

Conversion of Glycosylated Platycoside E to Deapiose-Xylosylated Platycodin D by Cytolase PCL5

Kyung-Chul Shin^{1,†}, Dae Wook Kim^{2,†}, Hyun Sim Woo², Deok-Kun Oh^{1,3}, Yeong-Su Kim^{2,*}

¹ Research Institute of Bioactive-Metabolome Network, Konkuk University, Seoul 05029, Korea; hidex2@naver.com (K.-C.S.); deokkun@konkuk.ac.kr (D.-K.O.)

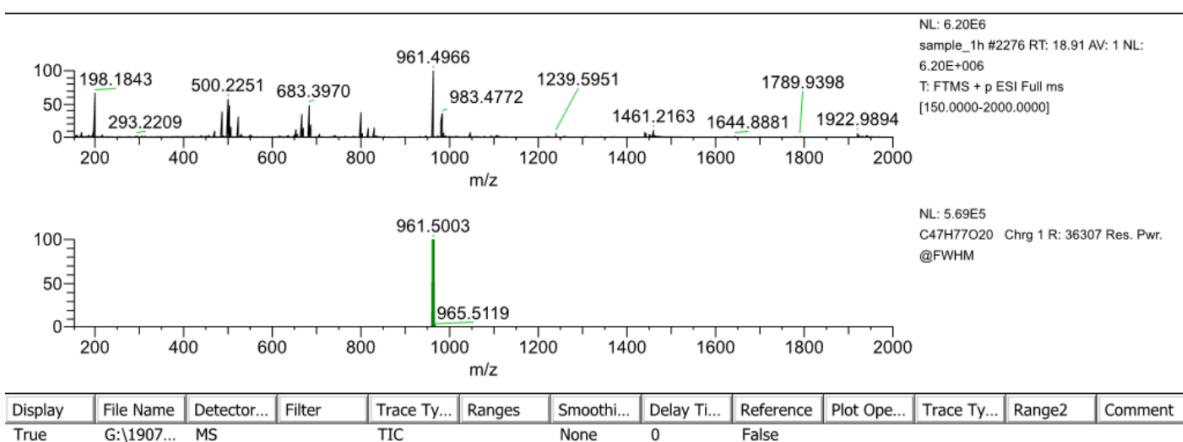
² Forest Plant Industry Department, Baekdudaegan National Arboretum, Bonghwa 36209, Korea; dwking@bdna.or.kr (D.W.K.); whs0428@bdna.or.kr (H.S.W.)

³ Department of Bioscience and Biotechnology, Konkuk University, Seoul 05029, Korea; deokkun@konkuk.ac.kr (D.-K.O.)

* Correspondence: yskim@bdna.or.kr; Tel.: +82-54-679-2740; Fax: +82-54-679-0636

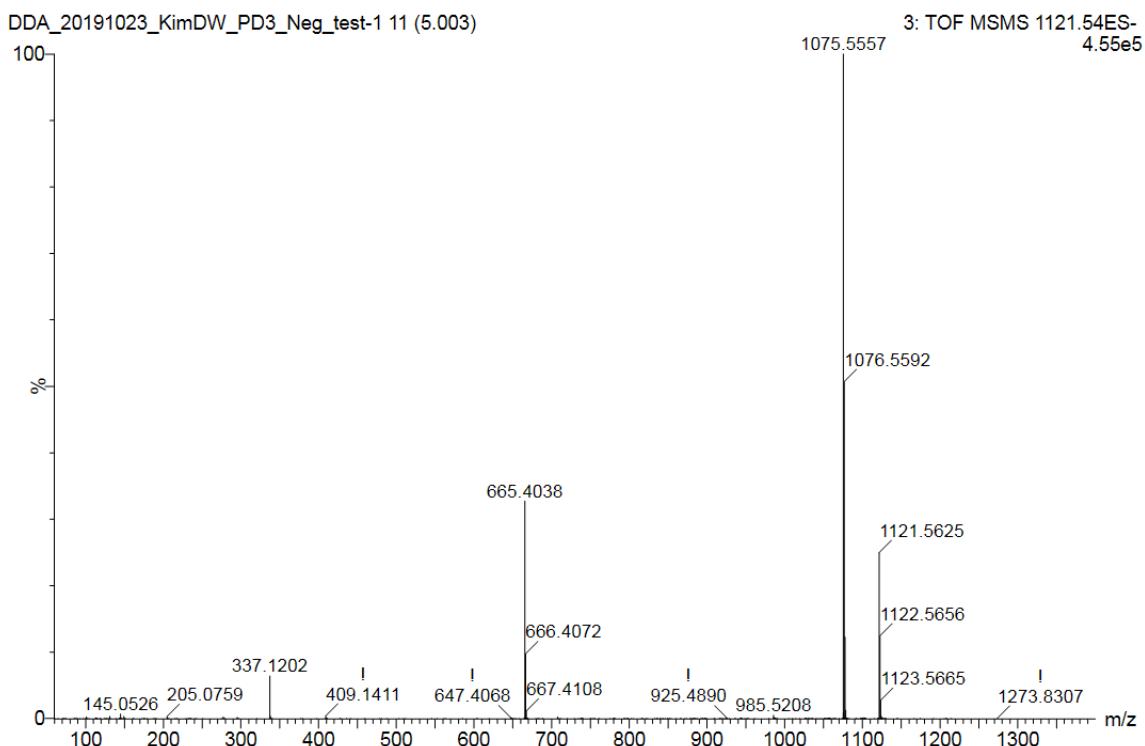
† These authors contributed equally to this work.

Supplementary Materials



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	961.4966	C ₄₇ H ₇₇ O ₂₀	88.2892529843...	9.5	-3.77	C47H77O20	961.50027
2		C ₅₄ H ₇₃ O ₁₅	78.8906328156...	18.5	2.34	C54H73O15	961.49440
3		C ₄₀ H ₆₁ O ₂₅	30.7046751588...	0.5	-9.88	C40H61O25	961.50614
4		C ₆₁ H ₆₉ O ₁₀	16.5483883676...	27.5	8.44	C61H69O10	961.48852
5		C ₆₅ H ₆₉ O ₇	0	31.5	-7.42	C65H69O7	961.50378
6		C ₇₂ H ₆₅ O ₂	0	40.5	-1.32	C72H65O2	961.49791

Figure S1. LCMS and HRMS analysis of deapi-dexyl-platycodin D (**1'**).



Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

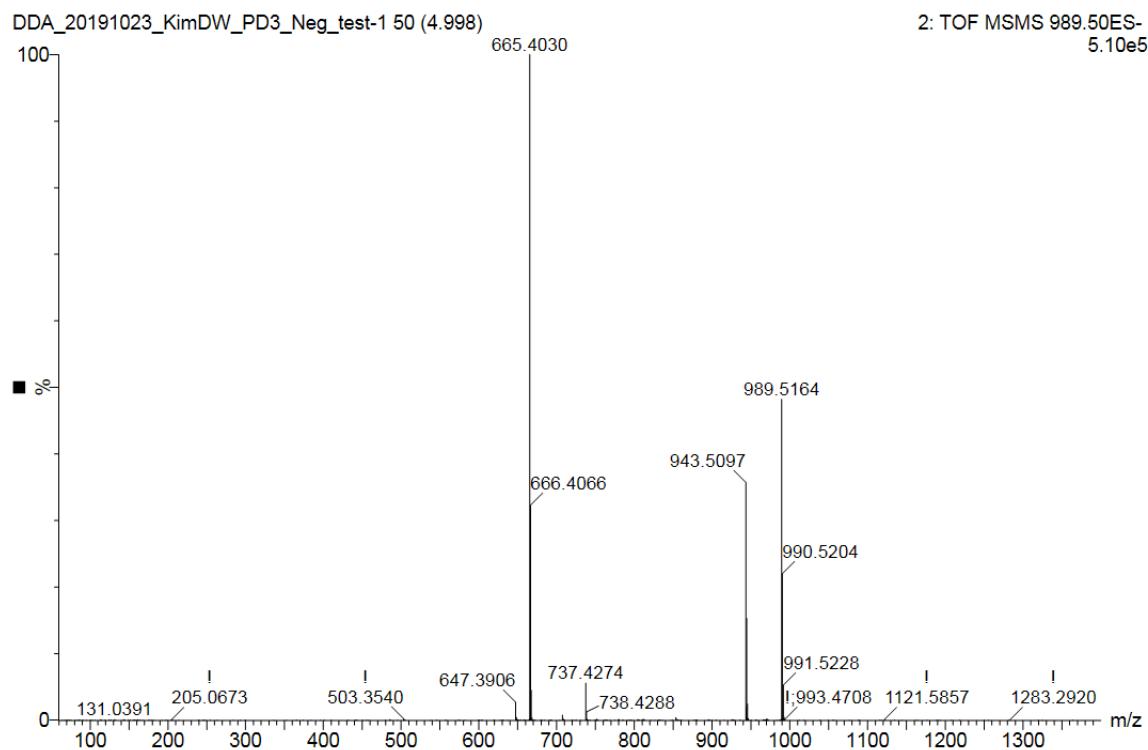
485 formula(e) evaluated with 2 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-50

	Minimum:	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1121.5436	60.00	100.00	1121.5439	-0.3	-0.3	2.5	212.6	0.300	74.06	C46 H89 O30
			1121.5380	5.6	5.0	11.5	213.6	1.349	25.94	C53 H85 O25

Figure S2. LCMS and HRMS analysis of deapi-patycodin D (**2'**).



Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

406 formula(e) evaluated with 2 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-50

	Minimum:	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
989.4985	60.00	100.00	989.4957	2.8	2.8	-1.5	221.4	0.853	42.60	C48 H77 O21
	Maximum:		989.5016	-3.1	-3.1	20.0	221.1	0.555	57.40	C41 H81 O26

Figure S3. LCMS and HRMS analysis of deapi-dexyl-platycodin D (**3'**)