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Supplementary materials

Synthesis and Structural Characterization of a New 1,2,3-Triazole Derivative of Pentacyclic Triterpene

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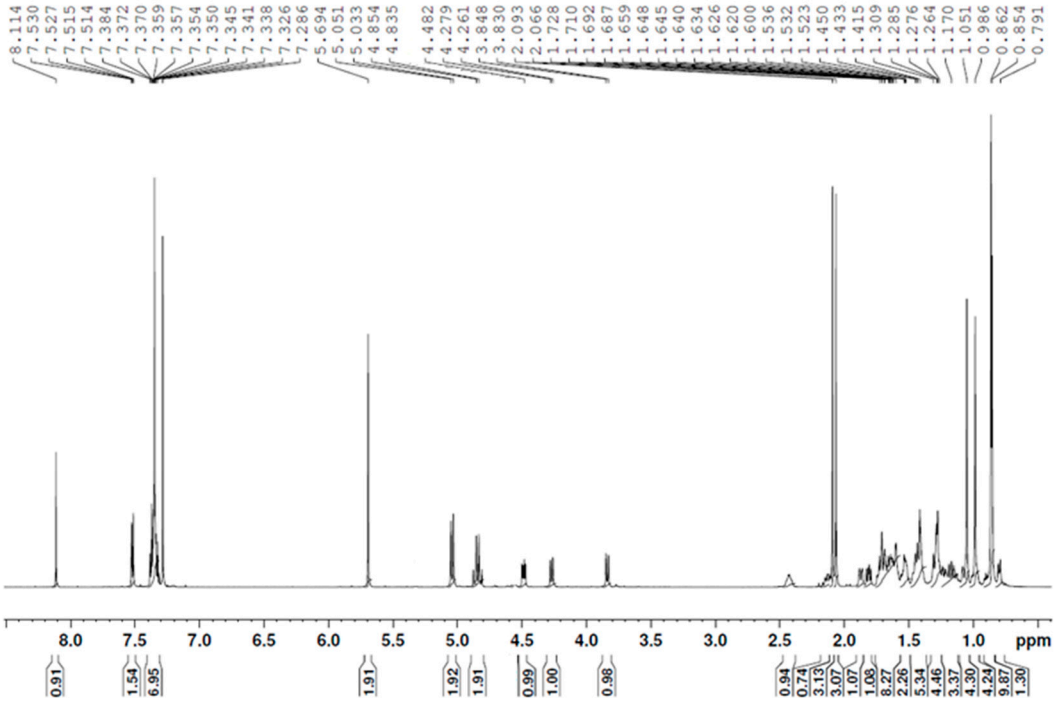

Figure S1. [1]H NMR, 3,28-O,O′-diacetyl-30-(1-phenylthiomethyl-1H-1,2,3-triazol-4-yl)carbonylbetulin **4.**

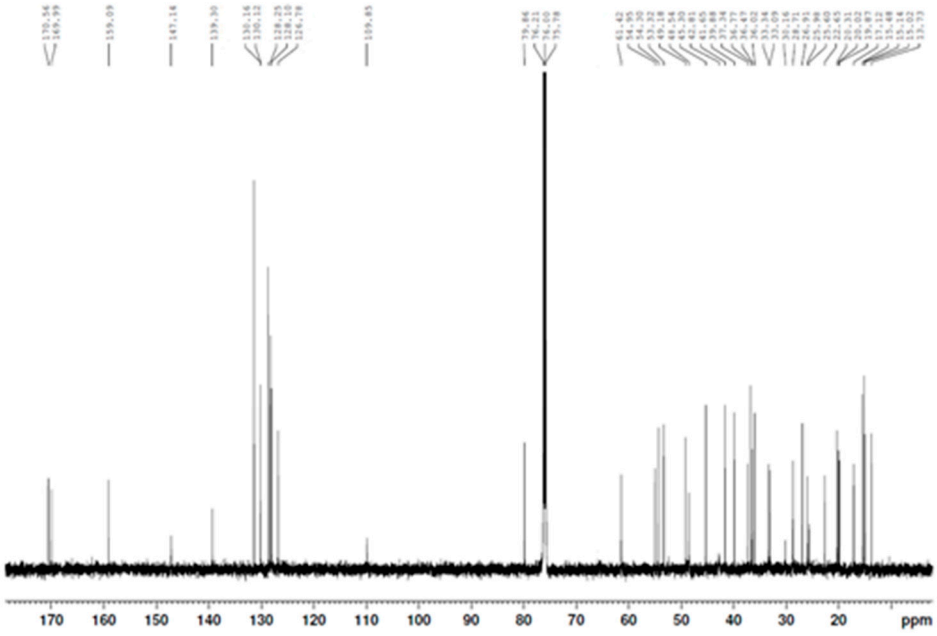

Figure S2. [13]C NMR, 3,28-O,O′-diacetyl-30-(1-phenylthiomethyl-1H-1,2,3-triazol-4-yl)carbonylbetulin **4.**

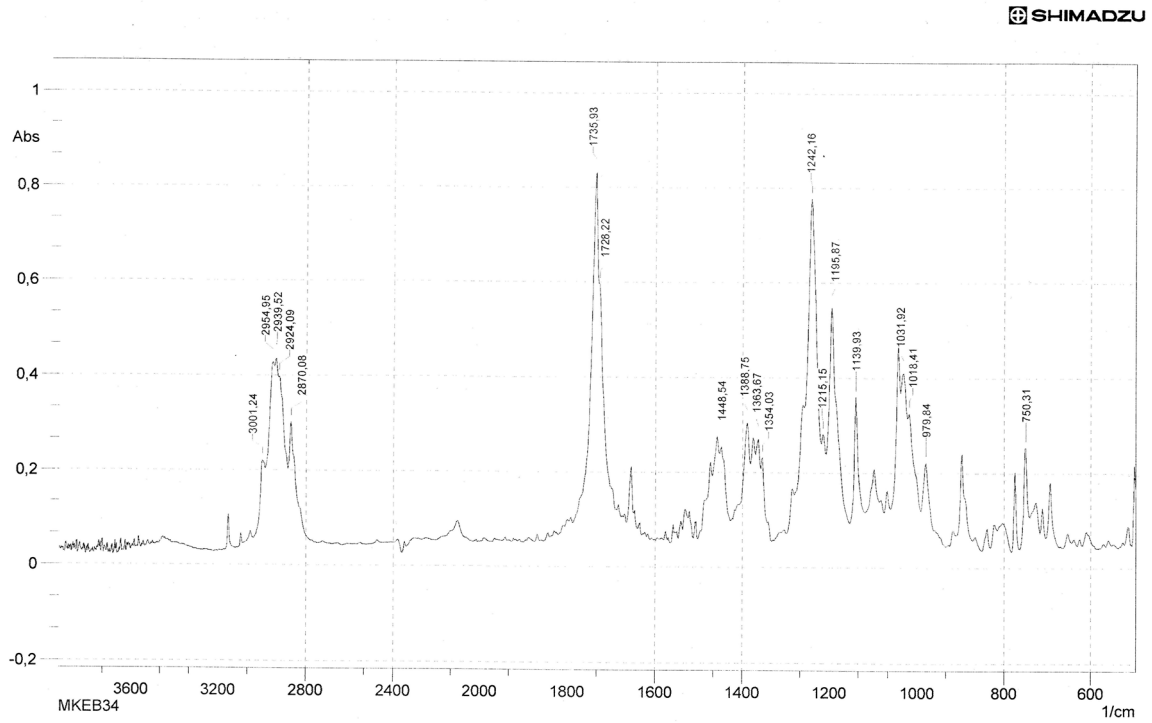

Figure S3. IR, 3,28-O,O′-diacetyl-30-(1-phenylthiomethyl-1H-1,2,3-triazol-4-yl)carbonylbetulin **4.**

Analysis Name D:\Data\PM_20171204\MK EB 34 Pa.d
Method low_mass.m
Sample Name AN 40_18
Comment
Operator KM
Instrument impact II
1825265.10082

Acquisition Parameter

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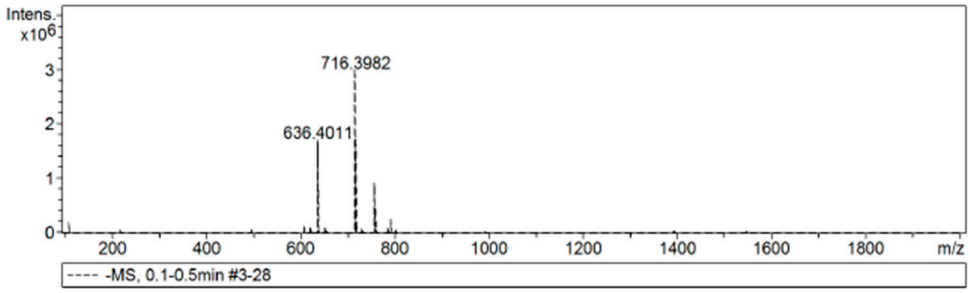
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C



#	m/z	Res.	S/N	I	I %	FWHM
1	636.4011	44867	35549.0	1651740	56.3	0.0142
2	716.3982	38401	56744.8	2935886	100.0	0.0187
3	758.4196	44798	17168.0	933896	31.8	0.0169

Figure S4. HR-MS, 3,28-O,O′-diacetyl-30-(1-phenylthiomethyl-1H-1,2,3-triazol-4-yl)carbonylbetulin **4.**

Table S1. Selected bond lengths (Å) for compounds **4**.

Compound 4.	
Distance (Å)	
S1-C38	1.822(3)
S1-C39	1.782(3)
O1-C3	1.451(3)
O1-C33	1.340(3)
O2-C33	1.203(4)
O3-C28	1.453(3)
O3-C31	1.333(4)
O4-C31	1.194(4)
O5-C30	1.435(4)
O5-C35	1.342(3)
O6-C35	1.211(3)
N1-N2	1.305(4)
N1-C36	1.364(4)
N2-N3	1.348(3)
N3-C37	1.344(4)
N3-C38	1.461(4)
C18-C19	1.541(4)
C19-C20	1.511(4)
C19-C21	1.572(4)
C20-C29	1.330(4)
C20-C30	1.502(4)
C31-C32	1.493(4)
C35-C36	1.466(4)
C36-C37	1.372(4)
C39-C40	1.383(4)
C39-C44	1.387(4)
C40-C41	1.388(5)
C41-C42	1.379(5)
C42-C43	1.390(5)
C43-C44	1.376(4)

Table S2. Selected angle (degree) for compounds **4**.

Compound 4.	
Angle (degree)	
C38-S1-C39	101.1(1)
C3-O1-C33	117.9(2)
C28-O3-C31	118.6(2)
C30-O5-C35	116.3(2)
N2-N1-C36	108.2(3)
N1-N2-N3	107.8(2)
N2-N3-C37	110.9(2)
N2-N3-C38	120.3(2)
C37-N3-C38	128.6(2)
O1-C3-C2	109.4(2)
O1-C3-C4	108.4(2)
C20-C19-C21	110.7(2)

C19-C20-C29	126.4(3)
C19-C20-C30	110.9(2)
C29-C20-C30	122.6(3)
C19-C21-C22	106.0(2)
O3-C28-C17	109.1(2)
C39-S1-C38-N3	77.6(2)
C38-S1-C39-C40	-114.2(3)
C38-S1-C39-C44	66.1(3)
C31-O3-C28-C17	-125.0(3)
C28-O3-C31-C32	-179.1(2)
N2-N1-C36-C35	-178.9(3)
N1-N2-N3-C38	-176.6(2)
C38-N3-C37-C36	175.4(3
N2-N3-C38-S1	107.4(3)
C37-N3-C38-S1	-67.8(3)
C2-C1-C10-C5	51.0(3)
C1-C2-C3-O1	-178.6(2)
C1-C2-C3-C4	59.8(3)
O1-C3-C4-C5	-179.9(2)
C2-C3-C4-C5	-57.8(3)
C16-C17-C28-O3	67.9(3)
C18-C17-C28-O3	-171.5(2)
C22-C17-C28-O3	-61.6(3)
C21-C19-C20-C29	95.9(3)
C21-C19-C20-C30	-81.0(3)
C20-C19-C21-C22	-128.6(2)
C19-C21-C22-C17	-27.3(3)
S1-C39-C40-C41	178.4(2)
S1-C39-C44-C43	-178.2(2)

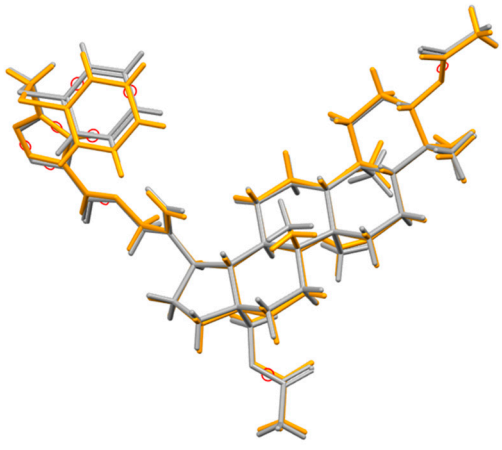


Figure S5. Atom by atom superimposition of X-ray structure (yellow) and calculate structure (grey).

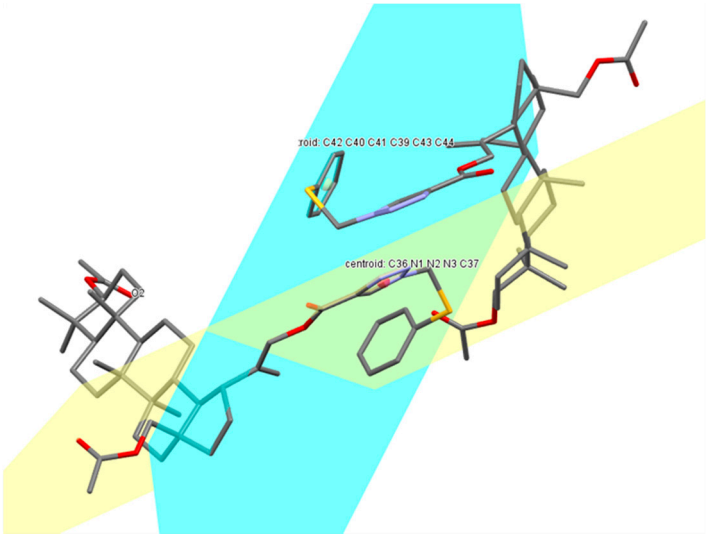


Figure S6. Intermolecular orientation of triazole and phenyl centroids showing π···π interactions.

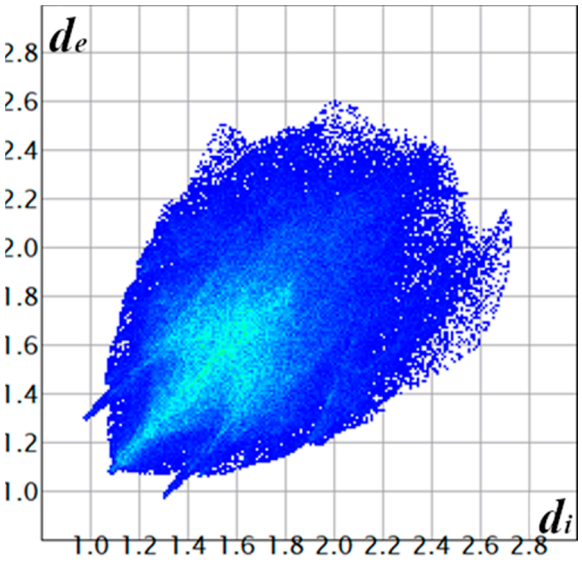


Figure S7. The full 2D fingerprint plot for **4.**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

Bond precision: C-C = 0.0040 A Wavelength=1.54184

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alpha=90 beta=90 gamma=90
Temperature: 100 K

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Sum formula	C44 H61 N3 O6 S	C44 H61 N3 O6 S
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Dx,g cm-3	1.262	1.262
Z	4	4
Mu (mm-1)	1.131	1.131
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F000'	1645.85	
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Click on the hyperlinks for more details of the test.
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Alert level C

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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        81 Report
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Alert level G

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       96 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      4.6 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       16 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by        3 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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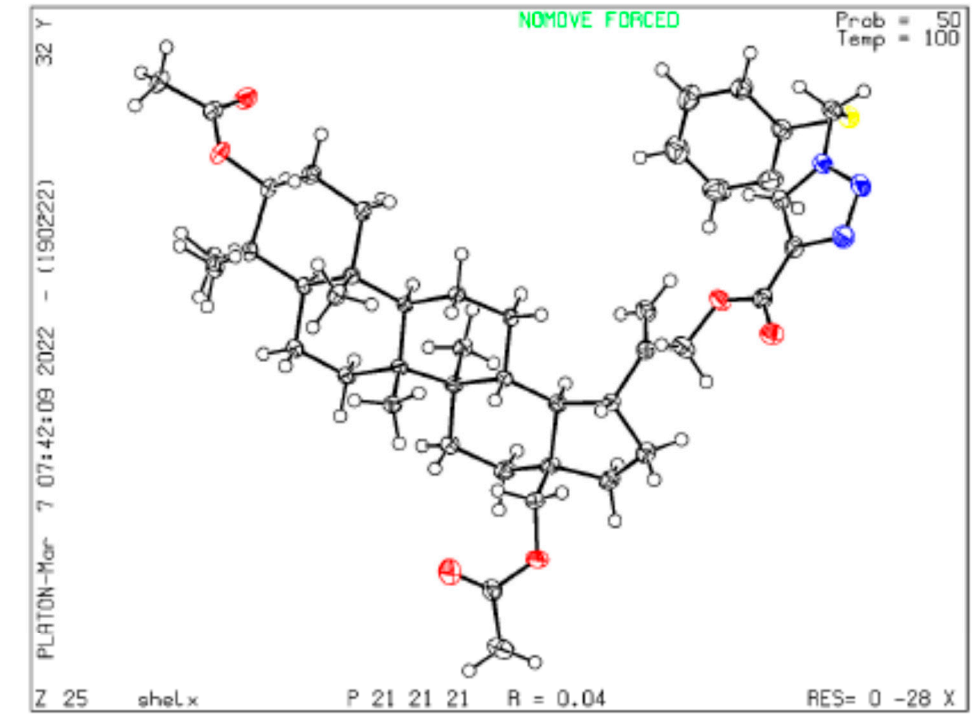
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