ELECTRONIC SUPPORTING INFORMATION

Hetero-layered Hybrid Dendrimers with Optimized Sugar Head Groups for Enhancing Carbohydrate-Protein Interactions

Rahul S. Bagul[a], Maryam Hosseini[a], Tze Chieh Shiao[a], Nadim K. Saadeh[b] and René Roy[a]*

[a]*Pharmaqam and Nanoqam, Department of Chemistry, University du Québec à Montréal, P.O. Box 8888, Succ. Centre-ville, Montréal, Québec H3C 3P8, CANADA.*
E-mail: roy.rene@uqam.ca

[b] *Department of Chemistry (Mass Spectrometry), MAASS Chemistry Building, 801, rue Sherbrooke Ouest, Centre-ville, Montréal, Québec, H3A OB8, CANADA. Fax: +1-514-398-3797; Tel: +1-514-398-6178.*

Content

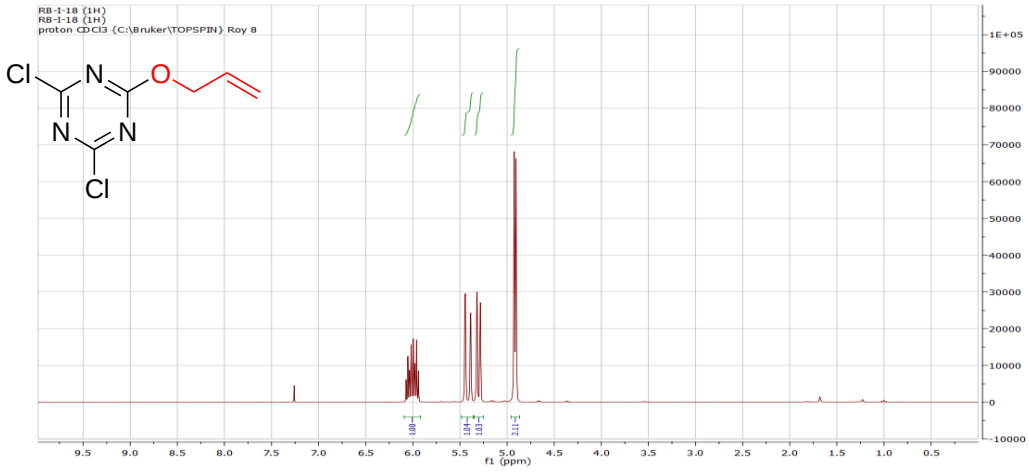


Figure S1. ^{1}H NMR spectrum of **2** (300 MHz, $CDCl_3$)

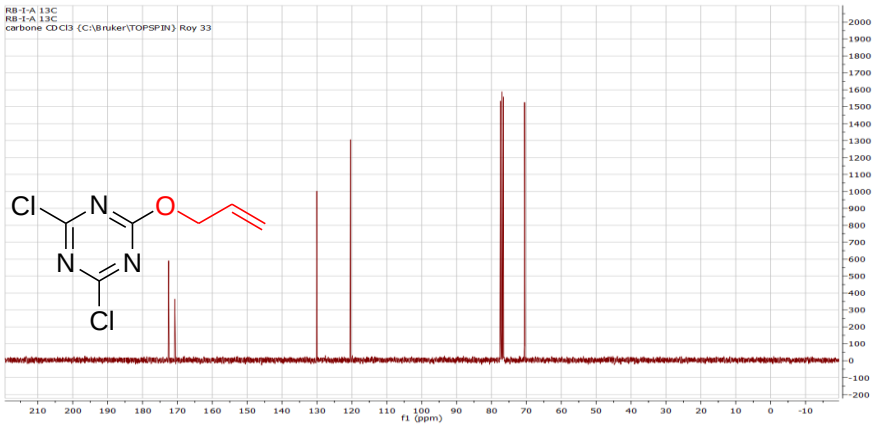


Figure S2. ^{13}C NMR spectrum of **2** (75 MHz, $CDCl_3$)

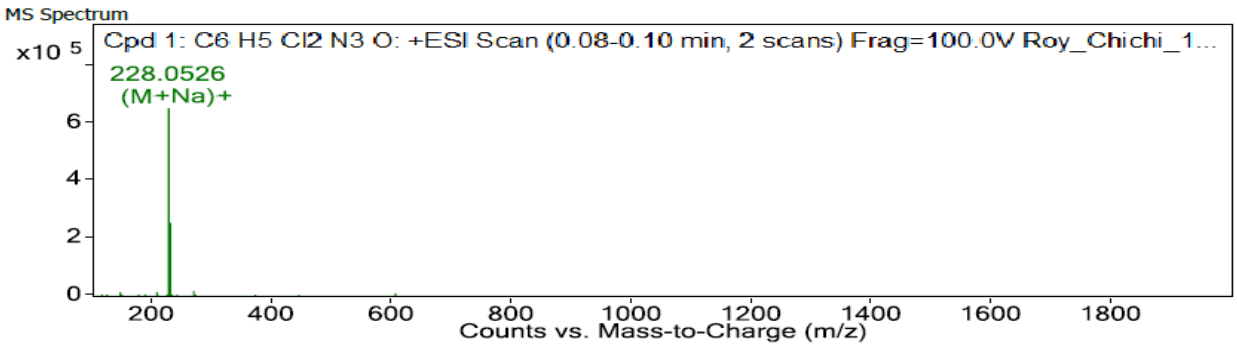


Figure S3. ESI-MS spectrum of 2

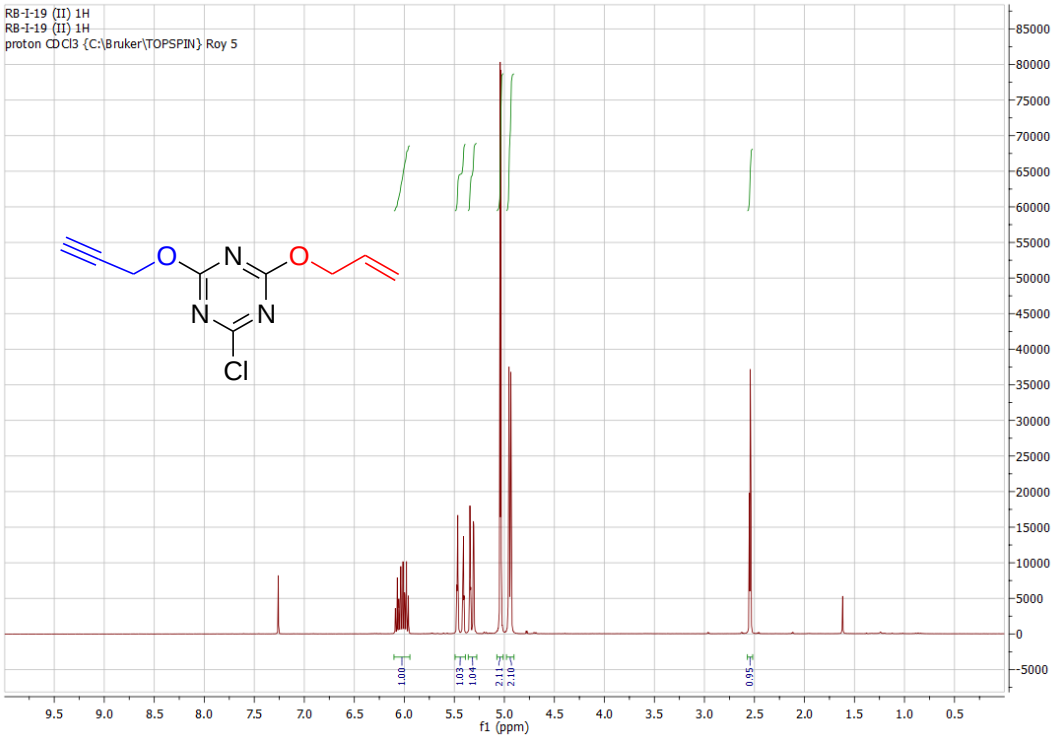


Figure S4. ^{1}H NMR spectrum of **3** (300 MHz, $CDCl_3$)

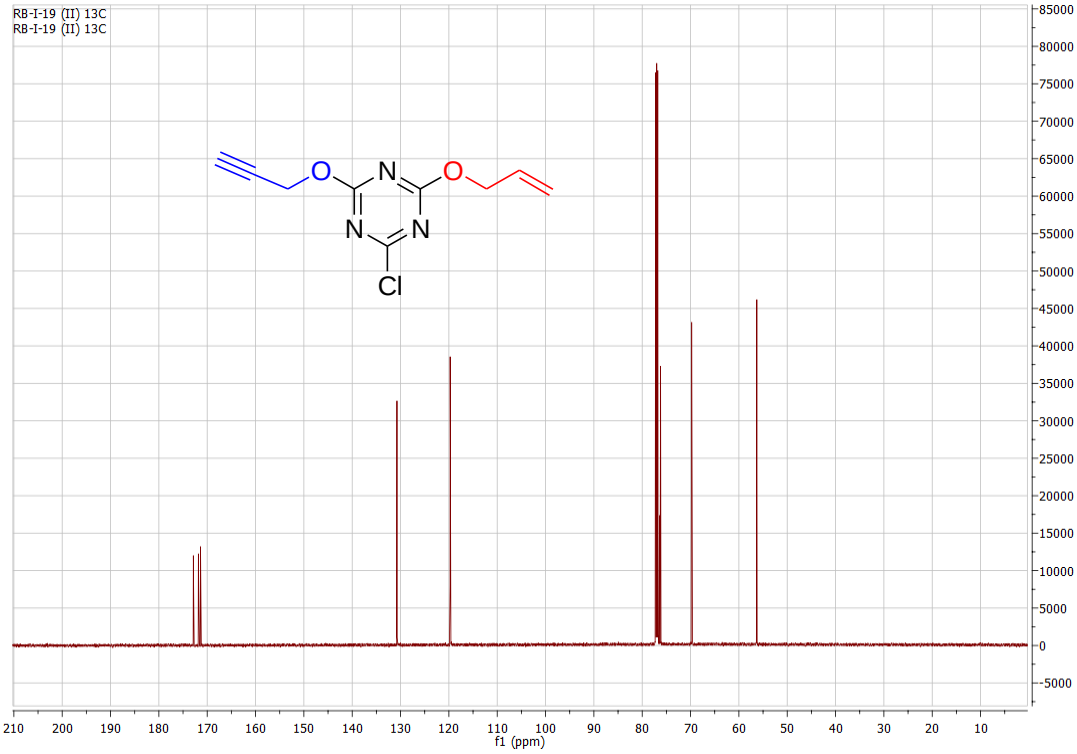


Figure S5. ^{13}C NMR spectrum of **3** (150 MHz, $CDCl_3$)

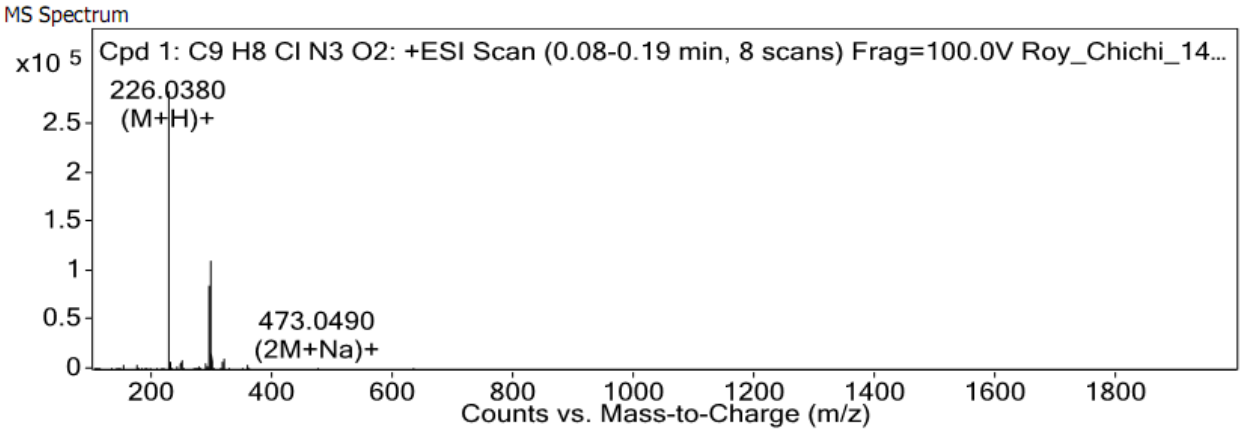


Figure S6. ESI-MS spectrum of 3

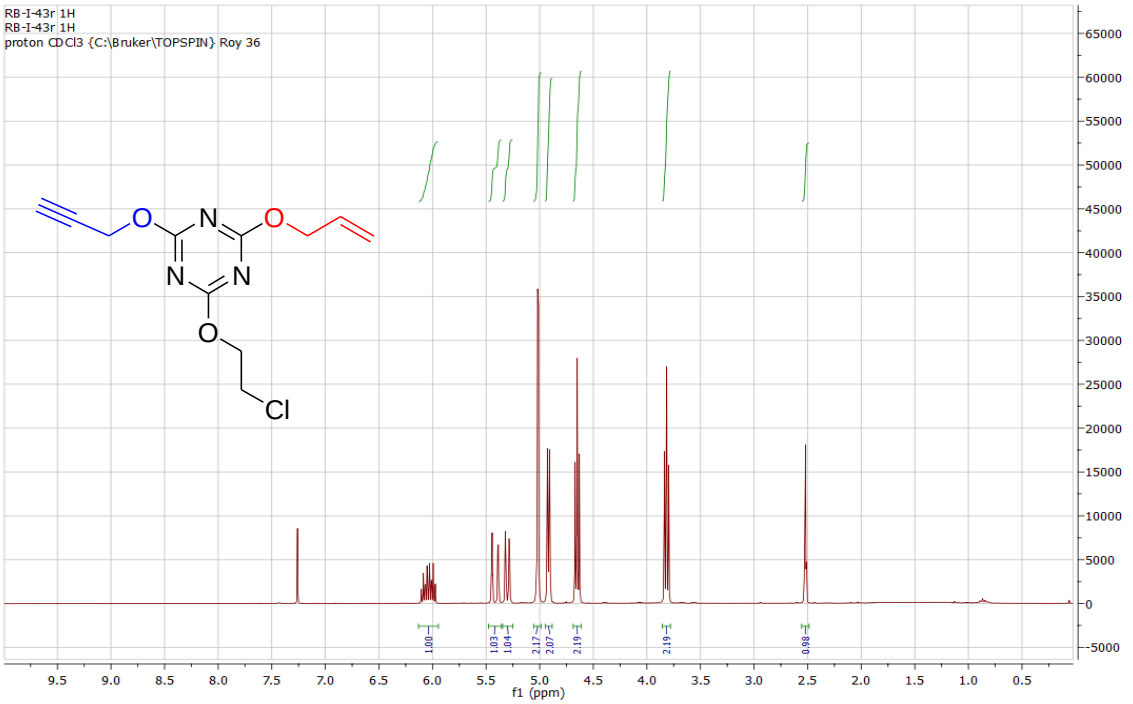


Figure S7. ^{1}H NMR spectrum of **4** (300 MHz, $CDCl_3$)

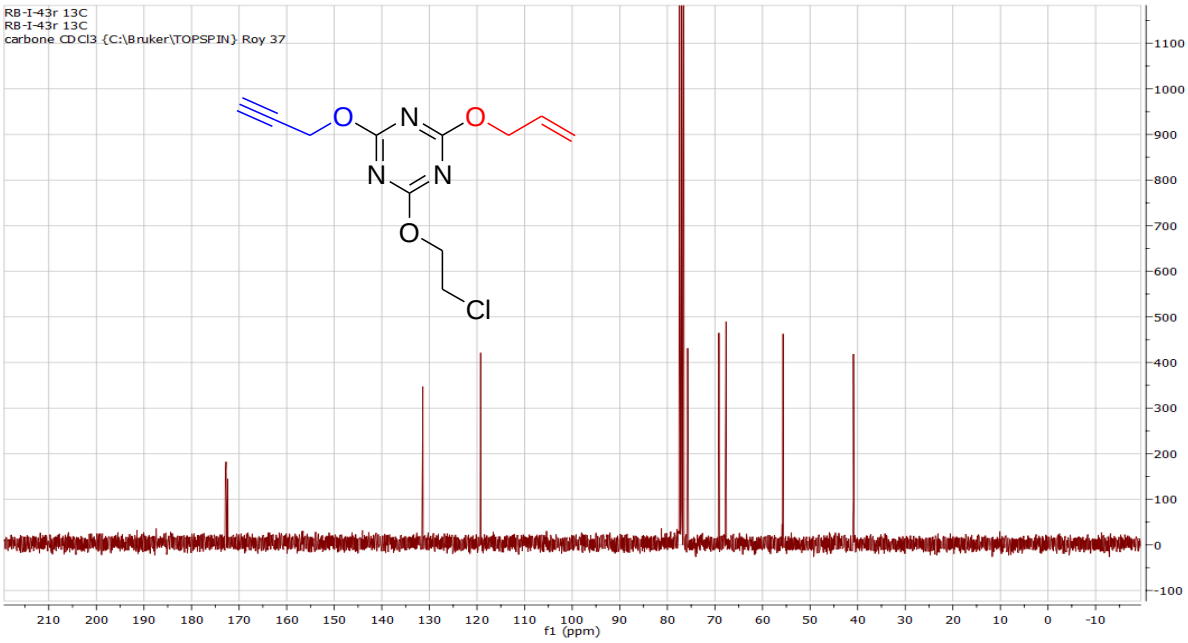


Figure S8. ^{13}C NMR spectrum of **4** (75 MHz, $CDCl_3$)

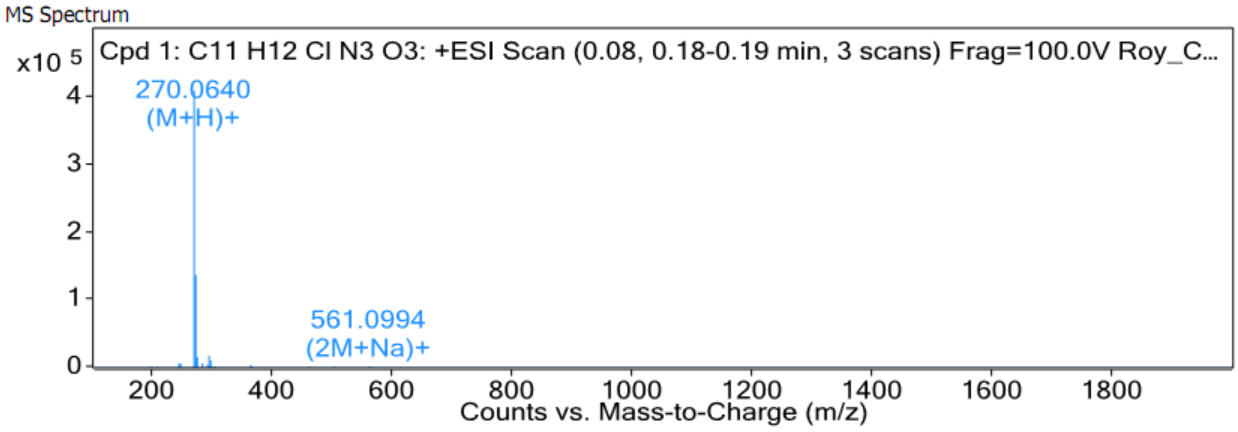


Figure S9. ESI-MS spectrum of **4**

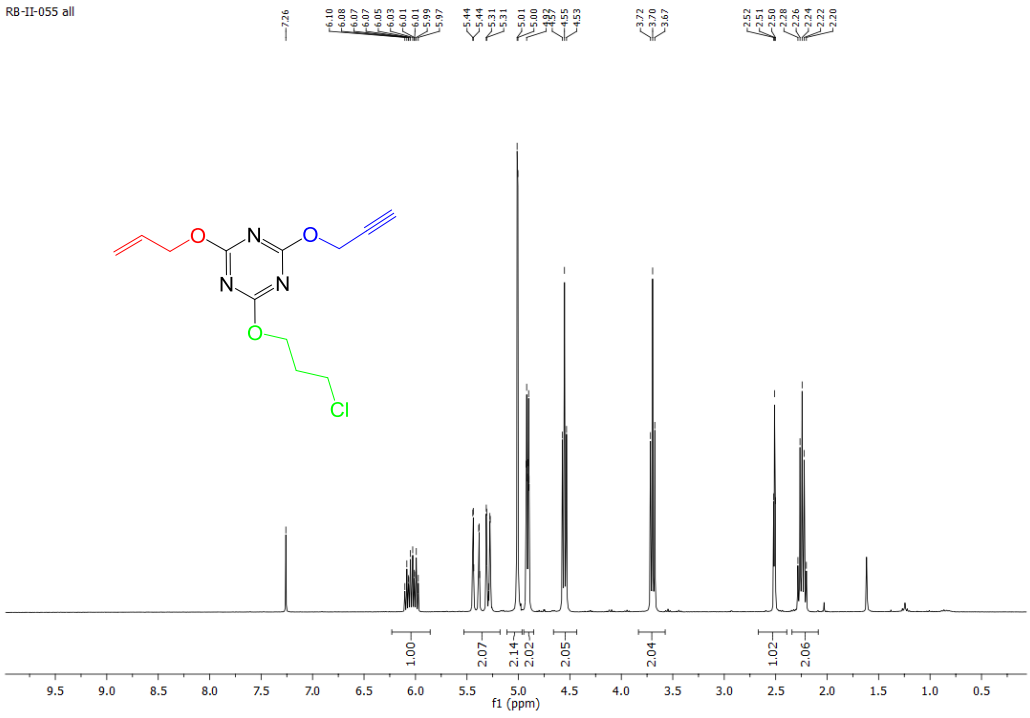


Figure S10. ^{1}H NMR spectrum of **5** (300 MHz, $CDCl_3$)

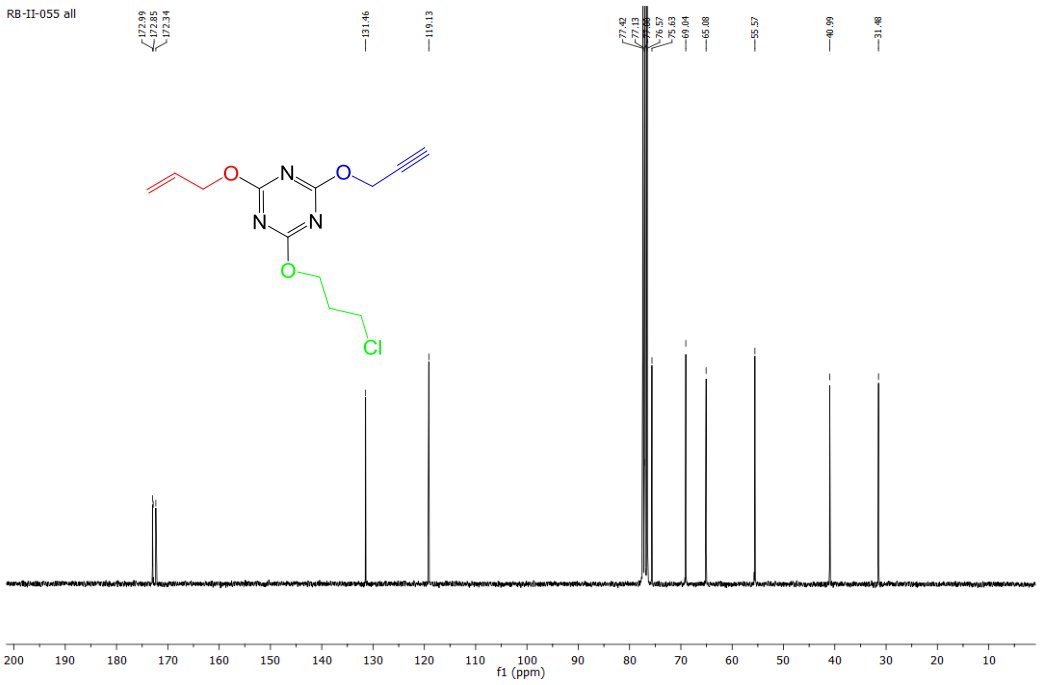


Figure S11. ^{13}C NMR spectrum of **5** (75 MHz, $CDCl_3$)

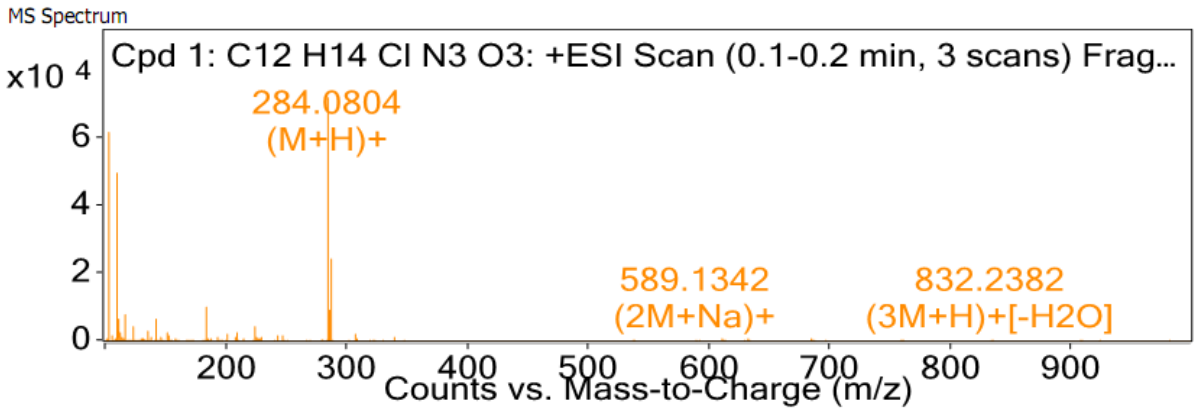


Figure S12. ESI-MS spectrum of **5**

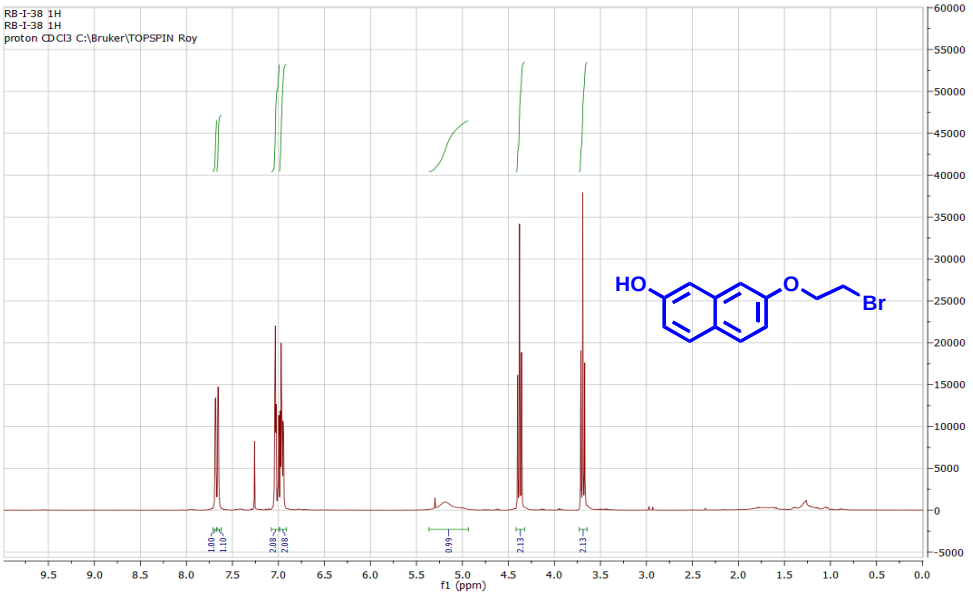


Figure S13. ^{1}H NMR spectrum of **7** (300 MHz, $CDCl_3$).

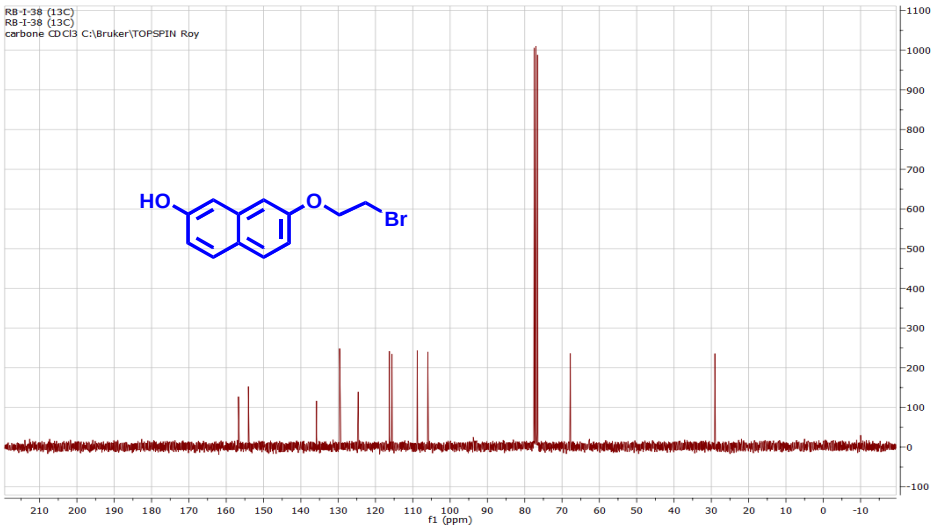


Figure S14. ^{13}C NMR spectrum of **7** (75 MHz, $CDCl_3$).

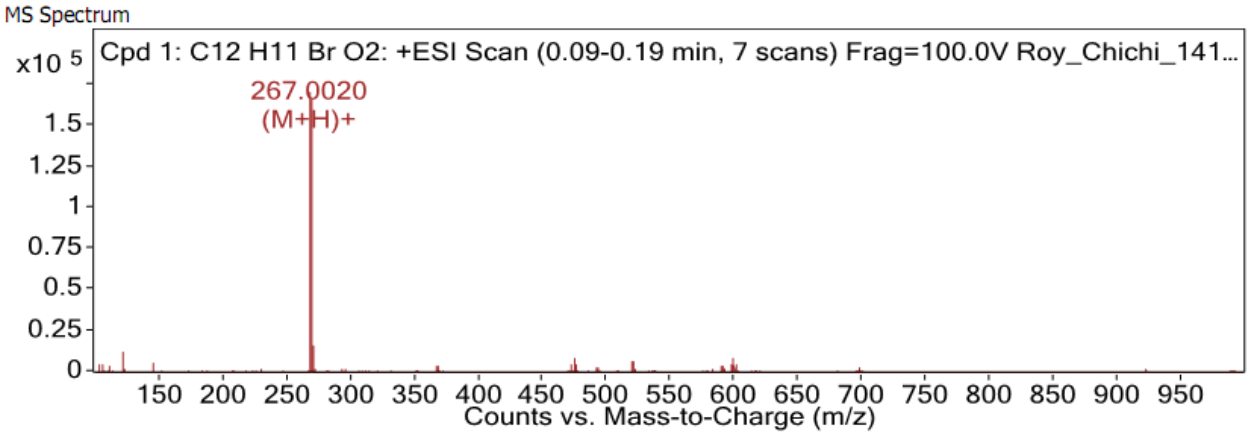


Figure S15. ESI-MS spectrum of compound **7**

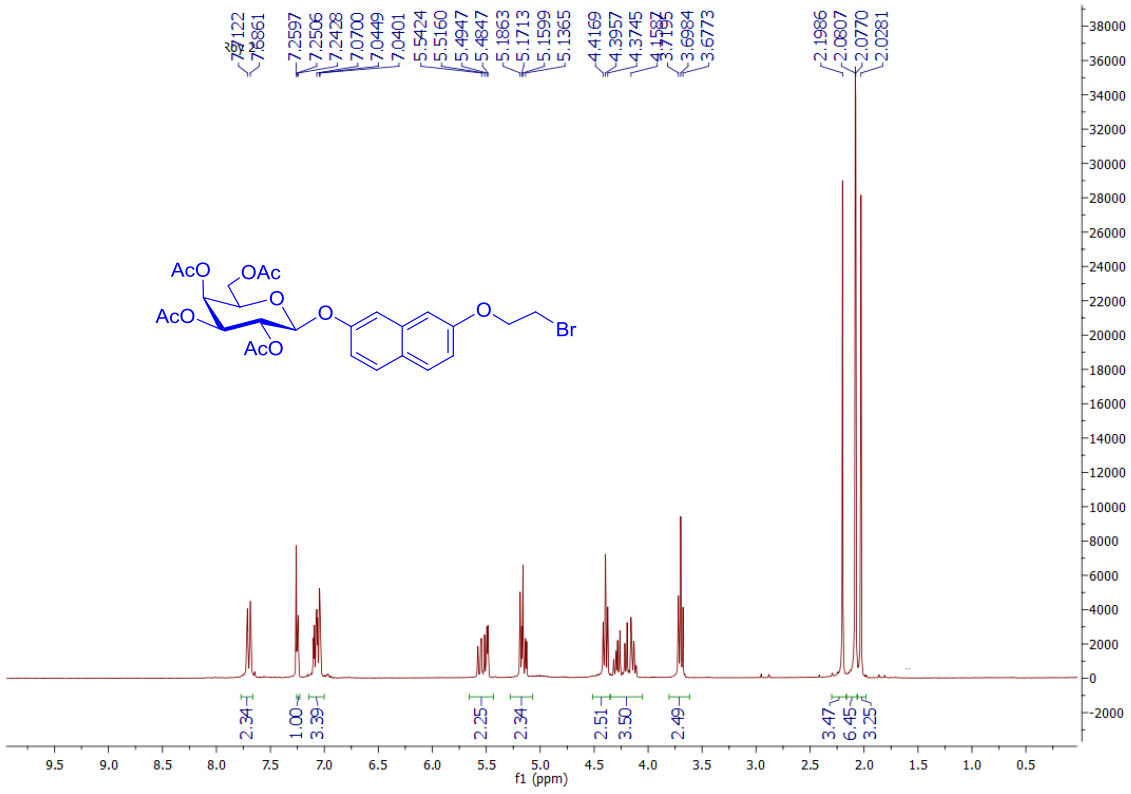


Figure S16. ^{1}H NMR spectrum of **9** (300 MHz, $CDCl_3$).

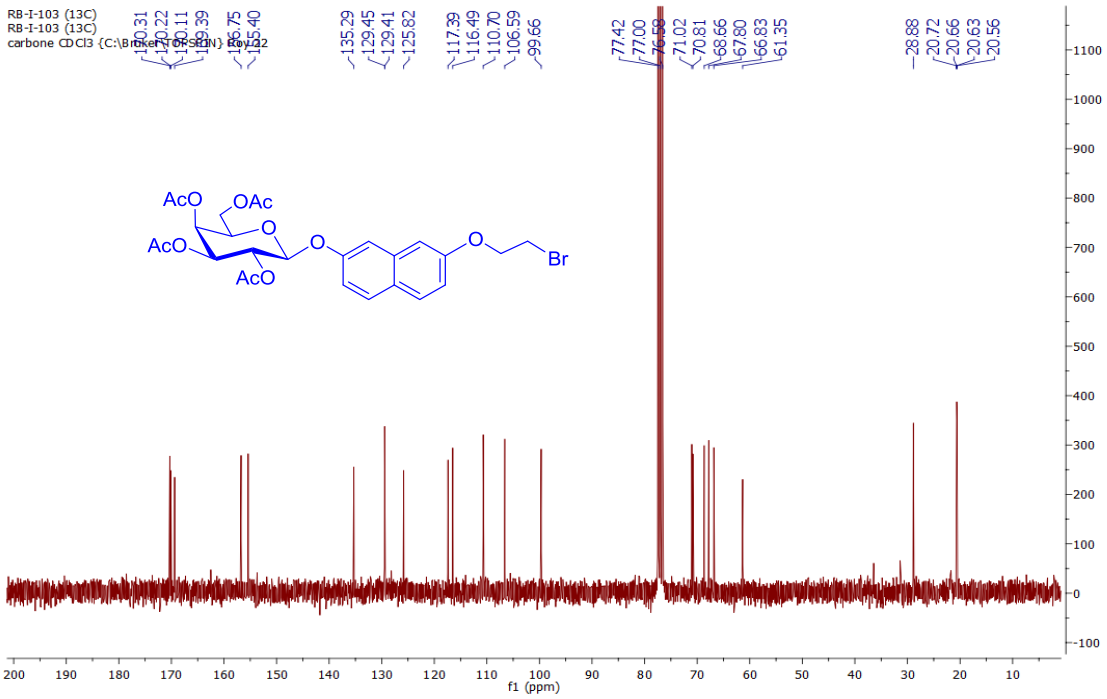


Figure S17. ^{13}C NMR spectrum of **9** (75 MHz, $CDCl_3$).

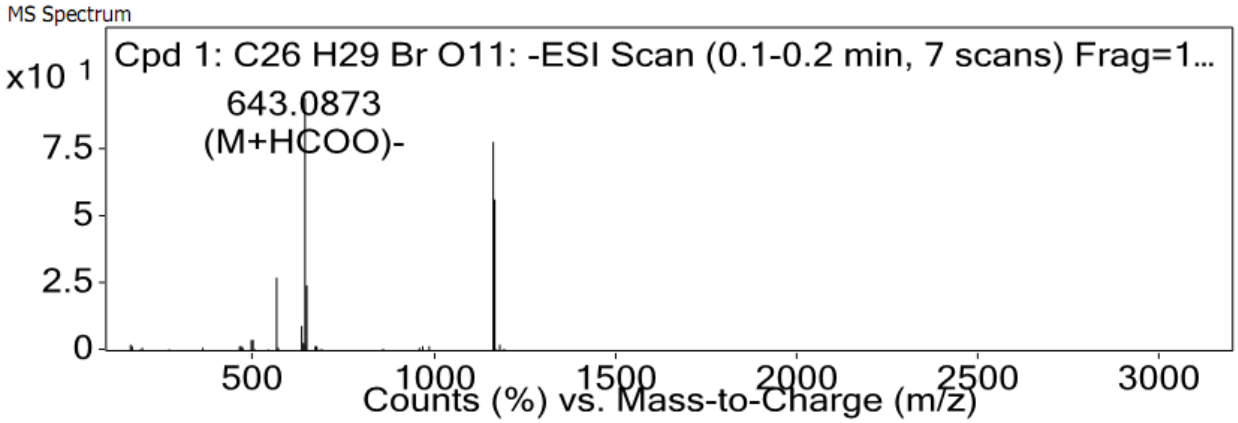


Figure S18. ESI-MS spectrum of **9**

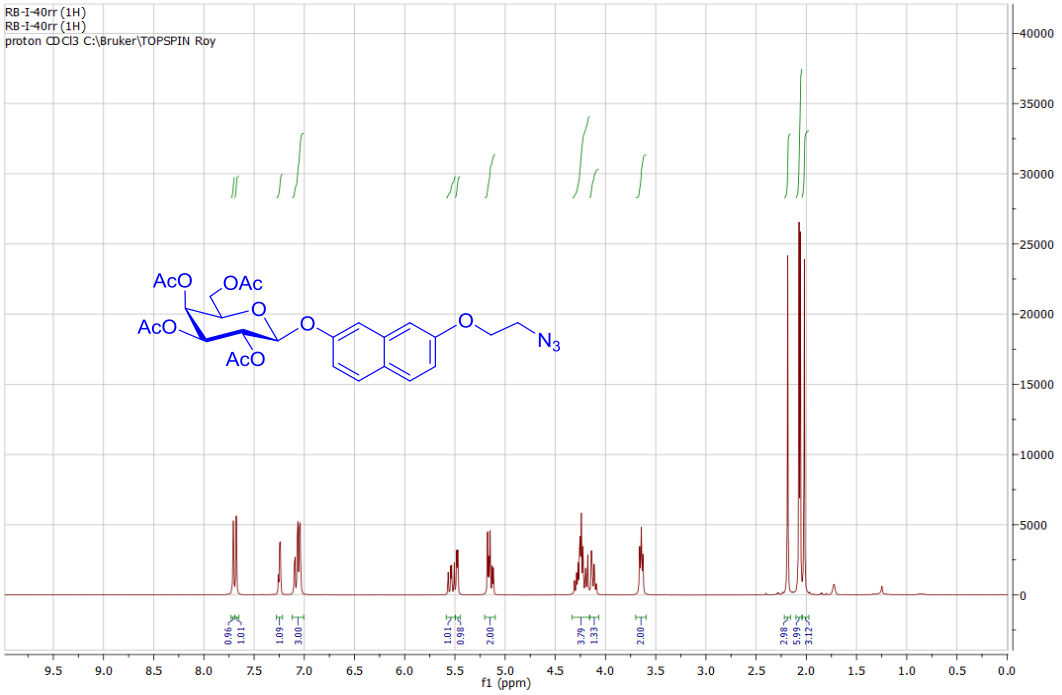


Figure S19. ^{1}H NMR spectrum of **10** (300 MHz, $CDCl_3$).

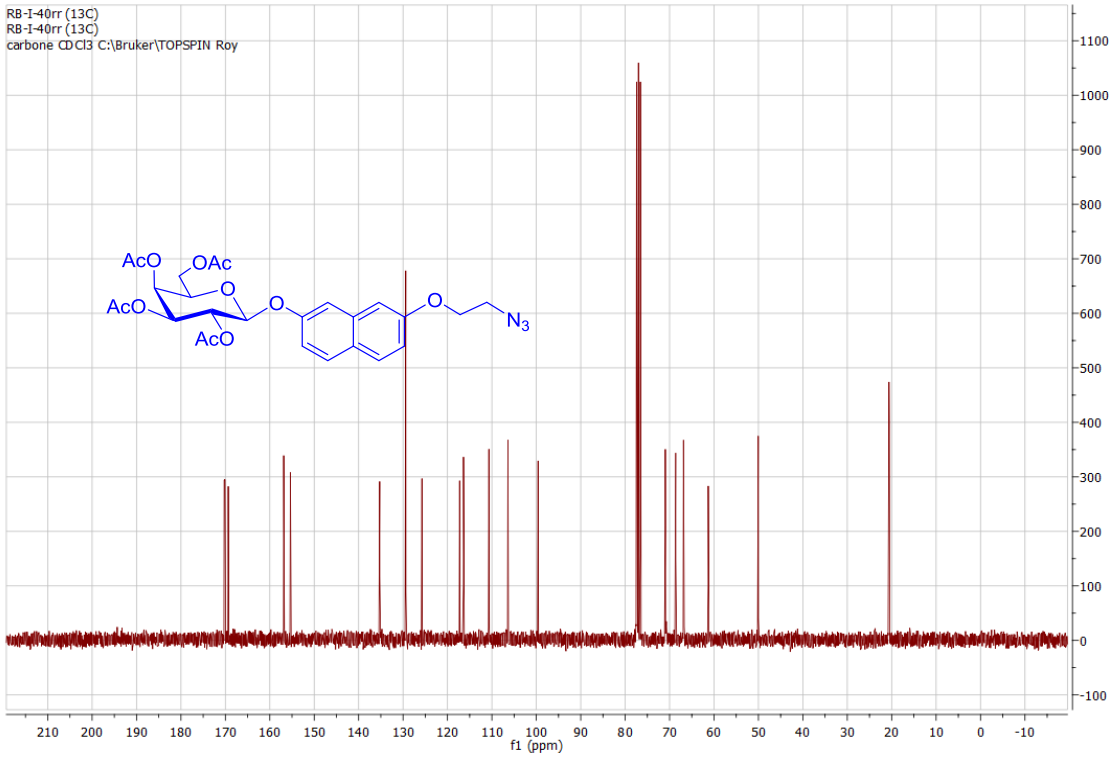


Figure S20. ^{13}C NMR spectrum of **10** (75 MHz, $CDCl_3$)

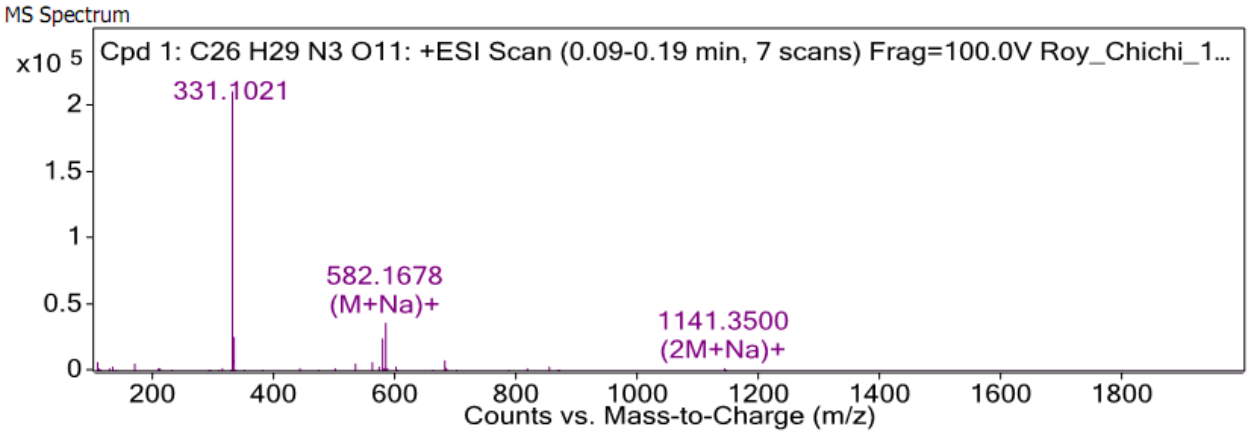


Figure S21. ESI-MS spectrum of compoud **10**

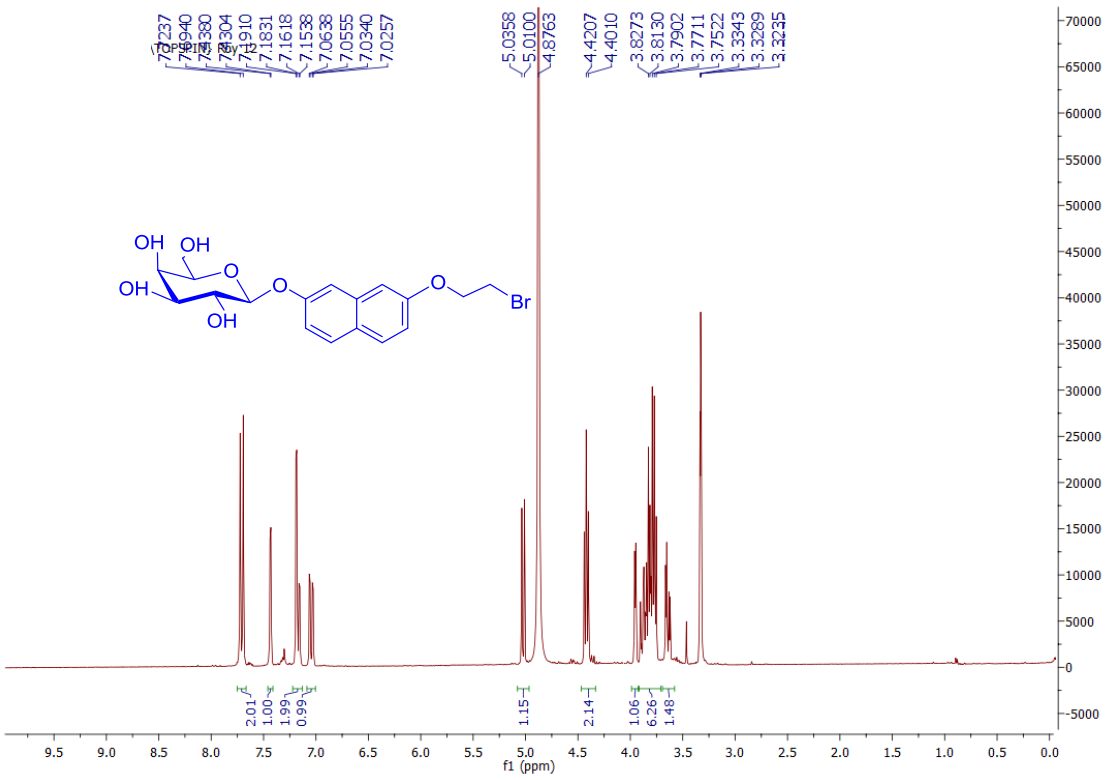


Figure S22. ^{1}H NMR spectrum of **11** (300 MHz, MeOH-d_4).

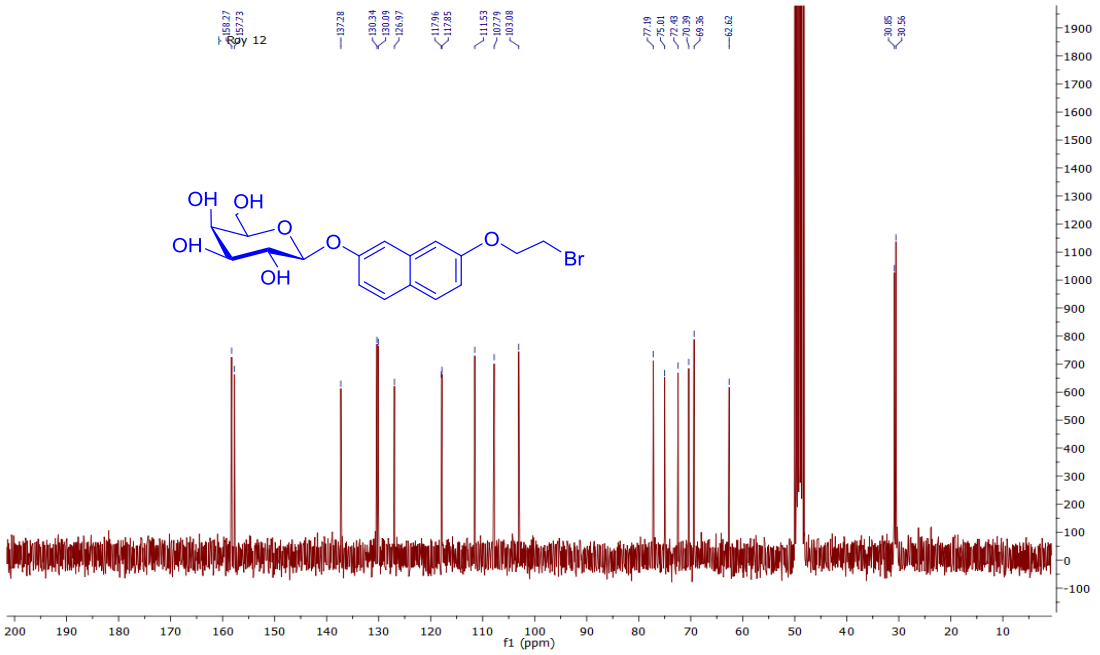


Figure S23. ^{13}C NMR spectrum of **11** (75 MHz, MeOH-d_4).

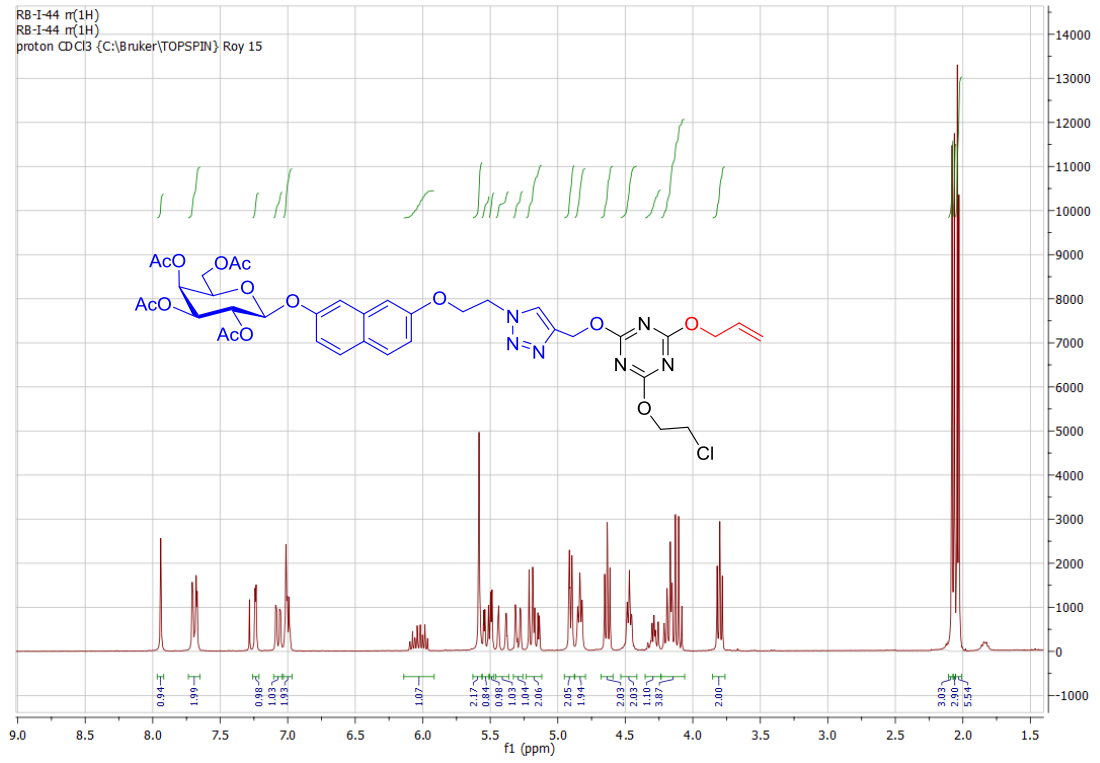


Figure S24. ^{1}H NMR Spectrum of **12** (300 MHz, $CDCl_3$)

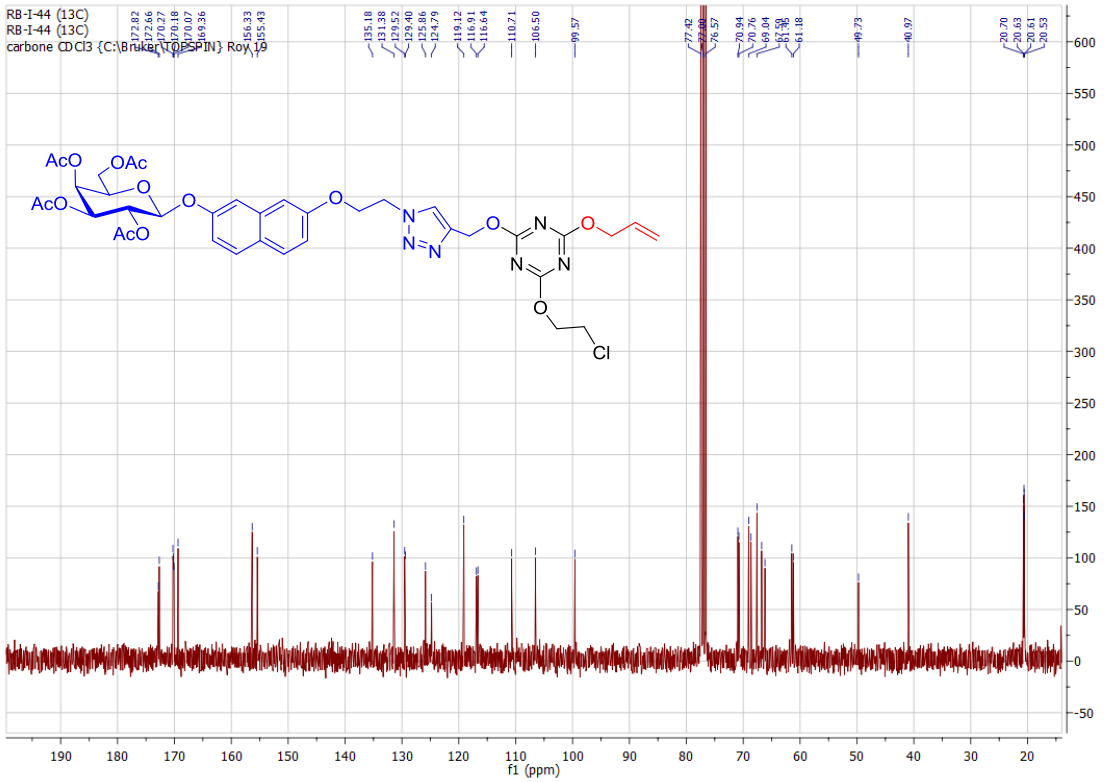


Figure S25. ^{13}C NMR spectrum of **12** (75 MHz, $CDCl_3$)

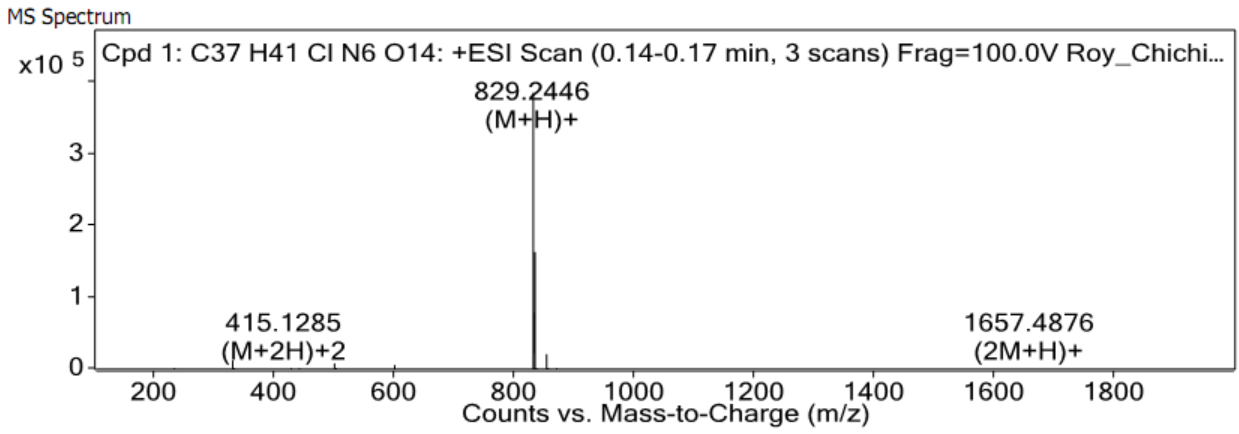


Figure S26. ESI-MS spectrum of compound **12**

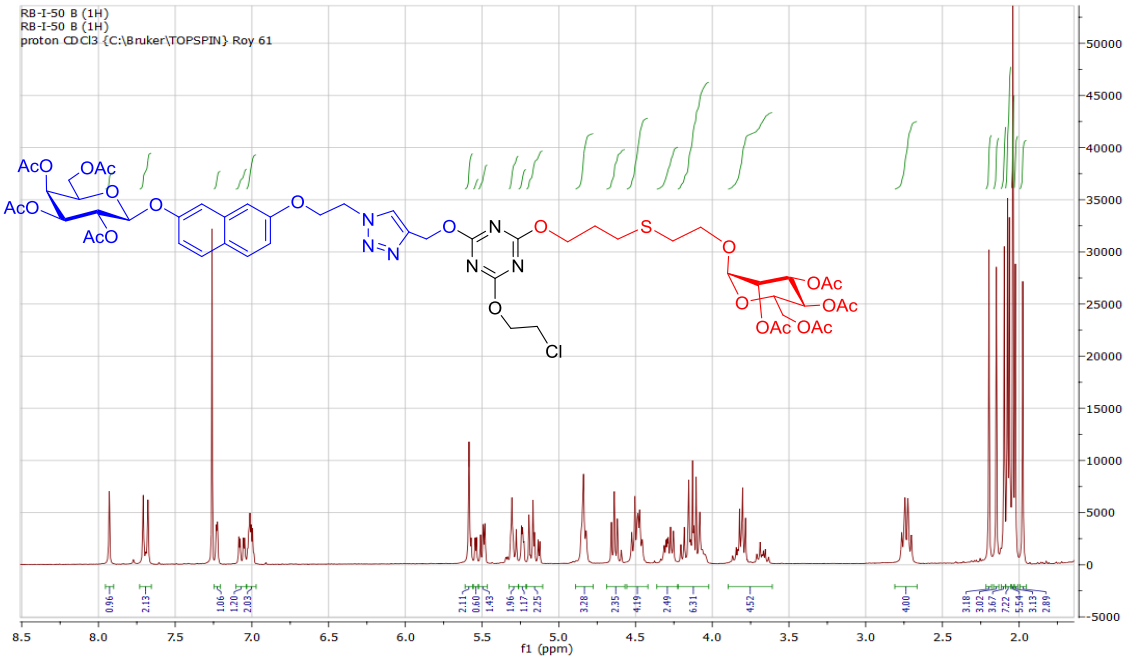


Figure S27. ^{1}H NMR Spectrum of **14** (300 MHz, $CDCl_3$)

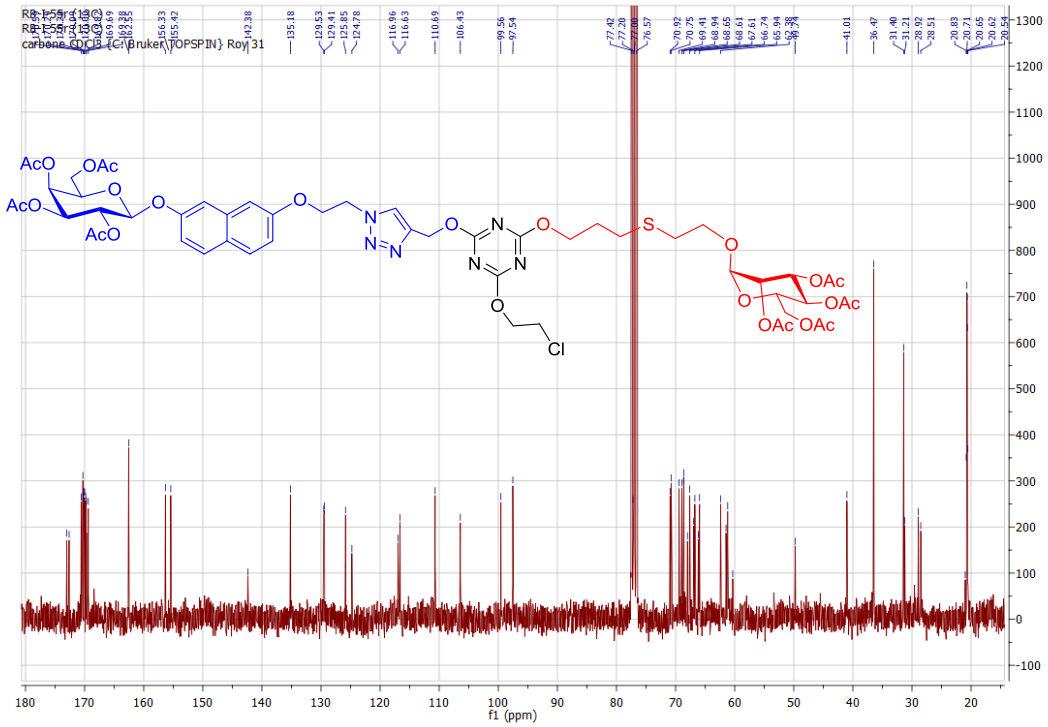


Figure S28. ^{13}C NMR Spectrum of **14** (75 MHz, $CDCl_3$)

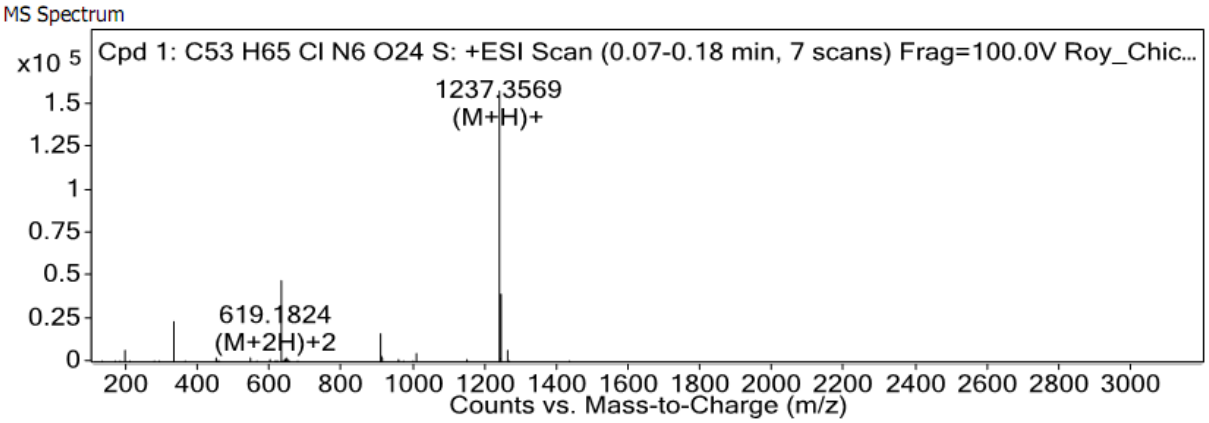


Figure S29. ESI-MS spcterum of compound **14**

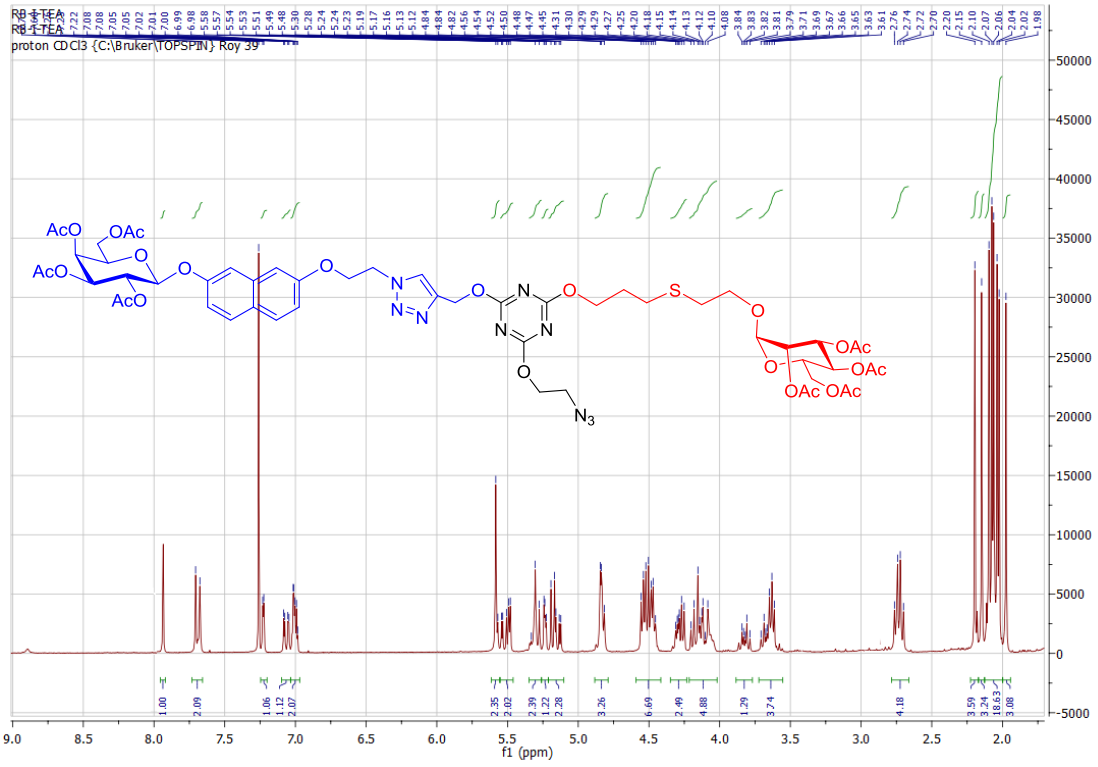


Figure S30. ^{1}H NMR Spectrum of **15** (300 MHz, $CDCl_3$)

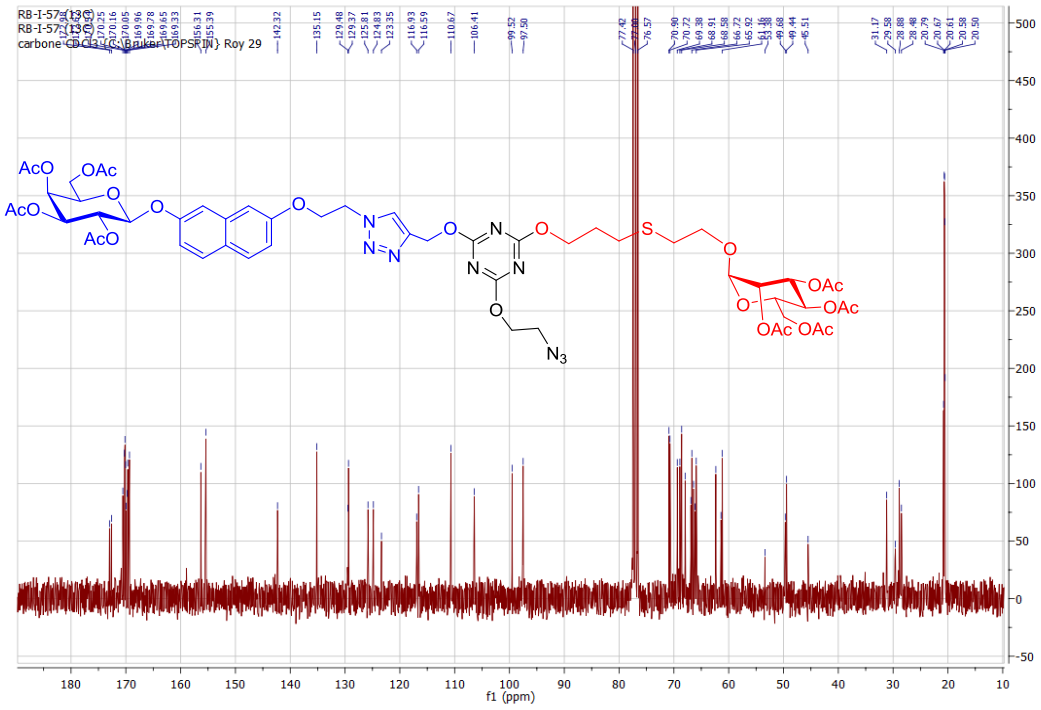


Figure S31. ^{13}C NMR Spectrum of **15** (75MHz, $CDCl_3$)

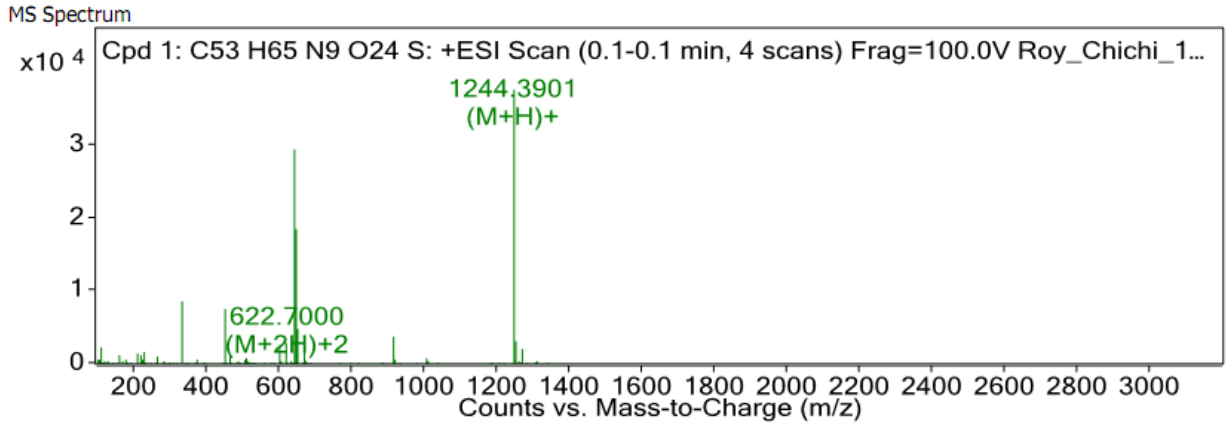


Figure S32. HRMS spectrum of compound **15**

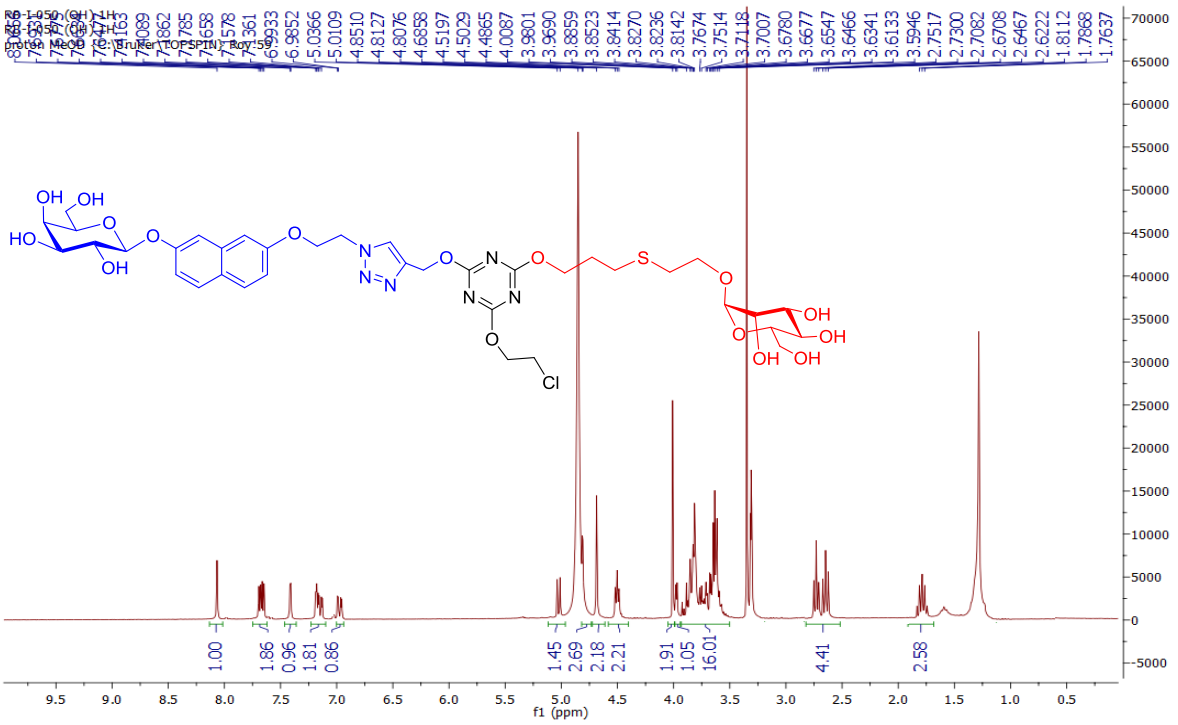


Figure S33. ^{1}H NMR Spectrum of **16** (300MHz, MeOH-d_4)

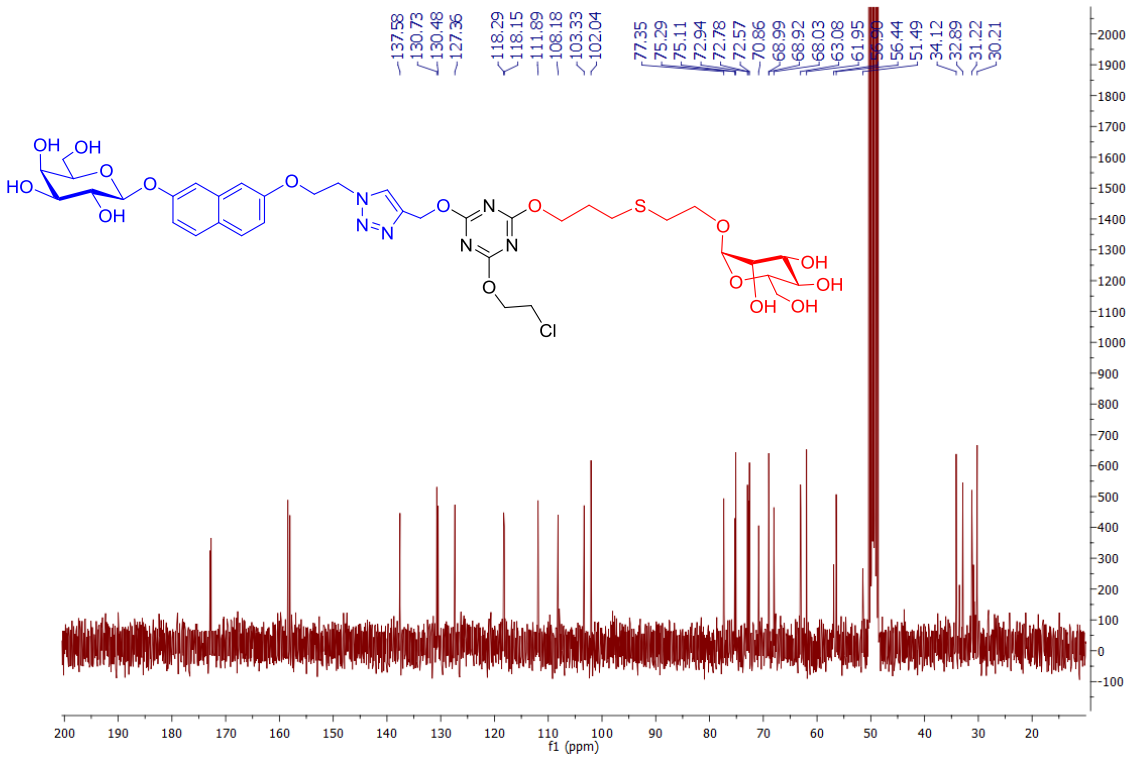


Figure S34. ^{13}C NMR spectrum of **16** (75 MHz, MeOH-d_4)

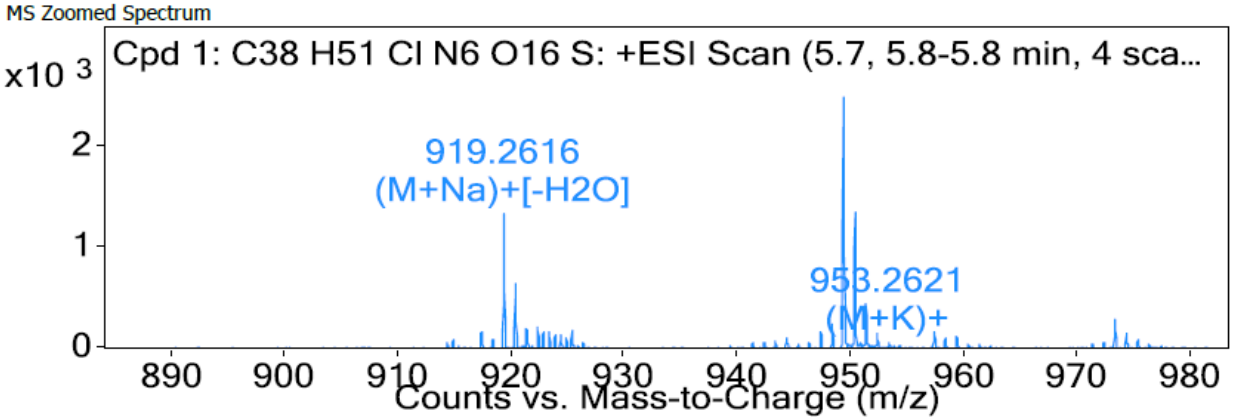


Figure S35. HRMS of compound **16**

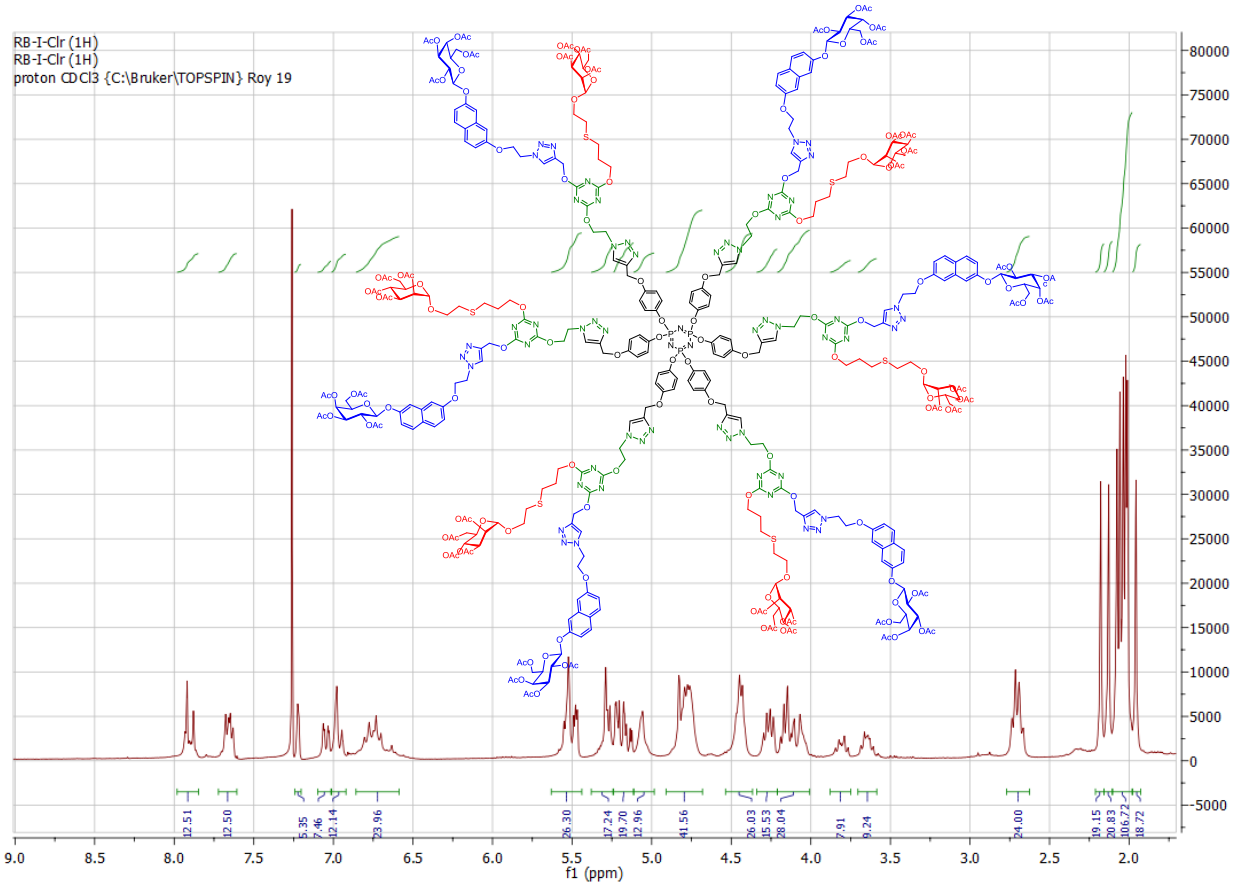


Figure S36. ^{1}H NMR spectrum of **18** (300 MHz, $CDCl_3$)

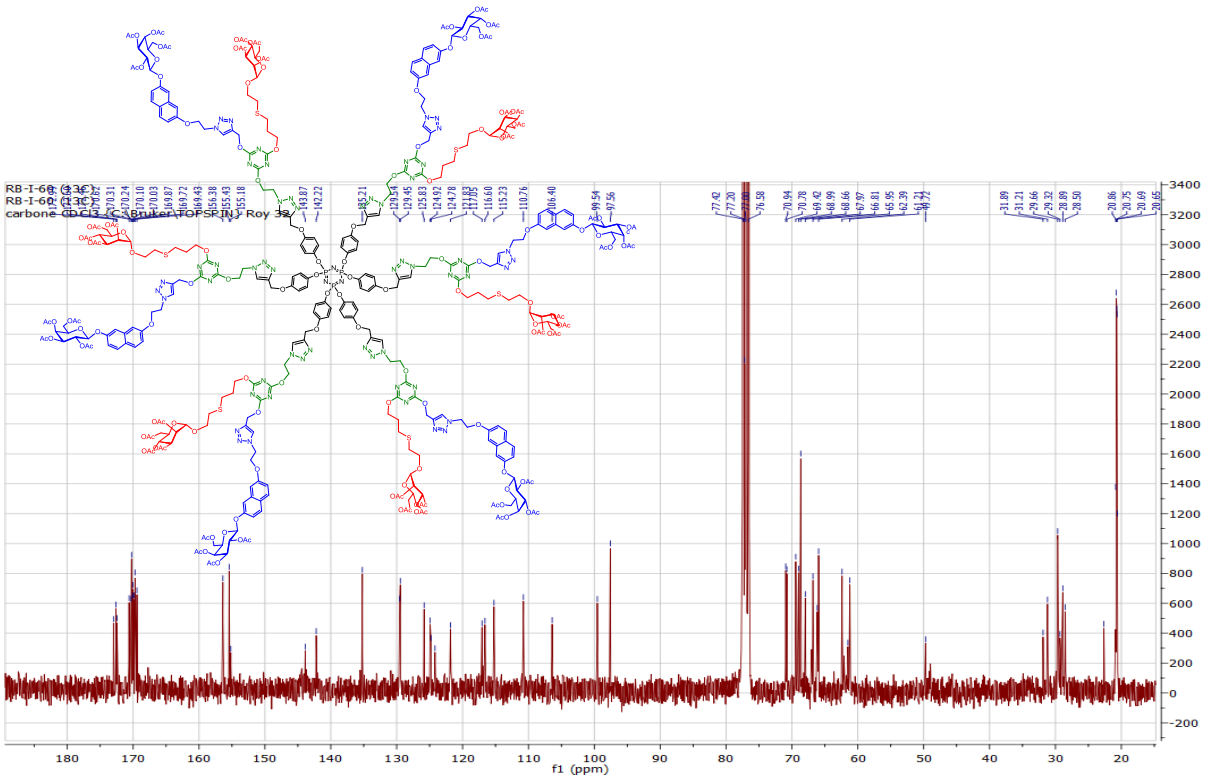


Figure S37. ^{13}C NMR spectrum of **18** (75 MHz, $CDCl_3$)

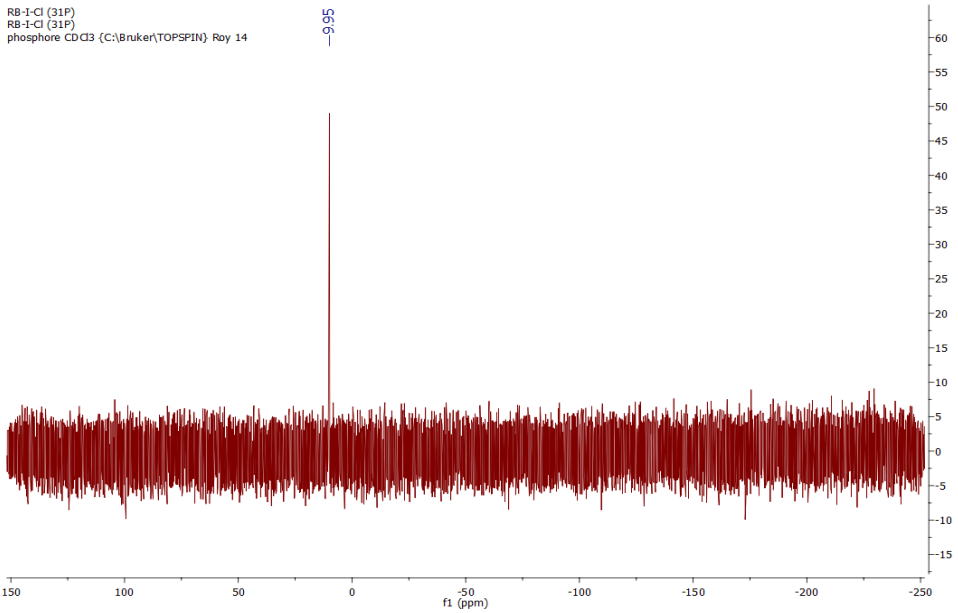


Figure S38. $^{31}P\{^{1}H\}$ NMR spectrum of **18** (122 MHz, $CDCl_3$)

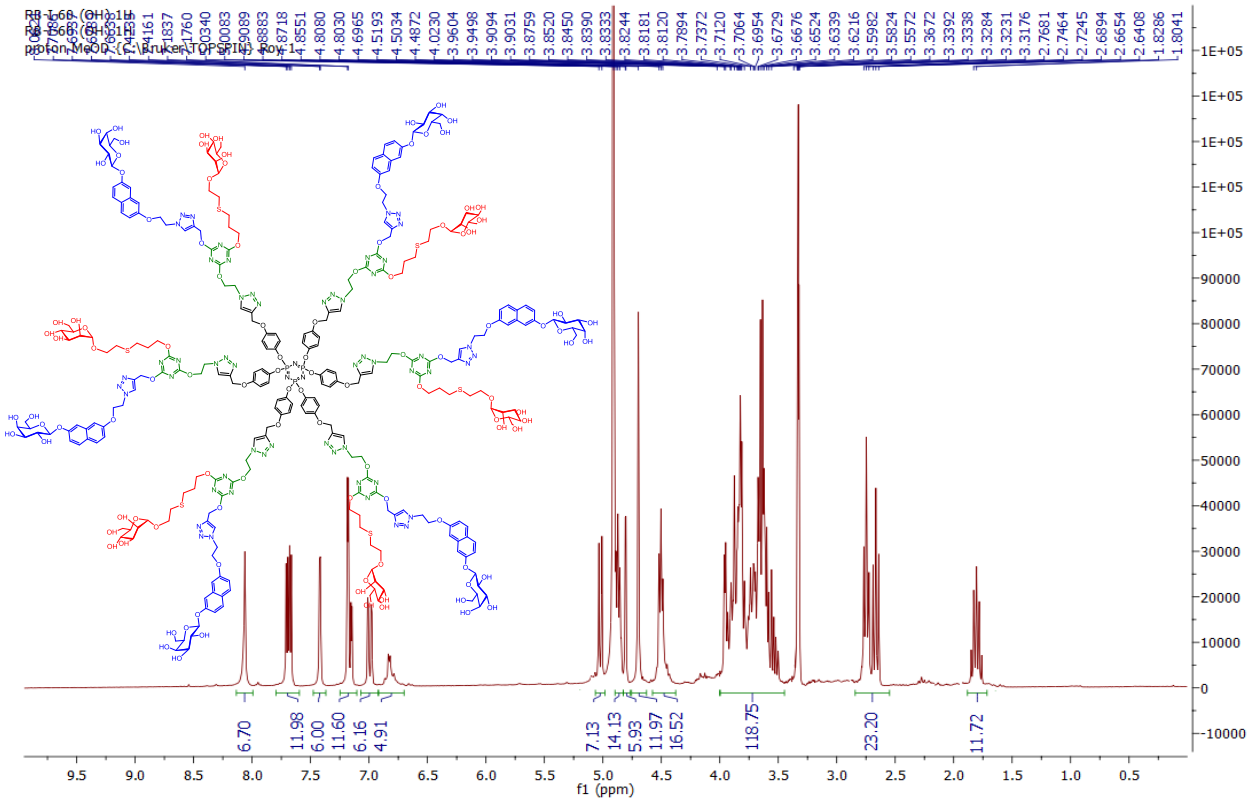


Figure S39. ^{1}H NMR spectrum of **19** (300 MHz, MeOH-d_4)

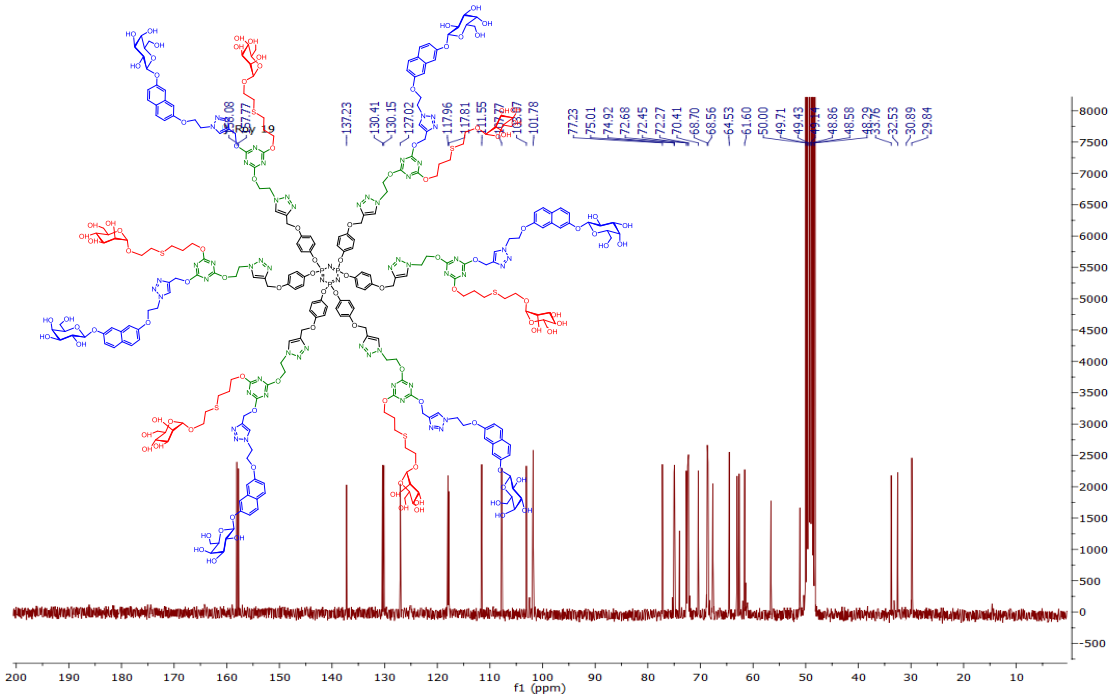


Figure S40. ^{13}C NMR spectrum of **19** (75 MHz, MeOH-d_4)

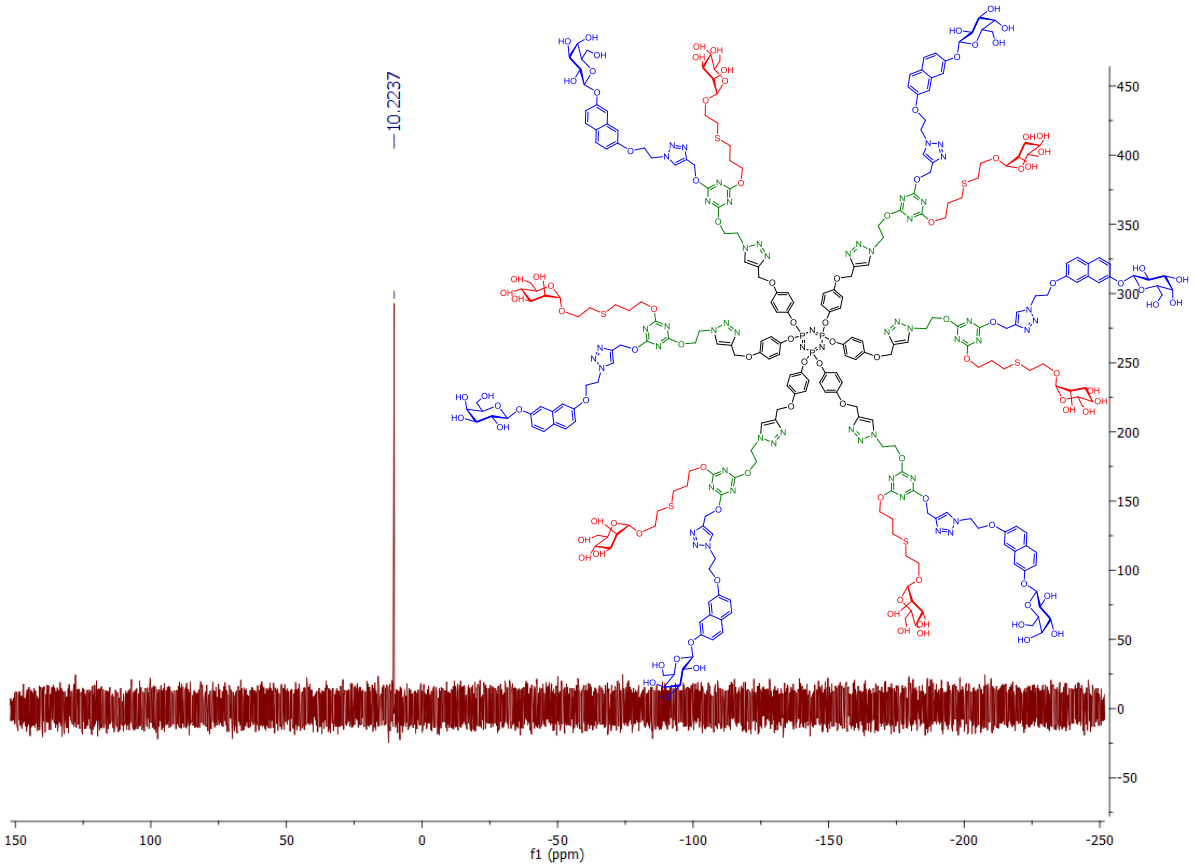


Figure S41. $^{31}P\{^{1}H\}$ NMR spectrum of **19** (122 MHz, MeOH-d_4)

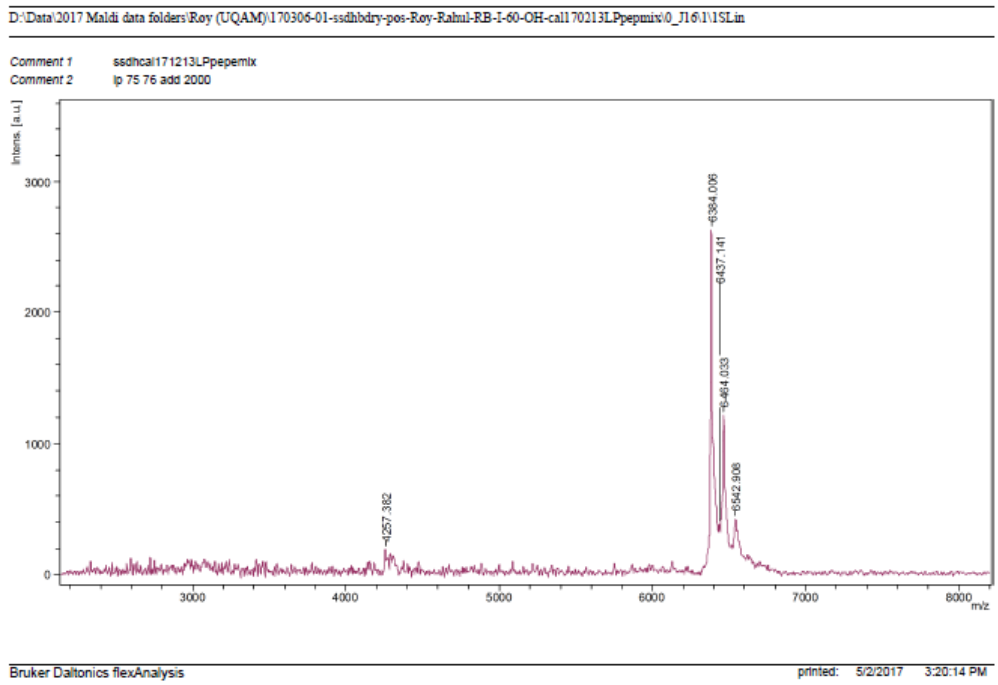


Figure S42. MALDI-TOF spectrum of **19**

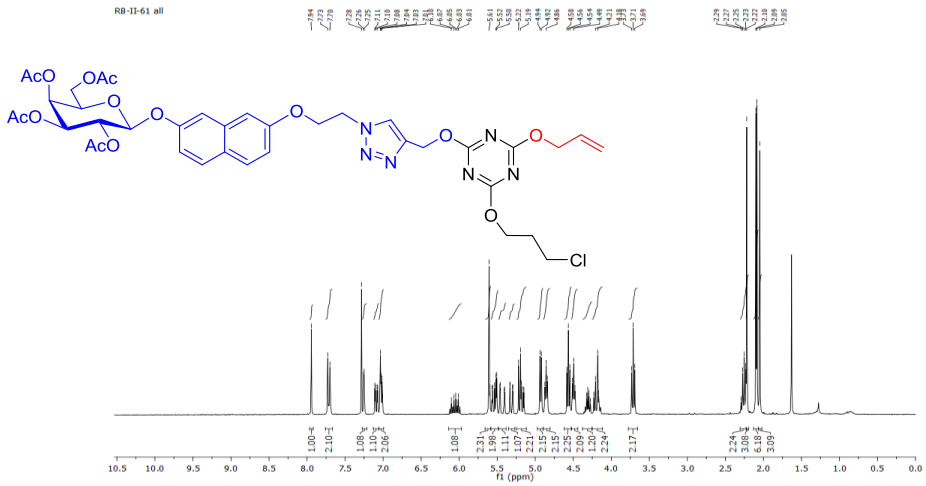


Figure S43. ^{1}H NMR spectrum of **20** (300 MHz, $CDCl_3$)

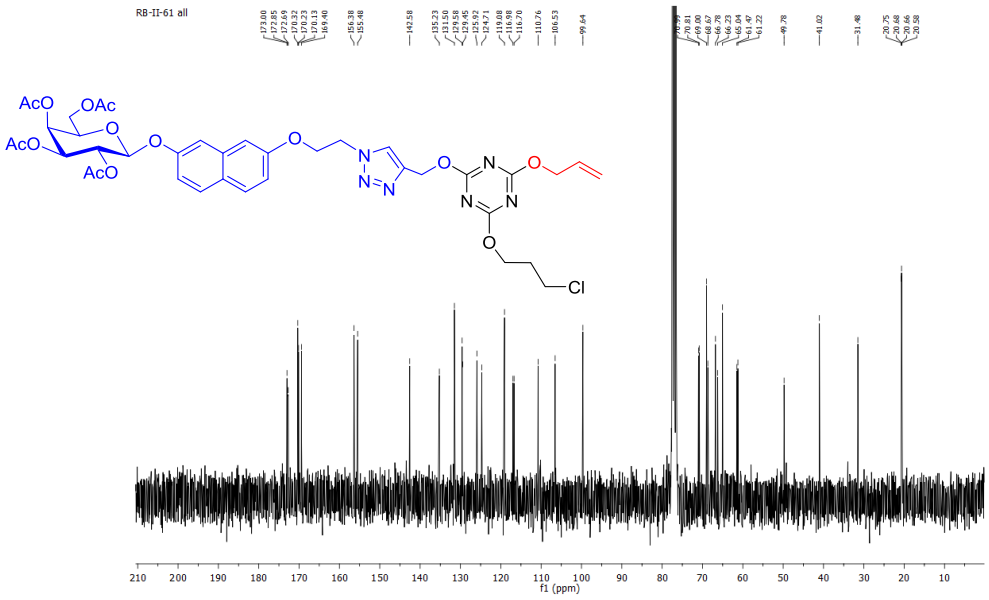


Figure S44. ^{13}C NMR spectrum of **20** (75 MHz, $CDCl_3$)

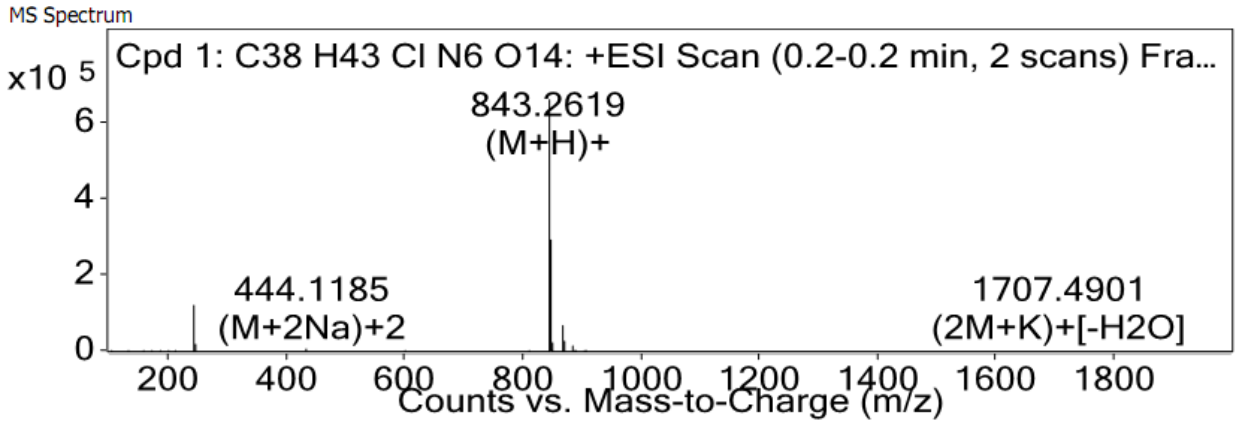


Figure S45. HRMS spectrum of compound **20**

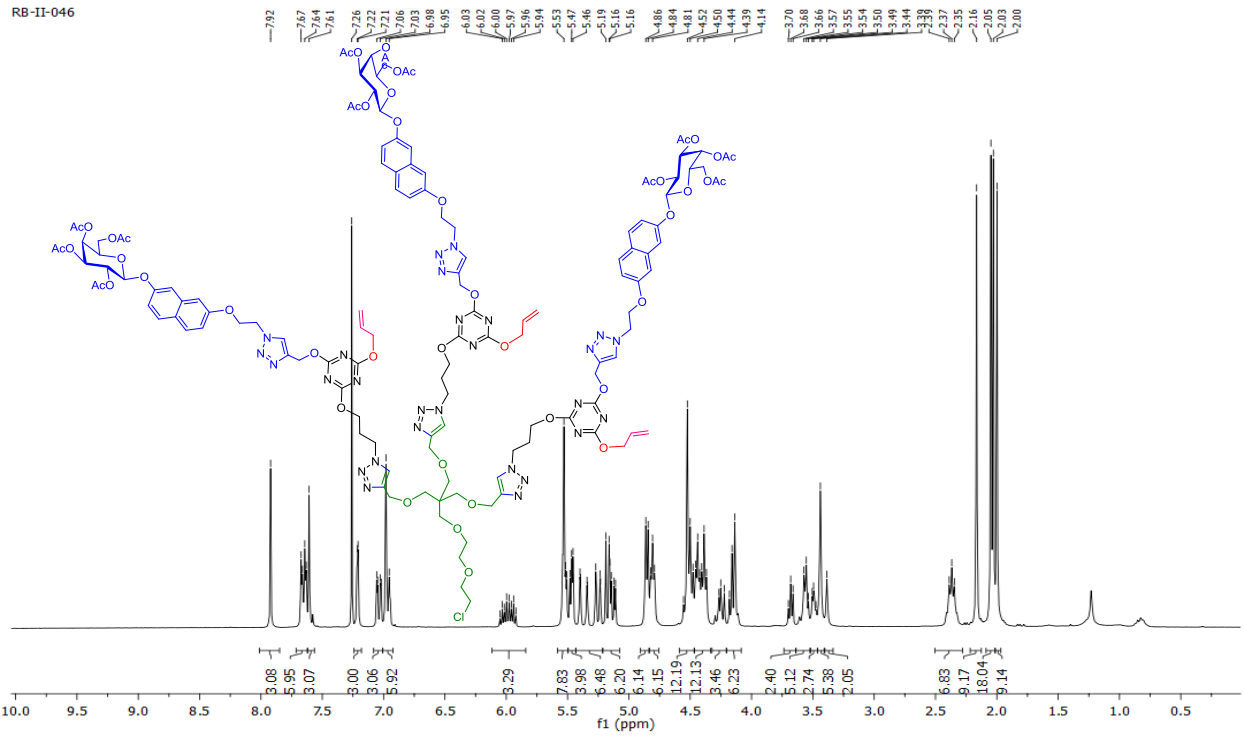


Figure S46. ^{1}H NMR of Dendron **23**(300 MHz, $CDCl_3$)

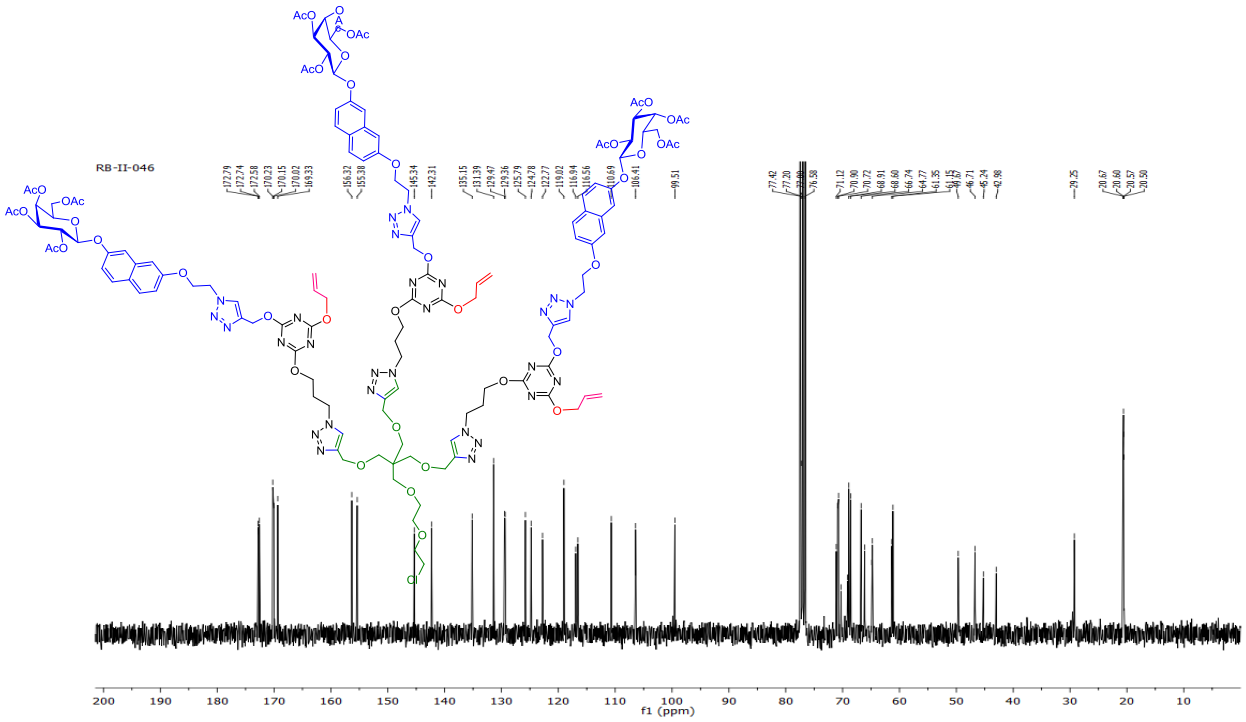


Figure S47. ^{13}C NMR spectrum of Dendron **23** (75 MHz, $CDCl_3$) \

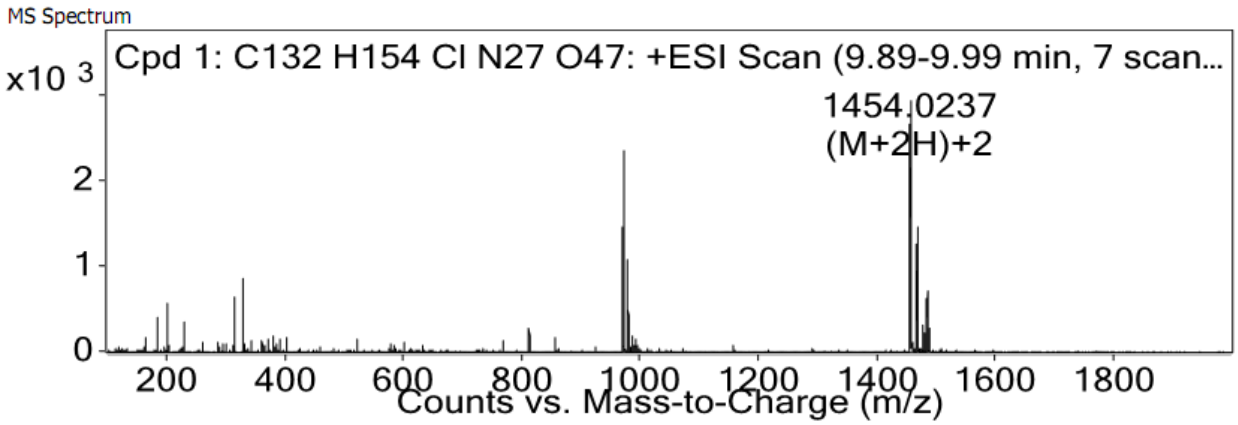


Figure S48. HRMS spectrum of compound **23**

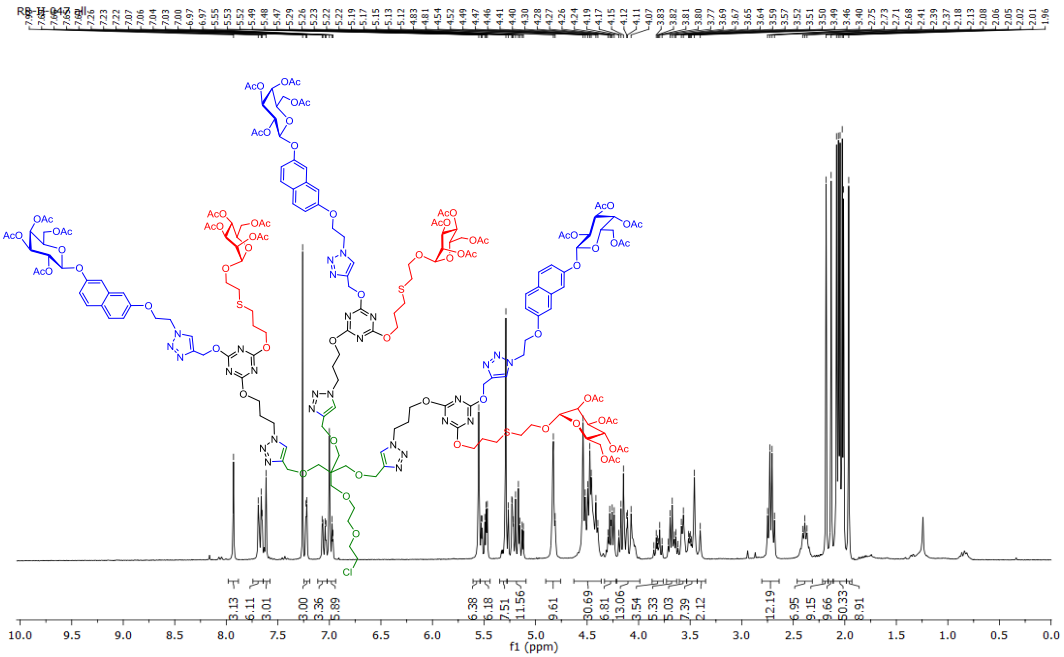


Figure S49. ^{1}H NMR of Dendron **24** (300 MHz, $CDCl_3$)]

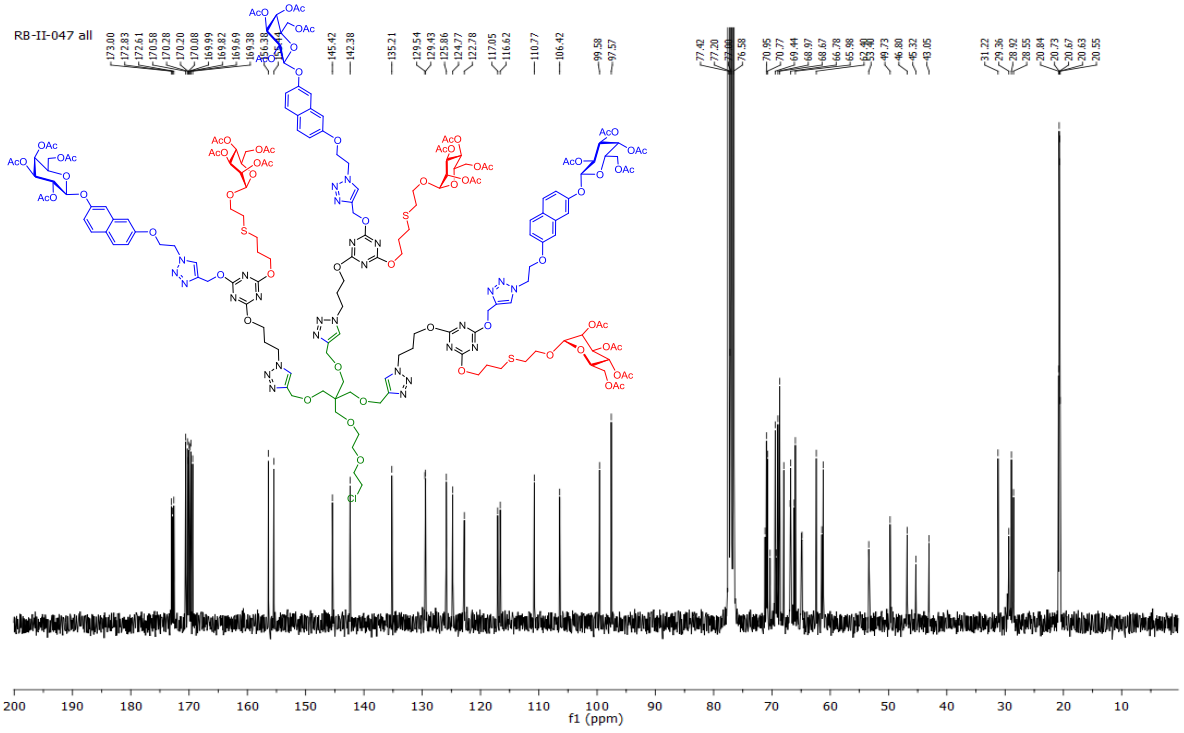
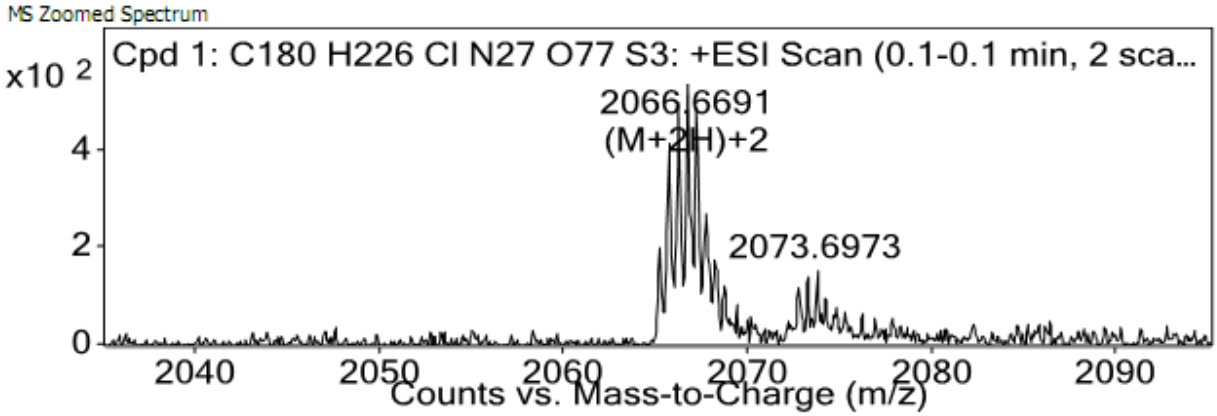


Figure S50. ^{13}C NMR spectrum of dendron **24** (75 MHz, $CDCl_3$)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
338.3402			1	3647		
610.1825			1	10231		
611.1833			1	6031		
612.18			1	4746		
684.2002			1	5795		
685.2019			1	4274		
686.1964			1	3036		
758.2202			1	3998		
759.2164			1	2972		
2065.1538	2065.1797	-12.58	2	206	C180 H228 Cl N27 O77 S3	(M+2H)+2

--- End Of Report ---

Figure S51. HRMS spectrum of compoud **24**

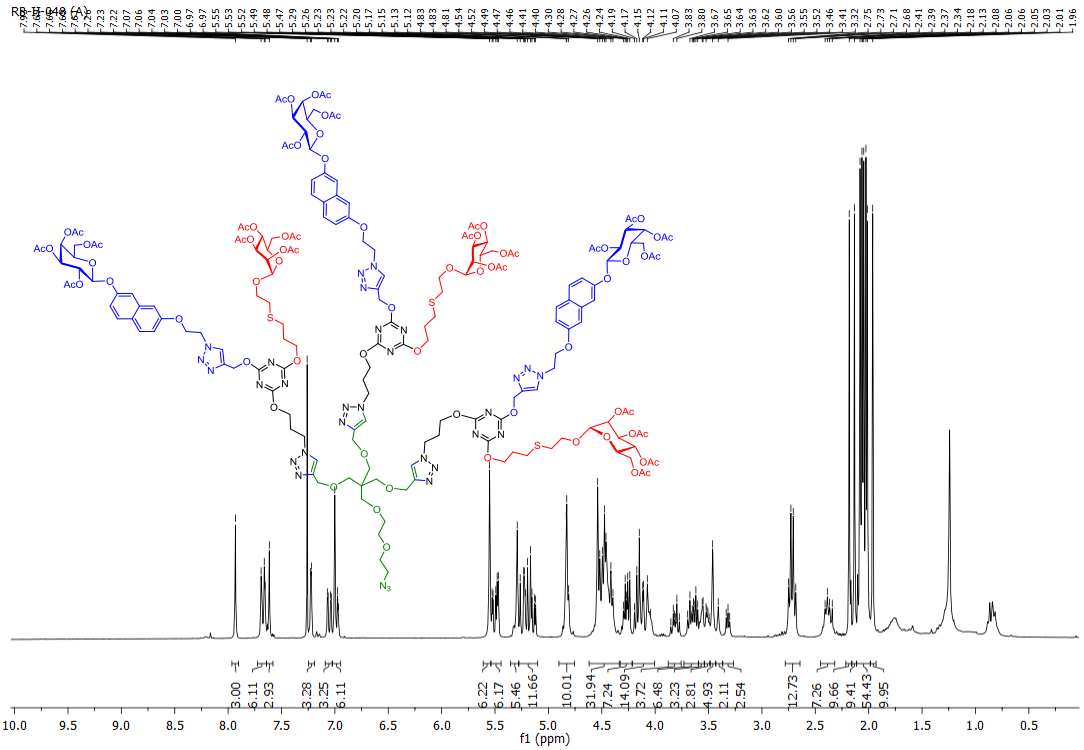


Figure S52. ^{1}H NMR spectrum of dendron **25** (300 MHz, $CDCl_3$)

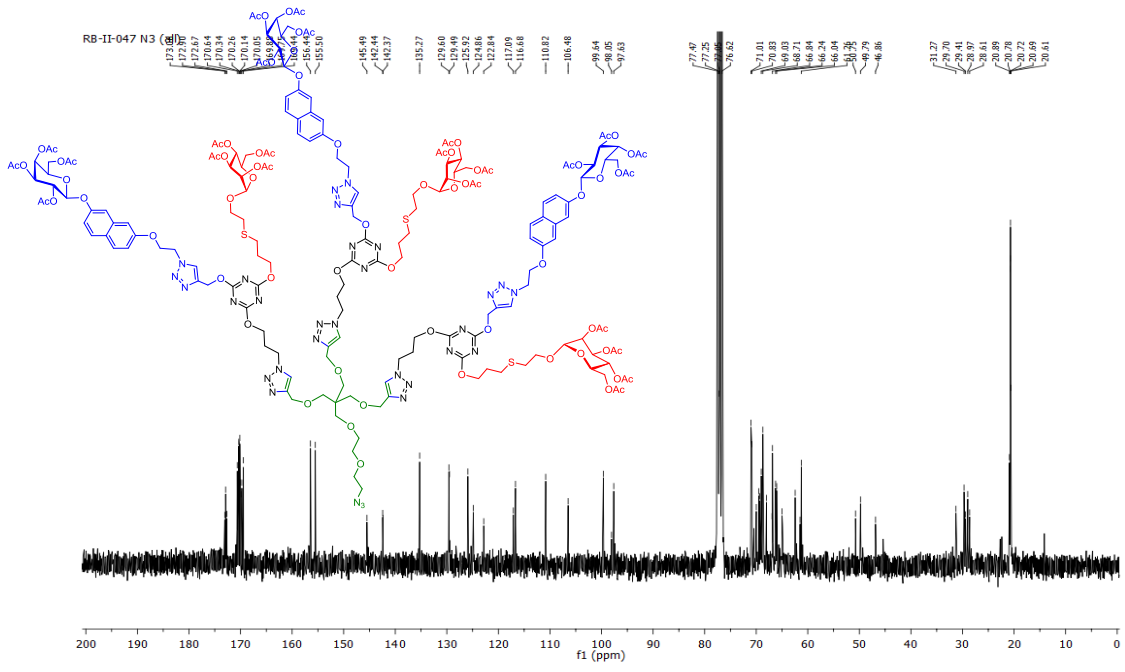
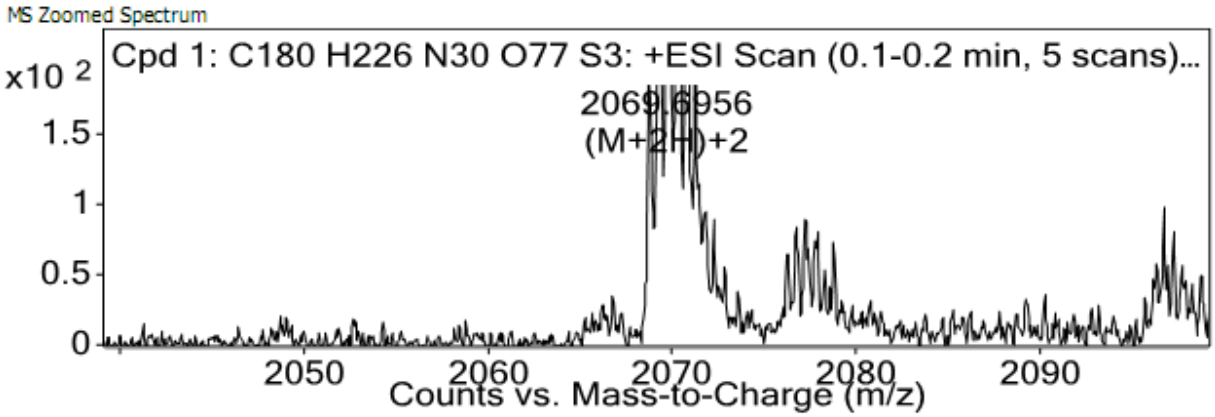


Figure S53. ^{13}C NMR spectrum of dendron **25** (75 MHz, $CDCl_3$)

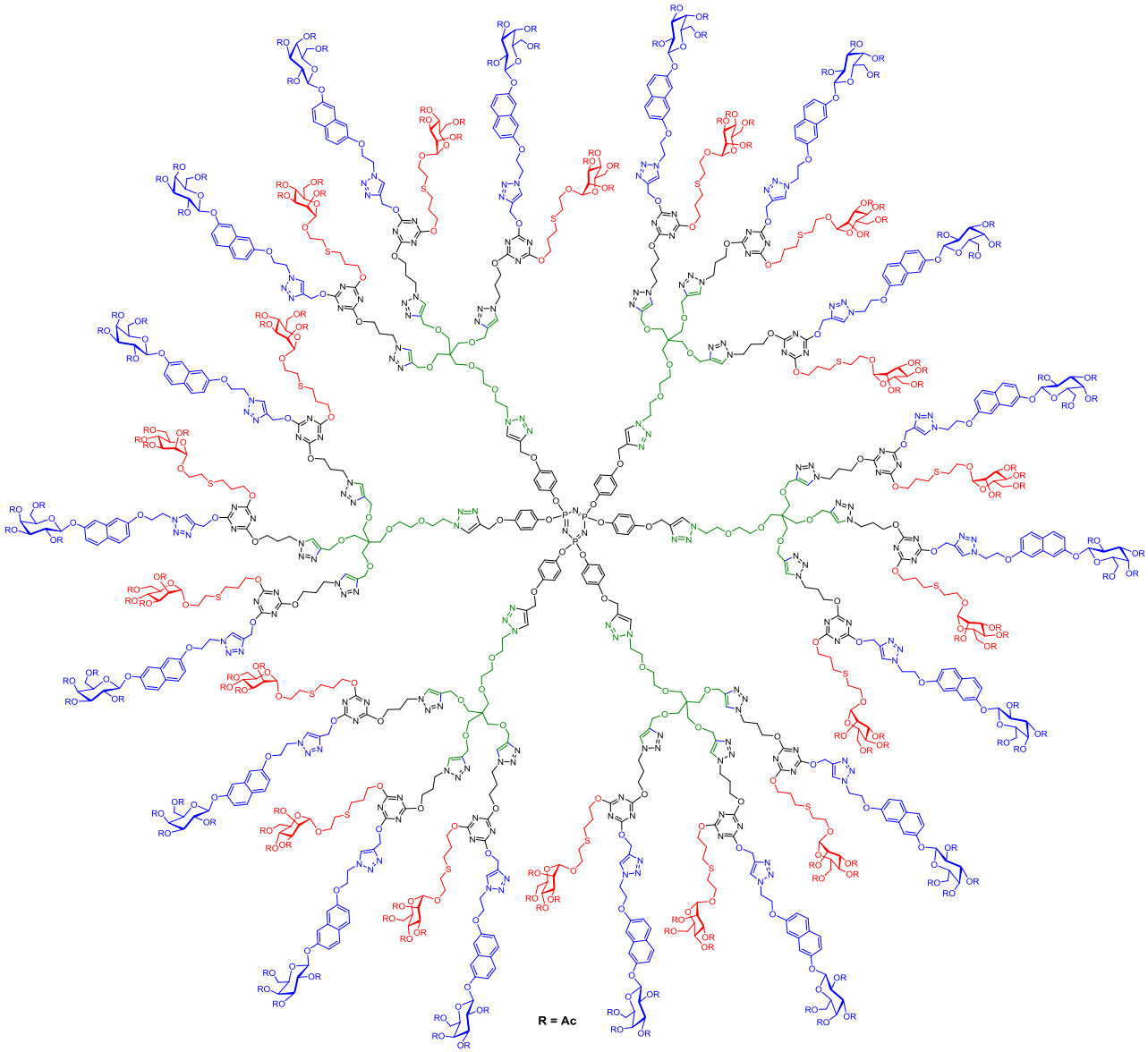


MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
109.0245				790		
109.9423				445		
110.0202				10156		
110.15				353		
110.5219				1220		
111.0189				1626		
112.0169				535		
2069.1782	2069.2015	-11.23	2	445	C180 H228 N30 O77 S3	(M+2H)+2
2069.6956	2069.7026	-3.39	2	496	C180 H228 N30 O77 S3	(M+2H)+2
2070.2258	2070.2037	10.69	2	402	C180 H228 N30 O77 S3	(M+2H)+2

--- End Of Report ---

Figure S54. HRMS spectrum of compound **25**


R = Ac

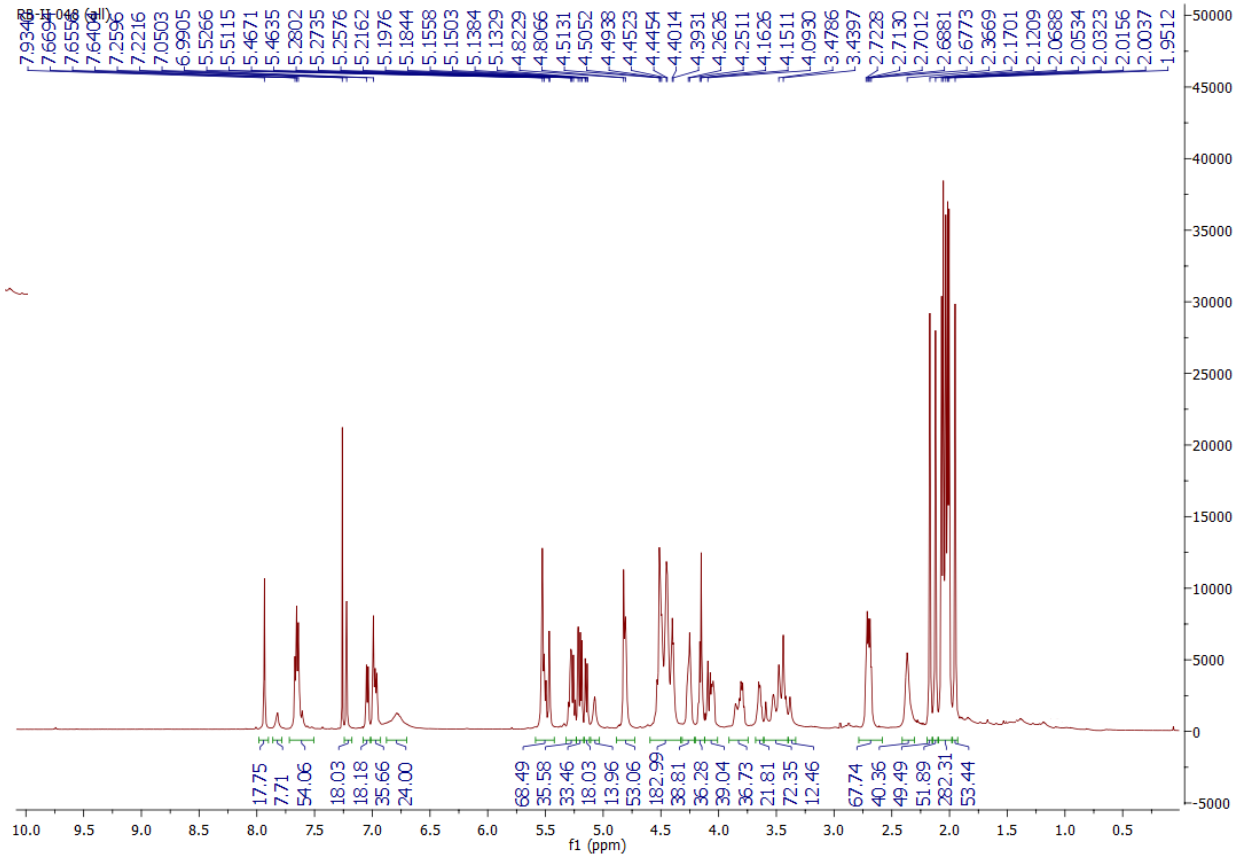


Figure S55. ^{1}H NMR spectrum of second generation hybrid dendrimer **26 (**600 MHz, $CDCl_3$**)**

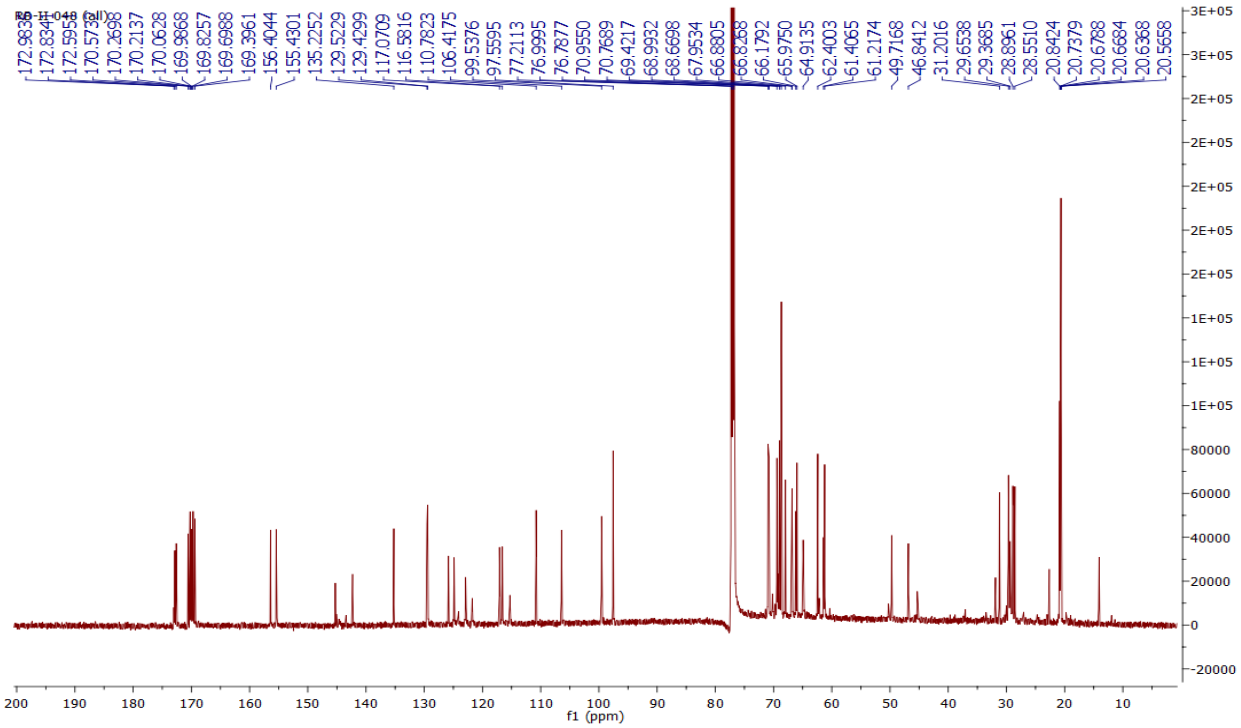


Figure S56. ^{13}C NMR spectrum of second generation hybrid dendrimer **26 (**150 MHz, $CDCl_3$**)**

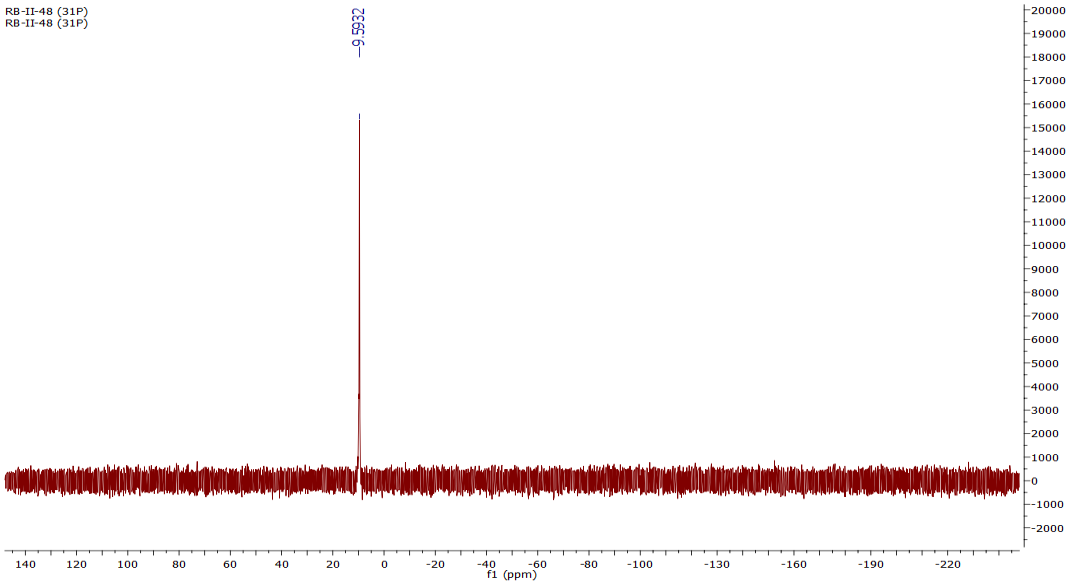


Figure S57. $^{31}P\{^{1}H\}$-NMR spectrum of second generation hybrid dendrimer **26 (**122 MHz, $CDCl_3$**)**

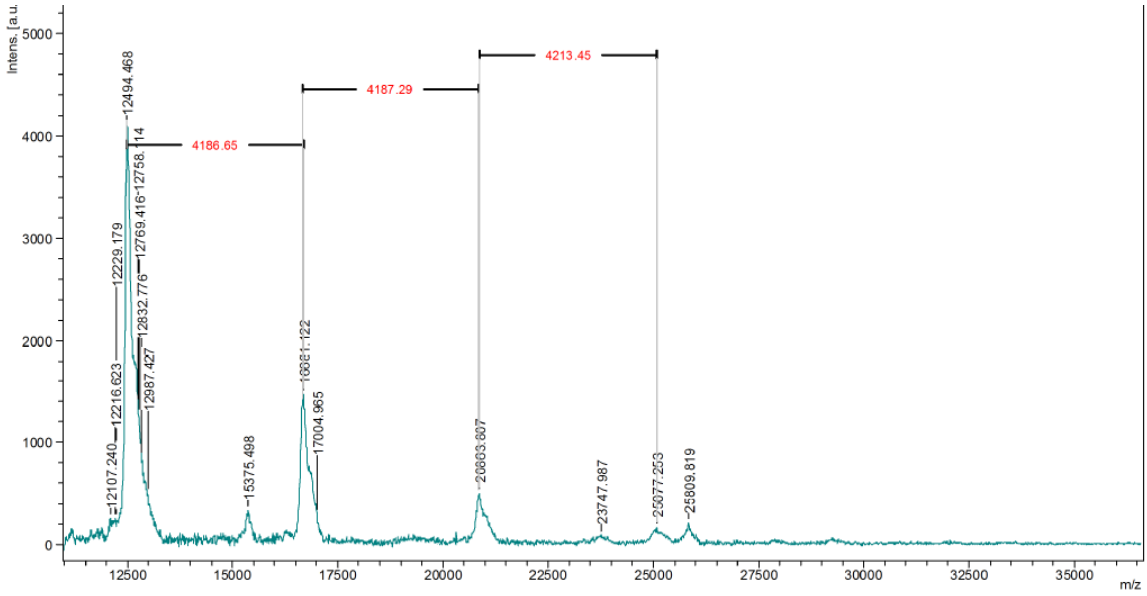
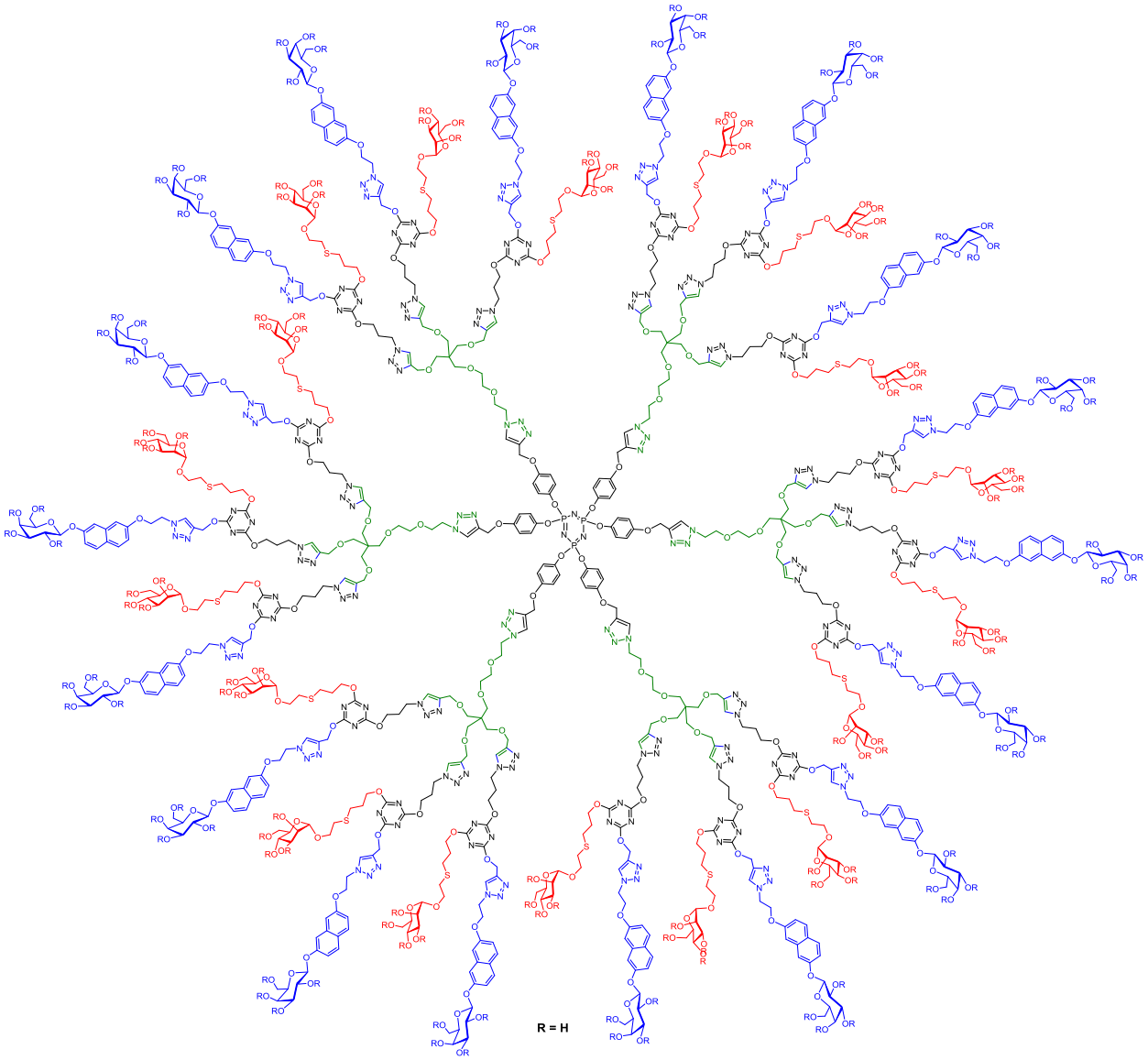


Figure S58. MALDI-TOF analysis of compound **26**


R = H

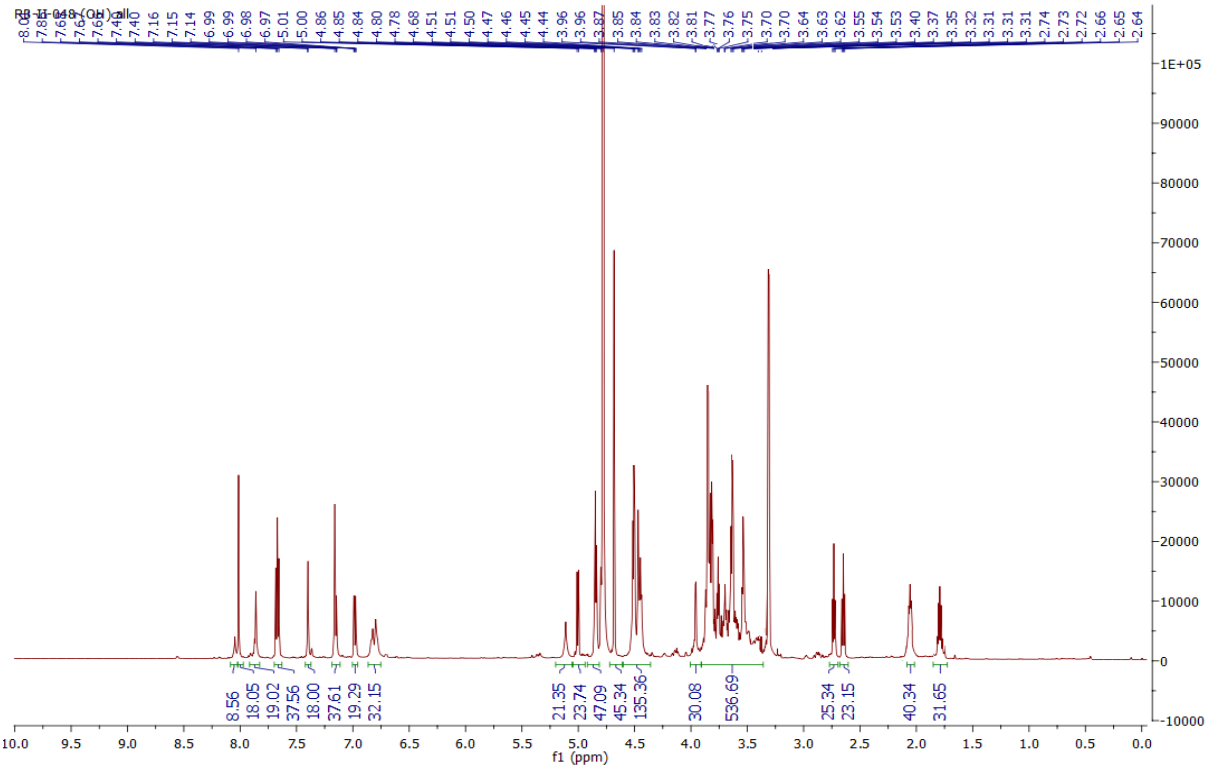


Figure S59. ^{1}H NMR spectrum of second generation hybrid dendrimer **27** (600 MHz, MeOH-d_4)

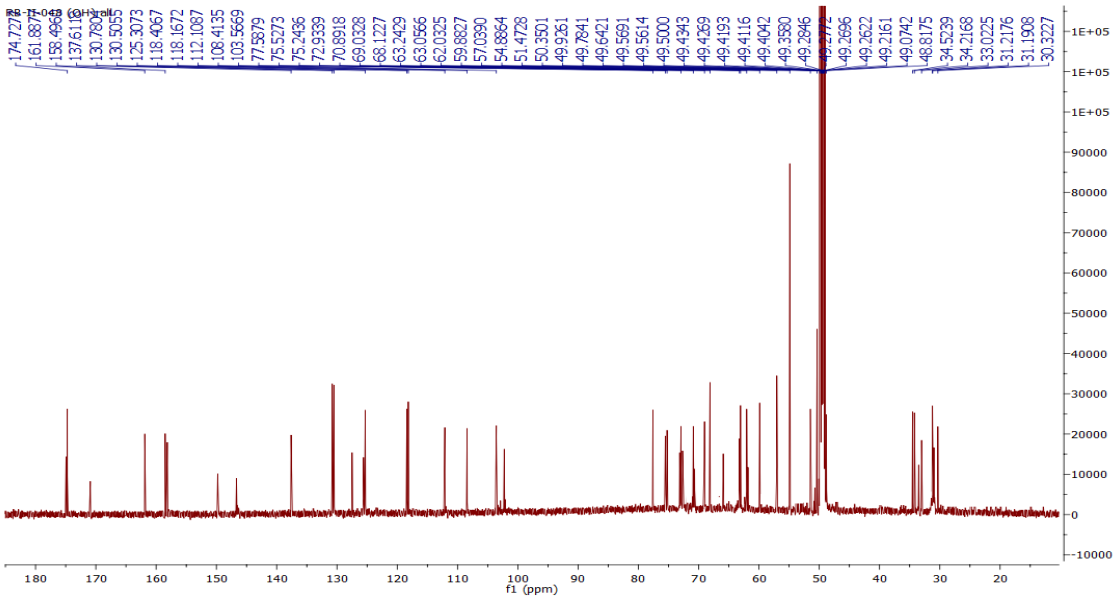


Figure S60. ^{13}C NMR spectrum of second generation hybrid dendrimer **27** (150 MHz, MeOH-d_4)

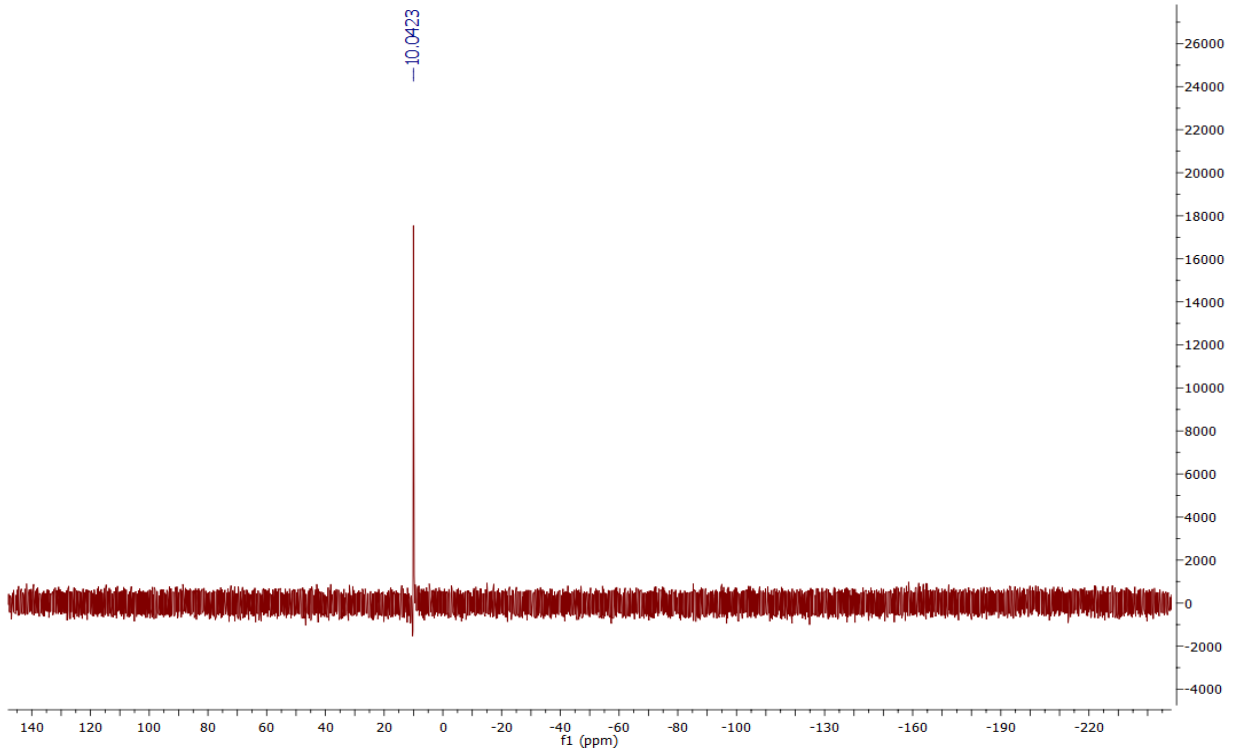


Figure S61. $^{31}P\{^{1}H\}$ NMR spectrum of second generation hybrid dendrimer **27 (**122 MHz, MeOH-d_4**).**

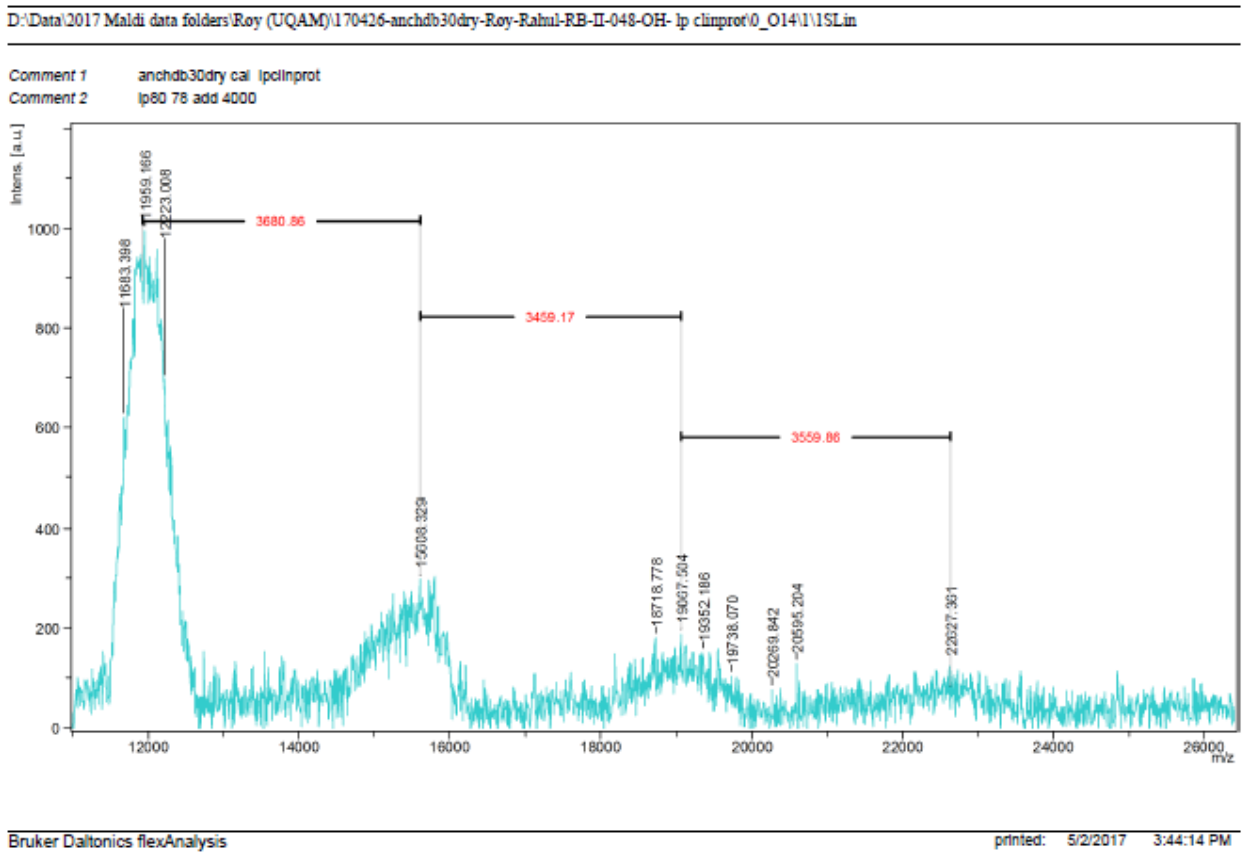


Figure S62. MALDI-TOF analysis of **27**

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	206.6	Peak 1:	176.4	100.0	46.53
PdI:	0.021	Peak 2:	0.000	0.0	0.000
Intercept:	0.942	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

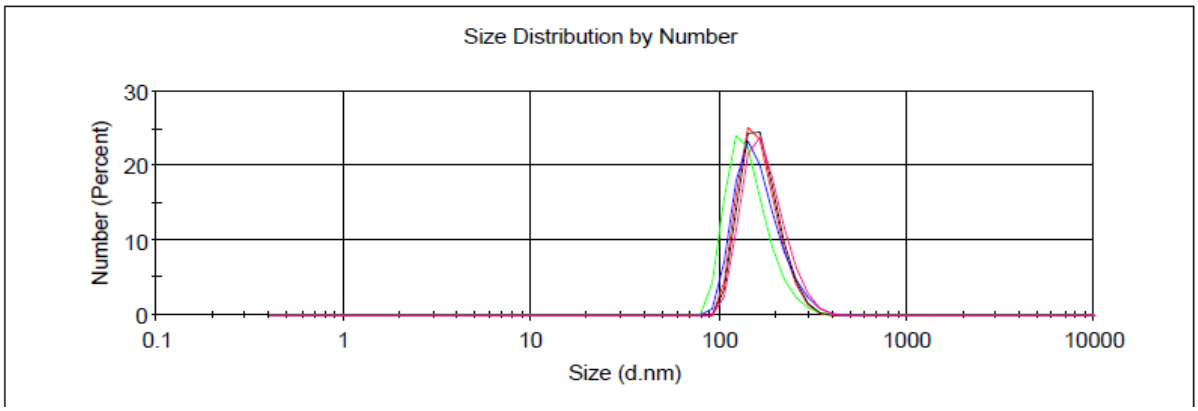


Figure S63. DLS curves of kinetics of ConA in the presence of monomer **16** as function of time (curves for few initial points are shown).

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	196.9	Peak 1:	153.1	100.0	47.10
PdI:	0.055	Peak 2:	0.000	0.0	0.000
Intercept:	0.922	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

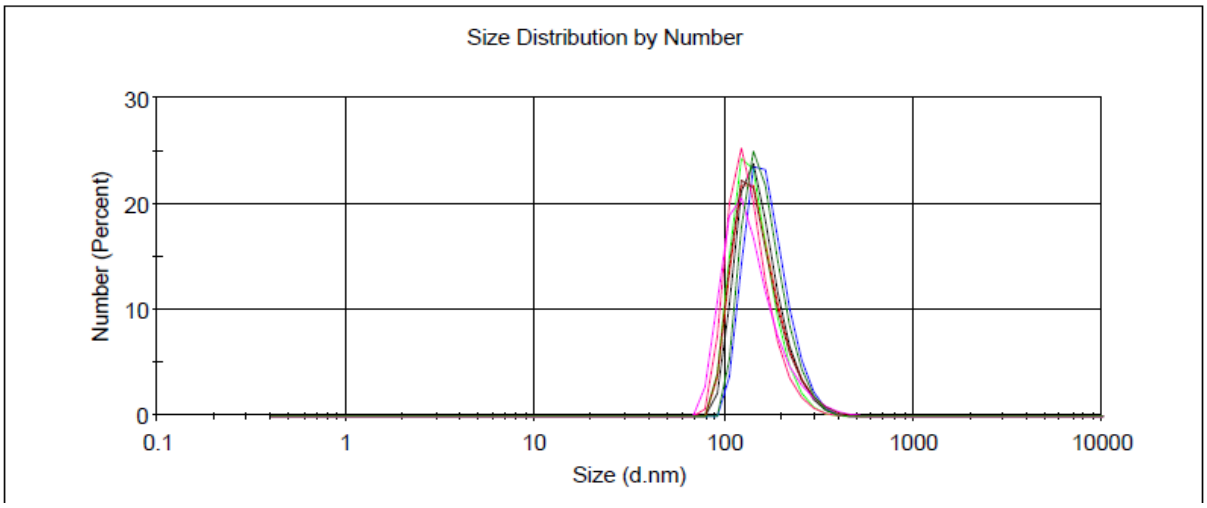


Figure S64. DLS curves of kinetics of LecA in the presence of monomer **16** as function of time (curves for few initial points are shown).

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	291.3	Peak 1:	221.1	100.0	55.85
PdI:	0.340	Peak 2:	5227	0.0	718.9
Intercept:	0.941	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

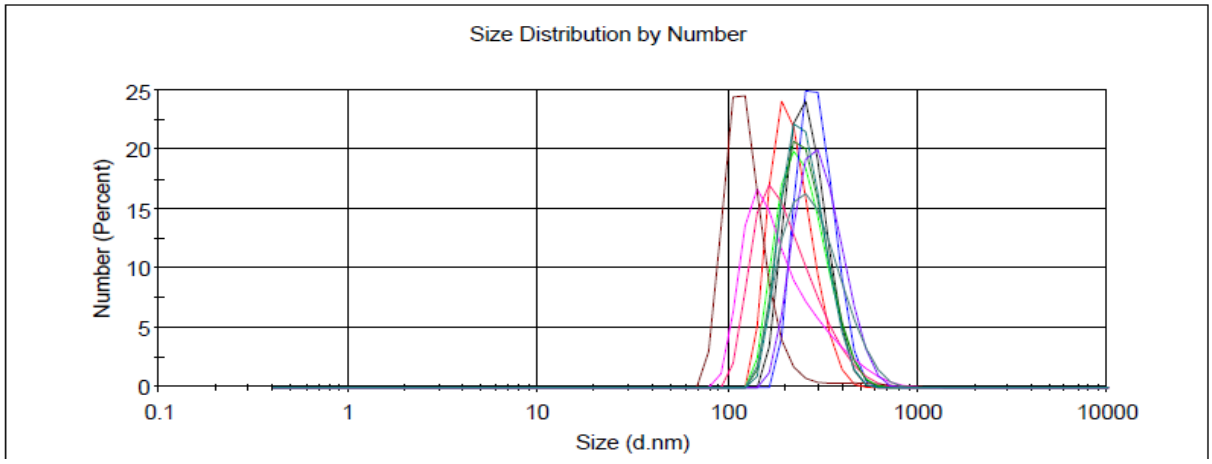


Figure S65. DLS curves of kinetics of ConA in the presence of glycodendrimer **19** as function of time (curves for few initial points are shown).

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	1719	Peak 1:	1140	100.0	232.0
PdI:	0.389	Peak 2:	0.000	0.0	0.000
Intercept:	0.952	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

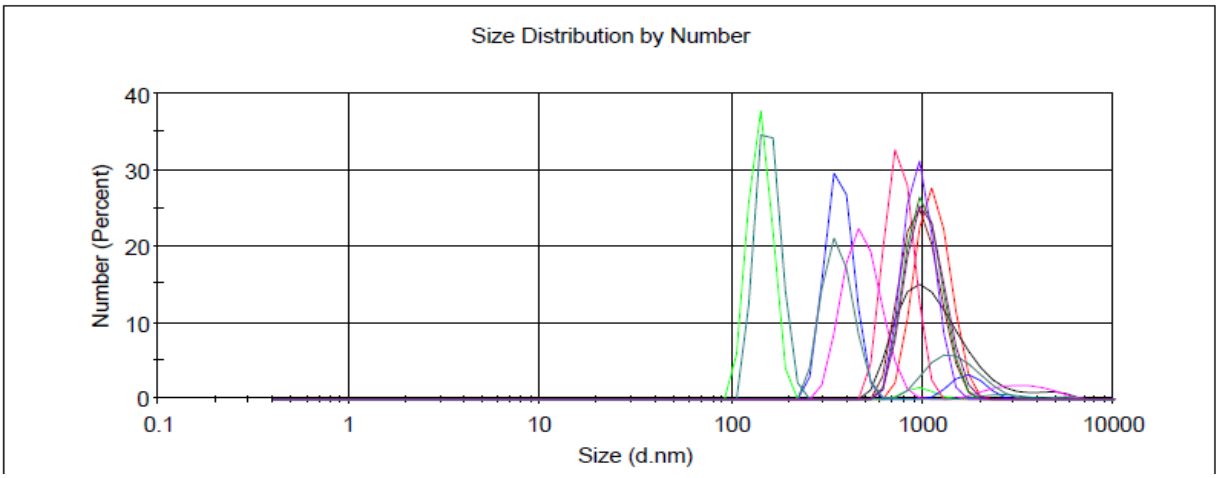


Figure S66. DLS curves of kinetics of ConA in the presence of glycodendrimer **27** as a function of time (curves for few initial points are shown).

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	350.3	Peak 1:	150.2	100.0	98.73
PdI:	0.274	Peak 2:	0.000	0.0	0.000
Intercept:	0.950	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

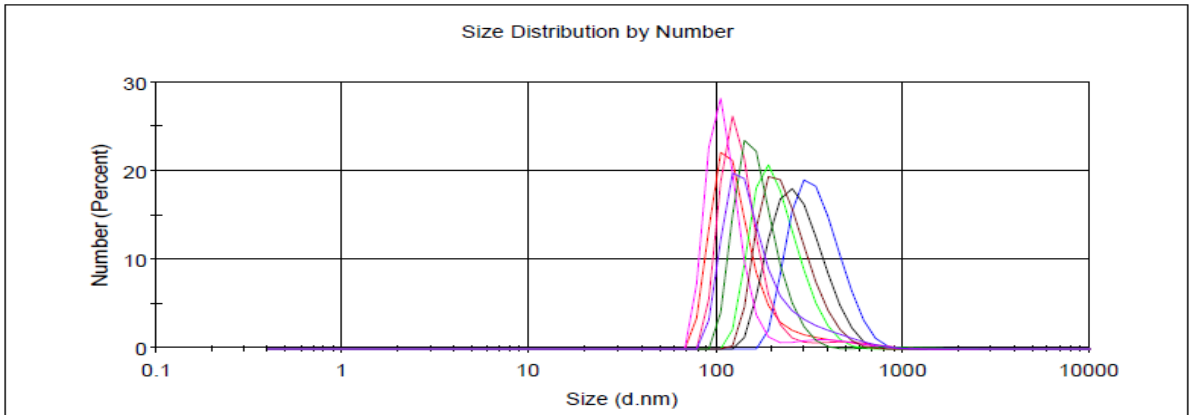


Figure S67. DLS curves of kinetics of LecA in the presence of glycodendrimer **19** as function of time (curves for few initial points are shown).

Results

			Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm):	1779	Peak 1:	1140	96.2	308.5
PdI:	0.438	Peak 2:	5200	3.8	727.8
Intercept:	0.910	Peak 3:	0.000	0.0	0.000

Result quality : Refer to quality report

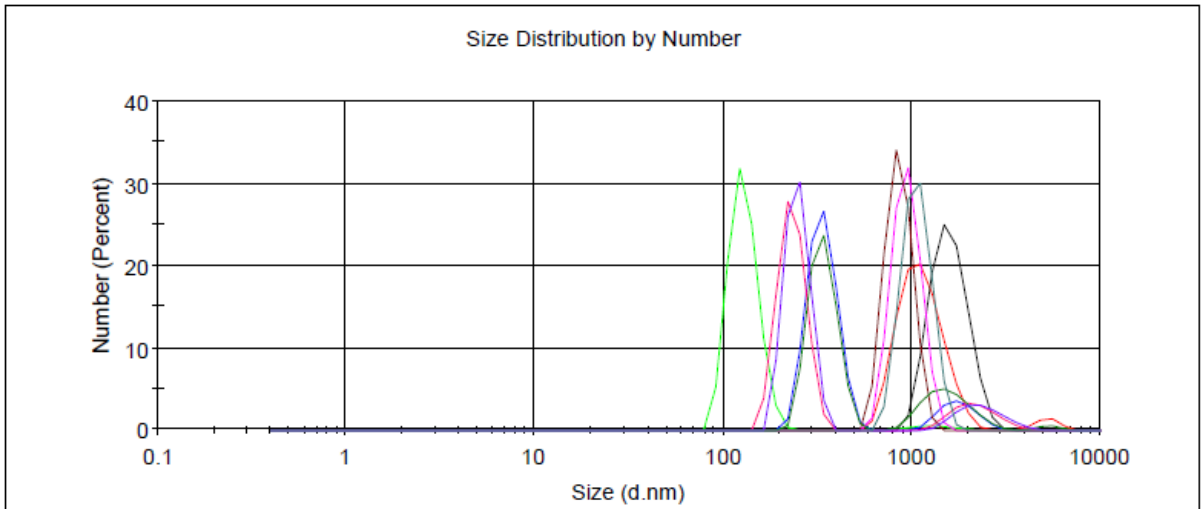


Figure S68. DLS curves of kinetics of LecA in the presence of glycodendrimer **27** as function of time (curves for few initial points are shown).