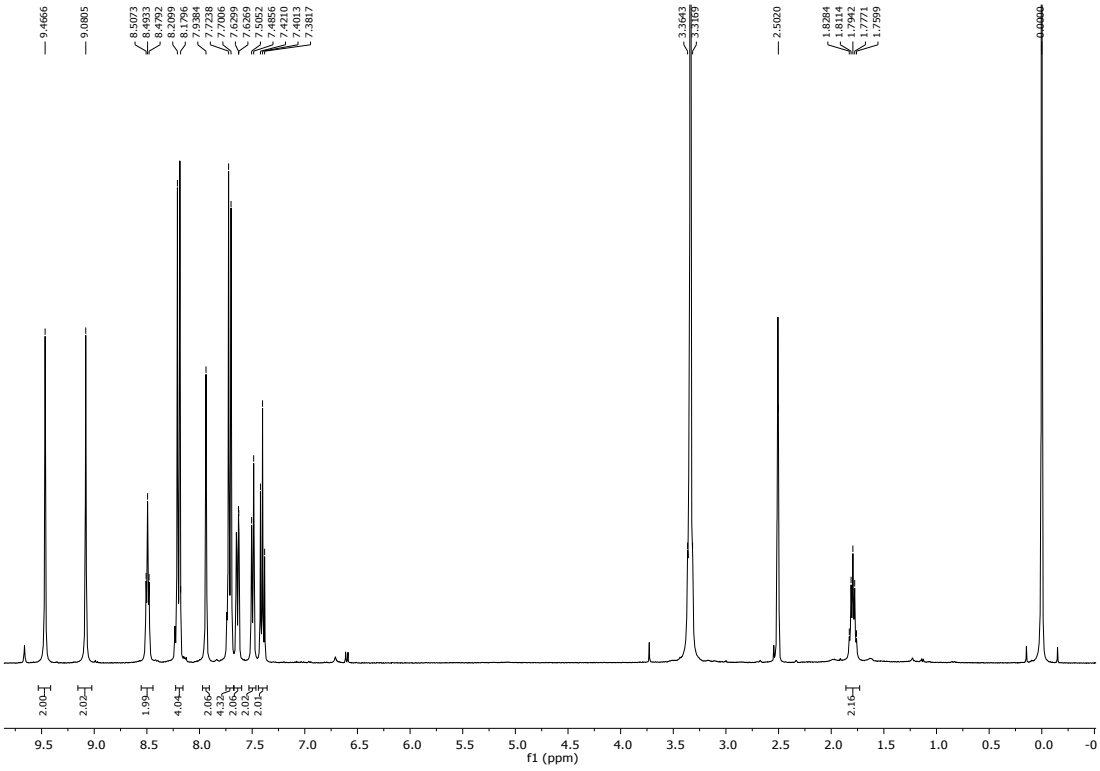


Figure S8. [1]H NMR spectra of **8b** in DMSO-d_6.

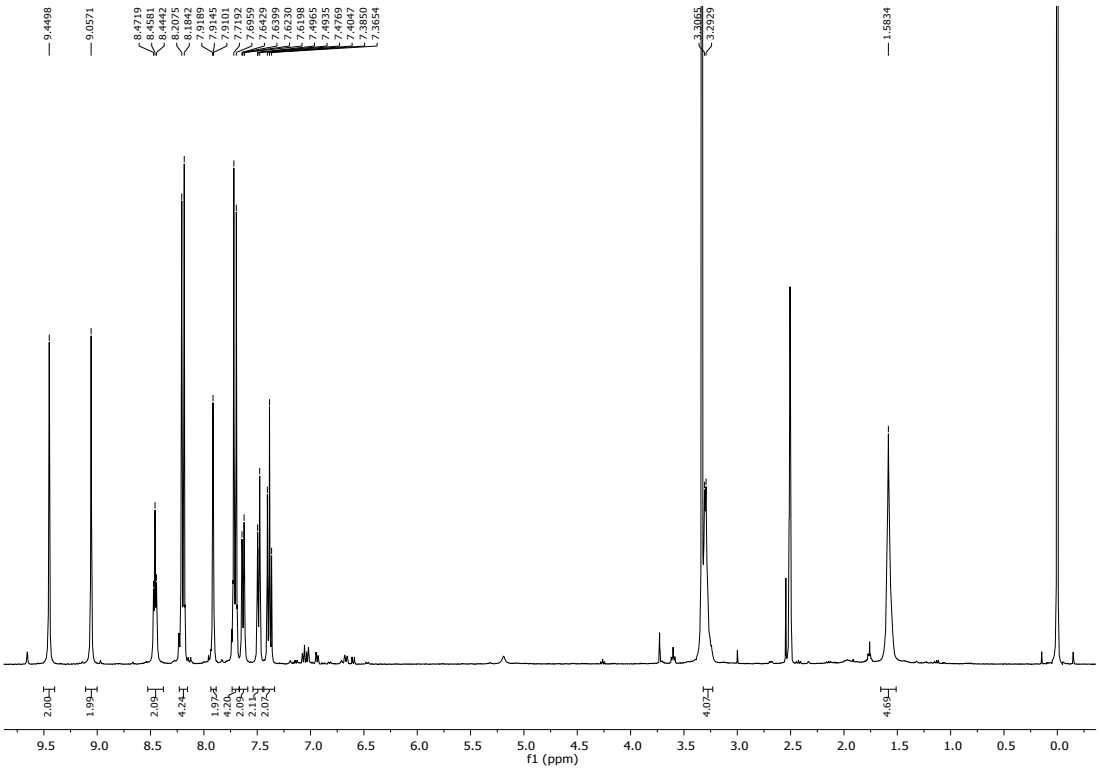


Figure S9. [1]H NMR spectra of **8c** in DMSO-d_6.

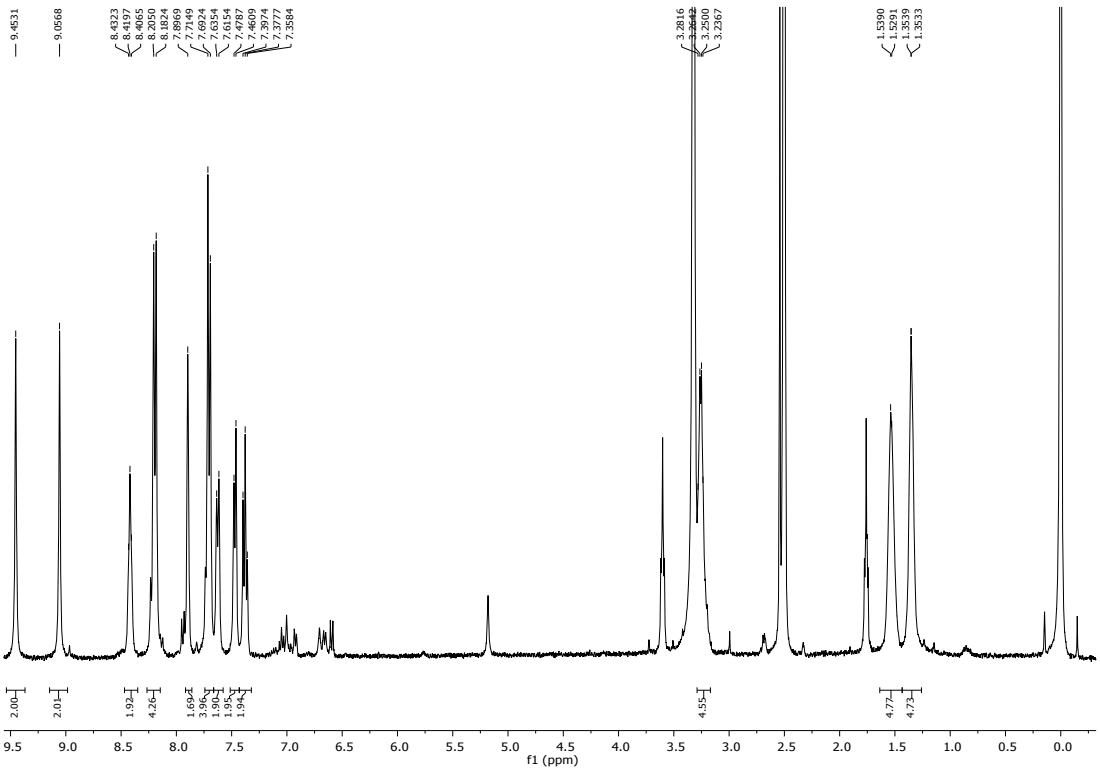


Figure S10. [1]H NMR spectra of **8d** in DMSO-d_6.

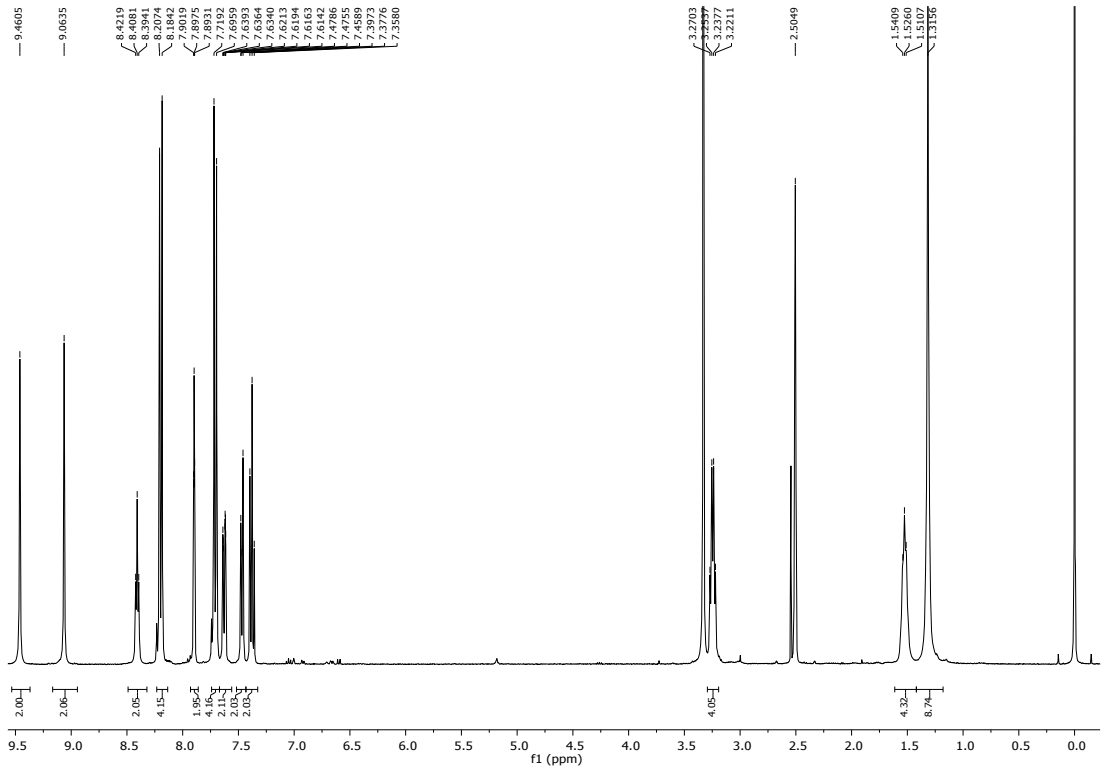
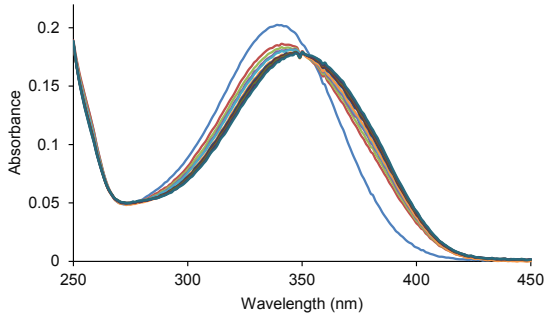
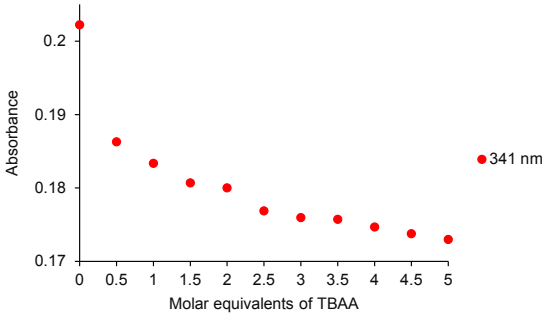


Figure S11. ^{1}H NMR spectra of **8e** in DMSO-d_6.

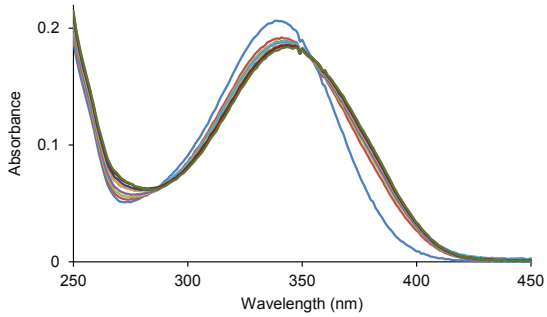
a)


Absorbance
0.2
0.15
0.1
0.05
0
250
300
350
400
450
Wavelength (nm)

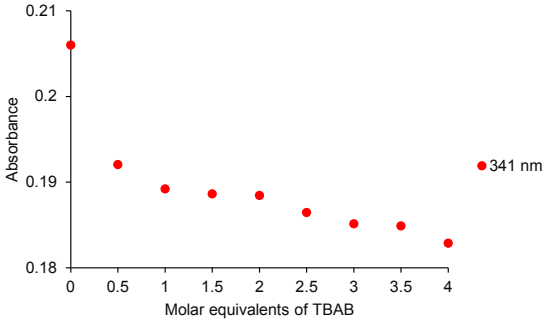
b)


Absorbance
0.2
0.19
0.18
0.17
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Molar equivalents of TBAA
341 nm

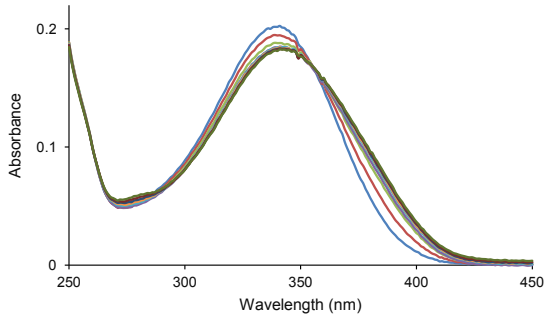
c)


Absorbance
0.2
0.1
0
250
300
350
400
450
Wavelength (nm)

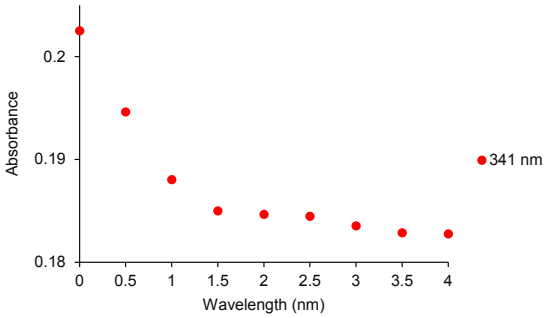
d)


Absorbance
0.21
0.2
0.19
0.18
0
0.5
1
1.5
2
2.5
3
3.5
4
Molar equivalents of TBAB
341 nm

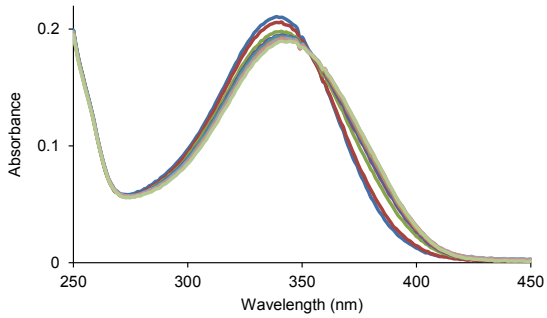
e)


Absorbance
0.2
0.1
0
250
300
350
400
450
Wavelength (nm)

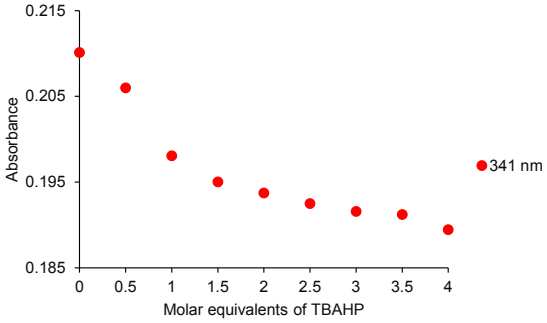
f)


Absorbance
0.2
0.19
0.18
0
0.5
1
1.5
2
2.5
3
3.5
4
Wavelength (nm)
341 nm

g)


Absorbance
0.2
0.1
0
250
300
350
400
450
Wavelength (nm)

h)


Absorbance
0.215
0.205
0.195
0.185
0
0.5
1
1.5
2
2.5
3
3.5
4
Molar equivalents of TBAHP
341 nm

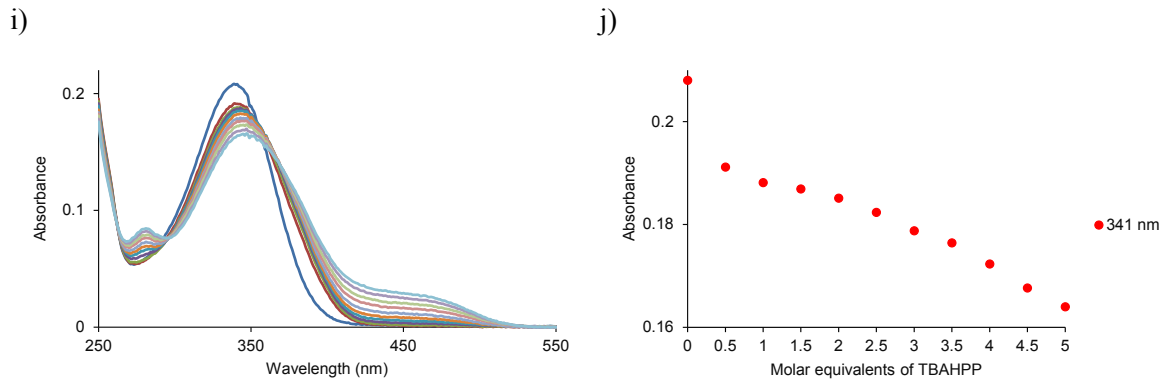
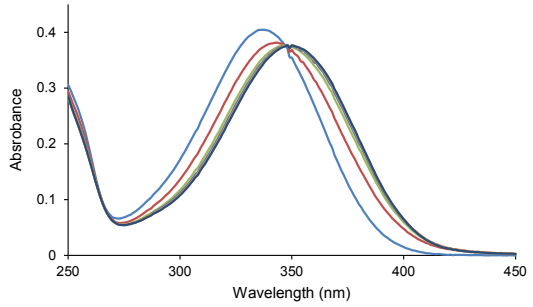
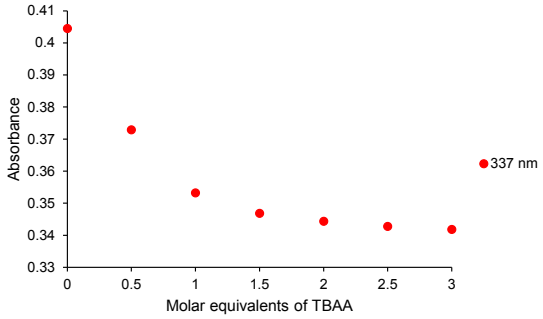


Figure S12. UV-vis spectra and absorbance profiles obtained by the titration of the *ortho* mono-ureabenzamide with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

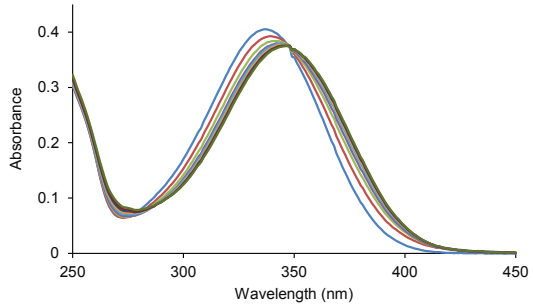
a)


Absrobance
Wavelength (nm)

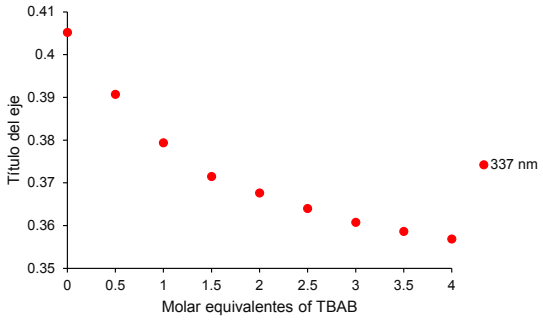
b)


Absorbance
Molar equivalents of TBAA
337 nm

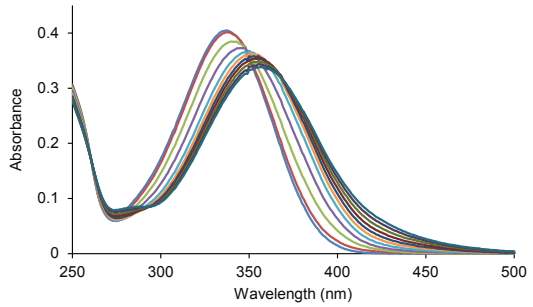
c)


Absorbance
Wavelength (nm)

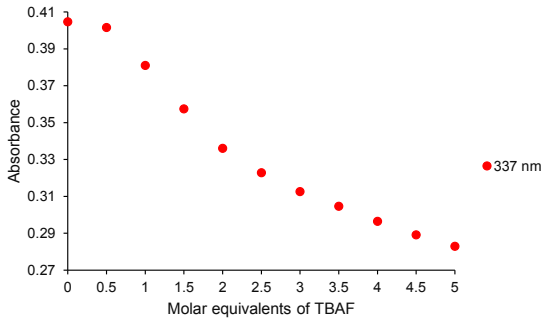
d)


Título del eje
Molar equivalentes of TBAB
337 nm

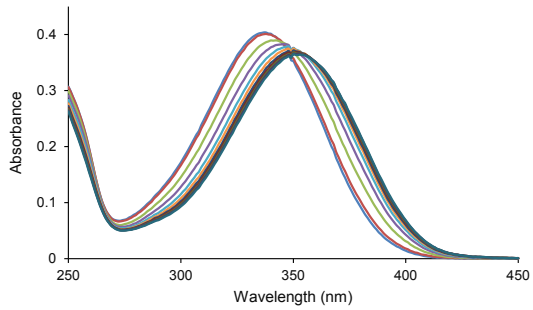
e)


Absorbance
Wavelength (nm)

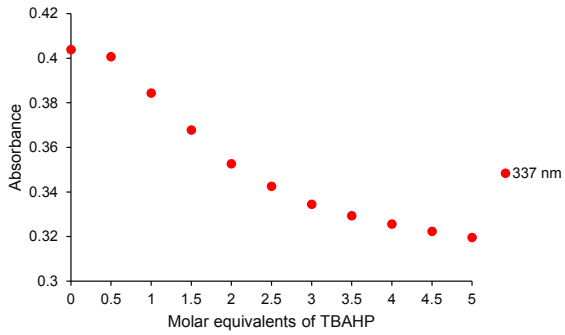
f)


Absorbance
Molar equivalents of TBAF
337 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
337 nm

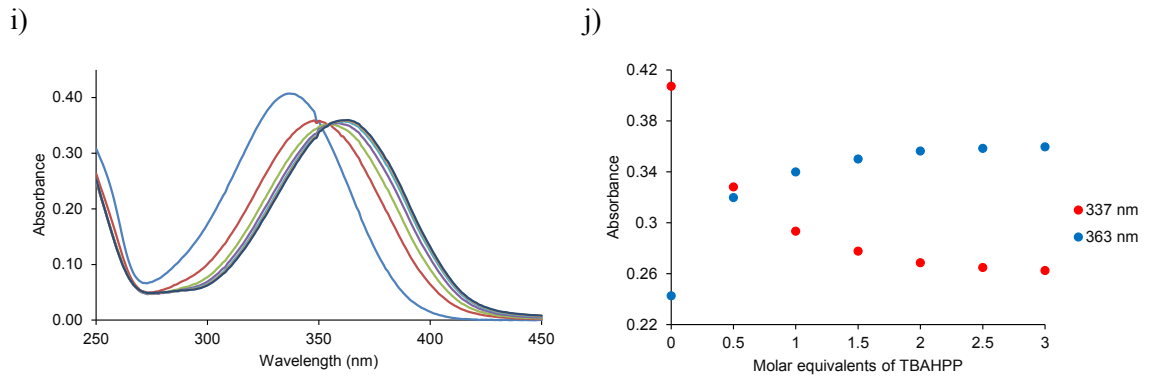
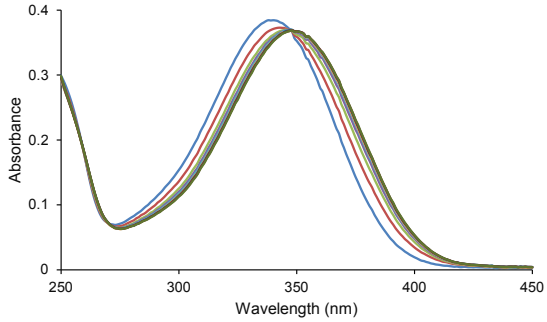
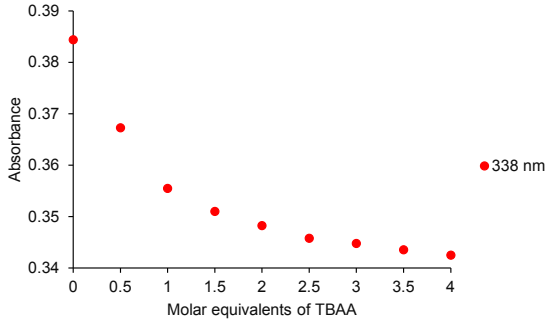


Figure S13. UV-vis spectra and absorbance profiles obtained by the titration of **4a** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

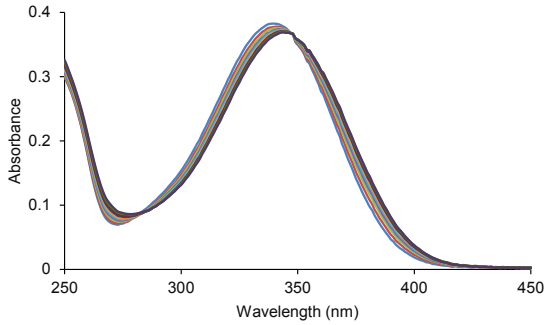
a)


Absorbance
Wavelength (nm)

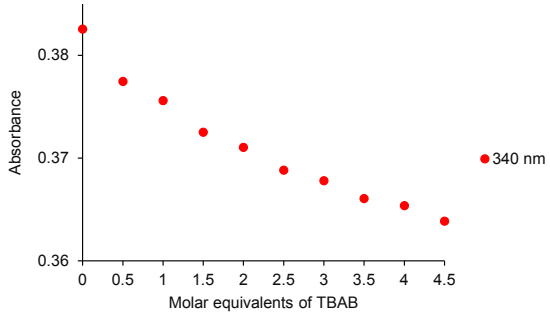
b)


Absorbance
Molar equivalents of TBAA
338 nm

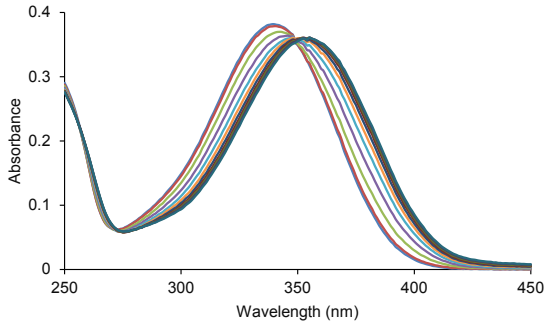
c)


Absorbance
Wavelength (nm)

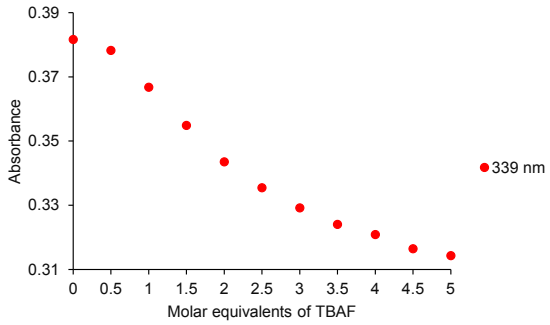
d)


Absorbance
Molar equivalents of TBAB
340 nm

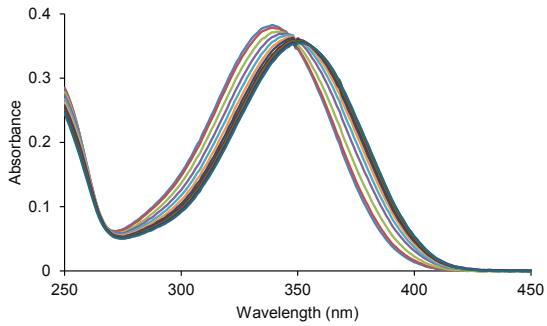
e)


Absorbance
Wavelength (nm)

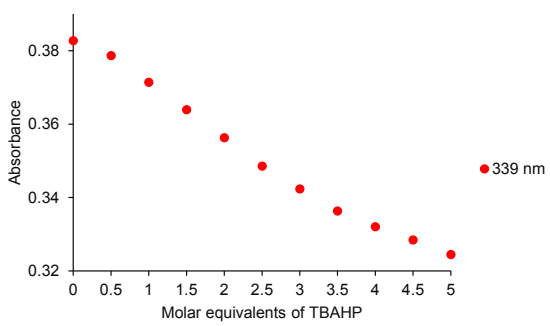
f)


Absorbance
Molar equivalents of TBAF
339 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
339 nm

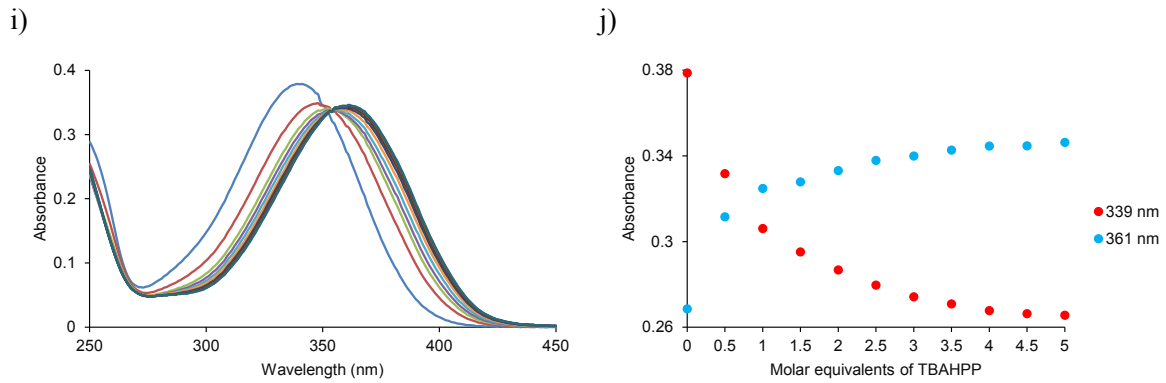
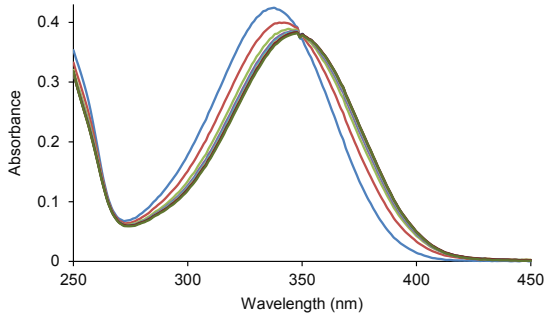
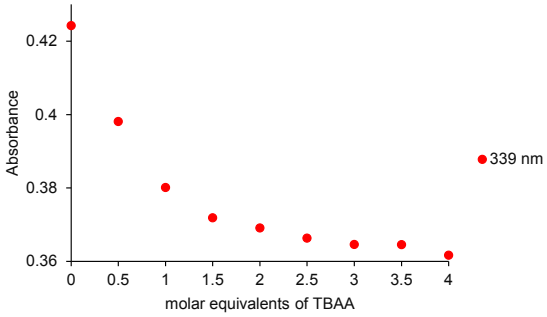


Figure S14. UV-vis spectra and absorbance profiles obtained by the titration of **4b** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

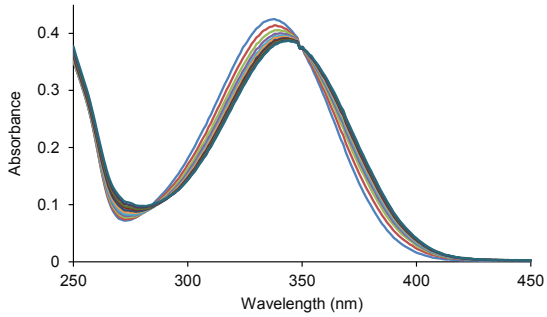
a)


Absorbance
0.4
0.3
0.2
0.1
0
250
300
350
400
450
Wavelength (nm)

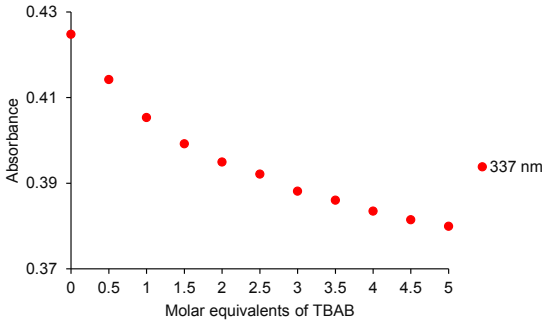
b)


Absorbance
0.42
0.4
0.38
0.36
0
0.5
1
1.5
2
2.5
3
3.5
4
molar equivalents of TBAA
339 nm

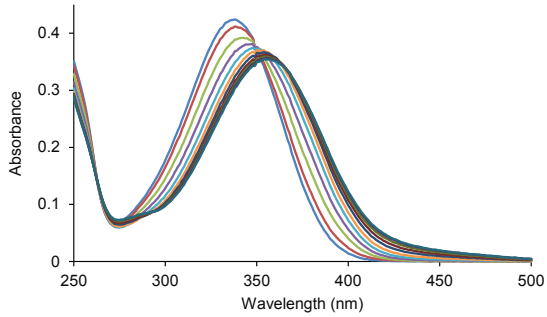
c)


Absorbance
0.4
0.3
0.2
0.1
0
250
300
350
400
450
Wavelength (nm)

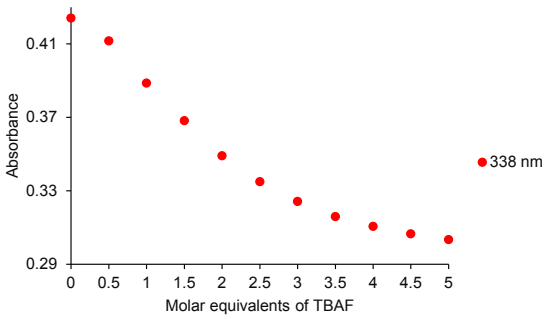
d)


Absorbance
0.43
0.41
0.39
0.37
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Molar equivalents of TBAB
337 nm

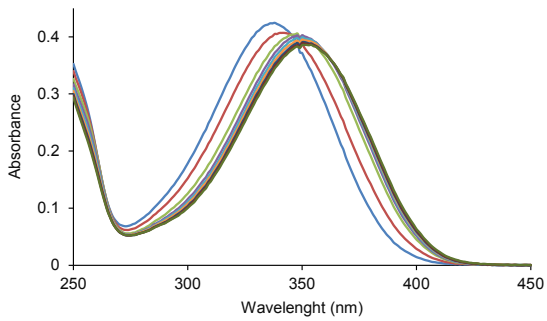
e)


Absorbance
0.4
0.3
0.2
0.1
0
250
300
350
400
450
500
Wavelength (nm)

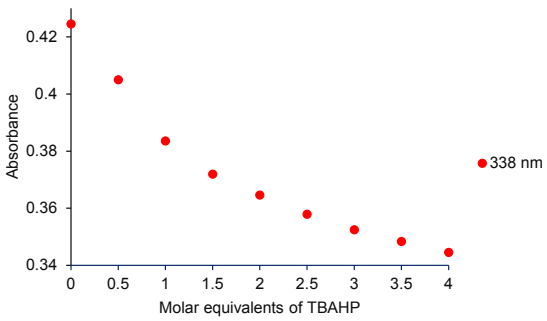
f)


Absorbance
0.41
0.37
0.33
0.29
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Molar equivalents of TBAF
338 nm

g)


Absorbance
0.4
0.3
0.2
0.1
0
250
300
350
400
450
Wavelenght (nm)

h)


Absorbance
0.42
0.4
0.38
0.36
0.34
0
0.5
1
1.5
2
2.5
3
3.5
4
Molar equivalents of TBAHP
338 nm

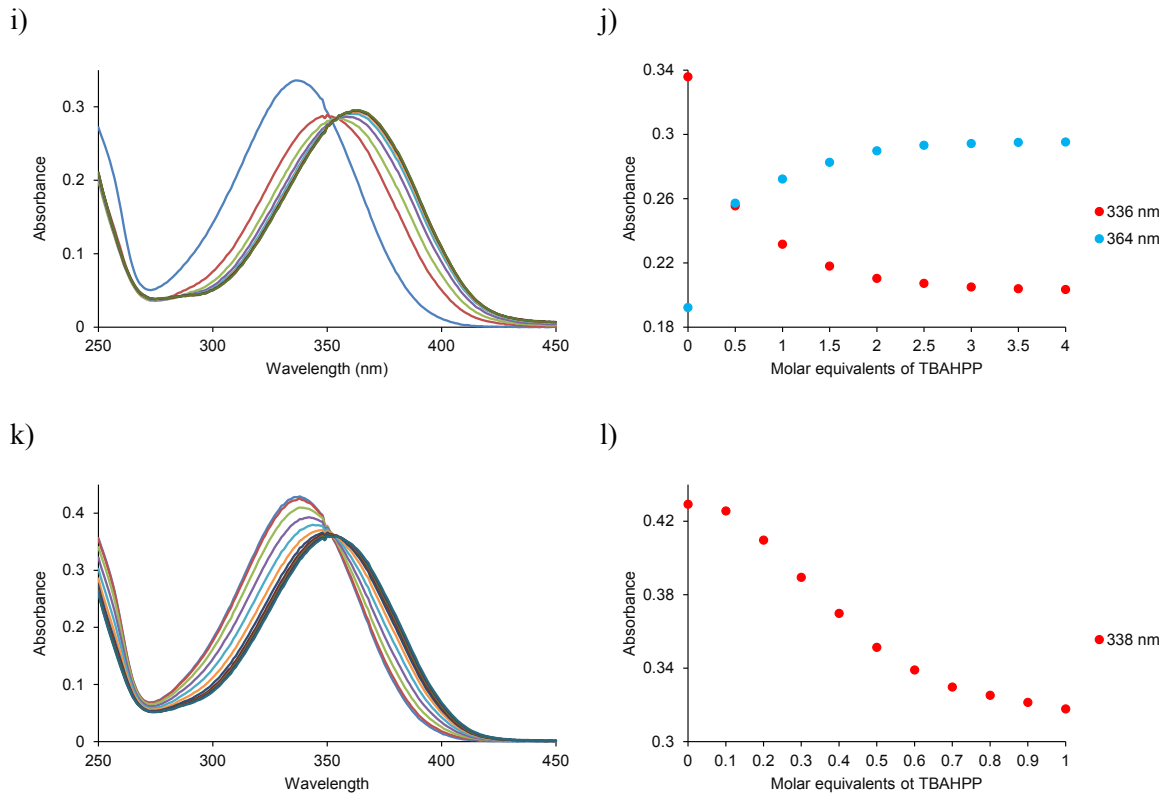
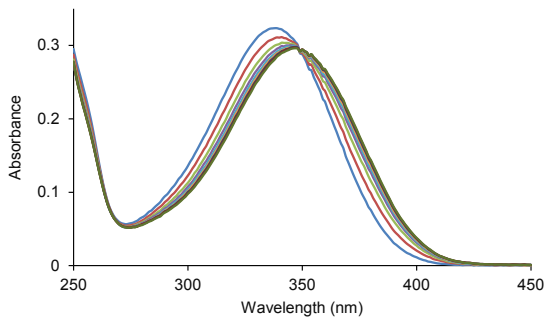
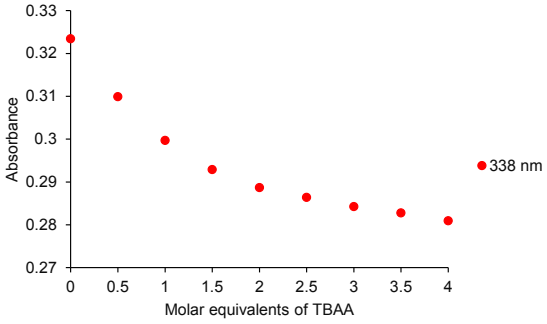


Figure S15. UV-vis spectra and absorbance profiles obtained by the titration of **4c** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i, j, k and l).

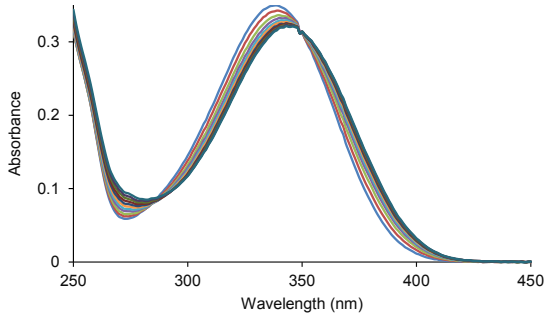
a) b)


Absorbance
Wavelength (nm)

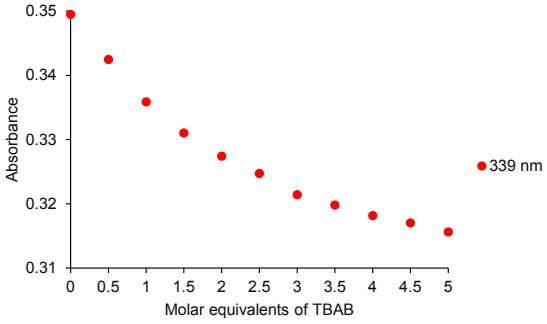
c)


Absorbance
Molar equivalents of TBAA
338 nm

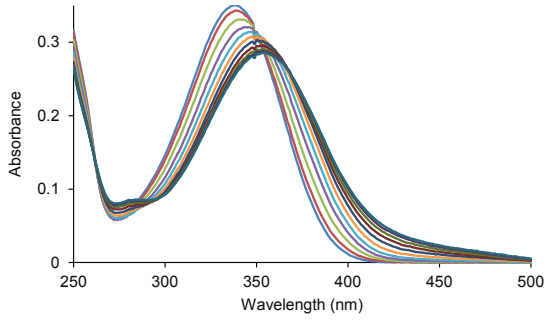
d)


Absorbance
Wavelength (nm)

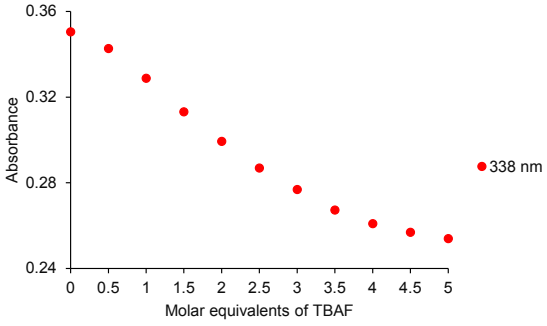
e)


Absorbance
Molar equivalents of TBAB
339 nm

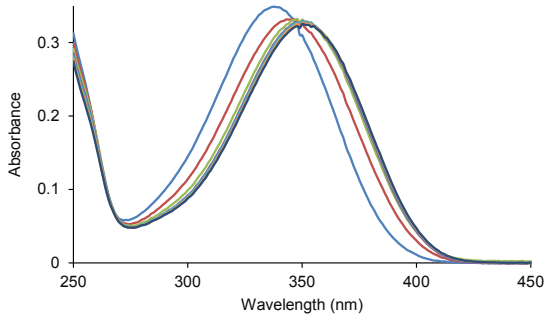
f)


Absorbance
Wavelength (nm)

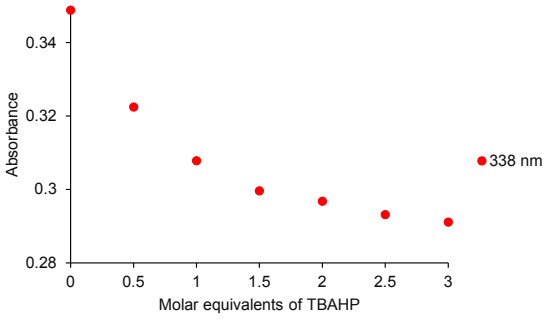
g)


Absorbance
Molar equivalents of TBAF
338 nm

h)


Absorbance
Wavelength (nm)

i)


Absorbance
Molar equivalents of TBAHP
338 nm

j)

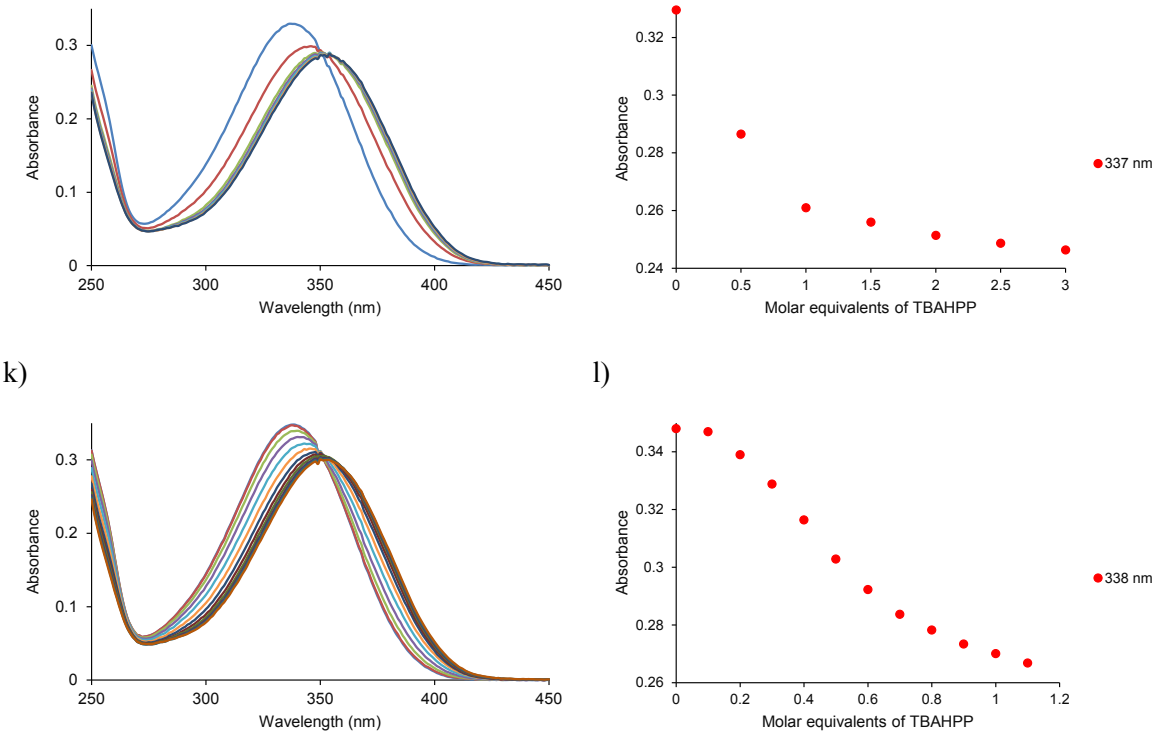
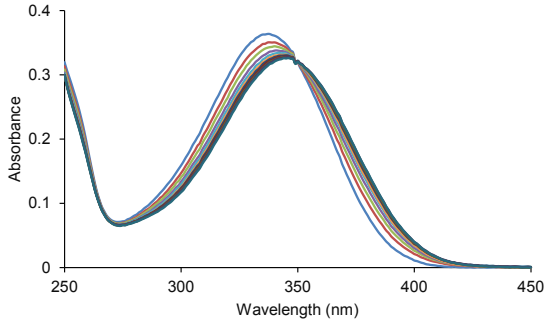
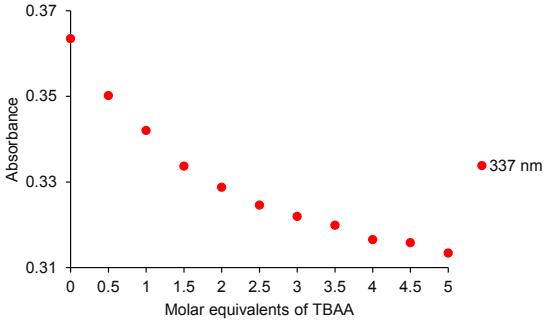


Figure S16. UV-vis spectra and absorbance profiles obtained by the titration of **4d** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i, j, k and l).

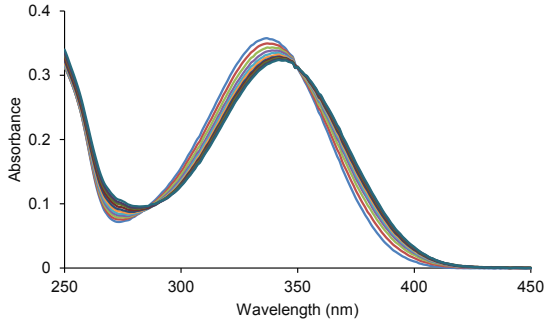
a) b)

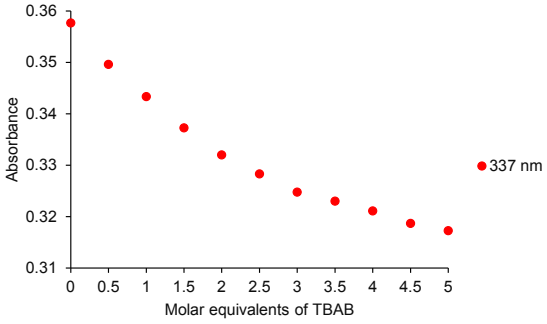

Absorbance
Wavelength (nm)


Absorbance
Molar equivalents of TBAA
337 nm

c)

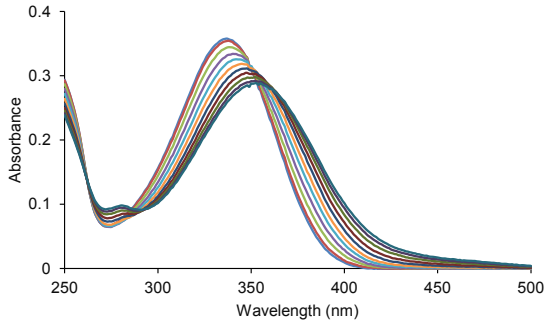
d)

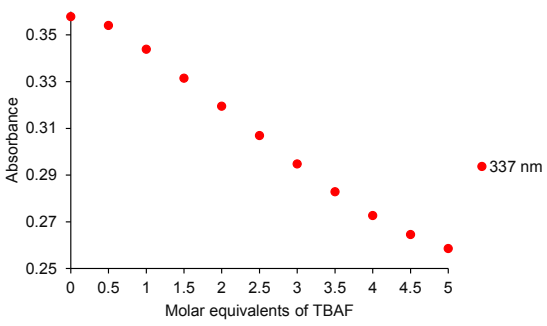

Absorbance
Wavelength (nm)


Absorbance
Molar equivalents of TBAB
337 nm

e)

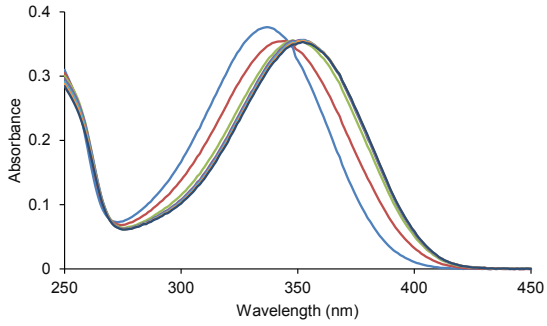
f)

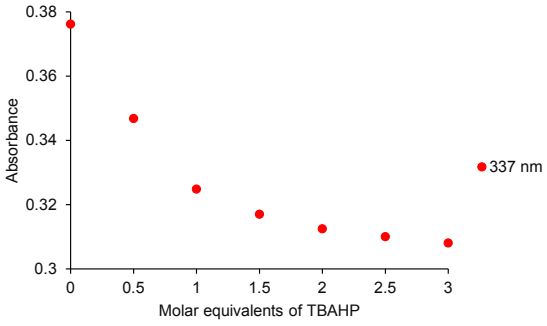

Absorbance
Wavelength (nm)


Absorbance
Molar equivalents of TBAF
337 nm

g)

h)


Absorbance
Wavelength (nm)


Absorbance
Molar equivalents of TBAHP
337 nm

i)

j)

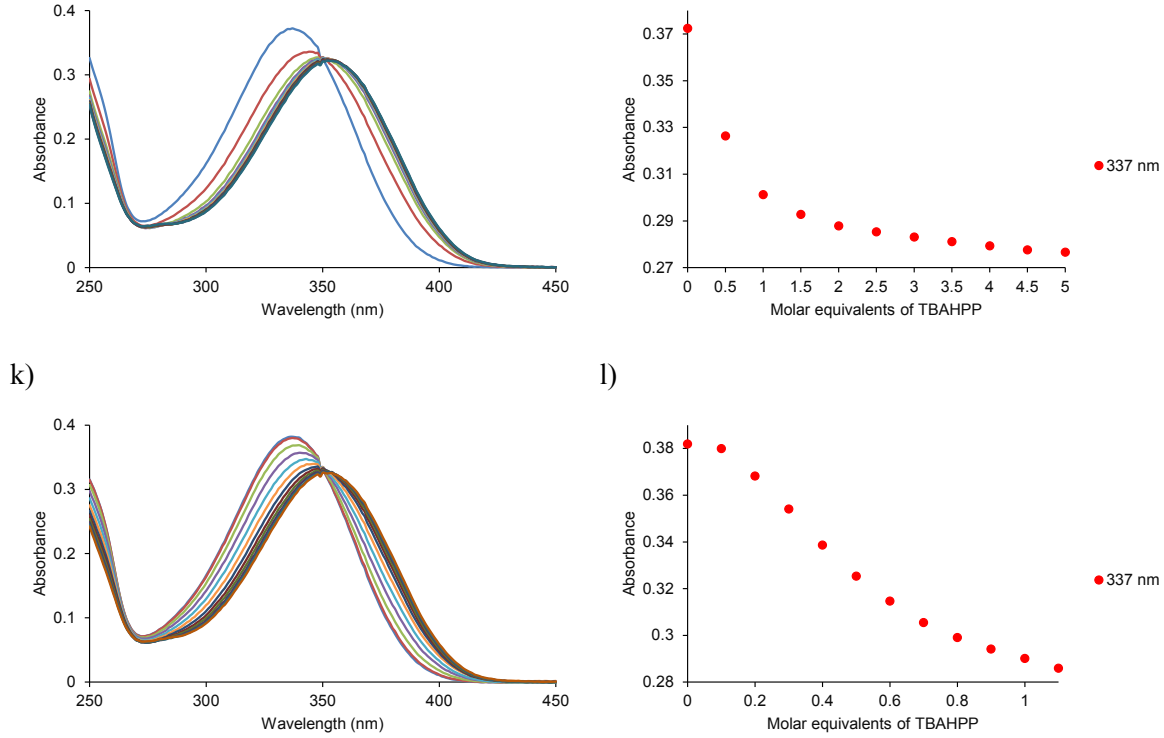
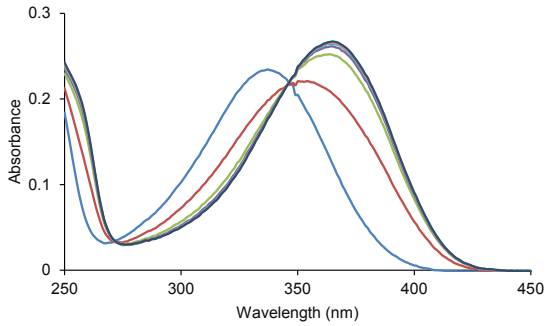
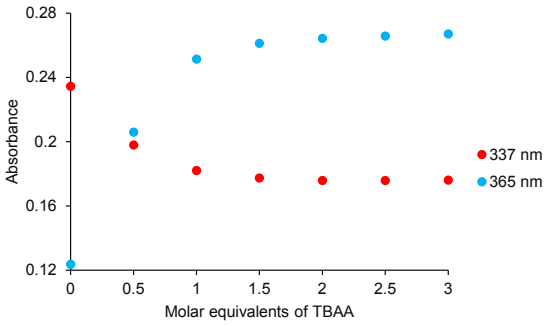


Figure S17. UV-vis spectra and absorbance profiles obtained by the titration of **4e** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i, j, k and l).

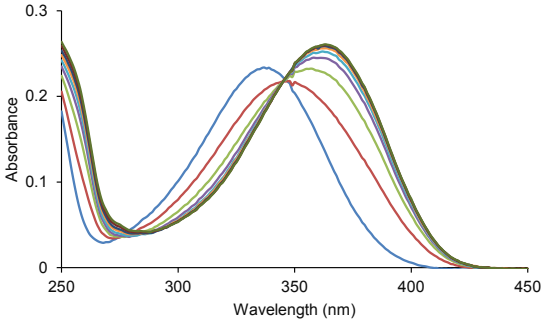
a)


Absorbance
Wavelength (nm)

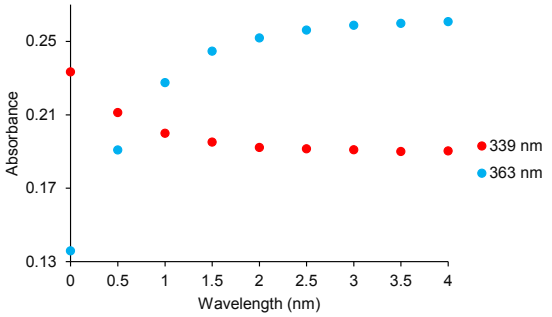
b)


Absorbance
Molar equivalents of TBAA
337 nm
365 nm

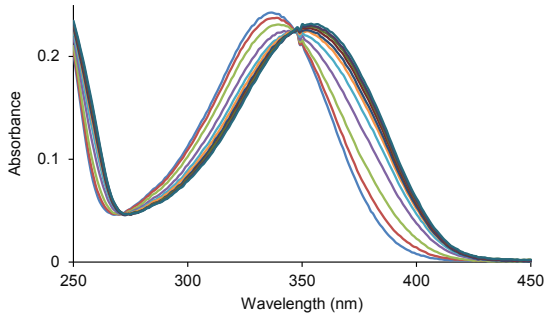
c)


Absorbance
Wavelength (nm)

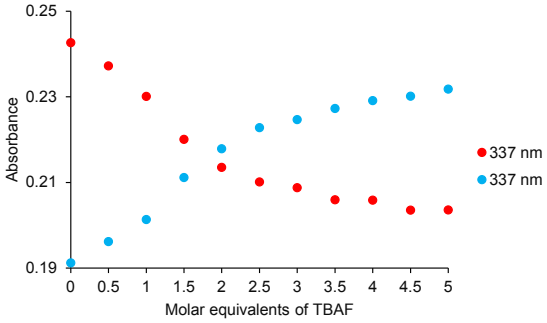
d)


Absorbance
Wavelength (nm)
339 nm
363 nm

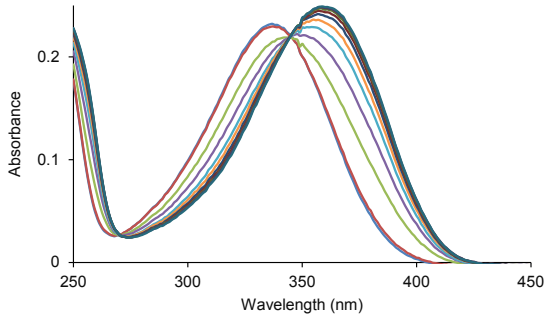
e)


Absorbance
Wavelength (nm)

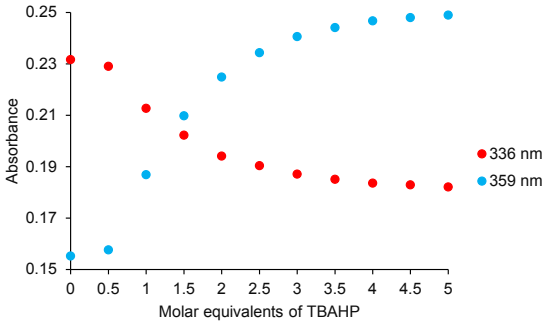
f)


Absorbance
Molar equivalents of TBAF
337 nm
337 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
336 nm
359 nm

i)

j)

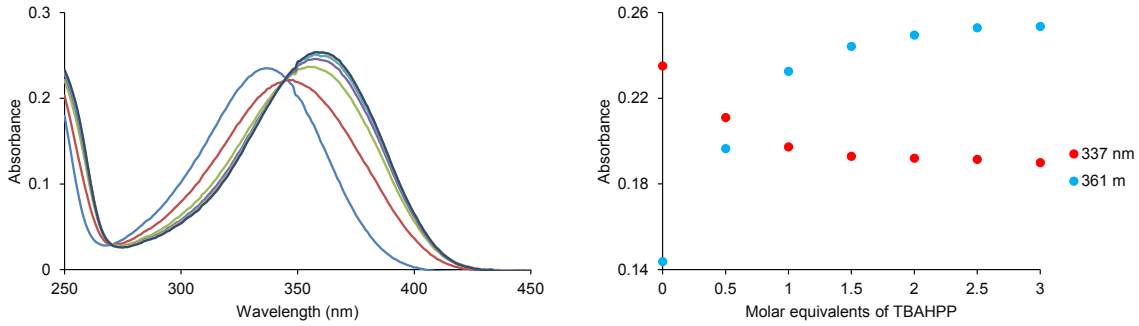
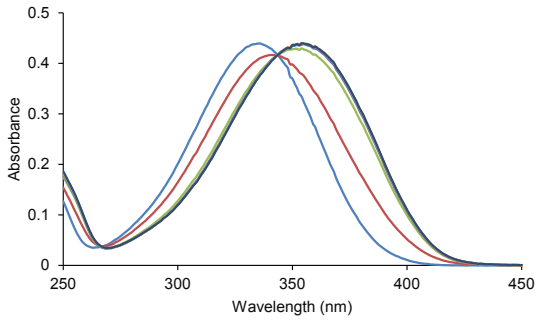
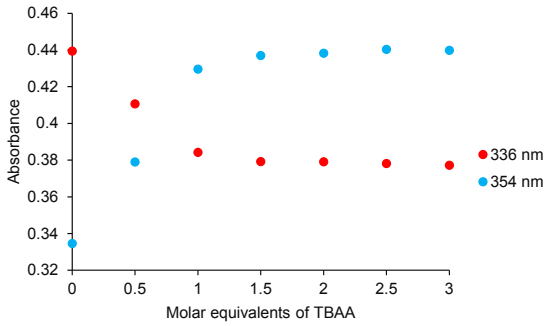


Figure S18. UV-vis spectra and absorbance profiles obtained by the titration of the *meta* mono-ureabenzamide with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j)

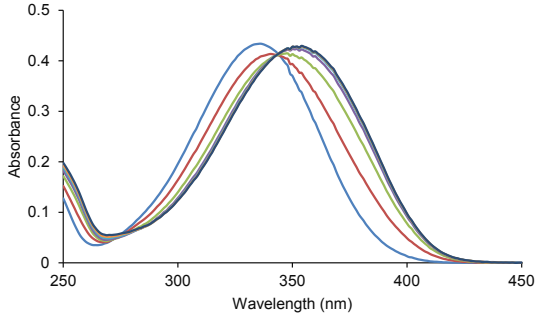
a)


Absorbance
Wavelength (nm)

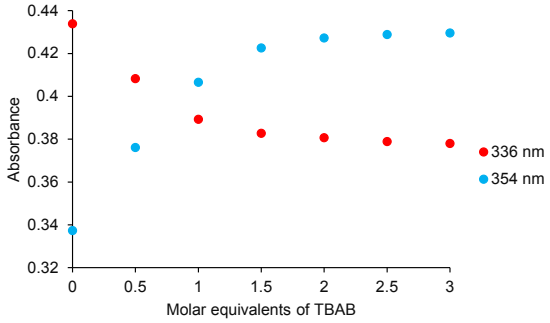
b)


Absorbance
Molar equivalents of TBAA
336 nm
354 nm

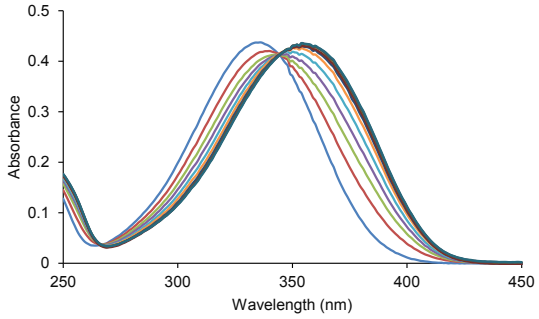
c)


Absorbance
Wavelength (nm)

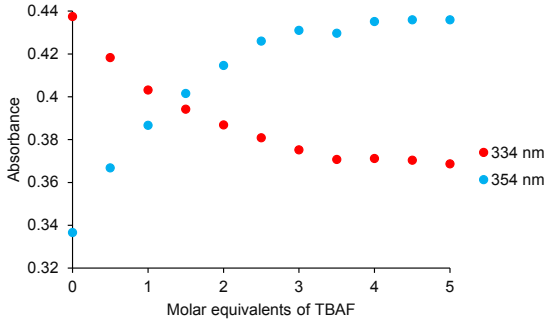
d)


Absorbance
Molar equivalents of TBAB
336 nm
354 nm

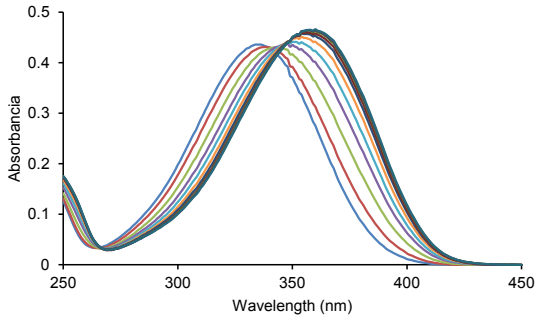
e)


Absorbance
Wavelength (nm)

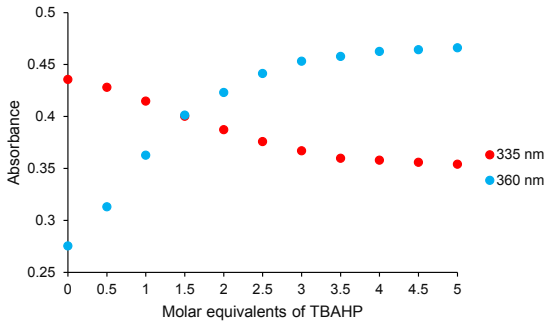
f)


Absorbance
Molar equivalents of TBAF
334 nm
354 nm

g)


Absorbancia
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
335 nm
360 nm

i)

j)

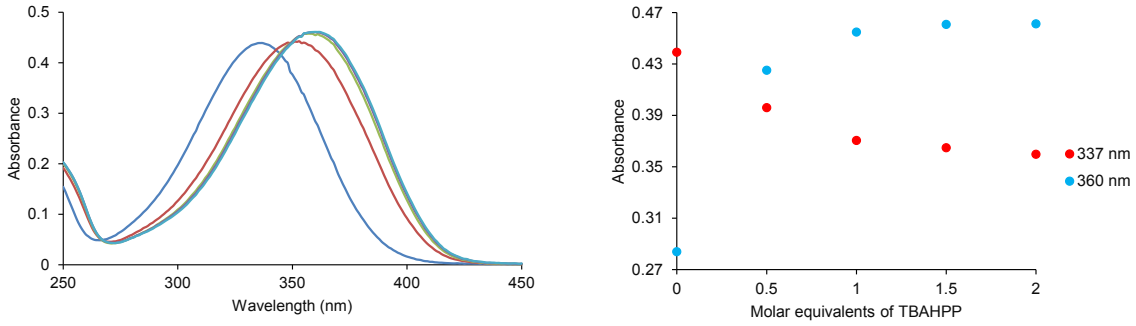
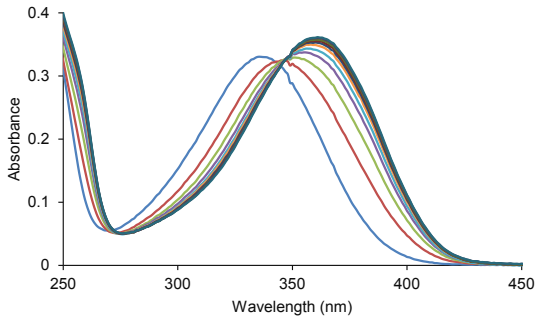
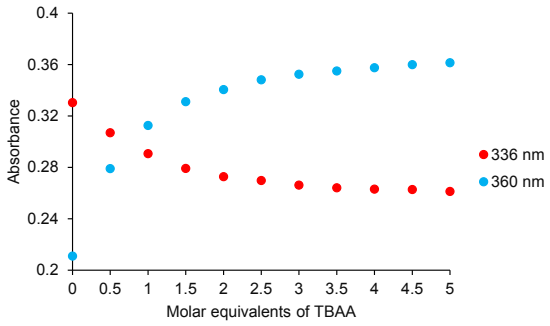


Figure S19. UV-vis spectra and absorbance profiles obtained by the titration of **8a** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

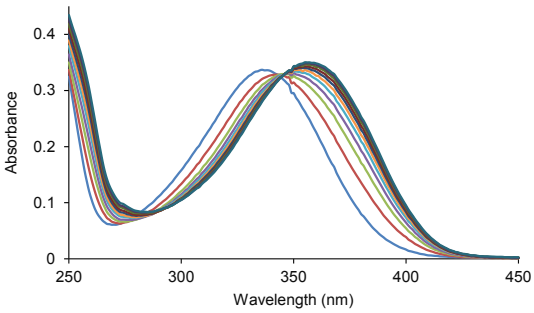
a)


Absorbance
Wavelength (nm)

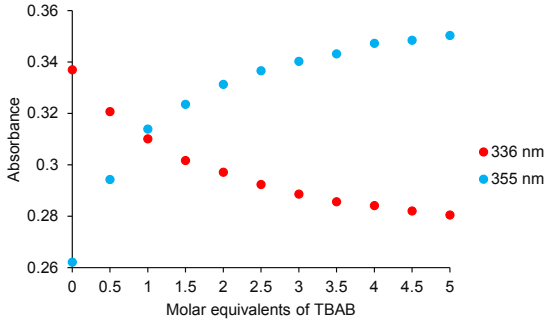
b)


Absorbance
Molar equivalents of TBAA
336 nm
360 nm

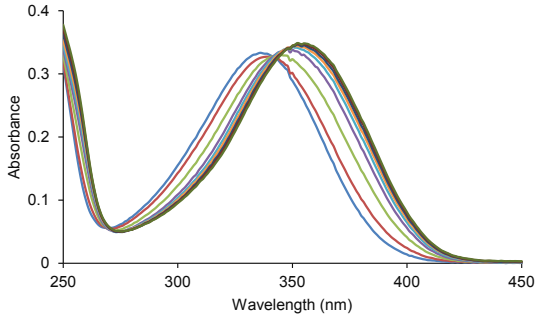
c)


Absorbance
Wavelength (nm)

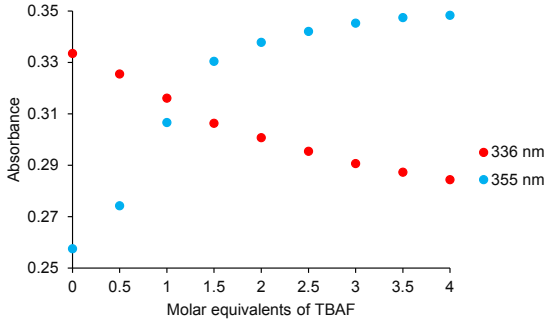
d)


Absorbance
Molar equivalents of TBAB
336 nm
355 nm

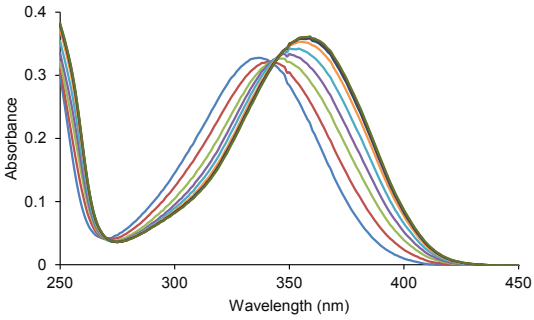
e)


Absorbance
Wavelength (nm)

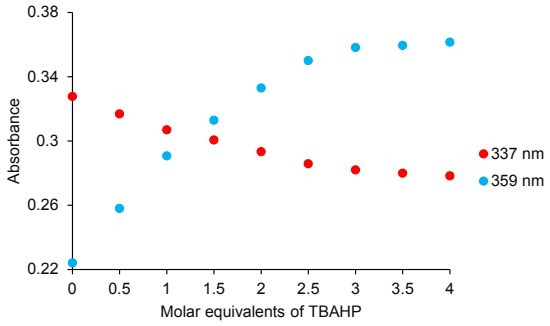
f)


Absorbance
Molar equivalents of TBAF
336 nm
355 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
337 nm
359 nm

i)

j)

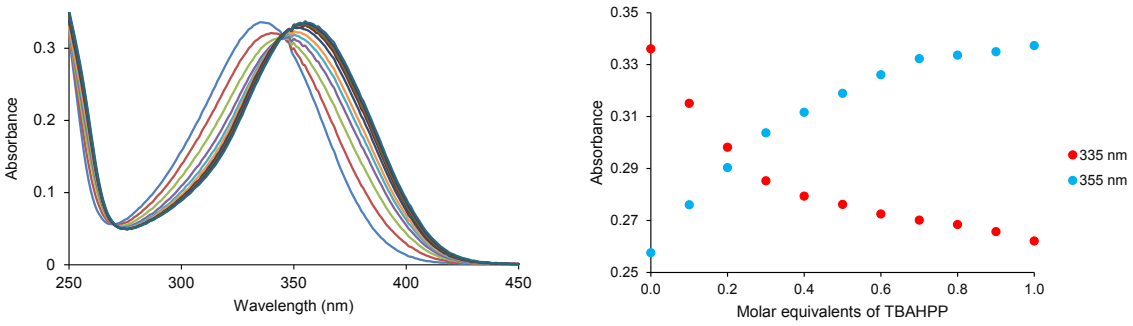
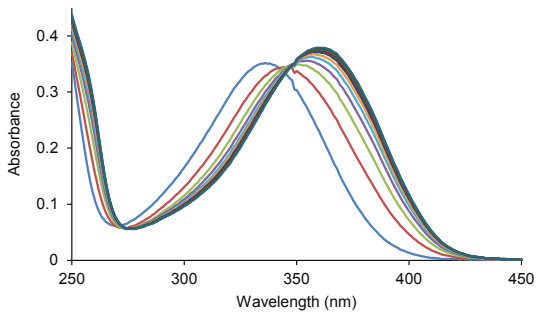
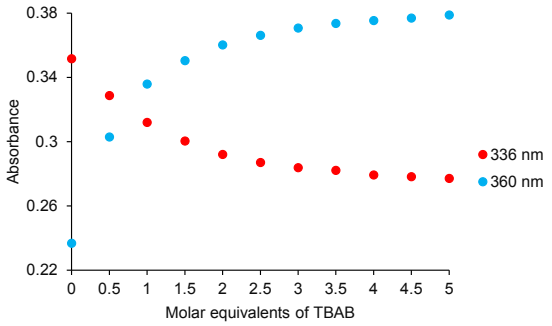


Figure S20. UV-vis spectra and absorbance profiles obtained by the titration of **8b** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

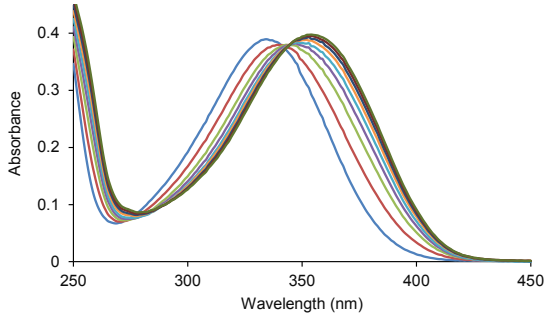
a)


Absorbance
Wavelength (nm)

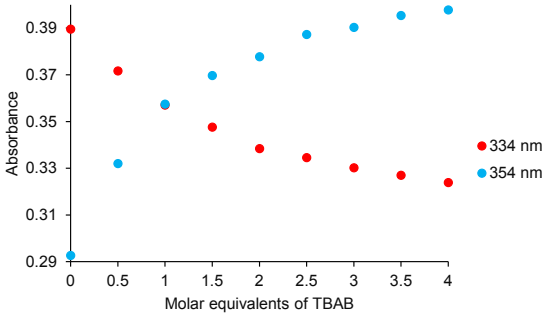
b)


Absorbance
Molar equivalents of TBAB
336 nm
360 nm

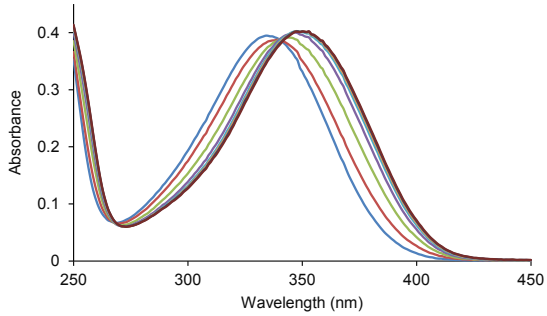
c)


Absorbance
Wavelength (nm)

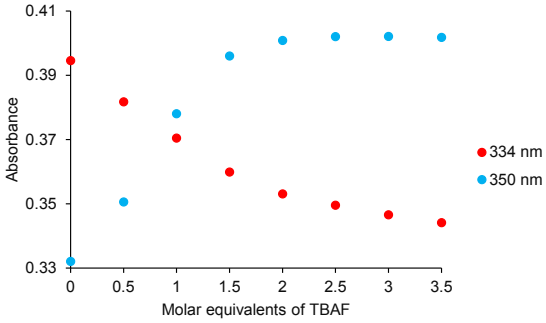
d)


Absorbance
Molar equivalents of TBAB
334 nm
354 nm

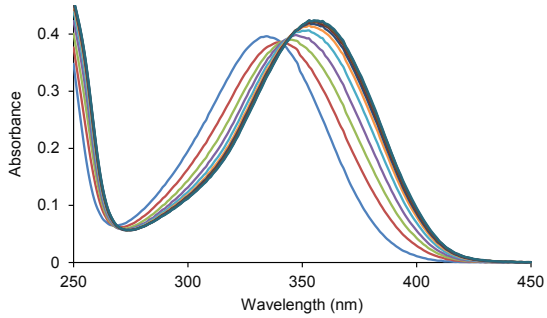
e)


Absorbance
Wavelength (nm)

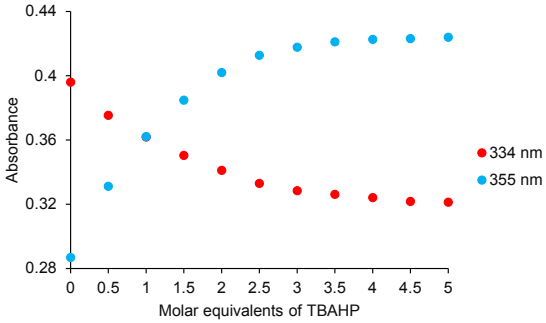
f)


Absorbance
Molar equivalents of TBAF
334 nm
350 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
334 nm
355 nm

i)

j)

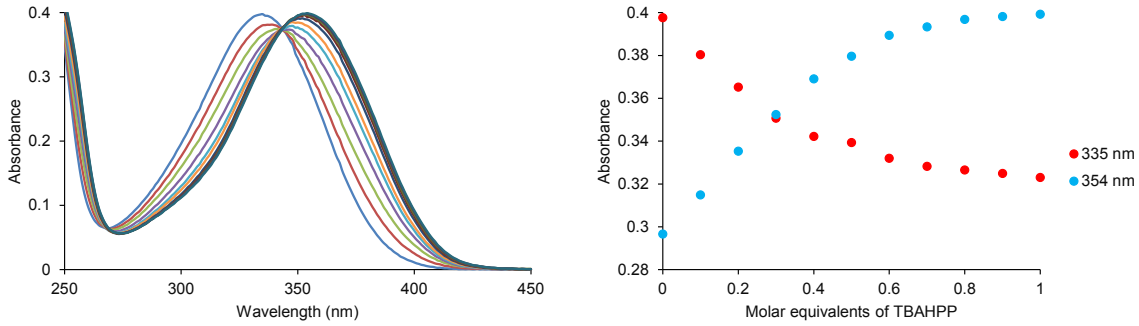
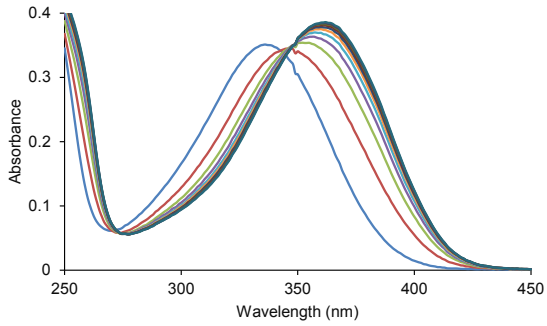
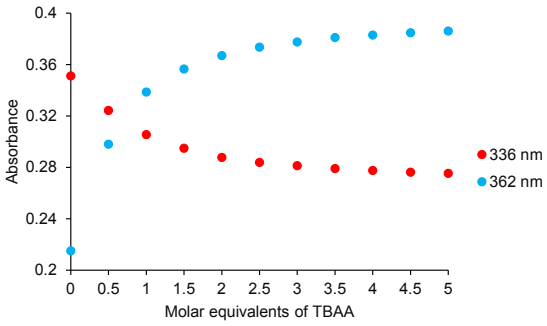


Figure S21. UV-vis spectra and absorbance profiles obtained by the titration of **8c** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

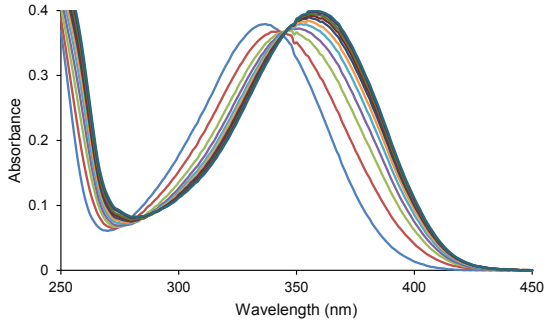
a)


Absorbance
Wavelength (nm)

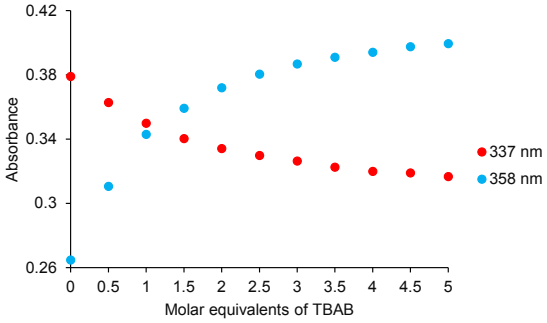
b)


Absorbance
Molar equivalents of TBAA
336 nm
362 nm

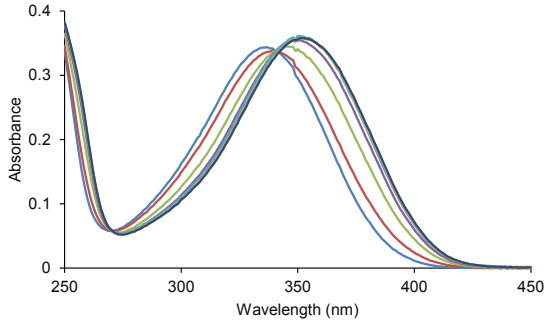
c)


Absorbance
Wavelength (nm)

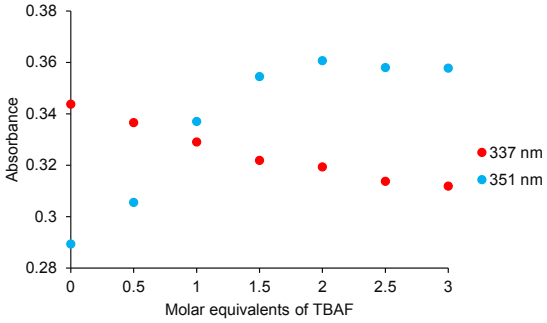
d)


Absorbance
Molar equivalents of TBAB
337 nm
358 nm

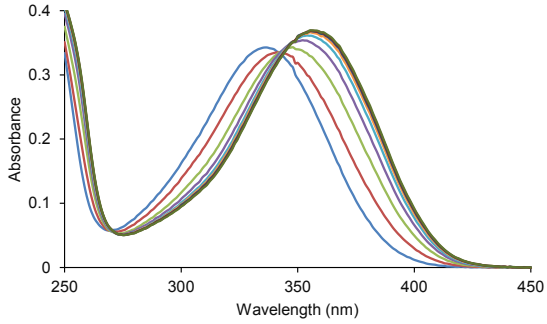
e)


Absorbance
Wavelength (nm)

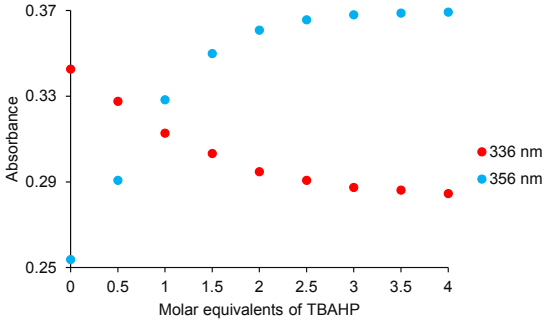
f)


Absorbance
Molar equivalents of TBAF
337 nm
351 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
336 nm
356 nm

i)

j)

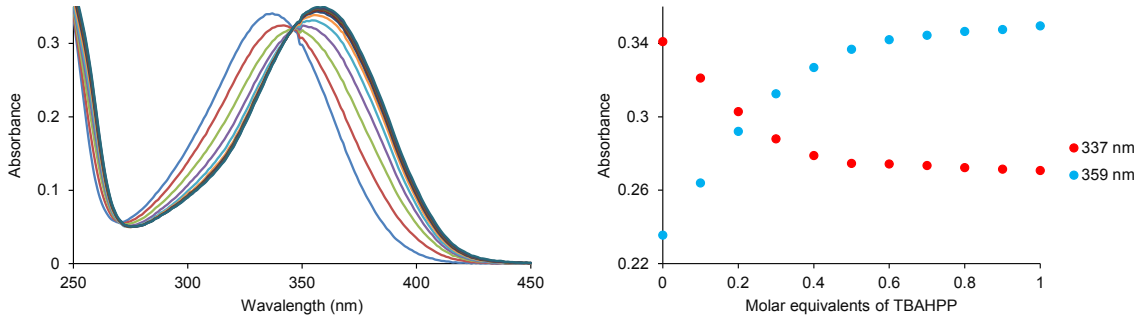
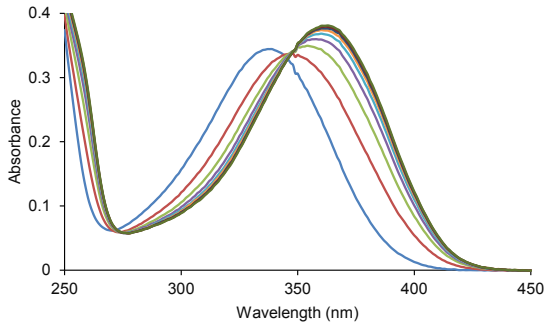
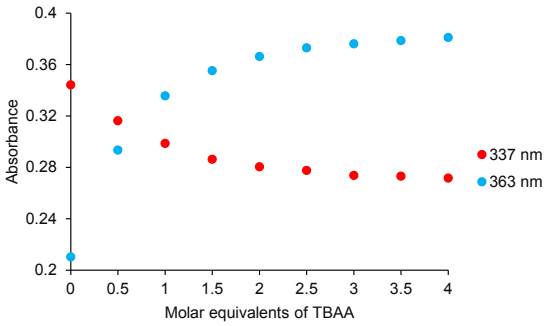


Figure S22. UV-vis spectra and absorbance profiles obtained by the titration of **8d** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

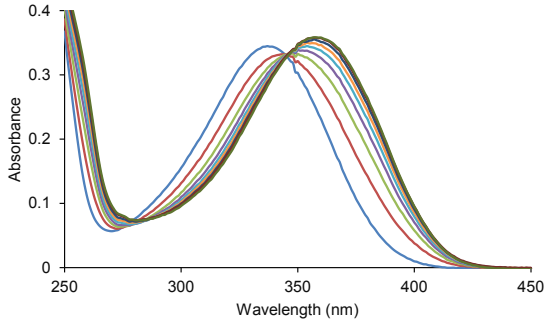
a)


Absorbance
Wavelength (nm)

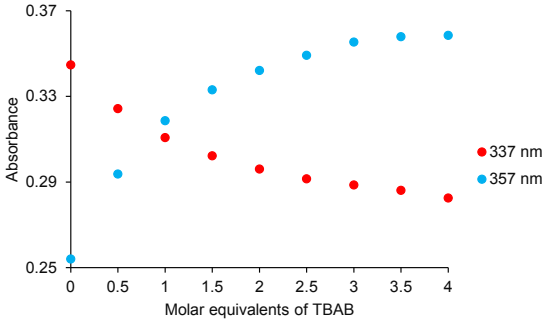
b)


Absorbance
Molar equivalents of TBAA
337 nm
363 nm

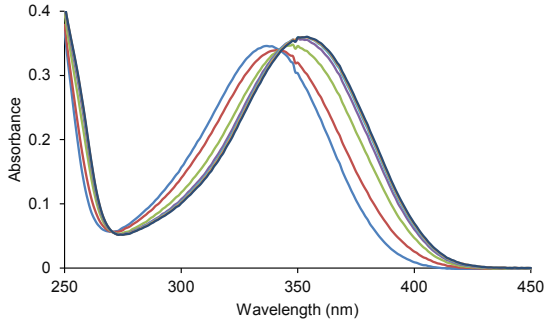
c)


Absorbance
Wavelength (nm)

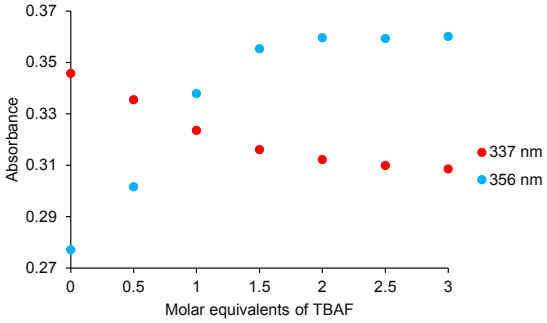
d)


Absorbance
Molar equivalents of TBAB
337 nm
357 nm

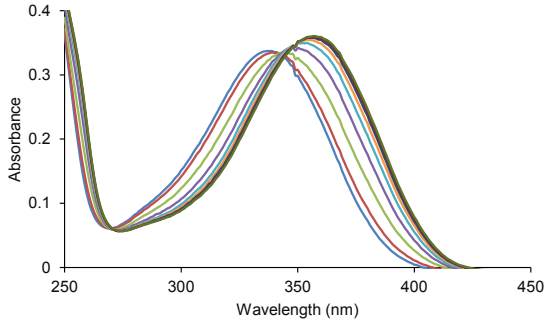
e)


Absorbance
Wavelength (nm)

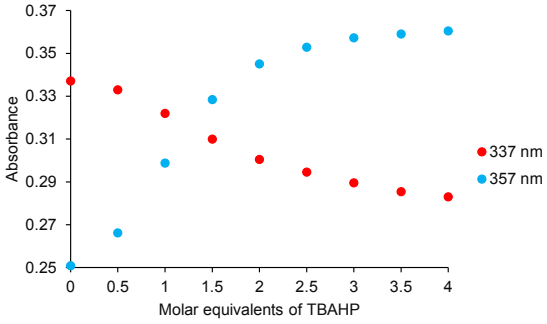
f)


Absorbance
Molar equivalents of TBAF
337 nm
356 nm

g)


Absorbance
Wavelength (nm)

h)


Absorbance
Molar equivalents of TBAHP
337 nm
357 nm

i)

j)

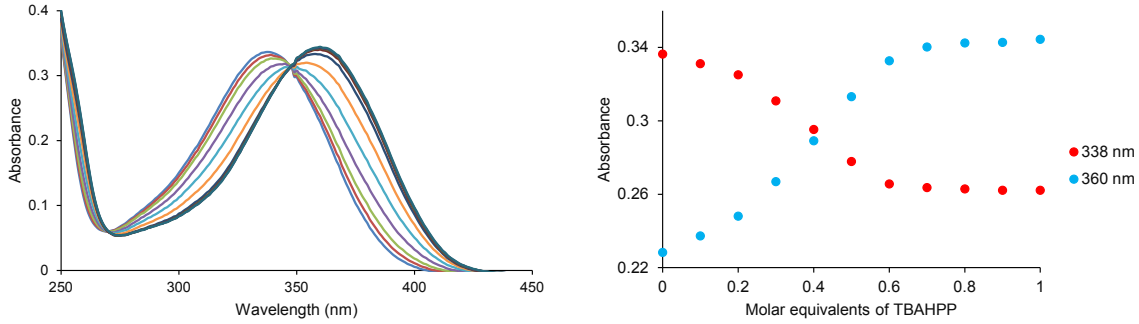


Figure S23. UV-vis spectra and absorbance profiles obtained by the titration of **8e** with TBAA (a and b), TBAB (c and d), TBAF (e and f), TBAHP (g and h) and TBAHPP (i and j).

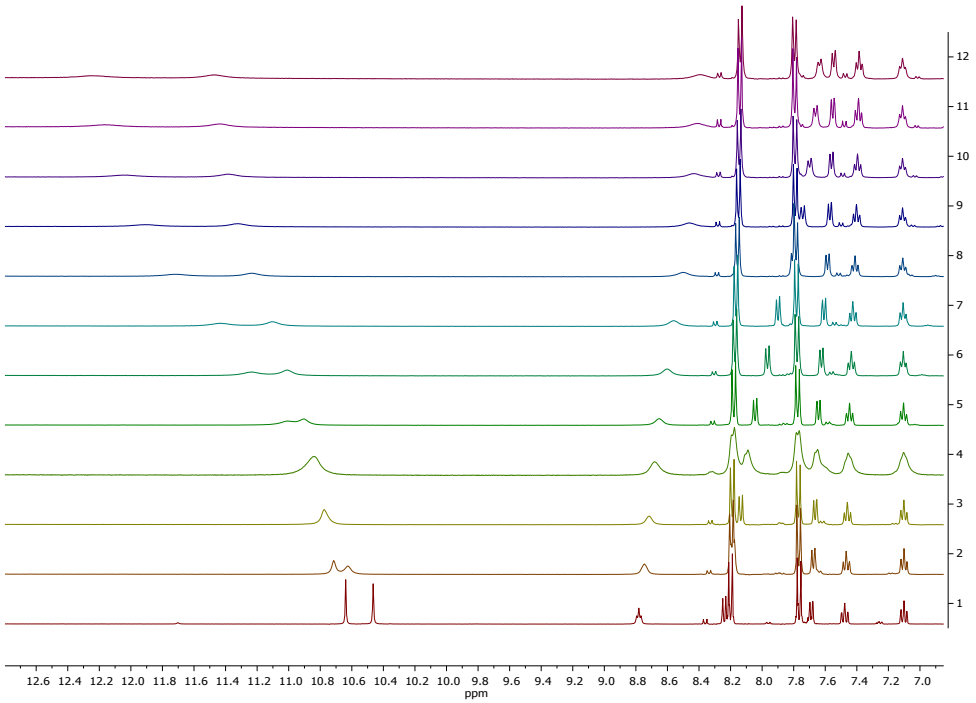


Figure S24. ^{1}H NMR spectra obtained by titration of *ortho* mono-ureylbenzamide with TBAA in DMSO-d_6.

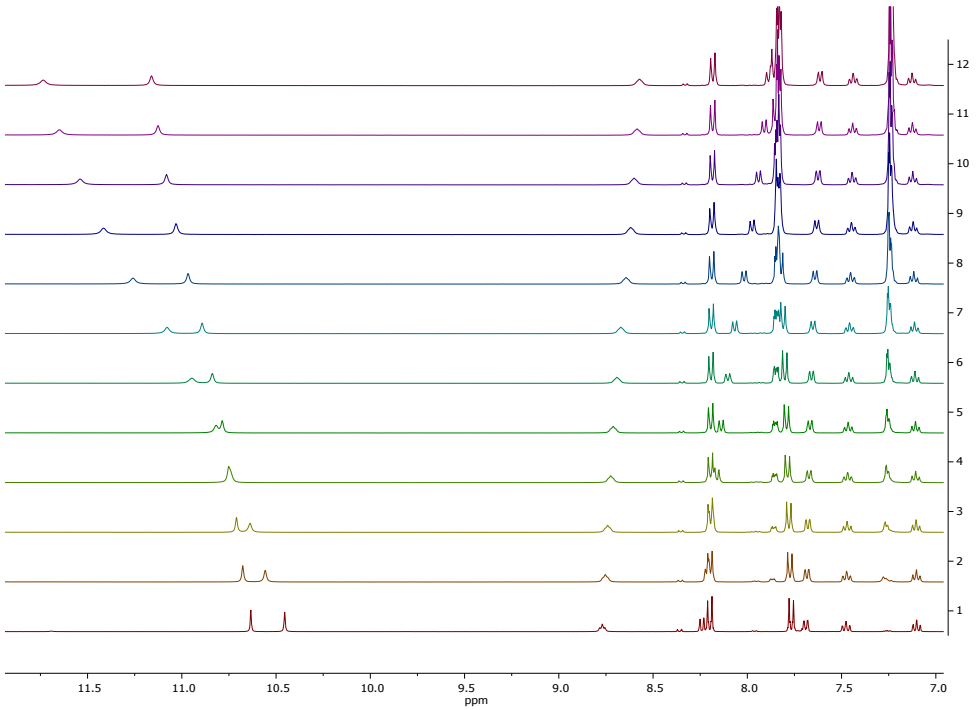


Figure S25. ^{1}H NMR spectra obtained by titration of *ortho* mono-ureabenzamide with TBAB in DMSO-d_6.

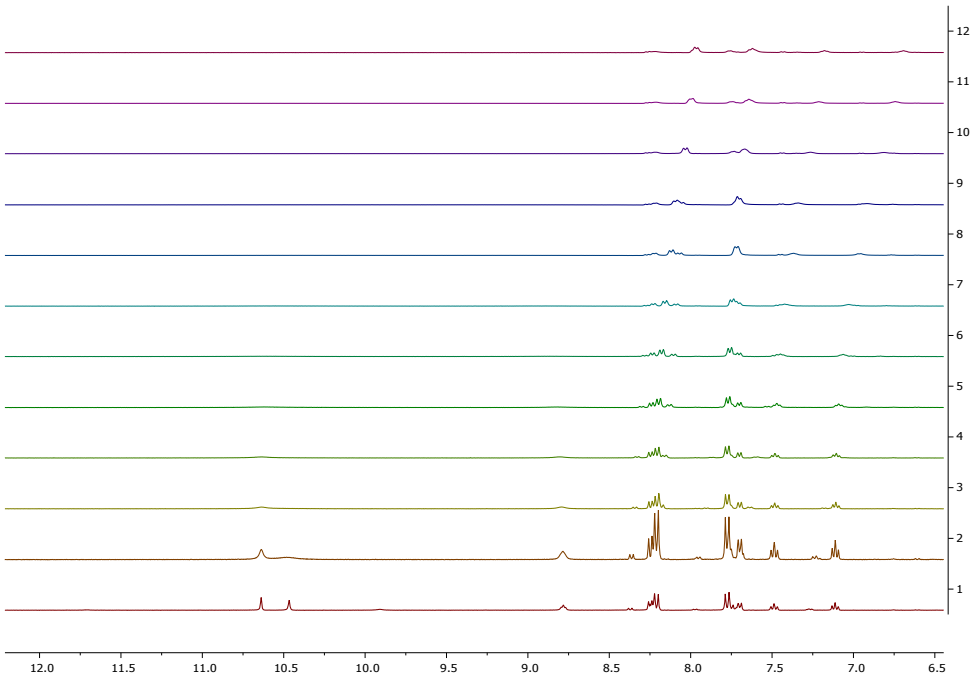


Figure S26. ^{1}H NMR spectra obtained by titration of *ortho* mono-ureabenzamide with TBAF in DMSO-d_6.

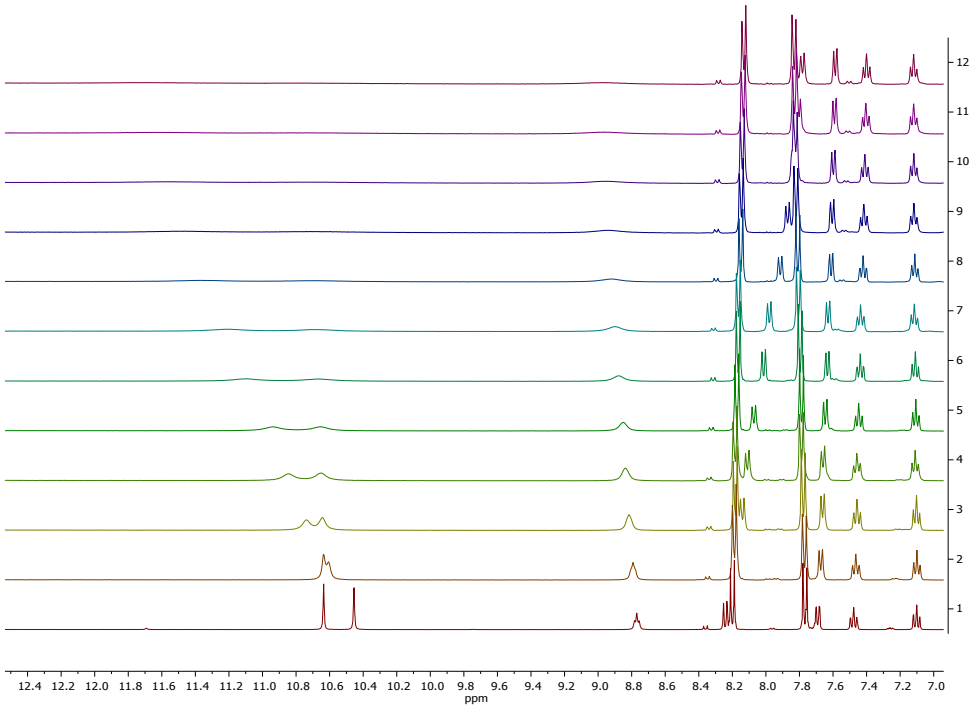


Figure S27. ^{1}H NMR spectra obtained by titration of *ortho* mono-ureabenzamide with TBAHP in DMSO-d_6.

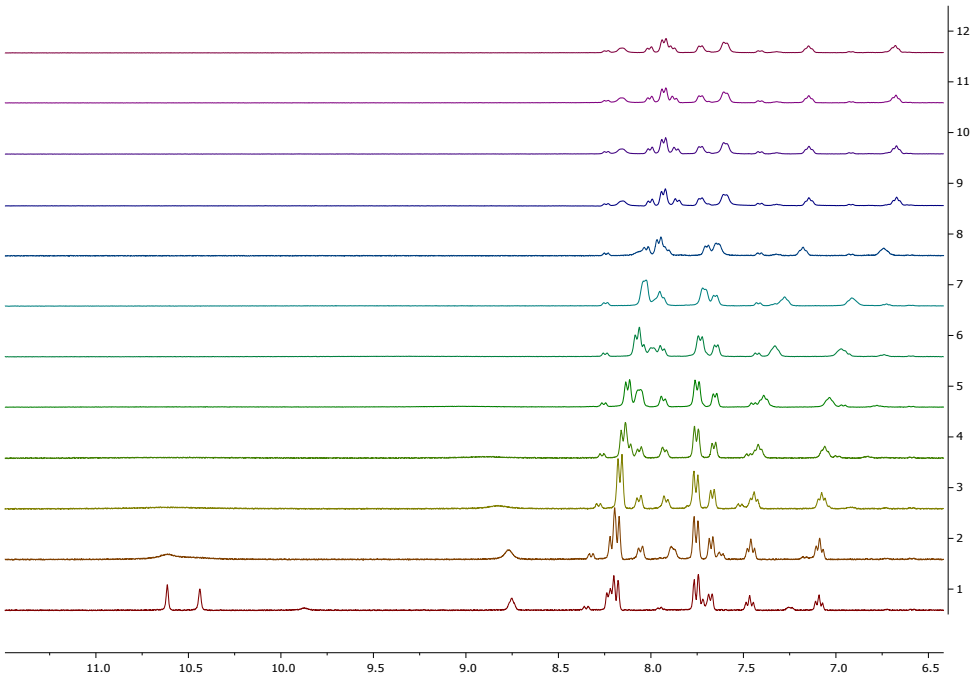


Figure S28. ^{1}H NMR spectra obtained by titration of *ortho* mono-ureylbenzamide with TBAHPP in DMSO-d_6.

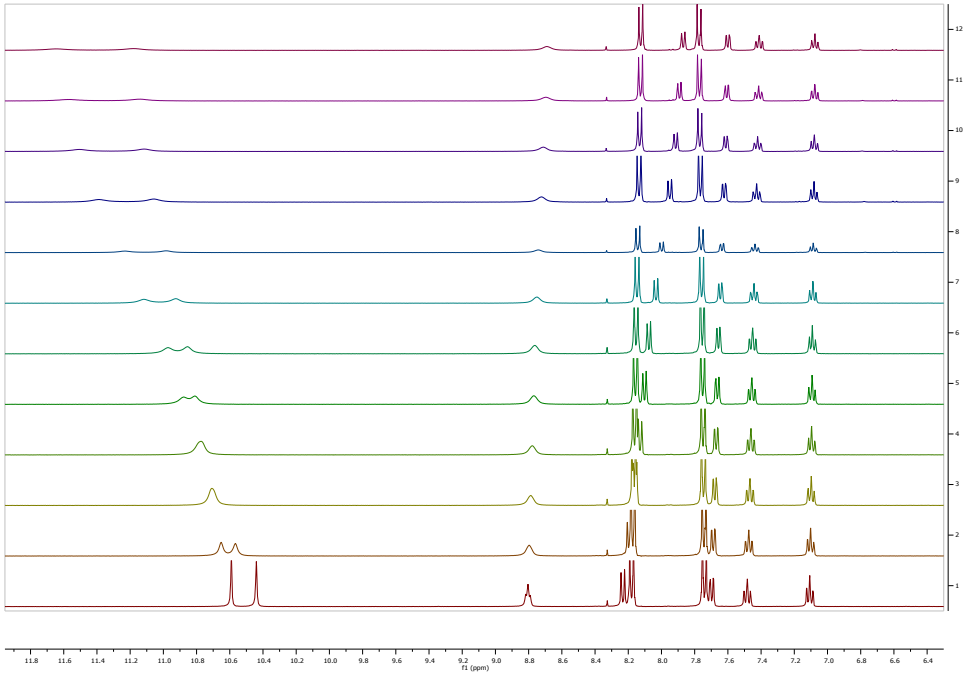


Figure S29. ^{1}H NMR spectra obtained by titration of **4b** with TBAA in DMSO-d_6.

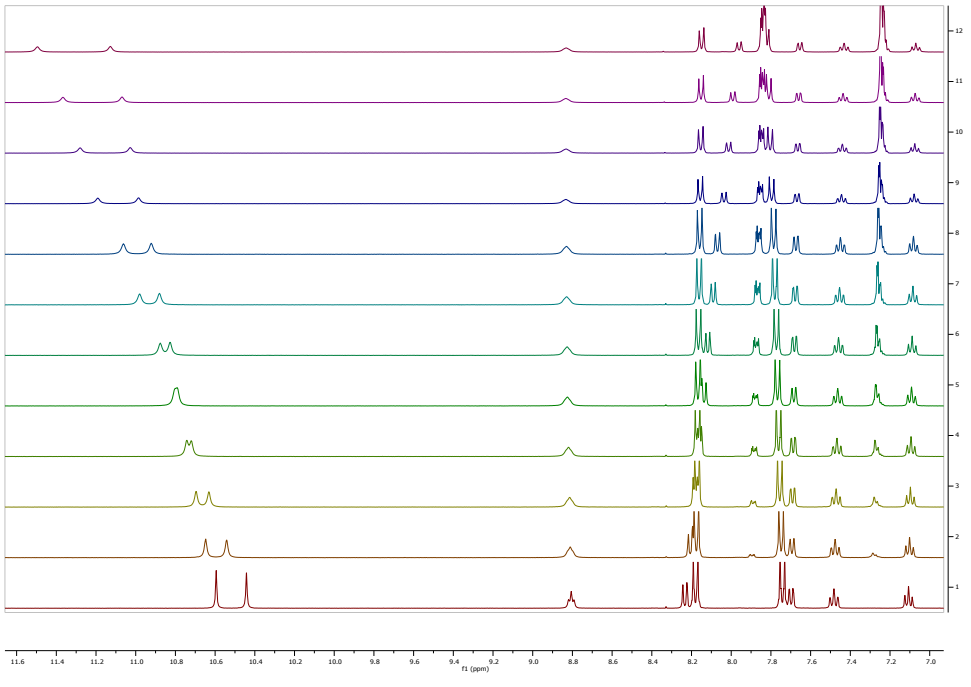


Figure S30. ^{1}H NMR spectra obtained by titration of **4b** with TBAB in DMSO-d_6.

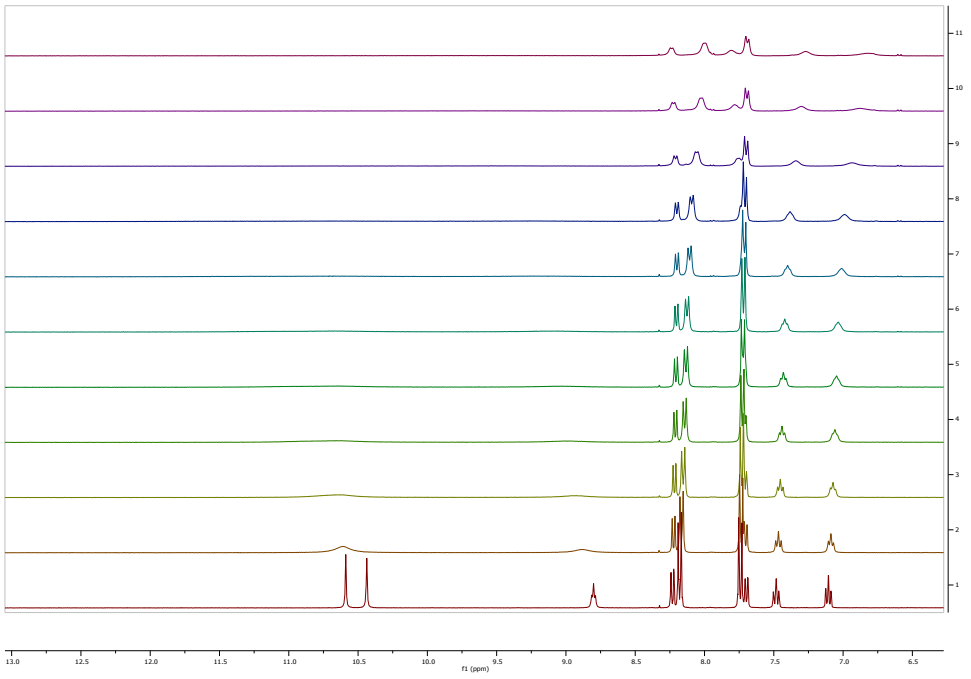


Figure S31. ^{1}H NMR spectra obtained by titration of **4b** with TBAF in DMSO-d_6.

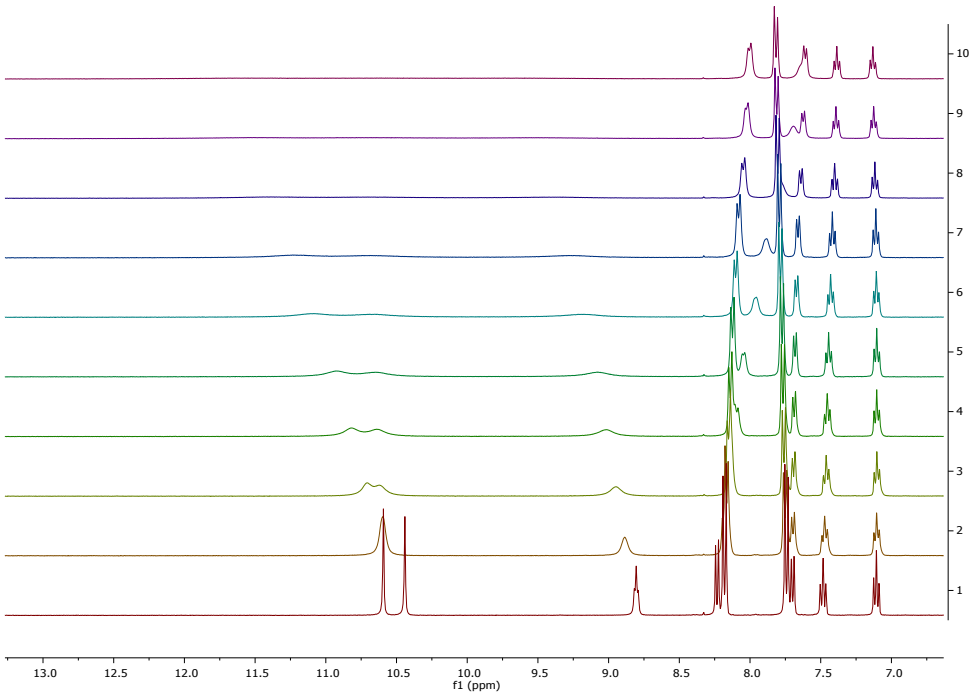


Figure S32. ^{1}H NMR spectra obtained by titration of **4b** with TBAHP in DMSO-d_6.

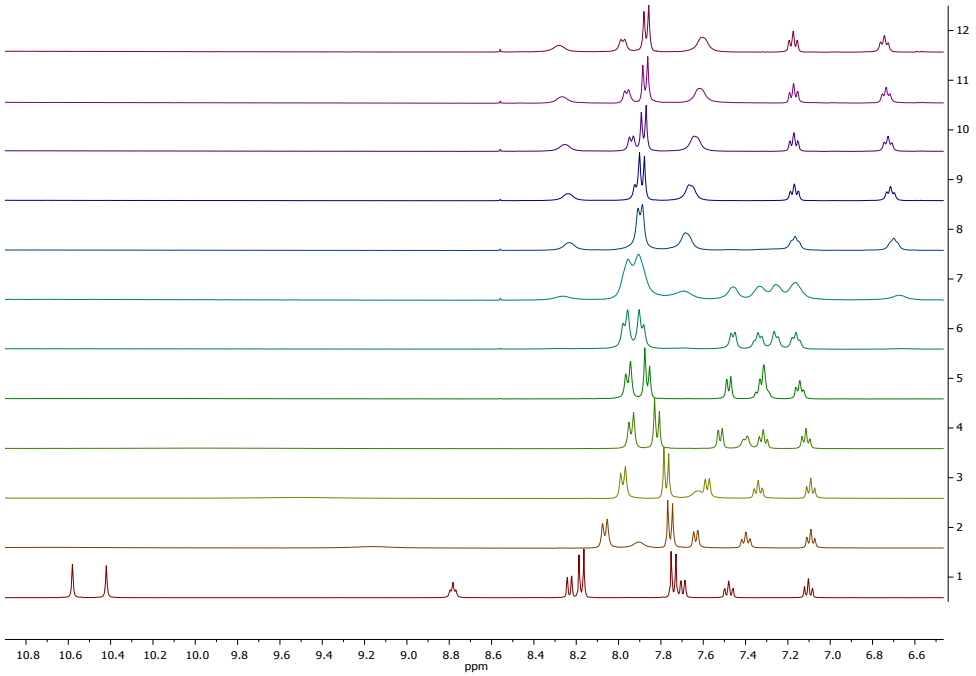


Figure S33. ^{1}H NMR spectra obtained by titration of **4b** with TBAHPP in DMSO-d_6.

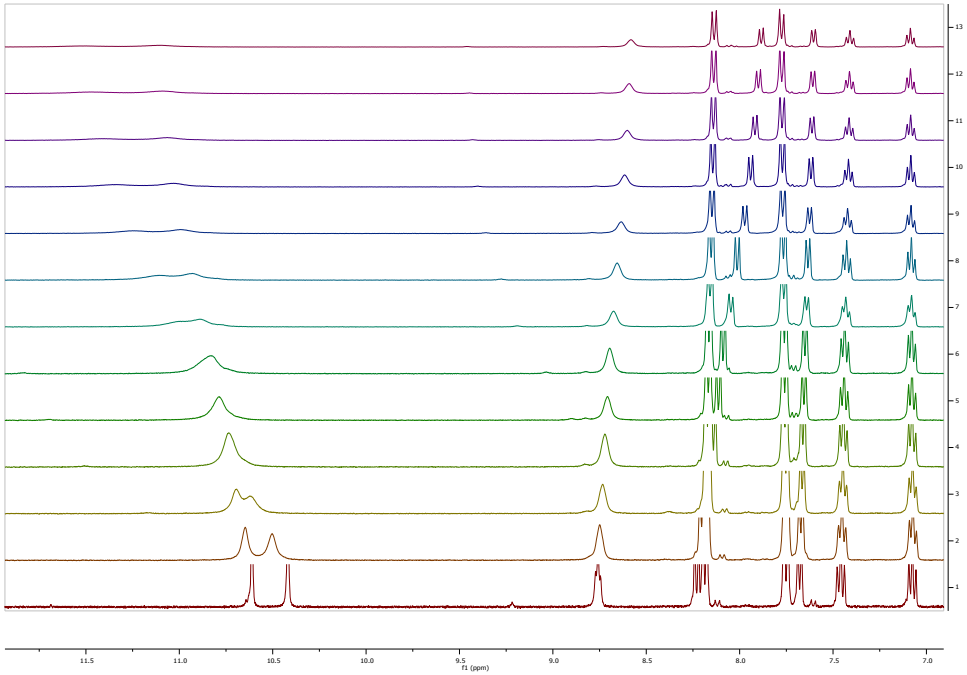


Figure S34. ^{1}H NMR spectra obtained by titration of **4c** with TBAA in DMSO-d_6.

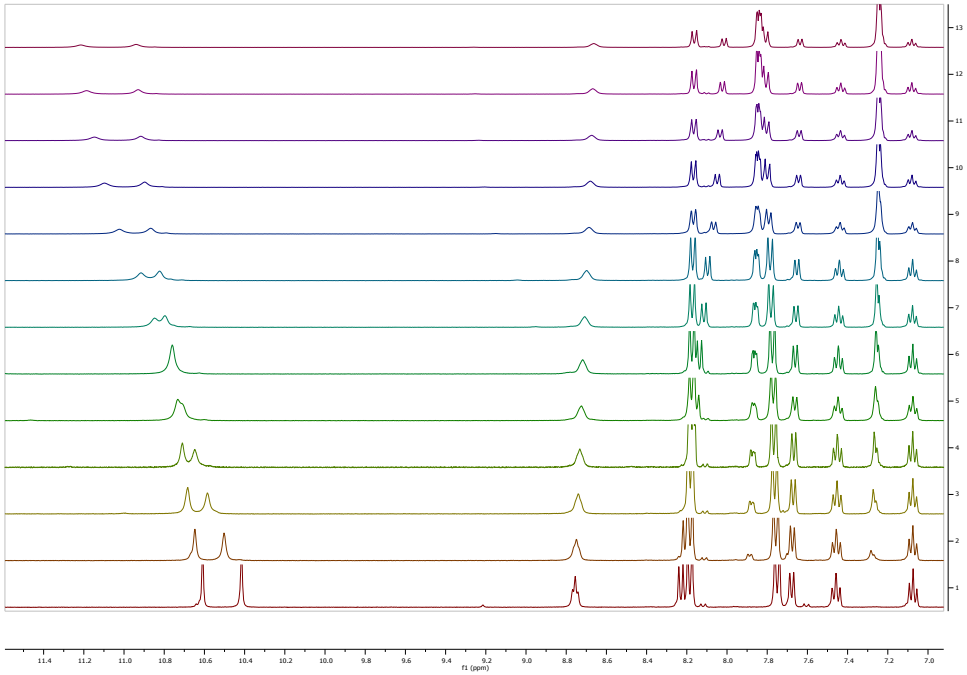


Figure S35. ^{1}H NMR spectra obtained by titration of **4c** with TBAB in DMSO-d_6.

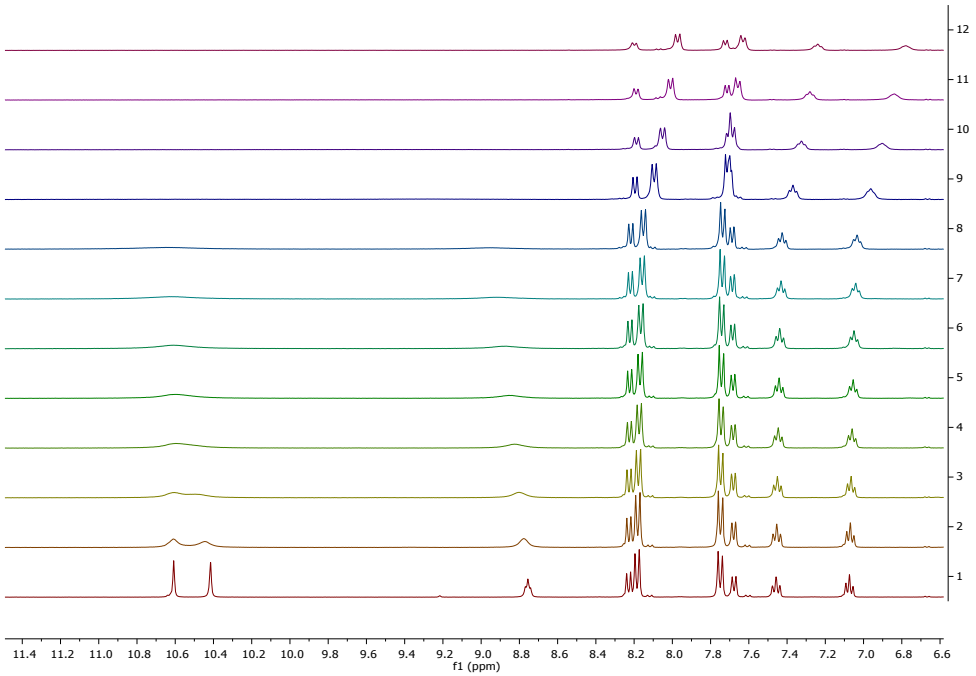


Figure S36. [1]H NMR spectra obtained by titration of **4c** with TBAF in DMSO-d_6.

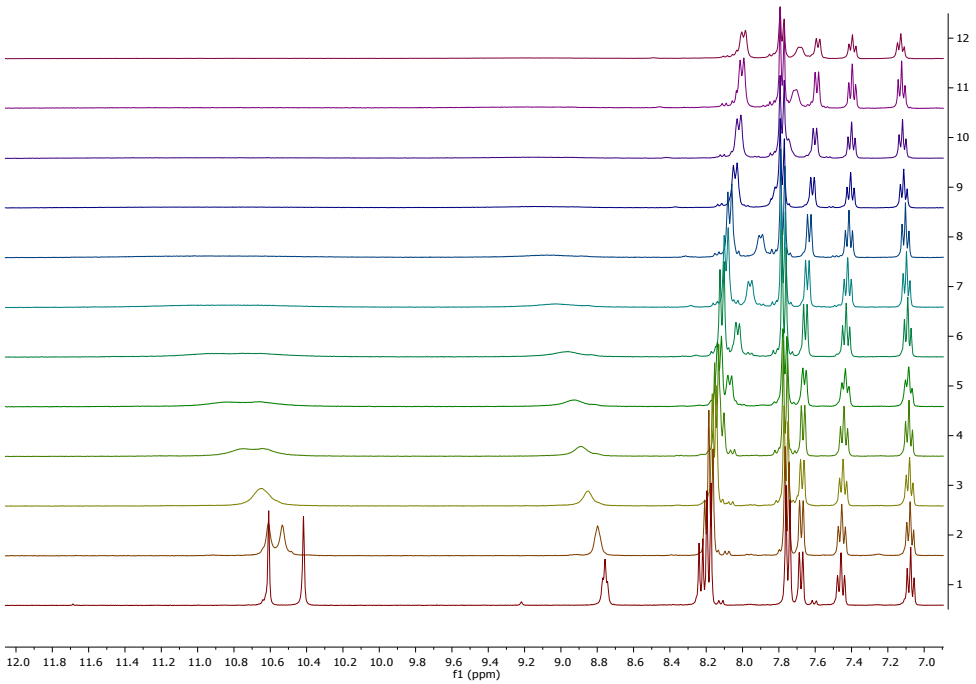


Figure S37. [1]H NMR spectra obtained by titration of **4c** with TBAHP in DMSO-d_6.

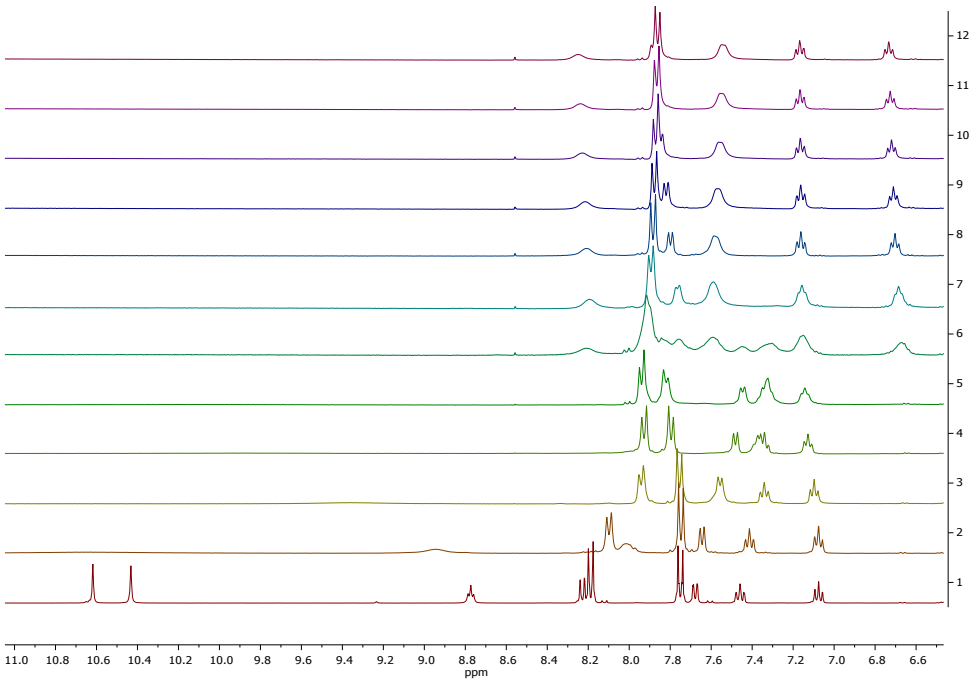


Figure S38. ^{1}H NMR spectra obtained by titration of **4c** with TBAHPP in DMSO-d_6.

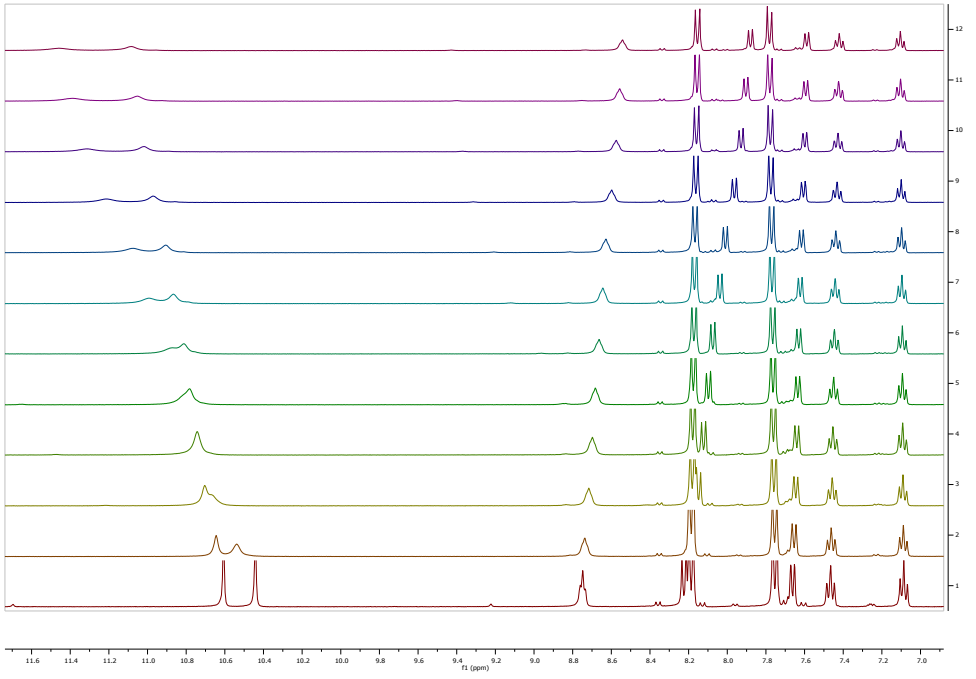


Figure S39. ^{1}H NMR spectra obtained by titration of **4d** with TBAA in DMSO-d_6.

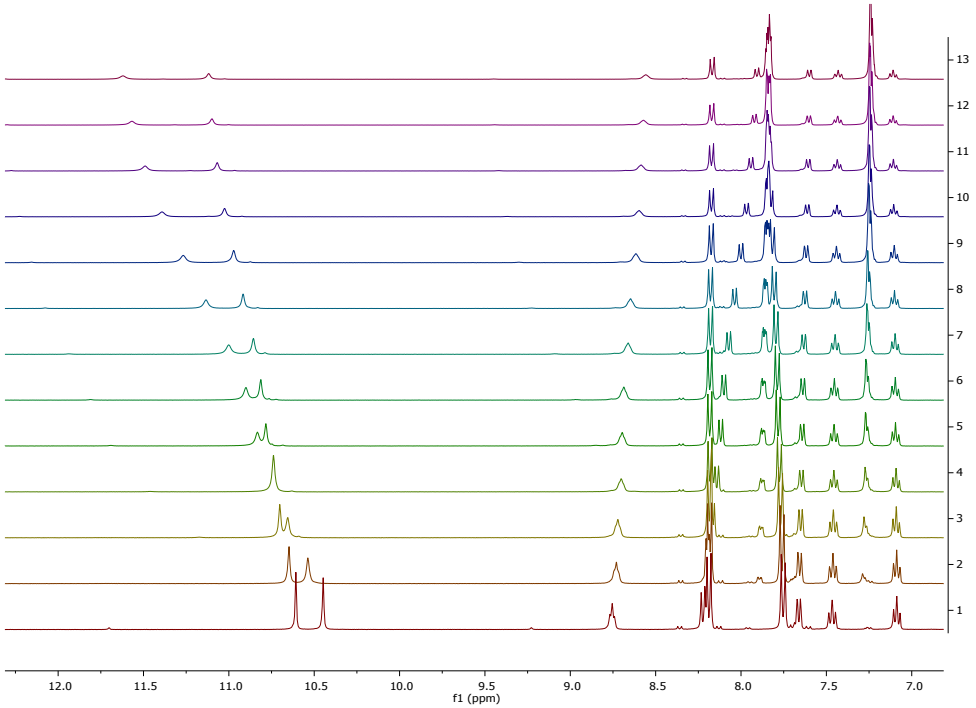


Figure S40. ^{1}H NMR spectra obtained by titration of **4d** with TBAB in DMSO-d_6.

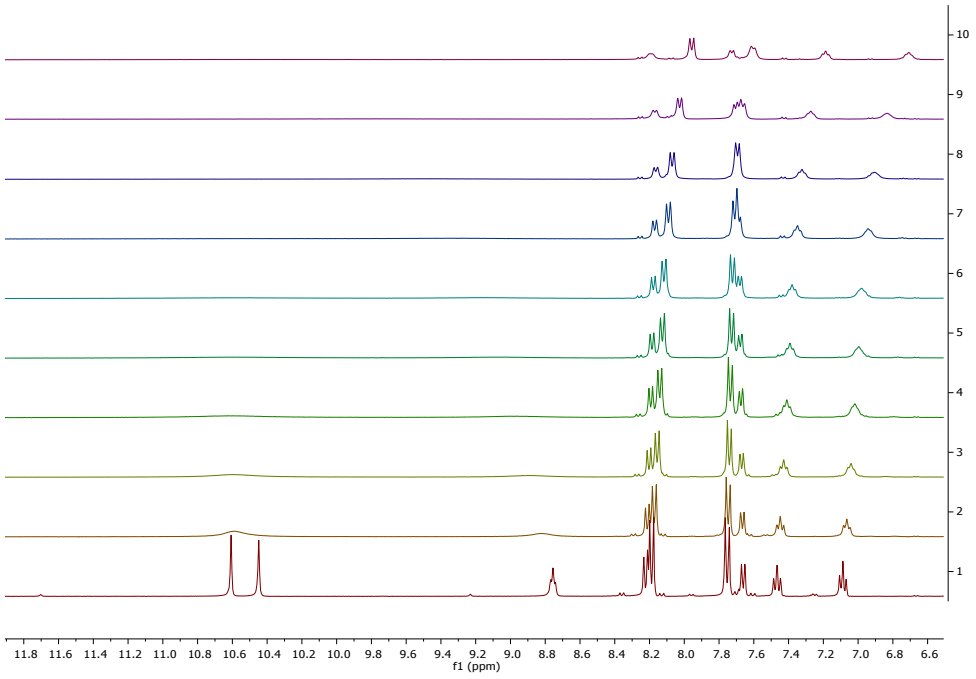


Figure S41. ^{1}H NMR spectra obtained by titration of **4d** with TBAF in DMSO-d_6.

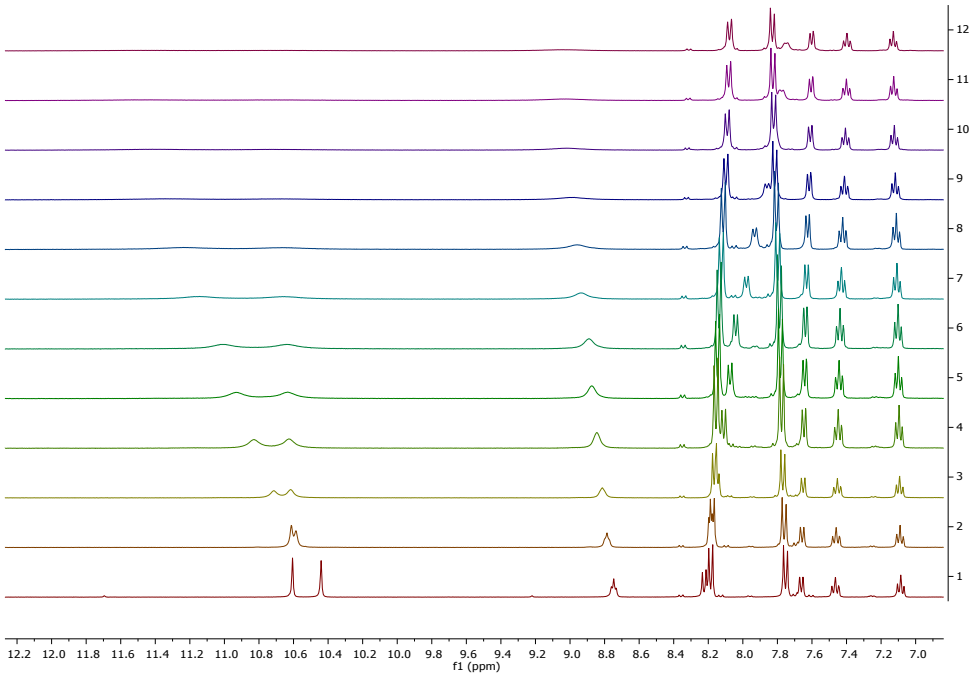


Figure S42. ^{1}H NMR spectra obtained by titration of **4d** with TBAHP in DMSO-d_6.

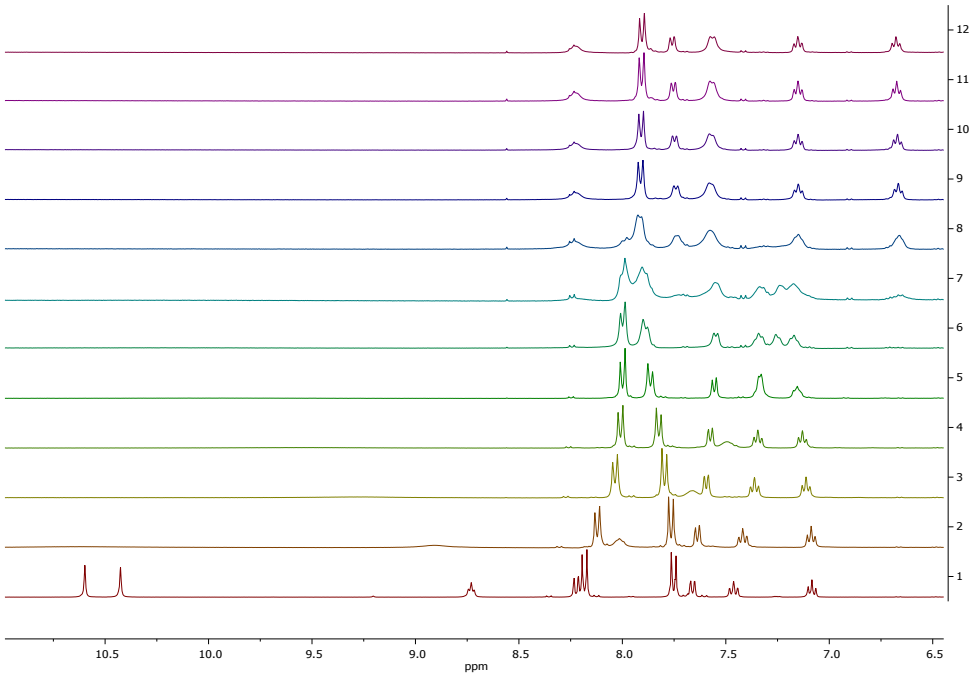


Figure S43. ^{1}H NMR spectra obtained by titration of **4d** with TBAHPP in DMSO-d_6.

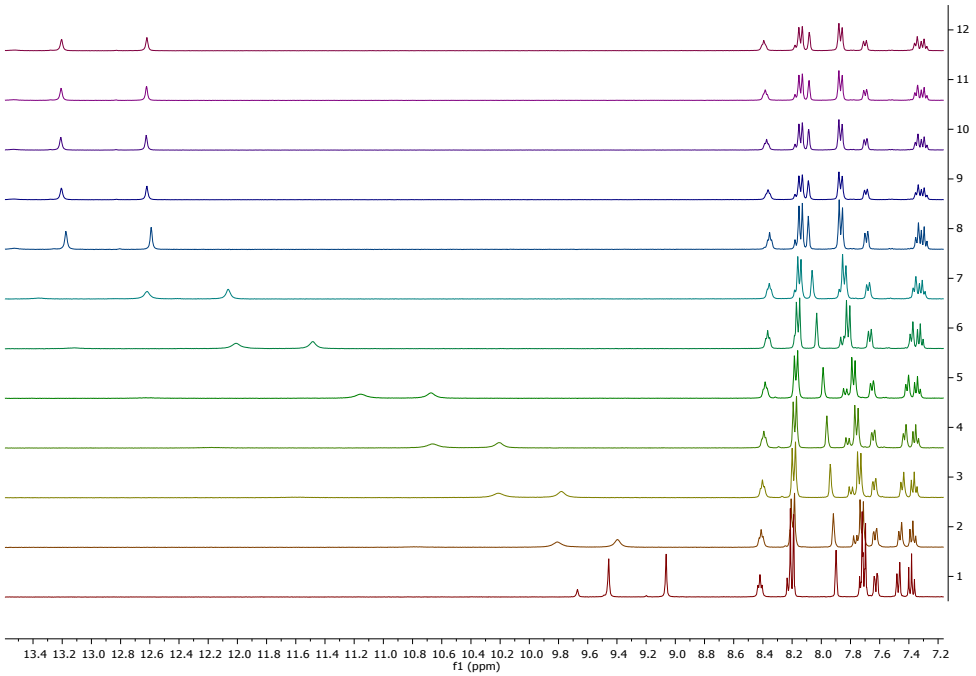


Figure S44. ^{1}H NMR spectra obtained by titration of *meta* mono-ureylbenzamide with TBAA in DMSO-d_6.

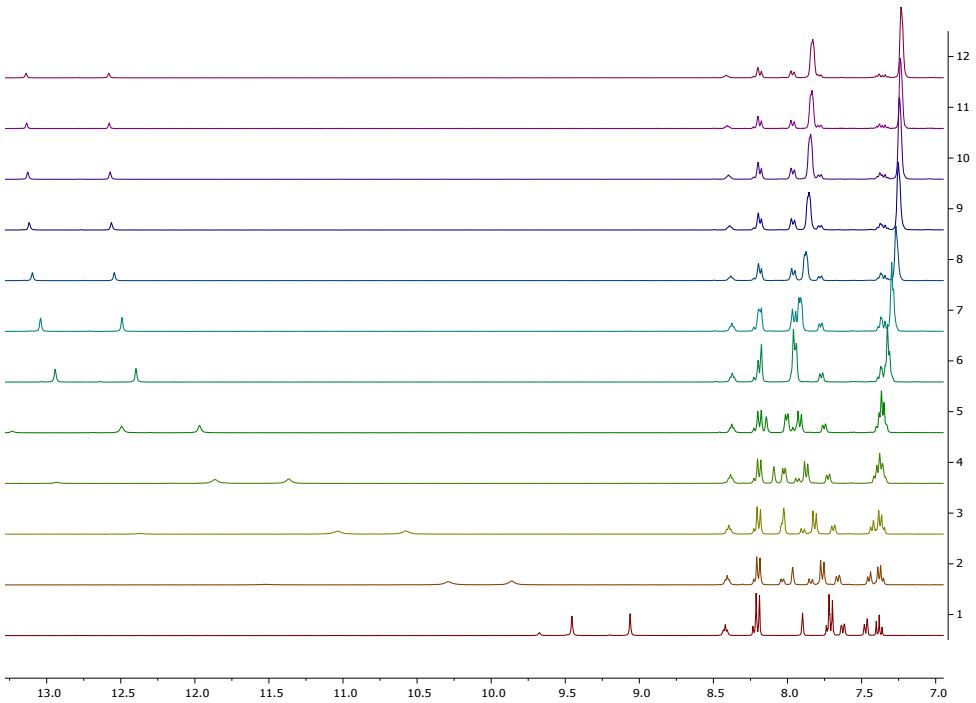


Figure S45. ^{1}H NMR spectra obtained by titration of *meta* mono-ureabenzamide with TBAB in DMSO-d_6.

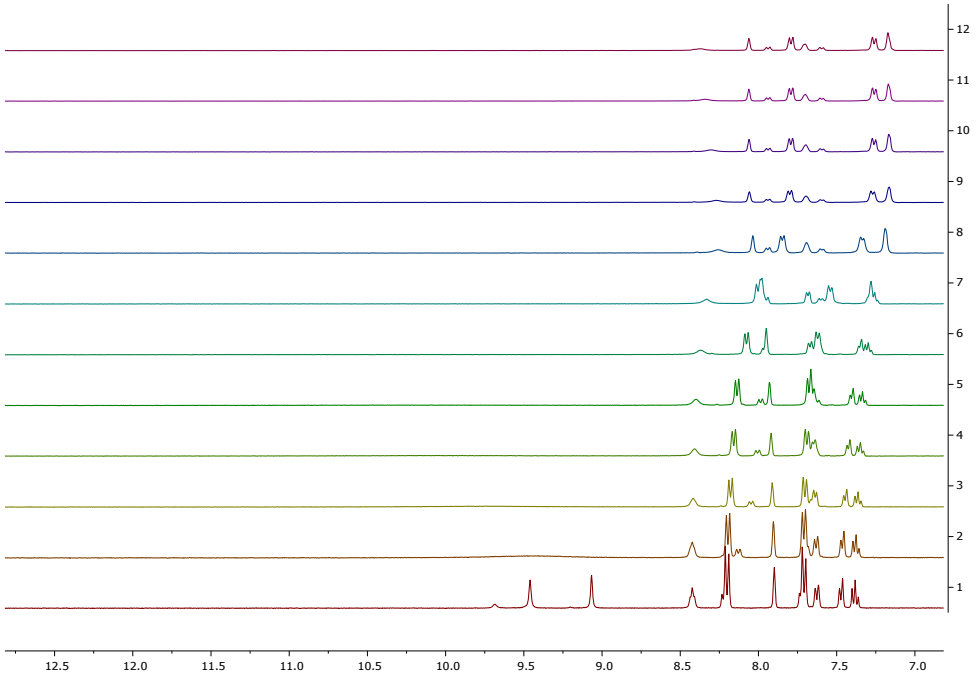


Figure S46. ^{1}H NMR spectra obtained by titration of *meta* mono-ureabenzamide with TBAF in DMSO-d_6.

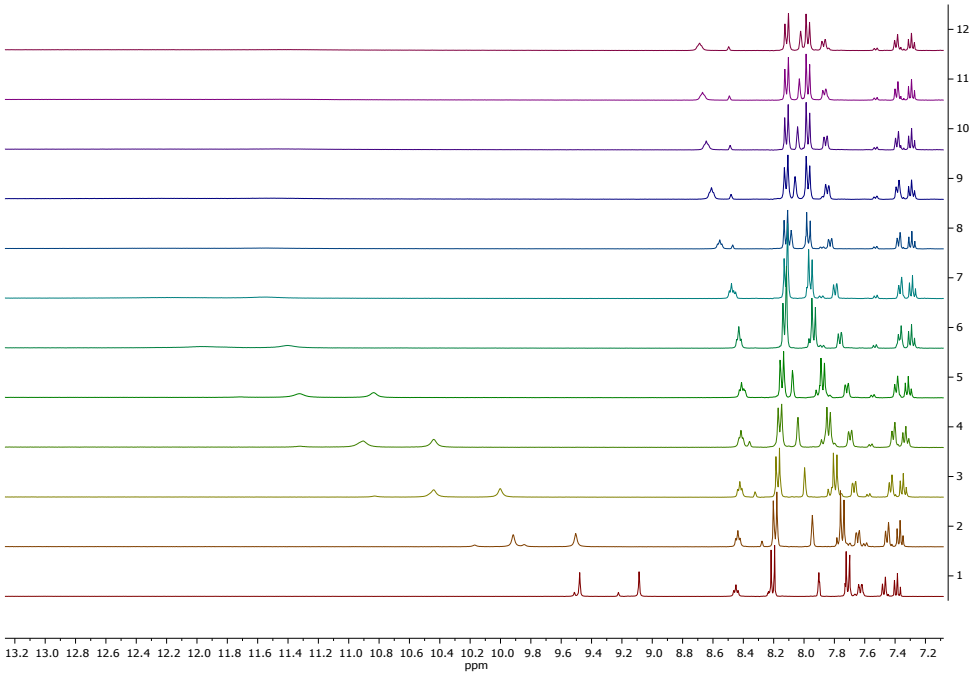


Figure S47. ^{1}H NMR spectra obtained by titration of *meta* mono-ureabenzamide with TBAHP in DMSO-d_6.

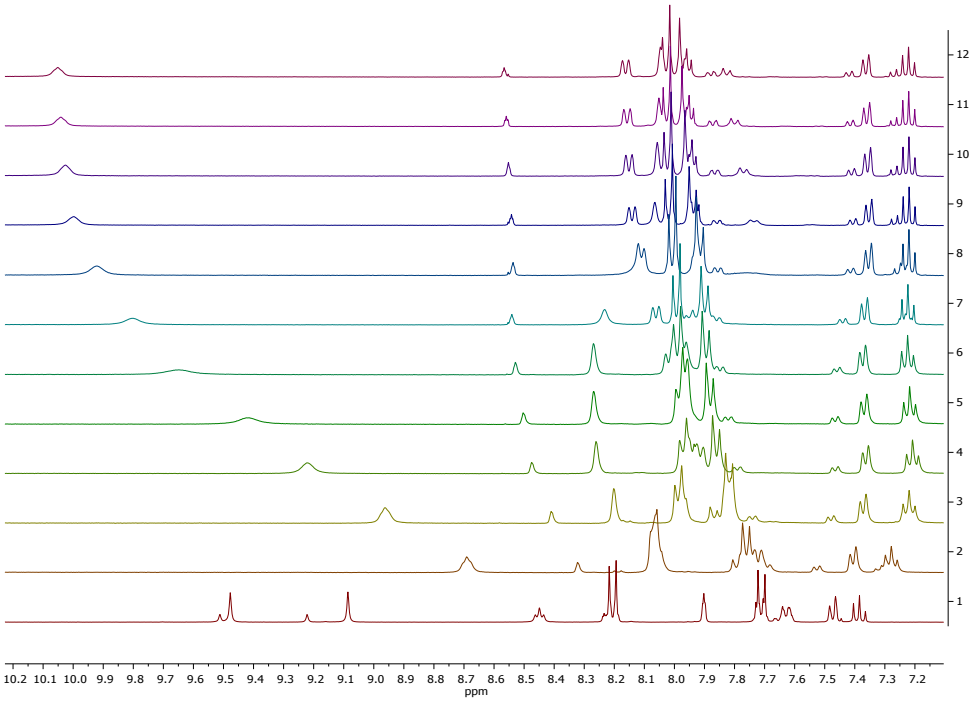


Figure S48. ^{1}H NMR spectra obtained by titration of *meta* mono-ureabenzamide with TBAHPP in DMSO-d_6.

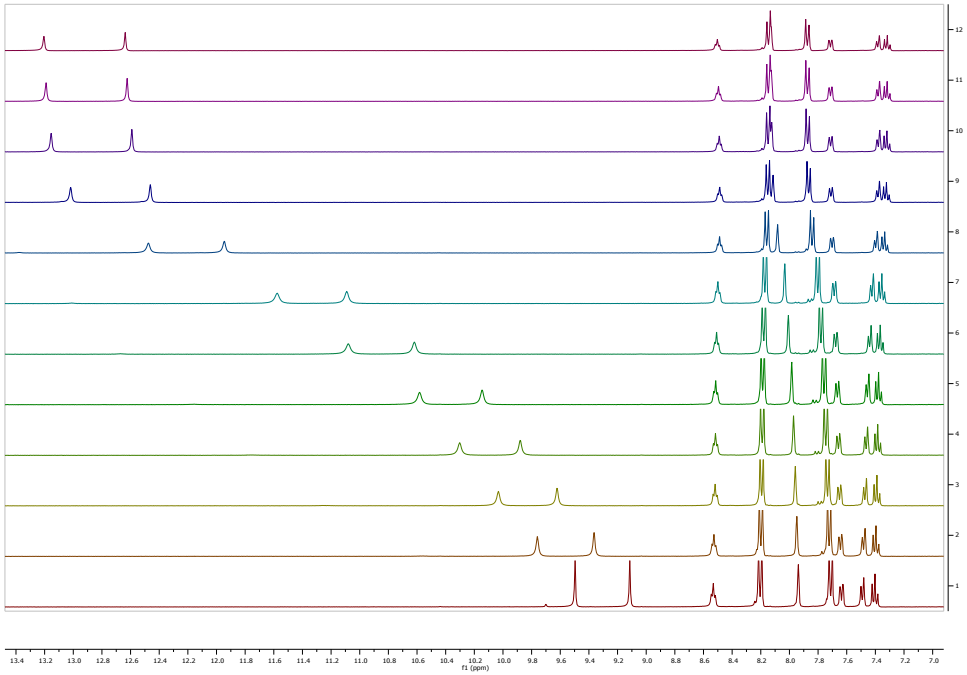


Figure S49. ^{1}H NMR spectra obtained by titration of **8b** with TBAA in DMSO-d_6.

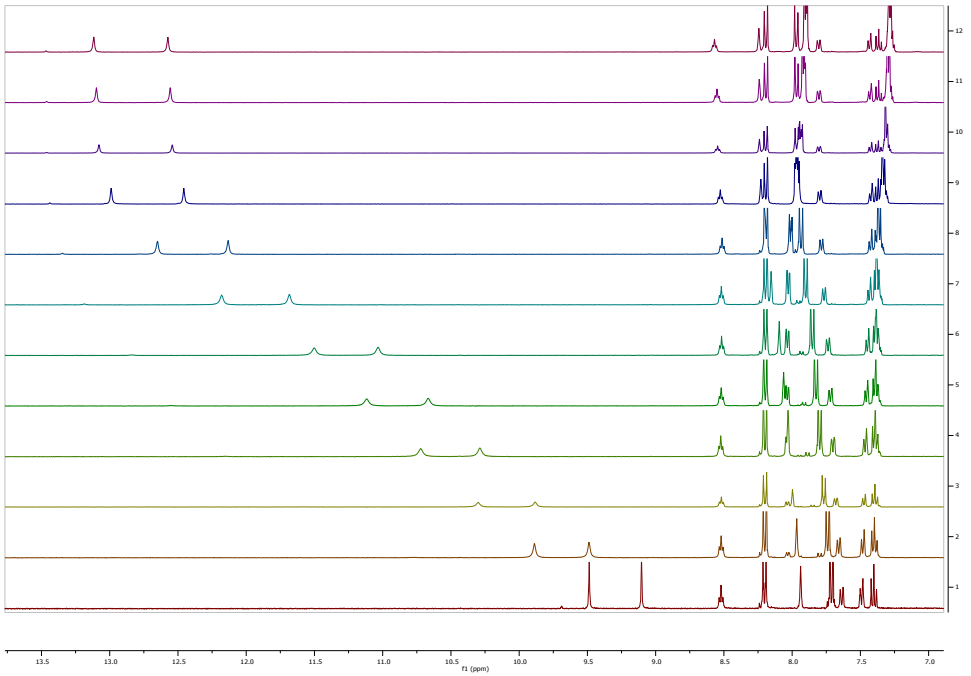


Figure S50. ^{1}H NMR spectra obtained by titration of **8b** with TBAB in DMSO-d_6.

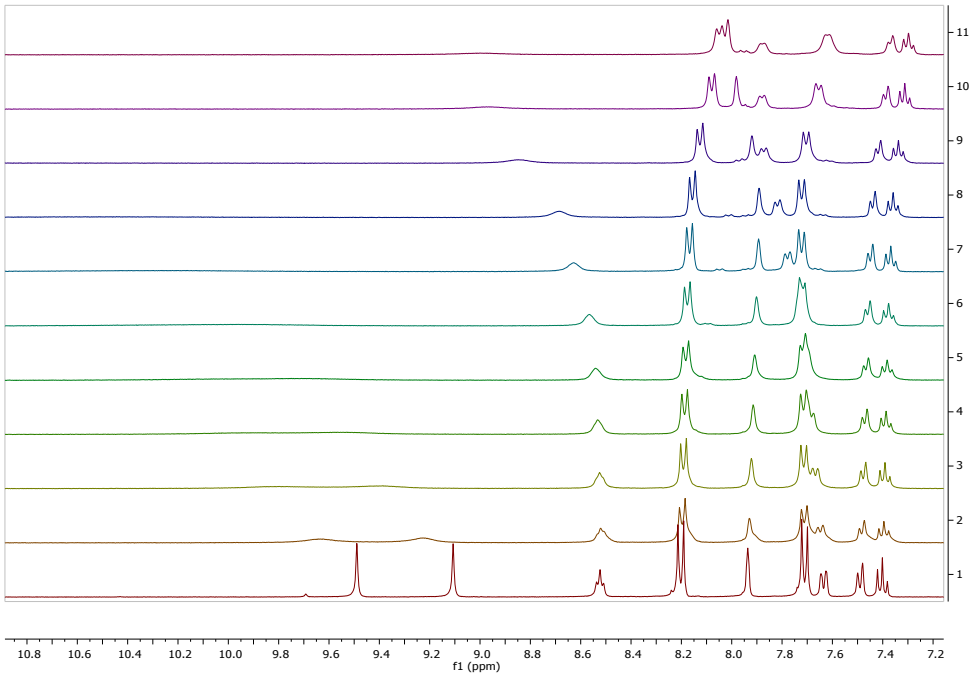


Figure S51. ^{1}H NMR spectra obtained by titration of **8b** with TBAF in DMSO-d_6.

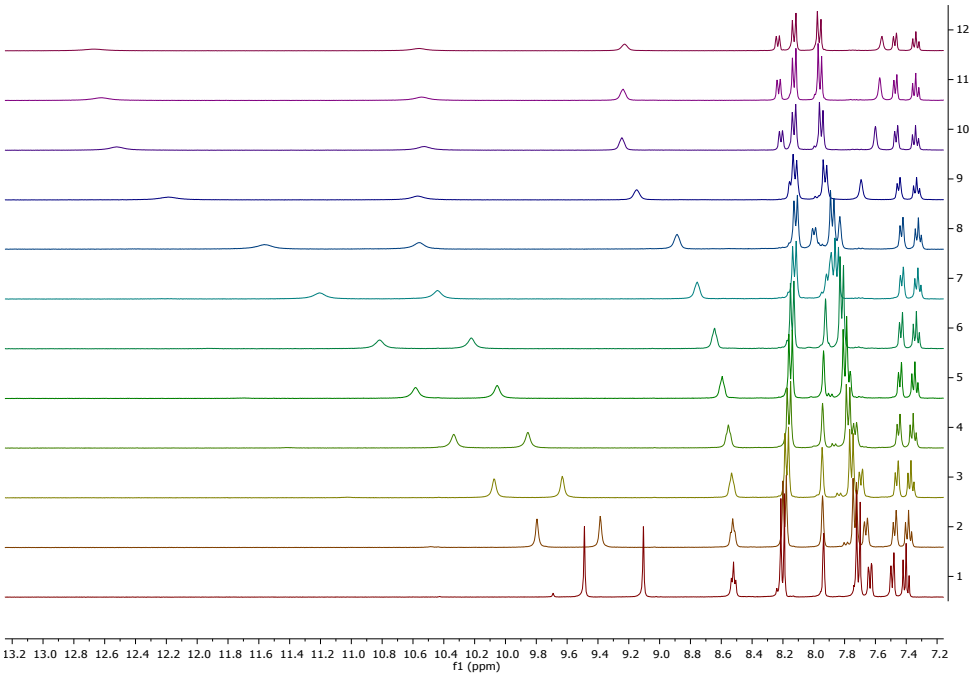


Figure S52. ^{1}H NMR spectra obtained by titration of **8b** with TBAHP in DMSO-d_6.

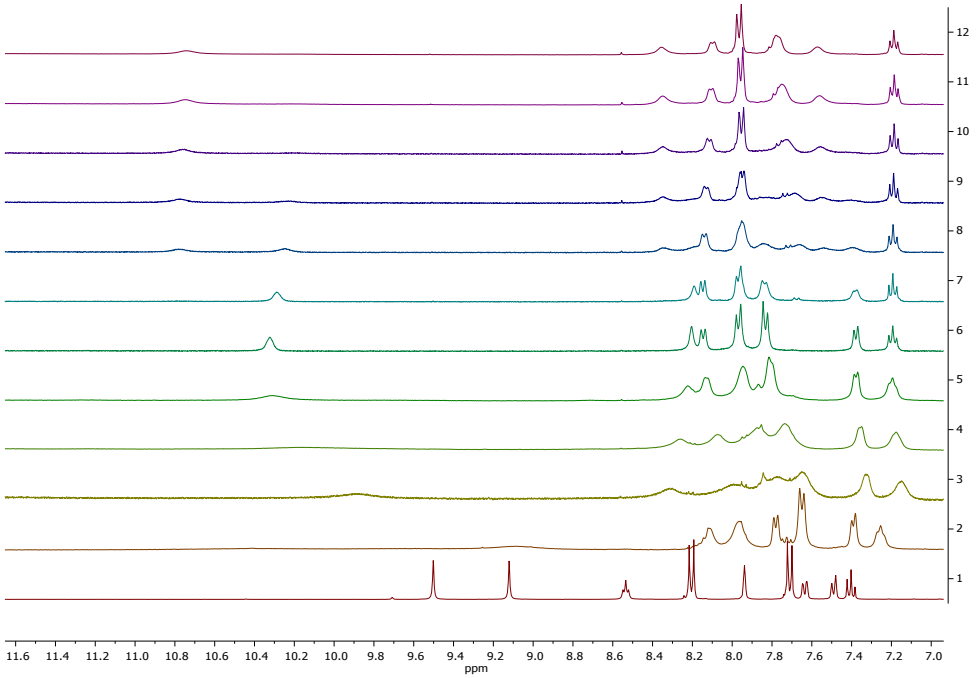


Figure S53. ^{1}H NMR spectra obtained by titration of **8b** with TBAHPP in DMSO-d_6.

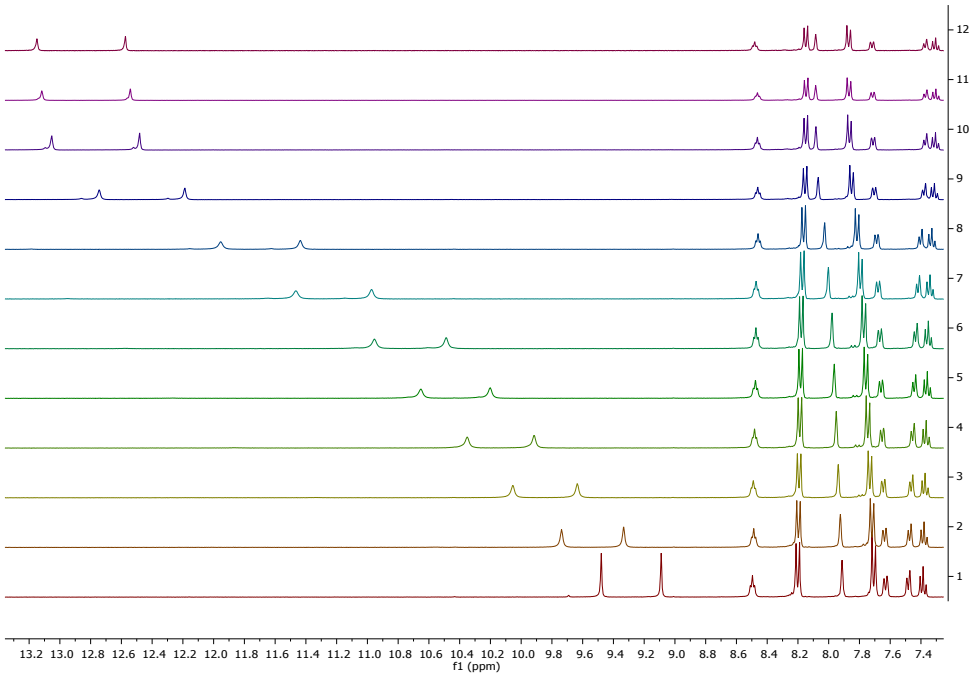


Figure S54. ^{1}H NMR spectra obtained by titration of **8c** with TBAA in DMSO-d_6.

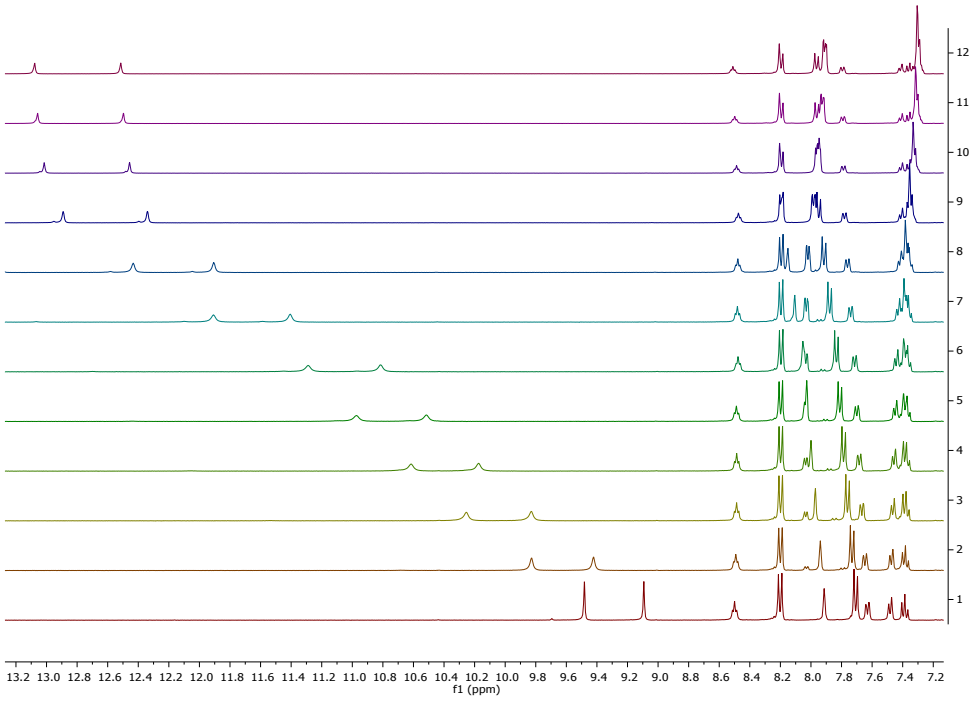


Figure S55. ^{1}H NMR spectra obtained by titration of **8c** with TBAB in DMSO-d_6.

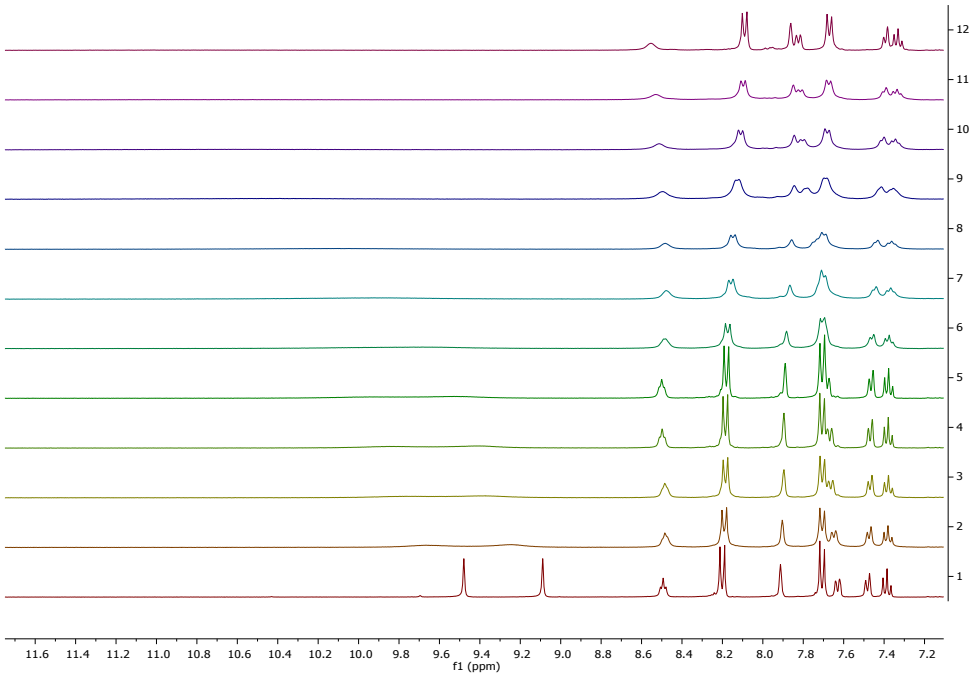


Figure S56. ^{1}H NMR spectra obtained by titration of **8c** with TBAF in DMSO-d_6.

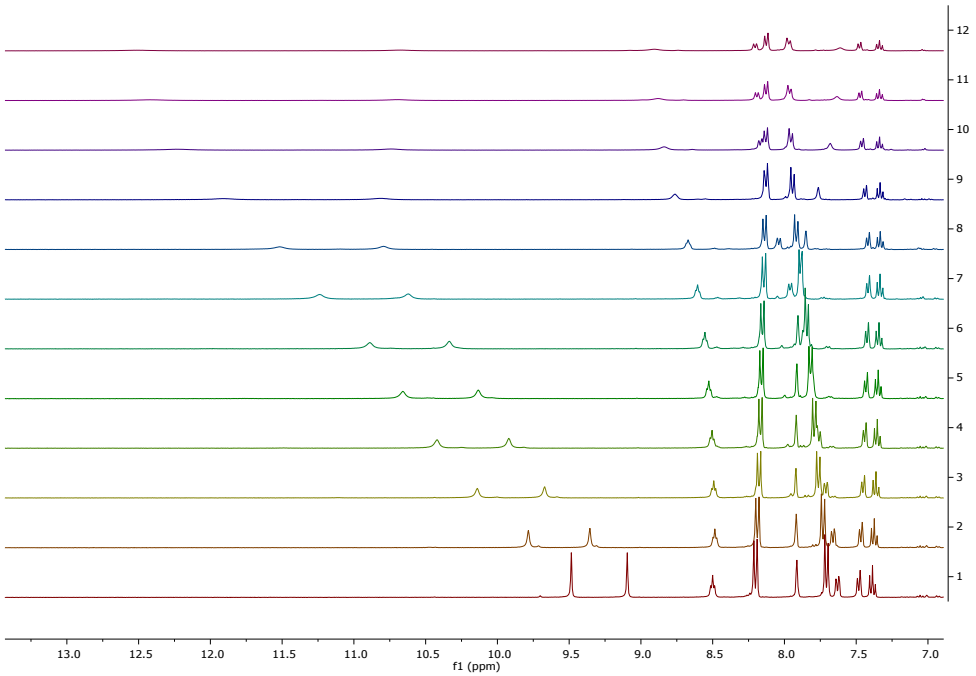


Figure S57. ^{1}H NMR spectra obtained by titration of **8c** with TBAHP in DMSO-d_6.

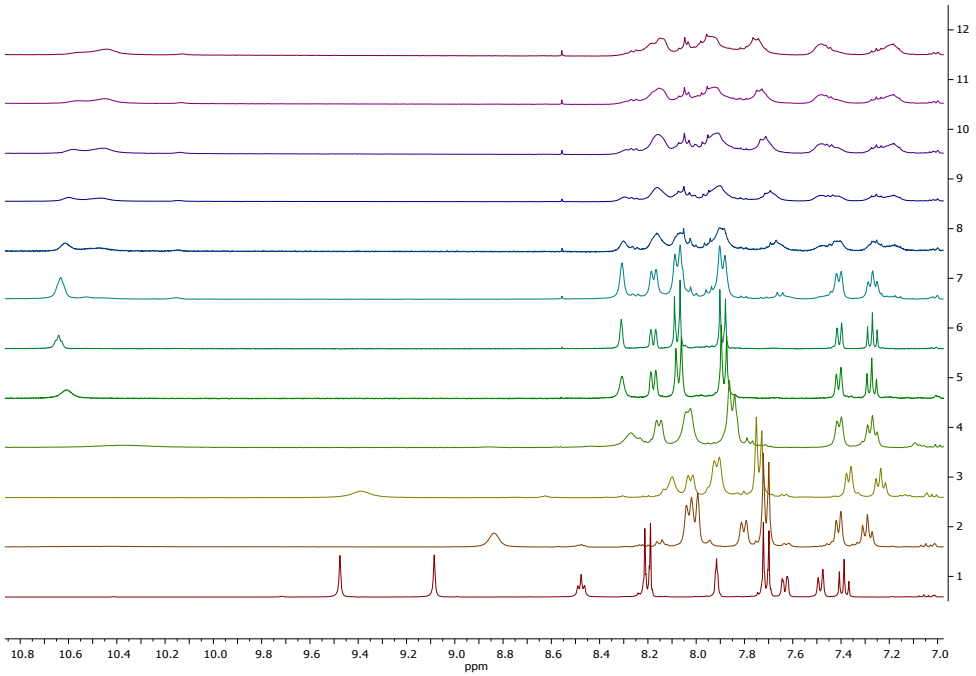


Figure S58. ^{1}H NMR spectra obtained by titration of **8c** with TBAHPP in DMSO-d_6.

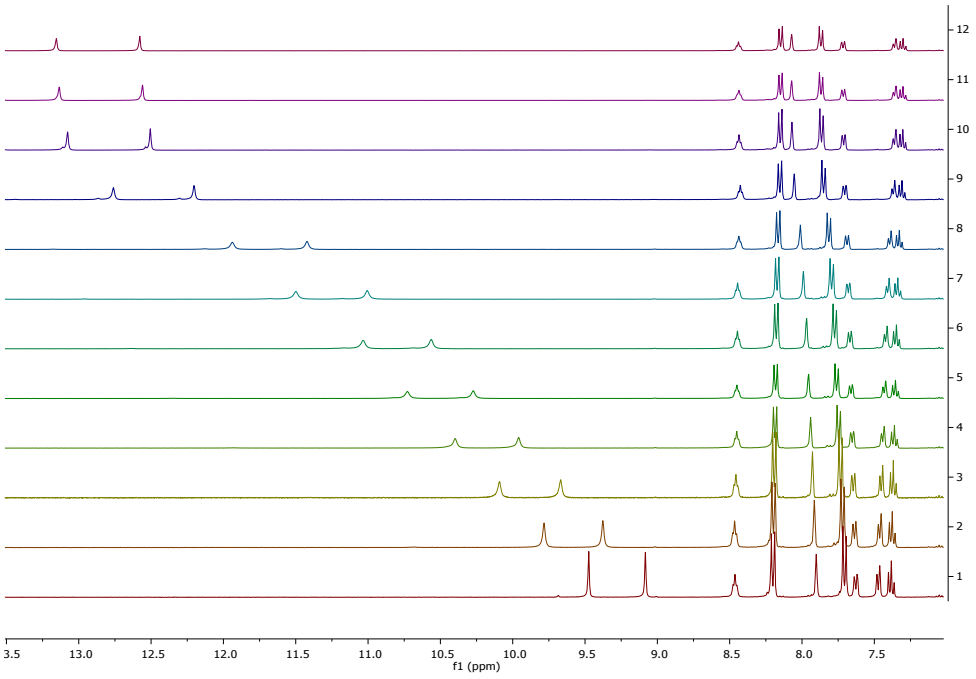


Figure S59. ^{1}H NMR spectra obtained by titration of **8d** with TBAA in DMSO-d_6.

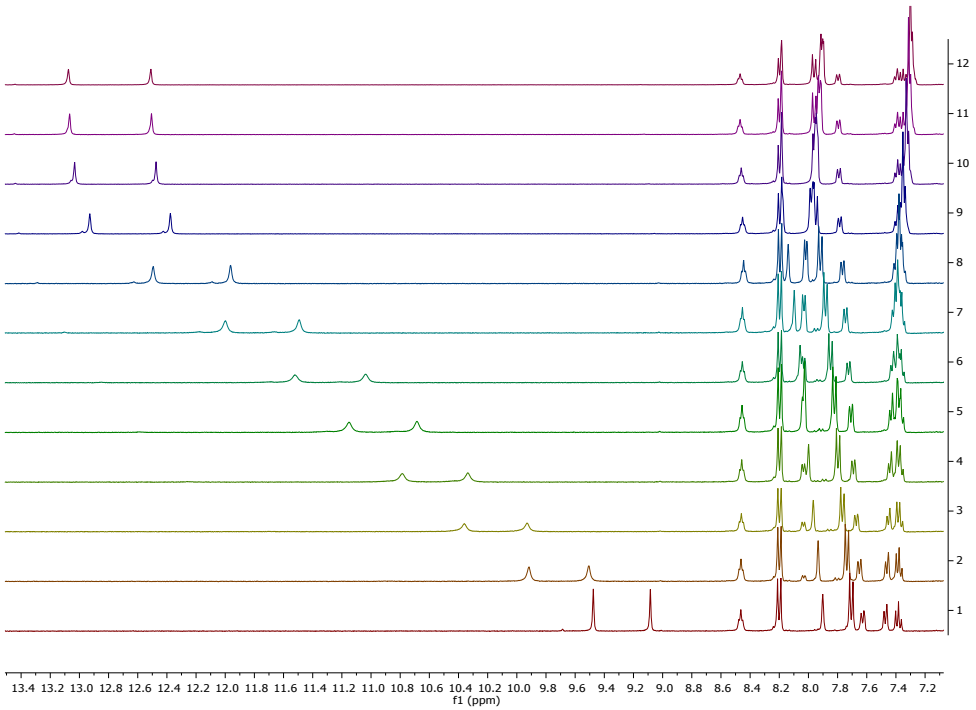


Figure S60. ^{1}H NMR spectra obtained by titration of **8d** with TBAB in DMSO-d_6.

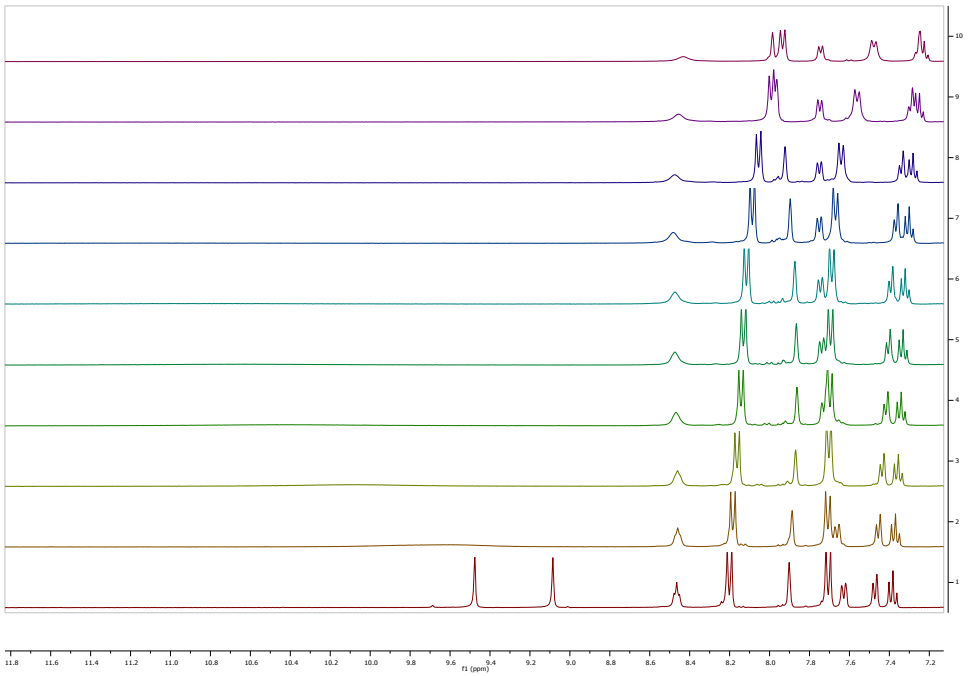


Figure S61. ^{1}H NMR spectra obtained by titration of **8d** with TBAF in DMSO-d_6.

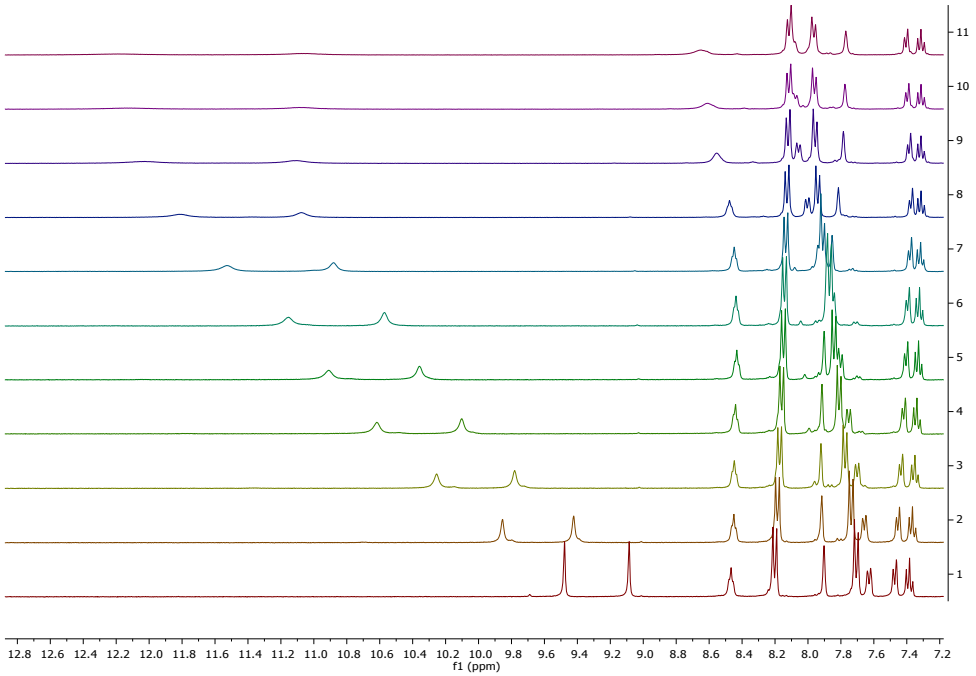


Figure S62. [1]H NMR spectra obtained by titration of **8d** with TBAHP in DMSO-d_6.

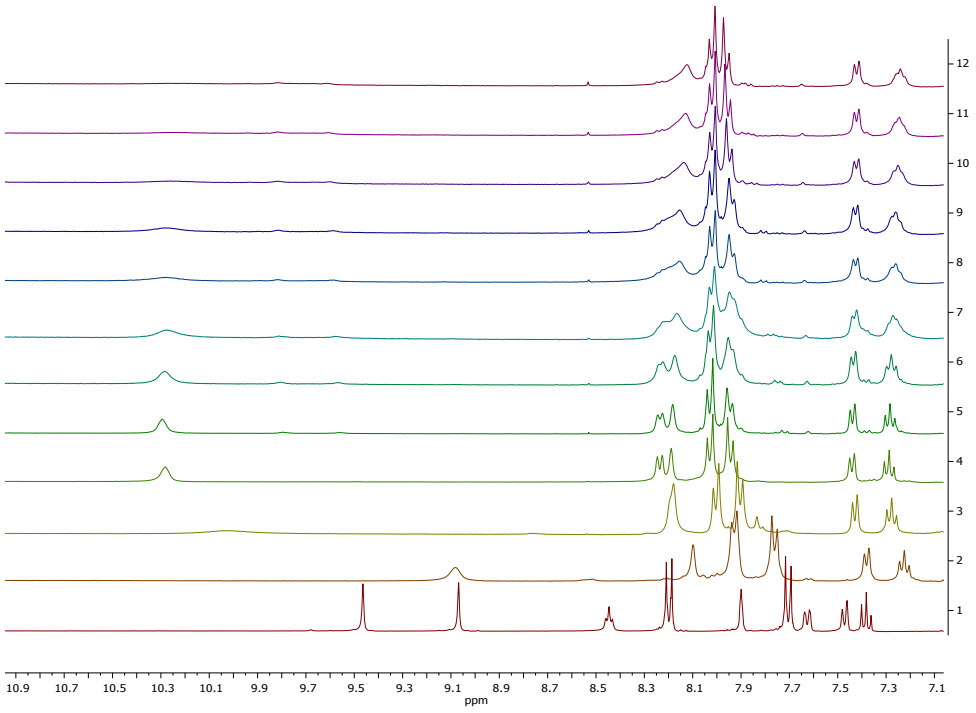


Figure S63. [1]H NMR spectra obtained by titration of **8d** with TBAHPP in DMSO-d_6.

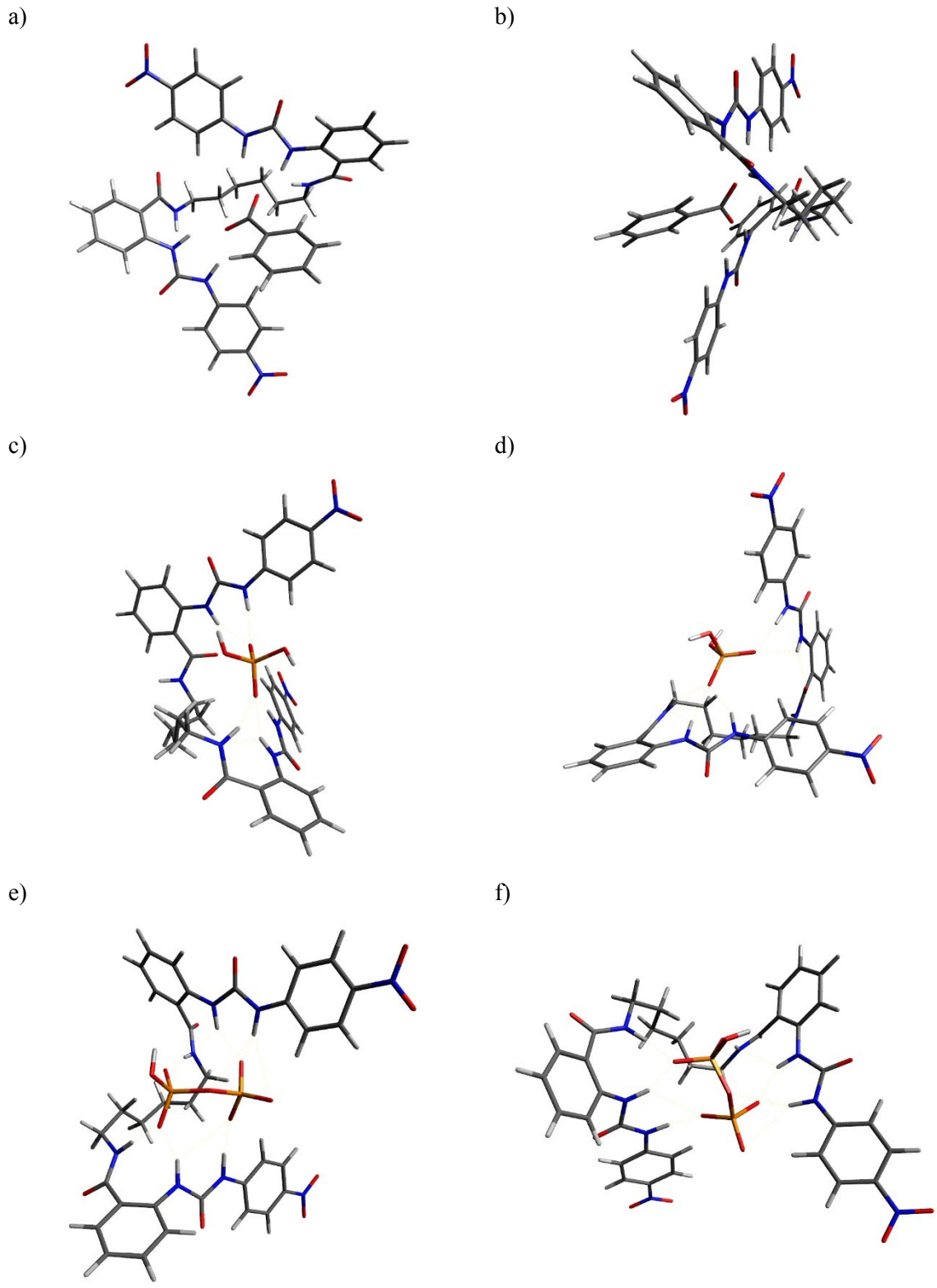


Figure S64. Optimized geometries for the complexes **4d**-BnO^- (a and b), **4d**-$H_2PO_4^-$ (c and d) and **4d**-$HP_2O_7^{3-}$ (e and f) by DFT.

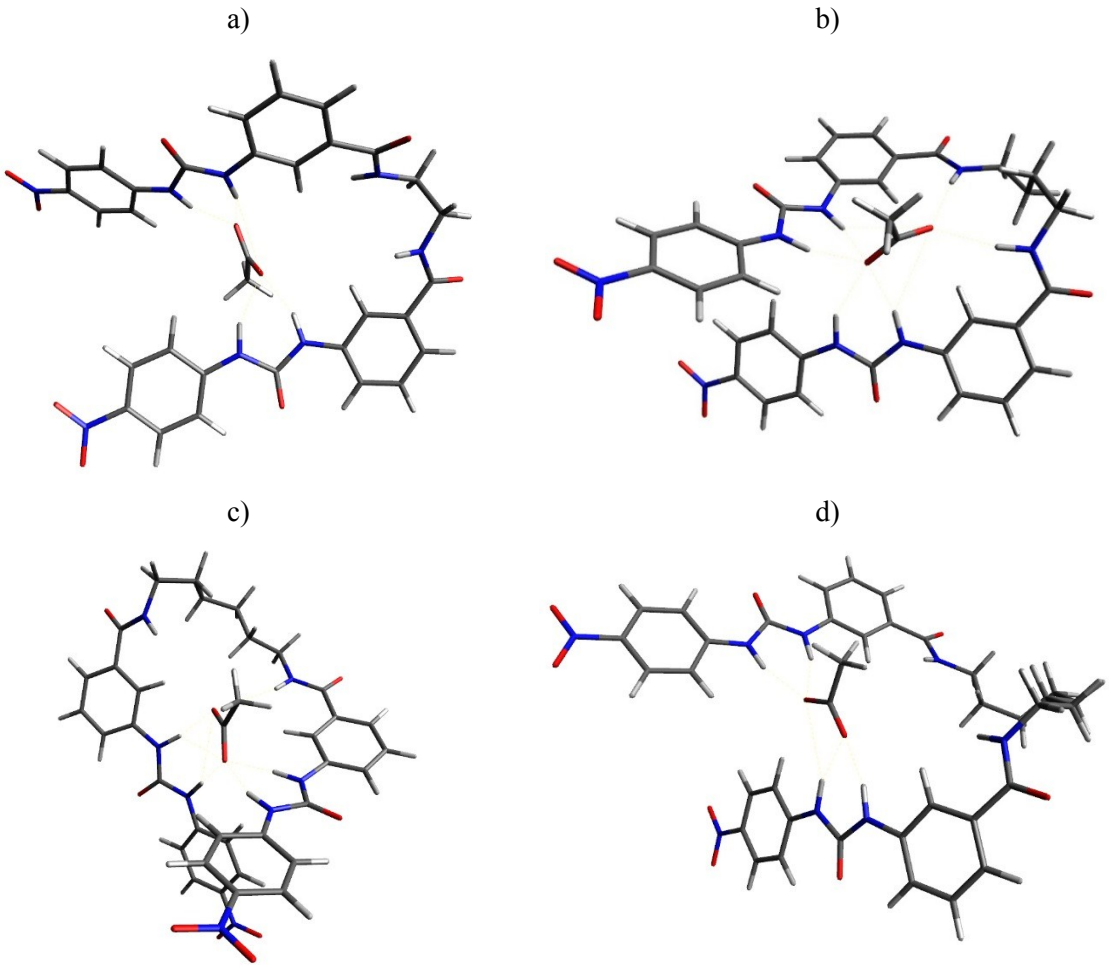


Figure S65. Optimized geometries for the complexes **8a**-AcO^- (a), **8c**- AcO^- (b), **8d**-AcO^- (c) and **8e**- AcO^- (d) by DFT.

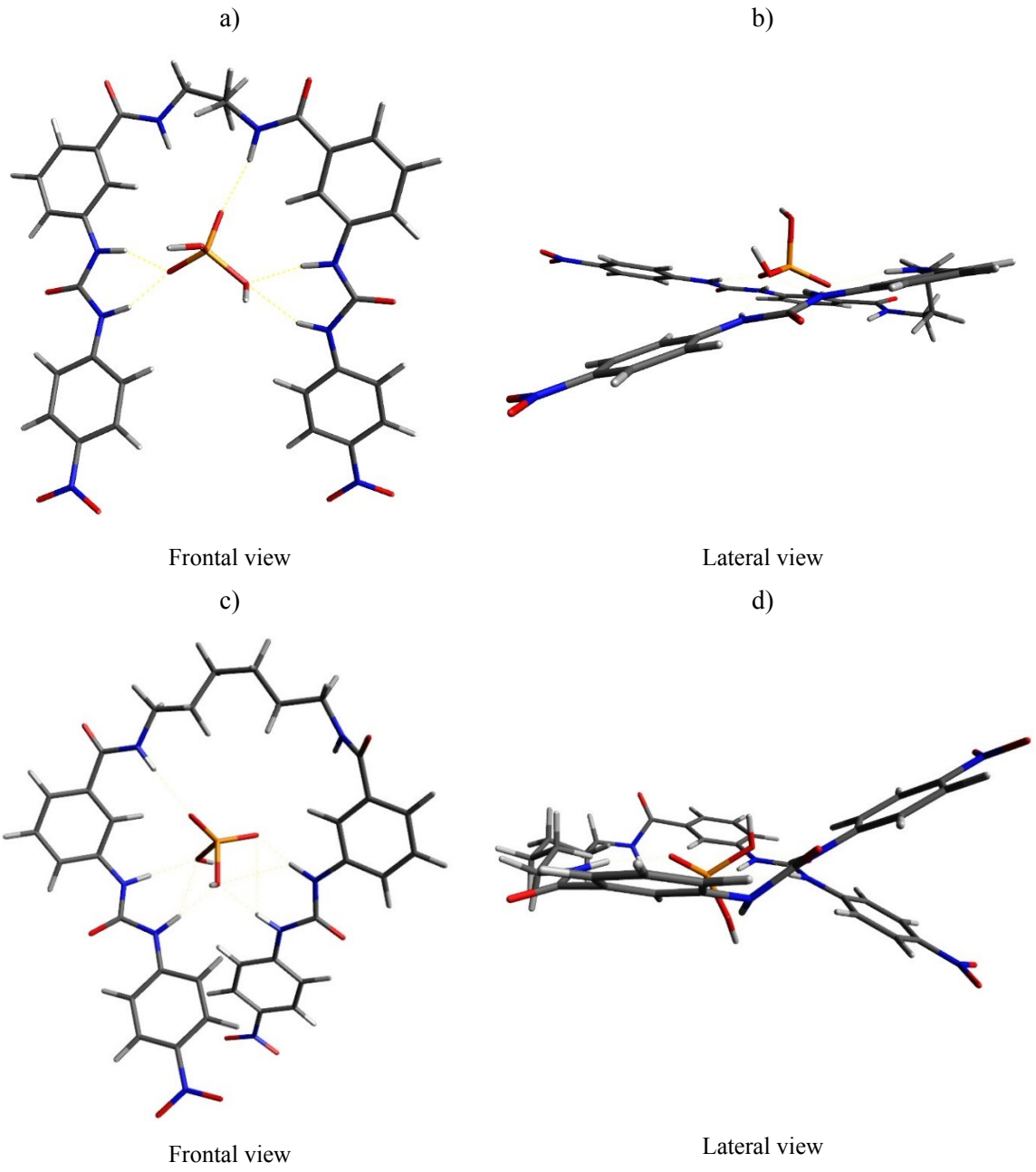


Figure S66. Optimized geometries for the complexes **8b**-$H_2PO_4^-$ (a and b), and **8d**-$H_2PO_4^-$ (c and d).

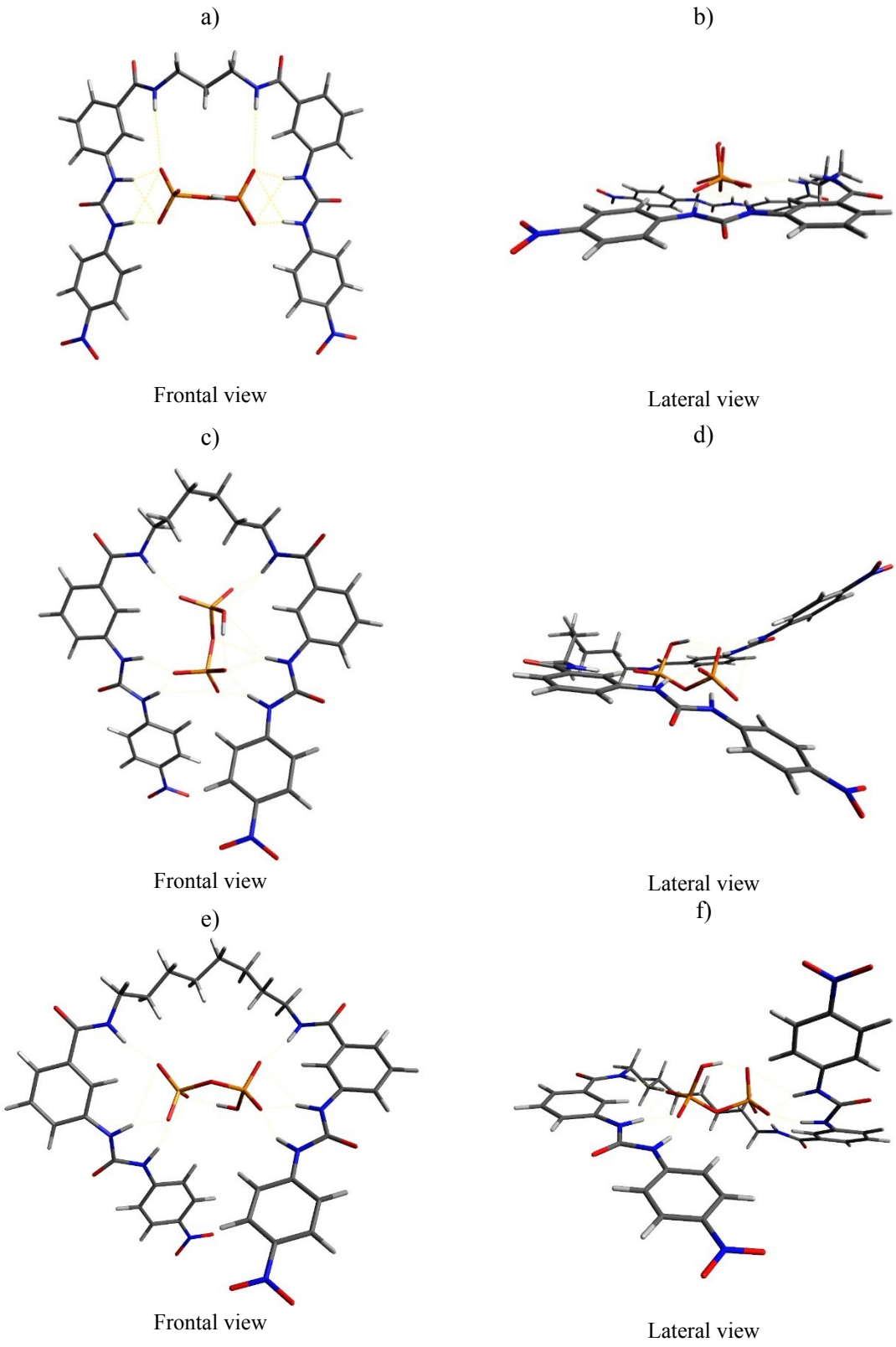


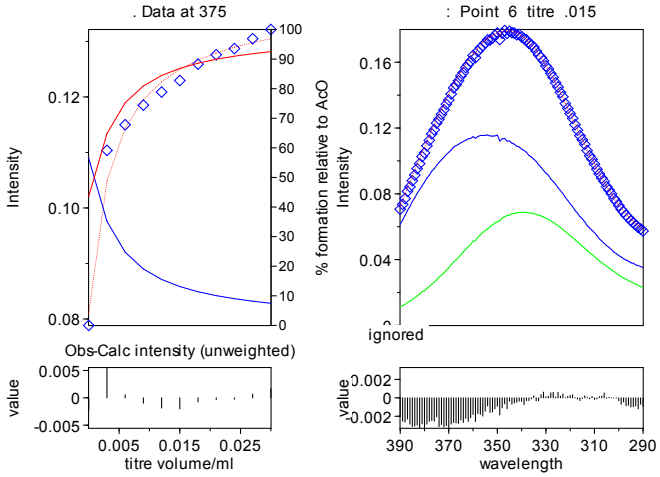
Figure S67. Optimized geometries for the complexes **8b**-$HP_2O_7^{3-}$ (a and b), **8d**-$HP_2O_7^{3-}$ (c and d) and **8e**-$HP_2O_7^{3-}$.

UV-Vis data fitting with HypSpec

HypSpec. Refinement concluded at 7/1/2018 10:32:27 PM
Project title: ***ortho*** **monourea-AcO**.HQD

Converged in 1 iterations with sigma = 1.6884E-03

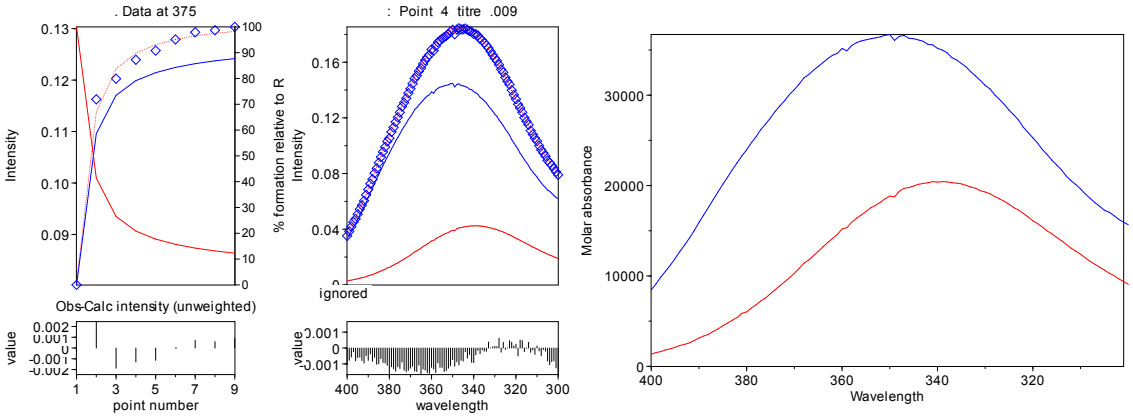
Log beta	value	standard deviation
AR2	10.112	0.0172



HypSpec. Refinement concluded at 7/11/2018 7:18:34 PM
Project title: ***ortho*** **monourea-BzO**.HQD

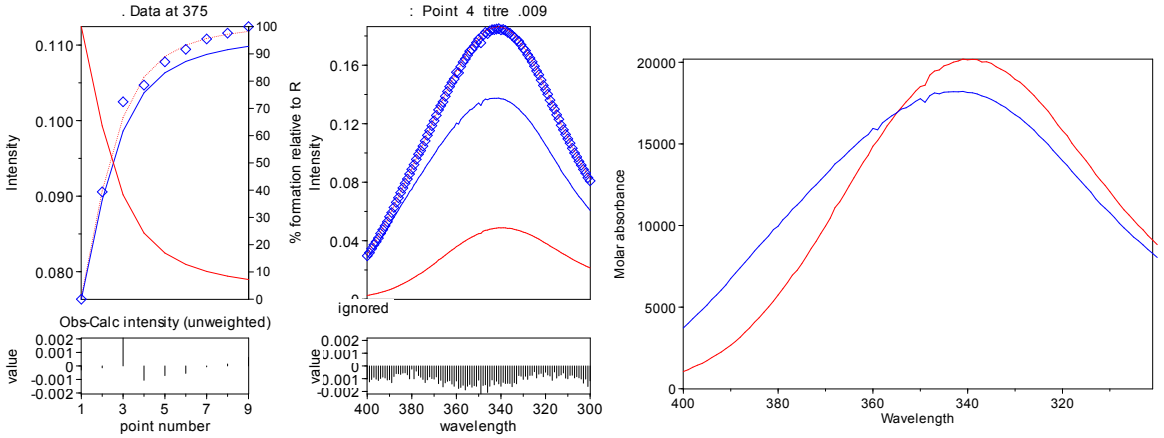
Converged in 1 iterations with sigma = 1.1235E-03

Log beta	value	standard deviation
R2A	10.9186	0.0179



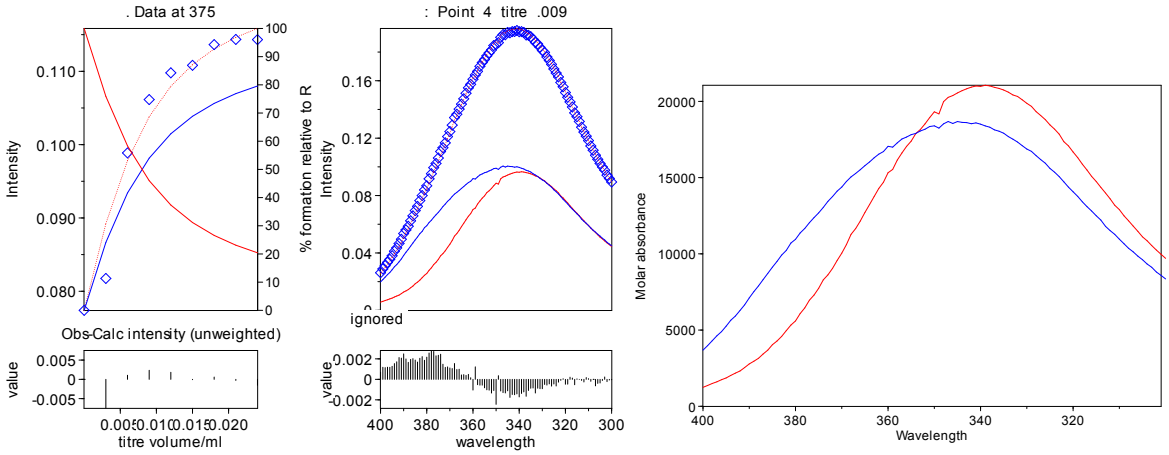
HypSpec. Refinement concluded at 7/11/2018 7:44:00 PM
Project title: ***ortho* monourea-F**.HQD
Converged in 1 iterations with sigma = 6.6153E-04

Log beta	value	standard deviation
RA	5.6247	0.0103



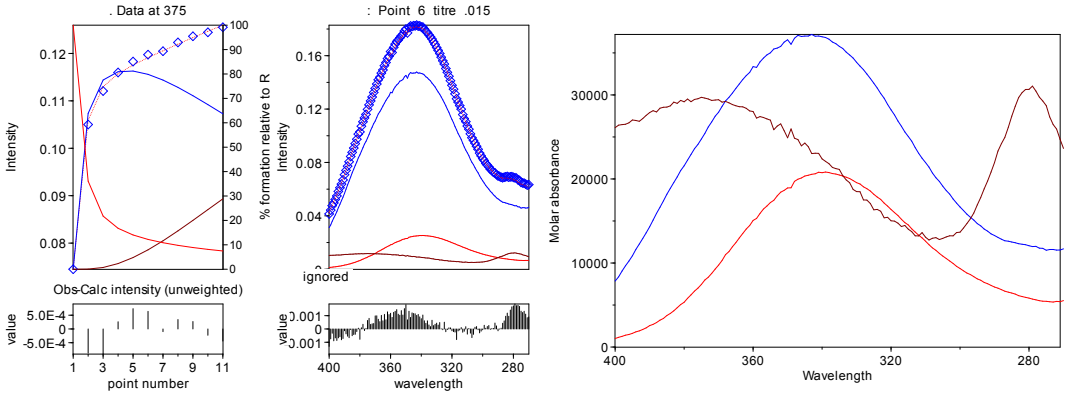
HypSpec. Refinement concluded at 7/11/2018 10:10:08 PM
Project title: ***ortho* monourea-HP**.HQD
Converged in 1 iterations with sigma = 1.5920E-03

Log beta	value	standard deviation
RA	5.0884	0.0182



HypSpec. Refinement concluded at 7/12/2018 12:16:39 AM
Project title: ***ortho* monourea-HPP**.HQD
Converged in 1 iterations with sigma = 7.7532E-04

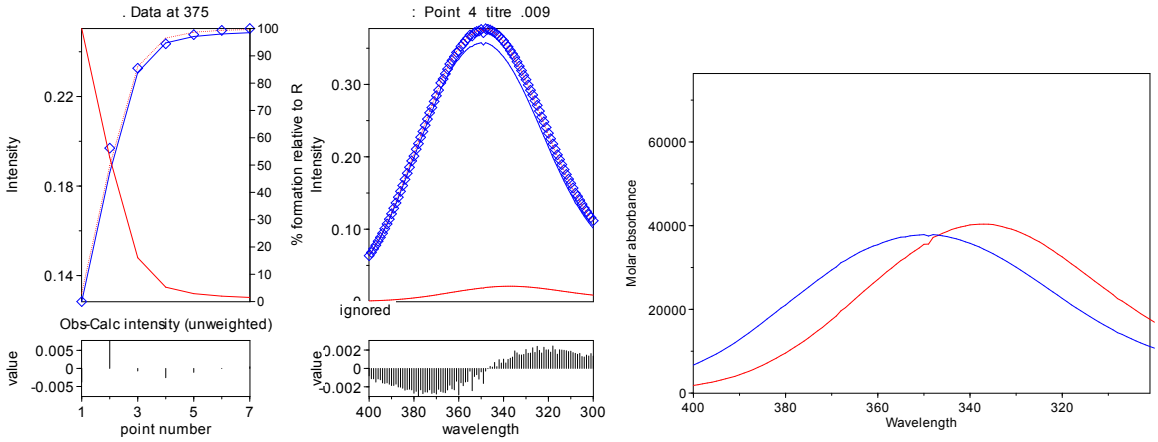
Log beta	value	standard deviation
R2A	11.1353	0.0261
R2A3	19.543	0.044



Project title: **4a-AcO**. HQD
Converged in 1 iterations with sigma = 2.3631E-03

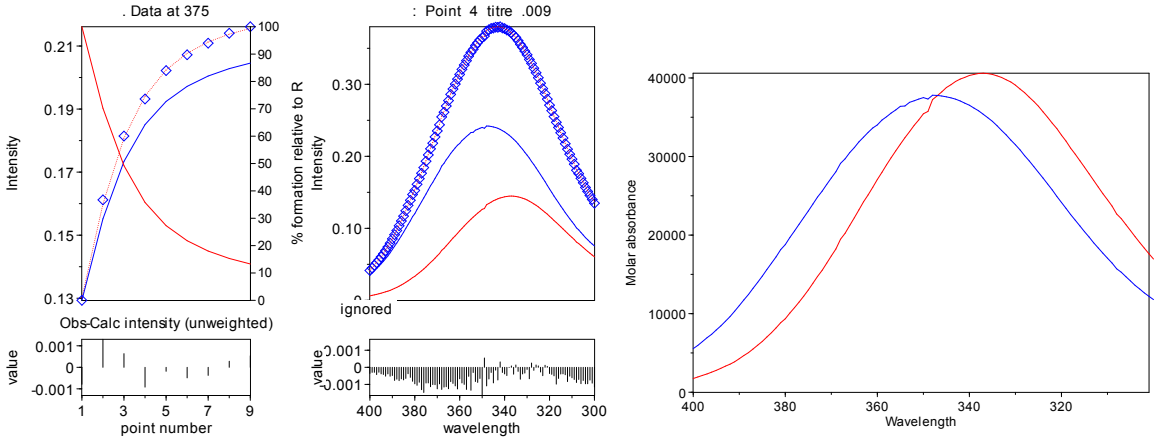
Log beta	value	standard deviation
RA	6.5136	0.0232

R2A was ignored



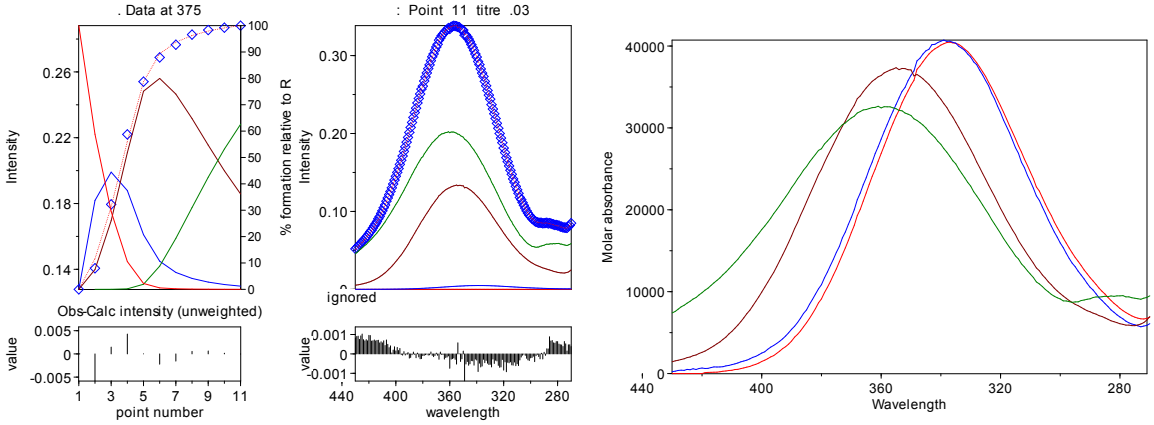
HypSpec. Refinement concluded at 7/16/2018 10:08:36 PM
Project title: **4a-BzO**.HQD
Converged in 1 iterations with sigma = 8.0351E-04

Log beta	value	standard deviation
RA	5.3221	0.0044



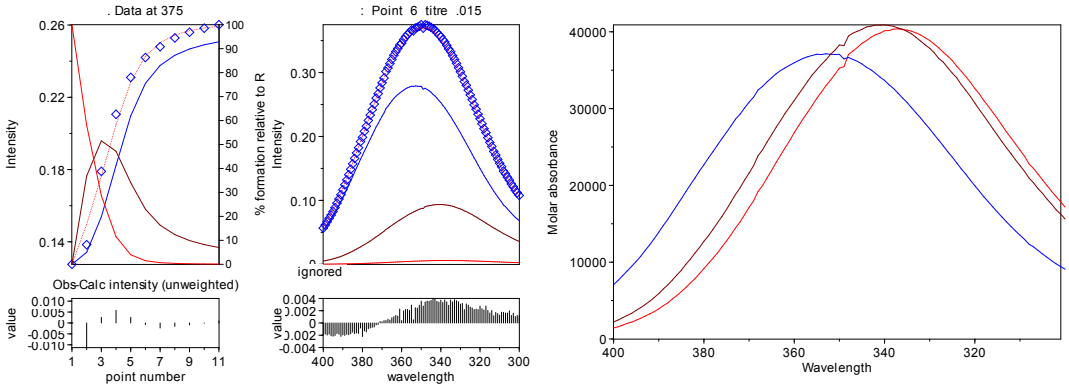
HypSpec. Refinement concluded at 7/12/2018 1:10:04 AM
Project title: **4a-F**.HQD
Converged in 1 iterations with sigma = 1.3994E-03

Log beta	value	standard deviation
RA	6.6423	0.0566
RA2	12.8742	0.0467
RA4	22.6292	0.0725



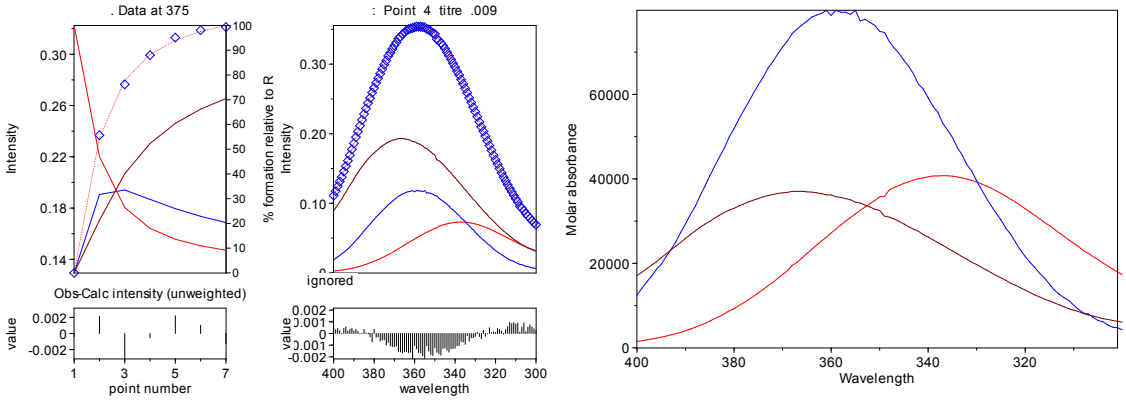
HypSpec. Refinement concluded at 7/12/2018 1:55:33 PM
Project title: **4a-HP**.HQD
Converged in 2 iterations with sigma = 3.0051E-03

Log beta	value	standard deviation
RA2	11.9467	0.1105
RA	6.3086	0.1417



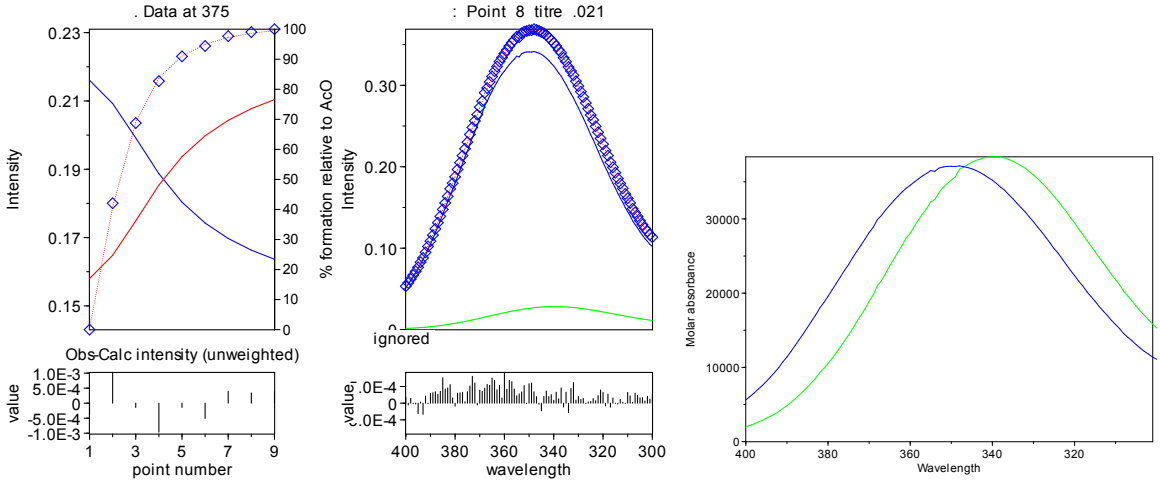
HypSpec. Refinement concluded at 7/12/2018 2:16:17 PM
Project title: **4a-HPP**.HQD
Converged in 1 iterations with sigma = 1.3920E-03

Log beta	value	standard deviation
R2A	10.7467	0.0725
RA	5.5468	0.0372



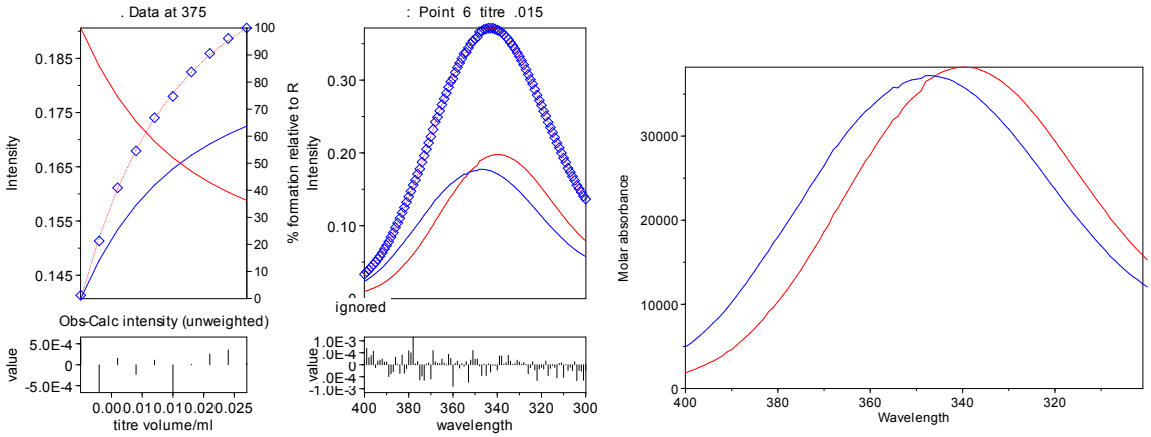
HypSpec. Refinement concluded at 7/2/2018 7:18:40 PM
Project title: **4b-AcO**.HQD
Converged in 1 iterations with sigma = 5.5868E-04

Log beta	value	standard deviation
AcOR	5.6886	0.0035



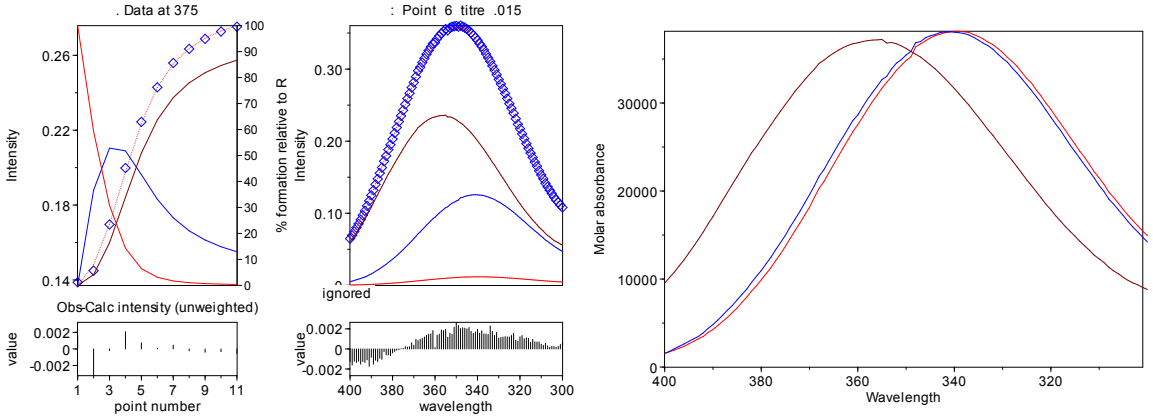
HypSpec. Refinement concluded at 7/11/2018 7:58:54 PM
Project title: **4b-BzO**.HQD
Converged in 3 iterations with sigma = 3.9648E-04

Log beta	value	standard deviation
RA	4.6615	0.004



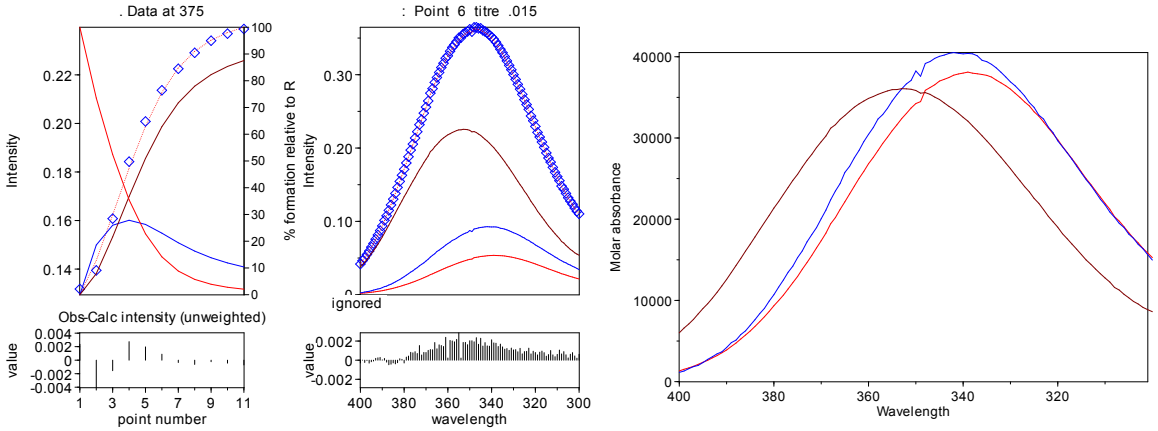
HypSpec. Refinement concluded at 7/11/2018 7:41:09 PM
Project title: **4b-F**.HQD
Converged in 1 iterations with sigma = 1.1825E-03

Log beta	value	standard deviation
RA	6.0777	0.054
RA2	11.4123	0.0395



HypSpec. Refinement concluded at 7/12/2018 2:34:42 PM
Project title: **4b-HP**.HQD
Converged in 1 iterations with sigma = 1.5268E-03

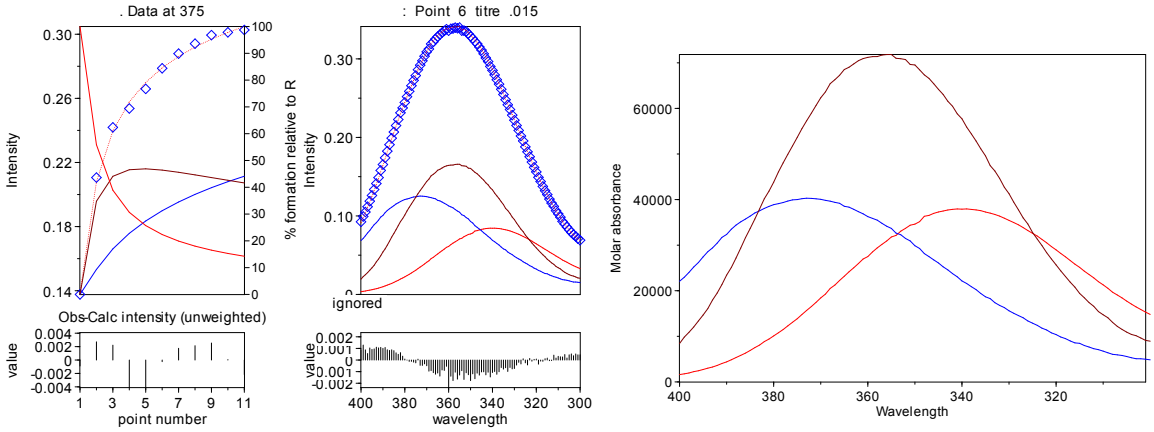
Log beta	value	standard deviation
RA	5.2076	0.1246
RA2	10.6405	0.055



HypSpec. Refinement concluded at 7/12/2018 2:56:30 PM

Project title: **4b-HPP**.HQD
Converged in 1 iterations with sigma = 1.7395E-03

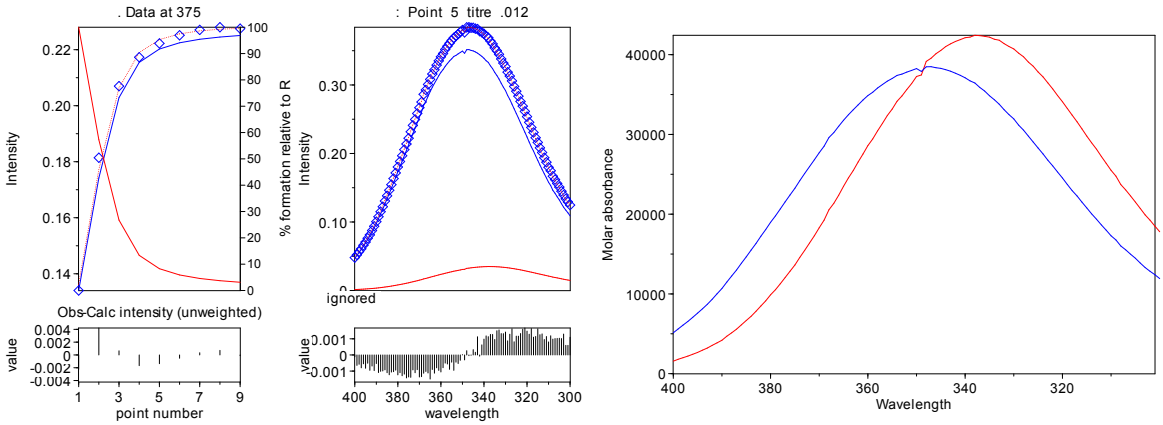
Log beta	value	standard deviation
RA	4.8563	0.0608
R2A	10.38	0.0528



HypSpec. Refinement concluded at 7/12/2018 8:59:30 PM
Project title: **4c-AcO**.HQD

Converged in 1 iterations with sigma = 1.2113E-03

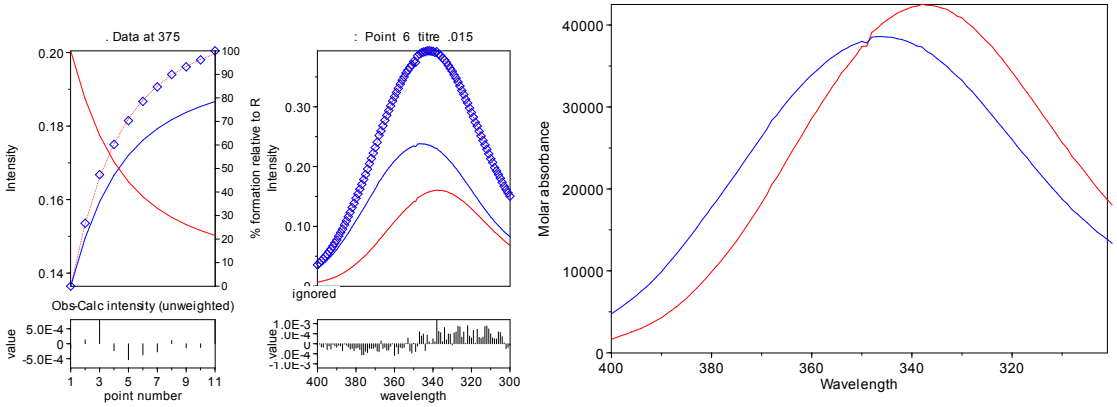
Log beta	value	standard deviation
RA	6.0115	0.0079



HypSpec. Refinement concluded at 7/13/2018 1:31:01 AM
Project title: **4c-BzO**.HQD

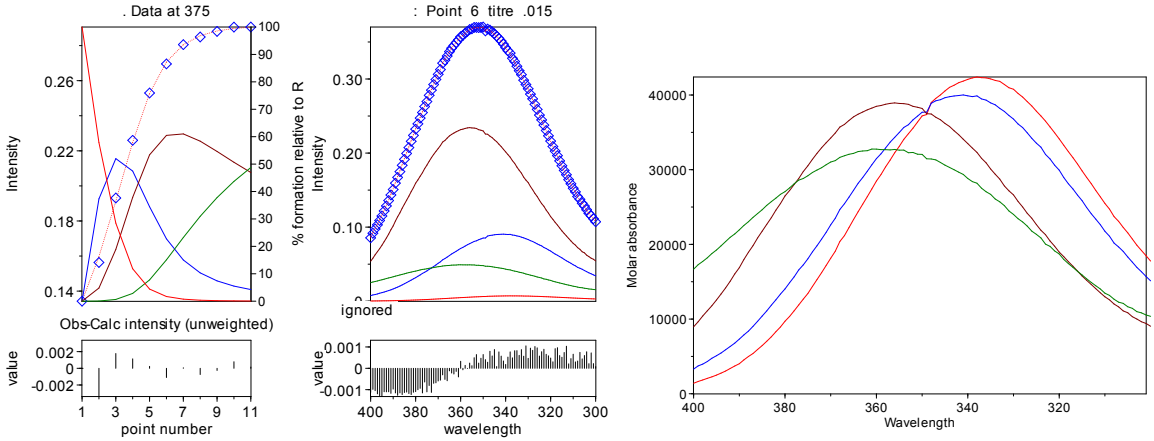
Converged in 1 iterations with sigma = 4.2902E-04

Log beta	value	standard deviation
RA	4.9409	0.0024



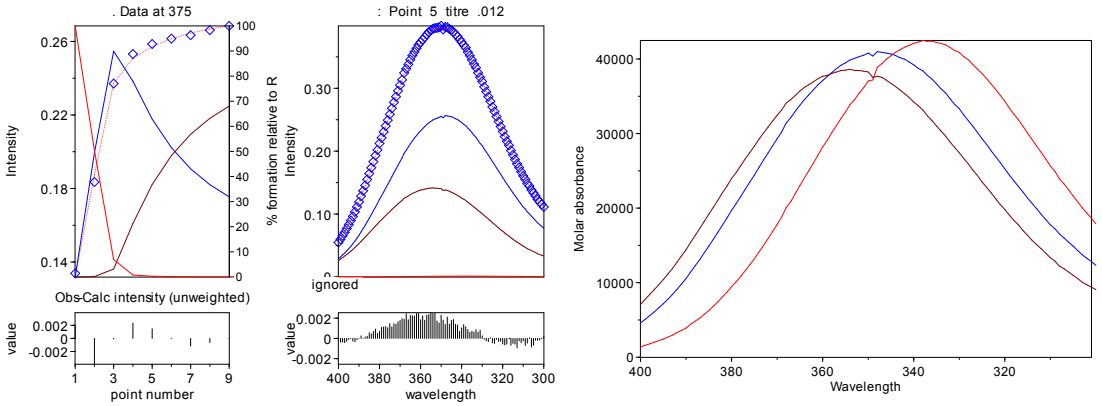
HypSpec. Refinement concluded at 7/13/2018 5:28:20 PM
Project title: **4c-F**.HQD
Converged in 1 iterations with sigma = 1.0976E-03

Log beta	value	standard deviation
RA	6.3429	0.0725
RA2	11.9841	0.0669
RA3	16.5973	0.1061



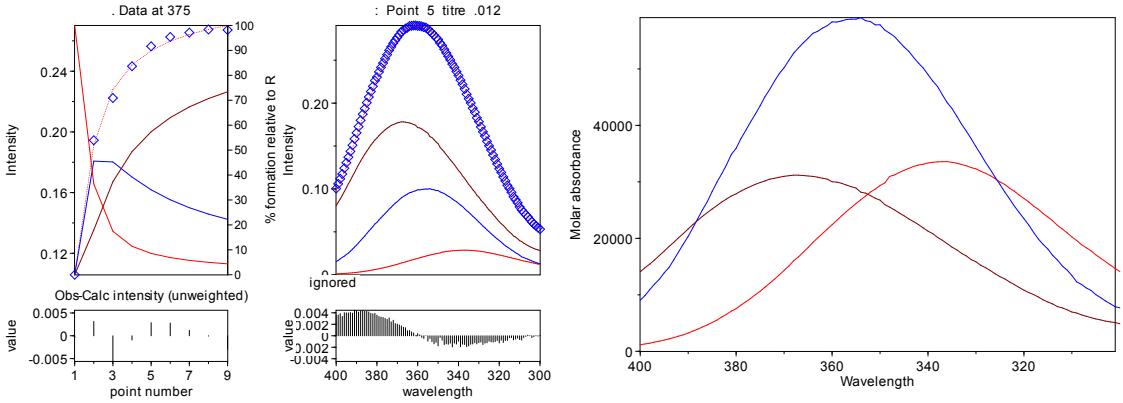
HypSpec. Refinement concluded at 7/13/2018 12:22:45 PM
Project title: **4c-HP**.HQD
Converged in 1 iterations with sigma = 1.3262E-03

Log beta	value	standard deviation
RA	7.5367	0.0647
RA2	12.5037	0.0817



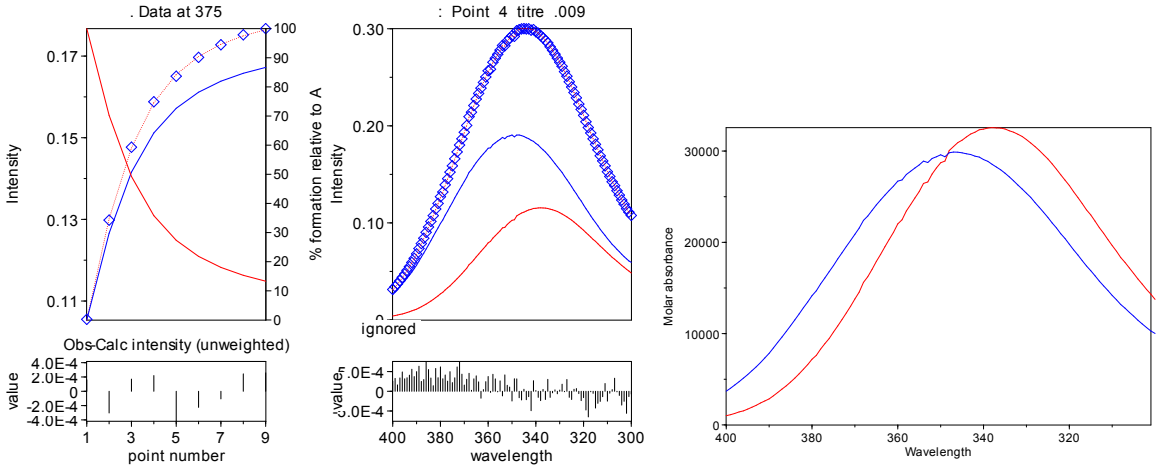
HypSpec. Refinement concluded at 7/13/2018 12:42:57 PM
Project title: **4c-HPP**.HQD
Converged in 1 iterations with sigma = 1.9796E-03

Log beta	value	standard deviation
R2A	11.2708	0.0967
RA	5.7287	0.0508



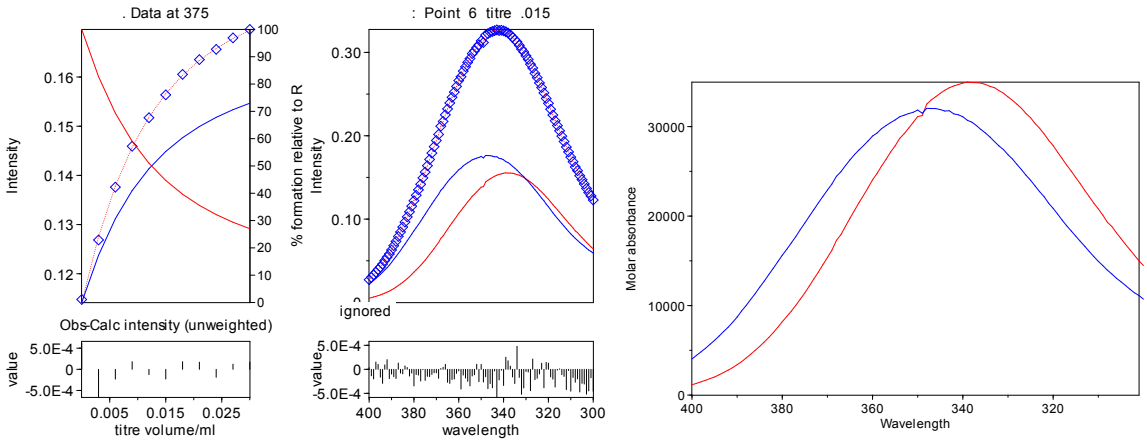
HypSpec. Refinement concluded at 6/27/2018 6:56:14 PM
Project title: **4d-AcO**.HQD
Converged in 5 iterations with sigma = 3.2722E-04

Log beta	value	standard deviation
RA	5.3213	0.0021



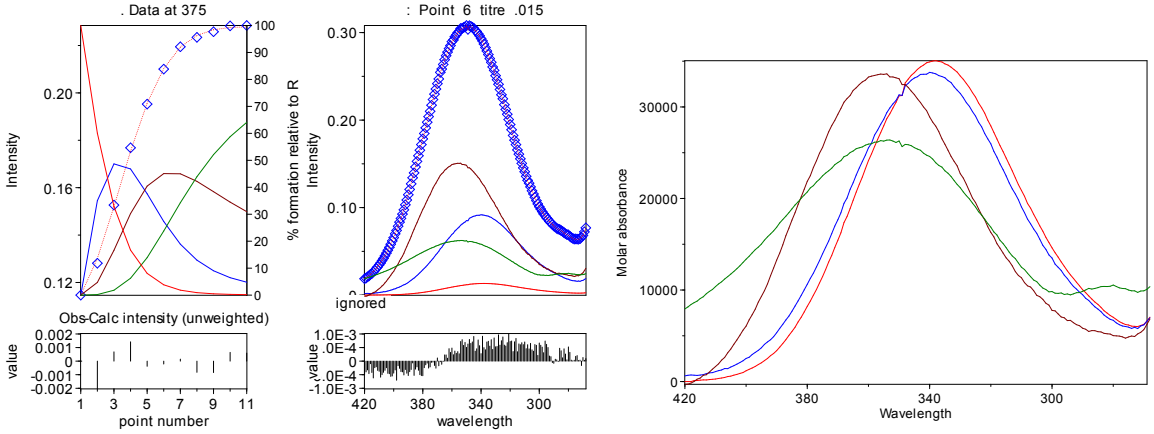
HypSpec. Refinement concluded at 7/13/2018 4:53:49 PM
Project title: **4d-BzO**.HQD
Converged in 1 iterations with sigma = 3.5907E-04

Log beta	value	standard deviation
RA	4.8055	0.0026



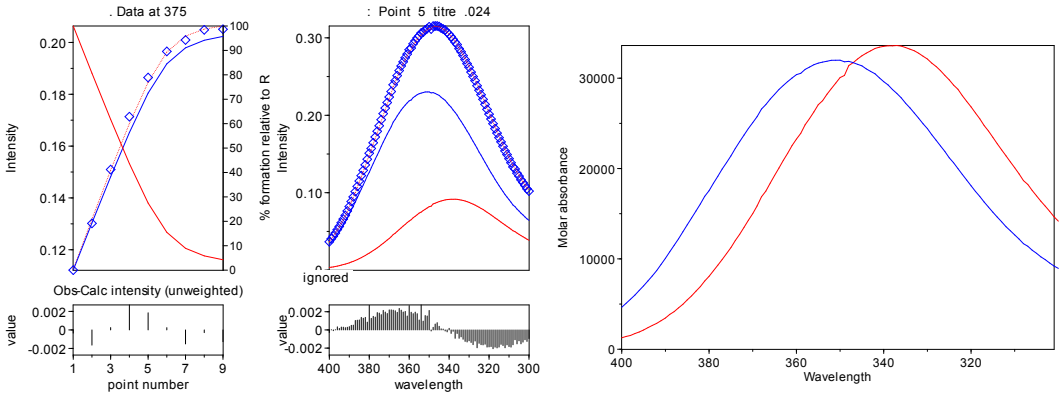
HypSpec. Refinement concluded at 7/13/2018 5:23:13 PM
Project title: **4d-F**.HQD
Converged in 1 iterations with sigma = 6.0485E-04

Log beta	value	standard deviation
RA	6.0699	0.0385
RA2	11.503	0.0329
RA3	16.441	0.0362



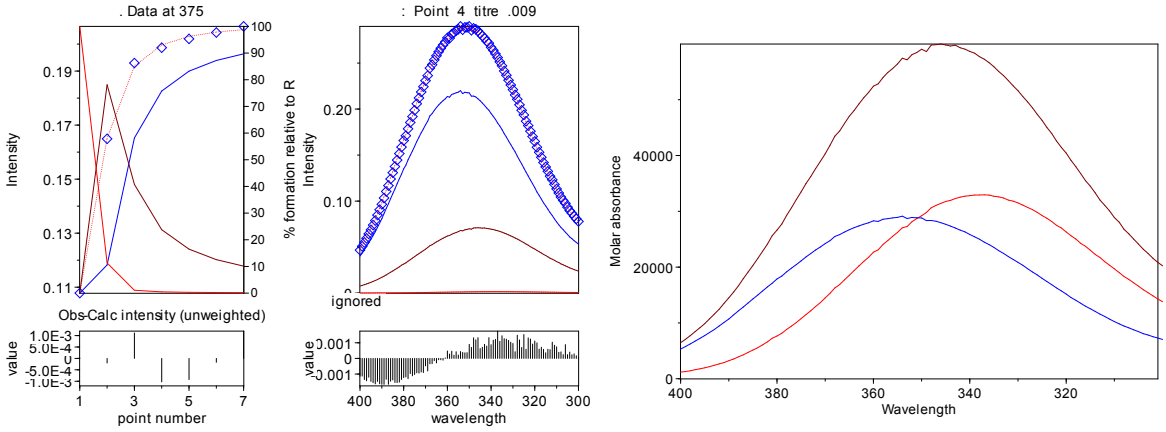
HypSpec. Refinement concluded at 7/13/2018 8:32:37 PM
Project title: **4d-HP**.HQD
Converged in 1 iterations with sigma = 1.2110E-03

Log beta	value	standard deviation
RA	6.5516	0.0223



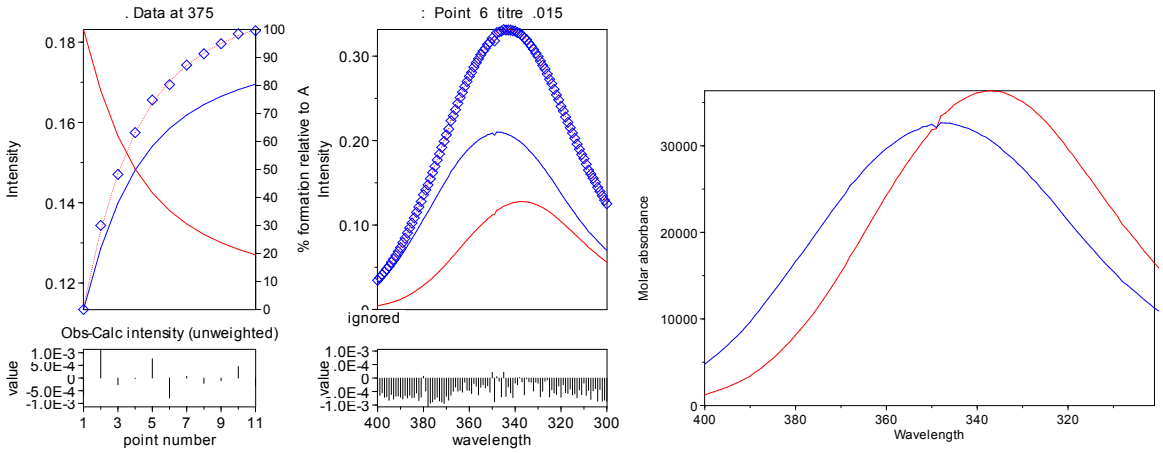
HypSpec. Refinement concluded at 7/27/2018 1:12:08 PM
Project title: **4d-HPP**.HQD
Converged in 13 iterations with sigma = 8.0323E-04

Log beta	value	standard deviation
RA	7.4043	0.4431
R2A	13.9196	0.8996



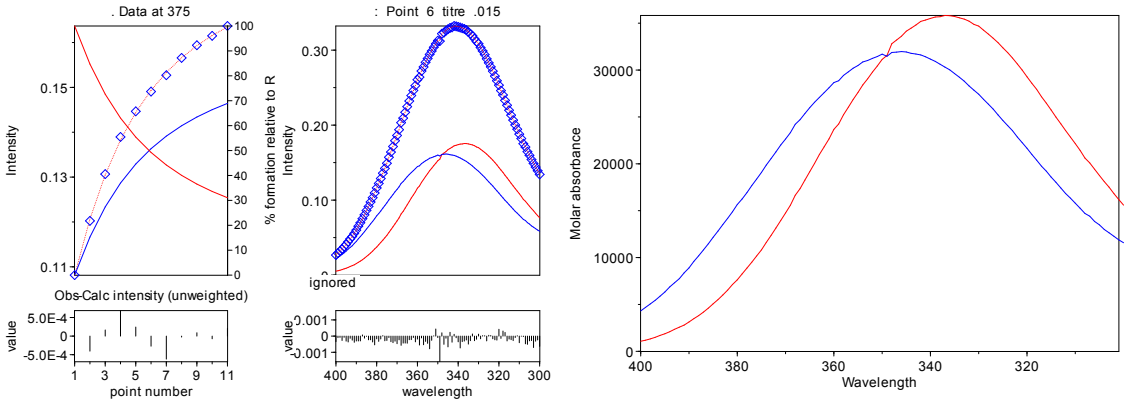
HypSpec. Refinement concluded at 6/27/2018 7:02:20 PM
Project title: **4e-AcO**.HQD
Converged in 1 iterations with sigma = 5.4968E-04

Log beta	value	standard deviation
RA	4.9966	0.0029



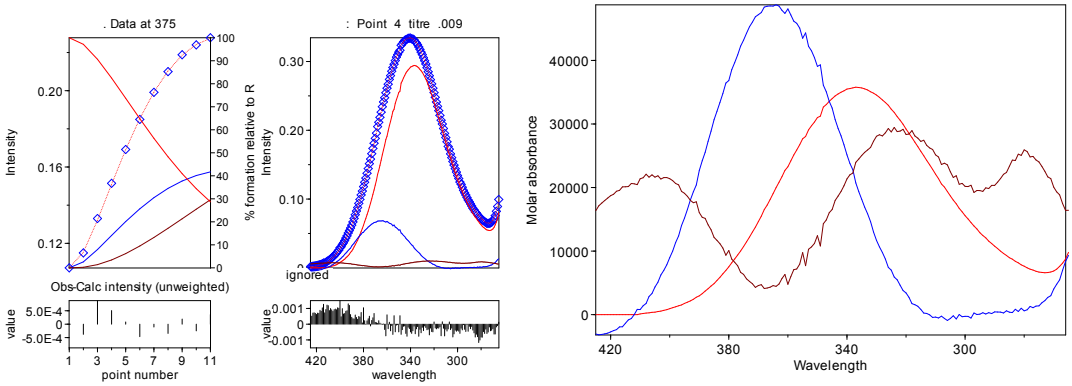
HypSpec. Refinement concluded at 7/14/2018 11:05:25 AM
Project title: **4e-BzO**.HQD
Converged in 1 iterations with sigma = 4.5496E-04

Log beta	value	standard deviation
RA	4.716	0.0033



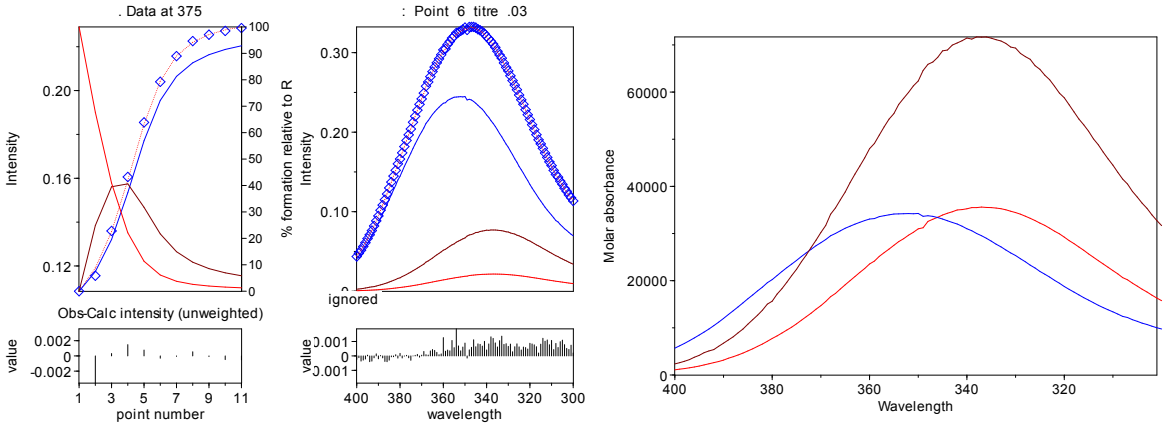
HypSpec. Refinement concluded at 7/15/2018 1:03:30 AM
Project title: **4e-F**.HQD
Converged in 1 iterations with sigma = 7.4362E-04

Log beta	value	standard deviation
RA2	9.1398	0.0205
RA3	13.4794	0.0271



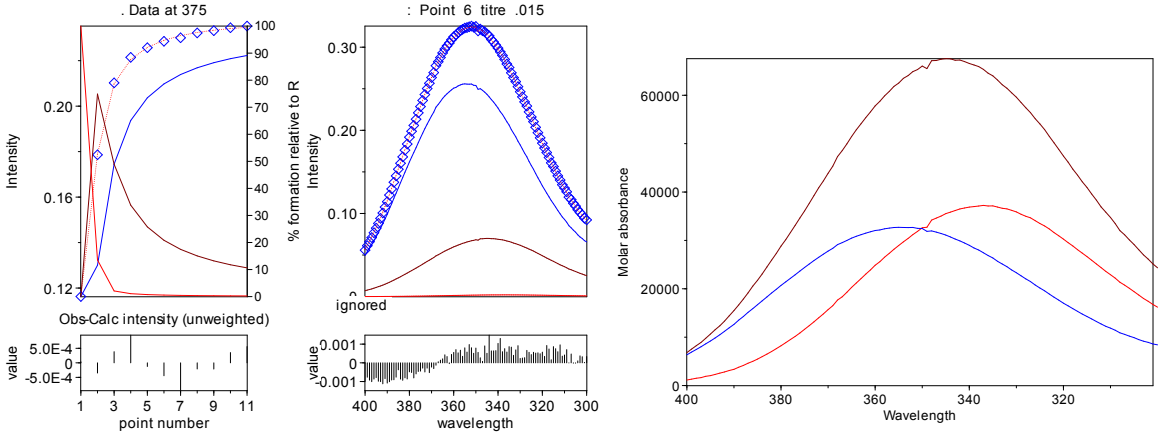
HypSpec. Refinement concluded at 7/27/2018 12:35:43 PM
Project title:**4e-HP**.HQD
Converged in 1 iterations with sigma = 9.4836E-04

Log beta	value	standard deviation
RA	6.8461	0.0233
R2A	12.2405	0.0705



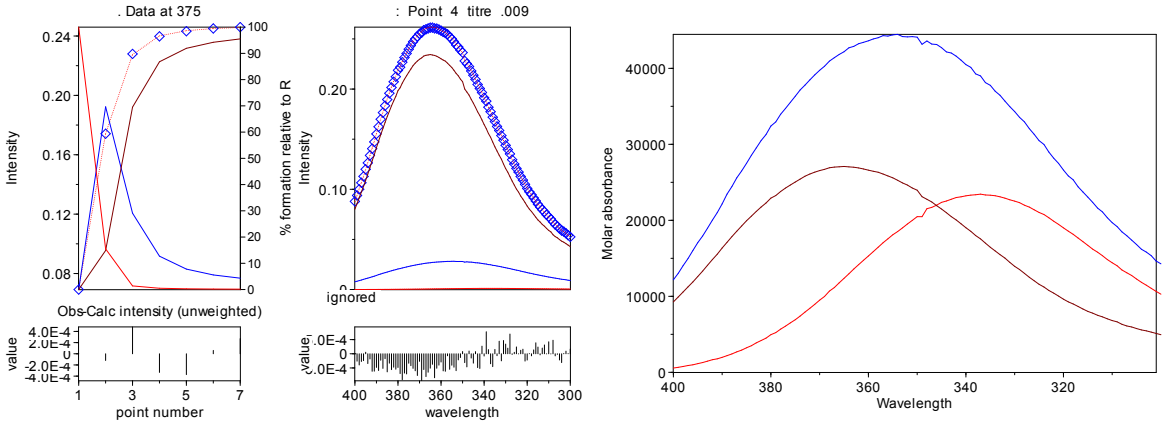
HypSpec. Refinement concluded at 7/27/2018 1:17:20 PM
Project title: **4e-HPP**.HQD
Converged in 1 iterations with sigma = 6.0791E-04

Log beta	value	standard deviation
RA	6.9454	0.1227
R2A	13.3239	0.2539



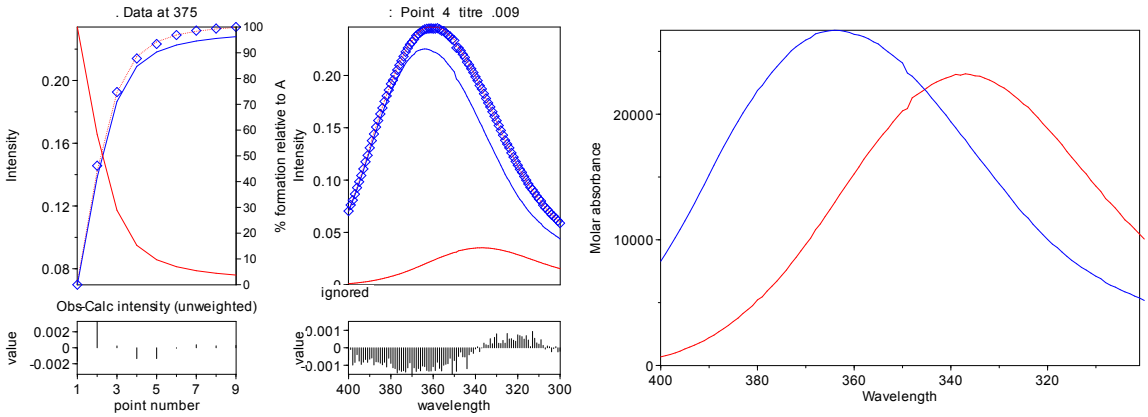
HypSpec. Refinement concluded at 7/16/2018 9:03:08 PM
Project title: ***meta* monourea-AcO**.HQD
Converged in 10 iterations with sigma = 3.3610E-04

Log beta	value	standard deviation
R2A	13.6786	0.3541
RA	7.4988	0.1747



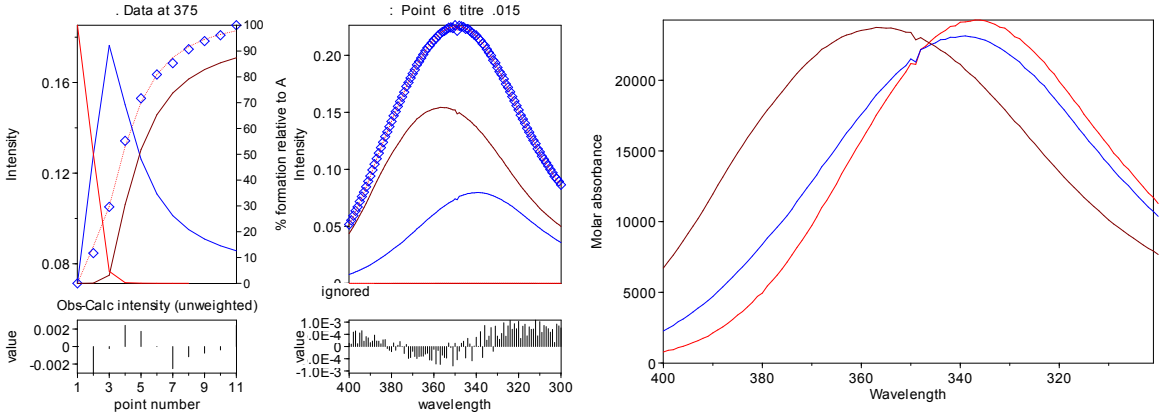
HypSpec. Refinement concluded at 7/16/2018 9:10:51 PM
Project title: ***meta* monourea-BzO**.HQD
Converged in 1 iterations with sigma = 1.0129E-03

Log beta	value	standard deviation
RA	5.9308	0.0044



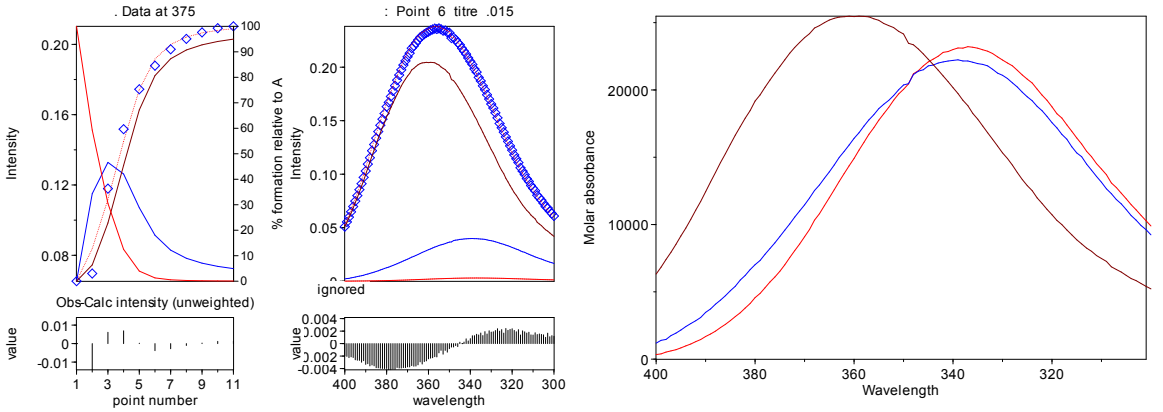
HypSpec. Refinement concluded at 7/16/2018 10:13:07 PM
Project title: ***meta* monourea-F**.HQD
Converged in 1 iterations with sigma = 1.1001E-03

Log beta	value	standard deviation
RA	8.1146	0.2203
R2A	13.4648	0.2154



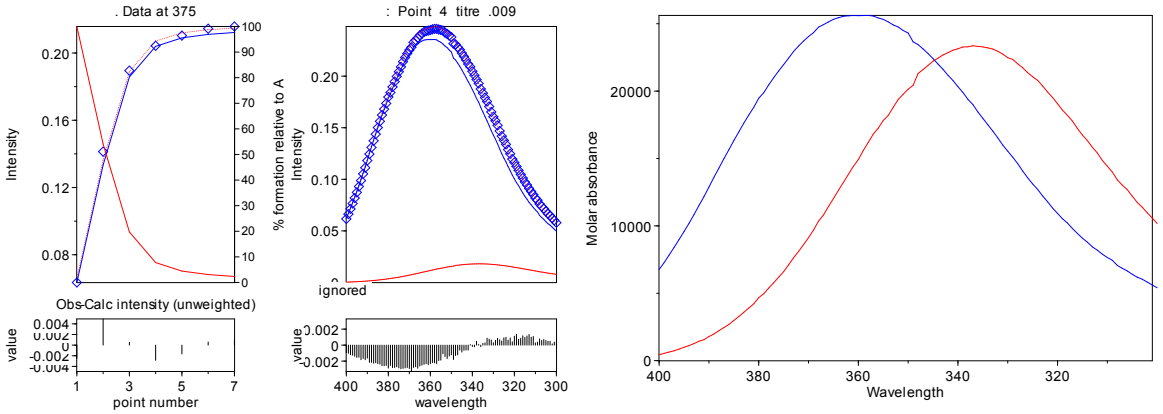
HypSpec. Refinement concluded at 7/16/2018 4:03:04 PM
Project title: ***meta* monourea-HP**.HQD
Converged in 1 iterations with sigma = 3.2188E-03

Log beta	value	standard deviation
RA	6.2976	0.1743
RA2	12.1015	0.1277



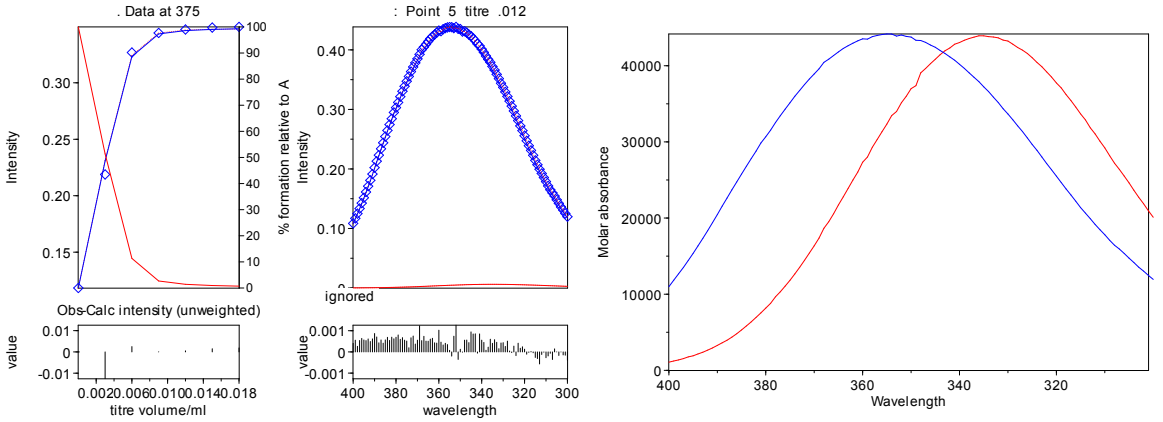
HypSpec. Refinement concluded at 7/16/2018 3:59:06 PM
Project title: ***meta* monourea-HPP**.HQD
Converged in 1 iterations with sigma = 1.5852E-03

Log beta	value	standard deviation
RA	6.3148	0.012



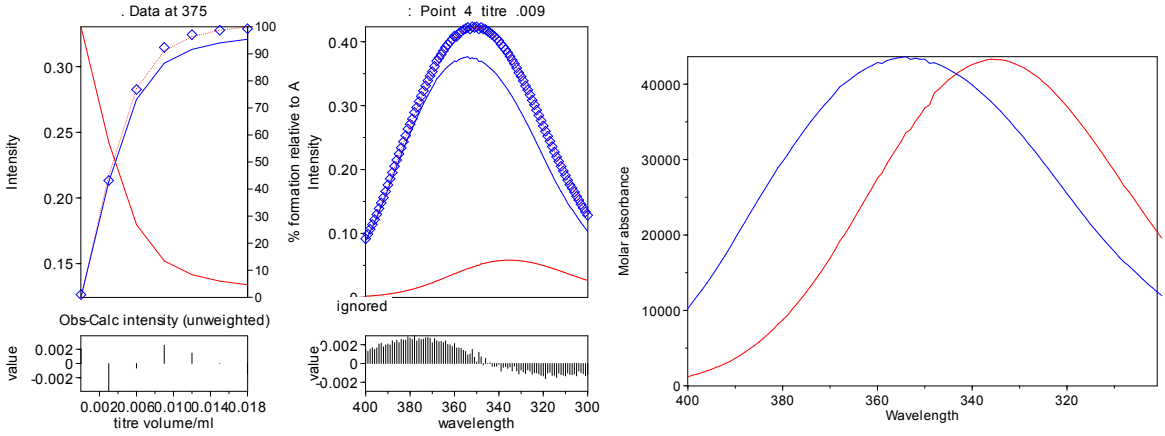
HypSpec. Refinement concluded at 6/20/2018 12:00:35 AM
Project title: **8a-AcO**.HQD
Converged in 1 iterations with sigma = 3.0414E-03

Log beta	value	standard deviation
RA	6.8399	0.0229



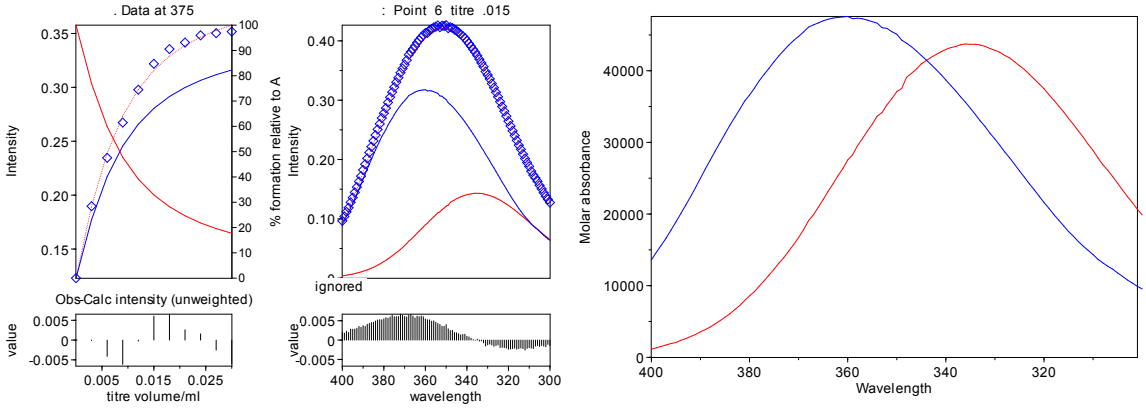
HypSpec. Refinement concluded at 6/20/2018 12:02:02 AM
Project title: **8a-BzO**.HQD
Converged in 1 iterations with sigma = 1.4155E-03

Log beta	value	standard deviation
RA	6.007	0.0062



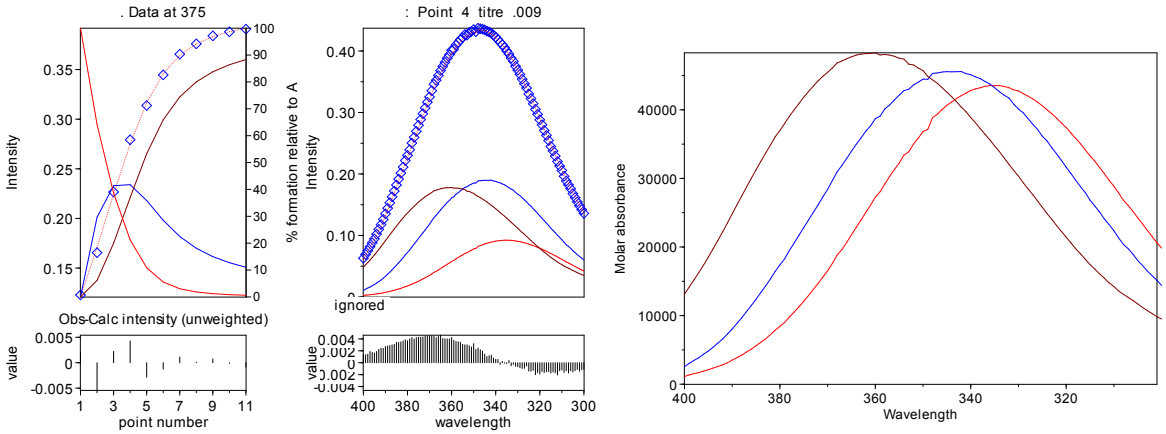
HypSpec. Refinement concluded at 6/20/2018 12:03:17 AM
Project title: **8a-F**.HQD
Converged in 1 iterations with sigma = 2.6858E-03

Log beta	value	standard deviation
RA	5.0498	0.0042



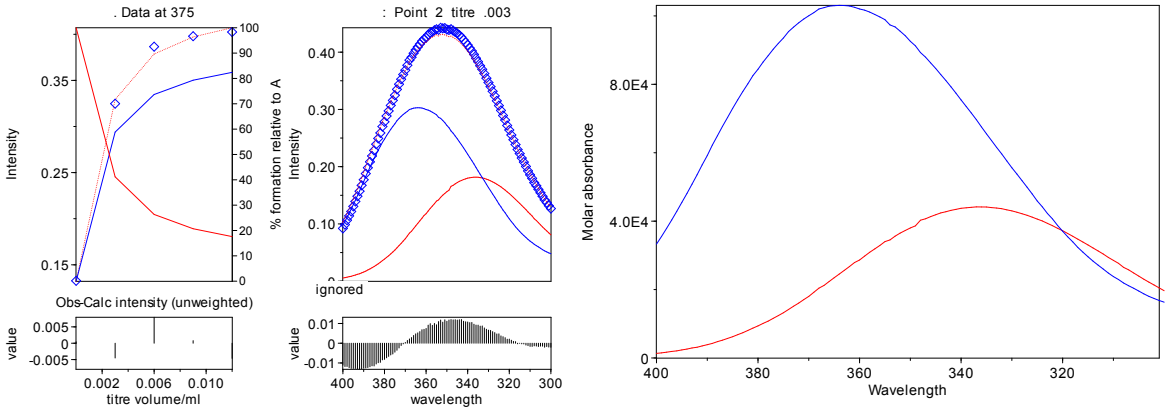
HypSpec. Refinement concluded at 6/20/2018 12:04:19 AM
Project title: **8a-HP**.HQD
Converged in 1 iterations with sigma = 1.7125E-03

Log beta	value	standard deviation
RA	5.7596	0.0522
RA2	11.1726	0.0384



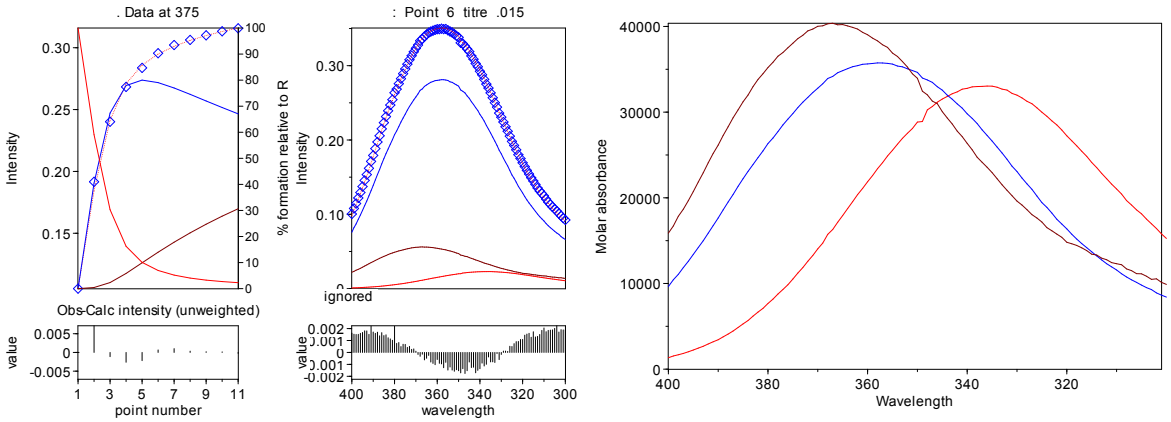
HypSpec. Refinement concluded at 6/20/2018 12:06:12 AM
Project title: **8a-HPP**.HQD
Converged in 1 iterations with sigma = 4.8826E-03

Log beta	value	standard deviation
R2A	10.9266	0.0215



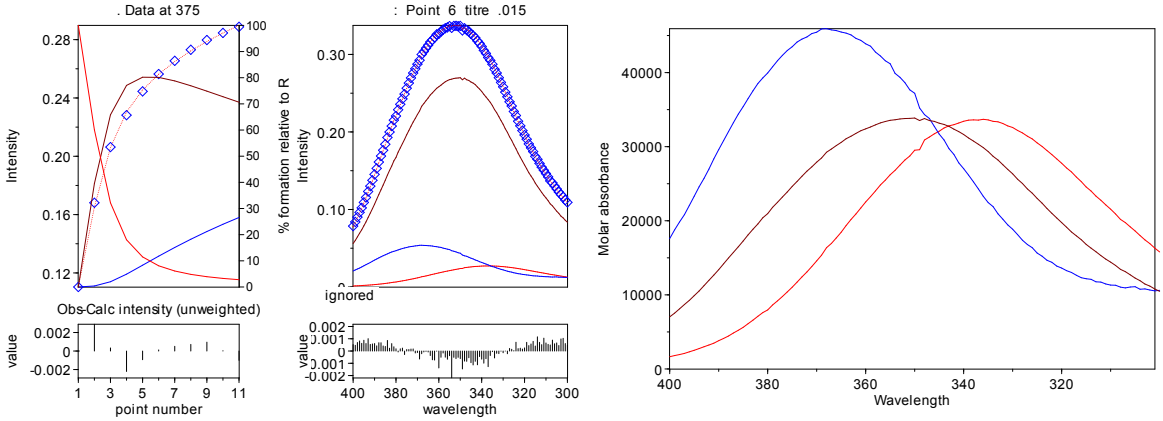
HypSpec. Refinement concluded at 7/27/2018 6:03:40 PM
Project title: **8b-AcO**.HQD
Converged in 18 iterations with sigma = 2.1723E-03

Log beta	value	standard deviation
RA	5.9012	0.0502
RA2	9.9955	0.2095



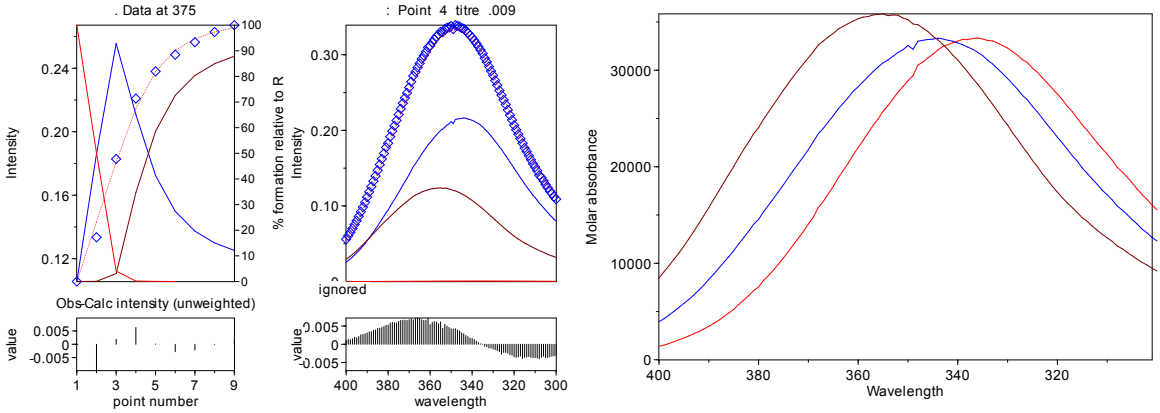
HypSpec. Refinement concluded at 7/27/2018 6:11:44 PM
Project title: **8b-AcO**.HQD
Converged in 1 iterations with sigma = 1.0627E-03

Log beta	value	standard deviation
RA2	9.8359	0.0969
RA	5.8317	0.0365



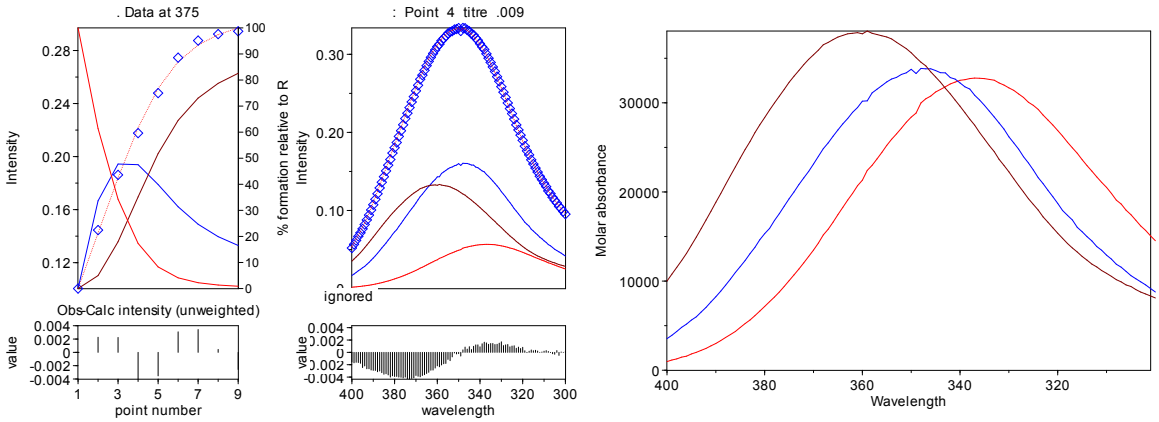
HypSpec. Refinement concluded at 7/27/2018 6:21:17 PM
Project title: **8b-F**.HQD
Converged in 1 iterations with sigma = 2.8643E-03

Log beta	value	standard deviation
RA	8.3741	1.3363
RA2	13.9112	1.3345



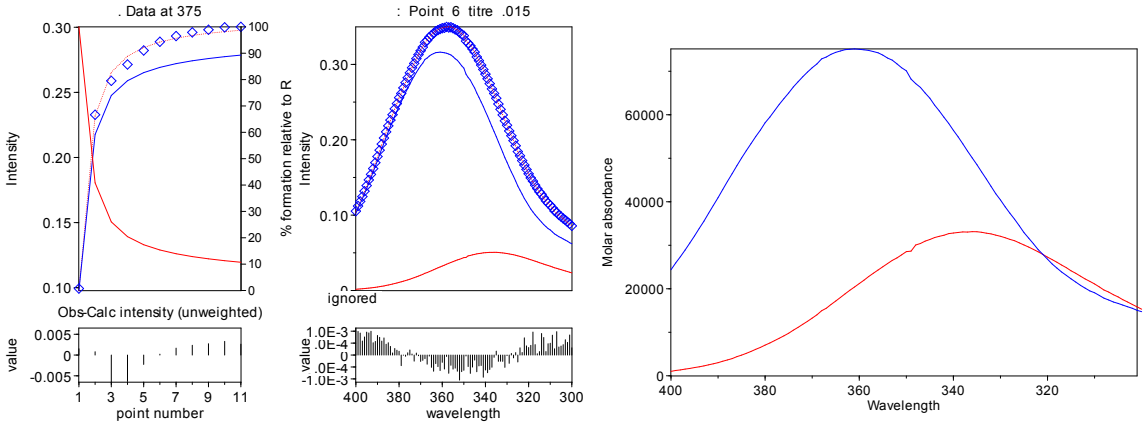
HypSpec. Refinement concluded at 7/27/2018 6:23:45 PM
Project title: **8b-HP**.HQD
Converged in 1 iterations with sigma = 1.6268E-03

Log beta	value	standard deviation
RA	5.9323	0.0086
RA2	11.2953	0.0139



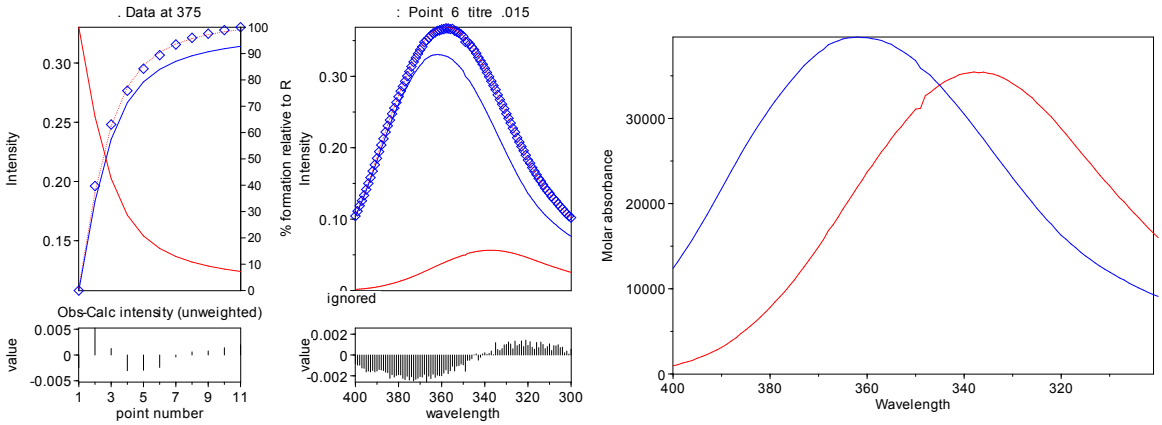
HypSpec. Refinement concluded at 7/27/2018 6:26:11 PM
Project title: **8b-HPP**.HQD
Converged in 1 iterations with sigma = 3.5916E-03

Log beta	value	standard deviation
R2A	10.9397	0.0129



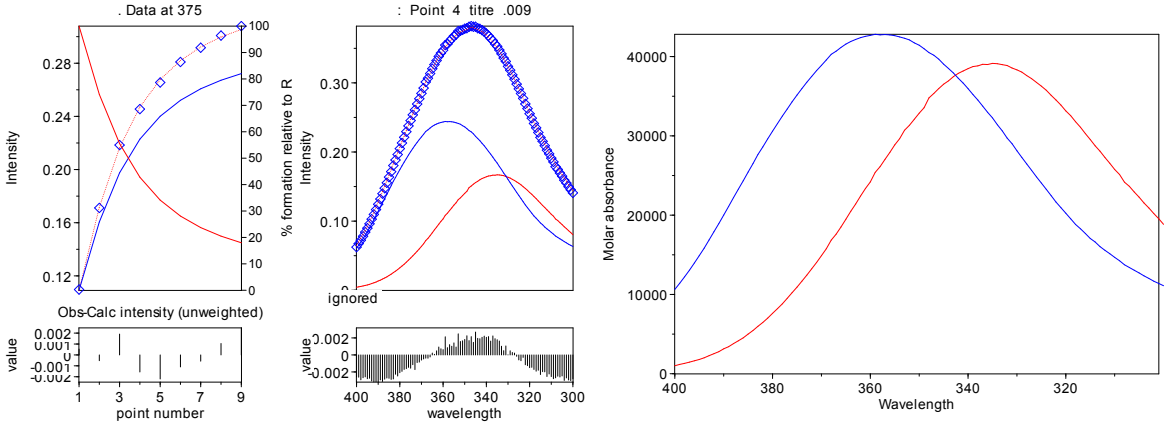
HypSpec. Refinement concluded at 7/27/2018 4:10:56 PM
Project title: **8c-AcO**.HQD
Converged in 1 iterations with sigma = 2.8907E-03

Log beta	value	standard deviation
RA	5.5024	0.0063



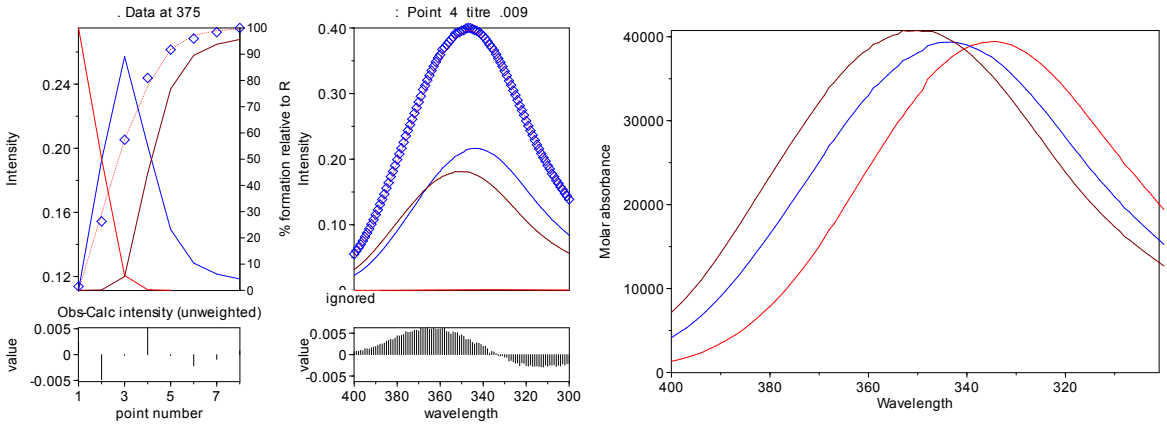
HypSpec. Refinement concluded at 7/27/2018 6:31:32 PM
Project title: **8c-BzO**.HQD
Converged in 1 iterations with sigma = 1.9667E-03

Log beta	value	standard deviation
RA	5.1599	0.0053



HypSpec. Refinement concluded at 7/27/2018 6:33:50 PM
Project title: **8c-F**.HQD
Converged in 1 iterations with sigma = 2.0366E-03

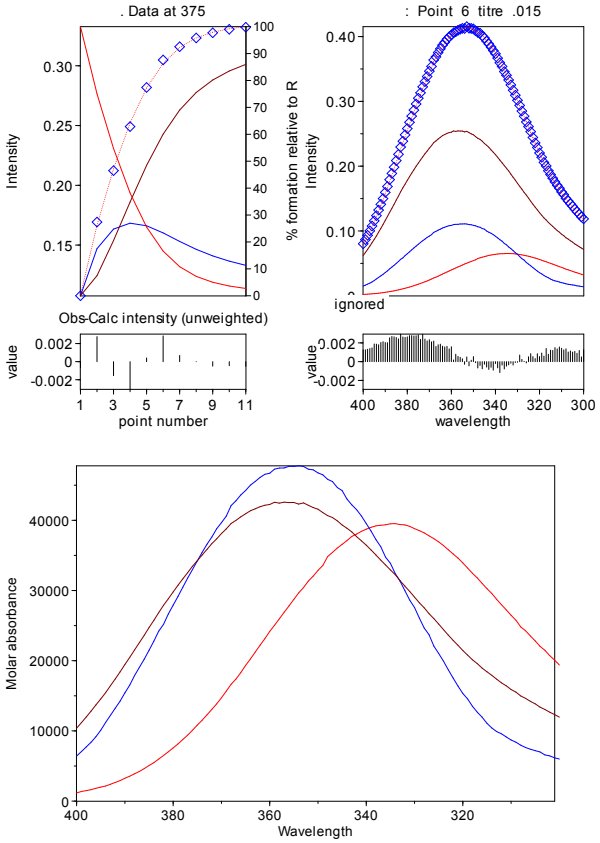
Log beta	value	standard deviation
RA	8.5803	0.3322
RA2	14.7355	0.3469



HypSpec. Refinement concluded at 7/27/2018 6:36:03 PM
Project title: **8c-HP**.HQD

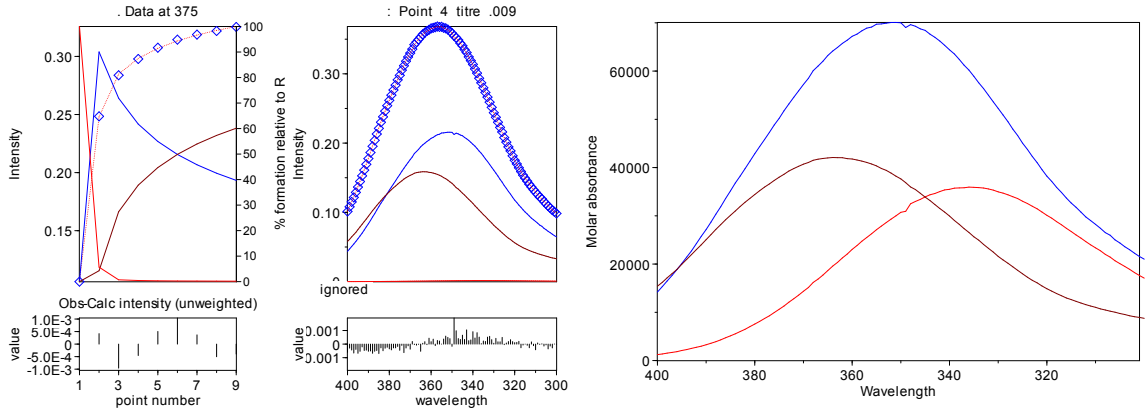
Converged in 1 iterations with sigma = 1.1649E-03

Log beta	value	standard deviation
RA	5.1227	0.0357
RA2	10.5076	0.0272



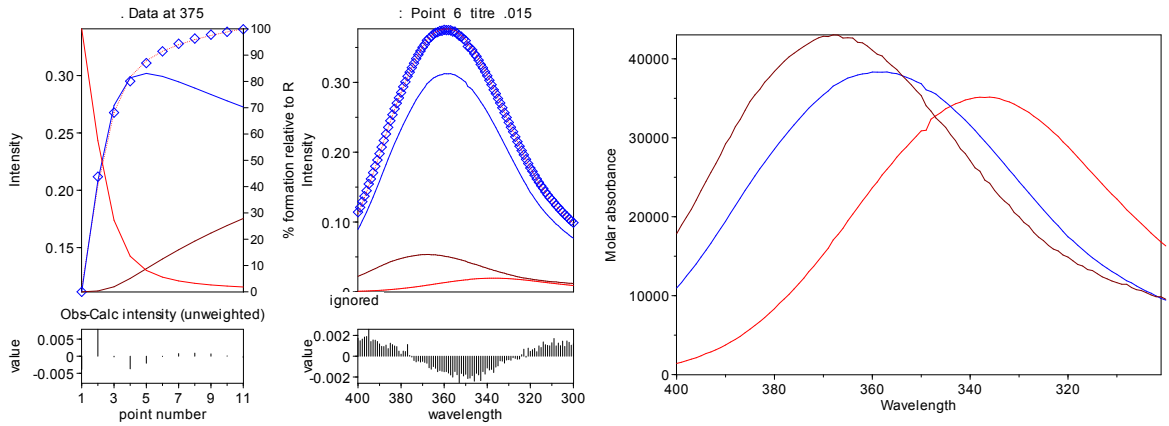
HypSpec. Refinement concluded at 7/27/2018 6:39:00 PM
Project title: **8c-HPP**.HQD
Converged in 1 iterations with sigma = 5.5535E-04

Log beta	value	standard deviation
R2A	14.2928	0.1251
RA	7.0242	0.0666



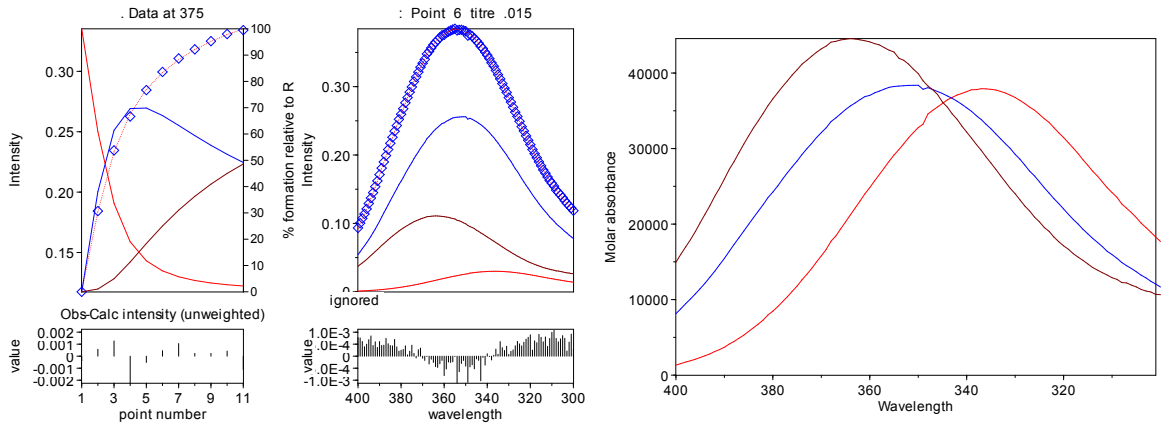
HypSpec. Refinement concluded at 7/27/2018 4:59:23 PM
Project title: **8d-AcO**.HQD
Converged in 1 iterations with sigma = 2.3691E-03

Log beta	value	standard deviation
RA	6.0131	0.053
RA2	10.0431	0.251



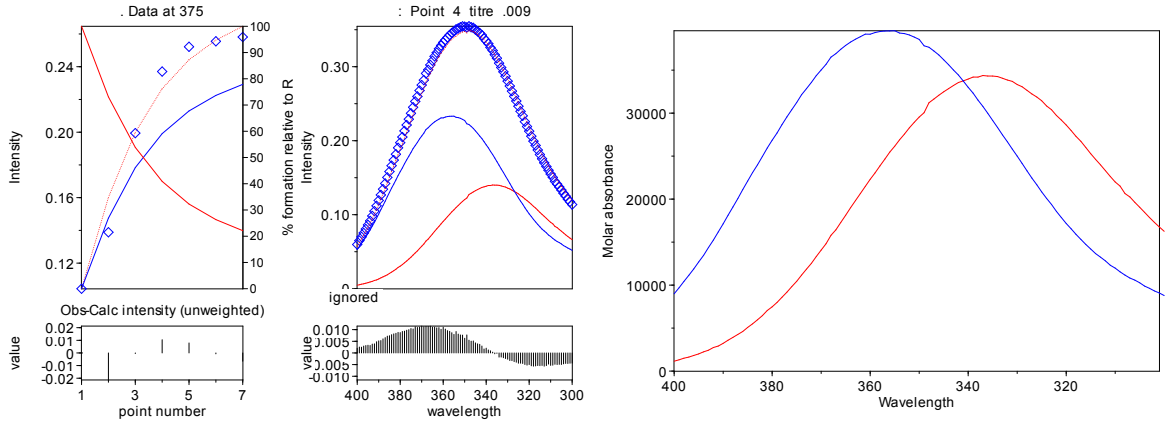
HypSpec. Refinement concluded at 7/27/2018 5:02:04 PM
Project title: **8d-BzO**.HQD
Converged in 1 iterations with sigma = 7.2912E-04

Log beta	value	standard deviation
RA	5.8043	0.0265
RA2	10.2551	0.0469



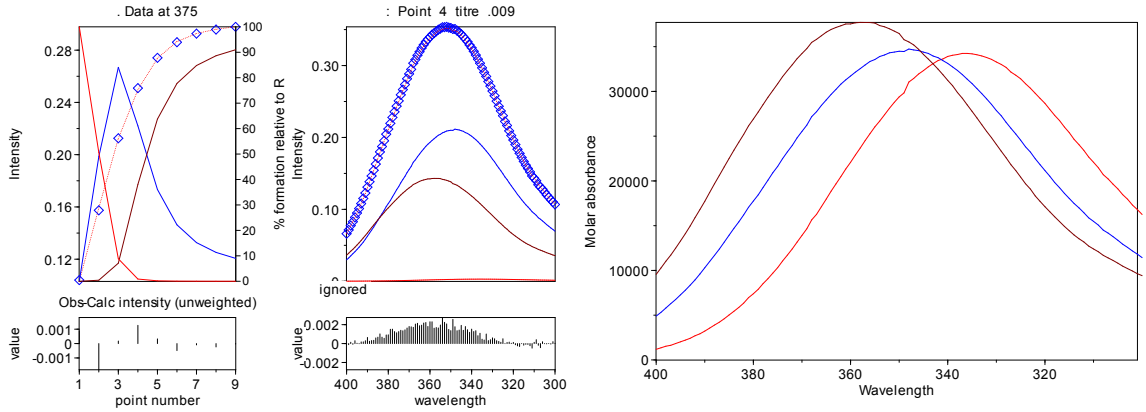
HypSpec. Refinement concluded at 7/27/2018 5:46:17 PM
Project title: **8d-F**.HQD
Converged in 1 iterations with sigma = 6.2726E-03

Log beta	value	standard deviation
RA	5.2025	0.0241



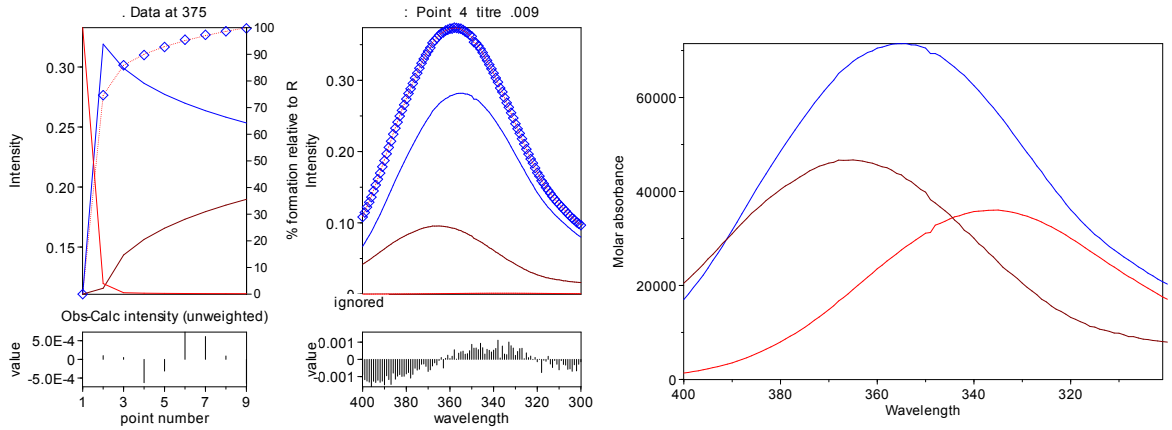
HypSpec. Refinement concluded at 7/27/2018 5:48:19 PM
Project title: **8d-HP**.HQD
Converged in 1 iterations with sigma = 7.9146E-04

Log beta	value	standard deviation
RA	7.7392	0.0651
RA2	13.427	0.069



HypSpec. Refinement concluded at 7/27/2018 5:50:29 PM
Project title: **8d-HPP**.HQD
Converged in 1 iterations with sigma = 5.7763E-04

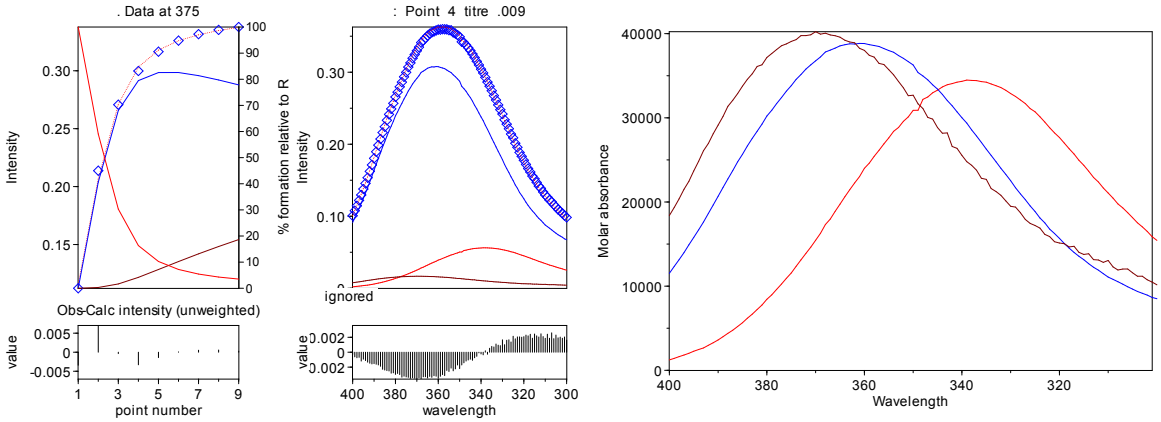
Log beta	value	standard deviation
R2A	14.5334	0.1374
RA	6.8037	0.0864



HypSpec. Refinement concluded at 7/27/2018 6:43:09 PM
Project title: **8e-AcO**.HQD
Converged in 9 iterations with sigma = 2.2555E-03

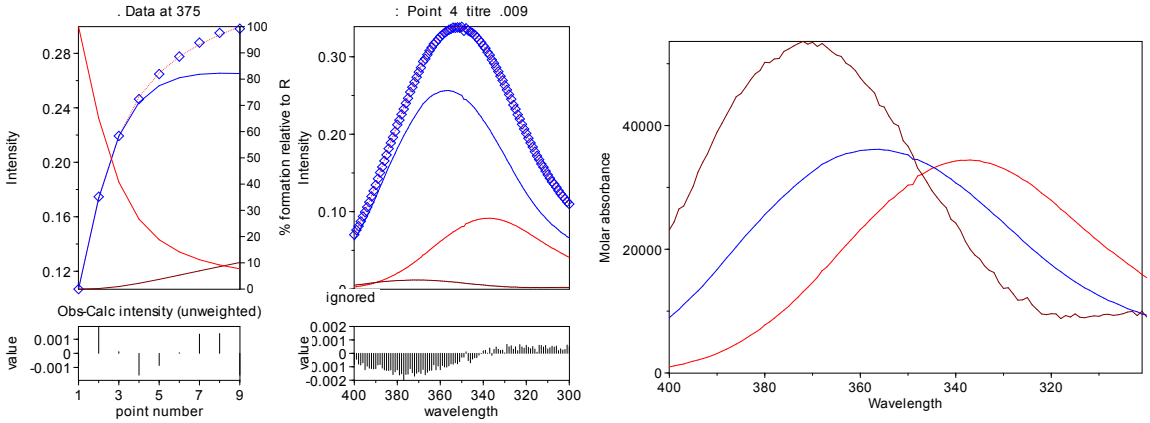
standard

Log beta	value	standard deviation
RA	5.8949	0.0612
RA2	9.8228	0.487



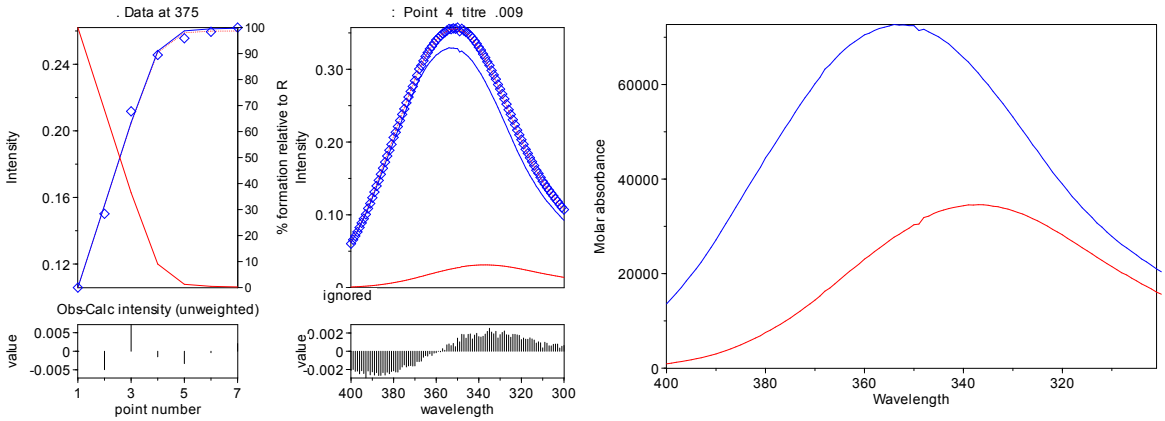
HypSpec. Refinement concluded at 7/27/2018 6:46:41 PM
Project title: **8d-BzO**.HQD
Converged in 2 iterations with sigma = 9.4409E-04

Log beta	value	standard deviation
RA	5.5558	0.0469
RA2	9.1766	0.3959



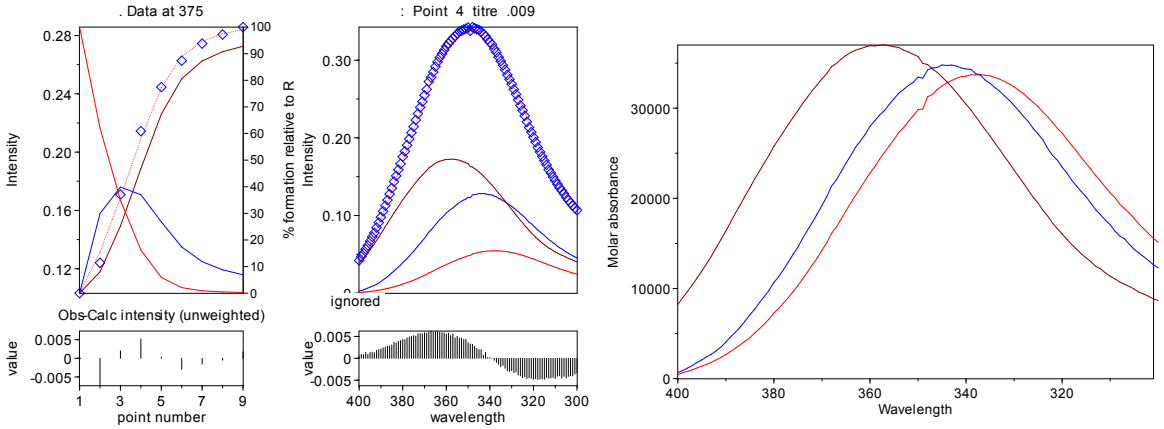
HypSpec. Refinement concluded at 7/27/2018 7:15:25 PM
Project title: **8d-F**.HQD
Converged in 1 iterations with sigma = 2.6001E-03

Log beta	value	standard deviation
R2A3	24.3516	0.0773



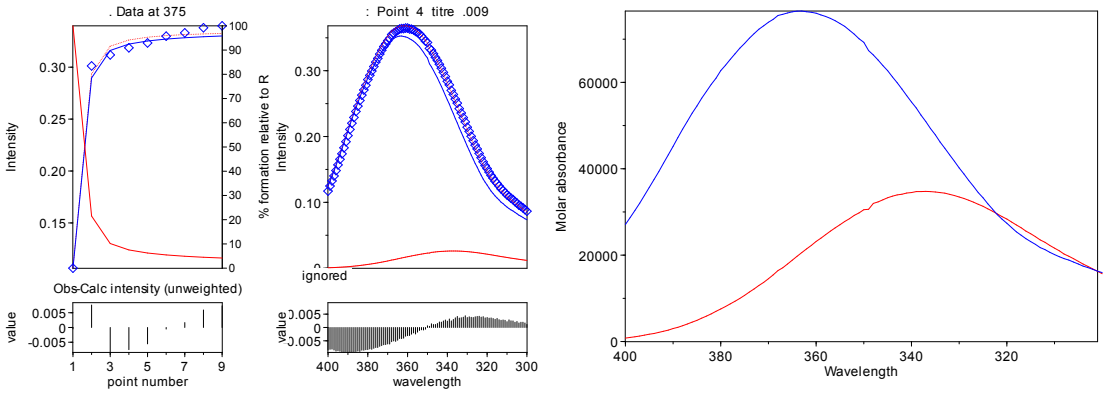
HypSpec. Refinement concluded at 7/27/2018 7:18:24 PM
Project title: **8d-HP**.HQD
Converged in 1 iterations with sigma = 2.6383E-03

Log beta	value	standard deviation
RA	6.0709	0.0324
RA2	11.8855	0.0434



HypSpec. Refinement concluded at 7/27/2018 8:15:36 PM
Project title: **8d-HPP**.HQD
Converged in 1 iterations with sigma = 4.8244E-03

Log beta	value	standard deviation
R2A	11.8986	0.0297



^{1}H NMR data fitting with HypNMR

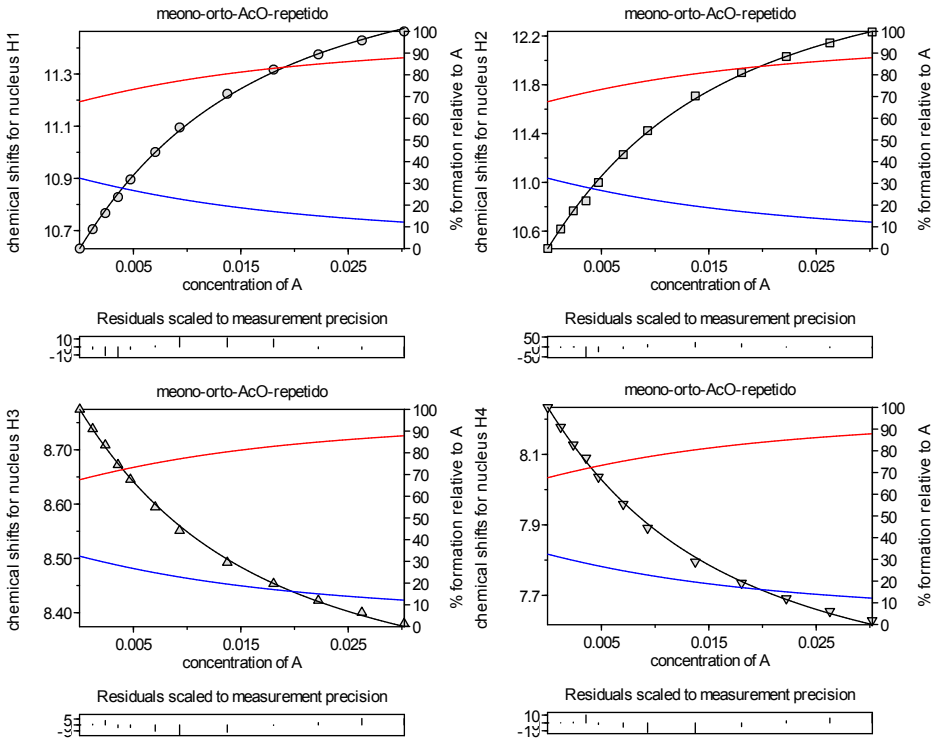
Project title: ***ortho* monourea-AcO**

Converged in 3 iterations with sigma = 8.078370

	value	standard deviation	Comments
1 log beta(AR)	1.9021	0.0087	1.902(9)

***ortho* monourea-AcO** chemical shifts

nucleus	R	AR
H1	10.6313	11.8729
H2	10.4578	13.0781
H3	8.7744	8.1858
H4	8.2335	7.3264
H5	8.1934	8.0881
H6	7.7588	7.8002
H7	7.6814	7.4667
H8	7.4694	7.3317
H9	7.0946	7.1064



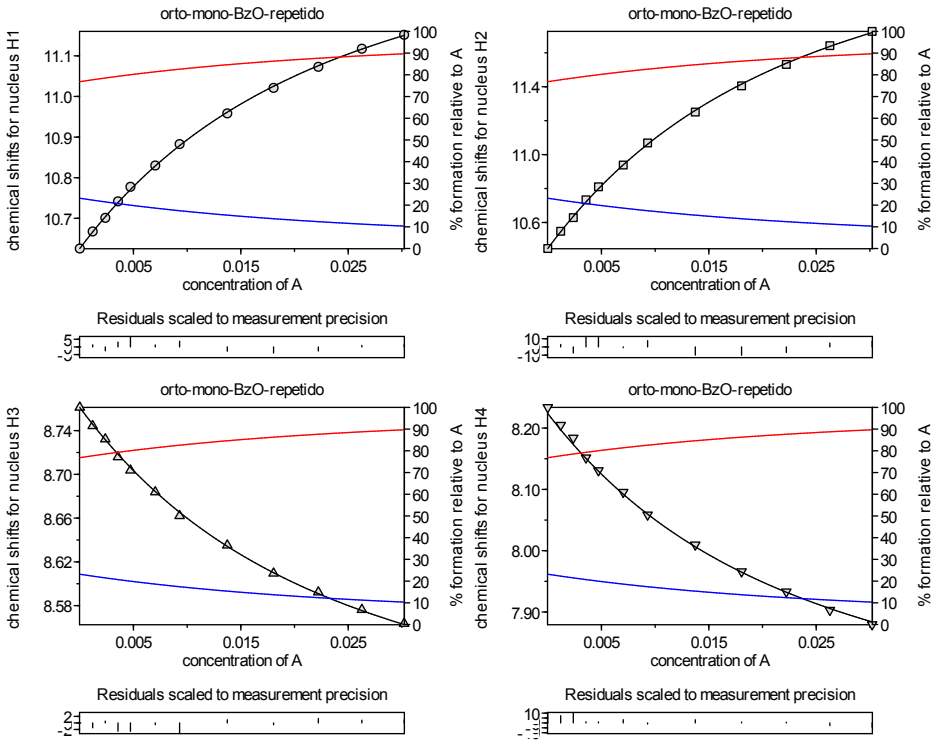
Project title: ***ortho*** **monourea-BzO**

Converged in 4 iterations with sigma = 3.664169

	value	standard deviation	Comments
1 log beta(AR)	1.7011	0.0065	1.701(7)

ortho **monourea-BzO** chemical shifts

nucleus	R	AR
H1	10.6256	11.5357
H2	10.4464	12.6541
H3	8.7612	8.4169
H4	8.2238	7.6342
H5	8.1908	8.1628
H6	7.7592	7.9605
H7	7.6814	7.5492
H8	7.4681	7.4027
H9	7.0934	7.1355

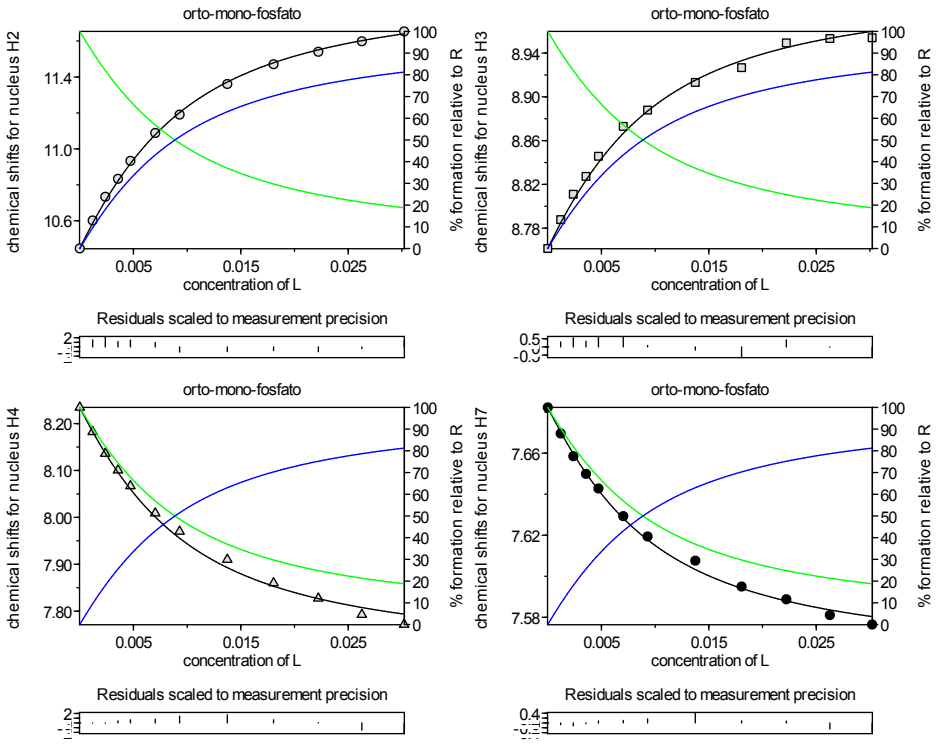


Project title: ***ortho* monourea-HP**
Converged in 5 iterations with sigma = 0.658406

	value	standard deviation	Comments
1 log beta(LR)	2.2252	0.0108	2.23(1)

***ortho* monourea-HP** chemical shifts

nucleus	R	LR
H2	10.4460	11.4133
H3	8.7614	8.9287
H4	8.2346	7.9080
H5	8.1915	8.1486
H6	7.7597	7.8058
H7	7.6823	7.6042
H8	7.4686	7.4185
H9	7.0933	7.1119

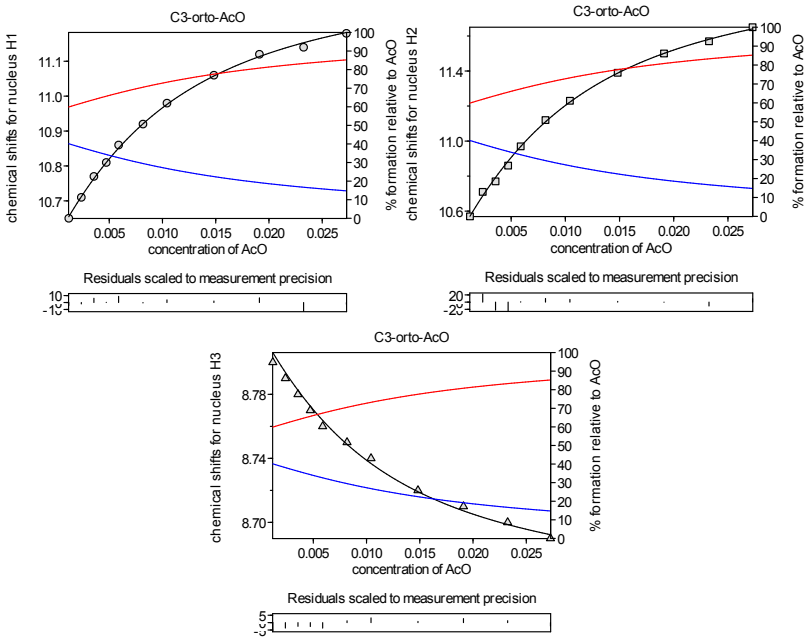


Project title: **4b-AcO**
Converged in 1 iterations with sigma = 9.299599

	value	standard deviation	Comments
1 log beta(AcOR)	2.0857	0.0155	2.09(2)

4b-AcO chemical shifts

nucleus	R	AcOR	Δδ
H1	10.5900	11.3917	0.8
H2	10.4400	12.0646	1.62
H3	8.8200	8.6472	-0.17

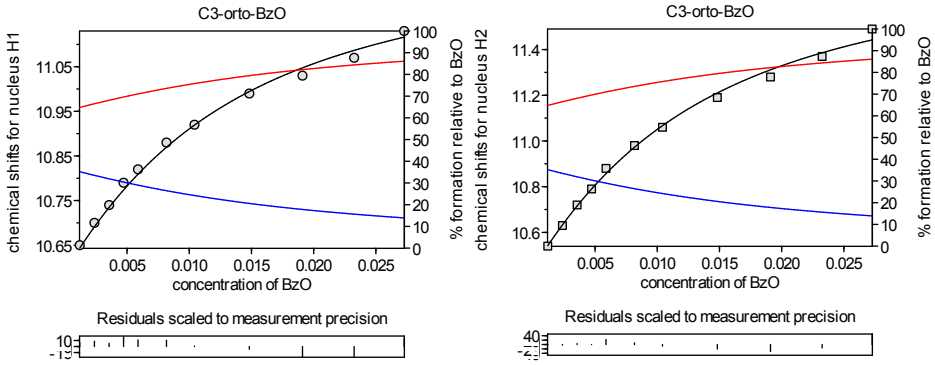


Project title: **4b-BzO**
Converged in 1 iterations with sigma = 17.769959

	value	standard deviation	Comments
1 log beta(BzOR)	1.99	0.036	1.99(4)

4b-BzO chemical shifts

nucleus	R	BzOR
H1	10.5900	11.3456
H2	10.4400	11.8792
H3	no change	



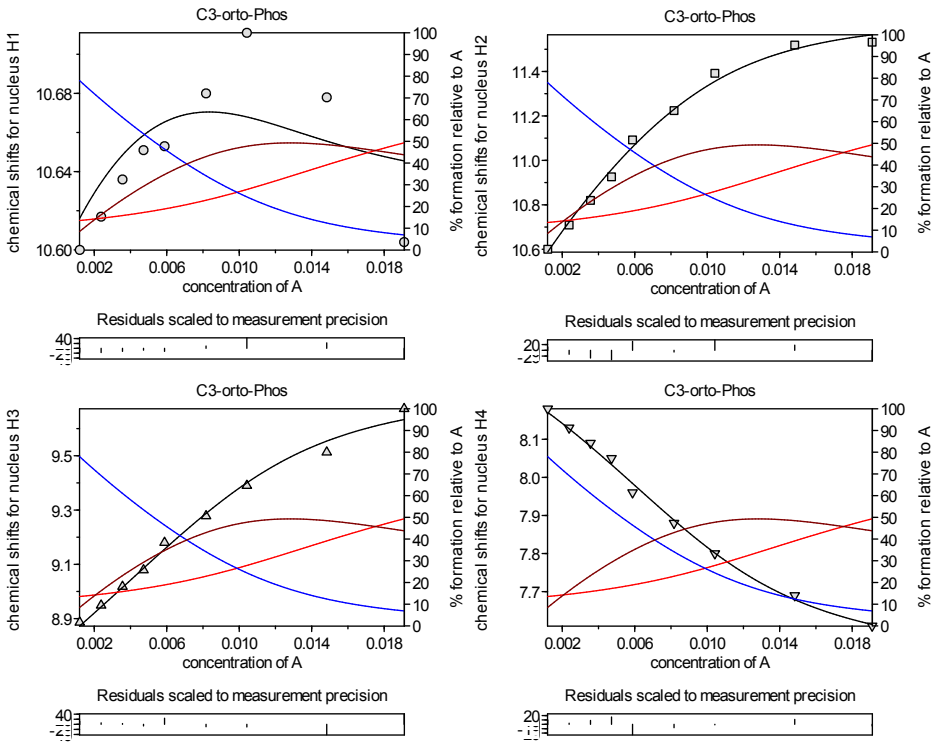
Project title: **4b-HP**
Converged in 1 iterations with sigma = 25.206265

	value	standard deviation	Comments
1 log beta(AR)	3.0616	excessive	relative error on beta = 163%
2 log beta(A2R)	5.5893	excessive	relative error on beta = 122%

4b-HP chemical shifts

nucleus	R	AR	A2R	$\Delta\delta_{01}$	$\Delta\delta_{12}$	$\Delta\delta_{02}$
H1	10.59	10.74	10.62	0.15	-0.12	0.03
H2	10.44	11.31	11.68	0.87	0.37	1.24

H3	8.80	9.19	9.80	0.39	0.61	1.00
H4	8.21	8.00	7.48	-0.21	-0.52	-0.73



Project title: **4c-AcO**
Converged in 1 iterations with sigma = 14.407662

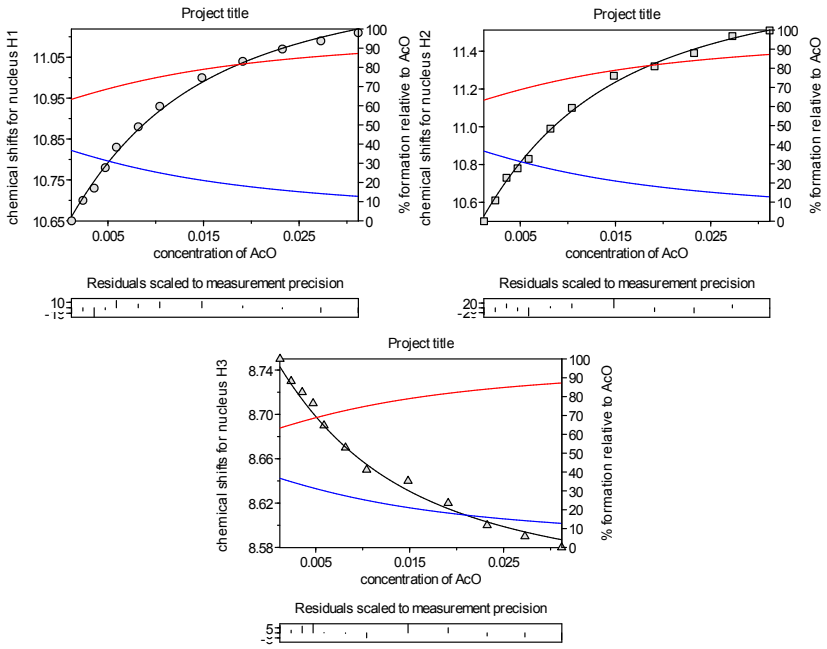
	value	standard deviation	Comments
log beta(AcOR)	2.0187	0.0241	2.02(2)

log beta(AcO2R) was ignored

4c-AcO chemical shifts

nucleus	R	AcOR	$\Delta\delta_{01}$
H1	10.6100	11.2983	0.6883

H2	10.4200	11.8966	1.4766
H3	8.7600	8.5260	-0.234



Project title: **4c-BzO**
Converged in 1 iterations with sigma = 0.515915

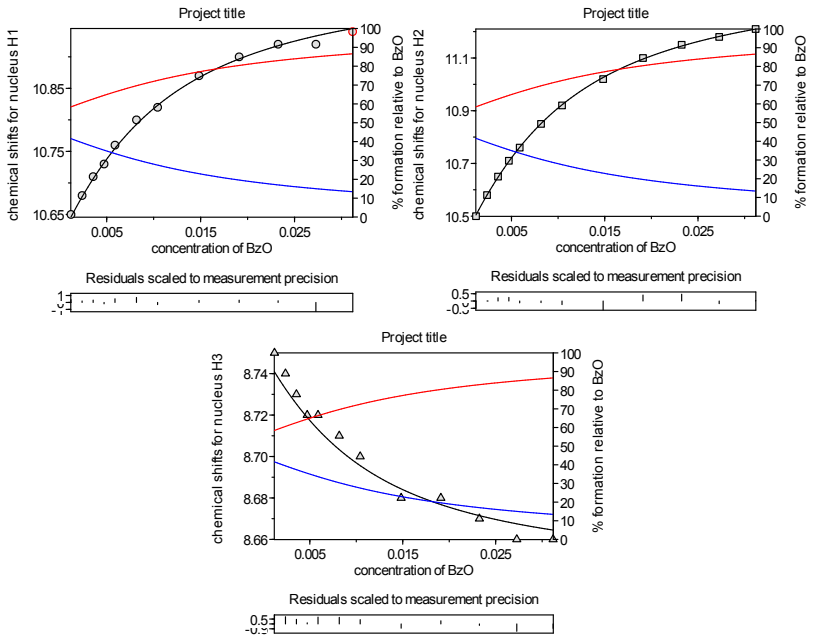
	value	standard deviation	Comments
log beta(BzOR)	2.1131	0.0122	2.11(1)

log beta(BzO2R) was ignored

4c-BzO chemical shifts

nucleus	R	BzOR	$\Delta\delta_{01}$
H1	10.6100	11.0405	0.43

H2	10.4200	11.4351	1.0151
H3	8.7500	8.6401	-0.11



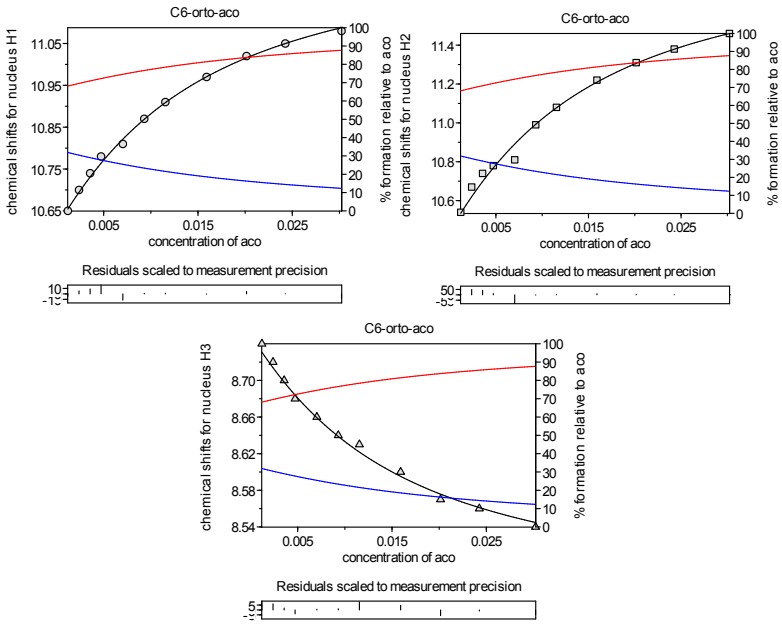
Project title: **4d-AcO**
Converged in 1 iterations with sigma = 20.371878

	value	standard deviation	Comments
log beta(acoR)	1.922	0.0405	1.92(4)

4d-AcO chemical shifts

nucleus	R	AcOR	Δδ
H1	10.61	11.30	0.69

H2	10.44	11.92	1.48
H3	8.75	8.45	-0.30



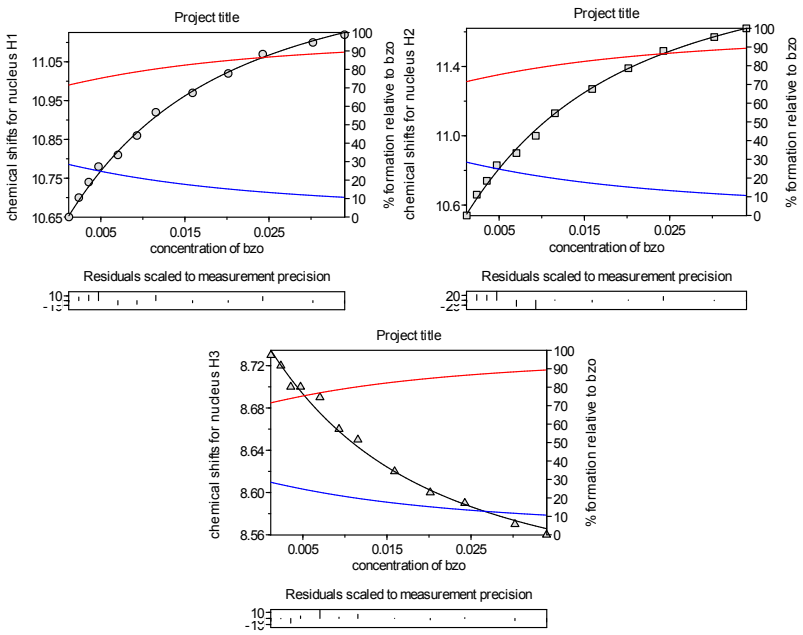
Project title: **4d-BzO**
Converged in 1 iterations with sigma = 13.574154

	value	standard deviation	Comments
log beta(bzoR)	1.8487	0.0218	1.85(2)

4d-BzO chemical shifts

nucleus	R	bzoR	$\Delta\delta_{01}$
H1	10.61	11.37	0.76

H2	10.45	12.17	1.72
H3	8.75	8.48	-0.27



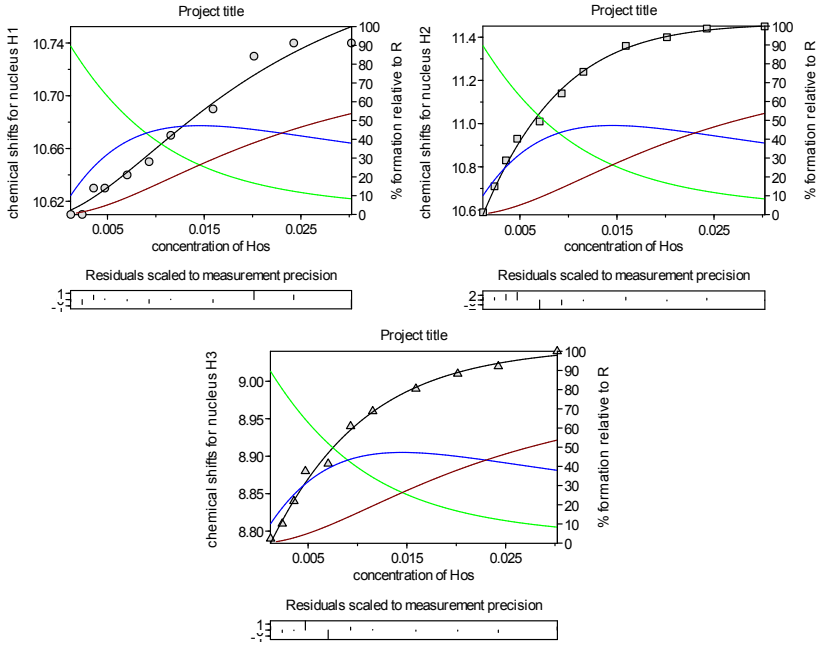
Project title: **4d-HP**
Converged in 23 iterations with sigma = 1.426437

	value	standard deviation	Comments
log beta(HosR)	2.3084	excessive	relative error on beta = 73%
log beta(Hos2R)	4.1095	excessive	relative error on beta = 191%

4d-HP chemical shifts

nucleus	R	fosR	fos2R	$\Delta\delta_{01}$	$\Delta\delta_{12}$	$\Delta\delta_{02}$

H1	10.61	10.63	10.86	0.02	0.23	0.25
H2	10.44	11.78	11.37	1.34	-0.41	0.93
H3	8.75	9.08	9.05	0.33	-0.03	0.3



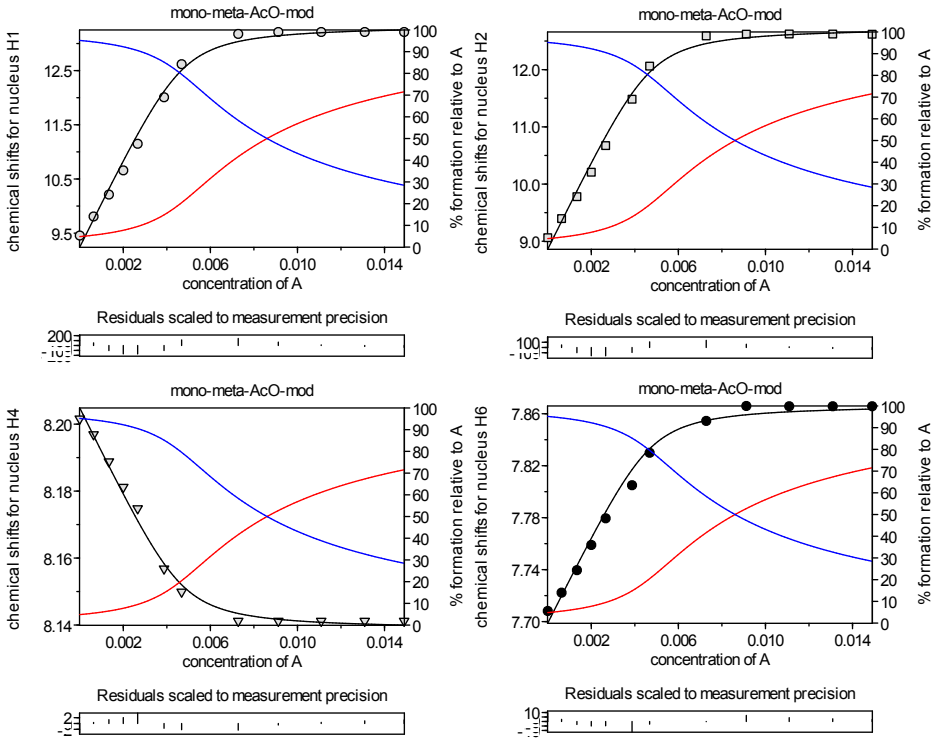
Project title: ***meta*** **monourea-AcO**

Converged in 1 iterations with sigma = 63.217288

	value	standard deviation	Comments
1 log beta(AR)	3.611	0.0629	3.61(6)

meta **monourea-AcO** chemical shifts

nucleus	R	RA
H1	9.2429	13.3427
H2	8.8631	12.7461
H3	8.4200	0.0000
H4	8.2048	8.1385
H5	7.8909	8.0943
H6	7.6989	7.8674
H7	7.6190	7.6971
H8	7.4772	7.3425
H9	7.3856	7.2917

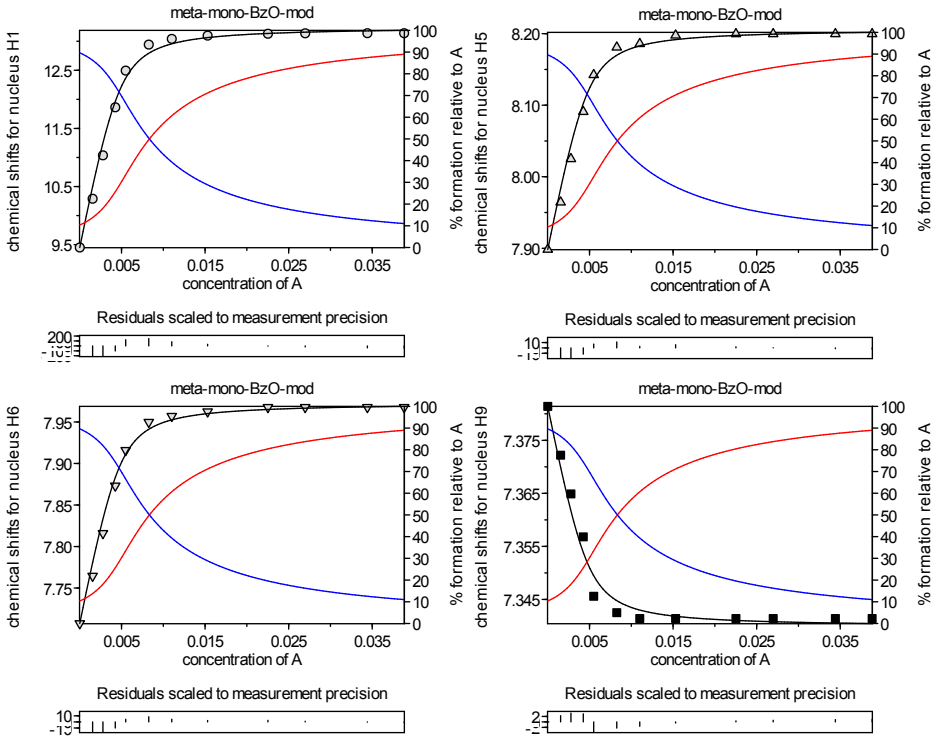


Project title: ***meta*** **monourea-BzO**
Converged in 1 iterations with sigma = 61.501691

	value	standard deviation	Comments
log beta(AR)	3.2543	0.0349	3.25(3)

meta **monourea-BzO** chemical shifts

nucleus	R	AR
H1	9.4513	13.2474
H2	9.0621	12.6802
H5	7.8983	8.2067
H6	7.7073	7.9730
H7	7.6256	7.7867
H8	7.4710	7.3816
H9	7.3814	7.3398

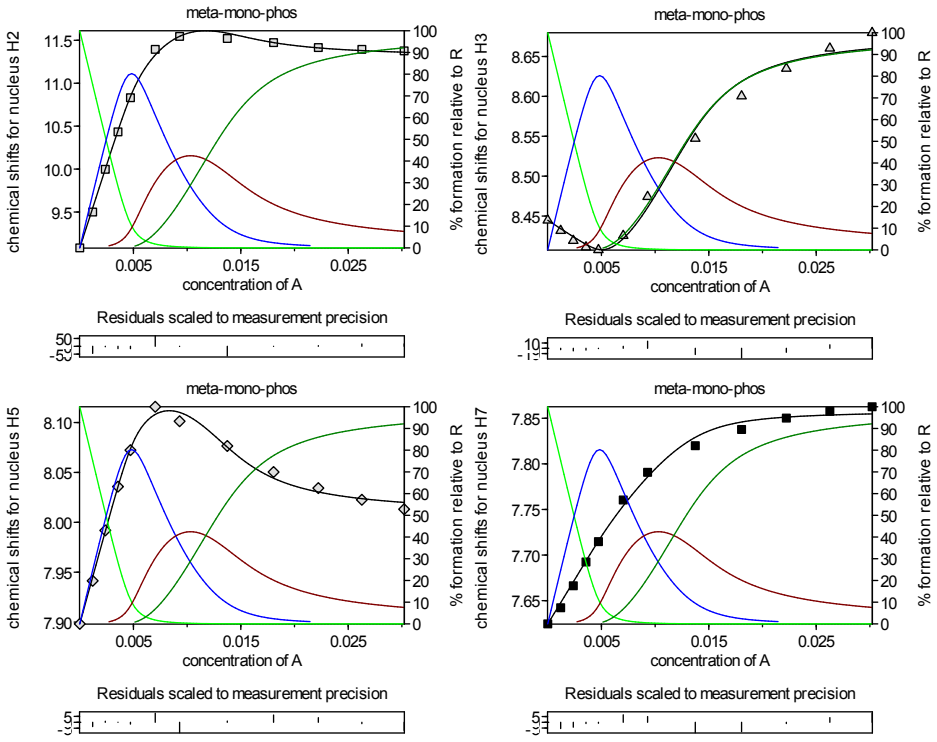


Project title: ***meta* monourea-HP**
Converged in 5 iterations with sigma = 15.447629

	value	standard deviation	Comments
1 log beta(AR)	5.0253	excessive	relative error on beta = 41%
2 log beta(A2R)	8.2075	excessive	relative error on beta = 54%
3 log beta(A3R)	11.047	fixed	

***meta* monourea-HP** chemical shifts

nucleus	R	AR	A2R	A3R
H1	9.4742	11.3975	13.1452	11.8403
H2	9.0829	10.9443	12.2436	11.2898
H3	8.4447	8.4025	8.4005	8.6820
H4	8.2012	8.1370	8.1014	8.1075
H5	7.8982	8.0869	8.1864	8.0060
H6	7.7069	7.8810	8.0188	7.9561
H7	7.6245	7.7176	7.8114	7.8588
H8	7.4696	7.3822	7.3276	7.3890
H9	7.3805	7.3031	7.2592	7.2866

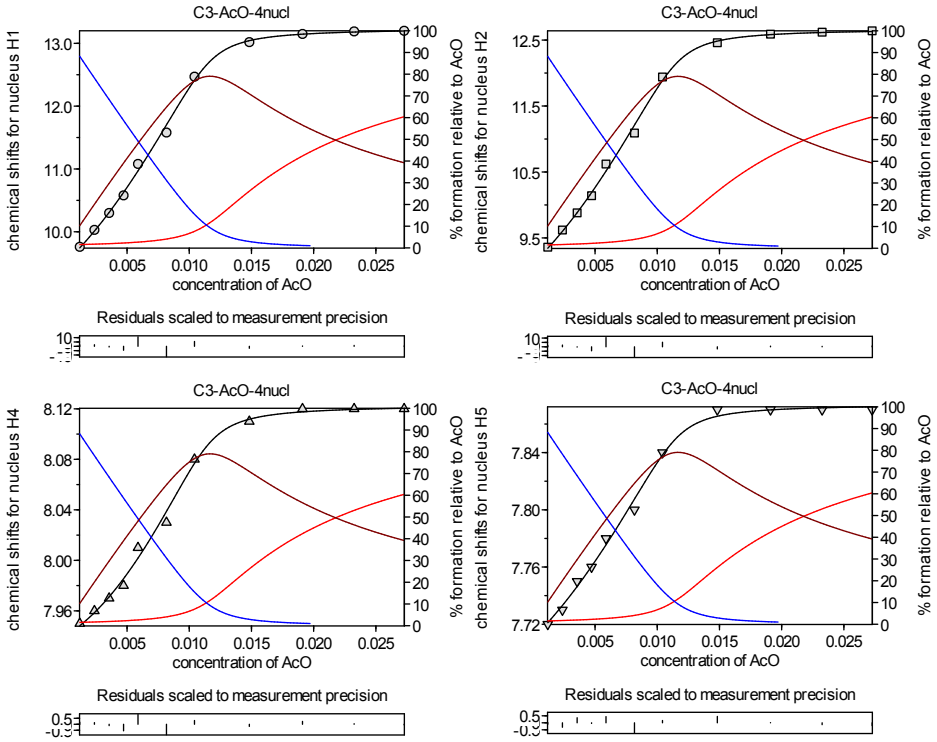


Project title: **8b-AcO**
Converged in 4 iterations with sigma = 4.153617

	value	standard deviation	Comments
1 log beta(AcOR)	4.0706	0.12	4.1(1)
2 log beta(AcO2R)	7.5661	0.16	7.6(2)

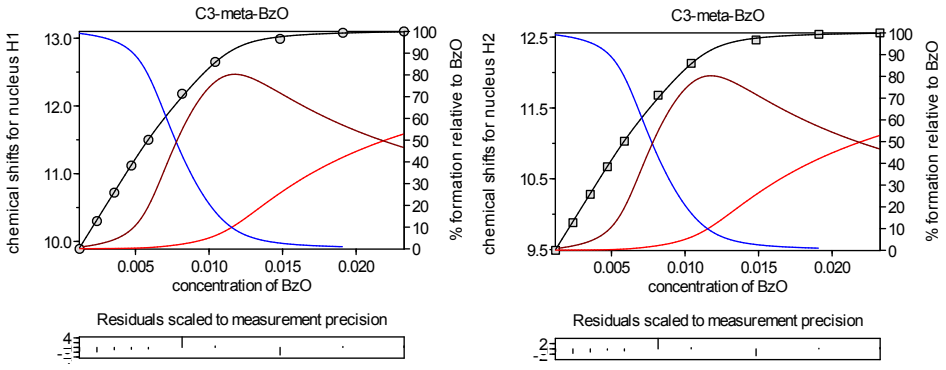
8b-AcO chemical shifts

Nucleus	R	AcOR	AcO2R
H1	9.5000	10.6550	13.2460
H2	9.1100	10.2190	12.6774
H4	7.9400	7.9760	8.1233
H5	7.7100	7.7630	7.8742



Project title: **8b-BzO**
Converged in 5 iterations with sigma = 2.057031

	value	standard deviation	Comments
1 log beta(BzOR)	5.3415	0.37	5.3(4)
2 log beta(BzO2R)	8.8922	0.65	8.9(7)



chemical shifts

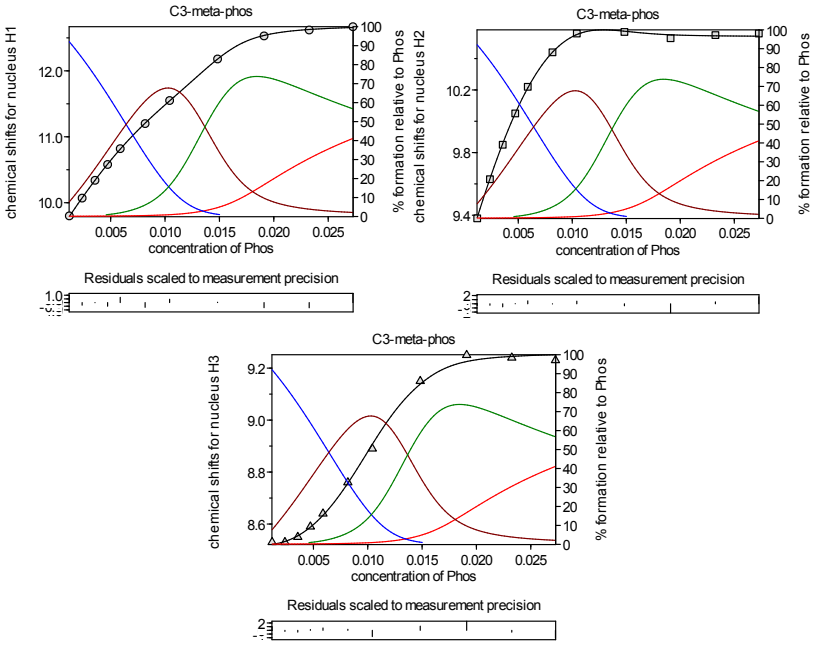
nucleus	R	BzOR	BzO2R
H1	9.4900	11.5700	13.1289
H2	9.1000	11.1000	12.5883

Project title: **8b-HP**
Converged in 1 iterations with sigma = 1.226338

	value	standard deviation	Comments
1 log beta(PhosR)	5.0811	excessive	relative error on beta = 90%
2 log beta(Phos2R)	9.4263	excessive	relative error on beta = 183%
3 log beta(Phos3R)	12.6259	excessive	relative error on beta = 182%

8b-HP chemical shifts

nucleus	R	PhosR	Phos2R	Phos3R	$\Delta\delta_{01}$	$\Delta\delta_{12}$	$\Delta\delta_{23}$	$\Delta\delta_{03}$
H1	9.49	11.02	11.66	12.71	1.53	0.64	1.05	3.22
H2	9.11	10.53	10.62	10.54	1.42	0.09	-0.08	1.43
H3	8.52	8.51	9.04	9.26	-0.01	0.53	0.22	0.74

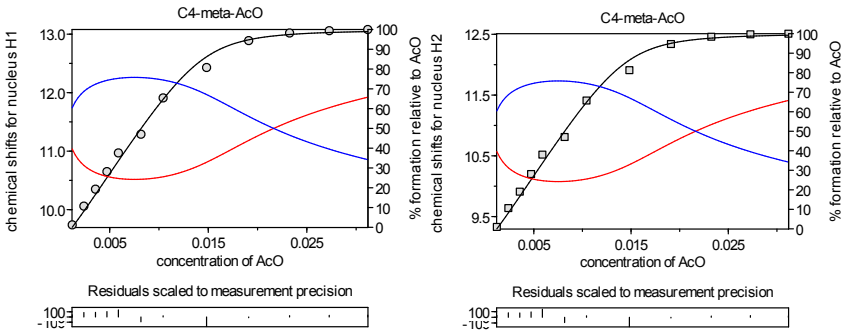


Project title: **8c-AcO**
Converged in 1 iterations with sigma = 91.232749

	value	standard deviation	Comments
1 log beta(AcO2R)	5.4566	0.0779	5.46(8)

8c-AcO chemical shifts

nucleus	R	AcO_2R	Δδ
H1	9.48	13.07	3.59
H2	9.09	12.51	3.42
H3	8.50	no change	

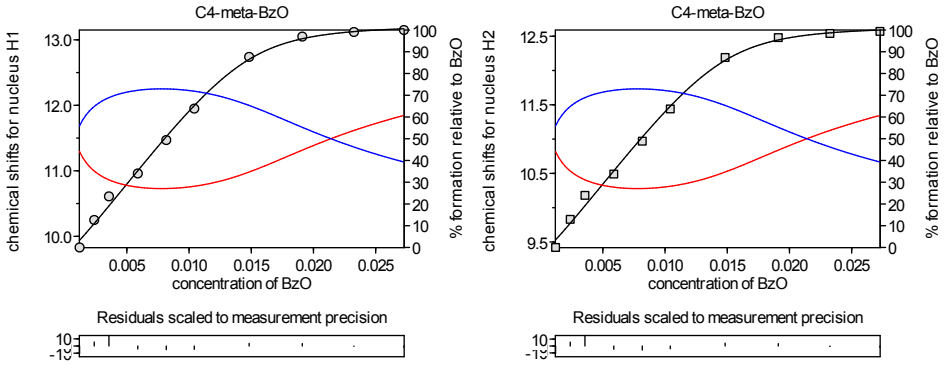


Project title: **8c-BzO**
Converged in 6 iterations with sigma = 7.950490

	value	standard deviation	Comments
1 log beta(BzO2R)	5.3276	0.0975	5.33(1)

8c-BzO chemical shifts

nucleus	R	BzO2R
H1	9.7434	13.2275
H2	9.3456	12.6454



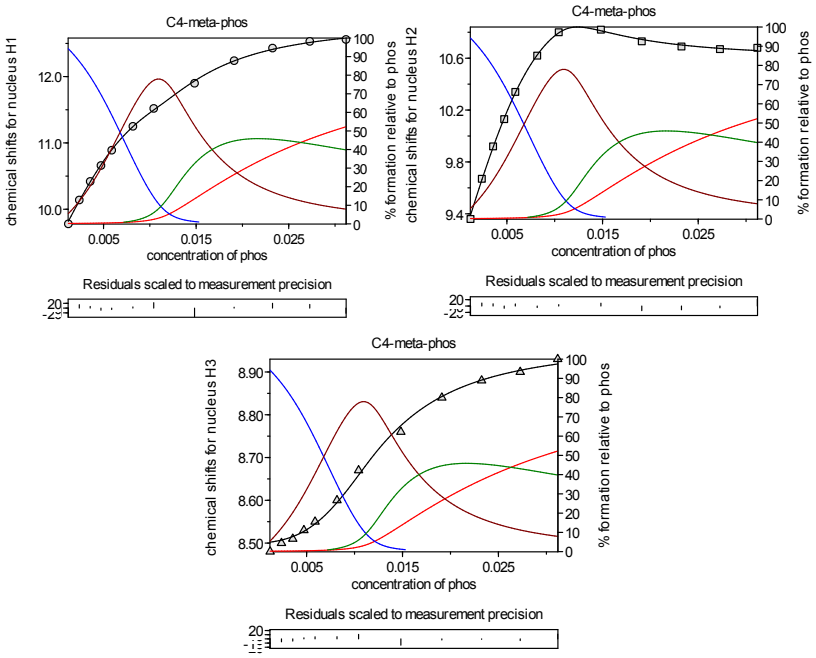
Project title: **8c-HP**
Converged in 1 iterations with sigma = 18.153318

	value	standard deviation	Comments
log beta(phosR)	4.93	excessive	relative error on beta = 141%
log beta(phos2R)	8.96	excessive	relative error on beta = 269%

log beta(phos3R) 11.27 excessive relative error on beta = 261%

8c-HP chemical shifts

nucleus	R	phosR	phos2R	phos3R	$\Delta\delta_{01}$	$\Delta\delta_{12}$	$\Delta\delta_{23}$	$\Delta\delta_{03}$
H1	9.49	11.16	11.58	12.88	1.67	0.42	1.30	3.39
H2	9.10	10.57	10.92	10.58	1.47	0.35	-0.34	1.48
H3	8.50	8.51	8.70	8.98	0.01	0.19	0.28	0.48



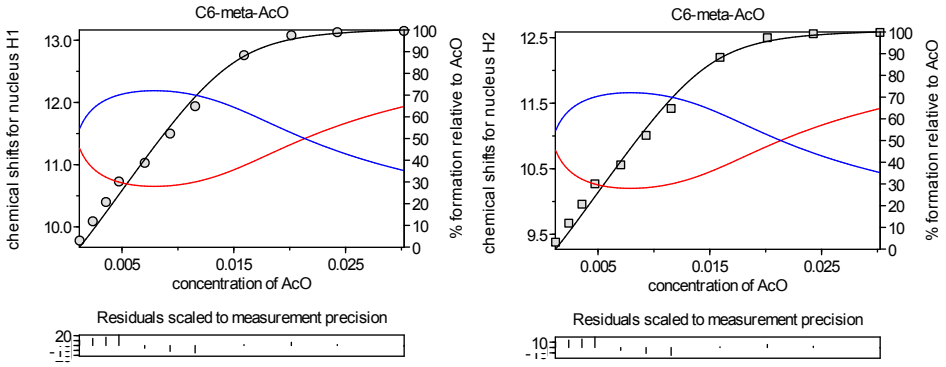
Project title: **8d-AcO**
Converged in 1 iterations with sigma = 12.212353

value	standard deviation	Comments

1 log beta(AcO2R)	5.2886	0.0971	5.29(1)

C6-meta-AcO chemical shifts

nucleus	R	AcO2R	Δδ
H1	9.47	13.21	3.74
H2	9.08	12.63	3.55
H3	8.47	no change	

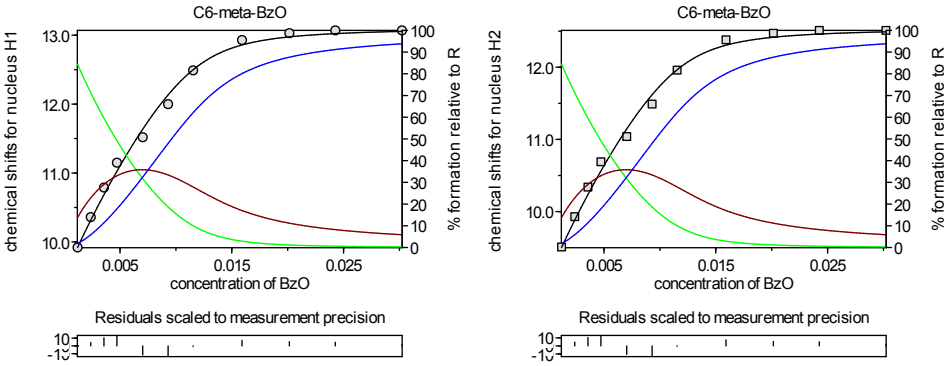


Project title: **8d-BzO**
Converged in 1 iterations with sigma = 8.367374

	value	standard deviation	Comments
1 log beta(BzO2R)	5.9089	0.0885	5.91(9)
2 log beta(BzOR)	3.0023	0.0604	3.0(6)

8d-BzO chemical shifts

nucleus	R	BzOR	BzO2R	$\Delta\delta_{01}$	$\Delta\delta_{12}$	$\Delta\delta_{02}$
H1	9.48	12.20	13.12	2.72	0.92	3.64
H2	9.08	11.70	12.55	2.62	0.85	3.47
H3	no change					



Project title: **8d-HP**
Converged in 1 iterations with sigma = 4.577521

	value	standard deviation	Comments
log beta(fosR)	2.50		fixed
log beta(fos2R)	4.4724	excessive	relative error on beta = 133%

log beta(fos3R) was ignored

8d-HP chemical shifts

nucleus	R	fosR	fos2R
H1	9.4800	12.8756	11.9990
H2	9.0900	12.2900	10.5342
H3	8.4700	8.2716	8.9214