Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2017

Electronic Supplementary Information

Sensitive and selective ratiometric fluorescent detection of monosaccharides in aqueous solutions at physiological pH using self-assembled peptides with different aromatic side chains

Lok Nath Neupane, Pramod Kumar Mehta and Keun-Hyeung Lee*

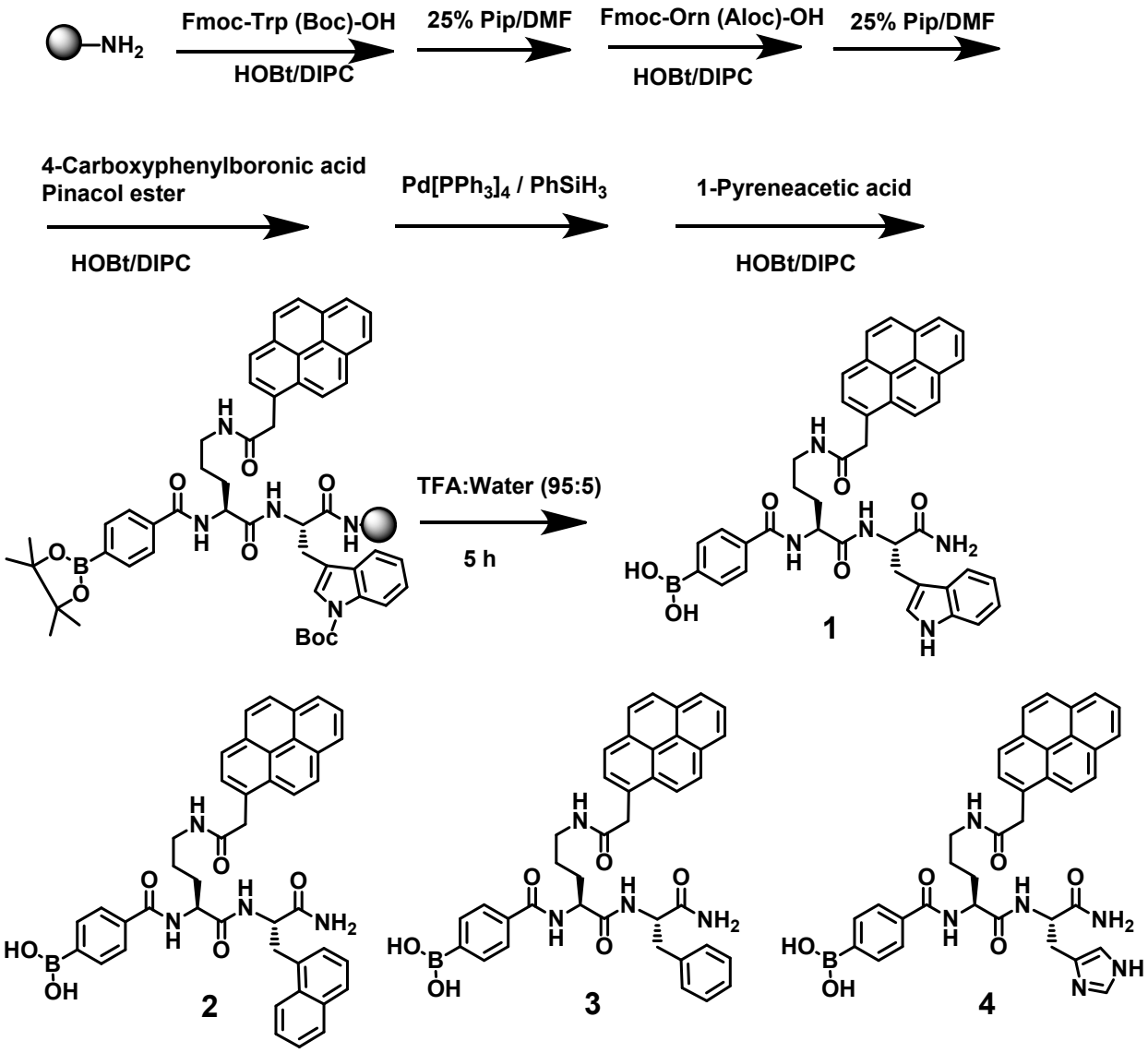
Bioorganic Chemistry Laboratory, Center for Design and Applications of Molecular Catalysts, Department of Chemistry and Chemical Engineering, Inha University, Incheon 402-751, South Korea

E-mail:leekh@inha.ac.kr

Contents:

Scheme S1. Synthesis scheme	S3
Figure S1. HPLC Chromatogram of **1**	S4
Figure S2. ESI-mass spectrum of **1**	S5
Figure S3. ^{1}H NMR of **1**	S6
Figure S4. ^{13}C NMR of **1**	S7
Figure S5. Elemental analysis of **1**	S8
Figure S6. HPLC Chromatogram of **2**	S9
Figure S7. ESI-mass spectrum of **2**	S10
Figure S8. ^{1}H NMR of **2**	S11
Figure S9. ^{13}C NMR of **2**	S12
Figure S10. Elemental analysis of **2**	S13
Figure S11. HPLC Chromatogram of **3**	S14
Figure S12. ESI-mass spectrum of **3**	S15
Figure S13. ^{1}H NMR of **3**	S16
Figure S14. ^{13}C NMR of **3**	S17
Figure S15. Elemental analysis of **3**	S18
Figure S16. HPLC Chromatogram of **4**	S19
Figure S17. ESI-mass spectrum of **4**	S20
Figure S18. ^{1}H NMR of **4**	S21

Figure S19. ^{13}C NMR of **4** S22
Figure S20. Elemental analysis of **4** S23
Figure S21. Fluorescence emission spectra of **3** and **4** in different percentage of DMSO S24
Figure S22. Fluorescence spectra and intensity correlation function of **1**-**4** for particle size analysis S25
Figure S23. UV-vis absorbance spectra of **1-4** in different percentage of DMSO S26
Figure S24. Fluorescence spectra of **1** in the presence of D-glucose and D-galactose S27
Figure S25. Fluorescence emission spectra of **2** in the presence of D-glucose and D-galactose S28
Figure S26. Fluorescence emission spectra of **3** in the presence of D-glucose and D-galactose S29
Figure S27. Fluorescence emission spectra of **4** in the presence of D-glucose and D-galactose S30
Figure S28. UV-visible absorption spectra of **1-4** in the presence of D-fructose S31
Figure S29. Fluorescence spectra and intensity correlation function of **1**-**4** in the presence of D-Fructose for particle size analysis S32
Figure S30. Fluorescence spectra of **2** in the presence of pinanediol S33
Figure S31. UV-visible absorption spectra of **1**-**3** in the presence of pinanediol S34
Figure S32. Fluorescence spectra and UV-visible absorption spectra of **4** in the presence of pinanediol S35
Figure S33. Fluorescence spectra and intensity correlation function of **1-4** in the presence of pinanediol S36
Figure S34. ESI mass of **1** in the presence of D-fructose S37
Figure S35. ESI mass of **2** in the presence of D-fructose S38
Figure S36. Fitting curve of **1**–**4** in the presence of monosaccharides S39
Figure S37. Fitting curve of **1**–**4** in the presence of pinanediol S40
Figure S38. Linear intensity ratio change of **1**–**4** in the presence of D-Fructose S41



Scheme S1. Synthesis scheme of **1–4.**

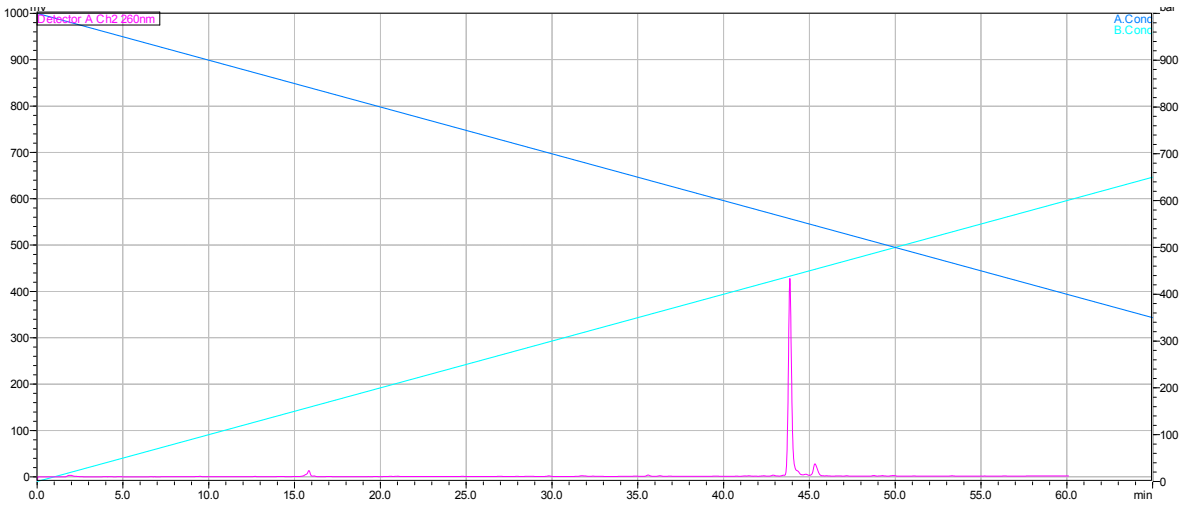


Figure S1. HPLC chromatogram of **1.**

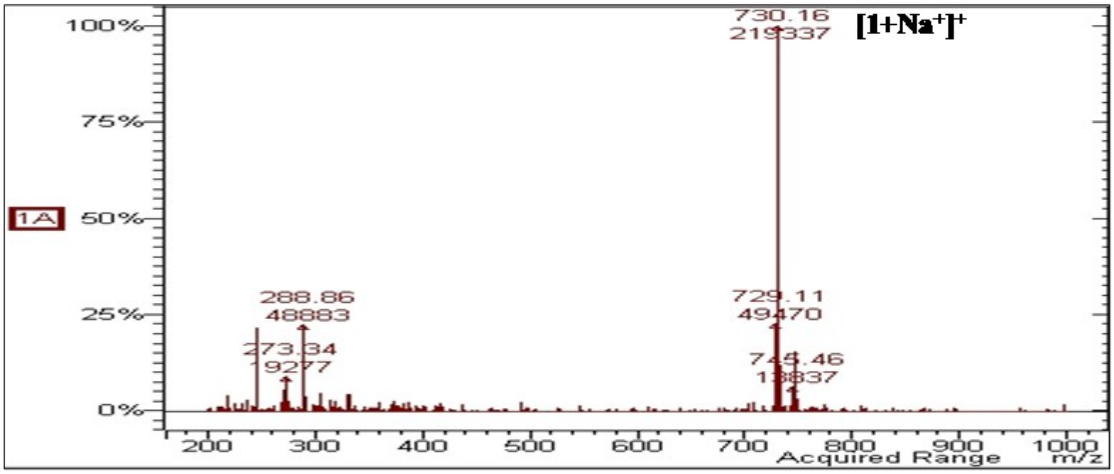


Figure S2. ESI-Mass spectrum of **1.**

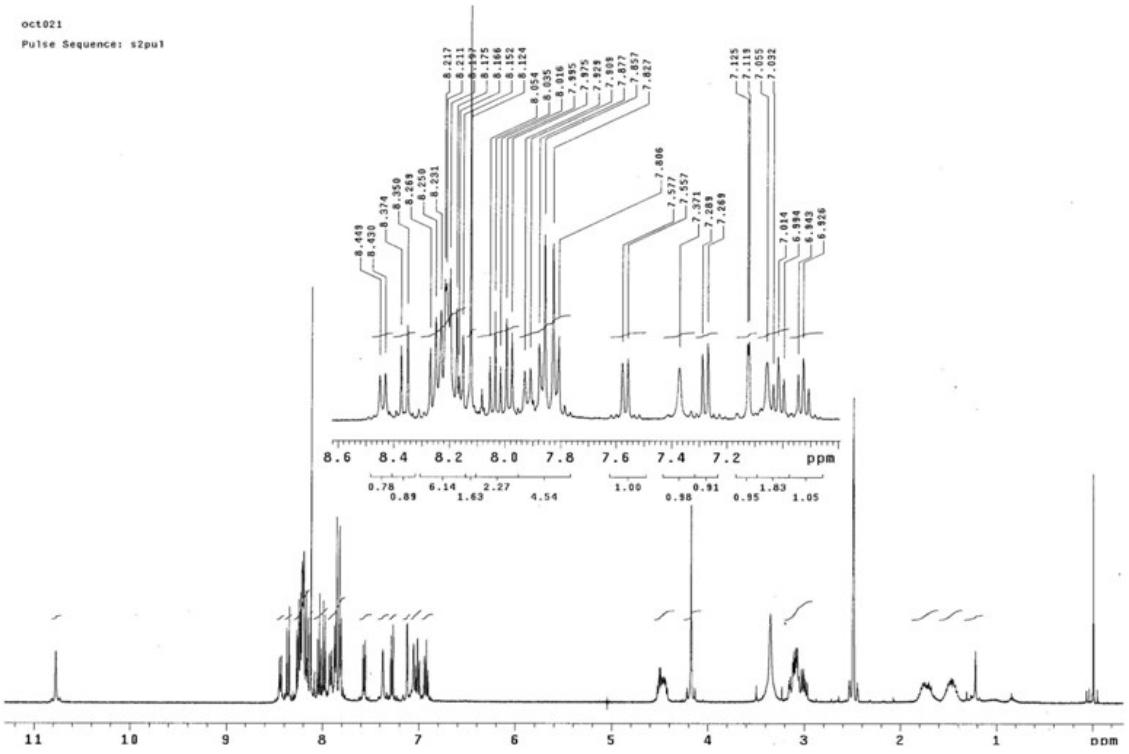


Figure S3. ^{1}H NMR of **1.**

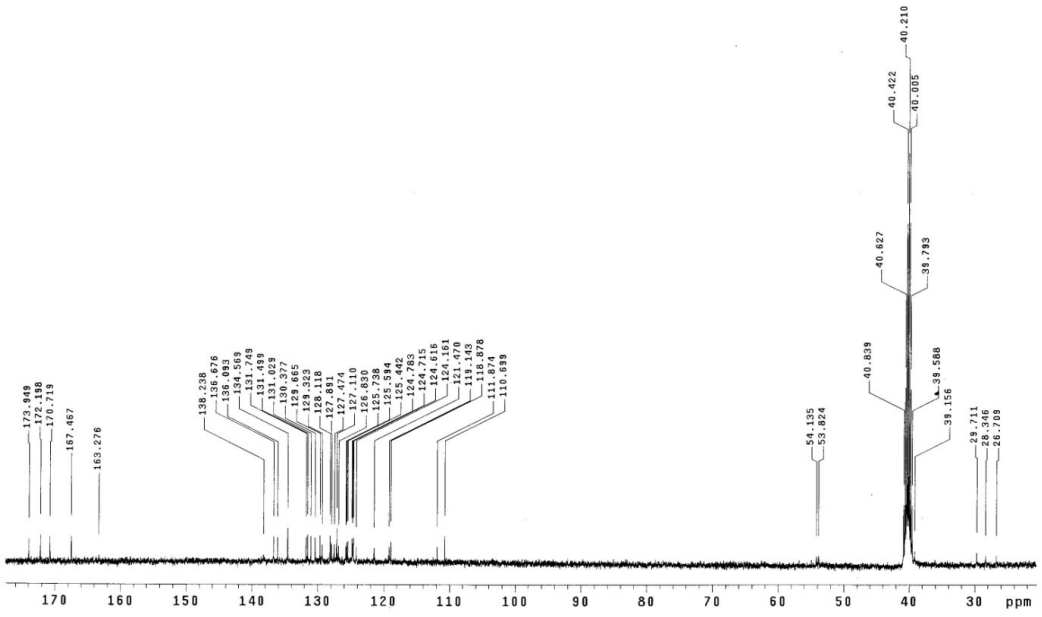
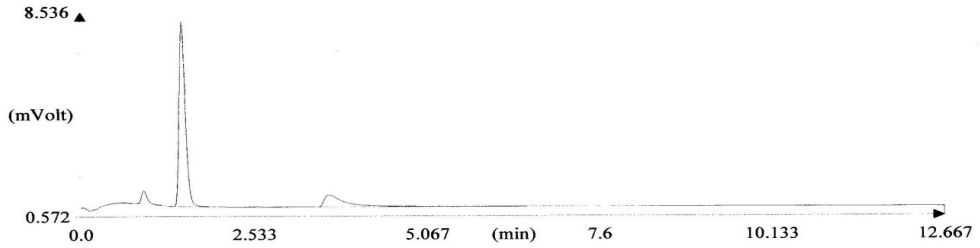


Figure S4. ^{13}C NMR of **1.**



Operator ID:
Company name: ThermoFinnigan
Method filename: C:\Program Files\Thermo Electron\Eager 300 for EA1112\원소분석기2\2012\chns\20130111.
Method name: NCHS
Analysed: 2013-01-10 16:56
Printed: 2013-01-14 14:53
Elemental Analyser method:
Sampler method:
Sample ID: BOPW (# 16)
Analysis type: UnkNown
Chromatogram filename: S192.dat
Calibration method: K Factors
Sample weight: .141
Protein factor: 6.25

Element Name		Ret.Time	Area	BC	Area ratio	K f
Nitrogen	10.7560	55	30620	RS	14.851270	.201
Carbon	66.0790	88	454739	RS	1.000000	.481
Hydrogen	5.1169	218	111096	RS	4.093203	.146
Totals	81.9519		596454			

Figure S5. Elemental analysis of **1.**

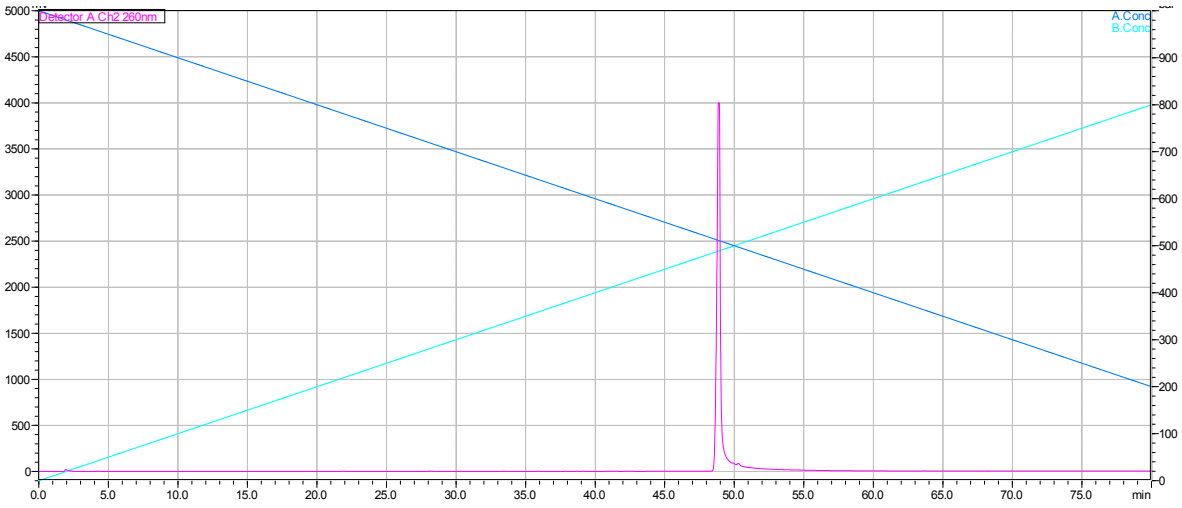


Figure S6. HPLC Chromatogram of **2.**

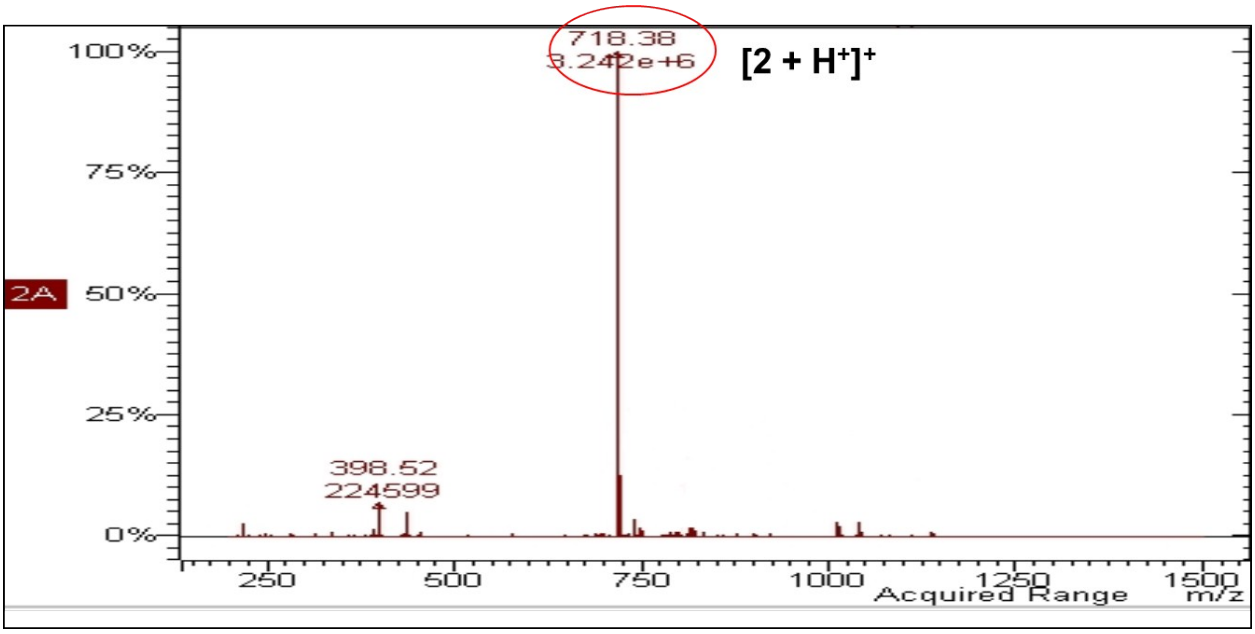


Figure S7. ESI-Mass spectrum of **2.**

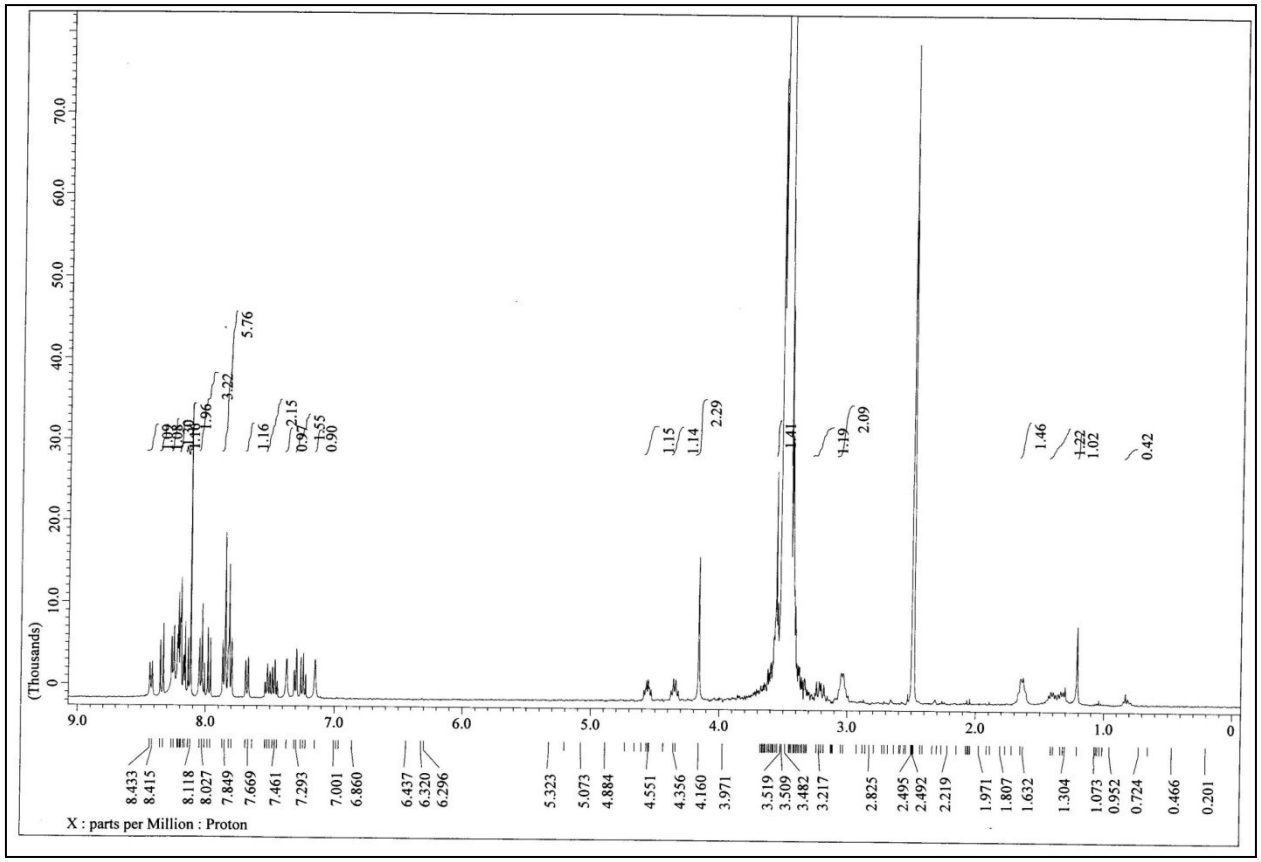


Figure S8. ^{1}H NMR of **2.**

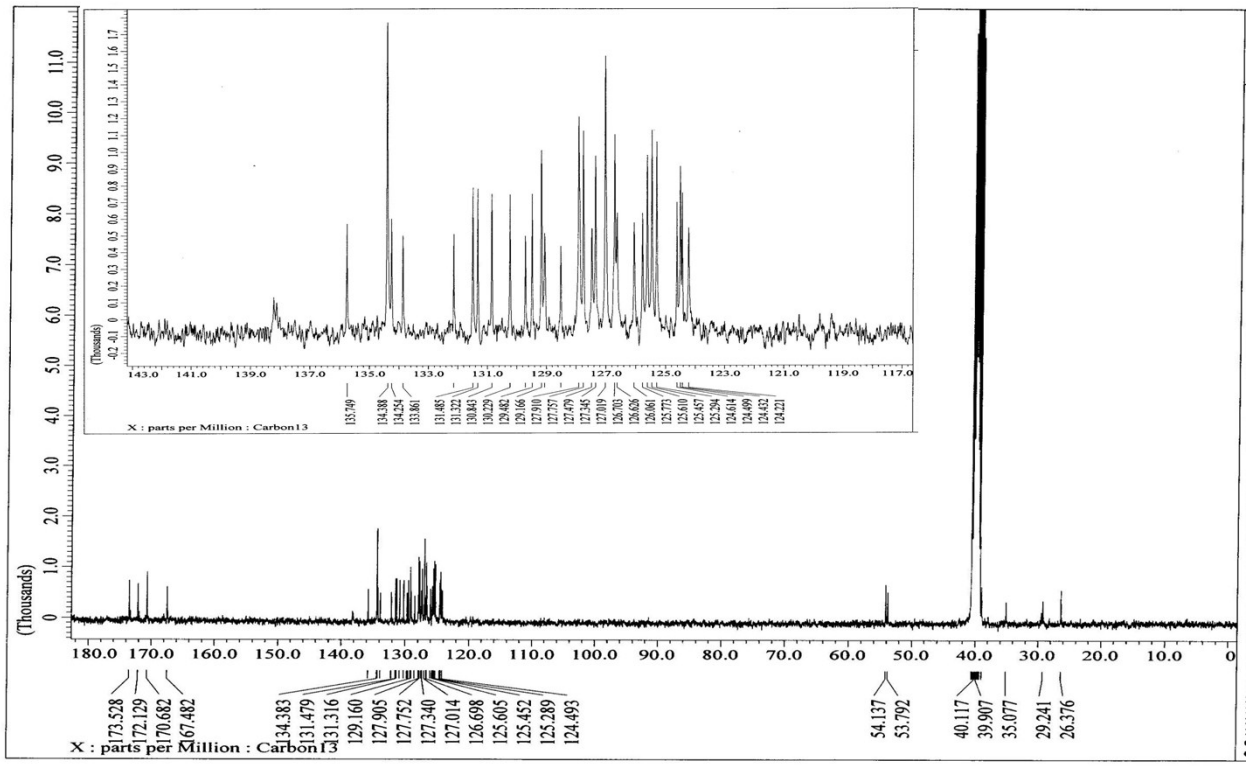
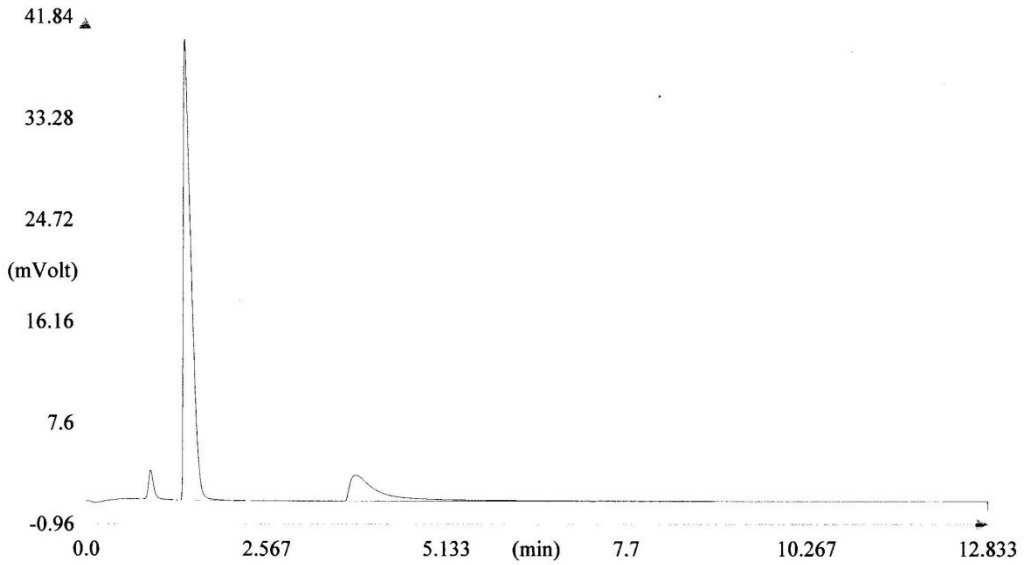


Figure S9. ^{13}C NMR of **2.**



Operator ID:	
Company name:	ThermoFinnigan
Method filename:	E:\Eager for FLASH\INHA\NCHS\N C H S system 151021.mth
Method name:	NCHS
Analysed:	2015-10-29 15:30
Printed:	2015-10-30 13:44
Elemental Analyser method:	
Sampler method:	
Sample ID:	BOPNaI (# 22)
Analysis type:	UnkNown
Chromatogram filename:	Q133.dat
Calibration method:	K Factors
Sample weight:	.85
Protein factor:	6.25

Element Name	Ret.Time	Area	BC	Area rati
Nitrogen	7.3703	55	125076 RS	23.3957
Carbon	70.6648	85	2926244 RS	1.0000
Hydrogen	5.5180	231	685209 RS	4.2705
Totals	83.5531		3736529	

Figure S10. Elemental analysis of **2.**

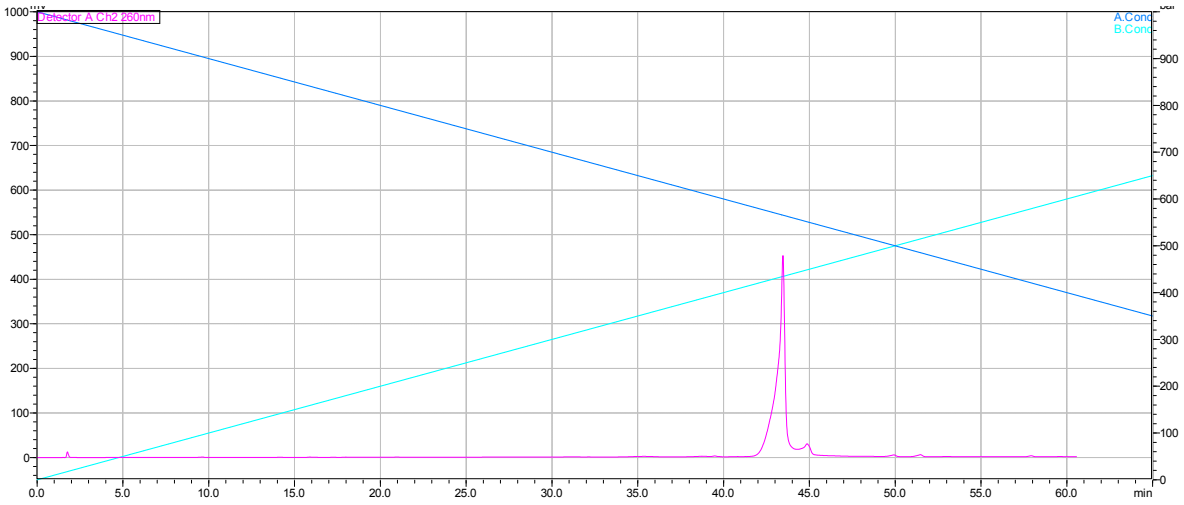


Figure S11. HPLC Chromatogram of **3.**

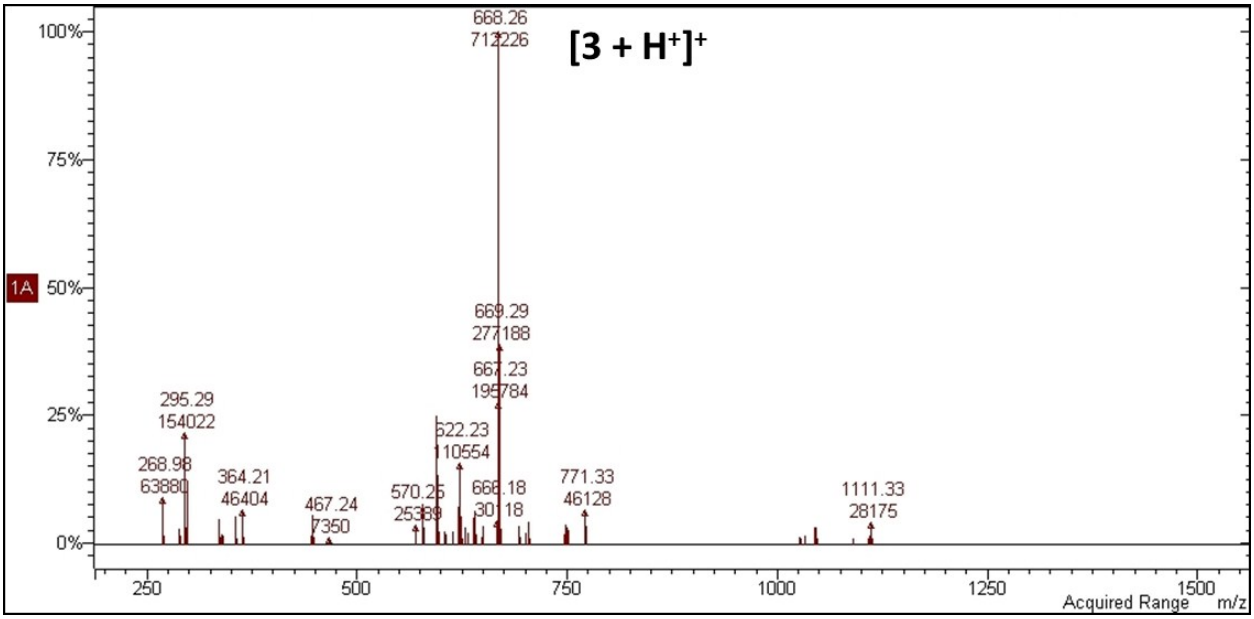


Figure S12. ESI-Mass spectrum of **3.**

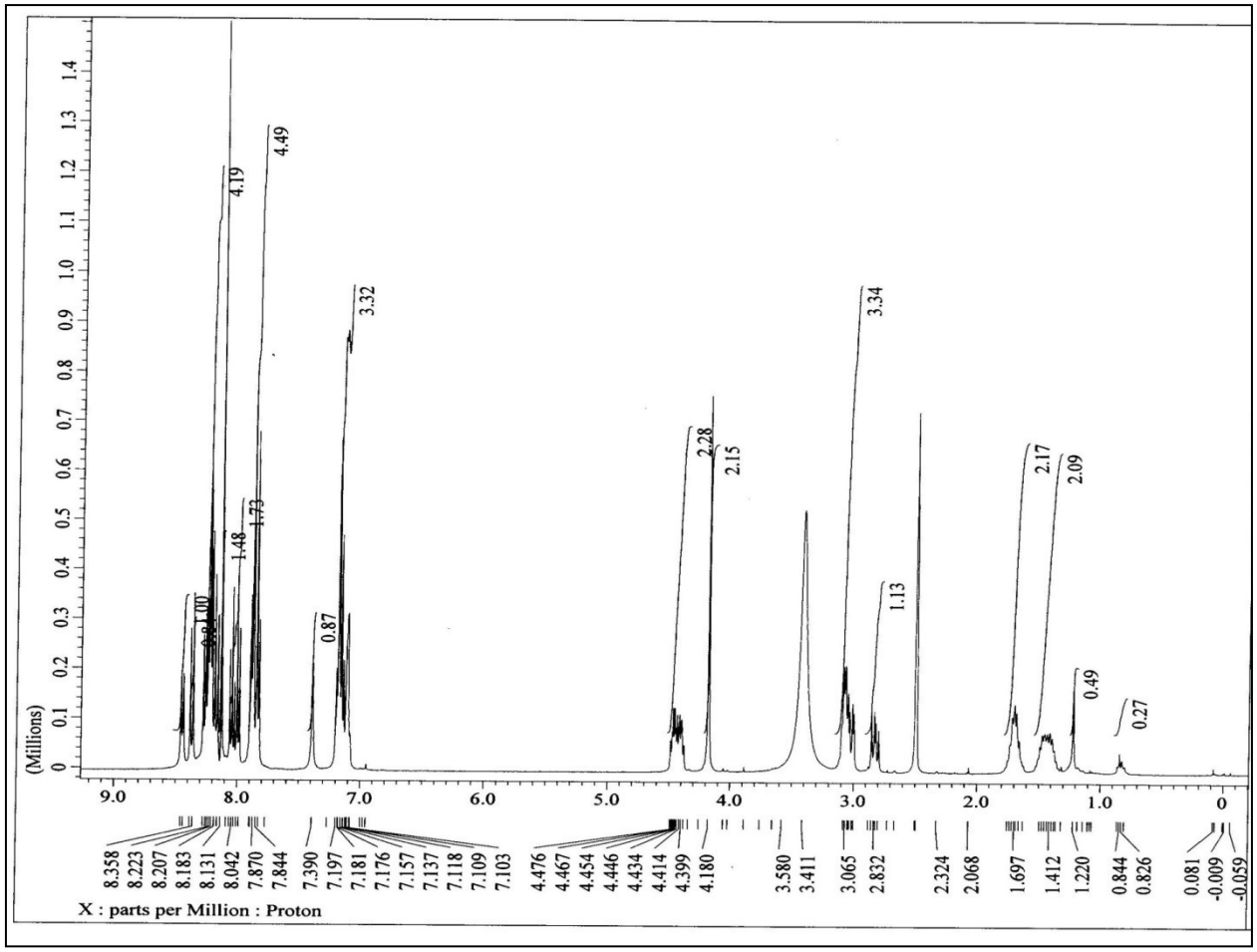


Figure S13. ^{1}H NMR of **3.**

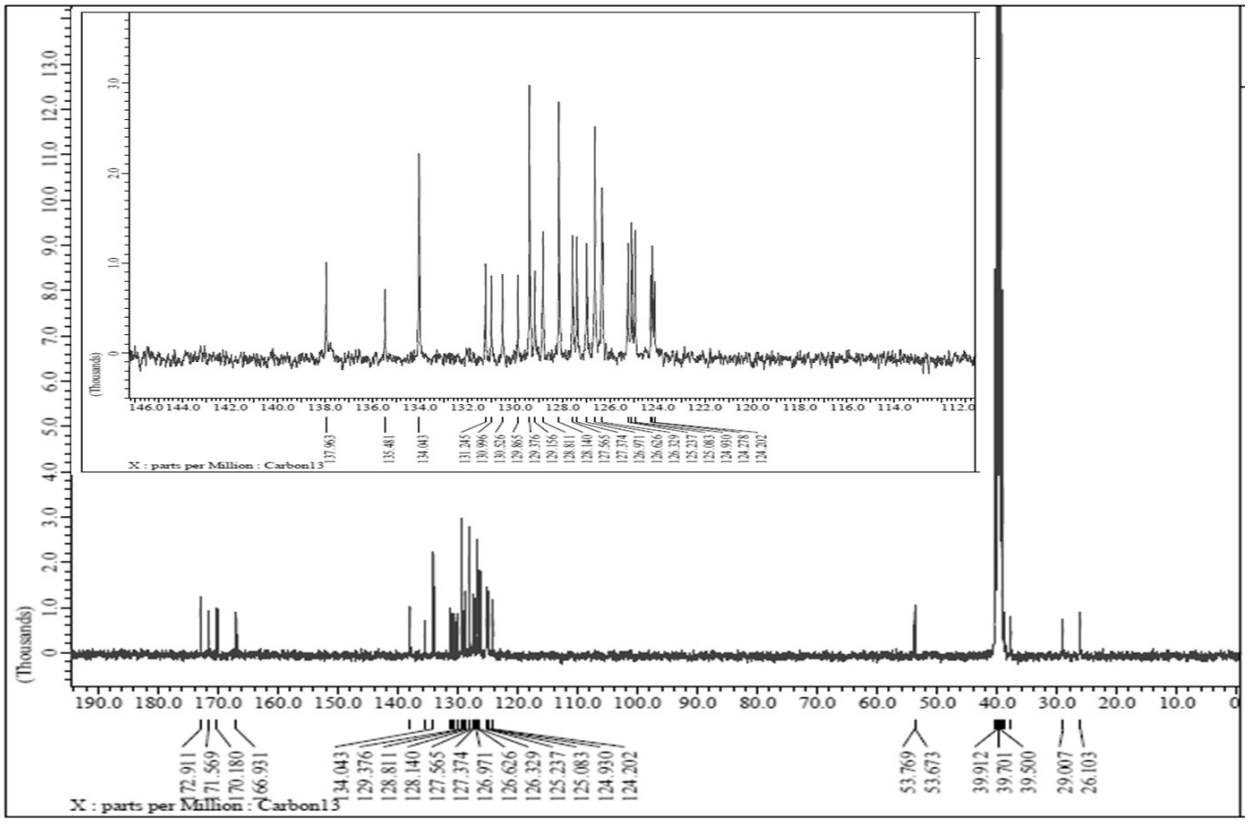
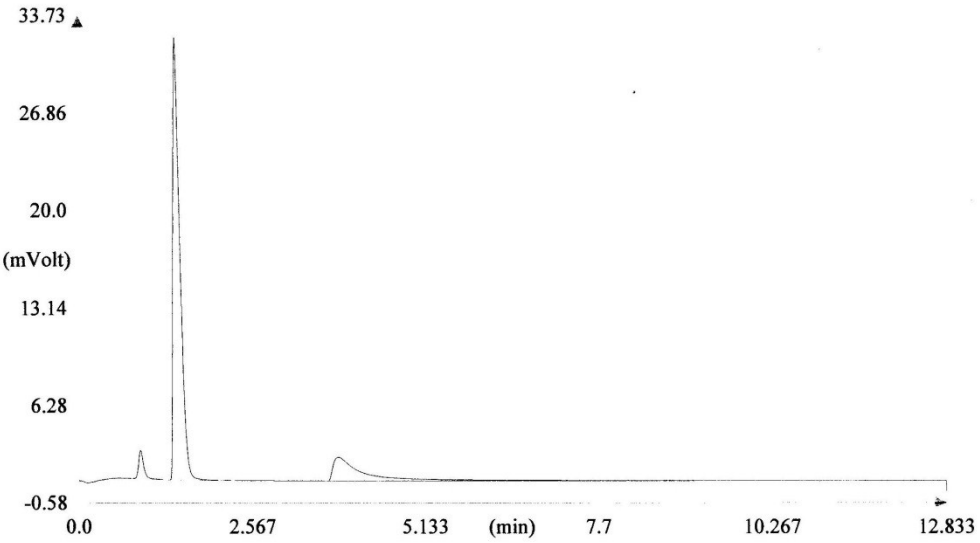


Figure S14. ^{13}C NMR of **3.**



Operator ID:	
Company name:	ThermoFinnigan
Method filename:	E:\Eager for FLASH\INHA\NCHS\N C H S system 151021.mth
Method name:	NCHS
Analysed:	2015-10-29 15:43
Printed:	2015-10-30 13:44
Elemental Analyser method:	
Sampler method:	
Sample ID:	BOPF (# 23)
Analysis type:	UnkNown
Chromatogram filename:	Q134.dat
Calibration method:	K Factors
Sample weight:	.665
Protein factor:	6.25

Element Name	Ret.Time	Area	BC	Area rati
Nitrogen	7.8835	55 105239	RS	20.9970
Carbon	68.1799	85 2209710	RS	1.0000
Hydrogen	5.5325	230 537481	RS	4.1112
Totals	81.5959	2852430		

Figure S15. Elemental analysis of **3.**

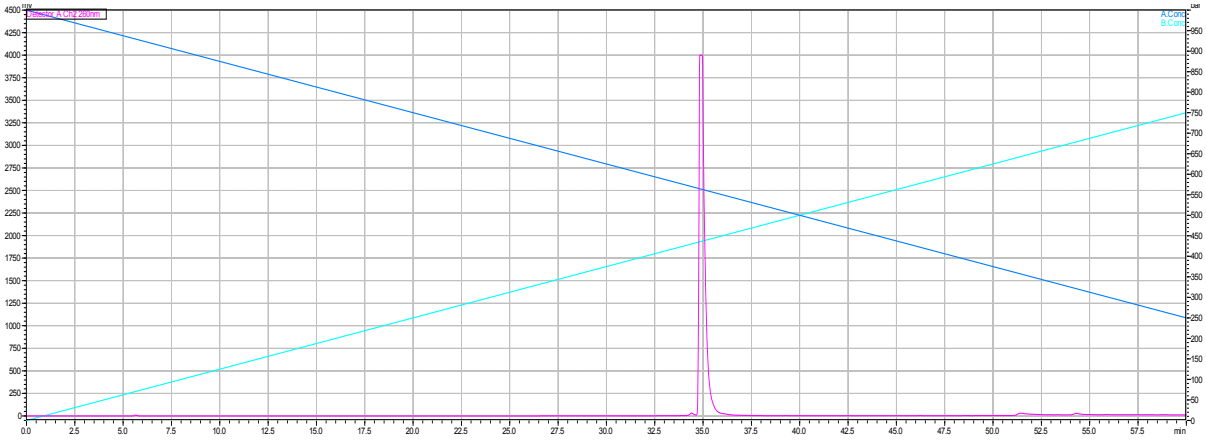


Figure S16. HPLC Chromatogram of **4.**

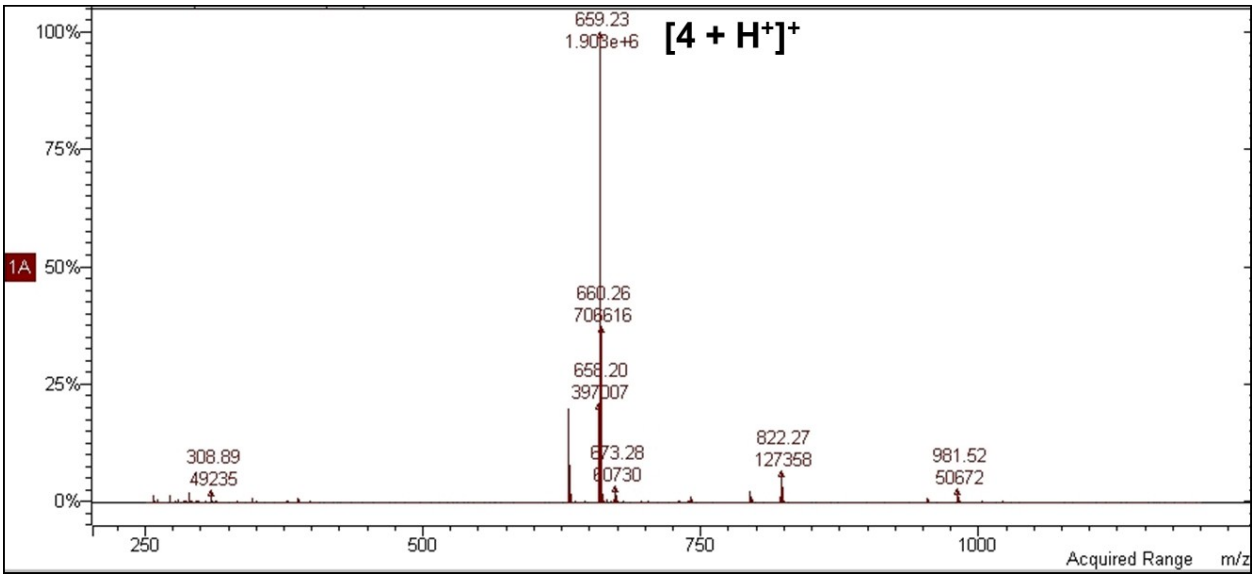


Figure S17. ESI-Mass spectrum of **4.**

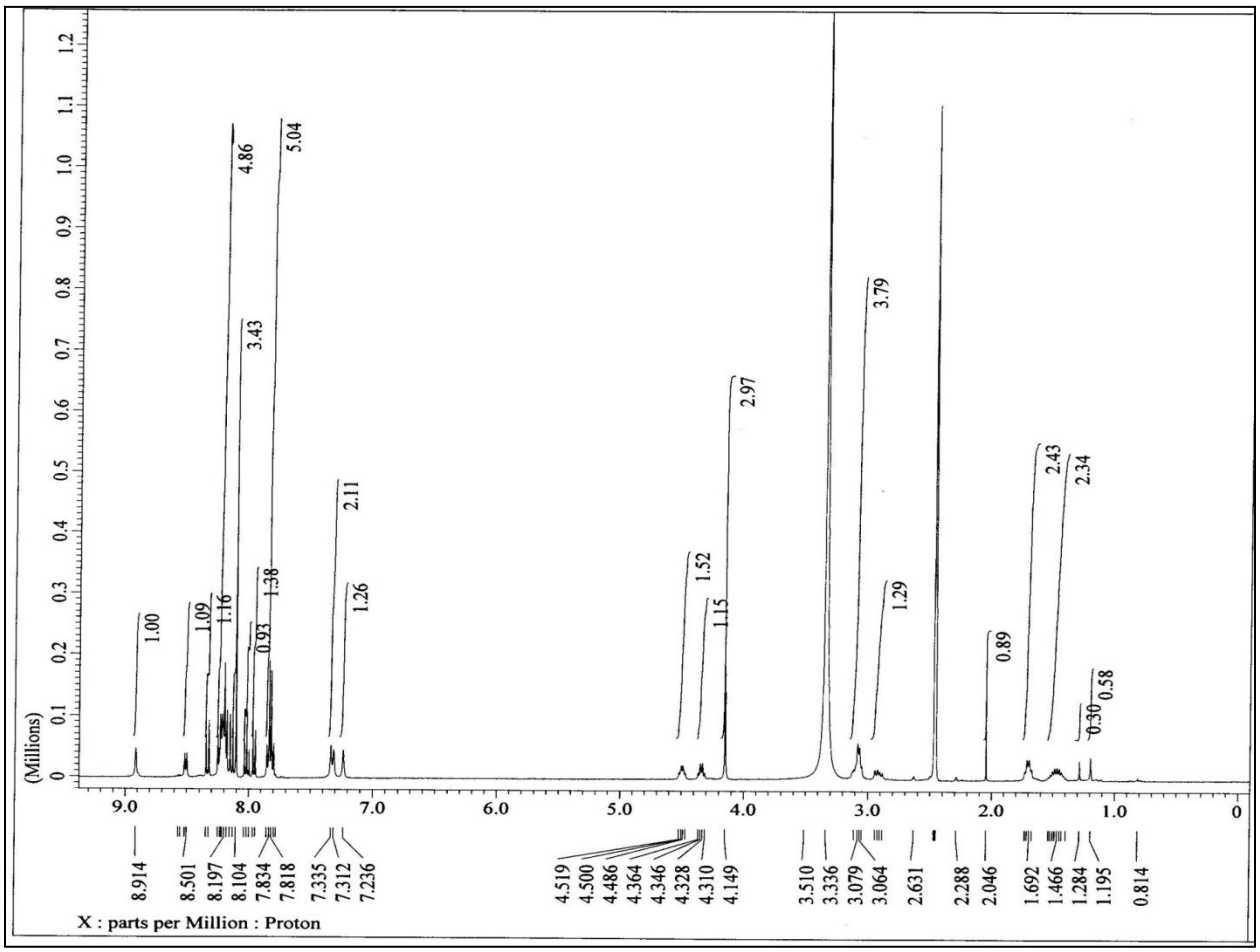


Figure S18. ^{1}H NMR of **4.**

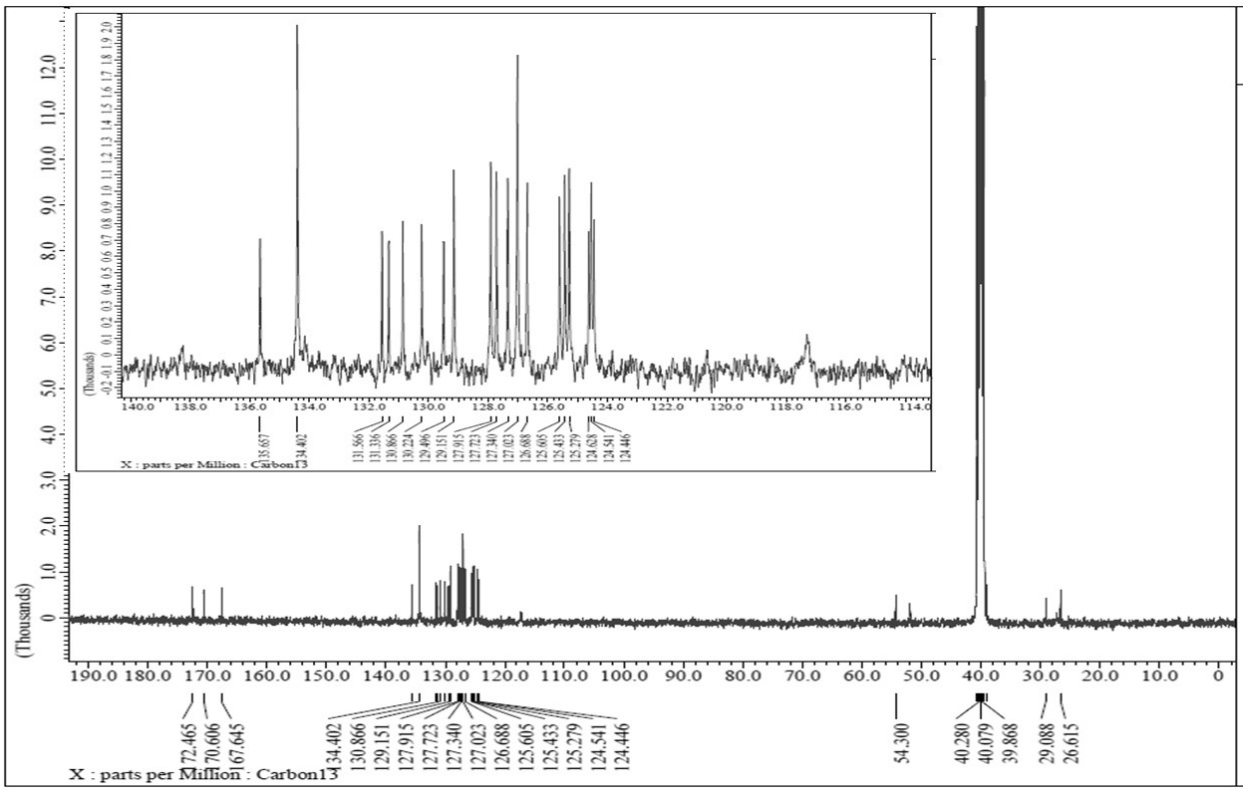
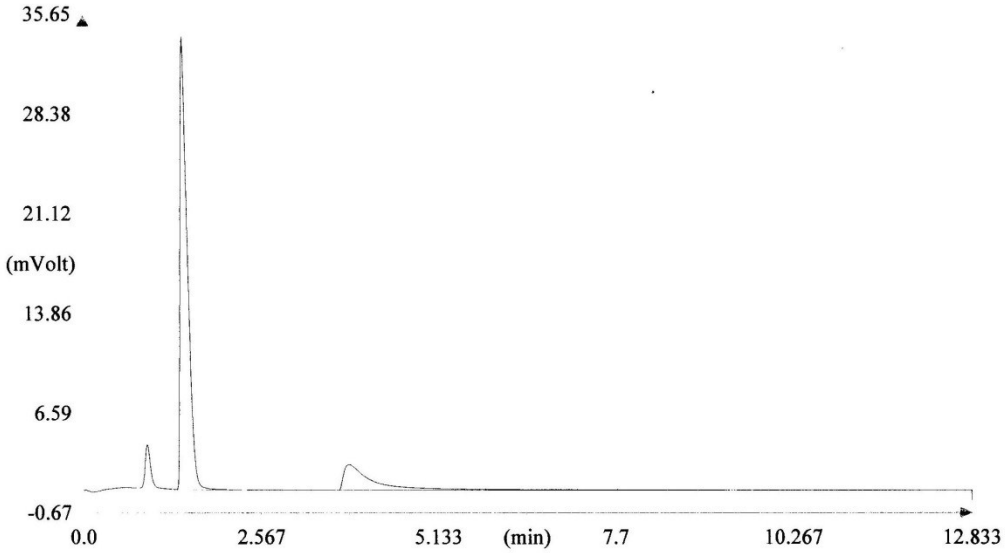


Figure S19. ^{13}C NMR of **4.**



Operator ID:	
Company name:	ThermoFinnigan
Method filename:	E:\Eager for FLASH\INHA\NCHS\N C H S system 151021.mth
Method name:	NCHS
Analysed:	2015-10-29 15:17
Printed:	2015-10-30 13:44
Elemental Analyser method:	
Sampler method:	
Sample ID:	BOPH (# 21)
Analysis type:	UnkNown
Chromatogram filename:	Q132.dat
Calibration method:	K Factors
Sample weight:	.875
Protein factor:	6.25

Element Name	Ret.Time	Area	BC	Area rati
Nitrogen	10.0026	55	173351 RS	13.8391
Carbon	56.2631	85	2399022 RS	1.0000
Hydrogen	4.5324	230	579365 RS	4.1407
Totals	70.7981		3151738	

Figure S20. Elemental analysis of **4.**

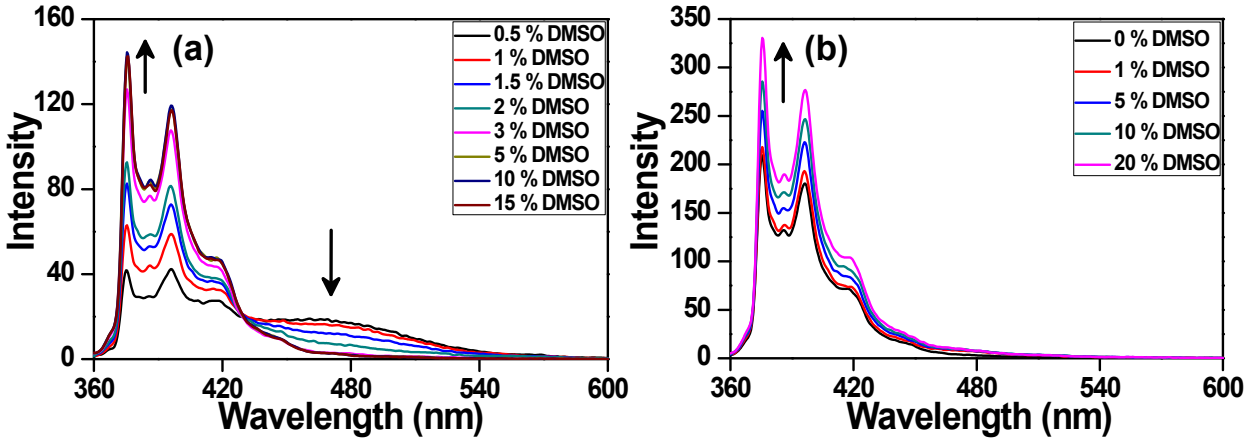


Figure S21. Fluorescence spectra of (a) **3** (10 μM) and (b) **4** (10 μM) in aqueous buffered solution (50 mM phosphate, pH 7.4) containing different percentage of DMSO (λ_{ex} = 342 nm, slit = 12/2.5 nm).

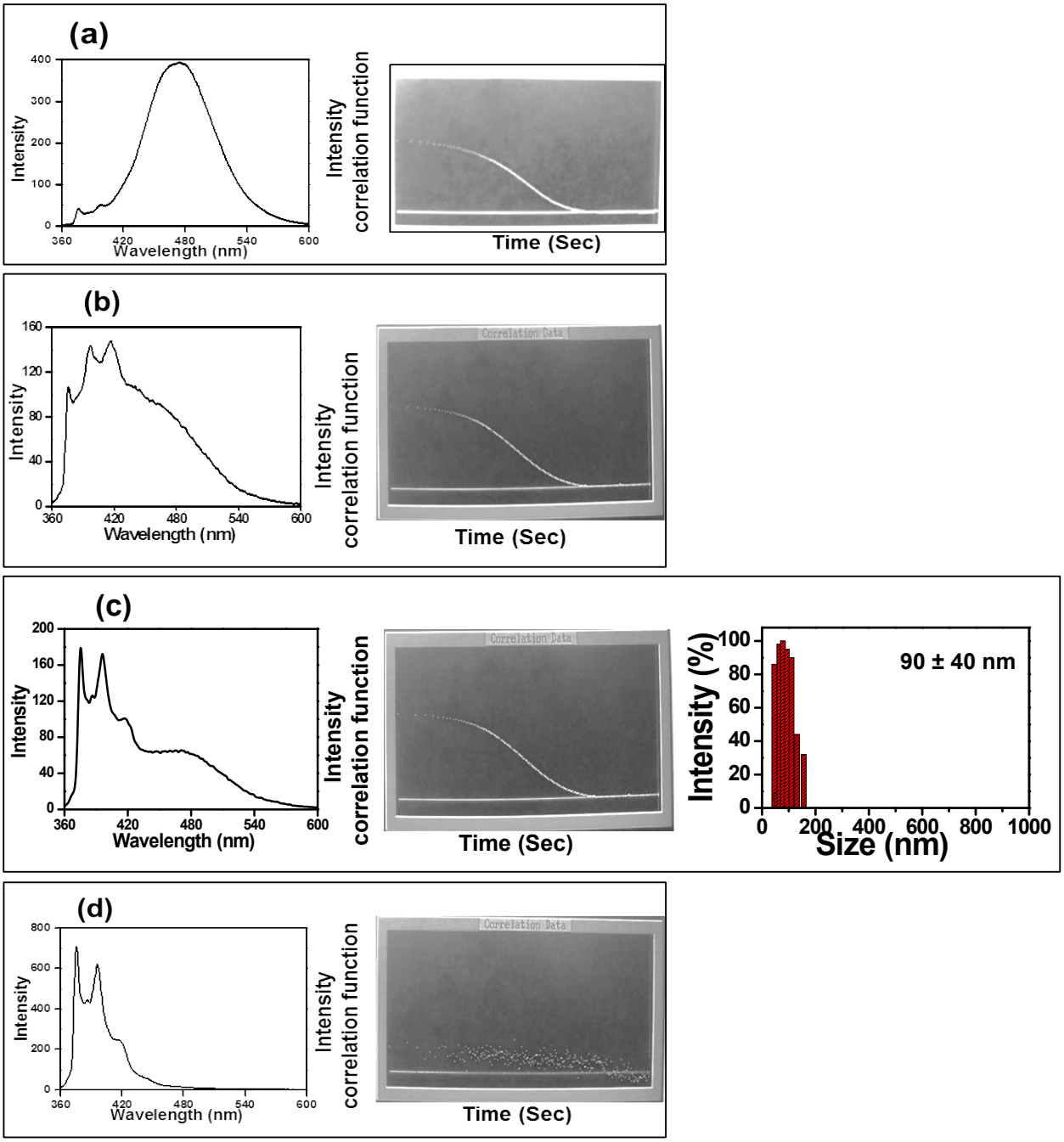


Figure S22. Fluorescence emission spectra and intensity correlation function of (a) **1** (b) **2** (c) **3,** and (d) **4** for particle size analysis in phosphate buffer solutions containing DMSO (3 %, 10 %, 3 %, and 0 %, respectively) at pH 7.4. The concentration of each compound is 30 μM.

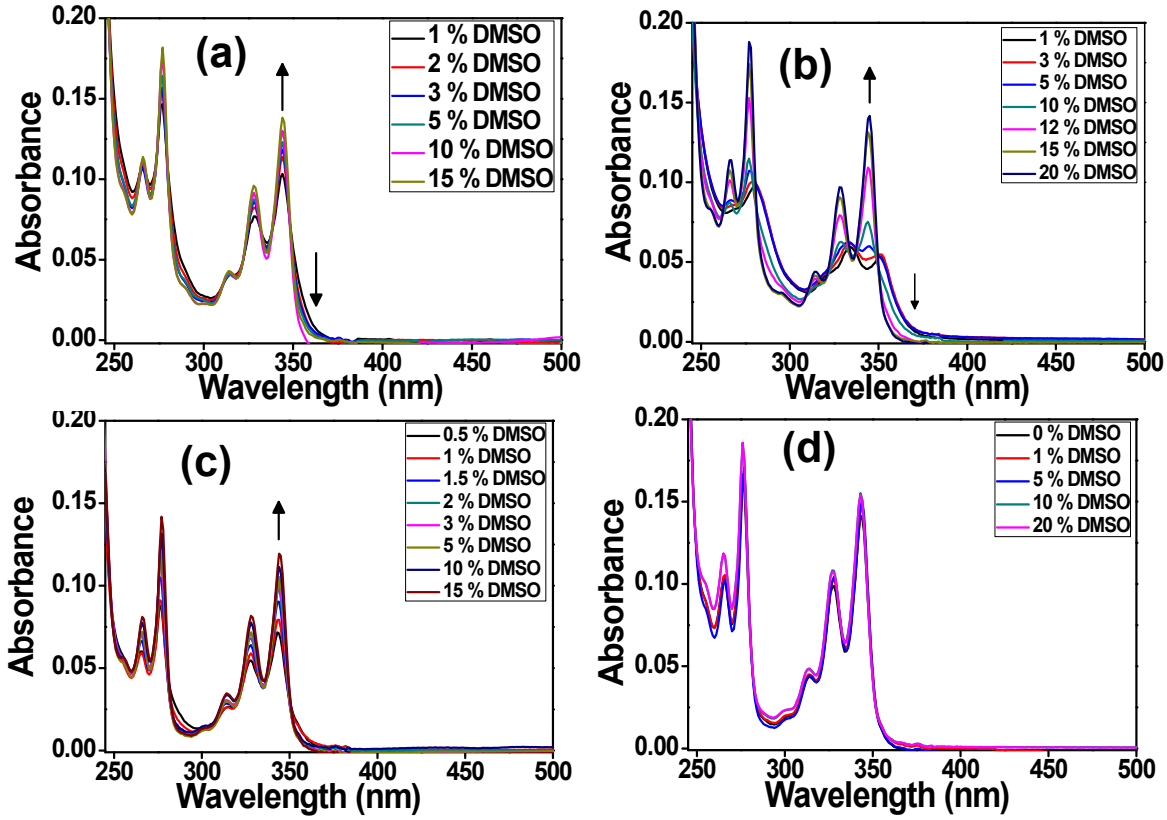


Figure S23. UV-visible absorption spectra of (a) **1** (b) **2** (c) **3,** and (d) **4** in aqueous buffered solutions (50 mM phosphate, pH 7.4) containing different percentage of DMSO. The concentration of each compound is 10 μM.

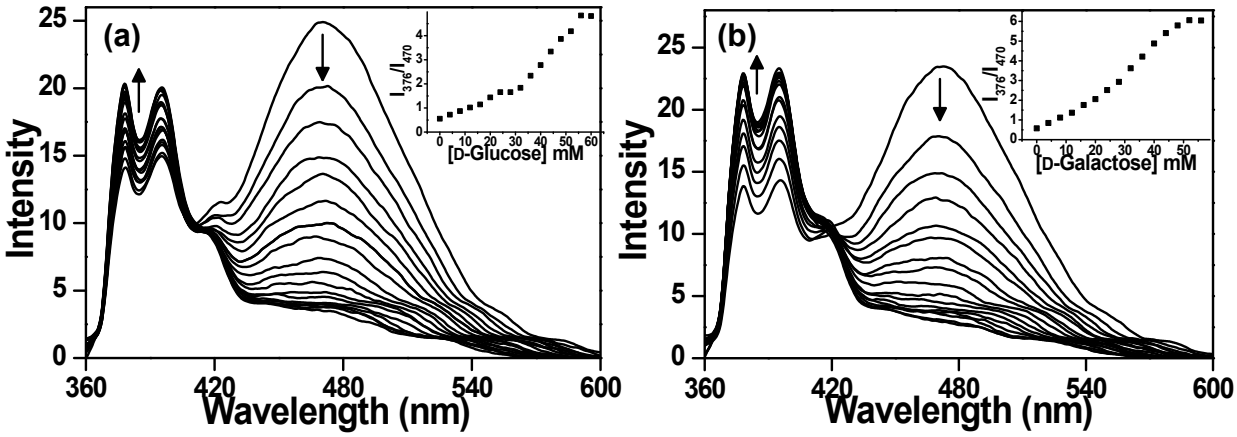


Figure S24. Fluorescence spectra of **1** (10 μM) upon the gradual addition of (a) D-glucose and (b) D-galactose in aqueous buffered solutions (H_2O–DMSO, 99:1, v/v, 50 mM phosphate at pH 7.4), λ_{ex} = 342 nm, slit = 12/2.5 nm.

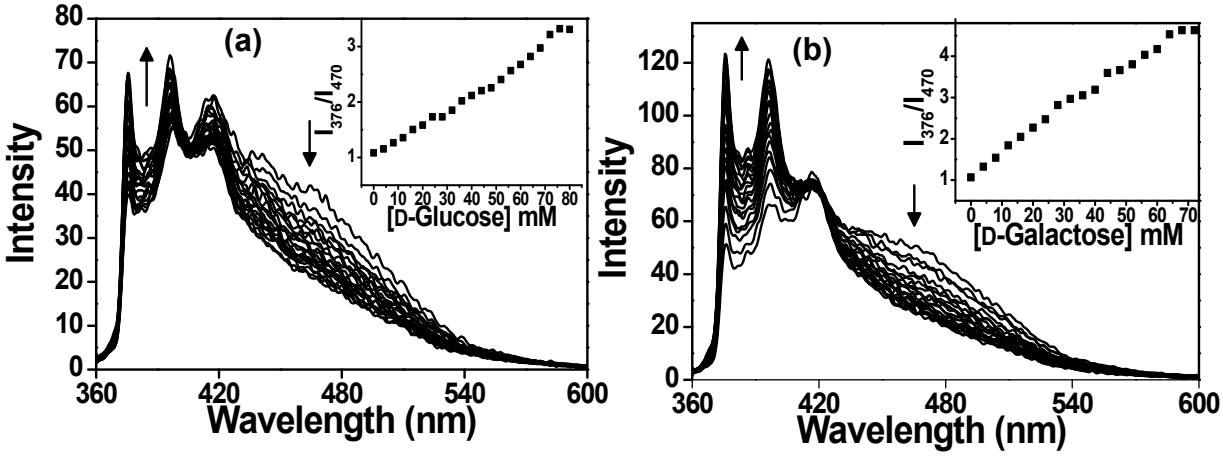


Figure S25. Fluorescence spectra of **2** (10 μM) upon the gradual addition of (a) D-glucose mM) and (b) D-galactose in aqueous buffered solutions (H_2O–DMSO, 95:5, v/v, 50 mM phosphate at pH 7.4), λ_{ex} = 342 nm, slit = 12/2.5 nm.

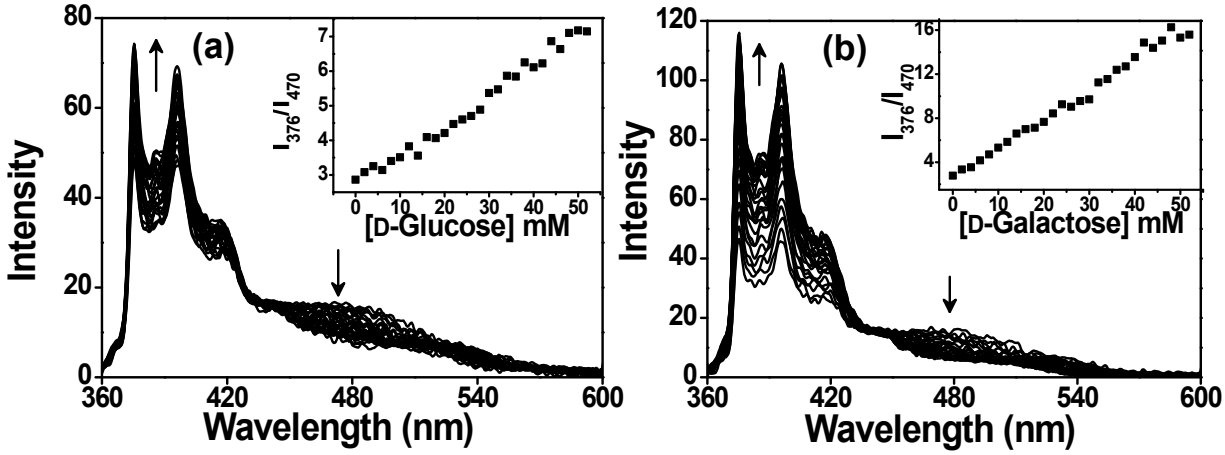


Figure S26. Fluorescence spectra of **3** (10 μM) upon the gradual addition of (a) D-glucose mM) and (b) D-galactose in aqueous buffered solutions (H_2O–DMSO, 99.5:0.5, v/v, 50 mM phosphate at pH 7.4), λ_{ex} = 342 nm, slit = 12/2.5 nm.

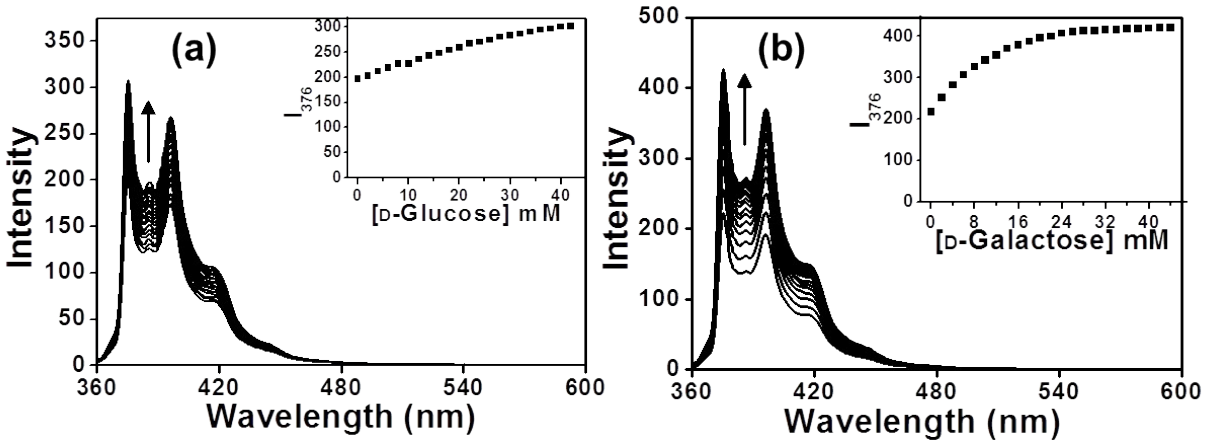


Figure S27. Fluorescence spectra of **4** (10 μM) upon the gradual addition of (a) D-glucose mM) and (b) D-galactose in aqueous buffered solutions (50 mM phosphate, pH 7.4), λ_{ex} = 342 nm, slit = 12/2.5 nm.

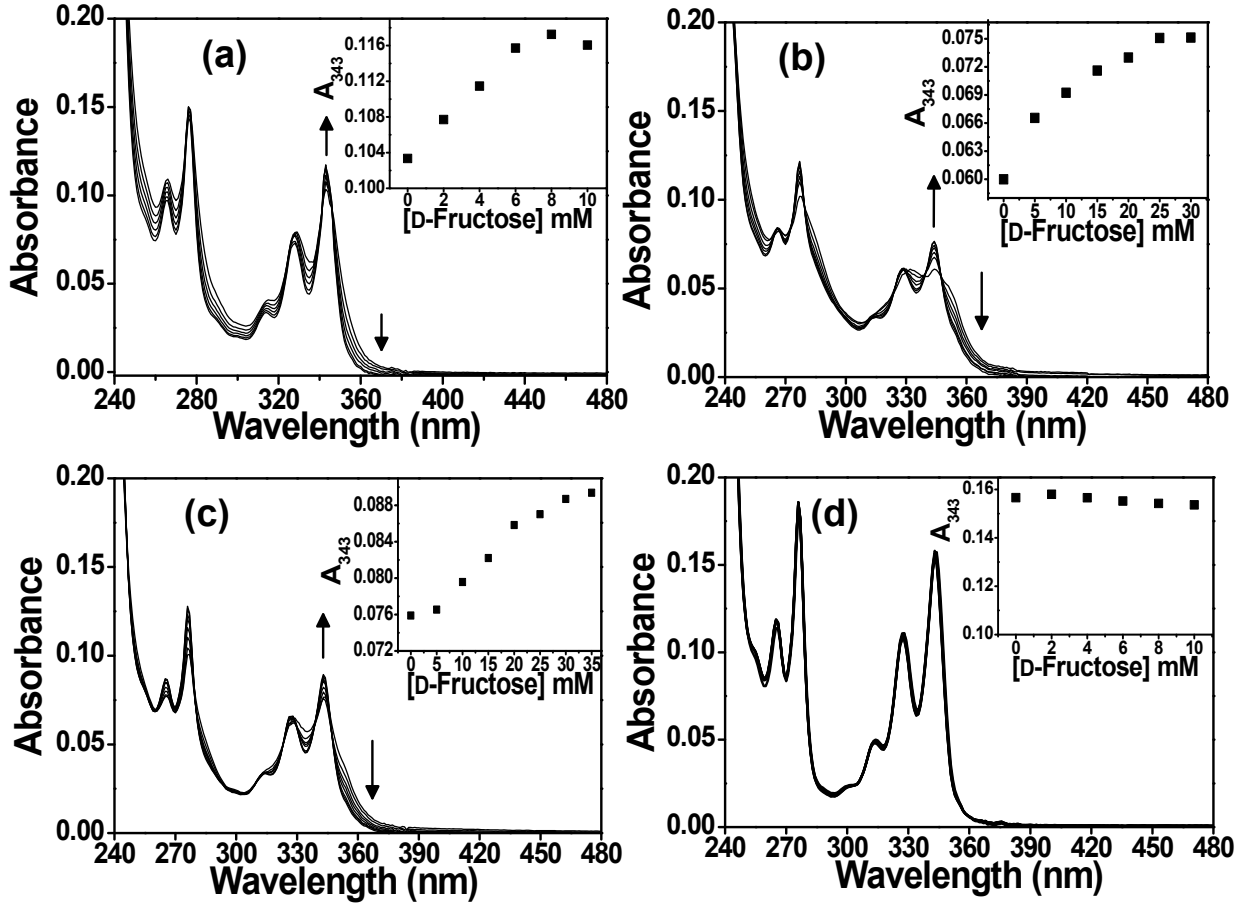


Figure S28. UV-visible absorption spectra of (a) **1** (b) **2** (c) **3** and (d) **4** upon the gradual addition of D-fructose in aqueous buffered solutions containing 1%, 5 %, 0.5 % and 0 % DMSO, respectively. The concentration of each compound is 10 μM.

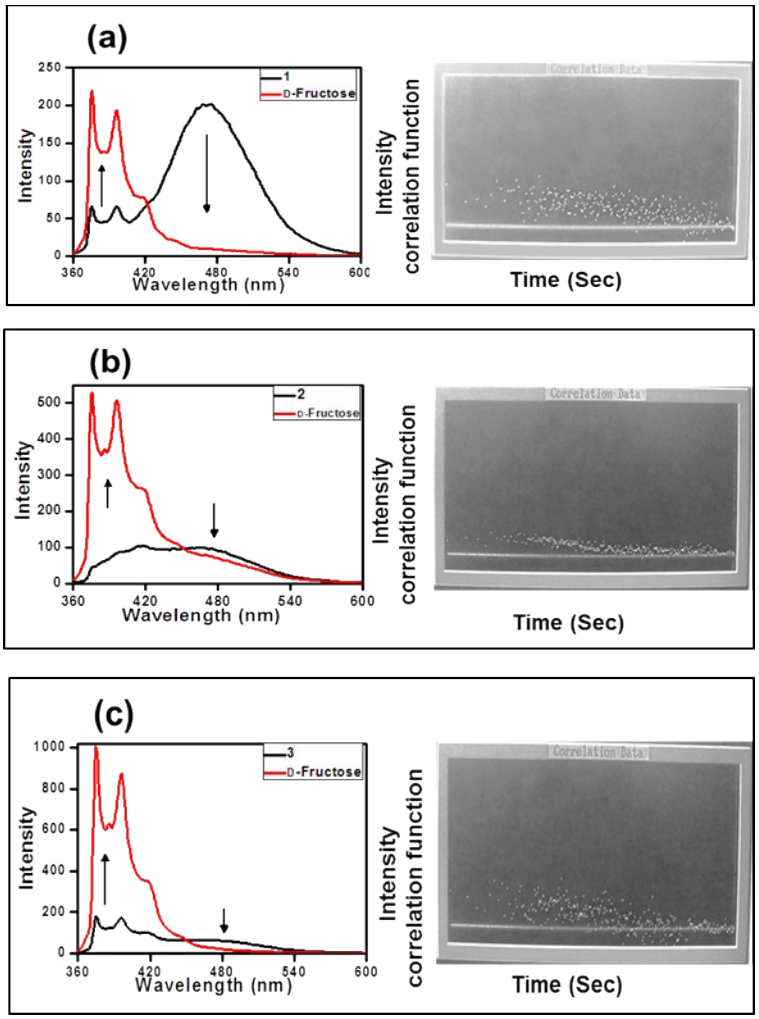


Figure S29. Fluorescence emission spectra and intensity correlation function of (a) **1** (b) **2,** and (c) **3** in the presence of D-fructose (60 mM) for particle size analysis in phosphate buffer solution containing DMSO (3 %, 10 %, and 3 %, respectively) at pH 7.4. The concentration of each compound is 30 μM.

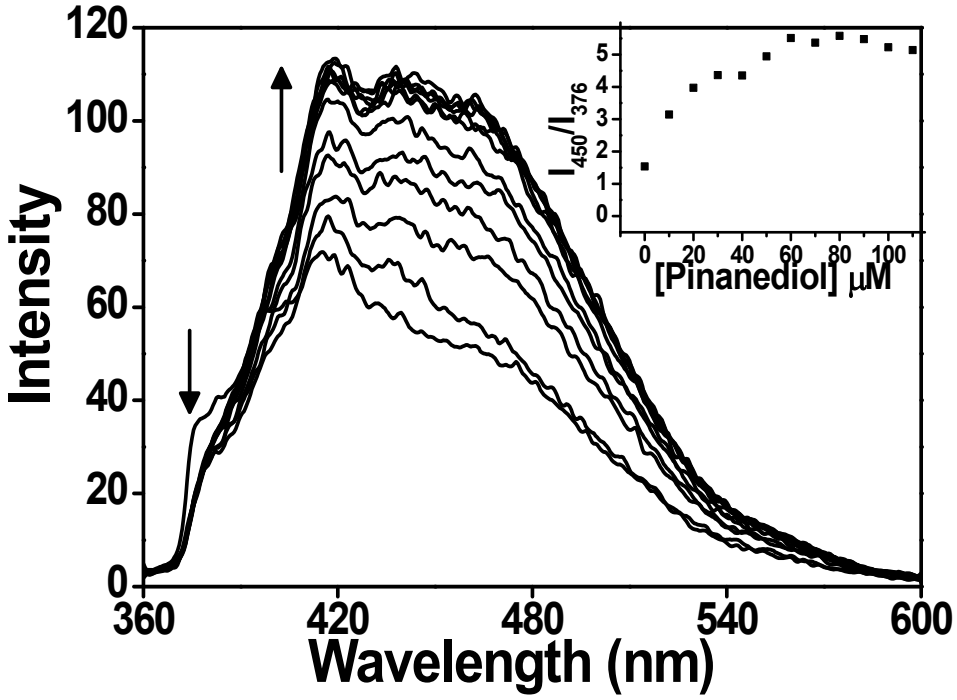


Figure S30. Fluorescence spectra of **2** (10 μM) upon the gradual addition of pinanediol in aqueous buffered solutions (50 mM phosphate buffer, pH 7.4) containing 5 % DMSO (λ_{ex} = 342 nm, slit = 12/2.5 nm).

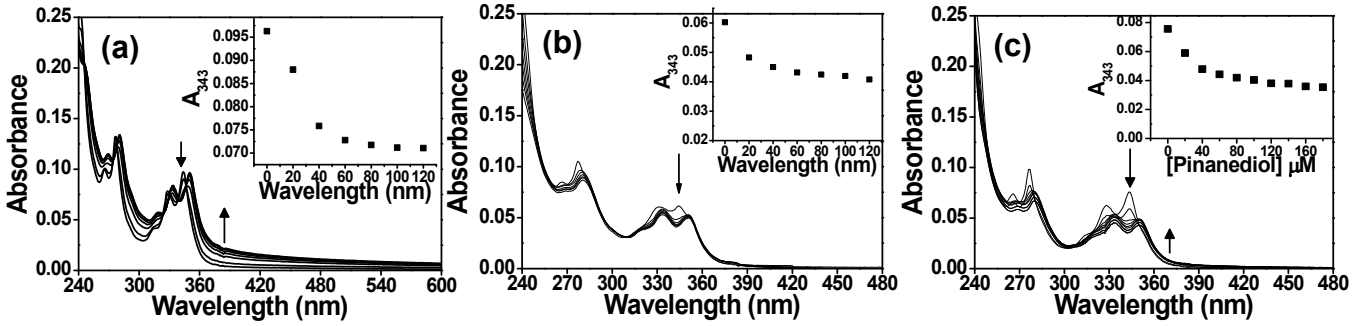


Figure S31. UV-visible absorption spectra of (a) **1** (b) **2** and (c) **3** upon the addition of pinanediol in aqueous buffered solutions (50 mM phosphate, pH 7.4) containing DMSO (1 %, 5% and 0.5 %, respectively). The concentration of each compound is 10 μM.

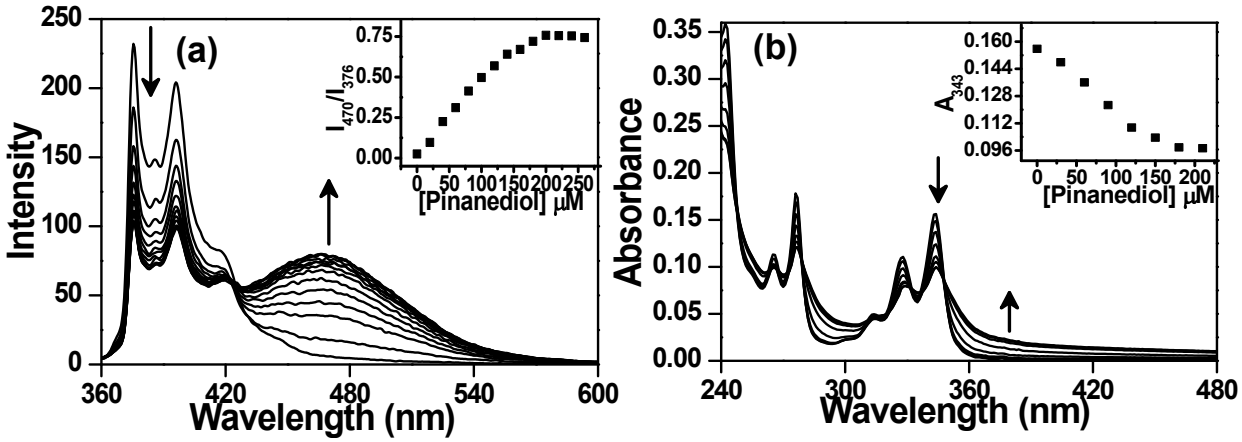


Figure S32. (a) Fluorescence spectra of **4** (10 μM) upon the gradual addition of pinanediol (λ_{ex} = 342 nm, slit = 12/2.5 nm). (b) UV-visible absorption spectra of **4** (10 μM) upon the gradual addition of pinanediol in aqueous buffered solutions (50 mM phosphate, pH 7.4).

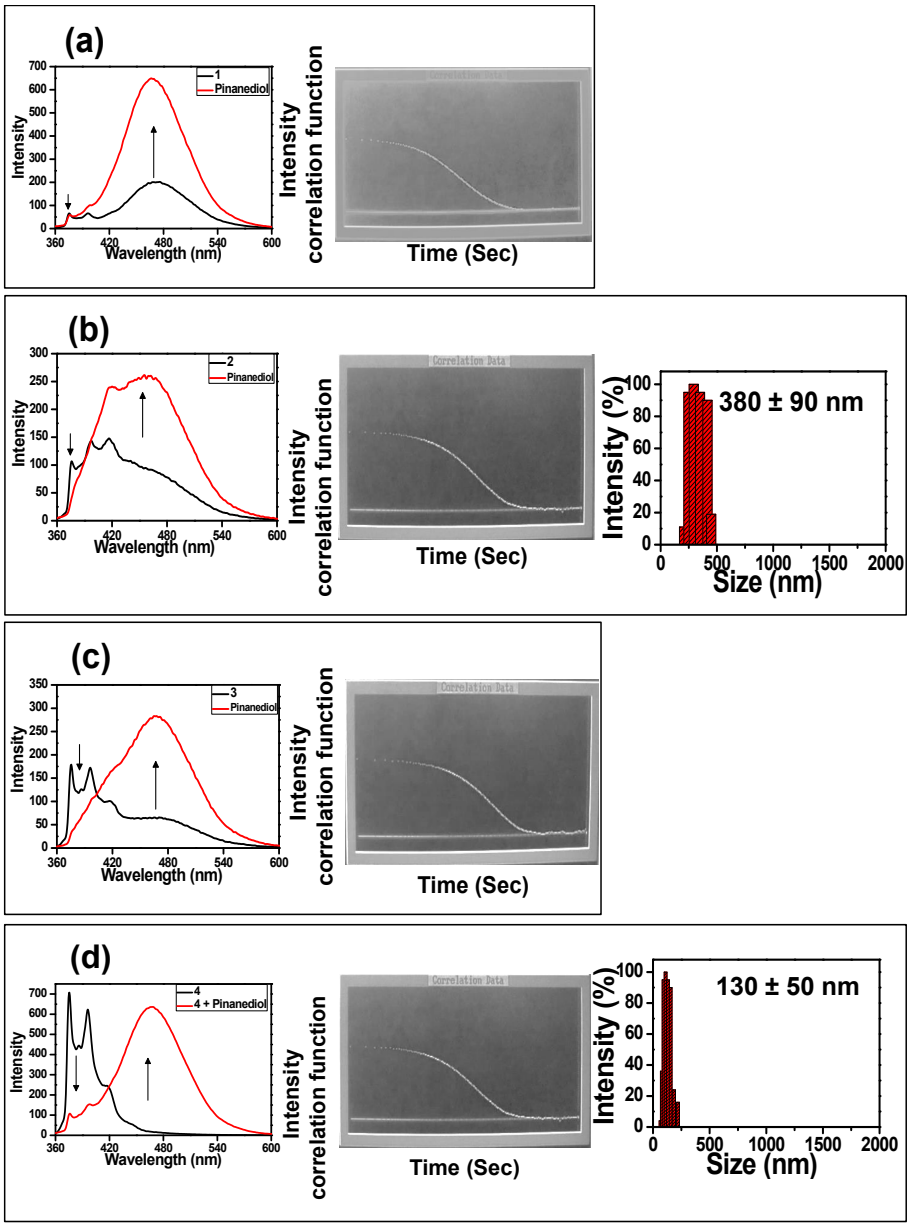


Figure S33. Fluorescence emission spectra and intensity correlation function of (a) **1** (b) **2** (c) **3,** and (d) **4** in the presence of pinanediol (0.2 mM) for particle size analysis in phosphate buffer solution containing DMSO (3 %, 10%, 3 % and 0 %, respectively) at pH 7.4. The concentration of each compound is 30 μM.

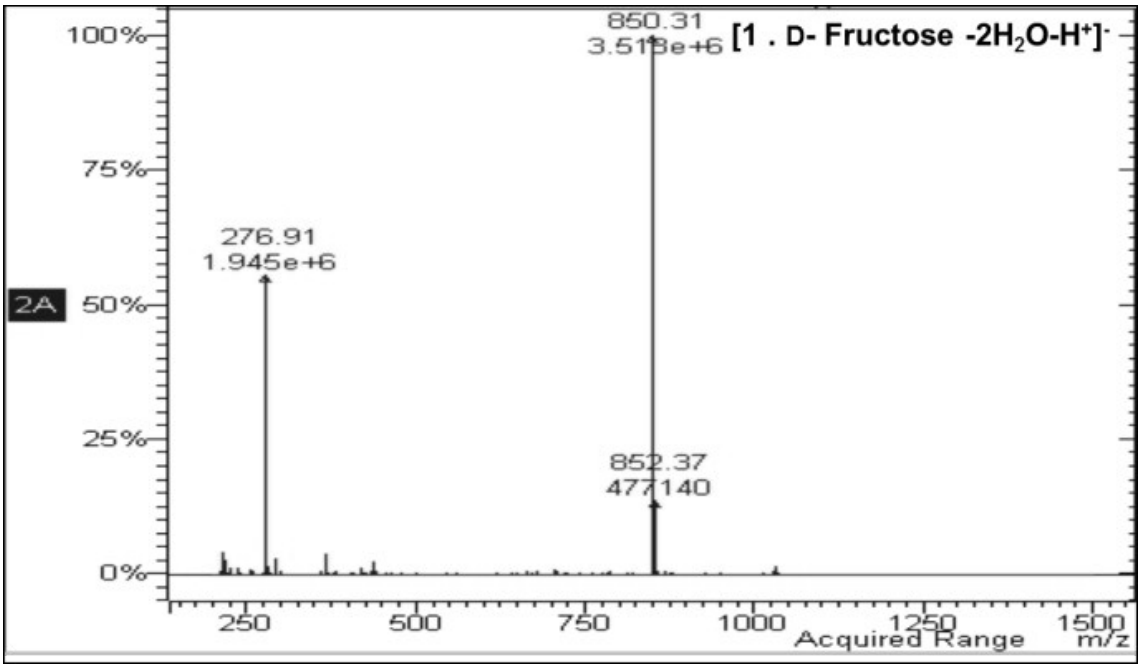


Figure S34. ESI-mass spectrum of **1** in the presence of D-fructose.

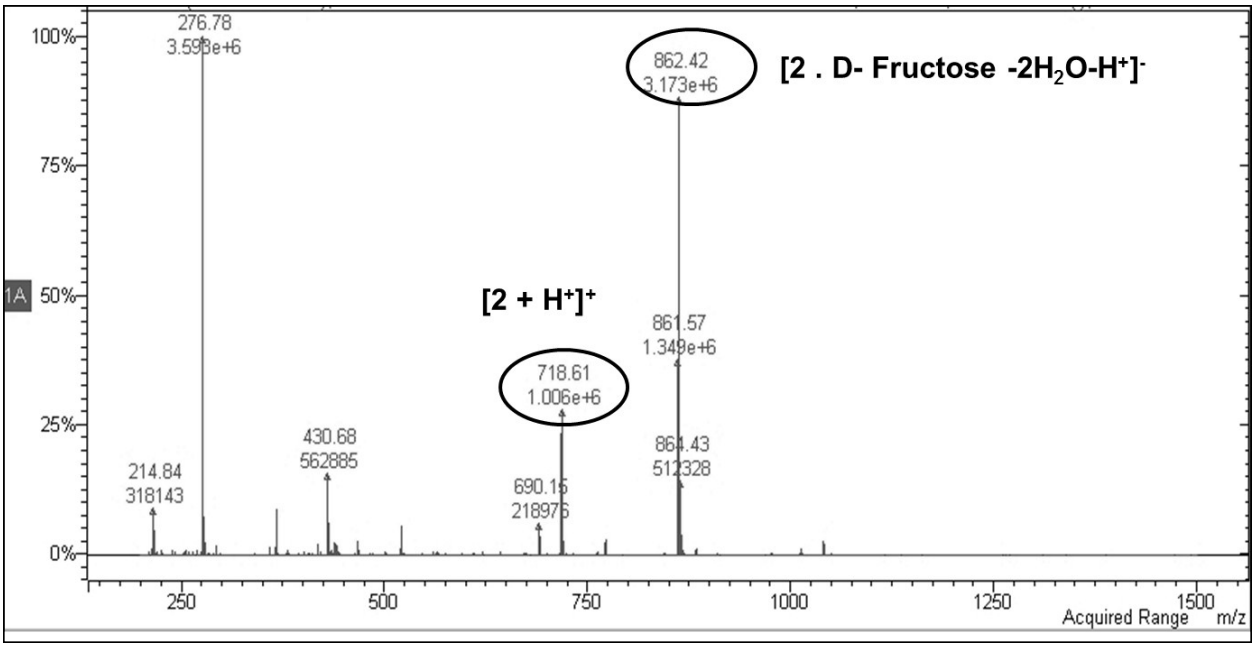


Figure S35. ESI mass spectrum of **2** in the presence of D-fructose.

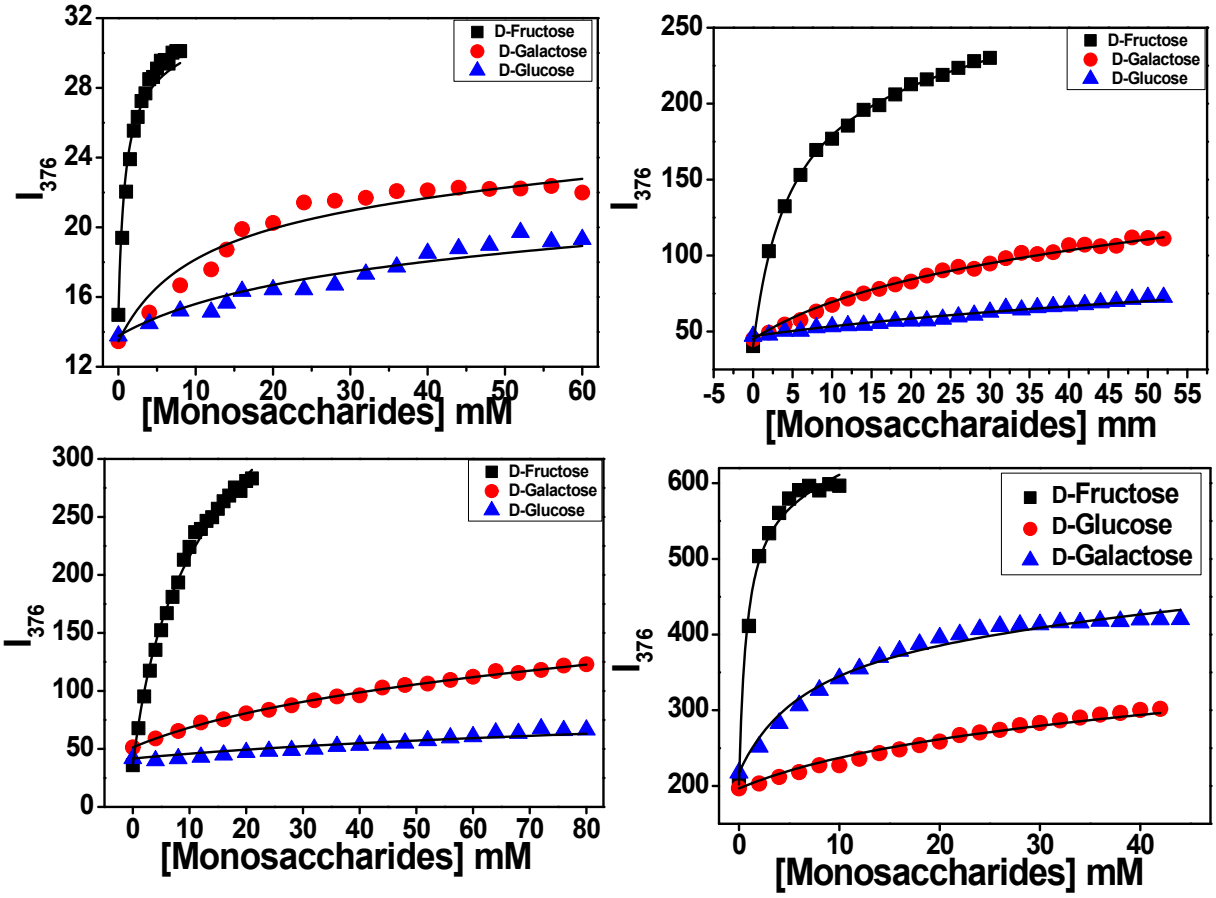


Figure S36. Fitting curve of (a) **1** (b) **2** (c) **3,** and (d) **4** in the presence of monosaccharides.

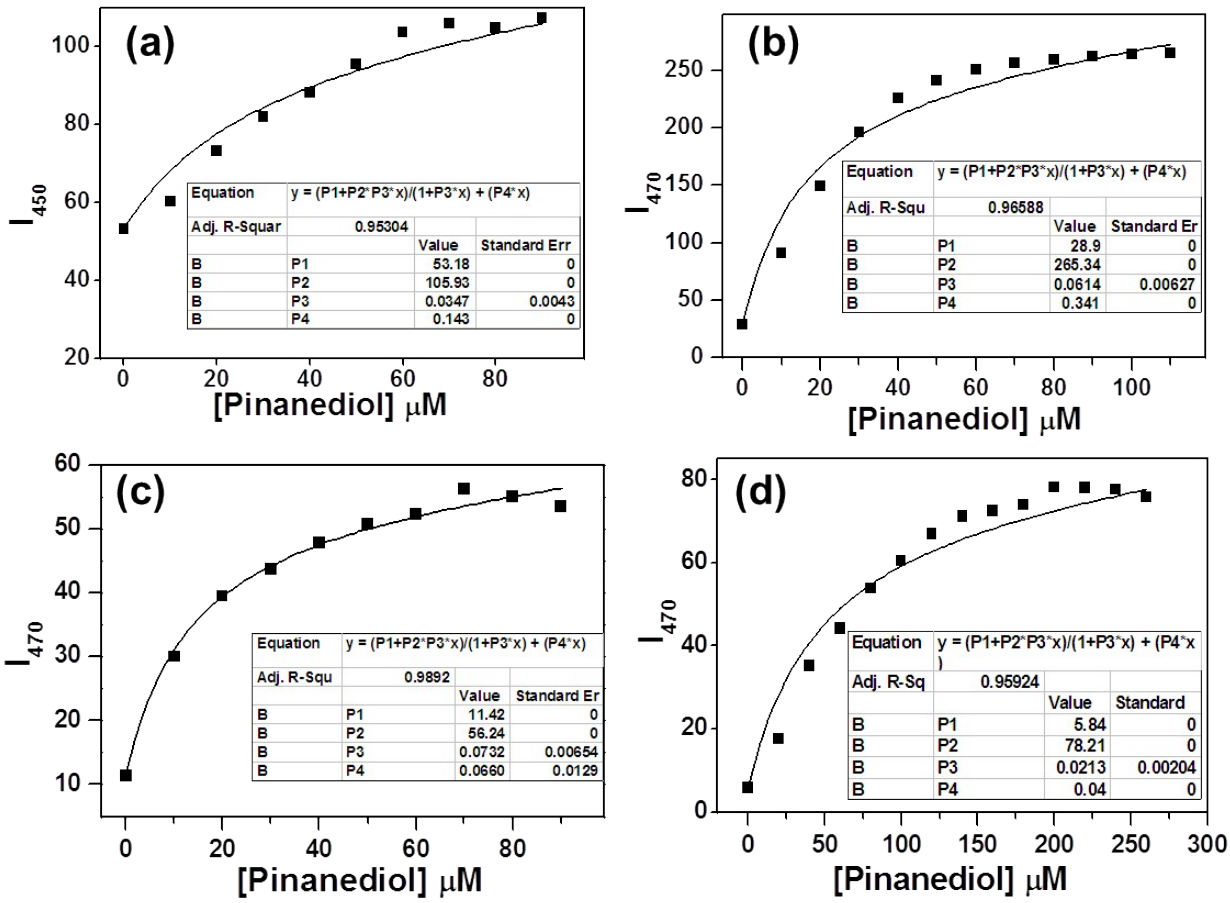


Figure S37. Fitting curve of (a) **1** (b) **2** (c) **3,** and (d) **4** in the presence of pinanediol.

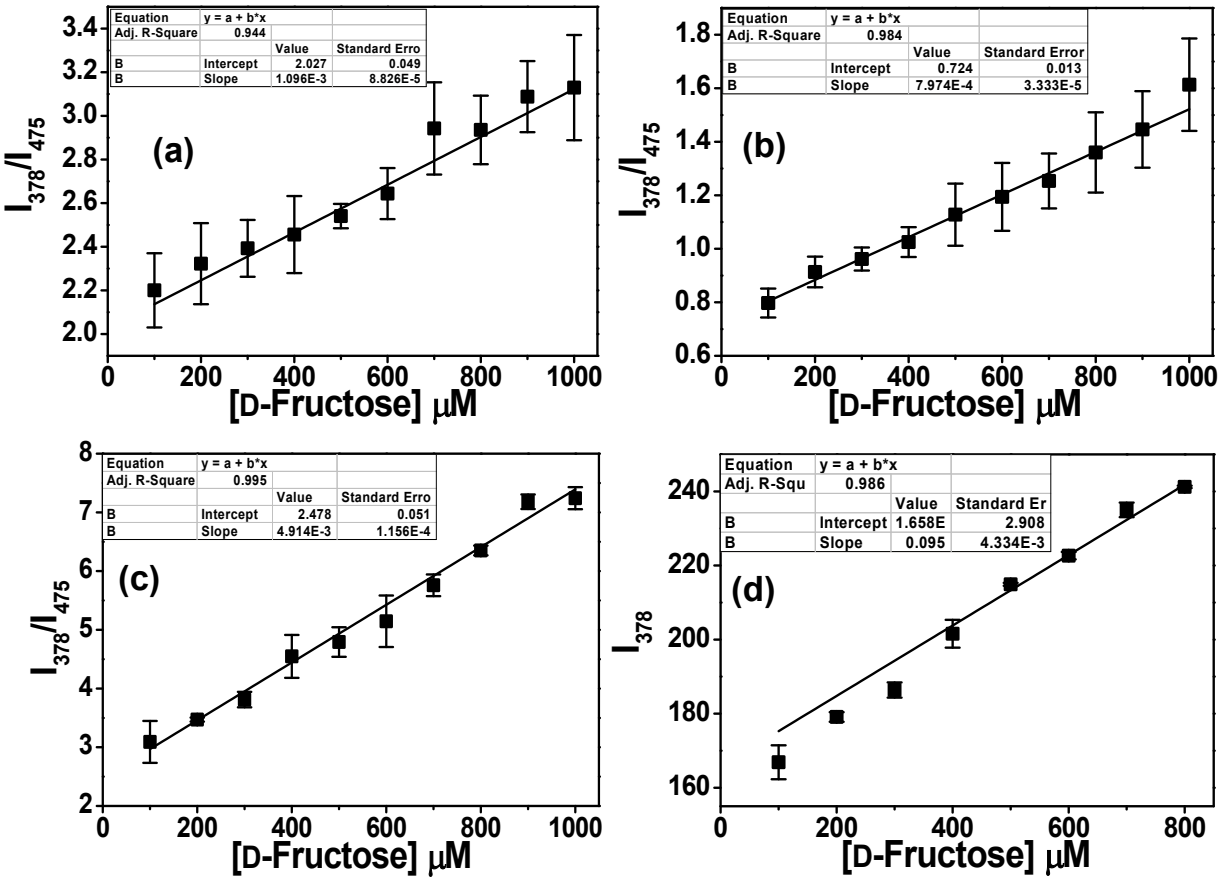


Figure S38. The emission intensity ratio (I_{378}/I_{475}) of (a) **1** (b) **2** (c) **3**, and (d) **4** with increasing concentration of D-fructose in aqueous buffered solution. The concentration of peptides is 10 μM.