

Effect of Dendrimer Generation and Aglyconic Linkers on the Binding Properties of Mannosylated Dendrimers Prepared by a Combined Convergent and Onion Peel Approach

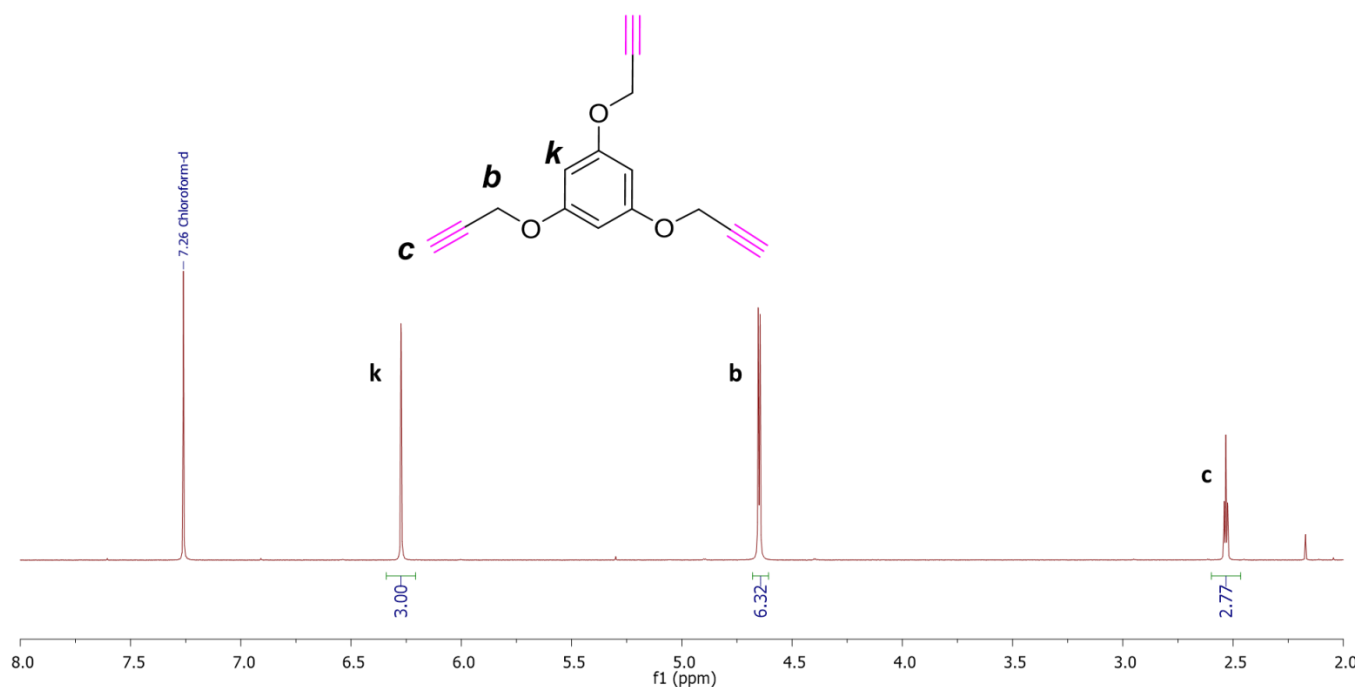
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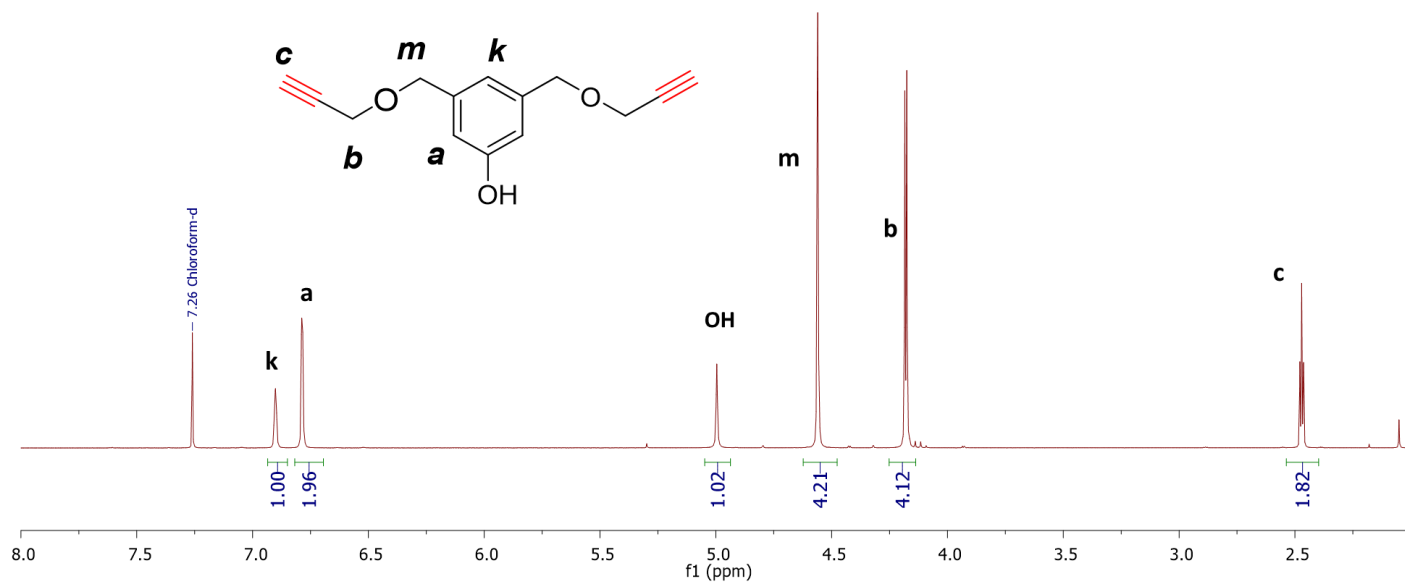
² Glycovax Pharma Inc., 424 Guy, Suite 202, Montreal, Quebec, Canada, H3J 1S6

* Correspondence: rroy@glycovax.com;

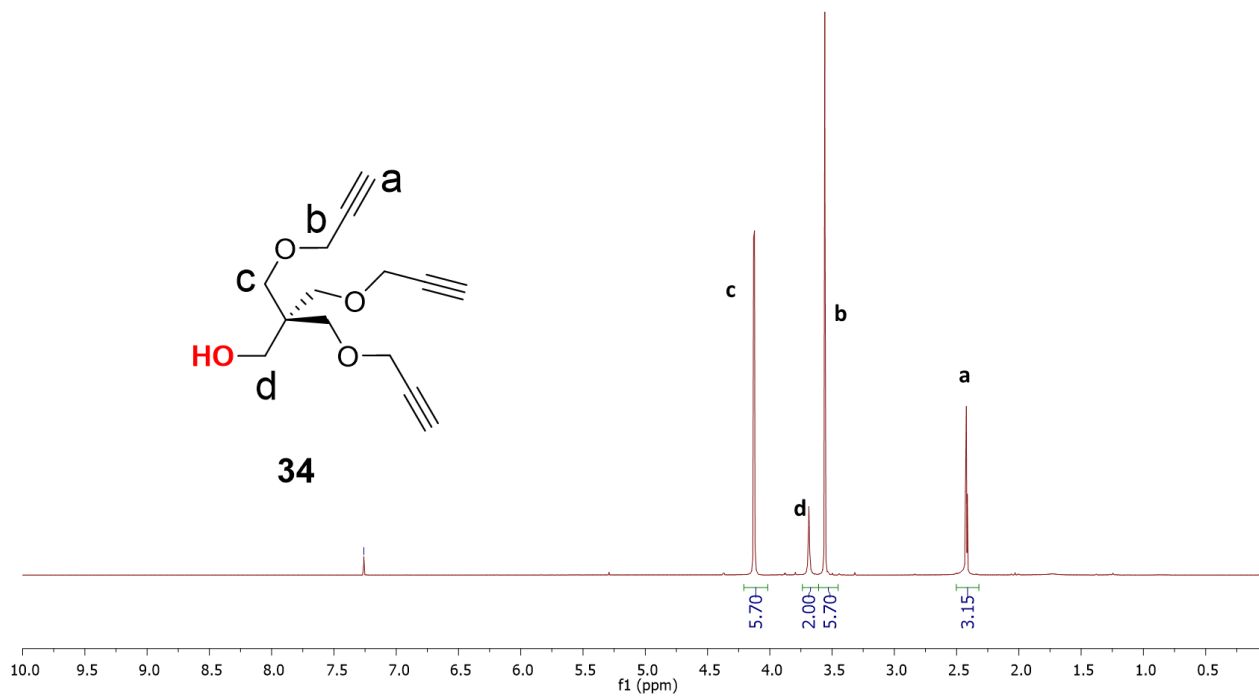
Supplementary material



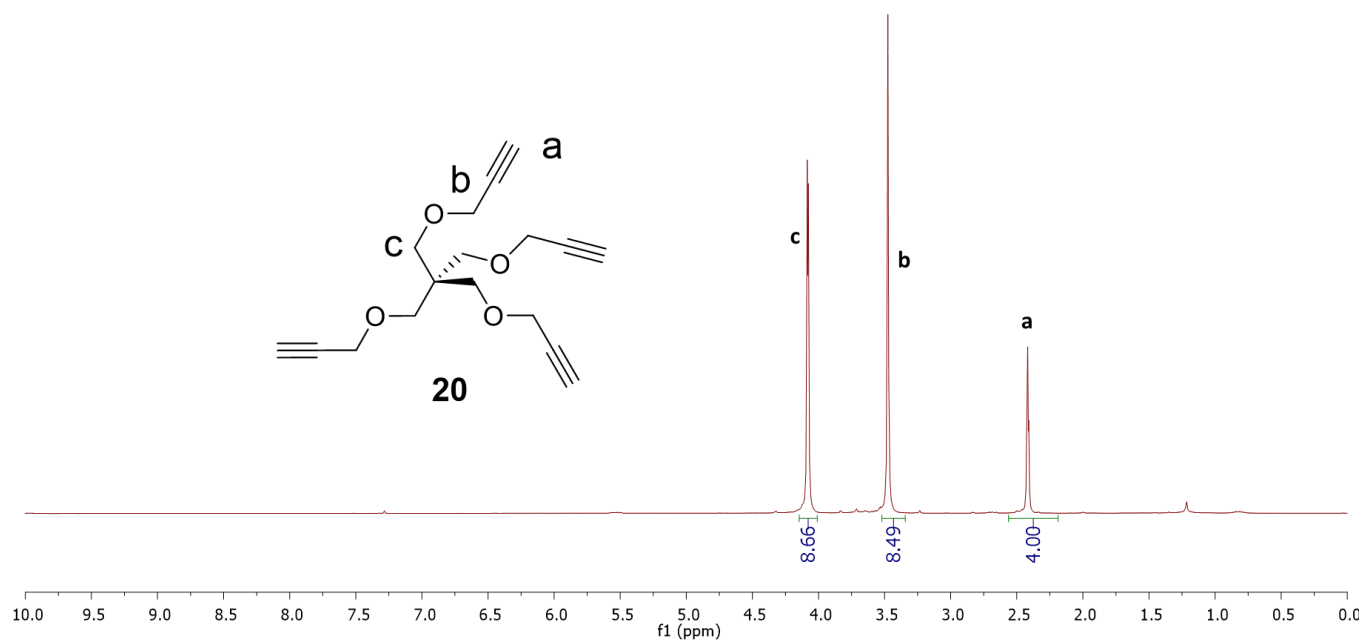
¹H- NMR spectrum of compound 2.



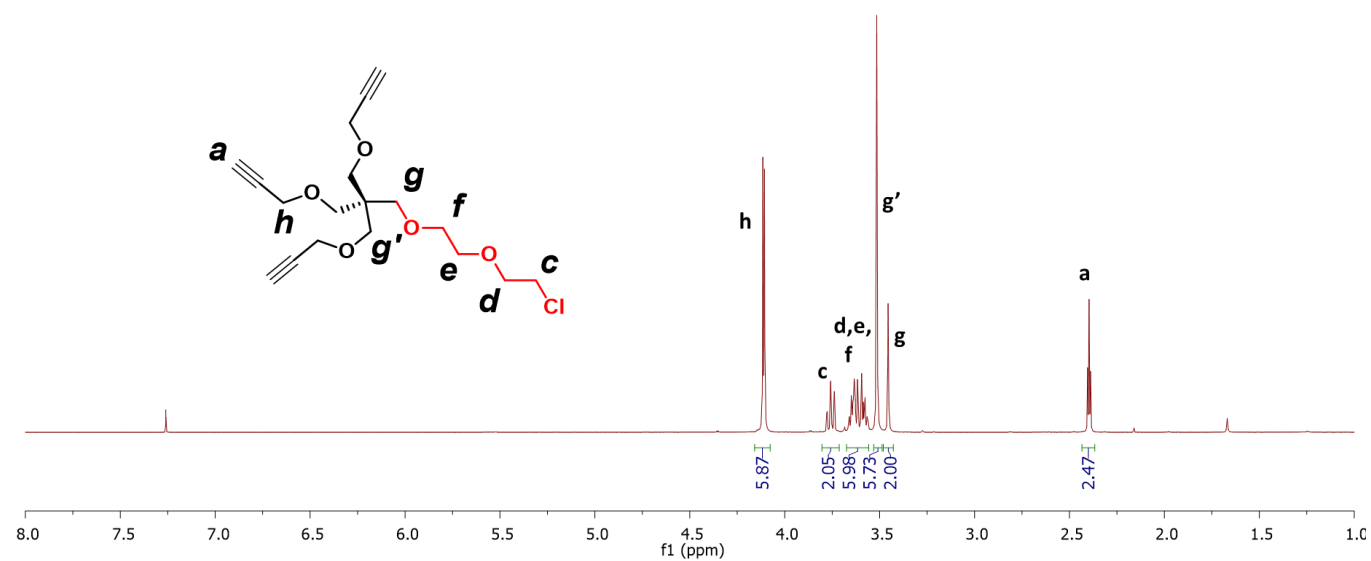
¹H- NMR spectrum of compound 7.



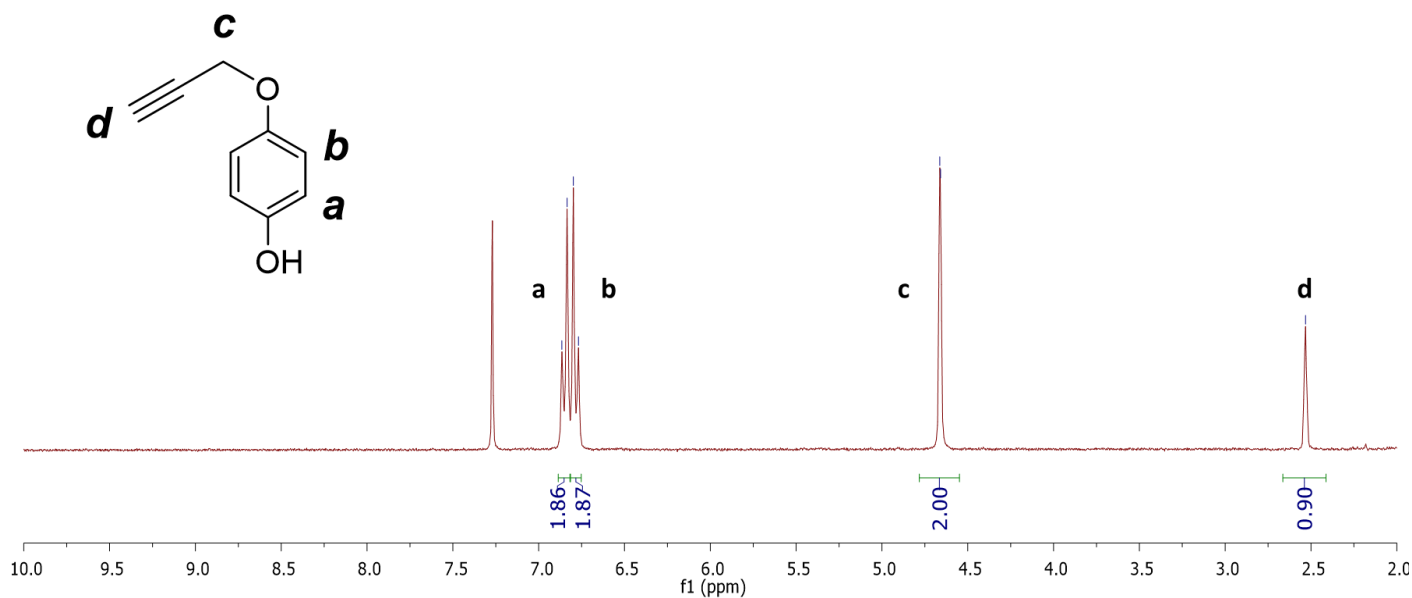
¹H- NMR spectrum of compound 9.



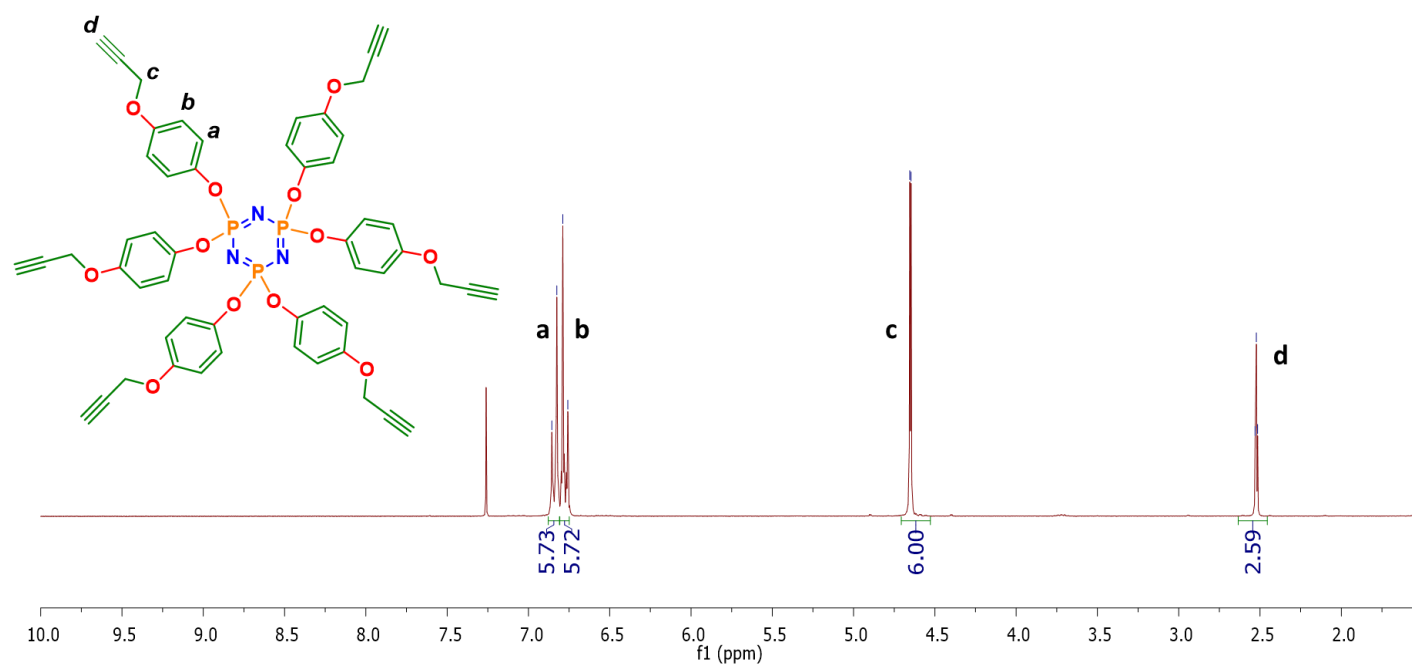
¹H- NMR spectrum of compound 10.



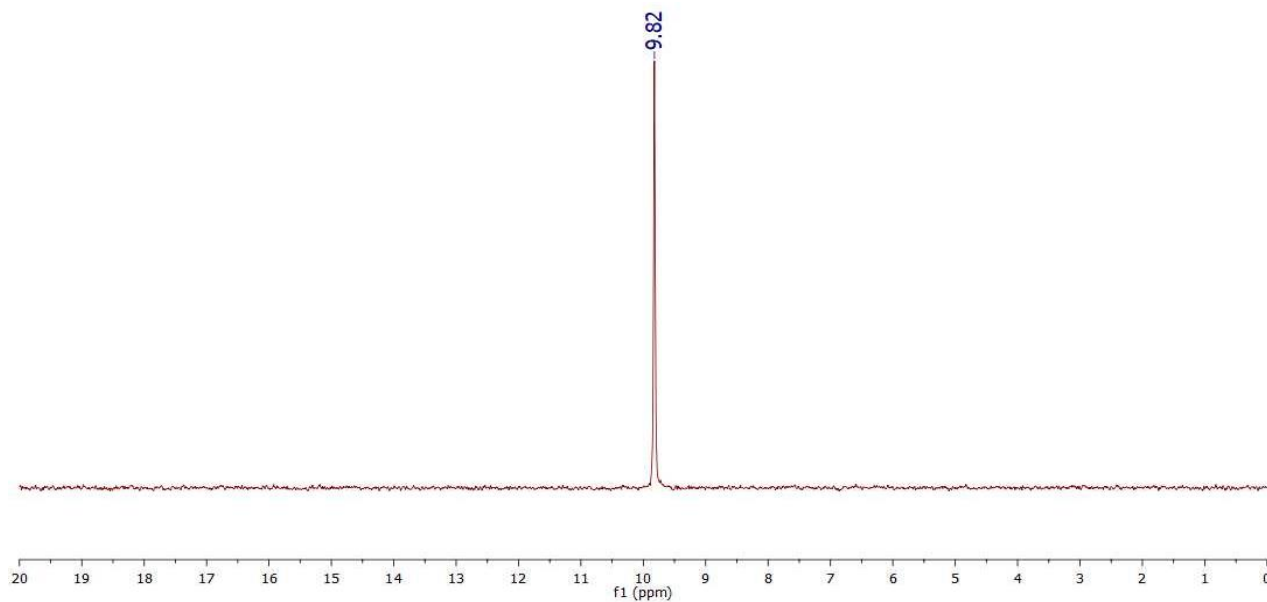
¹H- NMR spectrum of compound 11.



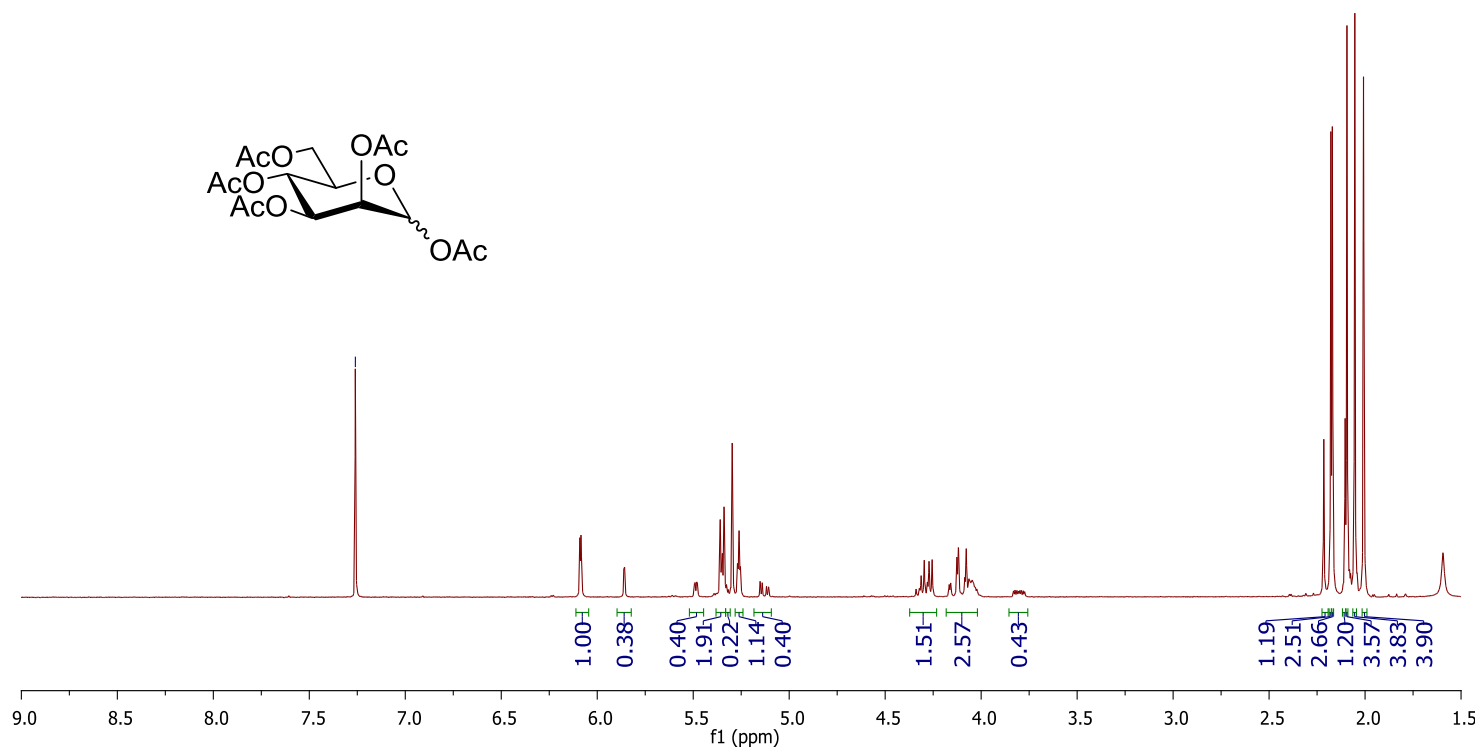
¹H-NMR spectrum of compound 13.



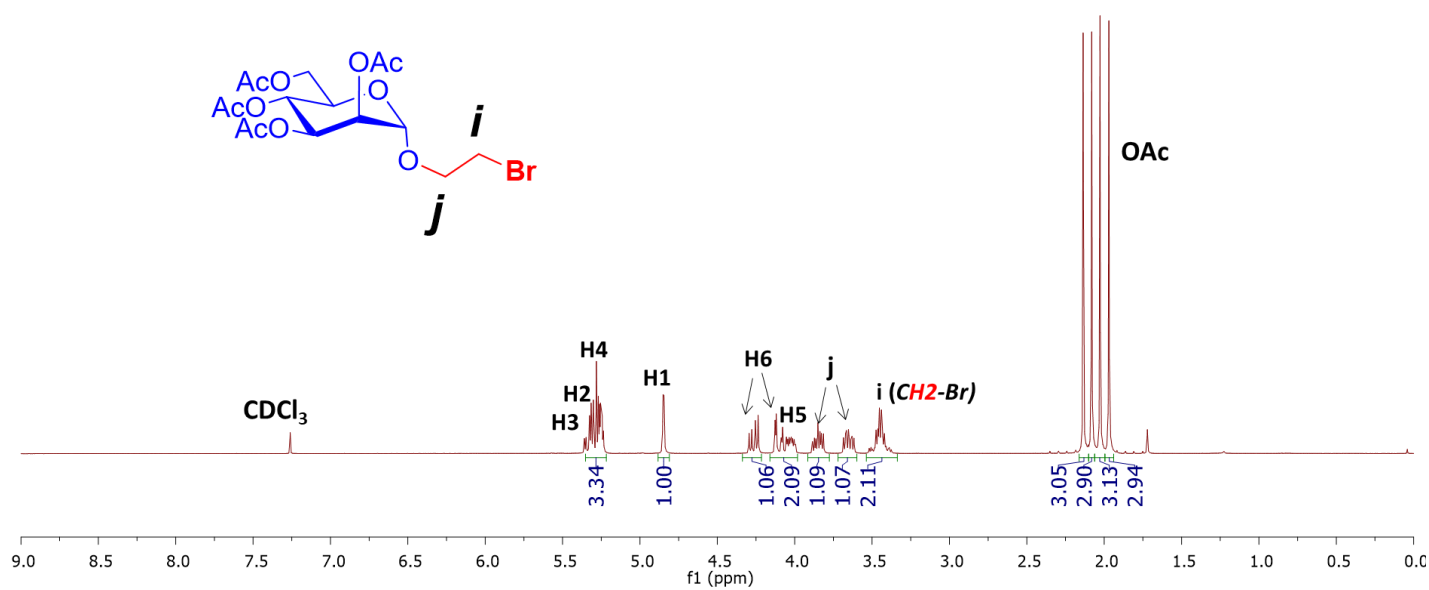
¹H-NMR spectrum of compound 15.



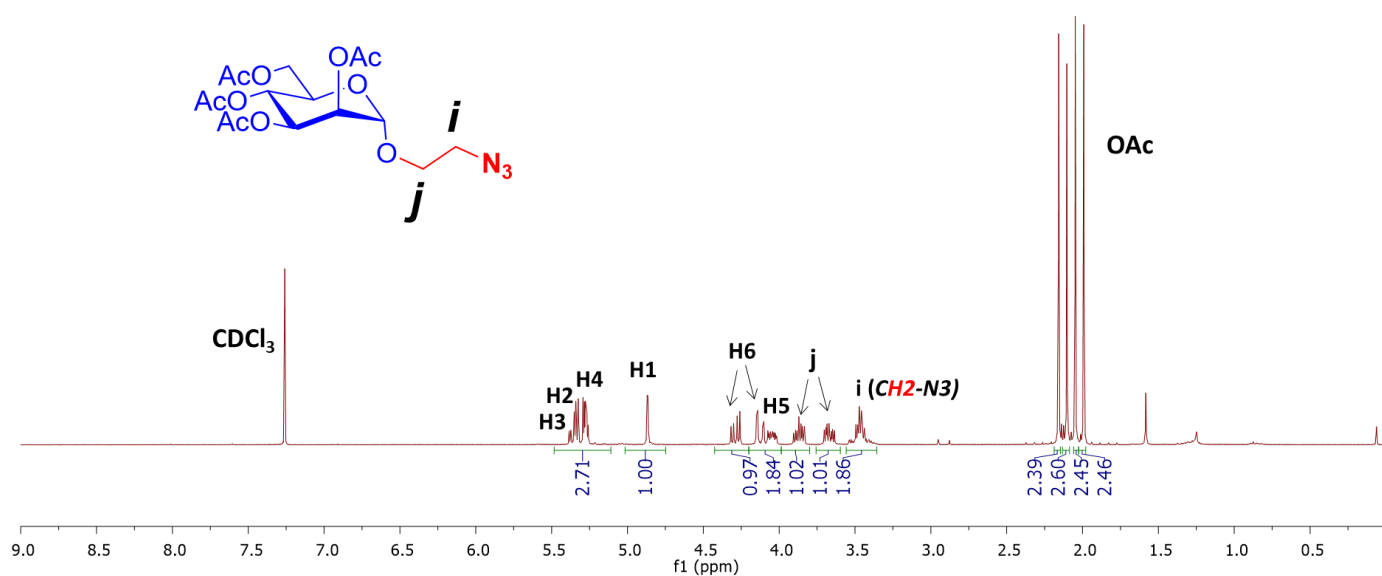
³¹P- NMR spectrum of compound 15.



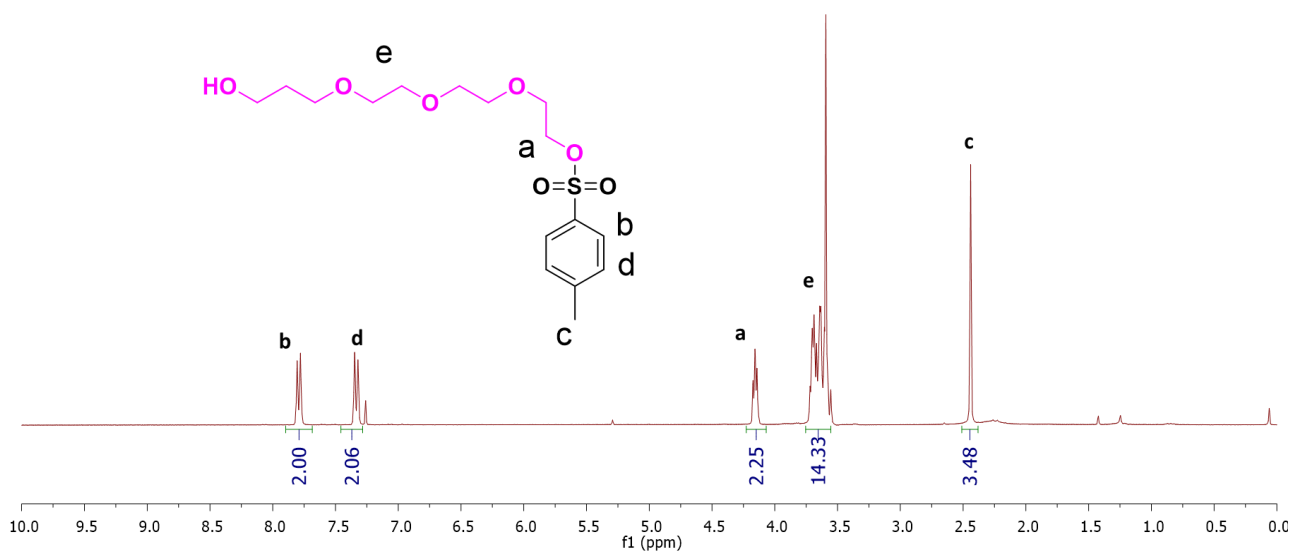
¹H-NMR spectrum of compound 17.



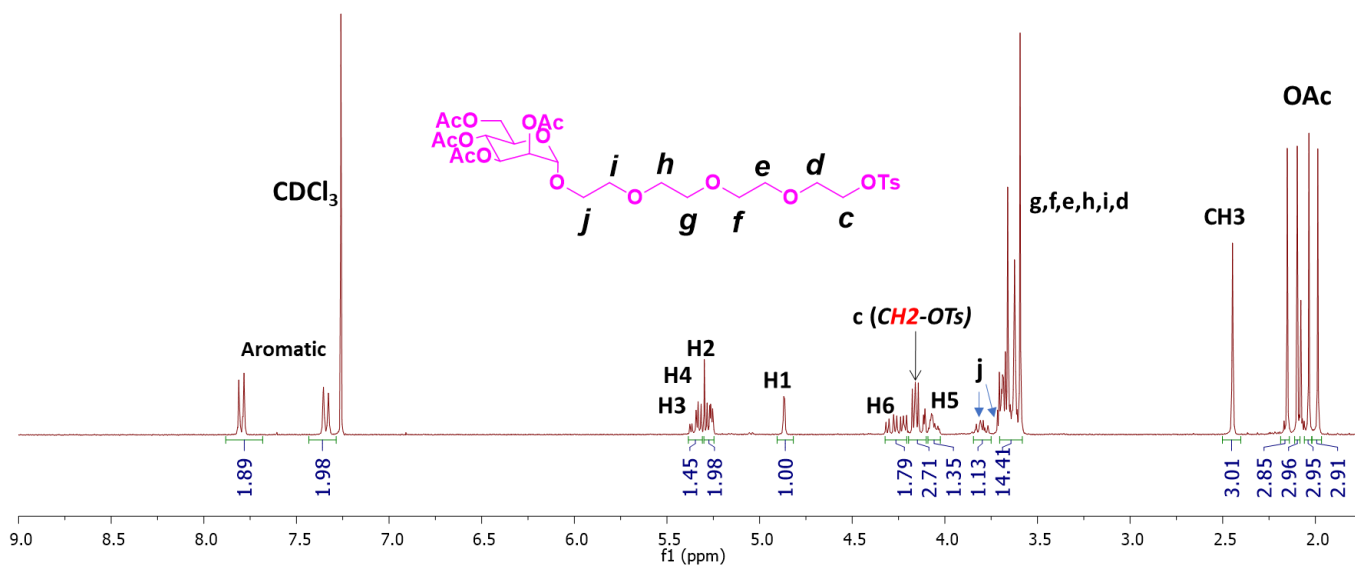
¹H-NMR spectrum of compound 18.



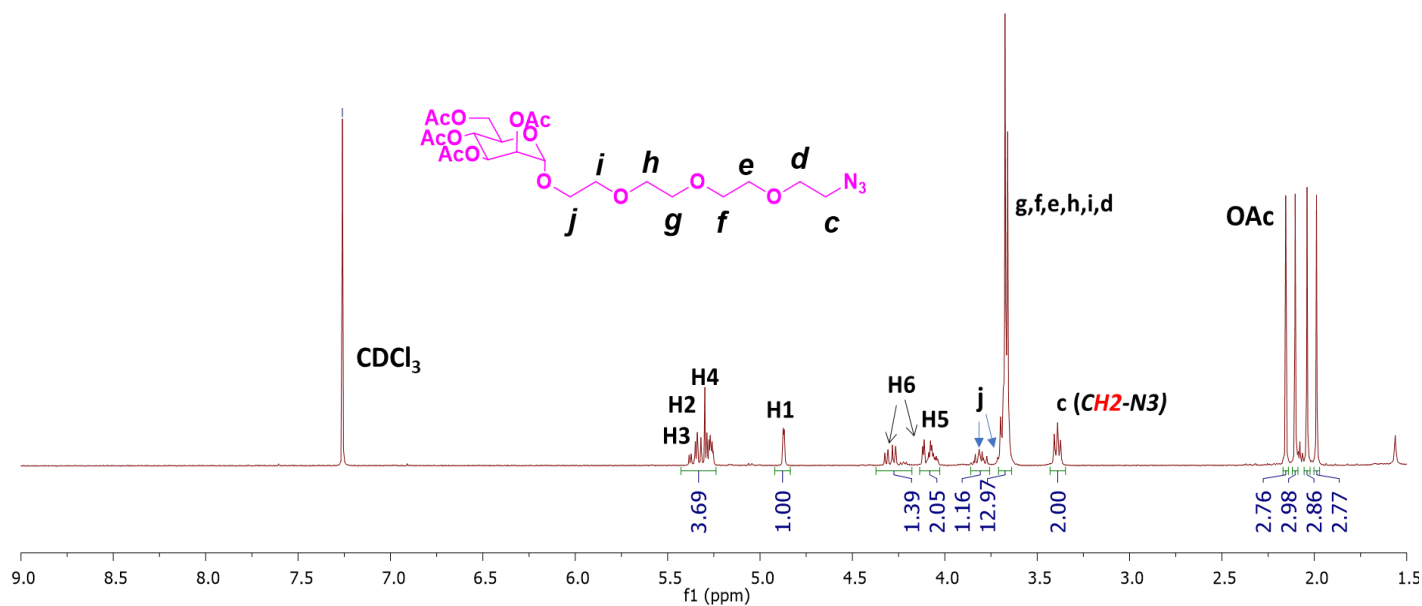
¹H-NMR spectrum of compound 19.



¹H-NMR spectrum of compound 20.



¹H-NMR spectrum of compound 21.



¹H-NMR spectrum of compound 22.

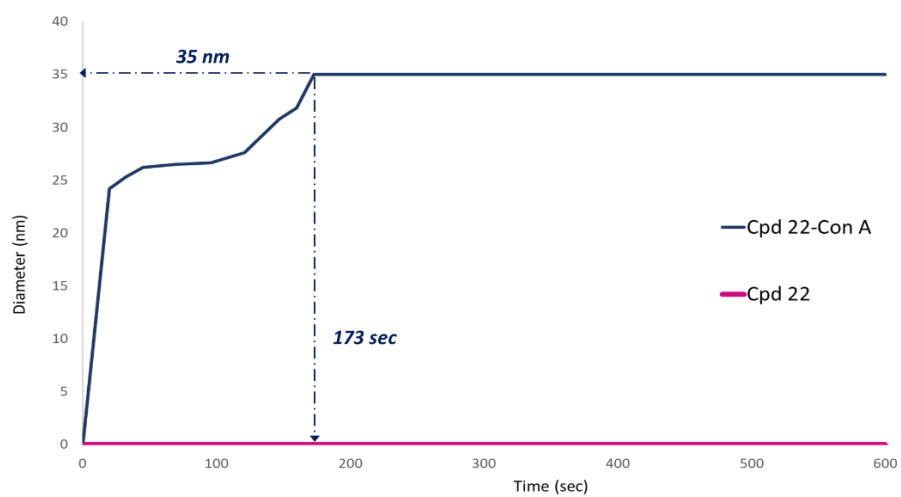
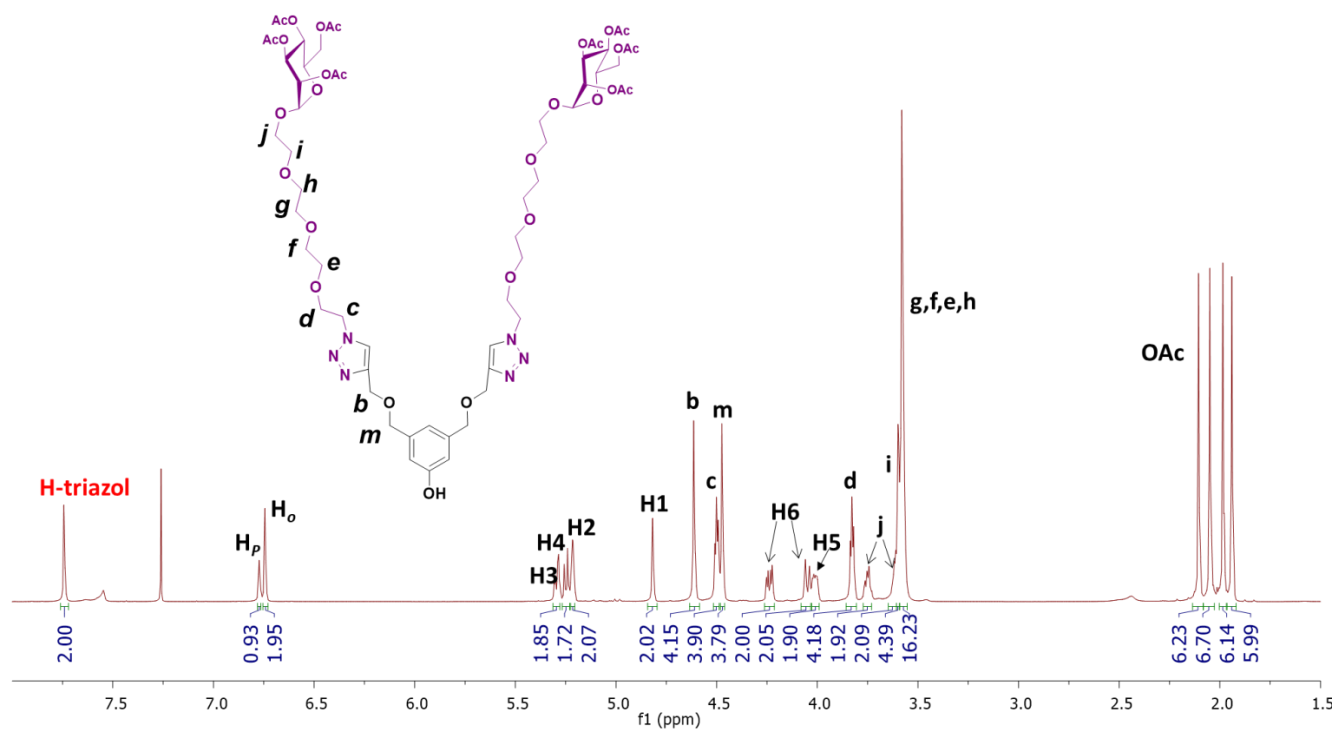
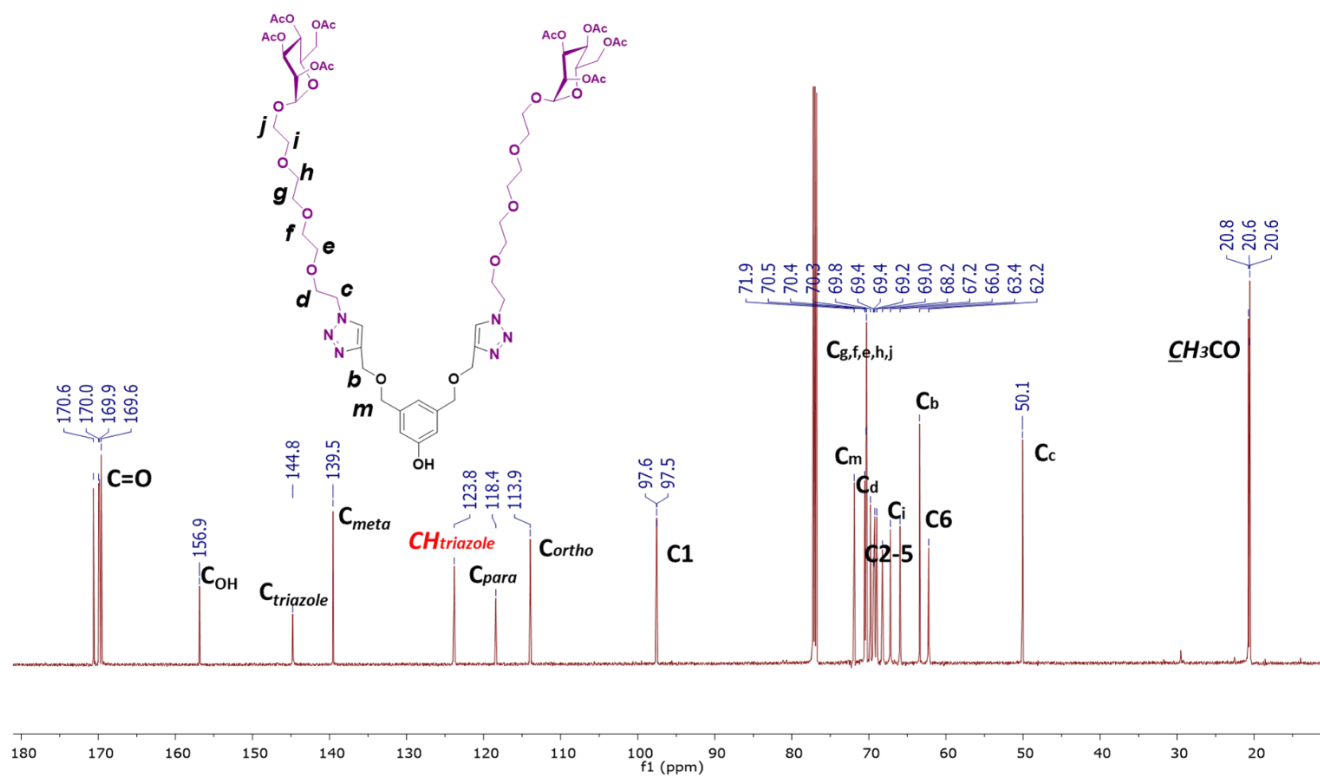


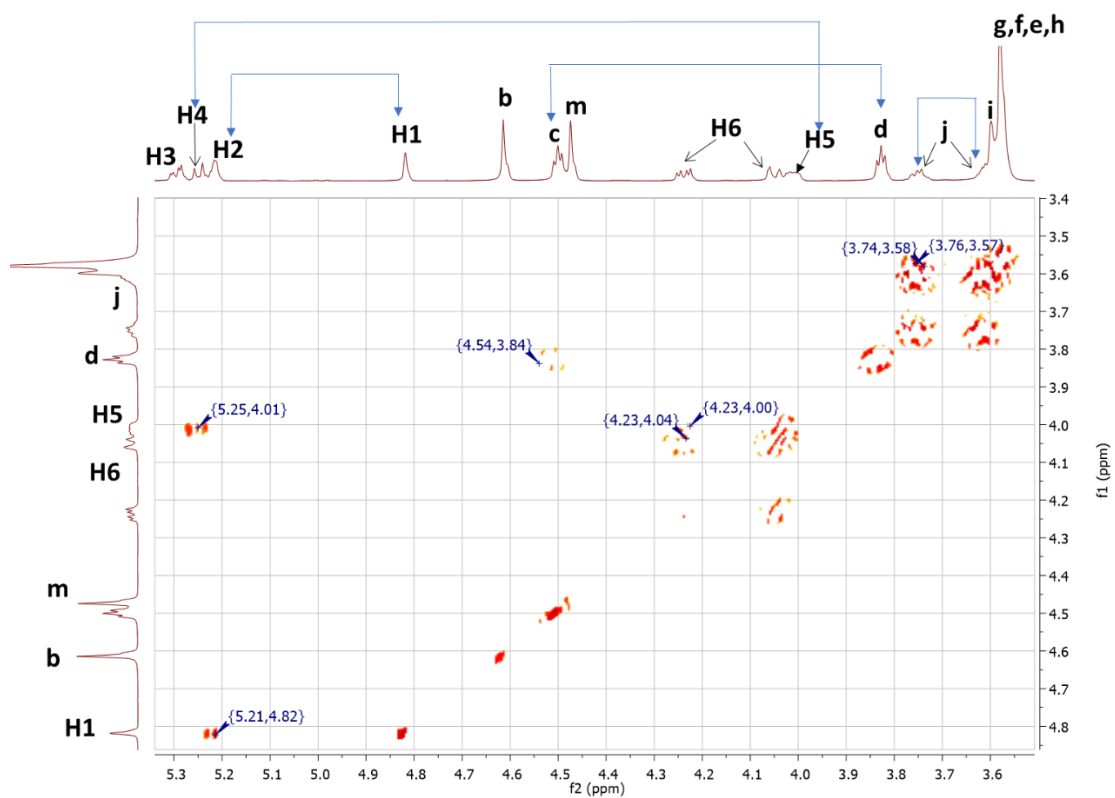
Fig 1. Synthesis DLS of Cpd 22 (deprotected monomer) Crosslinked with Con A.



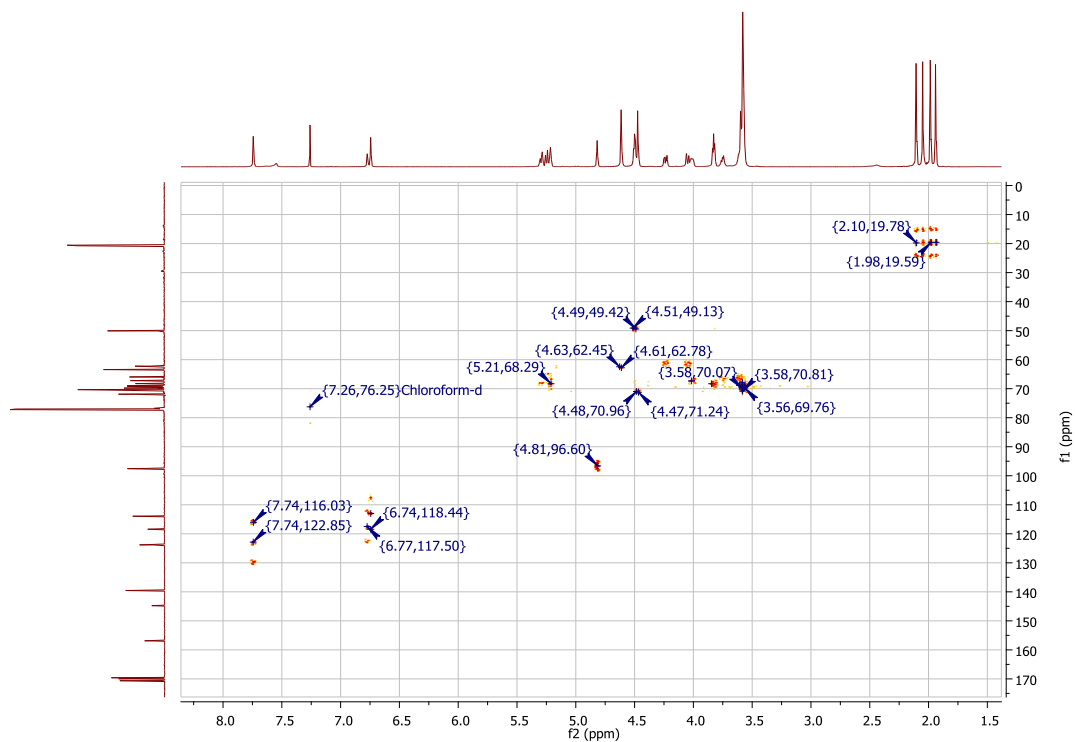
¹H-NMR spectrum of compound 23.



¹³C-NMR spectrum of compound 23.



2D NMR – COSY: ¹H-¹H correlation spectrum of compound 23.

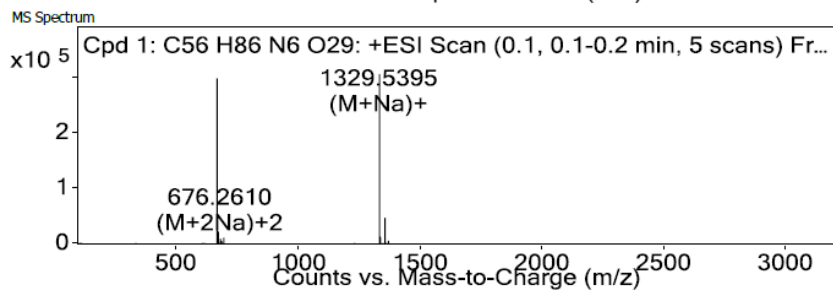
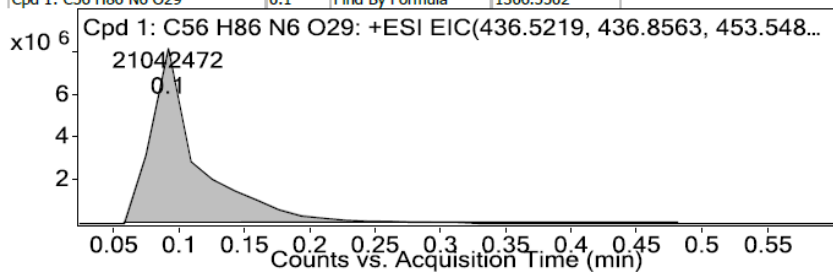


2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 23.

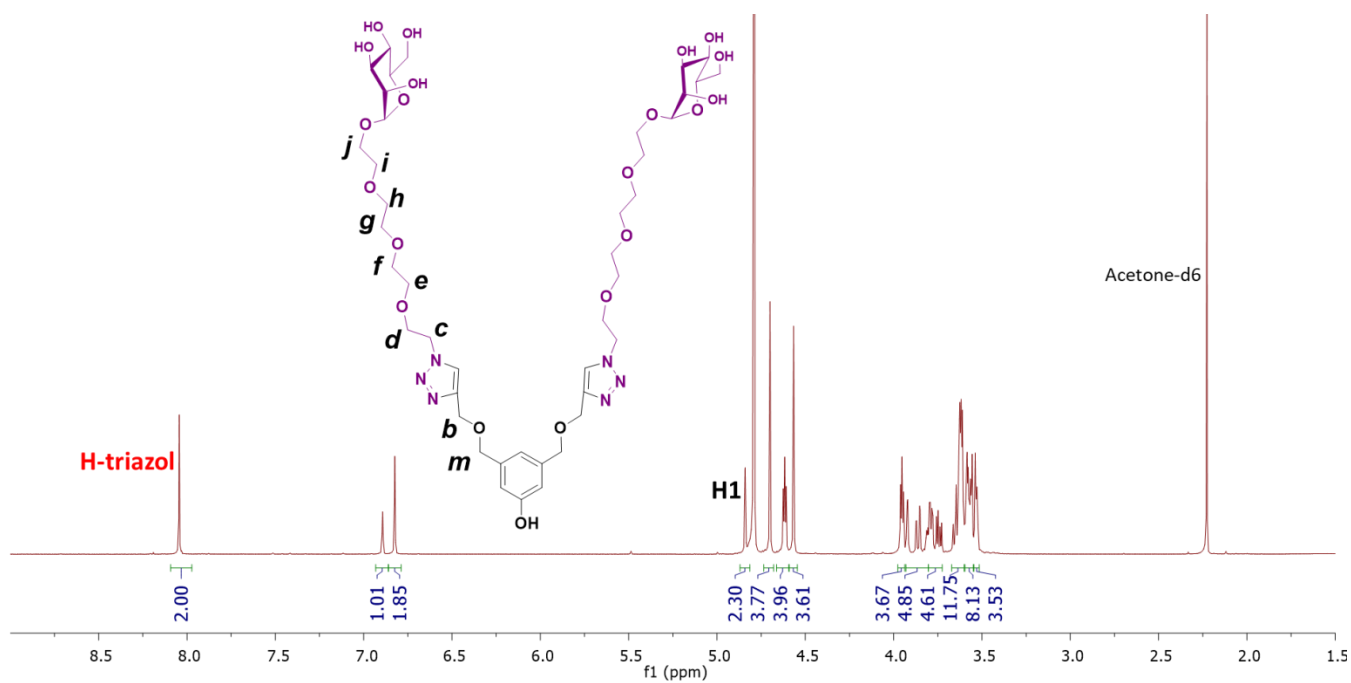
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C56 H86 N6 O29	0.1	1306.5502	304616	C56 H86 N6 O29	1306.5439	4.83

Compound Label	RT	Algorithm	Mass
Cpd 1: C56 H86 N6 O29	0.1	Find By Formula	1306.5502



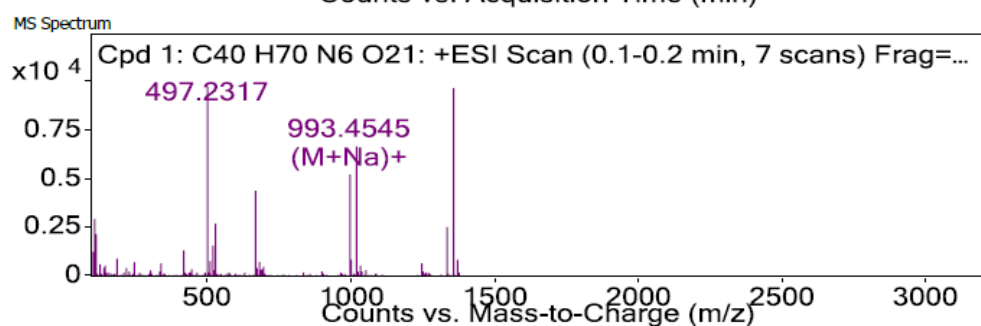
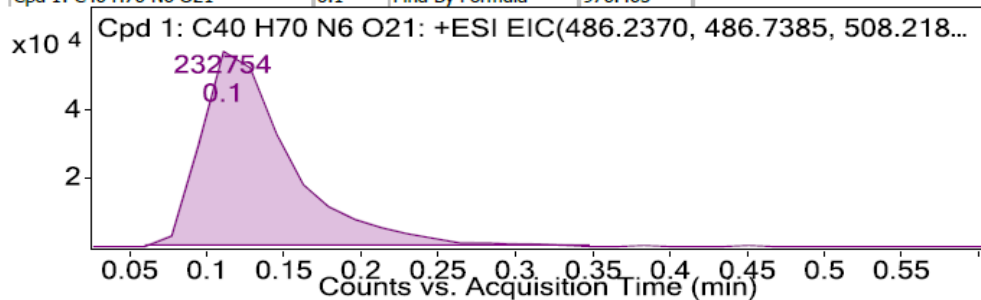
HRMS of compound 23.



Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C ₄₀ H ₇₀ N ₆ O ₂₁	0.1	970.465	5215	C ₄₀ H ₇₀ N ₆ O ₂₁	970.4594	5.74

Compound Label	RT	Algorithm	Mass
Cpd 1: C ₄₀ H ₇₀ N ₆ O ₂₁	0.1	Find By Formula	970.465



HRMS of compound 24.

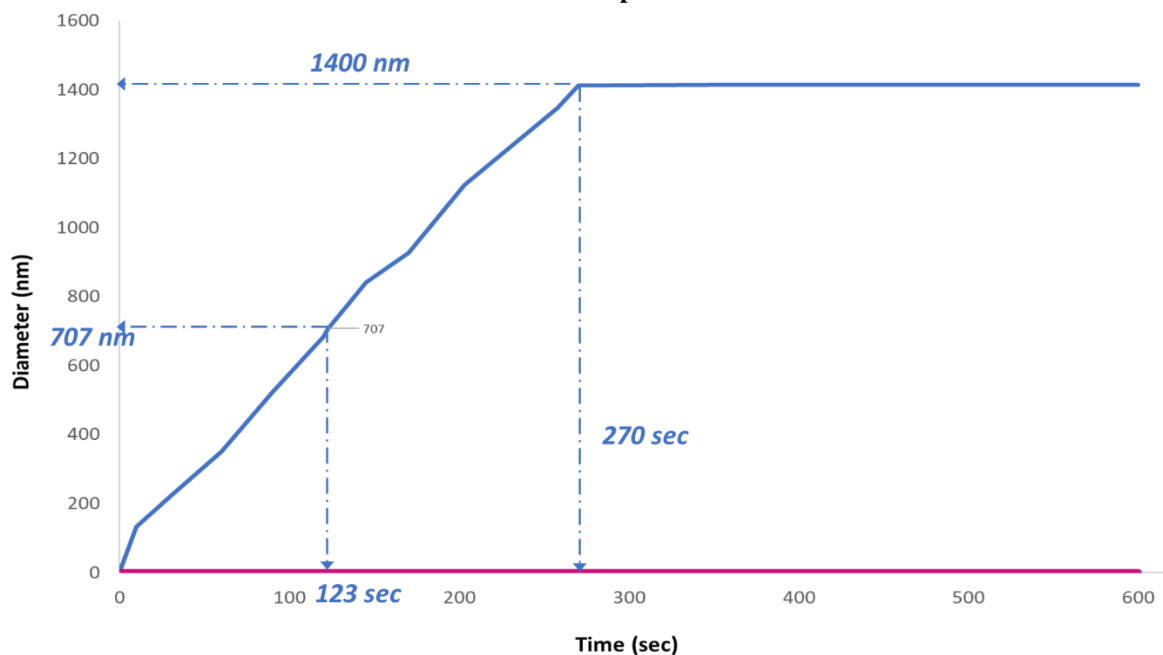
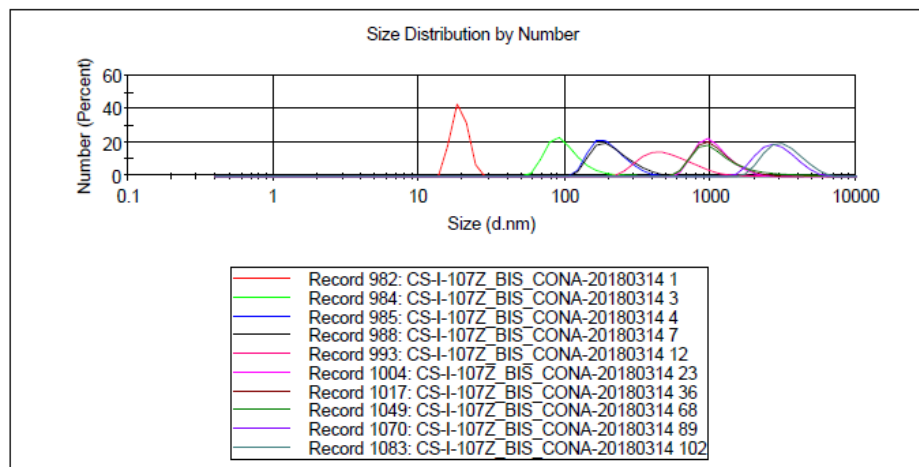


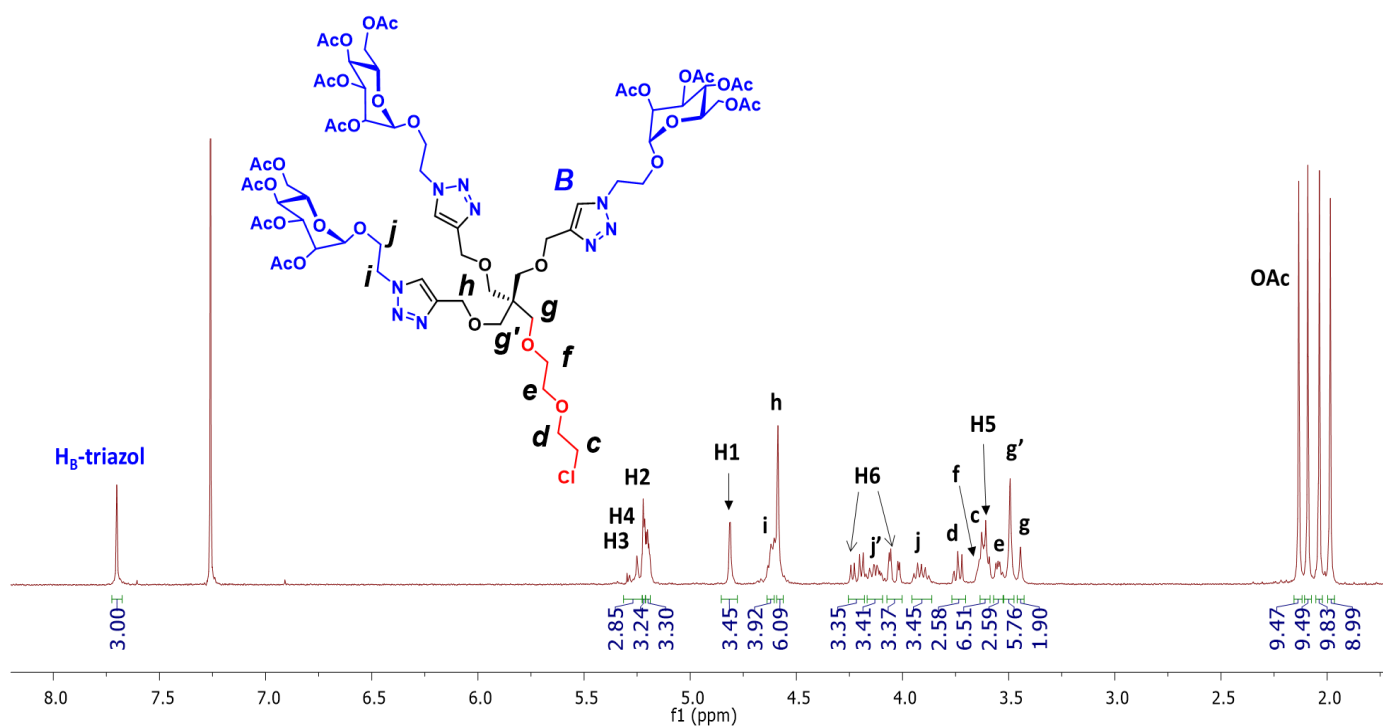
Fig 2. Synthesis DLS of Cpd 24 (Bis) Crosslinked with Con A.

		Size (d.nm):	% Number:	St Dev (d.nm):
Z-Average (d.nm): 2979	Peak 1:	3253	100.0	940.0
Pdl: 0.279	Peak 2:	0.000	0.0	0.000
Intercept: 0.861	Peak 3:	0.000	0.0	0.000

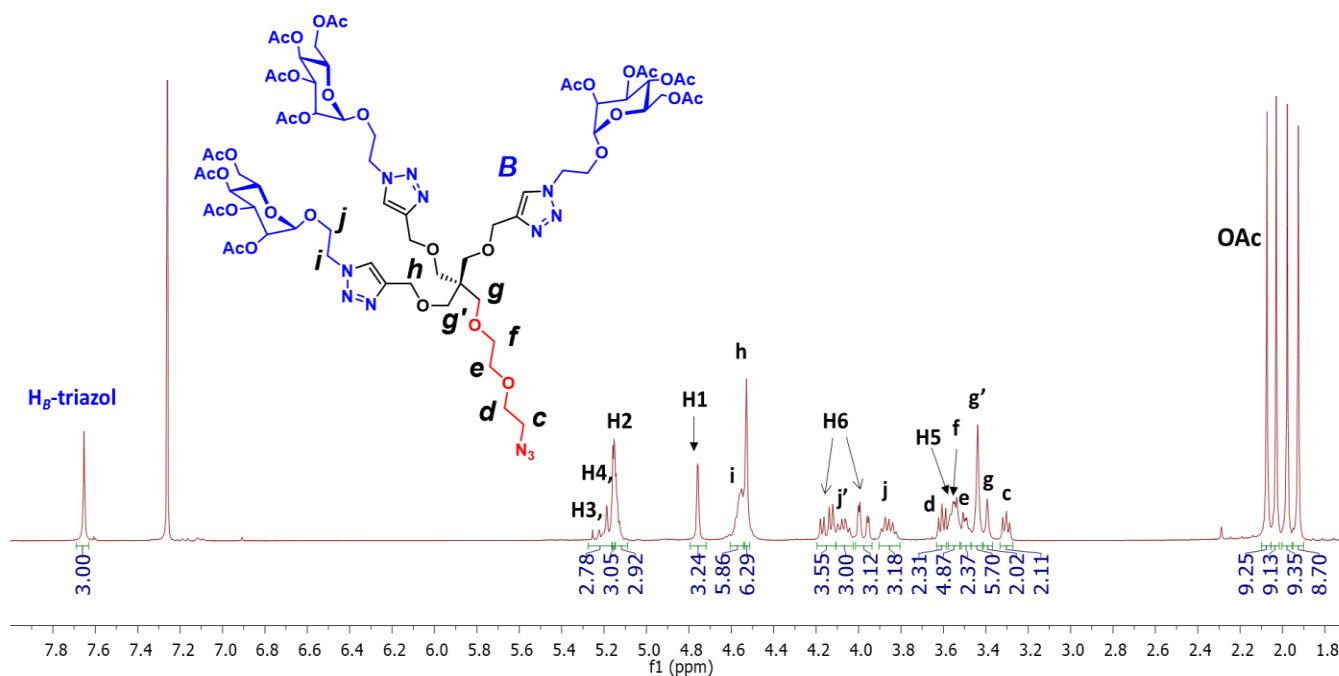
Result quality : Refer to quality report



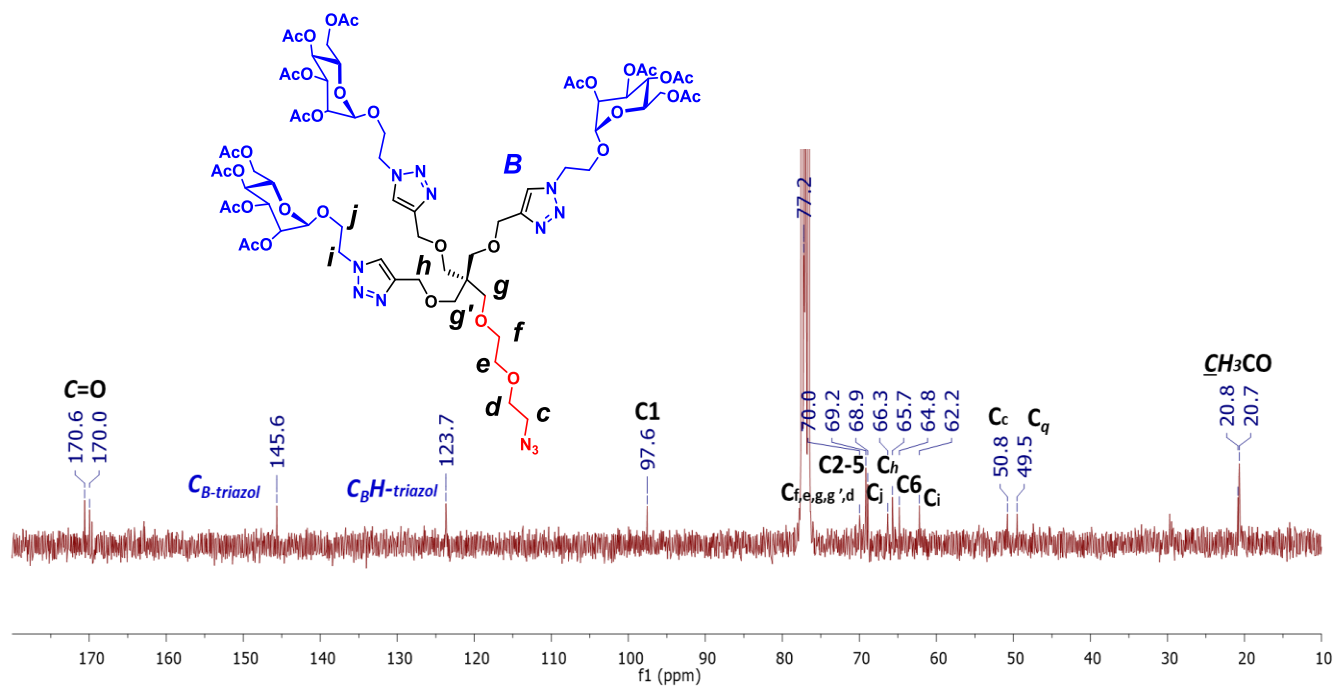
DLS-Size distribution of compound 24.

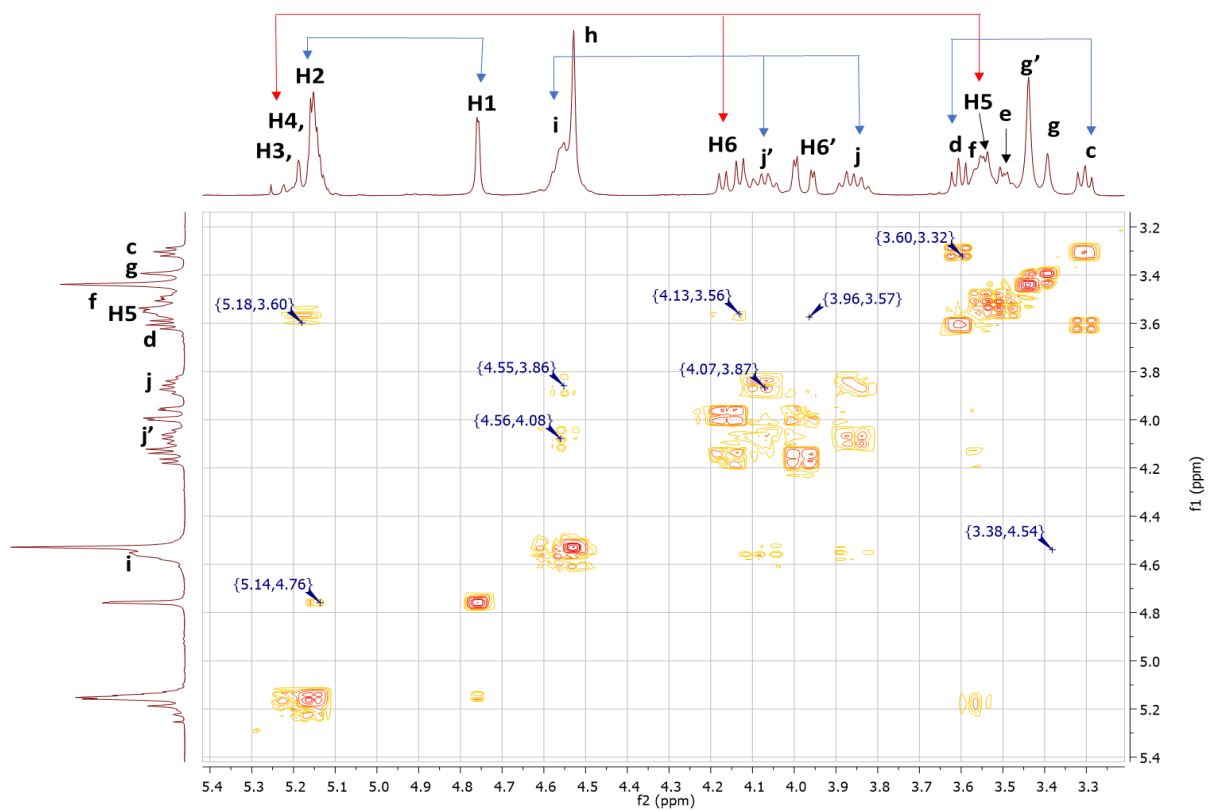
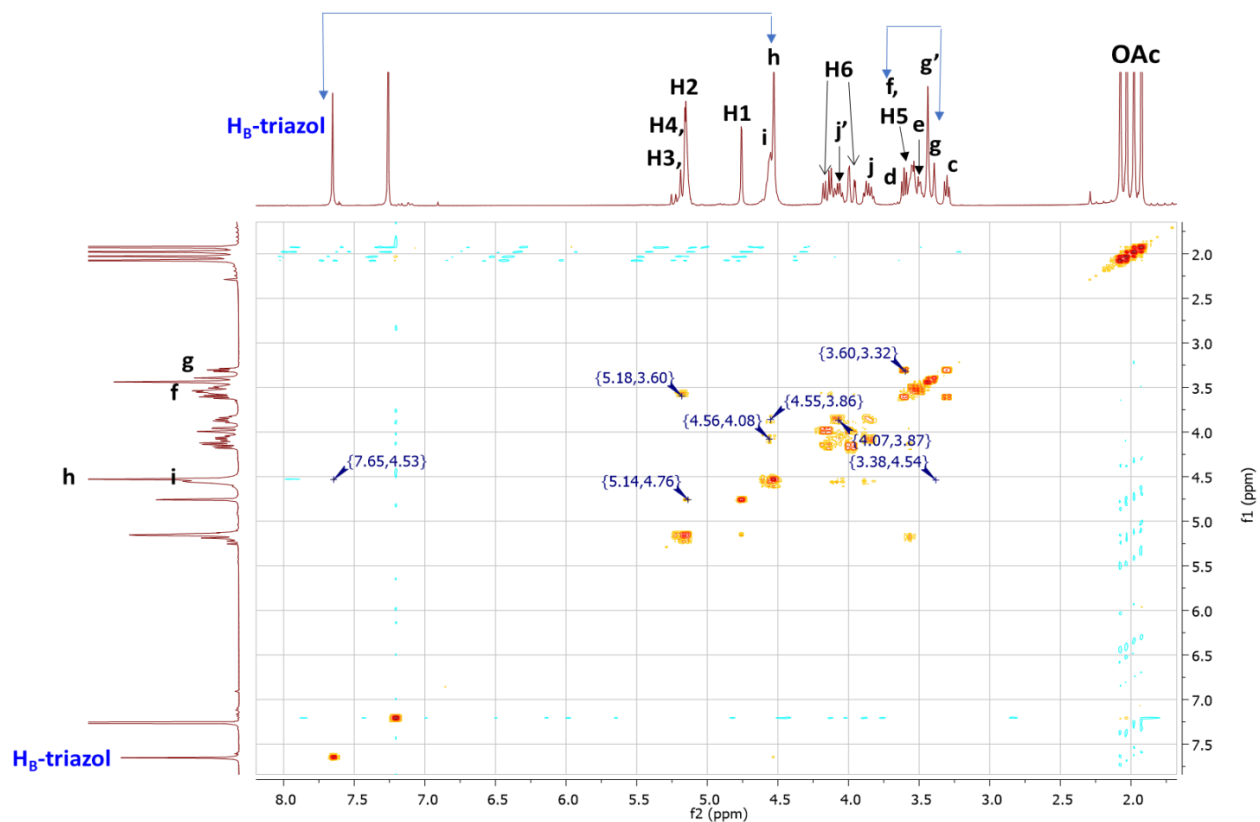


^1H - NMR spectrum of compound 25.

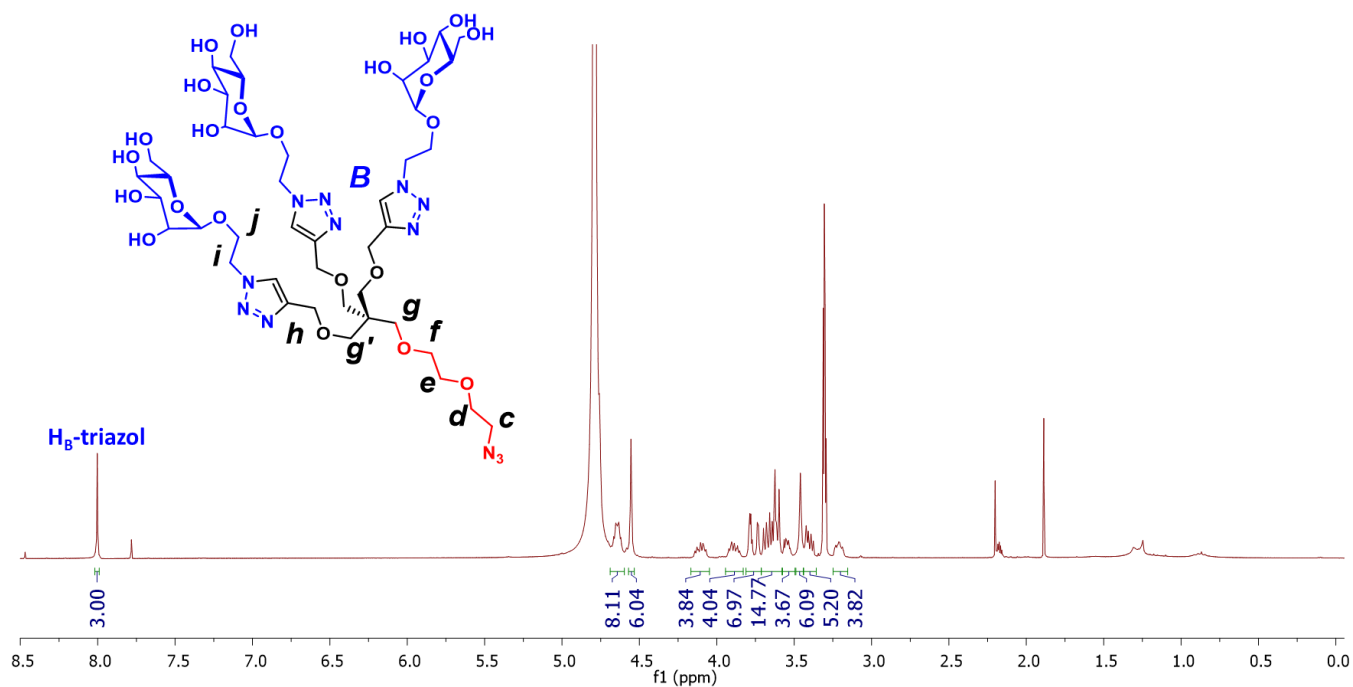


¹H-NMR spectrum of compound 26.

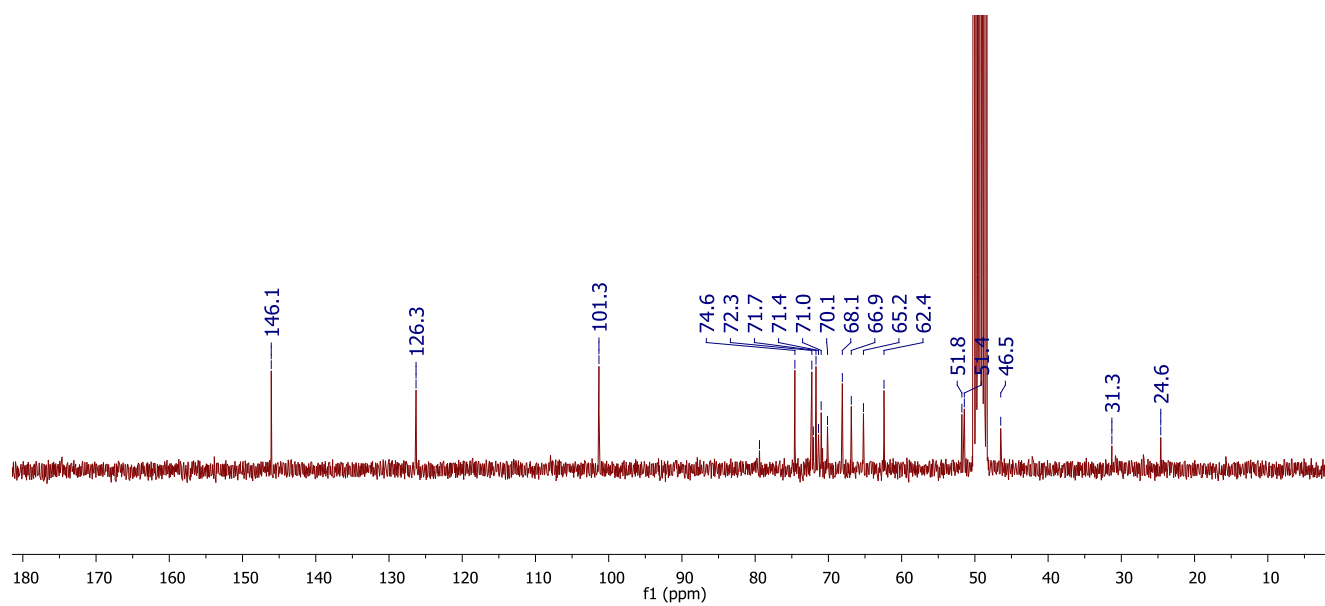




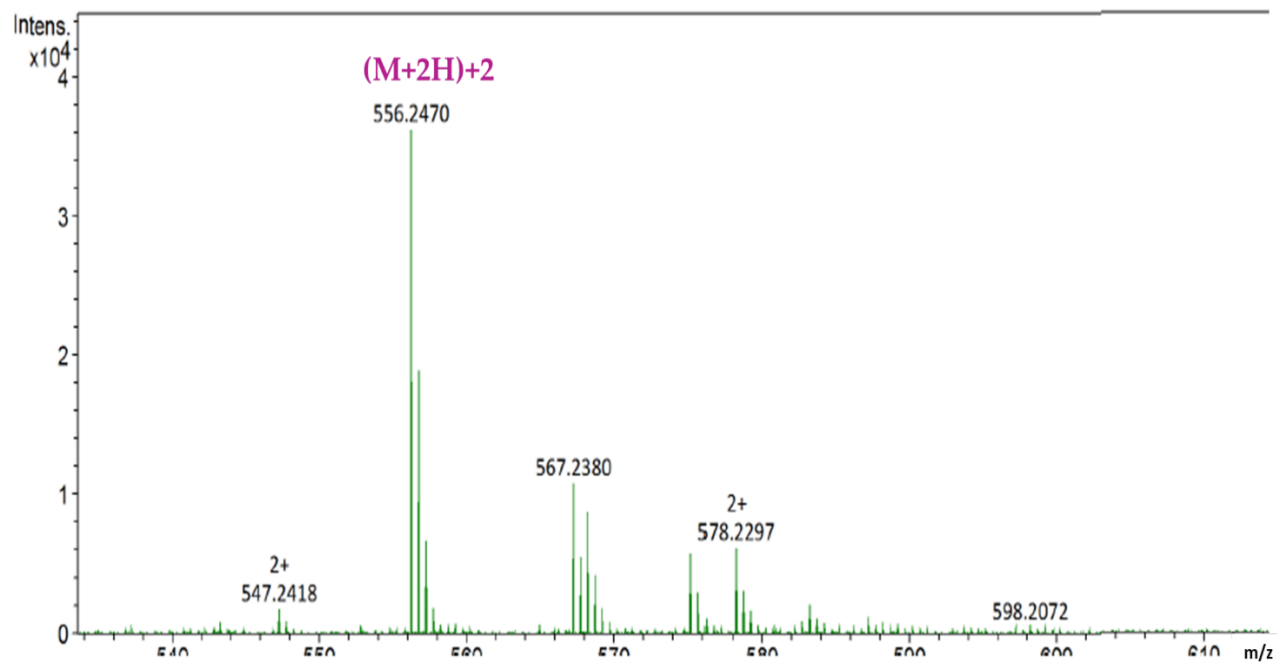
2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 26.



^1H - NMR spectrum of compound 27.



^{13}C - NMR spectrum of compound 27.



HRMS of compound 27.

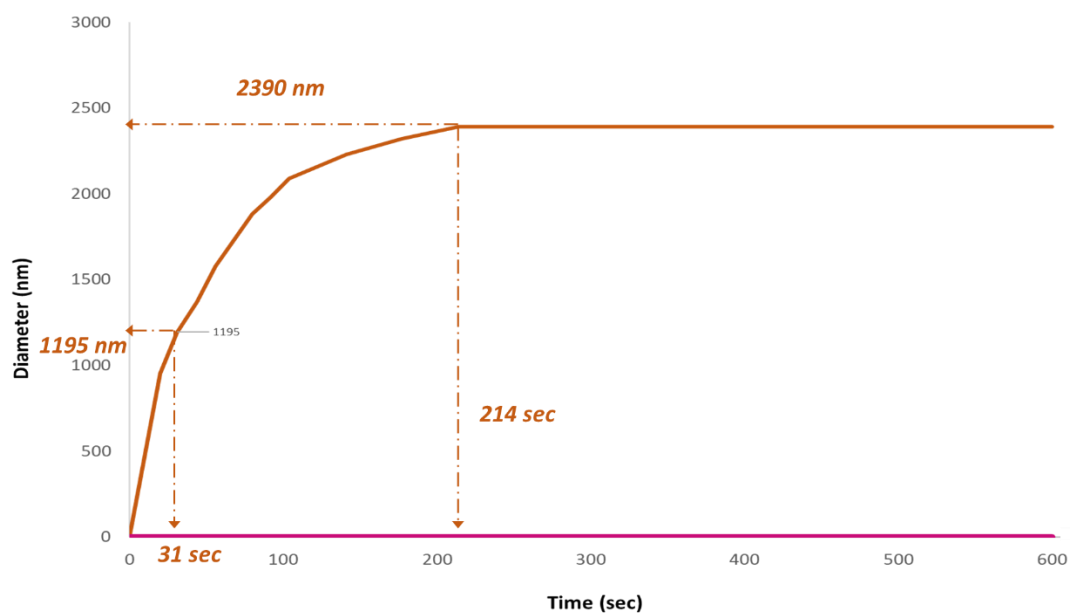
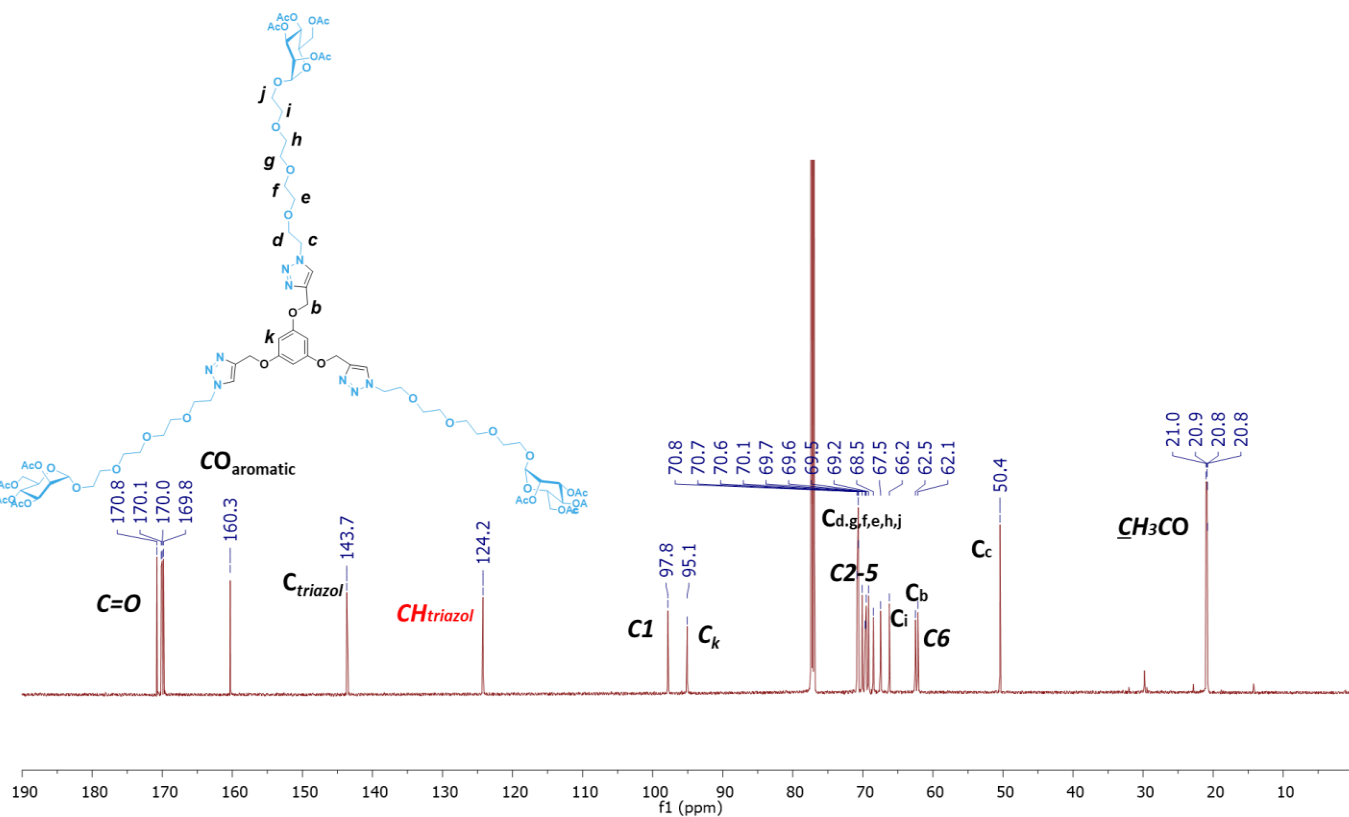
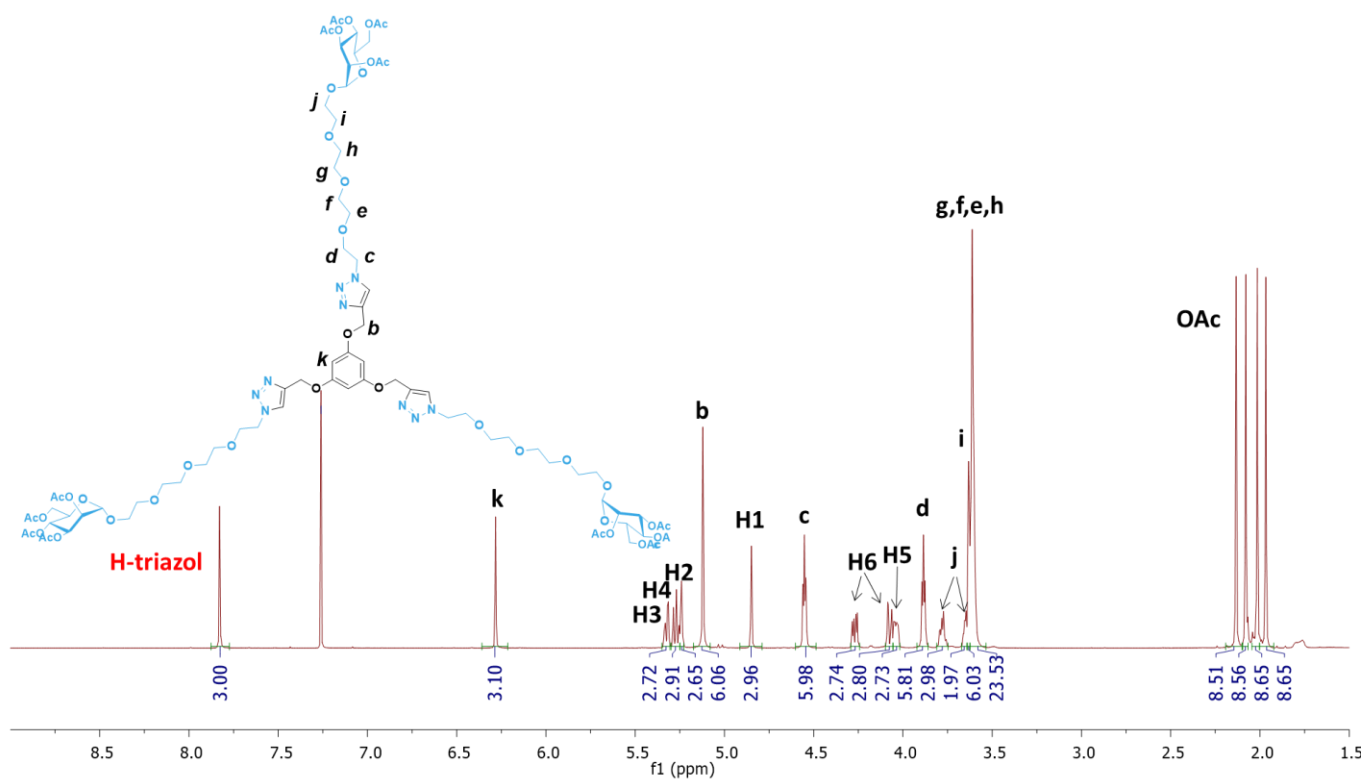
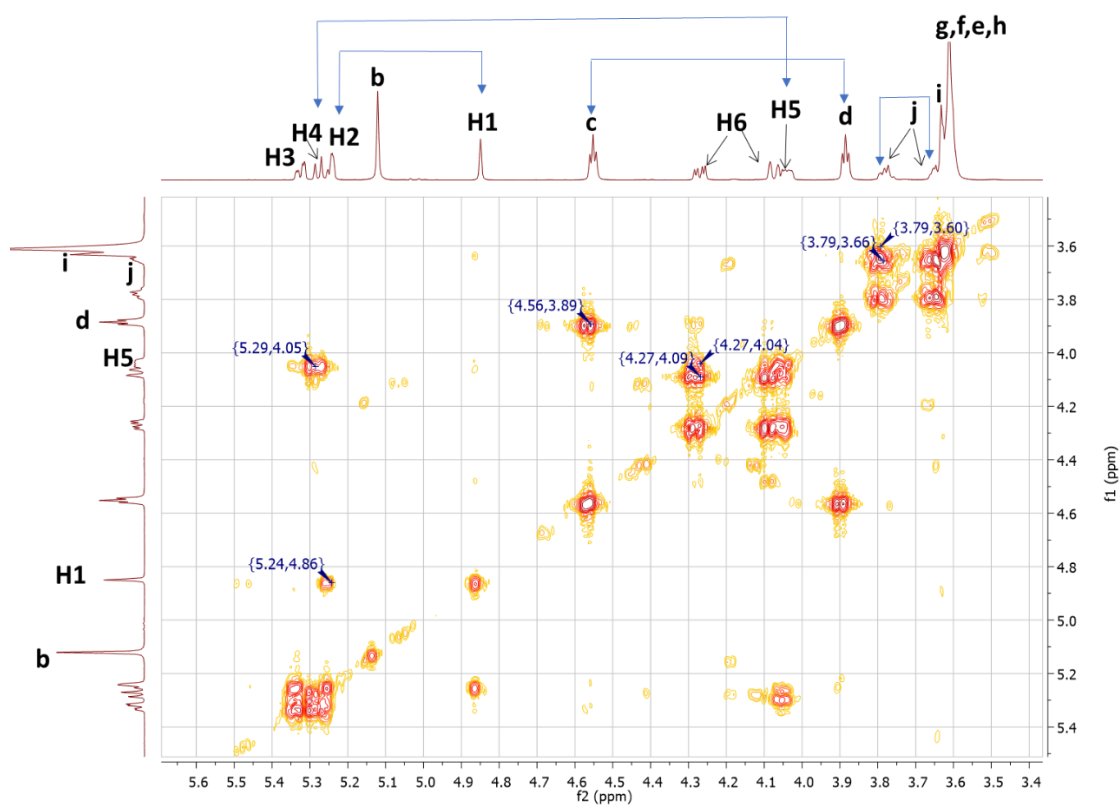
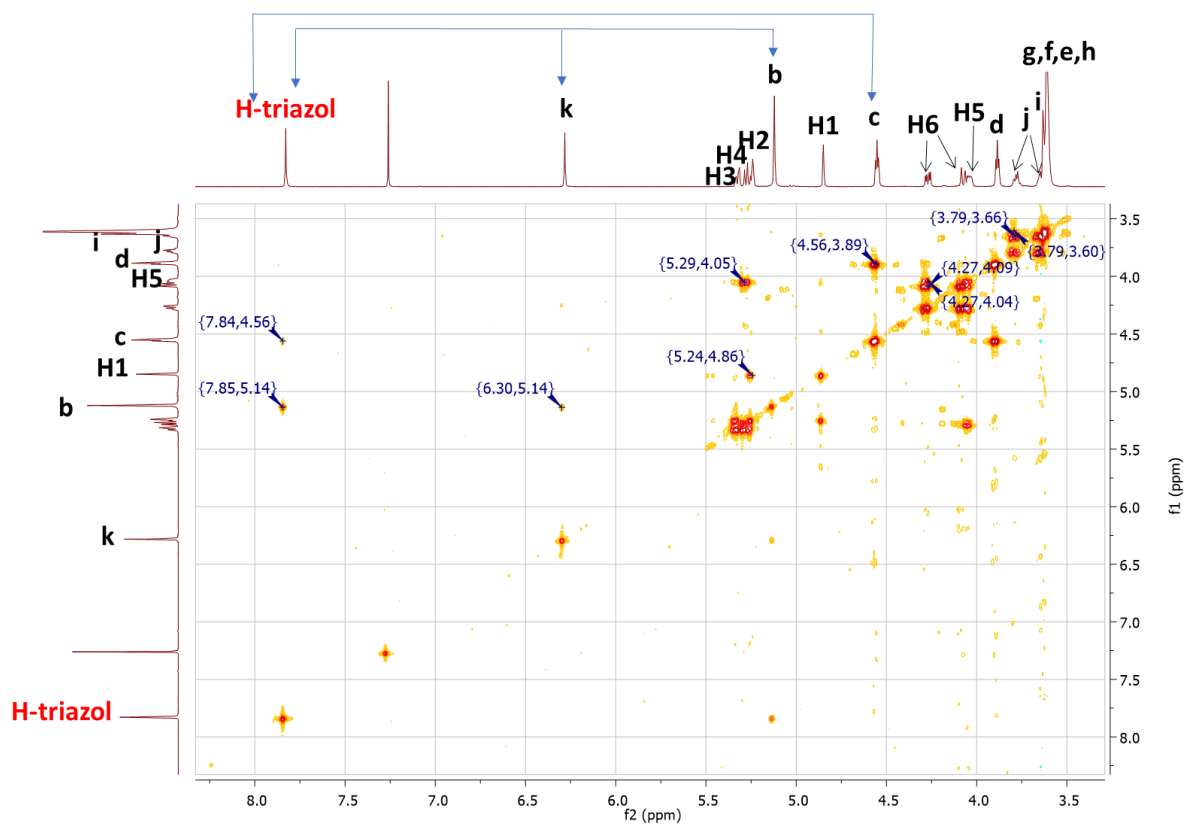


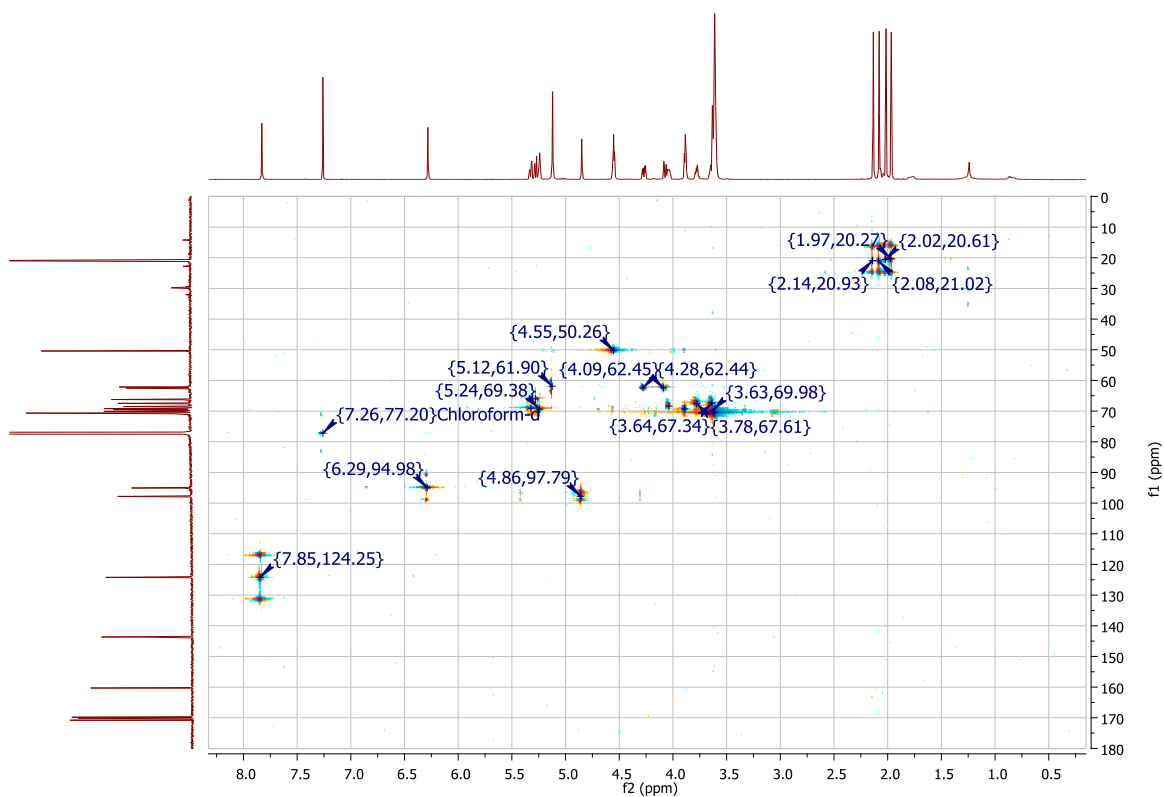
Fig 3. Synthesis DLS of Cpd 27 (Trivalent dendron) Crosslinked with Con A.



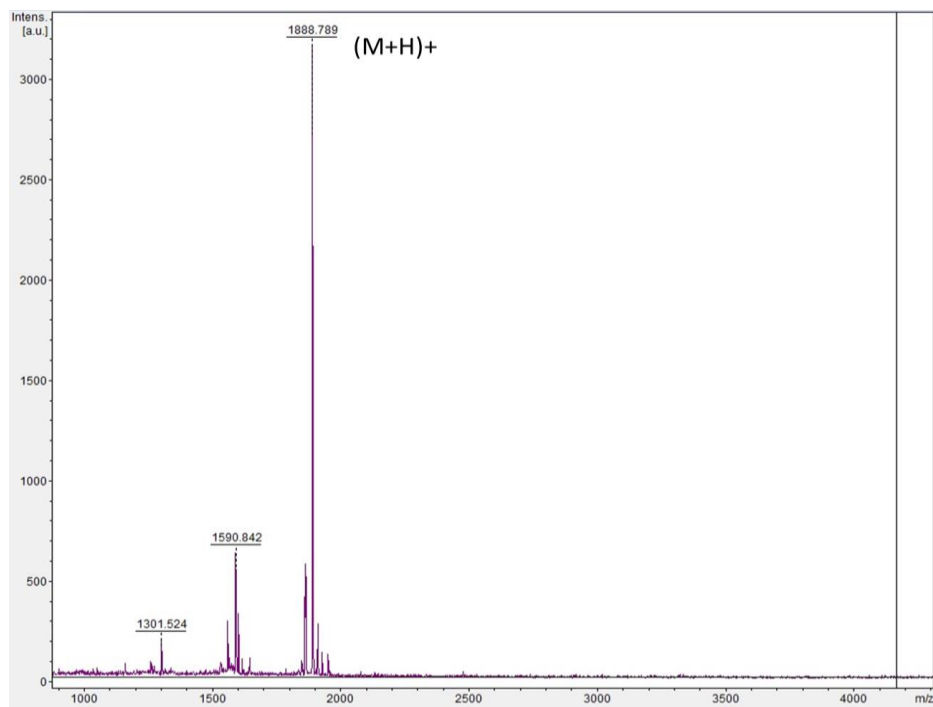
¹H- and ¹³C- NMR spectrum of compound 28.



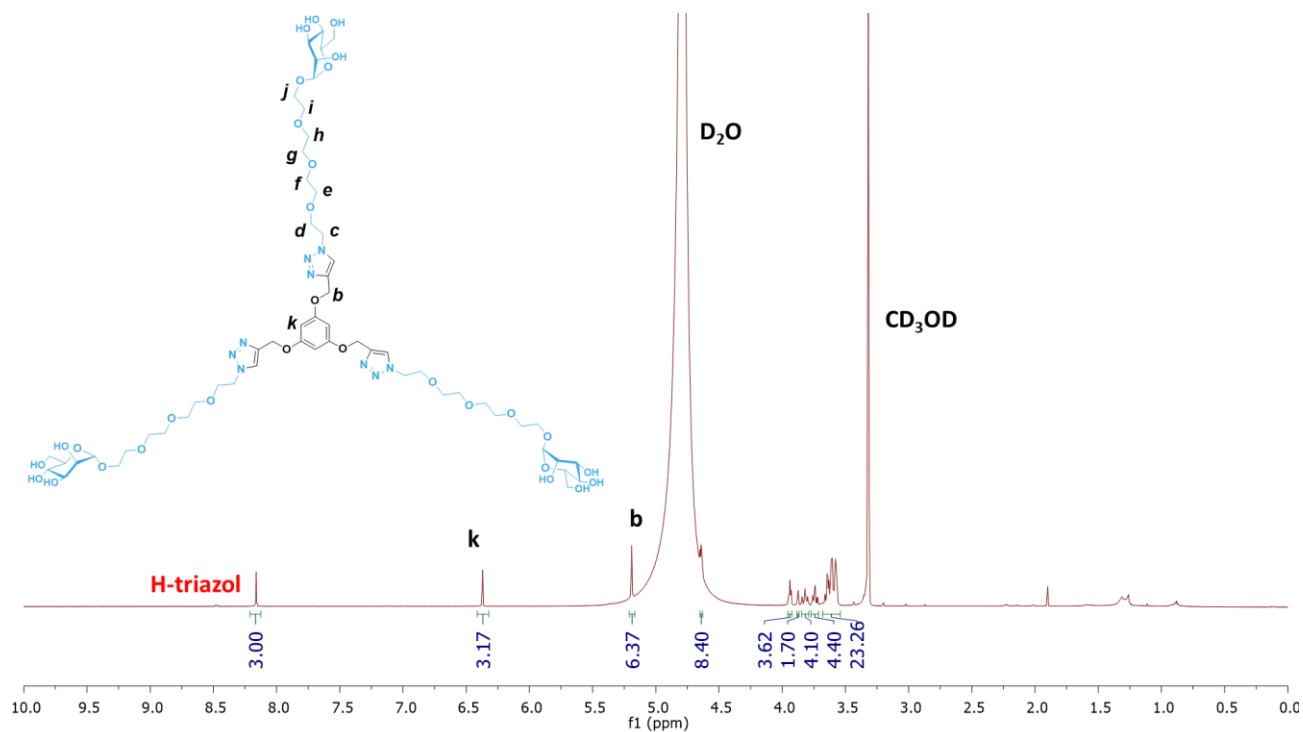
2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 28.



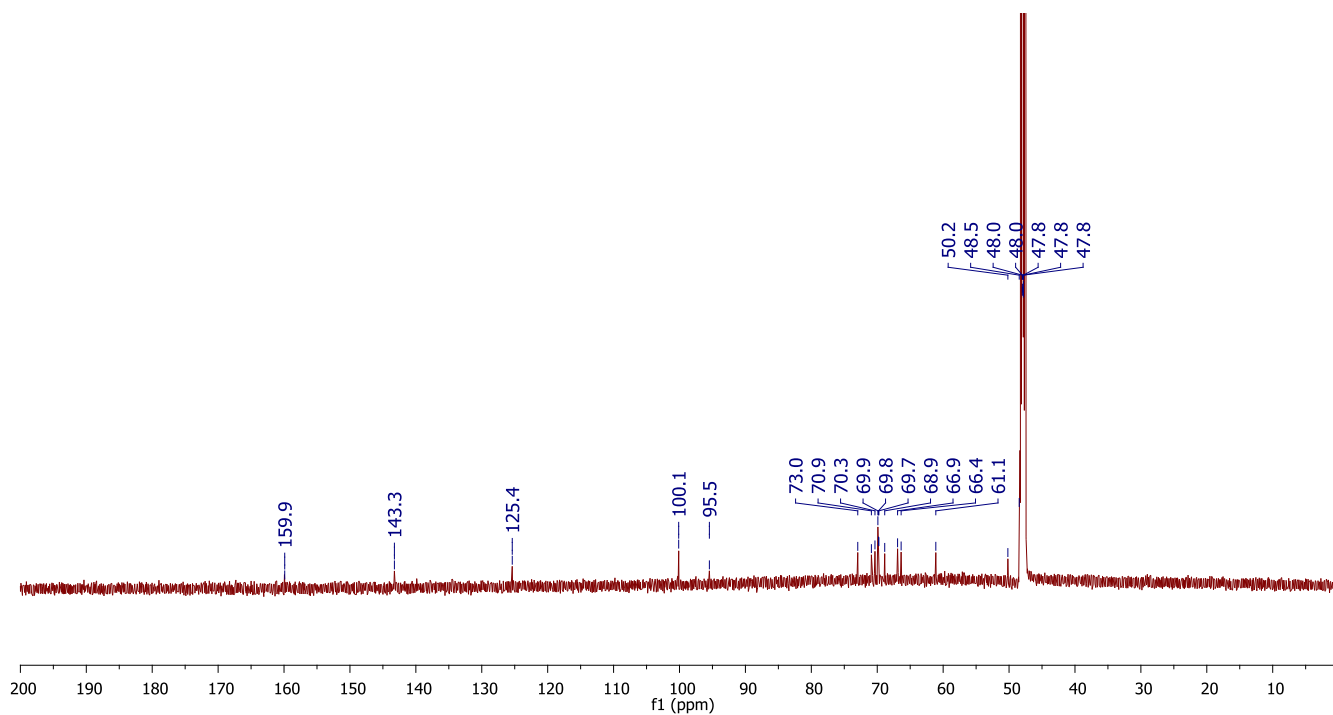
2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 28.



HRMS of compound 28.



¹H- NMR spectrum of compound 29.



¹³C- NMR spectrum of compound 29.

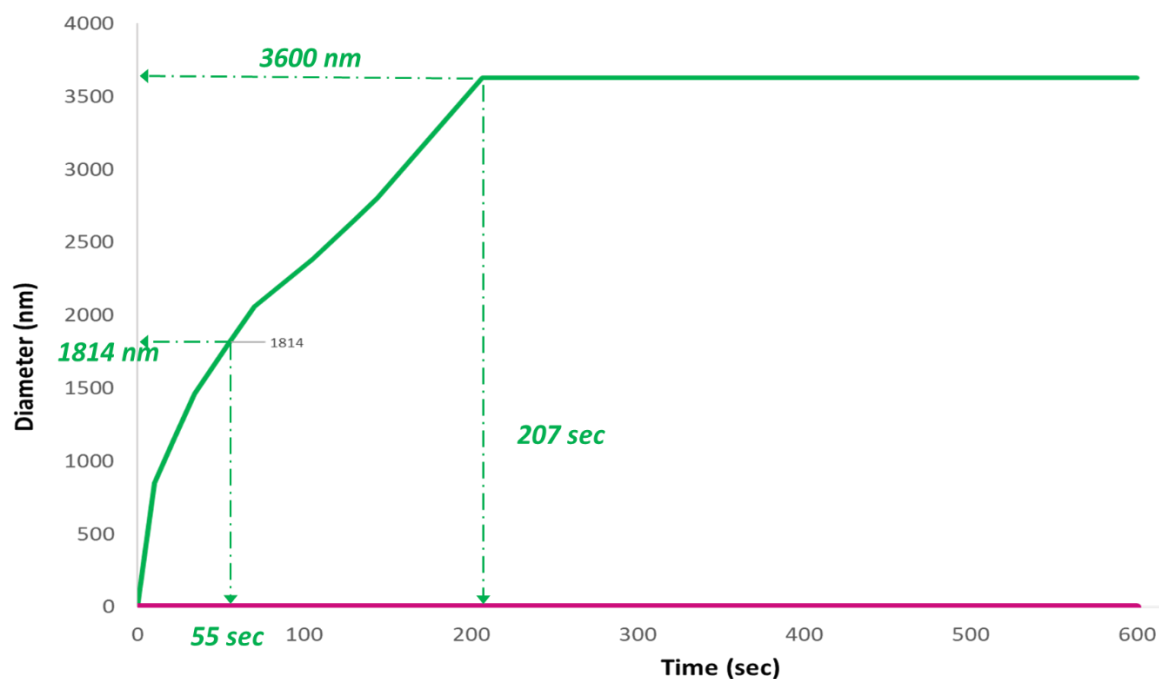
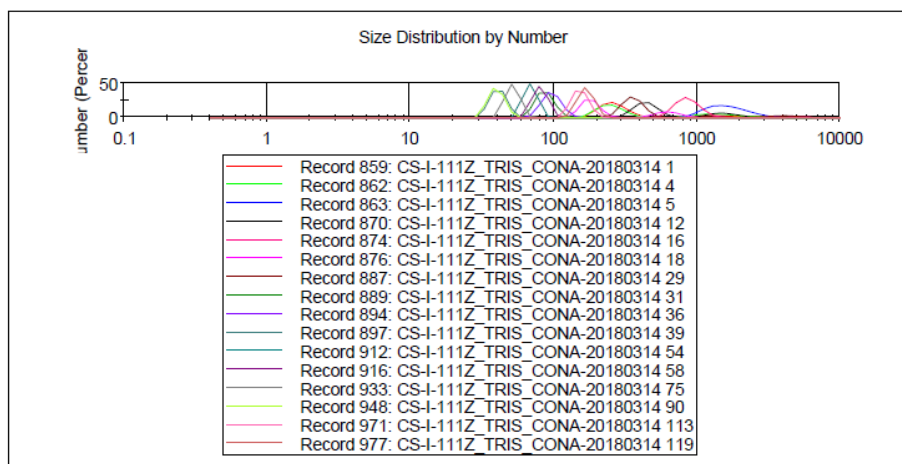
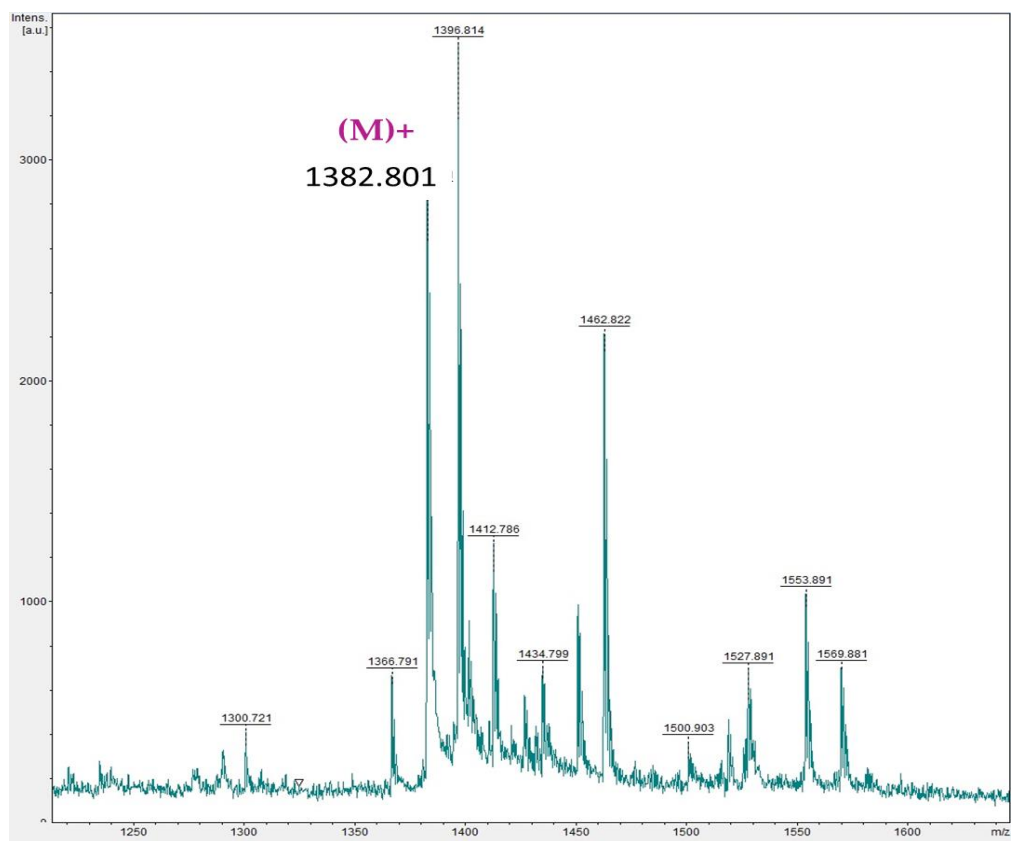


Fig 4. Synthesis DLS of Cpd 29 (Tis) Crosslinked with Con A.

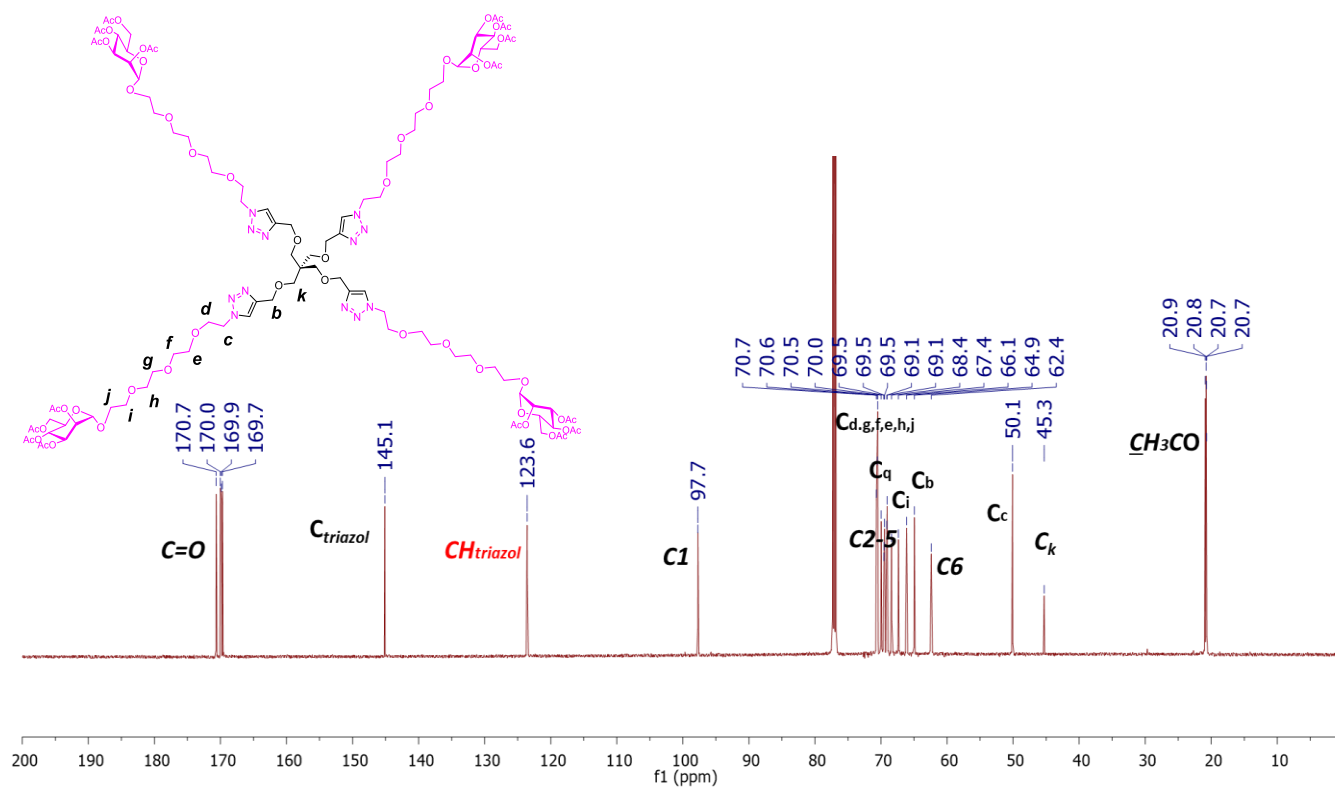
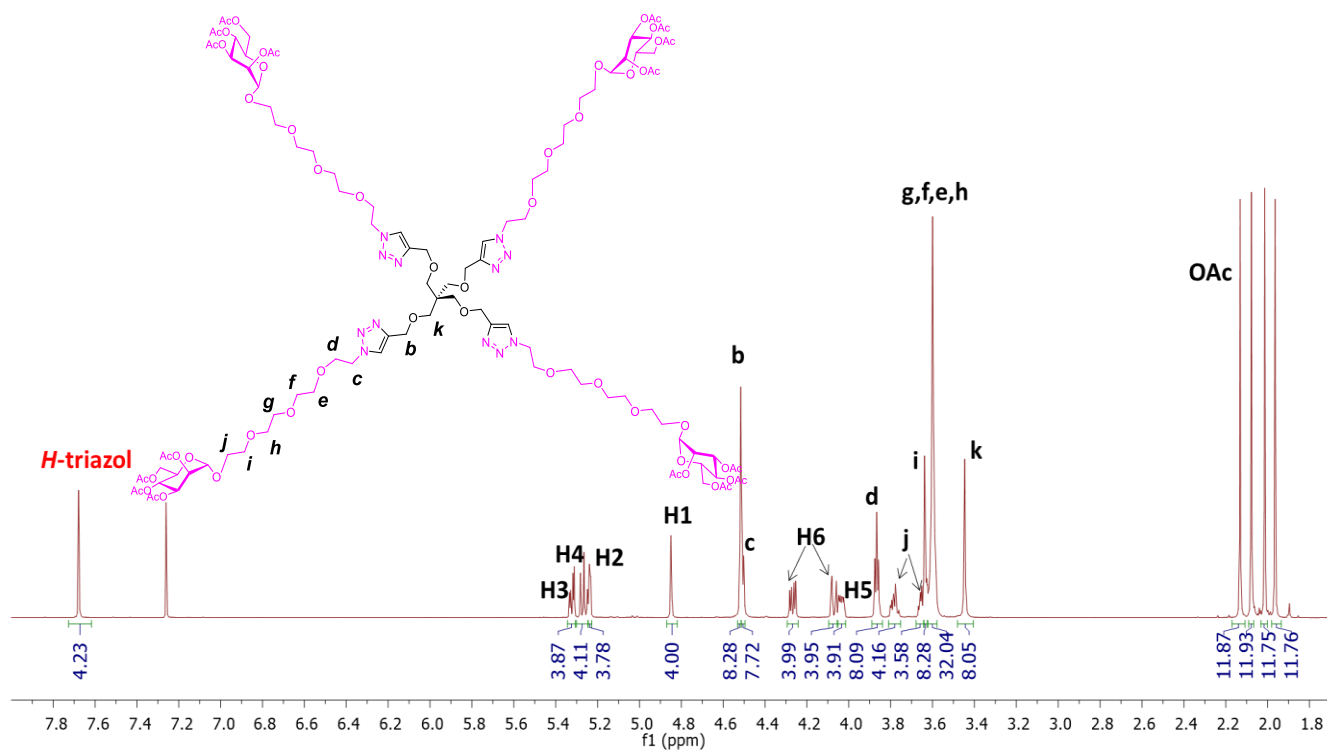
	Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm): 8048	Peak 1: 167.9	100.0	21.81
Pdl: 0.457	Peak 2: 0.000	0.0	0.000
Intercept: 0.831	Peak 3: 0.000	0.0	0.000
Result quality : Refer to quality report			



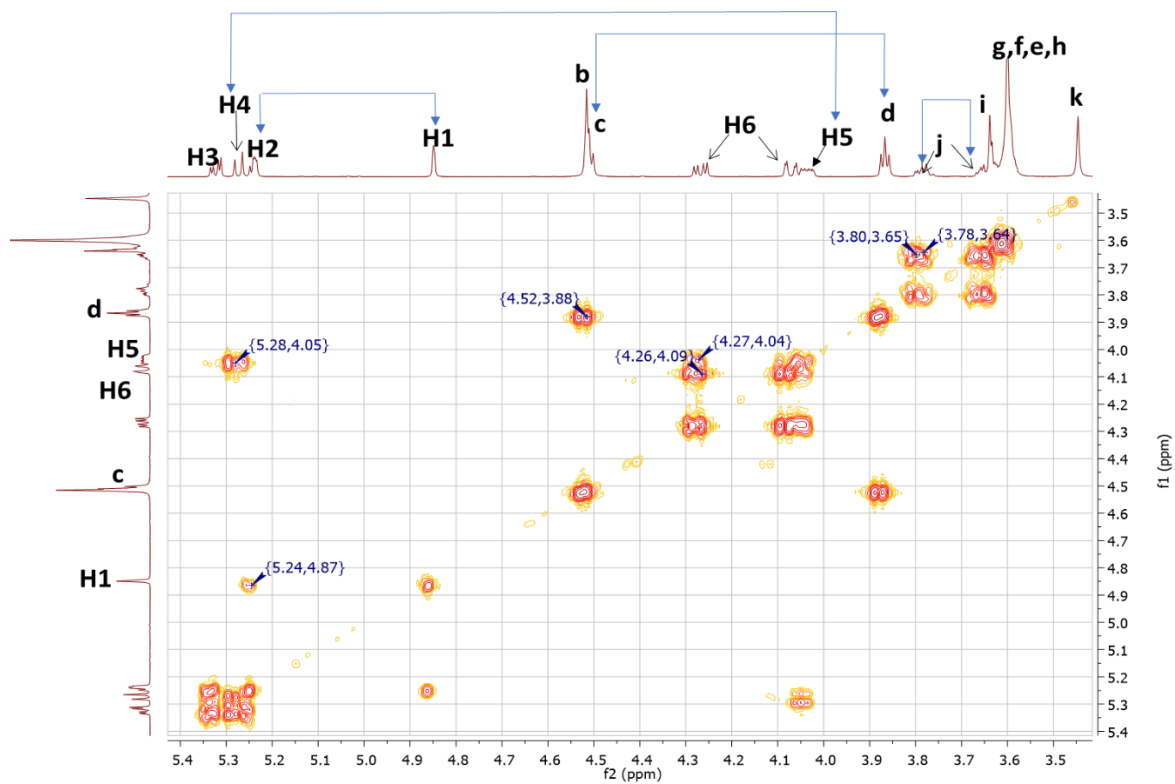
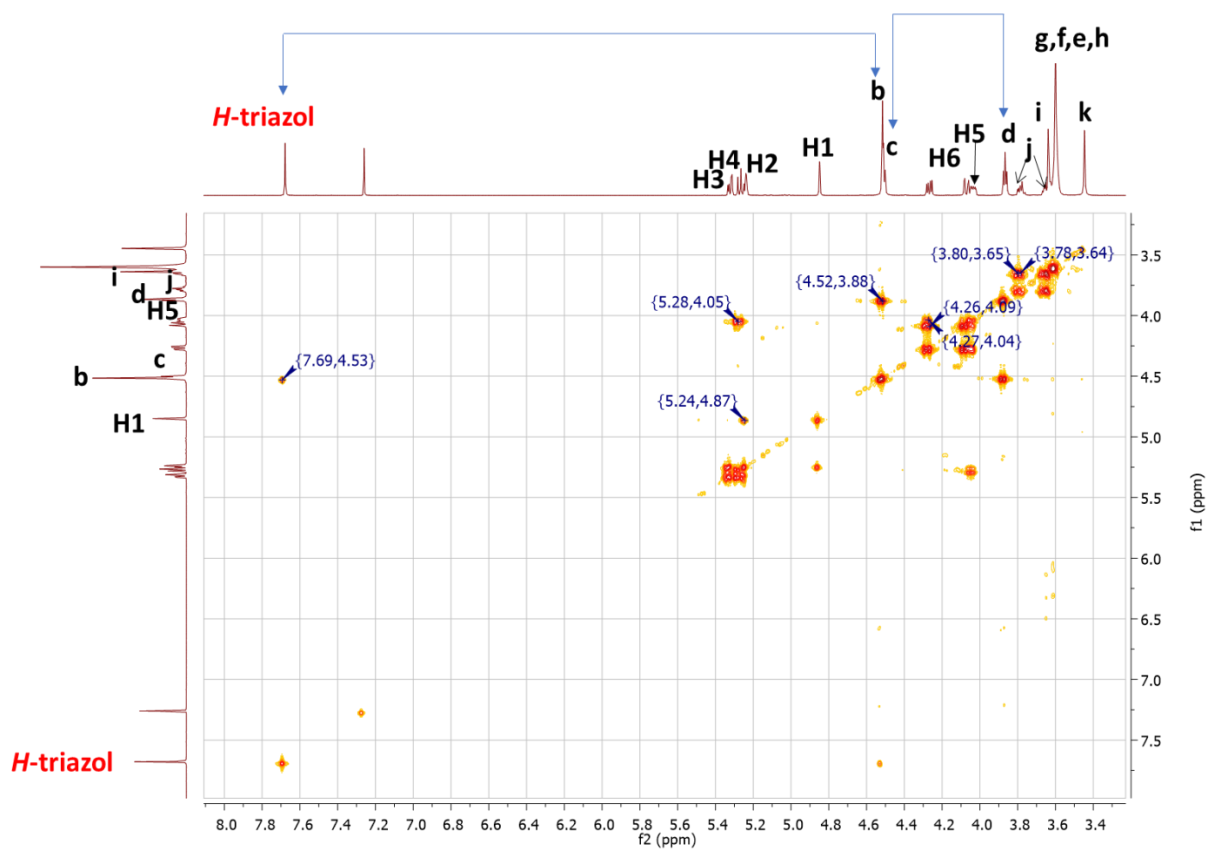
DLS-Size distribution of compound 29.



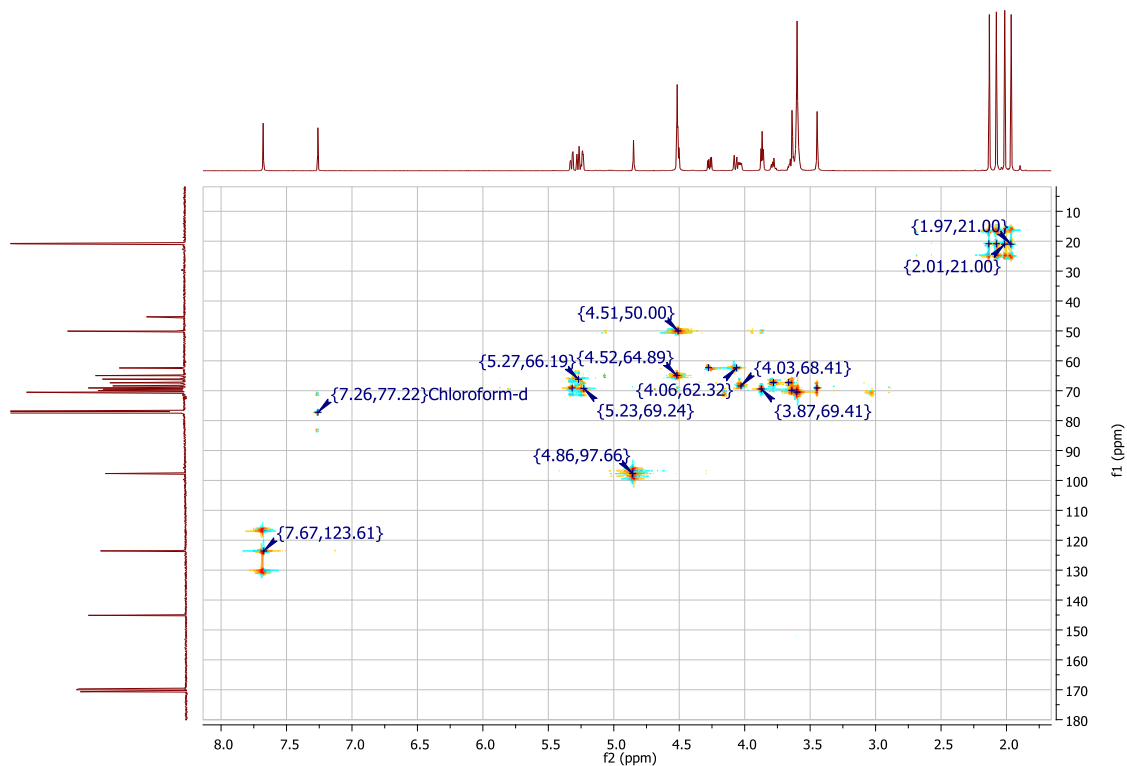
HRMS of compound 29.



¹H- and ¹³C- NMR spectrum of compound 30.



2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 30.

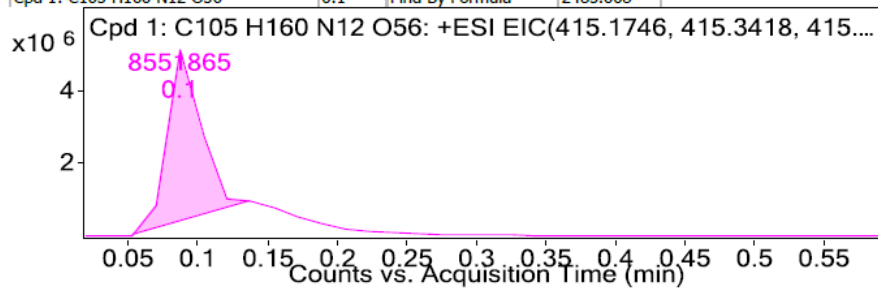


2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 30.

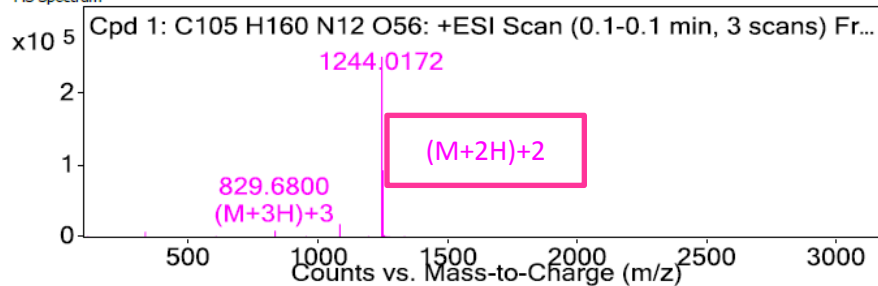
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C105 H160 N12 O56	0.1	2485.008	9337	C105 H160 N12 O56	2485.0041	1.58

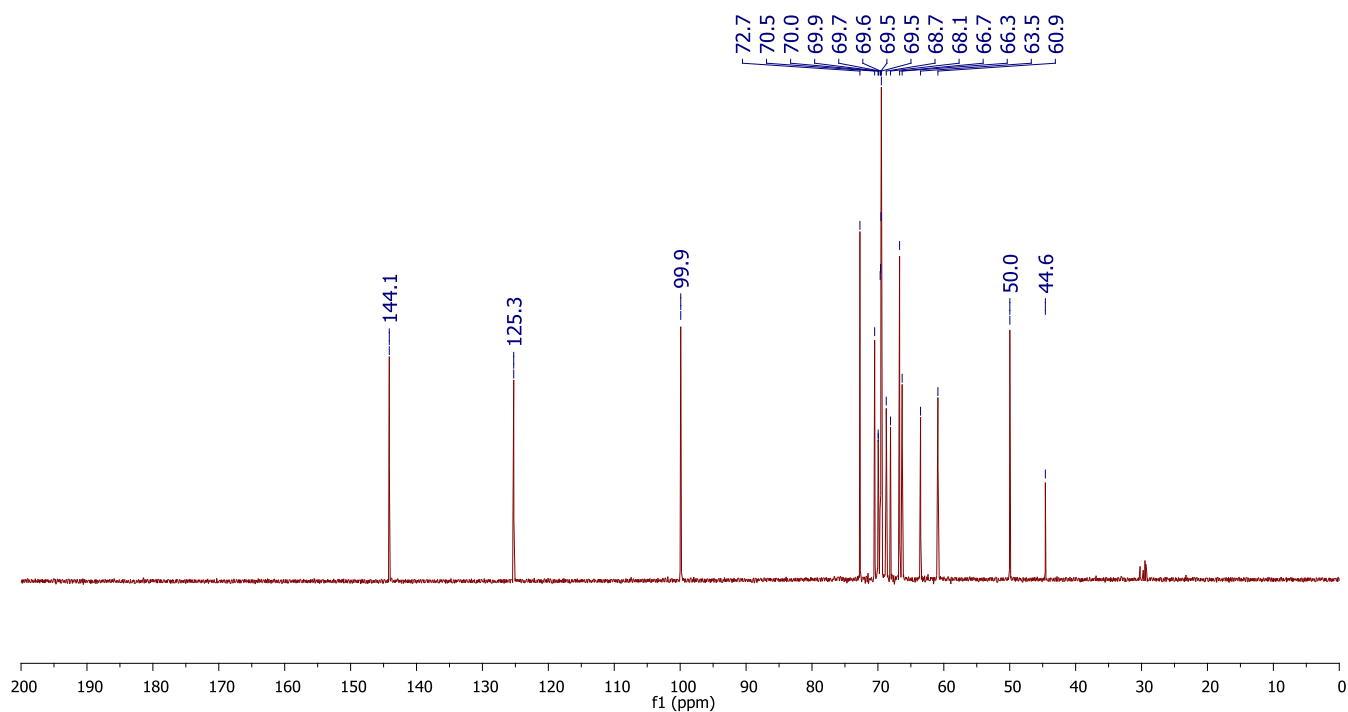
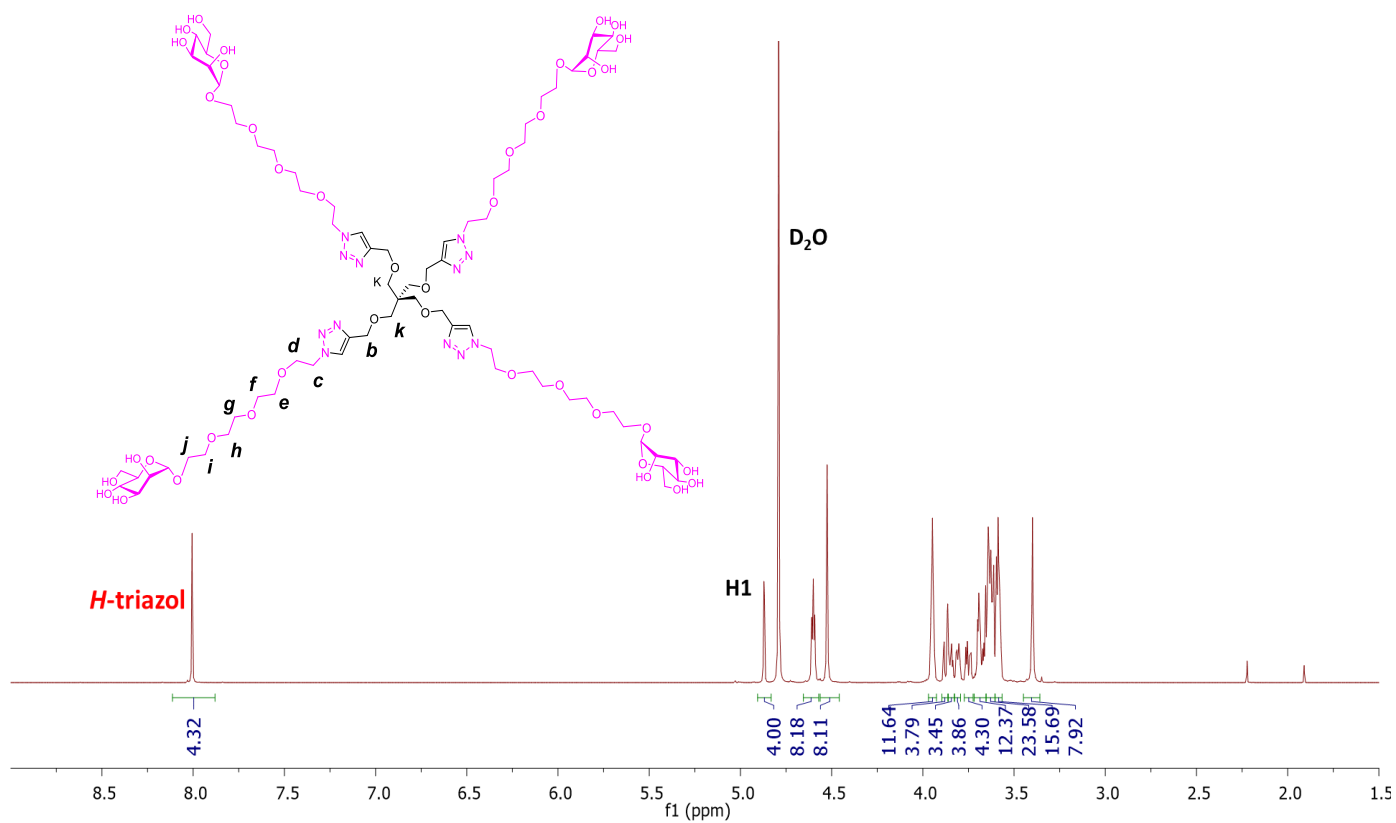
Compound Label	RT	Algorithm	Mass
Cpd 1: C105 H160 N12 O56	0.1	Find By Formula	2485.008



MS Spectrum



HRMS of compound 30.

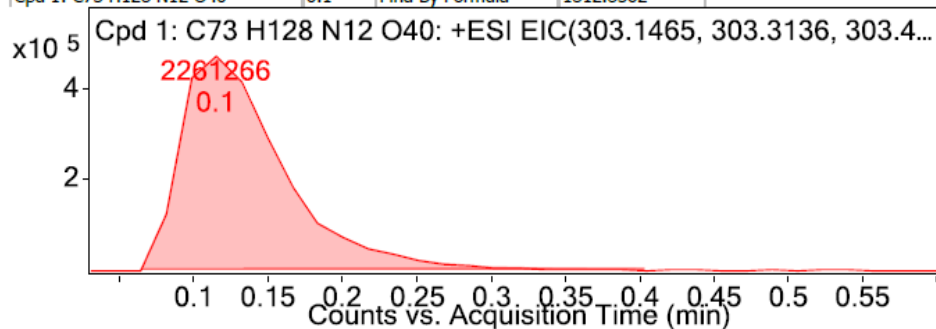


¹H- and ¹³C- NMR spectrum of compound 31.

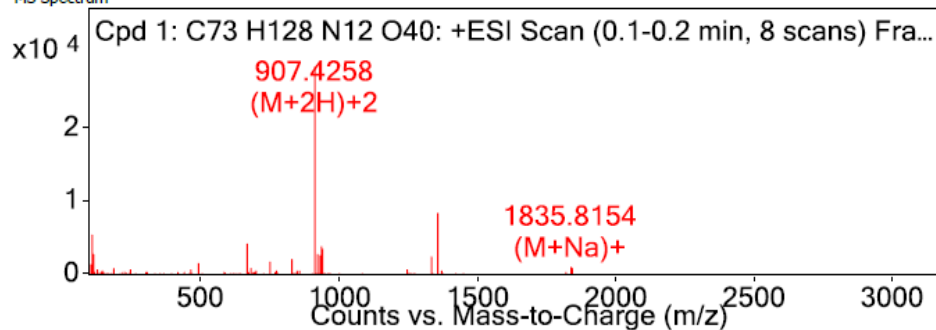
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C73 H128 N12 O40	0.1	1812.8362	28364	C73 H128 N12 O40	1812.8351	0.6

Compound Label	RT	Algorithm	Mass
Cpd 1: C73 H128 N12 O40	0.1	Find By Formula	1812.8362



MS Spectrum



HRMS of compound 31.

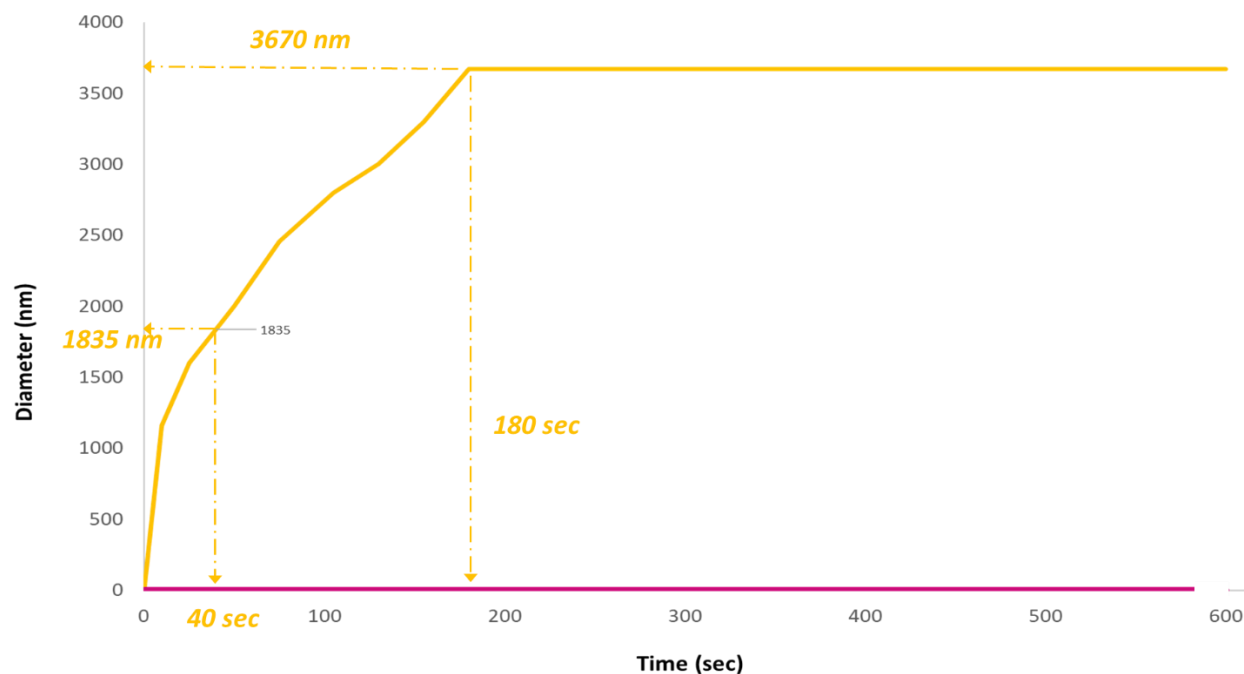
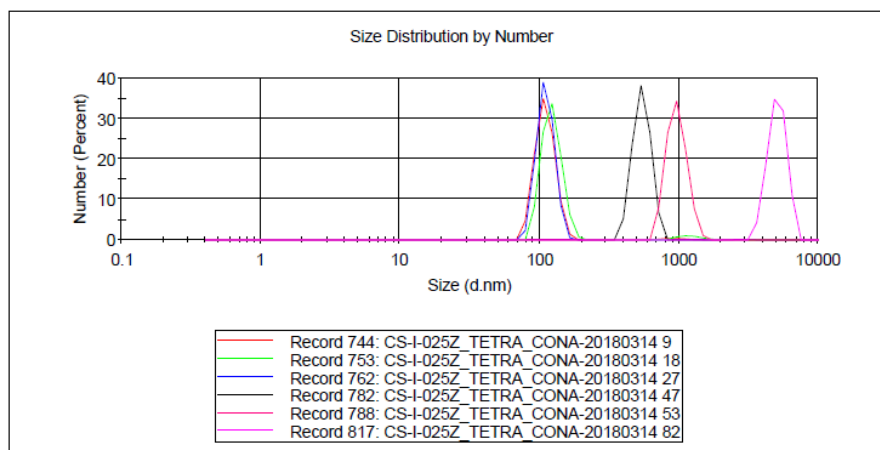


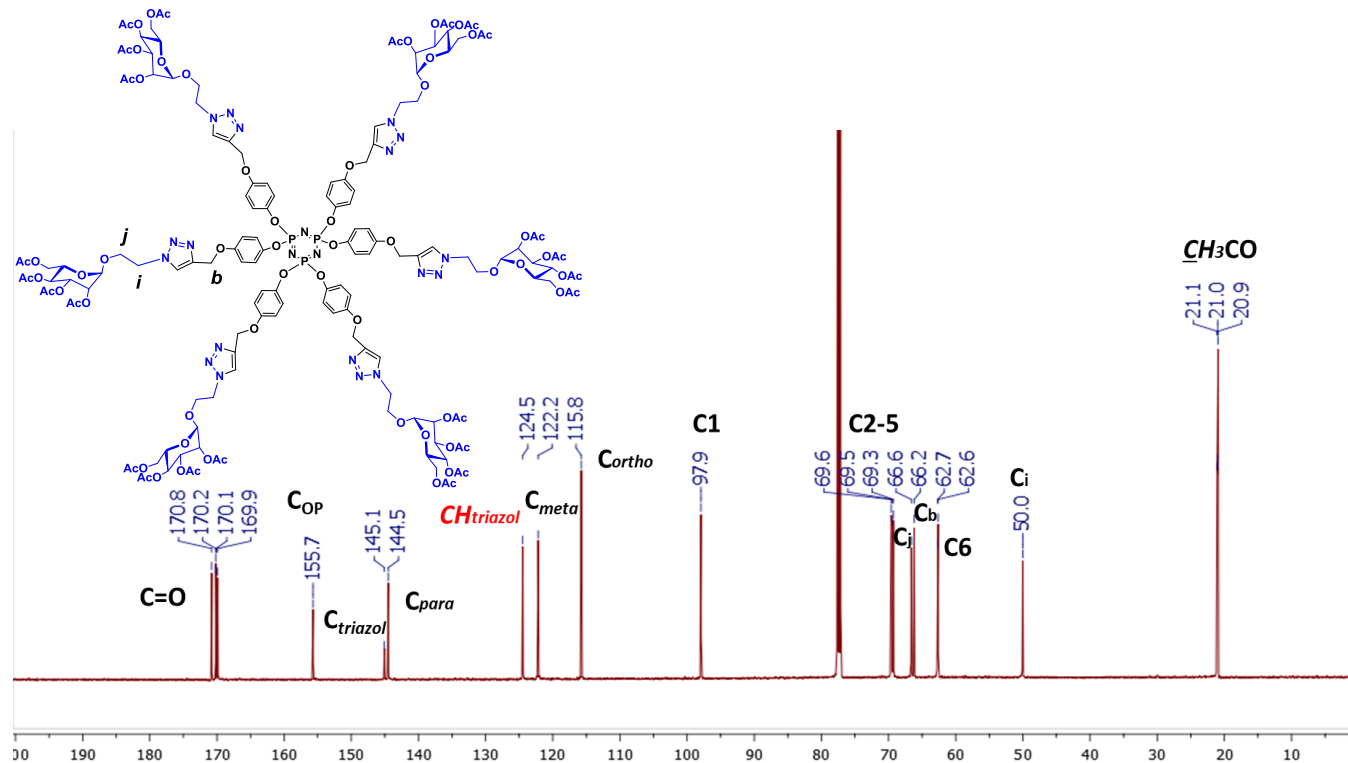
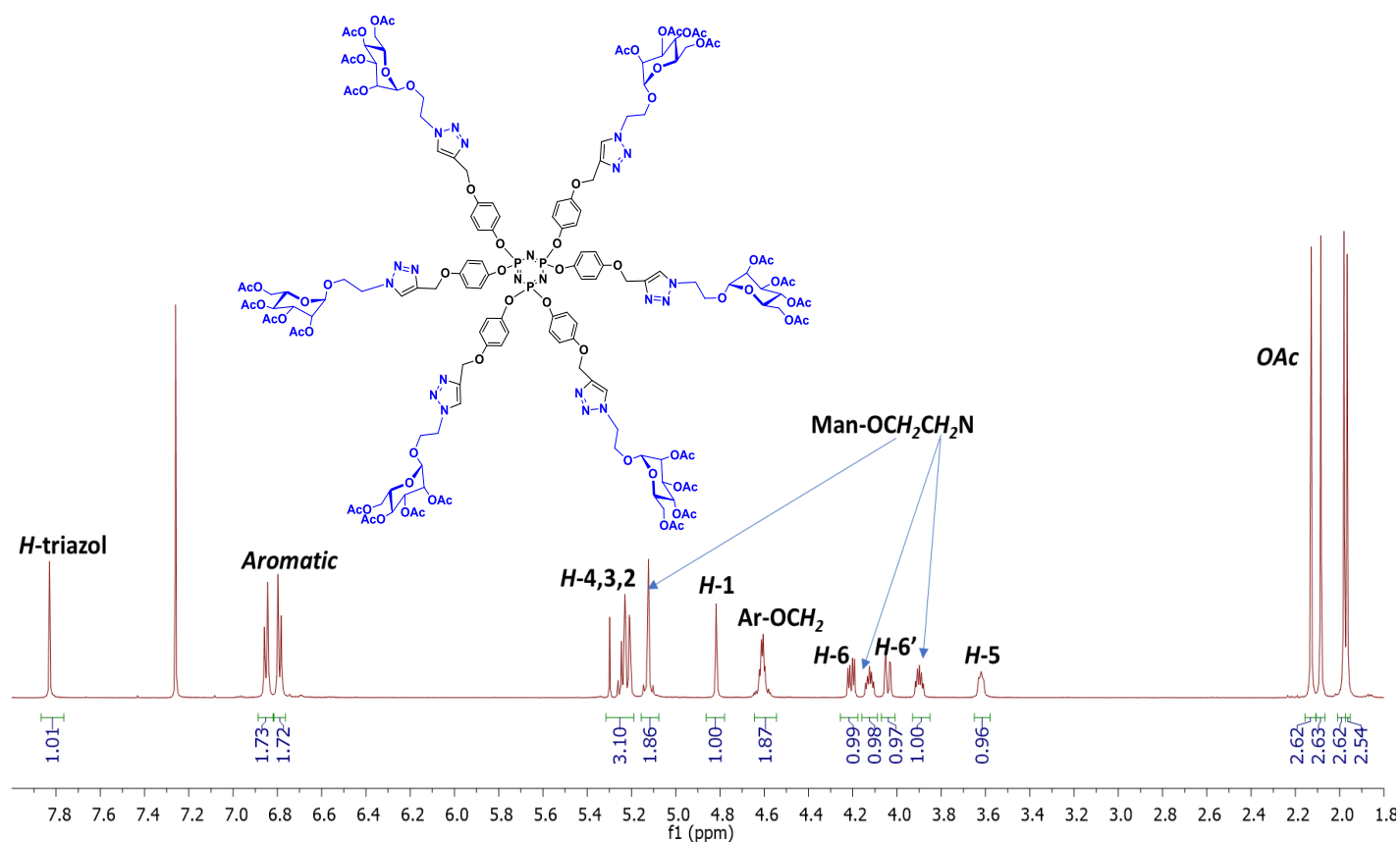
Fig 5. Synthesis DLS of Cpd **31** (Tetra) Crosslinked with Con A.

Results

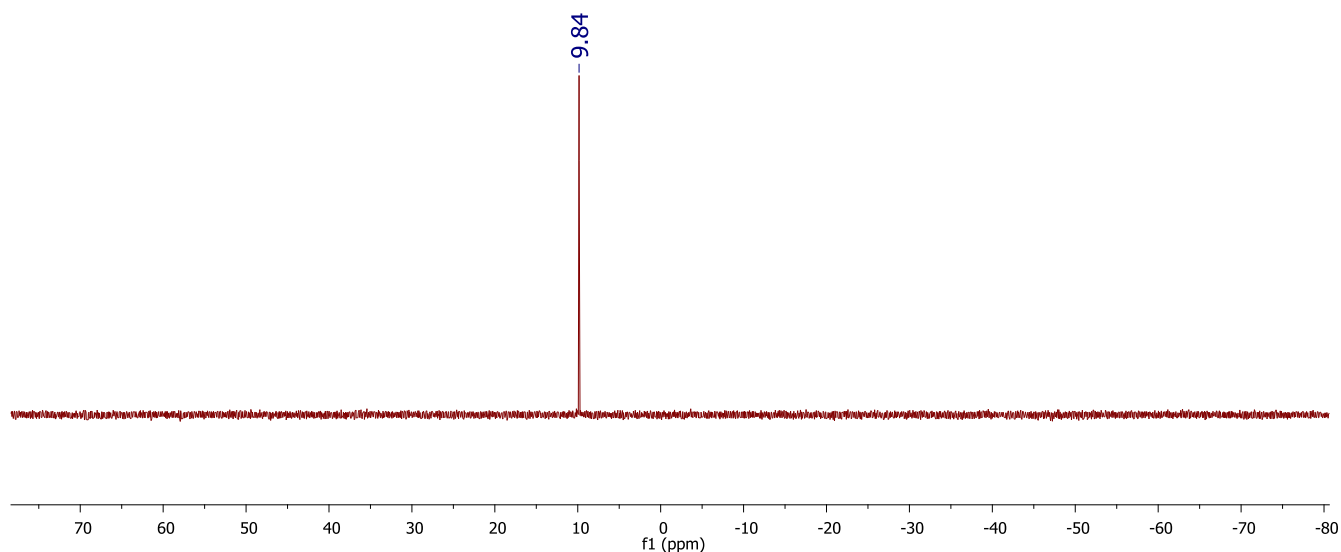
	Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm): 5235	Peak 1: 5051	100.0	747.9
Pdl: 0.030	Peak 2: 0.000	0.0	0.000
Intercept: 0.894	Peak 3: 0.000	0.0	0.000
Result quality : Refer to quality report			



DLS-Size distribution of compound 31.



¹H- and ¹³C- NMR spectrum of compound 33

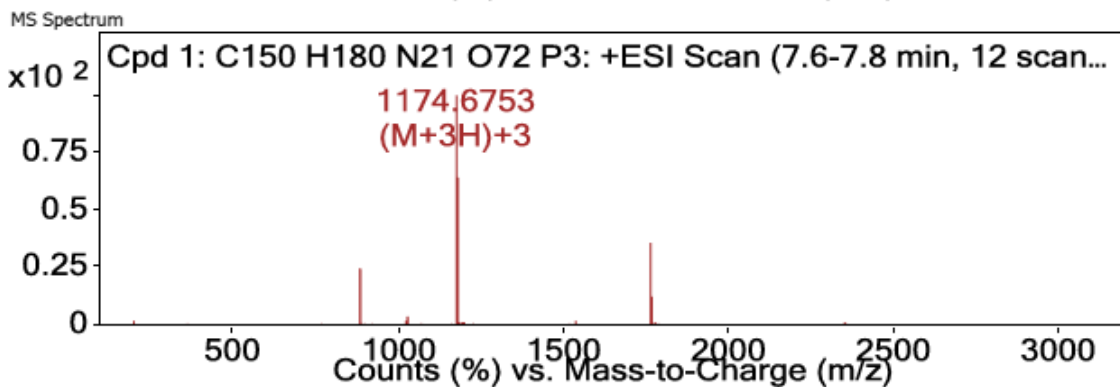
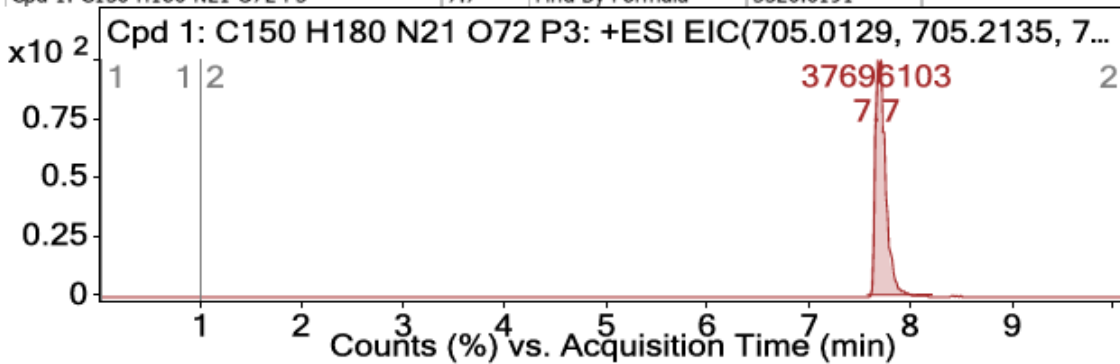


^{31}P - NMR spectrum of compound 33.

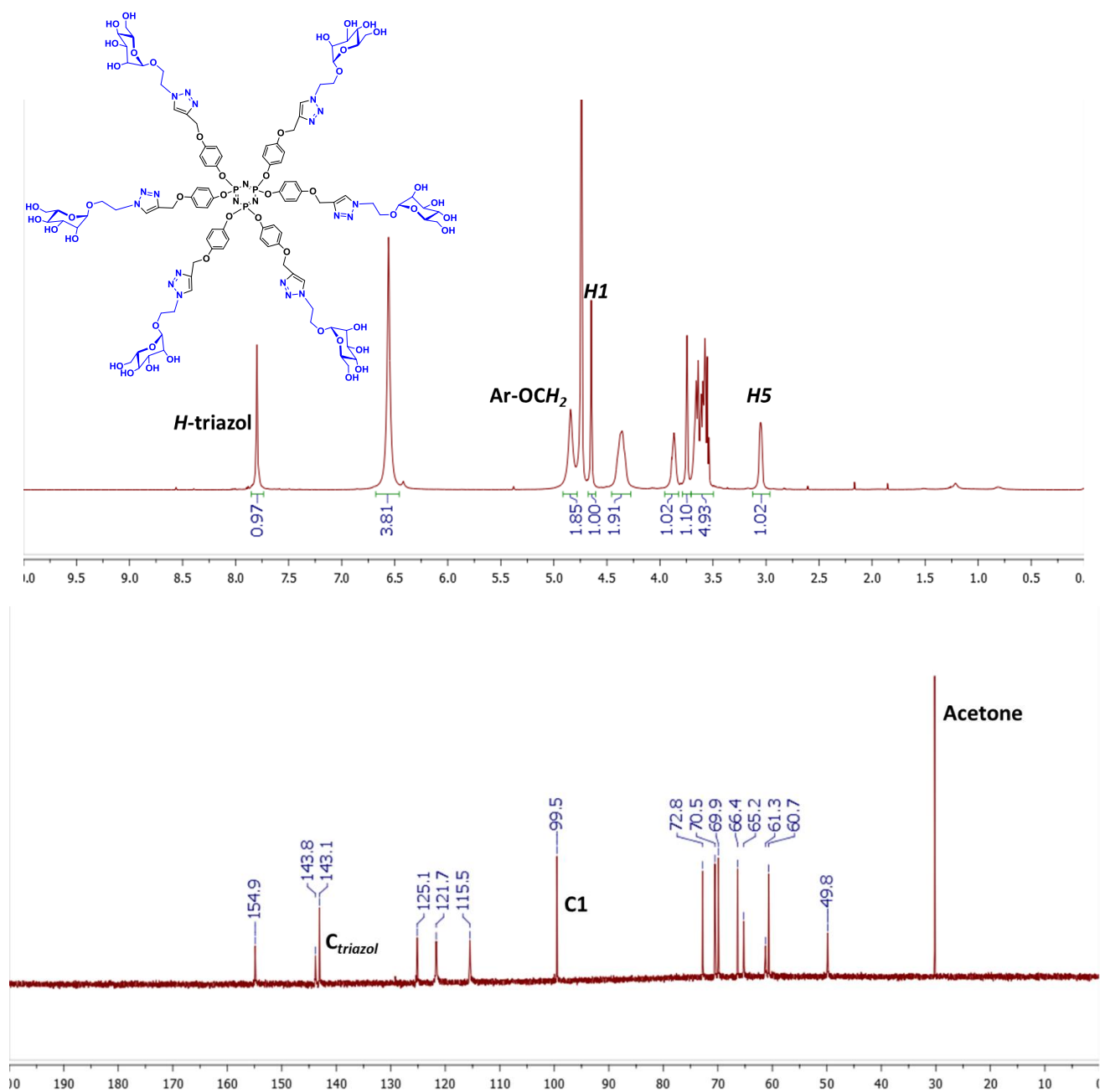
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C150 H180 N21 O72 P3	7.7	3520.0191	167714	C150 H180 N21 O72 P3	3520.0282	-2.59

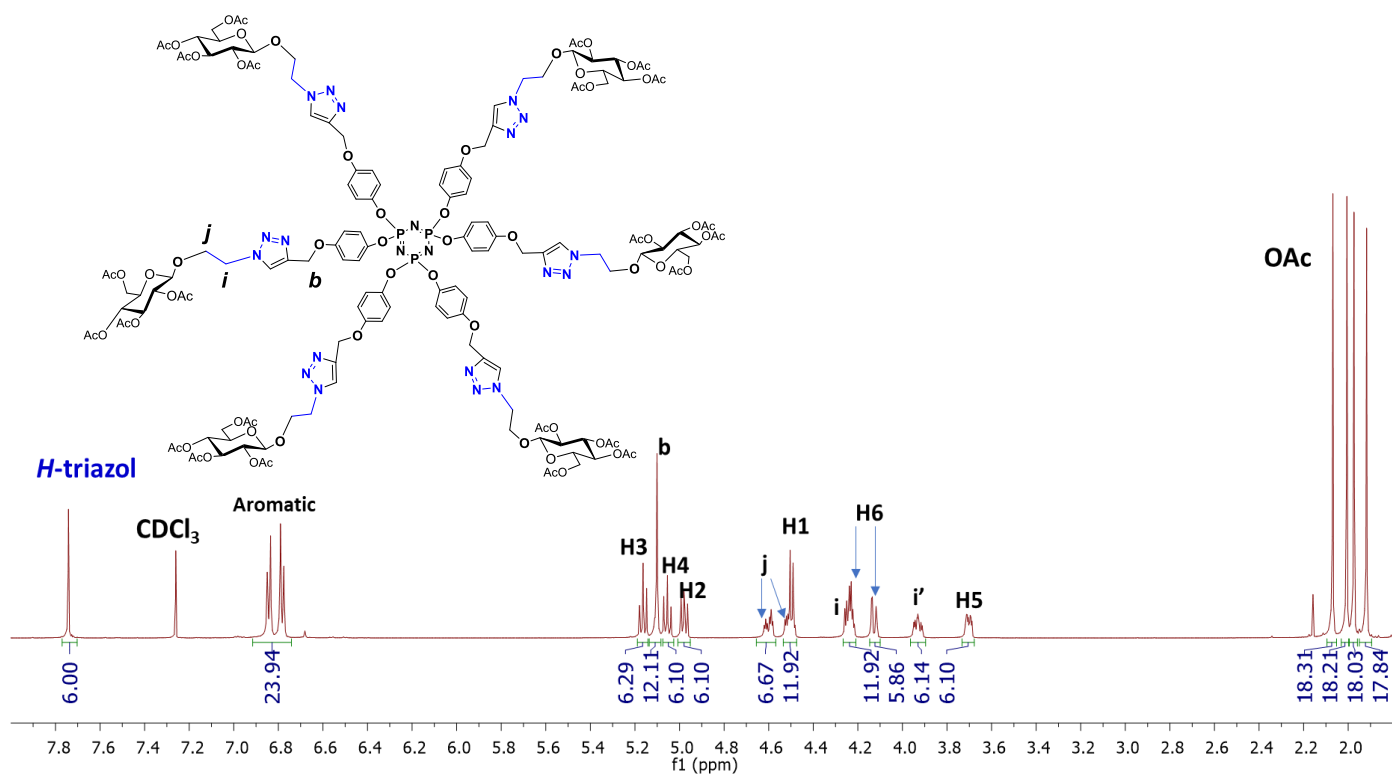
Compound Label	RT	Algorithm	Mass
Cpd 1: C150 H180 N21 O72 P3	7.7	Find By Formula	3520.0191



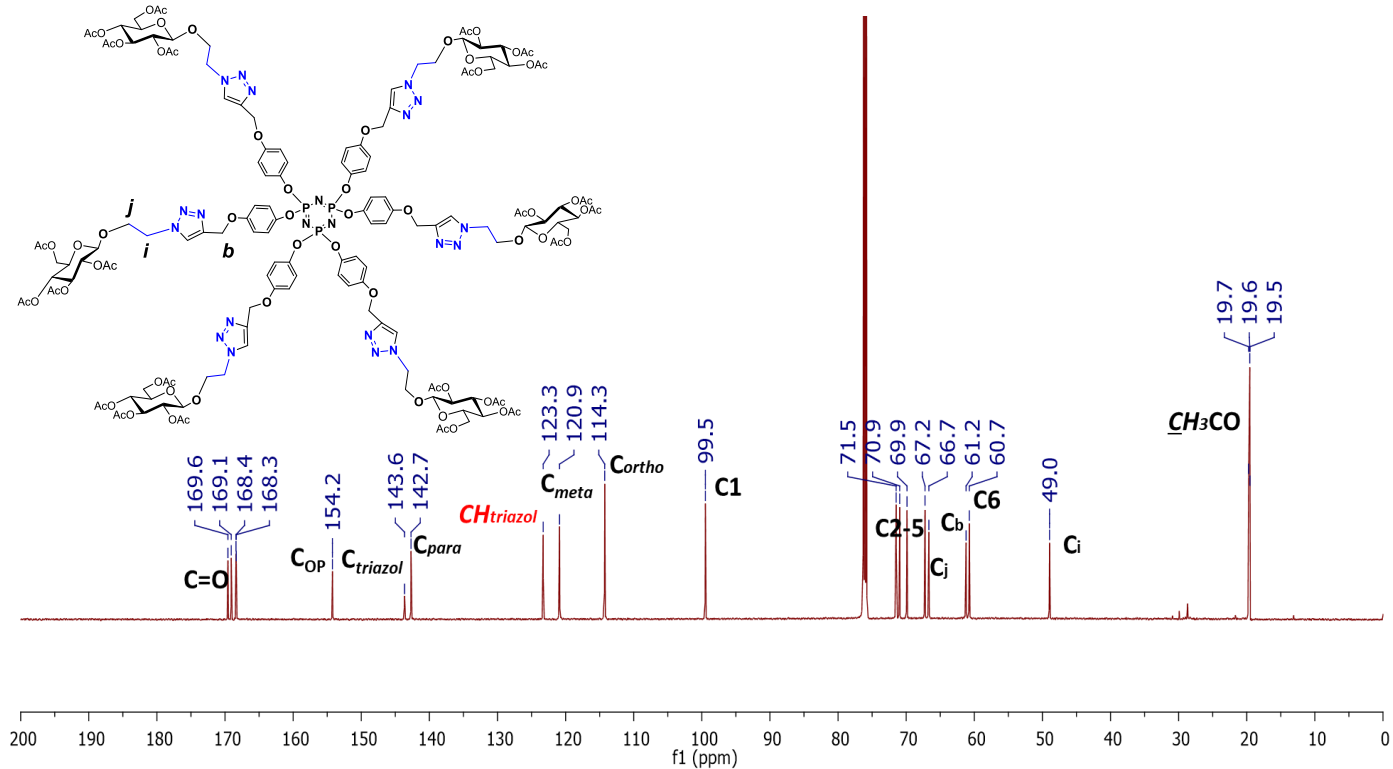
HRMS of compound 33.



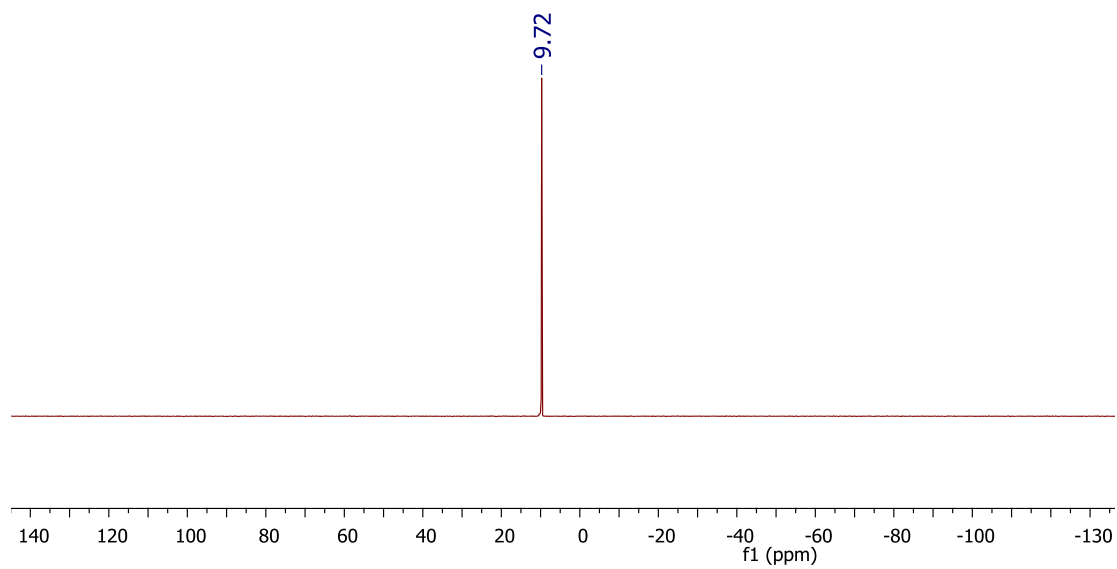
^1H - and ^{13}C - NMR spectrum of compound 34.



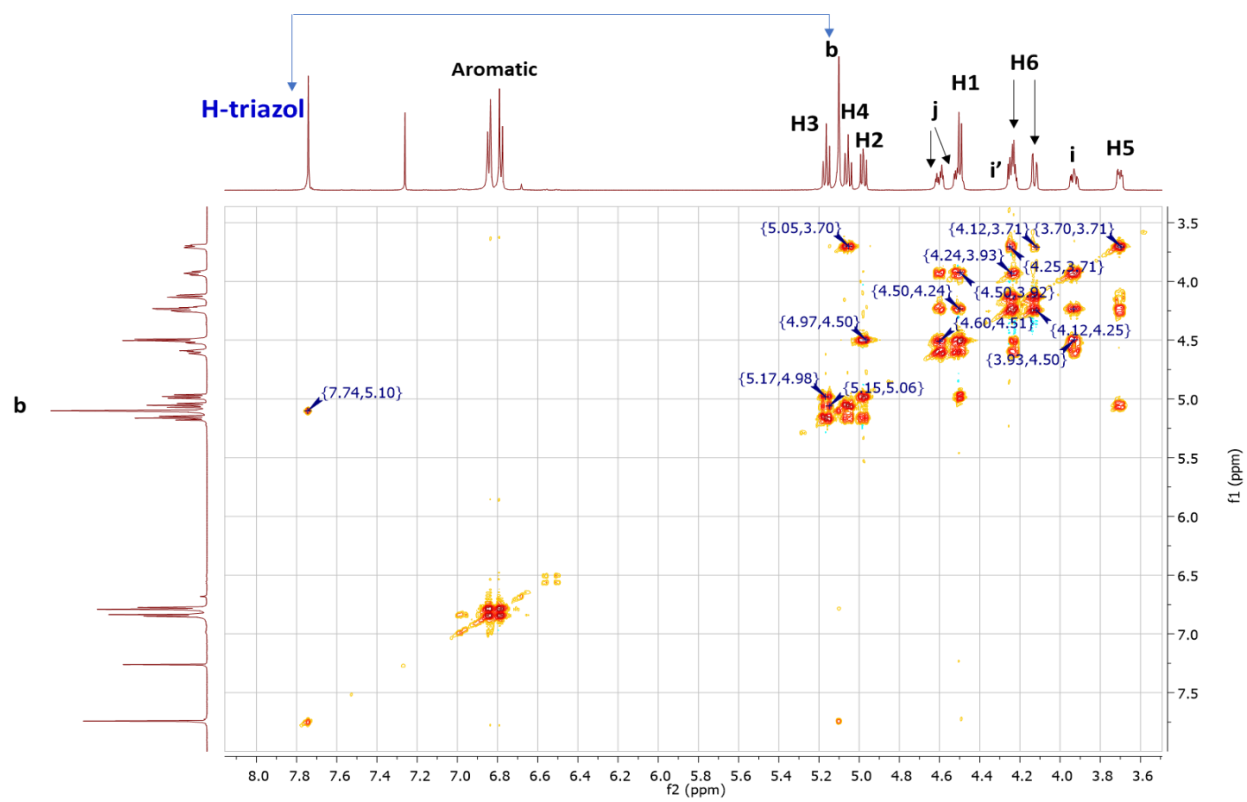
¹H-NMR spectrum of compound 35.

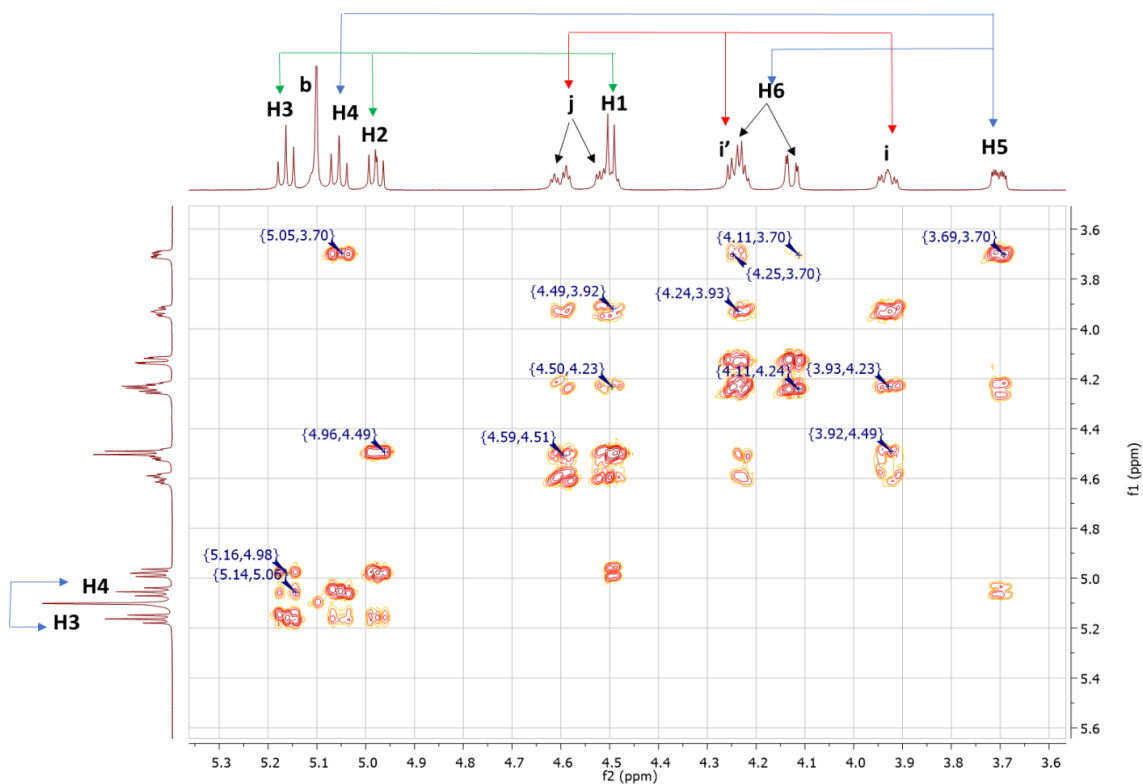


¹³C-NMR spectrum of compound 35.

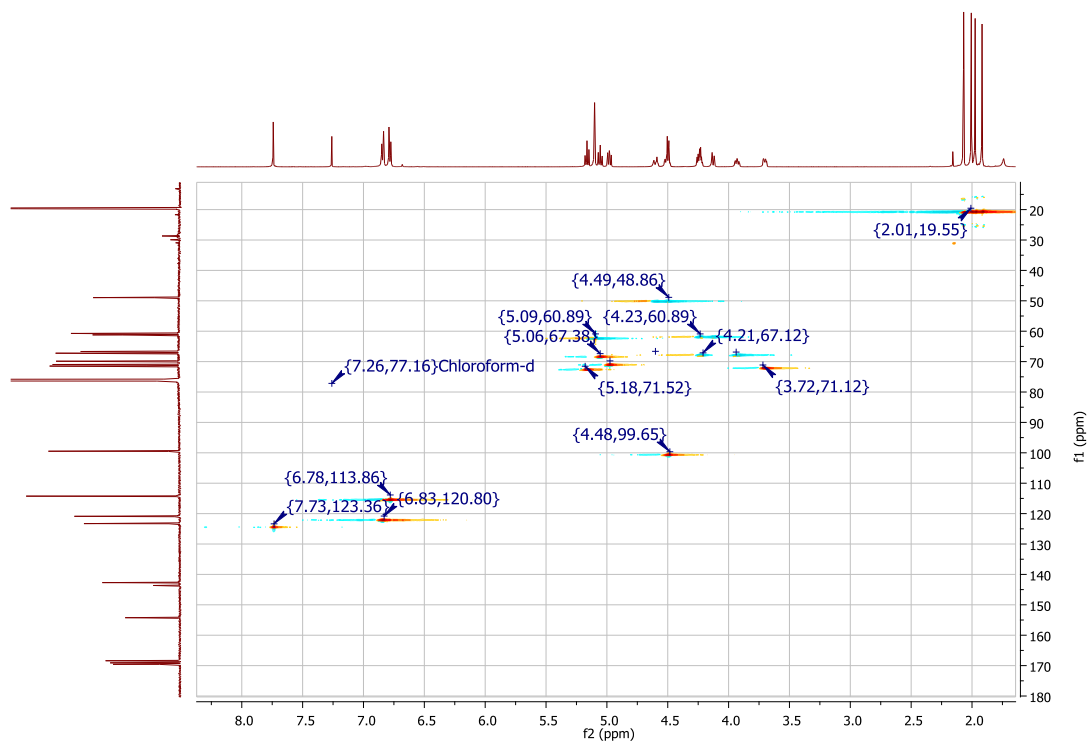


^{31}P - NMR spectrum of compound 35.

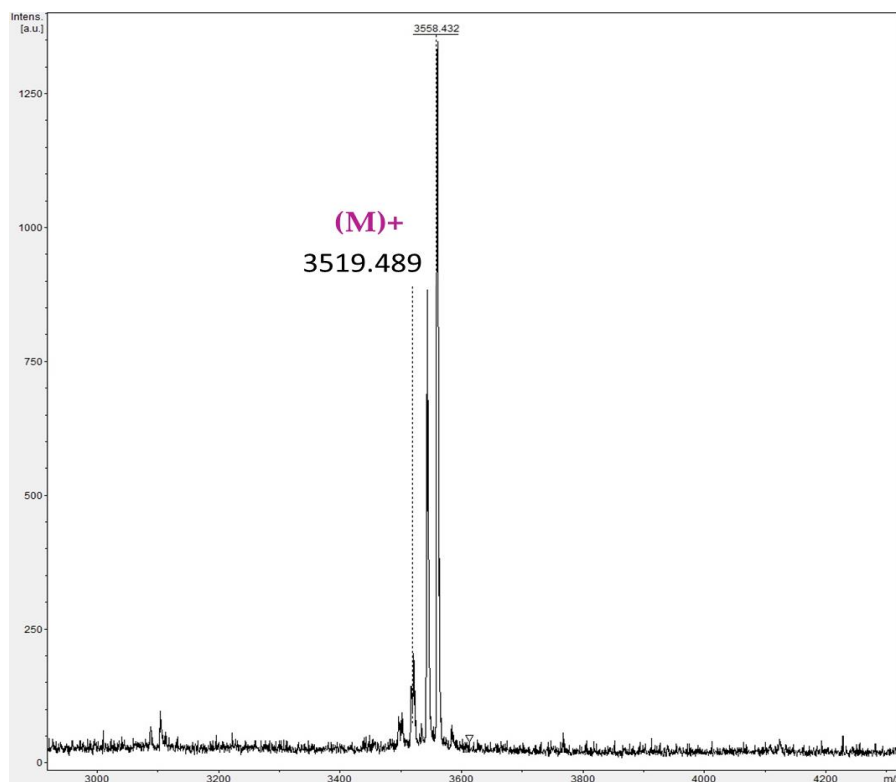




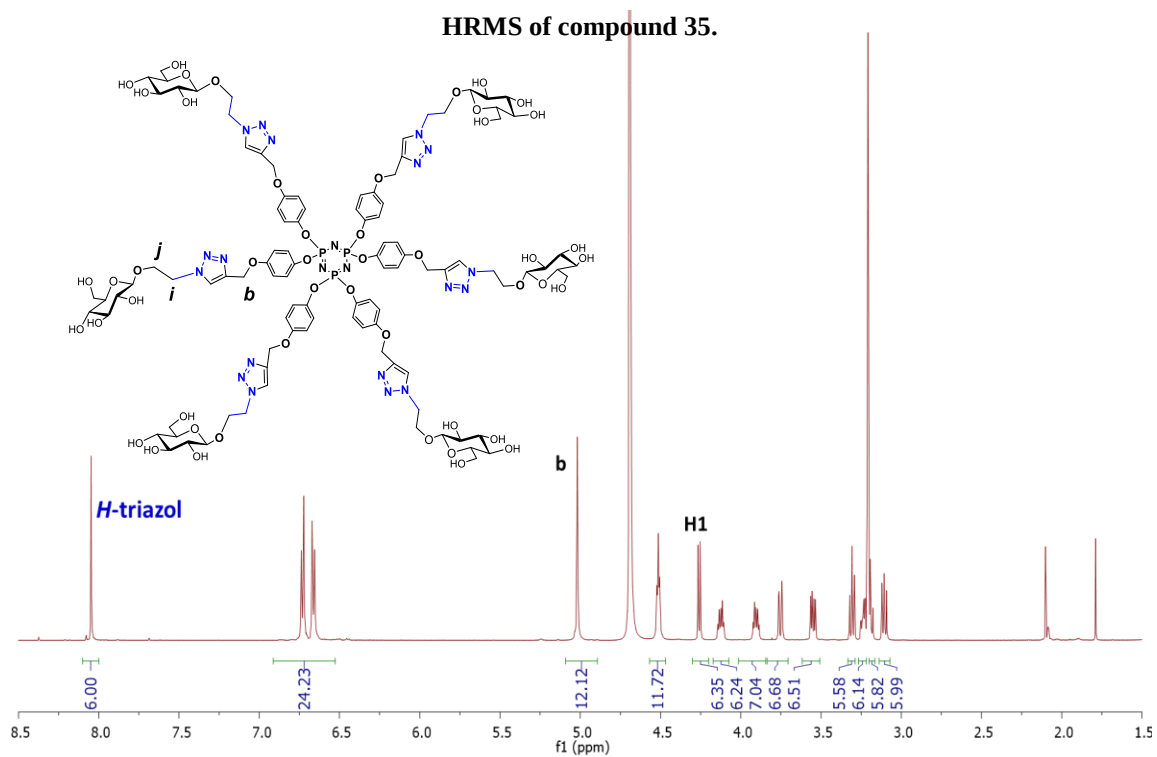
2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 35.



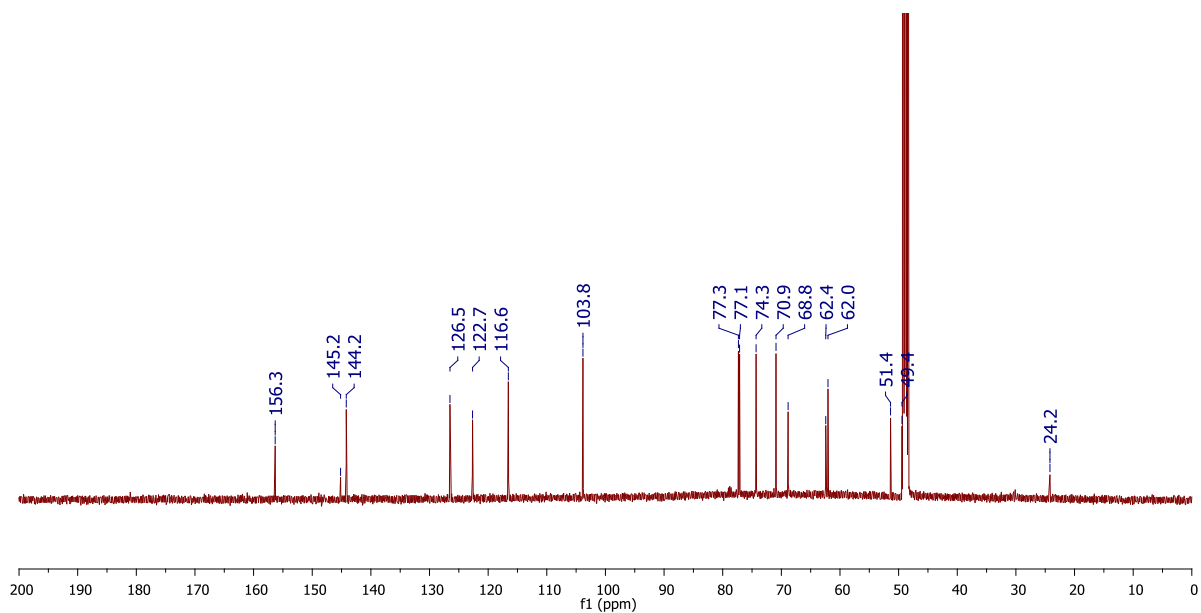
2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 35.



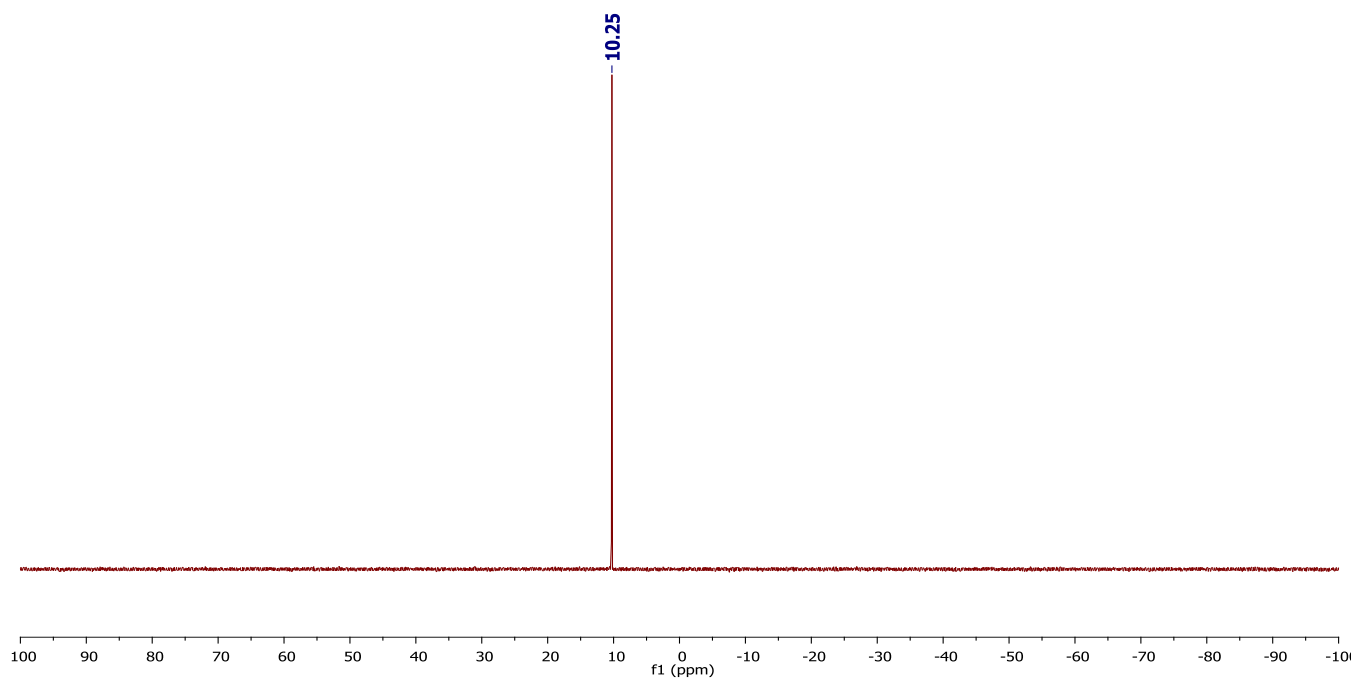
HRMS of compound 35.



¹H- NMR spectrum of compound 36.



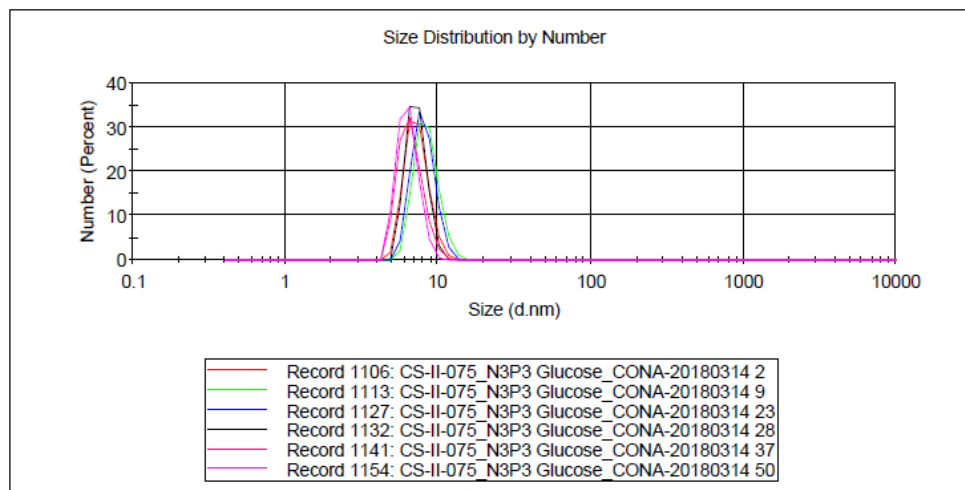
^{13}C - NMR spectrum of compound 36.



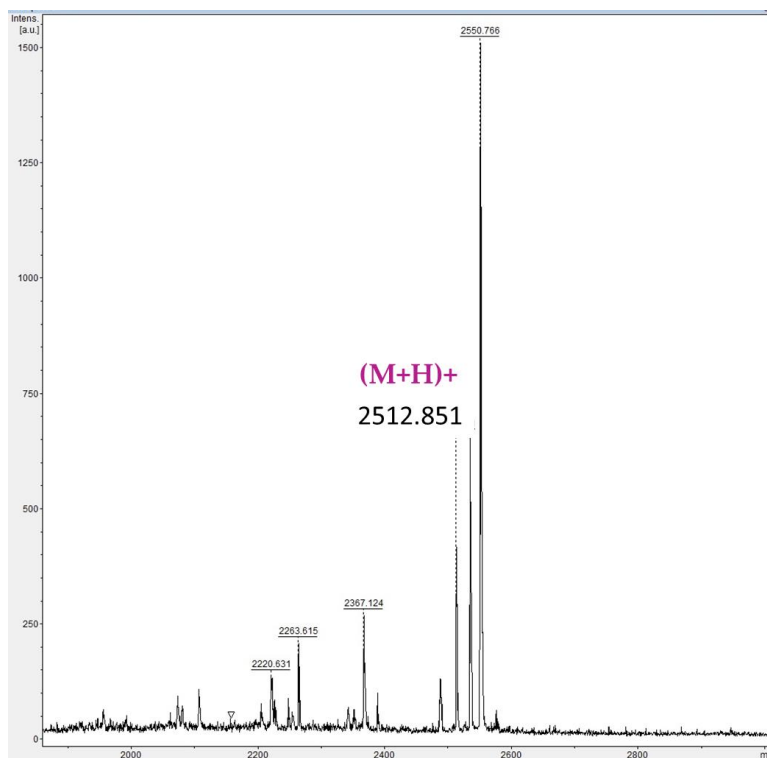
^{31}P - NMR spectrum of compound 36.

		Size (d.nm):	% Number:	St Dev (d.nm):
Z-Average (d.nm): 85.49	Peak 1:	6.344	100.0	1.006
Pdl: 0.579	Peak 2:	0.000	0.0	0.000
Intercept: 0.900	Peak 3:	0.000	0.0	0.000

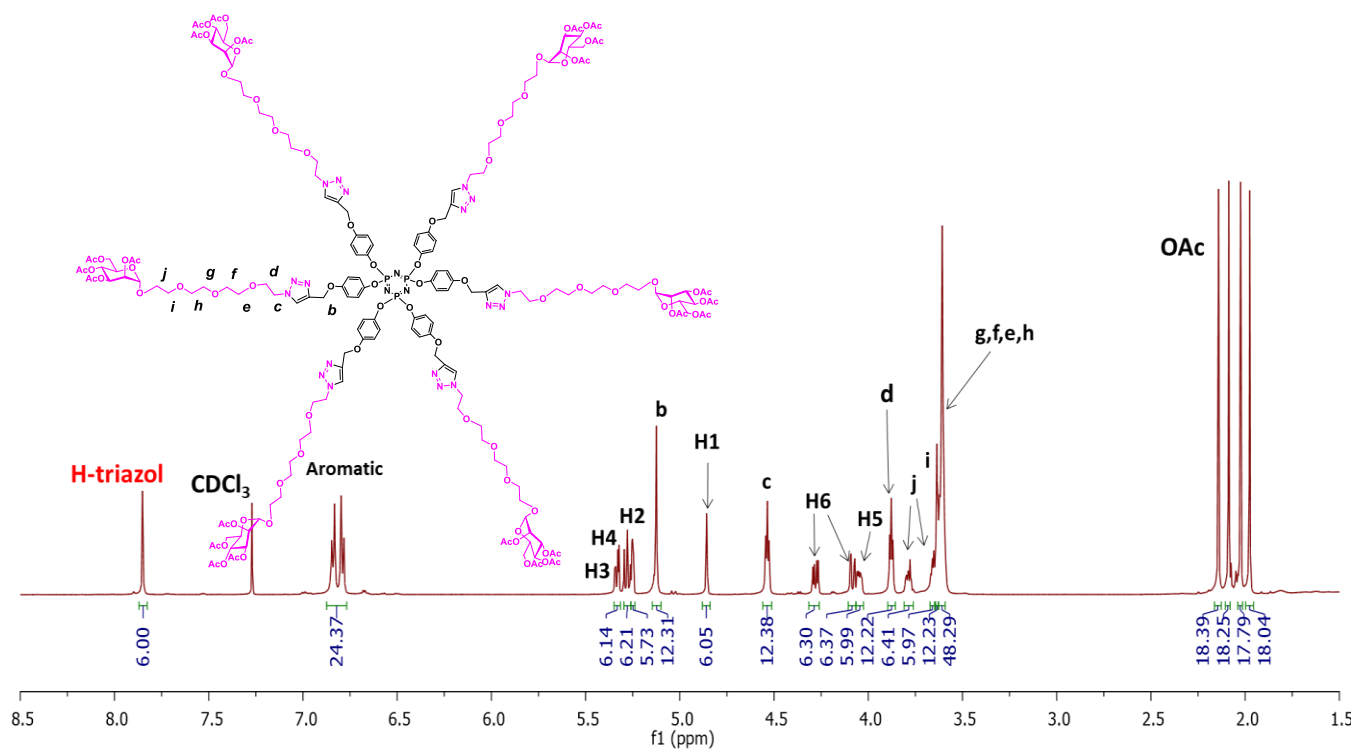
Result quality : Refer to quality report



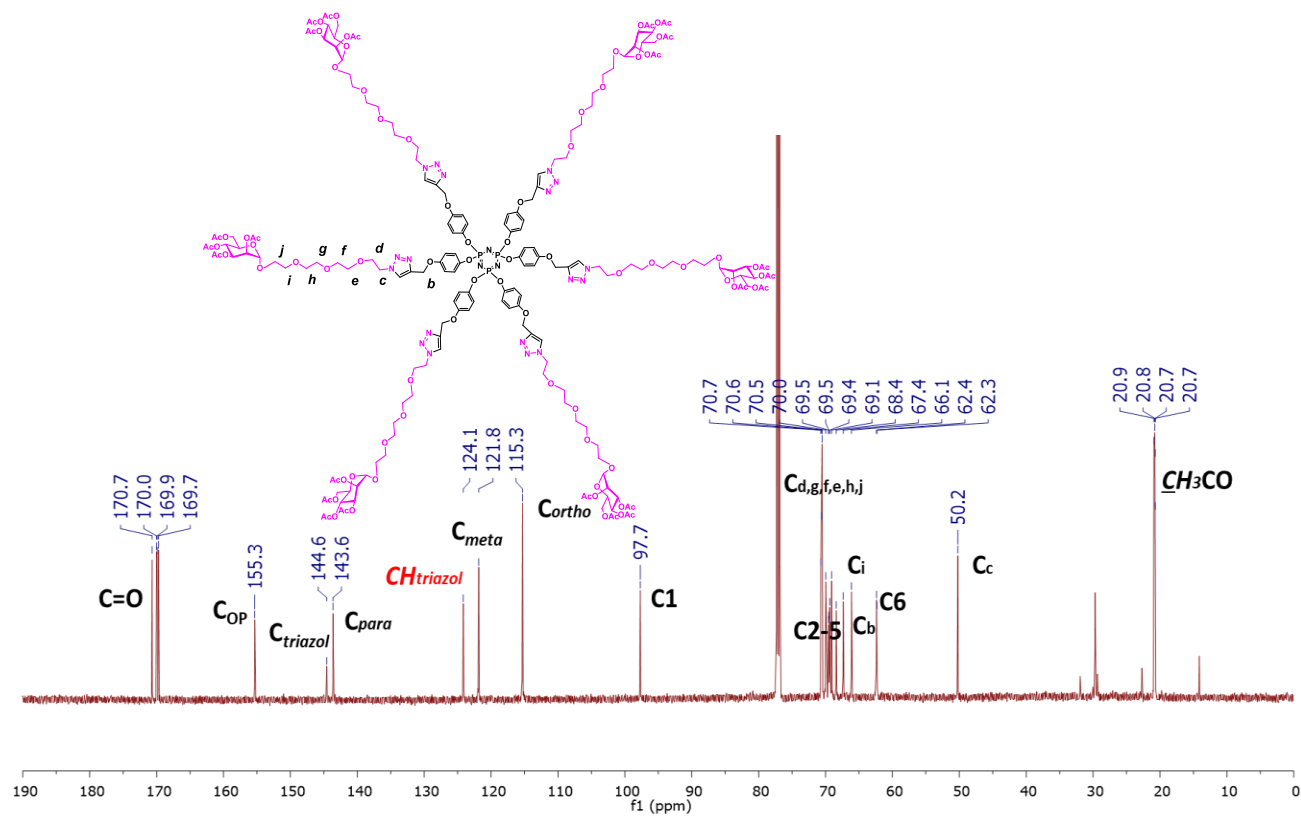
DLS- Qualitative Size distribution of compound 36 showing no cross-linking to Con A (no change in particle size).



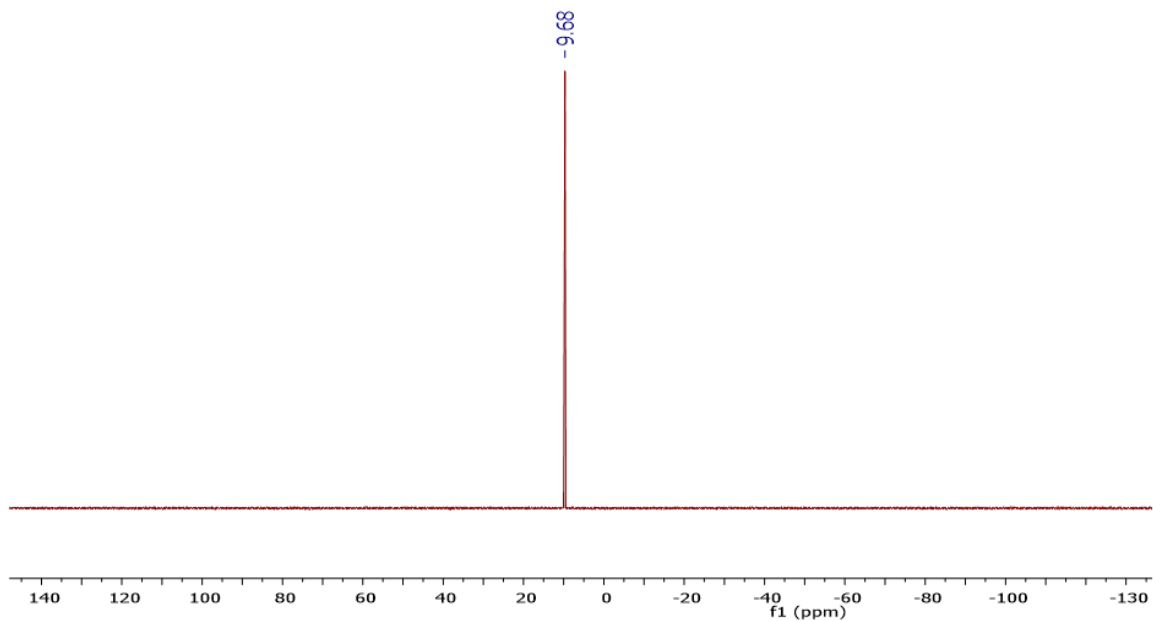
HRMS of compound 36.



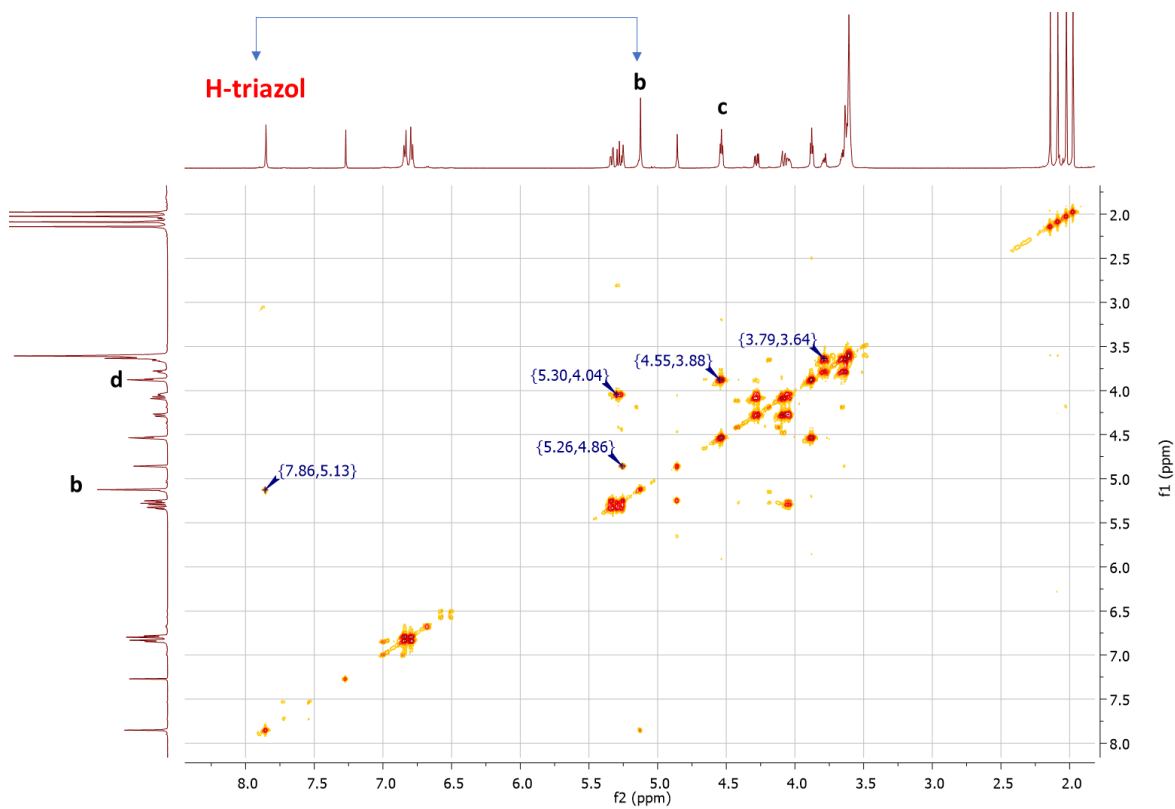
¹H-NMR spectrum of compound 37.

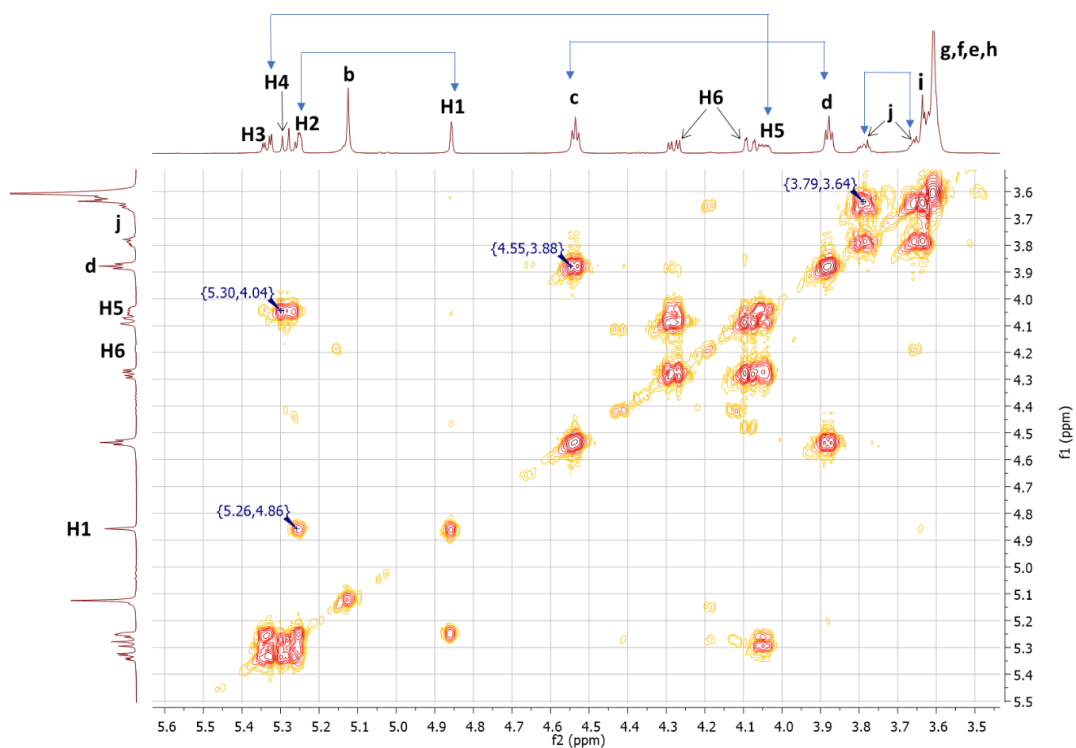


¹³C-NMR spectrum of compound 37.

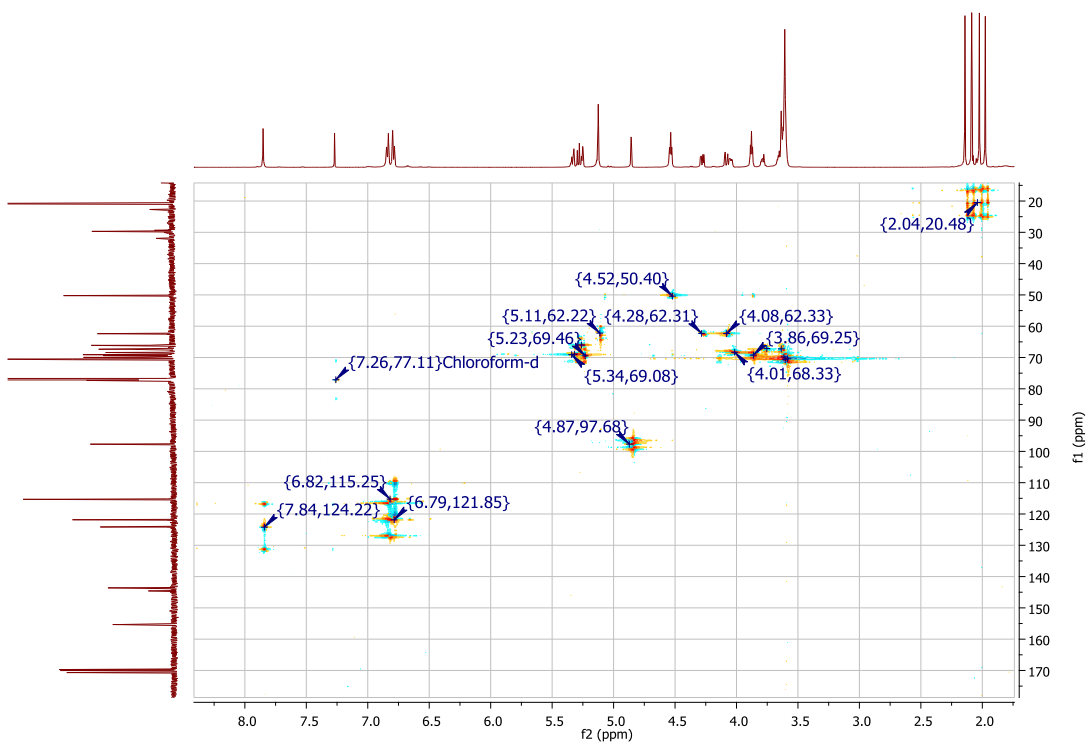


^{31}P - NMR spectrum of compound 37.





2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 37.

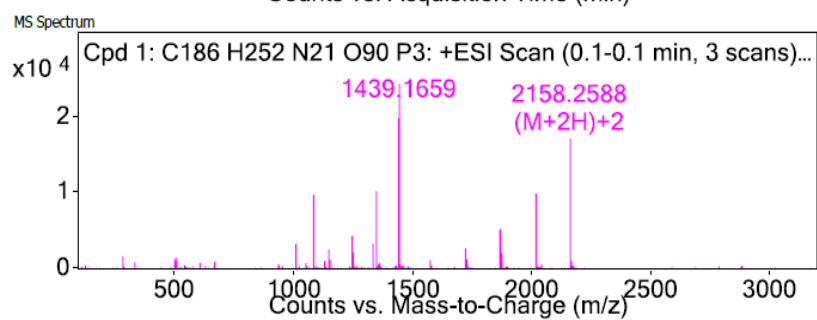
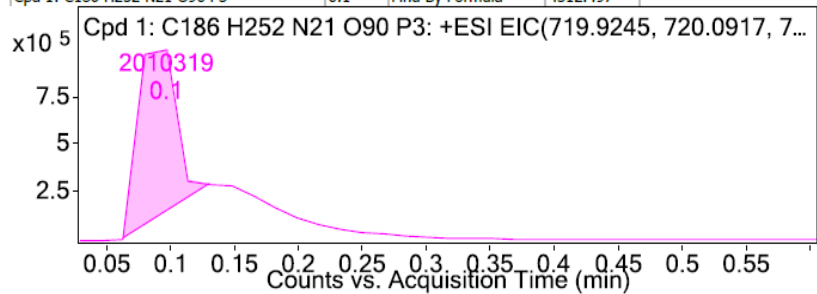


2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 37.

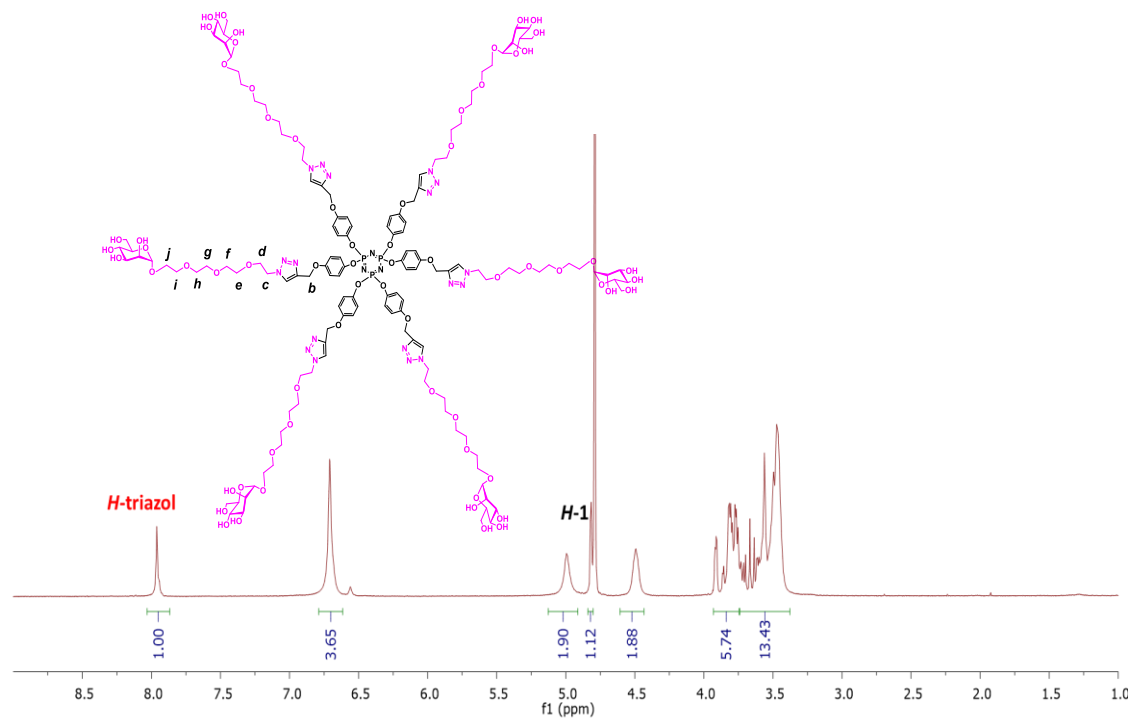
Compound Table

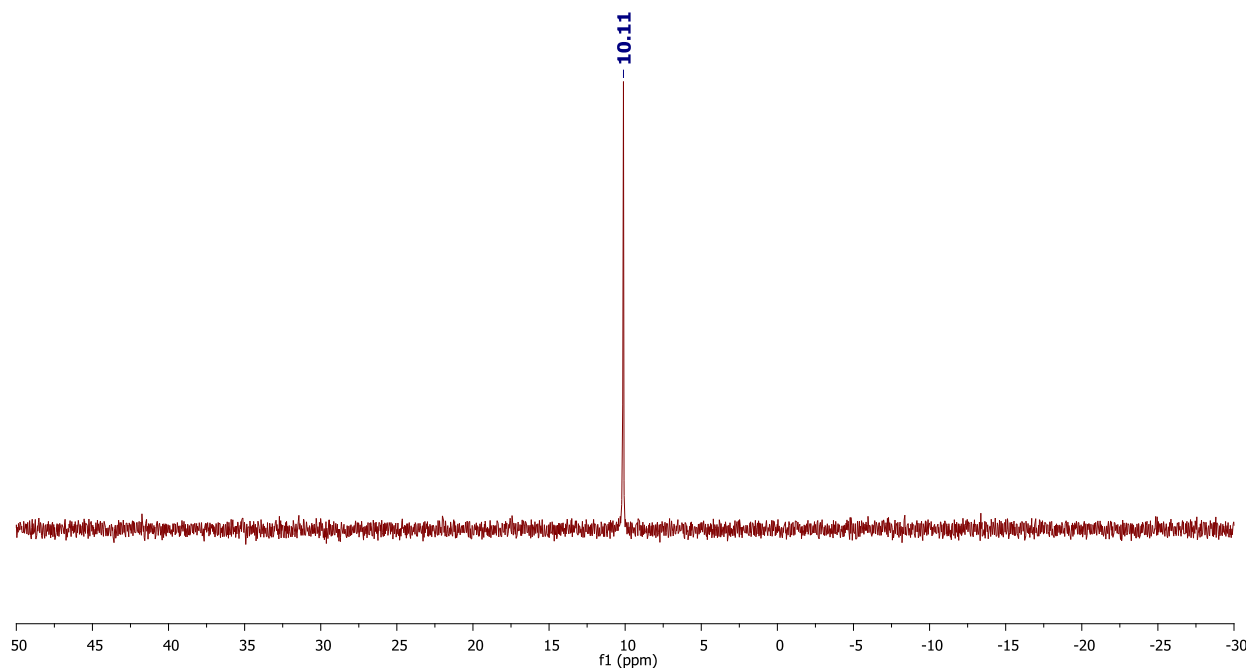
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C186 H252 N21 O90 P3	0.1	4312.497	17070	C186 H252 N21 O90 P3	4312.5001	-0.71

Compound Label	RT	Algorithm	Mass
Cpd 1: C186 H252 N21 O90 P3	0.1	Find By Formula	4312.497



HRMS of compound 37.

¹H- NMR spectrum of compound 38.

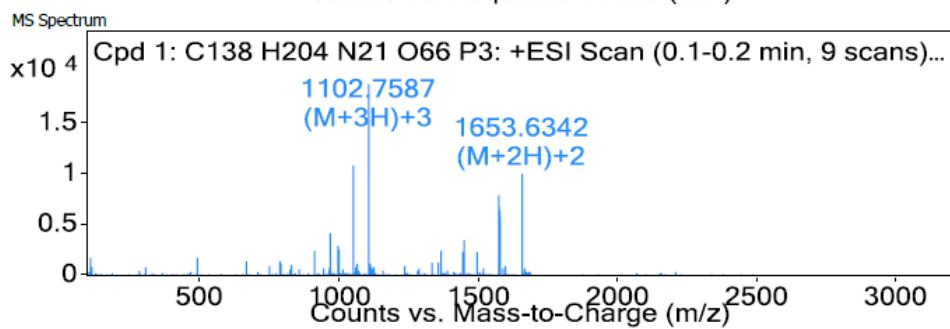
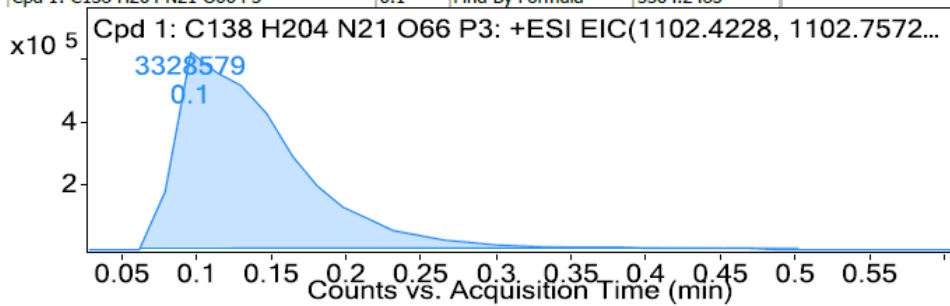


^{31}P - NMR spectrum of compound 38.

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C138 H204 N21 O66 P3	0.1	3304.2485	18873	C138 H204 N21 O66 P3	3304.2465	0.59

Compound Label	RT	Algorithm	Mass
Cpd 1: C138 H204 N21 O66 P3	0.1	Find By Formula	3304.2485



HRMS of compound 38.

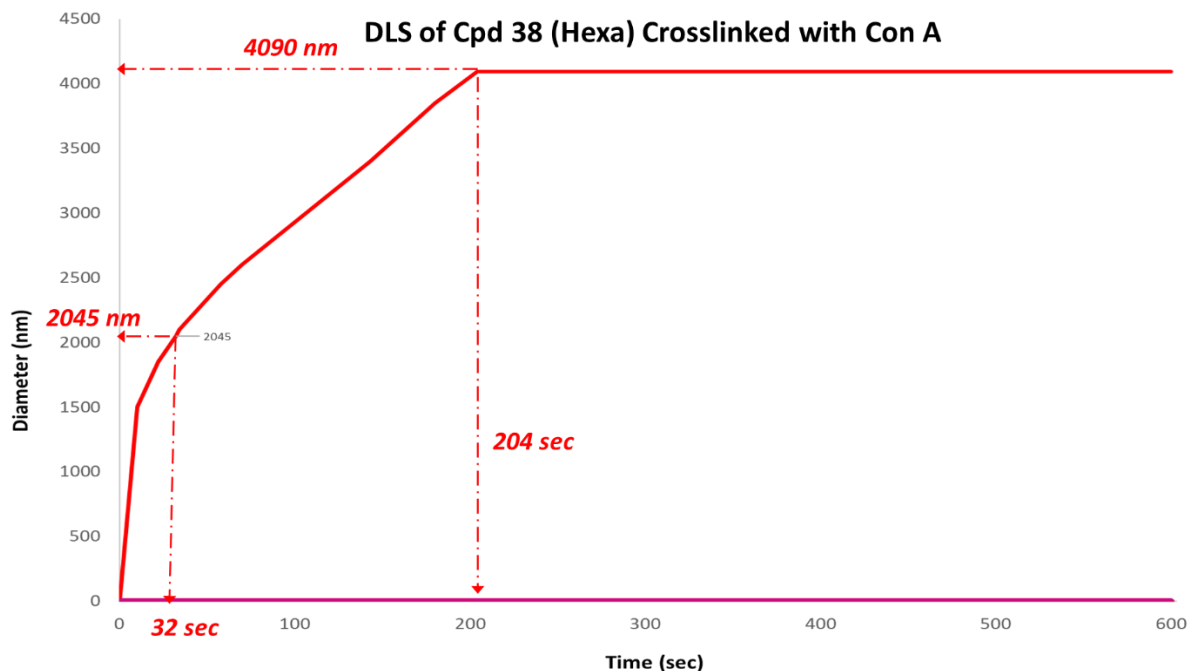
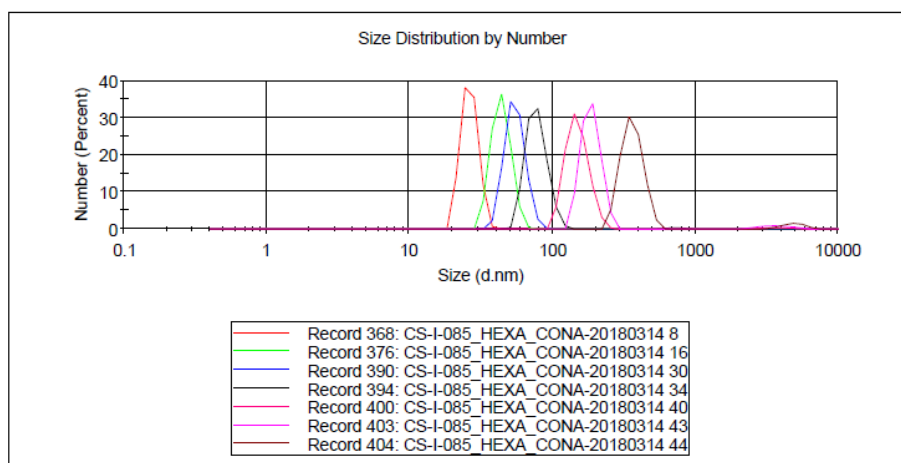
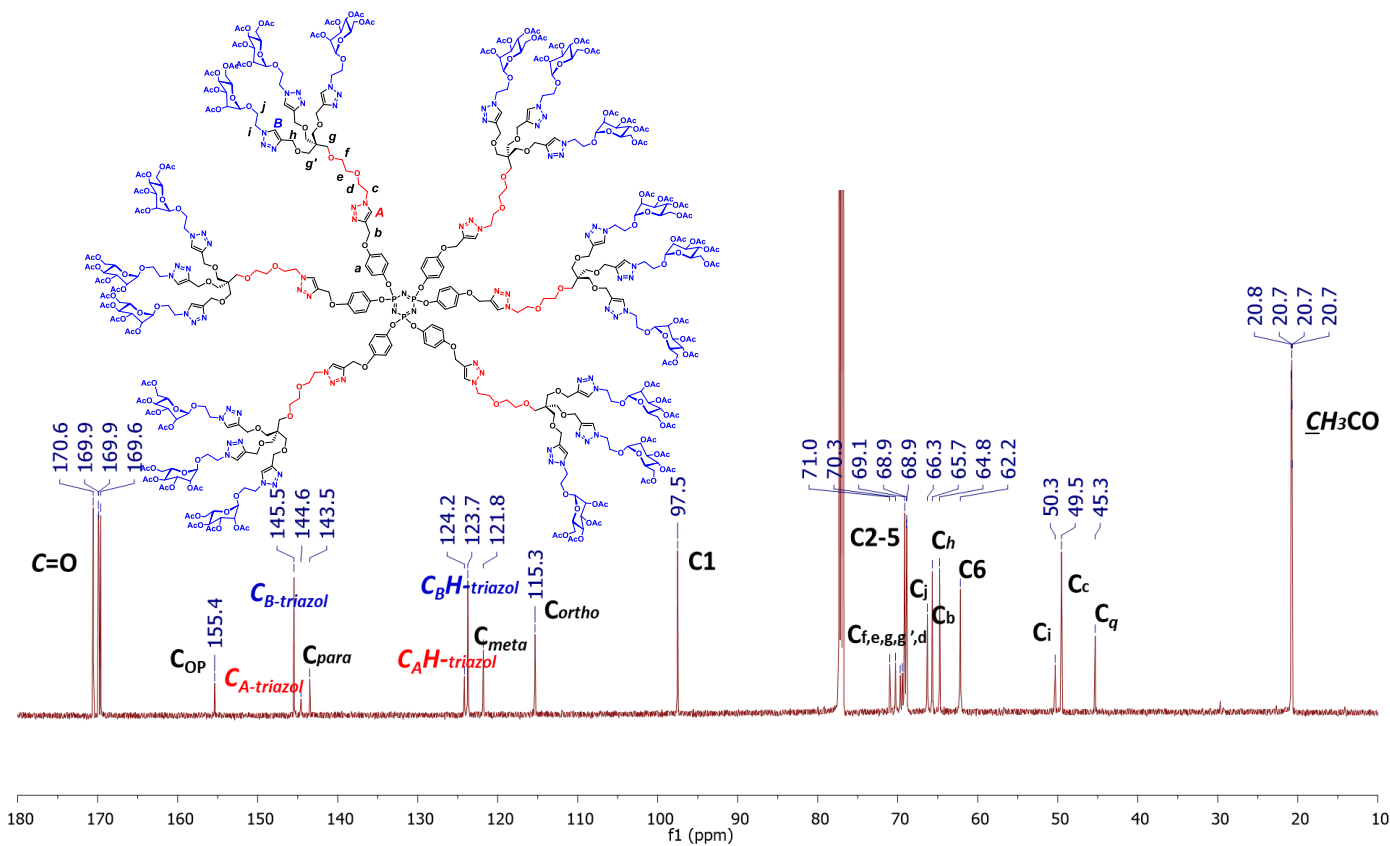


Fig 6. Synthesis DLS of Cpd 38 (Hexa) Crosslinked with Con A.

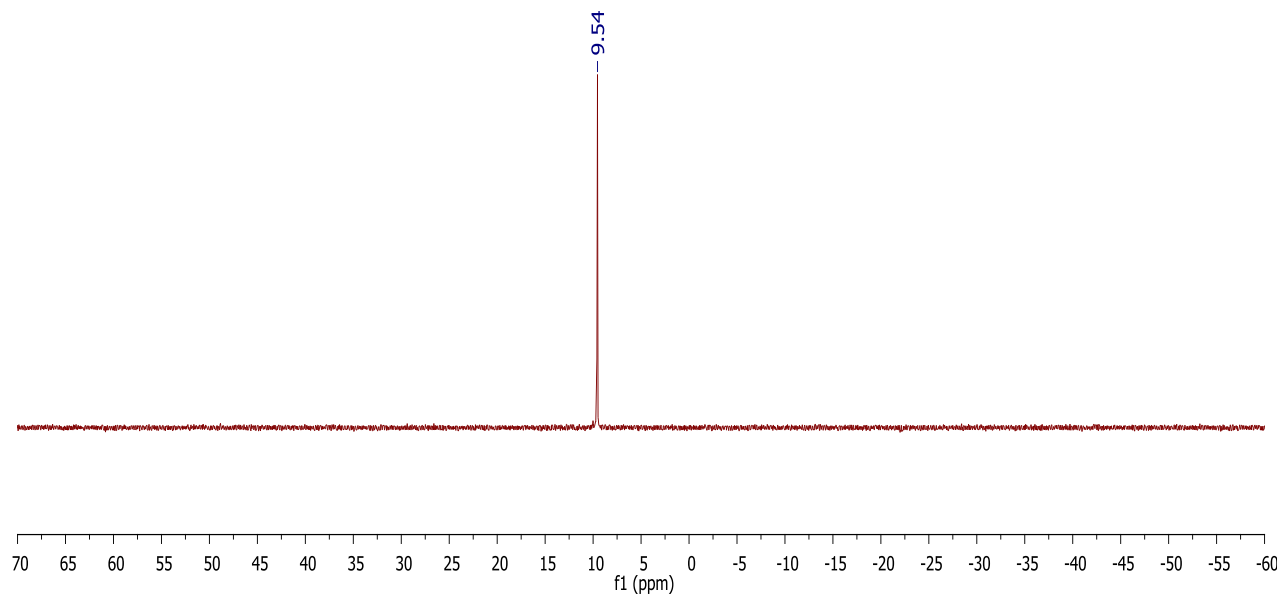
	Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm): 3303	Peak 1: 4827	5.1	834.8
Pdl: 0.574	Peak 2: 361.8	94.9	62.63
Intercept: 0.805	Peak 3: 0.000	0.0	0.000
Result quality : Refer to quality report			



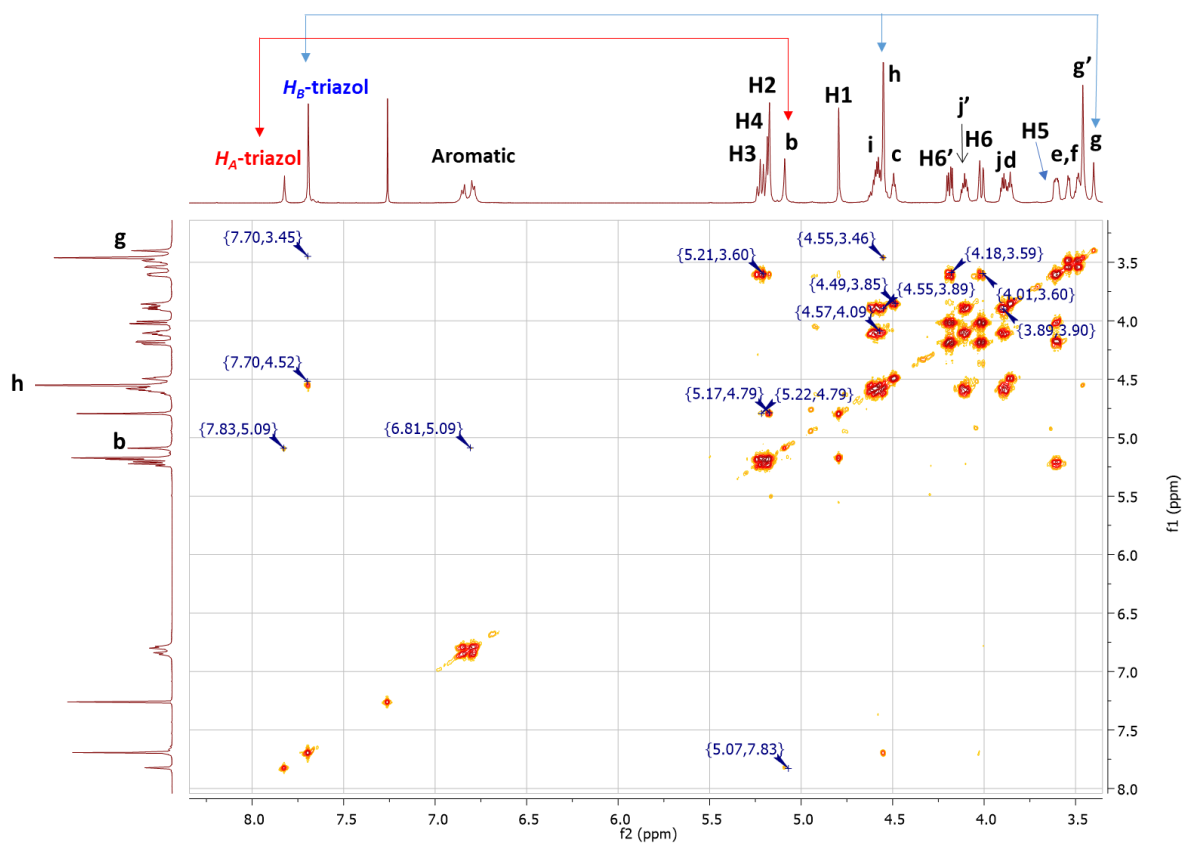
DLS-Size distribution of compound 38.

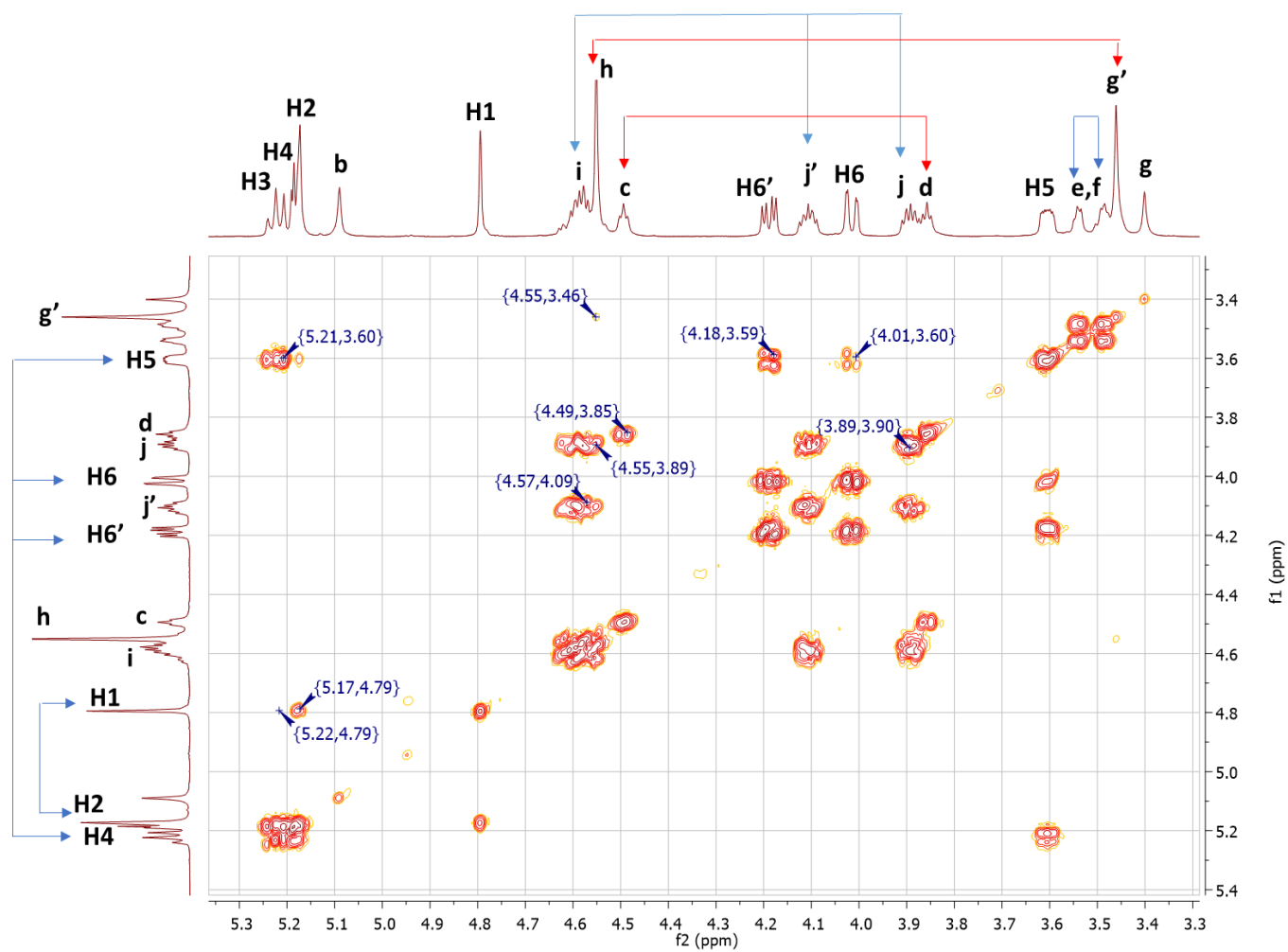


¹H- and ¹³C- NMR spectrum of compound 39.

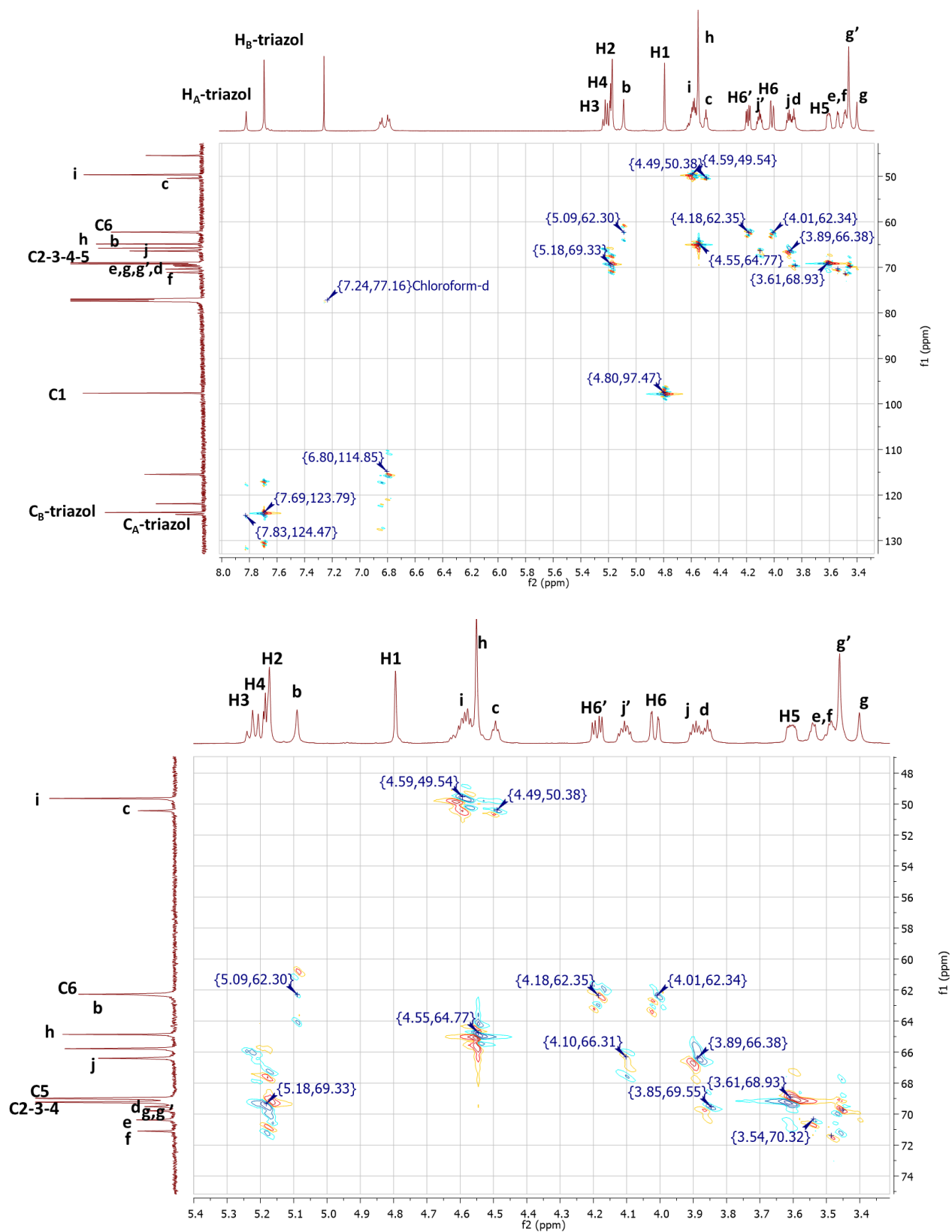


^{31}P - NMR spectrum of compound 39.

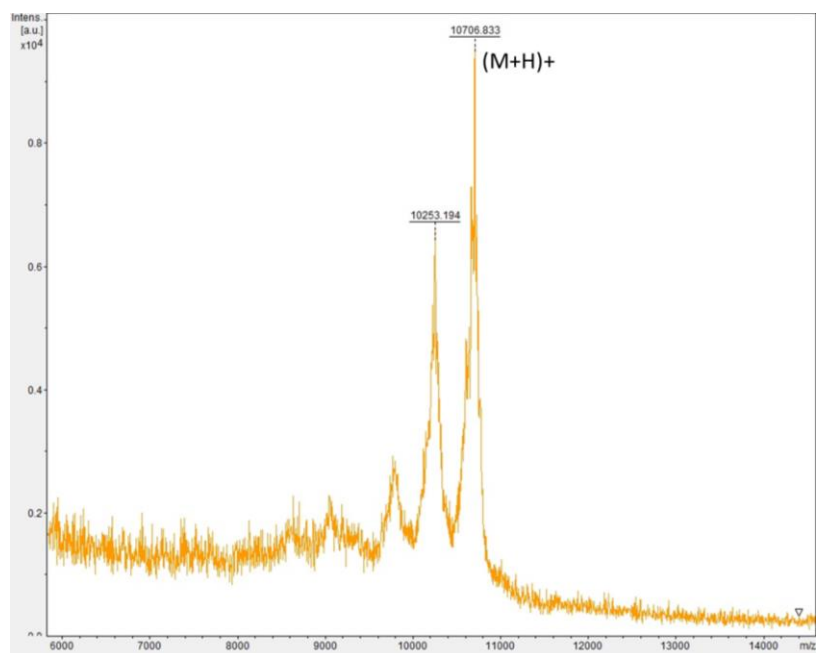




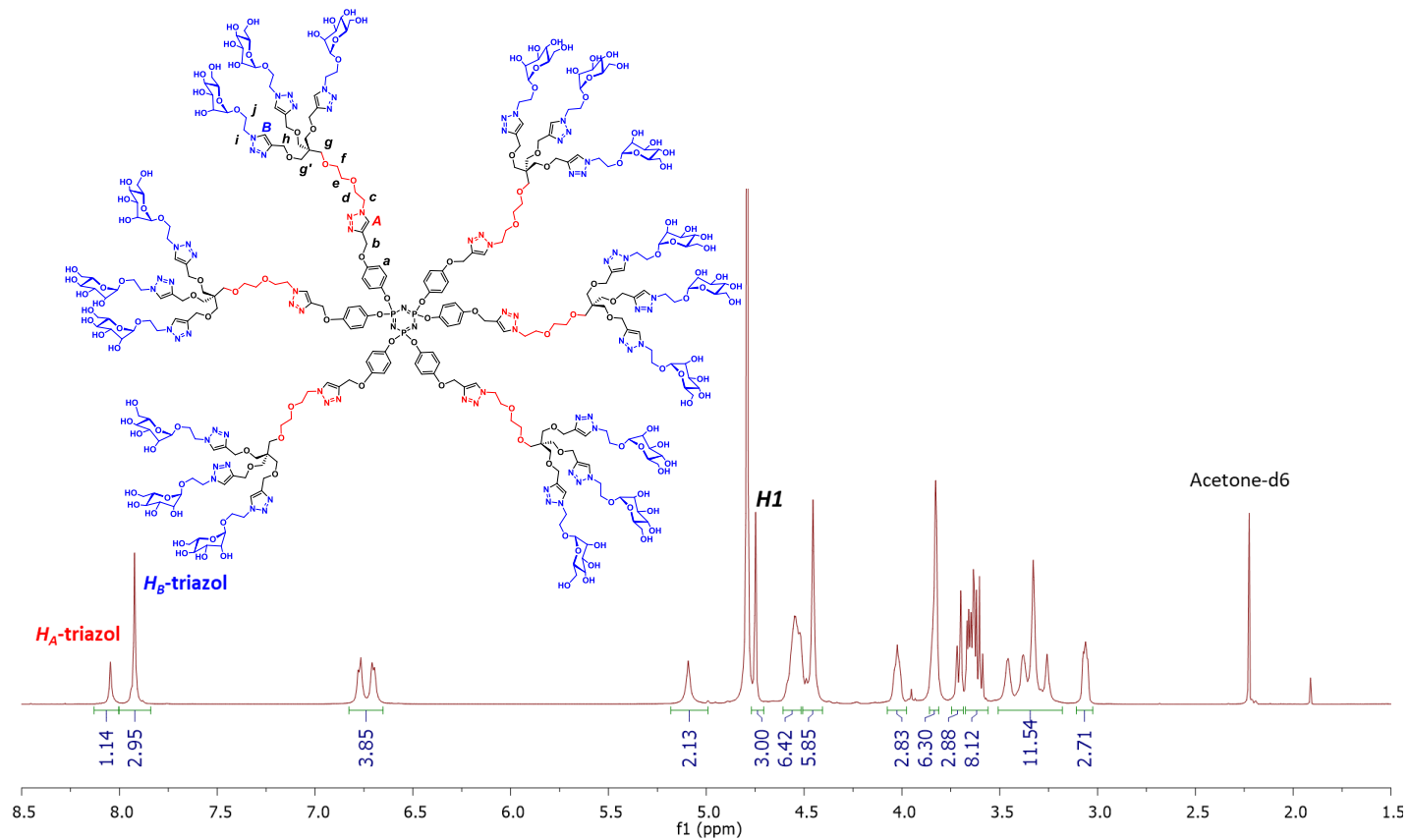
2D NMR – COSY: ^1H - ^1H correlation spectrum of compound 39.

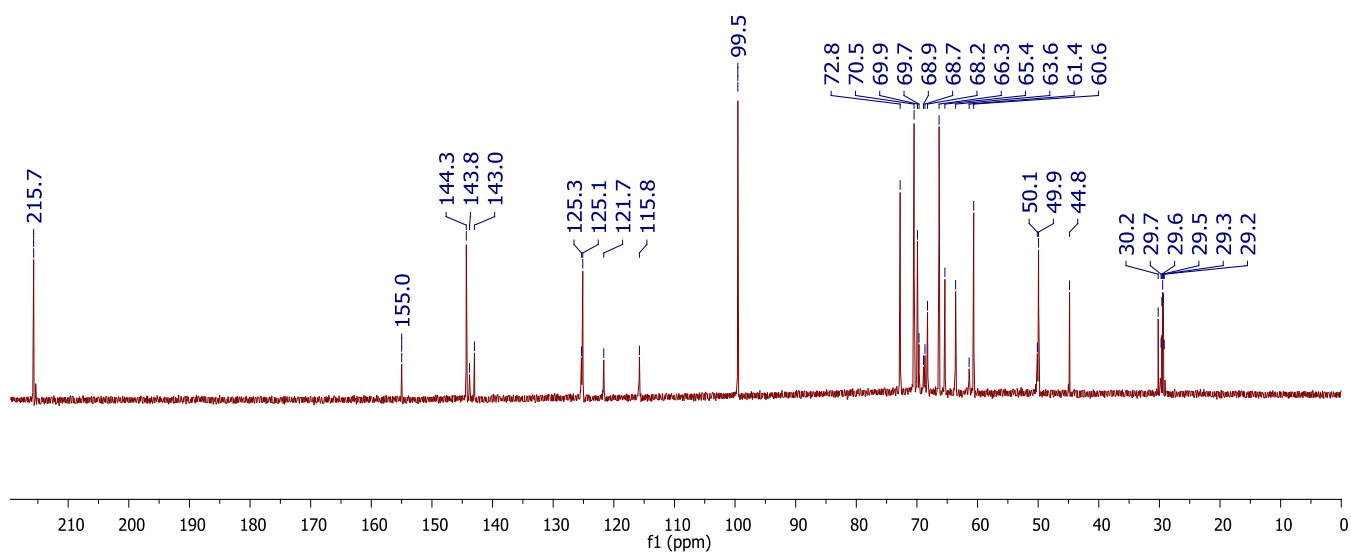


2D NMR – HSQC: ^1H - ^{13}C correlation spectrum of compound 39.

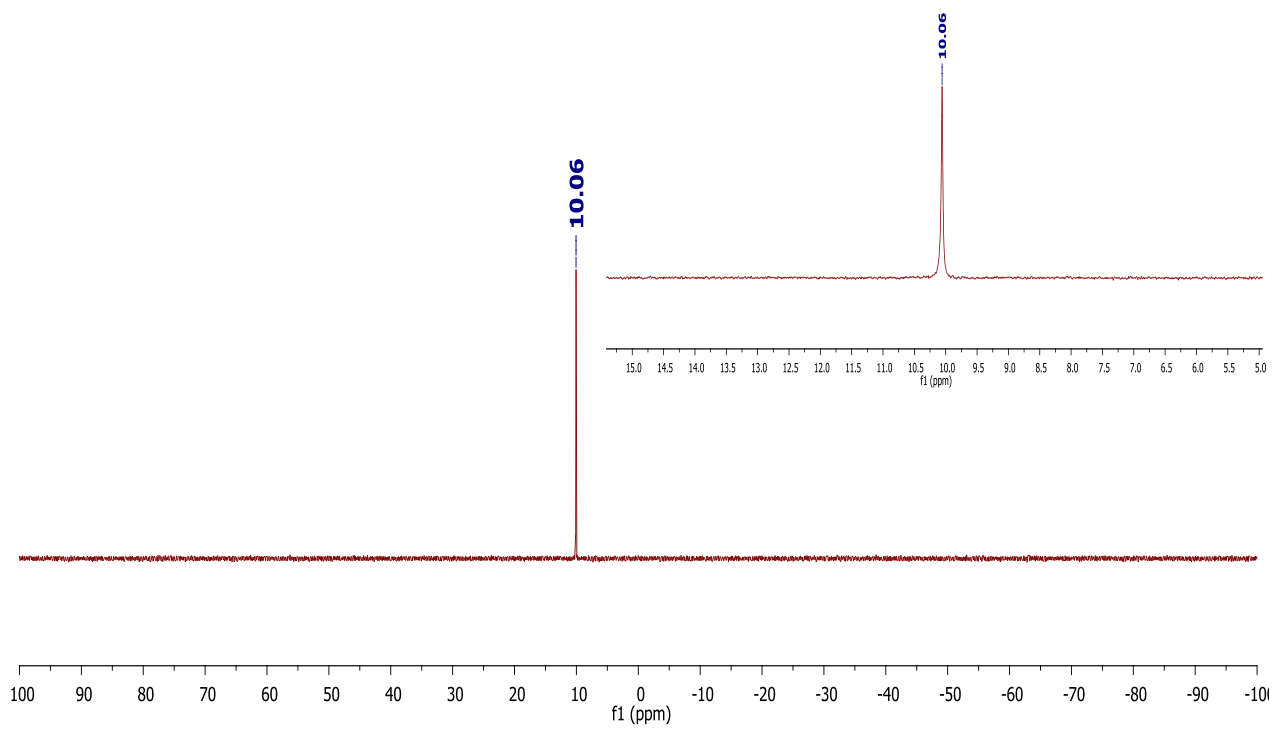


HRMS of compound 39.

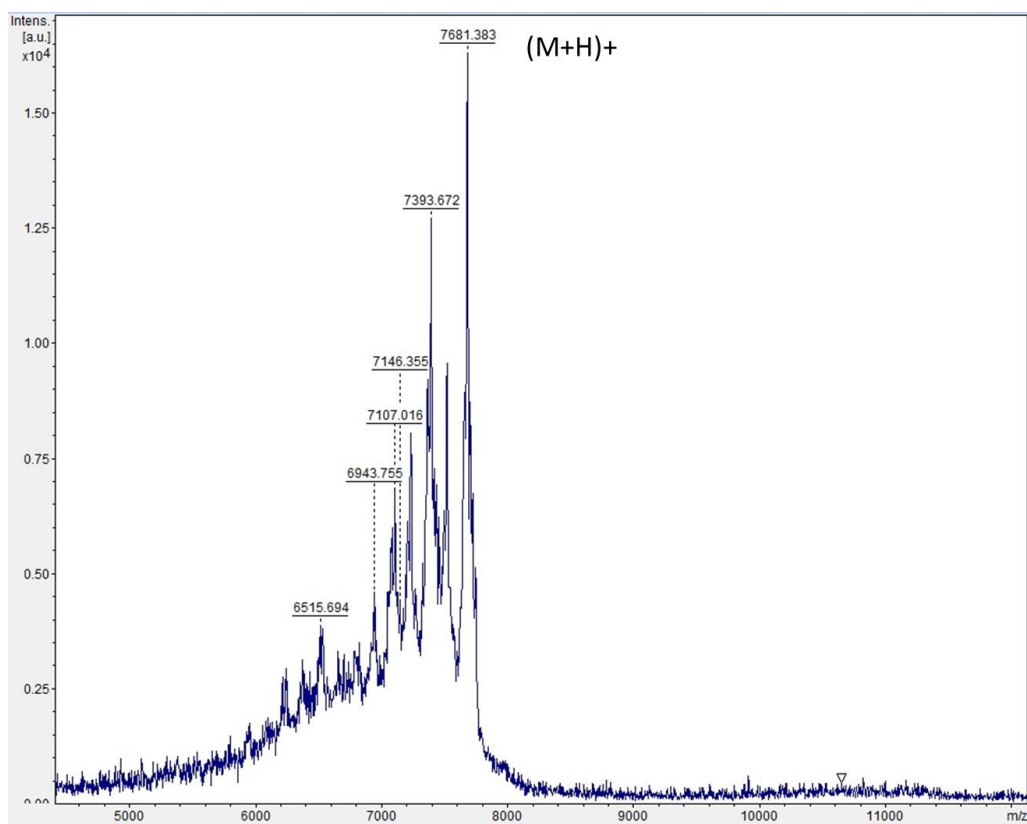




^1H - and ^{13}C - NMR spectrum of compound 40.



^{31}P - NMR spectrum of compound 40.



HRMS of compound 40.

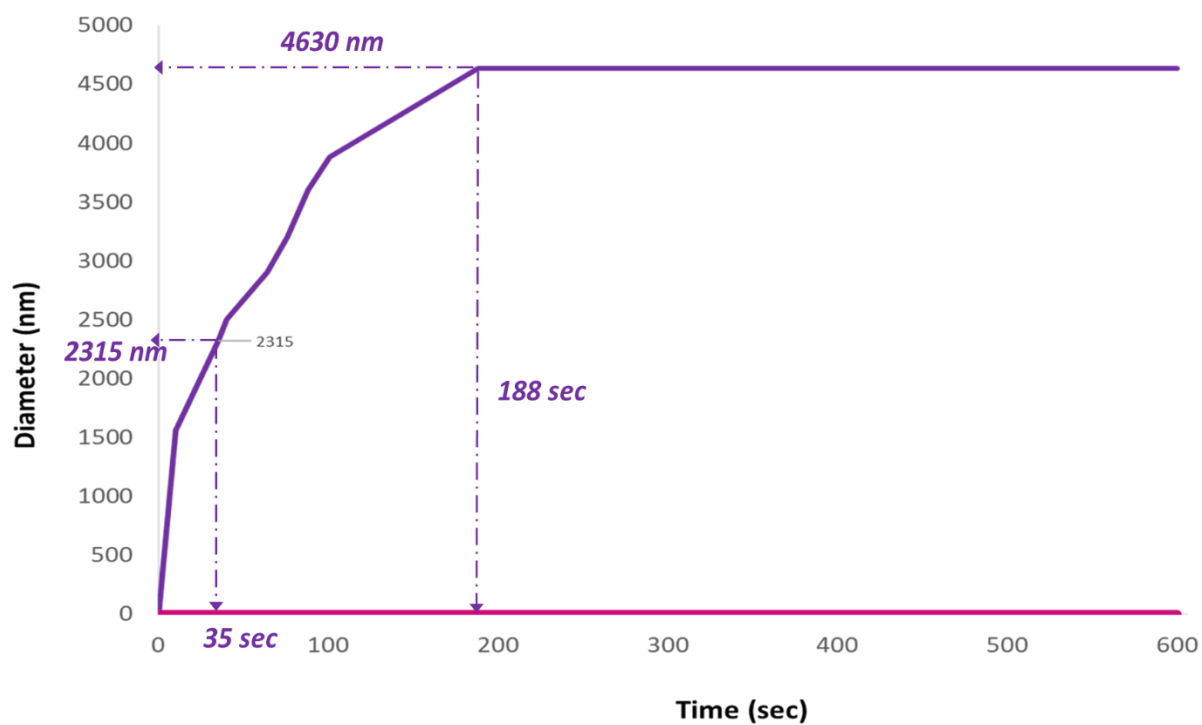
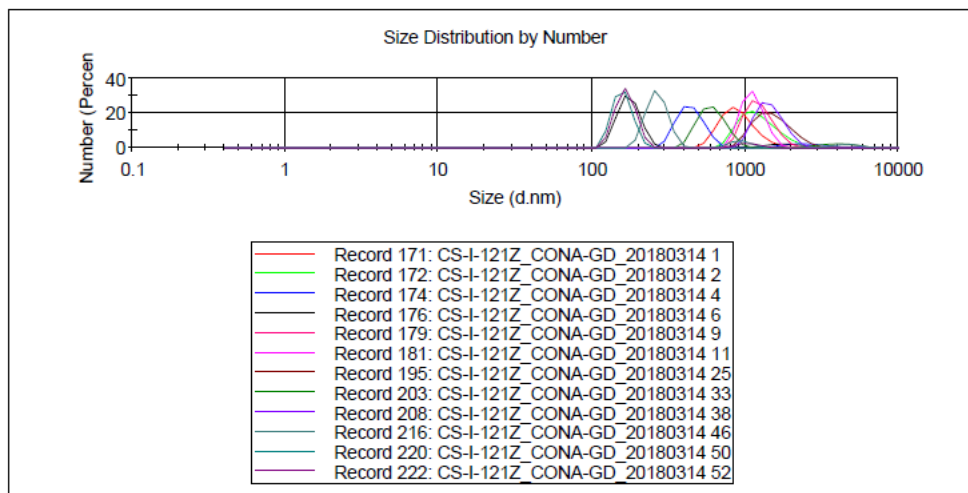


Fig 7. Synthesis DLS of Cpd 40 (G1) Crosslinked with Con A.

	Size (d.nm):	% Number:	St Dev (d.n...
Z-Average (d.nm): 5030	Peak 1: 1054	8.1	183.0
Pdl: 0.525	Peak 2: 166.4	91.9	25.29
Intercept: 0.876	Peak 3: 0.000	0.0	0.000

Result quality : Refer to quality report



DLS of compound 40.

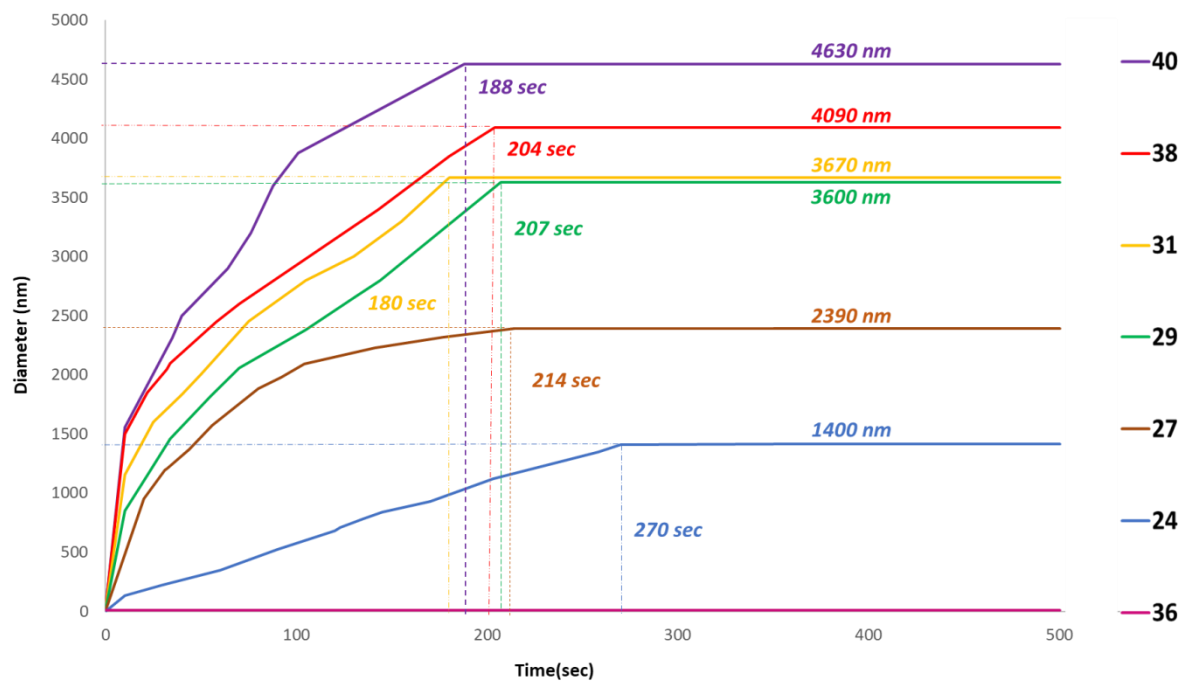


Fig 2. DLS of Cpds 24; 27; 29; 31; 38 and 40 Crosslinked with Con A.

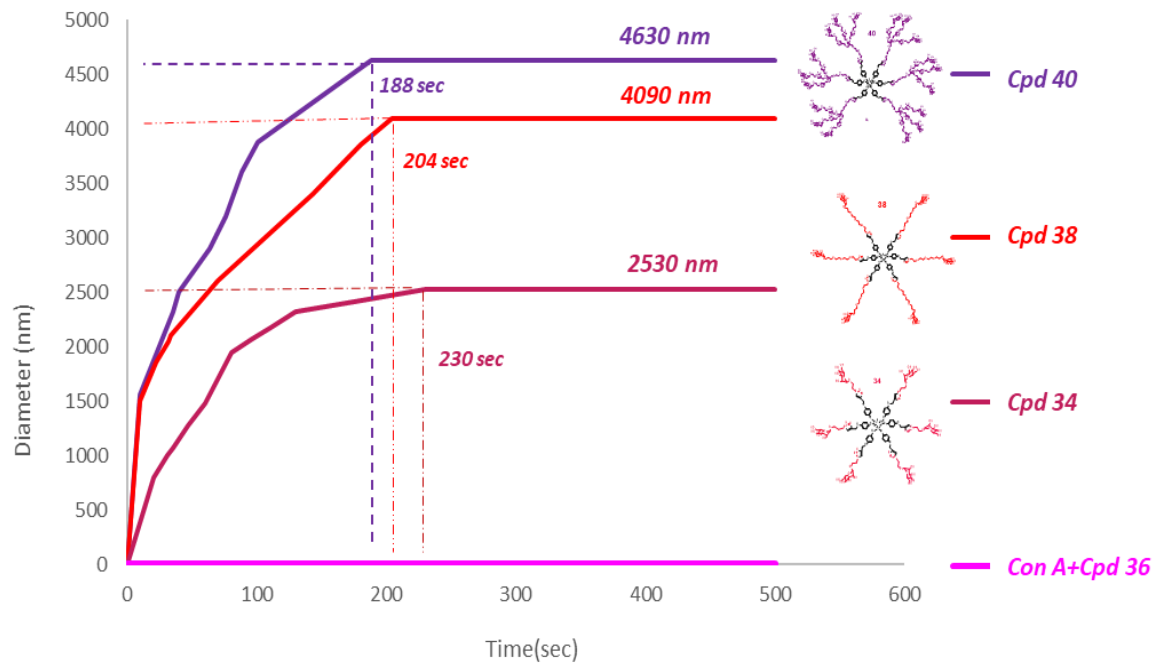


Fig 3. DLS of phosphorylated Cpd 34; 36; 38 and 40 Crosslinked with Con A.