Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

"A Selective Fluorescent Chemosensor for Phosphoserine"

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I. Binding Titrations

Titrations with Zn^{2+}

Sensor **1**

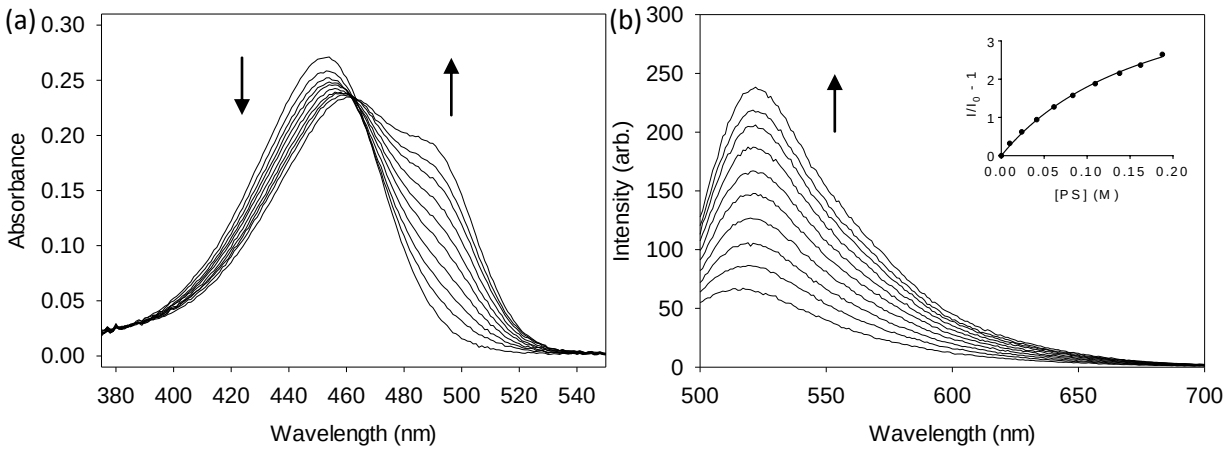


Figure S1. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) and zinc acetate (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM phosphoserine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

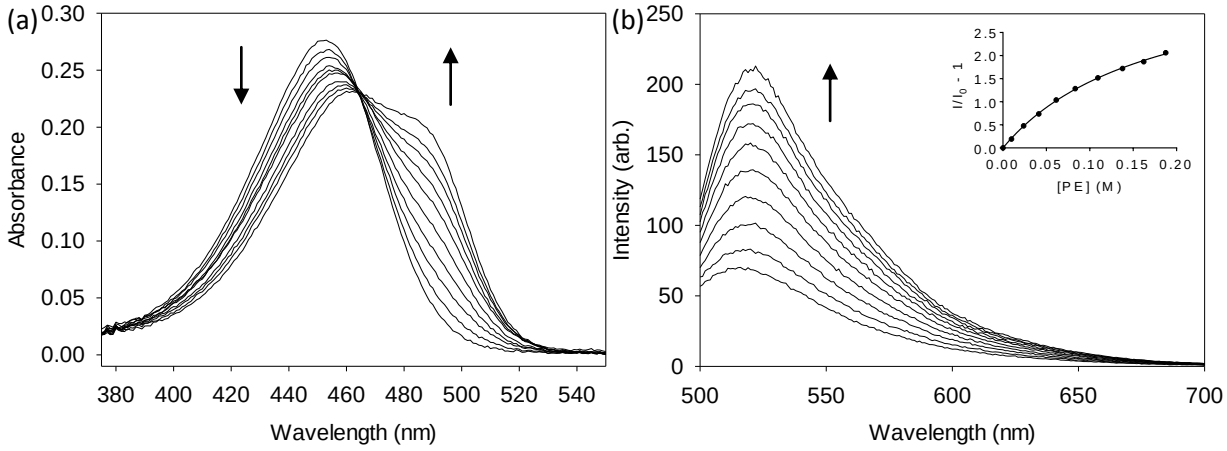


Figure S2. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) and zinc acetate (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM phosphoethanolamine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

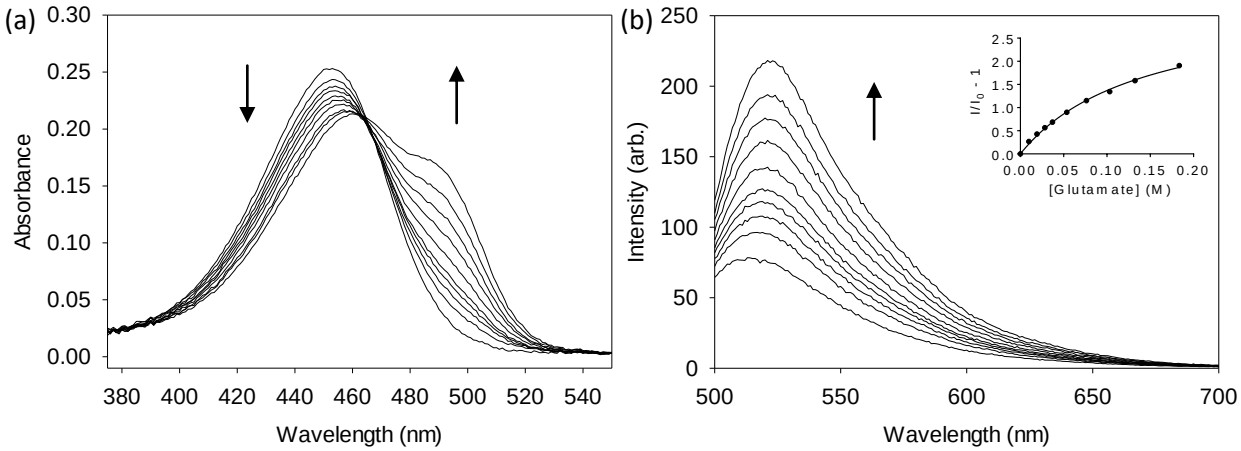


Figure S3. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) and zinc acetate (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM glutamate. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

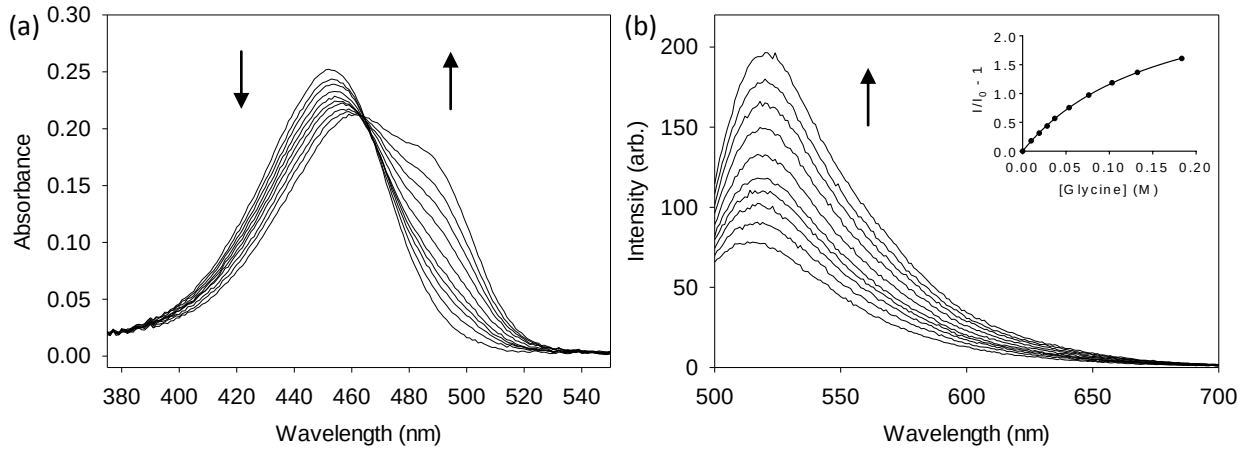


Figure S4. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) and zinc acetate (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM glycine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

Sensor **2**

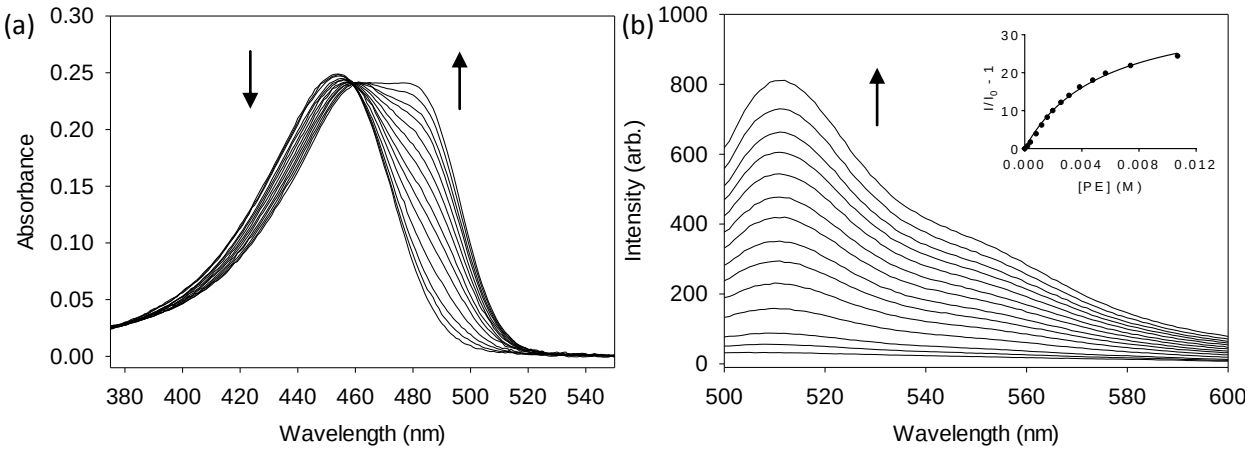


Figure S5. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) and zinc acetate (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 100 mM phosphoethanolamine. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

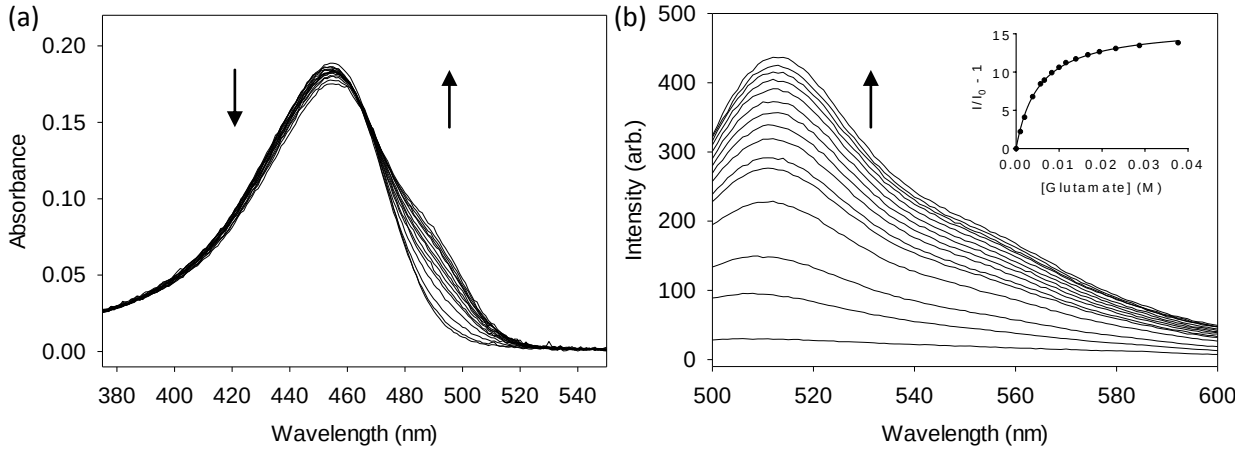


Figure S6. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) and zinc acetate (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M glutamate. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

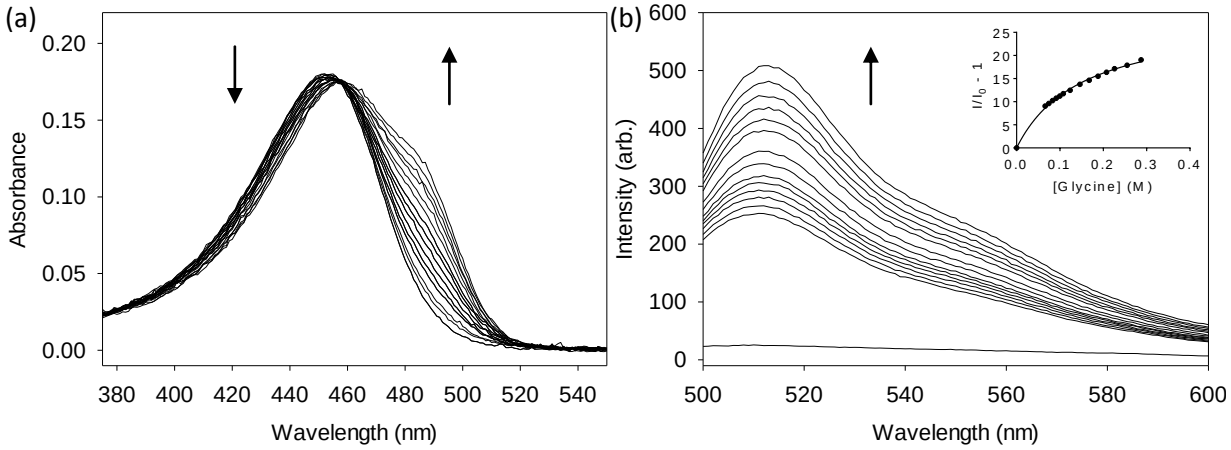


Figure S7. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) and zinc acetate (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M glycine. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

Titrations without Zn^{2+}

Sensor **1**

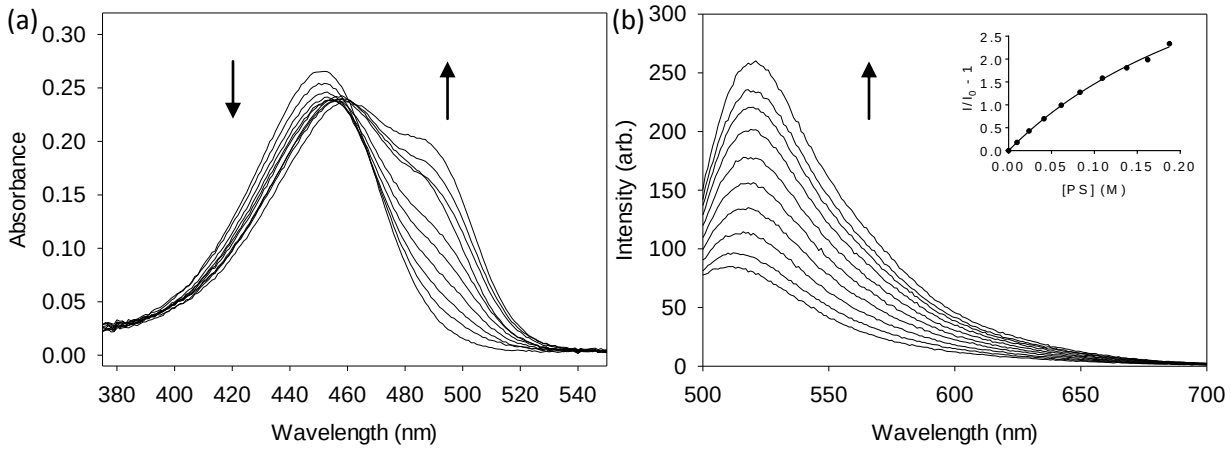


Figure S8. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM phosphoserine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

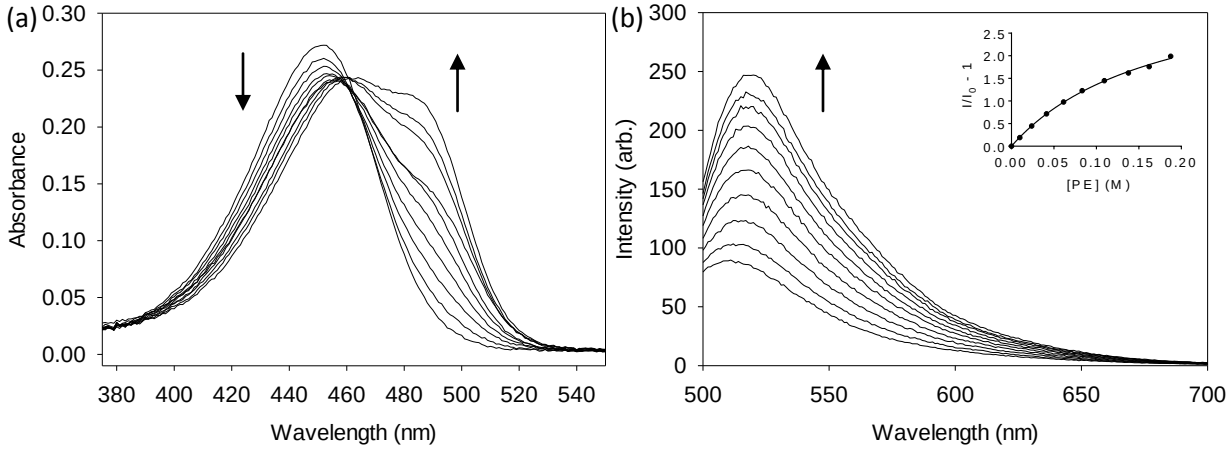


Figure S9. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM phosphoethanolamine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

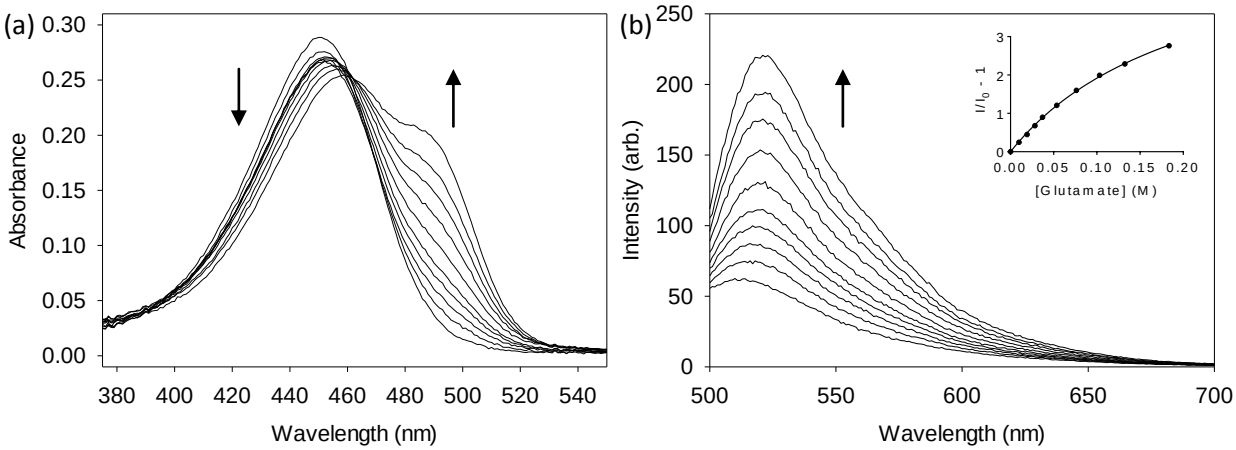


Figure S10. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM glutamate. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

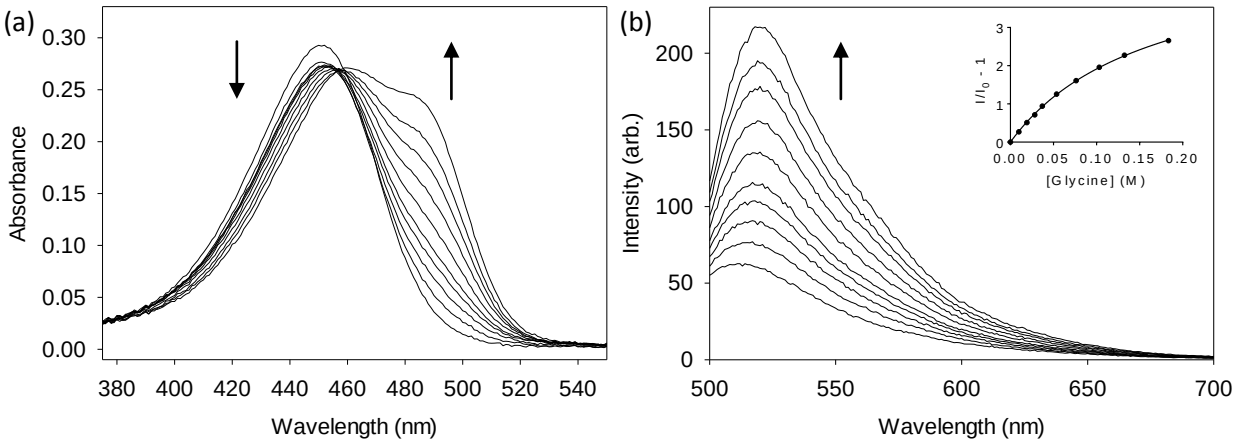


Figure S11. (a) UV/Vis and (b) fluorescence titration of sensor **1** (10 μM) in 3:97 DMSO/buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 500 mM glycine. λ_{em} = 521 nm. Inset is the fit to a binding isotherm.

Sensor **2**

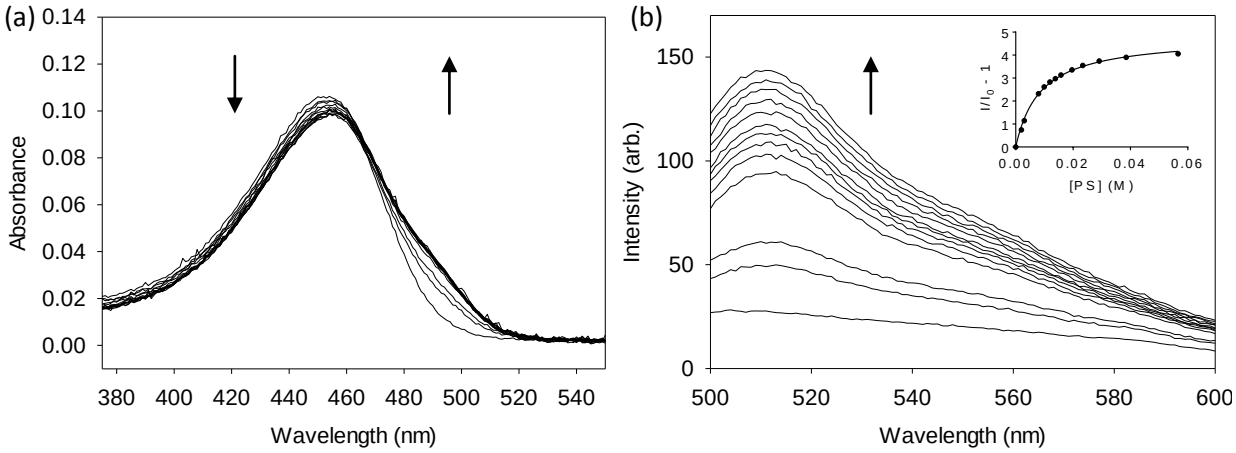


Figure S12. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M phosphoserine. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

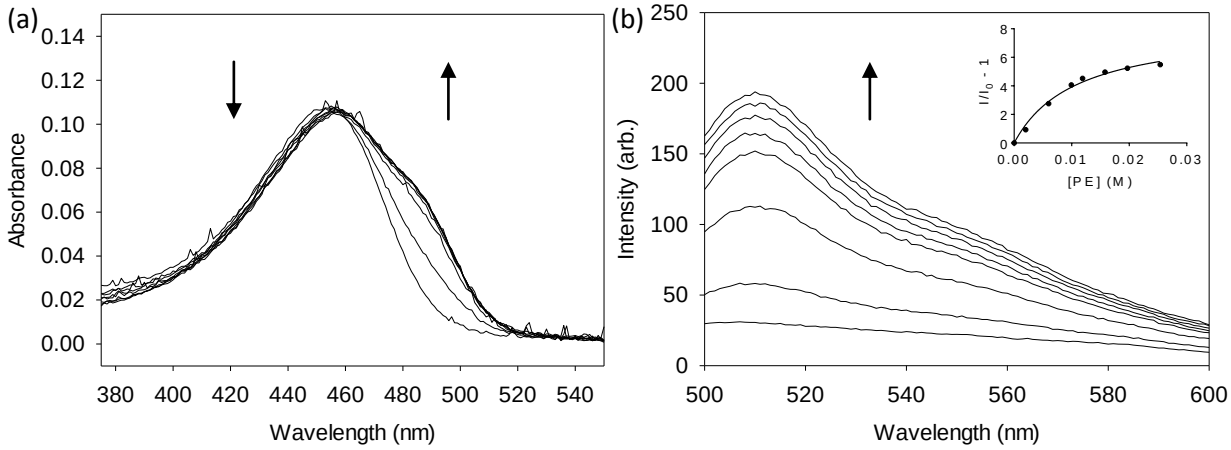


Figure S13. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M phosphoethanolamine. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

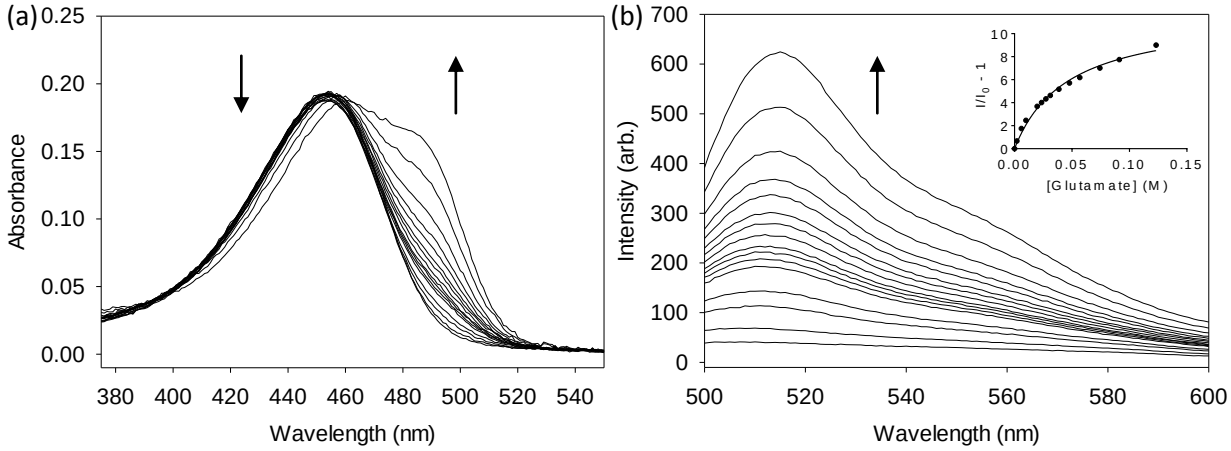


Figure S14. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M glutamate. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

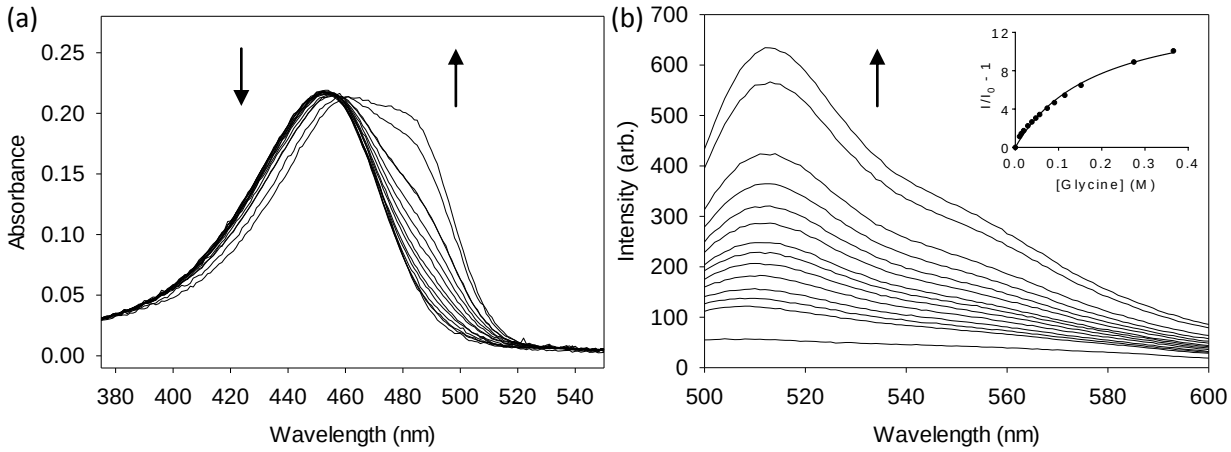
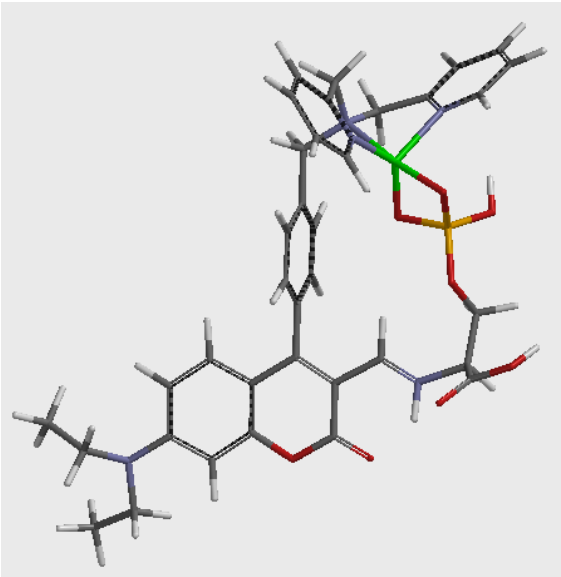


Figure S15. (a) UV/Vis and (b) fluorescence titration of sensor **2** (10 μM) in buffer (50 mM HEPES, 100 mM NaCl, pH 7.4) adding aliquots of 1 M glycine. λ_{em} = 513 nm. Inset is the fit to a binding isotherm.

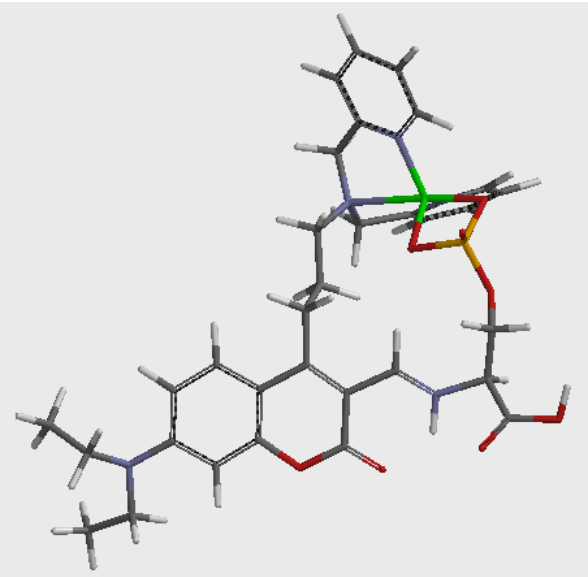
II. Molecular Modeling

Models were constructed using Spartan '10.

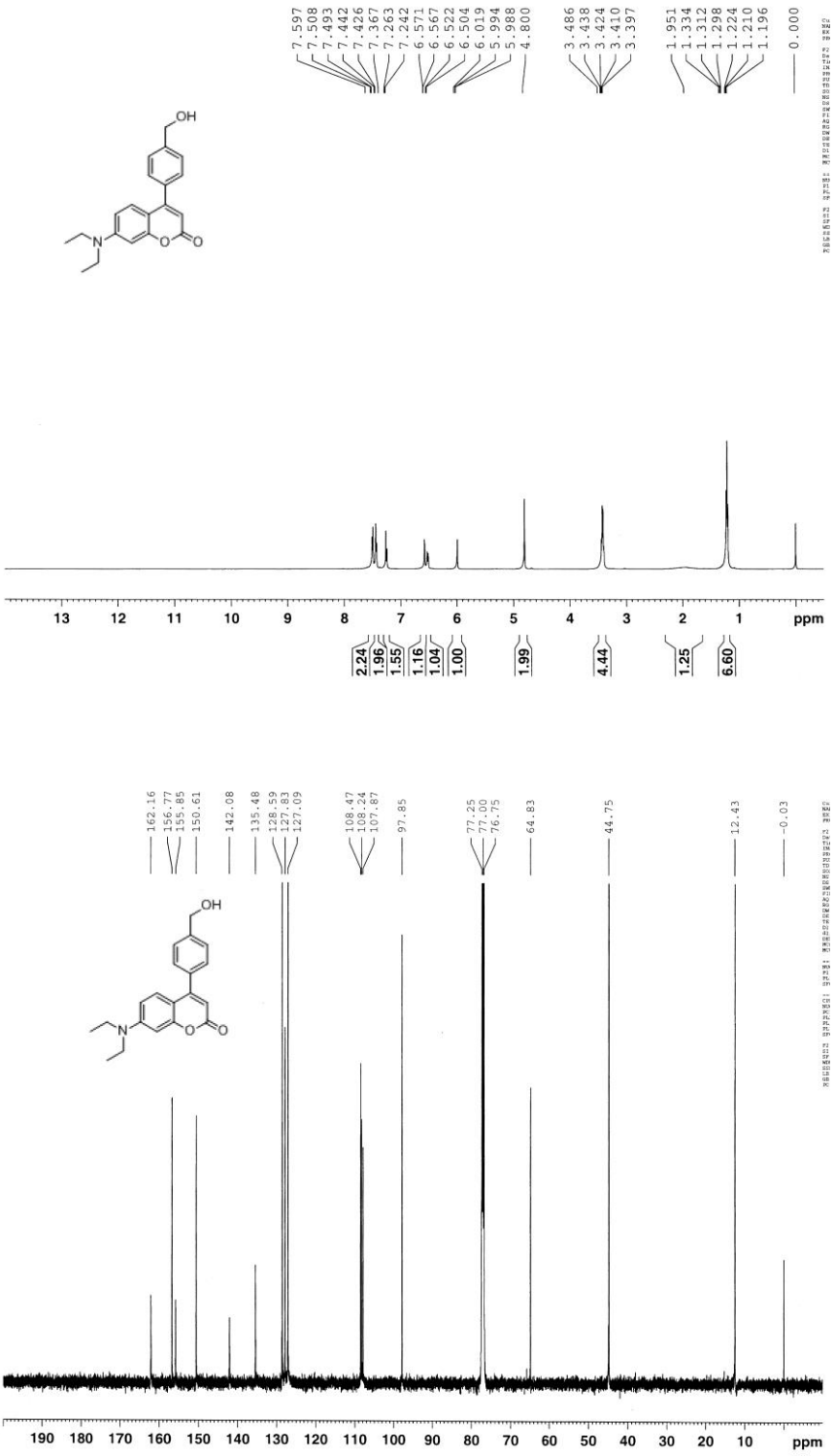
Sensor **1** + phosphoserine

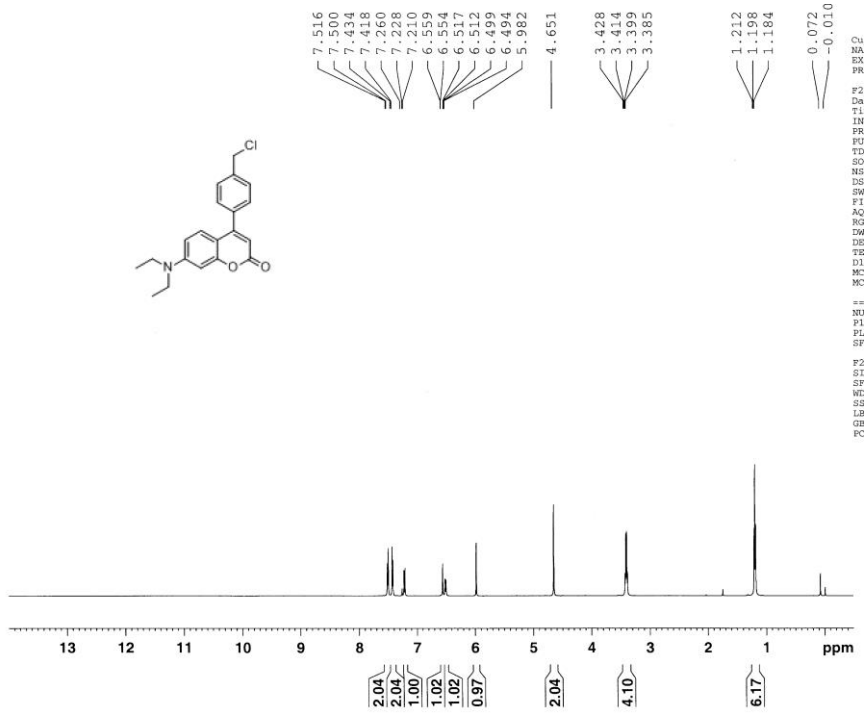


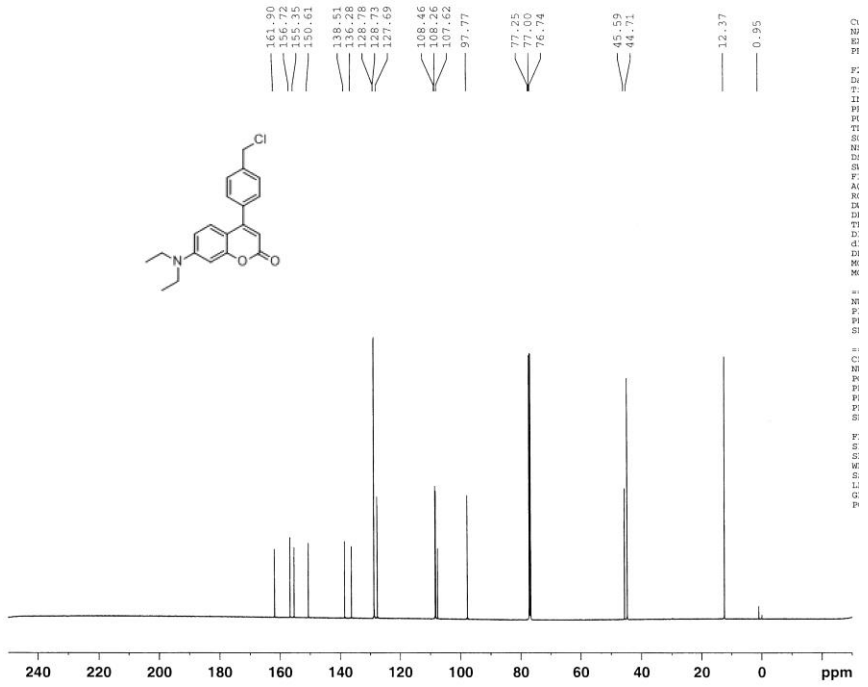
Sensor **2** + phosphoserine

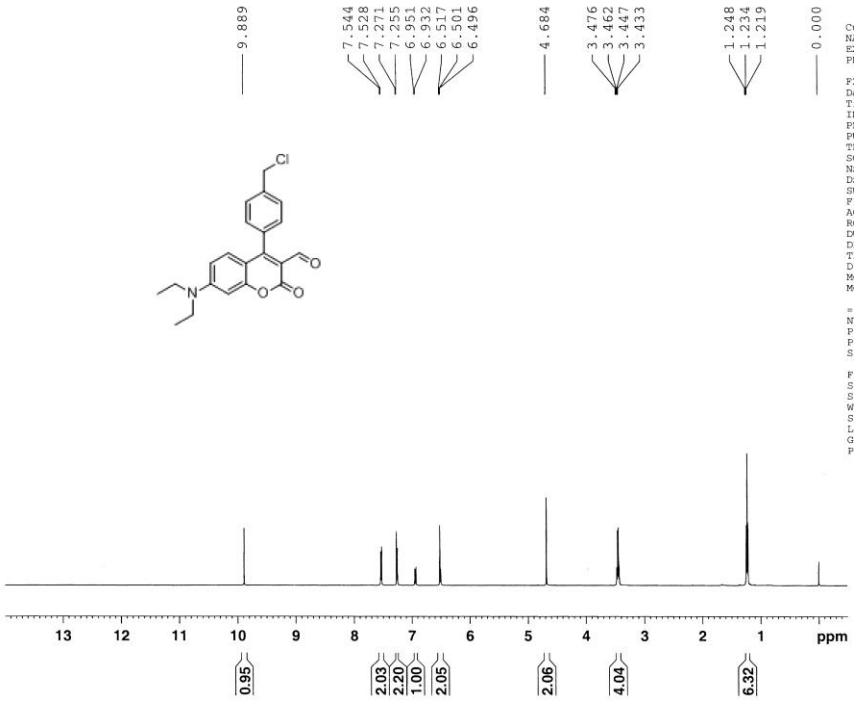


III. NMR Spectra





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7.271
7.255
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6.501
6.496
4.684
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3.462
3.447
3.433
1.248
1.234
1.219
0.000
Cl
O
N
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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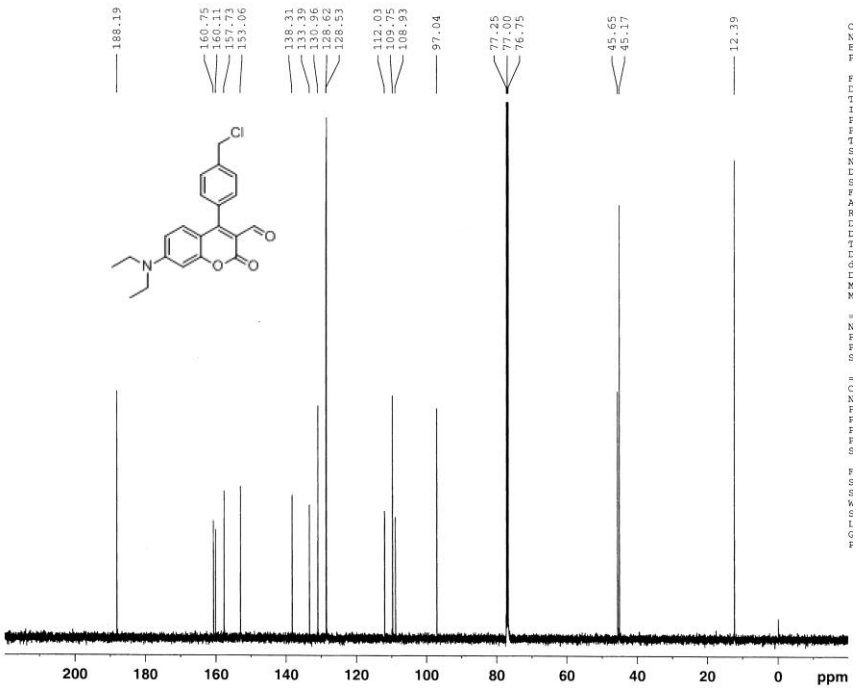
2.03
2.20
1.00
2.05
2.06
4.04
6.32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160.11
157.73
153.06
138.31
133.39
130.96
128.62
128.53
112.03
109.75
108.93
97.04
77.25
77.00
76.75
45.65
45.17
12.39
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N
O
O
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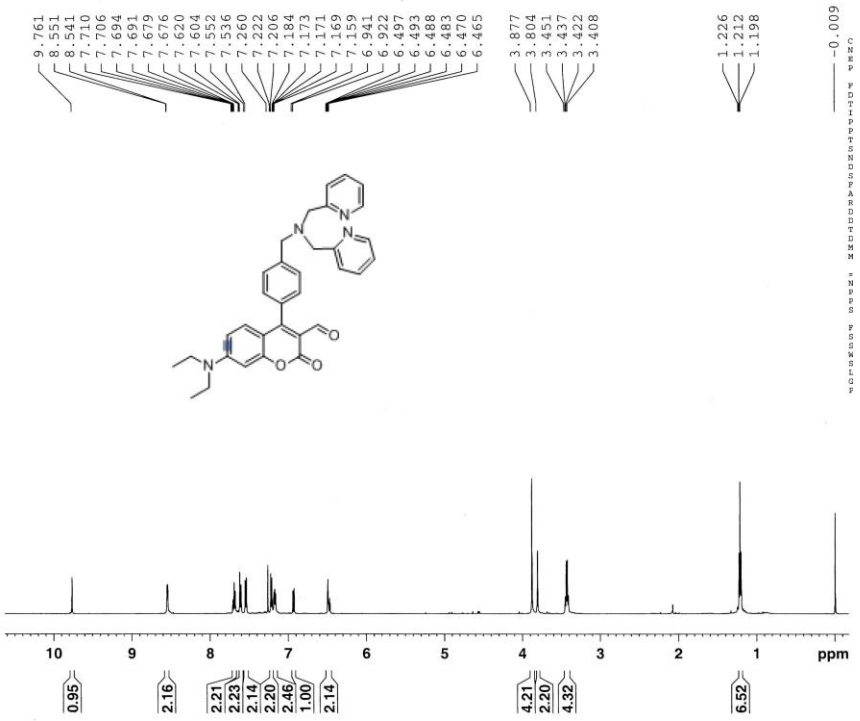
140
120
100
80
60
40
20
0
ppm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7.536
7.260
7.222
7.206
7.184
7.173
7.171
7.169
7.159
6.941
6.922
6.497
6.493
6.488
6.483
6.470
6.465
3.877
3.804
3.451
3.437
3.422
3.408
1.226
1.212
1.198
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10
9
8
7
6
5
4
3
2
1
ppm
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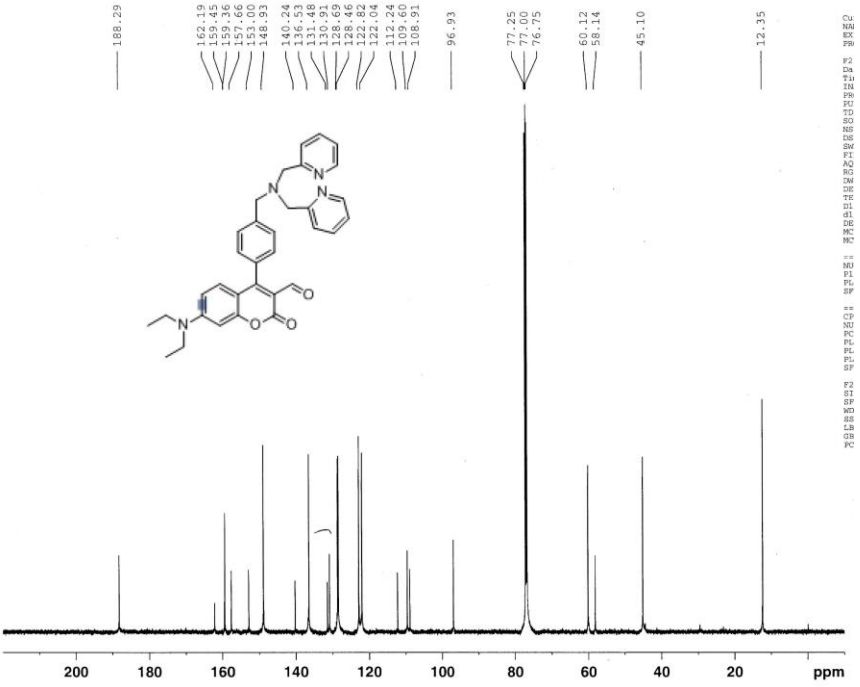
2.14
4.21
2.20
4.32
6.52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153.00
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122.82
122.04
112.24
109.60
108.91
96.93
77.25
77.00
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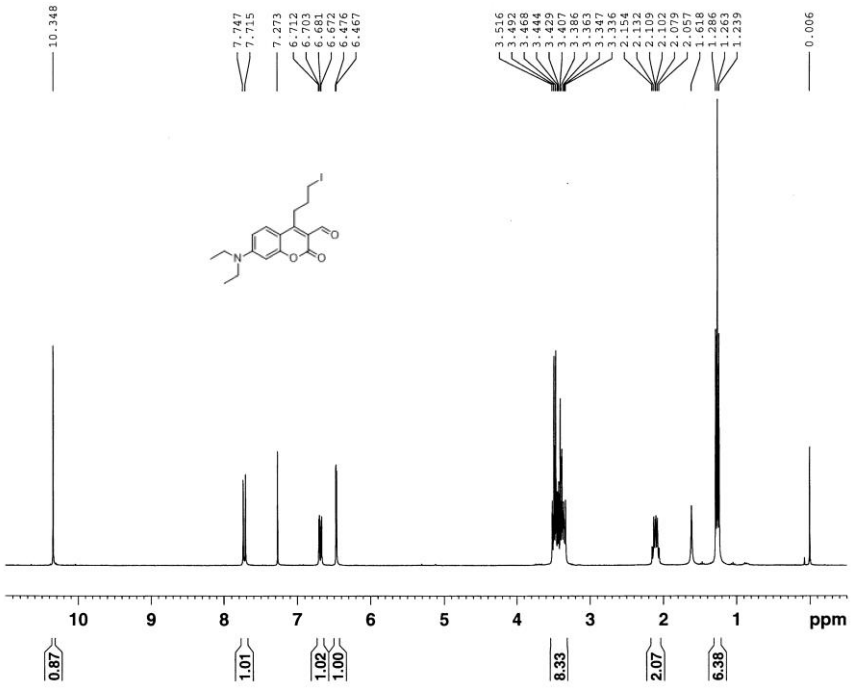
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3.468
3.444
3.429
3.407
3.386
3.363
3.347
3.336
2.154
2.132
2.109
2.102
2.079
2.057
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1.286
1.263
1.239
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9
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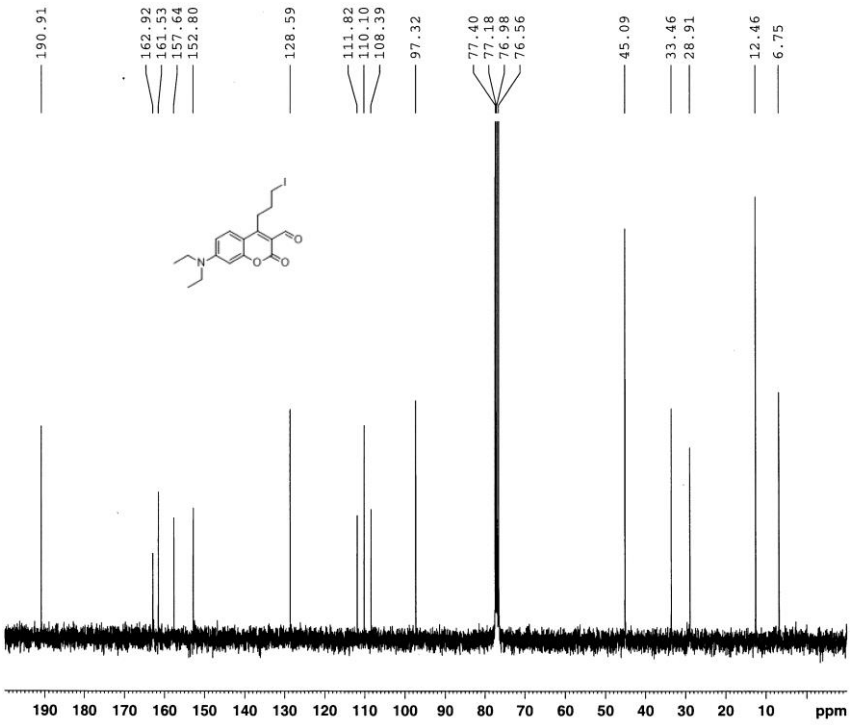
6.38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76.56
45.09
33.46
28.91
12.46
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30
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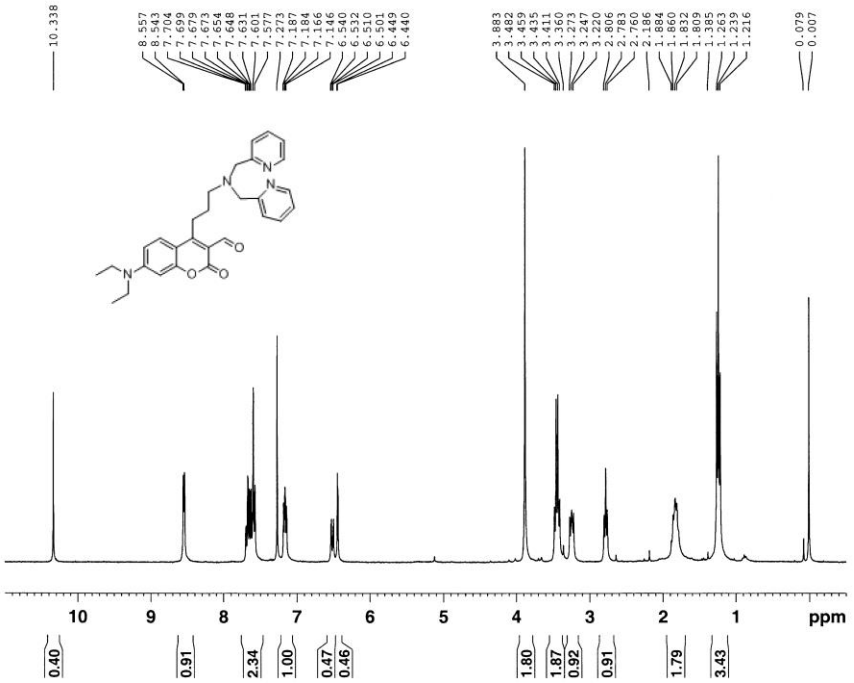
10
ppm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7.184
7.166
7.146
6.540
6.532
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6.501
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3.482
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3.360
3.273
3.247
3.220
2.806
2.783
2.760
2.186
2.164
1.860
1.832
1.809
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10
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8
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4
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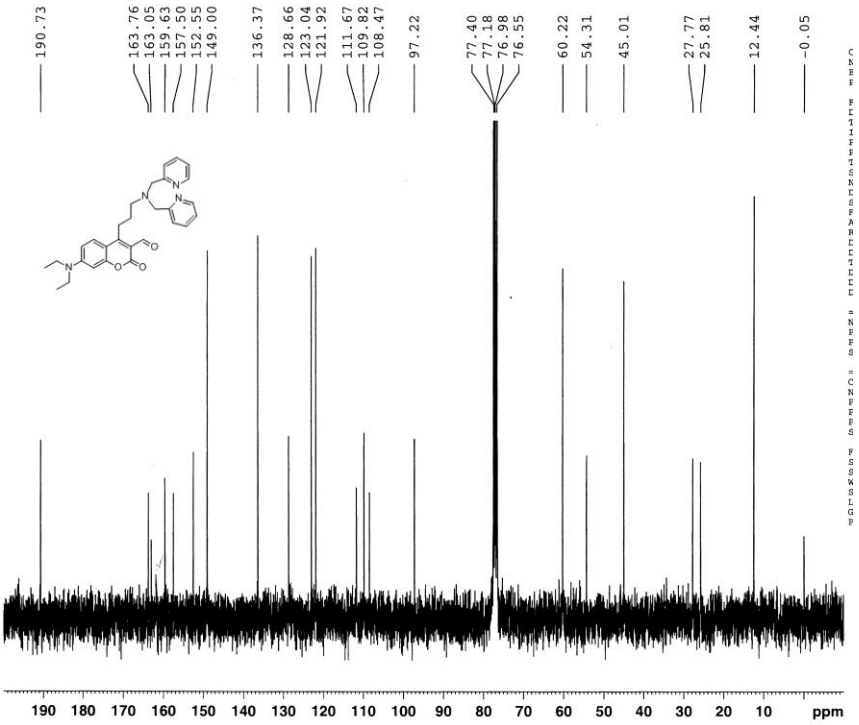
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97.22
77.40
77.18
76.98
76.55
60.22
54.31
45.01
27.77
25.81
12.44
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180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm