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PII: S0008-6215(15)00035-X

DOI: [10.1016/j.carres.2015.01.022](https://doi.org/10.1016/j.carres.2015.01.022)

Reference: CAR 6939

To appear in: *Carbohydrate Research*

Received Date: 21 July 2014

Revised Date: 14 January 2015

Accepted Date: 31 January 2015

Please cite this article as: Tyagi M, Taxak N, Bharatam PV, Nandanwar H, Ravindranathan Kartha KP, Mechanochemical click reaction as a tool for making carbohydrate-based triazole-linked self-assembling materials (CTSAMs), *Carbohydrate Research* (2015), doi: 10.1016/j.carres.2015.01.022.

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# Mechanochemical click reaction as a tool for making carbohydrate-based triazole-linked self-assembling materials (CTSAMs)

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**Abstract-**Various glycosides in which glycosylated triazole residues are anchored on to a central phenyl ring have been prepared under green reaction conditions by a solvent-free mechanochemical method. Some of the glycosides exhibited the ability to form gels when in contact with long chain hydrocarbons, e.g. hexane, heptane and octane, and this property was phase-selective. Thus, from a mixture of hexane-water, the compounds preferably absorbed the alkane to form a gel. The gelation ability was found to increase with an increasing number of substituents on the phenyl ring but only up to tetra-substitution. The hexa-substituted phenyl derivative did not swell in the hydrocarbon solvents investigated. The spontaneous self-assembling properties of these compounds in hexane have been investigated by transmission electron microscopy (TEM). Molecular modelling was used to optimize the structural geometry of these carbohydrate-based triazole-linked self-assembling materials (CTSAMs) and to rationalize their behaviour.

**Keywords:** CTSAMs, mechanochemical click reaction, nano bioorganomaterials, organogelators.

## 1. Introduction

'Click reactions' usually between azides and alkynes<sup>1-4</sup> have found extensive applications in supramolecular chemistry,<sup>5-9</sup> material science,<sup>10-12</sup> and medicinal chemistry<sup>13-21</sup>. Because of the ease with which these reactions can be performed, they have been widely applied in the synthesis of complex molecules such as large dendrimers,<sup>22</sup> catenanes, and rotaxanes<sup>23</sup> which have been utilized in making nano-scale devices such as molecular machines, molecular walkers and other devices.<sup>24</sup> Click chemistry has also been well explored in carbohydrate chemistry. Thus, some of the glycopolymers<sup>25-29</sup> so prepared have been found important in developing antiviral vaccines,<sup>30</sup> bacterial/lectininhibitors,<sup>31-33</sup> and multivalent inhibitors.<sup>34-39</sup> In addition to providing access to such large dendritic structures, it has also been proved an excellent tool for generating macrocyclic frameworks composed of glycoconjugates<sup>40-42</sup> with potential applications in the field of supramolecular chemistry<sup>5-9</sup> and molecular-assembly<sup>43,44</sup>. Interestingly, the cyclized/organized structures have also been demonstrated to be often superior to their uncyclized counterparts in biological activity, which has implications in medicinal chemistry.<sup>45</sup> In synthetic carbohydrate chemistry, other important areas where click chemistry has found application include preparation of carbohydrate-fused heterocycles as carbohydrate mimetics<sup>46-48</sup> through intramolecular cyclisation, and synthesis of glycopolymers<sup>49,50</sup> and pseudo-oligosaccharides<sup>51,52</sup> which have potential uses in lectin-binding and mycobacterial inhibition. In addition, click chemistry has enabled conjugation of carbohydrates with other bio macromolecules such as proteins, DNA and RNA.<sup>53</sup>  
<sup>55</sup> Recently, the syntheses of several 1,5-disubstituted carbohydrate-linked triazoles under metal-free click conditions were also reported.<sup>56-59</sup>

In spite of these advances, the application of click chemistry in generating nanostructured self-assembling materials is still at exploratory stage. Because of the possibility for self-assembly through  $\pi$ - $\pi$  stacking as well as hydrogen bonding interactions in compounds carrying triazole residues, this method

can also be potentially useful for making phase-selective gelators that find effective application in oil spill cleanup and recovery processes. We have been recently involved in developing new solvent-free approaches for the synthesis of biologically important molecules.<sup>60</sup> The current work describes the synthesis of certain triazole-linked sugar derivatives by ball milling in the absence of solvent and in an examination of some of the structures so generated by TEM for studying their self-assembly properties. Moreover, as the 1,2,3-triazole residue has been an important pharmacophore, forming a structural component of many biologically active compounds,<sup>13-21</sup> the compounds have been evaluated for their antimicrobial activity.

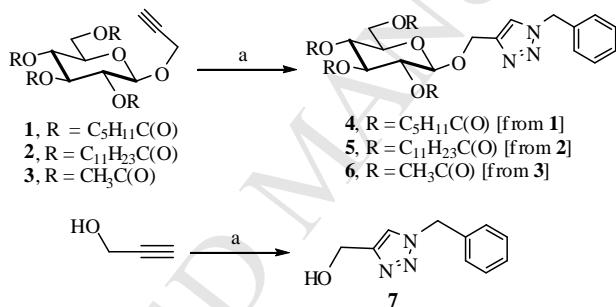
Recently we noted that 1,2-*cis*- and 1,2-*trans*-linked long chain alkyl glycosides, known traditionally for their surfactant properties, differed significantly in their molecular self-assembly and could be studied by TEM.<sup>61</sup> It was therefore reasoned that triazole-linked carbohydrates bearing such alkyl residues, either on the carbohydrate moiety or the triazole residue, should be capable of assembling efficiently, a useful addition to their physical/physicochemical properties. Substitution of the alkyl chain in the glycolipid by a phenyl moiety, capable of organization by  $\pi$ - $\pi$  stacking, might therefore potentially alter the organization-pattern considerably. Recently, CuAAC reaction has been proven to be an excellent tool for the preparation of aromatic core-linked glycopolymers in addition to the normal dendrimers, which are explored in the area of drug delivery, biosensors, nanomaterials, etc.<sup>26,62,63</sup> Besides, click reaction was also widely explored in the preparation of self-assembling materials<sup>64-68</sup> and molecular gelators.<sup>69-71</sup> These gelators and other materials have further been shown to be suitable for their applications in metal ion-binding, drug delivery, etc. In fact, it was during the span of our work that most of the reports in this research area started to appear in the literature. Till date there has been no report on the effect of sugar residues, bearing lipophilic protection and also anchored on to an aromatic core, on the self-assembling behaviour of glycoclusters. This work describes the application of click reaction in the

preparation of carbohydrate-based triazole-linked self-assembling materials (CTSAMs), in particular the effect of the anchored sugar residue on its gelation/self-assembling properties. In our initial study, a small library of carbohydrate derivatives formed through ‘click chemistry’ were synthesised under green reaction conditions and subsequently analysed by TEM.

## 2. Results and Discussion

### 2.1 Solution-phase synthesis of monovalent carbohydrate-based triazole-linked compounds

The required propargyl glucoside derivatives **1**, **2** and **3** were synthesised using literature methods.<sup>60,72</sup> They were then reacted with benzyl azide, generated *in situ* from a mixture of benzyl bromide and NaN<sub>3</sub>,<sup>73</sup> to yield the corresponding sugar-linked triazoles **4**, **5** and **6** (Scheme 1).



Reagents and conditions: (a) BnBr (2 mol equiv); NaN<sub>3</sub> (10 mol equiv); CuSO<sub>4</sub>·5H<sub>2</sub>O (0.4 mol equiv), sodium ascorbate; *t*-BuOH-H<sub>2</sub>O (1:1), rt, 1 h, 73 - 80%

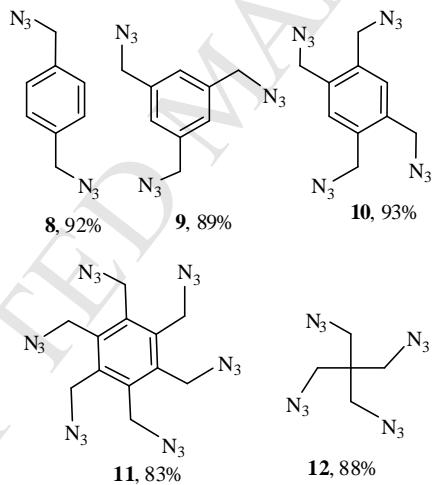
**Scheme 1.** Synthesis of triazole-linked carbohydrate derivatives

The sugar-linked triazole **4** thus obtained was found to form gels when in contact with hexane. The gels obtained were soft and possessed shear-thinning properties and tendency to form clear solution on extensive dilution and/or on subjecting to ultrasound irradiation. Neither the acetyl analogue of **4**, namely **6**, nor the *N*-benzyl-triazolyl methanol **7** formed gels under these conditions. This clearly indicated the role played by the lipophilic moieties present on the sugar in the formation of gel-structures. The dodecyl analogue **5** also formed gels which were marginally stronger than those formed by **4**.

Therefore it became evident that the longer lipophilic chains present in **5** helped the association of molecules more effectively. Nevertheless, the organized structures formed did not appear to be large enough to be visible under TEM.

## 2.2 Synthesis of polyvalent triazole compounds under mechanochemical azide alkyne click reaction using Cu<sup>I</sup> (CuSO<sub>4</sub>-sodium ascorbate) and their physicochemical properties

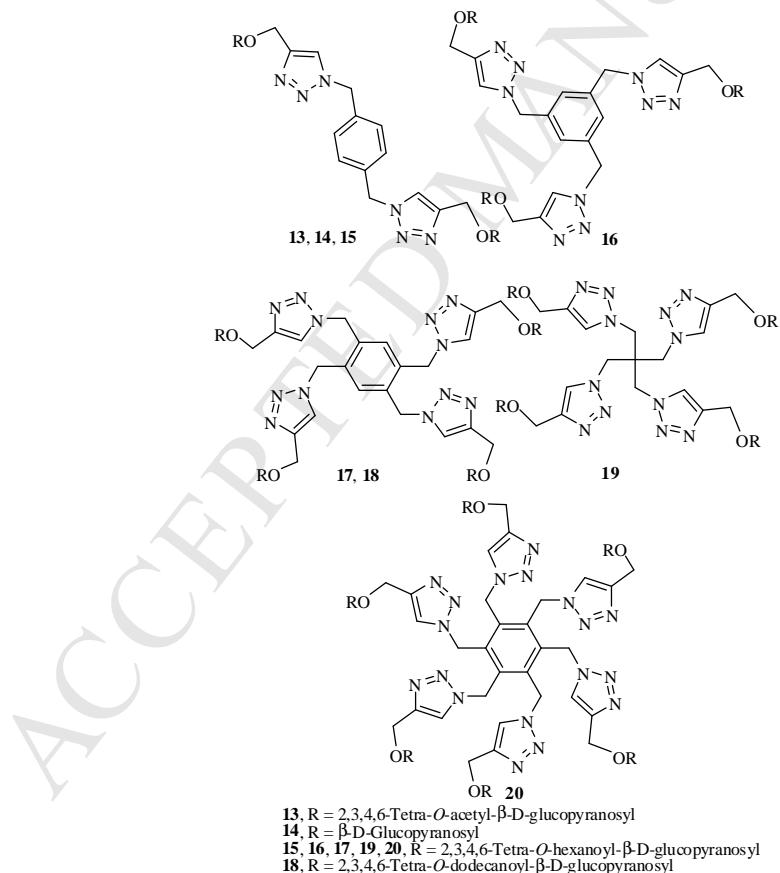
In attempts to obtain molecules with improved gelation ability, the syntheses of various other sugar-linked triazole compounds were undertaken. As multiple sites of reaction were present in some of the cases targeted, for ensuring the homogeneity of each of the compounds formed, the one-pot two-step procedure mentioned above was modified in these cases. Thus the aromatic azides required for this purpose (**8**, **9**, **10**, **11**, **12**, Fig 1) were synthesized<sup>74-79</sup> and then reacted with the desired propargyl



**Figure 1.** Structures of various clickable azides synthesized under conventional conditions

glycosides by co-grinding under the optimized solvent-free mechanochemical click reaction conditions.<sup>80</sup> The usual aqueous solution-phase CuAAC reaction was not chosen for this purpose, because of the insolubility of the lipophilic substrates in the reaction medium. Various triazole-linked glycoclusters (Fig 2) were thus obtained in excellent yields (85-92%) and were characterized by <sup>1</sup>H and <sup>13</sup>C NMR

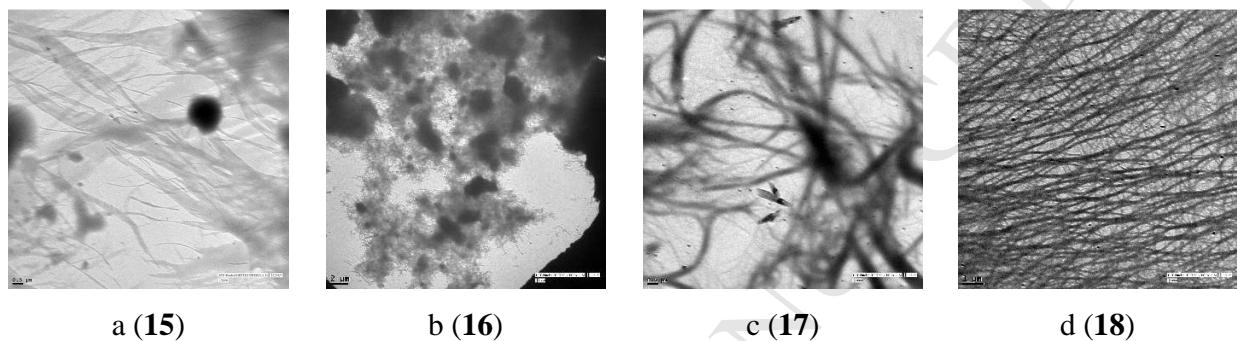
spectroscopic methods. In the  $^1\text{H}$  NMR spectra, the compounds were clearly distinguishable by the ratio of the triazolyl hydrogen to the phenyl ring-hydrogens in the respective structures. When qualitatively evaluated, the gelation ability of the compounds prepared was found to be in the order **18>17>16>15>4**. Thus it was apparent that the gelation ability of a compound increased with increasing number of lipophilic sugar residues anchored on to the core structural element, namely, the phenyl ring up to the level of tetra-substitution (derivatives **17** and **18**). The hexa-substituted phenyl derivative **20** did not form a gel. Likewise, the pentaerythritol-derived **19** also failed to gel. The latter observations were supportive of our initial contention that the phenyl ring would help in the organization of individual structural units into an ordered arrangement and that the sugar-linked triazole units must preferably lie on the same side



**Figure 2.** Structures of various sugar-linked triazole derivatives synthesized by mechanochemical CuAAC reaction

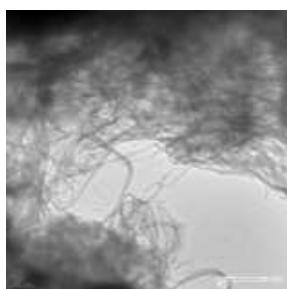
of the phenyl ring to which they are anchored. It appears that the tetrahedrally arranged core structural motif in **19**, prevents it from forming effective ordered arrangements necessary for holding the solvent molecules that eventually leads to a gel-like structure. This also appeared true of the hexa-substituted phenyl derivative **20** wherein due to the steric crowding not all of the anchored sugar-bearing triazolyl residues are in a position to align on the same phase of the phenyl ring. This appears to be limiting the scope of structural association crucial for the gelation to occur. These observations along with the fact that analogues **13**, **14** and **16** devoid of the lipophilic protecting groups on the sugar moieties did not yield gels indicate that both the presence of phenyl ring as well as the fatty (long chain) substituents on the sugar ring were prerequisites for the molecules to form organized structures capable of gelation. Moreover, In view of the foregoing observations an examination of the morphological features of the structures formed in hexane was undertaken. The nano-architecture of these gels could indeed be clearly seen in the TEM images obtained (Fig 3). Thus, compounds **16/17/18** taken up in hexane (equal concentration, w/v) gave TEM patterns typical of those produced by organic polymers.<sup>81,82</sup> It was noticed that an estradiol-based low-molecular-weight gelator described in the literature possesses the triazole-bearing tetra-substituted phenyl residue characteristic of **17/18** described here.<sup>69</sup> Likewise, a click nucleoside-lipid-linked triazolyl glucoside that forms a hydrogel has similarly been reported to have a supramolecular structure stabilized by a network of fibers.<sup>71</sup> Some of the other triazole-linked compounds described in the literature, although are not sugar-bearing, have been found to have polyaromatic units in their structure that allows them to form assemblies of various descriptions such as lamellae,<sup>65</sup> spheres,<sup>65,68</sup> fibres,<sup>67,69,71</sup> etc and find applications in liquid crystals,<sup>64</sup> aggregation-induced-emission (AIE)-active molecules,<sup>67</sup> selective metal ion-binding,<sup>68,70</sup> nucleic acid delivery,<sup>71</sup> etc. The tetra-substituted phenyl derivative **18** bearing the longest alkanoyl chains on the sugar residues gave relatively the densest gel as

can be seen from the TEM images shown in Fig 3. It may be recalled that among these compounds, **18** had the highest molecular weight and hence the lowest molar concentration in the gel prepared and yet had formed comparatively the densest gel. The disubstituted phenyl derivative **15**, only marginally thick in hexane, was investigated after taking up in moist methanolic hexane, where it formed a stronger gel as compared to hexane alone as the solvent. The acetylated and deacetylated analogues **13** and **14**,



**Figure 3.** Transmission electron micrographs: a. **15**; b. **16**; c. **17** and d. **18** (for sample preparation, moist MeOH-Hex was used for **15** and hexane only for others). For a larger image please see Supplementary Information.

respectively, did not yield any gel under such conditions. Dispersion of the tris-triazolyl compound **16** in hexane was thin initially (Fig 3b), but gave a rather firm gel (Fig 4) on standing for 3-5 days (in closed vials). The gel could be easily cut into cubes with a surgical knife. On dilution and application of the



**Figure 4.** Transmission electron micrographs for the gel made by **16** on standing for 3-5 days (For a larger image please see Supplementary Information.)

solution for imaging (TEM), the sample, for most part, appeared as a smooth film but otherwise had the pattern shown in Fig 4. Further, it was observed that compound **18** dissolved in polar solvents such as DMSO, DMF, AcOH, MeNO<sub>2</sub>, etc giving clear colorless solutions (Table 1). While it formed gels in alkanes such as hexane, heptane and octane, it dissolved in alcohols such as methanol and *n*-octanol though in the latter case the resulting solution appeared slightly viscous. Aromatic solvents such as

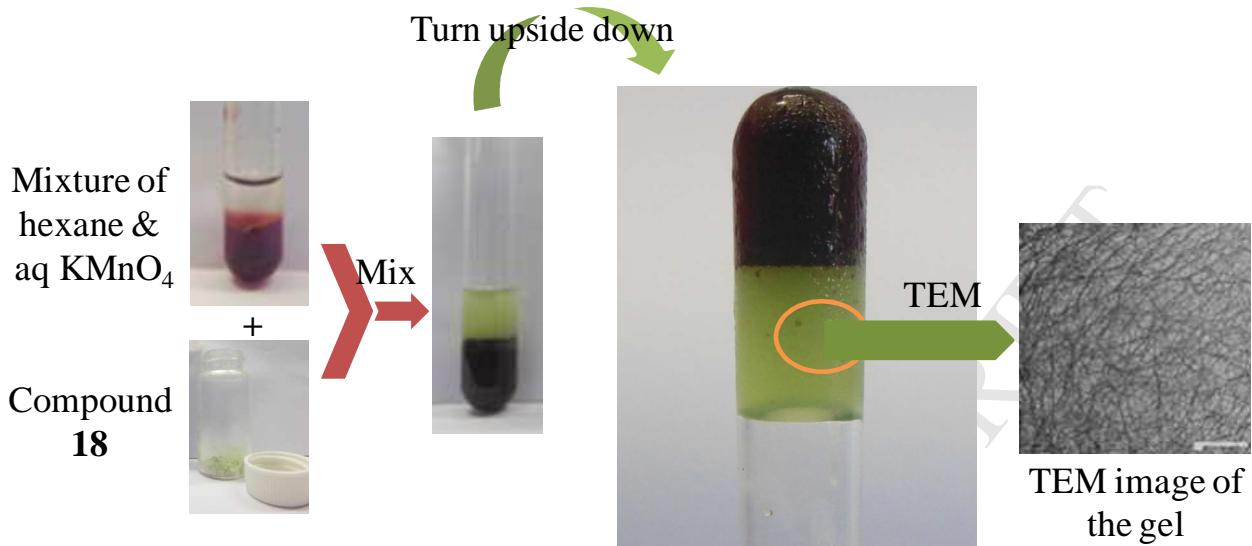
**Table 1.** Interaction of **18** with various solvents\*

Entry	Solvent	Observation	Hansen's solvent parameters <sup>⑧</sup>		
			$\delta_d$	$\delta_p$	$\delta_h$
1	Hexane	Quickly absorbs, forms clear thick gel	7.28	0.00	0.00
2	Heptane	Quickly absorbs, forms clear thick gel	7.48	0.00	0.00
3	Octane	Quickly absorbs, forms clear thick gel	7.58	0.00	0.00
4	Octanol	Dissolves; solution, marginally viscous	-- <sup>#</sup>	-- <sup>#</sup>	-- <sup>#</sup>
5	Methanol	Dissolves; does not gel	7.38	6.01	10.90
6	Toluene	Dissolves; does not gel	8.80	0.68	0.98
7	DMSO	Dissolves; does not gel	9.00	8.02	4.99
8	AcOH	Dissolves; does not gel	7.09	3.91	6.60
9	Water	Insoluble	7.63	7.82	20.68
10	Water-Hexane	Absorbs hexane and leaves water at the bottom			

\* 20 mg of **18** was taken up in 2 mL of the respective solvent and the nature of the interaction was noted;

<sup>@</sup>  $\delta_d/\delta_p/\delta_h$  are the dispersion/polar/H-bonding contributions to  $\delta$ , the Hildebrand solubility parameter ( $\text{MPa}^{1/2}$ ); <sup>#</sup> values for octanol were not available but the respective values reported for decanol are: 8.60, 1.32 and 4.89, respectively.<sup>83</sup>

toluene also dissolved **18**, giving clear solutions (Table 1). These observations clearly indicated possible ordered association between the fatty acyl chains present in the substance with the solvent molecules of matching attributes in agreement with the concept of “like seeks likes”. In general, mixing of **18** with organic non-polar solvents possessing Hildebrand’s polar and H-bonding parameters of zero (entries 1-3, Table 1) resulted in the formation of a gel whereas dissolution occurred in polar organic solvents possessing values greater than zero for these parameters. Thus, formation of a solution of slightly higher viscosity in octanol compared to methanol was also not unexpected. Details of the hydrophobic-hydrophobic (and other) interactions leading to the supramolecular assembly in these molecules have been rationalized further in Section 2. These observations led us to examine its possible application typical of those with phase-selective gelation abilities as used in oil-spill clean-up from water. In a qualitative evaluation thus, when **18** was added to a mixture (bi-phasic) of aqueous  $\text{KMnO}_4$  and hexane, the compound completely absorbed the organic liquid selectively, forming a gel capable of holding the aq permanganate solution over it upon turning the test tube upside down (Fig 5). The same was the case when  $\text{CuSO}_4$  was used in the place of  $\text{KMnO}_4$  (except for the fact that the aqueous layer in the latter case had the bluish appearance owing to the presence of  $\text{CuSO}_4$ ). Again, in the absence of the inorganic salts also the behavior of the biphasic system was identical to the above cases except for the fact that the aqueous layer remained colourless and therefore a visual demarcation of the two layers was more difficult.



**Figure 5.** Demonstration of the application of compound **18** as a phase-selective gelator: The compound absorbs hexane selectively from the bi-phasic mixture and generates a gel that can hold the aqueous permanganate solution over it.

Further, inspired by the various reports on the antimicrobial (antibacterial, antifungal, etc) activities of various 1,4-disubstituted 1,2,3-triazole derivatives,<sup>84-89</sup> the above compounds were also evaluated against bacterial strains in search of potential new antibacterial molecules. Also, as the triazole-linked compounds are known to act through different mechanisms, the possibility for finding compounds acting through novel mechanisms also existed. The compounds were tested against both gram positive and gram negative strains of various bacterial strains. The results of the screening experiments are summarized in Table 2. Thus, while compounds **4**, **16**, **18** and **19** were found to have moderate activities against the gram positive bacterial strains tested (Table 2), compounds **13**, **14**, **15**, **17** and **20** were inactive. Also, the activity was selective towards the gram positive strains as none of the compounds showed any activity against any gram negative strains tested (results not shown). In order to establish any structure activity

relationship for these molecules, therefore, the evaluation of a much wider range of compound-library would be required.

**Table 2.** Antibacterial activity of triazole-linked compounds

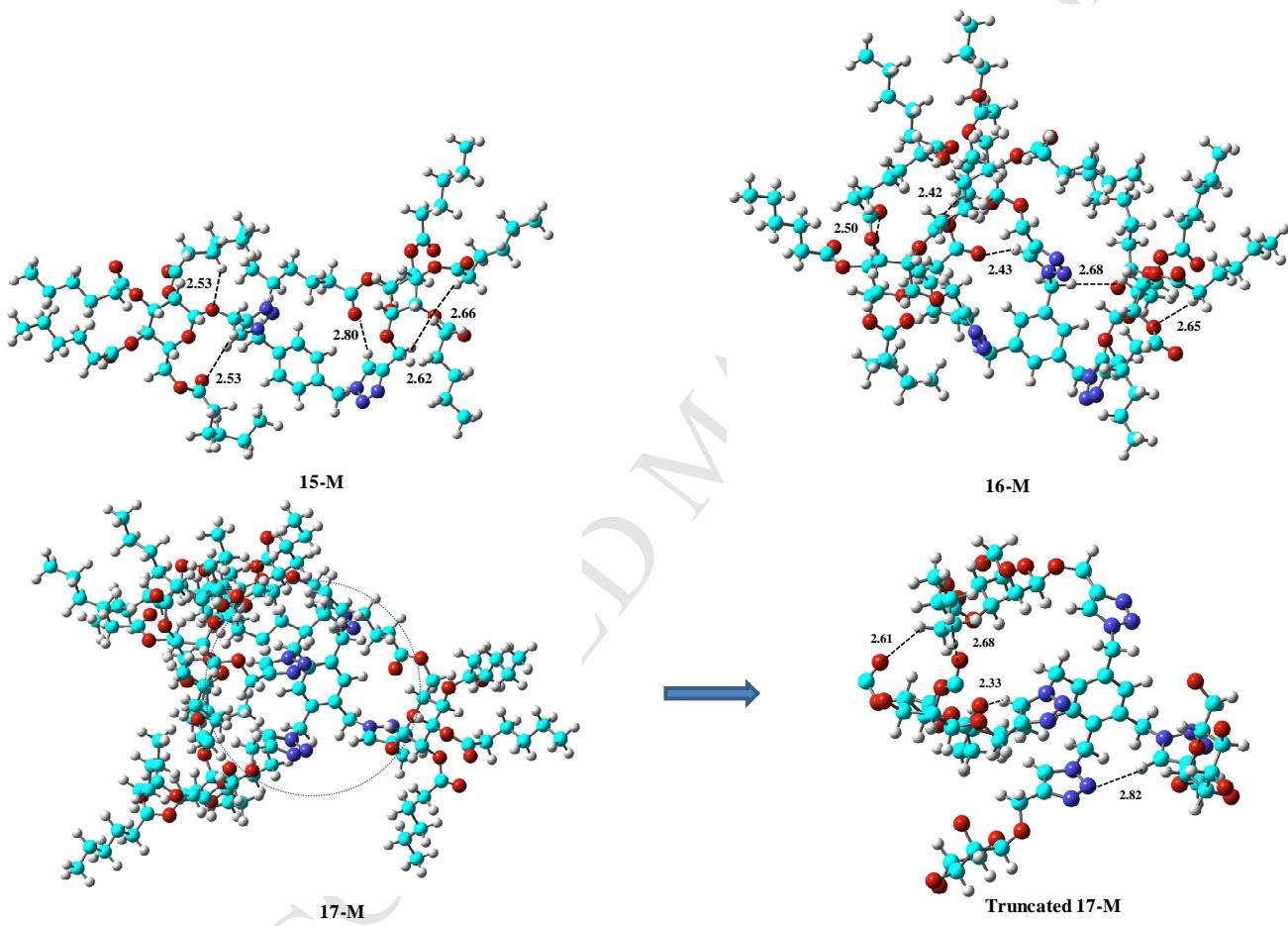
Compound	Bacterial strain		
	<i>Micrococcus luteus</i>	<i>Staphylococcus aureus</i>	<i>Bacillus subtilis</i>
	<i>MTCC-2470</i>	<i>MTCC-96</i>	(MIC, $\mu\text{g/ml}$ )
	(MIC, $\mu\text{g/ml}$ )	(MIC, $\mu\text{g/ml}$ )	
<b>4</b>	1000	125	250
<b>16</b>	250	500	500
<b>18</b>	1000	NAA	NAA
<b>19</b>	NAA	NAA	1000
Ampicillin	16	32	4
Amoxicillin	4	16	2

Test compounds: 1000 ( $\mu\text{g/ml}$ ); NAA: No Antimicrobial Activity; Compounds **13**, **14**, **15**, **17** and **20** were not active.

### 2.3 Quantum chemical analysis to rationalise the self-assembling property

In view of the interesting physicochemical properties exhibited by the compounds described above, attempts were made to rationalize the observations by TEM in terms of their electronic structures and the various inter- as well as intramolecular interactions that possibly existed in them. Initially, the monomeric structures of glycosides **15**, **16** and **17** were constructed and optimized employing the semi-empirical quantum chemical method, PM3 method using Gaussian03 package (for the details of methodology, see

supporting information and computational details provided in the experimental section). Recently, this method has been used for providing insights into the structural details of polymeric structures and supramolecular systems.<sup>43,61</sup> Fig 6 shows the optimized 3D geometries of these monomers, designated for easy differentiation from the dimers and trimers as, **15-M**, **16-M** and **17-M**. The optimized geometry of **15-M** showed the two triazole moieties above the plane of the benzene ring. It is characterized by a set of

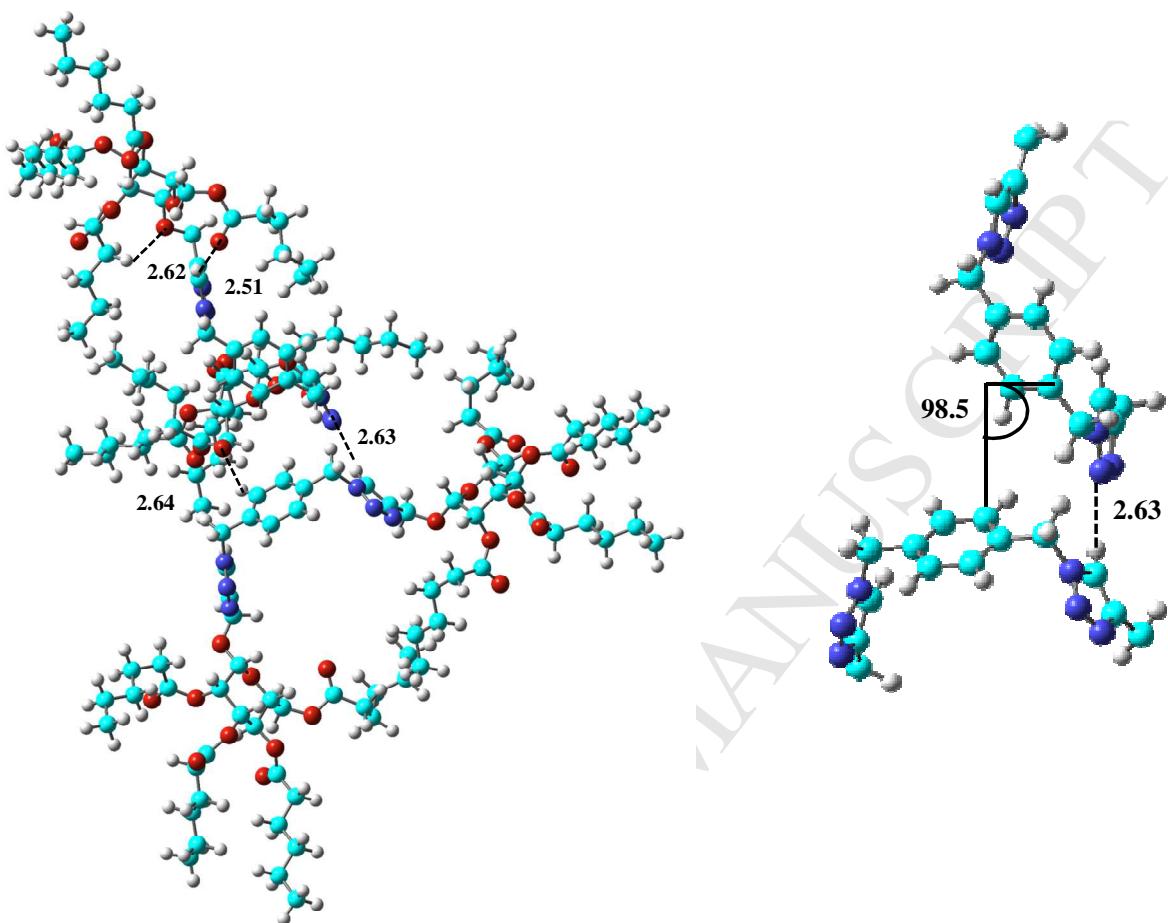


**Figure 6.** The optimized 3D geometries of monomeric structures of **15** (**15-M**) and **16** (**16-M**), showing characteristic intramolecular and intermolecular hydrogen bonding interactions. Owing to the difficulty in pointing out interactions in **17** (**17-M**), markings have been made on its truncated structure shown. All the bond distances are given in Å units.

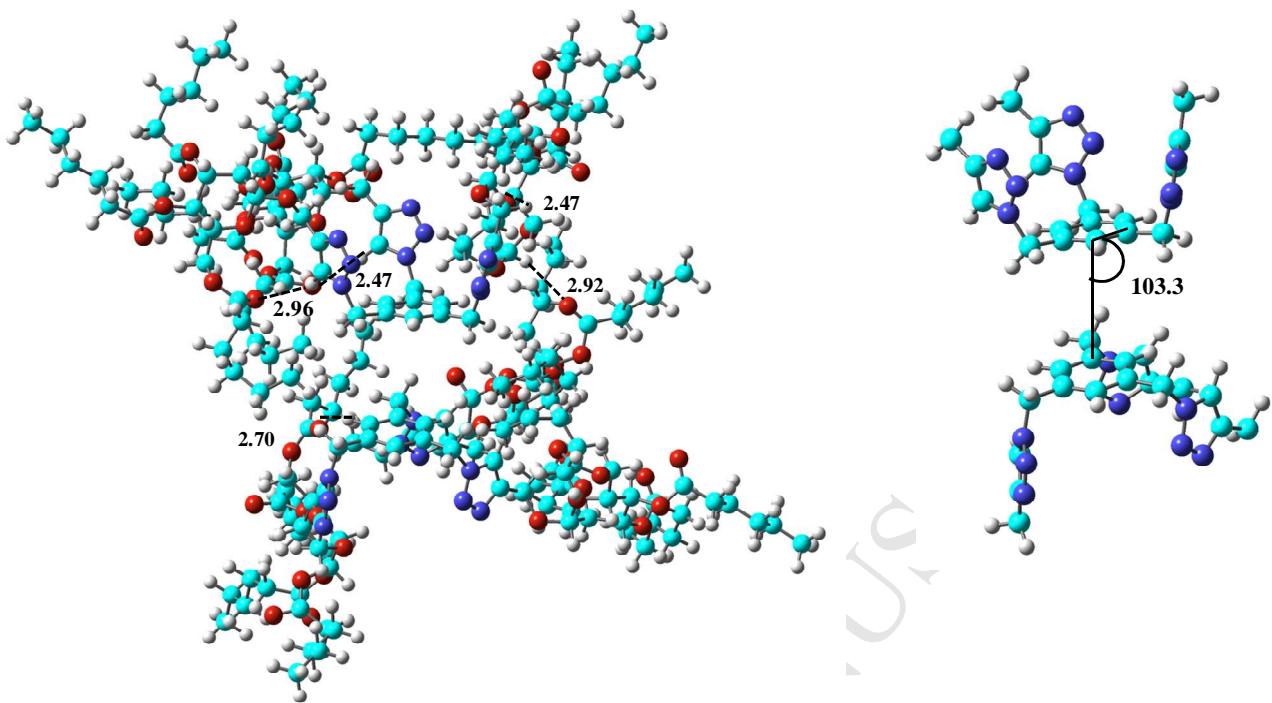
intramolecular H-bonding interactions amongst the sugar units as well as those between the C-H (triazole) and the carbonyl oxygen (of the 6-*O-n*-hexanoyl residue). The two H-bonding interactions, C-H<sub>triazole</sub>--O=C (of 6-*O-n*-hexanoyl residue) were observed with H-bond distances of 2.53 and 2.80 Å. The other weak interactions observed were between the methylene hydrogens (C-3 methylene, second from the acyl carbon of the 2-*O-n*-hexanoyl residue) and the anomeric oxygen [CH---O] with bond distances of 2.53 Å, triazolyl CH<sub>2</sub>--O(CO) (of 2-*O-n*-hexanoyl residue) with bond distances of 2.62 Å and between the methylene hydrogens (C-2 methylene next to the acyl carbon of the 3-*O-n*-hexanoyl residue) and O(CO) (of 2-*O-n*-hexanoyl residue) with the bond distance of 2.66 Å. The *n*-hexanoate chains at C-4 and C-5 of the sugar units were found to be involved in hydrophobic interactions. Likewise, the optimized geometry of **16-M** also showed the three triazole moieties connected to the benzene ring at 1, 3 and 5 positions, lying above the plane of the benzene ring. Several intramolecular H-bonding interactions, similar to those in **15-M**, were also indeed observed in this case. A strong intramolecular H-bonding interaction was observed between the C-H of the triazole unit and the O=C of the 6-*O-n*-hexanoyl residue (CH----O=C, 2.43 Å). The other intramolecular interactions observed were between the carbonyl oxygen of the 2-*O-n*-hexanoyl residue and the anomeric hydrogen (H-1) of the sugar moiety (2.42 Å). A similar interaction was also observed between the carbonyl oxygen of 3-*O-n*-hexanoyl residue and the H-4 of the sugar (2.50 Å). The C-2 methylene hydrogen of the 3-*O-n*-hexanoyl residue (that is, adjacent to the acyl carbon) was also observed to participate in an intramolecular H-bonding interaction with the ester oxygen of the 2-*O-n*-hexanoyl residue [CH---O(CO), 2.65 Å]. A characteristic intramolecular hydrogen bonding interaction (2.68 Å) between the hydrogen of benzylic methylene (PhCH<sub>2</sub> in the centre attached to the triazolyl nitrogen) and the carbonyl oxygen of the ester (6-*O-n*-hexanoyl residue) was also observed. These interactions give rise to the typical orientation of the three triazole rings connected to the central benzene ring in the optimized geometry of **16-M** (Fig 6). The optimized geometry of **17-M** was situated

above the plane of the benzene ring, while the fourth triazole moiety was oriented below the plane. This gave the geometry characterized by an arrangement, in which an intramolecular H-bonding interaction (2.82 Å) was observed between the two triazole units situated above the plane of the benzene ring while another intramolecular interaction was observed between the carbonyl oxygen of the 2-*O-n*-hexanoyl residue and a C-5 methylene hydrogen of the 3-*O-n*-hexanoyl residue (C=O---HC, 2.68 Å). To understand and determine the self-assembling property in these molecules, their dimeric structures (**15-D**, **16-D** and **17-D**) were constructed from the optimized geometries of the monomers, as shown in Fig 7 (a, b & c). The analysis of the dimeric structures provided an understanding of the orientation of the two monomeric units, especially with respect to the central benzene ring. Fig 7 (a, b & c) shows the optimized geometries of the dimeric structures. In **15-D**, the central benzene ring of the monomeric unit is oriented at an angle of 98.5° with respect to the benzene ring of the other monomeric unit. An important intermolecular H-bonding interaction between the two triazole rings (CH<sub>triazole</sub>---N<sub>triazole</sub>, 2.63 Å) was observed, resulting in this typical orientation of **15-D**. Other intramolecular and intermolecular H-bonding interactions in **15-D** are shown in Fig 7a. The optimized geometry of **16-D** was observed to be in a different orientation as compared to **15-D**. The two central benzene rings in **16-D** were observed to be aligned parallel to each other, with the bond angle between them observed to be 103.3°. The interactions remained similar to those observed in **16-M**, and are shown in Fig 7b. In **17-D**, the two benzene rings were observed to be oriented at an angle of 114.9°, with a characteristic intermolecular H-bonding interaction (2.86 Å) observed between the N<sub>triazole</sub> and the methylene hydrogen (connecting the phenyl and the triazole rings, Fig 7c). The optimized geometries of **15-D**, **16-D** and **17-D** show the sugar units with their *n*-hexanote chains covering the dimeric structures from both sides, thus, ruling out the possibility of trimeric structures. Thus, the different orientations of **15-D**, **16-D** and **17-D** and several interactions amongst them give an indication of their self-assembling property, and stabilization of these dimeric structures (Table

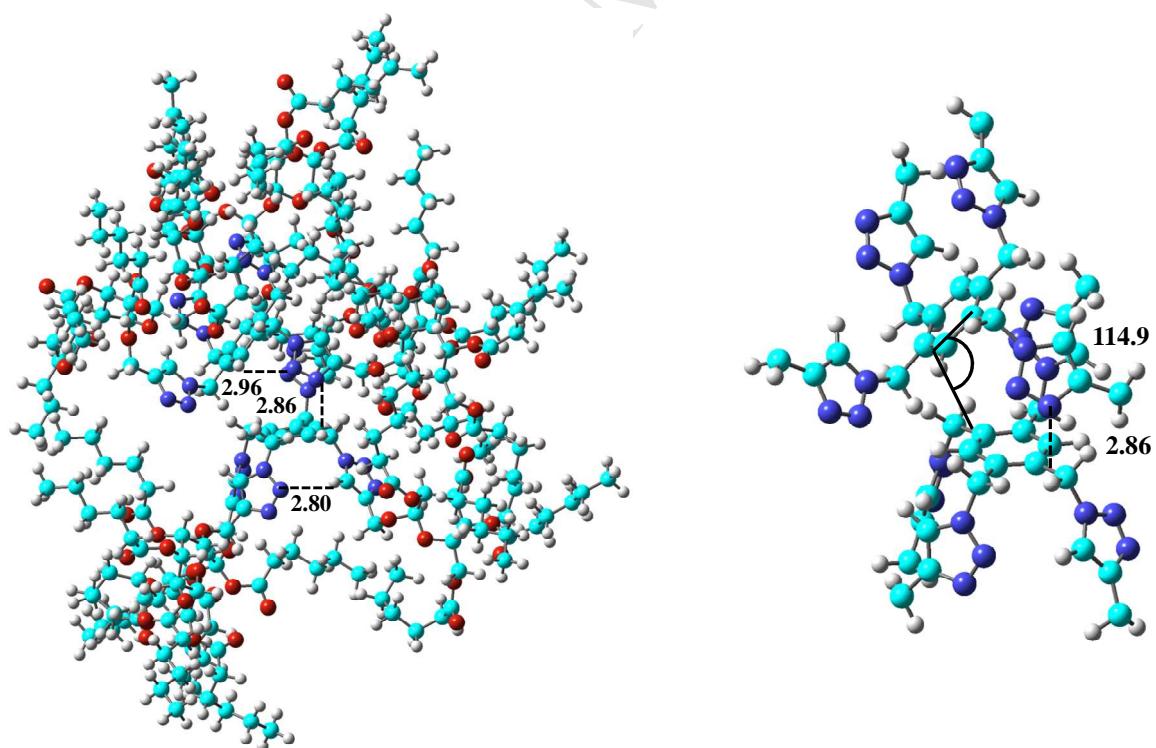
3).



**Figure 7a.** The optimized 3D geometries of dimeric structures of **15** (i. e. **15-D**) (showing the characteristic alignment of the two central benzene rings and the interactions in them. All the bond distances are given in Å units. Bond angles are given in degrees (°).



**Figure 7b.** The optimized 3D geometries of dimeric structures of **16** (i. e. **16-D**)



**Figure 7c.** The optimized 3D geometries of dimeric structures of **17** (i. e. **17-D**)

The energy details listed in Table 3 indicate a favourable formation of **16-D** and **17-D**, whereas no stabilization was observed in **15-D**. Thus, different intra- and intermolecular interactions, stabilization energies and distinct arrangement of dimeric structures confirm the self-assembling property of these molecules. The TEM analysis of the glucopyranosides synthesised indicate their self-assembling property (fibre like arrangement in **15**, **16** and **17**) which were rationalised in terms of their optimized geometries and H-bonding interactions in them. The self-assembling property of **15**, **16** and **17** can be judged on the basis of the thermodynamic factors (energy gain), along with the characteristic interactions. The dimerization of **16** (to give **16-D**) was observed to be a highly exothermic process (-15.59 kcal/mol) as compared to that of **17** (to give **17-D** with -7.07 kcal/mol), indicating its higher stability of formation.

**Table 3.** The absolute and stabilization energies of glucopyranosides **15-M**, **16-M**, **17-M**, **15-D**, **16-D** and **17-D** calculated using the PM3 method

Entry	Compound	Absolute Energy (kcal/mol)	Formulae	Dimerization Energy <sup>*</sup> (kcal/mol)
1	<b>15-M</b>	-1.313319	-	-
2	<b>16-M</b>	-1.996846	-	-
3	<b>17-M</b>	-2.667027	-	-
4	<b>15-D</b>	-2.626648	$E_{11-D} - 2E_{11-M}$	0.00
5	<b>16-D</b>	-4.018538	$E_{12-D} - 2E_{12-M}$	-15.59
6	<b>17-D</b>	-5.345318	$E_{13-D} - 2E_{13-M}$	-7.07

<sup>\*</sup>Dimerization energy is calculated by subtracting the summation of energies of monomers from the energy of the dimer.

This analysis supports the higher gelation ability of compound **17** over that of **16**, as discussed earlier. The oligomerization study, however, could not be extended beyond the above compounds due to the

excessive steric crowding and hindrances caused by the cluster of larger chains/groups and heavier substitutions on the central phenyl ring.

### 3. Conclusions

Application of ‘click reaction’ in making self-assembling glycocluster-materials has been demonstrated successfully. The preparation of these novel compounds were achieved under ‘green reaction conditions’ using a solvent-free mechanochemical method. Some of the compounds formed gels in organic solvents and this phase-selective gelation ability was demonstrated in a water-hexane system. Transmission electron micrographs clearly revealed the gel structures and were typical of organic polymer-derived gels. Geometry optimization studies on the monomeric forms of compounds **15**, **16** and **17** and their dimers (**15-D**, **16-D** and **17-D**) by Gaussian clearly indicated the role played by various inter- and intramolecular interactions. These interactions result in the specific arrangement of various structural elements present in these molecules that lead to self-assemblages, as observed by TEM. Some of the reported compounds possessed promising antibacterial activity.

## 4. Experimental

### 4.1 General

All reagents and chemicals were purchased from Aldrich Chemical Co (Milwaukee, WI, USA). Reactions were monitored by TLC, which was performed on 0.2 mm Merck pre-coated silica gel 60 F254 aluminium sheets. Compounds were detected by dipping the TLC plates in an ethanolic solution of sulphuric acid (5% v/v) and thereafter heating them. Melting points were recorded on a capillary melting point apparatus (Buchi). Specific rotations were obtained on Rudolph Research Autopol IV polarimeter at 20 °C. IR spectra were recorded on a Nicolet FT-IR Impact 410 instrument either as neat or KBr pellets. <sup>1</sup>H and <sup>13</sup>C NMR spectra were referenced to the internal standard tetramethylsilane, in the respective

deuterated solvents. Coupling constants (*J*) are reported in Hertz. High resolution mass spectra (HRMS) were recorded on a Bruker Maxis spectrometer.

#### **4.2 General procedure for the synthesis of CTSAMs by planetary ball-milling:**

The azide (1 mmol) and alkyne (1.1 mol equiv/per azide group) was taken in a stainless steel (SS) jar (capacity, 50 mL) containing 10 SS balls (10 mm o.d.) and sodium ascorbate (0.4 mol equiv/per azide functionality) was added to it followed by the addition of CuSO<sub>4</sub> (0.2 mol equiv/per azide functionality). The mixture was then ground in a planetary ball mill (Retsch PM-100, Retsch GmbH, Germany) at 500 rpm. After completion of the reaction the mixture was dissolved in EtOAc and was purified by column chromatography (EtOAc:Hex) to yield analytically pure product.

#### **4.3 Characterisation of compounds**

##### **Propargyl 2,3,4,6-tetra-*O*-hexanoyl- $\beta$ -D-glucopyranoside (1)**

This compound was prepared from propargyl  $\beta$ -D-glucopyranoside by literature methods.<sup>60,72</sup> Colourless syrup;  $[\alpha]_D$  -14.8 (*c* = 0.2, CHCl<sub>3</sub>); δ<sub>H</sub> (400 MHz, CDCl<sub>3</sub>); 5.28 (1H, t, *J* 9.5 Hz, *H*-3), 5.12 (1H, t, *J* 9.7 Hz, *H*-4), 5.03 (1H, d, *J* 8.2 Hz, *H*-2), 4.91 (1H, d, *J* 7.9 Hz, *H*-1), 4.36 (2H, s, OCH<sub>2</sub>), 4.20 (1H, m, *H*-6<sup>a</sup> & *H*-6b), 3.74 (1H, m, *H*-5), 2.23 (8H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.54 (8H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 1.25 (16H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (12H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>); δ<sub>C</sub> (100 MHz, CDCl<sub>3</sub>); 180.18, 173.49, 172.92, 172.17, 172.09, 160.39, 159.70, 98.05, 78.04, 75.48, 75.40, 72.36, 72.23, 72.03, 71.76, 70.66, 70.59, 70.40, 68.18, 68.05, 67.84, 61.64, 61.34, 55.69, 34.00, 33.95, 33.91, 33.85, 31.18, 31.15, 31.10, 29.03, 24.50, 24.39, 24.31, 24.13, 22.39, 22.24, 22.19, 22.17; IR (Neat) ν<sub>max</sub> 3311, 2957, 2931, 2872, 1750, 1458, 1379, 1225, 1161, 1095, 913, 743; HRMS: m/z calculated for C<sub>33</sub>H<sub>54</sub>O<sub>10</sub>: 610.3717, 633.3609 [M + Na]<sup>+</sup> Found 633.3610 [M + Na]<sup>+</sup>.

**Propargyl 2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranoside (2)**

This compound was prepared from propargyl  $\beta$ -D-glucopyranoside by literature methods.<sup>60,72</sup> Colourless syrup;  $[\alpha]_D$  -22.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 5.27 (1H, t,  $J$  9.5 Hz, H-3), 5.11 (1H, t,  $J$  9.7 Hz, H-4), 5.03 (1H, d,  $J$  8.0 Hz, H-2), 4.78 (1H, d,  $J$  8.0 Hz, H-1), 4.35 (2H, s, OCH<sub>2</sub>), 4.19 (1H, m, H-6a & H-6b), 3.72 (1H, m, H-5), 2.23 (8H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>9</sub>CH<sub>3</sub>)<sub>4</sub>), 1.54 (8H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>), 1.25 (64H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (12H, m, OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 202.92, 174.33, 173.42, 172.86, 172.15, 172.06, 101.88, 98.08, 78.09, 77.35, 77.03, 76.71, 75.39, 72.33, 72.09, 70.64, 68.06, 61.66, 60.12, 55.73, 51.40, 43.90, 34.37, 34.13, 34.09, 34.06, 33.99, 33.96, 31.90, 29.62, 29.58, 29.52, 24.48, 29.44, 29.34, 29.32, 29.26, 29.25, 29.13, 29.09, 29.05; IR (Neat)  $\nu_{max}$  3748, 3266, 2855, 2926, 2956, 1748, 1577, 1541, 1465, 1377, 1317, 1275, 1260, 1160, 1112, 1069, 913, 816, 764, 749; HRMS: m/z calculated C<sub>57</sub>H<sub>102</sub>O<sub>10</sub>: 946.7473, 969.7365 [M +Na]<sup>+</sup> Found 969.7345 [M +Na]<sup>+</sup>.

**1-Benzyl-4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (4)**

Greenish syrup;  $[\alpha]_D$  -11.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.27 (5H, s, PhH), 5.63 (2H, m, PhCH<sub>2</sub>), 5.01 (5H, m, H-4, H-3, H-2 & OCH<sub>2</sub>), 4.63 (1H, bs, H-1), 4.06 (1H, m, H-6a & H-6b), 3.63 (1H, m, H-5), 2.25-2.06 (8H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.52-1.44 (8H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 1.32-1.18 (16H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 0.80-0.76 (12H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 173.41, 172.78, 172.44, 172.12, 172.08, 134.39, 130.05, 129.90, 129.59, 129.53, 129.46, 129.16, 128.88, 128.79, 128.49, 128.26, 128.19, 128.11, 100.30, 72.38, 72.23, 72.06, 70.98, 70.73, 68.03, 67.38, 63.20, 61.62, 54.58, 34.25, 33.95, 33.90, 33.87, 31.88, 31.19, 31.15, 31.13, 31.06, 29.64, 24.43, 24.38, 24.33, 22.64, 22.25, 22.19, 14.06, 13.91, 13.88; IR (Neat)  $\nu_{max}$  2957, 2932, 2872, 2097, 1751, 1618, 1497, 1457, 1417, 1379, 1316, 1227, 1161, 1096, 1063, 913, 743, 655.

**1-Benzyl-4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (5)**

Colourless solid; mp 123-124 °C,  $[\alpha]_D$  -35.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.44 (1H, s, CH Triazole), 7.35 (3H, m, PhH), 7.27 (2H, d,  $J$  5.6 Hz, PhH), 5.51 (2H, s, CH<sub>2</sub>Ph), 5.20 (1H, t,  $J$  9.5 Hz, H-3), 5.08 (1H, t,  $J$  9.7 Hz, H-4), 5.03 (1H, d,  $J$  8.2 Hz, H-2), 4.90 (1H, d,  $J$  12.7 Hz, OCH<sub>2</sub>), 4.80 (1H, d,  $J$  12.7 Hz, OCH<sub>2</sub>), 4.64 (1H, d,  $J$  8.0 Hz, H-1), 4.19 (2H, dd,  $J$  12.4 Hz,  $J$  4.7 Hz, H-6a), 4.12 (2H, dd,  $J$  12.0 Hz,  $J$  1.6 Hz, H-6b), 3.68 (1H, m, H-5), 1.60 (8H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>9</sub>CH<sub>3</sub>)<sub>4</sub>), 1.56 (8H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>), 1.39 (64H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (12H, t,  $J$  6.4 Hz, OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 179.64, 173.48, 172.84, 172.13, 144.71, 134.43, 129.14, 128.82, 128.09, 122.72, 100.06, 72.35, 72.05, 70.91, 68.03, 62.99, 61.66, 54.22, 53.43, 42.53, 36.65, 34.08, 34.04, 33.97, 33.17, 32.00, 31.92, 29.87, 29.63, 29.60, 29.49, 29.46, 29.44, 29.36, 29.33, 29.27, 29.26, 29.13, 29.11, 29.08, 29.04, 29.81; IR (Neat)  $\nu_{max}$  2925, 2854, 1752, 1497, 1457, 1416, 1376, 1227, 1156, 1115, 1049, 912, 799, 722, 600, 527.

### **1-Benzyl-4-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (6)**

Colourless syrup;  $[\alpha]_D$  -18.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.44 (1H, s, CH Triazole), 7.36 (3H, m, PhH), 7.27 (2H, d,  $J$  5.6 Hz, PhH), 5.52 (2H, s, CH<sub>2</sub>Ph), 5.14 (1H, t,  $J$  9.5 Hz, H-3), 5.06 (1H, t,  $J$  9.7 Hz, H-4), 4.99 (1H, d,  $J$  8.2 Hz, H-2), 4.90 (1H, d,  $J$  12.7 Hz, OCH<sub>2</sub>), 4.80 (1H, d,  $J$  12.7 Hz, OCH<sub>2</sub>), 4.64 (1H, d,  $J$  8.0 Hz, H-1), 4.26 (2H, m, H-6a), 4.11 (2H, m, H-6b), 3.70 (1H, m, H-5), 2.07 (3H, s, OCOCH<sub>3</sub>), 2.03 (3H, s, OCOCH<sub>3</sub>), 1.98 (3H, s, OCOCH<sub>3</sub>), 1.85 (3H, s, OCOCH<sub>3</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 170.67, 170.21, 169.46, 169.36, 144.59, 144.51, 134.47, 129.18, 128.87, 128.41, 128.15, 127.72, 122.74, 122.69, 99.78, 72.33, 72.64, 71.85, 71.61, 71.15, 71.09, 70.86, 68.40, 68.25, 62.93, 61.78, 61.69, 61.59, 61.25, 55.15, 54.22, 53.47, 20.75, 20.60, 20.52; IR (Neat)  $\nu_{max}$  3446, 2969, 2532, 1743, 1645, 1498, 1434, 1366, 1227, 1130, 1047, 984, 905, 796, 724, 600, 527.

### **1-Benzyl-4-(hydroxymethyl)-1*H*-1,2,3-triazole (7)**

Colourless solid; mp 111-112.6 °C;  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.58 (1H, s, CH Triazole), 7.32 (3H, m, PhH), 7.24 (2H, m, PhH), 5.43 (2H, d, *J* 5.2 Hz, PhCH<sub>2</sub>), 4.68 (2H, d, *J* 4.5, CH<sub>2</sub>OH);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 148.26, 134.52, 129.09, 128.86, 128.74, 128.38, 128.30, 128.11, 122.04, 55.88, 55.84, 55.27, 54.13, 53.54, 50.72; IR (Neat)  $\nu_{max}$  3366, 3142, 2927, 2855, 1744, 1708, 1648, 1606, 1586, 1552, 1497, 1456, 1435, 1360, 1336, 1224, 1127, 1041, 1013, 913, 819, 795, 723, 697, 671, 582, 471.

**1,4-Bis[(4-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (13)**

Yellow solid; mp 126-126.5 °C;  $[\alpha]_D$  -28.9 (*c* = 0.2, CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.49 (1H, s, CH Triazole), 7.28 (2H, m, PhH), 5.52 (2H, d, *J* 2.3 Hz, PhCH<sub>2</sub>), 5.18 (1H, t, *J* 9.4 Hz, *H*-3), 5.07 (1H, t, *J* 9.8 Hz, *H*-4), 4.97 (1H, dd, *J* 9.4 Hz, *J* 8.0 Hz, *H*-2), 4.90 (2H, s, OCH<sub>2</sub>), 4.80 (2H, s, OCH<sub>2</sub>), 4.66 (1H, d, *J* 8.0 Hz, *H*-1), 4.23 (1H, dd, *J* 12.3 Hz, *J* 4.6 Hz, *H*-6a), 4.23 (1H, dd, *J* 12.3 Hz, *J* 2.2 Hz, *H*-6b), 3.72 (1H, m, *H*-5), 2.07 (3H, s, OCOCH<sub>3</sub>), 2.02 (3H, s, OCOCH<sub>3</sub>), 1.99 (3H, s, OCOCH<sub>3</sub>), 1.91 (3H, s, OCOCH<sub>3</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 170.68, 170.22, 169.46, 169.38, 144.77, 135.32, 128.75, 122.83, 100.03, 72.70, 71.88, 71.17, 68.27, 63.06, 61.78, 53.62, 22.74, 20.59; IR (Neat)  $\nu_{max}$  3445, 2957, 2872, 1749, 1368, 1228, 1164, 1047, 913, 749; HRMS: m/z calculated for C<sub>42</sub>H<sub>52</sub>N<sub>6</sub>O<sub>10</sub>: 960.3236, 983.3129 [M +Na]<sup>+</sup> Found 983.3086 [M +Na]<sup>+</sup>.

**1,4-Bis[(4-(β-D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (14)**

Yellowish solid; mp 135-135.8 °C;  $[\alpha]_D$  -38.8 (*c* = 0.2, CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 8.10 (1H, s, CH Triazole), 7.31 (2H, m, PhH), 5.54 (2H, s, PhCH<sub>2</sub>), 4.83 (2H, d, *J* 12.2 Hz, OCH<sub>2</sub>), 4.61 (2H, d, *J* 12.2 Hz, OCH<sub>2</sub>), 4.25 (1H, d, *J* 7.8 Hz, *H*-1), 3.70 (1H, d, *J* 12.1 Hz, *H*-6a), 3.60 (1H, dd, *J* 12.3 Hz, *J* 2.2 Hz, *H*-6b), 3.18-2.9 (4H, m, *H*-5, *H*-4, *H*-3, *H*-2);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 144.74, 136.32, 128.78, 124.71, 102.50, 77.10, 76.85, 73.68, 72.99, 72.21, 70.95, 70.38, 63.86, 61.87, 61.45, 52.88; IR (Neat)  $\nu_{max}$  3398, 2505, 2242, 2138, 2073, 1944, 1742, 1656, 1452, 1226, 1119, 1086, 975, 881, 822, 530.

**1,4-Bis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (15)**

Colourless solid; mp 120-120.6 °C;  $[\alpha]_D$  -18.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.47 (1H, s, CH Triazole), 7.28 (2H, m, PhH), 5.50 (2H, q,  $J$  15.02 Hz, PhCH<sub>2</sub>), 5.22 (1H, t,  $J$  9.4, H-3), 5.09 (1H, t,  $J$  9.6 Hz, H-4), 5.00 (1H, t,  $J$  8.2 Hz, H-2), 4.89 (2H, d,  $J$  12.5 Hz, OCH<sub>2</sub>), 4.79 (2H, d,  $J$  12.5 Hz, OCH<sub>2</sub>), 4.66 (1H, d,  $J$  8.2 Hz, H-1), 4.17 (2H, m, H-6a & H-6b), 3.70 (1H, m, H-5), 2.23 (8H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.55 (8H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 1.25 (16H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (12H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 173.41, 172.81, 172.10, 172.08, 144.82, 135.30, 128.67, 122.76, 100.22, 72.31, 72.09, 70.92, 68.05, 63.12, 61.64, 53.56, 33.96, 33.90, 31.21, 31.16, 31.08, 29.66, 29.24, 24.46, 24.42, 24.40, 24.37, 22.27, 22.21, 13.89, 13.84, 13.80; IR (Neat)  $\nu_{max}$  3479, 3267, 3122, 3066, 2957, 2932, 2872, 2319, 2102, 1747, 1516, 1458, 1416, 1379, 1318, 1287, 1245, 1166, 1097, 1067, 1051, 1011, 913, 846, 795, 781, 743, 667, 608, 507; HRMS: m/z calculated for C<sub>74</sub>H<sub>116</sub>N<sub>6</sub>O<sub>20</sub>: 1408.8244, 1431.8137 [M +Na]<sup>+</sup> Found 1431.8111 [M +Na]<sup>+</sup>.

**1,3,5-Tris[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (16)**

Colourless sticky solid;  $[\alpha]_D$  -8.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.37 (1H, s, CH Triazole), 7.35 (1H, s, PhH), 5.63 (2H, s, PhCH<sub>2</sub>), 5.23 (1H, t,  $J$  9.5 Hz, H-3), 5.10 (1H, t,  $J$  9.5 Hz, H-4), 4.99 (1H, t,  $J$  9.4 Hz, H-2), 4.89 (2H, d,  $J$  12.4 Hz, OCH<sub>2</sub>), 4.74 (2H, d,  $J$  12.4 Hz, OCH<sub>2</sub>), 4.67 (1H, d,  $J$  7.7 Hz, H-1), 4.19 (2H, m, H-6a & H-6b), 3.72 (1H, m, H-5), 2.27 (14H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.55 (11H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 1.25 (22H, m, (OCOCH<sub>2</sub>CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (16H, m, (OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 173.42, 172.81, 172.12, 144.30, 139.76, 130.55, 122.32, 100.28, 72.29, 70.95, 68.05, 63.05, 61.67, 48.98, 33.99, 33.96, 33.93, 33.90, 31.21, 31.17, 31.09, 24.48,

24.41, 24.37, 22.29, 22.23, 16.67, 13.91, 13.85, 13.82; IR (Neat)  $\nu_{\text{max}}$  3748, 2957, 2930, 2859, 1751, 1541, 1464, 1417, 1378, 1316, 1274, 1241, 1162, 1111, 1047, 913, 816, 764, 749, 609.

**1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (17)**

Colourless sticky solid;  $[\alpha]_D$  -4.9 ( $c = 0.2$ ,  $\text{CHCl}_3$ );  $\delta_{\text{H}}$  (400 MHz,  $\text{CDCl}_3$ ); 7.57 (1H, s,  $\text{CH}$  Triazole), 7.14 (1H, s,  $\text{PhH}$ ), 5.67 (2H, d,  $J$  15.2 Hz,  $\text{PhCH}_2$ ), 5.56 (2H, d,  $J$  15.2 Hz,  $\text{PhCH}_2$ ), 5.24 (1H, t,  $J$  9.5 Hz,  $H$ -3), 5.12 (1H, t,  $J$  9.7 Hz,  $H$ -4), 5.00 (1H, t,  $J$  8.8,  $H$ -2), 4.87 (2H, d,  $J$  12.5 Hz,  $\text{OCH}_2$ ), 4.78 (2H, d,  $J$  12.5 Hz,  $\text{OCH}_2$ ), 4.68 (1H, d,  $J$  7.9 Hz,  $H$ -1), 4.18 (2H, m,  $H$ -6a &  $H$ -6b), 3.74 (1H, m,  $H$ -5), 2.25 (10H, m,  $(\text{OCOCH}_2(\text{CH}_2)_3\text{CH}_3)_4$ ), 1.55 (10H, m,  $(\text{OCOCH}_2\text{CH}_2(\text{CH}_2)_2\text{CH}_3)_4$ ), 1.22 (22H, m,  $(\text{OCOCH}_2\text{CH}_2(\text{CH}_2)_2\text{CH}_3)_4$ ), 0.87 (16H, m,  $(\text{OCOCH}_2(\text{CH}_2)_3\text{CH}_3)_4$ );  $\delta_{\text{C}}$  (100 MHz,  $\text{CDCl}_3$ ); 173.48, 172.79, 172.12, 172.06, 144.83, 135.01, 132.28, 123.51, 100.44, 72.34, 72.12, 70.94, 68.03, 63.11, 61.52, 50.49, 33.97, 33.91, 31.56, 31.20, 31.17, 31.08, 30.90, 29.03, 24.48, 24.44, 24.40, 24.37, 22.63, 22.59, 22.27, 22.22, 14.09, 13.89, 13.84, 13.80; IR (Neat)  $\nu_{\text{max}}$  3479, 3142, 2957, 2932, 2872, 2256, 1447, 1462, 1416, 1379, 1316, 1273, 1227, 1163, 1096, 1048, 1012, 913, 888, 845, 795, 735, 647, 604, 496.

**1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (18)**

Colourless sticky solid;  $[\alpha]_D$  -3.4 ( $c = 0.2$ ,  $\text{CHCl}_3$ );  $\delta_{\text{H}}$  (400 MHz,  $\text{CDCl}_3$ ); 7.56 (1H, s,  $\text{CH}$  Triazole), 7.15 (1H, s,  $\text{PhH}$ ), 5.71 (2H, d,  $J$  15.2 Hz,  $\text{PhCH}_2$ ), 5.55 (2H, d,  $J$  15.2 Hz,  $\text{PhCH}_2$ ), 5.23 (1H, t,  $J$  9.5 Hz,  $H$ -3), 5.11 (1H, t,  $J$  9.7 Hz,  $H$ -4), 5.00 (1H, t,  $J$  8.1,  $H$ -2), 4.89 (2H, d,  $J$  9.6 Hz,  $\text{OCH}_2$ ), 4.81 (2H, d,  $J$  9.6 Hz,  $\text{OCH}_2$ ), 4.67 (1H, d,  $J$  8.0 Hz,  $H$ -1), 4.19 (2H, m,  $H$ -6a &  $H$ -6b), 3.70 (1H, m,  $H$ -5), 2.26 (10H, m,  $(\text{OCOCH}_2(\text{CH}_2)_9\text{CH}_3)_4$ ), 1.57 (10H, m,  $(\text{OCOCH}_2\text{CH}_2(\text{CH}_2)_8\text{CH}_3)_4$ ), 1.25 (113H, m,  $(\text{OCOCH}_2\text{CH}_2(\text{CH}_2)_8\text{CH}_3)_4$ ), 0.87 (21H, t,  $J$  6.2 Hz,  $(\text{OCOCH}_2(\text{CH}_2)_9\text{CH}_3)_4$ );  $\delta_{\text{C}}$  (100 MHz,  $\text{CDCl}_3$ ); 173.50, 172.80, 172.14, 172.06, 135.00, 134.59, 131.35, 72.36, 72.11, 70.90, 67.99, 63.08, 61.51, 52.27,

51.69, 50.51, 34.03, 33.97, 32.79, 31.92, 29.65, 29.60, 29.52, 29.46, 29.43, 29.37, 29.33, 29.15, 29.09, 25.74, 24.88, 24.80, 24.75, 22.69, 14.12; IR (Neat)  $\nu_{\text{max}}$  2956, 2925, 2855, 2102, 1750, 1711, 1617, 1465, 1415, 1378, 1275, 1260, 1158, 1113, 1063, 913, 764, 749.

**Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]methane (19)**

Colourless syrup;  $[\alpha]_D$  -18.9 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 8.15 (1H, s, CH Triazole), 5.23 (1H, t,  $J$  9.4 Hz, H-3), 5.12 (1H, t,  $J$  9.9 Hz, H-4), 5.01 (1H, t,  $J$  8.2 Hz, H-2), 4.96 (1H, d,  $J$  12.3 Hz, CH<sub>2</sub>), 4.79 (1H, d,  $J$  12.3 Hz, CH<sub>2</sub>), 4.69 (1H, d,  $J$  7.9 Hz, H-1), 4.37 (2H, s, CH<sub>2</sub>), 4.20 (2H, d,  $J$  2.6 Hz, H-6a & H-6b), 3.75 (1H, m, H-5), 2.34 (3H, t,  $J$  7.4 Hz, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 2.22 (8H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.55 (10H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.26 (21H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 0.87 (15H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 173.41, 172.81, 172.05, 143.65, 127.20, 100.00, 72.39, 72.18, 70.90, 68.03, 62.23, 61.61, 49.15, 46.57, 33.96, 33.91, 31.21, 31.18, 31.17, 31.09, 29.24, 24.47, 24.43, 24.39, 24.37, 22.28, 22.23, 13.89, 13.85, 13.80; IR (Neat)  $\nu_{\text{max}}$  3267, 3144, 2957, 2932, 2872, 2319, 1751, 1459, 1416, 1379, 1317, 1240, 1162, 1099, 1047, 913, 845, 797, 743, 667.

**1,2,3,4,5,6-Hexakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (20)**

Brown semi-solid;  $[\alpha]_D$  -4.4 ( $c = 0.2$ , CHCl<sub>3</sub>);  $\delta_H$  (400 MHz, CDCl<sub>3</sub>); 7.35 (1H, s, CH Triazole), 7.14 (1H, s, PhH), 5.89 (2H, d,  $J$  15.4 Hz, PhCH<sub>2</sub>), 5.81 (2H, d,  $J$  15.4 Hz, PhCH<sub>2</sub>), 5.22 (1H, t,  $J$  9.6 Hz, H-3), 5.11 (1H, t,  $J$  9.6 Hz, H-4), 4.97 (1H, t,  $J$  8.9, H-2), 4.67 (2H, m, OCH<sub>2</sub>&H-1), 4.25 (1H, d,  $J$  11.6 Hz, H-6a), 4.11 (1H, d,  $J$  9.2 Hz, H-6b), 3.73 (1H, m, H-5), 2.30 (8H, t,  $J$  7.4 Hz, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 2.23 (12H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.55 (20H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 1.26 (44H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>), 0.86 (32H, m, OCOCH<sub>2</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>)<sub>4</sub>);  $\delta_C$  (100 MHz, CDCl<sub>3</sub>); 173.60, 172.79, 172.12, 172.00, 137.45, 100.74, 72.48, 72.04, 70.89, 67.99, 67.59, 63.15, 61.34, 48.00, 47.81, 33.99,

33.94, 33.89, 31.31, 31.18, 31.10, 29.65, 24.47, 24.44, 24.36, 24.14, 22.65, 22.30, 22.65, 22.30, 22.25, 22.21, 13.87, 13.77; IR (Neat)  $\nu_{\text{max}}$  3784, 3427, 2957, 2932, 2872, 2097, 1746, 1635, 1457, 1416, 1379, 1275, 1259, 1222, 1165, 1110, 1064, 1064, 1016, 844, 764, 750, 723, 692.

**4.4 TEM analysis:** Philips TECNAI electron microscope was used for obtaining transmission micrographs at 120 Kv accelerating voltage. Compounds **15**, **16**, **17** and **18** were taken up in hexane/heptanes/octane and aliquots were applied onto copper grids coated with carbon film (Quantifoil on 200 square mesh copper grid of hole-shape R 2/2) and after allowing to dry was mounted on the microscope for recording the micrographs.

**4.5 Computational details:** All the geometries were optimized using semi-empirical PM3 (Parameterized Model number 3) method, using the Gaussian03 package, considering large size of glycol clusters. This method has been reported to be helpful, reliable and applicable in the optimization studies of large molecules, and save considerable computing time. PM3 method possesses higher computational efficiency in modelling larger systems, as compared to *ab initio* and Density Functional Theory (DFT) methods (which utilize longer time and computational power). PM3 provides improved description of the interaction between non-bonded atoms (hydrogen bonds and steric effects), and represents a middle pathway between the molecular mechanics (MM) method (giving mostly qualitative results) and *ab initio* methods (time-consuming but providing quantitative results). PM3 method has been indicated to provide insights into the structural details of dimers, polymeric structures and supramolecular systems and providing information about the interactions amongst them. The applicability of this method in the optimization studies of large molecules has been reported in previous studies, as it is reliable and saves considerable computing time.<sup>90-94</sup> PM3 method is utilized in modelling larger systems owing to its higher computational efficiency, as compared to *ab initio* and Density Functional Theory (DFT) methods (which utilize longer time and computational power). The interactions between non-bonded atoms (hydrogen

bonds and steric effects) can be inferred by this method.<sup>90-94</sup> Recently, we have reported the effectiveness of this method in providing insights into the structural details of monomers and their dimeric structures and supramolecular systems.<sup>43,61</sup> Hence, all the geometries of **15**, **16**, **17** and their dimeric structures were optimized using semi-empirical PM3 (Parameterized Model number 3) method,<sup>95-98</sup> using the Gaussian03 package (see Supplementary Information). Initially, the geometry optimizations of monomers, **15**, **16** and **17**, were computed using PM3 method. The optimized geometries were employed for the construction of dimers and thereafter, dimers were optimized. The dimerization energies were calculated in all the cases. The interactions were observed carefully in all the structures, which are responsible for the thread-like pattern in all the cases. The energy and geometric parameters used in the discussion are based on PM3 method unless otherwise specifically mentioned. However, it was not possible to extend calculation to explain polymeric behaviour of the molecules.

**4.6 MIC determination of the test compounds:** Minimum inhibitory concentration (MIC) was carried out as per previously described method.<sup>99</sup> All three Gram positive strains, viz. *Micrococcus luteus* MTCC-2470, *Staphylococcus aureus* MTCC-96 and *Bacillus subtilis* MTCC-121 were inoculated in 5 ml MHB independently and kept for incubation at 30 °C for 6-8 h (to reach OD<sub>600</sub> = 0.13). Antibiotics (100 µl) at a specific concentration were added in first well of 96-well micro titre plate and then exponentially diluted. Bacterial inocula equivalent to the 0.5 McFarland standards were prepared and 100 µl was added to give the final concentration of 5 x 10<sup>5</sup> cfu/ml, and incubated at 30 °C for 48 h. 20 µl of MTT dye (10 mg/ml wt/v in methanol) was added to each well and kept for incubation at 30 °C for 20 min. Bacterial growth indicated by purple coloration adhered to cells. The antibiotic concentration in the well at which no purple coloration observed, is the MIC of antibiotic. Similarly, the MIC of test compounds was also determined. Ampicillin and amoxicillin were used as the positive control to compare results obtained

from test compounds. Test assay, vehicle (DMSO) control, media control and cell control were done in triplicates (during each experiment) to validate the results.

**Acknowledgements:** MT and NT thank the Council of Scientific and Industrial Research (CSIR) and the Department of Science and Technology (DST), New Delhi, respectively, for financial support. We are grateful to Dr Alan Haines, UEA, Norwich for his kind help with the preparation of this manuscript.

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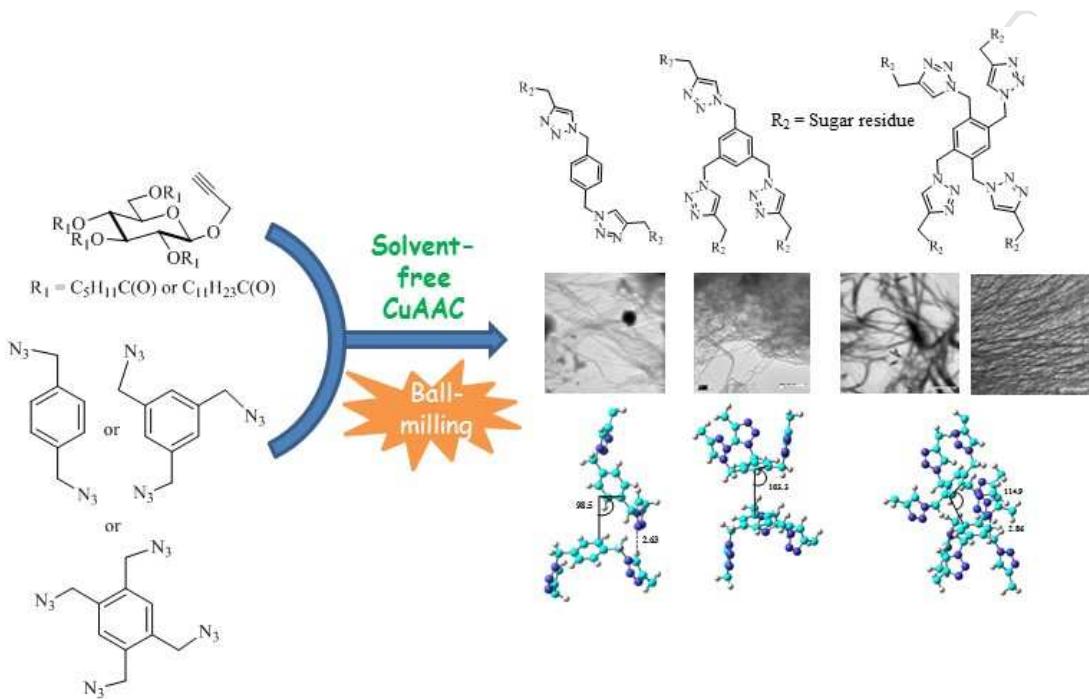
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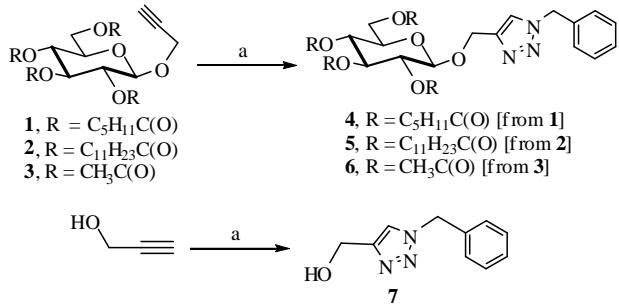
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**Graphical abstract**

**Mechanochemical click reaction as a tool for making carbohydrate-based triazole-linked self-assembling materials (CTSAMs)**

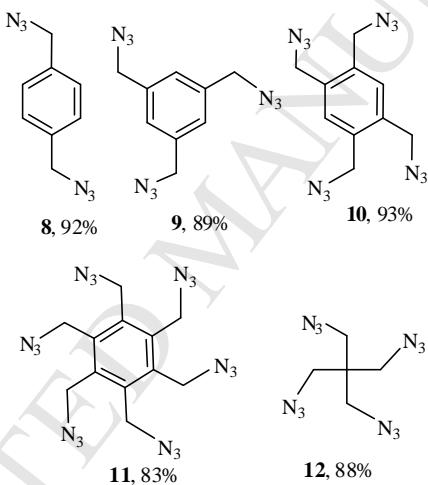
Mohit Tyagi, Nikhil Taxak, Prasad V. Bharatam, Hemraj Nandanwar, K. P. Ravindranathan Kartha\*



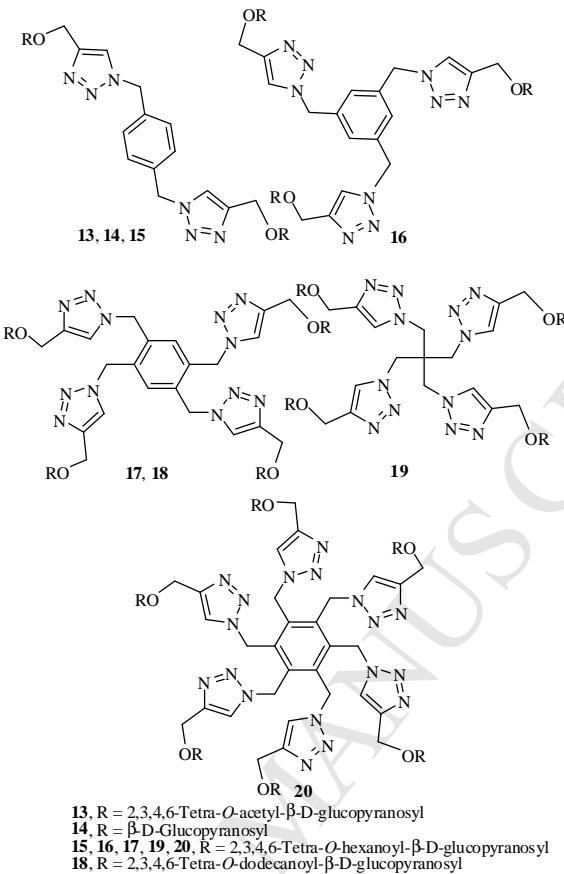
**Schemes, Figures and Tables:**

Reagents and conditions: (a) BnBr (2 mol equiv); NaN<sub>3</sub> (10 mol equiv); CuSO<sub>4</sub>·5H<sub>2</sub>O (0.4 mol equiv), sodium ascorbate; *t*-BuOH-H<sub>2</sub>O (1:1), rt, 1 h, 73 - 80%

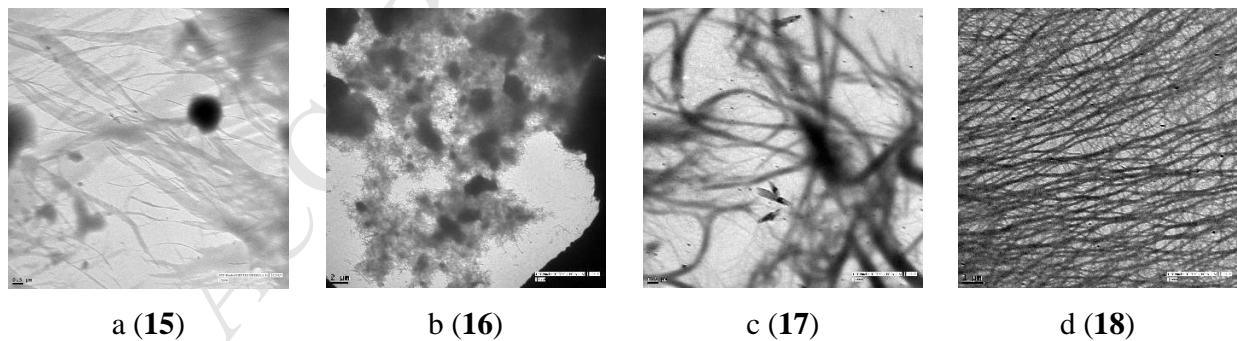
**Scheme 1.** Synthesis of triazole-linked carbohydrate derivatives



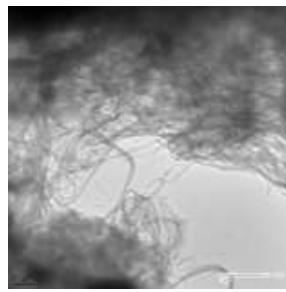
**Figure 1.** Structures of various clickable azides synthesized under conventional conditions



**Figure 2.** Structures of various sugar-linked triazole derivatives synthesized by mechanochemical CuAAC reaction



**Figure 3.** Transmission electron micrographs: a. **15**; b. **16**; c. **17** and d. **18** (for sample preparation, moist MeOH-Hex was used for **15** and hexane only for others). For a larger image please see Supplementary Information.



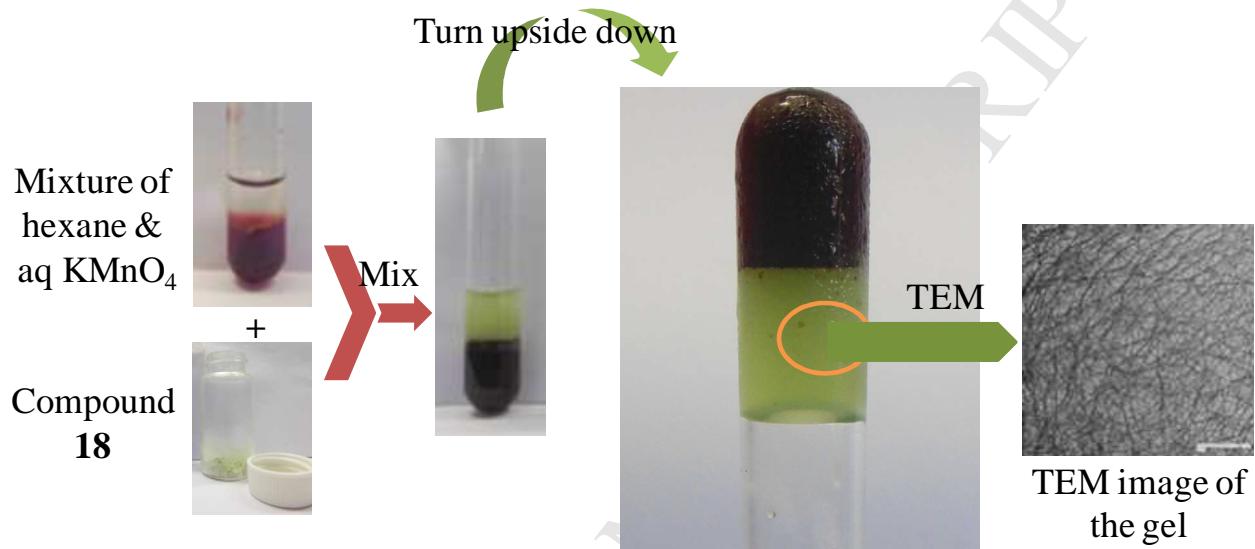
**Figure 4.** Transmission electron micrographs for the gel made by **16** on standing for 3-5 days (For a larger image please see Supplementary Information.)

**Table 1.** Interaction of **18** with various solvents\*

Entry	Solvent	Observation	Hansen's solvent parameters <sup>@</sup>		
			$\delta_d$	$\delta_p$	$\delta_h$
1	Hexane	Quickly absorbs, forms clear thick gel	7.28	0.00	0.00
2	Heptane	Quickly absorbs, forms clear thick gel	7.48	0.00	0.00
3	Octane	Quickly absorbs, forms clear thick gel	7.58	0.00	0.00
4	Octanol	Dissolves; solution, marginally viscous	-- <sup>#</sup>	-- <sup>#</sup>	-- <sup>#</sup>
5	Methanol	Dissolves; does not gel	7.38	6.01	10.90
6	Toluene	Dissolves; does not gel	8.80	0.68	0.98
7	DMSO	Dissolves; does not gel	9.00	8.02	4.99
8	AcOH	Dissolves; does not gel	7.09	3.91	6.60
9	Water	Insoluble	7.63	7.82	20.68
10	Water-Hexane	Absorbs hexane and leaves water at the bottom			

\* 20 mg of **18** was taken up in 2 mL of the respective solvent and the nature of the interaction was noted;

<sup>a</sup>  $\delta_d/\delta_p/\delta_h$  are the dispersion/polar/H-bonding contributions to  $\delta$ , the Hildebrand solubility parameter ( $\text{MPa}^{1/2}$ ); <sup>b</sup> values for octanol were not available but the respective values reported for decanol are: 8.60, 1.32 and 4.89, respectively.<sup>83</sup>



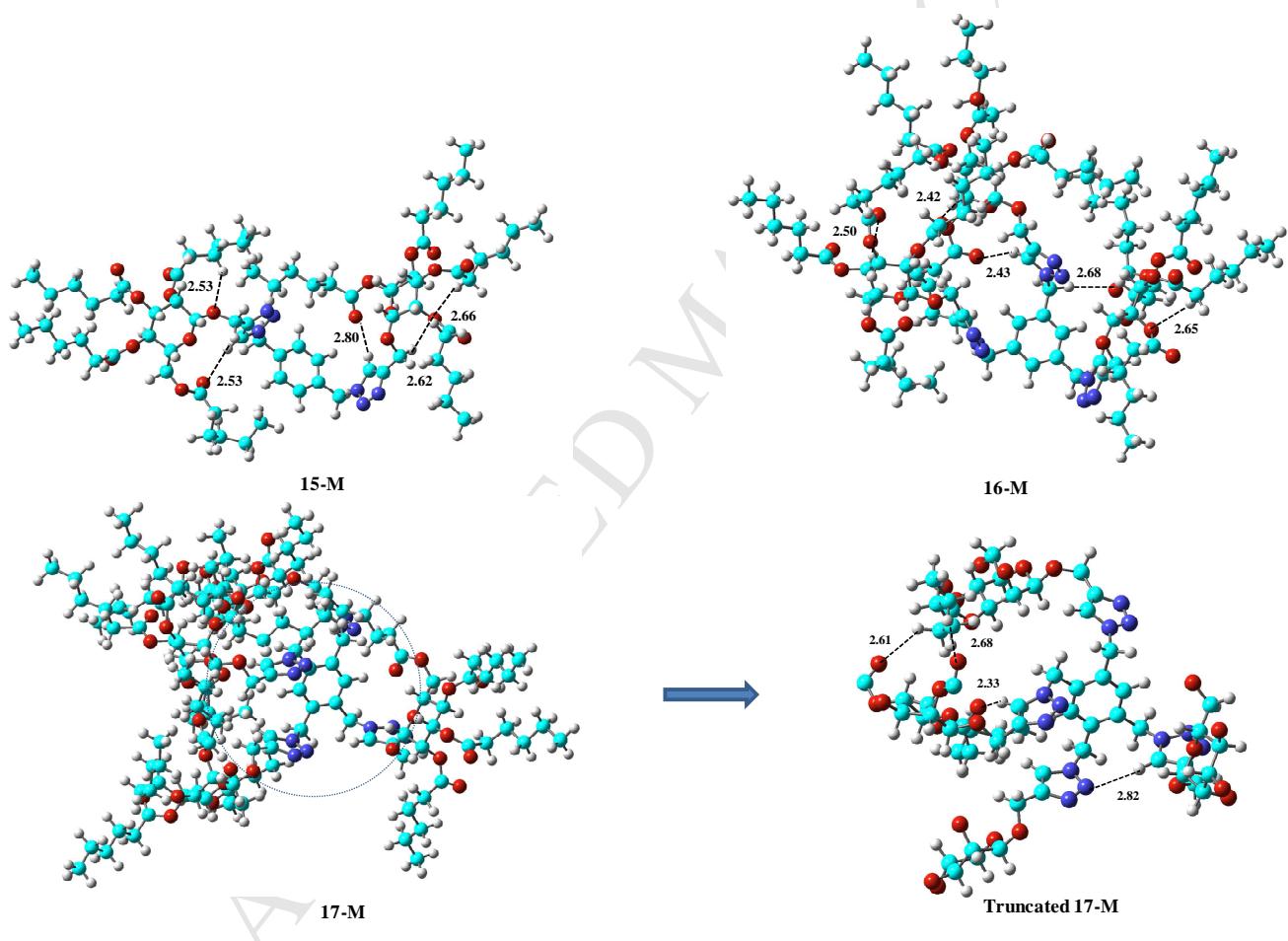
**Figure 5.** Demonstration of the application of compound **18** as a phase-selective gelator: The compound absorbs hexane selectively from the bi-phasic mixture and generates a gel that can hold the aq permanganate solution over it.

**Table 2.** Antibacterial activity of triazole-linked compounds

Compound	Bacterial strain		
	<i>Micrococcus luteus</i>	<i>Staphylococcus aureus</i>	<i>Bacillus subtilis</i>
	MTCC-2470 (MIC, $\mu\text{g}/\text{ml}$ )	MTCC-96 (MIC, $\mu\text{g}/\text{ml}$ )	MTCC-121 (MIC, $\mu\text{g}/\text{ml}$ )
<b>4</b>	1000	125	250

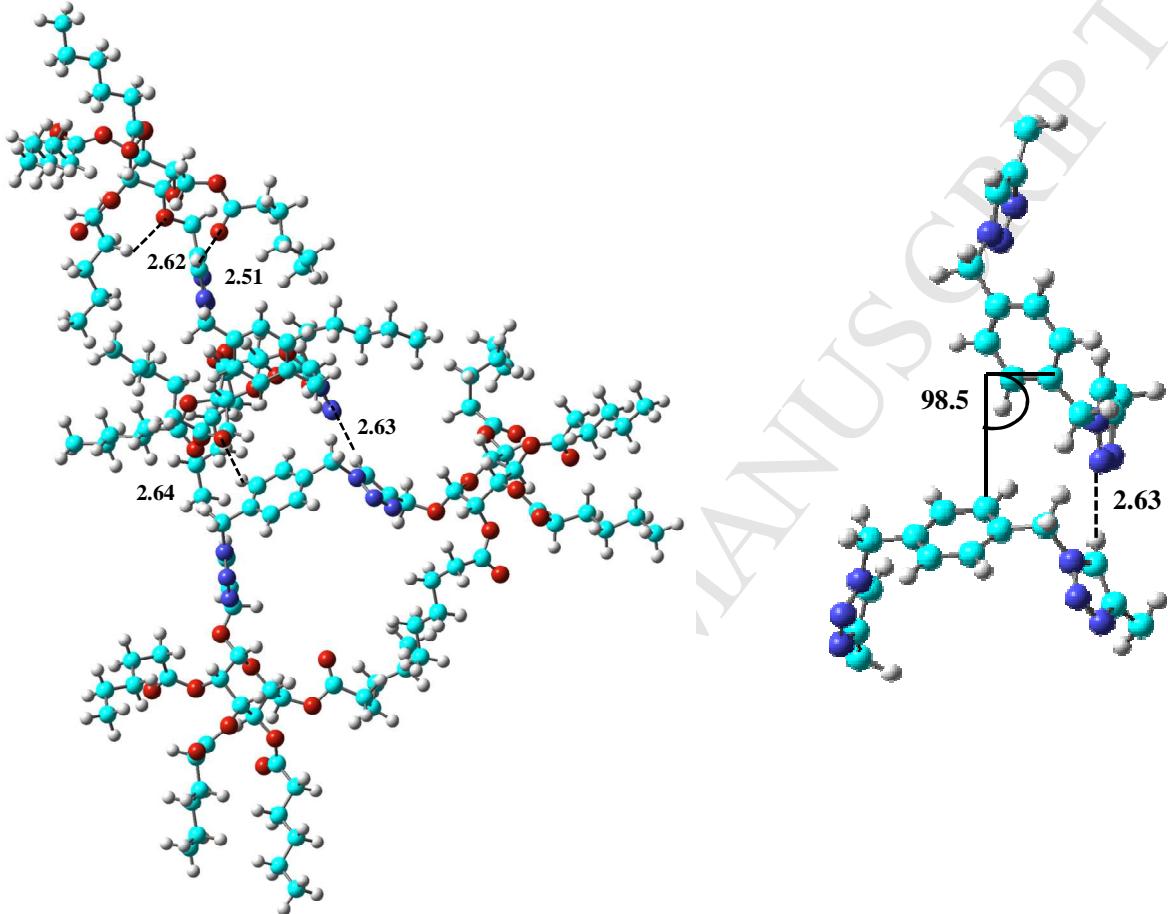
	<b>16</b>	250	500	500
<b>18</b>		1000	NAA	NAA
<b>19</b>		NAA	NAA	1000
Ampicillin		16	32	4
Amoxicillin		4	16	2

Test compounds: 1000 ( $\mu\text{g/ml}$ ); NAA: No Antimicrobial Activity; Compounds **13**, **14**, **15**, **17** and **20** were not active.

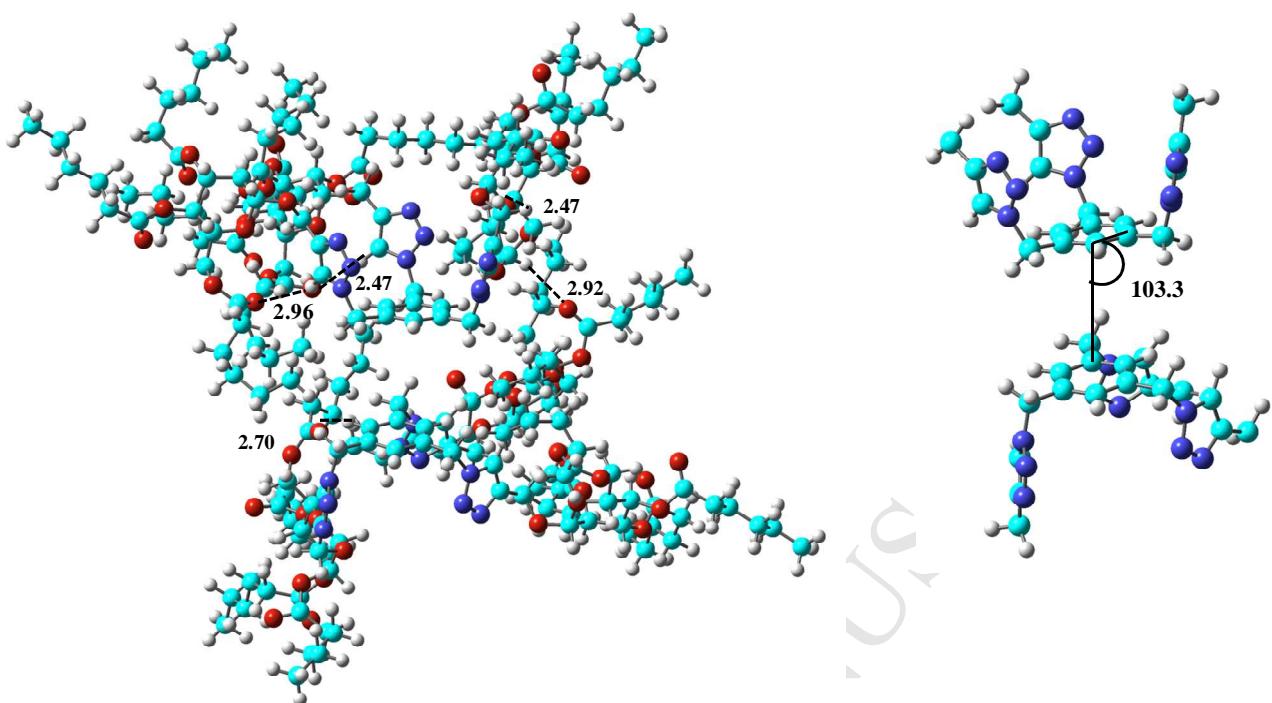


**Figure 6.** The optimized 3D geometries of monomeric structures of **15** (**15-M**) and **16** (**16-M**), showing characteristic intramolecular and intermolecular hydrogen bonding interactions. Owing to the difficulty in

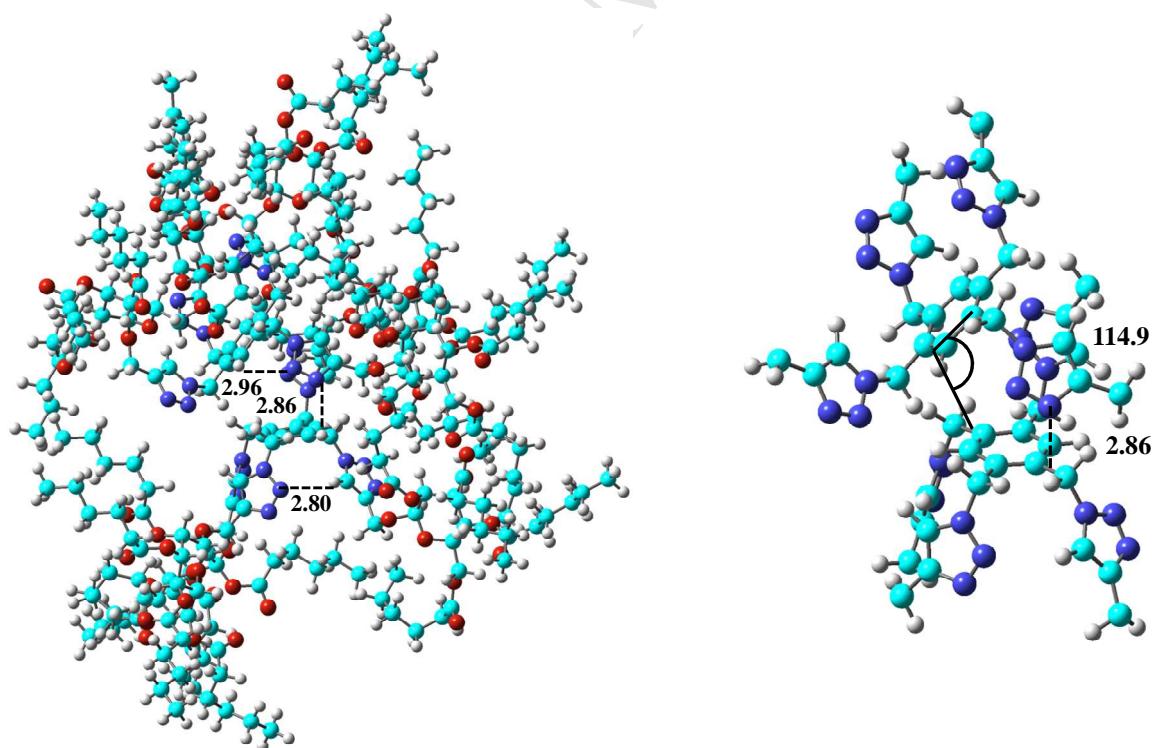
pointing out interactions in **17** (**17-M**), markings have been made on its truncated structure shown. All the bond distances are given in Å units.



**Figure 7a.** The optimized 3D geometries of dimeric structures of **15** (i. e. **15-D**) (showing the characteristic alignment of the two central benzene rings and the interactions in them. All the bond distances are given in Å units. Bond angles are given in degrees (°).



**Figure 7b.** The optimized 3D geometries of dimeric structures of **16** (i. e. **16-D**)



**Figure 7c.** The optimized 3D geometries of dimeric structures of **17** (i. e. **17-D**)

**Table 3.** The absolute and stabilization energies of glucopyranosides **15-M**, **16-M**, **17-M**, **15-D**, **16-D** and **17-D** calculated using the PM3 method

Entry	Compound	Absolute Energy (kcal/mol)	Formulae	Dimerization Energy <sup>*</sup>
				(kcal/mol)
1	<b>15-M</b>	-1.313319	-	-
2	<b>16-M</b>	-1.996846	-	-
3	<b>17-M</b>	-2.667027	-	-
4	<b>15-D</b>	-2.626648	$E_{11-D} - 2E_{11-M}$	0.00
5	<b>16-D</b>	-4.018538	$E_{12-D} - 2E_{12-M}$	-15.59
6	<b>17-D</b>	-5.345318	$E_{13-D} - 2E_{13-M}$	-7.07

\*Dimerization energy is calculated by subtracting the summation of energies of monomers from the energy of the dimer.

- Lipophilic polyvalent click-glycosides were made by solvent-free mechanochemical reaction.
- They self-assemble in long chain hydrocarbon solvents to form supramolecular structures.
- TEM observations were rationalized computationally by geometry optimisation.
- One compound showed phase-selective gelation ability in a biphasic mixture of hexane and water.
- Some of the compounds were moderately antimicrobial.

**Electronic Supplementary Material****Mechanochemical click reaction as a tool for making carbohydrate-based triazole-linked self-assembling materials (CTSAMs)**

**Mohit Tyagi, Nikhil Taxak, Prasad V. Bharatam, Hemraj Nandanwar, K. P. Ravindranathan Kartha\***

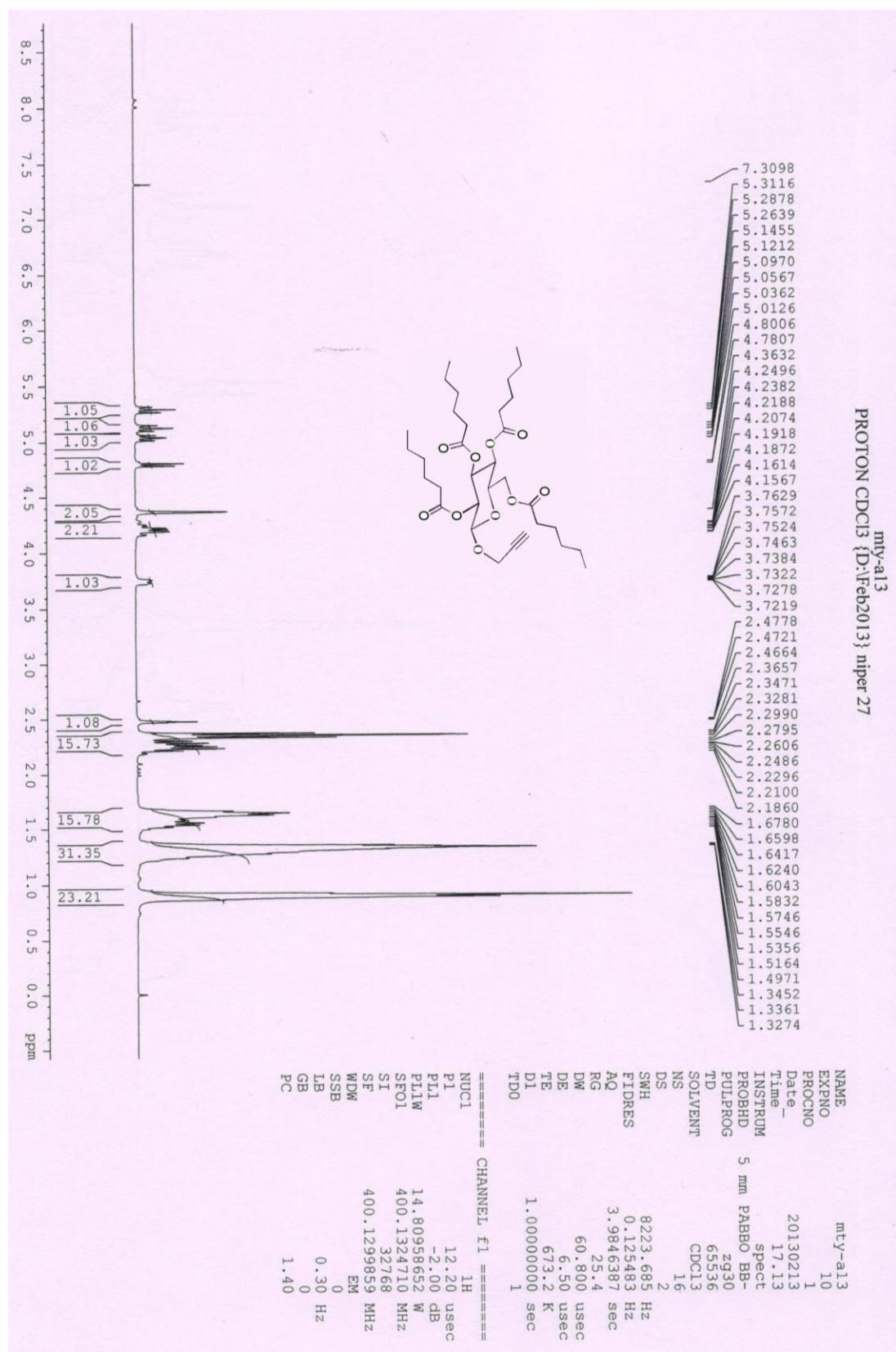
Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, SAS Nagar, Punjab 160062, India

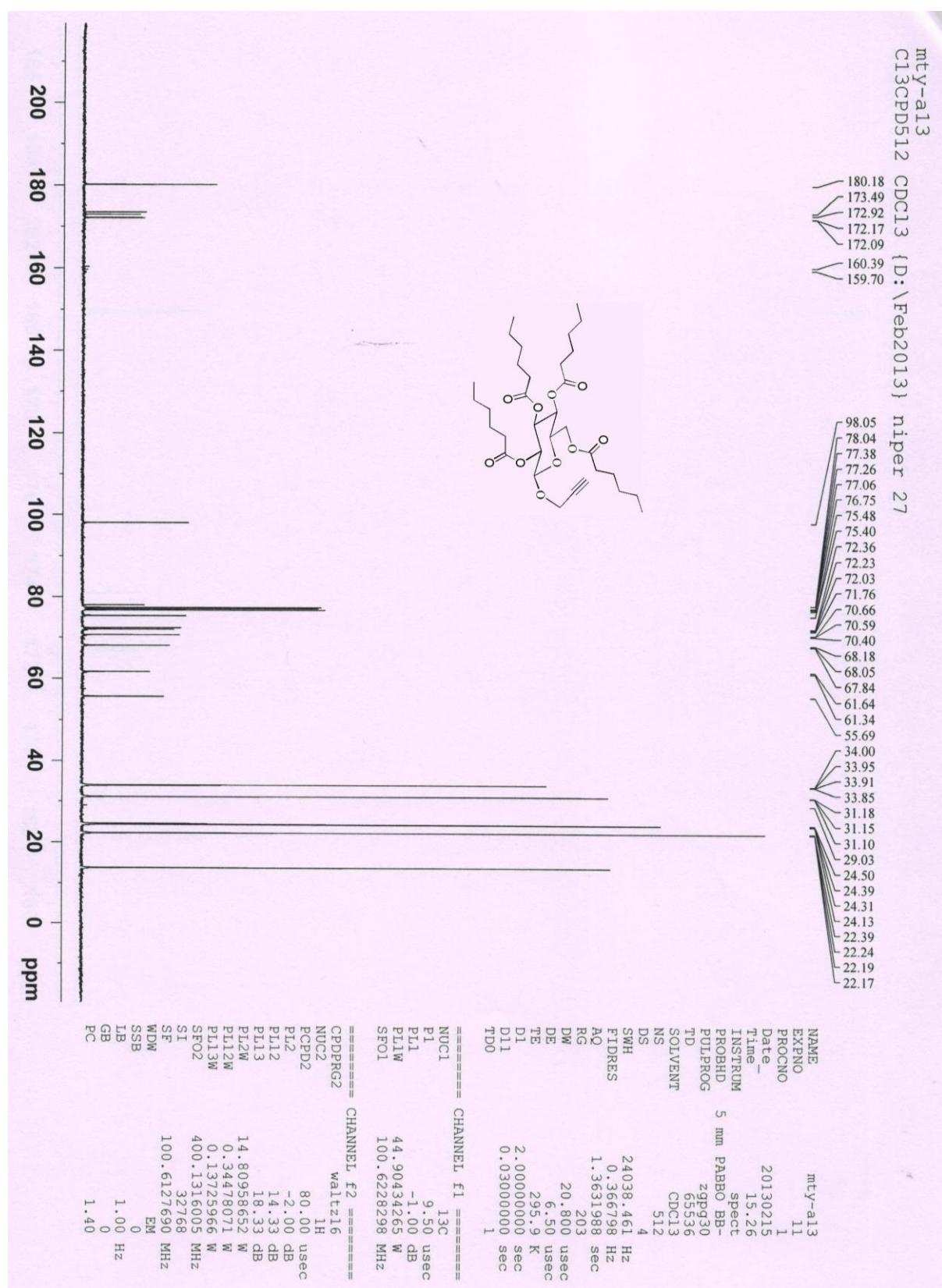
\*E-mail: rkartha@niper.ac.in

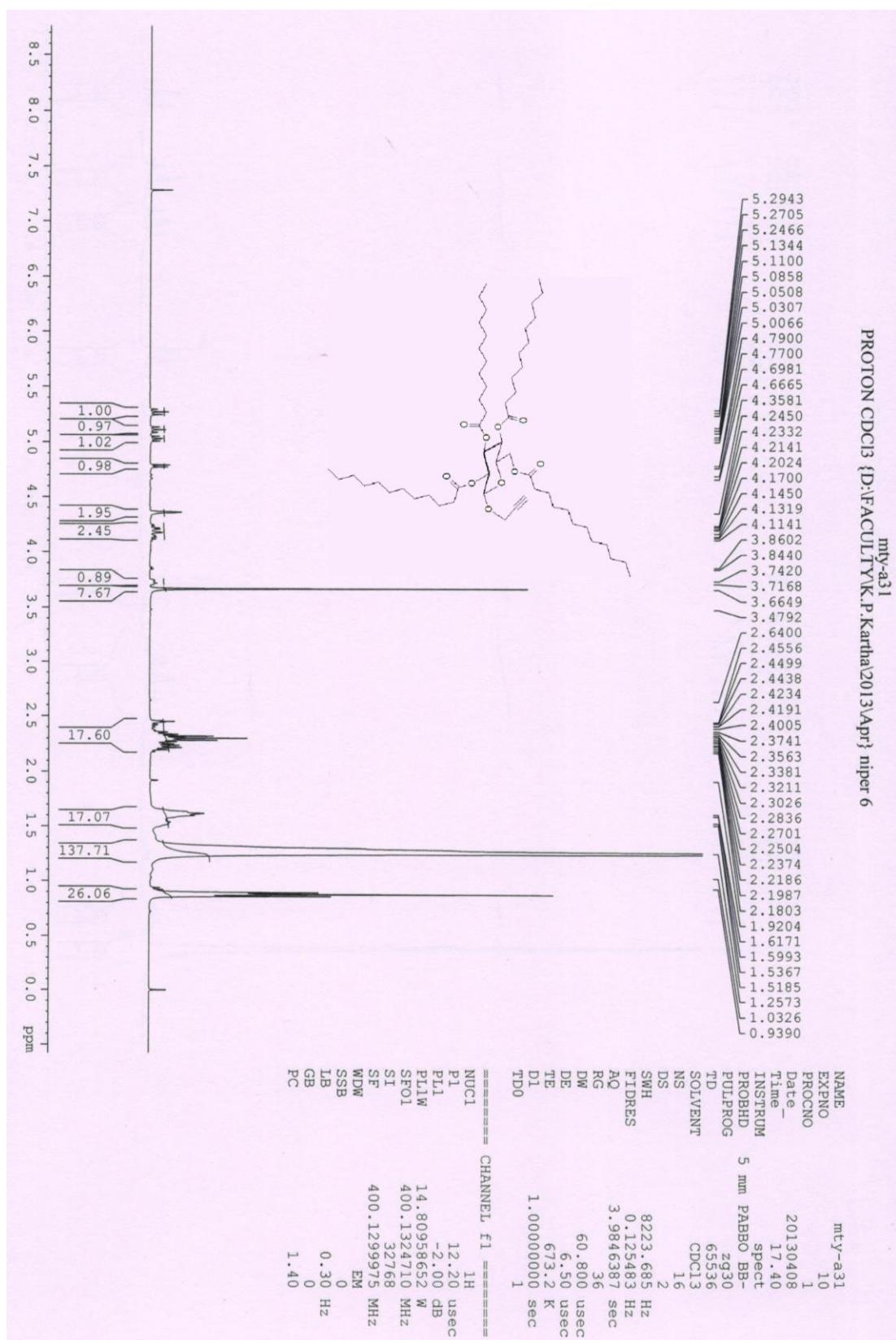
<i>Table of Contents</i>	Page
1. <sup>1</sup> H and <sup>13</sup> C NMR spectra	2
2. TEM images for compounds <b>15, 16, 17</b> and <b>18</b>	30
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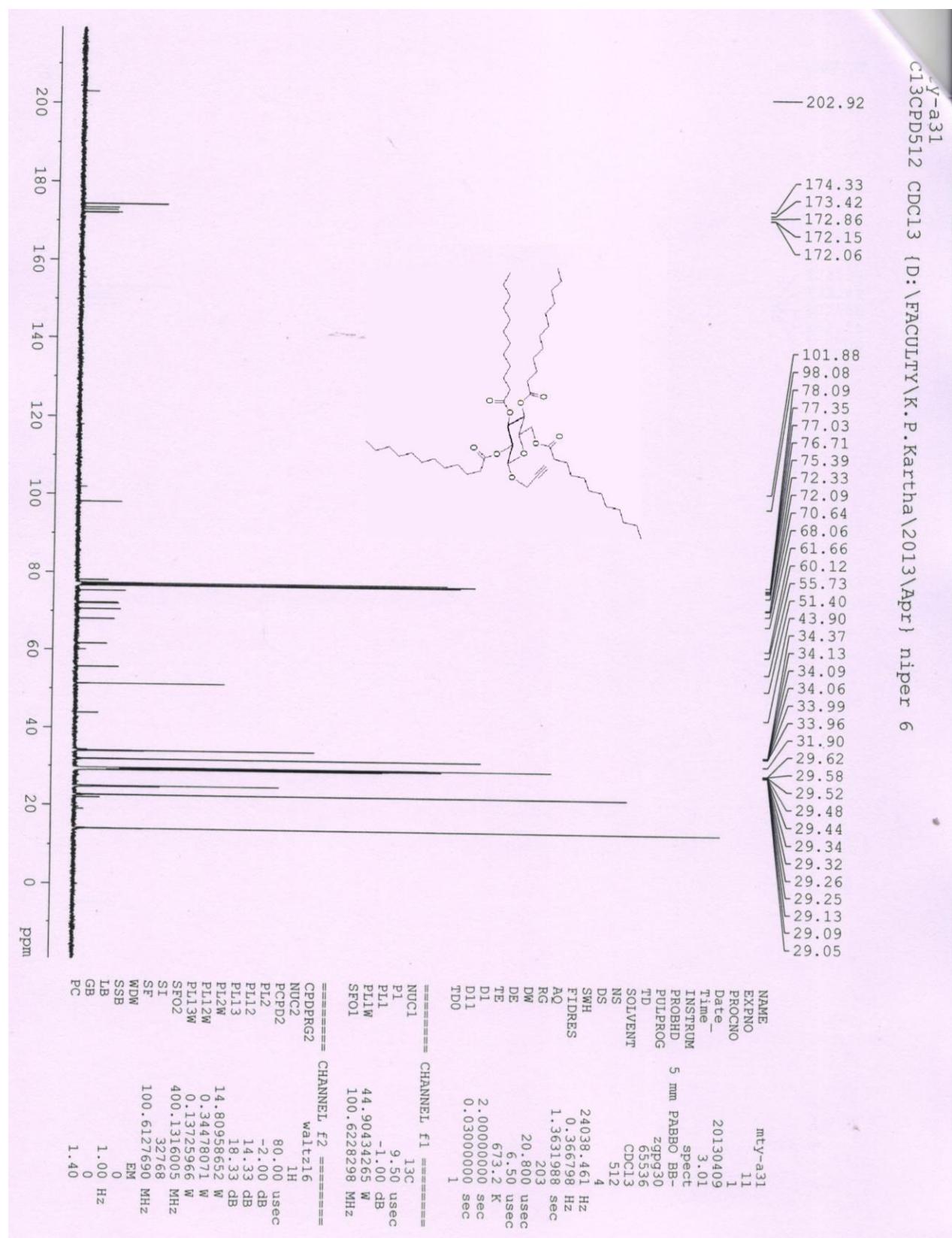
## 1. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra

### $^1\text{H}$ NMR spectrum of Propargyl 2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranoside (1)

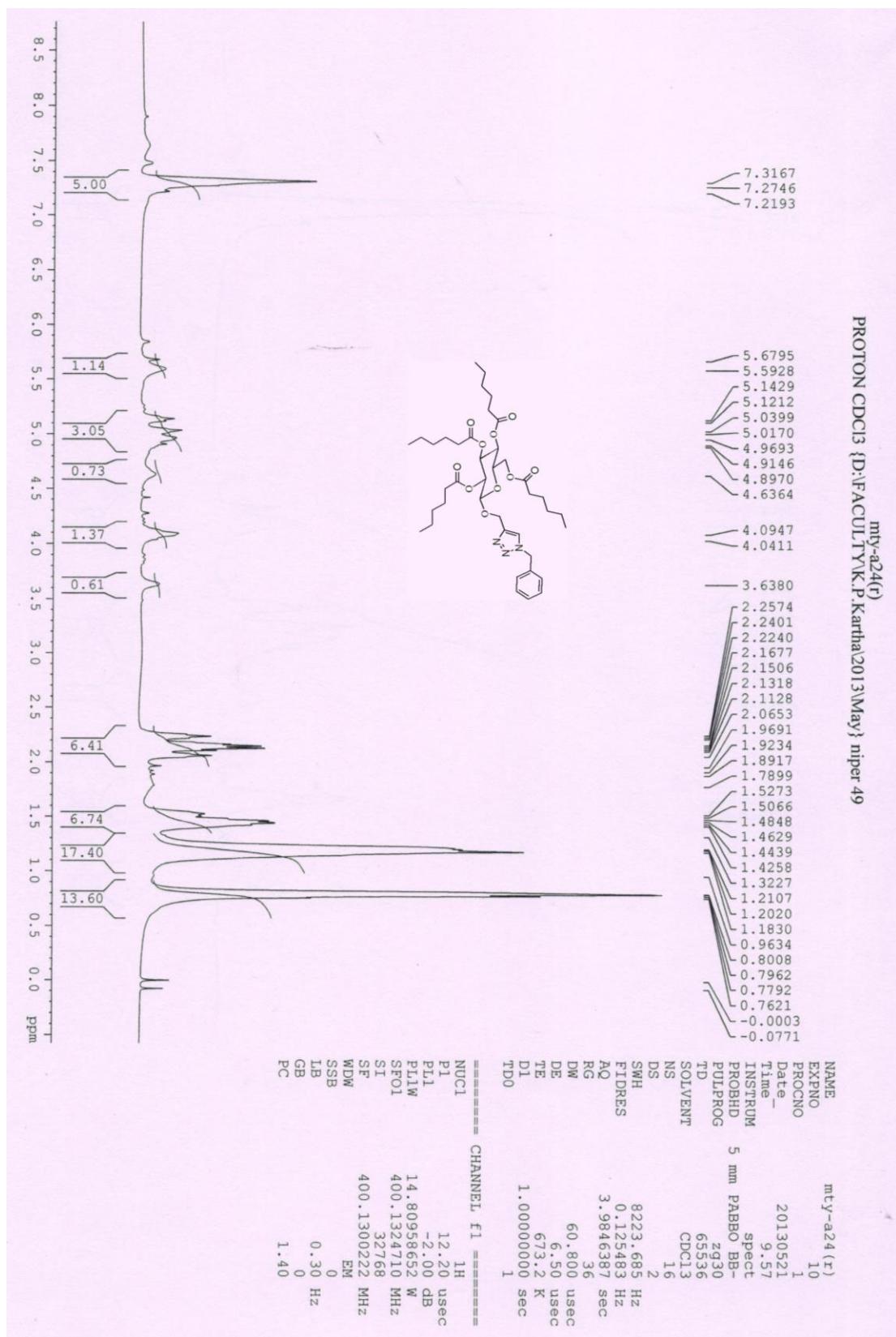


<sup>13</sup>C NMR spectrum of Propargyl 2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranoside (1)

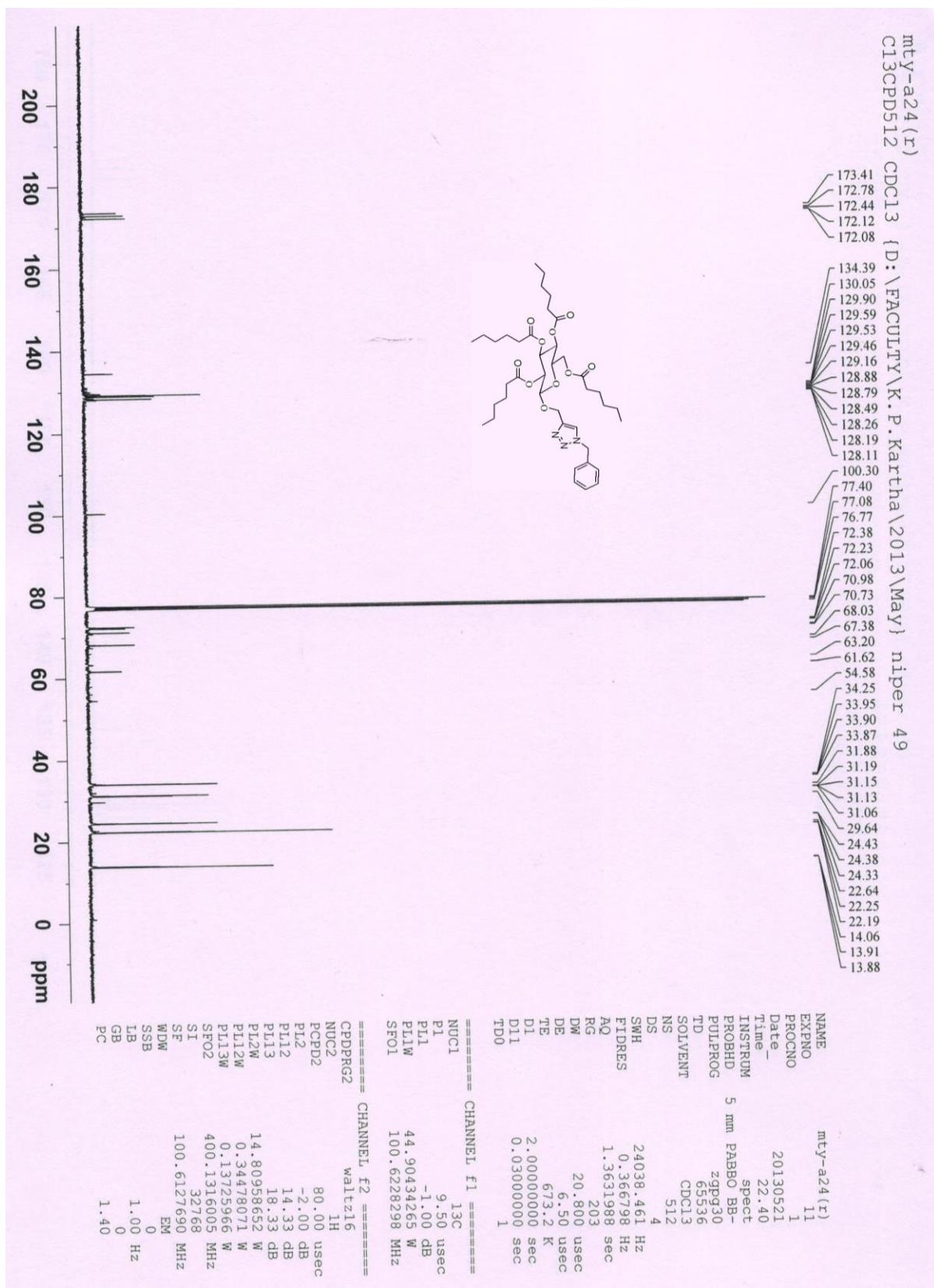
<sup>1</sup>H NMR spectrum of Propargyl 2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranoside (2)

**<sup>13</sup>C NMR spectrum of Propargyl 2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranoside (2)**

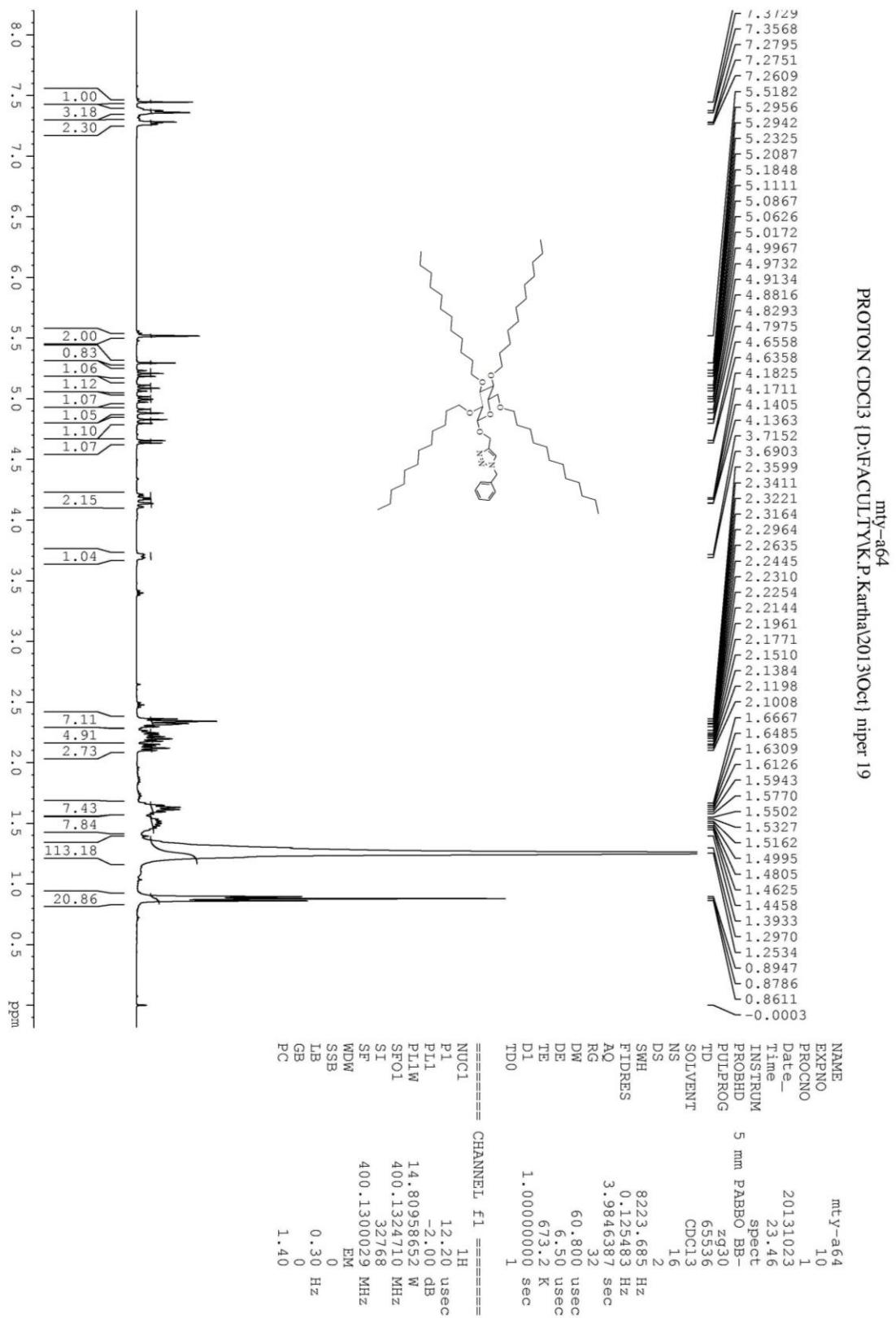
**<sup>1</sup>H NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (4)**



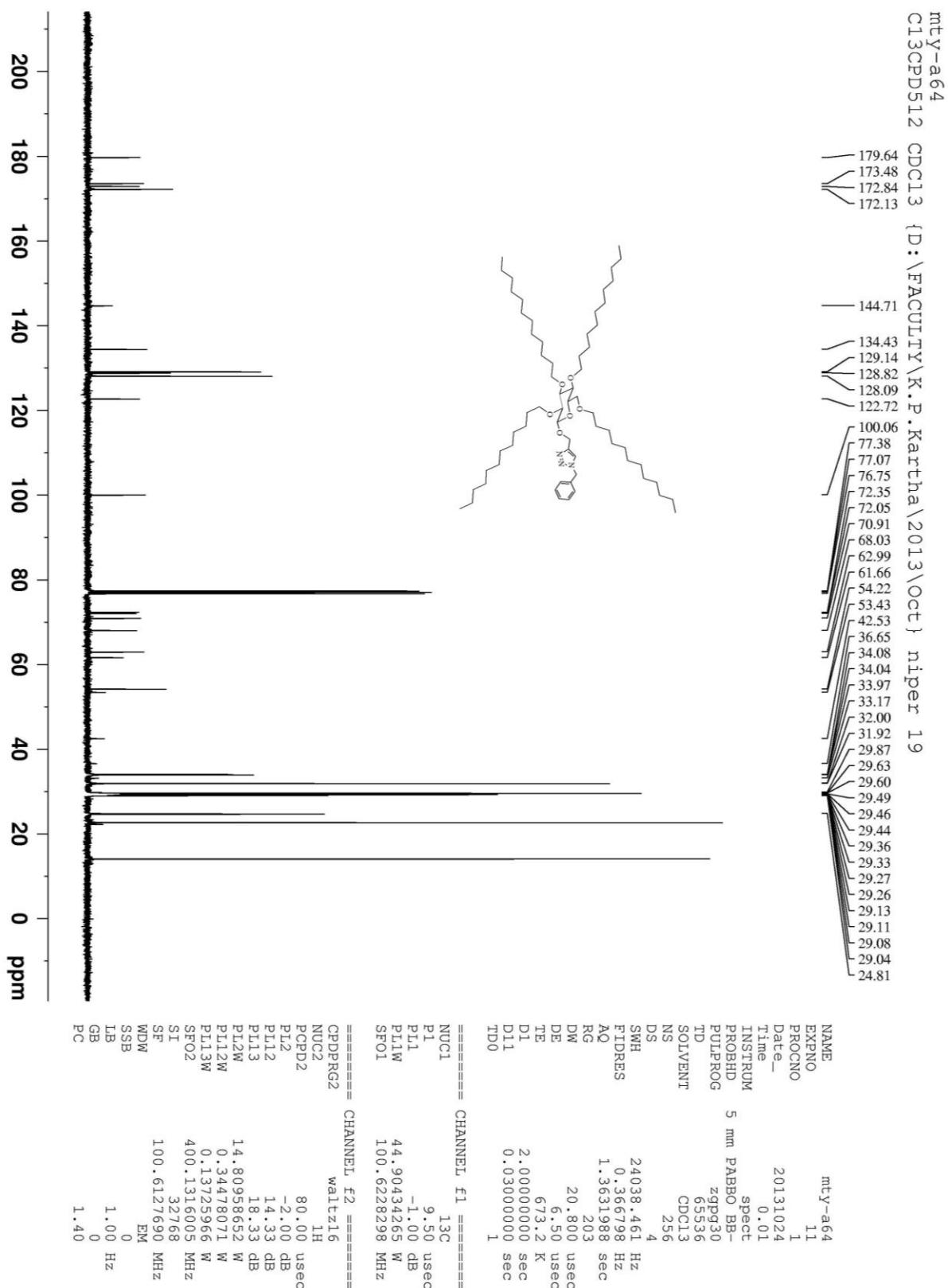
<sup>13</sup>C NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazole (4)



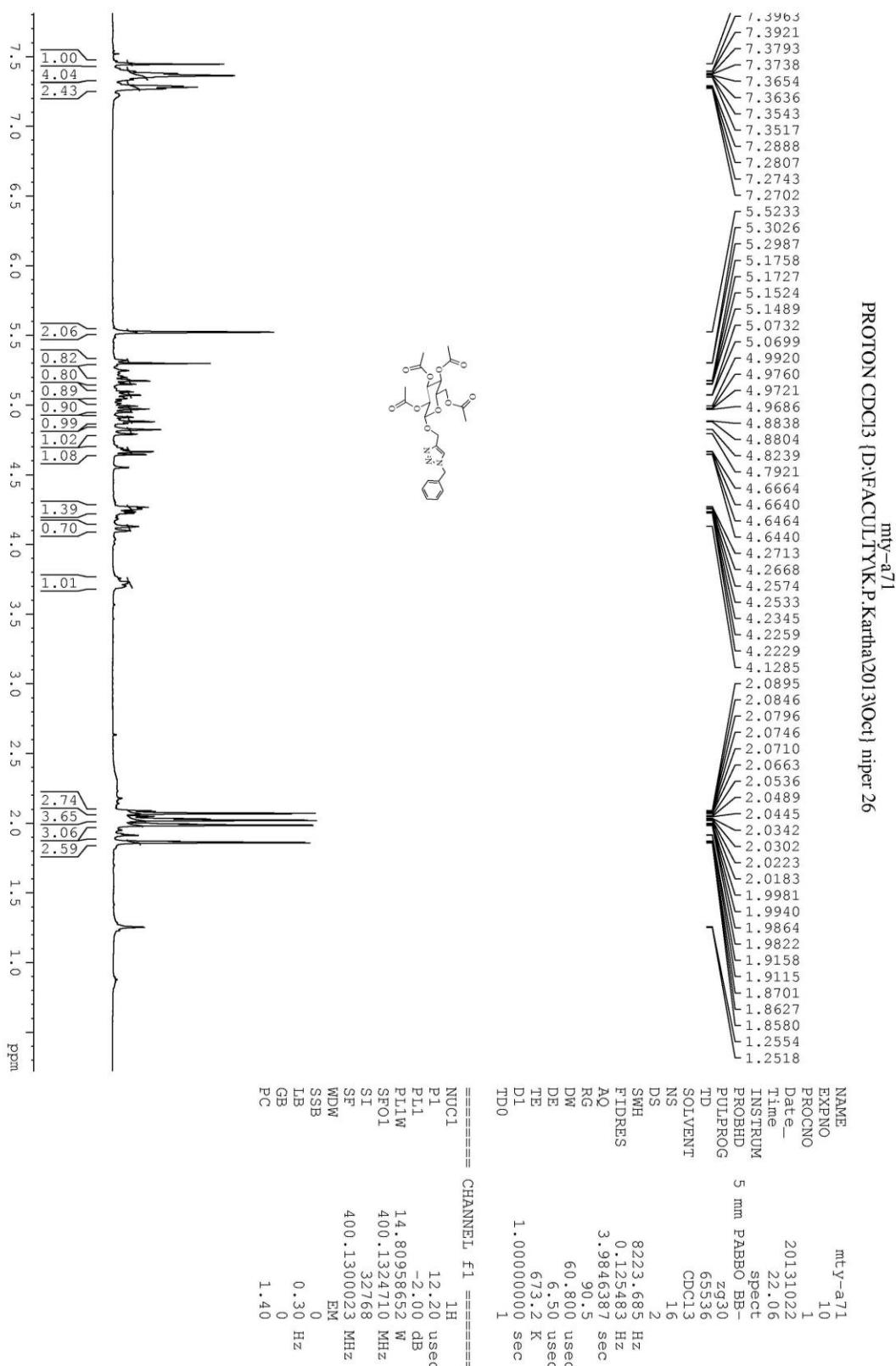
**<sup>1</sup>H NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (5)**



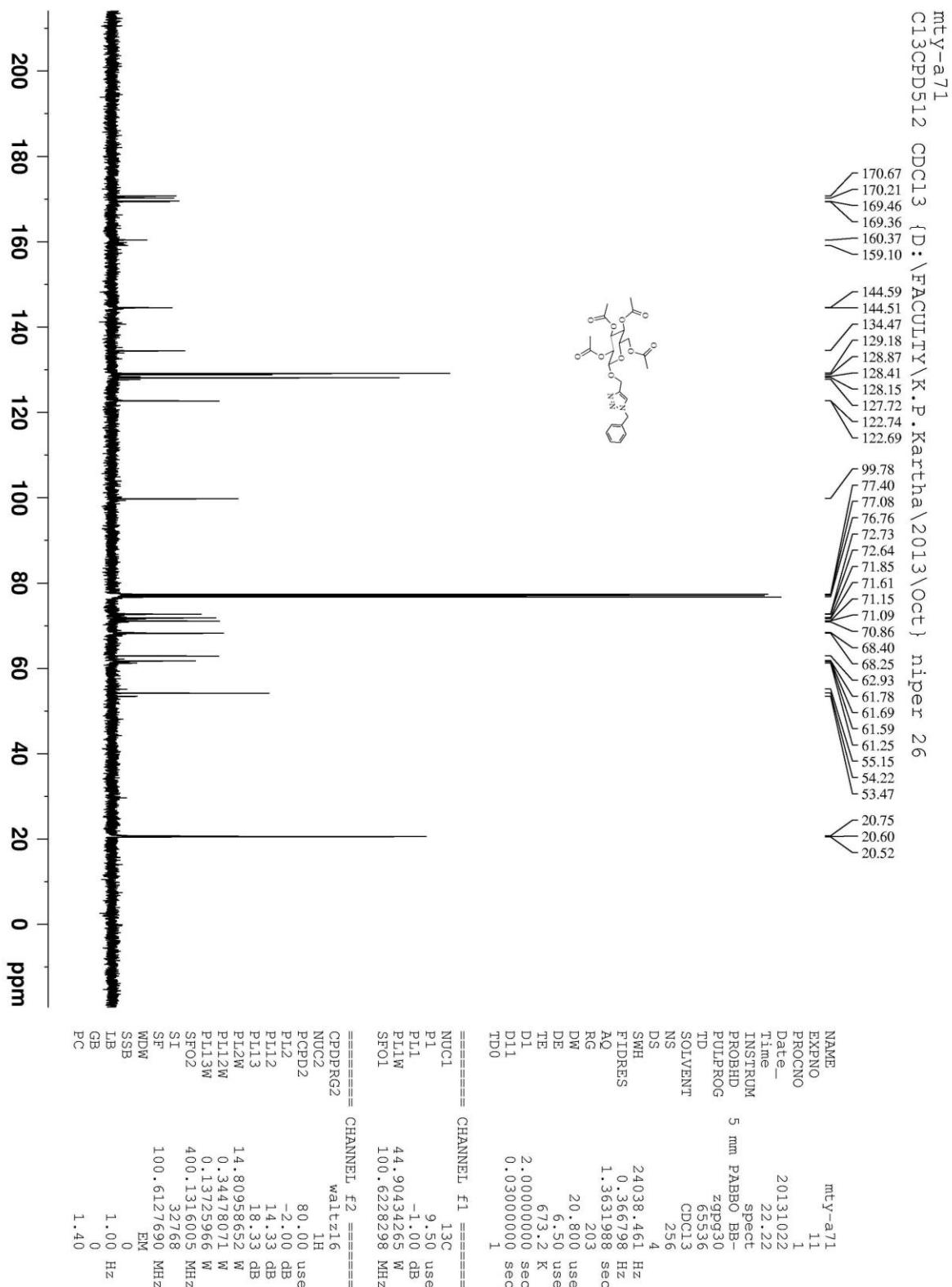
<sup>13</sup>C NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazole (5)

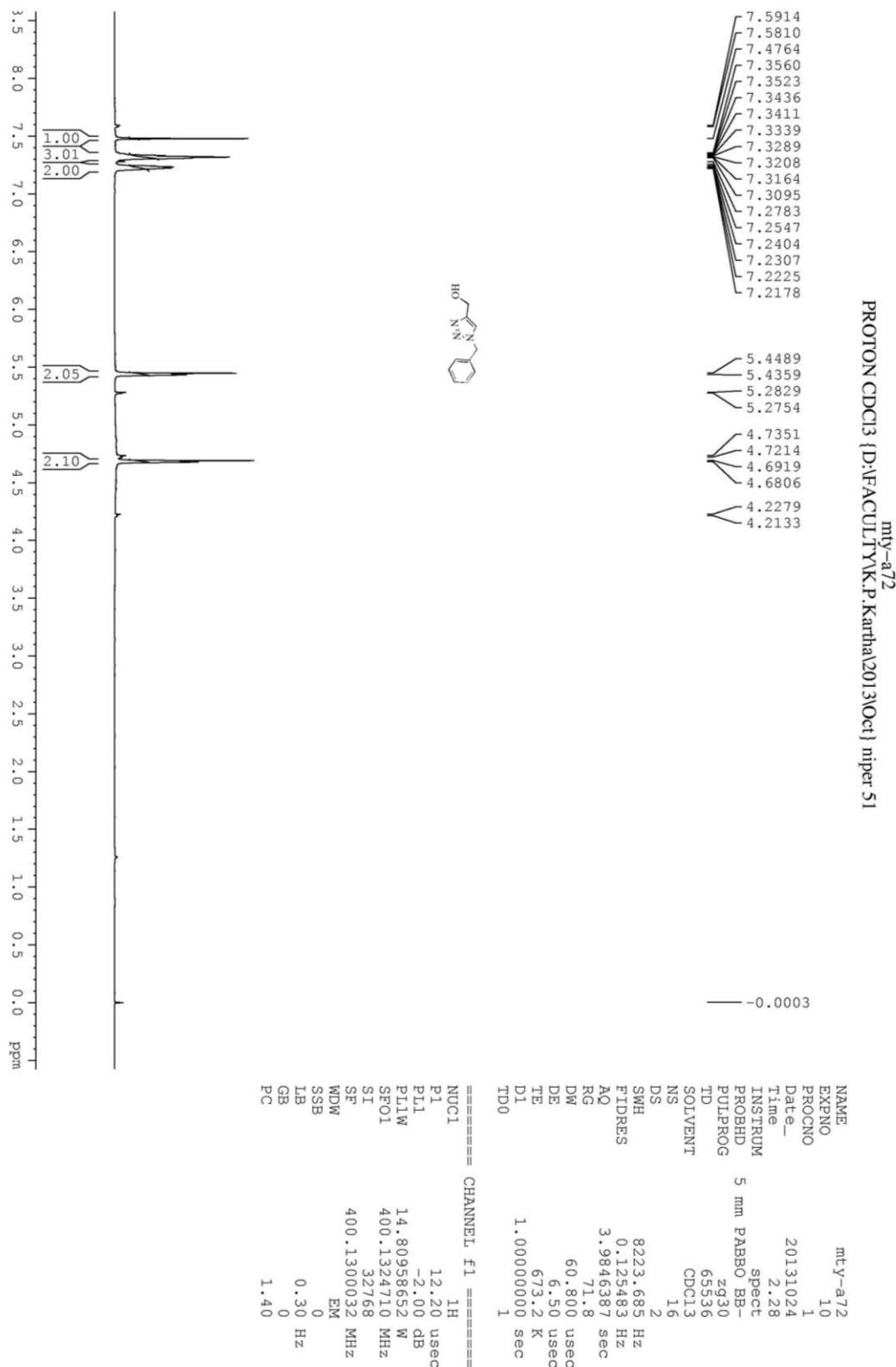


**<sup>1</sup>H NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-acetyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (6)**

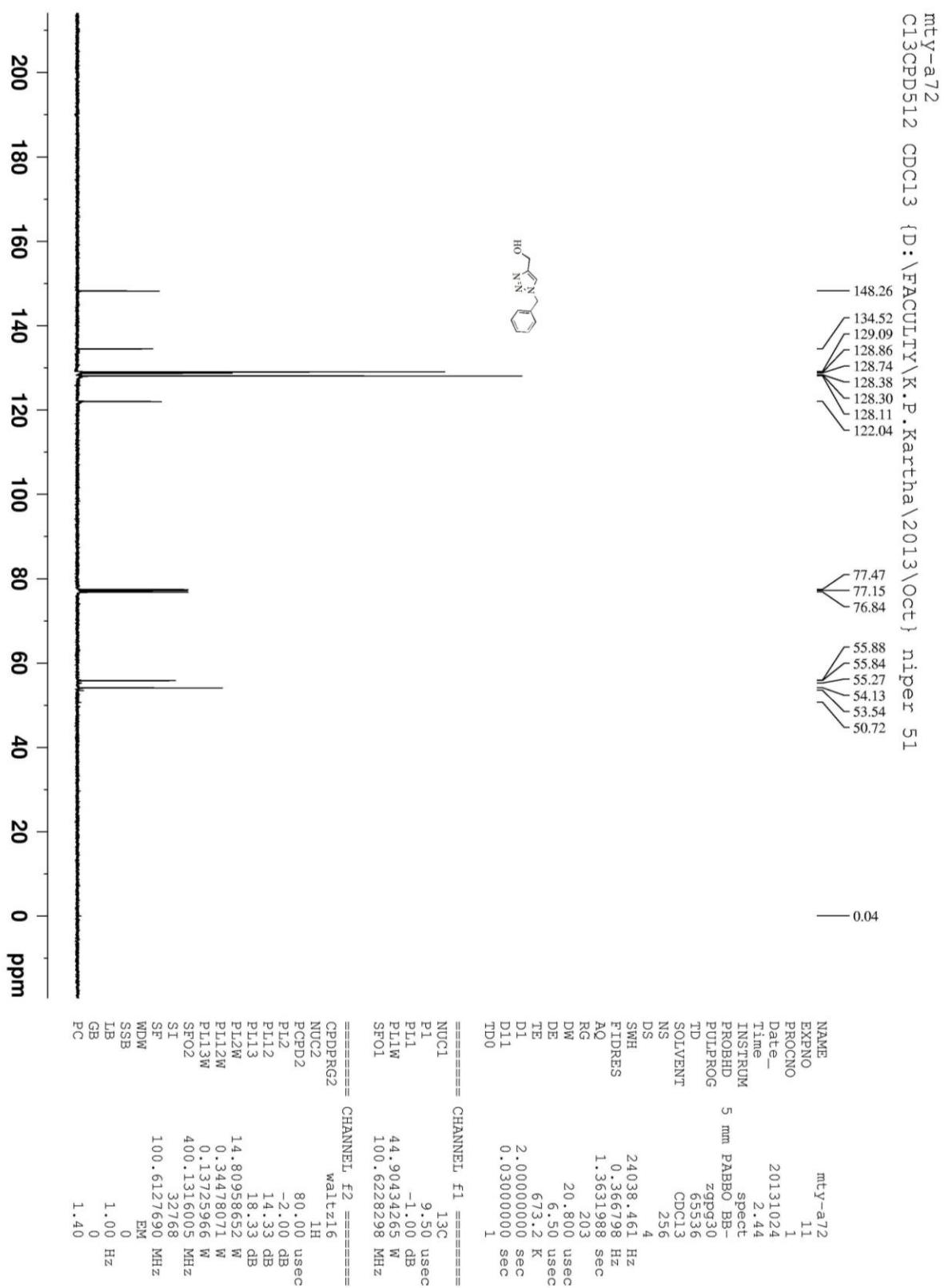


**<sup>13</sup>C NMR spectrum of 1-Benzyl-4-(2,3,4,6-tetra-O-acetyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazole (6)**

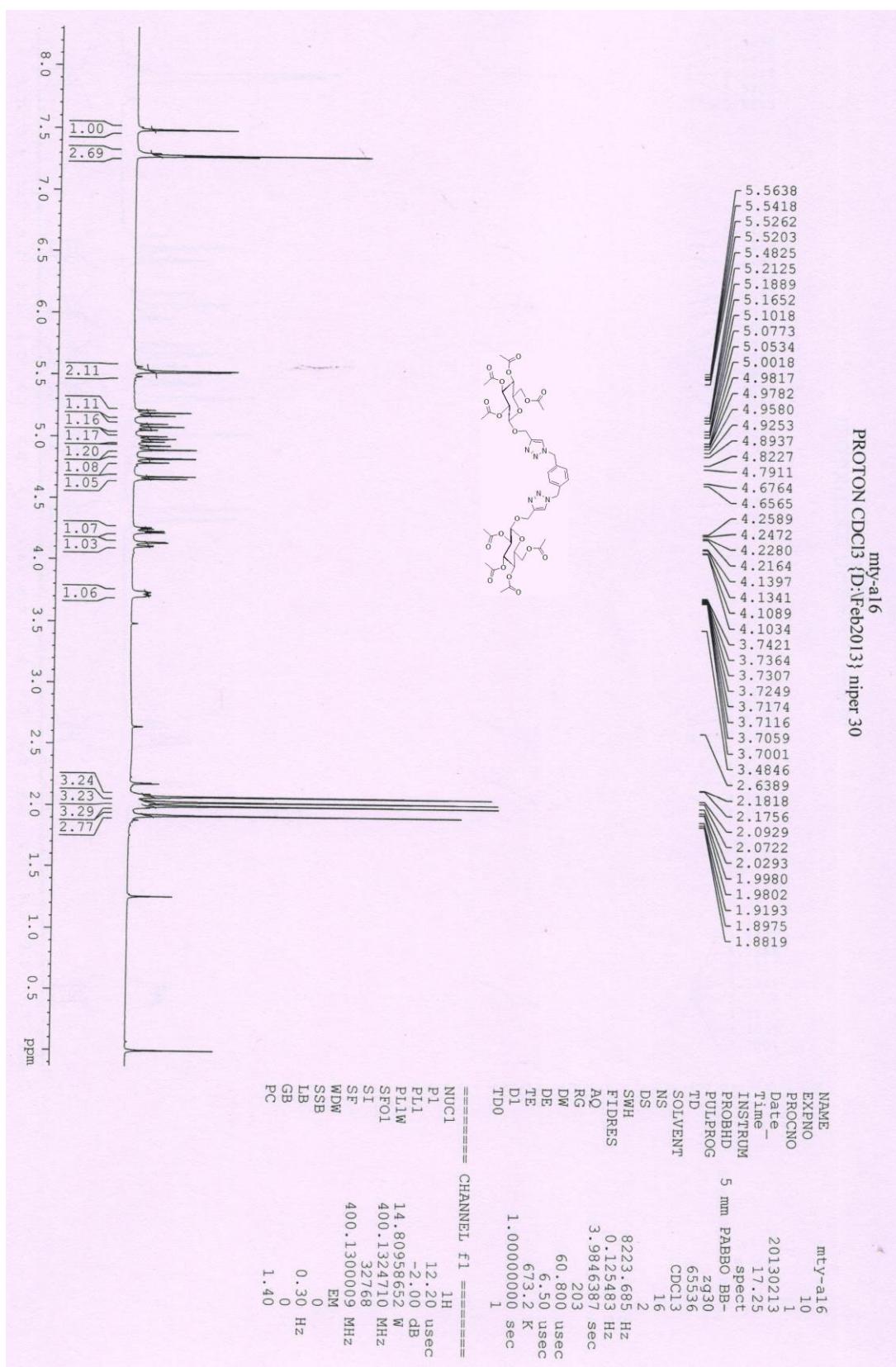


**<sup>1</sup>H NMR spectrum of 1-Benzyl-4-(hydroxymethyl)-1*H*-1,2,3-triazole (7)**

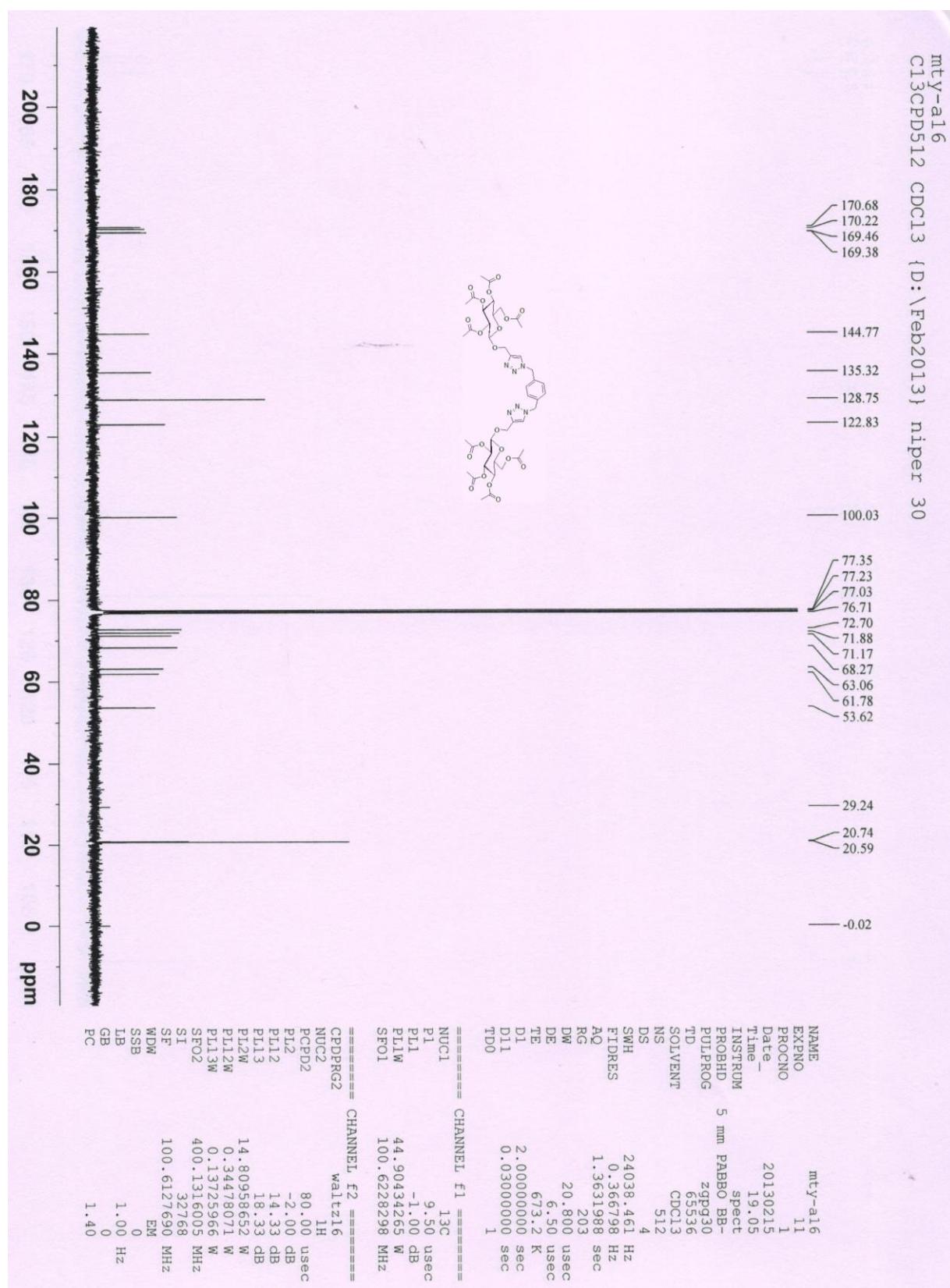
<sup>13</sup>C NMR spectrum of 1-Benzyl-4-(hydroxymethyl)-1*H*-1,2,3-triazole (7)



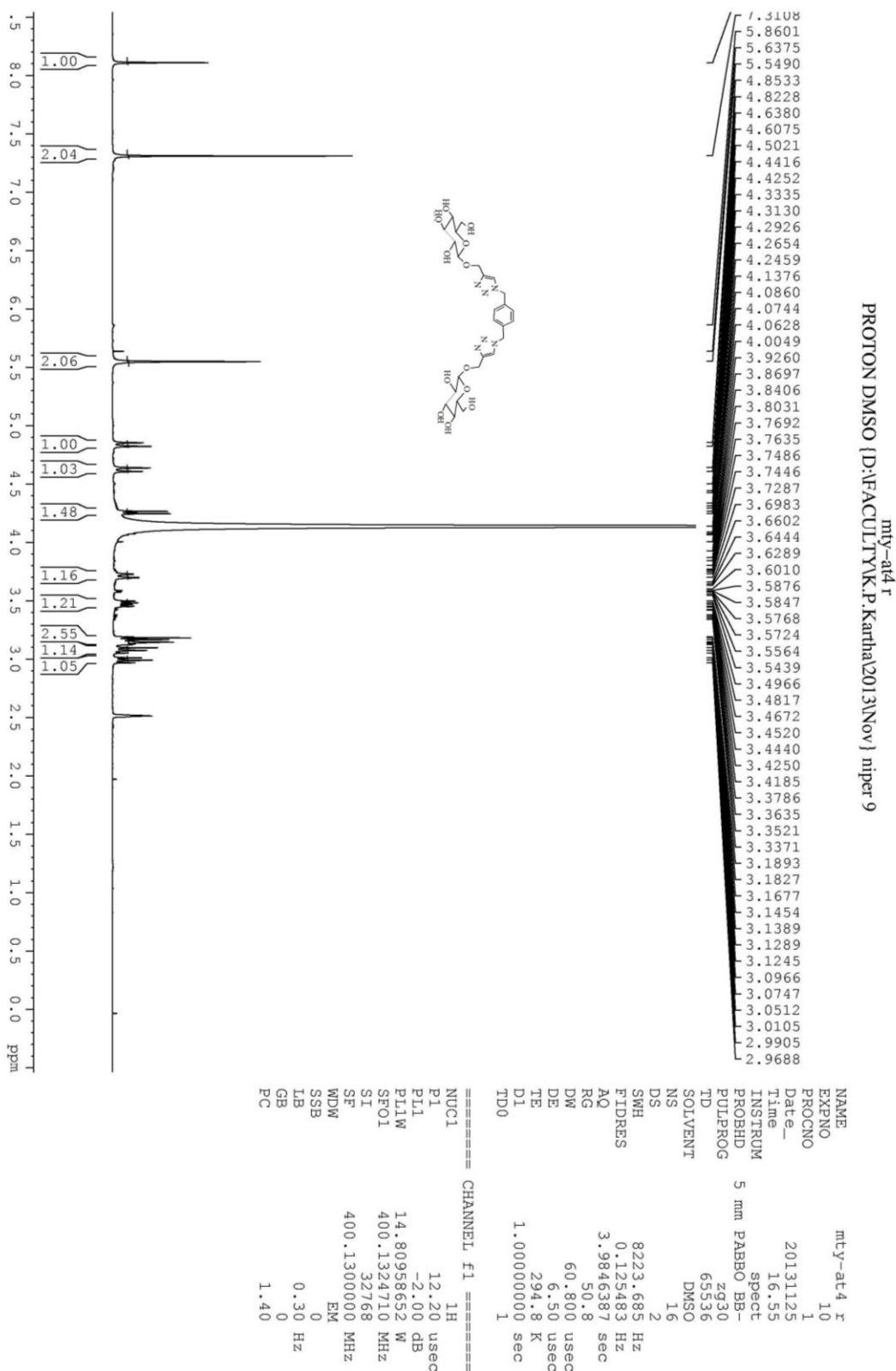
**<sup>1</sup>H NMR spectrum of 1,4-Bis[(4-(2,3,4,6-tetra-O-acetyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (13)**



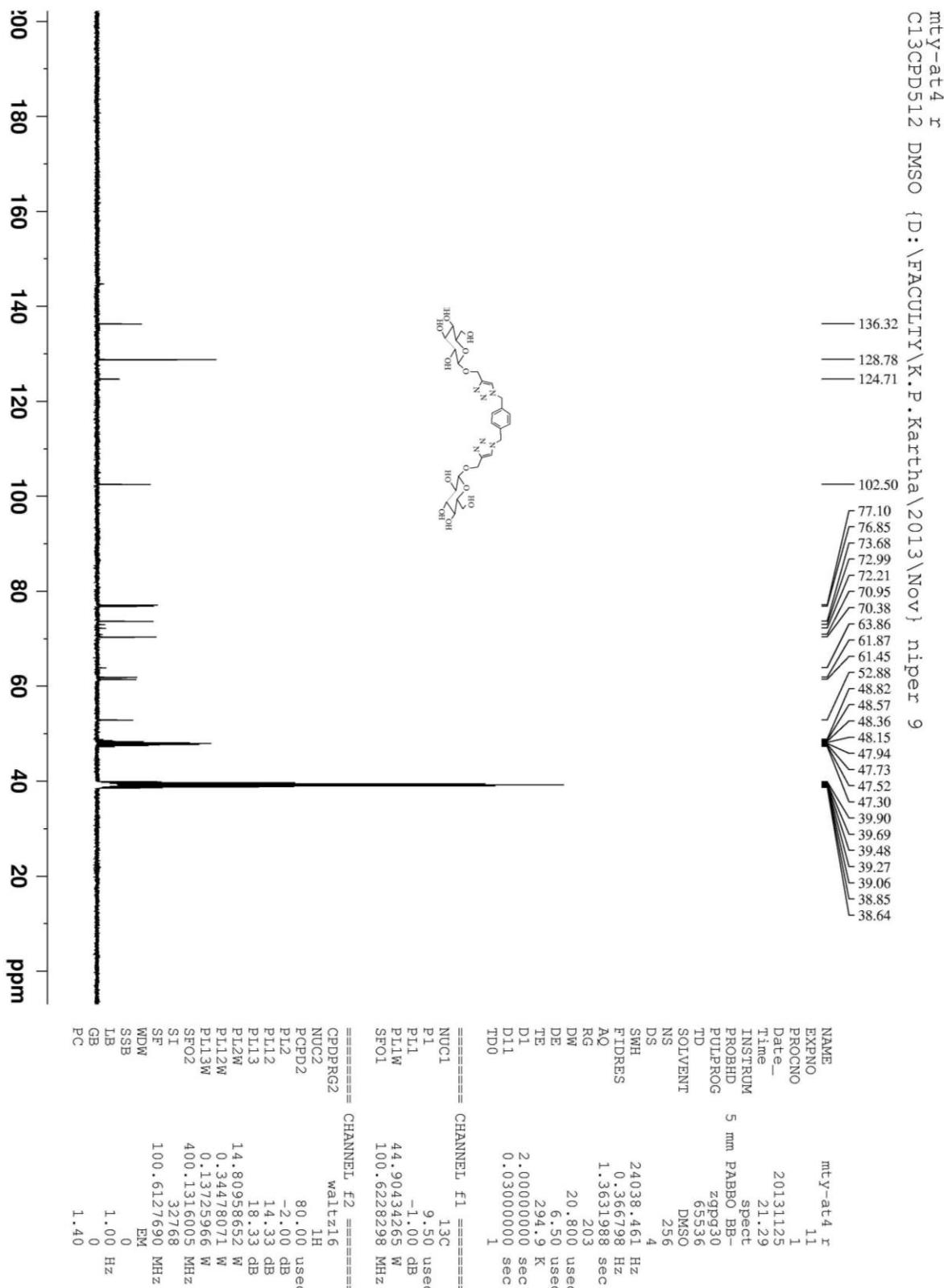
**<sup>13</sup>C NMR spectrum of 1,4-Bis[(4-(2,3,4,6-tetra-O-acetyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (13)**



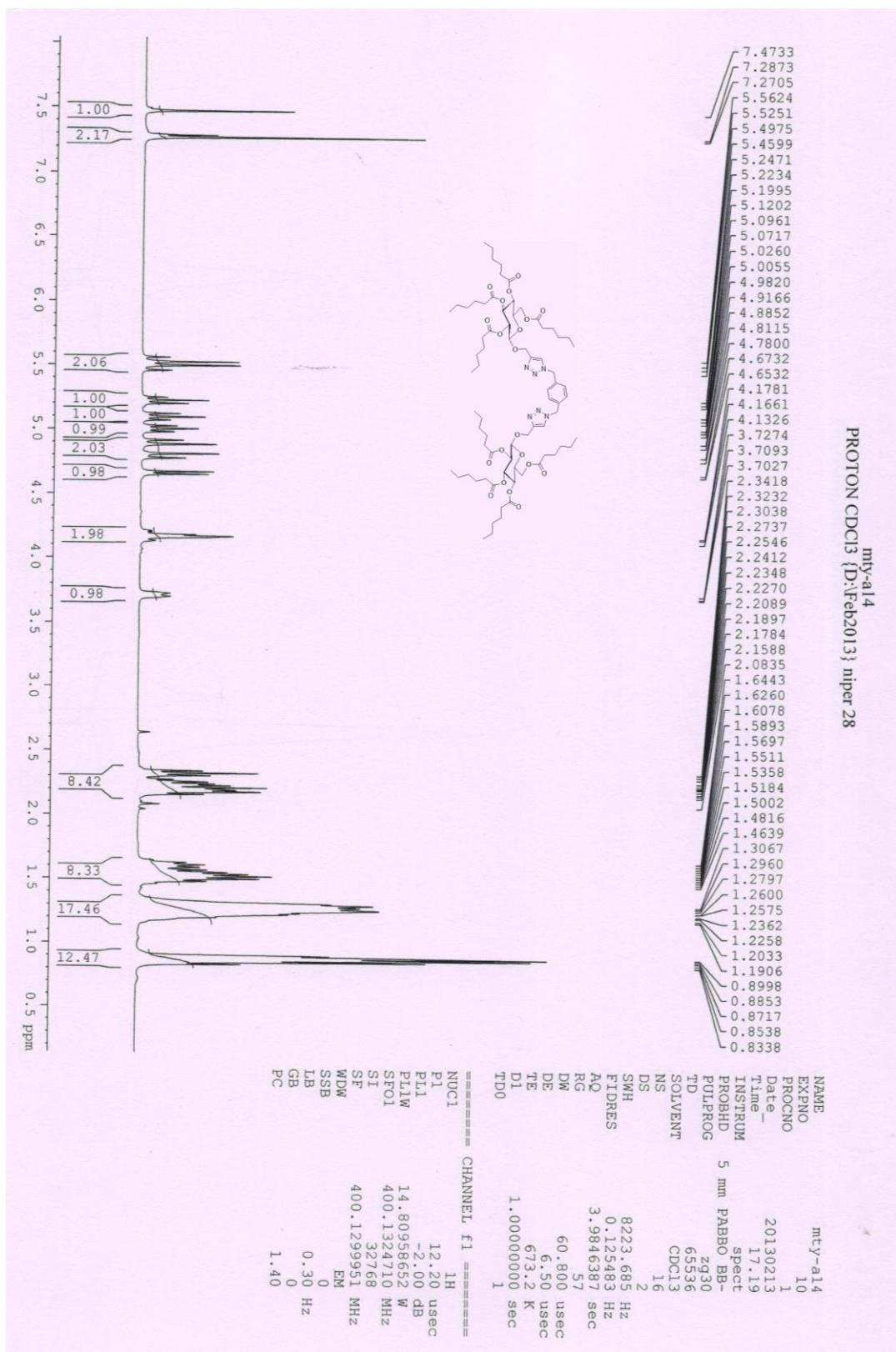
**<sup>1</sup>H NMR spectrum of 1,4-Bis[(4-( $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (14)**



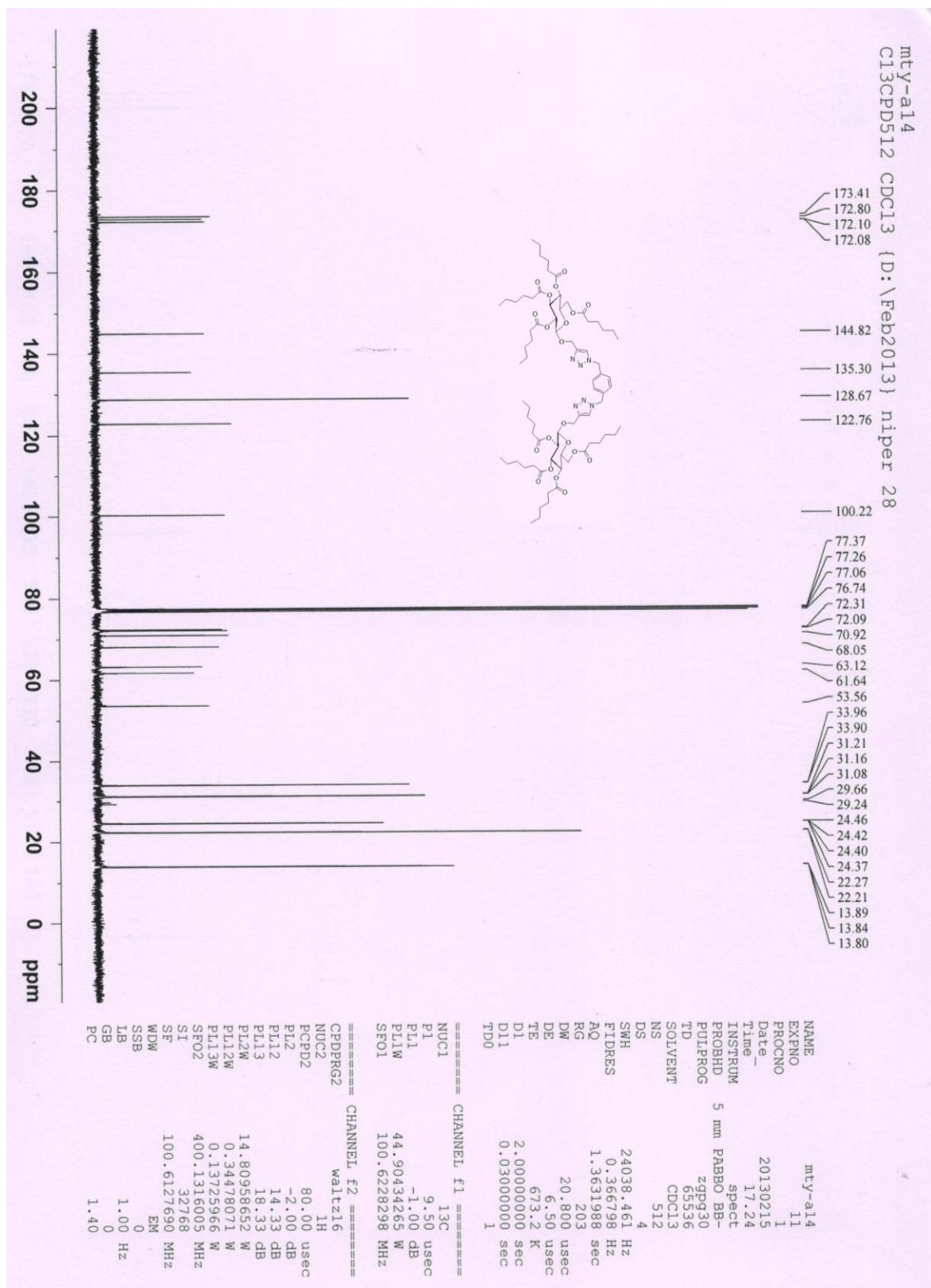
<sup>13</sup>C NMR spectrum of 1,4-Bis[(4-( $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (14)



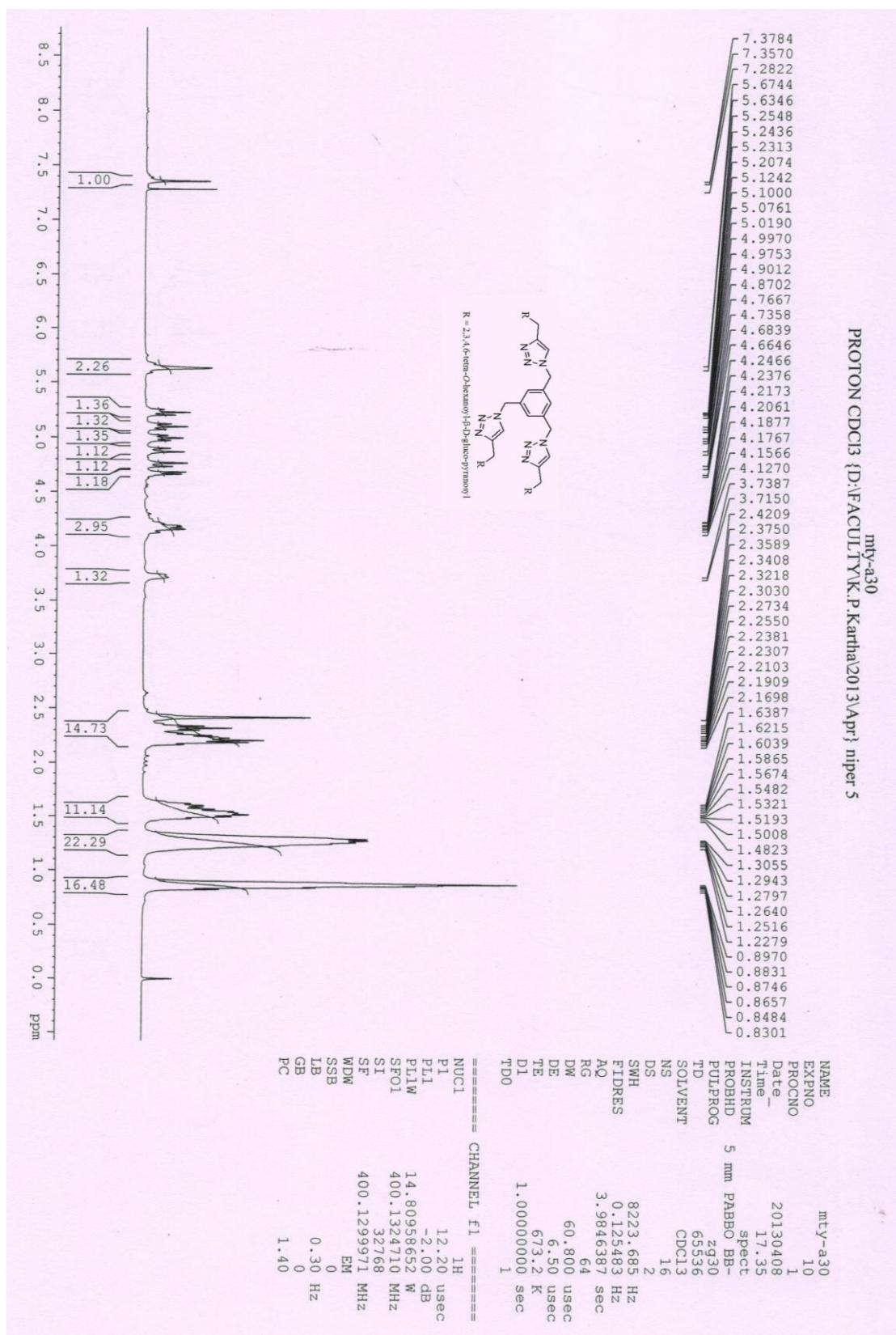
**<sup>1</sup>H NMR spectrum of 1,4-Bis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (15)**



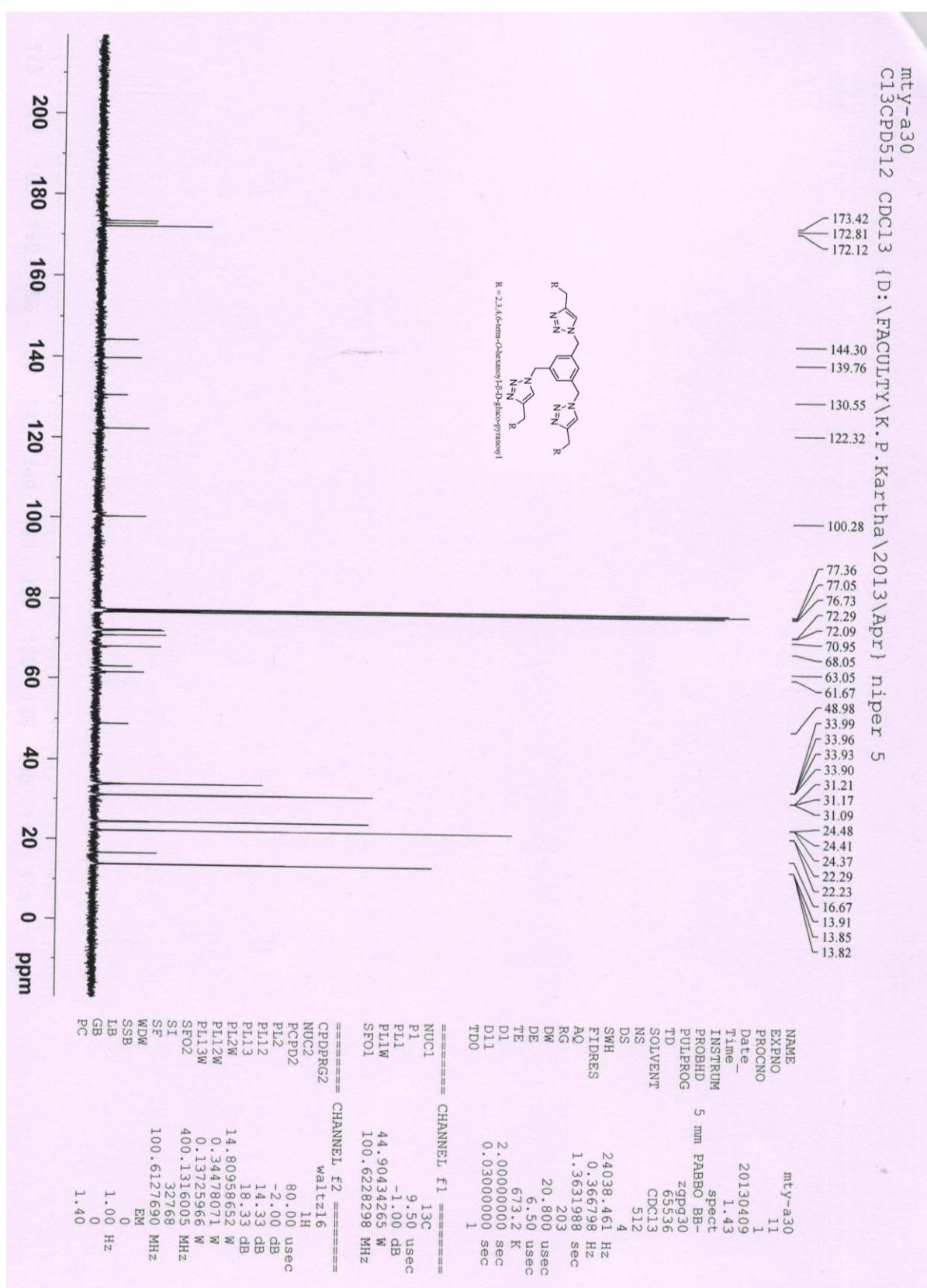
<sup>13</sup>C NMR spectrum of 1,4-Bis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (15)



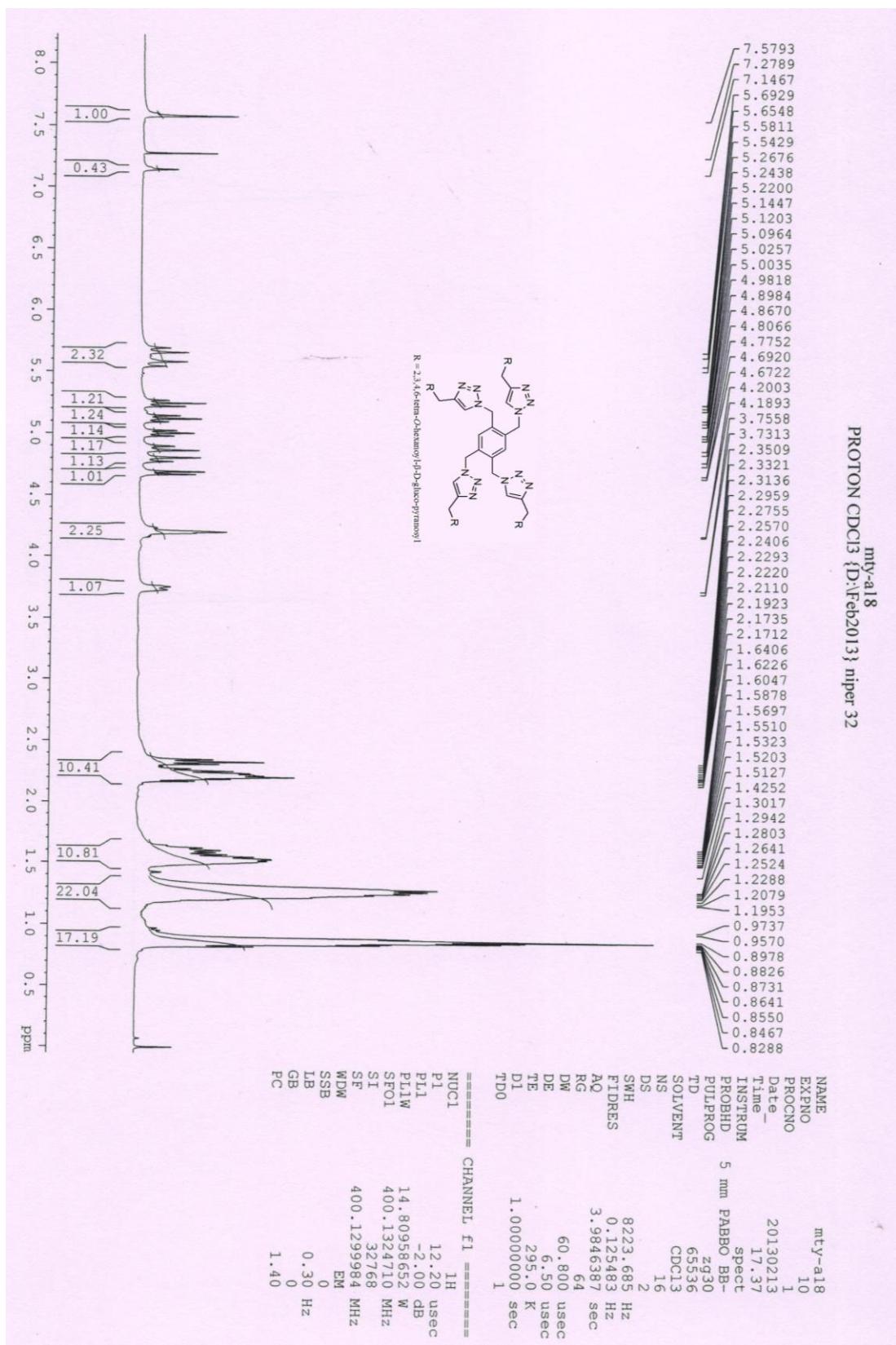
**<sup>1</sup>H NMR spectrum of 1,3,5-Tris[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (16)**



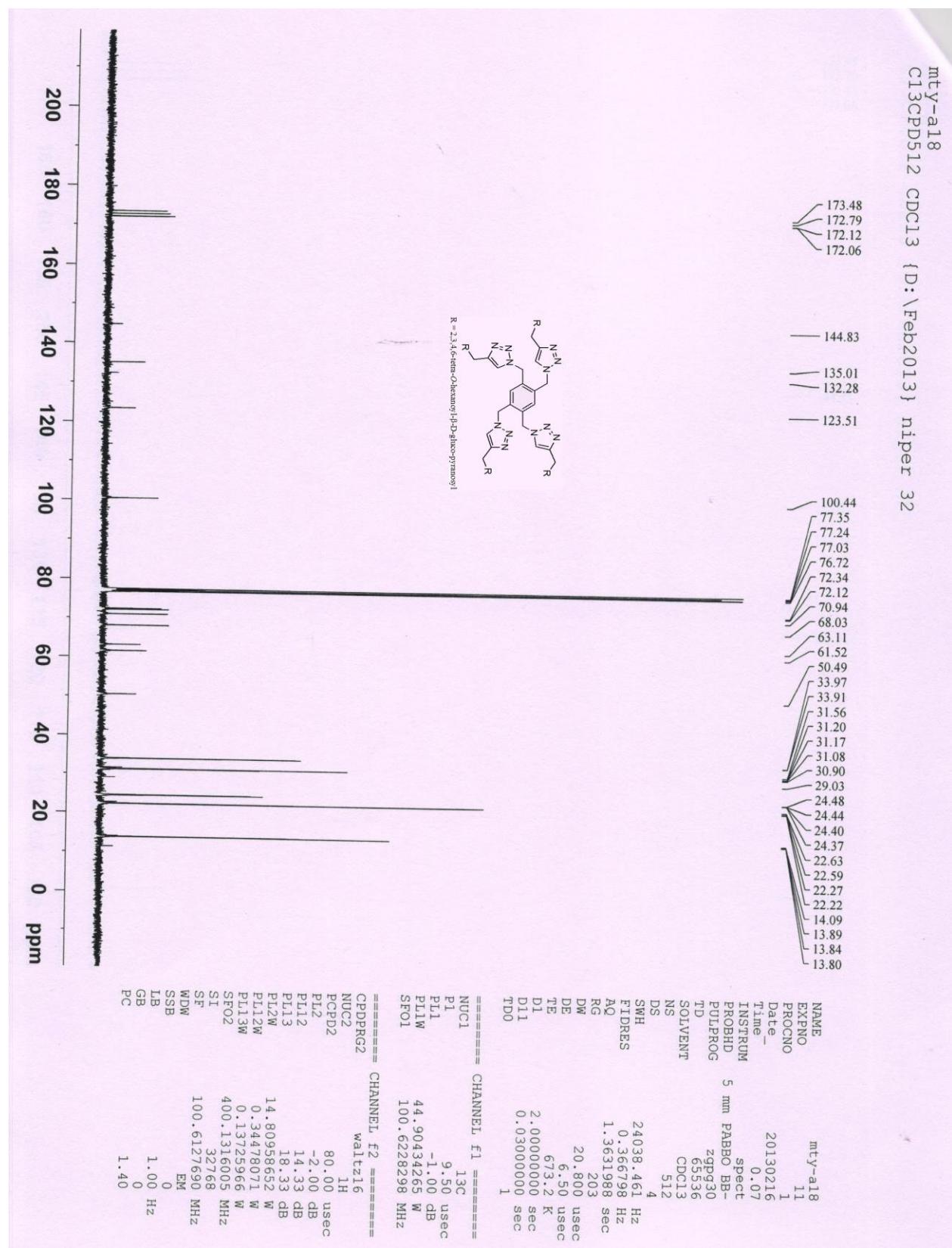
<sup>13</sup>C NMR spectrum of 1,3,5-Tris[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1*H*-1,2,3-triazol-1-yl)methyl]benzene (16)



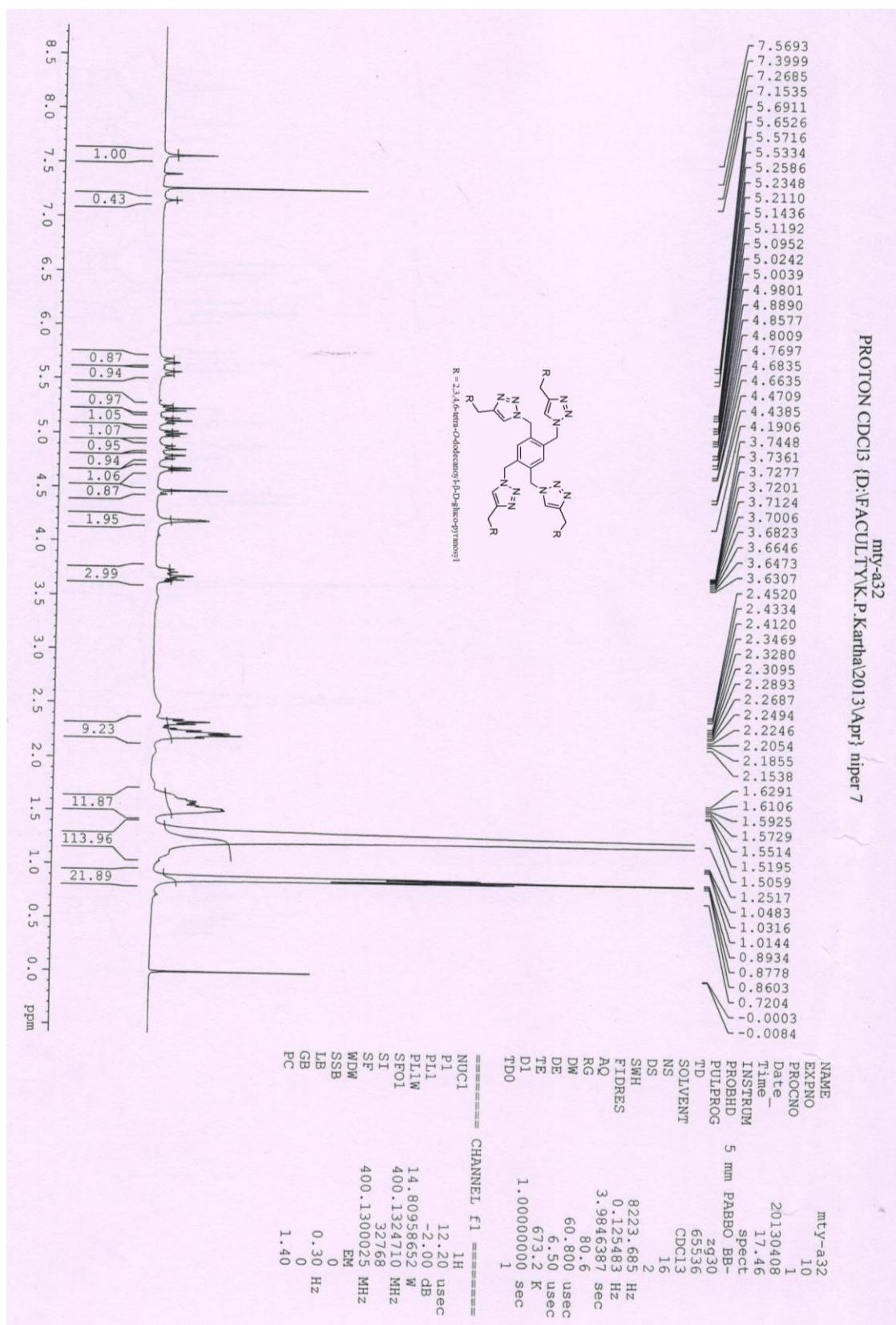
**<sup>1</sup>H NMR spectrum of 1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (17)**



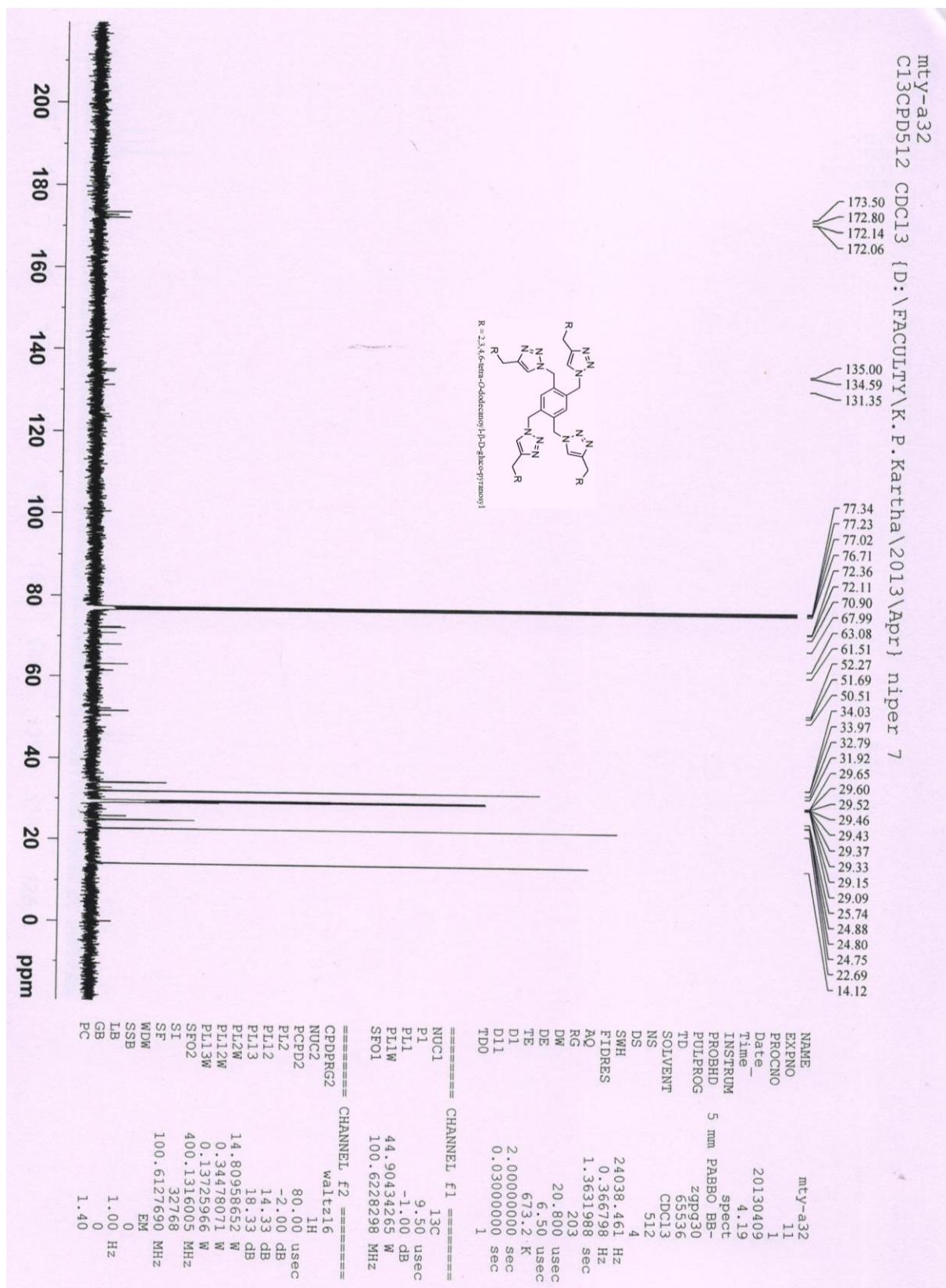
**<sup>13</sup>C NMR spectrum of 1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (17)**



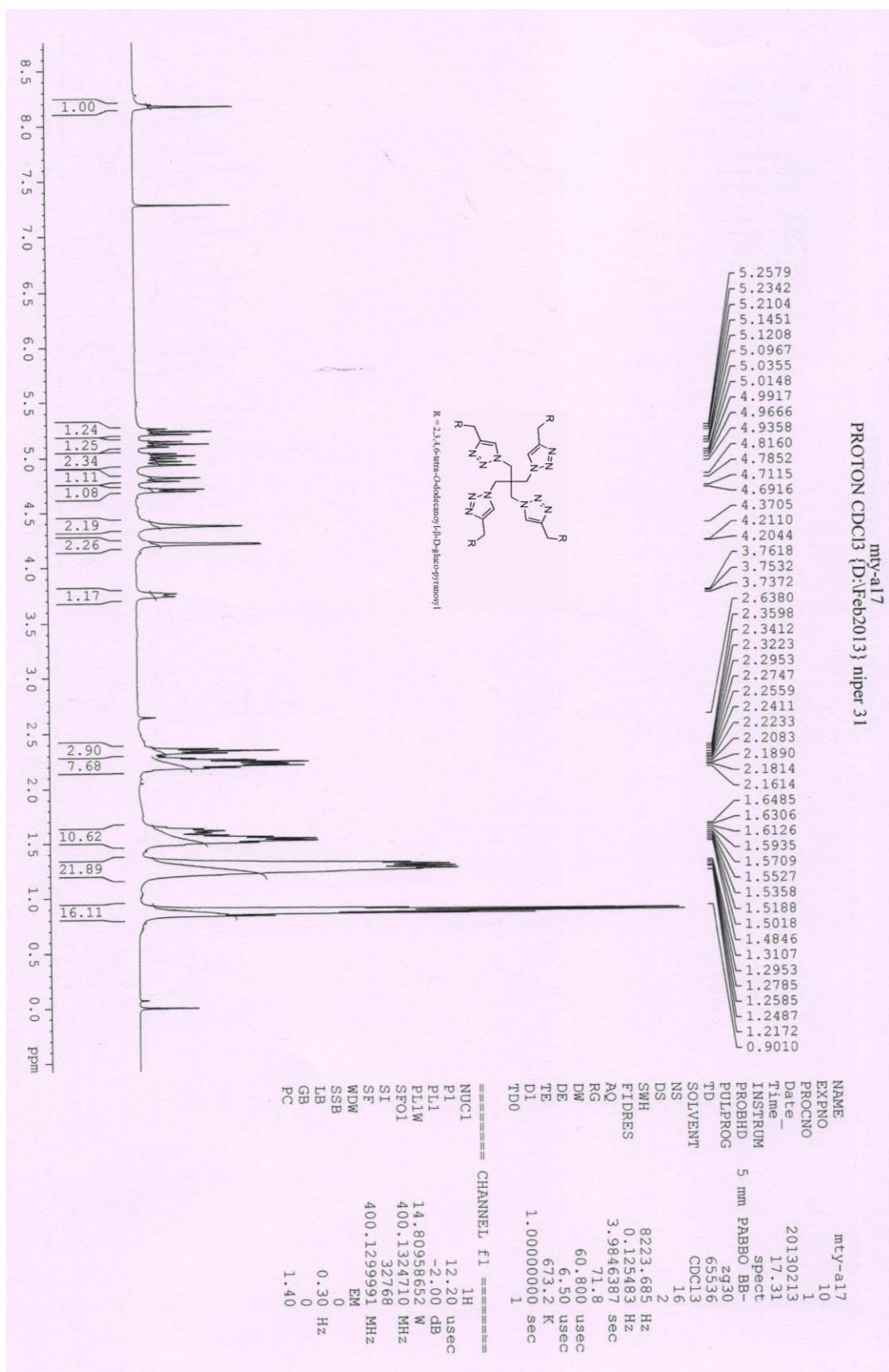
**<sup>1</sup>H NMR spectrum of 1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (18)**



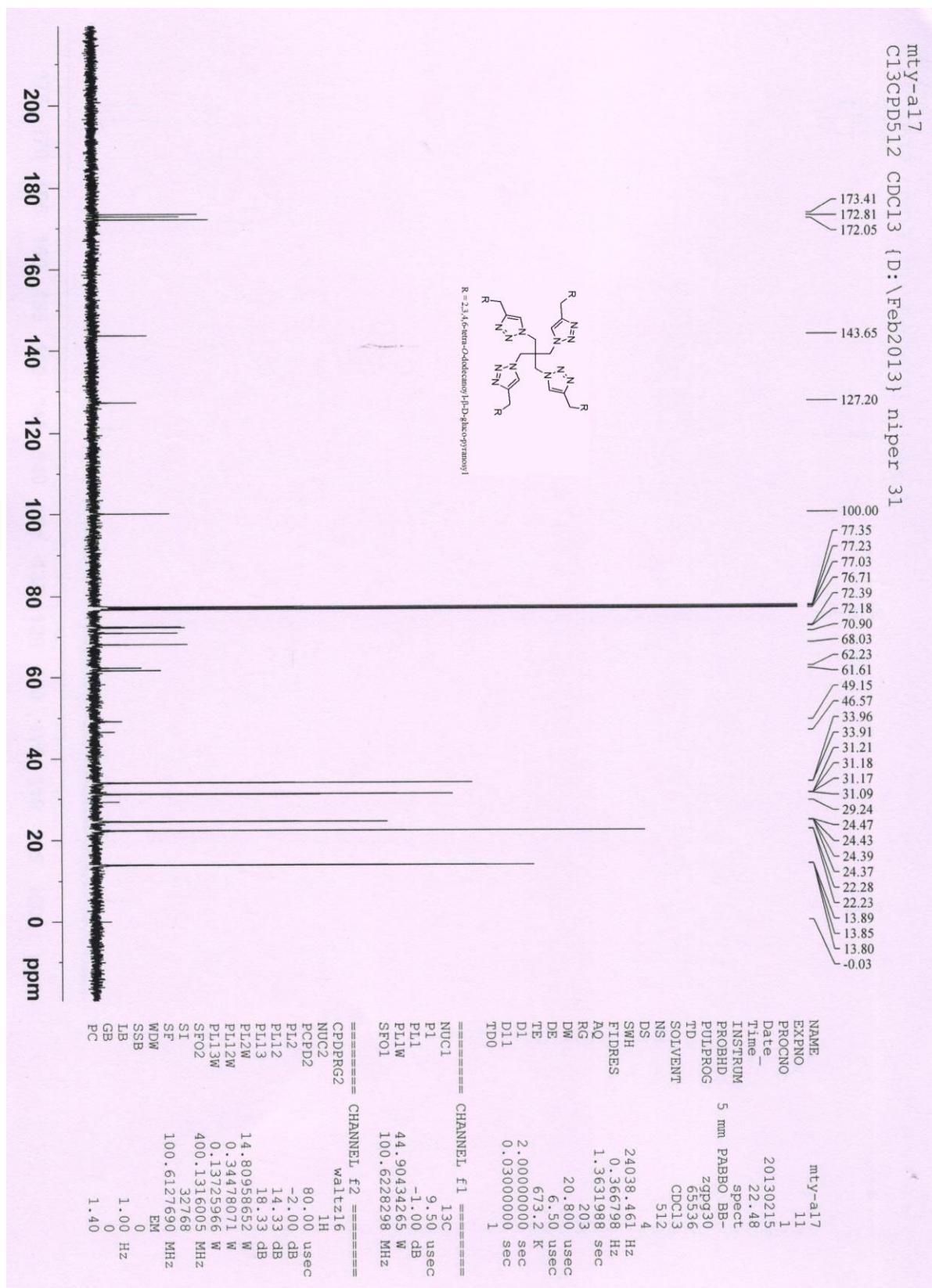
<sup>13</sup>C NMR spectrum of 1,2,4,5-Tetrakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (18)



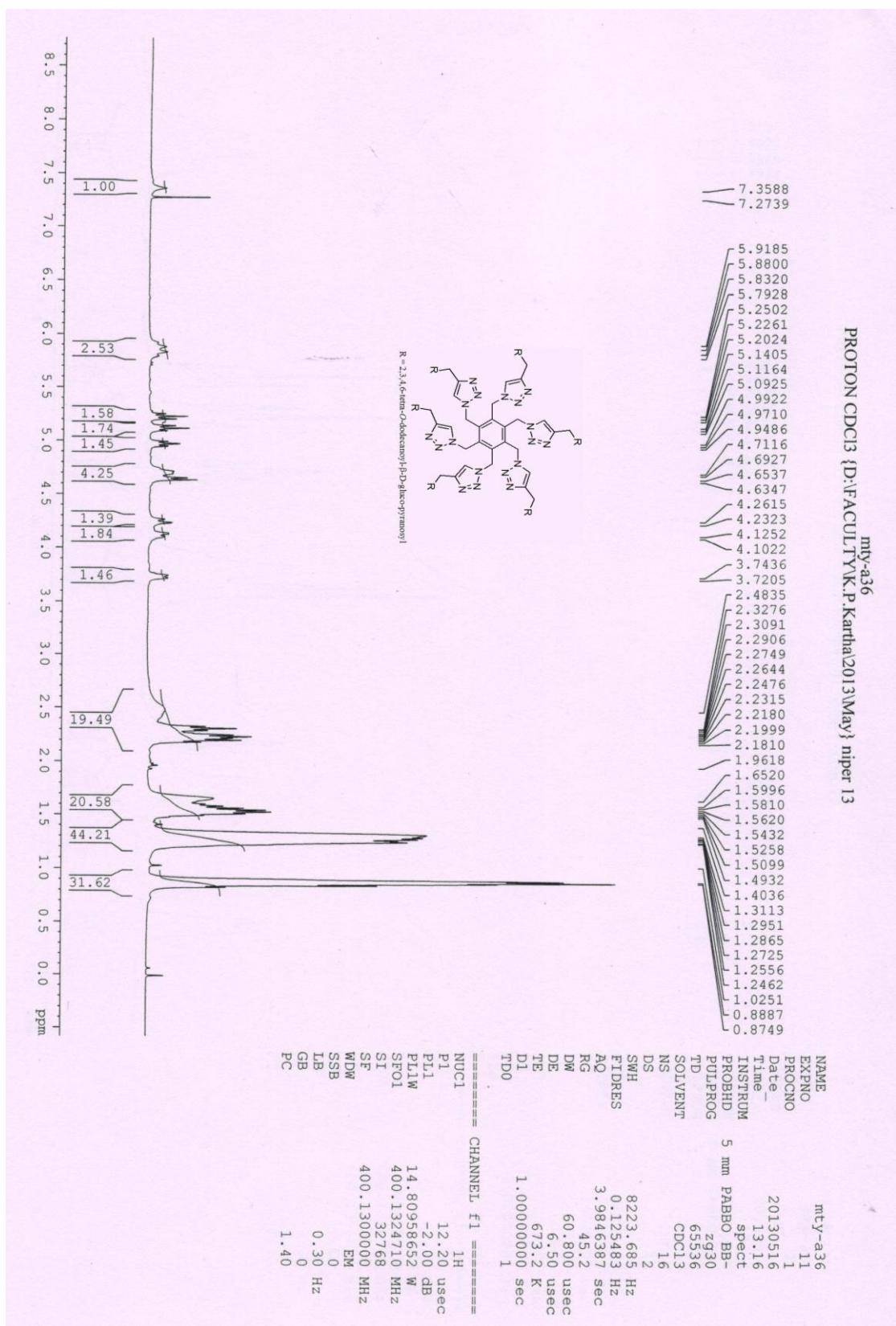
**<sup>1</sup>H NMR spectrum of Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]methane (19)**



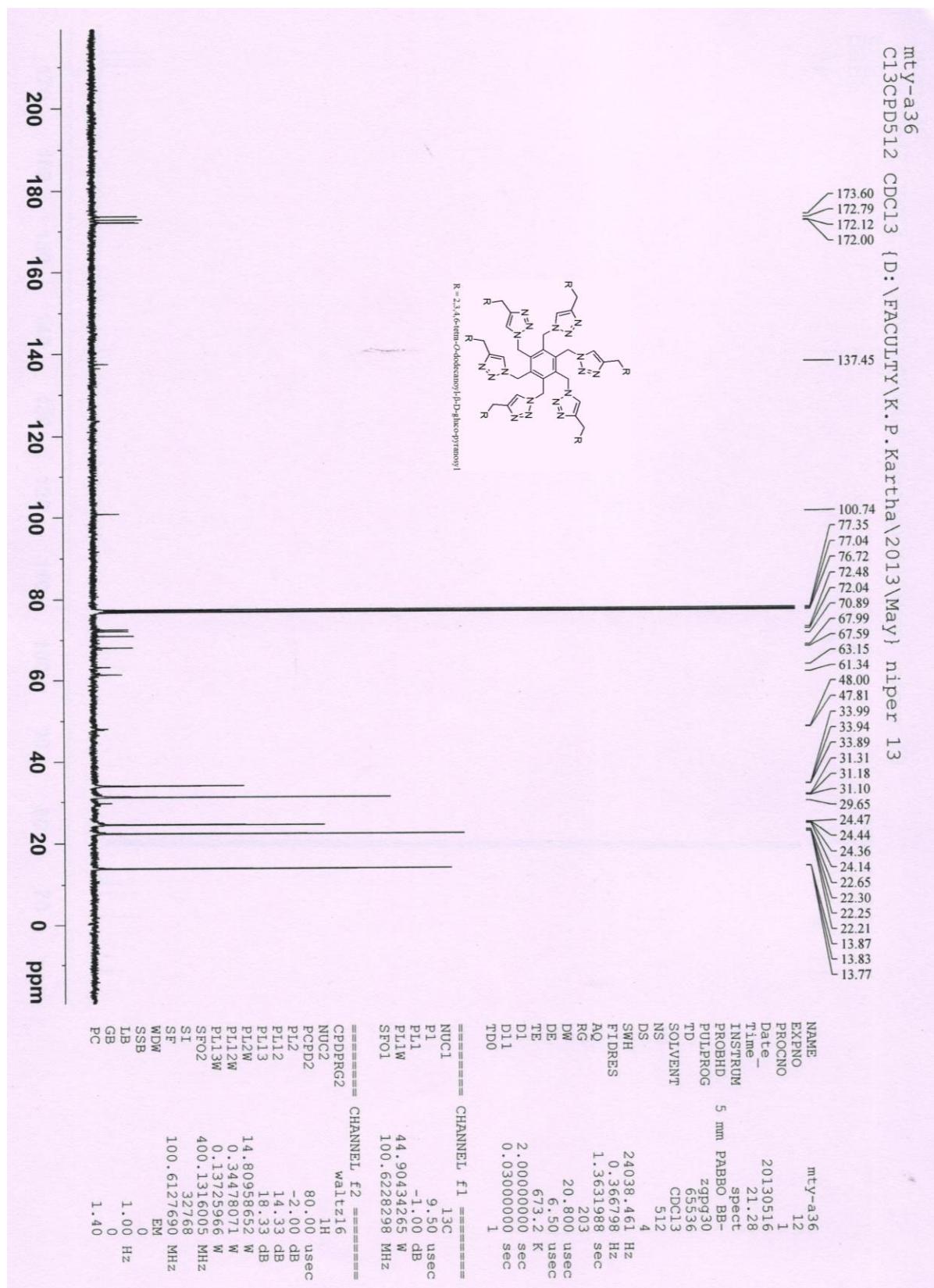
<sup>13</sup>C NMR spectrum of Tetrakis[(4-(2,3,4,6-tetra-O-hexanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]methane (19)

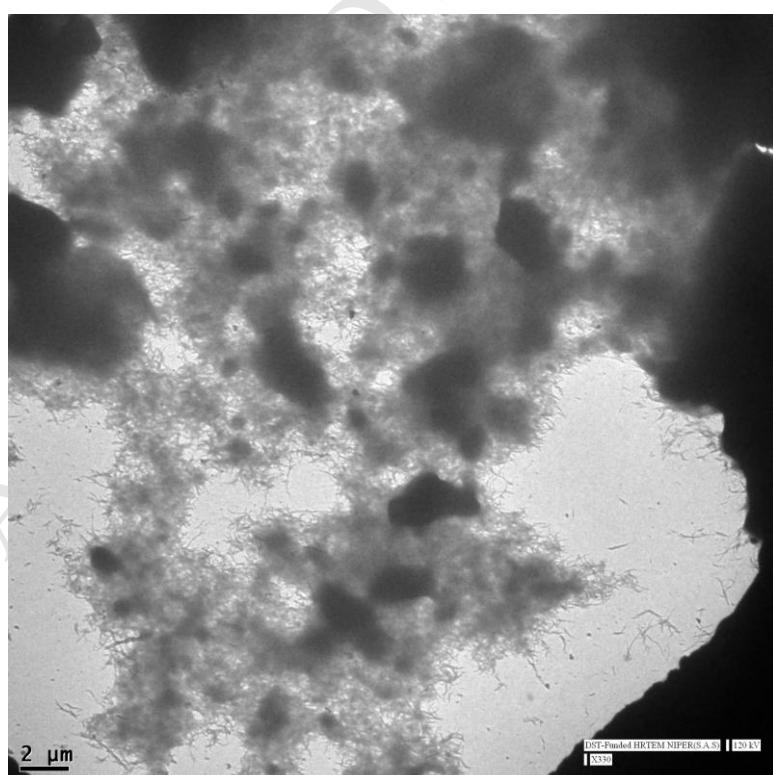
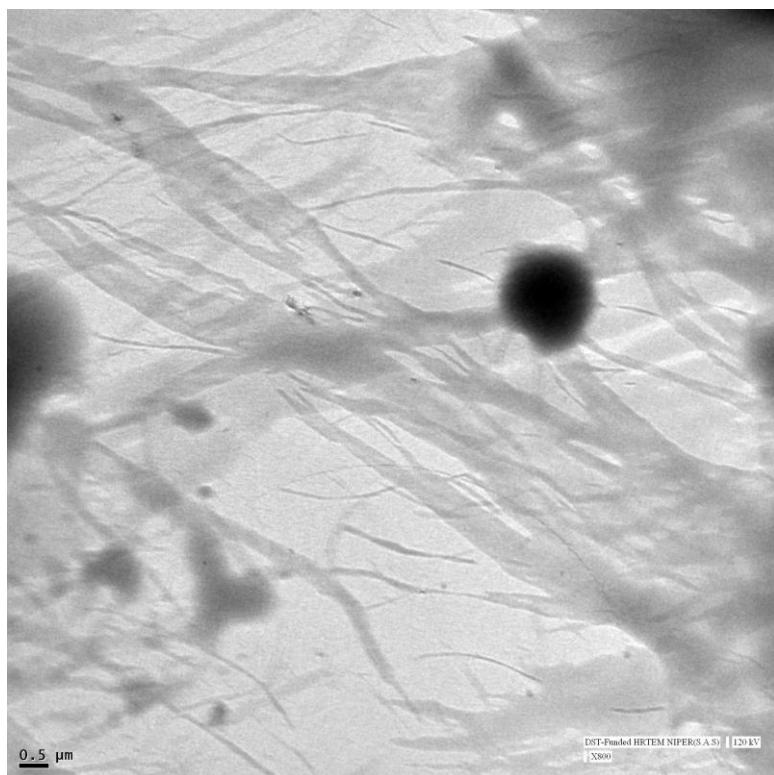


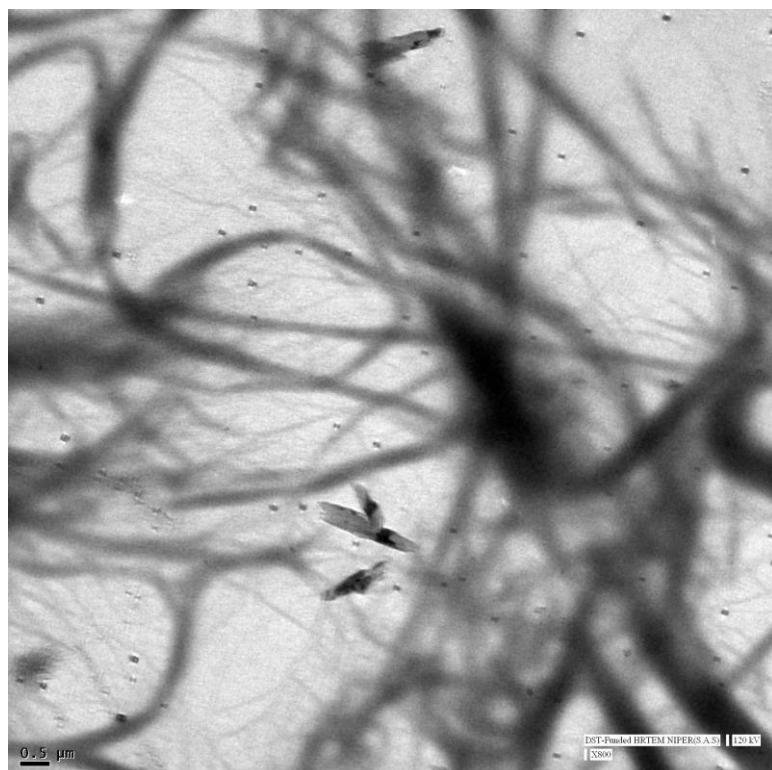
**<sup>1</sup>H NMR spectrum of 1,2,3,4,5,6-Hexakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (20)**



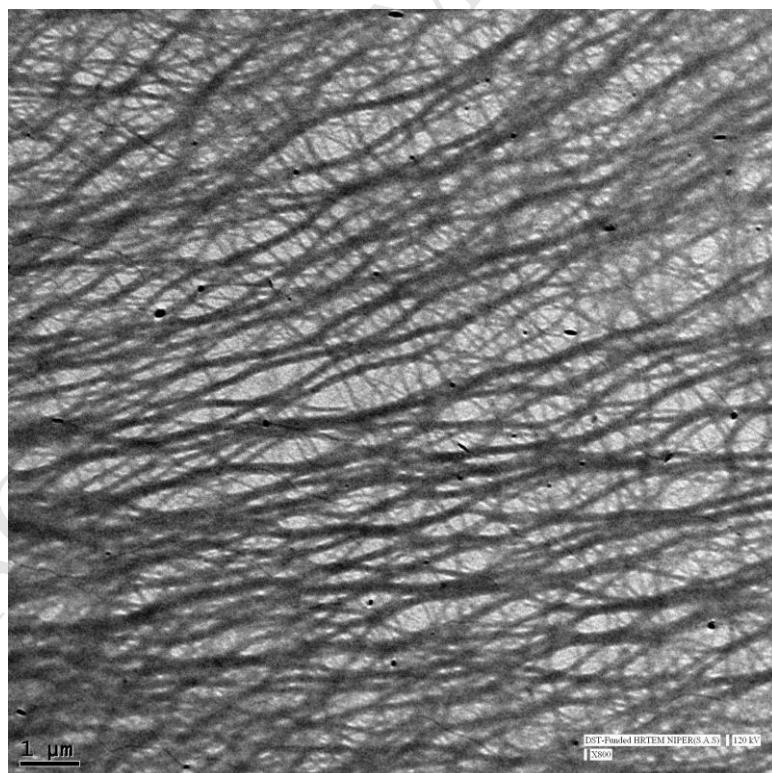
<sup>13</sup>C NMR spectrum of 1,2,3,4,5,6-Hexakis[(4-(2,3,4,6-tetra-O-dodecanoyl- $\beta$ -D-glucopyranosyloxymethyl)-1H-1,2,3-triazol-1-yl)methyl]benzene (20)



**2. TEM Images for compounds 14, 15, 16 and 17**

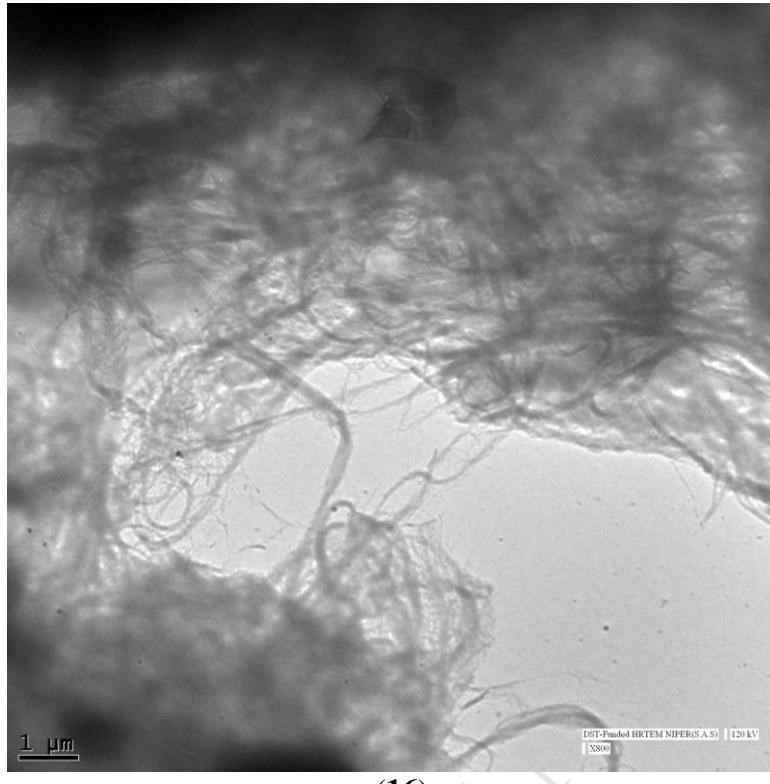


c (17)



d (18)

**Figure 3** Transmission electron micrographs: a. **15**; b. **16**; c. **17** and d. **18** (for sample preparation, moist MeOH-Hex was used for **16** and hexane only for others)



(16)

**Figure 4** Transmission electron micrograph for the gel made by **16** on standing for 3-5 days

### 3. XYZ Coordinates of the geometries optimized using PM3 method

#### Monomer 15 (15-M)

1	6	0	-3.565856	0.044728	-1.584344
2	6	0	-2.667252	0.195340	-0.411424
3	1	0	-3.102737	-0.548568	-2.395158
4	1	0	-3.830924	1.040066	-1.991334
5	7	0	-1.387600	-0.379872	-0.337001
6	6	0	-2.900755	0.838740	0.795296
7	7	0	-0.854663	-0.138235	0.795292
8	7	0	-1.741286	0.604431	1.536104
9	6	0	-1.500089	1.026652	2.934860
10	6	0	-0.408781	2.046989	3.038997
11	1	0	-2.450776	1.431741	3.337782
12	1	0	-1.246629	0.119427	3.537743
13	6	0	0.854229	1.656084	3.484348
14	6	0	-0.640583	3.381900	2.709226
15	6	0	1.875655	2.589132	3.597444
16	6	0	0.389679	4.312301	2.797678
17	1	0	-1.634286	3.715910	2.366605
18	6	0	1.653155	3.918447	3.236215
19	1	0	2.863461	2.269293	3.956571
20	6	0	2.777457	4.906169	3.318280
21	7	0	3.687479	4.785443	2.155681
22	1	0	2.392012	5.945417	3.368845

23	1	0	3.371618	4.735423	4.239777
24	6	0	4.544107	3.715967	1.875300
25	7	0	3.729306	5.697525	1.128659
26	6	0	5.102360	4.039652	0.649167
27	7	0	4.553618	5.273793	0.255468
28	6	0	6.078096	3.281369	-0.176522
29	1	0	6.477697	3.899974	-1.009453
30	1	0	6.928572	2.949386	0.448613
31	1	0	4.688104	2.837738	2.511785
32	1	0	-3.778441	1.391394	1.145192
33	1	0	6.979116	4.049763	-4.413147
34	6	0	7.621082	4.022907	-3.510025
35	6	0	8.361715	2.693115	-3.473634
36	1	0	6.922318	4.097741	-2.645193
37	6	0	8.563429	5.215592	-3.521542
38	6	0	8.845161	2.359432	-2.082660
39	1	0	7.702218	1.882862	-3.855739
40	1	0	9.236641	2.715612	-4.154407
41	1	0	9.235971	5.179962	-2.640509
42	1	0	9.229689	5.165145	-4.406455
43	6	0	7.788309	6.523810	-3.528171
44	8	0	9.802755	2.817131	-1.495977
45	8	0	8.267970	1.450059	-1.228028
46	1	0	7.124680	6.573093	-2.641407
47	1	0	7.113670	6.558850	-4.406771
48	6	0	8.719557	7.714731	-3.544086
49	6	0	7.176660	0.645179	-1.645191
50	1	0	9.377079	7.726099	-2.664557
51	1	0	8.158317	8.657761	-3.546419
52	1	0	9.364445	7.713880	-4.432990
53	6	0	7.510876	-0.858364	-1.424718
54	6	0	5.887639	0.925737	-0.804984
55	1	0	6.943934	0.818244	-2.729090
56	6	0	7.648545	-1.191976	0.087650
57	1	0	6.657309	-1.451502	-1.847593
58	8	0	8.512814	-1.339034	-2.295598
59	8	0	6.055371	0.635029	0.563181
60	8	0	5.367360	2.213970	-0.811394
61	1	0	5.037777	0.350788	-1.250863
62	8	0	7.710367	-2.622429	0.155248
63	6	0	6.357012	-0.730415	0.835247
64	1	0	8.554723	-0.693683	0.523767
65	6	0	9.853030	-1.030636	-2.274679
66	6	0	8.663297	-3.245201	0.911635
67	6	0	6.525398	-0.807168	2.371391
68	1	0	5.493310	-1.357816	0.495335
69	6	0	10.680751	-0.609662	-1.085802
70	8	0	10.249118	-1.238387	-3.403526
71	6	0	8.759602	-4.728860	0.629429
72	8	0	9.322155	-2.604368	1.706137
73	8	0	5.436680	-1.516335	2.946392
74	1	0	7.380392	-1.445170	2.657932
75	1	0	6.685938	0.193267	2.822442
76	1	0	10.026287	-0.286651	-0.246562
77	1	0	11.269832	0.287898	-1.366259
78	6	0	11.604842	-1.725254	-0.616721
79	1	0	9.107289	-5.244893	1.547145
80	1	0	7.763161	-5.154580	0.397558
81	6	0	9.726348	-4.970315	-0.522436
82	6	0	4.436581	-0.856925	3.601522

83	1	0	11.047358	-2.689542	-0.564203
84	1	0	11.916412	-1.510479	0.425691
85	6	0	12.838049	-1.889912	-1.489542
86	1	0	9.279054	-4.616669	-1.473499
87	1	0	10.648282	-4.356897	-0.385022
88	6	0	10.094596	-6.439884	-0.634512
89	6	0	3.341365	-1.786694	4.080889
90	8	0	4.507041	0.345233	3.766118
91	1	0	12.546619	-2.018472	-2.551665
92	1	0	13.449757	-0.965835	-1.459227
93	6	0	13.668280	-3.081338	-1.036774
94	1	0	10.525049	-6.800118	0.321917
95	1	0	9.182989	-7.048620	-0.798947
96	6	0	11.086013	-6.667788	-1.765077
97	1	0	3.736769	-2.811821	4.232233
98	1	0	2.991661	-1.446159	5.076637
99	6	0	2.185910	-1.805128	3.089240
100	1	0	13.053259	-4.005653	-1.075433
101	1	0	13.955125	-2.960458	0.026795
102	6	0	14.904430	-3.248521	-1.890817
103	1	0	10.650900	-6.320924	-2.723549
104	1	0	11.988802	-6.041913	-1.605857
105	6	0	11.477217	-8.124150	-1.871201
106	1	0	1.771259	-0.777622	2.971154
107	1	0	2.562209	-2.094447	2.088341
108	6	0	1.083516	-2.764768	3.512194
109	1	0	14.648331	-3.406786	-2.946959
110	1	0	15.500417	-4.110264	-1.564432
111	1	0	15.552662	-2.363429	-1.842112
112	1	0	11.949059	-8.485848	-0.947842
113	1	0	12.190905	-8.285282	-2.689139
114	1	0	10.606278	-8.764525	-2.064557
115	1	0	1.521958	-3.699922	3.916515
116	1	0	0.502828	-3.076413	2.618163
117	6	0	0.133589	-2.155281	4.532741
118	1	0	0.702293	-1.770101	5.402839
119	1	0	-0.375604	-1.264334	4.095785
120	6	0	-0.898957	-3.161152	4.989007
121	1	0	-1.453711	-3.589723	4.135531
122	1	0	-0.436904	-3.999921	5.526346
123	1	0	-1.632878	-2.703350	5.663763
124	1	0	-3.601585	-4.582958	-1.628093
125	6	0	-4.066798	-4.071212	-0.761021
126	6	0	-5.578326	-4.172986	-0.901069
127	1	0	-3.744153	-3.012480	-0.832063
128	6	0	-3.545331	-4.687756	0.527249
129	6	0	-6.318055	-3.258656	0.045980
130	1	0	-5.871895	-3.944406	-1.949955
131	1	0	-5.913329	-5.212717	-0.710846
132	1	0	-3.962785	-4.151608	1.403399
133	1	0	-3.900664	-5.733765	0.622182
134	6	0	-2.025550	-4.650268	0.571279
135	8	0	-6.526645	-3.421634	1.229632
136	8	0	-6.949322	-2.090191	-0.300716
137	1	0	-1.665648	-3.615069	0.404885
138	1	0	-1.610843	-5.246892	-0.265725
139	6	0	-1.495146	-5.170561	1.887500
140	6	0	-6.891368	-1.590536	-1.627805
141	1	0	-1.797214	-4.529783	2.734648
142	1	0	-0.397030	-5.202798	1.887826

143	1	0	-1.855575	-6.185351	2.100227
144	6	0	-8.294234	-1.053701	-2.032245
145	6	0	-5.919019	-0.374592	-1.740866
146	1	0	-6.569326	-2.394913	-2.340613
147	6	0	-8.705550	0.167785	-1.161508
148	1	0	-8.229085	-0.728463	-3.103697
149	8	0	-9.249852	-2.077568	-2.209039
150	8	0	-6.305260	0.699870	-0.915386
151	8	0	-4.705514	-0.683753	-1.120832
152	1	0	-5.823969	-0.063248	-2.812531
153	8	0	-9.875228	0.703849	-1.793172
154	6	0	-7.581570	1.250163	-1.217129
155	1	0	-8.888378	-0.146453	-0.099124
156	6	0	-9.790773	-2.881190	-1.231153
157	6	0	-10.971905	1.043258	-1.049965
158	6	0	-7.820374	2.342377	-0.150115
159	1	0	-7.543954	1.698101	-2.242193
160	6	0	-10.010598	-2.534014	0.220444
161	8	0	-10.128934	-3.899675	-1.798342
162	6	0	-12.202569	1.288499	-1.895592
163	8	0	-10.881893	1.123208	0.158609
164	8	0	-7.137043	3.536490	-0.500212
165	1	0	-8.873520	2.675446	-0.165403
166	1	0	-7.584282	1.976180	0.868704
167	1	0	-9.385112	-1.662964	0.515745
168	1	0	-9.655664	-3.380284	0.843722
169	6	0	-11.475044	-2.237025	0.513702
170	1	0	-12.866960	1.998472	-1.362690
171	1	0	-11.934084	1.779238	-2.852089
172	6	0	-12.920845	-0.029513	-2.153207
173	6	0	-5.975781	3.890916	0.128754
174	1	0	-11.892860	-1.555409	-0.263638
175	1	0	-11.536647	-1.669221	1.464273
176	6	0	-12.330913	-3.488797	0.615774
177	1	0	-12.324688	-0.657458	-2.846006
178	1	0	-12.991078	-0.619358	-1.208615
179	6	0	-14.309533	0.202297	-2.723936
180	6	0	-5.383148	5.166536	-0.432099
181	8	0	-5.541475	3.211050	1.037147
182	1	0	-12.216397	-4.111178	-0.294811
183	1	0	-11.977315	-4.121857	1.454389
184	6	0	-13.796080	-3.131243	0.813265
185	1	0	-14.901753	0.843620	-2.039977
186	1	0	-14.239848	0.766409	-3.675557
187	6	0	-15.032463	-1.116441	-2.950265
188	1	0	-4.280539	5.038861	-0.525111
189	1	0	-5.757553	5.345016	-1.459987
190	6	0	-5.699369	6.370988	0.444757
191	1	0	-14.148529	-2.504392	-0.033482
192	1	0	-13.913426	-2.501306	1.717408
193	6	0	-14.655046	-4.369795	0.929893
194	1	0	-14.447447	-1.752843	-3.643841
195	1	0	-15.084335	-1.685365	-1.998519
196	6	0	-16.423844	-0.896246	-3.498784
197	1	0	-5.537347	7.293267	-0.149415
198	1	0	-6.778772	6.367966	0.696089
199	6	0	-4.881422	6.439281	1.727631
200	1	0	-14.586215	-4.996230	0.030495
201	1	0	-15.712058	-4.109673	1.069163
202	1	0	-14.354575	-4.991750	1.783622

203	1	0	-17.041020	-0.301104	-2.812524
204	1	0	-16.941819	-1.849766	-3.662613
205	1	0	-16.401135	-0.365638	-4.460004
206	1	0	-4.818463	5.437038	2.197494
207	1	0	-5.430695	7.073005	2.452359
208	6	0	-3.484473	7.017552	1.544245
209	1	0	-3.517249	7.883858	0.853291
210	1	0	-3.135987	7.427014	2.513454
211	6	0	-2.477933	6.003757	1.049316
212	1	0	-2.386429	5.142110	1.734081
213	1	0	-2.757919	5.599391	0.062977
214	1	0	-1.477749	6.446502	0.951694
215	1	0	1.057709	0.599178	3.726759
216	1	0	0.199344	5.355202	2.510893

**Monomer 16 (16-M)**

1	6	0	0.224429	1.191119	0.203353
2	6	0	1.039277	0.400269	-0.753338
3	1	0	0.848869	1.647319	0.995613
4	1	0	-0.537354	0.548367	0.694364
5	7	0	2.391140	0.087022	-0.532509
6	6	0	0.692507	-0.125895	-1.988224
7	7	0	2.863356	-0.571088	-1.518176
8	7	0	1.866989	-0.725762	-2.447249
9	6	0	2.031552	-1.425977	-3.742619
10	6	0	2.168653	-2.907860	-3.566810
11	1	0	1.144964	-1.193211	-4.368252
12	1	0	2.920467	-1.005725	-4.261633
13	6	0	3.410242	-3.512584	-3.760110
14	6	0	1.063773	-3.680738	-3.213069
15	6	0	3.546839	-4.890121	-3.588269
16	6	0	1.210825	-5.051481	-2.998717
17	1	0	0.076938	-3.209539	-3.093946
18	6	0	2.451731	-5.658050	-3.193238
19	6	0	0.040003	-5.874979	-2.549265
20	6	0	4.878322	-5.539747	-3.823865
21	7	0	-0.488805	-5.416192	-1.245736
22	1	0	0.316187	-6.946082	-2.459815
23	1	0	-0.787533	-5.816127	-3.300290
24	7	0	5.702294	-5.554140	-2.594968
25	1	0	4.748724	-6.580903	-4.185046
26	1	0	5.441159	-4.993427	-4.609048
27	7	0	0.096783	-5.713135	-0.036398
28	6	0	-1.477473	-4.438935	-1.062343
29	6	0	6.197108	-4.435156	-1.916617
30	7	0	5.984714	-6.694237	-1.880691
31	7	0	-0.476120	-5.023227	0.863186
32	6	0	-1.471484	-4.198708	0.300738
33	6	0	6.788374	-4.959391	-0.779301
34	7	0	6.621542	-6.356233	-0.831615
35	6	0	-2.306647	-3.244377	1.077367
36	6	0	7.449777	-4.265142	0.358460
37	1	0	-1.682046	-2.420357	1.472636
38	1	0	7.674635	-4.963945	1.193687
39	1	0	8.399672	-3.799644	0.032952
40	1	0	6.093264	-3.398924	-2.252081
41	1	0	-2.116971	-4.028569	-1.863466

42	1	0	-0.255047	-0.082175	-2.535090
43	1	0	7.569924	-4.842337	4.615905
44	6	0	8.388382	-4.643410	3.895459
45	6	0	8.814111	-3.187553	4.026470
46	1	0	7.948799	-4.827942	2.887674
47	6	0	9.532651	-5.611972	4.146706
48	6	0	9.546040	-2.705197	2.797057
49	1	0	7.923180	-2.548809	4.215887
50	1	0	9.475289	-3.053375	4.906186
51	1	0	10.379115	-5.389340	3.465683
52	1	0	9.931373	-5.472124	5.171795
53	6	0	9.080026	-7.051096	3.955705
54	8	0	10.697803	-2.921010	2.483052
55	8	0	9.014757	-1.918349	1.804794
56	1	0	8.682152	-7.187237	2.929646
57	1	0	8.233148	-7.274249	4.634869
58	6	0	10.211963	-8.021863	4.204589
59	6	0	7.709540	-1.372483	1.924707
60	1	0	11.052596	-7.847514	3.519768
61	1	0	9.883659	-9.059488	4.063704
62	1	0	10.602053	-7.936556	5.227608
63	6	0	7.749429	0.154534	1.633999
64	6	0	6.722628	-1.981233	0.873929
65	1	0	7.297217	-1.547443	2.953288
66	6	0	8.150914	0.429067	0.157557
67	1	0	6.714627	0.552482	1.807444
68	8	0	8.399540	0.896488	2.644320
69	8	0	7.132609	-1.732753	-0.450170
70	8	0	6.522024	-3.357889	0.950823
71	1	0	5.693274	-1.592915	1.076081
72	8	0	7.940376	1.831361	-0.037544
73	6	0	7.184666	-0.349973	-0.790918
74	1	0	9.215112	0.121039	-0.025408
75	6	0	9.744068	0.913284	2.928764
76	6	0	8.859480	2.584016	-0.713070
77	6	0	7.660771	-0.337826	-2.265560
78	1	0	6.152886	0.078232	-0.706856
79	6	0	10.887422	0.654554	1.979279
80	8	0	9.825771	1.255187	4.091381
81	6	0	8.573109	4.066853	-0.620624
82	8	0	9.781588	2.047330	-1.293323
83	8	0	7.118226	0.779673	-2.949512
84	1	0	8.746543	-0.148575	-2.352424
85	1	0	7.438974	-1.299484	-2.772374
86	1	0	10.529455	0.125692	1.068664
87	1	0	11.600352	-0.041944	2.466687
88	6	0	11.593505	1.943828	1.581405
89	1	0	9.024916	4.574943	-1.496075
90	1	0	7.477247	4.267201	-0.682339
91	6	0	9.140595	4.621714	0.678836
92	6	0	5.953235	0.667387	-3.655277
93	1	0	10.846104	2.726158	1.310346
94	1	0	12.170944	1.757611	0.653079
95	6	0	12.525220	2.473204	2.659156
96	1	0	8.564252	4.228343	1.541009
97	1	0	10.183141	4.253918	0.830238
98	6	0	9.113341	6.140641	0.686962
99	6	0	5.372417	1.997107	-4.080543
100	8	0	5.516985	-0.434520	-3.928806
101	1	0	11.980621	2.590098	3.617987

102	1	0	13.327820	1.735696	2.861619
103	6	0	13.132488	3.805434	2.246749
104	1	0	9.663189	6.538197	-0.189981
105	1	0	8.069004	6.500199	0.573256
106	6	0	9.719066	6.689710	1.969117
107	1	0	5.931355	2.357350	-4.967025
108	1	0	4.319516	1.851143	-4.420317
109	6	0	5.389494	3.044242	-2.976132
110	1	0	12.325603	4.543861	2.052544
111	1	0	13.670395	3.694369	1.284241
112	6	0	14.071444	4.335132	3.306584
113	1	0	9.160999	6.303042	2.845109
114	1	0	10.755700	6.311109	2.087695
115	6	0	9.714809	8.201398	1.978700
116	1	0	5.026060	2.604905	-2.023609
117	1	0	6.427953	3.376169	-2.772416
118	6	0	4.530772	4.243280	-3.348630
119	1	0	13.555636	4.489226	4.263801
120	1	0	14.506019	5.297799	3.008679
121	1	0	14.903274	3.642798	3.492859
122	1	0	10.295581	8.614025	1.142944
123	1	0	10.150243	8.594256	2.906267
124	1	0	8.696305	8.604072	1.897832
125	1	0	4.853225	4.655458	-4.325431
126	1	0	4.693488	5.059938	-2.607322
127	6	0	3.054903	3.878780	-3.392470
128	1	0	2.924568	2.991610	-4.053109
129	1	0	2.719328	3.555360	-2.384951
130	6	0	2.207261	5.034721	-3.868155
131	1	0	2.279001	5.890982	-3.182144
132	1	0	2.512038	5.383041	-4.863766
133	1	0	1.148176	4.752807	-3.926837
134	1	0	-1.877366	1.110376	4.564883
135	6	0	-2.481515	1.202924	3.639910
136	6	0	-3.592671	0.161115	3.671168
137	1	0	-1.779898	0.999672	2.803531
138	6	0	-3.029084	2.617506	3.529217
139	6	0	-4.013251	-0.299352	2.298043
140	1	0	-3.273571	-0.724062	4.266042
141	1	0	-4.496055	0.563347	4.191713
142	1	0	-3.615254	2.727772	2.592577
143	1	0	-3.751576	2.803642	4.358566
144	6	0	-1.926660	3.664939	3.571776
145	8	0	-3.910081	0.290599	1.241689
146	8	0	-4.604857	-1.500752	2.023329
147	1	0	-1.352184	3.667445	2.610682
148	1	0	-1.188919	3.416937	4.359819
149	6	0	-2.495977	5.046787	3.807808
150	6	0	-4.756841	-2.484914	3.034518
151	1	0	-3.205796	5.330627	3.017989
152	1	0	-1.701996	5.804847	3.823927
153	1	0	-3.030519	5.107480	4.766048
154	6	0	-6.250138	-2.781837	3.330857
155	6	0	-4.178733	-3.851144	2.524857
156	1	0	-4.224647	-2.183281	3.974394
157	6	0	-6.973117	-3.278523	2.047979
158	1	0	-6.279798	-3.588123	4.111544
159	8	0	-6.911852	-1.787402	4.096769
160	8	0	-4.810439	-4.287601	1.345550
161	8	0	-2.820569	-3.899331	2.236201

162	1	0	-4.249689	-4.606200	3.346800
163	8	0	-8.260334	-3.719251	2.496125
164	6	0	-6.210737	-4.514498	1.470081
165	1	0	-7.031279	-2.468232	1.277773
166	6	0	-7.452797	-0.635716	3.587000
167	6	0	-9.403076	-3.307289	1.862359
168	6	0	-6.704670	-4.817556	0.037115
169	1	0	-6.360117	-5.398499	2.139431
170	6	0	-8.369153	0.055722	4.576891
171	8	0	-7.199372	-0.275583	2.458600
172	6	0	-10.636777	-3.543775	2.707379
173	8	0	-9.342596	-2.835460	0.747373
174	8	0	-6.413410	-6.159321	-0.323189
175	1	0	-7.808935	-4.810215	0.001142
176	1	0	-6.327079	-4.070415	-0.692222
177	1	0	-9.192077	-0.654584	4.831995
178	1	0	-8.858422	0.913418	4.070998
179	6	0	-7.656016	0.527873	5.833071
180	1	0	-11.468354	-3.874006	2.053492
181	1	0	-10.469216	-4.369939	3.428254
182	6	0	-11.013771	-2.265058	3.442399
183	6	0	-5.353116	-6.443708	-1.139091
184	1	0	-7.121932	-0.312923	6.318693
185	1	0	-8.419759	0.857012	6.566826
186	6	0	-6.690713	1.670187	5.555450
187	1	0	-10.142241	-1.873767	4.018755
188	1	0	-11.266442	-1.469093	2.713121
189	6	0	-12.183700	-2.498889	4.383763
190	6	0	-5.177590	-7.926254	-1.386414
191	8	0	-4.683502	-5.540136	-1.598369
192	1	0	-5.874302	1.327915	4.876826
193	1	0	-7.209130	2.482535	5.006982
194	6	0	-6.092916	2.214437	6.843517
195	1	0	-13.062174	-2.865831	3.815940
196	1	0	-11.937716	-3.304583	5.104923
197	6	0	-12.542793	-1.225148	5.133153
198	1	0	-4.091796	-8.142224	-1.510684
199	1	0	-5.507351	-8.502091	-0.499124
200	6	0	-5.946912	-8.385460	-2.617577
201	1	0	-5.490768	1.427430	7.339603
202	1	0	-6.900617	2.465667	7.559924
203	6	0	-5.241796	3.436869	6.584447
204	1	0	-11.651634	-0.842473	5.671909
205	1	0	-12.817602	-0.429024	4.412734
206	6	0	-13.676800	-1.456792	6.105554
207	1	0	-6.009943	-9.492593	-2.601058
208	1	0	-6.994286	-8.029040	-2.549685
209	6	0	-5.344728	-7.929415	-3.939625
210	1	0	-4.437168	3.229865	5.857919
211	1	0	-4.766929	3.794738	7.506536
212	1	0	-5.835692	4.266264	6.177447
213	1	0	-14.583902	-1.804623	5.593538
214	1	0	-13.935646	-0.534833	6.641595
215	1	0	-13.417417	-2.212775	6.858721
216	1	0	-5.081632	-6.846129	-3.898491
217	1	0	-6.129339	-8.010365	-4.718261
218	6	0	-4.135781	-8.742265	-4.385411
219	1	0	-4.277915	-9.811183	-4.128326
220	1	0	-4.069752	-8.711699	-5.491335
221	6	0	-2.833464	-8.241170	-3.802418

222	1	0	-2.627213	-7.195355	-4.094775
223	1	0	-2.844736	-8.271685	-2.700429
224	1	0	-1.984820	-8.849412	-4.139497
225	1	0	-3.080144	-2.805353	0.415835
226	1	0	1.889717	4.342617	1.901515
227	6	0	1.630848	4.692169	0.881214
228	6	0	0.273619	5.378399	0.939327
229	1	0	1.571738	3.775772	0.257710
230	6	0	2.737951	5.592727	0.357424
231	6	0	-0.347154	5.534115	-0.429232
232	1	0	-0.409516	4.800272	1.613315
233	1	0	0.366700	6.383719	1.397179
234	1	0	2.511955	5.910098	-0.682899
235	1	0	2.789089	6.526235	0.952623
236	6	0	4.078580	4.874859	0.395152
237	8	0	-0.026091	6.310391	-1.305335
238	8	0	-1.417617	4.824721	-0.909100
239	1	0	4.017638	3.937323	-0.198200
240	1	0	4.314221	4.560553	1.431083
241	6	0	5.189169	5.743981	-0.148490
242	6	0	-2.122182	3.921948	-0.071258
243	1	0	5.001533	6.019564	-1.200582
244	1	0	6.157629	5.215088	-0.122857
245	1	0	5.306281	6.673312	0.423305
246	6	0	-3.647995	4.055833	-0.342634
247	6	0	-1.740860	2.432448	-0.340282
248	1	0	-1.916221	4.144196	1.017006
249	6	0	-4.028763	3.512059	-1.750389
250	1	0	-4.172839	3.438136	0.436001
251	8	0	-4.167681	5.311894	0.040084
252	8	0	-2.118987	1.988309	-1.621605
253	8	0	-0.356526	2.289648	-0.497379
254	1	0	-2.173600	1.790335	0.474481
255	8	0	-5.460909	3.511138	-1.782476
256	6	0	-3.526602	2.038134	-1.847126
257	1	0	-3.574595	4.142173	-2.560180
258	6	0	-3.957674	6.521819	-0.576590
259	6	0	-6.132009	3.984711	-2.873328
260	6	0	-3.744540	1.415987	-3.244367
261	1	0	-4.049392	1.426641	-1.064689
262	6	0	-3.569183	6.765682	-2.013444
263	8	0	-4.213048	7.359166	0.266029
264	6	0	-7.615272	4.151552	-2.621719
265	8	0	-5.531694	4.224628	-3.902611
266	8	0	-4.292681	0.111218	-3.107635
267	1	0	-4.549540	1.928990	-3.799028
268	1	0	-2.828290	1.443770	-3.867121
269	1	0	-3.227409	5.821532	-2.492628
270	1	0	-2.690049	7.442474	-2.029045
271	6	0	-4.715577	7.360456	-2.819711
272	1	0	-8.155895	4.034147	-3.582543
273	1	0	-7.996342	3.351645	-1.956029
274	6	0	-7.883101	5.523804	-2.018066
275	6	0	-3.488630	-0.990411	-3.128580
276	1	0	-5.660457	6.806922	-2.609569
277	1	0	-4.512678	7.193720	-3.897141
278	6	0	-4.920894	8.845073	-2.568135
279	1	0	-7.501566	5.561077	-0.977528
280	1	0	-7.308643	6.305228	-2.569816
281	6	0	-9.364933	5.857488	-2.042033

282	6	0	-4.186924	-2.257741	-2.682525
283	8	0	-2.331866	-0.893747	-3.495056
284	1	0	-5.039188	9.041355	-1.483248
285	1	0	-4.017647	9.409696	-2.875257
286	6	0	-6.139524	9.359371	-3.319281
287	1	0	-9.752021	5.803936	-3.079865
288	1	0	-9.934938	5.096718	-1.471999
289	6	0	-9.620632	7.241824	-1.466525
290	1	0	-3.416328	-3.050709	-2.504539
291	1	0	-4.666501	-2.083075	-1.696671
292	6	0	-5.223306	-2.746397	-3.682306
293	1	0	-7.042511	8.794423	-3.003760
294	1	0	-6.028371	9.158775	-4.403476
295	6	0	-6.348502	10.838177	-3.085049
296	1	0	-9.247420	7.291391	-0.424150
297	1	0	-9.032235	7.997377	-2.027823
298	6	0	-11.090078	7.594461	-1.507606
299	1	0	-5.782786	-3.585072	-3.217344
300	1	0	-5.971672	-1.946904	-3.854306
301	6	0	-4.647369	-3.187790	-5.021414
302	1	0	-6.498199	11.062088	-2.020381
303	1	0	-7.229723	11.206586	-3.625469
304	1	0	-5.485680	11.427305	-3.423323
305	1	0	-11.478995	7.593097	-2.534641
306	1	0	-11.271203	8.592874	-1.089643
307	1	0	-11.693945	6.882126	-0.929750
308	1	0	-3.920521	-2.436089	-5.389959
309	1	0	-5.470648	-3.193754	-5.763359
310	6	0	-4.003167	-4.567493	-5.002626
311	1	0	-4.583512	-5.261943	-4.350662
312	1	0	-4.056093	-5.009201	-6.017622
313	6	0	-2.560503	-4.534011	-4.554617
314	1	0	-1.917766	-4.006724	-5.270899
315	1	0	-2.453156	-4.020220	-3.578737
316	1	0	-2.148890	-5.554345	-4.419578
317	1	0	2.570377	-6.737212	-3.027069
318	1	0	4.281387	-2.899672	-4.036204

**Monomer 17 (17-M)**

1	6	0	-0.334382	1.815187	-2.249247
2	6	0	0.299020	0.622238	-1.630438
3	1	0	0.378994	2.402018	-2.859654
4	1	0	-0.750022	2.484164	-1.467867
5	7	0	1.638262	0.245455	-1.838677
6	6	0	-0.286901	-0.355026	-0.843190
7	7	0	1.891278	-0.851595	-1.246692
8	7	0	0.735781	-1.281793	-0.630891
9	6	0	0.648238	-2.482546	0.228682
10	6	0	1.523959	-2.356834	1.440625
11	1	0	-0.411907	-2.619710	0.528584
12	1	0	0.929268	-3.369973	-0.386670
13	6	0	2.593764	-3.226888	1.685382
14	6	0	1.273331	-1.316319	2.332663
15	6	0	3.437400	-2.983172	2.769525
16	6	0	2.854898	-4.425463	0.818510
17	6	0	2.120656	-1.063859	3.412363
18	1	0	0.392944	-0.673361	2.178198
19	6	0	3.223296	-1.900278	3.626737

20	1	0	4.292861	-3.653366	2.946508
21	7	0	2.270131	-5.651365	1.410814
22	1	0	2.404411	-4.293895	-0.194686
23	6	0	1.795171	0.103426	4.301424
24	6	0	4.157384	-1.715331	4.788202
25	6	0	0.999117	-6.178740	1.123463
26	7	0	2.806694	-6.307722	2.488025
27	7	0	1.754231	1.379752	3.555496
28	1	0	2.531557	0.202733	5.130714
29	1	0	0.795201	-0.052771	4.781380
30	7	0	5.527359	-1.339654	4.378916
31	1	0	3.779591	-0.930814	5.483284
32	1	0	4.202258	-2.659392	5.372593
33	6	0	0.826489	-7.185684	2.056419
34	7	0	1.987200	-7.204709	2.859032
35	7	0	2.877265	2.062828	3.144902
36	6	0	0.617469	1.945058	2.962141
37	6	0	5.923528	-0.199593	3.668493
38	7	0	6.638694	-2.048795	4.779695
39	6	0	-0.277800	-8.161795	2.283324
40	7	0	2.508155	3.012293	2.384817
41	6	0	1.109167	3.004880	2.219278
42	6	0	7.306120	-0.275819	3.649190
43	7	0	7.669365	-1.441772	4.352370
44	1	0	0.007758	-9.165271	1.916184
45	1	0	-0.517811	-8.238912	3.362315
46	6	0	0.354856	3.962223	1.365048
47	6	0	8.315924	0.638291	3.052367
48	1	0	0.584154	3.784258	0.295926
49	1	0	8.403903	1.568213	3.657369
50	1	0	9.313249	0.160129	3.004884
51	1	0	5.245914	0.540049	3.234697
52	1	0	-0.419311	1.606298	3.133262
53	1	0	0.350805	-5.844582	0.302300
54	1	0	-1.315593	-0.450010	-0.480504
55	1	0	3.951334	-4.566829	0.646771
56	1	0	9.146786	4.819928	2.910224
57	6	0	9.814965	3.966415	3.141491
58	6	0	10.688864	3.684379	1.927136
59	1	0	9.137554	3.102717	3.338454
60	6	0	10.629040	4.280809	4.386126
61	6	0	11.254717	2.284527	1.957575
62	1	0	10.102285	3.839956	0.994819
63	1	0	11.530641	4.404226	1.878110
64	1	0	11.333580	3.451903	4.602034
65	1	0	11.264262	5.172413	4.210316
66	6	0	9.723765	4.516012	5.585018
67	8	0	12.184829	1.873343	2.618427
68	8	0	10.796826	1.218352	1.222278
69	1	0	9.088618	3.623600	5.756791
70	1	0	9.019973	5.344899	5.370733
71	6	0	10.525906	4.826513	6.828365
72	6	0	9.803395	1.393985	0.224230
73	1	0	11.207239	4.004671	7.086134
74	1	0	9.871005	4.993591	7.692934
75	1	0	11.138085	5.729239	6.700647
76	6	0	10.266113	0.715596	-1.096980
77	6	0	8.443328	0.721060	0.611210
78	1	0	9.621629	2.485164	0.036295
79	6	0	10.326938	-0.831673	-0.950031

80	1	0	9.505680	0.971901	-1.881149
81	8	0	11.369323	1.361584	-1.696278
82	8	0	8.540730	-0.674687	0.739117
83	8	0	7.858439	1.148288	1.802498
84	1	0	7.671583	1.022474	-0.139710
85	8	0	10.534983	-1.331337	-2.276916
86	6	0	8.939883	-1.345092	-0.451689
87	1	0	11.139203	-1.132886	-0.236233
88	6	0	12.668990	1.378008	-1.247293
89	6	0	11.481354	-2.287102	-2.521056
90	6	0	8.964030	-2.845738	-0.070790
91	1	0	8.173088	-1.149277	-1.245537
92	6	0	13.356935	0.348292	-0.386032
93	8	0	13.169403	2.364421	-1.748910
94	6	0	11.753413	-2.478988	-3.997486
95	8	0	12.004209	-2.875629	-1.596186
96	8	0	8.011168	-3.567979	-0.836106
97	1	0	9.902367	-3.338708	-0.381191
98	1	0	8.843844	-3.003476	1.020893
99	1	0	12.611599	-0.324162	0.093194
100	1	0	13.865645	0.871527	0.449904
101	6	0	14.356522	-0.479546	-1.182219
102	1	0	12.079680	-3.525012	-4.167155
103	1	0	10.827946	-2.346778	-4.592252
104	6	0	12.827507	-1.499893	-4.452752
105	6	0	6.732082	-3.722098	-0.376227
106	1	0	13.902274	-0.807657	-2.146279
107	1	0	14.564163	-1.414797	-0.623575
108	6	0	15.662485	0.250153	-1.449883
109	1	0	12.421183	-0.468164	-4.461286
110	1	0	13.665585	-1.479546	-3.716256
111	6	0	13.357236	-1.862847	-5.829489
112	6	0	5.789320	-4.298748	-1.411832
113	8	0	6.449675	-3.429438	0.767682
114	1	0	15.467286	1.230020	-1.930787
115	1	0	16.168275	0.485080	-0.491766
116	6	0	16.578247	-0.582775	-2.333846
117	1	0	13.747645	-2.900824	-5.827371
118	1	0	12.530984	-1.856900	-6.568328
119	6	0	14.452304	-0.900381	-6.262465
120	1	0	6.226409	-5.210976	-1.862890
121	1	0	4.857646	-4.623298	-0.890049
122	6	0	5.475751	-3.264105	-2.483536
123	1	0	16.069555	-0.810110	-3.294913
124	1	0	16.769793	-1.566104	-1.860079
125	6	0	17.885929	0.128185	-2.598257
126	1	0	14.058876	0.135599	-6.278453
127	1	0	15.268326	-0.895712	-5.510003
128	6	0	15.003114	-1.265989	-7.621966
129	1	0	5.054452	-2.351897	-2.013309
130	1	0	6.418411	-2.941626	-2.970144
131	6	0	4.520616	-3.785664	-3.546301
132	1	0	17.728337	1.091627	-3.101256
133	1	0	18.543907	-0.473089	-3.238463
134	1	0	18.430890	0.332485	-1.666997
135	1	0	15.437245	-2.274736	-7.625894
136	1	0	15.791489	-0.568410	-7.932092
137	1	0	14.222884	-1.244084	-8.394469
138	1	0	4.906342	-4.727710	-3.983544
139	1	0	4.492366	-3.056349	-4.384200

140	6	0	3.111433	-3.994160	-3.013478
141	1	0	3.064779	-4.921979	-2.406232
142	1	0	2.849102	-3.170912	-2.316551
143	6	0	2.085063	-4.059245	-4.119879
144	1	0	2.120752	-3.170571	-4.772502
145	1	0	2.207534	-4.945801	-4.766119
146	1	0	1.066922	-4.123382	-3.698418
147	1	0	-0.261200	6.157436	-3.859324
148	6	0	-1.104806	5.676748	-3.323978
149	6	0	-1.369199	6.445126	-2.035750
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152	6	0	-1.984458	5.598579	-0.949427
153	1	0	-0.421066	6.888847	-1.656933
154	1	0	-2.051601	7.309350	-2.225321
155	1	0	-3.161831	5.112486	-3.727097
156	1	0	-2.689982	6.678026	-4.411361
157	6	0	-2.026464	4.972953	-5.565504
158	8	0	-2.669582	4.602471	-1.065196
159	8	0	-1.863689	5.838056	0.391275
160	1	0	-1.805515	3.884224	-5.424399
161	1	0	-1.110244	5.405517	-6.013218
162	6	0	-3.192966	5.120952	-6.517662
163	6	0	-1.015259	6.867421	0.875251
164	1	0	-4.101860	4.650218	-6.115896
165	1	0	-2.978968	4.648234	-7.484916
166	1	0	-3.427589	6.176984	-6.710569
167	6	0	-1.810948	7.996076	1.580928
168	6	0	-0.084331	6.283877	1.995308
169	1	0	-0.385501	7.293072	0.050908
170	6	0	-2.622947	7.427153	2.776734
171	1	0	-1.062523	8.742761	1.958840
172	8	0	-2.495529	8.878431	0.705142
173	8	0	-0.820798	5.729787	3.058821
174	8	0	0.809745	5.290481	1.609748
175	1	0	0.618804	7.083135	2.338102
176	8	0	-3.112545	8.579655	3.472754
177	6	0	-1.665574	6.652848	3.739959
178	1	0	-3.440192	6.749040	2.422240
179	6	0	-3.729742	8.638725	0.158503
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181	6	0	-2.498491	5.799976	4.723703
182	1	0	-1.012734	7.376210	4.289567
183	6	0	-4.347311	9.889086	-0.435626
184	8	0	-4.218640	7.530888	0.189753
185	6	0	-4.817344	10.107293	4.167914
186	8	0	-5.142505	7.701245	3.813720
187	8	0	-1.752931	5.498140	5.893072
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189	1	0	-2.925953	4.903977	4.226912
190	1	0	-4.403849	10.661412	0.368726
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192	6	0	-3.586393	10.418218	-1.640201
193	1	0	-5.524889	10.091461	5.020741
194	1	0	-3.932523	10.678227	4.516447
195	6	0	-5.450626	10.790602	2.963894
196	6	0	-1.201529	4.259058	6.063305
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198	1	0	-3.994143	11.415440	-1.903138
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205	1	0	-3.217988	8.508235	-2.610118
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207	6	0	-3.036846	10.098850	-4.071557
208	1	0	-6.420900	12.342265	4.124564
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210	6	0	-6.353278	12.938424	2.042100
211	1	0	0.363961	3.387143	7.250486
212	1	0	-0.003492	5.075290	7.665449
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214	1	0	-1.952982	10.239852	-3.888664
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221	1	0	-2.302879	4.291138	8.511160
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224	1	0	-2.730711	9.645303	-6.168242
225	1	0	-4.315757	9.155756	-5.552869
226	1	0	-7.290054	14.554637	3.148506
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228	1	0	-5.674343	14.940395	2.541295
229	1	0	-2.144842	1.954570	7.317150
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252	1	0	2.491436	0.260647	-5.114872
253	1	0	2.979683	0.901906	-6.685852
254	6	0	3.123182	-1.246716	-6.518102
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256	1	0	2.649388	-2.089857	-5.985247
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265	8	0	-3.141834	1.112844	-2.086262
266	8	0	-1.311436	1.320091	-3.163238
267	1	0	-2.577465	2.994727	-2.841914
268	8	0	-6.701608	1.504141	-2.905069
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271	6	0	-5.831113	0.689458	-6.230683
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273	6	0	-4.915085	0.582176	-0.597522
274	1	0	-4.613742	2.512539	-1.601581
275	6	0	-5.712982	-0.751199	-5.801092
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287	6	0	-9.628559	0.930702	-4.131690
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295	6	0	-3.170761	1.837473	2.470819
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299	6	0	-9.108406	-2.338710	-6.803760
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323	6	0	-2.988187	0.254850	5.355047
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326	6	0	-1.734062	-0.258206	4.686047
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329	1	0	-0.870057	-0.260566	5.380602
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331	6	0	-0.455416	-6.244566	-2.906978
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334	6	0	-1.055236	-6.264765	-4.303391
335	6	0	-2.460157	-6.862685	-1.472190
336	1	0	-0.879455	-5.508654	-0.919179
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338	1	0	-1.913531	-6.965834	-4.344868
339	1	0	-1.479856	-5.263616	-4.549561
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342	8	0	-3.179742	-6.847603	-0.304885
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345	6	0	-0.610344	-6.630735	-6.736281
346	6	0	-2.779647	-6.016657	0.774886
347	1	0	-1.437413	-7.345954	-6.839677
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355	8	0	-4.353429	-4.155953	0.425478
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359	8	0	-6.118671	-5.353413	2.364158
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361	1	0	-5.455905	-6.854485	1.011067
362	6	0	-5.127900	-4.288439	-0.698539
363	6	0	-7.434503	-5.632614	2.090955
364	6	0	-5.365371	-8.147538	3.500250
365	1	0	-4.131248	-6.351326	3.808456
366	6	0	-5.098684	-3.023068	-1.531459
367	8	0	-5.755796	-5.301385	-0.910286
368	6	0	-8.339515	-4.445858	2.349814
369	8	0	-7.760123	-6.735054	1.707827
370	8	0	-6.166632	-7.718979	4.589911
371	1	0	-6.141972	-8.427843	2.764697
372	1	0	-4.792624	-9.059242	3.763261
373	1	0	-4.778928	-2.149583	-0.914572
374	1	0	-6.133768	-2.789728	-1.858567
375	6	0	-4.173003	-3.163052	-2.732520
376	1	0	-9.256772	-4.794527	2.864294
377	1	0	-7.861196	-3.719641	3.037446
378	6	0	-8.689126	-3.777451	1.027577
379	6	0	-5.652912	-7.701172	5.857408

380	1	0	-3.238360	-3.700978	-2.447375
381	1	0	-3.849329	-2.149471	-3.051418
382	6	0	-4.841631	-3.868122	-3.902047
383	1	0	-7.760514	-3.475545	0.499686
384	1	0	-9.189682	-4.504280	0.356063
385	6	0	-9.582243	-2.565041	1.236448
386	6	0	-6.683343	-7.326813	6.900907
387	8	0	-4.480047	-7.960120	6.039571
388	1	0	-5.167652	-4.884572	-3.603212
389	1	0	-5.774427	-3.326709	-4.189487
390	6	0	-3.908725	-3.943319	-5.100027
391	1	0	-10.524658	-2.864711	1.736746
392	1	0	-9.094595	-1.846385	1.925785
393	6	0	-9.886175	-1.888656	-0.090846
394	1	0	-6.166427	-6.917793	7.799962
395	1	0	-7.329182	-6.515522	6.512948
396	6	0	-7.530058	-8.524235	7.314006
397	1	0	-2.980803	-4.496002	-4.825638
398	1	0	-3.574736	-2.923110	-5.384419
399	6	0	-4.576855	-4.611299	-6.279713
400	1	0	-8.937358	-1.632106	-0.606061
401	1	0	-10.405516	-2.598841	-0.764883
402	6	0	-10.722810	-0.642393	0.086972
403	1	0	-8.469029	-8.156825	7.774484
404	1	0	-7.841102	-9.102136	6.421868
405	6	0	-6.806085	-9.434003	8.295729
406	1	0	-4.942982	-5.614969	-6.026051
407	1	0	-3.878681	-4.718034	-7.120132
408	1	0	-5.437986	-4.027004	-6.637228
409	1	0	-11.731800	-0.874323	0.450846
410	1	0	-10.828906	-0.101841	-0.869801
411	1	0	-10.268808	0.054625	0.804068
412	1	0	-5.853898	-9.788338	7.851274
413	1	0	-7.411101	-10.344696	8.473370
414	6	0	-6.530163	-8.729447	9.615534
415	1	0	-6.034150	-7.754154	9.404923
416	1	0	-7.485523	-8.474340	10.115183
417	6	0	-5.672823	-9.572223	10.530366
418	1	0	-6.152686	-10.532544	10.761386
419	1	0	-4.696555	-9.795378	10.079533
420	1	0	-5.485397	-9.060694	11.482968

**15-D**

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4	6	0	-1.141397	-1.572538	-2.262473
5	6	0	-1.832060	-2.159079	-3.323174
6	6	0	-2.379586	-1.355934	-4.324301
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17	6	0	-8.602442	-6.688832	-2.413797
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19	6	0	-8.052469	-5.551226	-1.498729
20	8	0	-11.734077	-3.593338	0.710389
21	1	0	-11.530956	-5.520187	1.001315
22	1	0	-10.087464	-4.598537	1.521779
23	8	0	-8.651244	-7.942667	-1.747772
24	1	0	-7.968217	-6.755587	-3.337506
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26	1	0	-7.931093	-4.615613	-2.102052
27	6	0	-5.946510	-4.951591	-0.546840
28	6	0	-5.006660	-4.663967	-1.667279
29	1	0	-6.428123	-4.011462	-0.210867
30	1	0	-5.399671	-5.388773	0.308031
31	7	0	-5.327138	-4.747272	-3.033112
32	6	0	-3.685275	-4.251273	-1.586522
33	7	0	-4.324318	-4.422607	-3.751619
34	7	0	-3.283085	-4.114656	-2.920038
35	6	0	-1.961370	-3.650130	-3.399616
36	1	0	-1.183264	-4.145419	-2.782758
37	1	0	-1.815274	-3.994939	-4.444499
38	6	0	-4.032058	3.685561	-1.187934
39	7	0	-4.500254	3.711910	-2.513765
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42	7	0	-2.572953	2.774458	-2.557981
43	6	0	-1.390515	2.101072	-3.140839
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45	1	0	-1.215058	2.504824	-4.159717
46	6	0	-4.783180	4.188483	-0.003456
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49	6	0	10.732979	0.268055	0.889150
50	6	0	9.363036	-0.026931	0.394861
51	1	0	10.821592	0.124469	1.982416
52	1	0	11.000905	1.317410	0.655641
53	7	0	8.280077	-0.309431	1.243925
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55	7	0	7.230601	-0.555581	0.563264
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60	1	0	6.325249	-1.807824	-1.840758
61	6	0	4.176885	-0.405481	-1.343937
62	6	0	5.442955	1.487923	-2.138334
63	6	0	3.049841	0.397174	-1.219506
64	6	0	4.326239	2.300073	-1.978563
65	1	0	6.375625	1.927318	-2.530362
66	6	0	3.132809	1.763784	-1.494429
67	1	0	2.102040	-0.046689	-0.883800
68	6	0	1.956511	2.656519	-1.244513
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74	6	0	1.679574	2.470522	2.387858
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77	1	0	2.222210	3.245880	4.320652
78	1	0	1.245664	1.737522	4.370486
79	1	0	3.586813	2.493390	1.186515
80	1	0	-3.050246	-4.057352	-0.721369
81	1	0	9.425557	0.020662	-1.859102
82	1	0	-2.086040	2.855048	-0.397632
83	6	0	-11.249252	-2.324009	0.880033
84	6	0	-12.340421	-1.277163	0.936416
85	1	0	-11.896650	-0.270968	0.724469
86	1	0	-13.071066	-1.465482	0.125204
87	6	0	-13.051855	-1.264679	2.281681
88	1	0	-13.970068	-0.649644	2.190591
89	1	0	-13.404073	-2.288364	2.520016
90	6	0	-12.196402	-0.745141	3.429536
91	1	0	-11.171112	-1.161491	3.360921
92	1	0	-12.614761	-1.139251	4.377122
93	6	0	-12.137394	0.774013	3.520978
94	1	0	-13.133394	1.208836	3.302215
95	1	0	-11.913850	1.062676	4.567398
96	6	0	-11.096567	1.383048	2.609402
97	1	0	-10.088780	1.009963	2.835010
98	1	0	-11.297107	1.151391	1.544340
99	1	0	-11.071978	2.476121	2.703856
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101	6	0	-13.327312	-5.973978	-1.415526
102	6	0	-14.547609	-5.538465	-2.196825
103	1	0	-15.129708	-4.829250	-1.575209
104	1	0	-14.262323	-4.978316	-3.110956
105	6	0	-15.390626	-6.751811	-2.562245
106	1	0	-14.763345	-7.503021	-3.097126
107	1	0	-15.737017	-7.267259	-1.642063
108	6	0	-16.581775	-6.357913	-3.418475
109	1	0	-17.205079	-5.614196	-2.882305
110	1	0	-16.238194	-5.848691	-4.341490
111	6	0	-17.418735	-7.575430	-3.778971
112	1	0	-16.795377	-8.311557	-4.325294
113	1	0	-17.746436	-8.094237	-2.855543
114	6	0	-18.619837	-7.193169	-4.613553
115	1	0	-19.277578	-6.493491	-4.080781
116	1	0	-19.220110	-8.074265	-4.873671
117	1	0	-18.322490	-6.709373	-5.553517
118	8	0	-13.297200	-6.643756	-0.402621
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121	6	0	-14.869706	-10.613926	-1.517353
122	1	0	-14.833930	-12.192521	-0.027014
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124	6	0	-13.401730	-10.238704	-1.384580
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126	1	0	-15.469720	-9.707293	-1.745808
127	6	0	-12.895652	-9.569375	-2.651488
128	1	0	-12.795633	-11.139631	-1.162353
129	1	0	-13.264003	-9.563044	-0.515345
130	6	0	-11.447459	-9.125169	-2.499115
131	1	0	-12.995135	-10.258289	-3.514060
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134	1	0	-11.322239	-8.511981	-1.579766
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139	6	0	-6.683244	-11.450250	-5.526080
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143	1	0	-6.671876	-12.322442	-4.842379
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145	6	0	-6.098935	-9.940310	-3.608188
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157	6	0	-8.104531	5.272926	-2.735265
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163	1	0	-10.353264	4.458213	-1.416023
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165	6	0	-9.997311	2.360518	-1.025085
166	8	0	-9.369090	6.877587	-1.378964
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173	1	0	-11.602115	1.164684	-0.187971
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242	6	0	-1.557448	10.194583	7.263404
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251	6	0	2.292073	4.783727	7.556350
252	6	0	2.257875	1.600891	7.334050
253	1	0	4.376685	2.027492	7.312624
254	1	0	3.494486	2.685101	8.701744
255	1	0	1.310615	4.281947	7.679864

256	1	0	2.636917	5.017605	8.583843
257	6	0	2.117663	6.068458	6.761772
258	8	0	1.142948	1.647556	7.808179
259	8	0	2.267527	0.529505	6.473641
260	1	0	1.775542	5.832732	5.733586
261	1	0	3.095716	6.575310	6.641104
262	6	0	1.131745	6.997100	7.432486
263	6	0	3.470448	0.096608	5.856464
264	1	0	0.143860	6.529489	7.541392
265	1	0	0.990364	7.924601	6.851607
266	1	0	1.467023	7.288208	8.436679
267	6	0	3.630377	-1.437186	6.052855
268	6	0	3.449864	0.322690	4.310338
269	1	0	4.357112	0.629829	6.290587
270	6	0	2.470437	-2.192228	5.345919
271	1	0	4.603053	-1.740800	5.583882
272	8	0	3.949336	-1.793680	7.379587
273	8	0	2.408312	-0.368744	3.665106
274	8	0	3.324300	1.651155	3.898868
275	1	0	4.450692	0.051540	3.891248
276	8	0	2.805265	-3.581249	5.432051
277	6	0	2.432128	-1.783428	3.839691
278	1	0	1.489540	-1.954886	5.839513
279	6	0	3.131351	-1.665687	8.480966
280	6	0	1.852358	-4.503833	5.772908
281	6	0	1.138271	-2.276729	3.134822
282	1	0	3.346450	-2.189219	3.312860
283	6	0	1.646236	-1.917555	8.539589
284	8	0	3.863561	-1.423519	9.417334
285	6	0	2.440873	-5.865171	6.070751
286	8	0	0.683247	-4.177293	5.806172
287	8	0	1.446455	-3.397020	2.322212
288	1	0	0.403557	-2.698696	3.843818
289	1	0	0.632481	-1.465207	2.573229
290	1	0	1.203800	-2.005086	7.523341
291	1	0	1.151344	-1.038356	9.001538
292	6	0	1.370324	-3.173886	9.354814
293	1	0	2.085450	-6.579489	5.301471
294	1	0	3.547054	-5.855156	5.989575
295	6	0	2.015454	-6.314837	7.460843
296	6	0	1.816225	-3.183376	1.014006
297	1	0	1.753401	-3.049869	10.387527
298	1	0	1.933325	-4.036091	8.927289
299	6	0	-0.114172	-3.497758	9.382369
300	1	0	2.314655	-5.549351	8.214775
301	1	0	0.907908	-6.365403	7.522197
302	6	0	2.616451	-7.662486	7.819602
303	6	0	2.959575	-4.061788	0.560294
304	8	0	1.204665	-2.368753	0.354112
305	1	0	-0.679666	-2.653920	9.825827
306	1	0	-0.499544	-3.606045	8.347478
307	6	0	-0.378557	-4.773779	10.167191
308	1	0	2.308846	-8.426009	7.077045
309	1	0	3.722599	-7.617657	7.760537
310	6	0	2.186860	-8.089138	9.215085
311	1	0	2.890972	-5.063698	1.029594
312	1	0	2.903181	-4.229933	-0.533496
313	6	0	4.267643	-3.375507	0.938262
314	1	0	0.001897	-4.666342	11.202422
315	1	0	0.197297	-5.615520	9.724832

316	6	0	-1.851804	-5.111886	10.188907
317	1	0	2.511145	-7.330889	9.956283
318	1	0	1.079712	-8.106630	9.279599
319	6	0	2.750828	-9.443876	9.577508
320	1	0	4.367684	-2.425348	0.362995
321	1	0	4.227190	-3.068379	2.011604
322	6	0	5.478832	-4.258136	0.691035
323	1	0	-2.443810	-4.312167	10.653579
324	1	0	-2.040575	-6.032109	10.756265
325	1	0	-2.247200	-5.263276	9.175550
326	1	0	2.411663	-10.223298	8.882179
327	1	0	2.441158	-9.746551	10.585885
328	1	0	3.848814	-9.444147	9.557248
329	1	0	5.320749	-5.267120	1.124636
330	1	0	6.351267	-3.840291	1.236153
331	6	0	5.819151	-4.376422	-0.787885
332	1	0	4.982815	-4.854484	-1.335998
333	1	0	5.922812	-3.361146	-1.236743
334	6	0	7.093382	-5.161852	-0.996195
335	1	0	7.941269	-4.713409	-0.447442
336	1	0	6.996551	-6.195309	-0.634257
337	1	0	7.369387	-5.206965	-2.056686
338	1	0	11.328245	-3.396622	2.838493
339	6	0	11.375902	-3.739009	1.785169
340	6	0	12.830592	-3.749307	1.333887
341	1	0	10.800249	-2.988882	1.205270
342	6	0	10.722367	-5.107481	1.668561
343	6	0	12.948839	-3.607409	-0.164525
344	1	0	13.392696	-2.932755	1.838605
345	1	0	13.327413	-4.692090	1.639701
346	1	0	10.916683	-5.543797	0.667727
347	1	0	11.183610	-5.808484	2.393250
348	6	0	9.223712	-5.018219	1.907170
349	8	0	12.681151	-4.427680	-1.016993
350	8	0	13.416809	-2.499713	-0.826471
351	1	0	8.743820	-4.448133	1.076882
352	1	0	9.016298	-4.438933	2.828398
353	6	0	8.589987	-6.387631	2.002844
354	6	0	13.897606	-1.369015	-0.115522
355	1	0	8.777136	-6.981652	1.097407
356	1	0	7.499645	-6.307769	2.118280
357	1	0	8.974888	-6.958973	2.857231
358	6	0	15.151548	-0.817718	-0.853802
359	6	0	12.865454	-0.198091	-0.097516
360	1	0	14.157909	-1.647319	0.939592
361	6	0	14.767483	-0.312720	-2.275025
362	1	0	15.544778	0.045999	-0.256266
363	8	0	16.277993	-1.656261	-0.725564
364	8	0	12.539346	0.260881	-1.389331
365	8	0	11.607269	-0.680551	0.275476
366	1	0	13.251245	0.631278	0.549444
367	8	0	15.946931	0.309785	-2.795119
368	6	0	13.644148	0.763282	-2.134494
369	1	0	14.410651	-1.162329	-2.916862
370	6	0	16.436892	-2.910714	-1.270615
371	6	0	16.338893	0.075919	-4.086573
372	6	0	13.065143	1.154526	-3.512150
373	1	0	14.053847	1.662567	-1.608482
374	6	0	15.896026	-3.405666	-2.587597
375	8	0	17.188032	-3.503309	-0.524648

376	6	0	17.741030	0.567745	-4.369209
377	8	0	15.571124	-0.465044	-4.856745
378	8	0	12.478749	2.446958	-3.449885
379	1	0	13.876271	1.314687	-4.244615
380	1	0	12.385968	0.373893	-3.908446
381	1	0	15.178975	-2.682871	-3.034659
382	1	0	15.307918	-4.329324	-2.407929
383	6	0	17.045975	-3.682416	-3.546467
384	1	0	17.682256	1.405840	-5.092182
385	1	0	18.214801	0.985059	-3.457061
386	6	0	18.583425	-0.568545	-4.930383
387	6	0	11.122201	2.604349	-3.426562
388	1	0	17.707344	-4.469408	-3.131894
389	1	0	17.685899	-2.774687	-3.644333
390	6	0	16.534230	-4.096079	-4.916206
391	1	0	18.576323	-1.430837	-4.223298
392	1	0	18.127270	-0.956031	-5.865527
393	6	0	20.010982	-0.123137	-5.195443
394	6	0	10.712856	4.057243	-3.302594
395	8	0	10.392244	1.636328	-3.512298
396	1	0	15.926608	-5.019225	-4.832318
397	1	0	15.848457	-3.321381	-5.316996
398	6	0	17.687081	-4.314348	-5.884317
399	1	0	20.018383	0.723078	-5.911625
400	1	0	20.469673	0.269264	-4.265522
401	6	0	20.843129	-1.274296	-5.739558
402	1	0	9.881894	4.132909	-2.564987
403	1	0	11.546379	4.657397	-2.885588
404	6	0	10.281777	4.641639	-4.641303
405	1	0	18.372450	-5.089230	-5.487023
406	1	0	18.297048	-3.388261	-5.959197
407	6	0	17.188567	-4.716358	-7.253642
408	1	0	20.852112	-2.109061	-5.009938
409	1	0	20.365178	-1.686759	-6.651379
410	6	0	22.257583	-0.837760	-6.045560
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412	1	0	11.027185	4.372046	-5.415936
413	6	0	8.897271	4.200845	-5.097385
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415	1	0	18.021869	-4.873839	-7.950163
416	1	0	16.536864	-3.947056	-7.689025
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420	1	0	8.764766	3.113208	-4.927895
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422	6	0	7.754307	4.973055	-4.451449
423	1	0	8.012568	6.048670	-4.378633
424	1	0	6.869175	4.927194	-5.116949
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2	6	0	-4.797099	-2.516628	0.040017
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5	7	0	-4.052955	-3.581527	-0.496130
6	6	0	-3.903449	-1.497632	0.332053
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9	6	0	-1.363191	-1.304088	0.052521
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22	1	0	-1.109712	1.710189	-5.039598
23	1	0	-1.725869	2.458570	-3.537176
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26	1	0	2.459000	-2.520559	-2.937607
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28	6	0	-4.180830	1.282037	-3.662026
29	6	0	0.557242	-4.335011	-4.032611
30	7	0	1.326225	-3.303148	-5.900608
31	7	0	-4.559385	-0.134052	-5.365616
32	6	0	-5.155791	0.501996	-4.257552
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35	6	0	-6.563016	0.300622	-3.821866
36	6	0	-0.620894	-6.286790	-5.290066
37	1	0	-6.683669	-0.708175	-3.382525
38	1	0	-0.916877	-6.480594	-6.344306
39	1	0	-0.054308	-7.164352	-4.923966
40	1	0	0.349431	-4.521121	-2.974206
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47	6	0	-2.124448	-8.870791	-8.695010
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86	1	0	-1.160172	-10.890707	-2.474039
87	1	0	-1.674036	-12.237022	-3.501083
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91	6	0	-3.044043	-11.302819	1.821682
92	6	0	0.072369	-5.481942	1.152933
93	1	0	-2.104027	-12.256053	-0.437501
94	1	0	-0.588145	-12.775639	-1.184169
95	6	0	-2.262854	-14.067368	-1.618960
96	1	0	-3.880064	-10.932936	1.193584
97	1	0	-2.568158	-12.118251	1.227024
98	6	0	-3.584286	-11.851530	3.131195
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103	6	0	-2.110342	-14.948962	-0.388769
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113	1	0	-5.382009	-12.670386	2.246148
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115	6	0	-5.069981	-13.573676	4.182046
116	1	0	-2.371250	-5.600204	2.428407
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122	1	0	-4.260066	-13.953603	4.819018
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124	1	0	-5.612989	-12.816062	4.762743
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137	1	0	-9.169835	-2.312449	-1.071484
138	6	0	-11.055431	-2.187598	-0.006497
139	6	0	-9.645768	0.148242	-1.893812
140	1	0	-10.408065	-1.318644	-3.261756
141	1	0	-11.593901	-0.703429	-2.090282
142	1	0	-10.768382	-1.294054	0.586983
143	1	0	-12.137566	-2.055421	-0.243137
144	6	0	-10.870588	-3.443471	0.832199
145	8	0	-9.087383	0.427619	-0.852116
146	8	0	-9.332718	1.134536	-2.787549
147	1	0	-9.850528	-3.460883	1.293753
148	1	0	-10.923330	-4.345876	0.192065
149	6	0	-11.908752	-3.523130	1.930055
150	6	0	-9.711608	1.029110	-4.151619
151	1	0	-11.851001	-2.655985	2.603194
152	1	0	-11.769859	-4.423797	2.542163
153	1	0	-12.928918	-3.554581	1.522688
154	6	0	-10.681253	2.163658	-4.571335
155	6	0	-8.449695	1.233434	-5.062673
156	1	0	-10.167844	0.027941	-4.368113
157	6	0	-10.021554	3.554237	-4.359659
158	1	0	-10.907652	2.020218	-5.661577
159	8	0	-12.012710	2.009278	-4.105247
160	8	0	-7.829776	2.476198	-4.832775
161	8	0	-7.441060	0.283432	-4.942770
162	1	0	-8.747315	1.099418	-6.132256
163	8	0	-10.910451	4.484718	-4.989238
164	6	0	-8.652263	3.604899	-5.113686
165	1	0	-9.866555	3.764386	-3.270994
166	6	0	-12.452316	2.361964	-2.855855
167	6	0	-11.340190	5.603295	-4.324729
168	6	0	-7.846235	4.834882	-4.639350
169	1	0	-8.826184	3.641704	-6.218075
170	6	0	-13.965345	2.377720	-2.764067
171	8	0	-11.668769	2.634590	-1.973258
172	6	0	-12.561381	6.216583	-4.976140
173	8	0	-10.740622	5.995704	-3.346893
174	8	0	-6.852125	5.195424	-5.587104
175	1	0	-8.488414	5.734356	-4.636785
176	1	0	-7.449051	4.688212	-3.612669
177	1	0	-14.345158	3.108372	-3.518246
178	1	0	-14.258512	2.786580	-1.775243

179	6	0	-14.596138	1.010807	-2.972111
180	1	0	-12.475373	7.320995	-4.944359
181	1	0	-12.614271	5.945672	-6.050441
182	6	0	-13.819115	5.759857	-4.250030
183	6	0	-5.536237	4.910130	-5.349128
184	1	0	-14.271158	0.573564	-3.937114
185	1	0	-15.693943	1.141168	-3.060546
186	6	0	-14.287018	0.051585	-1.832728
187	1	0	-13.852032	4.646368	-4.186646
188	1	0	-13.800214	6.114491	-3.199719
189	6	0	-15.069709	6.267700	-4.948365
190	6	0	-4.602430	5.450620	-6.410577
191	8	0	-5.222177	4.298625	-4.347419
192	1	0	-13.190691	-0.148049	-1.784243
193	1	0	-14.545240	0.518537	-0.860763
194	6	0	-15.040104	-1.259733	-1.993602
195	1	0	-15.056629	7.375125	-4.995552
196	1	0	-15.083395	5.924984	-6.002919
197	6	0	-16.324437	5.791573	-4.232886
198	1	0	-3.667251	4.844299	-6.414491
199	1	0	-5.058183	5.326343	-7.412444
200	6	0	-4.267005	6.915936	-6.166945
201	1	0	-14.708909	-1.771583	-2.919019
202	1	0	-16.121413	-1.061166	-2.135207
203	6	0	-14.838828	-2.162579	-0.797673
204	1	0	-16.316399	4.684754	-4.157022
205	1	0	-16.324705	6.159901	-3.187577
206	6	0	-17.575626	6.253537	-4.944442
207	1	0	-3.767982	7.319503	-7.071272
208	1	0	-5.206814	7.494805	-6.065099
209	6	0	-3.390719	7.159817	-4.945292
210	1	0	-13.769998	-2.367687	-0.613901
211	1	0	-15.338425	-3.129124	-0.939208
212	1	0	-15.242286	-1.715642	0.120846
213	1	0	-17.625902	7.348939	-5.004007
214	1	0	-18.478823	5.911453	-4.423326
215	1	0	-17.623629	5.868679	-5.971880
216	1	0	-3.730349	6.533745	-4.087019
217	1	0	-3.538435	8.209028	-4.620114
218	6	0	-1.904372	6.938305	-5.188858
219	1	0	-1.612396	7.359049	-6.172231
220	1	0	-1.327913	7.515384	-4.437787
221	6	0	-1.492232	5.485521	-5.109109
222	1	0	-1.724024	5.039529	-4.124396
223	1	0	-2.009023	4.875039	-5.867798
224	1	0	-0.406153	5.377064	-5.268621
225	1	0	-6.820488	1.051056	-3.047882
226	1	0	-7.692305	-5.974762	1.937109
227	6	0	-7.219980	-5.397428	2.757886
228	6	0	-8.299300	-4.585144	3.459349
229	1	0	-6.492677	-4.720259	2.264173
230	6	0	-6.490527	-6.350287	3.691094
231	6	0	-7.720988	-3.491619	4.327673
232	1	0	-8.994855	-4.152000	2.695564
233	1	0	-8.924482	-5.241567	4.097395
234	1	0	-6.026873	-5.787853	4.527089
235	1	0	-7.210890	-7.047690	4.164097
236	6	0	-5.422163	-7.133075	2.943828
237	8	0	-7.144058	-3.611968	5.388497
238	8	0	-7.783010	-2.146121	4.069369

239	1	0	-4.721356	-6.433682	2.441473
240	1	0	-5.885318	-7.727285	2.131267
241	6	0	-4.649152	-8.039598	3.873990
242	6	0	-8.499990	-1.657220	2.947595
243	1	0	-4.111679	-7.461941	4.645955
244	1	0	-3.890237	-8.620622	3.322263
245	1	0	-5.300934	-8.757612	4.388374
246	6	0	-9.275078	-0.370526	3.353034
247	6	0	-7.563095	-1.275237	1.758804
248	1	0	-9.235626	-2.429819	2.576226
249	6	0	-8.312774	0.826495	3.606775
250	1	0	-9.949473	-0.113837	2.491509
251	8	0	-10.285084	-0.613920	4.309551
252	8	0	-6.727336	-0.179123	2.045031
253	8	0	-6.558097	-2.235488	1.589786
254	1	0	-8.190605	-1.098971	0.843053
255	8	0	-9.161927	1.969221	3.765337
256	6	0	-7.444714	1.020408	2.325571
257	1	0	-7.664373	0.637092	4.502763
258	6	0	-10.115970	-0.918026	5.639005
259	6	0	-8.941104	2.863844	4.773395
260	6	0	-6.370587	2.119840	2.477217
261	1	0	-8.122397	1.258753	1.462901
262	6	0	-8.919910	-0.615032	6.506536
263	8	0	-11.162119	-1.429982	5.985037
264	6	0	-10.085174	3.838396	4.953593
265	8	0	-7.909027	2.818722	5.413656
266	8	0	-6.360831	2.945086	1.319580
267	1	0	-6.642246	2.852841	3.256672
268	1	0	-5.370589	1.708386	2.726629
269	1	0	-8.052014	-0.304501	5.883548
270	1	0	-8.604710	-1.552880	7.008866
271	6	0	-9.222052	0.466370	7.534838
272	1	0	-9.686037	4.784493	5.371746
273	1	0	-10.538131	4.102075	3.977166
274	6	0	-11.130345	3.237877	5.884300
275	6	0	-5.520016	2.672871	0.280417
276	1	0	-9.762103	1.314514	7.052818
277	1	0	-8.262314	0.894411	7.889054
278	6	0	-10.018352	-0.042015	8.725239
279	1	0	-11.658040	2.405988	5.375177
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281	6	0	-12.129725	4.286693	6.341455
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288	1	0	-12.642021	4.731024	5.464674
289	6	0	-13.151321	3.686239	7.294747
290	1	0	-5.158647	3.074502	-1.800309
291	1	0	-6.864485	3.183273	-1.313575
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293	1	0	-10.968264	1.865318	9.116608
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295	6	0	-11.161924	0.603719	10.858985
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305	1	0	-13.635734	5.544512	8.309647
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320	6	0	16.902360	-5.911321	1.107351
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322	1	0	16.651188	-5.093166	1.813349
323	6	0	18.358416	-6.291421	1.250963
324	6	0	15.122426	-5.059715	-0.436988
325	1	0	16.794201	-6.309304	-1.020160
326	1	0	17.242884	-4.649032	-0.619415
327	1	0	18.626621	-7.123396	0.586234
328	1	0	18.588465	-6.604243	2.277396
329	1	0	19.022912	-5.451858	1.006773
330	6	0	14.799054	-4.609766	-1.855021
331	1	0	14.907666	-4.242871	0.292284
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333	6	0	13.378016	-4.091776	-1.919133
334	1	0	14.911380	-5.454022	-2.564089
335	1	0	15.517870	-3.833697	-2.188629
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338	6	0	12.101631	-2.058859	-1.497850
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341	1	0	11.289120	-2.763710	-1.187348
342	6	0	11.302197	-0.126433	-0.035683
343	1	0	13.351826	-0.460958	-0.651138
344	8	0	13.083640	-1.666595	0.804646
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349	6	0	11.050951	0.633780	-1.384582
350	1	0	11.602001	0.610392	0.754529
351	6	0	12.611916	-2.765718	1.474239
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353	1	0	11.549210	-3.086331	-3.904822
354	1	0	9.937112	-2.456922	-3.427207
355	6	0	9.575052	-0.669242	1.576150
356	8	0	10.076788	1.626741	-1.355532
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358	6	0	13.629464	-3.321017	2.451126

359	8	0	11.504415	-3.203175	1.252831
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361	6	0	10.184590	0.137103	2.695776
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366	6	0	13.953659	-2.365691	3.587852
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368	8	0	8.833705	-0.995186	-4.948331
369	6	0	9.151854	0.696109	3.665819
370	1	0	10.785818	0.967804	2.262798
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373	1	0	8.292149	1.702177	-0.438666
374	1	0	8.486666	0.196075	-1.392631
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376	1	0	14.814548	-2.774201	4.155159
377	6	0	12.773871	-2.163629	4.526611
378	1	0	9.407406	0.383646	-7.153455
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380	6	0	9.776712	-1.563322	-8.045896
381	1	0	9.555581	1.623275	4.120611
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384	6	0	7.100203	1.391967	-3.417276
385	7	0	8.254474	3.263285	-2.954137
386	1	0	11.927552	-1.682330	3.982618
387	1	0	12.385921	-3.144775	4.867543
388	6	0	13.159124	-1.313482	5.727032
389	1	0	10.186832	-1.223447	-9.018638
390	1	0	10.335852	-2.487288	-7.796261
391	6	0	8.299262	-1.896066	-8.204104
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398	1	0	13.463080	-0.302749	5.389174
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419	1	0	5.537905	1.373695	-5.624500
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421	1	0	7.828446	0.829520	-7.704212
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435	1	0	1.338160	4.794082	-3.275725
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443	6	0	4.503434	2.108388	0.824744
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448	7	0	4.361224	8.858320	-5.207377
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454	1	0	5.473994	10.160807	-3.153059
455	1	0	3.858833	10.299194	-2.380243
456	8	0	5.197043	8.739024	-1.797634
457	6	0	5.393603	-0.726254	2.752806
458	6	0	4.633927	8.608619	-0.527955
459	6	0	5.003195	-1.262065	4.166444
460	8	0	4.848424	-1.484215	1.699059
461	1	0	6.512764	-0.660964	2.692475
462	6	0	5.081947	9.678148	0.522164
463	8	0	3.241853	8.609553	-0.730019
464	1	0	5.013327	7.606292	-0.208496
465	8	0	3.622544	-1.096071	4.443953
466	6	0	5.363751	-2.774631	4.212508
467	1	0	5.633763	-0.716271	4.928438
468	6	0	5.276181	-2.843669	1.692897
469	8	0	4.725281	10.993770	0.123555
470	6	0	4.336175	9.313537	1.838097
471	1	0	6.189581	9.594558	0.678820
472	6	0	2.477268	8.310574	0.433750
473	6	0	3.190272	-0.080699	5.257760
474	6	0	4.785213	-3.548087	2.993423
475	1	0	6.485101	-2.838582	4.182149
476	8	0	5.179584	-3.346597	5.491674
477	6	0	4.665091	-3.468611	0.420550
478	1	0	6.396220	-2.884763	1.647325

479	6	0	5.683899	11.908790	-0.236039
480	6	0	2.800210	9.295553	1.602121
481	1	0	4.670280	8.286375	2.141661
482	8	0	4.829121	10.004004	2.965913
483	6	0	1.009193	8.423161	-0.044240
484	1	0	2.712727	7.262911	0.752154
485	6	0	4.065827	0.972652	5.896026
486	8	0	1.991209	-0.225286	5.379193
487	8	0	5.360909	-4.858537	3.063422
488	1	0	3.663516	-3.563667	3.024334
489	6	0	3.991053	-3.671421	6.097936
490	8	0	5.587999	-3.373421	-0.656354
491	1	0	4.568402	-4.564080	0.522640
492	1	0	3.665038	-3.052927	0.185246
493	6	0	7.160868	11.628221	-0.374261
494	8	0	5.104199	12.960148	-0.410192
495	8	0	2.227638	8.762834	2.800228
496	1	0	2.427817	10.329009	1.367688
497	6	0	4.715590	11.352753	3.215019
498	8	0	0.180899	7.481007	0.617007
499	1	0	0.540533	9.377213	0.260299
500	1	0	0.932679	8.343544	-1.148411
501	6	0	3.834621	2.354601	5.301447
502	1	0	5.147422	0.702406	5.794124
503	1	0	3.860437	0.979445	6.985531
504	6	0	4.576678	-5.963947	2.894009
505	6	0	2.632796	-3.807206	5.456771
506	8	0	4.271706	-3.871219	7.263163
507	6	0	5.498729	-2.363048	-1.565496
508	6	0	7.579813	11.509719	-1.833229
509	1	0	7.424966	10.695556	0.171822
510	1	0	7.722742	12.441915	0.127017
511	6	0	1.084878	9.301285	3.321593
512	6	0	3.543067	12.239903	2.878239
513	8	0	5.704148	11.660716	3.848465
514	6	0	-0.002606	6.233905	0.091658
515	1	0	4.687978	3.005076	5.582196
516	1	0	3.852897	2.303441	4.193105
517	6	0	2.538194	2.988575	5.778470
518	6	0	5.263949	-7.249510	3.299585
519	8	0	3.447017	-5.843071	2.461088
520	1	0	2.658009	-3.469248	4.397538
521	1	0	1.934080	-3.113342	5.969493
522	6	0	2.114862	-5.237072	5.520970
523	6	0	6.680963	-2.288803	-2.508225
524	8	0	4.521069	-1.636120	-1.576357
525	1	0	8.539483	10.957508	-1.885030
526	1	0	6.847426	10.885598	-2.396538
527	6	0	7.735268	12.862516	-2.508779
528	6	0	0.713230	8.689329	4.653572
529	8	0	0.490312	10.175550	2.723307
530	1	0	2.969791	11.819847	2.022354
531	1	0	3.926081	13.220478	2.528931
532	6	0	2.623251	12.427625	4.077575
533	6	0	-0.859954	5.346581	0.963579
534	8	0	0.465110	5.959568	-0.997357
535	1	0	1.673001	2.360215	5.482781
536	1	0	2.516746	3.023313	6.886623
537	6	0	2.369819	4.389997	5.213870
538	1	0	4.901062	-8.068504	2.646019

539	1	0	6.358047	-7.188336	3.135356
540	6	0	4.956517	-7.549102	4.761379
541	1	0	2.941029	-5.959848	5.327362
542	1	0	1.391861	-5.392967	4.684348
543	6	0	1.438561	-5.565413	6.840513
544	1	0	6.648352	-1.308588	-3.048377
545	1	0	7.622080	-2.275297	-1.919752
546	6	0	6.709653	-3.434790	-3.507724
547	1	0	6.795416	13.444586	-2.421054
548	1	0	8.506476	13.462919	-1.985223
549	6	0	8.108234	12.699940	-3.974012
550	1	0	-0.344712	8.932096	4.879330
551	1	0	0.765923	7.576946	4.596226
552	6	0	1.629630	9.214339	5.749382
553	1	0	2.402281	11.443590	4.554691
554	1	0	1.644394	12.802892	3.715702
555	6	0	3.182183	13.387899	5.114612
556	1	0	-1.801358	5.875885	1.220133
557	1	0	-1.177333	4.445335	0.374239
558	6	0	-0.136366	4.895251	2.222625
559	1	0	2.399907	4.358567	4.104688
560	1	0	3.221672	5.029444	5.519016
561	6	0	1.066704	5.006853	5.668334
562	1	0	5.513193	-6.849112	5.417016
563	1	0	3.878384	-7.357142	4.975121
564	6	0	5.301781	-8.984459	5.118982
565	1	0	2.135970	-5.395854	7.684819
566	1	0	0.580652	-4.873297	7.010764
567	6	0	0.939116	-7.001920	6.848983
568	1	0	7.659601	-3.370910	-4.078800
569	1	0	6.754222	-4.397487	-2.959876
570	6	0	5.528917	-3.461629	-4.469358
571	1	0	7.335871	12.097901	-4.494193
572	1	0	9.047567	12.118493	-4.062654
573	6	0	8.264040	14.040869	-4.654648
574	1	0	2.663394	8.846027	5.589410
575	1	0	1.700817	10.326218	5.685815
576	6	0	1.135838	8.792451	7.122746
577	1	0	4.197604	13.070553	5.427507
578	1	0	3.310545	14.394527	4.668181
579	6	0	2.270852	13.468319	6.329841
580	1	0	0.884730	4.538072	1.977374
581	1	0	0.007520	5.750295	2.916087
582	6	0	-0.915662	3.791167	2.924334
583	1	0	0.202394	4.420022	5.310661
584	1	0	0.950082	6.030019	5.272528
585	1	0	0.998736	5.070665	6.762174
586	1	0	4.771626	-9.685516	4.442672
587	1	0	6.381822	-9.169009	4.952266
588	6	0	4.935835	-9.285689	6.564339
589	1	0	1.780308	-7.699231	6.654514
590	1	0	0.221725	-7.147434	6.008115
591	6	0	0.267701	-7.341939	8.159731
592	1	0	4.580138	-3.319453	-3.911156
593	1	0	5.466135	-4.477879	-4.907116
594	6	0	5.616104	-2.451122	-5.605079
595	1	0	7.335310	14.625574	-4.614373
596	1	0	8.530840	13.921028	-5.712361
597	1	0	9.050452	14.645763	-4.183828
598	1	0	0.091257	9.131748	7.275180

599	1	0	1.101992	7.684120	7.186406
600	6	0	2.026465	9.355685	8.218843
601	1	0	2.152603	12.460175	6.781157
602	1	0	1.252280	13.775005	6.019074
603	6	0	2.810401	14.433738	7.360556
604	1	0	-1.951820	4.129128	3.127815
605	1	0	-0.461115	3.601729	3.924580
606	6	0	-0.938168	2.513319	2.100061
607	1	0	5.479963	-8.597891	7.241963
608	1	0	3.858828	-9.075249	6.731694
609	6	0	5.245796	-10.720666	6.924891
610	1	0	0.953843	-7.225996	9.009112
611	1	0	-0.092619	-8.378340	8.166694
612	1	0	-0.597463	-6.690233	8.346293
613	1	0	6.666348	-2.363023	-5.970252
614	1	0	5.036254	-2.826094	-6.472107
615	6	0	5.094722	-1.086401	-5.218543
616	1	0	3.068473	9.007207	8.073919
617	1	0	2.069529	10.461699	8.136306
618	6	0	1.533275	8.956478	9.590958
619	1	0	3.806423	14.134312	7.713178
620	1	0	2.153562	14.487787	8.238036
621	1	0	2.900779	15.450176	6.954770
622	1	0	-1.249729	2.762824	1.058346
623	1	0	0.087645	2.103568	2.014512
624	6	0	-1.864723	1.474555	2.686474
625	1	0	4.688156	-11.426740	6.295157
626	1	0	4.983062	-10.933910	7.968836
627	1	0	6.313238	-10.947532	6.802073
628	1	0	4.010418	-1.099247	-5.016499
629	1	0	5.592908	-0.708681	-4.304163
630	1	0	5.281546	-0.338546	-6.014663
631	1	0	0.515750	9.324284	9.779122
632	1	0	2.179769	9.362222	10.379456
633	1	0	1.512778	7.865186	9.712207
634	1	0	-1.561829	1.186659	3.701440
635	1	0	-2.903537	1.831574	2.738626
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1	6	0	-2.787917	0.436815	-2.661718
2	7	0	-2.873804	-0.962400	-2.742468
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5	6	0	-1.562173	0.802487	-3.196886
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7	6	0	1.335959	-0.486328	-2.769157
8	6	0	1.744602	-1.613211	-2.045278
9	6	0	2.412303	-1.435260	-0.834842
10	6	0	2.821901	-0.170331	-0.409518
11	6	0	2.491174	0.951306	-1.180834
12	6	0	1.722915	0.781305	-2.335541
13	1	0	0.542273	-1.605181	-4.445703
14	1	0	0.702511	0.158273	-4.737516
15	1	0	1.420156	1.665019	-2.918751
16	6	0	5.434453	-1.851650	0.502118
17	6	0	6.752667	-1.735270	0.092489
18	7	0	5.002423	-0.529195	0.672220

19	7	0	6.024739	0.331739	0.350107
20	7	0	7.044851	-0.359358	0.035778
21	6	0	3.604448	-0.081567	0.871773
22	1	0	3.138594	-0.717789	1.653863
23	1	0	3.606225	0.961672	1.267041
24	1	0	2.597115	-2.312361	-0.188005
25	8	0	7.569244	10.867999	-2.693029
26	6	0	7.799072	9.614004	-2.045938
27	6	0	8.162759	8.558655	-3.133739
28	6	0	6.417328	9.232122	-1.440842
29	1	0	8.599408	9.666038	-1.262933
30	8	0	8.163346	7.255727	-2.563223
31	6	0	9.588066	8.770012	-3.681436
32	1	0	7.404697	8.617889	-3.969969
33	6	0	6.365211	7.768133	-0.928132
34	1	0	5.641084	9.315770	-2.257413
35	6	0	6.910321	6.847155	-2.064420
36	8	0	9.668386	7.983447	-4.869070
37	1	0	9.757436	9.829789	-3.946941
38	1	0	10.359198	8.472539	-2.943219
39	8	0	7.120164	7.663432	0.268752
40	1	0	5.288255	7.500980	-0.746934
41	8	0	7.334207	5.610399	-1.552532
42	1	0	6.145427	6.779015	-2.879832
43	6	0	7.143246	4.491783	-2.403158
44	6	0	5.774104	3.922684	-2.265629
45	1	0	7.397552	4.711671	-3.465267
46	1	0	7.895368	3.786749	-2.005112
47	7	0	4.803944	3.944564	-3.281920
48	6	0	5.208273	3.281981	-1.173882
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50	7	0	3.922209	2.944308	-1.600835
51	6	0	2.859815	2.347072	-0.765456
52	1	0	3.205959	2.363545	0.295646
53	1	0	1.952865	3.002102	-0.805987
54	6	0	4.813810	-4.103740	-3.647606
55	7	0	3.956325	-4.379653	-4.726988
56	6	0	4.028980	-3.579728	-2.632415
57	7	0	2.757033	-4.055201	-4.444356
58	7	0	2.732616	-3.567104	-3.163187
59	6	0	1.506568	-3.009932	-2.539692
60	1	0	1.191406	-3.671584	-1.703509
61	1	0	0.687651	-3.027429	-3.296929
62	6	0	-3.836284	1.292328	-2.045167
63	6	0	6.291425	-4.302727	-3.625788
64	1	0	-4.553057	0.687359	-1.445127
65	1	0	6.558598	-5.018259	-2.821475
66	8	0	5.824305	10.148057	-0.542445
67	6	0	-8.695943	-2.553317	0.464491
68	6	0	-7.416554	-2.028997	1.005144
69	1	0	-9.121577	-3.349967	1.120675
70	1	0	-8.524516	-2.998745	-0.537463
71	7	0	-6.943717	-2.329420	2.295766
72	6	0	-6.488385	-1.187744	0.414157
73	7	0	-5.832782	-1.747415	2.513698
74	7	0	-5.506478	-1.020913	1.396308
75	6	0	-4.259254	-0.244643	1.241847
76	6	0	-3.035456	-1.110636	1.257864
77	1	0	-4.315977	0.305794	0.268950
78	1	0	-4.229355	0.525626	2.050441

79	6	0	-1.930575	-0.827009	2.068624
80	6	0	-2.997835	-2.224873	0.422008
81	6	0	-0.832231	-1.688352	2.049081
82	6	0	-1.883961	0.383270	2.956062
83	6	0	-1.910414	-3.096924	0.410661
84	1	0	-3.842770	-2.411496	-0.258716
85	6	0	-0.807662	-2.819986	1.230876
86	1	0	0.028398	-1.466460	2.697958
87	7	0	-1.064569	1.460368	2.355987
88	1	0	-2.911086	0.791759	3.150721
89	6	0	-1.958392	-4.279546	-0.517083
90	6	0	0.433148	-3.665023	1.200848
91	6	0	-1.518860	2.497822	1.533119
92	7	0	0.304220	1.472803	2.407494
93	7	0	-3.243129	-5.008305	-0.462065
94	1	0	-1.141088	-5.001691	-0.292095
95	1	0	-1.802610	-3.931842	-1.560893
96	7	0	0.833859	-4.172466	2.528947
97	1	0	0.300825	-4.544112	0.527788
98	1	0	1.273109	-3.064338	0.765535
99	6	0	-0.359580	3.134902	1.118387
100	7	0	0.719954	2.448336	1.702725
101	7	0	-3.584428	-5.878923	0.550527
102	6	0	-4.358307	-4.777140	-1.279986
103	6	0	0.103076	-5.015108	3.373788
104	7	0	2.081350	-3.941752	3.064319
105	6	0	-0.171690	4.307030	0.220343
106	7	0	-4.796923	-6.219167	0.387918
107	6	0	-5.352340	-5.571508	-0.734914
108	6	0	0.960708	-5.261230	4.434399
109	7	0	2.155223	-4.565072	4.171982
110	1	0	0.680703	4.126662	-0.472906
111	1	0	-1.080834	4.470922	-0.397001
112	6	0	-6.747623	-5.792967	-1.204206
113	6	0	0.772793	-6.103898	5.647907
114	1	0	-7.460827	-5.806952	-0.354409
115	1	0	1.070698	-7.155145	5.431855
116	1	0	1.389409	-5.742460	6.493782
117	1	0	-0.919781	-5.352453	3.193588
118	1	0	-4.367488	-4.120884	-2.153649
119	1	0	5.629969	3.049944	-0.191286
120	1	0	-1.119663	1.794045	-3.344891
121	1	0	-2.569894	2.712253	1.312341
122	1	0	-6.479841	-0.713158	-0.570512
123	1	0	4.305469	-3.226974	-1.634977
124	1	0	4.829409	-2.737710	0.705123
125	1	0	-1.477325	0.118859	3.964839
126	6	0	10.895084	7.718241	-5.405753
127	6	0	10.829797	6.727525	-6.548298
128	1	0	9.775472	6.457934	-6.789491
129	1	0	11.237025	7.222384	-7.451488
130	6	0	11.623909	5.466510	-6.238135
131	1	0	11.801285	4.915110	-7.183591
132	1	0	12.629812	5.747463	-5.865984
133	6	0	10.945797	4.551871	-5.225952
134	1	0	10.495436	5.151409	-4.409110
135	1	0	11.726362	3.930726	-4.743183
136	6	0	9.898750	3.627041	-5.832155
137	1	0	10.246409	3.244272	-6.813371
138	1	0	9.793064	2.729892	-5.189625

139	6	0	8.543994	4.280510	-5.987599
140	1	0	8.110198	4.560363	-5.012418
141	1	0	8.602123	5.200024	-6.592163
142	1	0	7.831715	3.600135	-6.483324
143	8	0	11.873442	8.287725	-4.965423
144	6	0	8.428080	11.920702	-2.551283
145	6	0	7.781651	13.211515	-3.008020
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147	1	0	6.740310	13.021618	-3.372308
148	6	0	7.778030	14.217267	-1.865818
149	1	0	7.370294	13.744145	-0.941511
150	1	0	8.819250	14.501788	-1.605588
151	6	0	6.971475	15.452425	-2.228083
152	1	0	7.379560	15.914155	-3.149712
153	1	0	5.928295	15.167732	-2.474107
154	6	0	6.977845	16.464042	-1.092979
155	1	0	6.566432	16.000699	-0.173920
156	1	0	8.021050	16.743162	-0.843031
157	6	0	6.183196	17.699706	-1.449827
158	1	0	6.591413	18.202265	-2.336862
159	1	0	6.189628	18.427446	-0.628433
160	1	0	5.133927	17.458289	-1.666056
161	8	0	9.546424	11.740155	-2.118409
162	1	0	11.871358	14.885743	1.920300
163	6	0	11.573201	13.831683	1.854376
164	6	0	10.089602	13.696147	1.597717
165	1	0	11.866796	13.347737	2.795421
166	1	0	12.166057	13.371678	1.052504
167	6	0	9.673469	12.236300	1.505154
168	1	0	9.517389	14.202289	2.400525
169	1	0	9.816893	14.223573	0.659639
170	6	0	8.183093	12.112046	1.237315
171	1	0	9.936684	11.703722	2.440841
172	1	0	10.248709	11.732503	0.701204
173	6	0	7.770905	10.654171	1.080964
174	1	0	7.606366	12.584042	2.057873
175	1	0	7.914837	12.685876	0.318377
176	6	0	6.326047	10.579866	0.660168
177	1	0	8.436238	10.131369	0.360026
178	1	0	7.891843	10.107770	2.039173
179	8	0	5.367903	10.986101	1.286922
180	1	0	1.409397	8.945393	4.937085
181	6	0	2.143209	8.991651	4.112085
182	6	0	2.843890	7.665168	3.929737
183	1	0	2.848193	9.802351	4.335821
184	1	0	1.585533	9.285659	3.204899
185	6	0	3.806789	7.680646	2.751064
186	1	0	3.392363	7.402169	4.856208
187	1	0	2.089813	6.863317	3.789489
188	6	0	4.527497	6.344072	2.640369
189	1	0	4.540005	8.503852	2.867366
190	1	0	3.255475	7.910974	1.806545
191	6	0	5.318552	6.204345	1.350281
192	1	0	5.189306	6.196353	3.517296
193	1	0	3.784230	5.521694	2.683003
194	6	0	6.609256	6.986786	1.349710
195	1	0	5.588341	5.141392	1.177527
196	1	0	4.674159	6.494932	0.489595
197	8	0	7.403626	7.129048	2.255336
198	1	0	5.111787	-2.082263	-7.235227

199	6	0	6.177869	-2.341885	-7.394266
200	6	0	6.247590	-3.636089	-8.192505
201	1	0	6.601345	-2.496014	-6.380896
202	6	0	6.881823	-1.185324	-8.086160
203	6	0	7.594381	-4.307101	-8.068331
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205	1	0	6.051156	-3.441326	-9.266007
206	1	0	7.944653	-1.440922	-8.272981
207	1	0	6.436863	-1.013545	-9.087140
208	6	0	6.794400	0.085526	-7.255443
209	8	0	8.645902	-3.965560	-8.568649
210	8	0	7.850554	-5.462409	-7.375545
211	1	0	7.242204	-0.086442	-6.256267
212	1	0	5.733094	0.342134	-7.065450
213	6	0	7.490090	1.240664	-7.938600
214	6	0	6.802589	-6.194524	-6.758254
215	1	0	8.552049	1.024924	-8.118414
216	1	0	7.444410	2.157731	-7.326652
217	1	0	7.034788	1.471084	-8.910652
218	6	0	7.041715	-7.714703	-6.998576
219	6	0	6.791061	-6.012228	-5.210287
220	1	0	5.805965	-5.889203	-7.173606
221	6	0	8.334913	-8.206949	-6.285162
222	1	0	6.161485	-8.259568	-6.566689
223	8	0	6.851311	-8.099869	-8.343641
224	8	0	7.998668	-6.426942	-4.616219
225	8	0	6.867134	-4.652202	-4.864973
226	1	0	5.906041	-6.544547	-4.777728
227	8	0	8.300255	-9.636151	-6.381391
228	6	0	8.272486	-7.815370	-4.774654
229	1	0	9.247022	-7.759377	-6.763217
230	6	0	7.651908	-7.790321	-9.417463
231	6	0	9.417878	-10.331879	-6.752928
232	6	0	9.631337	-8.042909	-4.080115
233	1	0	7.464680	-8.403491	-4.269429
234	6	0	9.127824	-7.478608	-9.403721
235	8	0	6.936752	-7.893927	-10.393854
236	6	0	9.123923	-11.777998	-7.089083
237	8	0	10.496322	-9.775457	-6.785870
238	8	0	9.381000	-7.955078	-2.679577
239	1	0	10.021959	-9.053085	-4.301043
240	1	0	10.384496	-7.301644	-4.415338
241	1	0	9.468838	-7.231337	-8.374139
242	1	0	9.299689	-6.559914	-10.001544
243	6	0	9.954177	-8.633705	-9.952974
244	1	0	10.031119	-12.383000	-6.888140
245	1	0	8.332063	-12.185506	-6.429933
246	6	0	8.714783	-11.890977	-8.551758
247	6	0	10.429382	-7.730529	-1.831164
248	1	0	9.606748	-9.598377	-9.514408
249	1	0	11.000863	-8.515146	-9.606189
250	6	0	9.930527	-8.719196	-11.470179
251	1	0	7.707575	-11.451034	-8.698845
252	1	0	9.397524	-11.280658	-9.189541
253	6	0	8.725211	-13.336923	-9.017435
254	6	0	9.990636	-7.502597	-0.401941
255	8	0	11.559930	-7.733336	-2.276304
256	1	0	8.885582	-8.753209	-11.839614
257	1	0	10.370483	-7.800605	-11.907960
258	6	0	10.688419	-9.944696	-11.957361

259	1	0	9.727375	-13.783353	-8.855607
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261	6	0	8.346006	-13.438738	-10.486686
262	1	0	10.757920	-6.881082	0.116675
263	1	0	9.056626	-6.905856	-0.387031
264	6	0	9.784088	-8.808350	0.351384
265	1	0	10.239190	-10.862999	-11.522583
266	1	0	11.730951	-9.918713	-11.582491
267	6	0	10.682791	-10.033079	-13.466530
268	1	0	7.339074	-13.004393	-10.647060
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271	1	0	9.159876	-8.602905	1.245974
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273	6	0	11.082705	-9.480467	0.776615
274	1	0	9.661170	-10.096818	-13.864387
275	1	0	11.227430	-10.919484	-13.815796
276	1	0	11.156403	-9.154769	-13.925033
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279	1	0	7.672827	-15.501737	-10.402433
280	1	0	11.809980	-9.473950	-0.059969
281	1	0	10.868951	-10.548969	0.977332
282	6	0	11.707312	-8.864150	2.022781
283	1	0	10.915219	-8.510456	2.713675
284	1	0	12.256210	-9.649041	2.580002
285	6	0	12.657835	-7.730589	1.711155
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289	1	0	6.798308	-3.341200	-3.416840
290	1	0	-0.197442	-10.271288	6.039032
291	6	0	0.590920	-9.689005	6.556360
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293	1	0	0.680129	-8.735795	5.985278
294	6	0	1.904536	-10.451135	6.501246
295	6	0	0.877503	-8.228387	8.573928
296	1	0	-0.957152	-9.217384	8.004148
297	1	0	0.307338	-10.291296	8.627310
298	1	0	2.683866	-9.925794	7.103403
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304	1	0	1.615565	-11.114219	4.458657
305	6	0	3.691576	-11.367741	5.002909
306	6	0	-0.963980	-6.656409	8.387213
307	1	0	4.494148	-10.840549	5.549660
308	1	0	4.028591	-11.492754	3.966358
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310	6	0	-1.580497	-5.878675	9.585446
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320	6	0	-1.064524	-3.711814	8.393951
321	1	0	0.182962	-4.598420	10.001050
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323	6	0	-0.999975	-3.124326	11.751077
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325	1	0	-2.153191	-3.520215	8.211829
326	6	0	0.580842	-6.537735	11.857524
327	8	0	-1.213333	-8.171895	12.061090
328	6	0	-1.932828	-2.696576	12.862241
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331	1	0	0.084953	-2.097305	9.379681
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333	1	0	0.764755	-5.641836	11.225041
334	1	0	1.383655	-7.256018	11.589944
335	6	0	0.659462	-6.175720	13.334381
336	1	0	-2.020512	-1.591794	12.842310
337	1	0	-2.958893	-3.086130	12.700371
338	6	0	-1.393259	-3.169564	14.204286
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341	1	0	-0.199283	-5.520393	13.610964
342	6	0	1.965729	-5.470525	13.659405
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344	1	0	-0.389364	-2.732332	14.387775
345	6	0	-2.334333	-2.804432	15.339104
346	6	0	-2.310433	0.178422	6.573646
347	8	0	-0.634982	-1.440408	5.868288
348	1	0	2.823385	-6.133948	13.429758
349	1	0	2.091519	-4.581338	13.007764
350	6	0	2.006571	-5.048220	15.120125
351	1	0	-2.485432	-1.706543	15.368849
352	1	0	-3.338485	-3.238787	15.159612
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355	1	0	-2.294069	0.513325	5.504554
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357	1	0	1.879802	-5.934303	15.773415
358	1	0	1.142302	-4.386881	15.344860
359	6	0	3.299585	-4.339474	15.453280
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362	6	0	-2.699137	-2.906945	17.816291
363	1	0	-3.940173	-1.245681	6.409267
364	1	0	-3.772252	-0.520507	8.014012
365	6	0	-4.749423	0.755929	6.568213
366	1	0	4.171402	-4.982805	15.274346
367	1	0	3.326777	-4.035515	16.507411
368	1	0	3.432720	-3.433965	14.846300
369	1	0	-2.815480	-1.817632	17.892985
370	1	0	-2.303887	-3.263004	18.776151
371	1	0	-3.703516	-3.334411	17.695921
372	1	0	-4.492903	1.728744	7.051406
373	1	0	-5.746093	0.475987	6.980991
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376	1	0	-5.303761	0.039828	4.600221
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378	1	0	-6.740795	2.026258	5.023110

379	1	0	-5.296139	3.065268	5.239746
380	1	0	-5.679804	2.369659	3.644380
381	1	0	-8.440967	-6.374198	2.742158
382	6	0	-9.249431	-5.901585	2.149973
383	6	0	-9.678294	-6.854767	1.040873
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385	6	0	-10.405104	-5.526682	3.065380
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389	1	0	-11.206160	-5.029630	2.480753
390	1	0	-10.867176	-6.440641	3.490721
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393	8	0	-9.810916	-6.466883	-1.479516
394	1	0	-9.523807	-3.667884	3.766600
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396	6	0	-11.078757	-4.280878	5.131782
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398	1	0	-11.894888	-3.758532	4.611275
399	1	0	-10.739440	-3.623075	5.943114
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405	1	0	-9.593235	-9.434953	-3.072586
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407	8	0	-7.973177	-6.656161	-3.604566
408	8	0	-6.722903	-7.070407	-1.842157
409	1	0	-7.462296	-8.545928	-2.831587
410	8	0	-10.826125	-8.462065	-5.075467
411	6	0	-8.843282	-7.134294	-4.626524
412	1	0	-10.896138	-6.703494	-3.879116
413	6	0	-12.279964	-8.229730	-1.704736
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421	8	0	-7.833423	-5.792592	-6.385133
422	1	0	-9.767230	-6.183728	-6.371608
423	1	0	-9.321040	-5.027918	-5.073084
424	1	0	-12.525397	-6.761321	-3.260062
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427	1	0	-12.003678	-9.195096	-7.665609
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429	6	0	-13.981992	-8.926507	-6.795512
430	6	0	-7.020237	-4.706121	-6.214432
431	1	0	-13.874922	-9.196991	-3.392693
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435	1	0	-14.185069	-8.047662	-7.439735
436	6	0	-14.672194	-10.157934	-7.357135
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441	6	0	-16.573686	-8.994450	-3.275521
442	1	0	-14.272203	-10.391845	-8.364072
443	1	0	-14.442141	-11.044697	-6.731973
444	6	0	-16.177729	-9.954896	-7.426881
445	1	0	-5.044092	-4.030647	-6.747197
446	1	0	-5.360576	-5.741813	-7.104950
447	6	0	-6.186783	-4.367261	-8.565688
448	1	0	-16.222342	-10.045312	-3.308850
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454	1	0	-5.417773	-4.782633	-9.248622
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456	6	0	-6.320416	-2.868762	-8.802202
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458	1	0	-18.661975	-9.553364	-3.139193
459	1	0	-18.326163	-7.899381	-2.607185
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464	1	0	-6.953656	-2.715047	-9.698301
465	6	0	-4.985484	-2.166160	-9.020624
466	1	0	-4.285184	-2.833175	-9.562180
467	1	0	-5.138025	-1.294423	-9.688625
468	6	0	-4.357514	-1.689357	-7.729839
469	1	0	-4.960625	-0.887880	-7.267513
470	1	0	-4.270654	-2.504329	-6.993076
471	1	0	-3.351112	-1.286768	-7.898042
472	1	0	-7.056684	-4.988075	-1.898402
473	1	0	-9.626536	-1.954188	3.984448
474	6	0	-10.062625	-0.943927	3.796930
475	6	0	-11.484121	-1.121263	3.277533
476	1	0	-9.421403	-0.484058	3.016734
477	6	0	-10.006544	-0.114915	5.070349
478	6	0	-11.877194	0.014700	2.367261
479	1	0	-11.575172	-2.093088	2.738650
480	1	0	-12.205368	-1.178113	4.118143
481	1	0	-10.528443	0.853205	4.921500
482	1	0	-10.557800	-0.635653	5.879727
483	6	0	-8.568711	0.139165	5.494750
484	8	0	-12.106271	1.169106	2.666267
485	8	0	-12.032338	-0.076761	1.009135
486	1	0	-8.077595	0.851273	4.781027
487	1	0	-7.979010	-0.797333	5.433669
488	6	0	-8.485359	0.707843	6.892967
489	6	0	-12.049112	-1.341752	0.361732
490	1	0	-8.962120	1.695610	6.954360
491	1	0	-7.431923	0.825594	7.202064
492	1	0	-8.973771	0.058853	7.631262
493	6	0	-13.152831	-1.310184	-0.734768
494	6	0	-10.721295	-1.650854	-0.398570
495	1	0	-12.244476	-2.161708	1.102407
496	6	0	-12.805369	-0.242459	-1.813586
497	1	0	-13.180646	-2.322202	-1.218212
498	8	0	-14.460990	-1.327995	-0.207257

499	8	0	-10.416649	-0.669601	-1.364403
500	8	0	-9.592036	-1.441204	0.403791
501	1	0	-10.792383	-2.673338	-0.853704
502	8	0	-13.786662	-0.401266	-2.844060
503	6	0	-11.392612	-0.563491	-2.398609
504	1	0	-12.813290	0.789192	-1.370919
505	6	0	-15.089383	-0.322533	0.487918
506	6	0	-14.378408	0.695754	-3.408641
507	6	0	-10.892796	0.572506	-3.317016
508	1	0	-11.433421	-1.533413	-2.957005
509	6	0	-14.870816	1.162450	0.349159
510	8	0	-15.930943	-0.869038	1.171253
511	6	0	-15.578642	0.338474	-4.257442
512	8	0	-13.916855	1.801179	-3.204834
513	8	0	-9.893733	0.051336	-4.183740
514	1	0	-11.687398	0.887787	-4.016227
515	1	0	-10.572766	1.457630	-2.732272
516	1	0	-14.009791	1.390542	-0.316274
517	1	0	-14.592159	1.575726	1.340755
518	6	0	-16.138699	1.826006	-0.170553
519	1	0	-15.343600	0.568171	-5.315946
520	1	0	-15.788680	-0.750281	-4.221784
521	6	0	-16.794381	1.127091	-3.792853
522	6	0	-8.617873	0.531230	-4.152720
523	1	0	-16.970720	1.672721	0.545584
524	1	0	-16.464265	1.334250	-1.116828
525	6	0	-15.923854	3.310416	-0.414395
526	1	0	-16.972016	0.945743	-2.706946
527	1	0	-16.597644	2.216529	-3.876492
528	6	0	-18.031904	0.759930	-4.593165
529	6	0	-7.665025	-0.240671	-5.040449
530	8	0	-8.346683	1.489784	-3.452271
531	1	0	-15.641084	3.814022	0.531551
532	1	0	-15.067591	3.463651	-1.103110
533	6	0	-17.174082	3.952331	-0.996315
534	1	0	-17.859060	0.954792	-5.670768
535	1	0	-18.230383	-0.328045	-4.515105
536	6	0	-19.241682	1.544382	-4.108935
537	1	0	-6.650662	0.216000	-4.964115
538	1	0	-7.573843	-1.269848	-4.635772
539	6	0	-8.094075	-0.299602	-6.498112
540	1	0	-18.030812	3.801143	-0.309893
541	1	0	-17.455842	3.439201	-1.940891
542	6	0	-16.968961	5.428115	-1.251555
543	1	0	-19.424204	1.329432	-3.036732
544	1	0	-19.030275	2.631841	-4.158795
545	6	0	-20.474212	1.216598	-4.920379
546	1	0	-7.499562	-1.093855	-7.010792
547	1	0	-9.147120	-0.637538	-6.567968
548	6	0	-7.937124	1.020973	-7.239759
549	1	0	-16.723434	5.968274	-0.327488
550	1	0	-17.872282	5.888996	-1.670995
551	1	0	-16.149401	5.606063	-1.960591
552	1	0	-20.336406	1.458380	-5.982722
553	1	0	-21.345597	1.781607	-4.565714
554	1	0	-20.727495	0.149793	-4.859045
555	1	0	-8.350697	1.850494	-6.632043
556	1	0	-8.563854	0.981283	-8.152820
557	6	0	-6.502066	1.331023	-7.646763
558	1	0	-5.963972	0.388747	-7.905382

559	1	0	-6.507805	1.935065	-8.575025
560	6	0	-5.730764	2.068831	-6.576360
561	1	0	-6.198953	3.030054	-6.323019
562	1	0	-5.672961	1.476979	-5.646357
563	1	0	-4.702392	2.278268	-6.897183
564	1	0	-9.000326	1.949489	0.647030
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566	6	0	-7.212776	2.717595	-0.257286
567	1	0	-7.516587	1.452444	1.468220
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569	6	0	-5.782332	3.095458	0.026884
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571	1	0	-7.702924	3.555324	-0.803256
572	1	0	-7.191199	3.817042	2.312717
573	1	0	-8.682322	4.315559	1.500949
574	6	0	-8.987522	2.977777	3.180558
575	8	0	-5.093560	2.835940	0.996421
576	8	0	-4.987860	3.813124	-0.828027
577	1	0	-8.577727	2.013568	3.569170
578	1	0	-10.029428	2.751186	2.876355
579	6	0	-8.977773	4.004315	4.289845
580	6	0	-5.443085	4.104409	-2.143309
581	1	0	-7.960722	4.176411	4.670965
582	1	0	-9.592731	3.672936	5.137273
583	1	0	-9.370175	4.976984	3.949934
584	6	0	-5.217998	5.604117	-2.471762
585	6	0	-4.644606	3.283766	-3.206069
586	1	0	-6.539287	3.873482	-2.235992
587	6	0	-3.717359	5.971967	-2.645187
588	1	0	-5.786126	5.827049	-3.410304
589	8	0	-5.936259	6.451108	-1.578415
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592	1	0	-5.131477	3.397132	-4.208180
593	8	0	-3.747187	7.242479	-3.317036
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595	1	0	-3.265155	6.040403	-1.606713
596	6	0	-5.422098	6.868583	-0.379414
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606	1	0	-1.025388	4.092596	-2.891655
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608	1	0	-5.816150	8.262199	1.208442
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624	6	0	-9.722517	7.110799	2.190240
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626	1	0	-4.985278	11.941331	-3.197267
627	6	0	-4.231942	12.843841	-1.375054
628	1	0	1.513138	5.721752	-5.936647
629	1	0	1.244202	4.262643	-6.904978
630	6	0	-0.076188	5.900704	-7.419608
631	1	0	-9.385856	6.328342	2.909363
632	1	0	-10.208407	6.555181	1.362799
633	6	0	-10.721869	8.028117	2.856874
634	1	0	-5.009201	12.431837	-0.700790
635	1	0	-3.293053	12.848890	-0.773207
636	6	0	-4.592220	14.256091	-1.774631
637	1	0	0.396560	5.774626	-8.414956
638	1	0	-1.094268	5.475517	-7.523058
639	6	0	-0.179690	7.385305	-7.095419
640	1	0	-10.274522	8.567841	3.702222
641	1	0	-11.580343	7.464590	3.244092
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643	1	0	-3.831226	14.699373	-2.430550
644	1	0	-4.682384	14.903035	-0.890887
645	1	0	-5.548973	14.295169	-2.311774
646	1	0	-0.465883	7.527525	-6.034181
647	1	0	-1.015901	7.807682	-7.687677
648	6	0	1.085138	8.177424	-7.407020
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655	1	0	-3.351231	2.012298	-1.354652
656	1	0	-3.953143	4.048215	4.649360
657	6	0	-3.079894	4.652030	4.992679
658	6	0	-2.752912	5.695960	3.940452
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660	6	0	-3.410874	5.277131	6.339684
661	6	0	-1.318252	6.161512	3.967975
662	1	0	-2.540165	5.859746	6.725077
663	1	0	-4.226382	6.017620	6.211252
664	6	0	-3.838792	4.229745	7.356654
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669	6	0	-2.666688	3.521584	8.000675
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671	1	0	-2.168463	2.823581	7.304291
672	1	0	-2.991163	2.925597	8.864363
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674	6	0	-1.743905	8.630726	1.432249
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676	1	0	-2.382006	6.545066	1.737361
677	6	0	-0.429347	9.448955	1.308314
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682	1	0	-1.042902	6.573234	-0.315487
683	8	0	-0.833959	10.736800	0.829418
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685	1	0	0.125271	9.494072	2.293409
686	6	0	-2.756227	9.557824	3.517324
687	6	0	-0.352362	11.880408	1.406493
688	6	0	1.874600	9.414927	0.143748
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690	6	0	-1.618667	10.308513	4.155950
691	8	0	-3.857893	9.339138	3.980685
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694	8	0	1.971605	10.189765	-1.042698
695	1	0	2.034697	10.185391	0.922133
696	1	0	2.689770	8.661261	0.272966
697	1	0	-1.704119	11.362289	3.791659
698	1	0	-0.638289	9.928235	3.784872
699	6	0	-1.636586	10.271736	5.675657
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704	1	0	-2.659478	10.463619	6.057617
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706	6	0	-1.111058	8.947610	6.205372
707	1	0	-2.293113	12.755866	2.882115
708	1	0	-1.155358	14.103501	2.961068
709	6	0	-2.997615	14.581159	1.924493
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711	8	0	3.010226	8.560461	-2.172558
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757	6	0	5.075172	-8.867653	7.166194
758	6	0	7.973939	-5.741805	3.539912
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762	1	0	4.151748	-9.204349	7.667039
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783	1	0	11.750822	-2.364013	1.103220
784	6	0	10.867258	-4.622470	7.092525
785	8	0	10.966168	-5.796189	4.942705
786	1	0	7.228677	-3.524890	-0.978380
787	1	0	8.587485	-2.357879	-0.853432
788	6	0	15.215731	-2.880287	3.687091
789	8	0	14.005362	-5.018894	3.786792
790	8	0	13.829378	-3.849275	0.343484
791	1	0	12.559443	-5.334908	0.573410
792	1	0	12.104120	-4.237260	-0.775628
793	1	0	10.992443	-3.556563	7.371407
794	1	0	11.765511	-5.141591	7.483640
795	6	0	9.597941	-5.175940	7.728644
796	1	0	15.596638	-2.690341	2.654861
797	1	0	14.879503	-1.894945	4.069743
798	6	0	16.323224	-3.433715	4.567640

799	6	0	14.252916	-2.749232	-0.354242
800	1	0	8.720596	-4.993003	7.064510
801	1	0	9.386438	-4.614356	8.660299
802	6	0	9.704722	-6.660182	8.043394
803	1	0	15.940084	-3.612976	5.592010
804	1	0	16.649484	-4.425696	4.194814
805	6	0	17.505051	-2.477907	4.612025
806	6	0	15.714191	-2.438365	-0.111029
807	8	0	13.472312	-2.139686	-1.055805
808	1	0	9.828415	-7.238038	7.104807
809	1	0	10.618128	-6.860683	8.639222
810	6	0	8.480343	-7.149057	8.800762
811	1	0	17.884323	-2.295287	3.586012
812	1	0	17.180475	-1.486991	4.989147
813	6	0	18.622232	-3.023882	5.486750
814	1	0	15.920065	-1.381972	-0.401522
815	1	0	15.925887	-2.512734	0.980116
816	6	0	16.636343	-3.360303	-0.897688
817	1	0	7.559153	-6.910162	8.221325
818	1	0	8.381496	-6.600032	9.757970
819	6	0	8.543598	-8.636910	9.059260
820	1	0	18.242302	-3.207365	6.511578
821	1	0	18.946659	-4.014017	5.108933
822	6	0	19.800061	-2.077026	5.533921
823	1	0	17.642519	-3.341006	-0.432962
824	1	0	16.290960	-4.409806	-0.820438
825	6	0	16.744750	-2.956062	-2.360697
826	1	0	8.586106	-9.207068	8.121110
827	1	0	7.657582	-8.980872	9.609535
828	1	0	9.427400	-8.910469	9.650219
829	1	0	20.222535	-1.905493	4.534860
830	1	0	20.604407	-2.473894	6.166266
831	1	0	19.516495	-1.096933	5.940182
832	1	0	15.738669	-2.951264	-2.827064
833	1	0	17.327197	-3.718761	-2.913916
834	6	0	17.395901	-1.590302	-2.519672
835	1	0	16.874794	-0.863808	-1.854653
836	1	0	18.442327	-1.625670	-2.157471
837	6	0	17.356910	-1.116481	-3.953605
838	1	0	17.879339	-1.812976	-4.622793
839	1	0	16.326420	-1.021664	-4.321384
840	1	0	17.835708	-0.134969	-4.061403