

Supplementary Materials

Bifunctional azido(thio)ureas from an *O*-protected 2-amino-2-deoxy-D-glucopyranose: synthesis and structural analyses

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Summary

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Table S1. Yield (%) and IR spectroscopic data (cm⁻¹) of **14-22**

Comp.	Yield	$\bar{\nu}_{\text{NH}}$	$\bar{\nu}_{\text{N=N=N}}$	$\bar{\nu}_{\text{C=O}}^{\text{a}}$	$\bar{\nu}_{\text{C=O}}^{\text{b}}$	$\delta_{\text{NH}}^{\text{c}}$	$\bar{\nu}_{\text{C-O-C}}^{\text{a}}$	$\bar{\nu}_{\text{C-O}}$
14	97	3349/3285	2117	1751	1652	1566	1225	1062
15	45	3337/3297	2112	1750	1598	1541	1238	1086
16	52	3322	2121	1754	1649	1585	1223	1090
17	65	3325/3154	2118	1752	1601	1549	1233	1081
18	64	3343/3184	2119	1732	1611	1549	1228	1085
19	64	3345/3182	2120	1731	1612	1550	1227	1086
20	69	3331	2113	1752	1597	1544	1241	1086
21	64	3331	2119	1750	1598	1569	1234	1087
22	54	3301	2118	1750	1729	1540	1241	1088

^aAcetate. ^bUrea amide I band. ^cUrea amide II band.**Table S2.** ¹H NMR data (δ , ppm) of **14-22**

Comp.	Ar-1	Ar-2	Ar-3	Ar-4	Ar-5
14^a	7.27 m/7.06m				
15^a	7.21 d	7.45 t	7.35 m	7.45 t	7.21 d
16^a	7.30 s	6.83 dd	7.21 t	6.65 dd	---
17^b	6.77 m	6.87 d	7.34 t	6.77 m	---
18^a	7.13 d	6.96 d	6.96 d	7.13 d	---
19^b	7.13 d	6.95 d	6.95 d	7.13 d	---
20^a	7.30 sa	7.31 m	7.19 m	---	---
21^a	8.21 d	7.57 d	7.57 d	8.21 d	---
22^c	7.31 d	7.20 d	7.15 t	---	---

^aIn CDCl₃ at 500 MHz. ^bIn CDCl₃ at 400 MHz. ^cIn DMSO-*d*₆ at 500 MHz.**Table S3.** Yield (%) and IR spectroscopic data of **34-36**

Urea	Yield	$\bar{\nu}_{\text{OH}}$	$\bar{\nu}_{\text{NH}}$	$\bar{\nu}_{\text{N=N=N}}$	$\bar{\nu}_{\text{C=O}}^{\text{a}}$	$\bar{\nu}_{\text{C=O}}^{\text{b}}$	$\delta_{\text{NH}}^{\text{c}}$	$\bar{\nu}_{\text{C-O}}$
34	40	3276	3351	2120	1619	1596	1561	1084
35	23	3304	3470	2110	1641	1598	1561	1090
36	79	3299	3299	2121	1638	1657	---	1073

^aAcetate. ^bUrea I amide band. ^c Urea amide II band.

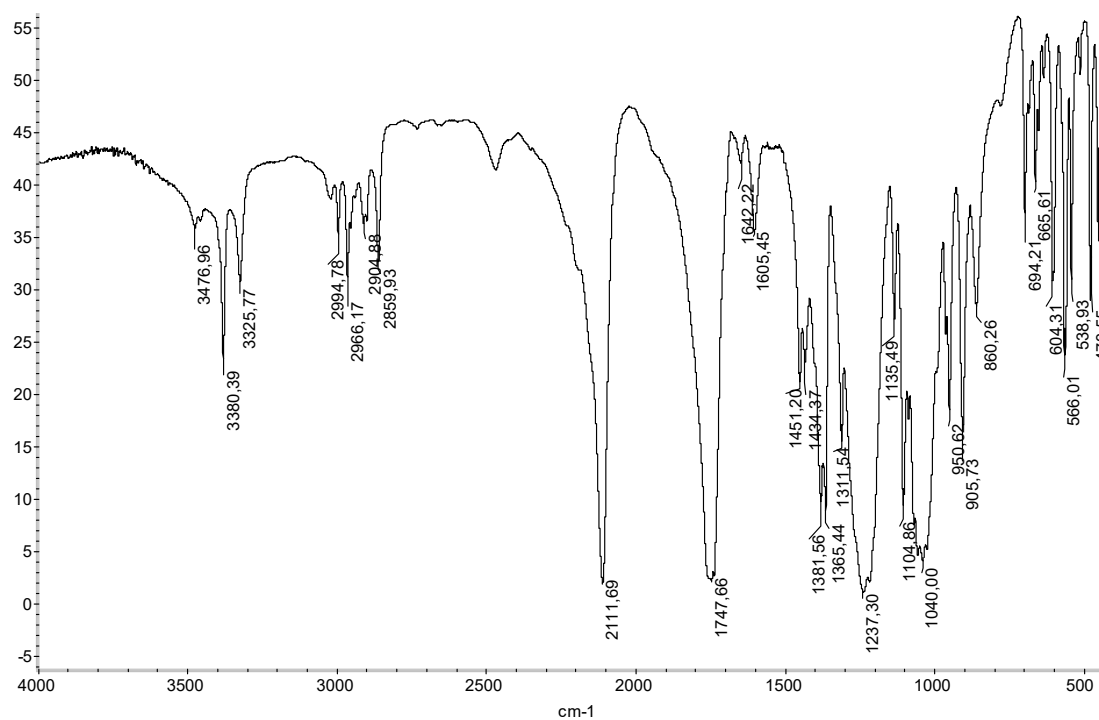


Figure S1 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-amino-2-deoxy-β-D-glucopyranosyl azide (**1**).

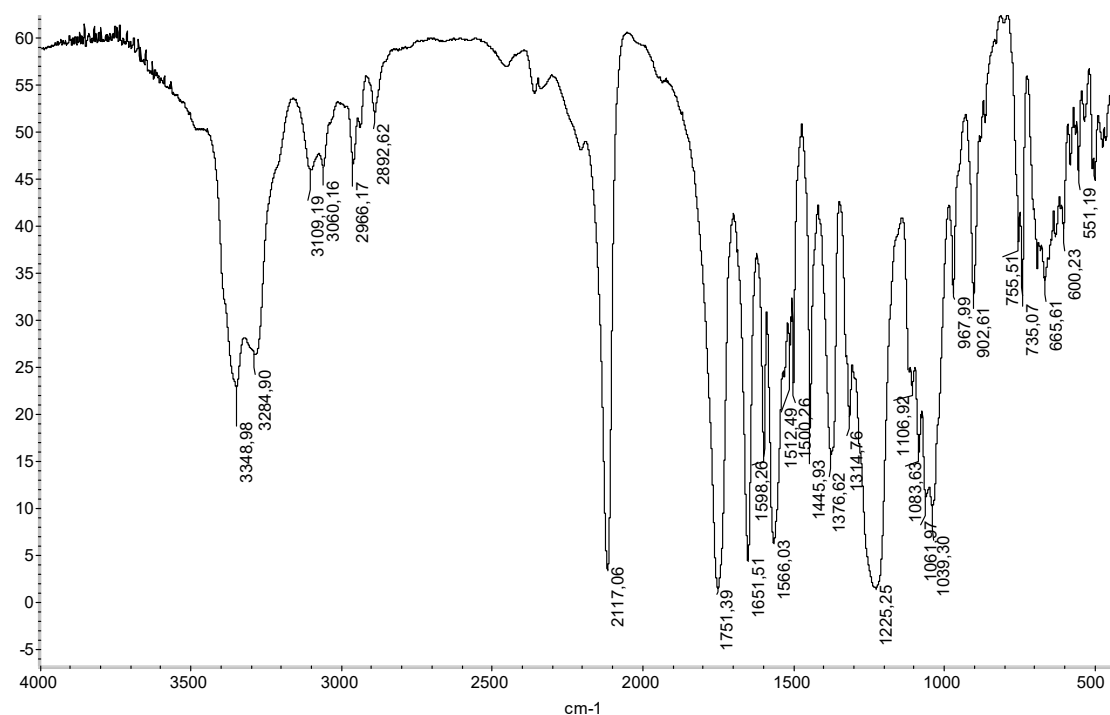


Figure S2 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-(3-phenylureido)-β-D-glucopyranosyl azide (**14**).

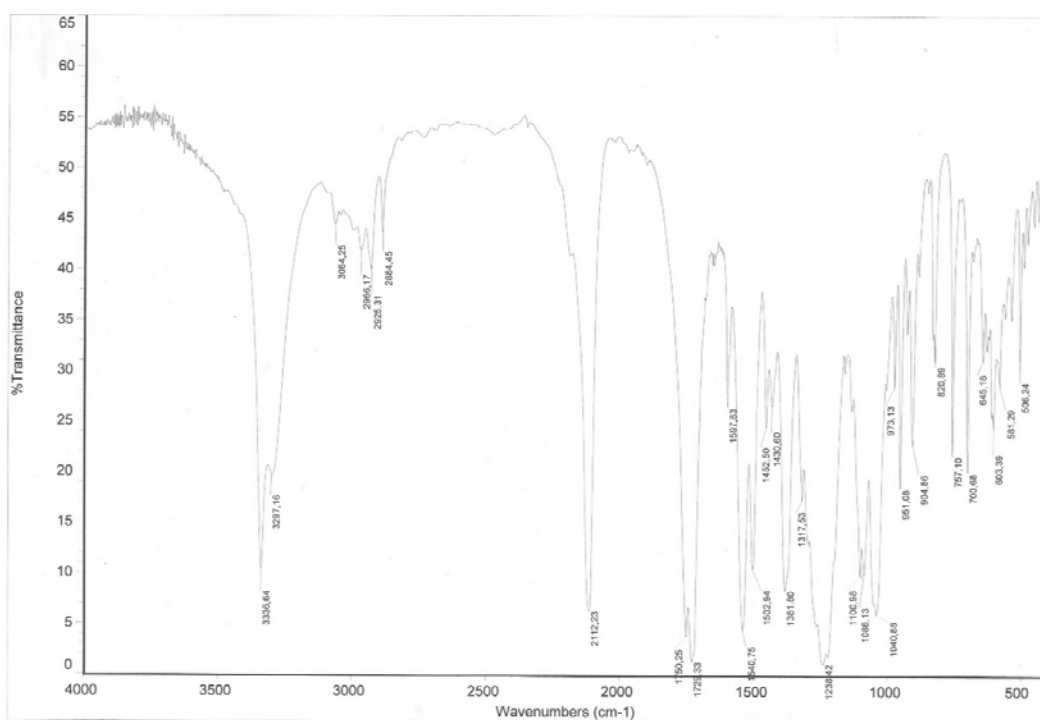


Figure S3 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-(3-phenylthioureido)-β-D-glucopyranosyl azide (15).

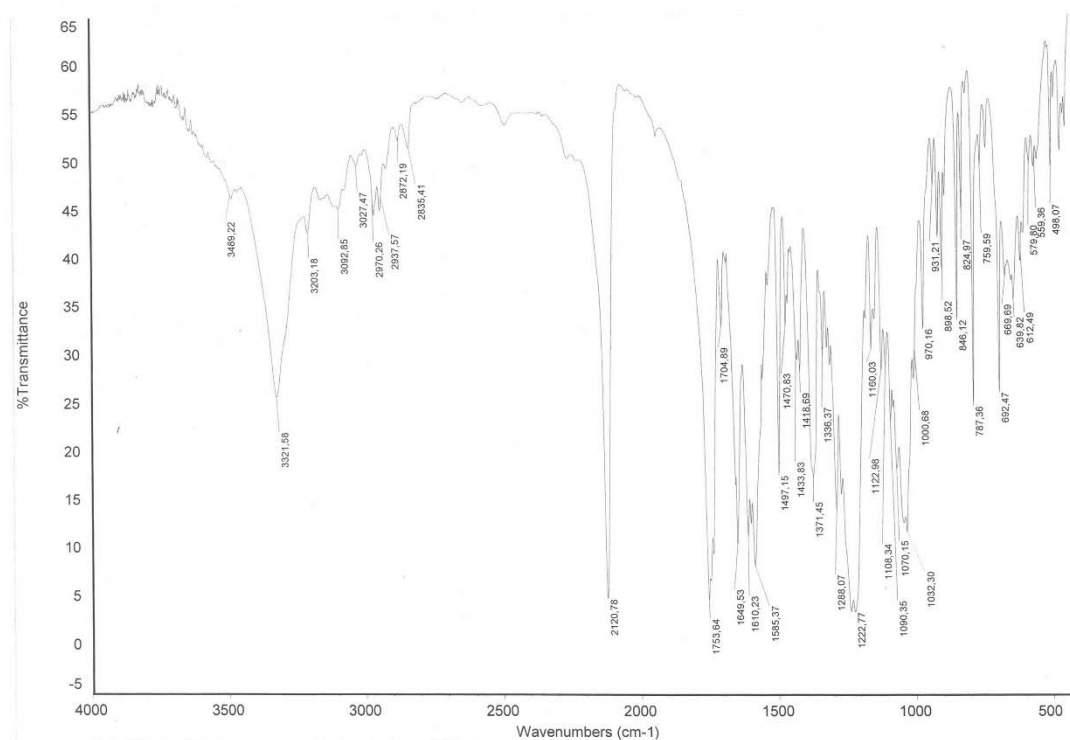


Figure S4 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)ureido]-β-D-glucopyranosyl azide (16).

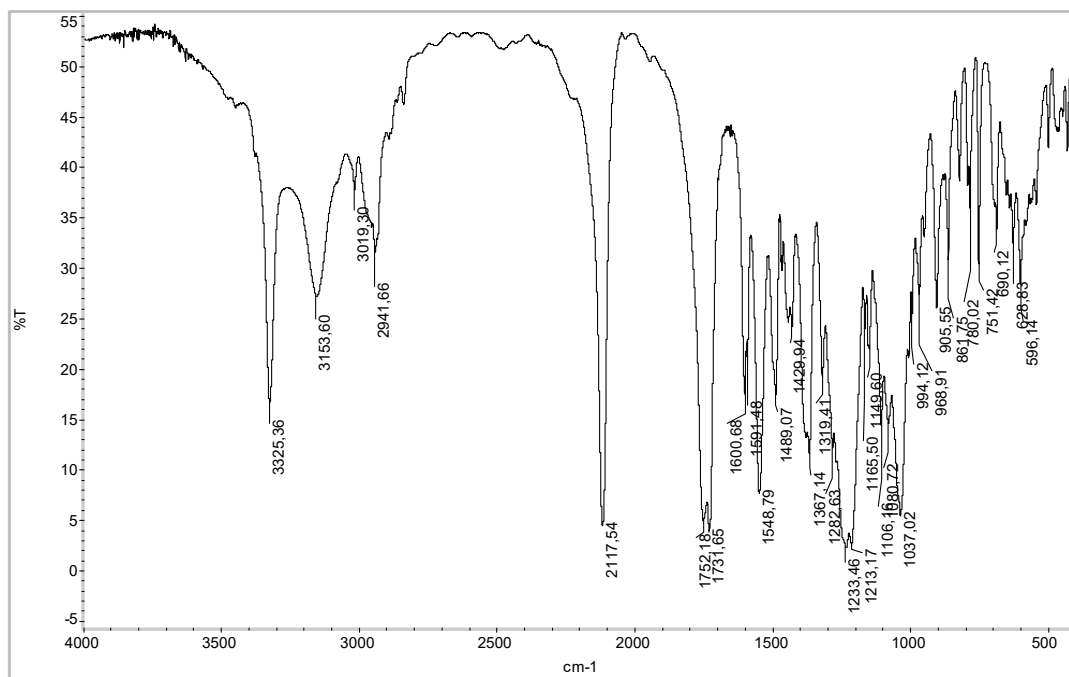


Figure S5 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)thioureido]-β-D-glucopyranosyl azide (**17**).

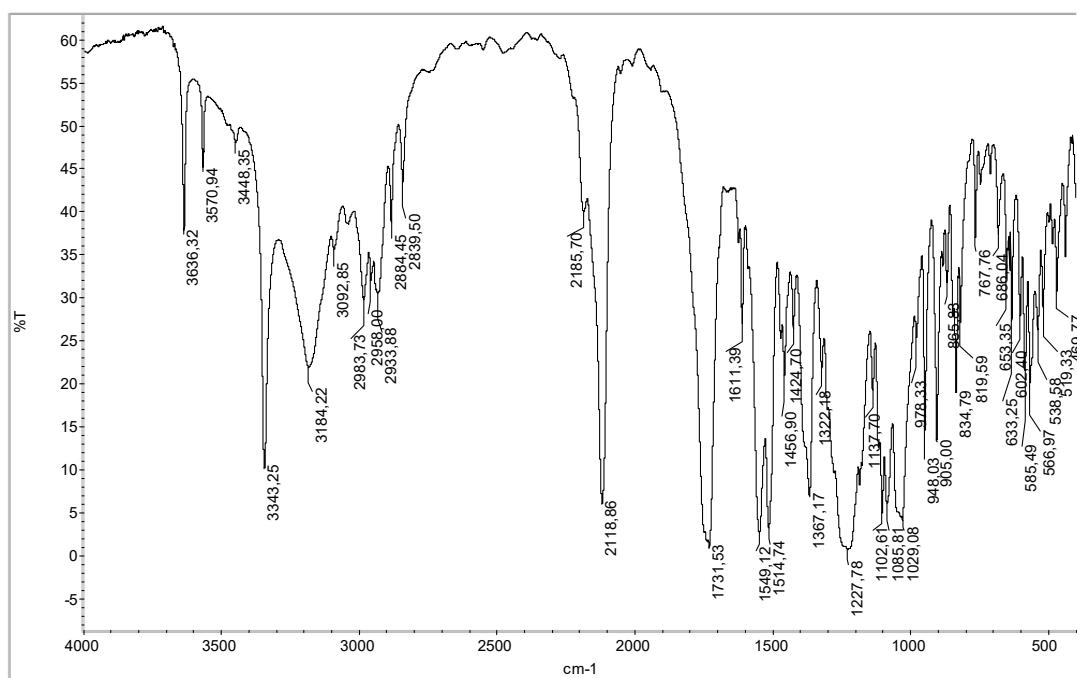


Figure S6 FT-IR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)ureido]-β-D-glucopyranosyl azide (**18**).

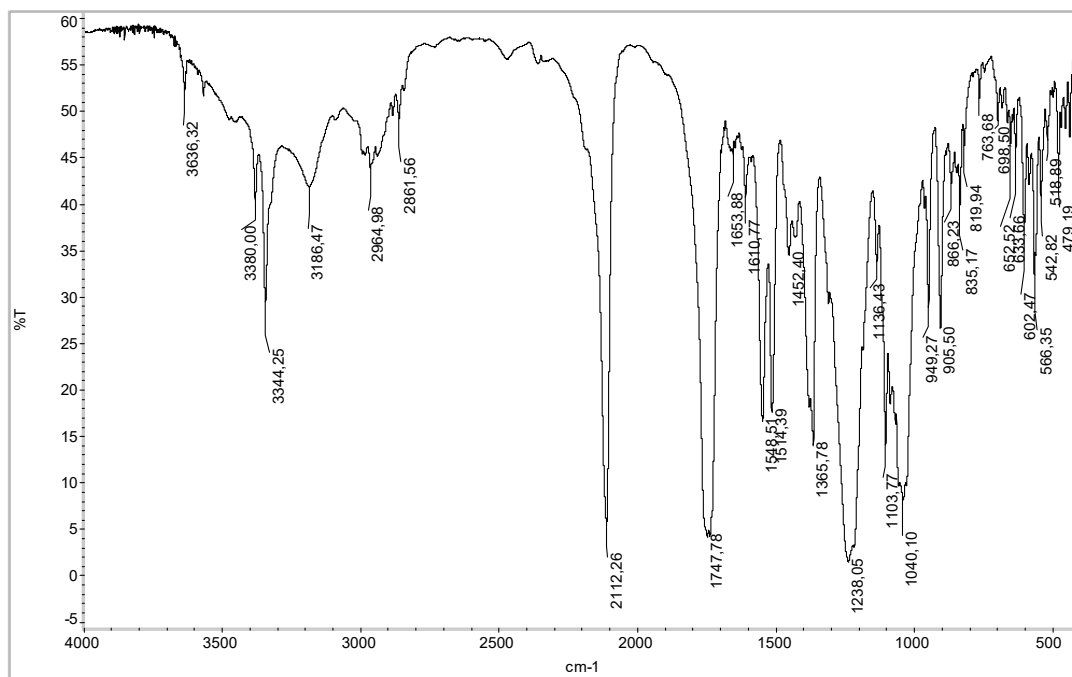


Figure S7 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)thiureido]-β-D-glucopyranosyl azide (**19**).

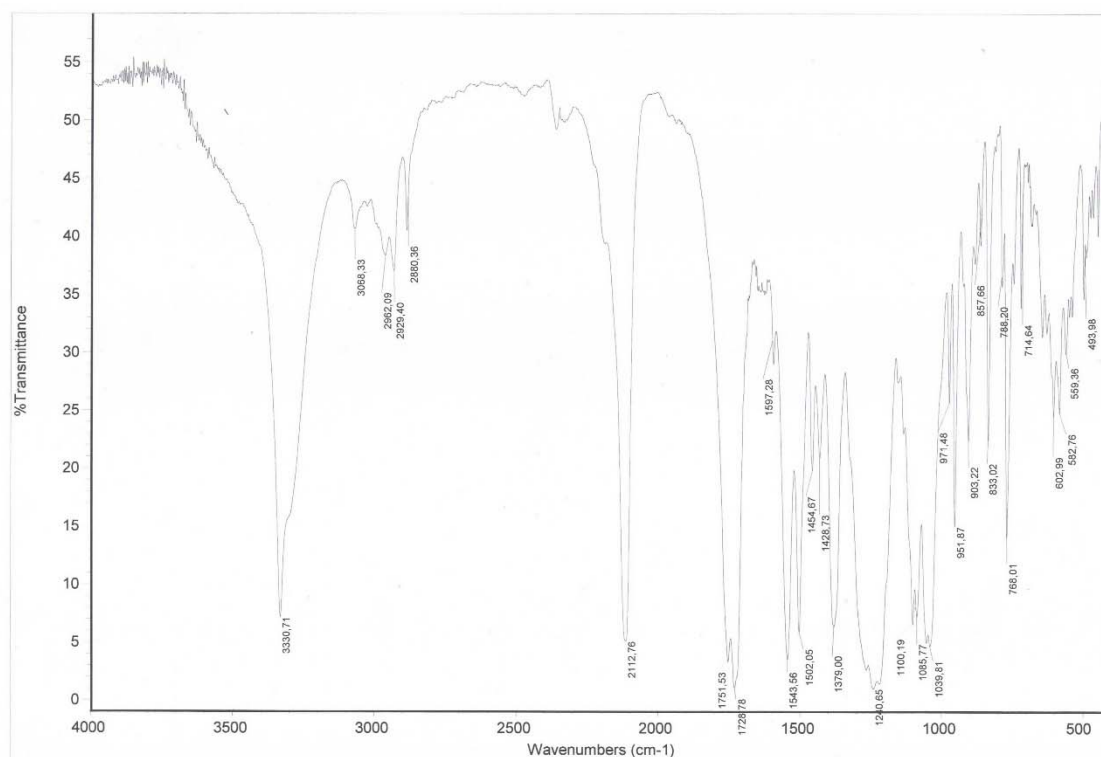


Figure S8 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-fluorophenyl)thiureido]-β-D-glucopyranosyl azide (**20**).

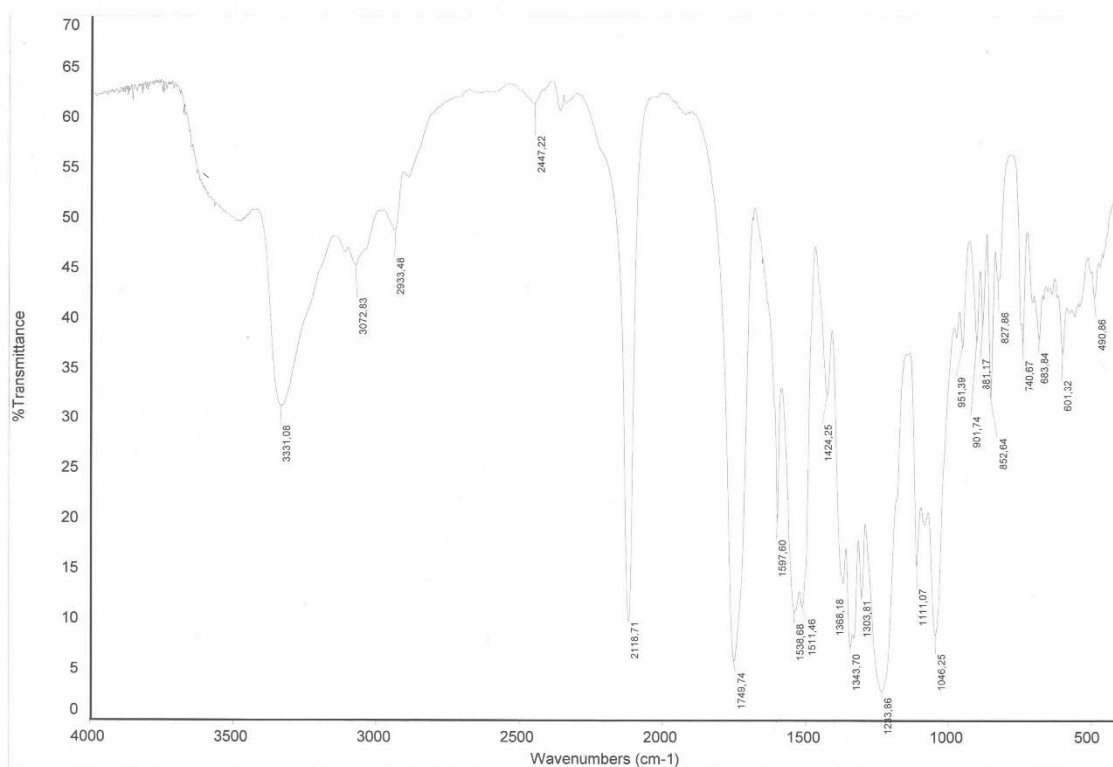


Figure S9 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-nitrophenyl)thioureido]-β-D-glucopyranosyl azide (**21**).

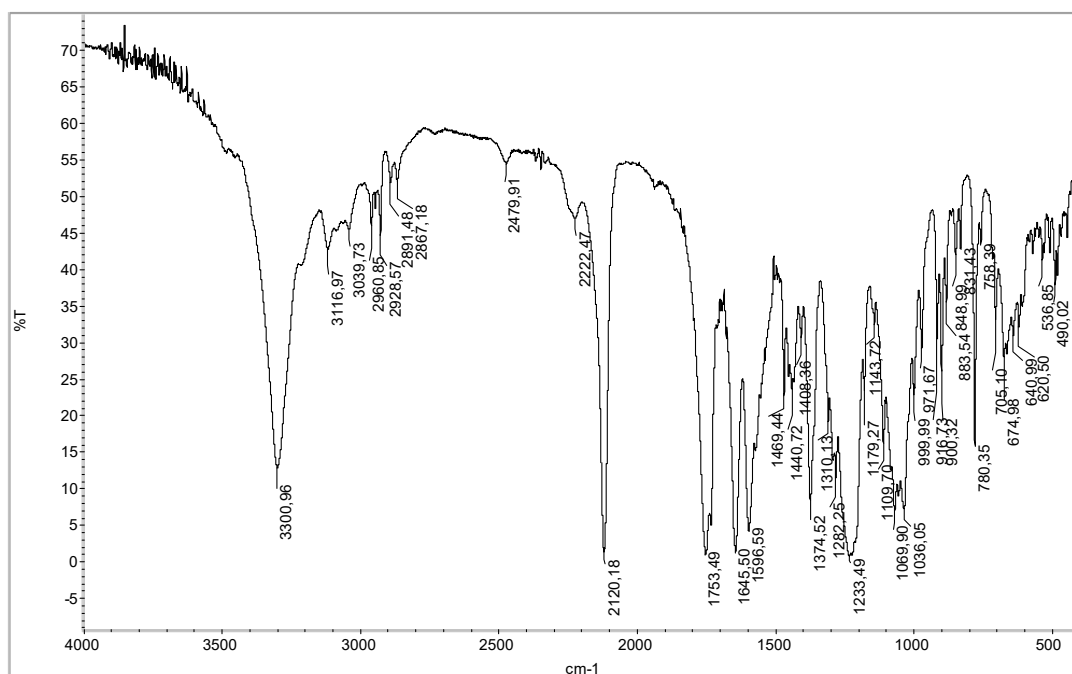


Figure S10 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]-β-D-glucopyranosyl azide (**22**).

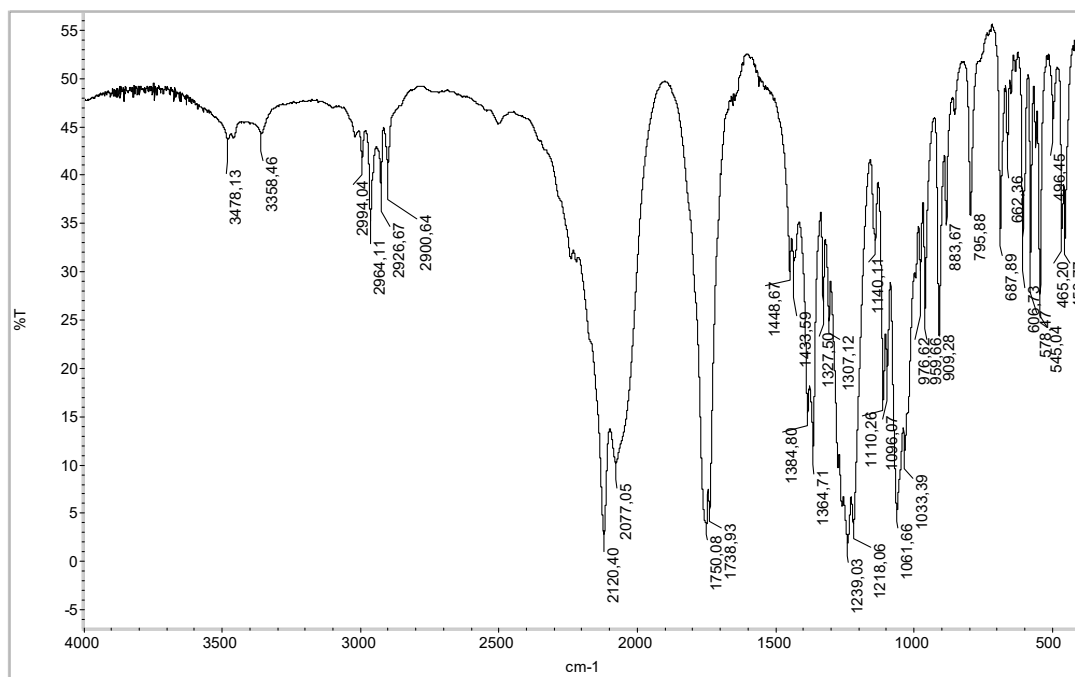


Figure S11 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-isothiocianato-β-D-glucopyranosyl azide (**23**).

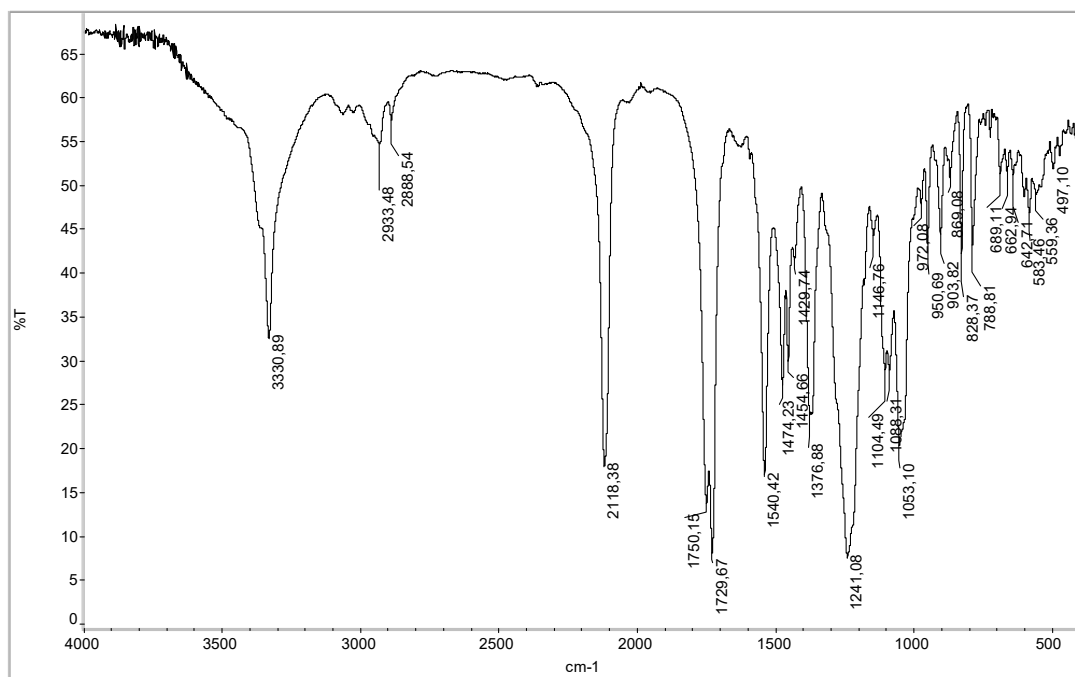


Figure S12 FT-IR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]-β-D-glucopyranosyl azide (**25**).

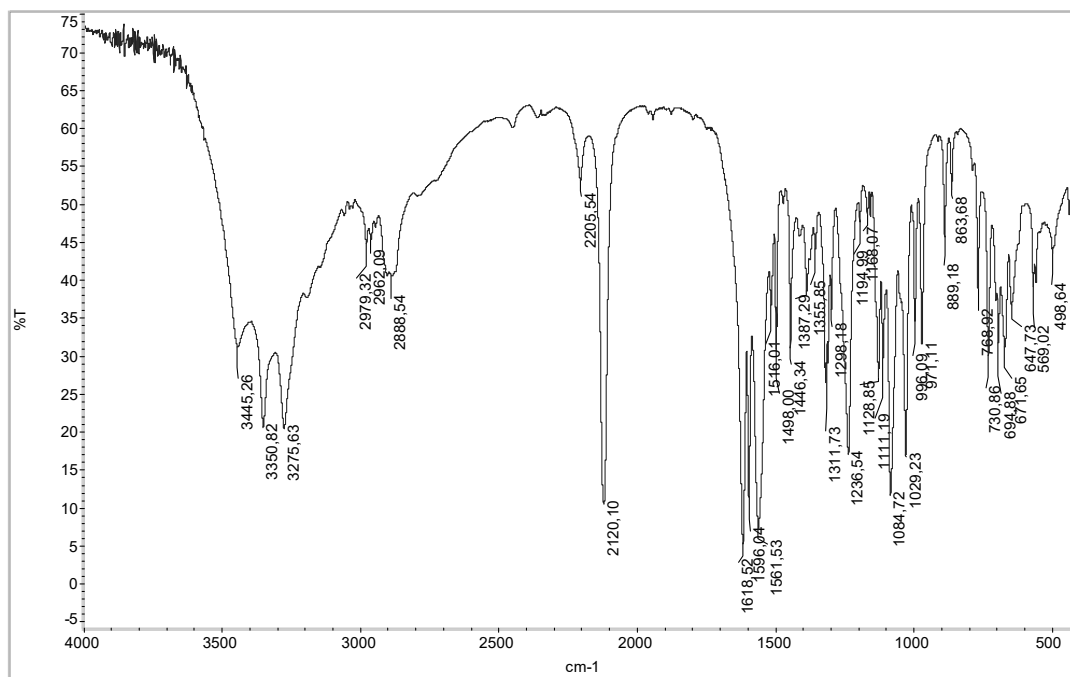


Figure S13 FT-IR spectrum of 2-deoxy-2-(3-phenylureido)-β-D-glucopyranosyl azide (**34**).

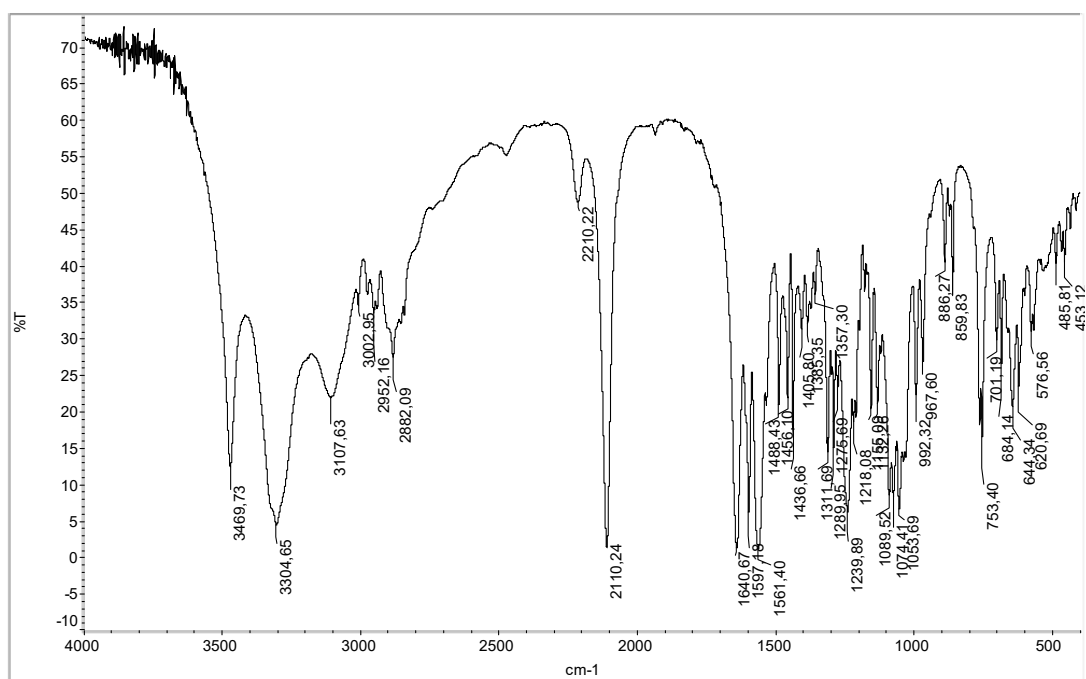


Figure S14 FT-IR spectrum of 2-deoxy-2-[3-(4-methoxyphenyl)ureido]-β-D-glucopyranosyl azide (**35**).

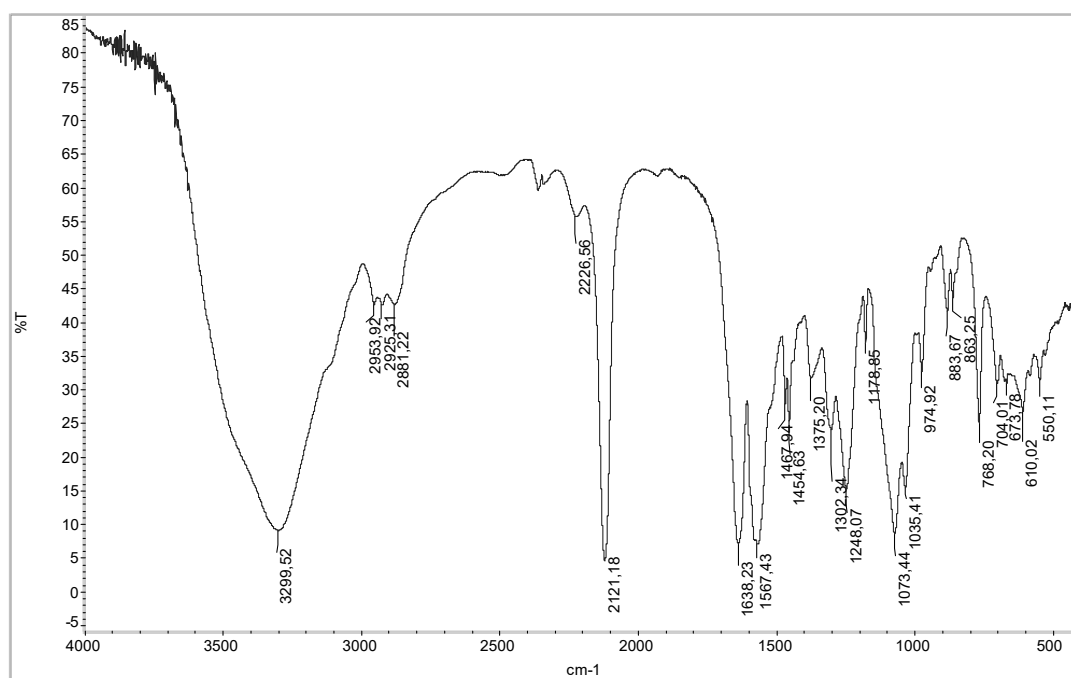


Figure S15 FT-IR spectrum of 2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]-β-D-glucopyranosyl azide (**36**).

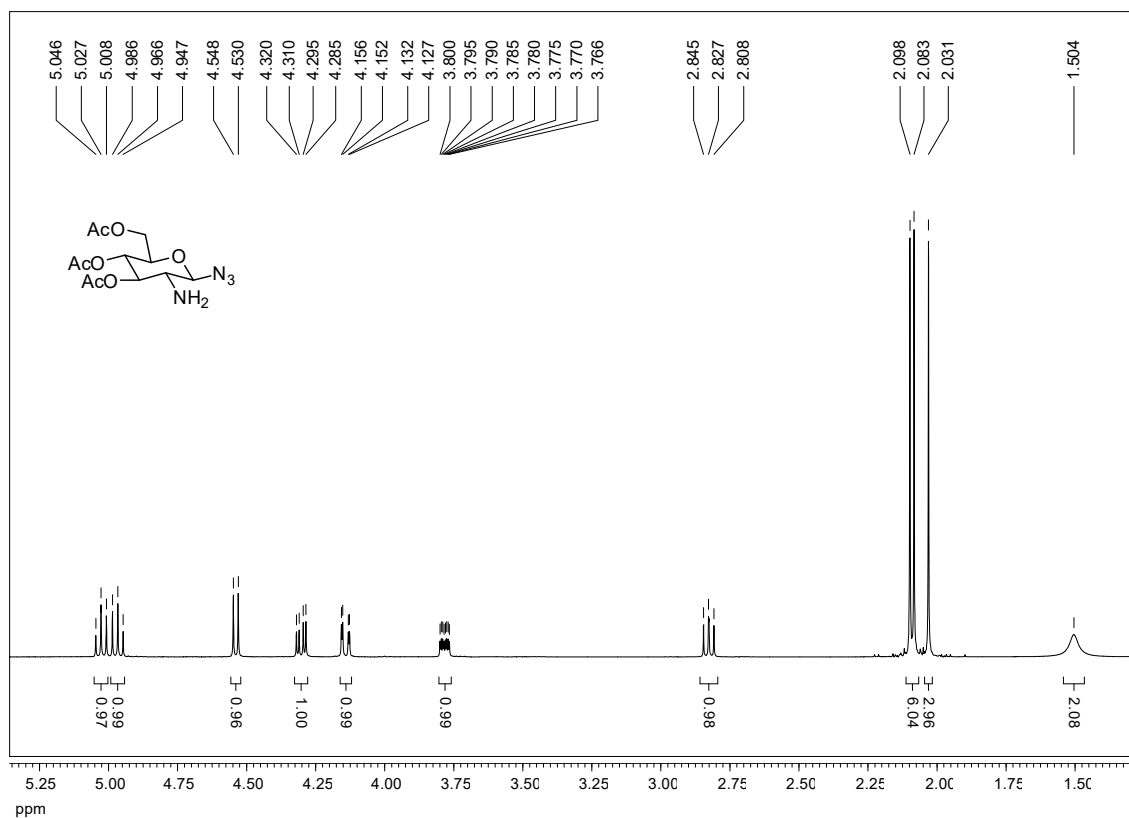


Figure S16 ¹H NMR spectrum of 3,4,6-tri-O-acetyl-2-amino-2-deoxy-β-D-glucopyranosyl azide (1) recorded in CDCl₃.

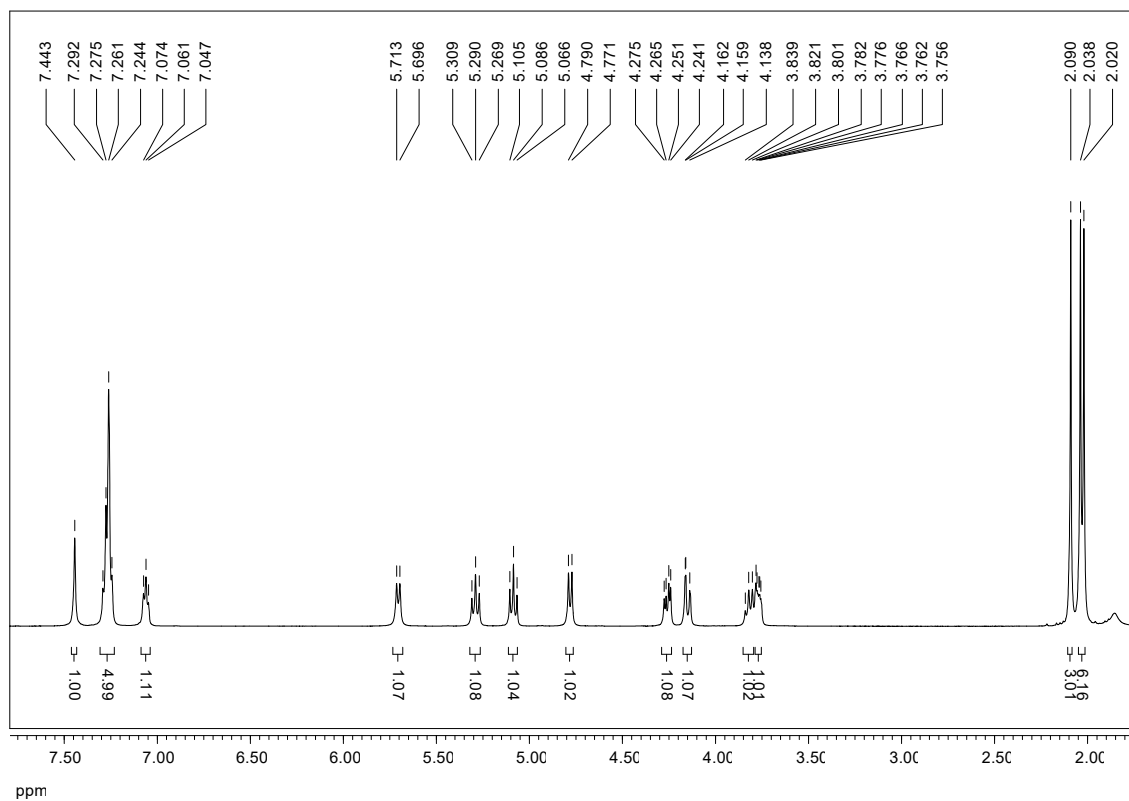


Figure S17 ¹H NMR spectrum of 3,4,6-tri-O-acetyl-2-deoxy-2-(3-phenylureido)-β-D-glucopyranosyl azide (14) recorded in CDCl₃.

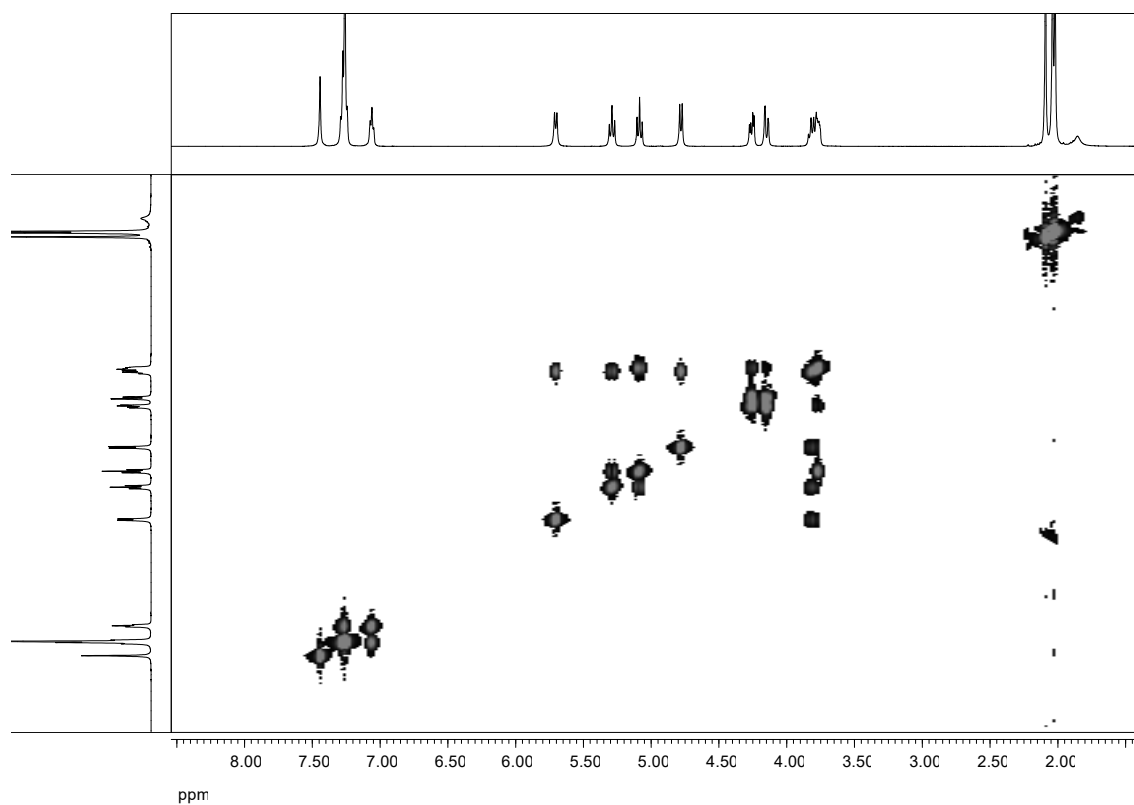


Figure S18 COSY spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**14**) recorded in CDCl_3 .

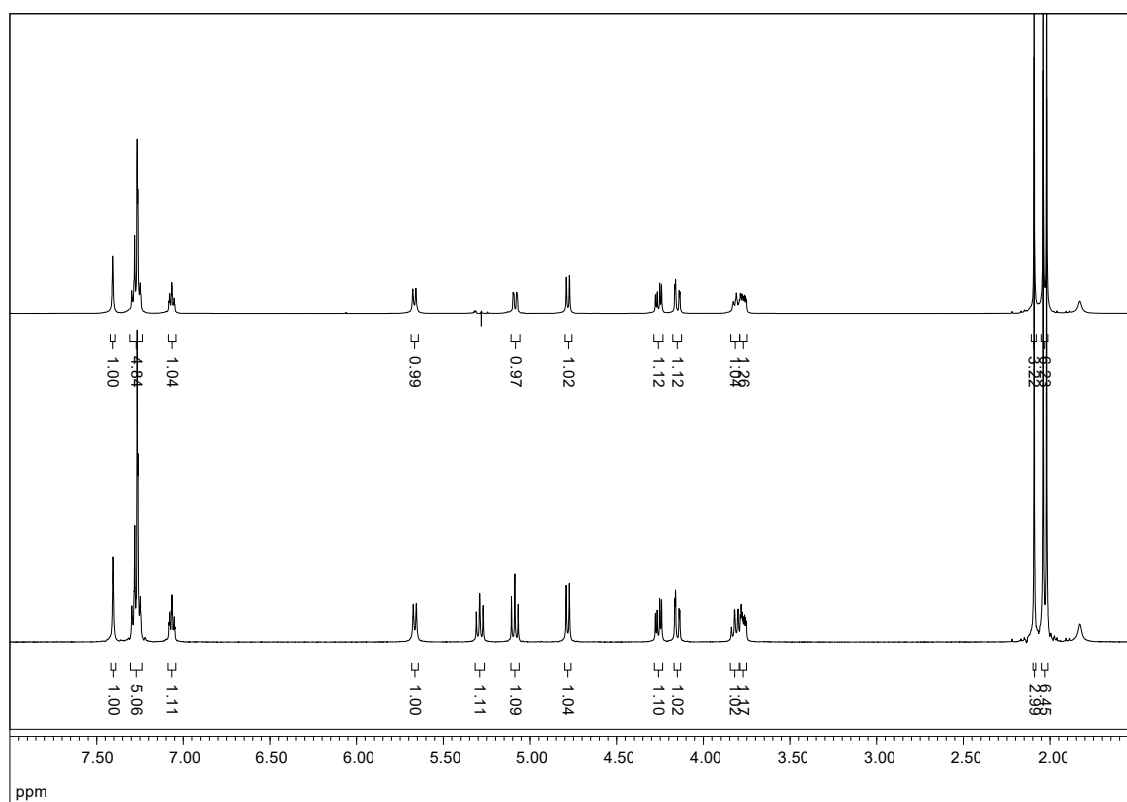


Figure S19 H-3 irradiation of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**14**) recorded in CDCl_3 .

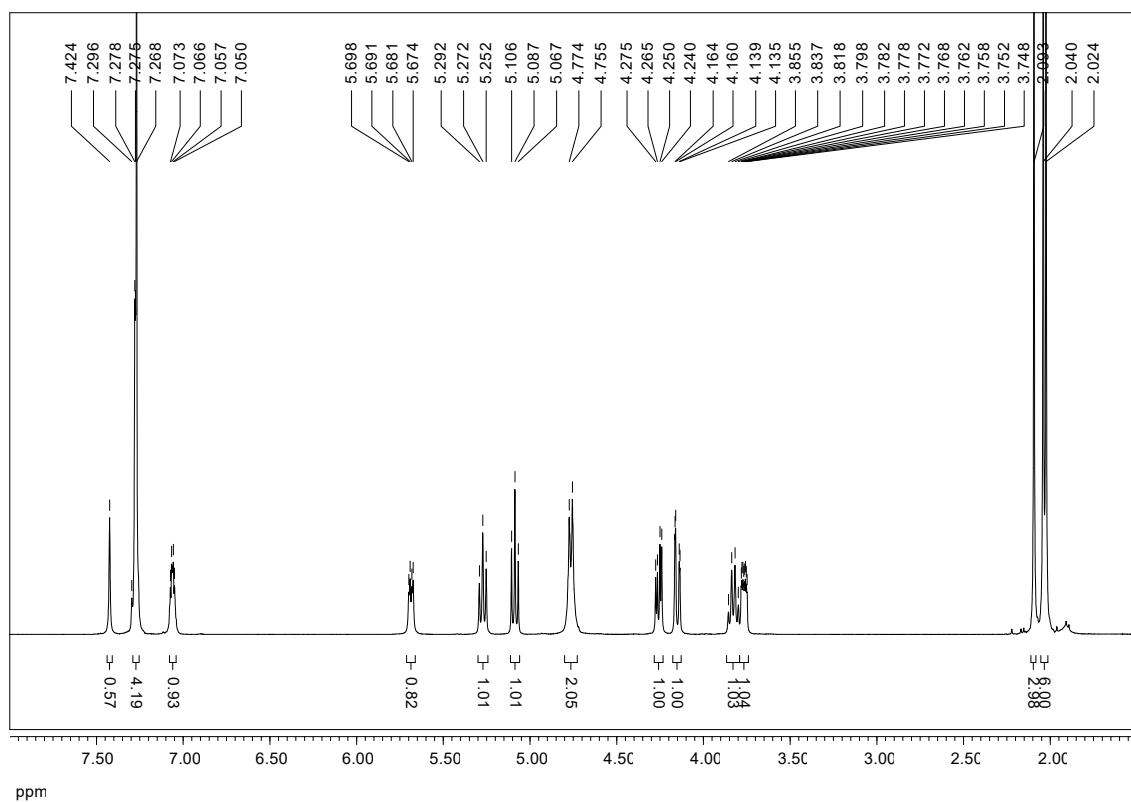


Figure S20 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**14**) recorded with isotopic exchange in D_2O .

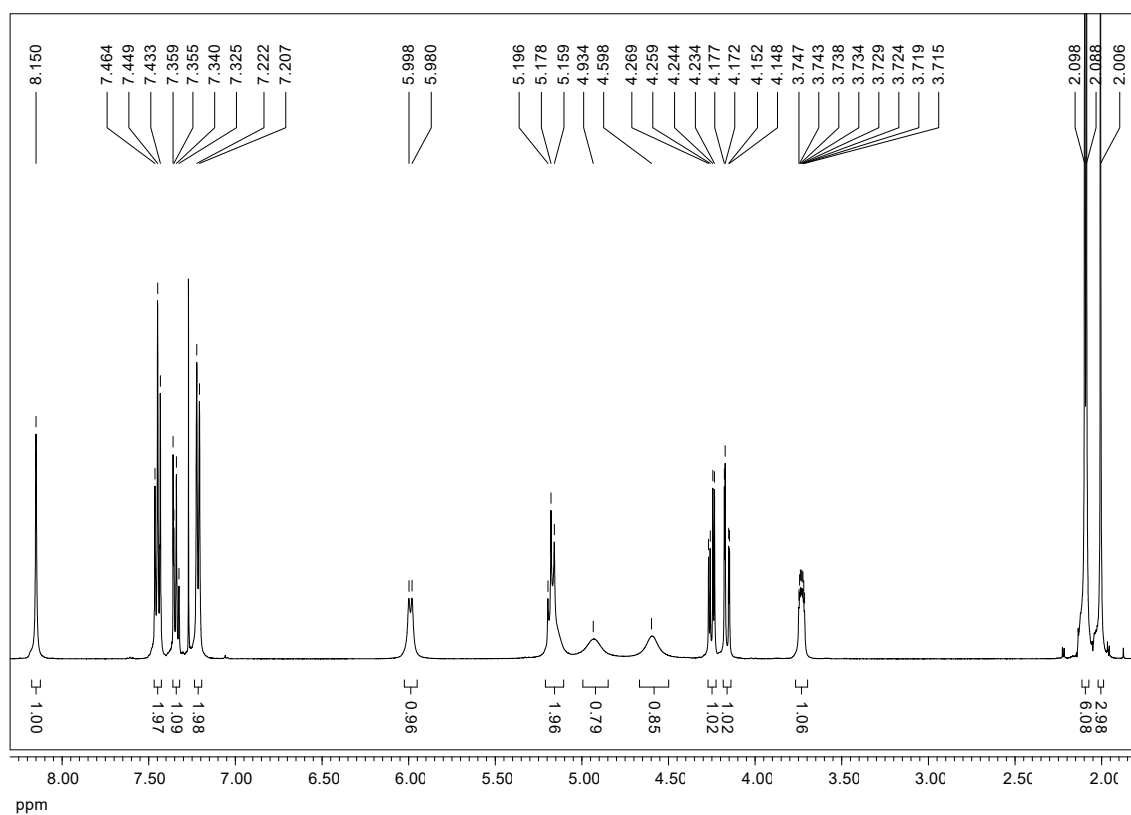


Figure S21 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in CDCl_3 .

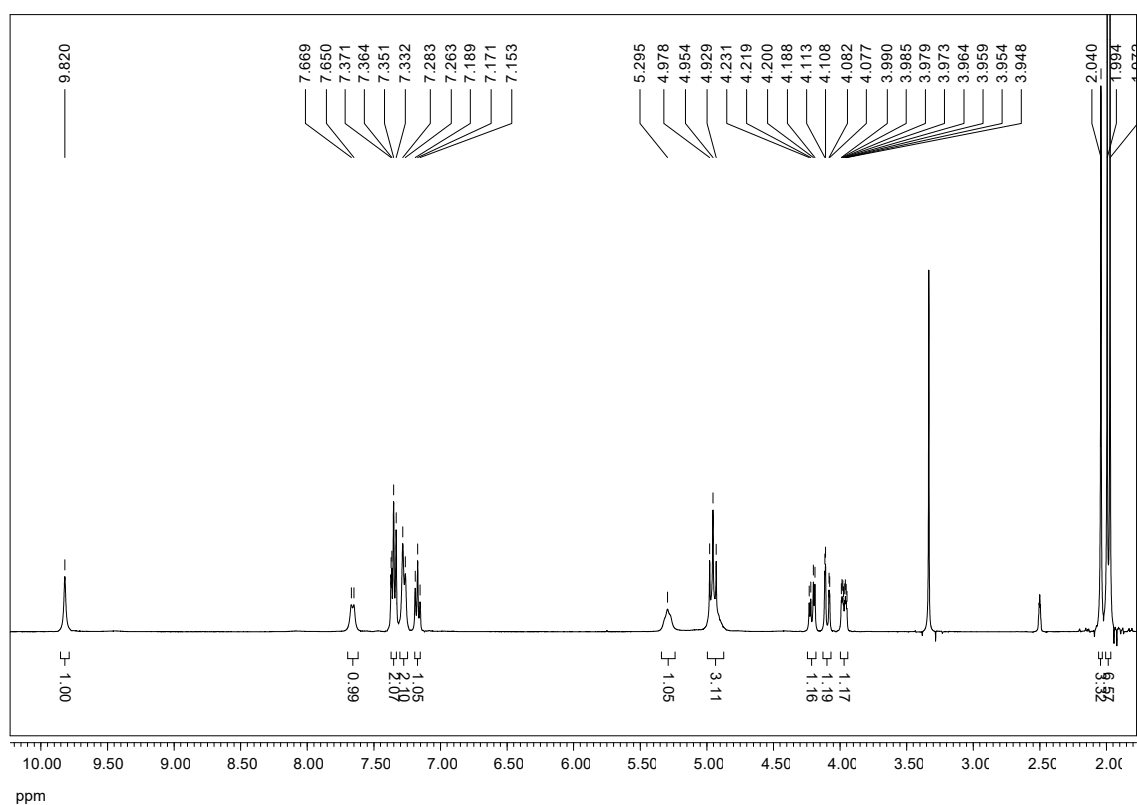


Figure S22 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in $\text{DMSO}-d_6$.

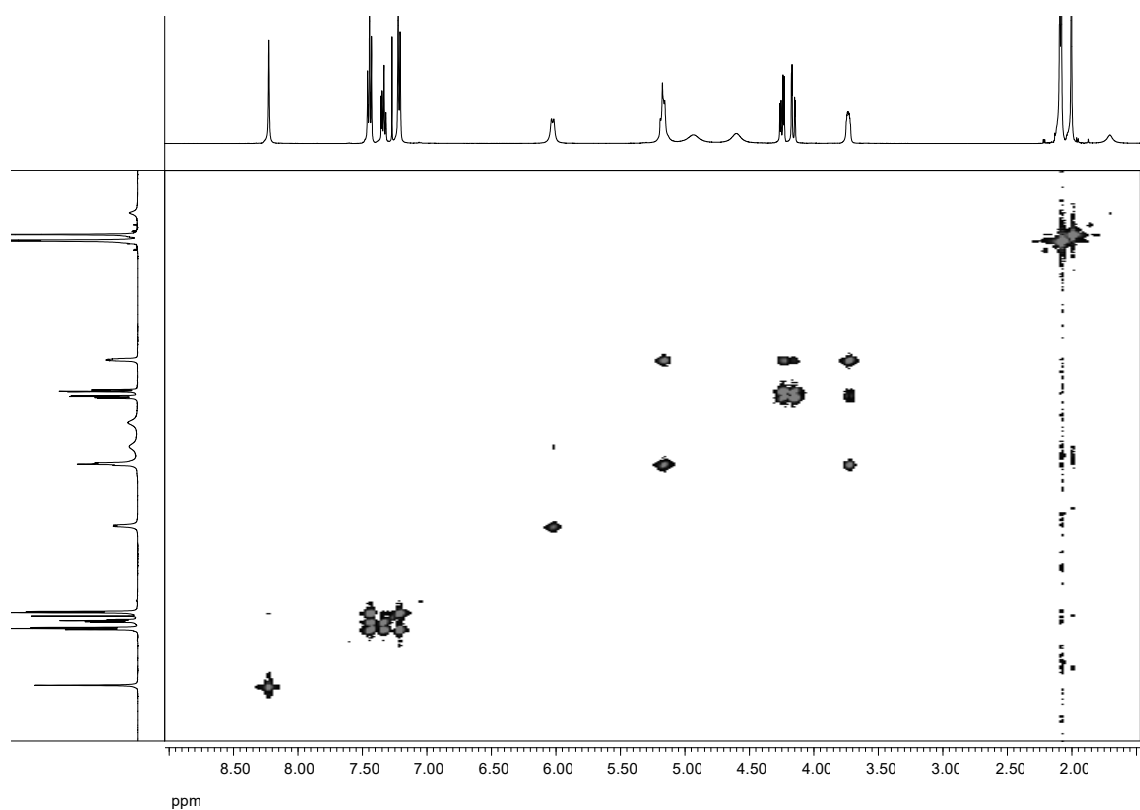


Figure S23 COSY spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in CDCl_3 .

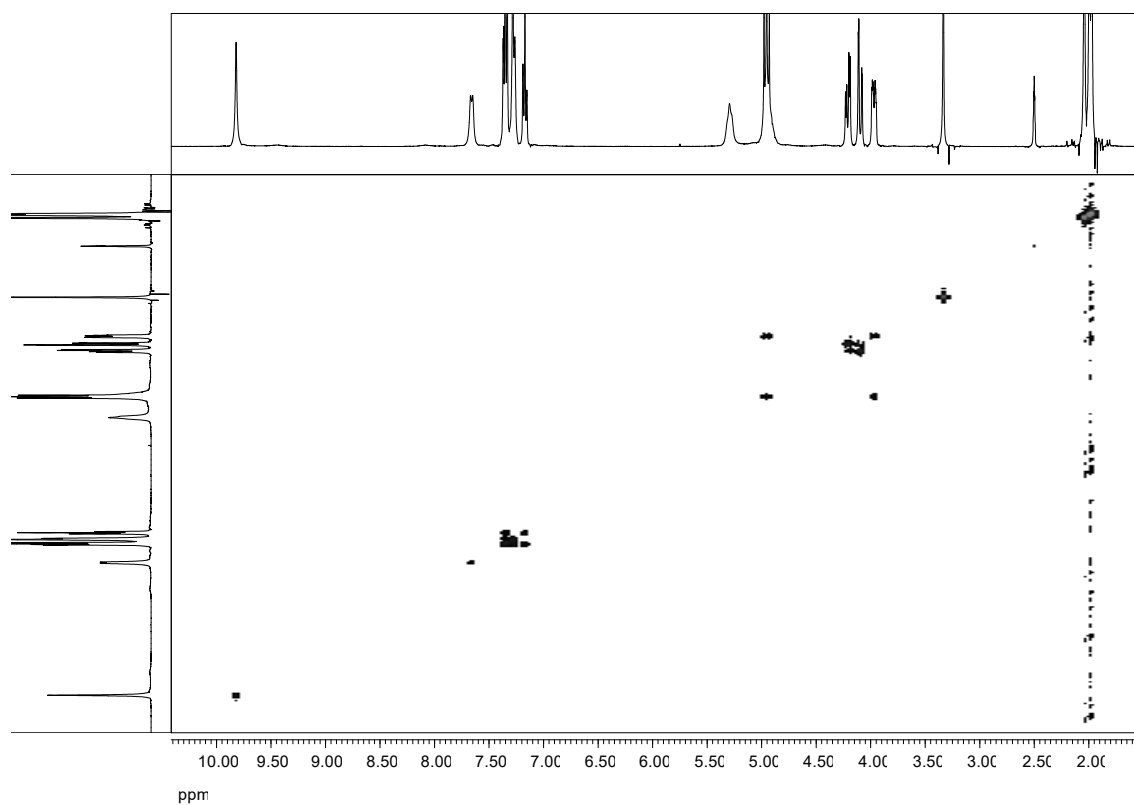


Figure S24 COSY spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in DMSO- d_6 .

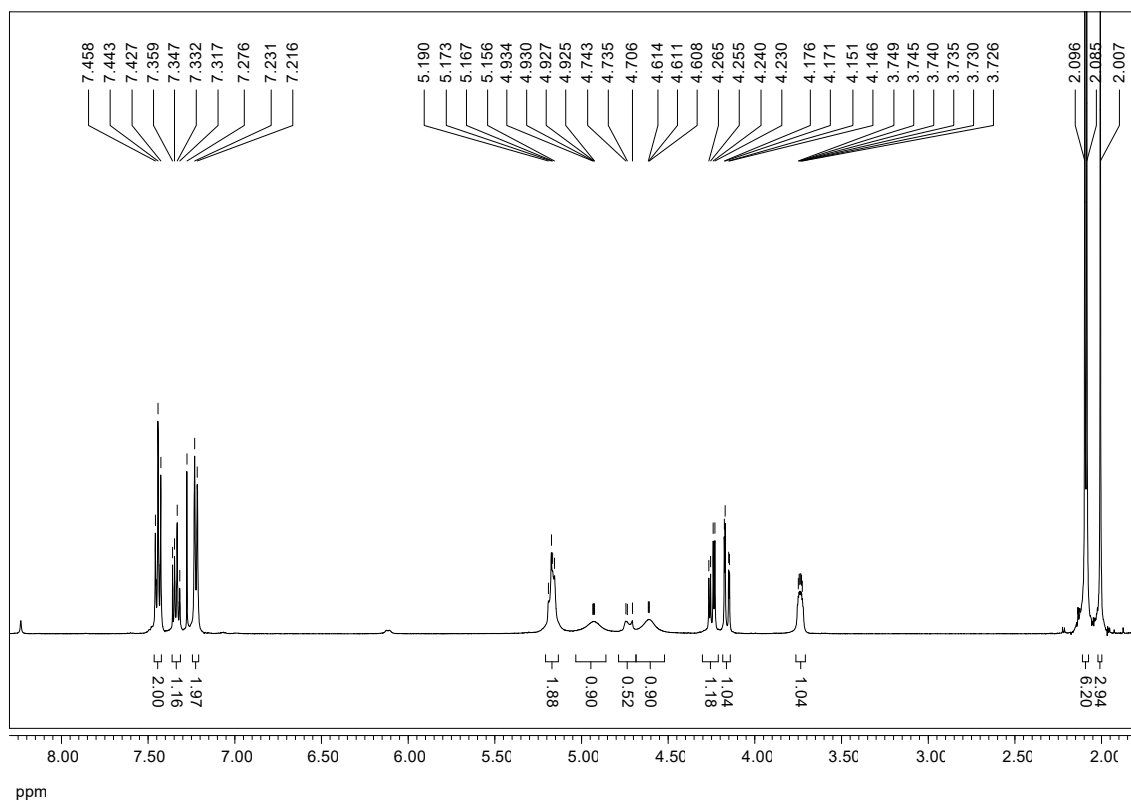


Figure S25 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded with isotopic exchange in D_2O .

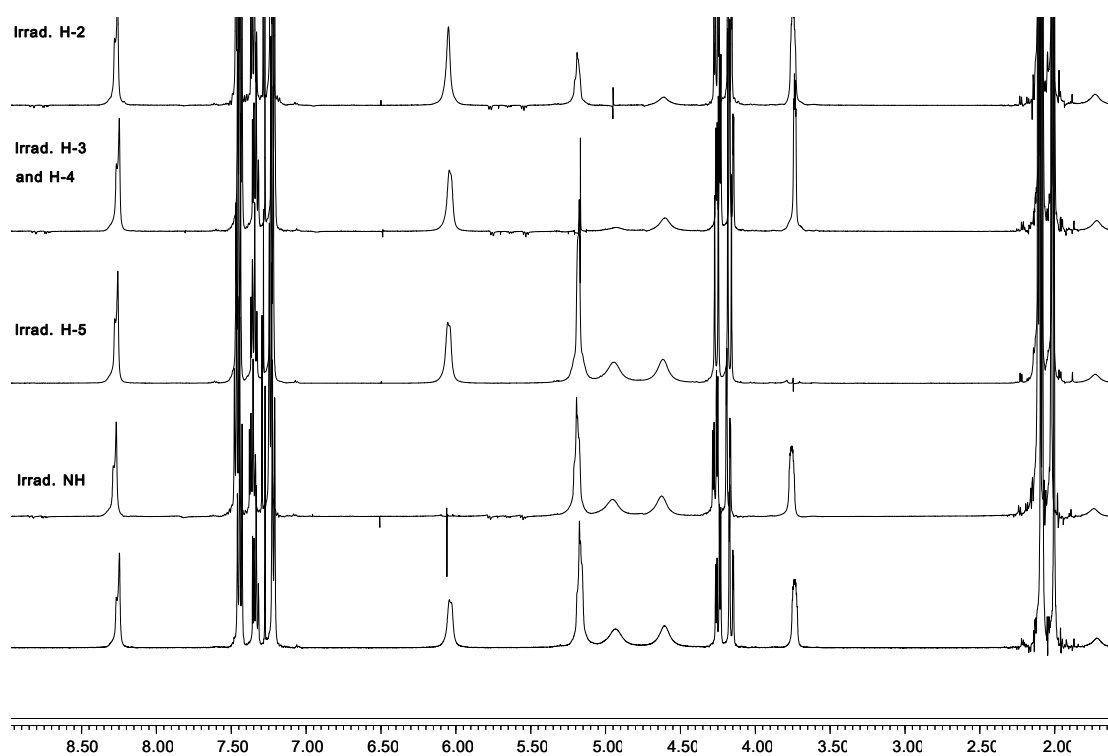


Figure S26 Selective proton irradiations of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in CDCl_3 .

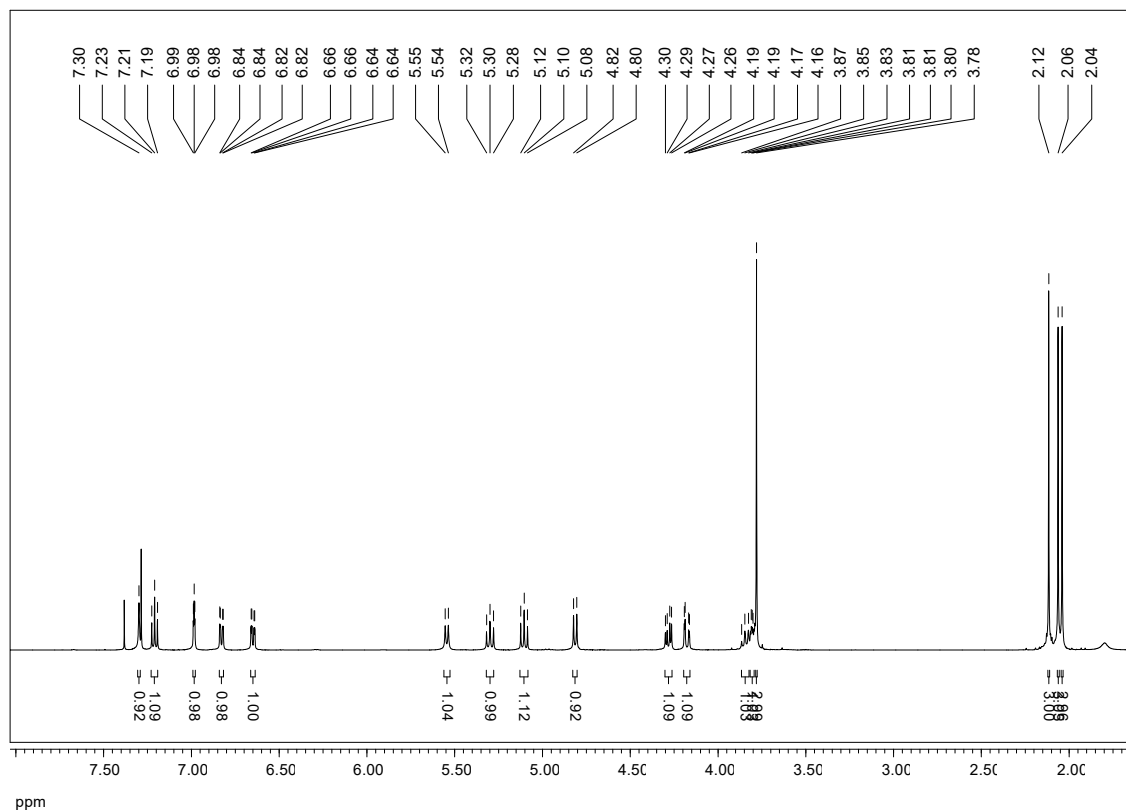


Figure S27 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**16**) recorded in CDCl_3 .

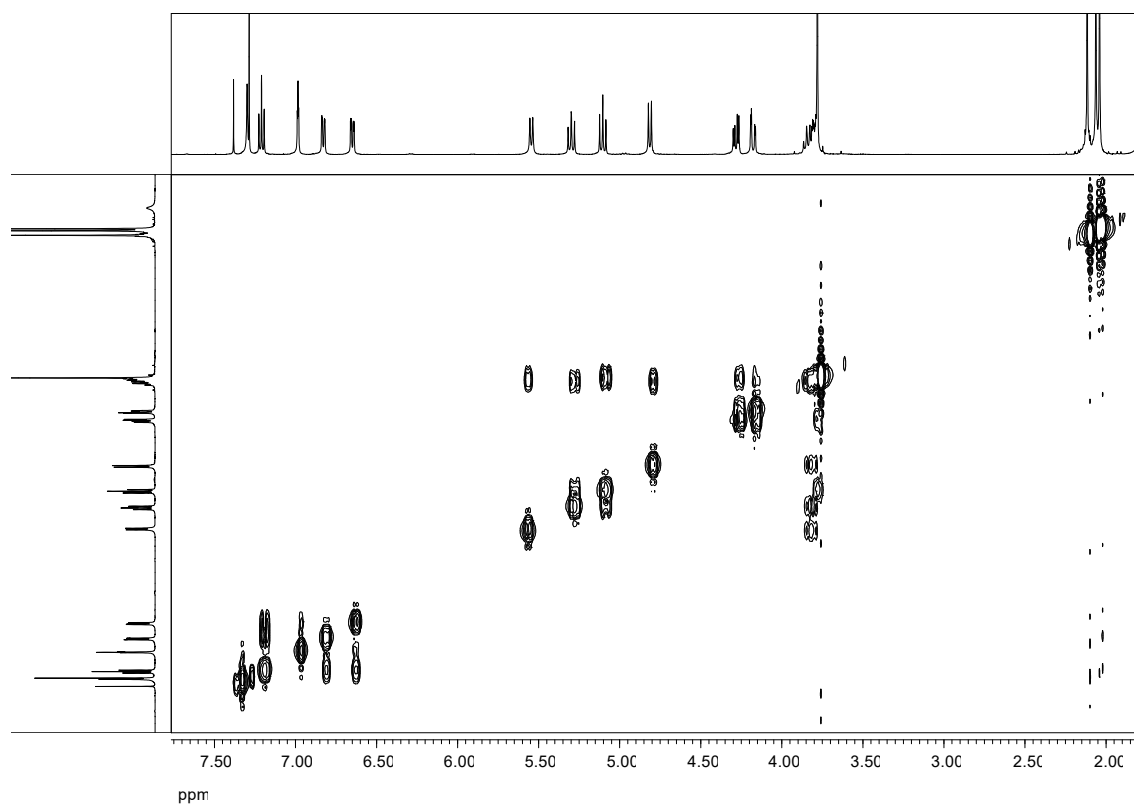


Figure S28 COSY spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**16**) recorded in CDCl_3 .

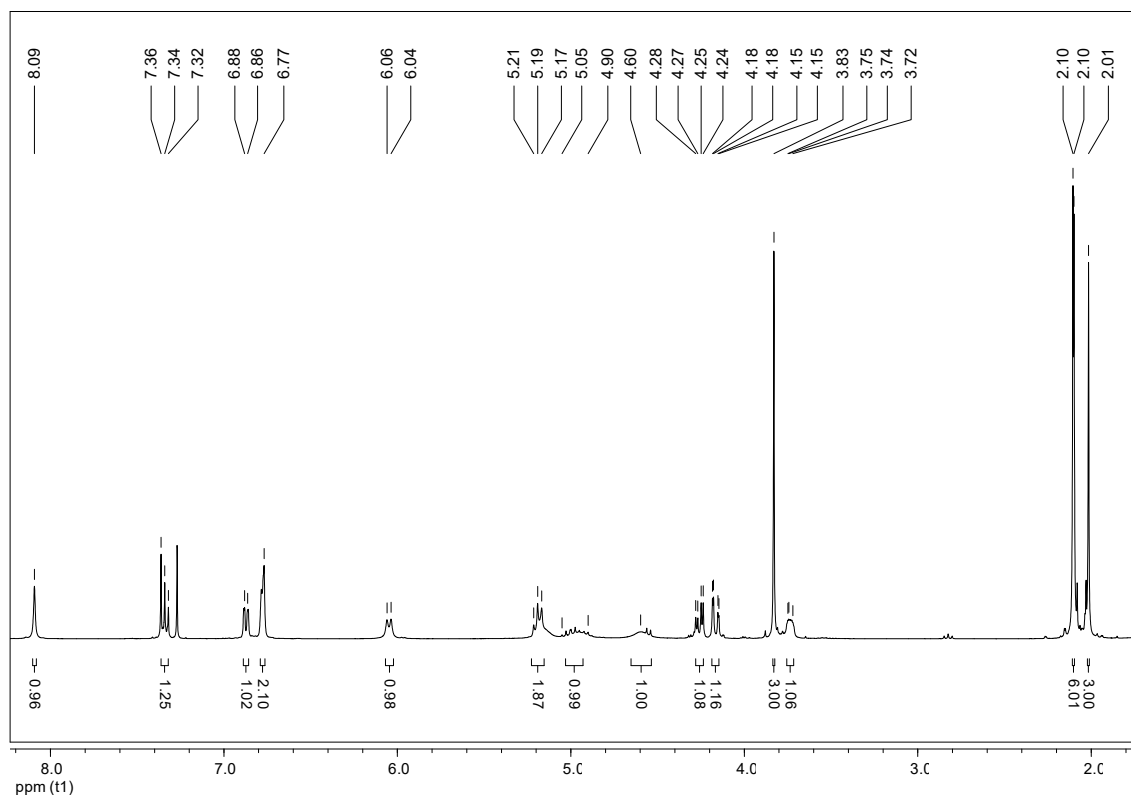


Figure S29 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)thioureido]- β -D-glucopyranosyl azide (**17**) recorded in CDCl_3 .

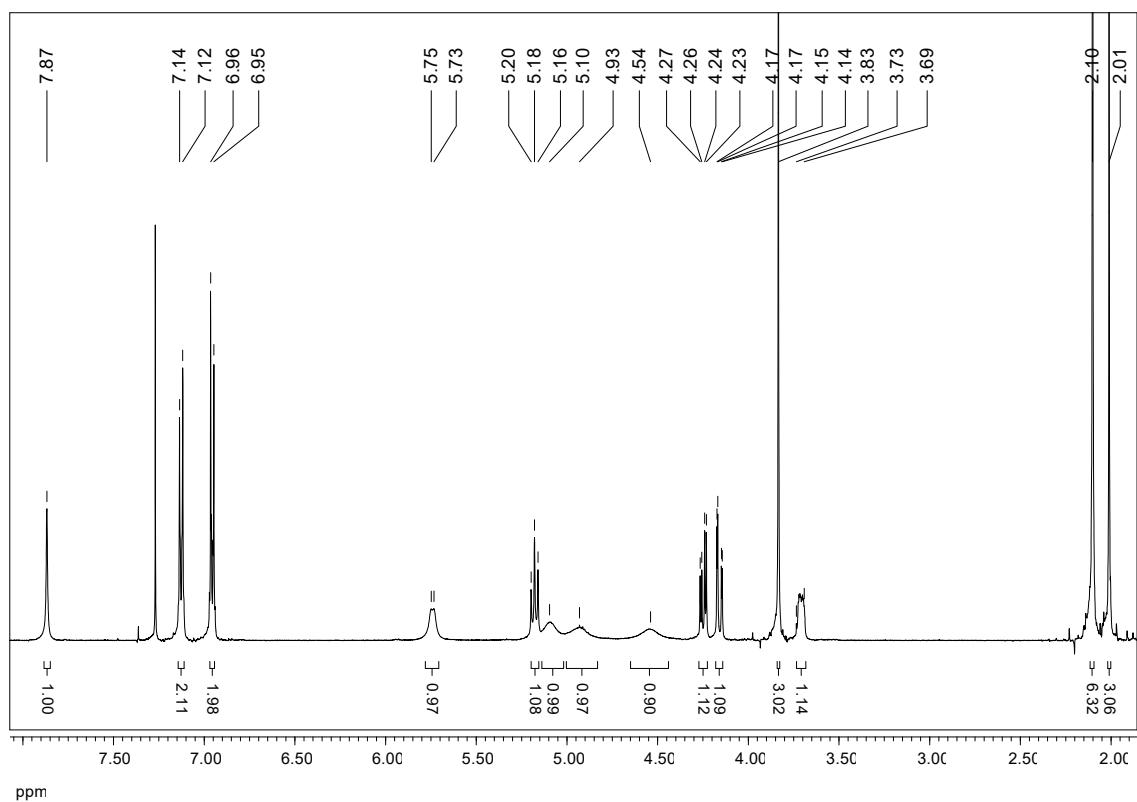


Figure S30 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**18**) recorded in CDCl_3 .

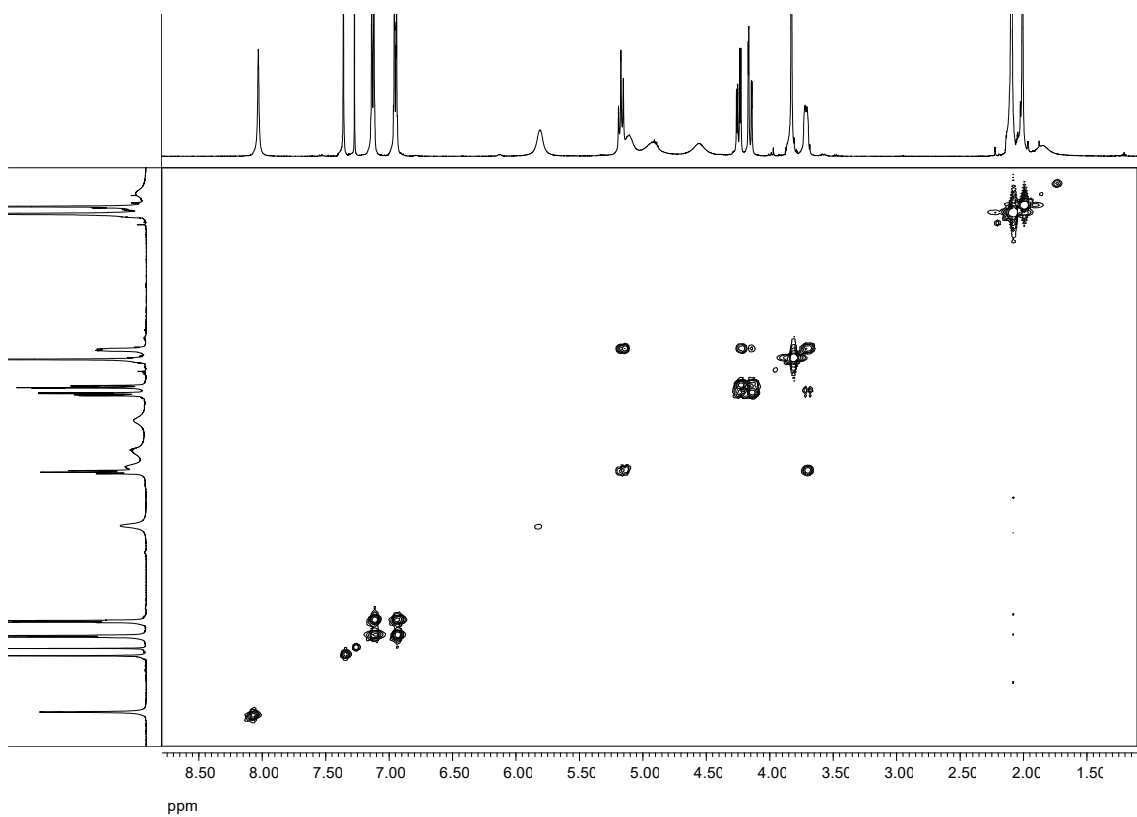


Figure S31 COSY spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**18**) recorded in CDCl_3 .

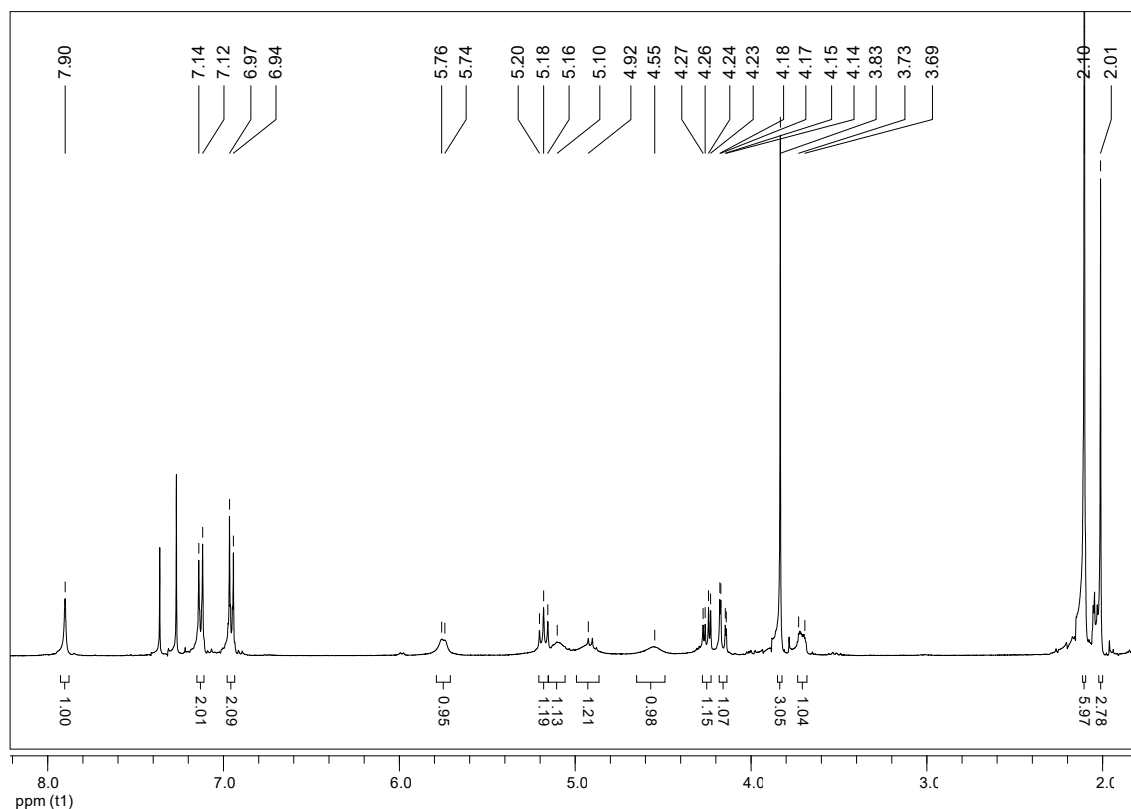


Figure S32 ¹H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)thioureido]-β-D-glucopyranosyl azide (**19**) recorded in CDCl₃.

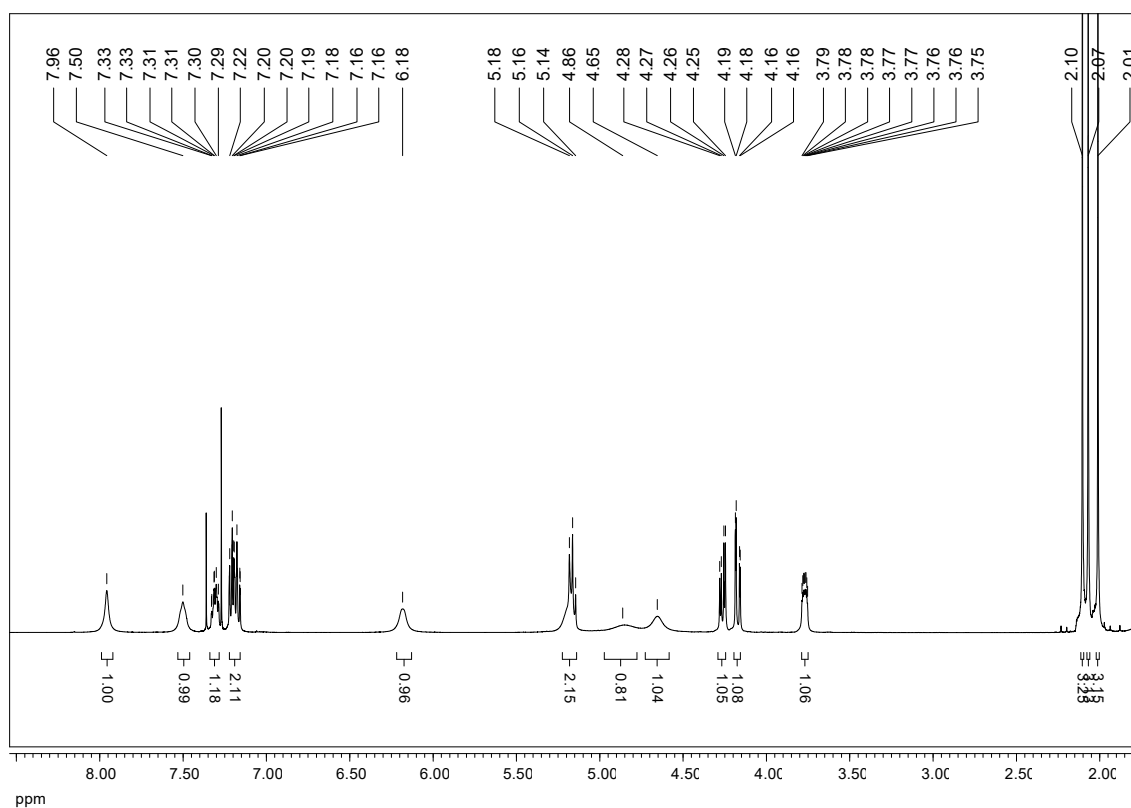


Figure S33 ¹H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-fluorophenyl)thioureido]-β-D-glucopyranosyl azide (**20**) recorded in CDCl₃.

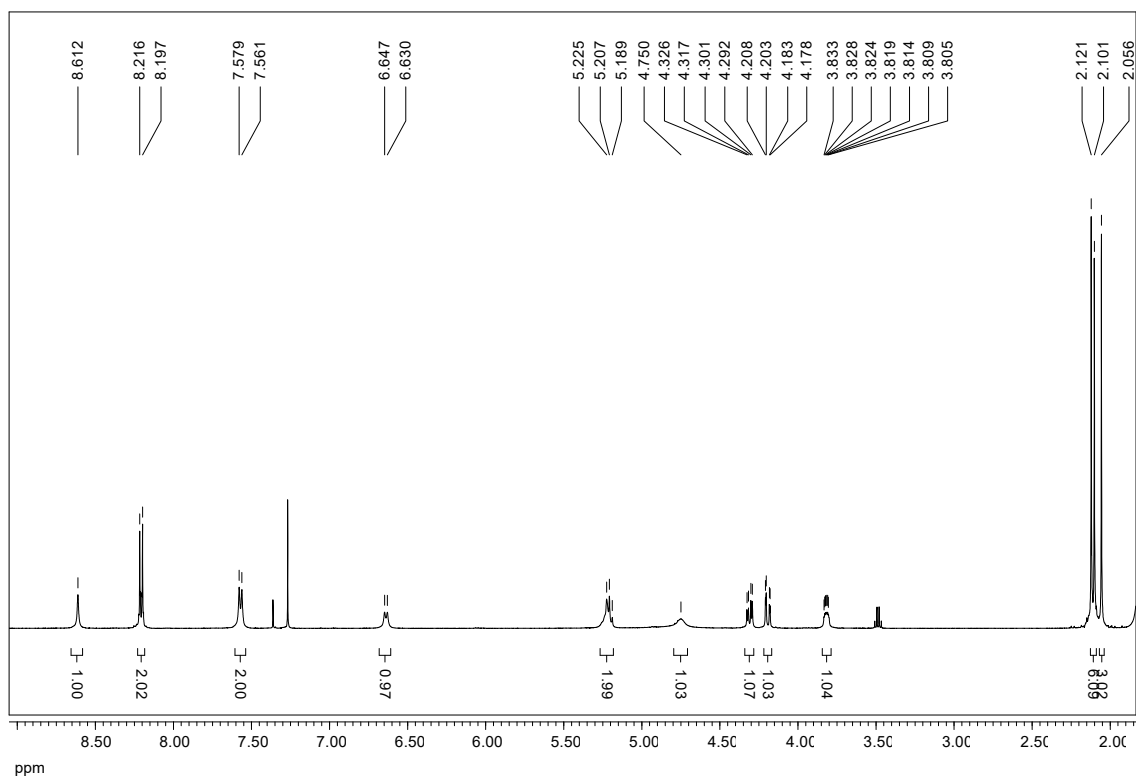


Figure S34 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-nitrophenyl)thioureido]- β -D-glucopyranosyl azide (**21**) recorded in CDCl_3 .

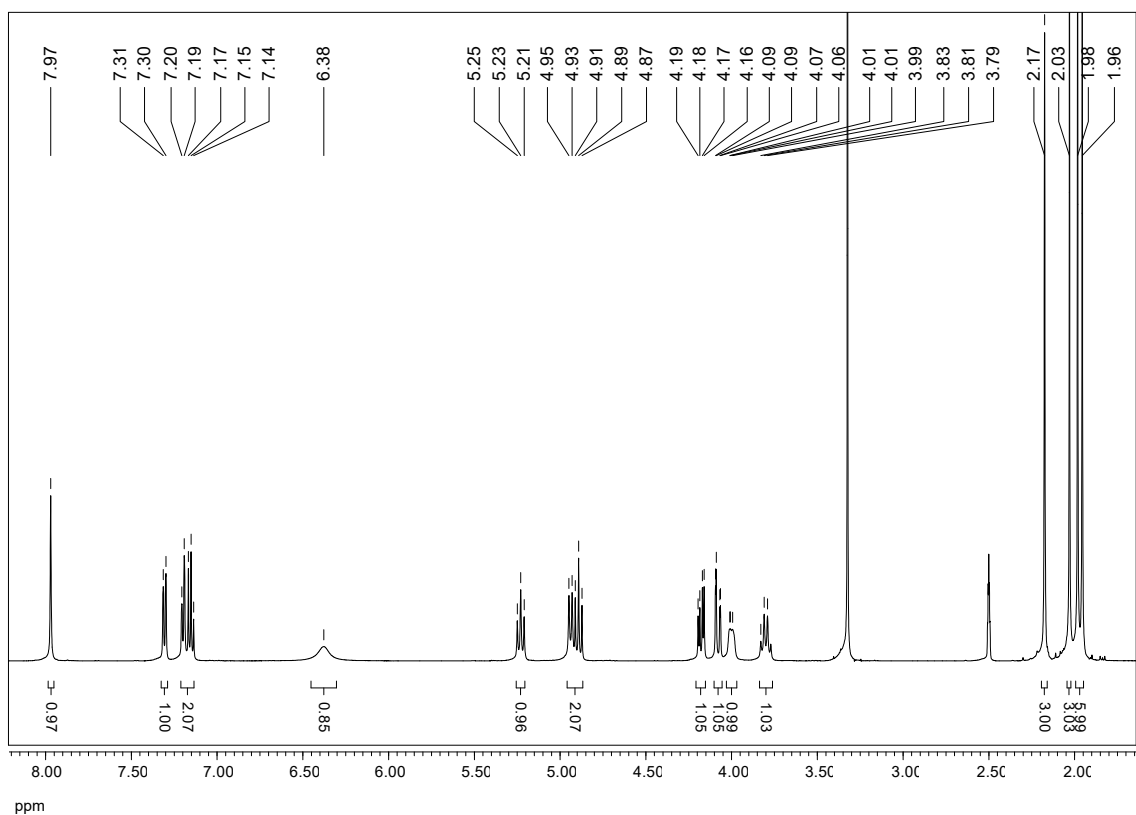


Figure S35 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) recorded in $\text{DMSO}-d_6$.

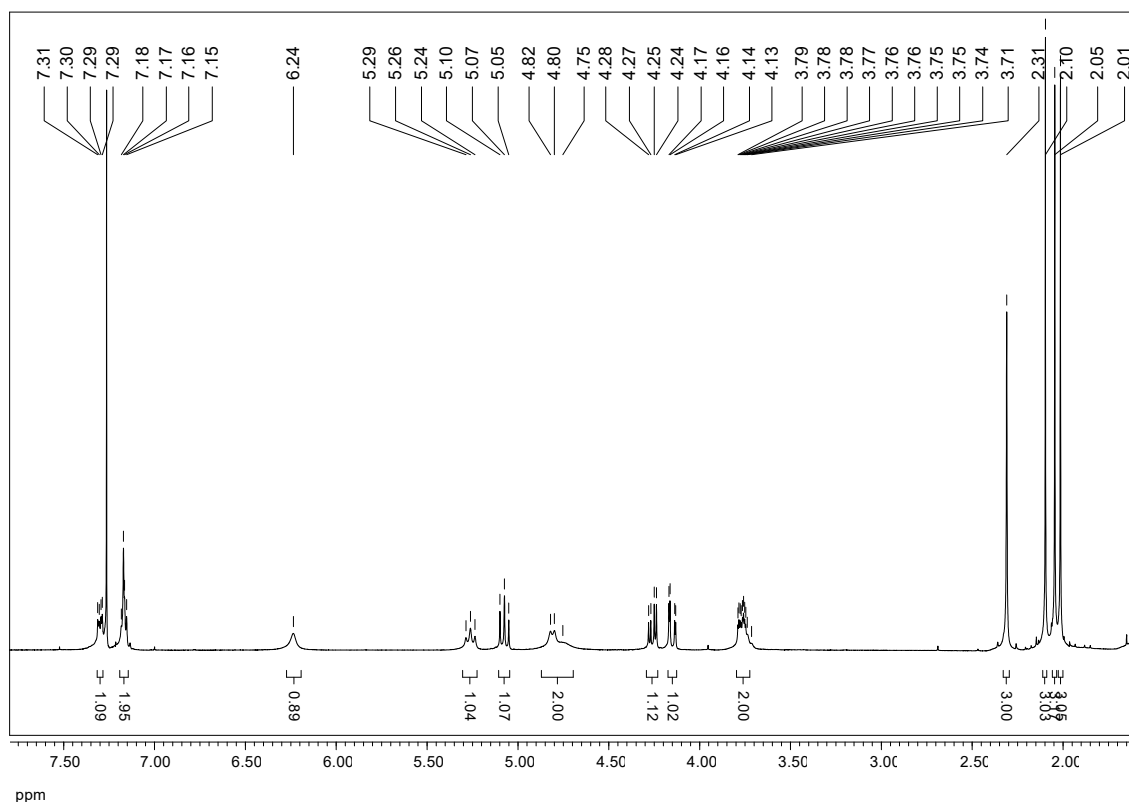


Figure S36 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) recorded in CDCl_3 .

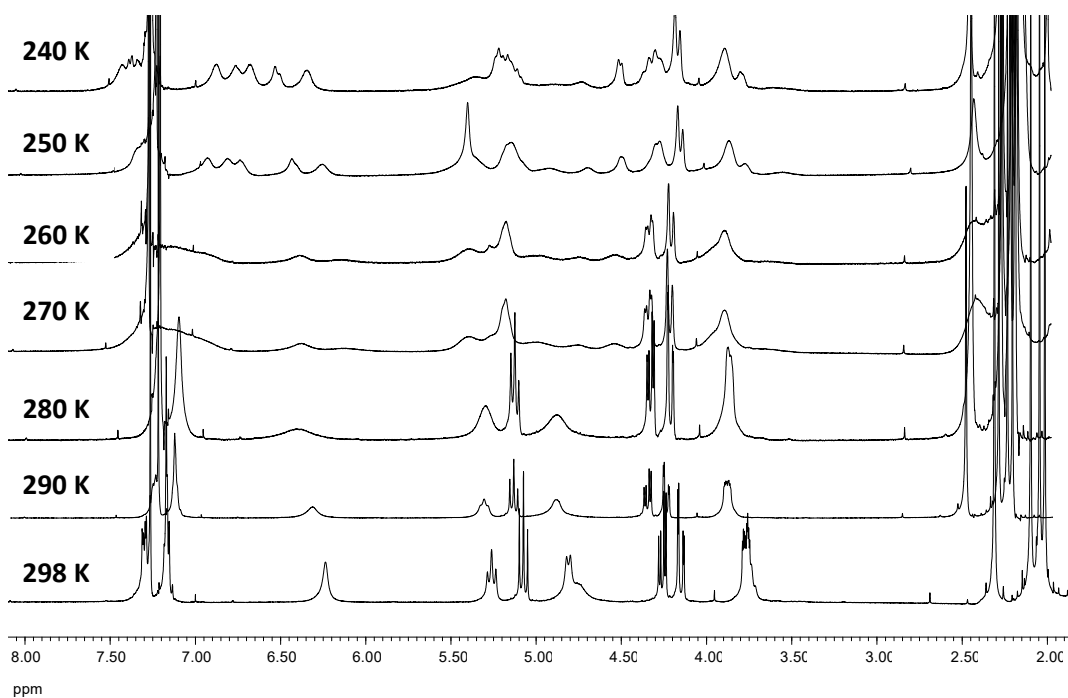


Figure S37 Variable-temperature ^1H NMR spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) recorded in CDCl_3 .

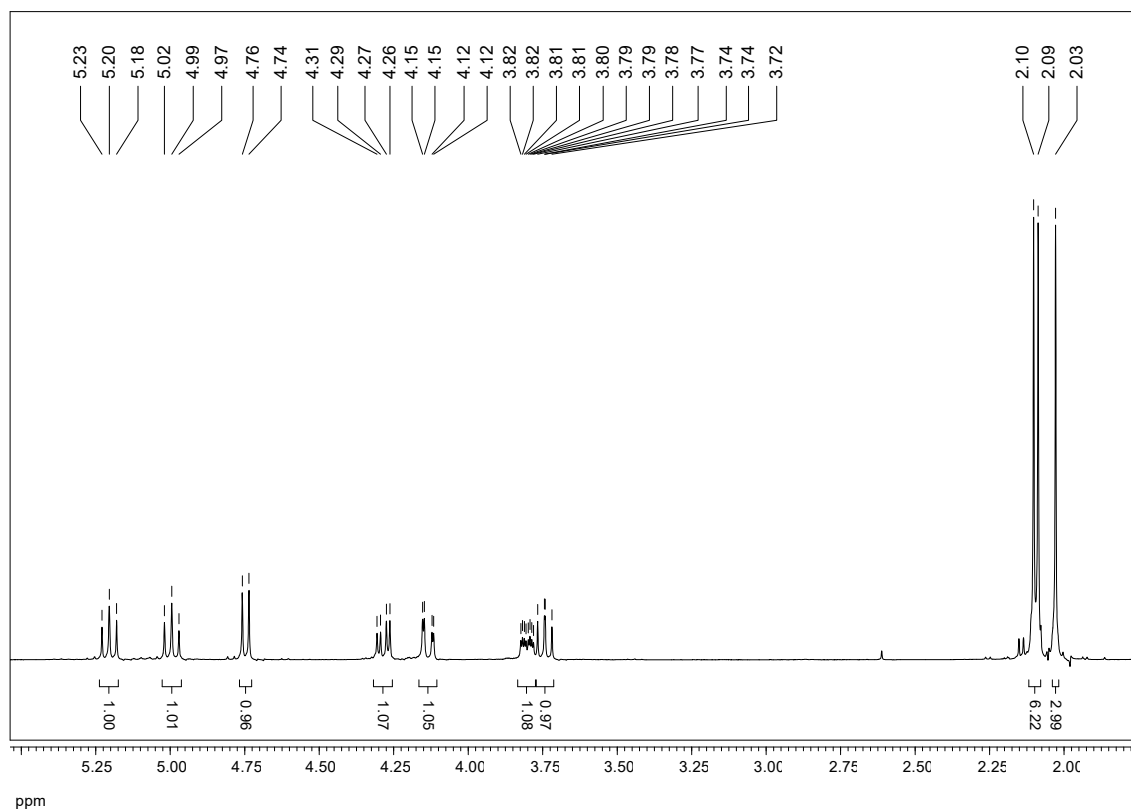


Figure S38 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-isothiocianato- β -D-glucopyranosyl azide (**23**) recorded in CDCl_3 .

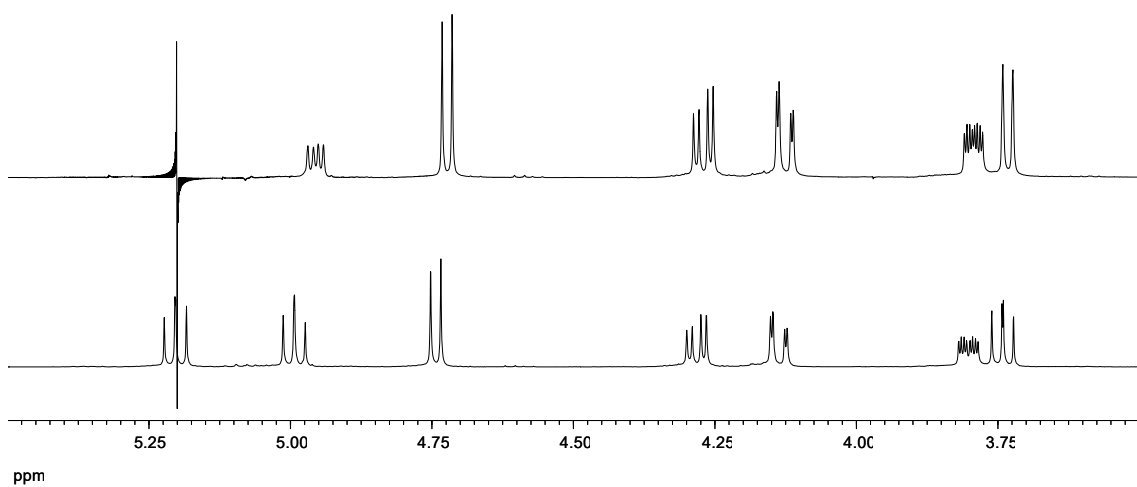


Figure S39 H-3 irradiation of 3,4,6-tri-*O*-acetyl-2-deoxy-2-isothiocianato- β -D-glucopyranosyl azide (**23**) recorded in CDCl_3 .

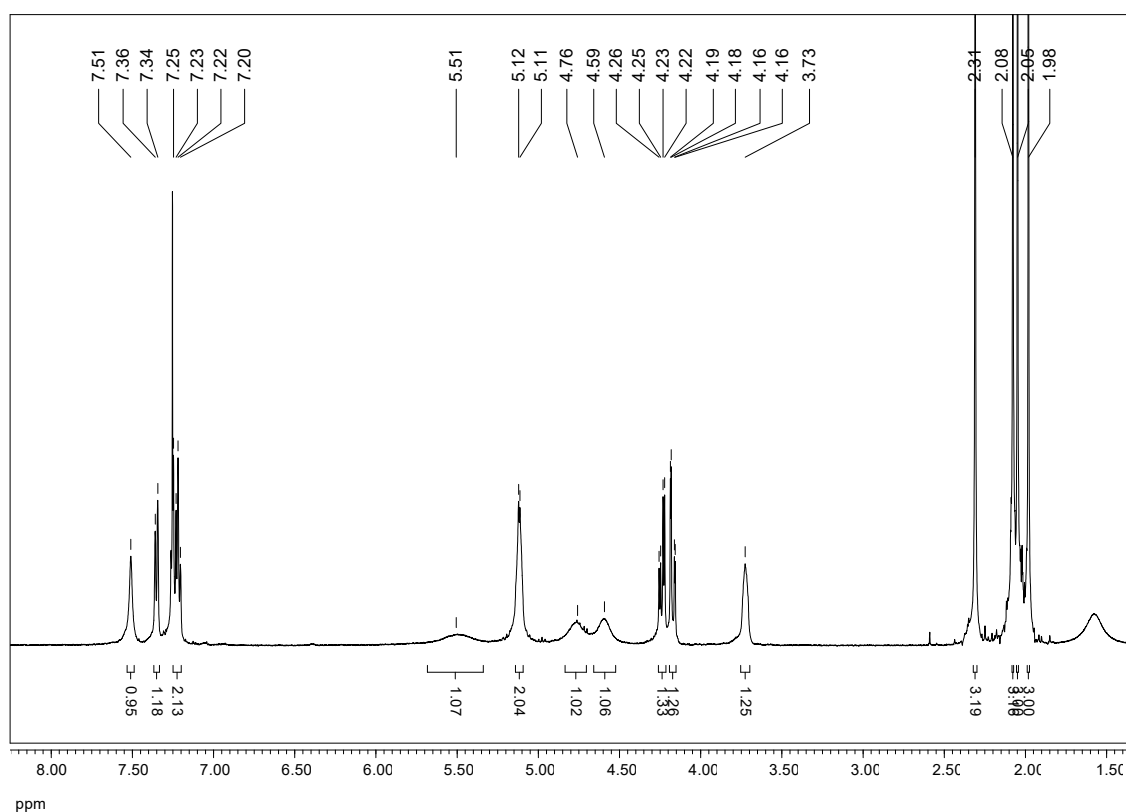


Figure S40 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 at 330K.

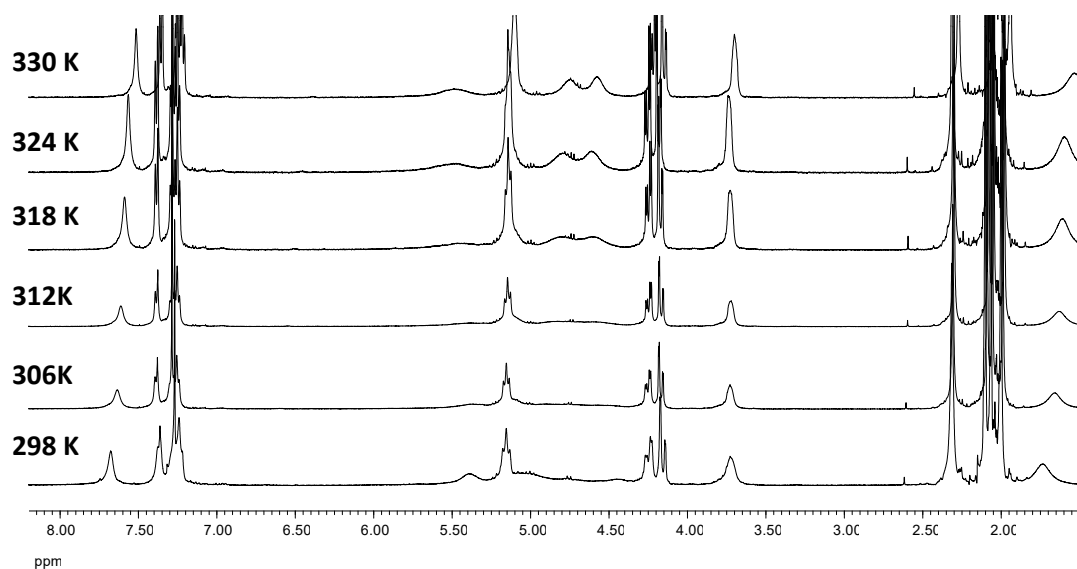


Figure S41 Variable-temperature ^1H NMR spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 .

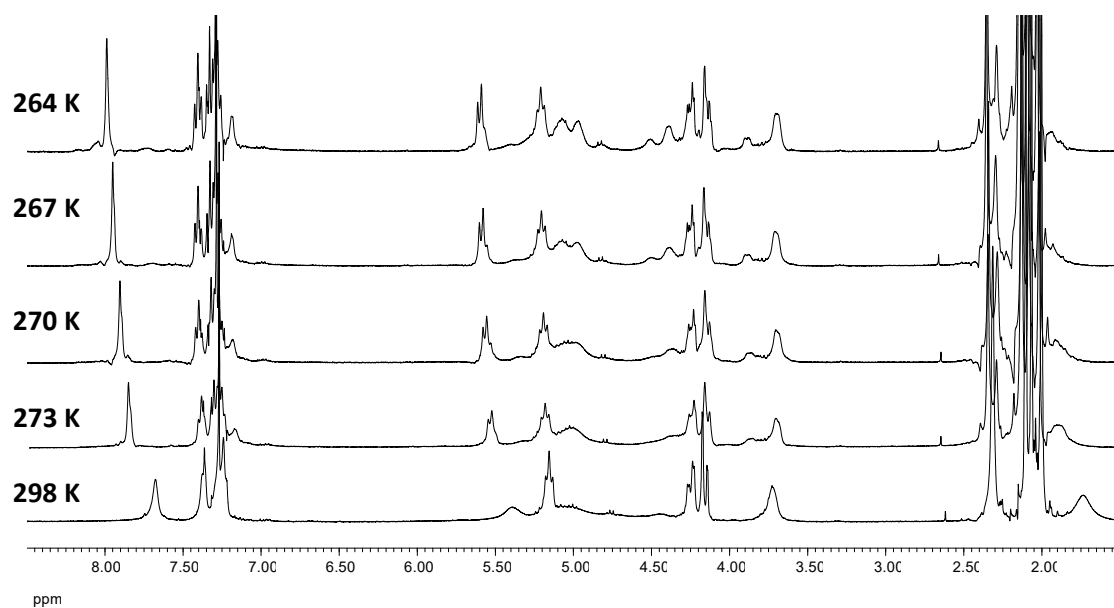


Figure S42 Variable-temperature ^1H NMR spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 .

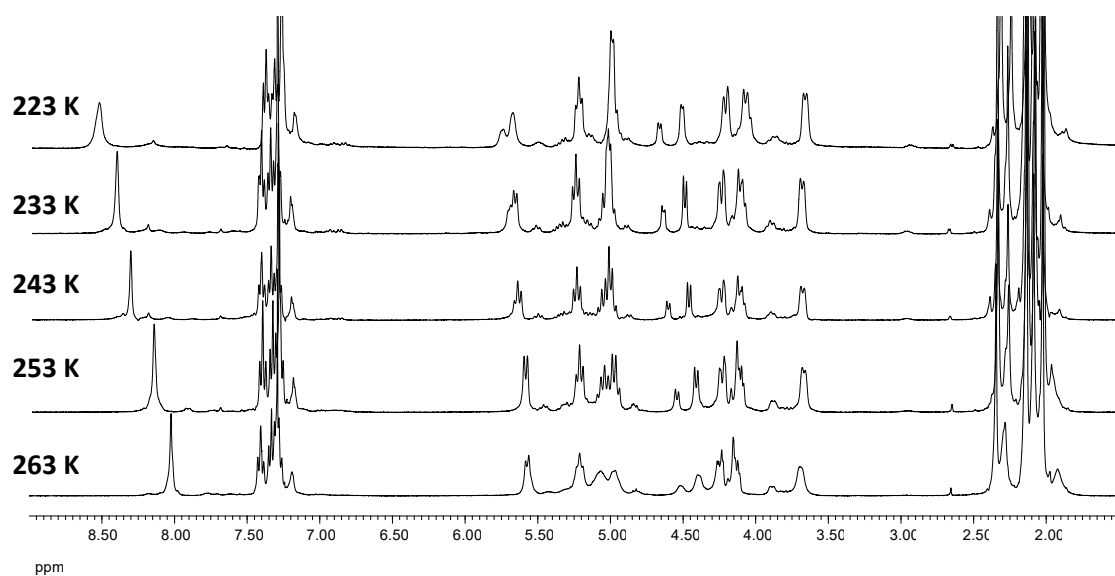


Figure S43 Variable-temperature ^1H NMR spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 .

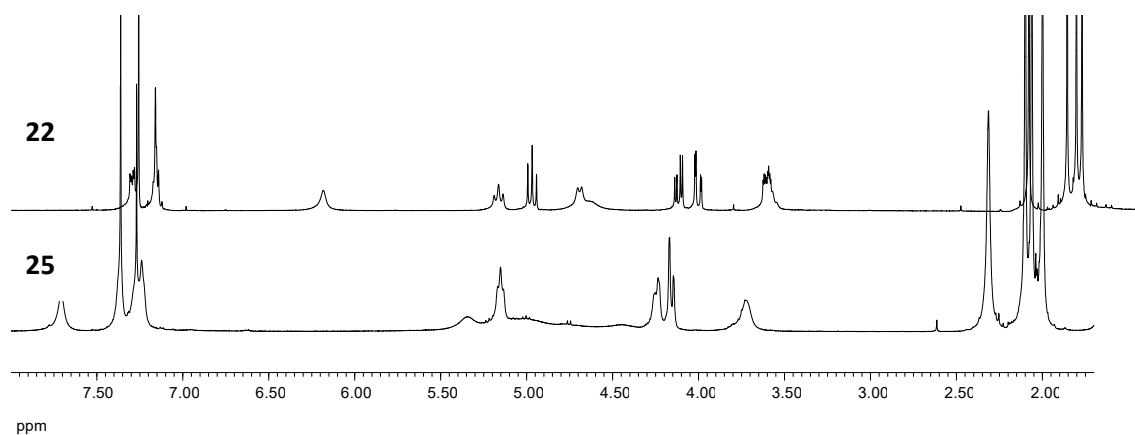


Figure S44 ^1H NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) and 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 at 330K.

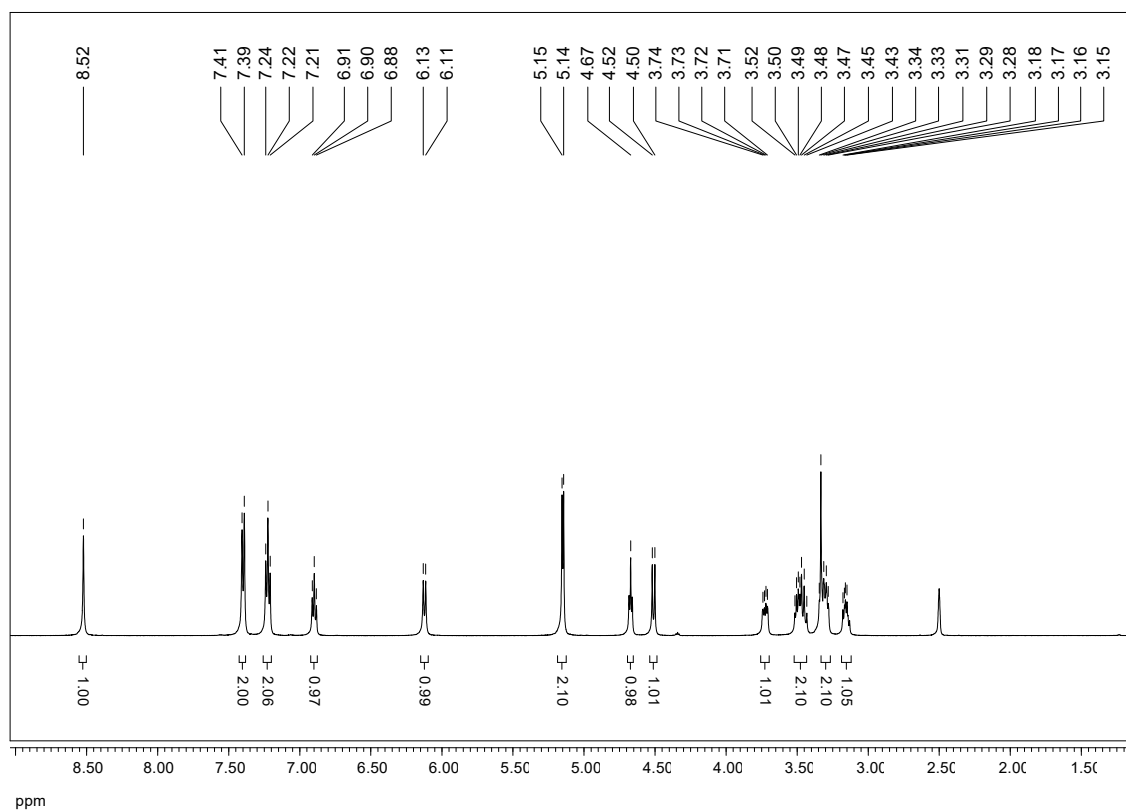


Figure S45 ^1H NMR spectrum of 2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**34**) recorded in $\text{DMSO}-d_6$.

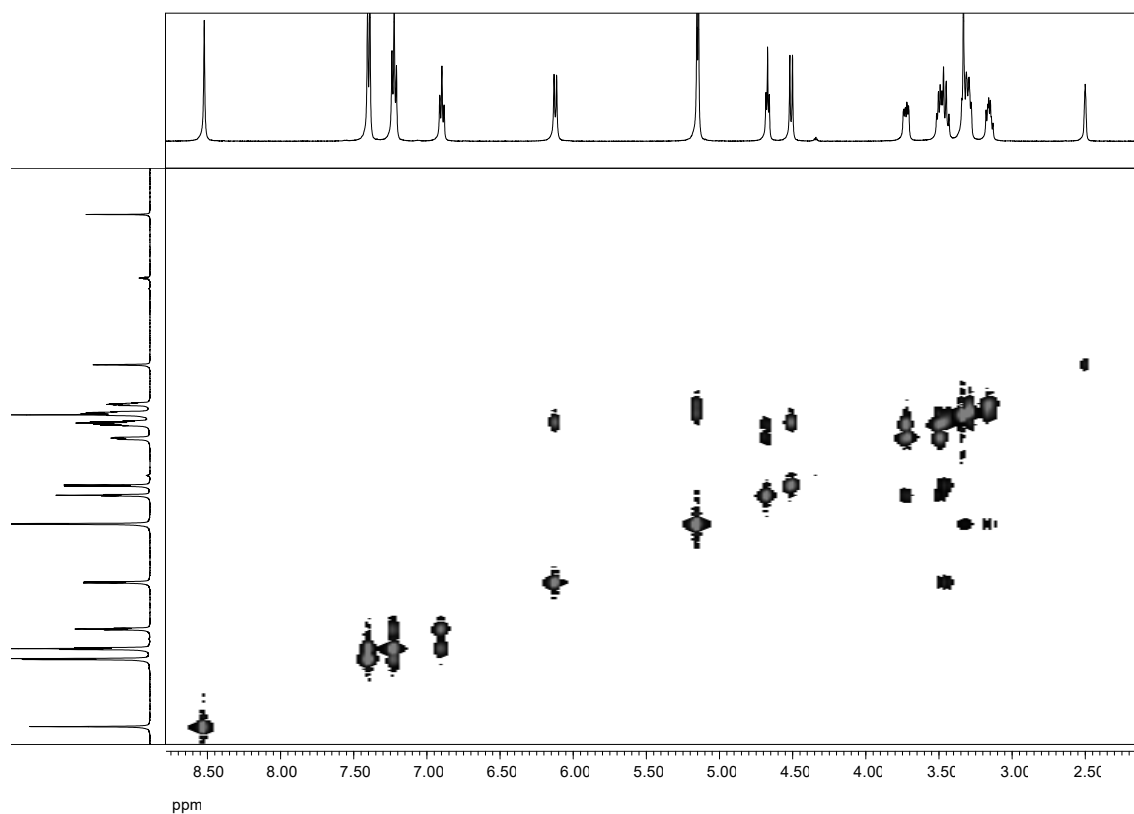


Figure S46 COSY spectrum 2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**34**) recorded in DMSO- d_6 .

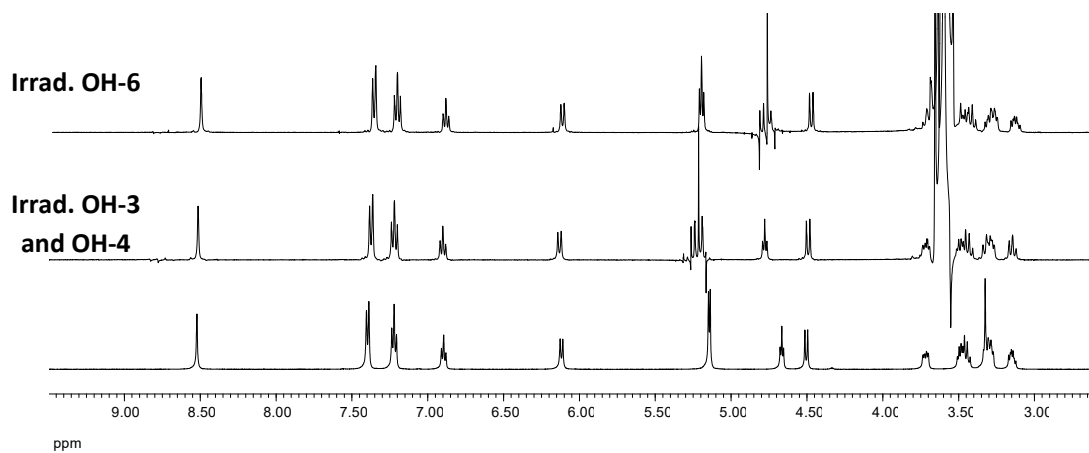


Figure S47 Selective proton irradiations of 2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**34**) recorded in DMSO- d_6 .

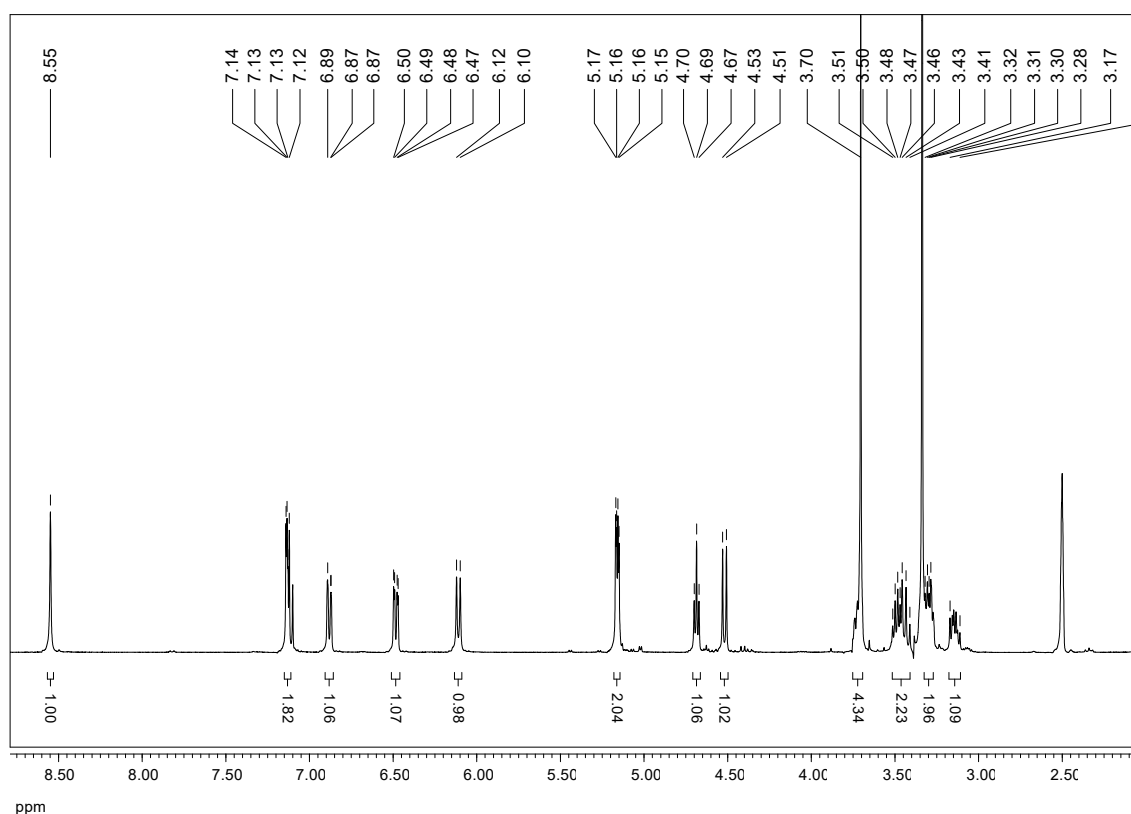


Figure S48 ^1H NMR spectrum of 2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**35**) recorded in $\text{DMSO}-d_6$.

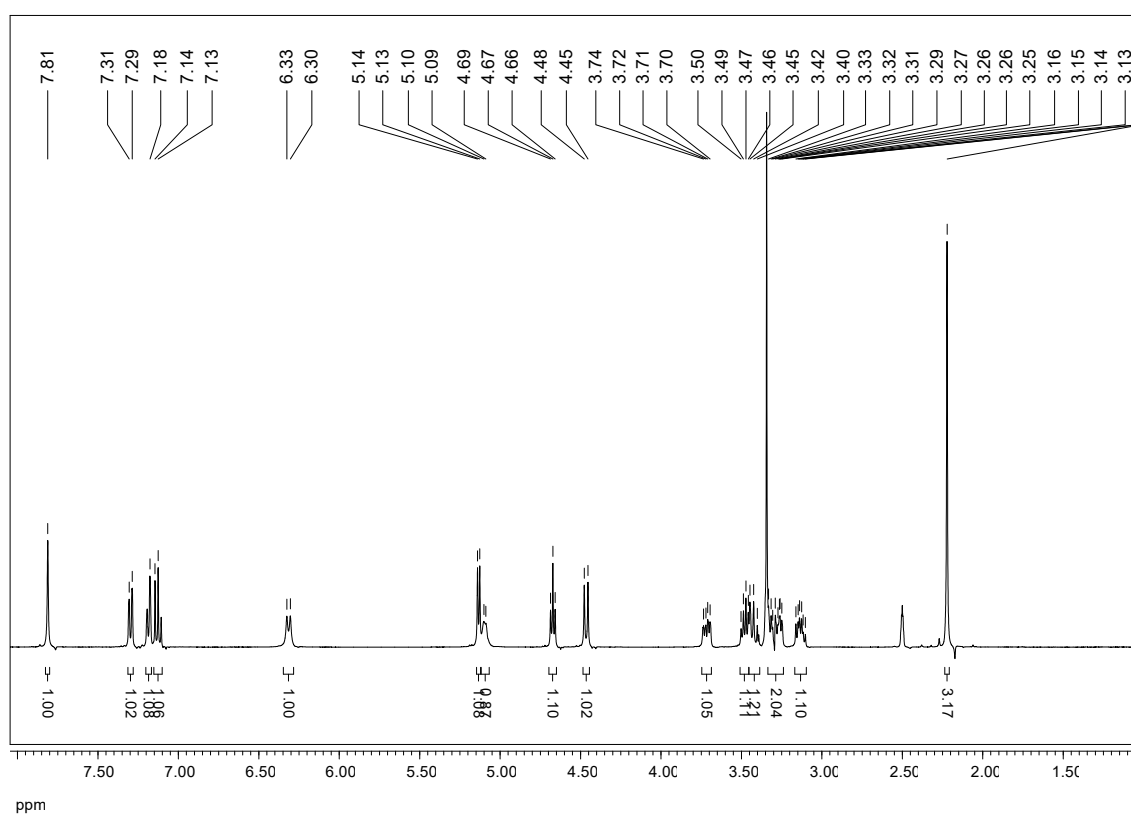


Figure S49 ^1H NMR spectrum of 2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**36**) recorded in $\text{DMSO}-d_6$.

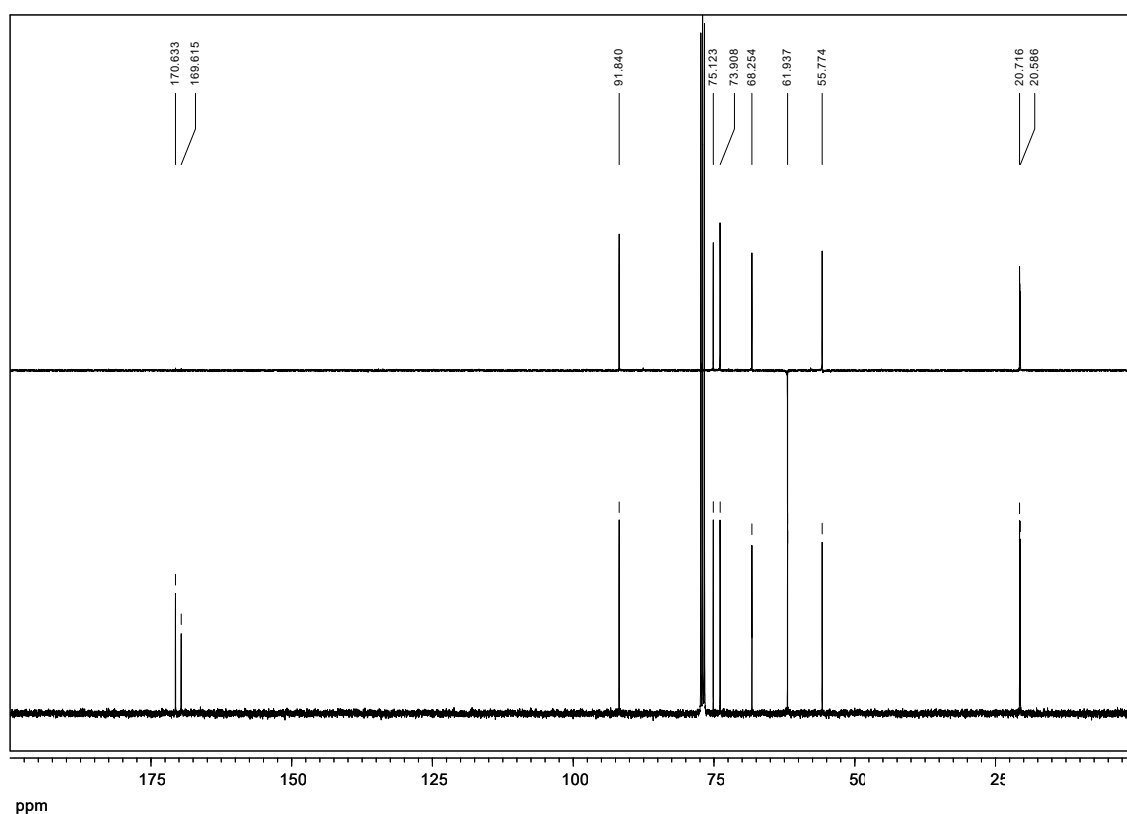


Figure S50 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-O-acetyl-2-amino-2-deoxy- β -D-glucopyranosyl azide (**1**) recorded in CDCl_3 .

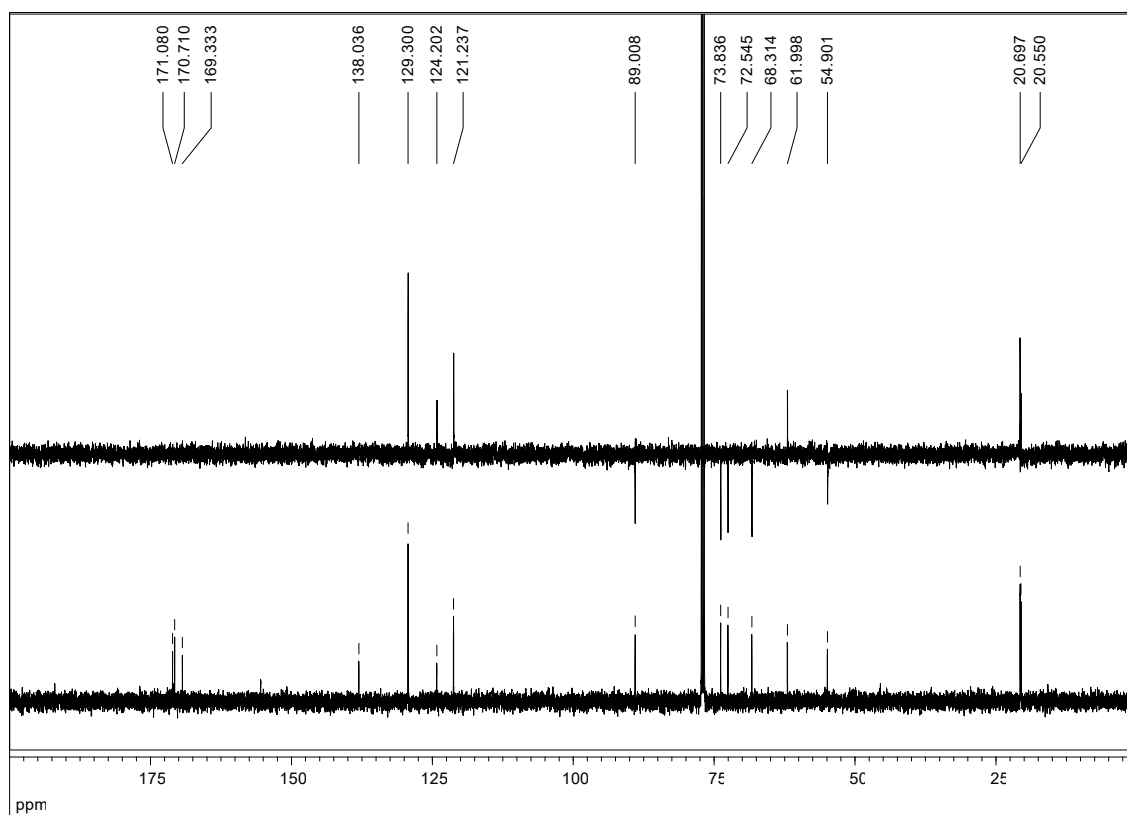


Figure S51 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-O-acetyl-2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**14**) recorded in CDCl_3 .

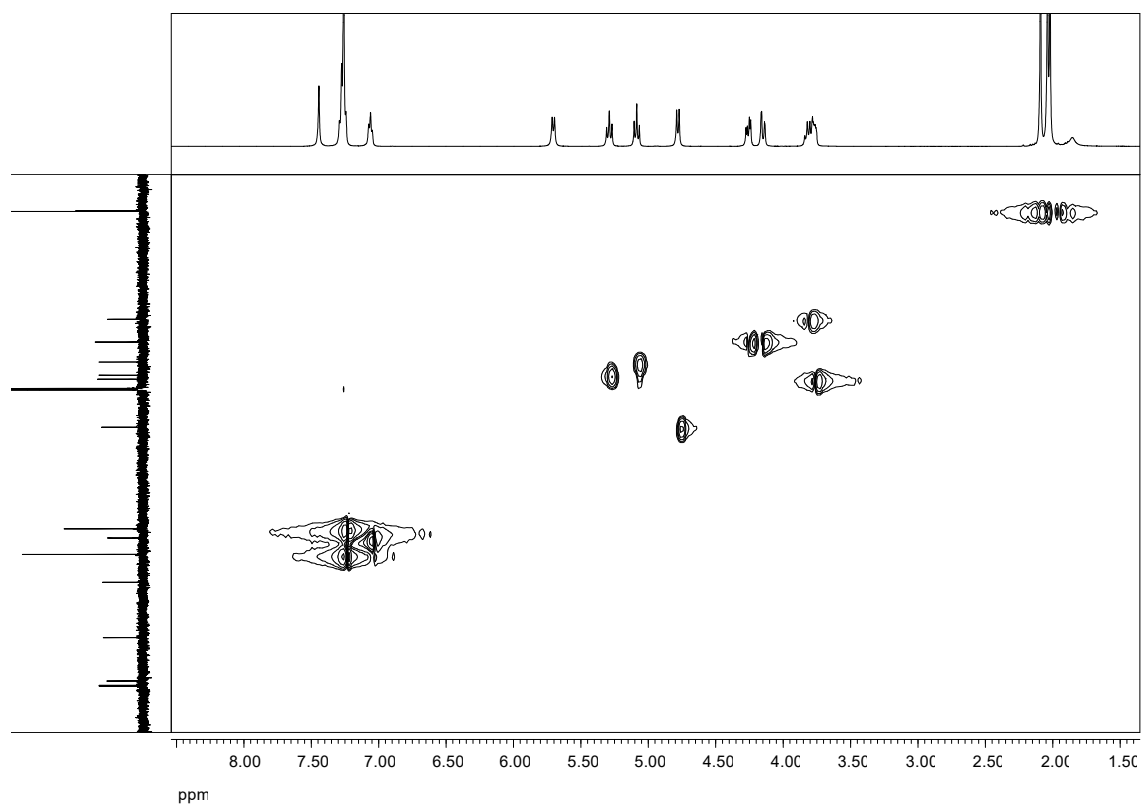


Figure S52 HMBC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**14**) recorded in DCl_3 .

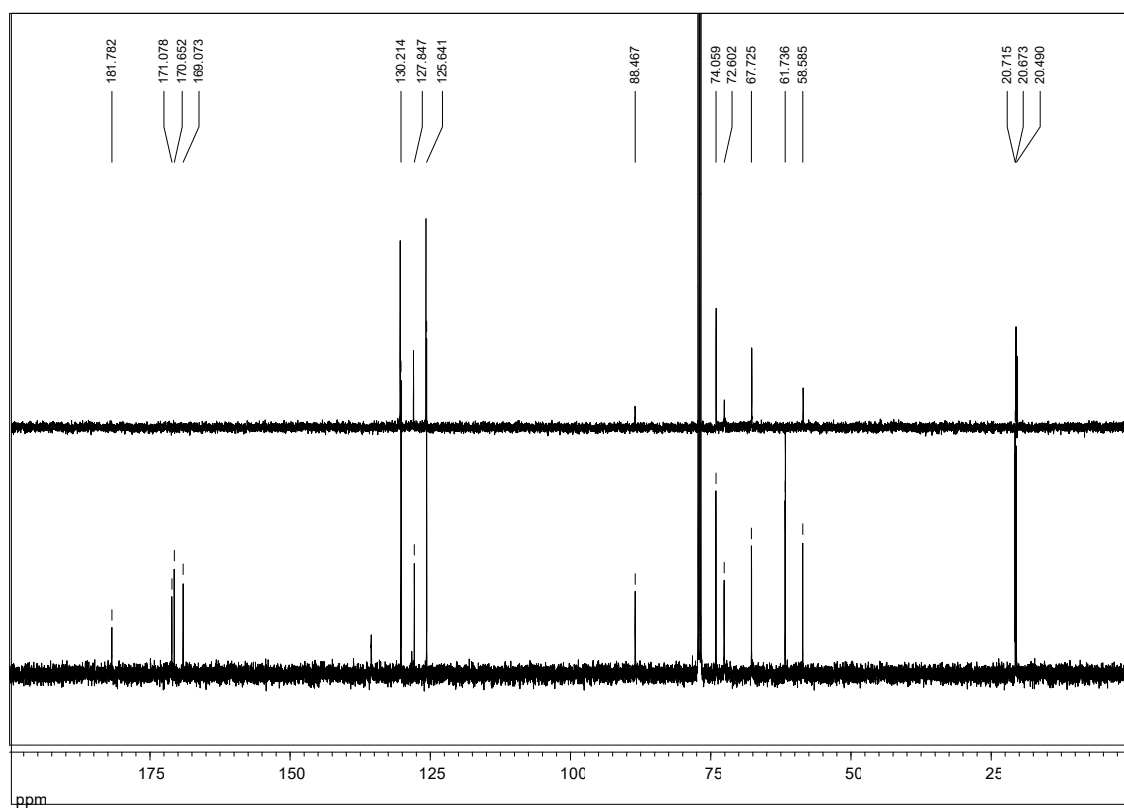


Figure S53 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in CDCl_3 .

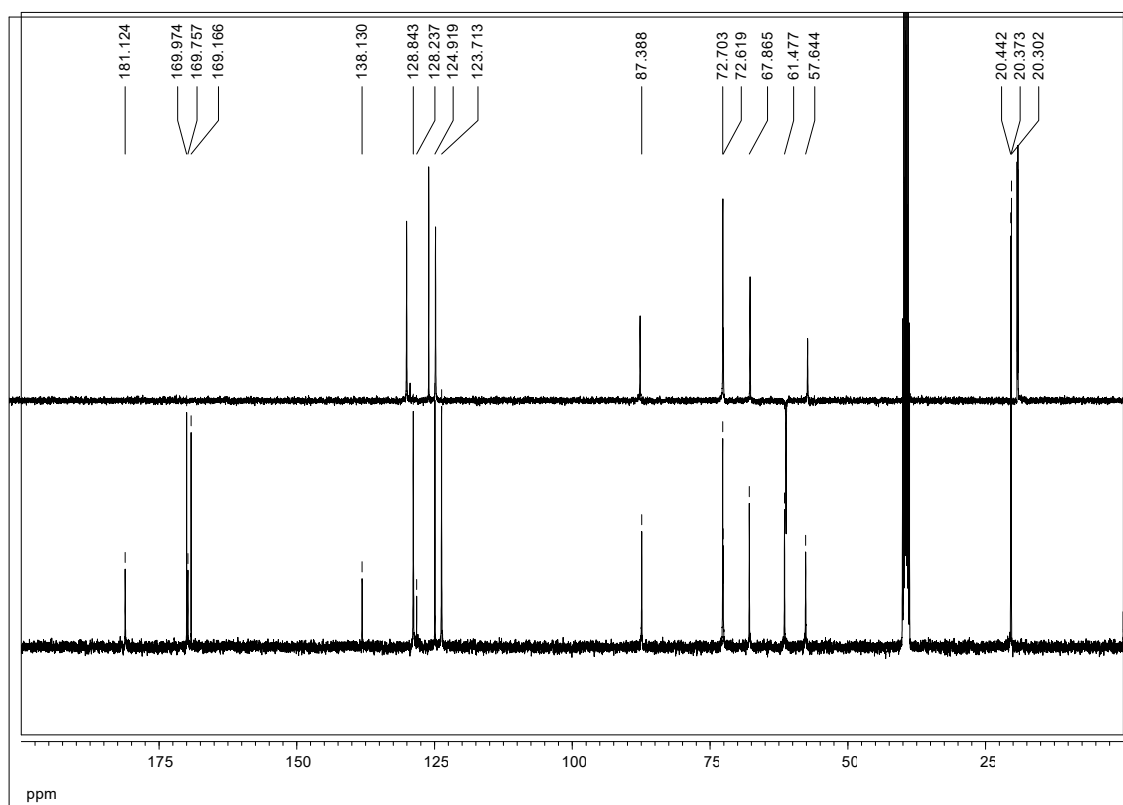


Figure S54 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)-β-D-glucopyranosyl azide (**15**) recorded in DMSO-*d*₆.

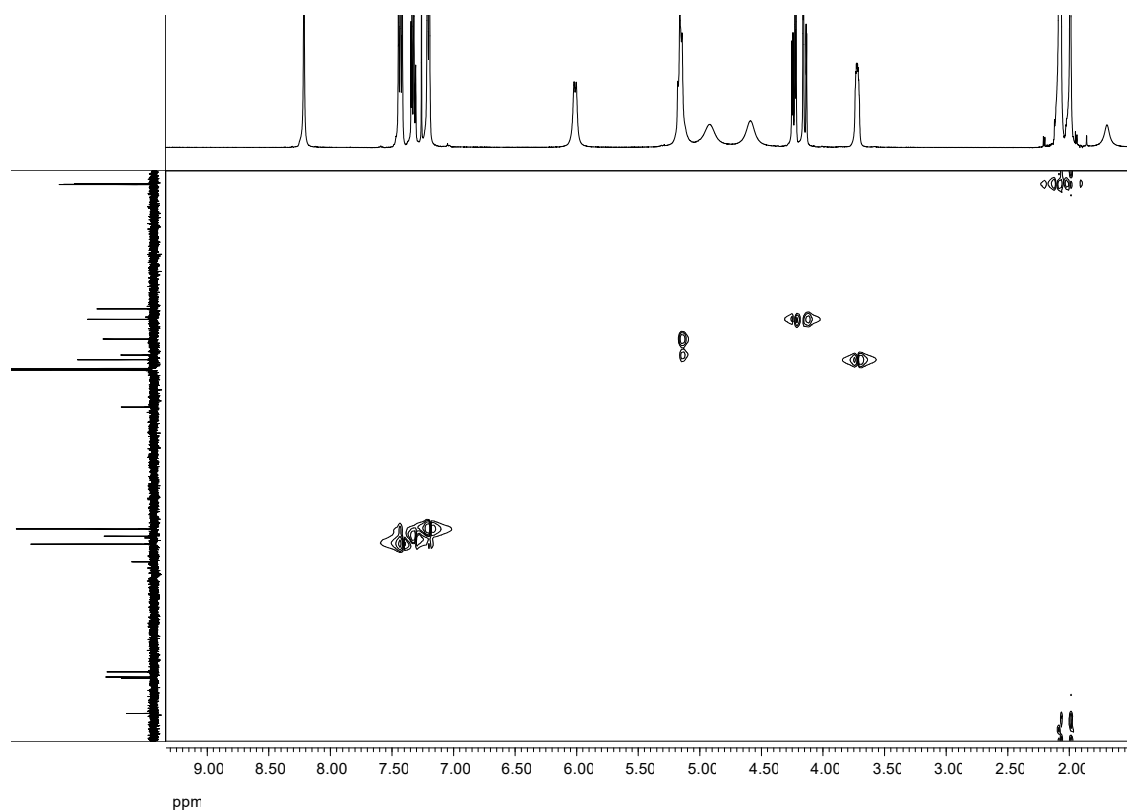


Figure S55 HMQC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)-β-D-glucopyranosyl azide (**15**) recorded in CDCl₃.

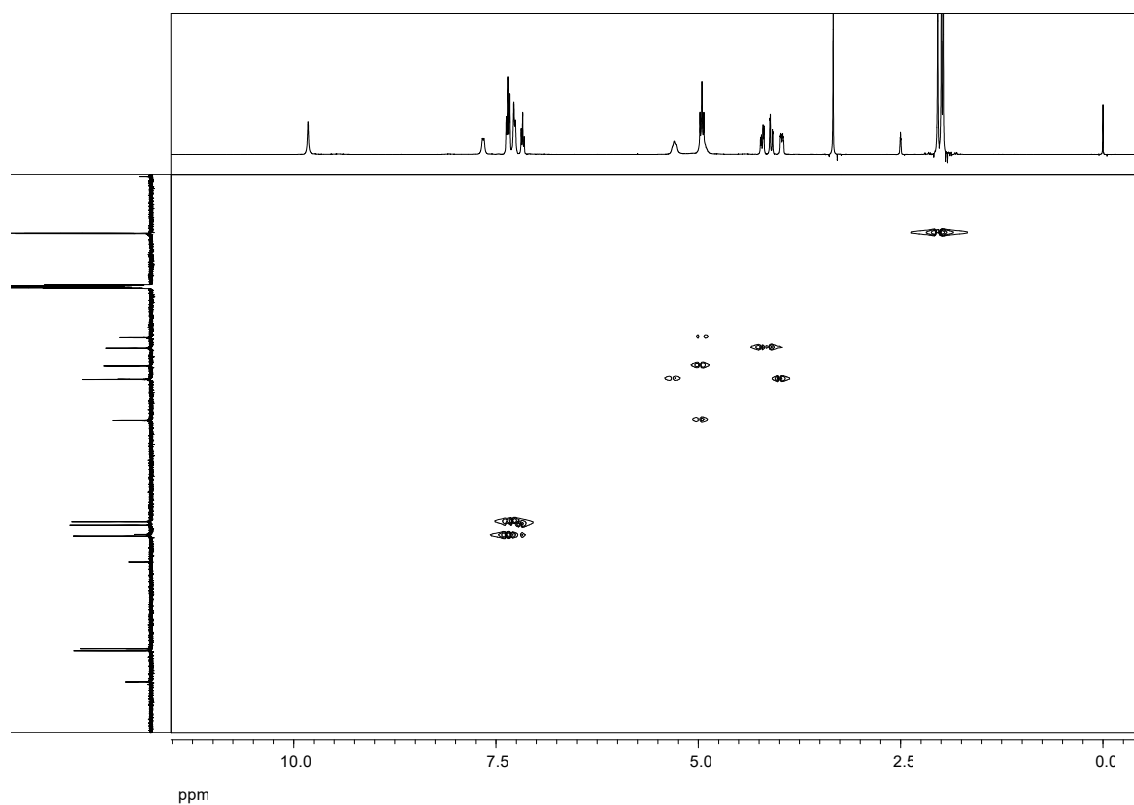


Figure S56 HMQC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-(3-phenylthioureido)- β -D-glucopyranosyl azide (**15**) recorded in DMSO-*d*₆.

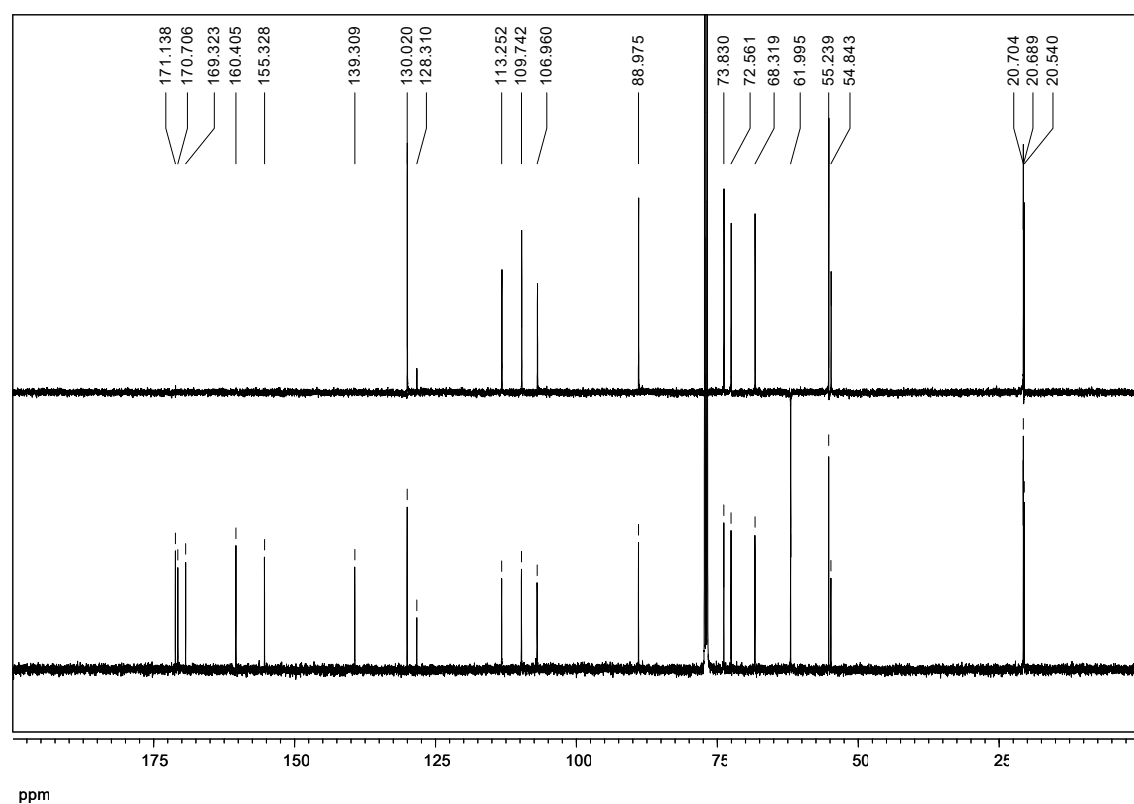


Figure S57 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**16**) recorded in CDCl_3 .

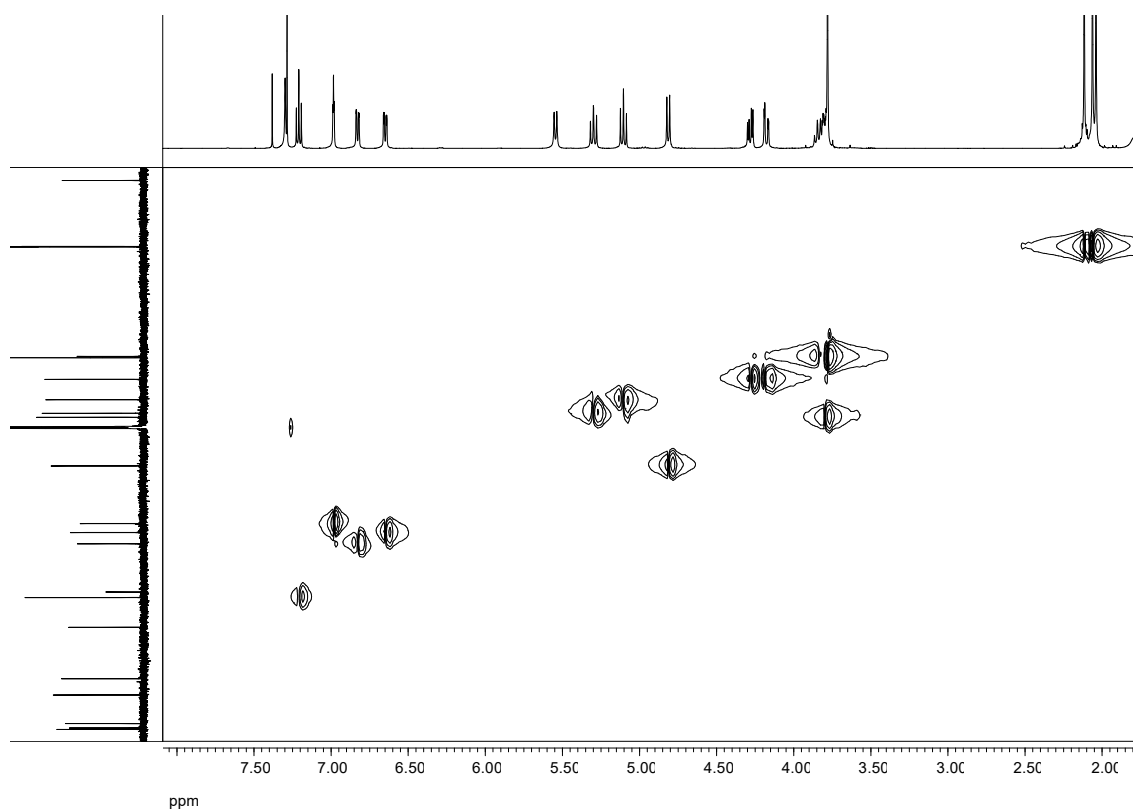


Figure S58 HMQC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**16**) recorded in CDCl_3 .

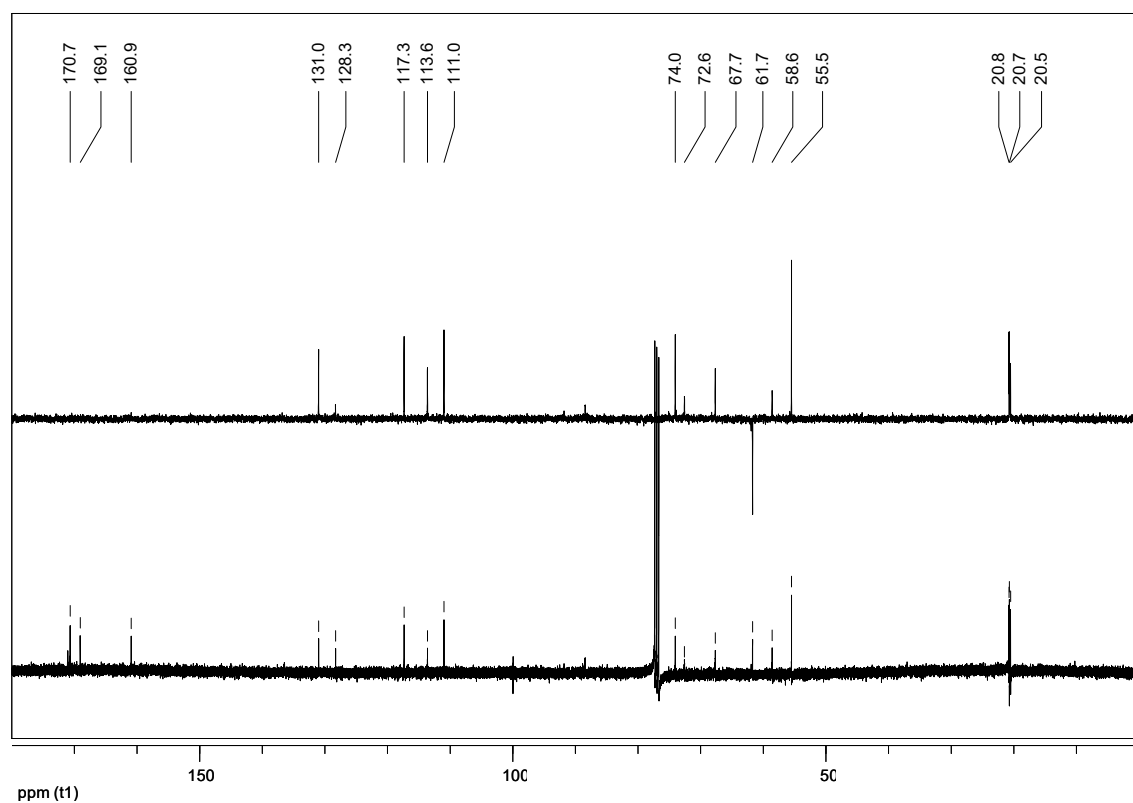


Figure S59 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(3-methoxyphenyl)thioureido]- β -D-glucopyranosyl azide (**17**) recorded in CDCl_3 .

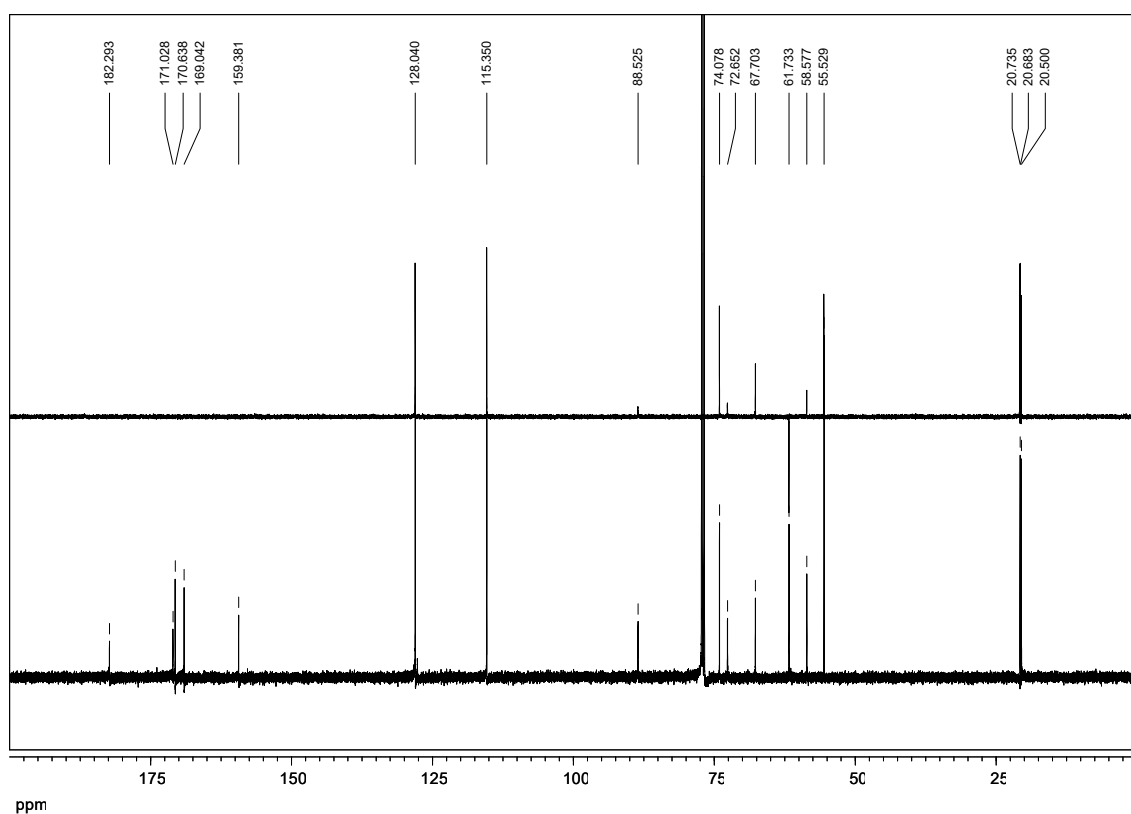


Figure S60 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**18**) recorded in CDCl_3 .

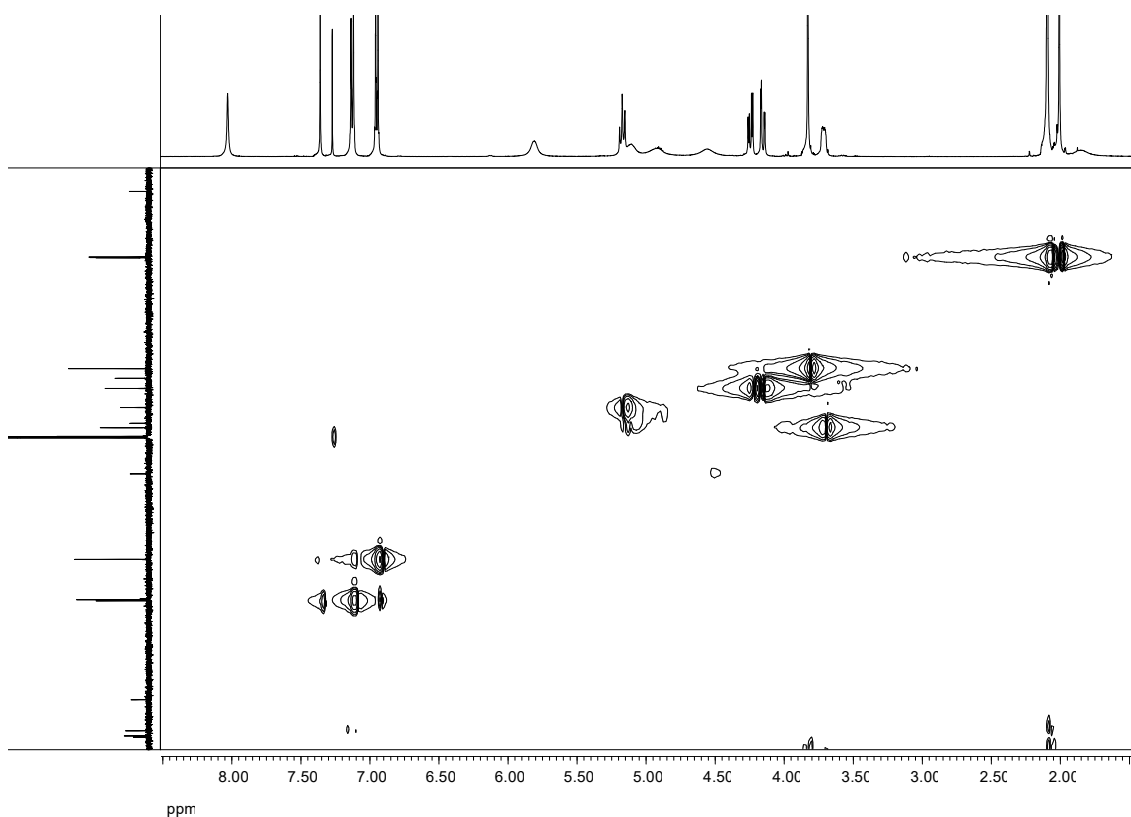


Figure S61 HMBC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**18**) recorded in CDCl_3 .

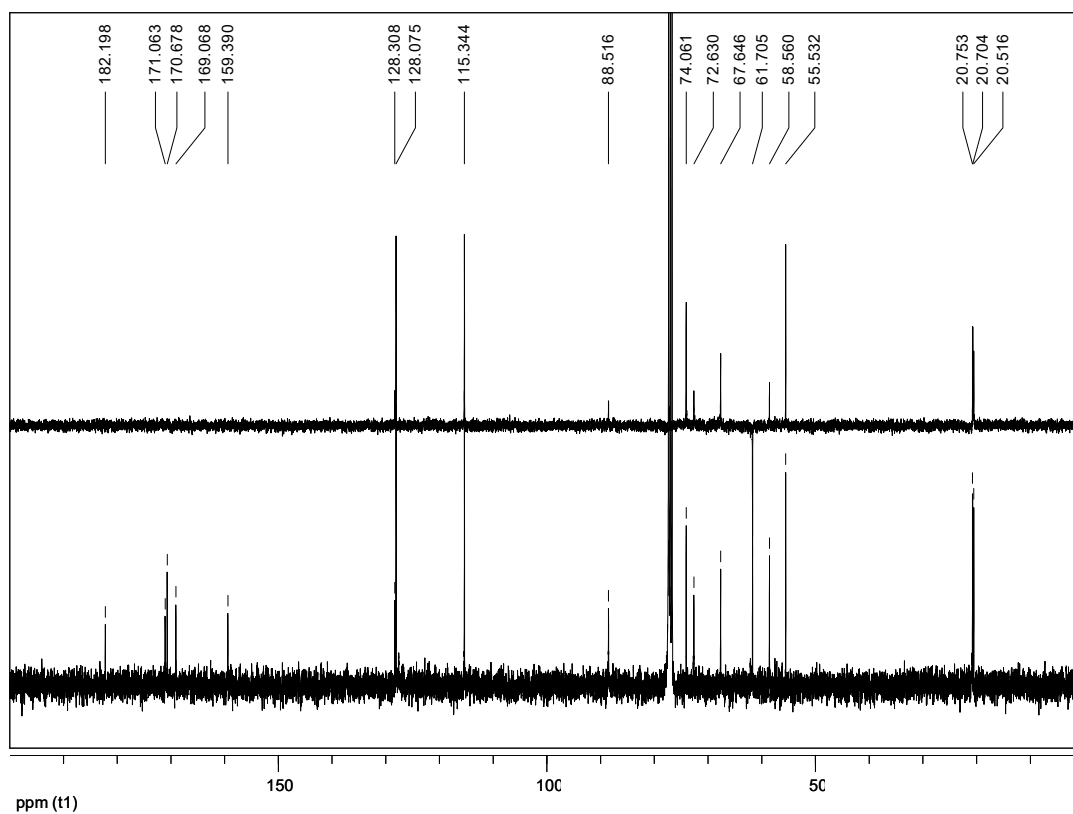


Figure S62 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-methoxyphenyl)thioureido]- β -D-glucopyranosyl azide (**19**) recorded in CDCl_3 .

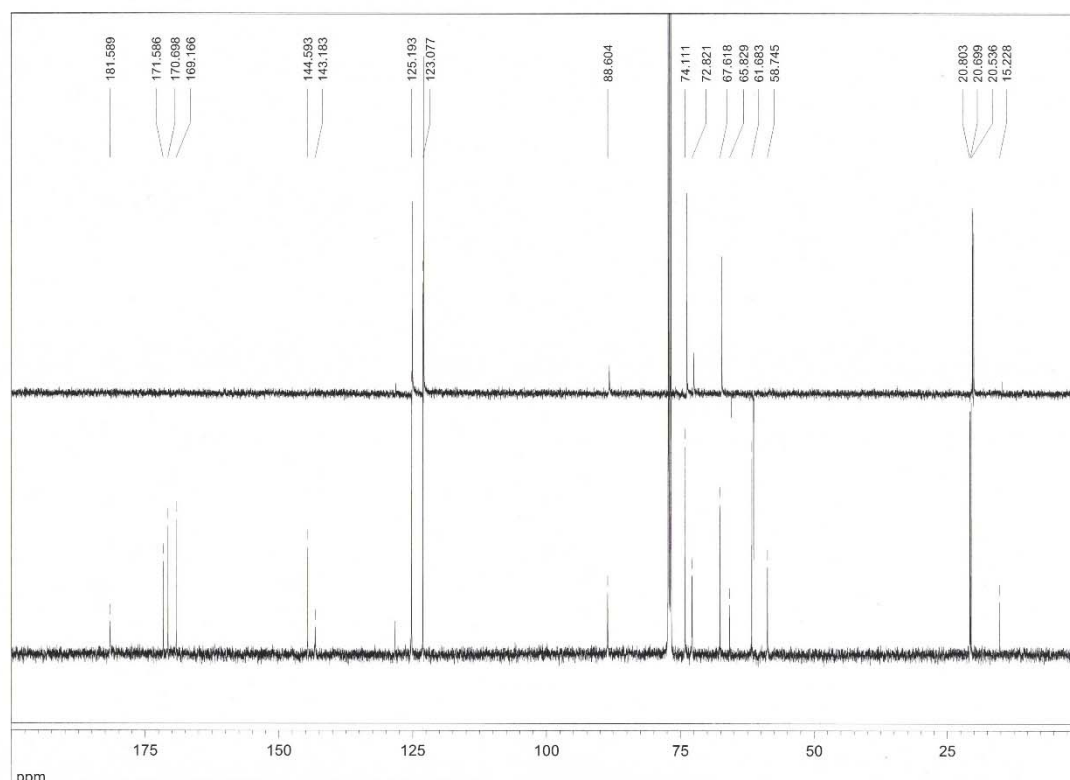


Figure S63 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-fluorophenyl)thioureido]- β -D-glucopyranosyl azide (**20**) recorded in CDCl_3 .

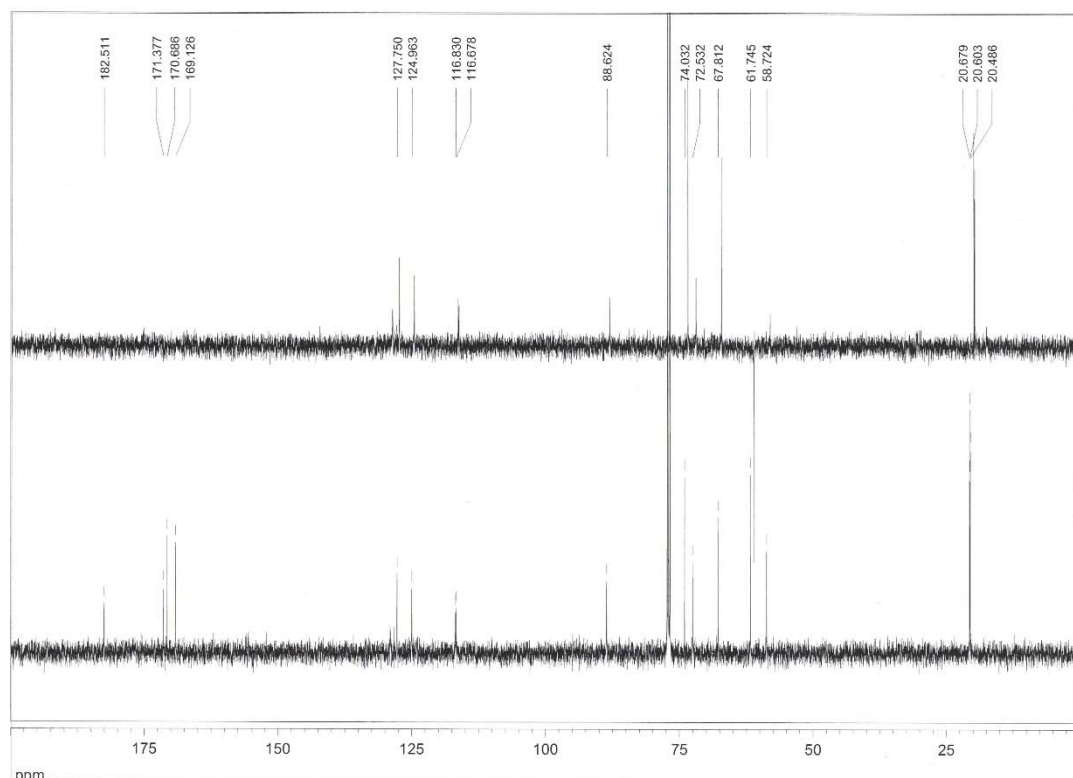


Figure S64 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(4-nitrophenyl)thioureido]- β -D-glucopyranosyl azide (**21**) recorded in CDCl_3 .

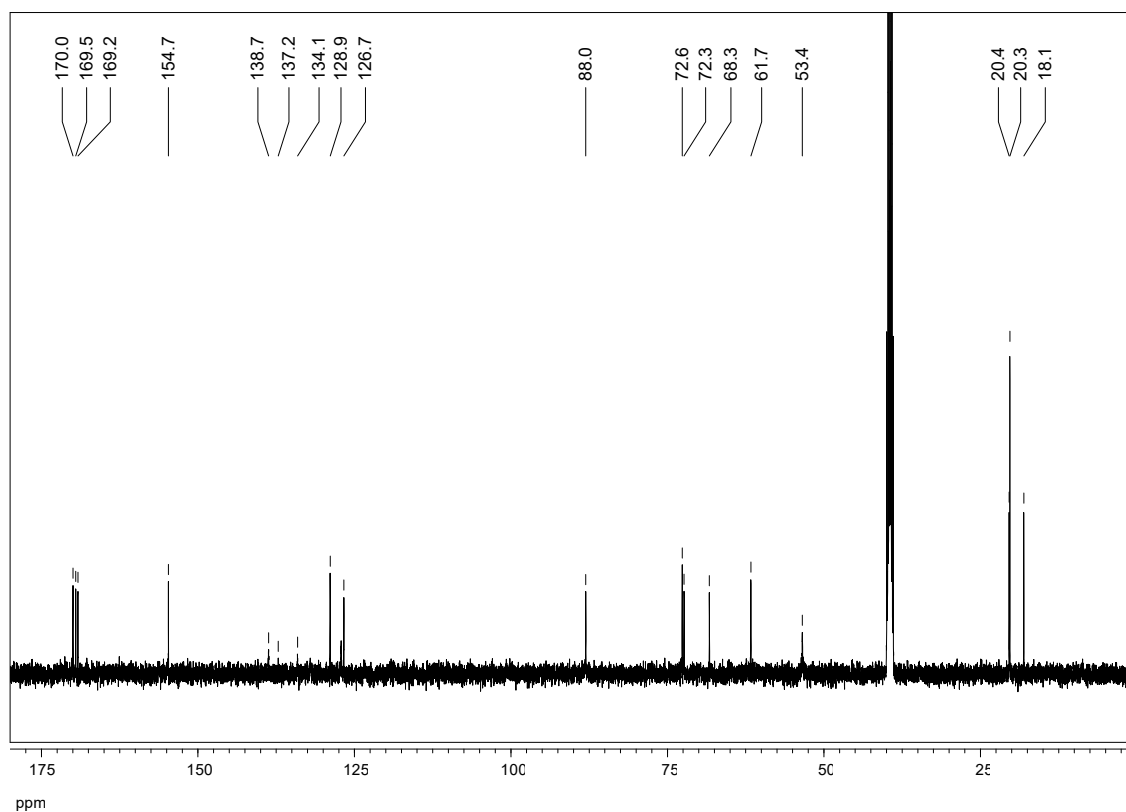


Figure S65 $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) recorded in $\text{DMSO}-d_6$.

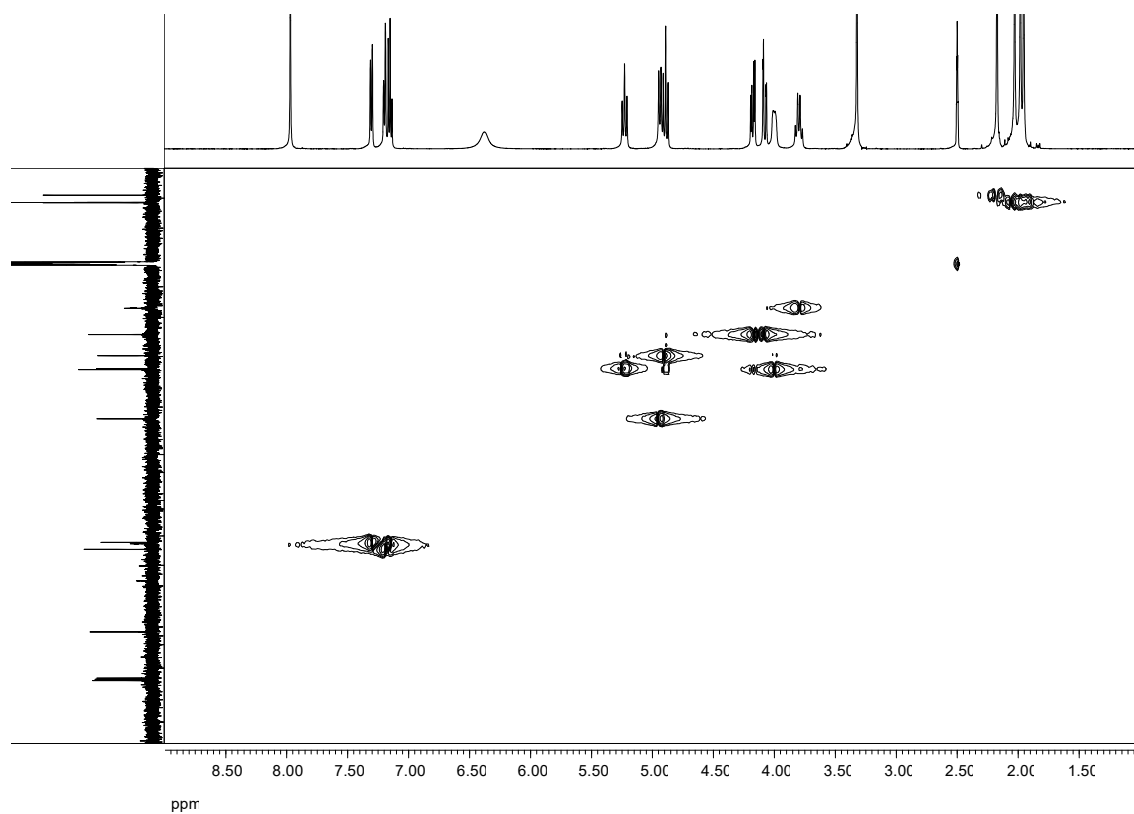


Figure S66 HMQC spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**22**) recorded in DMSO- d_6 .

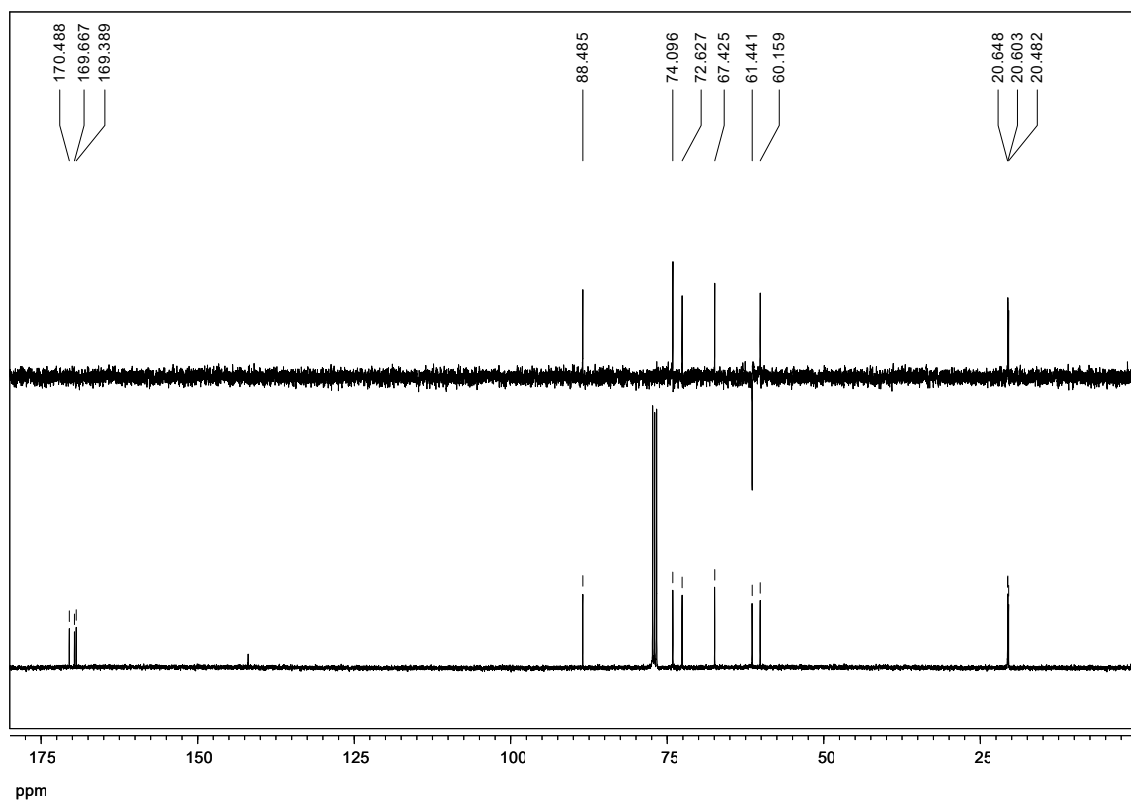


Figure S67 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 3,4,6-tri-*O*-acetyl-2-deoxy-2-isothiocianato- β -D-glucopyranosyl azide (**23**) recorded in CDCl_3 .

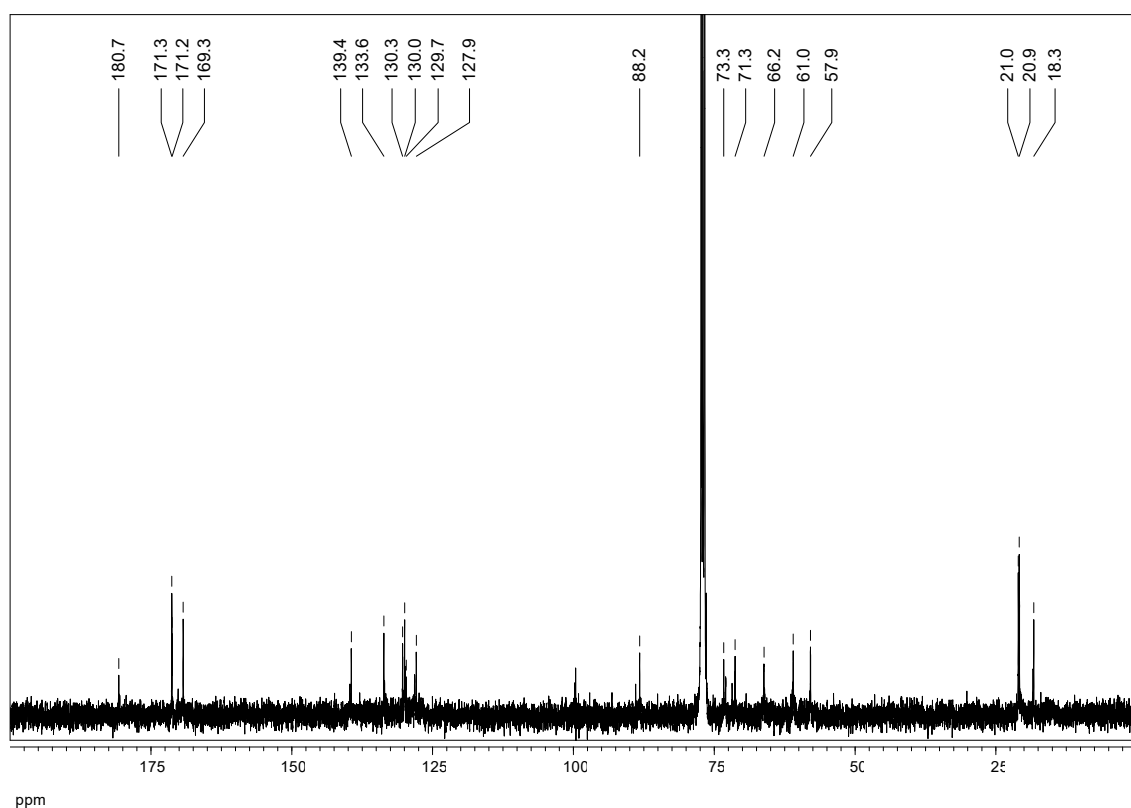


Figure S68 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]- β -D-glucopyranosyl azide (**25**) recorded in CDCl_3 at 223K.

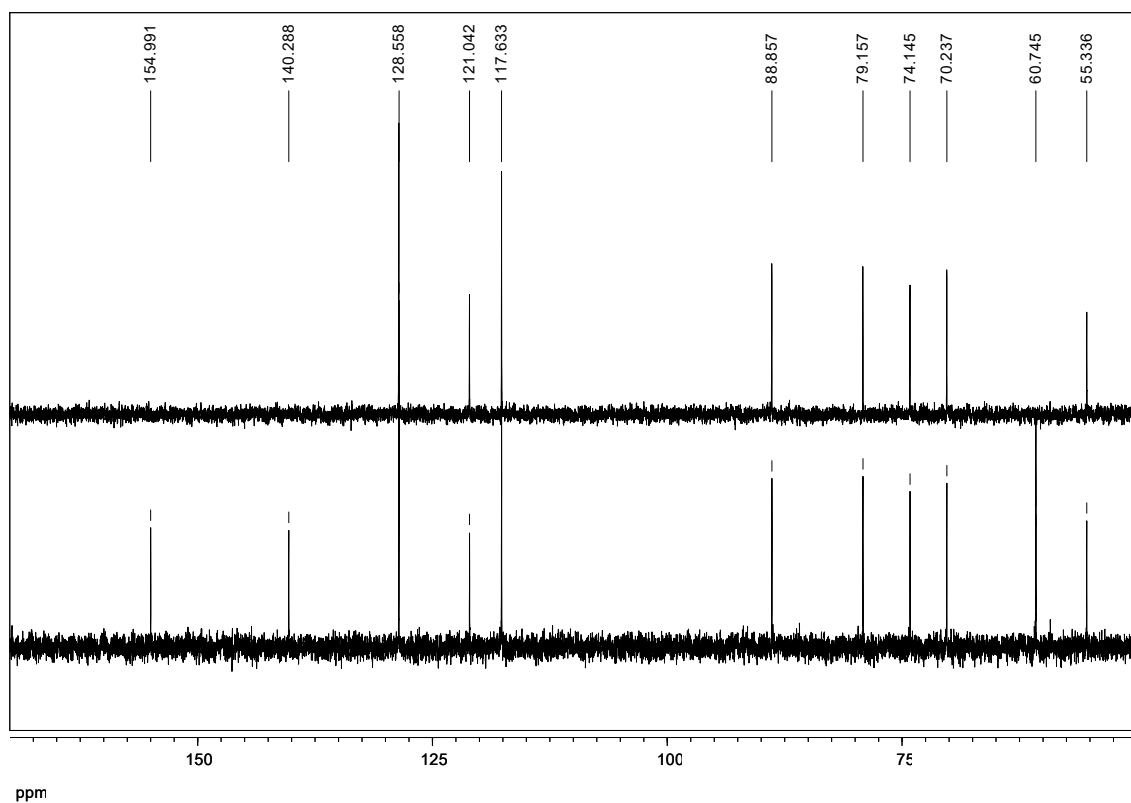


Figure S69 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**34**) recorded in $\text{DMSO}-d_6$.

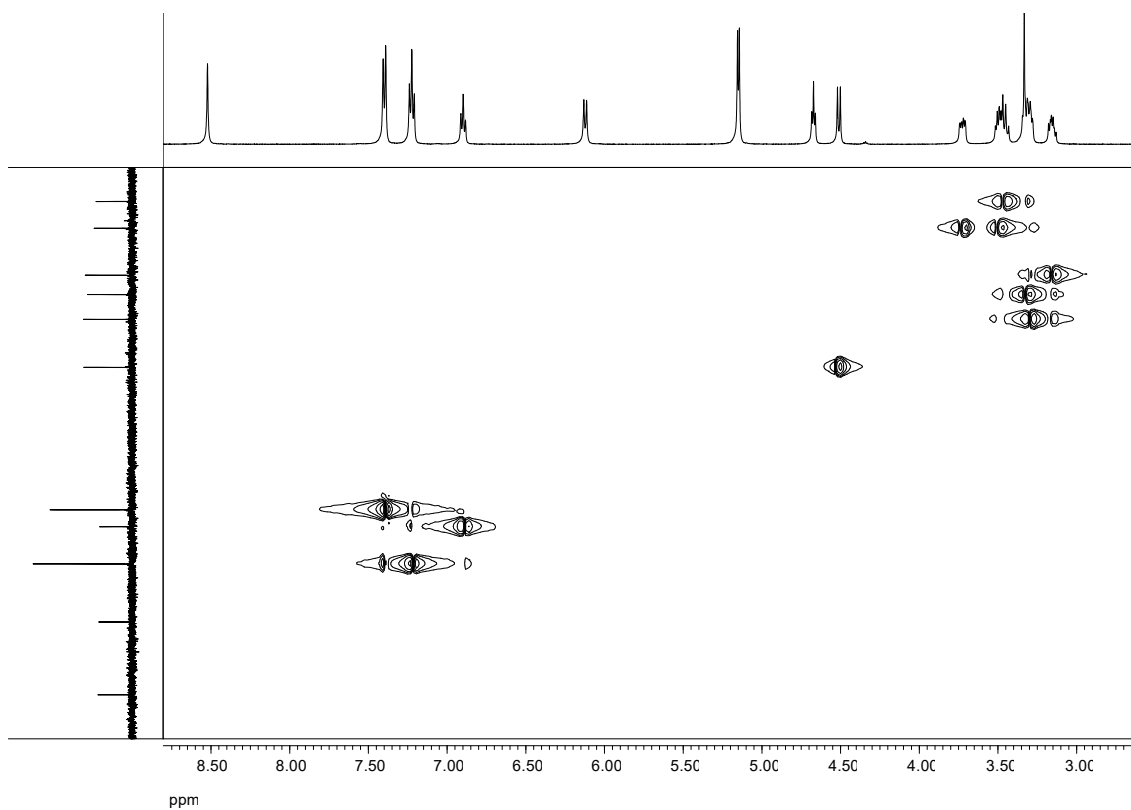


Figure S70 HMQC spectrum of 2-deoxy-2-(3-phenylureido)- β -D-glucopyranosyl azide (**34**) recorded in DMSO- d_6 .

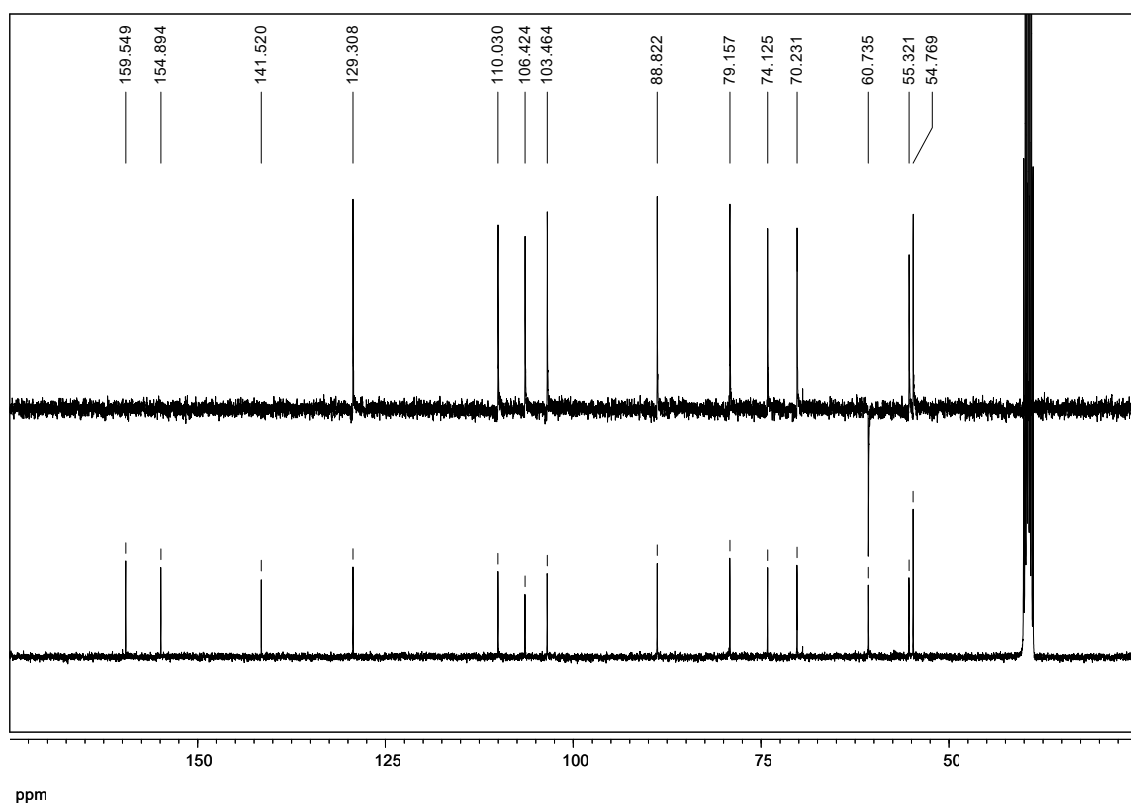


Figure S71 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 2-deoxy-2-[3-(4-methoxyphenyl)ureido]- β -D-glucopyranosyl azide (**35**) recorded in DMSO- d_6 .

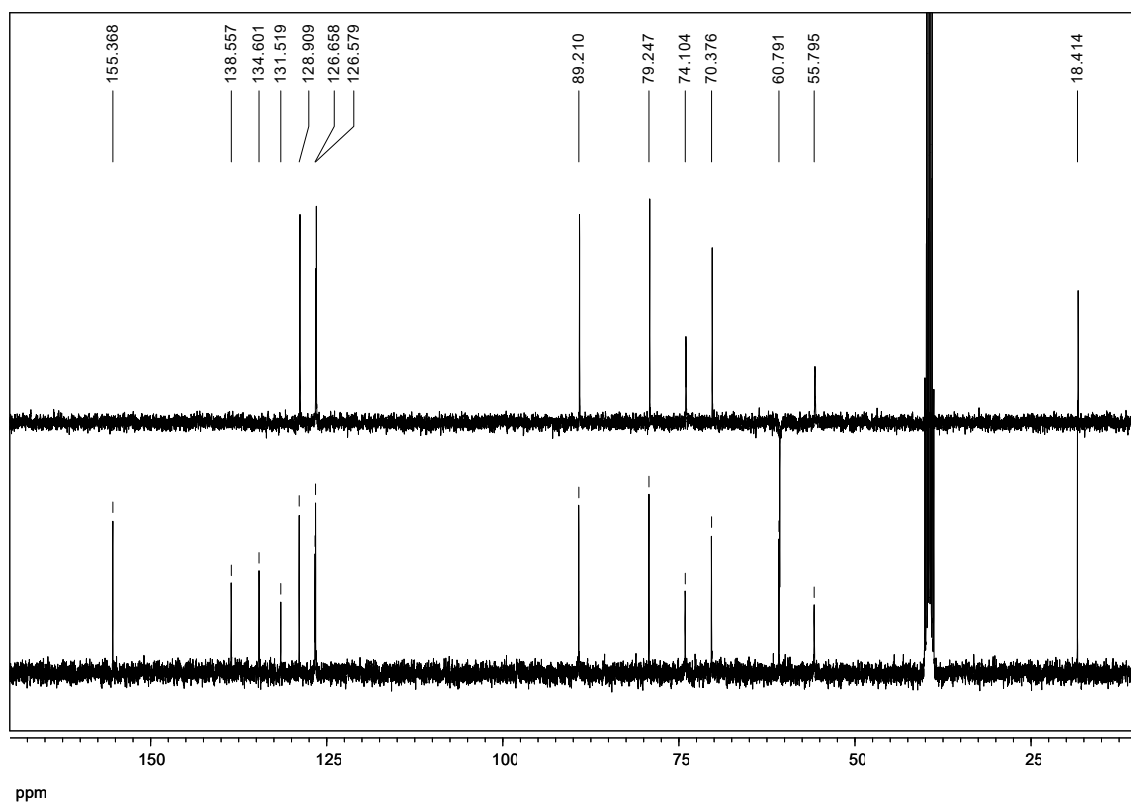



Figure S72 $^{13}\text{C}\{^1\text{H}\}$ NMR and DEPT spectra of 2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]- β -D-glucopyranosyl azide (**36**) recorded in $\text{DMSO}-d_6$.

PJC4NPhNCS PM-510 C19H22N6O9S Universidad de Sevilla
 Servicio de Espectrometría de Masas
 140124consogil06 5 (0.267) Cn (Top, 5, H); Sm (Mn, 2x2.00), Cm (2.6)
 24-Jan-2014 11:02:38
 Voltage FB+ 97.9

Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
533.1050	100.00	533.1067	-1.7	-3.1	11.5	1	C19 H22 N6 O9 Na S


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 ANÁLISIS TERAPEUTICO
 CENTRO DE INVESTIGACIÓN TECNOLÓGICA E INNOVACIÓN
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 AVDA. REINA MERCEDES, nº 4-B, 41012 SEVILLA, SPAIN

Centro de Investigación, Tecnología e Innovación
 Universidad de Sevilla
 Avda. Reina Mercedes, nº 4-B, 41012 Sevilla, Spain

SERVICIO DE ESPECTROMETRIA DE MASAS

141001_NMGNC5 1001/14 1422 41 NMGNC5 PM#513 C20H42N6O7S5

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530.0965
 Cal. H14 O1 N6 ClNa S = 536.0977
 -2.3953 ppm

Relative Abundance

m/z

513.0 513.5 514.0 514.5 515.0 515.5 516.0 516.5 517.0 517.5 518.0 518.5 519.0 519.5 520.0 520.5 521.0 521.5 522.0 522.5 523.0 523.5 524.0 524.5 525.0 525.5 526.0 526.5 527.0 527.5 528.0 528.5 529.0 529.5 530.0 530.5 531.0 531.5 532.0 532.5 533.0 533.5 534.0 534.5 535.0 535.5 536.0 536.5 537.0 537.5 538.0 538.5 539.0 539.5 540.0 540.5 541.0 541.5

SOI Espectrometría de Masas
 Tfno. 954559744; espectrometriademasas@us.es
 Apdo. 1152, 41080 Sevilla, Spain
 PGC07F106-EPM
 Rev.: 01

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Figure S74 Mass spectrum of 3,4,6-tri-*O*-acetyl-2-deoxy-2-[3-(2-chloro-6-methylphenyl)thioureido]-β-D-glucopyranosyl azide (**25**).

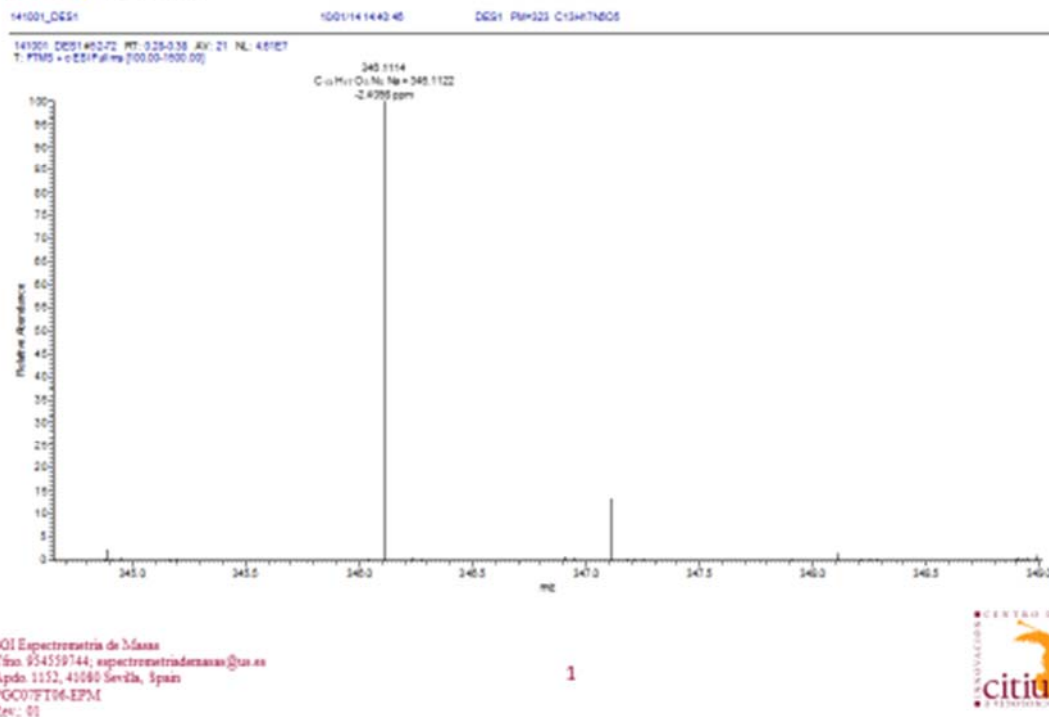


Figure S75 Mass spectrum of 2-deoxy-2-(3-phenylureido)-β-D-glucopyranosyl azide (**34**).

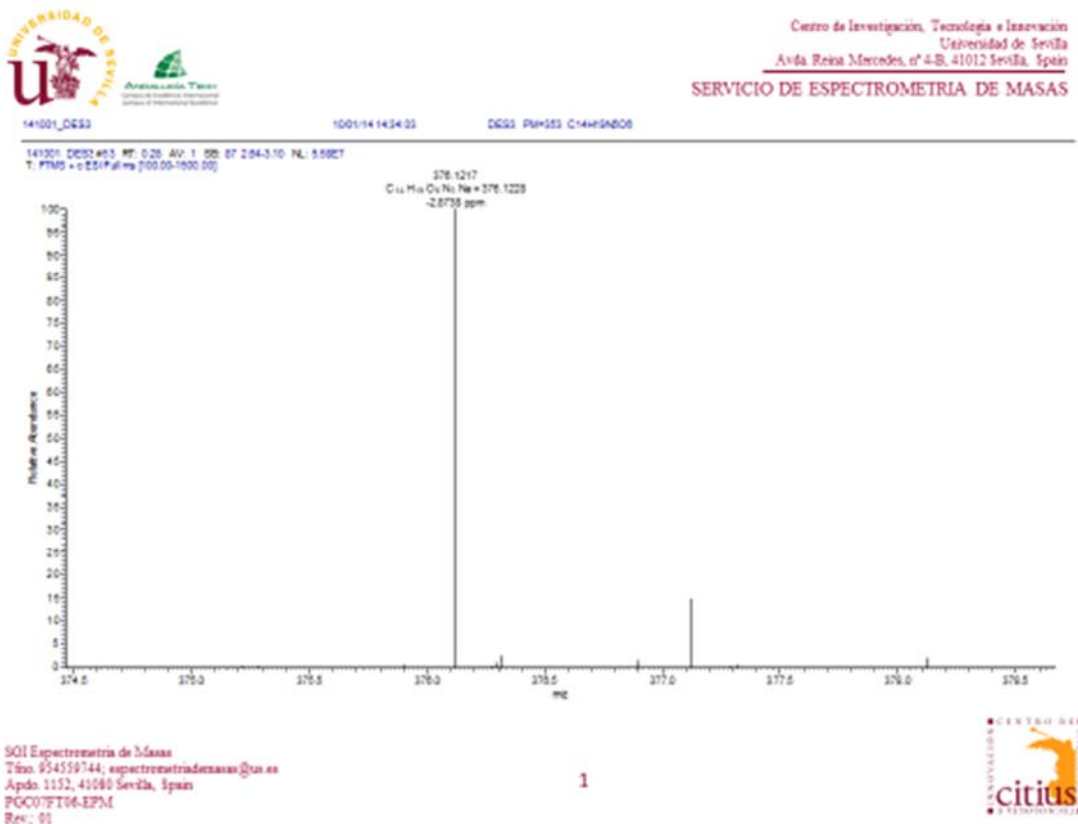


Figure S76 Mass spectrum of 2-deoxy-2-[3-(4-methoxyphenyl)ureido]-β-D-glucopyranosyl azide (**35**).

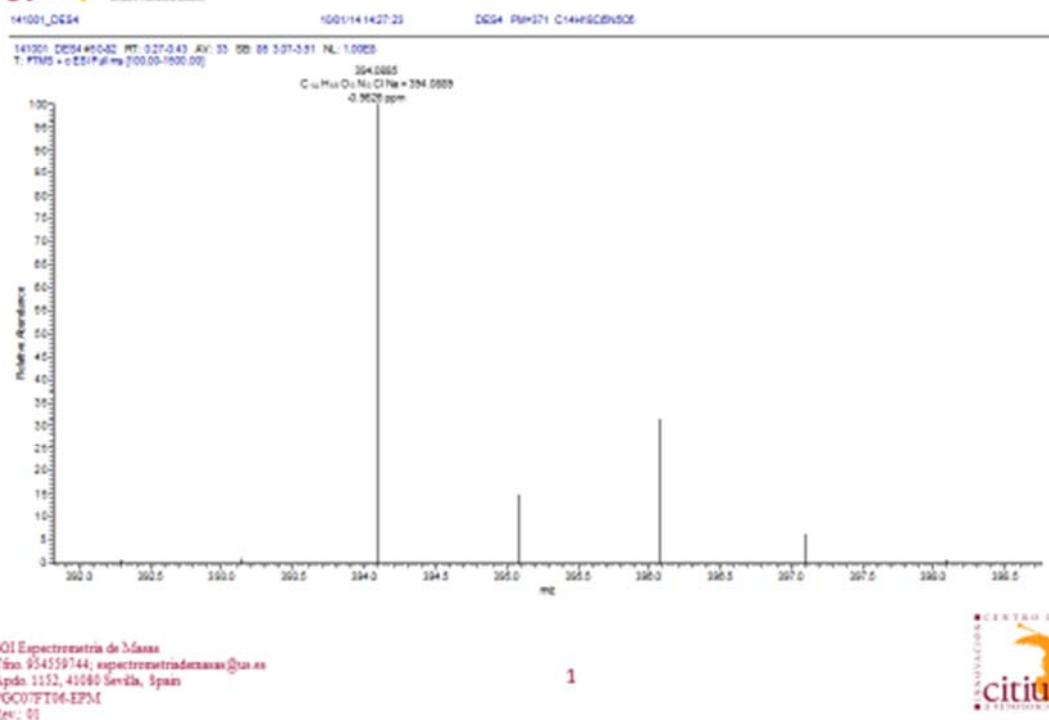


Figure S77 Mass spectrum of 2-deoxy-2-[3-(2-chloro-6-methylphenyl)ureido]-β-D-glucopyranosyl azide (**36**).

Cartesian coordinates and calculated energies at the M06-2X/6-311G(d,p) and M06-2X/def2-TZVP level in gas phase and CHCl₃ (SMD Model).

Structure 14 (Z,Z) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1613.2317991

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.698151	-1.244239	-0.802029
2	6	0	-0.004172	-0.032270	-0.159418
3	6	0	0.862919	1.206789	-0.360160
4	6	0	2.285272	0.970296	0.120049
5	6	0	2.842188	-0.300385	-0.517632
6	1	0	0.772015	-1.093151	-1.885934
7	1	0	0.887353	1.484217	-1.420136
8	1	0	2.302970	0.900250	1.210657
9	1	0	2.914145	-0.157038	-1.606628
10	1	0	-0.110200	-0.230701	0.913279
11	8	0	1.986443	-1.386424	-0.233317
12	6	0	4.211238	-0.653311	0.027612
13	1	0	4.148402	-0.851802	1.098931
14	1	0	4.913194	0.155602	-0.172516
15	8	0	4.683624	-1.807404	-0.655392
16	8	0	3.100149	2.060938	-0.310460
17	8	0	0.357754	2.312590	0.391928
18	7	0	-0.031296	-2.481742	-0.640707
19	6	0	4.575238	-2.993924	-0.001851
20	8	0	4.276076	-3.094761	1.149989
21	6	0	4.884666	-4.128101	-0.935776
22	1	0	5.791410	-3.914219	-1.500726
23	1	0	4.987811	-5.047260	-0.365653
24	1	0	4.059983	-4.223701	-1.644694
25	6	0	3.386955	3.037705	0.592586
26	8	0	3.028843	3.015245	1.731450
27	6	0	4.209701	4.114216	-0.056156
28	1	0	3.661551	4.533065	-0.901020
29	1	0	4.429043	4.886766	0.675628
30	1	0	5.134678	3.684688	-0.443039
31	6	0	-0.471354	3.181151	-0.214446
32	8	0	-0.891696	3.030256	-1.332187
33	6	0	-0.792012	4.327592	0.696861
34	1	0	-1.420777	3.960168	1.510182
35	1	0	0.125689	4.714377	1.140022
36	1	0	-1.319466	5.097477	0.140587
37	6	0	-2.421215	-0.333412	-0.082340
38	8	0	-2.328898	-1.053107	0.889135
39	7	0	-0.121279	-2.851700	0.542271
40	7	0	-0.253707	-3.294790	1.558692
41	7	0	-1.314173	0.181287	-0.728828
42	1	0	-1.421015	0.978299	-1.341422
43	7	0	-3.607568	0.060562	-0.660552
44	6	0	-4.913601	-0.287903	-0.269421
45	6	0	-5.206722	-1.017535	0.885860
46	6	0	-5.958022	0.144556	-1.093034
47	6	0	-6.533635	-1.299924	1.190908
48	1	0	-4.406188	-1.359500	1.522382
49	6	0	-7.275077	-0.145603	-0.772623
50	1	0	-5.731480	0.711020	-1.990926
51	6	0	-7.573320	-0.872027	0.374975
52	1	0	-6.750910	-1.867797	2.087988
53	1	0	-8.069003	0.197792	-1.425024
54	1	0	-8.601059	-1.101617	0.627148
55	1	0	-3.543547	0.587067	-1.518163

Structure 14 (Z,E) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1613.2307815

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.822801	-1.412991	-0.372813
2	6	0	-0.084034	-0.463041	0.433664
3	6	0	0.198064	0.969713	-0.007300
4	6	0	1.679694	1.289984	0.096944
5	6	0	2.486311	0.237865	-0.661155
6	1	0	0.568648	-1.346411	-1.438018
7	1	0	-0.126032	1.117538	-1.043603
8	1	0	1.980327	1.333241	1.146842
9	1	0	2.235319	0.294497	-1.731466
10	1	0	0.166381	-0.573722	1.494562
11	8	0	2.174339	-1.046756	-0.164593
12	6	0	3.979592	0.431838	-0.492536
13	1	0	4.257019	0.324791	0.557524
14	1	0	4.275658	1.409775	-0.870607
15	8	0	4.648675	-0.549254	-1.275723
16	8	0	1.919704	2.550302	-0.529593
17	8	0	-0.489217	1.903206	0.825613
18	7	0	0.649949	-2.806763	-0.029407
19	6	0	5.128369	-1.635827	-0.616078
20	8	0	5.182899	-1.722144	0.574026
21	6	0	5.564323	-2.685992	-1.596708
22	1	0	6.139230	-2.235099	-2.404769
23	1	0	6.144688	-3.444679	-1.078845
24	1	0	4.670032	-3.138795	-2.029587
25	6	0	2.040068	3.645313	0.268517
26	8	0	2.006977	3.605454	1.461401
27	6	0	2.228647	4.876845	-0.571004
28	1	0	1.397205	4.974976	-1.269755
29	1	0	2.288120	5.746594	0.077421
30	1	0	3.143674	4.780616	-1.157220
31	6	0	-1.685967	2.365343	0.409158
32	8	0	-2.233879	1.983914	-0.589513
33	6	0	-2.213011	3.393026	1.365953
34	1	0	-2.416320	2.908769	2.322660
35	1	0	-1.454121	4.156267	1.540457
36	1	0	-3.124209	3.827321	0.964166
37	6	0	-2.107922	-1.587754	1.164542
38	8	0	-1.524058	-2.121125	2.085825
39	7	0	1.000935	-3.077051	1.132146
40	7	0	1.299525	-3.445428	2.142988
41	7	0	-1.480688	-0.776754	0.250858
42	1	0	-2.032552	-0.183286	-0.355076
43	7	0	-3.467799	-1.754598	0.986454
44	6	0	-4.293330	-1.218159	-0.027257
45	6	0	-3.964235	-1.374040	-1.375028
46	6	0	-5.471935	-0.558847	0.321656
47	6	0	-4.791079	-0.842534	-2.356050
48	1	0	-3.069900	-1.924881	-1.640961
49	6	0	-6.308712	-0.057278	-0.666662
50	1	0	-5.720309	-0.439326	1.370149
51	6	0	-5.966526	-0.186335	-2.008006
52	1	0	-4.524366	-0.961517	-3.399206
53	1	0	-7.224142	0.449343	-0.385554
54	1	0	-6.613911	0.217360	-2.776375
55	1	0	-3.904117	-2.220775	1.767429

Structure 14 (E,Z) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1613.2257103

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.152619	0.814638	-1.129150
2	6	0	0.042460	-0.553228	-0.440613
3	6	0	-1.306950	-1.271536	-0.416892
4	6	0	-2.373673	-0.407476	0.233589
5	6	0	-2.416215	0.957331	-0.449875
6	1	0	-0.456809	0.666283	-2.172376
7	1	0	-1.617092	-1.511695	-1.439672
8	1	0	-2.171687	-0.302070	1.302977
9	1	0	-2.739763	0.831141	-1.493763
10	1	0	0.321931	-0.356261	0.601060
11	8	0	-1.128998	1.544098	-0.416538
12	6	0	-3.358905	1.911335	0.255333
13	1	0	-3.025014	2.076536	1.281269
14	1	0	-4.371404	1.509431	0.241375
15	8	0	-3.380765	3.143029	-0.454354
16	8	0	-3.642469	-1.028709	0.041362
17	8	0	-1.207279	-2.475139	0.330206
18	7	0	1.063981	1.603388	-1.192443
19	6	0	-2.614367	4.149654	0.041762
20	8	0	-2.055795	4.102648	1.096716
21	6	0	-2.585074	5.300962	-0.921418
22	1	0	-3.595975	5.543484	-1.247871
23	1	0	-2.115145	6.156628	-0.444505
24	1	0	-2.009890	5.004133	-1.800404
25	6	0	-4.161145	-1.741327	1.079835
26	8	0	-3.649850	-1.808809	2.156662
27	6	0	-5.441303	-2.405125	0.661843
28	1	0	-5.228936	-3.128482	-0.127058
29	1	0	-5.883768	-2.903277	1.519940
30	1	0	-6.127803	-1.663210	0.253190
31	6	0	-1.017691	-3.624834	-0.365501
32	8	0	-0.964163	-3.671031	-1.560871
33	6	0	-0.885570	-4.784678	0.575446
34	1	0	0.087213	-4.718486	1.066837
35	1	0	-1.653570	-4.729024	1.346632
36	1	0	-0.950404	-5.713953	0.016277
37	6	0	2.399427	-1.176805	-1.084062
38	8	0	3.077004	-1.475855	-2.037880
39	7	0	1.464684	1.958053	-0.074887
40	7	0	1.910562	2.324708	0.883732
41	7	0	1.022620	-1.403566	-1.076392
42	1	0	0.727671	-1.835734	-1.944342
43	7	0	2.882816	-0.646161	0.092745
44	6	0	4.204047	-0.237907	0.368240
45	6	0	5.225477	-0.229327	-0.583748
46	6	0	4.468953	0.204145	1.668088
47	6	0	6.490942	0.215010	-0.215320
48	1	0	5.029144	-0.574910	-1.586145
49	6	0	5.736915	0.639602	2.018660
50	1	0	3.668835	0.218790	2.401358
51	6	0	6.760004	0.647522	1.076647
52	1	0	7.278219	0.216767	-0.960001
53	1	0	5.921391	0.978678	3.030913
54	1	0	7.751536	0.987672	1.347496
55	1	0	2.278914	-0.696977	0.897913

Structure 14 (Z,Z) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1613.2672268

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.525891	-1.353224	-0.761570
2	6	0	-0.185179	-0.133096	-0.149513
3	6	0	0.683127	1.100795	-0.373537
4	6	0	2.091972	0.870567	0.144684
5	6	0	2.672102	-0.413651	-0.450130
6	1	0	0.609675	-1.234645	-1.847152
7	1	0	0.727158	1.346488	-1.439648
8	1	0	2.085307	0.817513	1.235845
9	1	0	2.784113	-0.290440	-1.536675
10	1	0	-0.289644	-0.305811	0.926983
11	8	0	1.801412	-1.497333	-0.171453
12	6	0	4.010917	-0.734771	0.165749
13	1	0	3.882014	-1.032846	1.209306
14	1	0	4.672665	0.133093	0.120653
15	8	0	4.571843	-1.814142	-0.583449
16	8	0	2.902223	1.962122	-0.287525
17	8	0	0.163263	2.221362	0.344984
18	7	0	-0.215015	-2.588936	-0.563374
19	6	0	5.762574	-2.265134	-0.151764
20	8	0	6.340032	-1.778831	0.783782
21	6	0	6.235784	-3.422616	-0.977190
22	1	0	6.278414	-3.131794	-2.028014
23	1	0	7.215987	-3.741917	-0.632085
24	1	0	5.520044	-4.241900	-0.886765
25	6	0	3.331131	2.853914	0.641764
26	8	0	3.099085	2.750978	1.812451
27	6	0	4.121763	3.945315	-0.011582
28	1	0	3.493456	4.460346	-0.740477
29	1	0	4.474301	4.643426	0.743390
30	1	0	4.966746	3.510237	-0.548071
31	6	0	-0.659775	3.072640	-0.299090
32	8	0	-1.023009	2.907260	-1.435136
33	6	0	-1.048901	4.210721	0.590112
34	1	0	-1.648780	3.820752	1.415354
35	1	0	-0.155779	4.669166	1.016681
36	1	0	-1.624350	4.938488	0.023806
37	6	0	-2.609391	-0.418717	-0.066510
38	8	0	-2.530569	-1.106384	0.936658
39	7	0	-0.303189	-2.922191	0.625219
40	7	0	-0.427713	-3.327282	1.659943
41	7	0	-1.498168	0.062097	-0.713966
42	1	0	-1.595671	0.736549	-1.461440
43	7	0	-3.789816	-0.045464	-0.664767
44	6	0	-5.097769	-0.372421	-0.271210
45	6	0	-5.409697	-1.086338	0.890681
46	6	0	-6.134846	0.064366	-1.105262
47	6	0	-6.742556	-1.348484	1.193640
48	1	0	-4.620832	-1.429720	1.540872
49	6	0	-7.457367	-0.204687	-0.787105
50	1	0	-5.892990	0.619104	-2.006414
51	6	0	-7.772777	-0.915723	0.367526
52	1	0	-6.970615	-1.903497	2.096694
53	1	0	-8.243384	0.143409	-1.447400
54	1	0	-8.805249	-1.128351	0.617204
55	1	0	-3.721519	0.497783	-1.514680

Structure 14 (Z,E) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1613.2653296

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.044171	-1.421461	0.560416
2	6	0	0.018756	-0.668229	-0.255929
3	6	0	-0.079823	0.816147	0.083922
4	6	0	-1.489905	1.327136	-0.152468
5	6	0	-2.481827	0.456606	0.619271
6	1	0	-0.839795	-1.320649	1.631629
7	1	0	0.187434	0.981702	1.132285
8	1	0	-1.720602	1.324686	-1.219964
9	1	0	-2.294760	0.564046	1.697180
10	1	0	-0.208623	-0.811966	-1.317672
11	8	0	-2.319466	-0.899388	0.240740
12	6	0	-3.915462	0.837352	0.313618
13	1	0	-4.126568	0.700815	-0.747521
14	1	0	-4.100062	1.870488	0.605437
15	8	0	-4.780878	0.018463	1.098456
16	8	0	-1.582075	2.653665	0.366309
17	8	0	0.799763	1.575874	-0.746455
18	7	0	-1.052628	-2.851315	0.301067
19	6	0	-5.353747	-1.045128	0.491151
20	8	0	-5.304513	-1.245249	-0.690319
21	6	0	-6.042716	-1.916043	1.497543
22	1	0	-6.646002	-1.310008	2.173544
23	1	0	-6.658876	-2.650295	0.984464
24	1	0	-5.279783	-2.426267	2.090139
25	6	0	-1.540478	3.689548	-0.509609
26	8	0	-1.502050	3.549034	-1.698786
27	6	0	-1.545898	4.994179	0.226113
28	1	0	-0.614025	5.085967	0.788428
29	1	0	-1.633110	5.812934	-0.483624
30	1	0	-2.369642	5.015589	0.940558
31	6	0	2.013769	1.901802	-0.252645
32	8	0	2.395062	1.559013	0.836397
33	6	0	2.791808	2.712969	-1.239356
34	1	0	3.027968	2.082055	-2.099358
35	1	0	2.186479	3.547347	-1.595889
36	1	0	3.709635	3.066848	-0.776531
37	6	0	1.934788	-2.041307	-0.855640
38	8	0	1.304107	-2.624174	-1.721791
39	7	0	-1.380109	-3.137494	-0.858515
40	7	0	-1.680479	-3.510451	-1.868345
41	7	0	1.356594	-1.144775	0.001827
42	1	0	1.938463	-0.603353	0.628132
43	7	0	3.286727	-2.258803	-0.679294
44	6	0	4.154635	-1.414451	0.068150
45	6	0	4.103746	-1.422350	1.461433
46	6	0	5.056434	-0.579772	-0.591317
47	6	0	4.933191	-0.576207	2.189272
48	1	0	3.416152	-2.095982	1.961148
49	6	0	5.900518	0.245554	0.143093
50	1	0	5.087447	-0.583634	-1.675547
51	6	0	5.833589	0.256799	1.533329
52	1	0	4.883715	-0.578793	3.271726
53	1	0	6.603895	0.888769	-0.372891
54	1	0	6.484267	0.909290	2.103126
55	1	0	3.692812	-2.766472	-1.454481

Structure 14 (E,Z) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1613.2620349

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.152426	0.816402	-1.158171
2	6	0	0.045435	-0.552519	-0.475856
3	6	0	-1.305549	-1.265997	-0.448970
4	6	0	-2.356964	-0.398151	0.221579
5	6	0	-2.407343	0.969552	-0.456244
6	1	0	-0.465469	0.677287	-2.198474
7	1	0	-1.624950	-1.496611	-1.469926
8	1	0	-2.133485	-0.290118	1.285752
9	1	0	-2.740145	0.851874	-1.497109
10	1	0	0.338150	-0.368489	0.563101
11	8	0	-1.113380	1.552057	-0.432763
12	6	0	-3.334815	1.920588	0.271266
13	1	0	-3.000413	2.063255	1.299630
14	1	0	-4.354023	1.536171	0.255642
15	8	0	-3.345870	3.167031	-0.421669
16	8	0	-3.629163	-1.019349	0.051220
17	8	0	-1.208064	-2.473946	0.296781
18	7	0	1.072297	1.602681	-1.224785
19	6	0	-2.566157	4.158898	0.065915
20	8	0	-1.997594	4.102294	1.120339
21	6	0	-2.525889	5.311928	-0.890183
22	1	0	-3.536359	5.577662	-1.201974
23	1	0	-2.033812	6.159605	-0.419734
24	1	0	-1.967745	5.007615	-1.778627
25	6	0	-4.156802	-1.696737	1.103511
26	8	0	-3.641820	-1.742191	2.184206
27	6	0	-5.443513	-2.352834	0.709420
28	1	0	-5.247173	-3.084006	-0.077177
29	1	0	-5.882338	-2.842866	1.574793
30	1	0	-6.130505	-1.607036	0.306441
31	6	0	-1.056908	-3.630488	-0.391774
32	8	0	-1.003794	-3.681249	-1.590095
33	6	0	-0.965444	-4.791146	0.547867
34	1	0	-0.019482	-4.725804	1.090248
35	1	0	-1.773775	-4.743035	1.278623
36	1	0	-1.003467	-5.720810	-0.014179
37	6	0	2.393781	-1.203828	-1.093476
38	8	0	3.104814	-1.529845	-2.022217
39	7	0	1.491797	1.947001	-0.113124
40	7	0	1.953137	2.306560	0.840937
41	7	0	1.022511	-1.390901	-1.135114
42	1	0	0.727383	-1.797567	-2.015653
43	7	0	2.854225	-0.663808	0.087318
44	6	0	4.171332	-0.265269	0.380685
45	6	0	5.161778	-0.095500	-0.591182
46	6	0	4.465234	0.020377	1.719259
47	6	0	6.425275	0.344370	-0.208552
48	1	0	4.947021	-0.312760	-1.625925
49	6	0	5.729644	0.458503	2.083322
50	1	0	3.691144	-0.098217	2.471335
51	6	0	6.722114	0.621676	1.120604
52	1	0	7.186026	0.470337	-0.970792
53	1	0	5.937740	0.674234	3.125038
54	1	0	7.710715	0.961225	1.404573
55	1	0	2.239441	-0.720027	0.887223

Structure 14 (Z,Z) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1613.4377789

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.648399	-1.180123	-0.829584
2	6	0	-0.075297	0.002986	-0.165119
3	6	0	0.764833	1.261501	-0.348233
4	6	0	2.187319	1.046805	0.130075
5	6	0	2.773908	-0.207092	-0.518892
6	1	0	0.720122	-1.004400	-1.909386
7	1	0	0.782215	1.552171	-1.403249
8	1	0	2.209041	0.949347	1.217296
9	1	0	2.850512	-0.040302	-1.603954
10	1	0	-0.170200	-0.218258	0.902893
11	8	0	1.934666	-1.310820	-0.265758
12	6	0	4.143025	-0.553897	0.028603
13	1	0	4.079867	-0.777059	1.092978
14	1	0	4.839534	0.267348	-0.131937
15	8	0	4.641421	-1.675416	-0.687647
16	8	0	2.930082	2.196483	-0.270242
17	8	0	0.226012	2.341606	0.416134
18	7	0	-0.060473	-2.432333	-0.697231
19	6	0	4.619752	-2.876051	-0.060506
20	8	0	4.334779	-3.022703	1.090489
21	6	0	5.002058	-3.969559	-1.013342
22	1	0	5.897743	-3.692388	-1.566552
23	1	0	5.157617	-4.891483	-0.462269
24	1	0	4.192748	-4.101912	-1.732334
25	6	0	3.846056	2.689658	0.594813
26	8	0	4.109661	2.171488	1.640217
27	6	0	4.467644	3.941243	0.051525
28	1	0	3.694509	4.693169	-0.104461
29	1	0	5.213130	4.305950	0.750663
30	1	0	4.923611	3.732972	-0.916097
31	6	0	-0.624444	3.190525	-0.184326
32	8	0	-1.004208	3.062086	-1.318700
33	6	0	-1.034804	4.288922	0.747441
34	1	0	-1.590428	3.855094	1.579402
35	1	0	-0.151803	4.774949	1.159621
36	1	0	-1.655233	5.002580	0.215456
37	6	0	-2.491289	-0.314404	-0.066730
38	8	0	-2.390006	-1.046744	0.894895
39	7	0	-0.127098	-2.843064	0.470005
40	7	0	-0.230408	-3.313472	1.472408
41	7	0	-1.391827	0.203999	-0.714650
42	1	0	-1.508626	0.978874	-1.350049
43	7	0	-3.681697	0.088758	-0.622712
44	6	0	-4.983678	-0.266369	-0.232530
45	6	0	-5.273515	-0.997187	0.918709
46	6	0	-6.027626	0.162858	-1.053709
47	6	0	-6.597003	-1.284977	1.222940
48	1	0	-4.473875	-1.335674	1.556368
49	6	0	-7.341114	-0.131192	-0.734532
50	1	0	-5.802945	0.730542	-1.949941
51	6	0	-7.636071	-0.860095	0.409370
52	1	0	-6.812331	-1.854519	2.118114
53	1	0	-8.135584	0.210344	-1.385452
54	1	0	-8.661942	-1.093540	0.660878
55	1	0	-3.625317	0.639820	-1.463677

Structure 14 (Z,E) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1613.4367736

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.751406	-1.403239	0.456755
2	6	0	0.166549	-0.501916	-0.386129
3	6	0	-0.118597	0.950728	-0.023958
4	6	0	-1.593465	1.268413	-0.171307
5	6	0	-2.426337	0.252820	0.612025
6	1	0	-0.517021	-1.270523	1.519764
7	1	0	0.187508	1.146768	1.008290
8	1	0	-1.880114	1.256329	-1.224663
9	1	0	-2.208442	0.372616	1.684101
10	1	0	-0.075478	-0.670646	-1.440048
11	8	0	-2.094613	-1.054466	0.202924
12	6	0	-3.914235	0.425437	0.384359
13	1	0	-4.158474	0.267349	-0.665401
14	1	0	-4.236184	1.419430	0.689694
15	8	0	-4.604921	-0.510452	1.201641
16	8	0	-1.784777	2.574070	0.370349
17	8	0	0.594936	1.832020	-0.889468
18	7	0	-0.568764	-2.814015	0.203452
19	6	0	-5.111310	-1.610270	0.594524
20	6	0	-5.629897	-2.579967	1.614942
21	1	0	-6.222272	-2.061119	2.366219
22	1	0	-6.216335	-3.346417	1.118264
23	1	0	-4.777515	-3.039215	2.117288
24	6	0	-2.638332	3.405983	-0.268098
25	8	0	-3.290354	3.080321	-1.217152
26	6	0	-2.646265	4.757028	0.382297
27	1	0	-1.658202	5.207539	0.287643
28	1	0	-3.391240	5.383617	-0.097140
29	1	0	-2.860072	4.652401	1.445339
30	6	0	1.779165	2.313030	-0.465254
31	8	0	2.283109	2.009171	0.581560
32	6	0	2.366310	3.254418	-1.471922
33	1	0	2.538080	2.717014	-2.404627
34	1	0	1.660733	4.057879	-1.680072
35	1	0	3.300440	3.653273	-1.089814
36	6	0	2.204346	-1.651015	-1.036123
37	8	0	1.633283	-2.242420	-1.931312
38	7	0	-0.918973	-3.162791	-0.933419
39	7	0	-1.220809	-3.588782	-1.915109
40	7	0	1.560739	-0.799483	-0.180052
41	1	0	2.098237	-0.192356	0.422020
42	7	0	3.561879	-1.801481	-0.842181
43	6	0	4.396155	-1.106405	0.060087
44	6	0	4.134860	-1.112769	1.428090
45	6	0	5.519081	-0.438430	-0.420402
46	6	0	4.969243	-0.424750	2.295863
47	1	0	3.287286	-1.672714	1.802636
48	6	0	6.364692	0.222480	0.456295
49	1	0	5.720501	-0.439053	-1.484740
50	6	0	6.086771	0.242684	1.815944
51	1	0	4.753513	-0.428515	3.356346
52	1	0	7.238179	0.733676	0.072564
53	1	0	6.740751	0.769883	2.497533
54	1	0	3.997629	-2.288657	-1.609560
55	8	0	-5.132161	-1.769276	-0.589591

Structure 14 (E,Z) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1613.4309394

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.177314	0.726712	-1.144367
2	6	0	0.133540	-0.600760	-0.426191
3	6	0	-1.148141	-1.431389	-0.386501
4	6	0	-2.291598	-0.648816	0.230178
5	6	0	-2.442710	0.698715	-0.476057
6	1	0	-0.466062	0.523563	-2.181763
7	1	0	-1.424210	-1.728310	-1.402516
8	1	0	-2.114389	-0.493923	1.296434
9	1	0	-2.748066	0.520783	-1.517347
10	1	0	0.392646	-0.358194	0.609980
11	8	0	-1.210142	1.387963	-0.455140
12	6	0	-3.462308	1.592085	0.199893
13	1	0	-3.154373	1.813126	1.220992
14	1	0	-4.439854	1.113377	0.207644
15	8	0	-3.588072	2.790487	-0.552752
16	8	0	-3.469233	-1.427844	0.044299
17	8	0	-0.941517	-2.597360	0.396733
18	7	0	0.968277	1.612392	-1.235089
19	6	0	-2.966331	3.894255	-0.072547
20	8	0	-2.424470	3.943926	0.991644
21	6	0	-3.061509	5.019268	-1.059938
22	1	0	-4.086501	5.127517	-1.410097
23	1	0	-2.712292	5.936292	-0.596566
24	1	0	-2.437539	4.779991	-1.921671
25	6	0	-4.352330	-1.492412	1.068290
26	8	0	-4.227493	-0.871373	2.083418
27	6	0	-5.478967	-2.423947	0.737605
28	1	0	-5.082294	-3.421926	0.553466
29	1	0	-6.184496	-2.442708	1.561659
30	1	0	-5.970304	-2.092173	-0.176616
31	6	0	-0.666894	-3.748764	-0.262259
32	8	0	-0.634517	-3.833318	-1.456081
33	6	0	-0.406735	-4.863391	0.703463
34	1	0	0.541240	-4.671049	1.207128
35	1	0	-1.186482	-4.895410	1.462315
36	1	0	-0.350614	-5.802645	0.163070
37	6	0	2.541631	-1.100442	-1.025004
38	8	0	3.255700	-1.458292	-1.933063
39	7	0	1.338520	2.039191	-0.137422
40	7	0	1.747474	2.471907	0.805143
41	7	0	1.179720	-1.373320	-1.044694
42	1	0	0.924568	-1.877844	-1.883942
43	7	0	2.981884	-0.461980	0.108506
44	6	0	4.282771	-0.002734	0.386032
45	6	0	5.323911	-0.023602	-0.539853
46	6	0	4.506197	0.519888	1.660808
47	6	0	6.566677	0.473921	-0.171723
48	1	0	5.160463	-0.428741	-1.524422
49	6	0	5.751053	1.009846	2.011527
50	1	0	3.691855	0.550974	2.376146
51	6	0	6.793594	0.989180	1.095054
52	1	0	7.369883	0.452925	-0.897103
53	1	0	5.903478	1.411815	3.004645
54	1	0	7.768418	1.371385	1.365946
55	1	0	2.344523	-0.405342	0.884576

Structure 14 (Z,Z) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1613.4730947

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.648157	-1.188201	-0.830843
2	6	0	-0.075898	-0.007001	-0.167575
3	6	0	0.759869	1.254154	-0.359247
4	6	0	2.179741	1.039112	0.128210
5	6	0	2.773439	-0.206332	-0.531355
6	1	0	0.704378	-1.030911	-1.912685
7	1	0	0.780421	1.535057	-1.416054
8	1	0	2.190816	0.928807	1.214100
9	1	0	2.844703	-0.036190	-1.614991
10	1	0	-0.160024	-0.219820	0.902339
11	8	0	1.937825	-1.319143	-0.278279
12	6	0	4.142921	-0.543554	0.017208
13	1	0	4.085504	-0.764306	1.081954
14	1	0	4.834965	0.280366	-0.151479
15	8	0	4.654534	-1.665152	-0.697794
16	8	0	2.925498	2.191713	-0.256363
17	8	0	0.211241	2.328399	0.401791
18	7	0	-0.057113	-2.446981	-0.661039
19	6	0	4.657239	-2.864830	-0.083725
20	8	0	4.365489	-3.025180	1.069444
21	6	0	5.070256	-3.944546	-1.034170
22	1	0	5.978647	-3.655990	-1.561846
23	1	0	5.221985	-4.873644	-0.492733
24	1	0	4.280579	-4.076647	-1.775930
25	6	0	3.811680	2.705769	0.623507
26	8	0	4.043986	2.204023	1.688760
27	6	0	4.443404	3.947150	0.080749
28	1	0	3.670906	4.690679	-0.118353
29	1	0	5.161986	4.335470	0.796283
30	1	0	4.937783	3.720819	-0.864684
31	6	0	-0.616087	3.194070	-0.210586
32	8	0	-0.947447	3.087136	-1.363500
33	6	0	-1.055724	4.271680	0.725881
34	1	0	-1.609851	3.820226	1.550132
35	1	0	-0.183540	4.771194	1.147733
36	1	0	-1.683938	4.983339	0.198884
37	6	0	-2.497984	-0.318428	-0.057915
38	8	0	-2.402965	-1.029107	0.928577
39	7	0	-0.114894	-2.824607	0.513545
40	7	0	-0.206795	-3.261678	1.533128
41	7	0	-1.398855	0.184856	-0.701842
42	1	0	-1.514225	0.857652	-1.446149
43	7	0	-3.685526	0.056198	-0.632565
44	6	0	-4.986813	-0.288356	-0.239028
45	6	0	-5.289204	-1.008180	0.917465
46	6	0	-6.027251	0.140394	-1.068108
47	6	0	-6.616422	-1.285613	1.220428
48	1	0	-4.498441	-1.345198	1.566869
49	6	0	-7.343883	-0.142959	-0.750835
50	1	0	-5.792077	0.700914	-1.966049
51	6	0	-7.649822	-0.861282	0.398743
52	1	0	-6.837764	-1.845898	2.120640
53	1	0	-8.133667	0.199338	-1.407983
54	1	0	-8.678692	-1.085845	0.648342
55	1	0	-3.629152	0.616290	-1.470827

Structure 14 (Z,E) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1613.4713098

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.752275	-1.426560	0.431772
2	6	0	0.168621	-0.525698	-0.405176
3	6	0	-0.108788	0.926272	-0.032443
4	6	0	-1.583032	1.248770	-0.175165
5	6	0	-2.414417	0.237920	0.615465
6	1	0	-0.508533	-1.321485	1.493966
7	1	0	0.199715	1.112021	1.000164
8	1	0	-1.872511	1.233916	-1.227260
9	1	0	-2.183216	0.347210	1.684499
10	1	0	-0.072336	-0.680082	-1.461138
11	8	0	-2.095289	-1.072874	0.191489
12	6	0	-3.899290	0.431381	0.398245
13	1	0	-4.156472	0.275580	-0.648456
14	1	0	-4.202259	1.430710	0.708220
15	8	0	-4.607878	-0.487553	1.226264
16	8	0	-1.771939	2.552521	0.370000
17	8	0	0.605231	1.804618	-0.899602
18	7	0	-0.586905	-2.839624	0.137598
19	6	0	-5.161120	-1.570142	0.644868
20	6	0	-5.750838	-2.480975	1.675660
21	1	0	-6.420602	-1.920286	2.327363
22	1	0	-6.284717	-3.290732	1.187202
23	1	0	-4.946450	-2.885904	2.291640
24	6	0	-2.565490	3.420848	-0.292791
25	8	0	-3.167399	3.130903	-1.289878
26	6	0	-2.576466	4.753807	0.384246
27	1	0	-1.582942	5.198619	0.306563
28	1	0	-3.308592	5.400282	-0.090126
29	1	0	-2.803832	4.630145	1.442887
30	6	0	1.778521	2.309671	-0.472973
31	8	0	2.274297	2.020735	0.585029
32	6	0	2.354970	3.253243	-1.476997
33	1	0	2.492287	2.731835	-2.424956
34	1	0	1.655269	4.072261	-1.647374
35	1	0	3.304838	3.636423	-1.116462
36	6	0	2.225771	-1.663482	-1.045526
37	8	0	1.664573	-2.256292	-1.955786
38	7	0	-0.937179	-3.148321	-1.005919
39	7	0	-1.244032	-3.532481	-2.004516
40	7	0	1.561768	-0.829544	-0.196087
41	1	0	2.082658	-0.251761	0.448174
42	7	0	3.575832	-1.811307	-0.836127
43	6	0	4.394544	-1.118126	0.085318
44	6	0	4.123217	-1.146908	1.451301
45	6	0	5.511757	-0.430387	-0.381296
46	6	0	4.945320	-0.461177	2.334287
47	1	0	3.280289	-1.720888	1.816529
48	6	0	6.342802	0.230705	0.510045
49	1	0	5.720885	-0.418423	-1.444402
50	6	0	6.056679	0.228093	1.869281
51	1	0	4.723483	-0.483044	3.393824
52	1	0	7.211854	0.759246	0.138511
53	1	0	6.700512	0.754034	2.562338
54	1	0	4.037516	-2.268789	-1.609351
55	8	0	-5.176115	-1.756491	-0.540731

Structure 14 (E,Z) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1613.4676889

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.179060	0.741656	-1.154585
2	6	0	0.136570	-0.585864	-0.441477
3	6	0	-1.143827	-1.418356	-0.413535
4	6	0	-2.281250	-0.637833	0.217893
5	6	0	-2.440206	0.711091	-0.484365
6	1	0	-0.470675	0.544067	-2.190579
7	1	0	-1.420543	-1.699716	-1.432955
8	1	0	-2.087910	-0.486277	1.281413
9	1	0	-2.742176	0.536953	-1.526178
10	1	0	0.401359	-0.357411	0.595528
11	8	0	-1.206220	1.405237	-0.458854
12	6	0	-3.463144	1.591551	0.200466
13	1	0	-3.168615	1.796142	1.228409
14	1	0	-4.441810	1.114453	0.185371
15	8	0	-3.583458	2.806505	-0.533904
16	8	0	-3.462578	-1.413836	0.041376
17	8	0	-0.939861	-2.592502	0.361267
18	7	0	0.970385	1.630198	-1.243521
19	6	0	-2.987652	3.908740	-0.036568
20	8	0	-2.469338	3.955390	1.045367
21	6	0	-3.062874	5.039581	-1.013665
22	1	0	-4.077789	5.143010	-1.395360
23	1	0	-2.737445	5.959290	-0.536878
24	1	0	-2.408764	4.811875	-1.857352
25	6	0	-4.324602	-1.515995	1.076809
26	8	0	-4.172811	-0.932171	2.114594
27	6	0	-5.453690	-2.436251	0.742371
28	1	0	-5.058915	-3.439059	0.573785
29	1	0	-6.169462	-2.448802	1.558649
30	1	0	-5.934508	-2.109429	-0.179697
31	6	0	-0.687421	-3.747604	-0.293059
32	8	0	-0.649949	-3.829846	-1.490715
33	6	0	-0.459363	-4.868159	0.667994
34	1	0	0.472418	-4.682952	1.205288
35	1	0	-1.265456	-4.904209	1.400080
36	1	0	-0.389914	-5.806307	0.125940
37	6	0	2.539700	-1.108581	-1.016381
38	8	0	3.283838	-1.505555	-1.894160
39	7	0	1.356660	2.042611	-0.148035
40	7	0	1.779476	2.465537	0.792687
41	7	0	1.183905	-1.343495	-1.080931
42	1	0	0.925514	-1.835255	-1.927241
43	7	0	2.965120	-0.445714	0.106630
44	6	0	4.269700	-0.006176	0.390135
45	6	0	5.260810	0.138262	-0.579996
46	6	0	4.546470	0.346720	1.712658
47	6	0	6.510413	0.619074	-0.211149
48	1	0	5.056834	-0.124578	-1.605163
49	6	0	5.796095	0.827488	2.063871
50	1	0	3.770953	0.244648	2.463982
51	6	0	6.790311	0.964358	1.103059
52	1	0	7.273399	0.725480	-0.972376
53	1	0	5.991624	1.095574	3.094492
54	1	0	7.768829	1.336656	1.376613
55	1	0	2.325364	-0.386106	0.883791

Structure 15 (Z,Z) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1936.1742609

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.934271	-1.306328	-0.791247
2	6	0	0.115006	-0.155618	-0.175967
3	6	0	0.843370	1.165366	-0.423049
4	6	0	2.278981	1.096807	0.067238
5	6	0	2.965537	-0.120275	-0.548951
6	1	0	0.982806	-1.186854	-1.881108
7	1	0	0.848341	1.407804	-1.492145
8	1	0	2.300661	1.048186	1.158873
9	1	0	3.012217	0.006197	-1.641333
10	1	0	0.033121	-0.327806	0.901648
11	8	0	2.233580	-1.286881	-0.234313
12	6	0	4.369469	-0.313889	-0.013062
13	1	0	4.340273	-0.494593	1.062656
14	1	0	4.978326	0.560591	-0.240329
15	8	0	4.953714	-1.426324	-0.679263
16	8	0	2.973653	2.258835	-0.383550
17	8	0	0.202814	2.225840	0.285068
18	7	0	0.341089	-2.607723	-0.577999
19	6	0	4.990115	-2.600226	0.004041
20	8	0	4.720648	-2.704563	1.162897
21	6	0	5.408443	-3.717853	-0.907200
22	1	0	6.250091	-3.408918	-1.525940
23	1	0	5.660479	-4.591977	-0.312811
24	1	0	4.570627	-3.951832	-1.567170
25	6	0	3.153774	3.274940	0.504905
26	8	0	2.805625	3.227092	1.645632
27	6	0	3.848580	4.427234	-0.162969
28	1	0	3.248724	4.775085	-1.004877
29	1	0	3.990840	5.226139	0.559417
30	1	0	4.810194	4.095642	-0.556690
31	6	0	-0.747782	2.937158	-0.351305
32	8	0	-1.096569	2.718946	-1.482217
33	6	0	-1.303091	3.999344	0.548392
34	1	0	-1.926203	3.514090	1.302977
35	1	0	-0.493746	4.512094	1.067427
36	1	0	-1.904190	4.691039	-0.035386
37	6	0	-2.350484	-0.438477	-0.058887
38	7	0	0.421401	-3.000148	0.597729
39	7	0	0.452348	-3.468491	1.611611
40	7	0	-1.215351	-0.082406	-0.731151
41	1	0	-1.324102	0.567696	-1.500394
42	7	0	-3.473140	-0.119603	-0.768147
43	6	0	-4.827374	-0.352328	-0.416398
44	6	0	-5.331763	-0.001929	0.833829
45	6	0	-5.674791	-0.883106	-1.386331
46	6	0	-6.677812	-0.202688	1.107436
47	1	0	-4.670089	0.414560	1.579504
48	6	0	-7.023714	-1.065317	-1.108517
49	1	0	-5.270739	-1.164083	-2.352881
50	6	0	-7.528617	-0.731556	0.141942
51	1	0	-7.064680	0.064400	2.083328
52	1	0	-7.675588	-1.479024	-1.868258
53	1	0	-8.578028	-0.881964	0.363227
54	1	0	-3.332454	0.139437	-1.735077
55	16	0	-2.341984	-1.172401	1.438350

Structure 15 (Z,E) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1936.1805349

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.447062	-1.273356	0.230340
2	6	0	0.162445	-0.067159	-0.510509
3	6	0	-0.388016	1.214410	0.109093
4	6	0	-1.906767	1.199243	0.095486
5	6	0	-2.416878	-0.080067	0.757761
6	1	0	-0.142276	-1.253416	1.285235
7	1	0	-0.040884	1.321912	1.143036
8	1	0	-2.271812	1.279916	-0.931702
9	1	0	-2.133789	-0.073868	1.821072
10	1	0	-0.132200	-0.116808	-1.562523
11	8	0	-1.852620	-1.210581	0.121459
12	6	0	-3.922098	-0.209011	0.642380
13	1	0	-4.212851	-0.265641	-0.407925
14	1	0	-4.405705	0.637038	1.129394
15	8	0	-4.333745	-1.385942	1.326966
16	8	0	-2.381397	2.301335	0.867052
17	8	0	0.035998	2.347319	-0.639822
18	7	0	0.024074	-2.546528	-0.274619
19	6	0	-4.588279	-2.480612	0.563885
20	8	0	-4.636161	-2.464610	-0.629425
21	6	0	-4.791158	-3.685241	1.437215
22	1	0	-5.425614	-3.435725	2.286781
23	1	0	-5.224745	-4.488356	0.847516
24	1	0	-3.817953	-3.996907	1.821864
25	6	0	-2.808323	3.406613	0.195447
26	8	0	-2.872888	3.475202	-0.994328
27	6	0	-3.177759	4.489730	1.168091
28	1	0	-2.294394	4.774796	1.741517
29	1	0	-3.565495	5.345043	0.621822
30	1	0	-3.921941	4.115761	1.871990
31	6	0	1.168880	2.970508	-0.246516
32	8	0	1.810918	2.636506	0.711428
33	6	0	1.495309	4.097974	-1.179190
34	1	0	1.865939	3.669424	-2.113083
35	1	0	0.595684	4.667438	-1.410300
36	1	0	2.260737	4.727409	-0.733626
37	6	0	2.408774	-0.523623	-1.437602
38	7	0	-0.450490	-2.840872	-1.386045
39	7	0	-0.828515	-3.221067	-2.365378
40	7	0	1.600162	-0.082989	-0.444806
41	1	0	2.033009	0.271507	0.400232
42	7	0	3.722660	-0.629767	-1.092253
43	6	0	4.238492	-0.754285	0.228188
44	6	0	3.655967	-1.643650	1.134130
45	6	0	5.356235	-0.011111	0.595945
46	6	0	4.190994	-1.769346	2.409255
47	1	0	2.798910	-2.233315	0.824289
48	6	0	5.897768	-0.160592	1.867581
49	1	0	5.786109	0.683697	-0.115910
50	6	0	5.313266	-1.032596	2.778204
51	1	0	3.741004	-2.460722	3.111640
52	1	0	6.770423	0.416244	2.148992
53	1	0	5.731501	-1.141569	3.771330
54	1	0	4.330117	-0.860618	-1.864632
55	16	0	1.899338	-0.878468	-2.992939

Structure 15 (E,Z) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1936.1716117

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.144503	0.800149	-0.992003
2	6	0	-0.048307	-0.573089	-0.288478
3	6	0	-1.424495	-1.234124	-0.332001
4	6	0	-2.488581	-0.321166	0.253761
5	6	0	-2.439179	1.033399	-0.449159
6	1	0	-0.386083	0.657911	-2.051899
7	1	0	-1.690993	-1.469271	-1.367984
8	1	0	-2.338688	-0.208133	1.330571
9	1	0	-2.702613	0.903509	-1.509106
10	1	0	0.197329	-0.388276	0.762606
11	8	0	-1.134344	1.570459	-0.343717
12	6	0	-3.385198	2.034639	0.182814
13	1	0	-3.110617	2.203110	1.225318
14	1	0	-4.410246	1.673405	0.109651
15	8	0	-3.310810	3.253751	-0.544461
16	8	0	-3.767836	-0.896809	0.001315
17	8	0	-1.416315	-2.435469	0.426891
18	7	0	1.101339	1.545878	-0.978651
19	6	0	-2.538572	4.237329	-0.012382
20	8	0	-2.058311	4.187739	1.080464
21	6	0	-2.387921	5.364869	-0.992180
22	1	0	-3.354502	5.621282	-1.424329
23	1	0	-1.945438	6.221047	-0.490540
24	1	0	-1.734555	5.032578	-1.801188
25	6	0	-4.371871	-1.568700	1.020691
26	8	0	-3.924442	-1.635548	2.125700
27	6	0	-5.652467	-2.189193	0.541669
28	1	0	-5.426218	-2.928025	-0.228735
29	1	0	-6.157891	-2.661022	1.379571
30	1	0	-6.287401	-1.426167	0.090809
31	6	0	-1.257369	-3.599594	-0.253220
32	8	0	-1.131202	-3.654477	-1.442684
33	6	0	-1.258721	-4.761448	0.694403
34	1	0	-0.320524	-4.752907	1.252492
35	1	0	-2.073975	-4.659015	1.410264
36	1	0	-1.339706	-5.686426	0.130315
37	6	0	2.282382	-1.251663	-0.873467
38	7	0	1.432686	1.903555	0.161878
39	7	0	1.826286	2.270418	1.142642
40	7	0	0.921646	-1.464232	-0.896458
41	1	0	0.617818	-1.923566	-1.747167
42	7	0	2.728682	-0.750257	0.316083
43	6	0	4.015280	-0.217015	0.577406
44	6	0	4.566708	0.739873	-0.272810
45	6	0	4.685307	-0.597773	1.734854
46	6	0	5.797712	1.297579	0.037459
47	1	0	4.026794	1.032511	-1.164932
48	6	0	5.912139	-0.021592	2.044911
49	1	0	4.249518	-1.349188	2.383968
50	6	0	6.474444	0.922045	1.195279
51	1	0	6.227948	2.037779	-0.626046
52	1	0	6.430021	-0.320236	2.948134
53	1	0	7.433338	1.365535	1.433016
54	1	0	2.161103	-0.943410	1.129214
55	16	0	3.236655	-1.640929	-2.170363

Structure 15 (Z,Z) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1936.2129962

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.798164	-1.242266	-0.775009
2	6	0	0.091993	-0.035758	-0.127074
3	6	0	0.922274	1.214408	-0.412555
4	6	0	2.354996	1.024218	0.056343
5	6	0	2.934855	-0.243531	-0.569191
6	1	0	0.821230	-1.120279	-1.863774
7	1	0	0.926357	1.430502	-1.486333
8	1	0	2.392592	0.968570	1.146675
9	1	0	2.985265	-0.121567	-1.660691
10	1	0	0.039239	-0.199896	0.952372
11	8	0	2.103575	-1.347364	-0.252057
12	6	0	4.314104	-0.558269	-0.027931
13	1	0	4.271744	-0.709056	1.051412
14	1	0	5.005373	0.248009	-0.270600
15	8	0	4.799515	-1.734335	-0.672897
16	8	0	3.127301	2.130712	-0.406190
17	8	0	0.393450	2.338142	0.287710
18	7	0	0.102061	-2.496577	-0.538222
19	6	0	4.687613	-2.904313	-0.002701
20	8	0	4.345175	-2.986239	1.143319
21	6	0	5.051808	-4.054572	-0.891483
22	1	0	6.003129	-3.861128	-1.388166
23	1	0	5.105025	-4.967410	-0.303158
24	1	0	4.284190	-4.156765	-1.661920
25	6	0	3.427405	3.116625	0.479158
26	8	0	3.143014	3.069016	1.641485
27	6	0	4.145448	4.234243	-0.212513
28	1	0	3.467672	4.697710	-0.932657
29	1	0	4.470051	4.968620	0.520332
30	1	0	5.000343	3.840447	-0.763763
31	6	0	-0.465570	3.148532	-0.365413
32	8	0	-0.828044	2.950953	-1.496065
33	6	0	-0.888916	4.285825	0.508626
34	1	0	-1.459946	3.885804	1.349436
35	1	0	-0.009422	4.787467	0.914790
36	1	0	-1.501411	4.978630	-0.062709
37	6	0	-2.385230	-0.261520	-0.017970
38	7	0	0.226367	-2.910741	0.621967
39	7	0	0.290622	-3.384480	1.632520
40	7	0	-1.246701	0.135996	-0.637021
41	1	0	-1.334835	0.677329	-1.490348
42	7	0	-3.491536	-0.036498	-0.773191
43	6	0	-4.846265	-0.290098	-0.433875
44	6	0	-5.408489	0.207094	0.740143
45	6	0	-5.633340	-0.991092	-1.344598
46	6	0	-6.753148	-0.019046	1.004160
47	1	0	-4.795139	0.765180	1.434339
48	6	0	-6.982413	-1.199606	-1.079397
49	1	0	-5.183097	-1.376205	-2.253262
50	6	0	-7.544817	-0.719799	0.098136
51	1	0	-7.185778	0.365479	1.920420
52	1	0	-7.589162	-1.746233	-1.791645
53	1	0	-8.594036	-0.888872	0.309189
54	1	0	-3.334184	0.179256	-1.750805
55	16	0	-2.409101	-0.964564	1.513433

Structure 15 (Z,E) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1936.217831

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.650676	-1.331272	-0.340030
2	6	0	-0.121507	-0.288747	0.490696
3	6	0	0.254075	1.104436	-0.010195
4	6	0	1.761210	1.291538	0.024245
5	6	0	2.438065	0.160557	-0.749323
6	1	0	0.339107	-1.277095	-1.389427
7	1	0	-0.101013	1.249569	-1.035515
8	1	0	2.114680	1.318949	1.057364
9	1	0	2.147163	0.218539	-1.807666
10	1	0	0.169331	-0.386438	1.539536
11	8	0	2.034026	-1.089016	-0.213583
12	6	0	3.945969	0.231140	-0.634391
13	1	0	4.252670	0.127859	0.406920
14	1	0	4.307570	1.174013	-1.043326
15	8	0	4.514188	-0.812380	-1.423967
16	8	0	2.075380	2.516523	-0.635682
17	8	0	-0.319378	2.102738	0.830071
18	7	0	0.373990	-2.696950	0.076737
19	6	0	4.928949	-1.927814	-0.781495
20	8	0	4.972653	-2.032502	0.412237
21	6	0	5.317663	-2.986478	-1.768836
22	1	0	5.973670	-2.567165	-2.532135
23	1	0	5.806955	-3.807716	-1.251063
24	1	0	4.413588	-3.348881	-2.263335
25	6	0	2.423221	3.586191	0.125212
26	8	0	2.534987	3.540437	1.316859
27	6	0	2.648554	4.788637	-0.739159
28	1	0	1.745071	4.999270	-1.313718
29	1	0	2.907720	5.640751	-0.116005
30	1	0	3.453609	4.581134	-1.446318
31	6	0	-1.500520	2.642796	0.458015
32	8	0	-2.088485	2.317579	-0.539695
33	6	0	-1.954038	3.661349	1.455109
34	1	0	-2.225830	3.143190	2.377920
35	1	0	-1.139252	4.347853	1.686574
36	1	0	-2.815896	4.196563	1.064641
37	6	0	-2.324489	-1.084579	1.304096
38	7	0	0.902415	-2.995334	1.156551
39	7	0	1.348187	-3.376259	2.108160
40	7	0	-1.547469	-0.482506	0.382745
41	1	0	-1.998634	-0.078867	-0.431731
42	7	0	-3.627265	-1.236804	0.968740
43	6	0	-4.228887	-0.954576	-0.290583
44	6	0	-3.739654	-1.548113	-1.455092
45	6	0	-5.332134	-0.106323	-0.342708
46	6	0	-4.349383	-1.272013	-2.673100
47	1	0	-2.897832	-2.229582	-1.394824
48	6	0	-5.948576	0.146894	-1.562787
49	1	0	-5.695826	0.349234	0.571142
50	6	0	-5.453999	-0.426652	-2.729762
51	1	0	-3.968943	-1.732089	-3.577360
52	1	0	-6.809386	0.803749	-1.601260
53	1	0	-5.931268	-0.220493	-3.680250
54	1	0	-4.224123	-1.566754	1.714880
55	16	0	-1.765642	-1.618093	2.810314

Structure 15 (E,Z) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1936.2122043

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.253315	0.853984	-1.052546
2	6	0	-0.035715	-0.499867	-0.343014
3	6	0	-1.356145	-1.266463	-0.371552
4	6	0	-2.472497	-0.432976	0.234957
5	6	0	-2.537896	0.928214	-0.455953
6	1	0	-0.520737	0.687655	-2.101034
7	1	0	-1.616902	-1.520210	-1.403511
8	1	0	-2.310768	-0.311646	1.308390
9	1	0	-2.812486	0.790638	-1.510943
10	1	0	0.208902	-0.298510	0.704156
11	8	0	-1.268620	1.559205	-0.373933
12	6	0	-3.537749	1.844859	0.217991
13	1	0	-3.266235	1.999792	1.262653
14	1	0	-4.538803	1.421218	0.147231
15	8	0	-3.559965	3.090153	-0.475965
16	8	0	-3.709433	-1.101148	-0.000338
17	8	0	-1.247209	-2.461127	0.394530
18	7	0	0.943510	1.683130	-1.088108
19	6	0	-2.844617	4.109134	0.053097
20	8	0	-2.319900	4.064911	1.130693
21	6	0	-2.810864	5.271964	-0.891091
22	1	0	-3.816335	5.495586	-1.248438
23	1	0	-2.379527	6.135970	-0.391752
24	1	0	-2.198655	5.001044	-1.754275
25	6	0	-4.281643	-1.775322	1.031051
26	8	0	-3.829761	-1.790262	2.140443
27	6	0	-5.528131	-2.466600	0.572768
28	1	0	-5.279453	-3.166965	-0.226411
29	1	0	-5.981032	-2.993166	1.408791
30	1	0	-6.225131	-1.731664	0.166459
31	6	0	-1.020018	-3.619786	-0.270891
32	8	0	-0.892524	-3.676949	-1.463376
33	6	0	-0.945353	-4.769030	0.683361
34	1	0	-0.020226	-4.682194	1.257894
35	1	0	-1.780059	-4.729264	1.383770
36	1	0	-0.944604	-5.703928	0.128770
37	6	0	2.337564	-1.097353	-0.856632
38	7	0	1.307411	2.068972	0.029526
39	7	0	1.724934	2.469265	0.987497
40	7	0	0.997193	-1.297063	-0.975418
41	1	0	0.727792	-1.789615	-1.818735
42	7	0	2.729219	-0.511568	0.303290
43	6	0	4.036455	-0.030956	0.589527
44	6	0	4.598770	0.964751	-0.206816
45	6	0	4.712750	-0.508771	1.706136
46	6	0	5.854401	1.463853	0.109018
47	1	0	4.049346	1.334817	-1.064968
48	6	0	5.964846	0.008658	2.025186
49	1	0	4.260993	-1.285333	2.313295
50	6	0	6.540189	0.989059	1.225399
51	1	0	6.294916	2.234068	-0.512841
52	1	0	6.491672	-0.363948	2.895596
53	1	0	7.518010	1.385680	1.471185
54	1	0	2.112144	-0.601074	1.101365
55	16	0	3.387775	-1.592530	-2.070659

Structure 15 (Z,Z) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1936.3739915

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.843354	-1.246641	-0.813568
2	6	0	0.035886	-0.103407	-0.176388
3	6	0	0.773686	1.213016	-0.407330
4	6	0	2.206547	1.127858	0.079172
5	6	0	2.887351	-0.090953	-0.544676
6	1	0	0.891113	-1.103783	-1.900091
7	1	0	0.776095	1.466762	-1.472235
8	1	0	2.235627	1.057773	1.168240
9	1	0	2.943992	0.056805	-1.633652
10	1	0	-0.039429	-0.295746	0.897435
11	8	0	2.139454	-1.252338	-0.261403
12	6	0	4.282924	-0.318617	-0.001547
13	1	0	4.245658	-0.524550	1.067430
14	1	0	4.911324	0.550869	-0.186706
15	8	0	4.863350	-1.411804	-0.700413
16	8	0	2.856492	2.321956	-0.349868
17	8	0	0.133653	2.263809	0.313540
18	7	0	0.238148	-2.546794	-0.629762
19	6	0	4.932225	-2.600224	-0.053883
20	8	0	4.655092	-2.750199	1.098544
21	6	0	5.403003	-3.675299	-0.988185
22	1	0	6.290945	-3.345139	-1.524880
23	1	0	5.607089	-4.580023	-0.424641
24	1	0	4.619976	-3.865129	-1.723119
25	6	0	3.727068	2.909032	0.503923
26	8	0	4.033168	2.436464	1.559278
27	6	0	4.239851	4.198145	-0.064297
28	1	0	3.407105	4.884794	-0.214742
29	1	0	4.964563	4.628464	0.619241
30	1	0	4.695287	4.015091	-1.037123
31	6	0	-0.797026	2.996457	-0.323730
32	8	0	-1.113406	2.819005	-1.470455
33	6	0	-1.384481	4.027954	0.588833
34	1	0	-1.975579	3.516561	1.350108
35	1	0	-0.593051	4.575148	1.097952
36	1	0	-2.017630	4.698650	0.017124
37	6	0	-2.428056	-0.374163	-0.043560
38	7	0	0.313419	-2.969048	0.532303
39	7	0	0.341952	-3.451965	1.534163
40	7	0	-1.296942	-0.009670	-0.713534
41	1	0	-1.406577	0.626010	-1.492307
42	7	0	-3.552909	-0.060563	-0.747641
43	1	0	-4.723250	0.430494	1.621623
44	1	0	-5.374558	-1.031467	-2.341074
45	1	0	-7.113355	0.096753	2.134468
46	1	0	-7.773124	-1.335292	-1.843734
47	1	0	-8.649284	-0.788943	0.407275
48	1	0	-3.416768	0.202990	-1.712487
49	16	0	-2.412955	-1.118948	1.439675
50	6	0	-5.394044	0.041094	0.871071
51	6	0	-6.737764	-0.150614	1.150087
52	6	0	-7.601234	-0.644324	0.181130
53	6	0	-7.111148	-0.949580	-1.079526
54	6	0	-5.765384	-0.774674	-1.363502
55	6	0	-4.903918	-0.282194	-0.389256

Structure 15 (Z,E) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1936.3786132

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.427537	-1.280186	-0.211262
2	6	0	-0.226001	-0.095563	0.516972
3	6	0	0.313992	1.211132	-0.054662
4	6	0	1.829616	1.225491	-0.030795
5	6	0	2.371209	-0.036138	-0.705035
6	1	0	0.137102	-1.272278	-1.269402
7	1	0	-0.029480	1.349952	-1.084664
8	1	0	2.192617	1.285713	0.997234
9	1	0	2.085254	-0.018859	-1.767280
10	1	0	0.032045	-0.156410	1.577293
11	8	0	1.825545	-1.182309	-0.086584
12	6	0	3.877605	-0.149626	-0.597904
13	1	0	4.180562	-0.220912	0.445980
14	1	0	4.357914	0.710741	-1.060222
15	8	0	4.295035	-1.301675	-1.319001
16	8	0	2.239279	2.380712	-0.758648
17	8	0	-0.145691	2.298052	0.738463
18	7	0	-0.016509	-2.563779	0.291232
19	6	0	4.645111	-2.394131	-0.599827
20	8	0	4.741366	-2.407106	0.591167
21	6	0	4.886929	-3.563249	-1.508451
22	1	0	5.491973	-3.262814	-2.361853
23	1	0	5.370305	-4.359524	-0.951258
24	1	0	3.924742	-3.912143	-1.885693
25	6	0	3.288397	3.089050	-0.281137
26	8	0	3.934791	2.749585	0.666848
27	6	0	3.517241	4.319392	-1.106495
28	1	0	2.617074	4.933116	-1.104072
29	1	0	4.356832	4.873780	-0.699944
30	1	0	3.717490	4.032708	-2.138838
31	6	0	-1.272453	2.930236	0.348876
32	8	0	-1.861982	2.672323	-0.663697
33	6	0	-1.675781	3.959481	1.359198
34	1	0	-2.008242	3.439691	2.259309
35	1	0	-0.821666	4.577101	1.631228
36	1	0	-2.482821	4.564828	0.959465
37	6	0	-2.499929	-0.501811	1.397309
38	7	0	0.408412	-2.822064	1.427522
39	7	0	0.748794	-3.161594	2.430316
40	7	0	-1.658161	-0.134021	0.406166
41	1	0	-2.064888	0.178641	-0.465815
42	7	0	-3.808678	-0.583393	1.032765
43	6	0	-4.328345	-0.674865	-0.284432
44	6	0	-3.778618	-1.565848	-1.204687
45	6	0	-5.425696	0.100918	-0.638792
46	6	0	-4.320239	-1.659575	-2.477047
47	1	0	-2.940596	-2.186601	-0.909243
48	6	0	-5.975183	-0.015877	-1.907024
49	1	0	-5.836384	0.796807	0.081792
50	6	0	-5.420373	-0.889100	-2.831328
51	1	0	-3.892815	-2.354290	-3.188500
52	1	0	-6.832454	0.587309	-2.175916
53	1	0	-5.845275	-0.973494	-3.822719
54	1	0	-4.434662	-0.747434	1.805712
55	16	0	-2.039281	-0.796670	2.972634

Structure 15 (E,Z) (M06-2X/def2-TZVP, gas phase)

Energy (Hartrees): = -1936.368488

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.135826	0.777778	-0.983150
2	6	0	-0.014901	-0.586135	-0.271218
3	6	0	-1.378142	-1.270814	-0.318977
4	6	0	-2.466474	-0.373901	0.242583
5	6	0	-2.432800	0.978626	-0.462893
6	1	0	-0.370794	0.616517	-2.041364
7	1	0	-1.626243	-1.518907	-1.355548
8	1	0	-2.332371	-0.247152	1.319055
9	1	0	-2.686794	0.838264	-1.523424
10	1	0	0.223499	-0.391483	0.779214
11	8	0	-1.140785	1.536582	-0.353370
12	6	0	-3.401149	1.960712	0.160006
13	1	0	-3.128363	2.149804	1.198441
14	1	0	-4.414862	1.566549	0.102366
15	8	0	-3.373788	3.171728	-0.580556
16	8	0	-3.727028	-0.978248	-0.020586
17	8	0	-1.353643	-2.464531	0.448311
18	7	0	1.094063	1.547608	-0.979992
19	6	0	-2.687801	4.211123	-0.045264
20	8	0	-2.224181	4.205082	1.056242
21	6	0	-2.601499	5.342240	-1.025729
22	1	0	-3.572670	5.522090	-1.483111
23	1	0	-2.239302	6.231749	-0.520183
24	1	0	-1.905762	5.060748	-1.817248
25	6	0	-4.383174	-1.566227	1.012641
26	8	0	-3.988515	-1.553573	2.140044
27	6	0	-5.649731	-2.205542	0.527880
28	1	0	-5.414249	-2.947016	-0.235295
29	1	0	-6.161378	-2.670690	1.364124
30	1	0	-6.286619	-1.450898	0.066808
31	6	0	-1.186941	-3.633542	-0.216234
32	8	0	-1.088985	-3.705987	-1.407381
33	6	0	-1.137591	-4.782336	0.742742
34	1	0	-0.187082	-4.744274	1.276538
35	1	0	-1.935414	-4.694288	1.478286
36	1	0	-1.209092	-5.715490	0.193295
37	6	0	2.327052	-1.251529	-0.850051
38	7	0	1.432110	1.913382	0.151529
39	7	0	1.822145	2.285956	1.126459
40	7	0	0.967535	-1.462668	-0.872517
41	1	0	0.670568	-1.932789	-1.718504
42	7	0	2.778558	-0.731060	0.324979
43	6	0	4.046126	-0.156946	0.573535
44	6	0	4.619816	0.721797	-0.339490
45	6	0	4.674920	-0.413544	1.784985
46	6	0	5.828109	1.325319	-0.036878
47	1	0	4.114003	0.923208	-1.273680
48	6	0	5.879839	0.205709	2.083979
49	1	0	4.222770	-1.102286	2.488795
50	6	0	6.463680	1.071884	1.172638
51	1	0	6.271969	2.008058	-0.749733
52	1	0	6.363992	0.002663	3.030268
53	1	0	7.405995	1.550715	1.403063
54	1	0	2.193640	-0.859536	1.136356
55	16	0	3.271125	-1.680283	-2.133748

Structure 15 (Z,Z) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1936.4119175

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.732539	-1.203442	-0.766713
2	6	0	0.013233	-0.007866	-0.119998
3	6	0	0.827752	1.253612	-0.396380
4	6	0	2.256829	1.076982	0.078284
5	6	0	2.852691	-0.182525	-0.553211
6	1	0	0.754880	-1.077367	-1.854333
7	1	0	0.830523	1.473628	-1.468012
8	1	0	2.287227	1.003693	1.166872
9	1	0	2.896259	-0.045503	-1.643004
10	1	0	-0.040996	-0.177944	0.957691
11	8	0	2.037168	-1.297887	-0.248289
12	6	0	4.238676	-0.487942	-0.028458
13	1	0	4.209449	-0.682861	1.042432
14	1	0	4.914586	0.340810	-0.234633
15	8	0	4.749294	-1.619659	-0.728249
16	8	0	2.983111	2.22523	-0.358706
17	8	0	0.269874	2.358713	0.307378
18	7	0	0.048585	-2.465082	-0.538461
19	6	0	4.770395	-2.806683	-0.089776
20	8	0	4.493469	-2.945506	1.069634
21	6	0	5.182741	-3.901469	-1.023119
22	1	0	6.088431	-3.618935	-1.558768
23	1	0	5.340015	-4.820576	-0.466437
24	1	0	4.391262	-4.048677	-1.760042
25	6	0	3.882491	2.771501	0.486833
26	8	0	4.134346	2.309466	1.565332
27	6	0	4.503633	3.991687	-0.113005
28	1	0	3.726372	4.717862	-0.352176
29	1	0	5.217255	4.418914	0.585141
30	1	0	5.004553	3.722096	-1.043733
31	6	0	-0.575587	3.174015	-0.351314
32	8	0	-0.890988	3.007594	-1.501123
33	6	0	-1.052912	4.278969	0.533290
34	1	0	-1.596960	3.848181	1.375207
35	1	0	-0.198225	4.823561	0.935118
36	1	0	-1.699284	4.945905	-0.029157
37	6	0	-2.460851	-0.235045	-0.001807
38	7	0	0.149677	-2.876837	0.621308
39	7	0	0.196658	-3.342048	1.631649
40	7	0	-1.323960	0.153262	-0.627165
41	1	0	-1.411807	0.664332	-1.496760
42	7	0	-3.567195	-0.017708	-0.756668
43	1	0	-4.858920	0.740336	1.474904
44	1	0	-5.273422	-1.292331	-2.264299
45	1	0	-7.245164	0.346200	1.955020
46	1	0	-7.674459	-1.658033	-1.805563
47	1	0	-8.665729	-0.854932	0.319456
48	1	0	-3.410854	0.188772	-1.734931
49	16	0	-2.480973	-0.921575	1.526663
50	6	0	-5.475415	0.204984	0.767638
51	6	0	-6.818705	-0.017749	1.028653
52	6	0	-7.617140	-0.687383	0.109538
53	6	0	-7.062467	-1.136723	-1.080400
54	6	0	-5.715642	-0.930449	-1.343374
55	6	0	-4.919924	-0.263638	-0.418190

Structure 15 (Z,E) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1936.4156339

No imaginary frequencies

Standard orientation:						
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)			
			X	Y	Z	
1	6	0	0.571705	-1.326958	-0.328509	
2	6	0	-0.184869	-0.276886	0.501491	
3	6	0	0.236666	1.114090	0.036834	
4	6	0	1.744777	1.261014	0.087456	
5	6	0	2.397411	0.124898	-0.700865	
6	1	0	0.271386	-1.257351	-1.379413	
7	1	0	-0.106893	1.290095	-0.986469	
8	1	0	2.091606	1.247986	1.122297	
9	1	0	2.109215	0.213023	-1.757837	
10	1	0	0.082977	-0.404510	1.552949	
11	8	0	1.956270	-1.119867	-0.190867	
12	6	0	3.905674	0.142444	-0.586003	
13	1	0	4.212396	-0.004456	0.448524	
14	1	0	4.305469	1.084245	-0.958975	
15	8	0	4.435393	-0.888397	-1.416032	
16	8	0	2.056978	2.511231	-0.520485	
17	8	0	-0.324012	2.100413	0.897013	
18	7	0	0.261167	-2.689700	0.070855	
19	6	0	4.910912	-2.002148	-0.824785	
20	8	0	5.016272	-2.133860	0.363638	
21	6	0	5.279873	-3.029411	-1.848931	
22	1	0	5.884698	-2.579390	-2.635358	
23	1	0	5.815231	-3.845761	-1.373118	
24	1	0	4.364085	-3.409042	-2.305827	
25	6	0	3.001798	3.286862	0.054746	
26	8	0	3.640361	2.941295	1.010377	
27	6	0	3.125583	4.594206	-0.659427	
28	1	0	2.178995	5.131430	-0.587988	
29	1	0	3.923189	5.180184	-0.212832	
30	1	0	3.329317	4.417732	-1.715759	
31	6	0	-1.472362	2.697426	0.521315	
32	8	0	-2.041969	2.443274	-0.507455	
33	6	0	-1.924327	3.681110	1.550722	
34	1	0	-2.178521	3.138168	2.462918	
35	1	0	-1.114948	4.370412	1.789448	
36	1	0	-2.793299	4.220789	1.186503	
37	6	0	-2.428969	-0.985538	1.274726	
38	7	0	0.743618	-3.002989	1.164115	
39	7	0	1.148418	-3.387606	2.126929	
40	7	0	-1.612156	-0.421556	0.366444	
41	1	0	-2.031716	0.014640	-0.445638	
42	7	0	-3.735875	-1.068237	0.930500	
43	6	0	-4.343187	-0.782554	-0.319042	
44	6	0	-3.828477	-1.296162	-1.507442	
45	6	0	-5.509960	-0.024783	-0.335705	
46	6	0	-4.469965	-1.023933	-2.707121	
47	1	0	-2.944316	-1.921773	-1.486397	
48	6	0	-6.155515	0.224352	-1.537290	
49	1	0	-5.902595	0.365672	0.595384	
50	6	0	-5.633617	-0.266237	-2.727106	
51	1	0	-4.067064	-1.424718	-3.628734	
52	1	0	-7.064499	0.812291	-1.542971	
53	1	0	-6.134835	-0.064615	-3.664990	
54	1	0	-4.343670	-1.361179	1.681624	
55	16	0	-1.923479	-1.545421	2.779430	

Structure 15 (E,Z) (M06-2X/def2-TZVP, CHCl₃)

Energy (Hartrees): = -1936.4086464

No imaginary frequencies

Standard orientation:						
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)			
			X	Y	Z	
1	6	0	-0.202467	0.802000	-1.039145	
2	6	0	0.007844	-0.546052	-0.320894	
3	6	0	-1.312744	-1.308912	-0.355184	
4	6	0	-2.435597	-0.469262	0.225228	
5	6	0	-2.491299	0.885989	-0.475368	
6	1	0	-0.454614	0.624040	-2.088992	
7	1	0	-1.559183	-1.570777	-1.387627	
8	1	0	-2.286165	-0.333206	1.297842	
9	1	0	-2.755191	0.737393	-1.531159	
10	1	0	0.248186	-0.339505	0.725614	
11	8	0	-1.225229	1.514596	-0.387002	
12	6	0	-3.499259	1.802092	0.180697	
13	1	0	-3.226774	1.987634	1.219197	
14	1	0	-4.492064	1.356329	0.131630	
15	8	0	-3.556013	3.027218	-0.542898	
16	8	0	-3.662419	-1.148241	-0.016557	
17	8	0	-1.215383	-2.495241	0.421799	
18	7	0	0.993344	1.631118	-1.068721	
19	6	0	-2.935205	4.102926	-0.018096	
20	8	0	-2.436484	4.117163	1.073718	
21	6	0	-2.957020	5.249672	-0.978954	
22	1	0	-3.956805	5.379681	-1.391319	
23	1	0	-2.627971	6.155229	-0.477827	
24	1	0	-2.280996	5.022234	-1.805386	
25	6	0	-4.335067	-1.669936	1.035798	
26	8	0	-3.972217	-1.554895	2.172797	
27	6	0	-5.571500	-2.371763	0.574020	
28	1	0	-5.317701	-3.100801	-0.195272	
29	1	0	-6.052968	-2.858453	1.416754	
30	1	0	-6.250567	-1.642258	0.129550	
31	6	0	-1.008852	-3.665359	-0.223639	
32	8	0	-0.899341	-3.746072	-1.416883	
33	6	0	-0.929010	-4.800395	0.743878	
34	1	0	0.007589	-4.716658	1.298502	
35	1	0	-1.747859	-4.744270	1.460175	
36	1	0	-0.948863	-5.742536	0.204313	
37	6	0	2.380383	-1.149179	-0.836574	
38	7	0	1.350592	2.019400	0.046140	
39	7	0	1.753306	2.417455	1.005996	
40	7	0	1.038897	-1.349163	-0.943278	
41	1	0	0.769696	-1.839384	-1.786742	
42	7	0	2.780982	-0.567457	0.320284	
43	6	0	4.057981	-0.016853	0.590048	
44	6	0	4.631236	0.890465	-0.295534	
45	6	0	4.691637	-0.322247	1.787299	
46	6	0	5.848998	1.471912	0.013578	
47	1	0	4.116139	1.134234	-1.215448	
48	6	0	5.906776	0.275940	2.095471	
49	1	0	4.234451	-1.027338	2.471306	
50	6	0	6.491820	1.167967	1.208810	
51	1	0	6.292409	2.176518	-0.678620	
52	1	0	6.398224	0.036713	3.029998	
53	1	0	7.440928	1.630221	1.447868	
54	1	0	2.163715	-0.643080	1.117558	
55	16	0	3.410706	-1.651981	-2.051455	

Structure 25 (min 1) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -2435.0854761

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.528877	-1.381818	0.784478
2	6	0	-0.568618	-0.320331	0.219420
3	6	0	-1.138634	1.079630	0.456361
4	6	0	-2.567023	1.179979	-0.046993
5	6	0	-3.399362	0.043268	0.542571
6	1	0	-1.583561	-1.294431	1.876951
7	1	0	-1.119433	1.327136	1.524620
8	1	0	-2.579092	1.142758	-1.139292
9	1	0	-3.444731	0.153542	1.636772
10	1	0	-0.462025	-0.487860	-0.856870
11	8	0	-2.806995	-1.196538	0.210936
12	6	0	-4.808617	0.029014	-0.014177
13	1	0	-4.783046	-0.126489	-1.094007
14	1	0	-5.314368	0.963363	0.226879
15	8	0	-5.531910	-1.022223	0.613371
16	8	0	-3.127432	2.411895	0.404584
17	8	0	-0.376810	2.053979	-0.256725
18	7	0	-1.083006	-2.735024	0.532676
19	6	0	-5.688864	-2.168785	-0.099095
20	8	0	-5.405254	-2.279121	-1.253934
21	6	0	-6.260212	-3.247367	0.775527
22	1	0	-7.096146	-2.859810	1.356830
23	1	0	-6.570043	-4.085618	0.157453
24	1	0	-5.484950	-3.570688	1.472914
25	6	0	-3.201538	3.439095	-0.487269
26	8	0	-2.878154	3.346295	-1.632244
27	6	0	-3.743235	4.668001	0.184966
28	1	0	-3.051467	4.985550	0.966691
29	1	0	-3.863918	5.455811	-0.553400
30	1	0	-4.697296	4.439721	0.660834
31	6	0	0.690060	2.619831	0.340698
32	8	0	1.064736	2.331844	1.448693
33	6	0	1.325787	3.626101	-0.569302
34	1	0	1.832245	3.087981	-1.373746
35	1	0	0.560060	4.258012	-1.018731
36	1	0	2.048540	4.214404	-0.009792
37	6	0	1.877208	-0.724493	0.152350
38	7	0	-1.151188	-3.059823	-0.664347
39	7	0	-1.186344	-3.472942	-1.701981
40	7	0	0.736971	-0.412018	0.826066
41	1	0	0.854298	0.133290	1.670821
42	7	0	2.996264	-0.340533	0.847786
43	1	0	6.989505	1.198466	-0.750731
44	1	0	6.618004	-3.013496	-0.004003
45	1	0	7.974838	-1.090677	-0.757659
46	1	0	2.876360	0.461634	1.457997
47	16	0	1.907624	-1.483680	-1.327686
48	6	0	5.102481	0.505226	-0.022995
49	6	0	6.414347	0.339115	-0.432942
50	6	0	6.952665	-0.940030	-0.433289
51	6	0	6.187431	-2.018659	-0.012256
52	6	0	4.871545	-1.857626	0.417398
53	6	0	4.318559	-0.570738	0.397304
54	17	0	4.414286	2.112479	-0.032084
55	6	0	4.072182	-3.042452	0.881082
56	1	0	3.330481	-2.752558	1.626305
57	1	0	3.532122	-3.483263	0.039943
58	1	0	4.730745	-3.798470	1.309747

Structure 25 (min 2) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -2435.0888337

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.967418	-1.463002	-0.263864
2	6	0	0.211545	-0.397150	0.548783
3	6	0	0.619060	1.008240	0.104724
4	6	0	2.133139	1.175301	0.007470
5	6	0	2.747713	-0.002084	-0.746364
6	1	0	0.661964	-1.420054	-1.317434
7	1	0	0.188083	1.247783	-0.874676
8	1	0	2.560323	1.272253	1.009566
9	1	0	2.405107	0.024478	-1.791804
10	1	0	0.458045	-0.525148	1.606318
11	8	0	2.352654	-1.218093	-0.147151
12	6	0	4.262372	0.039923	-0.721538
13	1	0	4.622852	-0.036364	0.305594
14	1	0	4.617268	0.959112	-1.185795
15	8	0	4.754237	-1.048601	-1.493301
16	8	0	2.436555	2.336743	-0.771117
17	8	0	0.086426	1.899177	1.083407
18	7	0	0.676299	-2.815169	0.158476
19	6	0	5.190755	-2.138099	-0.808768
20	8	0	5.341252	-2.163848	0.375904
21	6	0	5.446283	-3.275709	-1.754847
22	1	0	6.018622	-2.930346	-2.615267
23	1	0	5.971452	-4.069345	-1.230400
24	1	0	4.484377	-3.644978	-2.115914
25	6	0	2.543220	3.528362	-0.134456
26	8	0	2.495507	3.644568	1.057238
27	6	0	2.675005	4.643466	-1.126300
28	1	0	1.685335	4.799877	-1.562652
29	1	0	3.001868	5.545588	-0.616086
30	1	0	3.362767	4.371431	-1.925572
31	6	0	-0.363271	3.107487	0.681051
32	8	0	-0.425123	3.440016	-0.471843
33	6	0	-0.722501	3.952496	1.864238
34	1	0	-1.240766	3.360836	2.617997
35	1	0	0.216715	4.308081	2.295850
36	1	0	-1.323556	4.798564	1.540347
37	6	0	-2.053384	-1.052189	1.335282
38	7	0	1.154689	-3.097981	1.269588
39	7	0	1.551247	-3.474417	2.243631
40	7	0	-1.217301	-0.530984	0.405407
41	1	0	-1.615880	-0.260696	-0.485369
42	7	0	-3.376055	-0.995475	0.997712
43	1	0	-5.223975	-1.252048	-3.189834
44	1	0	-4.401952	2.644129	-1.578706
45	1	0	-5.238374	1.223080	-3.421407
46	1	0	-3.984387	-1.543895	1.588295
47	16	0	-1.567789	-1.683636	2.802229
48	6	0	-4.361872	-1.188149	-1.232128
49	6	0	-4.860076	-0.615158	-2.394586
50	6	0	-4.862540	0.767084	-2.513692
51	6	0	-4.391267	1.565250	-1.477609
52	6	0	-3.915711	1.002319	-0.295894
53	6	0	-3.891691	-0.397704	-0.180814
54	17	0	-4.314818	-2.918682	-1.084439
55	6	0	-3.468615	1.861312	0.856843
56	1	0	-4.158264	1.751765	1.697480
57	1	0	-2.480150	1.567974	1.215223
58	1	0	-3.438655	2.910195	0.560059

Structure 25 (max 1) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -2435.0676817

Imaginary frequency -32.49

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.667021	-1.311793	0.753016
2	6	0	-0.438946	-0.791791	-0.010103
3	6	0	-0.395916	0.734028	0.059686
4	6	0	-1.718203	1.375418	-0.342600
5	6	0	-2.870298	0.684166	0.388128
6	1	0	-1.582623	-1.054422	1.816228
7	1	0	-0.164392	1.060426	1.081463
8	1	0	-1.842986	1.329120	-1.428232
9	1	0	-2.788446	0.906576	1.462592
10	1	0	-0.510749	-1.116926	-1.052822
11	8	0	-2.814361	-0.713542	0.187730
12	6	0	-4.219678	1.156628	-0.113254
13	1	0	-4.343770	0.891863	-1.164652
14	1	0	-4.310152	2.233267	0.025499
15	8	0	-5.233539	0.536917	0.667975
16	8	0	-1.744687	2.734254	0.102103
17	8	0	0.658179	1.137016	-0.807966
18	7	0	-1.804810	-2.751070	0.720248
19	6	0	-5.866735	-0.530566	0.115655
20	8	0	-5.733598	-0.867799	-1.022526
21	6	0	-6.734563	-1.204992	1.138721
22	1	0	-7.292108	-0.464313	1.710611
23	1	0	-7.404572	-1.900531	0.640706
24	1	0	-6.088082	-1.749539	1.829927
25	6	0	-1.210775	3.685512	-0.704163
26	8	0	-0.824758	3.464012	-1.816098
27	6	0	-1.141119	5.000673	0.010395
28	1	0	-0.303519	4.940862	0.709706
29	1	0	-0.965018	5.794581	-0.710582
30	1	0	-2.051332	5.181036	0.580284
31	6	0	1.447545	2.166356	-0.421802
32	8	0	1.328840	2.723800	0.635445
33	6	0	2.418405	2.510169	-1.506376
34	1	0	2.899703	1.605268	-1.877242
35	1	0	1.846575	2.962652	-2.320211
36	1	0	3.155953	3.210946	-1.123986
37	6	0	1.594568	-2.238389	0.021473
38	7	0	-2.137766	-3.188725	-0.392660
39	7	0	-2.451371	-3.697111	-1.337007
40	7	0	0.811308	-1.268383	0.534168
41	1	0	1.229649	-0.687926	1.250202
42	7	0	2.918808	-2.241356	0.601080
43	1	0	4.665184	1.857011	1.834055
44	1	0	5.732309	0.248943	-2.000117
45	1	0	5.911843	2.052106	-0.316601
46	1	0	2.879360	-2.494047	1.583170
47	16	0	1.138562	-3.308386	-1.135543
48	6	0	3.817205	-0.033954	1.301664
49	6	0	4.602303	1.086844	1.076871
50	6	0	5.288505	1.187388	-0.124108
51	6	0	5.180769	0.175564	-1.069290
52	6	0	4.391981	-0.952368	-0.850320
53	6	0	3.689242	-1.066371	0.363797
54	17	0	2.991319	-0.150528	2.847916
55	6	0	4.321681	-2.041237	-1.884267
56	1	0	4.201774	-3.015326	-1.410428
57	1	0	3.458028	-1.903595	-2.539301
58	1	0	5.222445	-2.033344	-2.498988

Structure 25 (min 1) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -2435.1230361

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.358700	-1.330046	0.770512
2	6	0	-0.508627	-0.185113	0.189449
3	6	0	-1.216751	1.140664	0.462439
4	6	0	-2.645801	1.106470	-0.048826
5	6	0	-3.370328	-0.111402	0.520940
6	1	0	-1.415481	-1.242069	1.861134
7	1	0	-1.229097	1.350244	1.537262
8	1	0	-2.655624	1.084318	-1.140890
9	1	0	-3.445480	-0.014264	1.613389
10	1	0	-0.416669	-0.331327	-0.890488
11	8	0	-2.646414	-1.286164	0.195505
12	6	0	-4.755307	-0.258168	-0.071724
13	1	0	-4.691040	-0.411738	-1.149617
14	1	0	-5.351344	0.626746	0.150010
15	8	0	-5.406723	-1.366182	0.547474
16	8	0	-3.312023	2.275102	0.426050
17	8	0	-0.555791	2.208731	-0.214399
18	7	0	-0.779589	-2.639892	0.515818
19	6	0	-5.446447	-2.531546	-0.137307
20	8	0	-5.077219	-2.651287	-1.271714
21	6	0	-6.014558	-3.622446	0.719207
22	1	0	-6.943095	-3.288275	1.183143
23	1	0	-6.185270	-4.510307	0.115462
24	1	0	-5.301948	-3.847504	1.515820
25	6	0	-3.541344	3.285185	-0.452589
26	8	0	-3.286134	3.214822	-1.620473
27	6	0	-4.143353	4.461361	0.252248
28	1	0	-3.424822	4.848920	0.977628
29	1	0	-4.391955	5.231821	-0.473245
30	1	0	-5.034627	4.150239	0.799119
31	6	0	0.378985	2.913138	0.457780
32	8	0	0.703788	2.664761	1.590222
33	6	0	0.920318	4.017613	-0.392864
34	1	0	1.331852	3.596281	-1.311679
35	1	0	0.104842	4.686970	-0.674233
36	1	0	1.685774	4.562276	0.154281
37	6	0	1.949794	-0.559654	0.158329
38	7	0	-0.872910	-2.991408	-0.667924
39	7	0	-0.920221	-3.415479	-1.701248
40	7	0	0.813327	-0.153860	0.767624
41	1	0	0.902823	0.357055	1.639237
42	7	0	3.062768	-0.348855	0.906904
43	1	0	6.906949	1.206649	-1.040702
44	1	0	6.786026	-2.911753	0.178699
45	1	0	8.003786	-1.014311	-0.839189
46	1	0	2.964004	0.196751	1.756779
47	16	0	1.999598	-1.265217	-1.370074
48	6	0	5.087384	0.518659	-0.139831
49	6	0	6.387675	0.367030	-0.597069
50	6	0	6.990356	-0.878508	-0.480747
51	6	0	6.304583	-1.944387	0.090705
52	6	0	5.000251	-1.794602	0.557056
53	6	0	4.387099	-0.543569	0.428603
54	17	0	4.308369	2.074916	-0.285215
55	6	0	4.249501	-2.935822	1.182258
56	1	0	3.941514	-2.687680	2.201008
57	1	0	3.344296	-3.159106	0.611628
58	1	0	4.870877	-3.830978	1.214343

Structure 25 (min 2) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -2435.1275939

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.945304	-1.457155	-0.245203
2	6	0	0.196334	-0.386179	0.564551
3	6	0	0.606402	1.010256	0.096910
4	6	0	2.122654	1.164053	0.020241
5	6	0	2.742668	-0.018084	-0.725375
6	1	0	0.636391	-1.420973	-1.295782
7	1	0	0.183424	1.222772	-0.890438
8	1	0	2.537843	1.250822	1.027655
9	1	0	2.413477	0.004533	-1.773740
10	1	0	0.450987	-0.500340	1.620722
11	8	0	2.331715	-1.233839	-0.125807
12	6	0	4.255196	0.025356	-0.670179
13	1	0	4.598438	-0.066965	0.360708
14	1	0	4.617448	0.954597	-1.107790
15	8	0	4.775196	-1.041370	-1.461813
16	8	0	2.452007	2.323086	-0.752346
17	8	0	0.064975	1.923781	1.052629
18	7	0	0.642682	-2.807095	0.201433
19	6	0	5.222642	-2.142051	-0.816677
20	8	0	5.315377	-2.224240	0.376131
21	6	0	5.582729	-3.214610	-1.799758
22	1	0	6.232224	-2.807843	-2.575601
23	1	0	6.072622	-4.035391	-1.281966
24	1	0	4.668947	-3.572204	-2.279168
25	6	0	2.587357	3.508179	-0.114754
26	8	0	2.489566	3.626879	1.076372
27	6	0	2.842526	4.610609	-1.092817
28	1	0	1.925740	4.773637	-1.664419
29	1	0	3.110904	5.517800	-0.557231
30	1	0	3.630895	4.325194	-1.789618
31	6	0	-0.372141	3.126167	0.620762
32	8	0	-0.394310	3.439762	-0.540593
33	6	0	-0.777256	3.990951	1.771987
34	1	0	-1.333318	3.417350	2.513298
35	1	0	0.139521	4.354706	2.243713
36	1	0	-1.360258	4.834361	1.409333
37	6	0	-2.078595	-1.030573	1.336284
38	7	0	1.133795	-3.079190	1.305024
39	7	0	1.544403	-3.437995	2.280998
40	7	0	-1.232971	-0.525348	0.417242
41	1	0	-1.616378	-0.266245	-0.485863
42	7	0	-3.390521	-0.996968	0.991330
43	1	0	-5.197811	-1.287689	-3.217526
44	1	0	-4.534383	2.623816	-1.569581
45	1	0	-5.311443	1.184160	-3.424902
46	1	0	-4.020715	-1.479365	1.618633
47	16	0	-1.599251	-1.639782	2.834804
48	6	0	-4.346069	-1.205121	-1.251552
49	6	0	-4.859781	-0.646678	-2.413591
50	6	0	-4.917999	0.736413	-2.520275
51	6	0	-4.480508	1.545135	-1.477381
52	6	0	-3.980902	0.992723	-0.299615
53	6	0	-3.911149	-0.405652	-0.192335
54	17	0	-4.242773	-2.939308	-1.112396
55	6	0	-3.543906	1.857686	0.850457
56	1	0	-4.180932	1.686654	1.722290
57	1	0	-2.520915	1.624631	1.154230
58	1	0	-3.598511	2.911874	0.578043

Structure 25 (min 1) (M06-2X/ def2-TZVP, gas phase)

Energy (Hartrees): = -2435.2920199

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.406395	-1.336980	0.796520
2	6	0	-0.478643	-0.260537	0.213409
3	6	0	-1.091660	1.119649	0.440722
4	6	0	-2.517453	1.177761	-0.068098
5	6	0	-3.321706	0.017502	0.520106
6	1	0	-1.466437	-1.223533	1.885693
7	1	0	-1.084840	1.366727	1.507500
8	1	0	-2.532835	1.127949	-1.158646
9	1	0	-3.381064	0.145557	1.611443
10	1	0	-0.375152	-0.441666	-0.860170
11	8	0	-2.684584	-1.204473	0.218791
12	6	0	-4.724072	-0.060189	-0.046691
13	1	0	-4.690240	-0.244622	-1.119672
14	1	0	-5.265410	0.863765	0.149390
15	8	0	-5.420805	-1.105497	0.618177
16	8	0	-3.059493	2.420653	0.371332
17	8	0	-0.344289	2.107465	-0.265877
18	7	0	-0.920527	-2.682237	0.582506
19	6	0	-5.603151	-2.263974	-0.060021
20	8	0	-5.326634	-2.413278	-1.212670
21	6	0	-6.197291	-3.306885	0.840008
22	1	0	-7.060172	-2.901351	1.365809
23	1	0	-6.477039	-4.174543	0.251158
24	1	0	-5.453725	-3.589631	1.585950
25	6	0	-3.857334	3.101026	-0.484793
26	8	0	-4.186091	2.678458	-1.554345
27	6	0	-4.262916	4.418416	0.104611
28	1	0	-3.373709	5.007658	0.326485
29	1	0	-4.902686	4.945260	-0.595729
30	1	0	-4.787774	4.249354	1.044681
31	6	0	0.666440	2.730168	0.367387
32	8	0	0.989265	2.491537	1.502024
33	6	0	1.319813	3.733449	-0.530905
34	1	0	1.779307	3.205539	-1.367348
35	1	0	0.571117	4.413300	-0.935192
36	1	0	2.076114	4.278434	0.025179
37	6	0	1.969366	-0.643110	0.149460
38	7	0	-0.985462	-3.049701	-0.598534
39	7	0	-1.016239	-3.489013	-1.620341
40	7	0	0.832107	-0.299182	0.807046
41	1	0	0.942639	0.256141	1.644499
42	7	0	3.091260	-0.266327	0.838910
43	1	0	7.030733	1.288865	-0.855291
44	1	0	6.734402	-2.901055	0.000348
45	1	0	8.046624	-0.980686	-0.821945
46	1	0	2.979591	0.529652	1.455580
47	16	0	1.999113	-1.425136	-1.311565
48	6	0	5.166197	0.589691	-0.081691
49	6	0	6.472379	0.430955	-0.508188
50	6	0	7.028272	-0.837056	-0.485834
51	6	0	6.287854	-1.914863	-0.026812
52	6	0	4.979245	-1.762639	0.418398
53	6	0	4.409204	-0.486674	0.375282
54	17	0	4.454273	2.173925	-0.116372
55	6	0	4.202335	-2.938479	0.929303
56	1	0	3.572989	-2.656261	1.773395
57	1	0	3.542024	-3.322520	0.149725
58	1	0	4.877271	-3.733967	1.240922

Structure 25 (min 2) (M06-2X/ def2-TZVP, gas phase)

Energy (Hartrees): = -2435.2929242

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.931484	-1.463692	-0.246757
2	6	0	0.186372	-0.389918	0.560718
3	6	0	0.621434	1.004220	0.115138
4	6	0	2.136642	1.148722	0.032586
5	6	0	2.747285	-0.041319	-0.703822
6	1	0	0.635915	-1.407990	-1.301852
7	1	0	0.205688	1.237440	-0.871607
8	1	0	2.552489	1.240415	1.039028
9	1	0	2.432022	-0.005295	-1.756734
10	1	0	0.423685	-0.525015	1.618750
11	8	0	2.317224	-1.249120	-0.119393
12	6	0	4.258329	-0.020872	-0.636252
13	1	0	4.587424	-0.156183	0.394220
14	1	0	4.635740	0.920361	-1.032951
15	8	0	4.766526	-1.067407	-1.451305
16	8	0	2.465726	2.300373	-0.743736
17	8	0	0.091860	1.911895	1.075872
18	7	0	0.610259	-2.812738	0.161464
19	6	0	5.313112	-2.137475	-0.826288
20	8	0	5.505447	-2.194349	0.351938
21	6	0	5.635524	-3.214467	-1.819034
22	1	0	6.195264	-2.798199	-2.655102
23	1	0	6.200999	-3.999956	-1.328112
24	1	0	4.701800	-3.619039	-2.210924
25	6	0	2.598458	3.491530	-0.118873
26	8	0	2.543508	3.621899	1.070955
27	6	0	2.784930	4.592223	-1.115694
28	1	0	1.819177	4.762863	-1.595065
29	1	0	3.108570	5.493589	-0.604850
30	1	0	3.498331	4.299364	-1.883515
31	6	0	-0.339206	3.119694	0.663522
32	8	0	-0.382146	3.448961	-0.491114
33	6	0	-0.715246	3.971903	1.833966
34	1	0	-1.263060	3.389187	2.572319
35	1	0	0.214226	4.313830	2.294072
36	1	0	-1.294648	4.825359	1.495021
37	6	0	-2.088288	-1.009449	1.334741
38	7	0	1.065976	-3.116704	1.272370
39	7	0	1.442765	-3.501383	2.245762
40	7	0	-1.241141	-0.502016	0.410207
41	1	0	-1.632823	-0.208937	-0.474753
42	7	0	-3.406894	-0.945182	0.989637
43	1	0	-5.272654	-1.290756	-3.174382
44	1	0	-4.411479	2.631728	-1.669963
45	1	0	-5.260524	1.173707	-3.472684
46	1	0	-4.013491	-1.499119	1.574947
47	16	0	-1.621174	-1.647957	2.796920
48	6	0	-4.402490	-1.185063	-1.225693
49	6	0	-4.898541	-0.637382	-2.398762
50	6	0	-4.887324	0.738240	-2.555053
51	6	0	-4.407851	1.556667	-1.542489
52	6	0	-3.935888	1.021216	-0.349537
53	6	0	-3.918582	-0.372778	-0.200131
54	17	0	-4.381947	-2.901108	-1.031257
55	6	0	-3.492781	1.908164	0.779722
56	1	0	-4.195983	1.835489	1.611907
57	1	0	-2.516397	1.614689	1.166402
58	1	0	-3.444565	2.945804	0.452606

Structure 25 (min 1) (M06-2X/ def2-TZVP, CHCl₃)

Energy (Hartrees): = -2435.3289242

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.288488	-1.294589	0.768414
2	6	0	-0.445984	-0.154601	0.175244
3	6	0	-1.159424	1.169652	0.434611
4	6	0	-2.590145	1.129160	-0.065992
5	6	0	-3.305015	-0.091907	0.513597
6	1	0	-1.341653	-1.192201	1.857255
7	1	0	-1.165104	1.387380	1.506610
8	1	0	-2.609054	1.095627	-1.156882
9	1	0	-3.371378	0.020875	1.604831
10	1	0	-0.353927	-0.315710	-0.901843
11	8	0	-2.575808	-1.262852	0.201361
12	6	0	-4.694112	-0.265644	-0.060679
13	1	0	-4.647014	-0.427364	-1.136545
14	1	0	-5.305947	0.608801	0.154631
15	8	0	-5.320314	-1.372029	0.583936
16	8	0	-3.215800	2.321653	0.401983
17	8	0	-0.493572	2.224653	-0.253650
18	7	0	-0.707303	-2.605869	0.532108
19	6	0	-5.392707	-2.539658	-0.085478
20	8	0	-5.053598	-2.675450	-1.228548
21	6	0	-5.953035	-3.615942	0.790747
22	1	0	-6.876157	-3.273881	1.257825
23	1	0	-6.131966	-4.512424	0.204608
24	1	0	-5.235605	-3.830120	1.584719
25	6	0	-4.052039	2.980373	-0.429601
26	8	0	-4.352826	2.569646	-1.516226
27	6	0	-4.534529	4.248853	0.197065
28	1	0	-3.679873	4.874687	0.455718
29	1	0	-5.190812	4.771323	-0.492295
30	1	0	-5.067801	4.016285	1.119812
31	6	0	0.407315	2.964146	0.420187
32	8	0	0.701271	2.759671	1.569978
33	6	0	0.958571	4.051351	-0.442854
34	1	0	1.348153	3.623773	-1.366696
35	1	0	0.151591	4.735561	-0.709904
36	1	0	1.738867	4.586192	0.090309
37	6	0	2.013776	-0.509791	0.147193
38	7	0	-0.784597	-2.972473	-0.644589
39	7	0	-0.820168	-3.401755	-1.671181
40	7	0	0.874092	-0.103747	0.748692
41	1	0	0.960017	0.416373	1.613244
42	7	0	3.123041	-0.272498	0.888370
43	1	0	6.973170	1.252501	-1.053235
44	1	0	6.832214	-2.851167	0.188545
45	1	0	8.059262	-0.968071	-0.836399
46	1	0	3.018848	0.285518	1.727646
47	16	0	2.070062	-1.242126	-1.358413
48	6	0	5.150579	0.579889	-0.154130
49	6	0	6.449680	0.418487	-0.606164
50	6	0	7.046484	-0.825669	-0.481540
51	6	0	6.355908	-1.883069	0.093534
52	6	0	5.054023	-1.725399	0.555908
53	6	0	4.447296	-0.474678	0.419719
54	17	0	4.383763	2.128228	-0.312689
55	6	0	4.302556	-2.859655	1.185539
56	1	0	4.005665	-2.611767	2.206564
57	1	0	3.391455	-3.075917	0.623699
58	1	0	4.917555	-3.757924	1.211720

Structure 25 (min 2) (M06-2X/ def2-TZVP, CHCl₃)

Energy (Hartrees): = -2435.3312857

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.921667	-1.448120	-0.241045
2	6	0	0.183563	-0.373959	0.569701
3	6	0	0.612188	1.014783	0.101257
4	6	0	2.127960	1.154358	0.027438
5	6	0	2.743467	-0.036236	-0.706749
6	1	0	0.615319	-1.400937	-1.291277
7	1	0	0.195420	1.222224	-0.888959
8	1	0	2.539749	1.237957	1.035600
9	1	0	2.433431	-0.005335	-1.760020
10	1	0	0.436847	-0.495894	1.624624
11	8	0	2.307804	-1.245786	-0.119912
12	6	0	4.252939	-0.010506	-0.620242
13	1	0	4.572195	-0.130226	0.414290
14	1	0	4.633829	0.927600	-1.020556
15	8	0	4.783438	-1.058206	-1.426484
16	8	0	2.469587	2.305948	-0.744823
17	8	0	0.078319	1.939090	1.046287
18	7	0	0.601464	-2.797487	0.192488
19	6	0	5.292344	-2.143222	-0.809763
20	8	0	5.415023	-2.237327	0.380704
21	6	0	5.676572	-3.188689	-1.809398
22	1	0	6.297540	-2.750482	-2.590125
23	1	0	6.204145	-3.996505	-1.311281
24	1	0	4.770679	-3.574410	-2.279737
25	6	0	2.630179	3.489751	-0.118865
26	8	0	2.532874	3.621925	1.071048
27	6	0	2.924936	4.576729	-1.100671
28	1	0	2.035178	4.740167	-1.711201
29	1	0	3.181701	5.488813	-0.570345
30	1	0	3.736295	4.276454	-1.762931
31	6	0	-0.375591	3.129834	0.613062
32	8	0	-0.409559	3.439570	-0.549405
33	6	0	-0.796416	3.991638	1.758595
34	1	0	-1.362066	3.414232	2.488332
35	1	0	0.108502	4.356399	2.249438
36	1	0	-1.376684	4.833495	1.392052
37	6	0	-2.094648	-0.991643	1.342302
38	7	0	1.073024	-3.085045	1.296797
39	7	0	1.467333	-3.448611	2.272370
40	7	0	-1.244753	-0.495599	0.424152
41	1	0	-1.627092	-0.219857	-0.472642
42	7	0	-3.403264	-0.958196	0.992496
43	1	0	-5.198559	-1.346504	-3.205199
44	1	0	-4.573147	2.595833	-1.637080
45	1	0	-5.330155	1.115788	-3.463577
46	1	0	-4.030084	-1.437524	1.623437
47	16	0	-1.625720	-1.601131	2.835055
48	6	0	-4.352420	-1.219318	-1.242900
49	6	0	-4.867161	-0.687371	-2.414615
50	6	0	-4.936262	0.689689	-2.549956
51	6	0	-4.509466	1.520745	-1.524011
52	6	0	-4.009675	0.996713	-0.336464
53	6	0	-3.925175	-0.395558	-0.202019
54	17	0	-4.241052	-2.938774	-1.070845
55	6	0	-3.592953	1.889562	0.795861
56	1	0	-4.249481	1.746849	1.657086
57	1	0	-2.580264	1.661807	1.132139
58	1	0	-3.636681	2.935084	0.494868

Structure 33 (min 1) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1317.3980826

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.703565	-0.048233	-0.097890
2	7	0	2.839480	0.372833	-0.693708
3	1	0	2.803708	0.592368	-1.677305
4	7	0	0.586647	0.137126	-0.891552
5	1	0	-3.471027	1.548866	0.681593
6	1	0	-2.911386	-2.662187	0.055466
7	1	0	-4.351765	-0.779986	0.754659
8	1	0	0.648644	0.923679	-1.526458
9	16	0	1.663473	-0.716446	1.425694
10	6	0	-1.556572	0.923515	-0.038095
11	6	0	-2.858704	0.708431	0.383269
12	6	0	-3.338351	-0.592918	0.421534
13	6	0	-2.526188	-1.649303	0.030261
14	6	0	-1.220729	-1.439049	-0.407016
15	6	0	-0.728033	-0.128484	-0.429274
16	17	0	-0.939539	2.558041	-0.070531
17	6	0	-0.353779	-2.589559	-0.833136
18	1	0	0.262780	-2.314423	-1.690335
19	1	0	0.321745	-2.869231	-0.020912
20	1	0	-0.964862	-3.453169	-1.095891
21	6	0	4.145673	0.264460	-0.071607
22	1	0	4.880032	0.697963	-0.749146
23	1	0	4.156340	0.808200	0.873199
24	1	0	4.398210	-0.778529	0.131598

Structure 33 (min 2) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1317.4029352

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.730877	0.123062	-0.129550
2	7	0	-1.612835	-0.535450	1.038962
3	1	0	-0.686092	-0.657267	1.422407
4	7	0	-0.558212	0.341973	-0.805589
5	1	0	3.674347	1.138869	0.752872
6	1	0	2.564891	-2.924037	-0.084915
7	1	0	4.241108	-1.282115	0.691775
8	1	0	-0.629007	1.026749	-1.544303
9	16	0	-3.190959	0.636146	-0.760747
10	6	0	1.683329	0.815778	0.039325
11	6	0	2.950929	0.404493	0.424089
12	6	0	3.256454	-0.948828	0.388073
13	6	0	2.311041	-1.870981	-0.043189
14	6	0	1.041623	-1.467475	-0.452946
15	6	0	0.721128	-0.100249	-0.396847
16	17	0	1.281643	2.507425	0.099260
17	6	0	0.033830	-2.460658	-0.964790
18	1	0	-0.732790	-2.667265	-0.213490
19	1	0	-0.481702	-2.065583	-1.841679
20	1	0	0.522409	-3.398397	-1.227420
21	6	0	-2.750165	-0.818077	1.895613
22	1	0	-2.396740	-1.395055	2.749094
23	1	0	-3.220030	0.105387	2.240995
24	1	0	-3.495396	-1.393894	1.346929

Structure 33 (max 1) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1317.3860344

Imaginary frequency -73.53

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.733565	-0.517785	-0.037275
2	7	0	-2.476924	-0.046787	-1.038707
3	1	0	-2.020639	0.022216	-1.936563
4	7	0	-0.390473	-0.773955	-0.454487
5	1	0	4.067624	-0.223472	0.154931
6	1	0	1.644213	3.299432	0.374601
7	1	0	3.876297	2.248077	0.481370
8	1	0	-0.147624	-1.715490	-0.165999
9	16	0	-2.297331	-0.839050	1.482845
10	6	0	1.967521	-0.468062	-0.111489
11	6	0	3.109642	0.277823	0.116452
12	6	0	2.996290	1.646284	0.295623
13	6	0	1.740009	2.228538	0.235820
14	6	0	0.576486	1.495074	0.003333
15	6	0	0.682616	0.099010	-0.171536
16	17	0	2.160864	-2.195492	-0.331580
17	6	0	-0.727179	2.255266	-0.063423
18	1	0	-1.182012	2.193591	-1.054045
19	1	0	-1.454631	1.894656	0.665892
20	1	0	-0.537354	3.307083	0.147953
21	6	0	-3.863333	0.341560	-0.892458
22	1	0	-4.223069	0.715420	-1.849127
23	1	0	-4.463889	-0.513563	-0.575865
24	1	0	-3.955468	1.119168	-0.129752

Structure 33 (max 2) (M06-2X/6-311G(d,p), gas phase)

Energy (Hartrees): = -1317.3843777

Imaginary frequency -66.19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.591508	-0.707616	-0.092693
2	7	0	2.306884	-0.101180	-1.036866
3	1	0	1.823166	0.107388	-1.897881
4	7	0	0.275828	-1.048475	-0.553081
5	1	0	-2.127247	2.767978	0.515385
6	1	0	-4.214048	-0.942498	0.037928
7	1	0	-4.263749	1.493895	0.527549
8	1	0	0.125681	-2.017206	-0.300208
9	16	0	2.151685	-1.125503	1.404560
10	6	0	-0.938787	1.066241	0.038231
11	6	0	-2.143949	1.705645	0.310184
12	6	0	-3.327939	0.993538	0.315607
13	6	0	-3.294426	-0.368474	0.042550
14	6	0	-2.102155	-1.023691	-0.225779
15	6	0	-0.882784	-0.306658	-0.226297
16	17	0	0.479187	2.092590	0.039807
17	6	0	-2.103933	-2.500839	-0.523032
18	1	0	-1.625859	-2.714645	-1.483331
19	1	0	-1.574778	-3.068428	0.250699
20	1	0	-3.124949	-2.877381	-0.561179
21	6	0	3.617131	0.462279	-0.793086
22	1	0	3.974780	0.923245	-1.711664
23	1	0	3.560086	1.208343	0.005293
24	1	0	4.306801	-0.321637	-0.476752

Structure 33 (min 1) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1317.423558

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.701360	-0.094968	-0.110880
2	7	0	2.846828	0.221683	-0.729692
3	1	0	2.810776	0.487683	-1.704032
4	7	0	0.589682	0.011501	-0.893710
5	1	0	-3.387963	1.698244	0.639789
6	1	0	-3.067761	-2.552853	0.118498
7	1	0	-4.397213	-0.569486	0.762083
8	1	0	0.692954	0.468498	-1.793236
9	16	0	1.639773	-0.589907	1.501698
10	6	0	-1.505274	0.949487	-0.061715
11	6	0	-2.819210	0.819856	0.362927
12	6	0	-3.373489	-0.451107	0.427575
13	6	0	-2.624574	-1.564901	0.065998
14	6	0	-1.307112	-1.438208	-0.369901
15	6	0	-0.740108	-0.158842	-0.424178
16	17	0	-0.795181	2.544537	-0.137370
17	6	0	-0.497144	-2.640336	-0.764061
18	1	0	-0.038155	-2.501653	-1.745576
19	1	0	0.309650	-2.804594	-0.044621
20	1	0	-1.124095	-3.531845	-0.791853
21	6	0	4.156302	0.152032	-0.108401
22	1	0	4.885520	0.517551	-0.829697
23	1	0	4.192903	0.773703	0.786901
24	1	0	4.405021	-0.874237	0.169483

Structure 33 (min 2) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1317.4273584

No imaginary frequencies

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.713941	0.083000	-0.133242
2	7	0	-1.569662	-0.410865	1.100817
3	1	0	-0.632123	-0.517705	1.466597
4	7	0	-0.571441	0.253381	-0.851068
5	1	0	3.613307	1.265167	0.733685
6	1	0	2.673154	-2.862388	0.006458
7	1	0	4.274706	-1.129316	0.740959
8	1	0	-0.674727	0.741561	-1.730280
9	16	0	-3.217688	0.461563	-0.812855
10	6	0	1.642150	0.841854	0.003542
11	6	0	2.920608	0.496232	0.416534
12	6	0	3.279941	-0.845221	0.419172
13	6	0	2.377556	-1.819225	0.008259
14	6	0	1.096021	-1.478947	-0.422182
15	6	0	0.726660	-0.124495	-0.419534
16	17	0	1.166610	2.519155	0.015102
17	6	0	0.118461	-2.523851	-0.883354
18	1	0	-0.685770	-2.657124	-0.153626
19	1	0	-0.348487	-2.229777	-1.825477
20	1	0	0.618282	-3.482702	-1.019556
21	6	0	-2.673335	-0.646316	2.014585
22	1	0	-2.261938	-1.067692	2.930307
23	1	0	-3.196710	0.283248	2.246518
24	1	0	-3.386059	-1.349718	1.582435

Structure 33 (max 1) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1317.4084235

Imaginary frequency -70.93

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.733565	-0.517785	-0.037275
2	7	0	-2.476924	-0.046787	-1.038707
3	1	0	-2.020639	0.022216	-1.936563
4	7	0	-0.390473	-0.773955	-0.454487
5	1	0	4.067624	-0.223472	0.154931
6	1	0	1.644213	3.299432	0.374601
7	1	0	3.876297	2.248077	0.481370
8	1	0	-0.147624	-1.715490	-0.165999
9	16	0	-2.297331	-0.839050	1.482845
10	6	0	1.967521	-0.468062	-0.111489
11	6	0	3.109642	0.277823	0.116452
12	6	0	2.996290	1.646284	0.295623
13	6	0	1.740009	2.228538	0.235820
14	6	0	0.576486	1.495074	0.003333
15	6	0	0.682616	0.099010	-0.171536
16	17	0	2.160864	-2.195492	-0.331580
17	6	0	-0.727179	2.255266	-0.063423
18	1	0	-1.182012	2.193591	-1.054045
19	1	0	-1.454631	1.894656	0.665892
20	1	0	-0.537354	3.307083	0.147953
21	6	0	-3.863333	0.341560	-0.892458
22	1	0	-4.223069	0.715420	-1.849127
23	1	0	-4.463889	-0.513563	-0.575865
24	1	0	-3.955468	1.119168	-0.129752

Structure 33 (max 2) (M06-2X/6-311G(d,p), CHCl₃)

Energy (Hartrees): = -1317.407627

Imaginary frequency -69.18

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.595366	-0.692767	-0.078932
2	7	0	2.310616	-0.133985	-1.038967
3	1	0	1.849394	-0.000705	-1.929941
4	7	0	0.280495	-1.052541	-0.515954
5	1	0	-2.157554	2.766510	0.478553
6	1	0	-4.215362	-0.964368	0.024464
7	1	0	-4.282683	1.478639	0.489693
8	1	0	0.136789	-2.024114	-0.264473
9	16	0	2.156901	-1.039297	1.452553
10	6	0	-0.951895	1.062851	0.032173
11	6	0	-2.162288	1.700967	0.286786
12	6	0	-3.341985	0.980506	0.291687
13	6	0	-3.298595	-0.385210	0.032962
14	6	0	-2.100571	-1.038301	-0.219007
15	6	0	-0.883628	-0.313459	-0.213924
16	17	0	0.464297	2.098295	0.023046
17	6	0	-2.093022	-2.515776	-0.509269
18	1	0	-1.604518	-2.732640	-1.464043
19	1	0	-1.567497	-3.078593	0.270325
20	1	0	-3.113059	-2.895285	-0.555961
21	6	0	3.646774	0.391282	-0.852530
22	1	0	3.982465	0.817751	-1.795306
23	1	0	3.643565	1.161309	-0.076183
24	1	0	4.326286	-0.405658	-0.544988