SUPPORTING INFORMATION to the paper entitled:

Deoxynivalenol-oligoglycosides: New ´Masked´ *Fusarium* Toxins Occurring in Malt, Beer and Breadstuff

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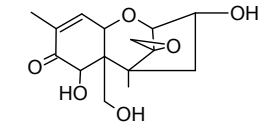
This document provides more detailed information to the main paper mentioned above. The following information is included:

Content page:

Figures S-1 – S-122: Possible Structures of Deoxynivalenol-glycosides.



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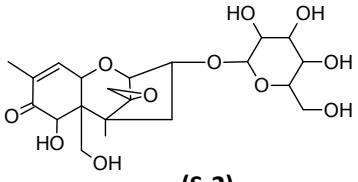

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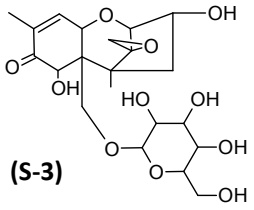

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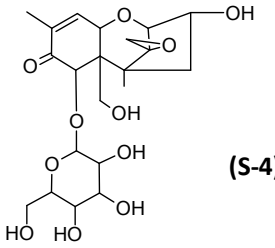

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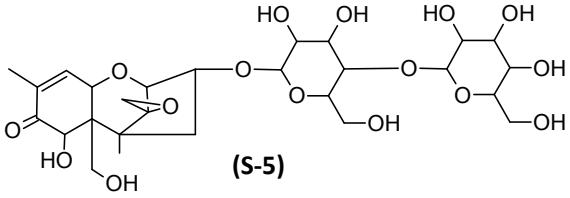

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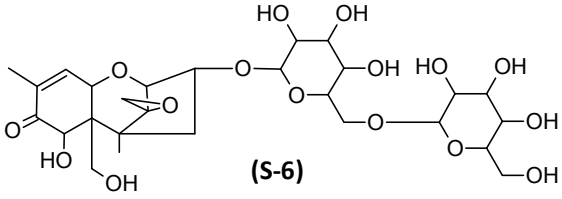

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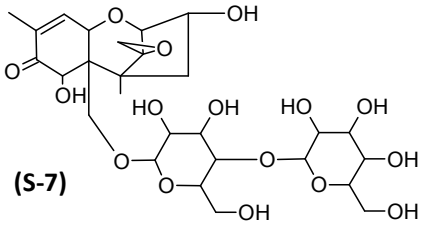

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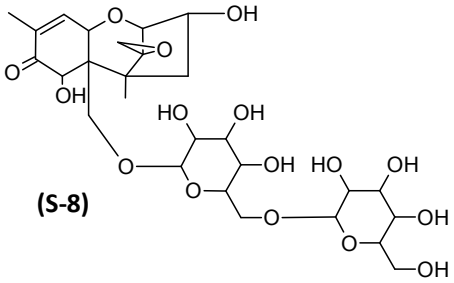

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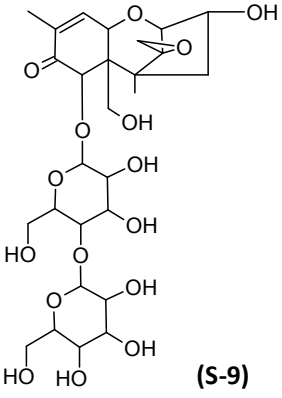

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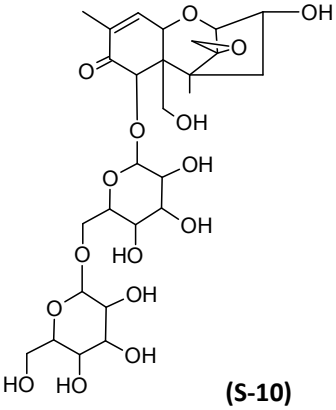

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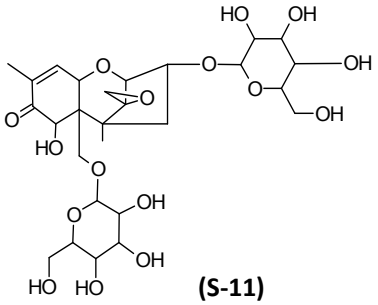

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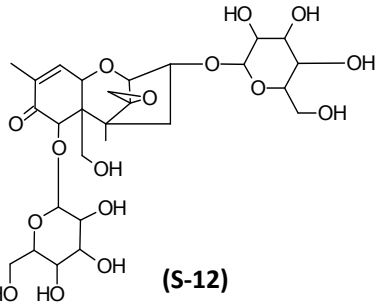

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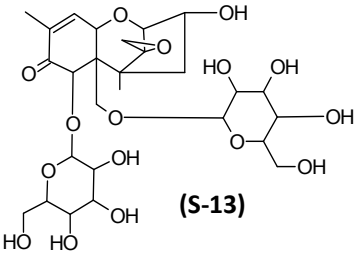

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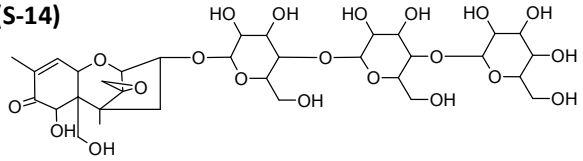

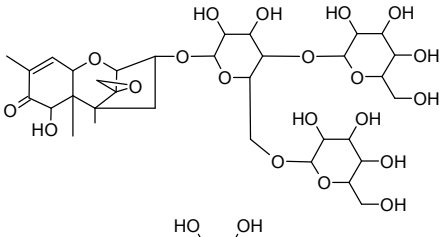

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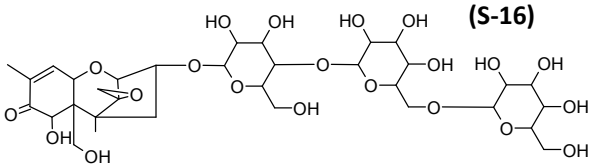

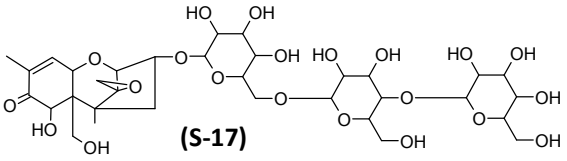

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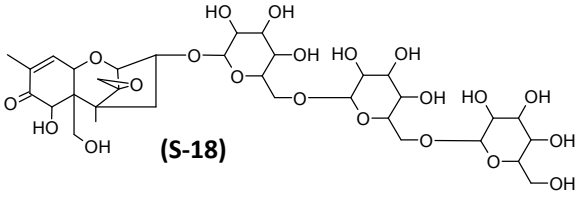

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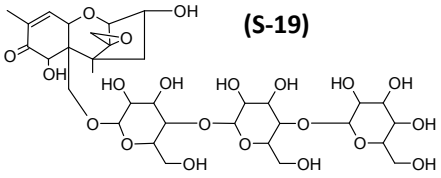

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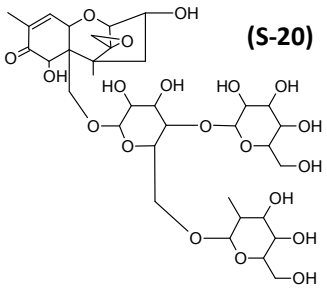

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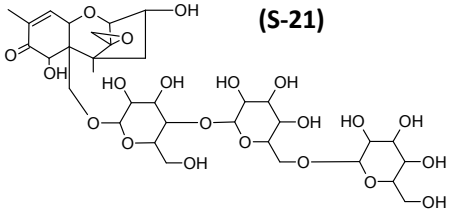

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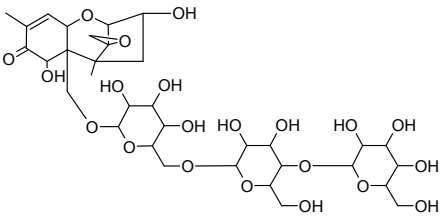

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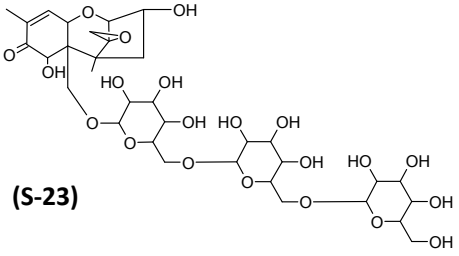

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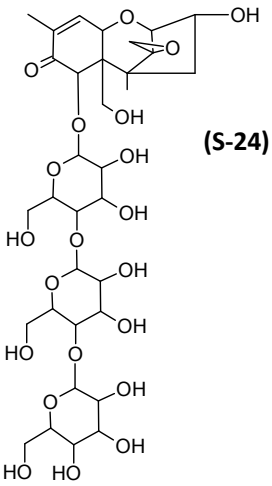

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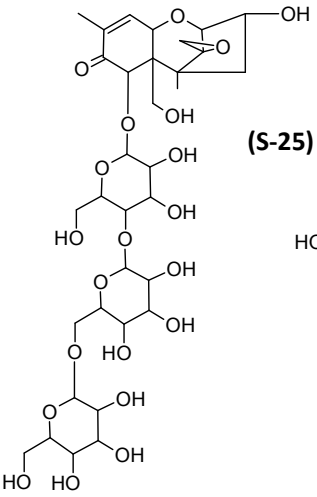

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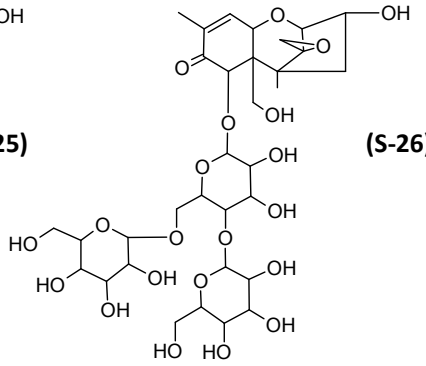

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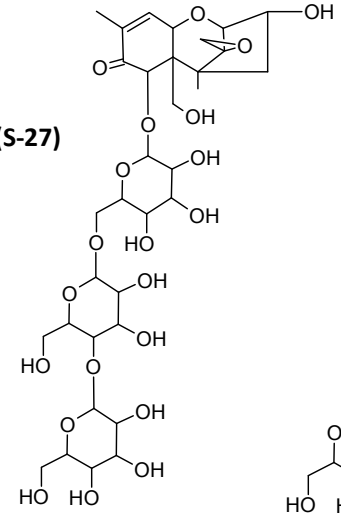

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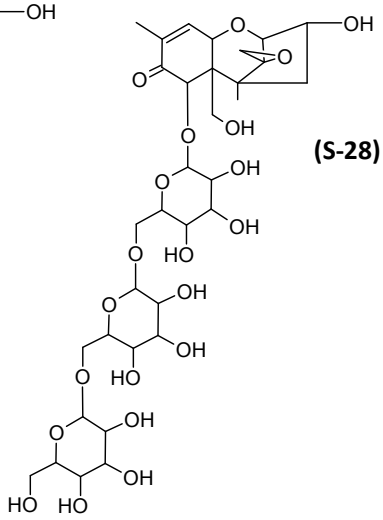

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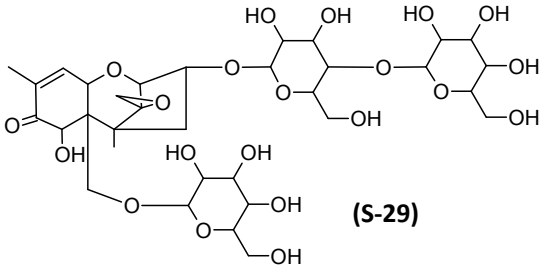

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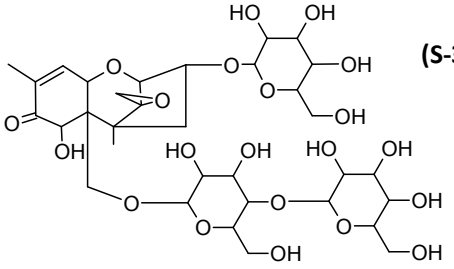

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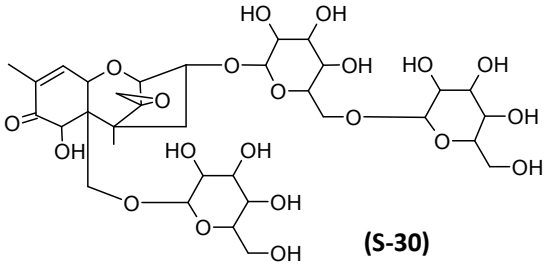

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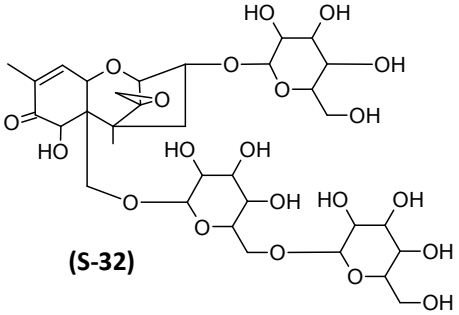

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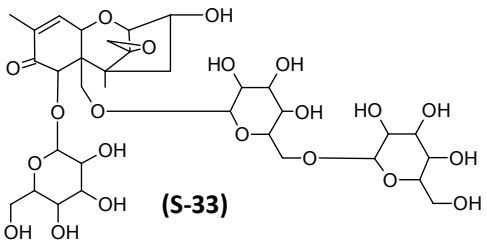

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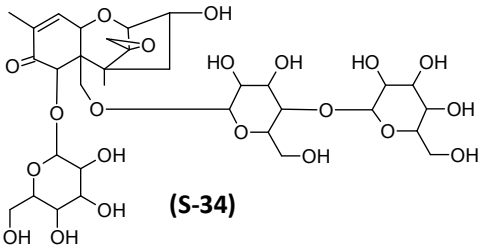

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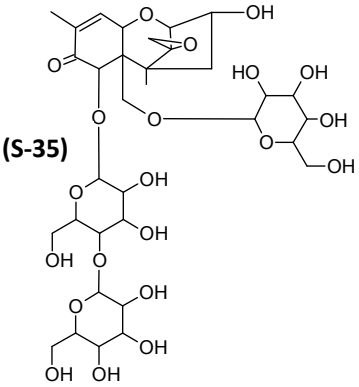

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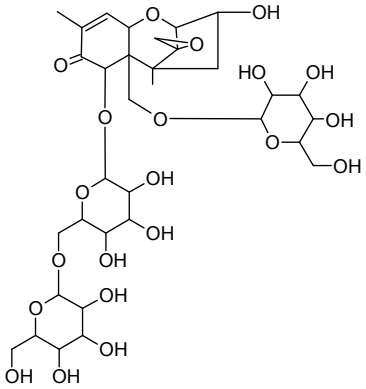

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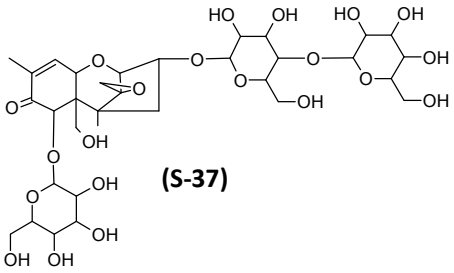

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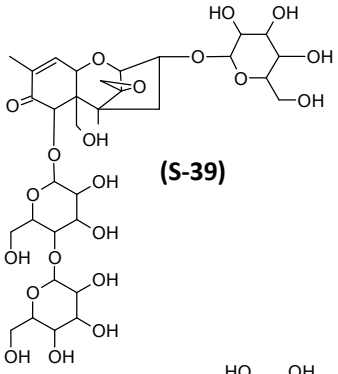

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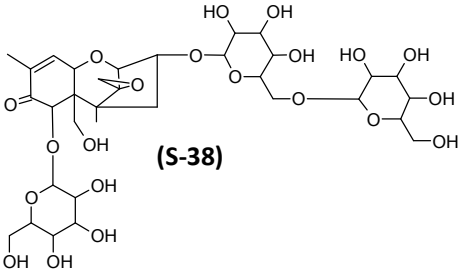

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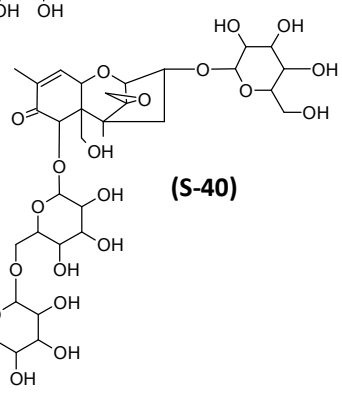

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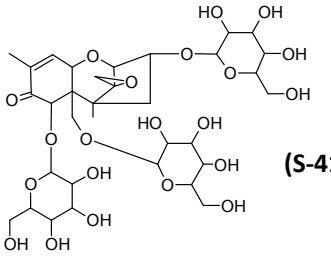

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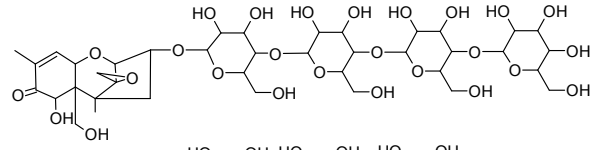

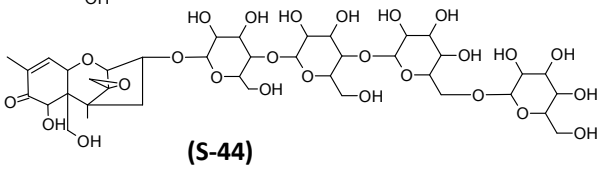

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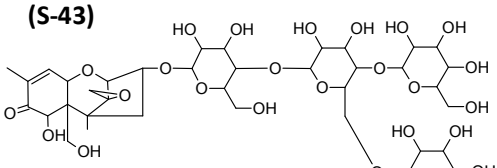

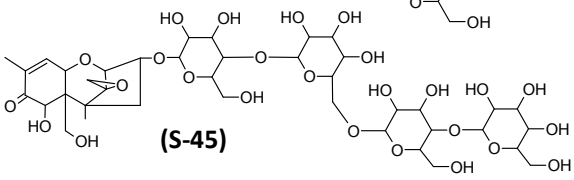

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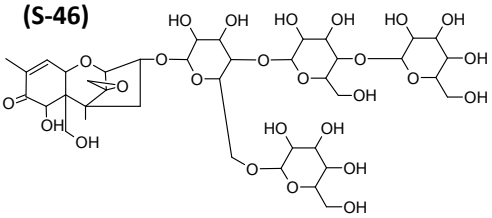

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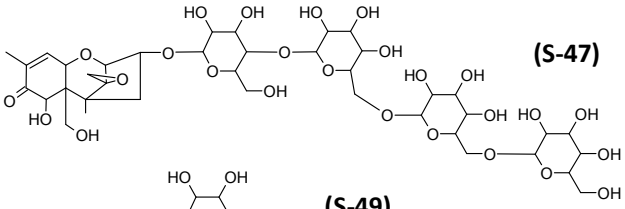

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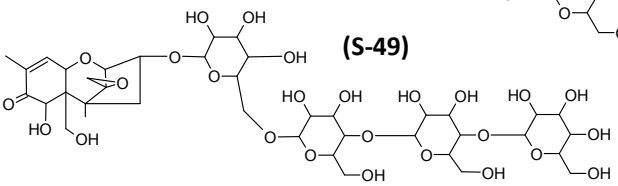

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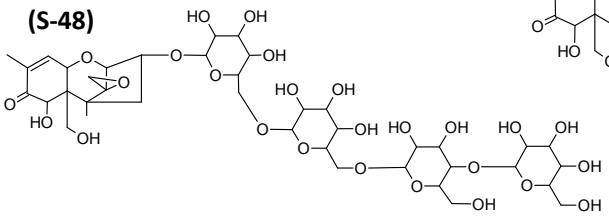

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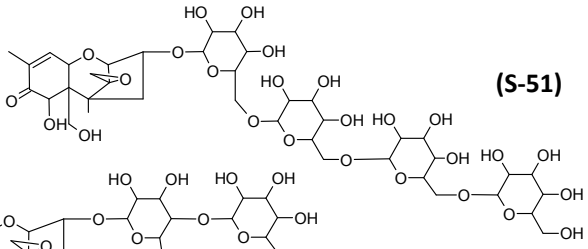

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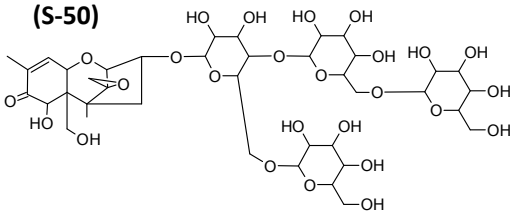

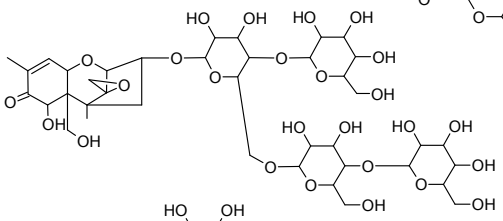

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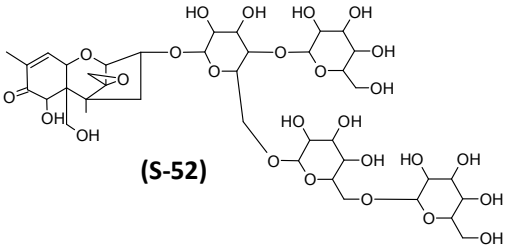

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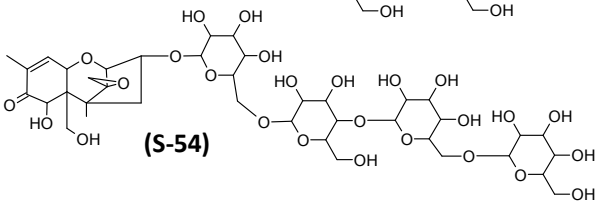

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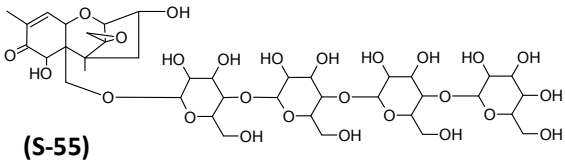

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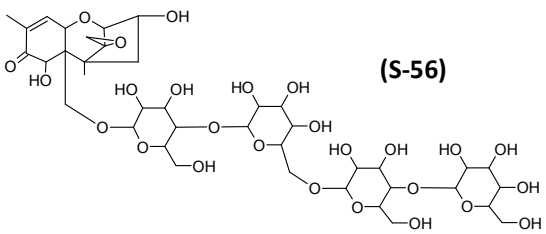

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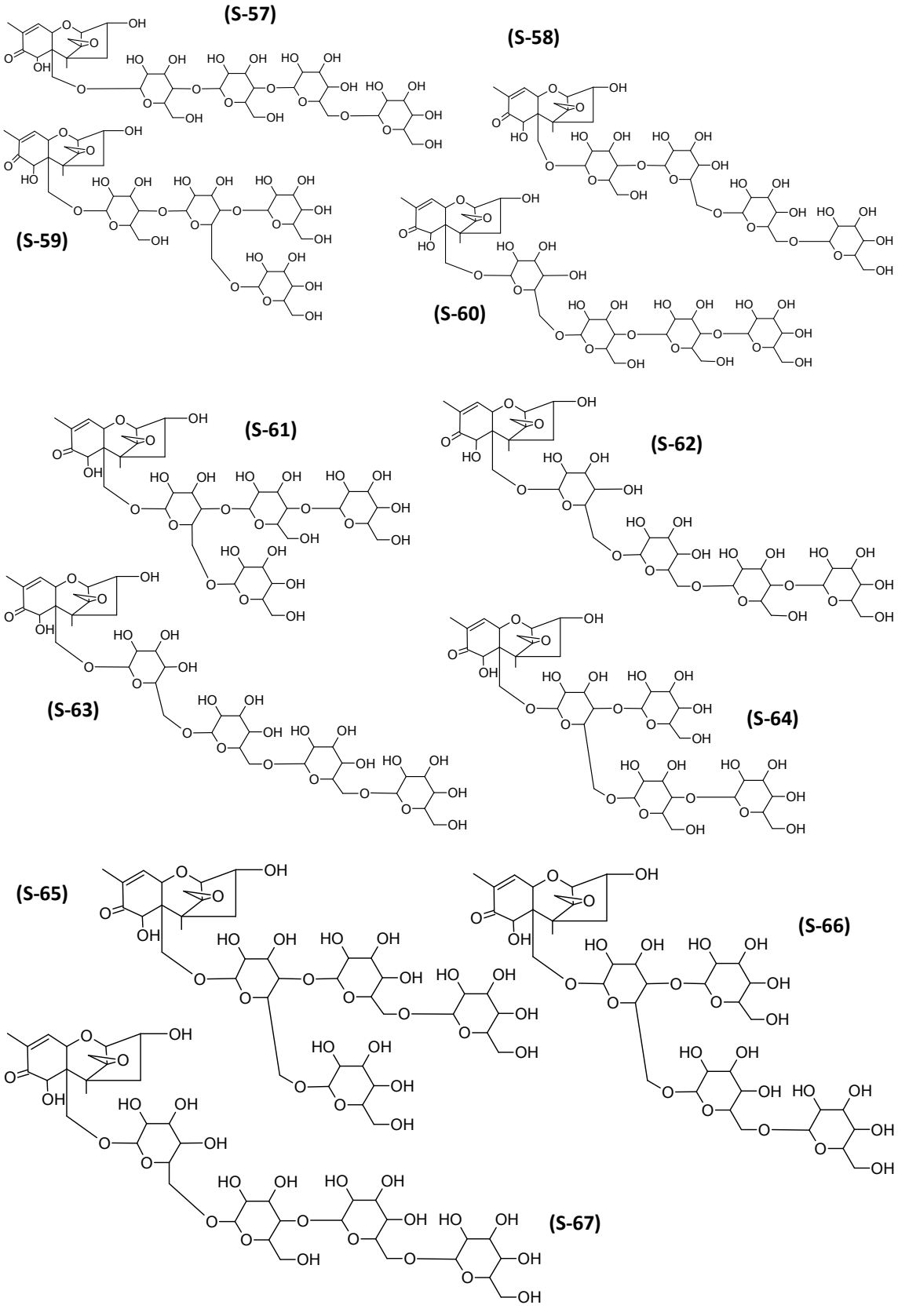
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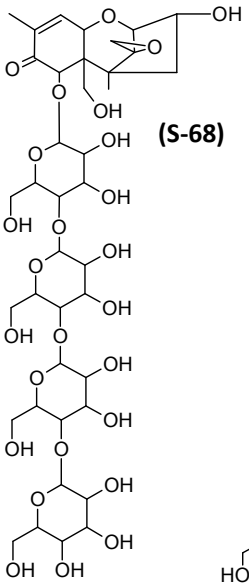

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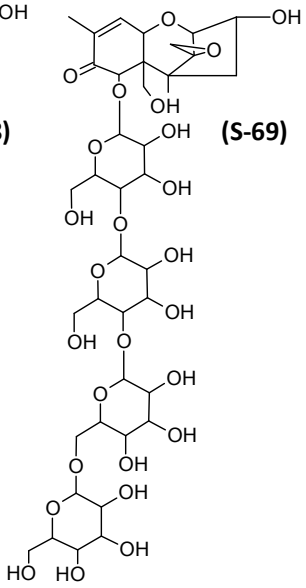

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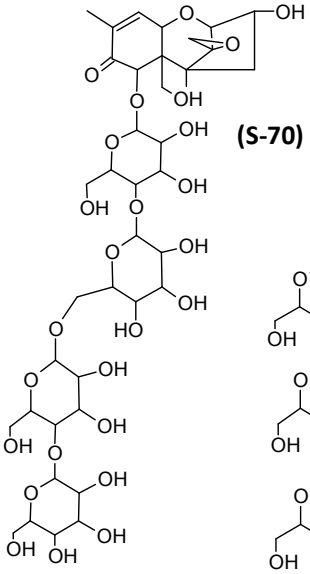

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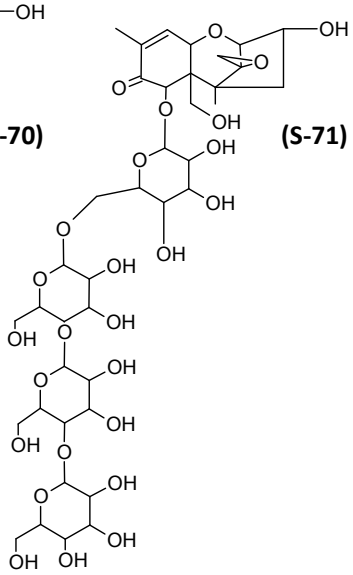

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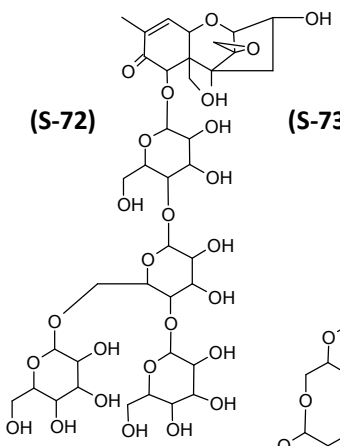

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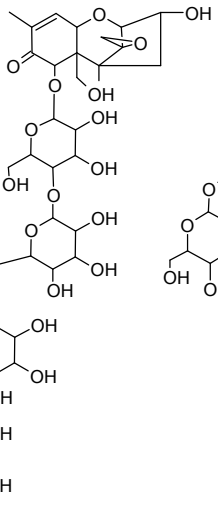

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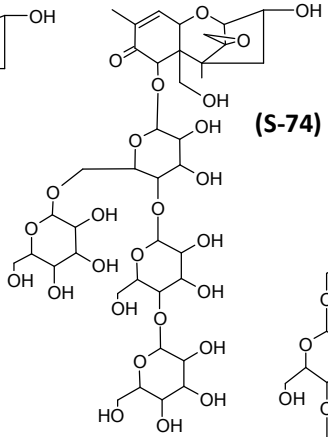

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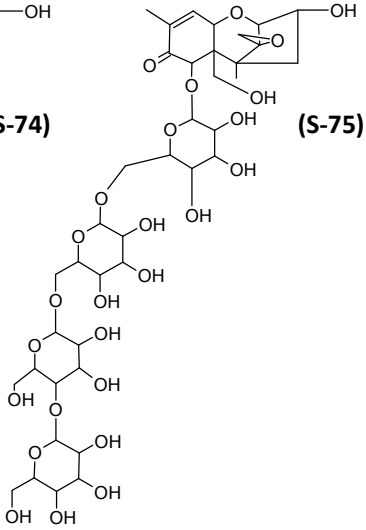

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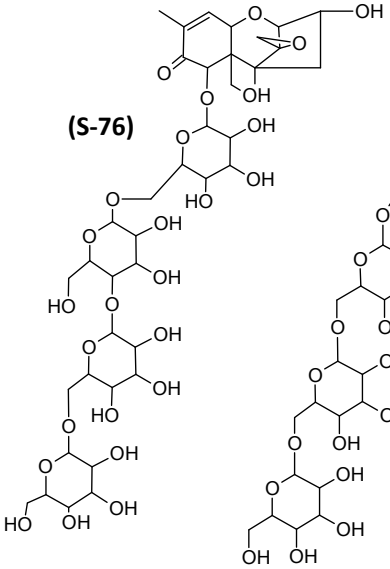

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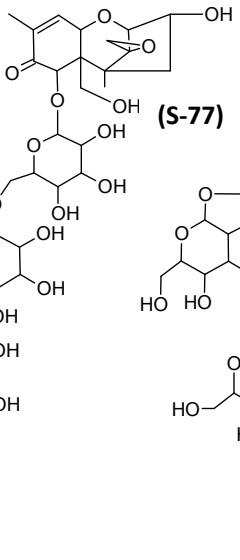

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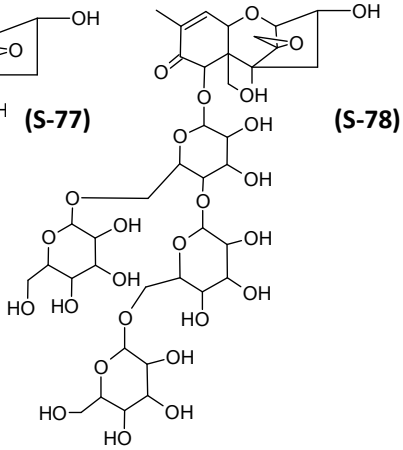

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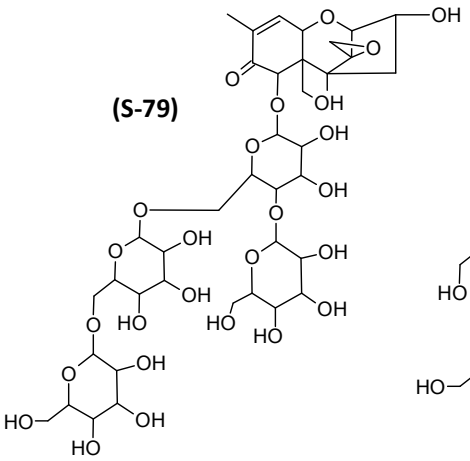

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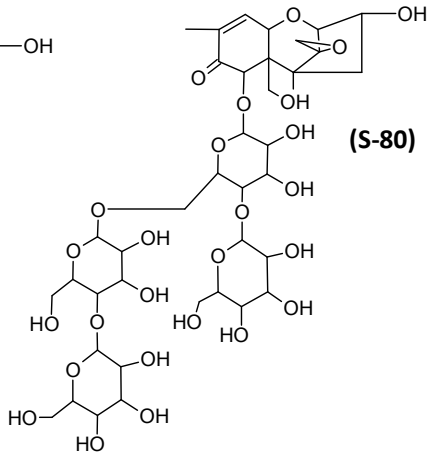

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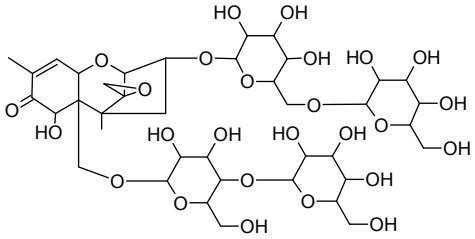

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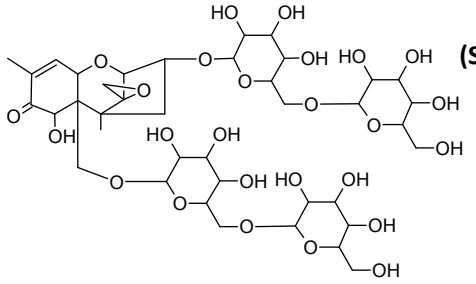

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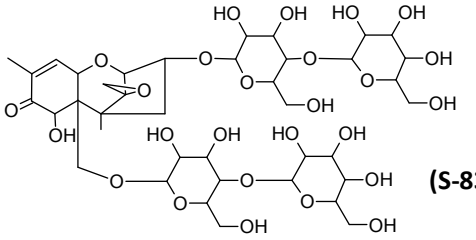

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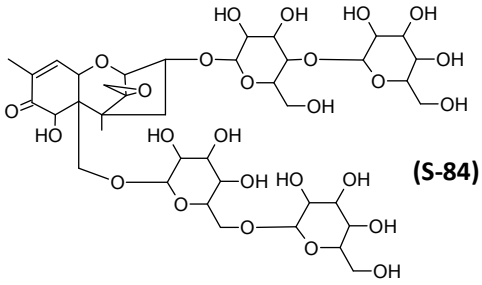

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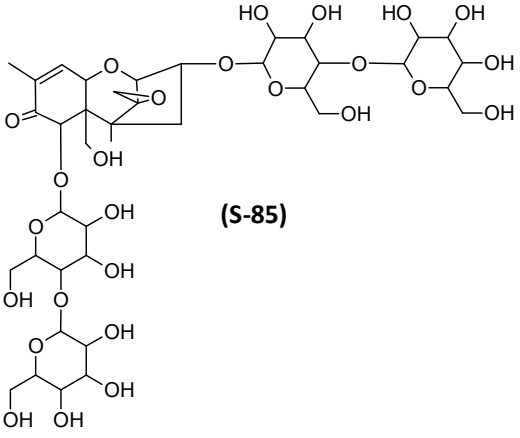

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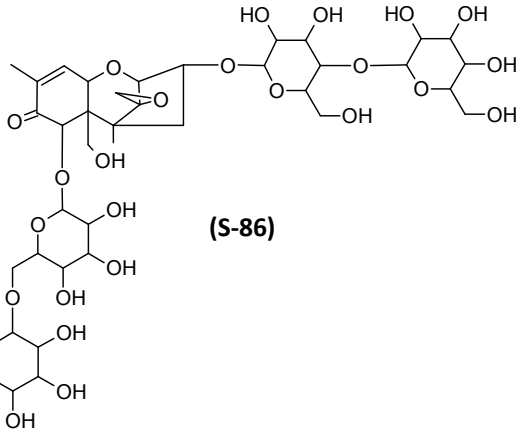

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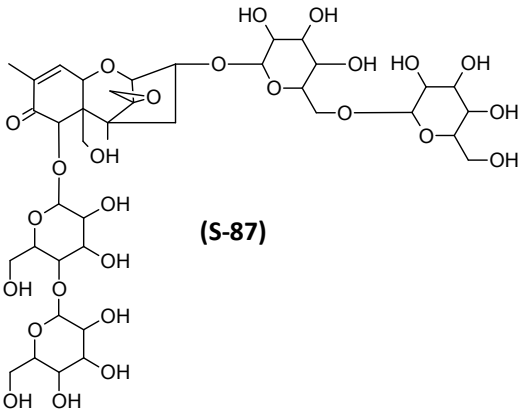

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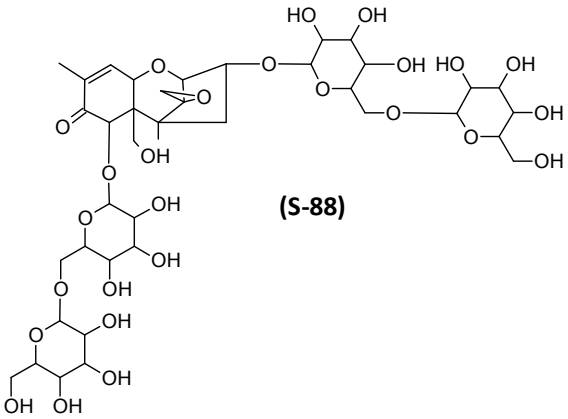

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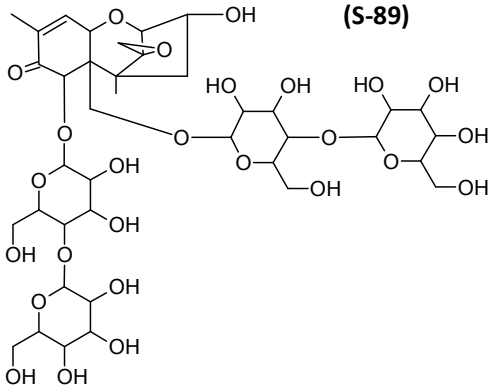

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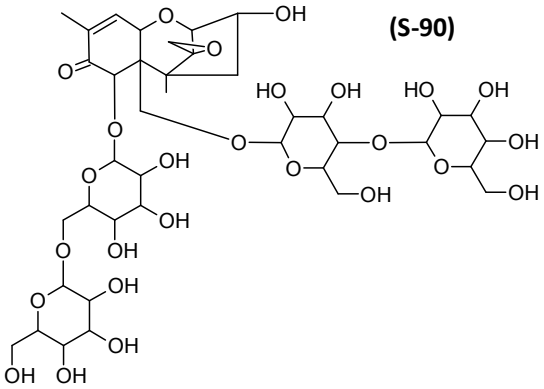

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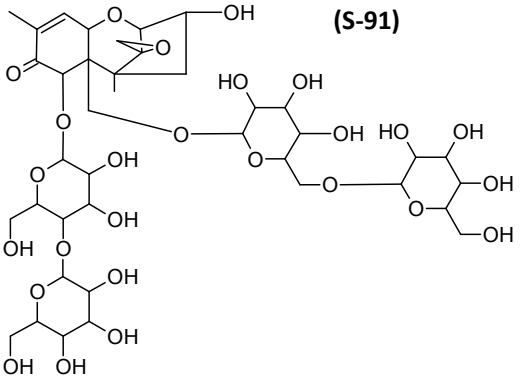

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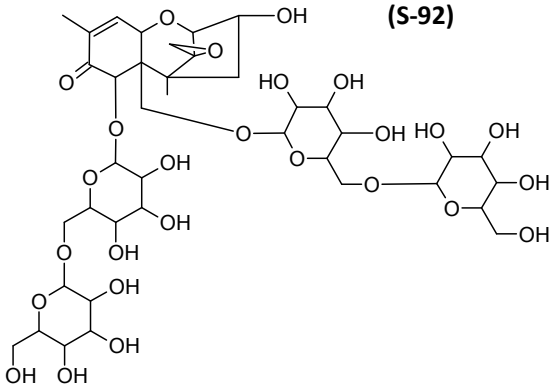

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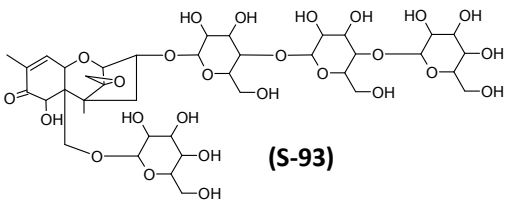

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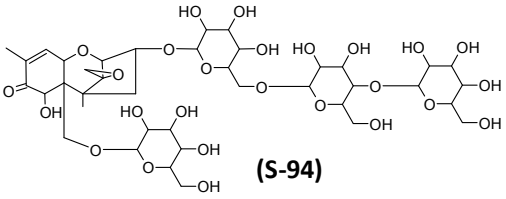

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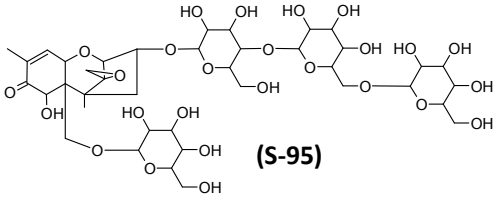

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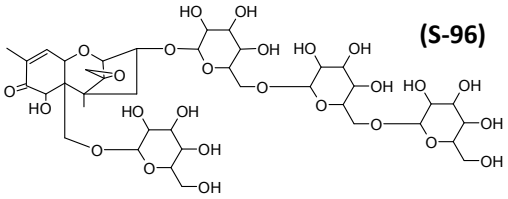

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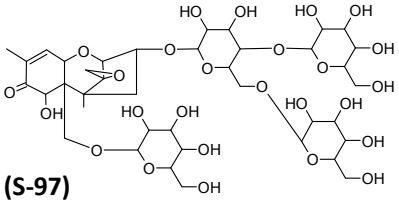

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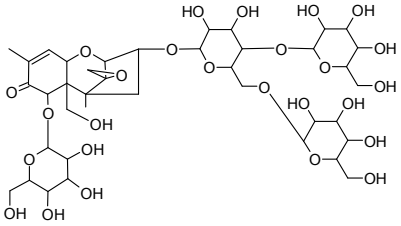

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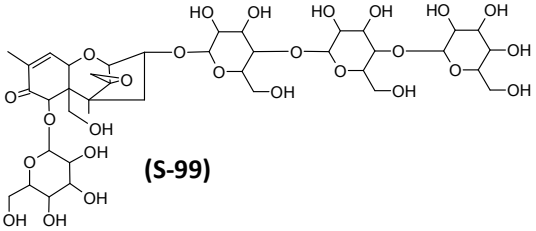

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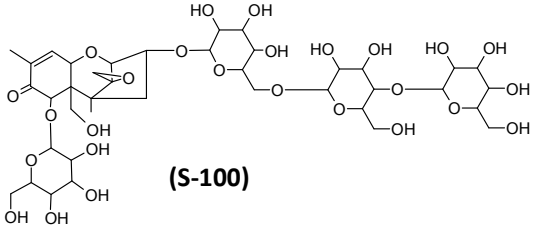

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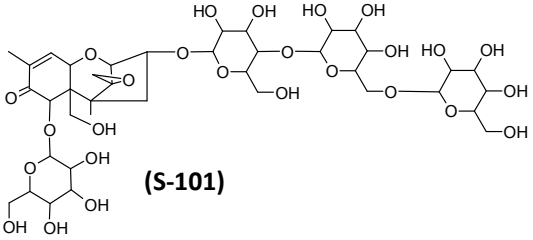

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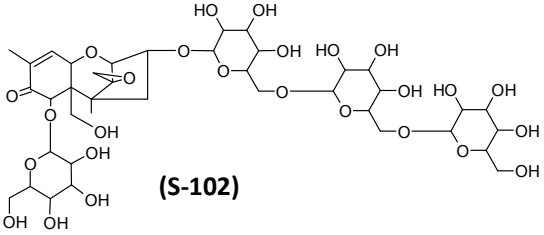

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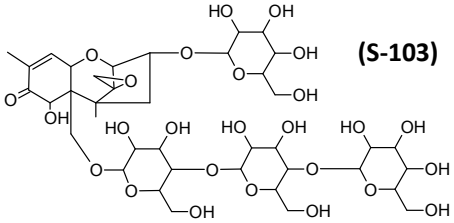

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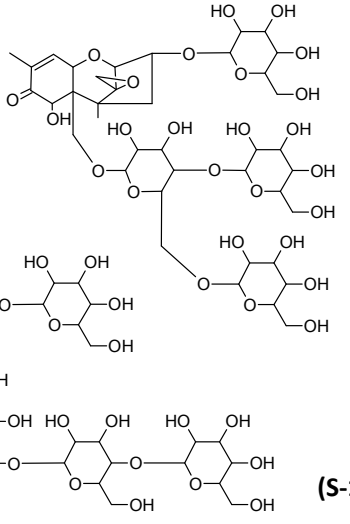

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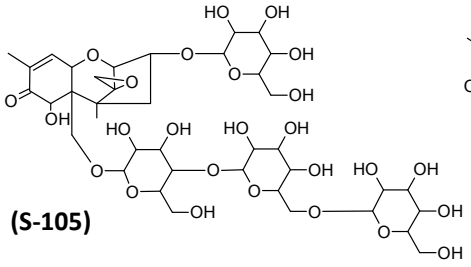

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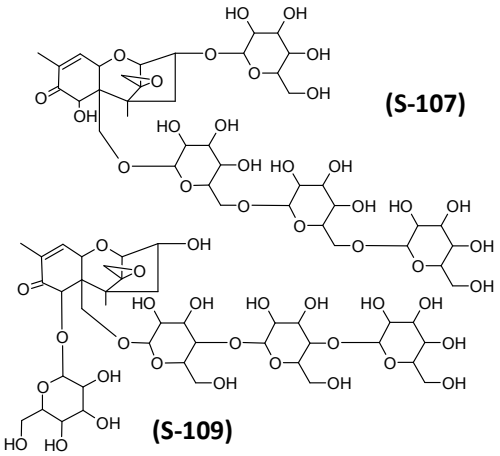
(S-106)



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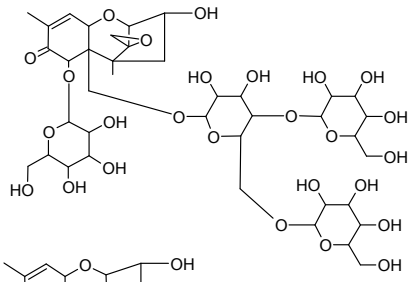

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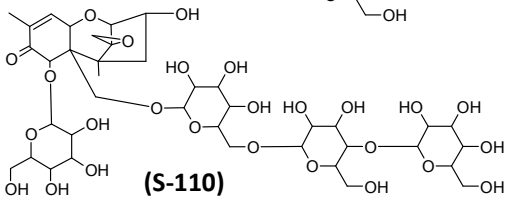
(S-109)



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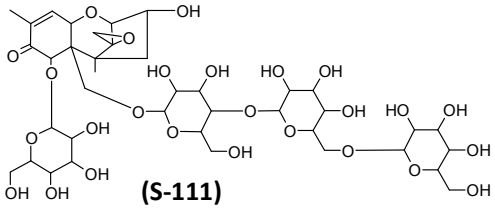

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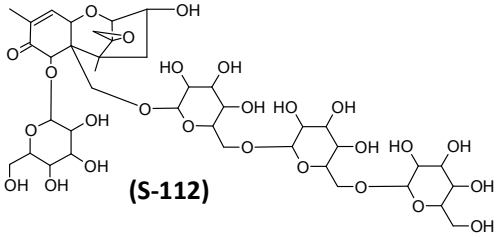

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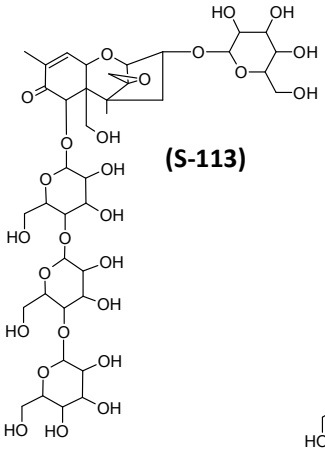

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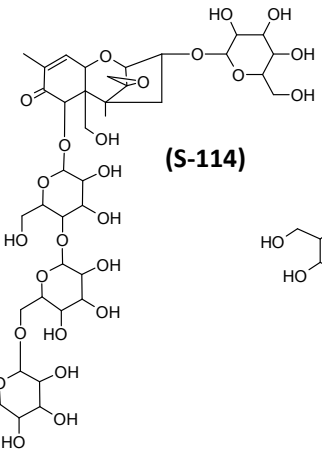

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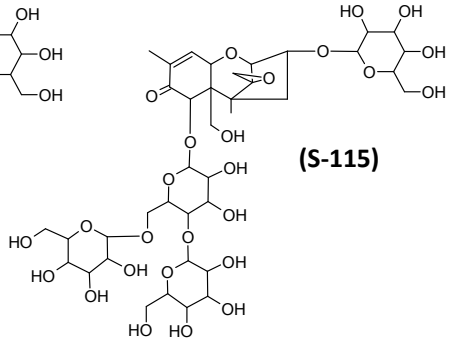

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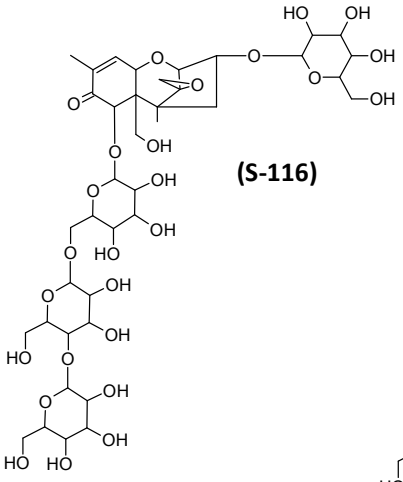

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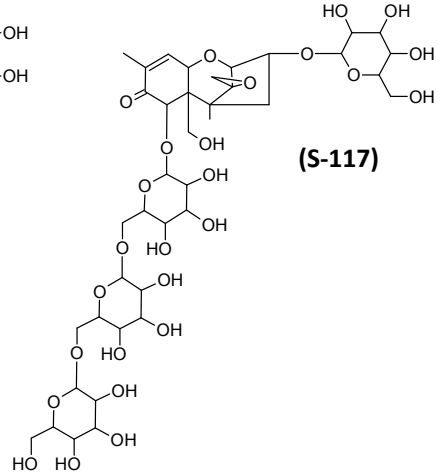

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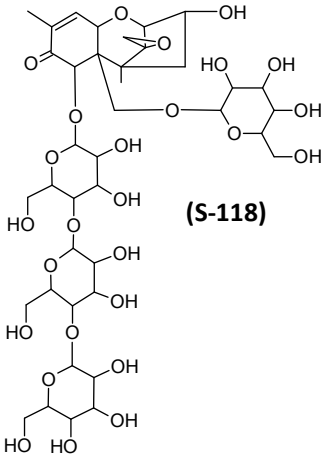

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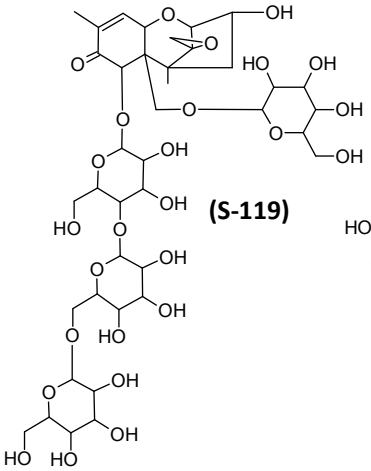

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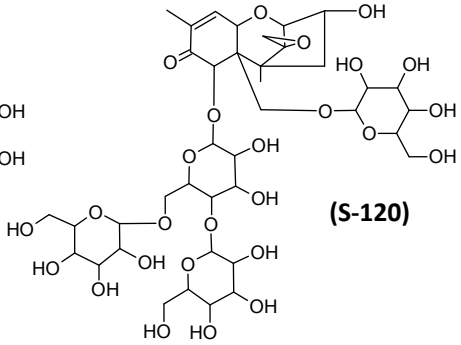

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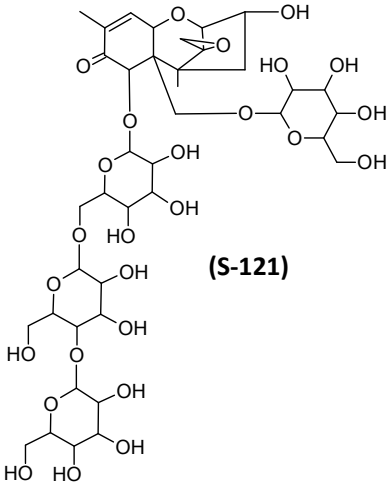

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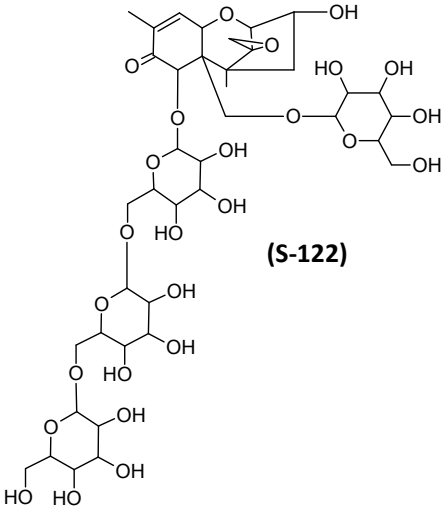

(S-122)

Table S-1: Summary of Calculated Exact Masses of Deoxynivalenol and its Glycosides, Together with Their Conceivable Diagnostic Fragments.

		M	[M+HCOO]-	[M-H]-	[M-CH2O-H]- from C6*	[M-CH2O-glucose-H] from C6*	[M-CH2O-2glucoses-H] from C6*	[M-CH2O-3glucoses-H] from C6*	[M-CH2O-4glucoses-H] from C6*	[M-glucose-H] from C7*	[M-2glucoses-H] from C7*	[M-3glucoses-H] from C7*	[M-4glucoses-H] from C7*
Deoxynivalenol with 1 glucose unit	Deoxynivalenol	C15H20O6	C16H21O8	C15H19O6	C14H17O5								
	(S-1)**	296.12599	341.12419	295.11871	265.10814								
	Deoxynivalenol-3-glucoside	C21H30O11	C22H31O13	C21H29O11	C20H27O10								
	(S-2)**	458.17881	503.17701	457.17153	427.16097								
	Deoxynivalenol-15-glucoside	C21H30O11	C22H31O13	C21H29O11		C14H17O5							
	(S-3)**	458.17881	503.17701	457.17153		265.1081							
	Deoxynivalenol-7-glucoside	C21H30O11	C22H31O13	C21H29O11						C15H19O6			
	(S-4)**	458.17881	503.17701	457.17153						295.11871			
Deoxynivalenol with 2 glucose units	Deoxynivalenol-3-diglucoside	C27H40O16	C28H41O18	C27H39O16	C26H37O15								
	(S-5, S-6)**	620.23163	665.22984	619.22436	589.21379								
	Deoxynivalenol-15-diglucoside	C27H40O16	C28H41O18	C27H39O16			C14H17O5						
	(S-7, S-8)**	620.23163	665.22984	619.22436			265.1081						
	Deoxynivalenol-7-diglucoside	C27H40O16	C28H41O18	C27H39O16							C15H19O6		
	(S-9, S-10)**	620.23163	665.22984	619.22436							295.11871		
	Deoxynivalenol-3-glucoside-15-glucoside	C27H40O16	C28H41O18	C27H39O16		C20H27O10							
	(S-11)**	620.23163	665.22984	619.22436		427.161							
	Deoxynivalenol-3-glucoside-7-glucoside	C27H40O16	C28H41O18	C27H39O16						C21H29O11			
	(S-12)**	620.23163	665.22984	619.22436						457.17153			
	Deoxynivalenol-7-glucoside -15-glucoside	C27H40O16	C28H41O18	C27H39O16						C21H29O11			
	(S-13)**	620.23163	665.22984	619.22436						457.17153			
Deoxynivalenol with 3 glucose units	Deoxynivalenol-3-triglucoside	C33H50O21	C34H51O23	C33H49O21	C32H47O20								
	(S-14–S-18)**	782.28446	827.28266	781.27718	751.26662								
	Deoxynivalenol-15-triglucoside	C33H50O21	C34H51O23	C33H49O21				C14H17O5					
	(S-19–S-23)**	782.28446	827.28266	781.27718				265.1081					
	Deoxynivalenol-7-triglucoside	C33H50O21	C34H51O23	C33H49O21								C15H19O6	
	(S-24–S-28)**	782.28446	827.28266	781.27718								295.11871	
	Deoxynivalenol-3-	C33H50O21	C34H51O23	C33H49O21		C26H37O15							

	diglucoside -15-glucoside (S-29, S-30)**	782.28446	827.28266	781.27718	589.2138						
	Deoxynivalenol-3-glucoside -15-diglucoside (S-31, S-32)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718		C20H27O10 427.161					
	Deoxynivalenol-7-glucoside -15-diglucoside (S-33, S-34)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718				C27H39O16 619.22436			
	Deoxynivalenol-7-diglucoside -15-glucoside (S-35, S-36)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718					C21H29O11 457.17153		
	Deoxynivalenol-3-diglucoside -7-glucoside (S-37, S-38)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718				C27H39O16 619.22436			
	Deoxynivalenol-3-glucoside -7-diglucoside (S-39, S-40)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718					C21H29O11 457.17153		
	Deoxynivalenol-3-glucoside-7-glucoside-15-glucoside (S-41)**	C33H50O21 782.28446	C34H51O23 827.28266	C33H49O21 781.27718				C27H39O16 619.22436			
Deoxynivalenol with 4 glucose units	Deoxynivalenol-3-tetraglucoside (S-42–S-54)**	C39H60O26 944.33728	C40H61O28 989.33548	C39H59O26 943.33	C38H57O25 913.31944						
	Deoxynivalenol-15-tetraglucoside (S-55–S-67)**	C39H60O26 944.33728	C40H61O28 989.33548	C39H59O26 943.33			C14H17O5 265.1081				
	Deoxynivalenol-7-tetraglucoside (S-68–S-80)**	C39H60O26 944.33728	C40H61O28 989.33548	C39H59O26 943.33						C15H19O6 295.11871	
	Deoxynivalenol-3-diglucoside-15-diglucoside (S-81–S-84)**	C39H60O26 944.33728	C40H61O28 989.33548	C39H59O26 943.33		C26H37O15 589.2138					
	Deoxynivalenol-3-diglucoside-7-diglucoside (S-85–S-88)**	C39H60O26 944.33728	C40H61O28 989.33548	C39H59O26 943.33					C27H39O16 619.22436		
	Deoxynivalenol-7-diglucoside-15-diglucoside	C39H60O26	C40H61O28	C39H59O26					C27H39O16		

(S-89–S-92)**	944.33728	989.33548	943.33				619.22436	
Deoxynivalenol-3-triglucoside-15-glucoside	C39H60O26	C40H61O28	C39H59O26	C32H47O20				
(S-93–S-97)**	944.33728	989.33548	943.33	751.2666				
Deoxynivalenol-3-triglucoside-7-glucoside	C39H60O26	C40H61O28	C39H59O26			C33H49O21		
(S-98–S-102)**	944.33728	989.33548	943.33			781.27718		
Deoxynivalenol-3-glucoside-15-triglucoside	C39H60O26	C40H61O28	C39H59O26		C20H27O10			
(S-103–S-107)**	944.33728	989.33548	943.33		427.161			
Deoxynivalenol-7-glucoside-15-triglucoside	C39H60O26	C40H61O28	C39H59O26			C33H49O21		
(S-108–S-112)**	944.33728	989.33548	943.33			781.27718		
Deoxynivalenol-3-glucoside-7-triglucoside	C39H60O26	C40H61O28	C39H59O26				C21H29O11	
(S-113–S-117)**	944.33728	989.33548	943.33				457.17153	
Deoxynivalenol-7-triglucoside-15-glucoside	C39H60O26	C40H61O28	C39H59O26				C21H29O11	
(S-118–S-122)**	944.33728	989.33548	943.33				457.17153	

* Calculated based on Berthiller et al., and Dall'Asta et al.[1,9]

** Possible structures of deoxynivalenol-glycosides are depicted in the Supporting information (S-1–S-122), page 2 – 13.