SUPPORTING INFORMATION

Modeling Plasma-Induced Modifications in Alginate Biopolymers at the Atomic Scale

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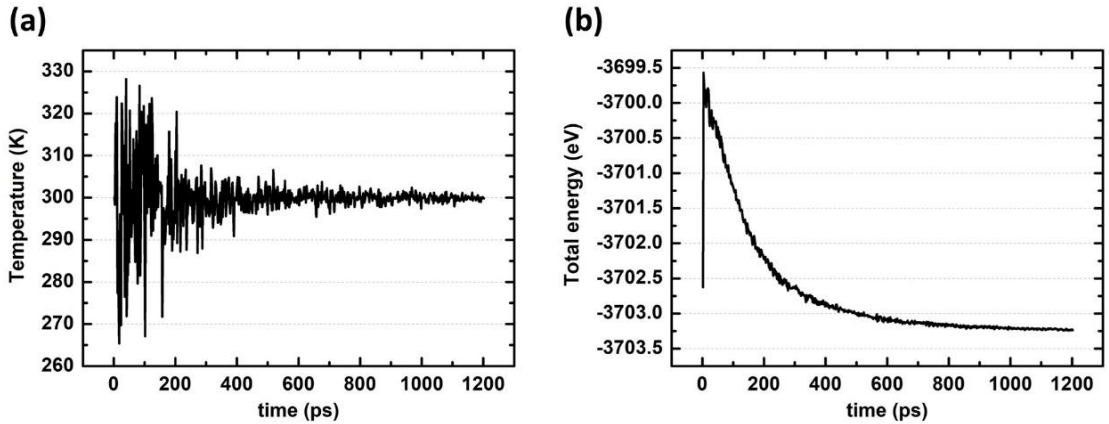
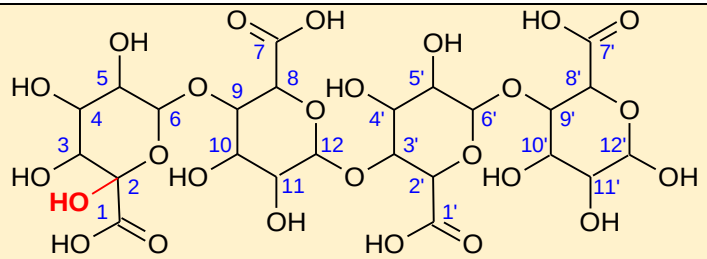
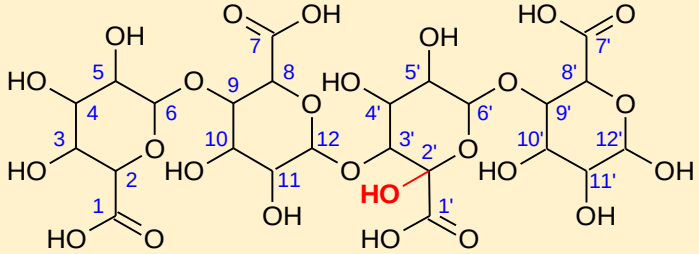
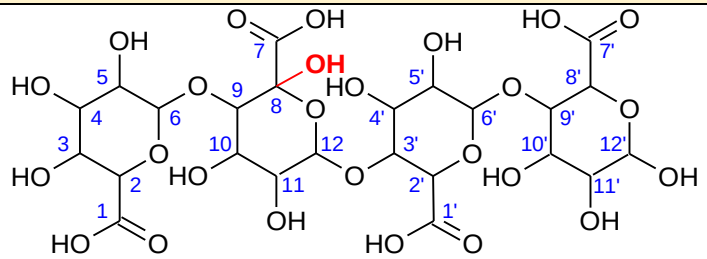
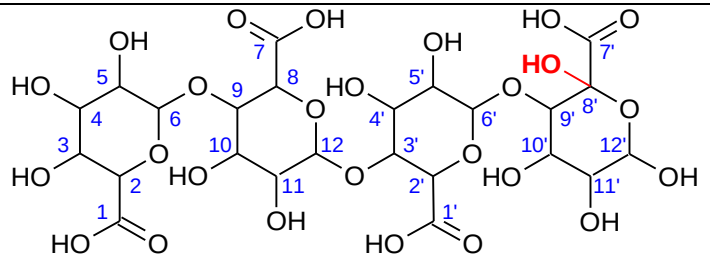
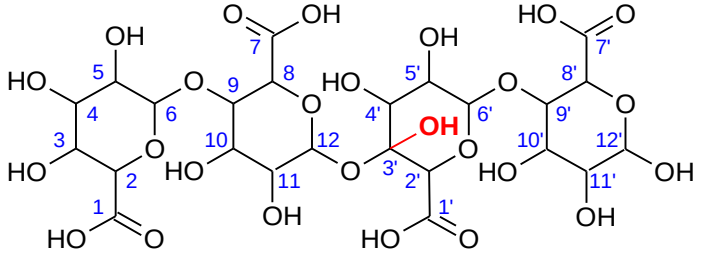
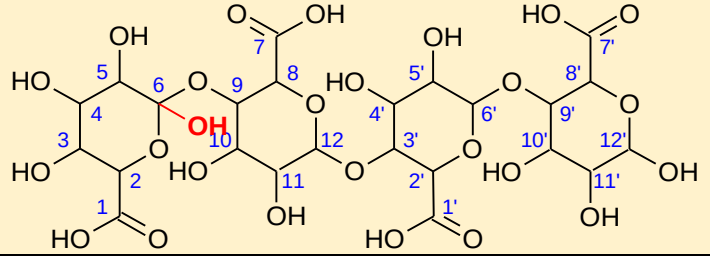
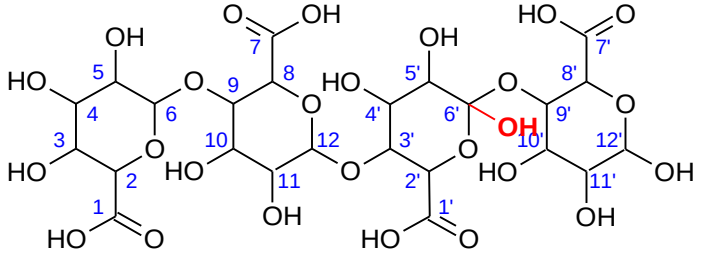
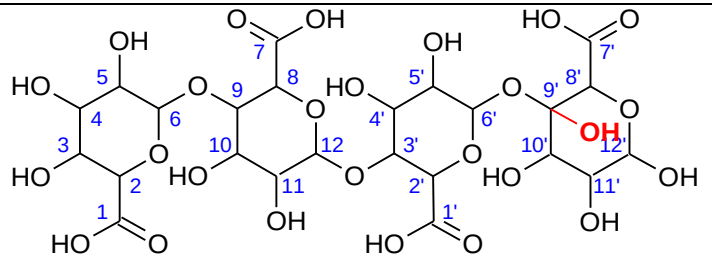
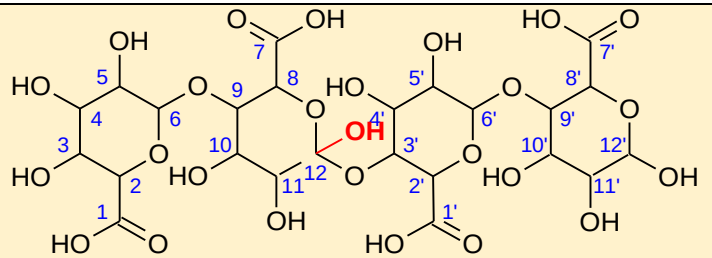
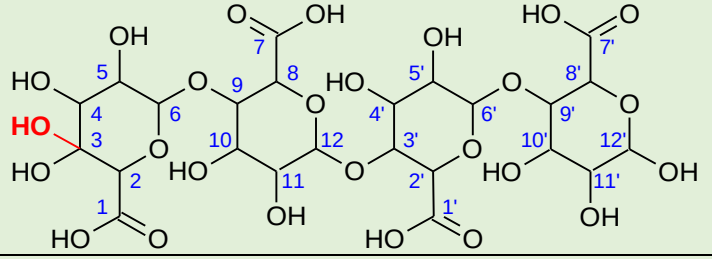
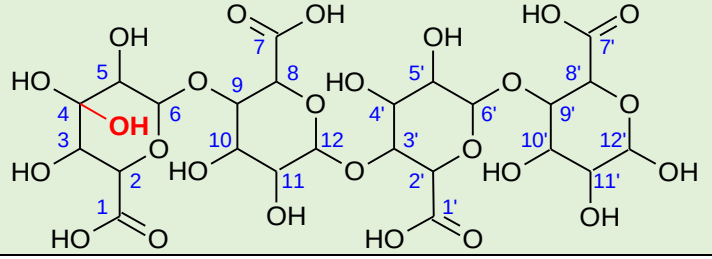


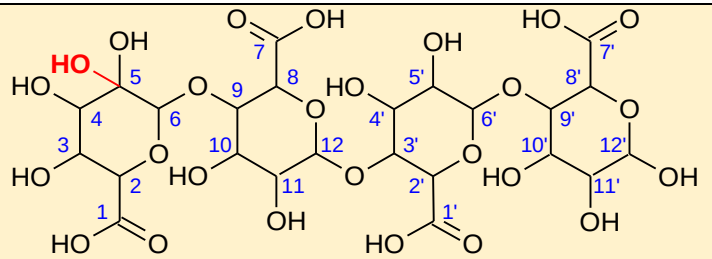
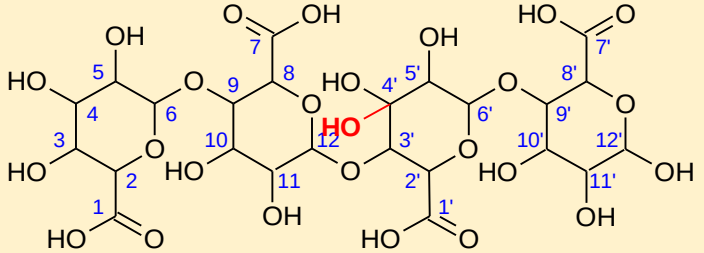
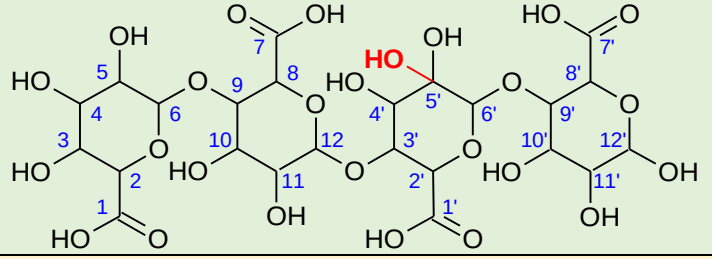
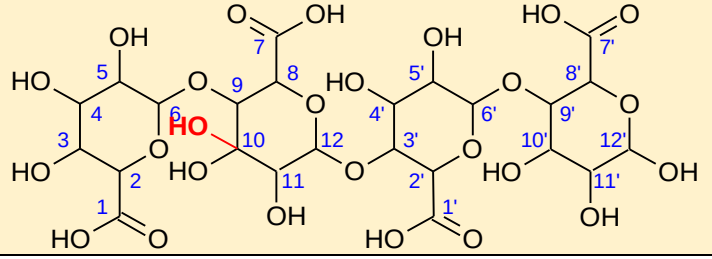
Figure S1. Time evolution of the temperature and total energy of the alginic acid model system, demonstrating that the equilibration time of 1200 ps was sufficient for obtaining a well-thermalized structure.

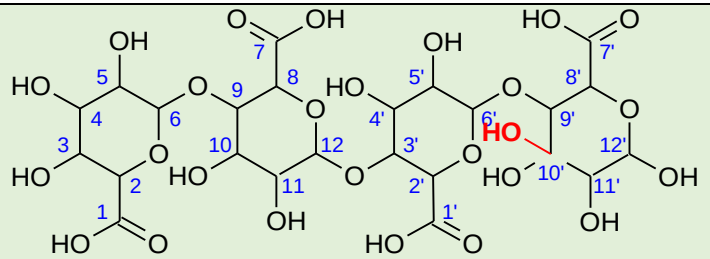
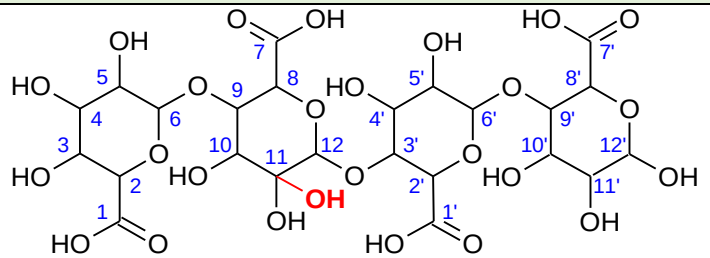
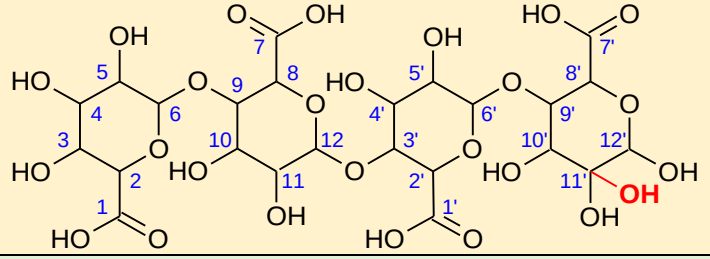
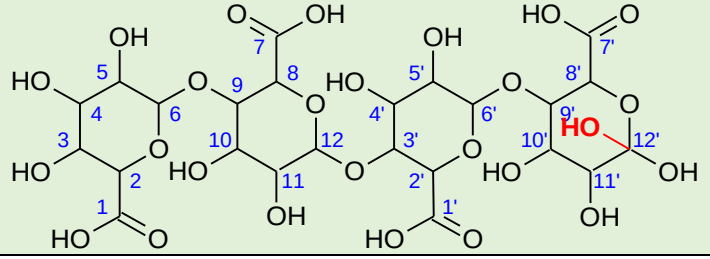
Table S1. Overview of all reaction mechanisms observed in the DFTB-MD simulations following the interaction of O atoms with the alginic acid tetramer. The numbering of the C atoms corresponds to Figure 1 in the main text. Note that most of the reactions are initiated by H-abstraction from different C or O atoms (1-75) and the last ones (76-85) are initiated by O addition. Color code: green = events that happen with frequency higher than 2.5%; yellow = events that happen with frequency between 2.5 and 1.5% (values included); white = events that happen with frequency lower than 1.5%.

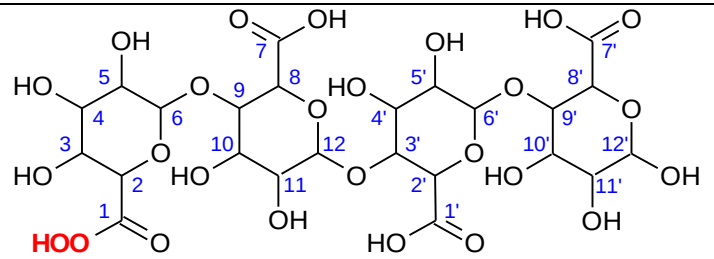
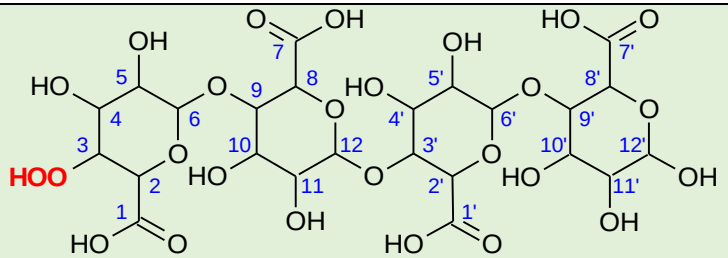
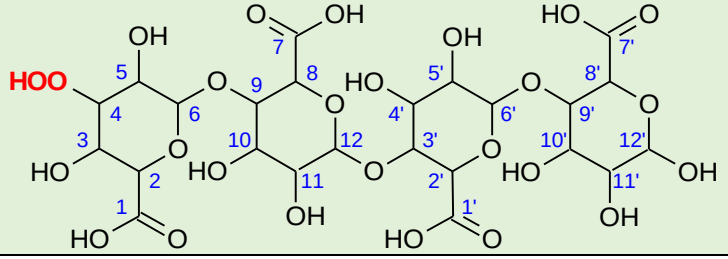
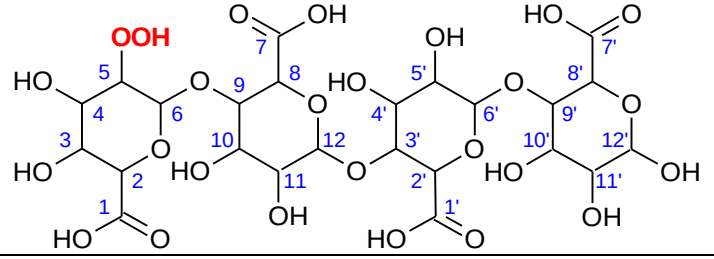
No.	H-abstraction	Number of events	Description	Structure	%
1	C_2H	5	C_2-OH is formed α-hydroxy acid $C_{24}H_{34}O_{26}$ (738 Da)		2.5
2	$C_{2'}H$	4	$C_{2'}$-OH is formed α-hydroxy acid $C_{24}H_{34}O_{26}$ (738 Da)		2.0
3	C_8H	1	C_8-OH is formed α-hydroxy acid $C_{24}H_{34}O_{26}$ (738 Da)		0.5

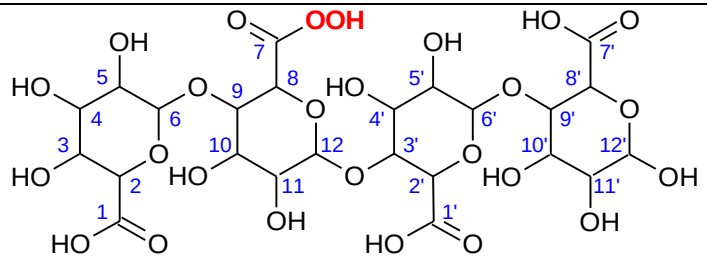
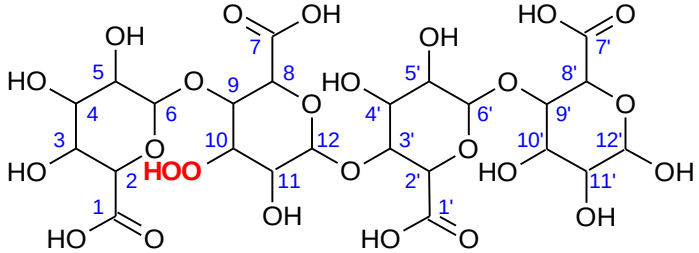
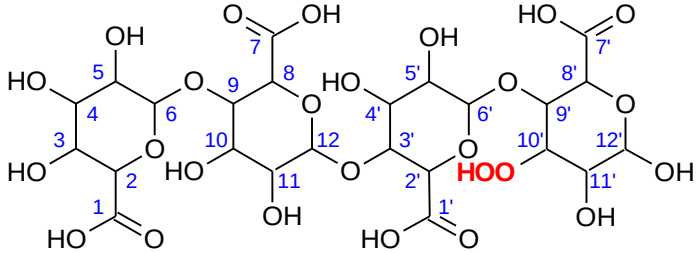
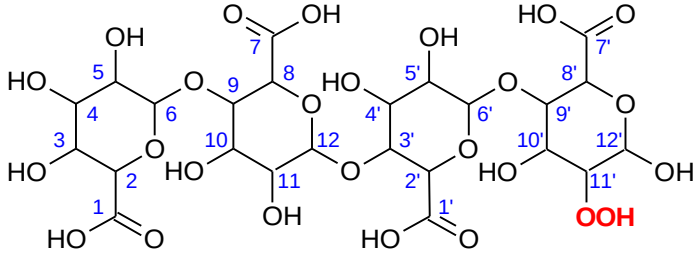
4	$C_{8'}H$	2	$C_{8'}$-OH is formed α-hydroxy acid $C_{24}H_{34}O_{26}$ (738 Da)		1.0
5	$C_{3'}H$	2	$C_{3'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		1.0
6	$C_{6}H$	4	C_{6}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		2.0
7	$C_{6'}H$	2	$C_{6'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		1.0

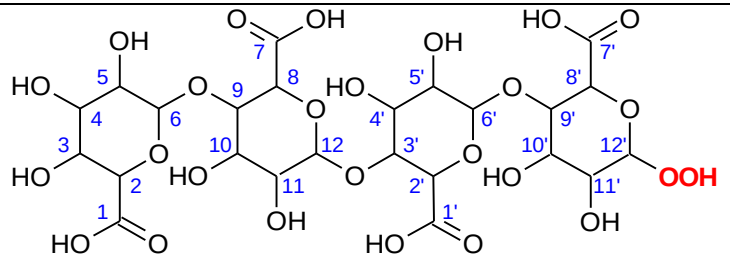
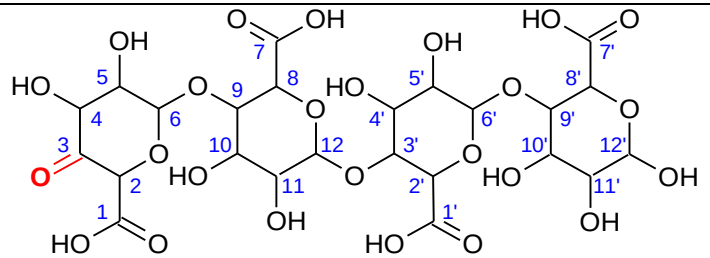
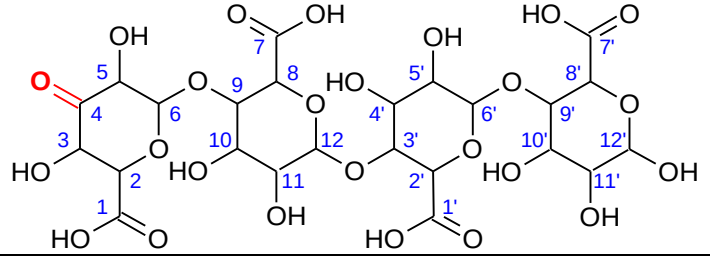
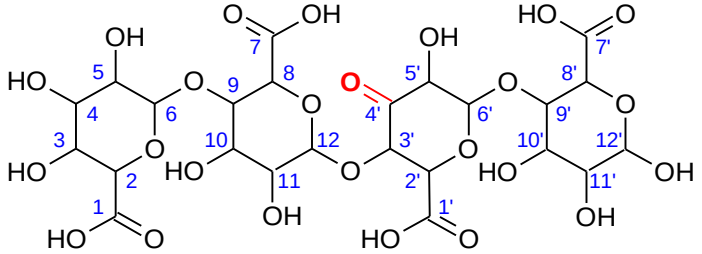
8	$C_{9'}H$	1	$C_{9'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		0.5
9	$C_{12}H$	4	C_{12}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		2.0
10	$C_{3}H$	6	C_{3}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		3.0
11	$C_{4}H$	6	C_{4}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		3.0

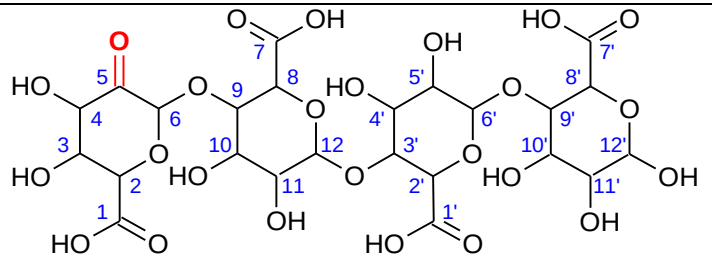
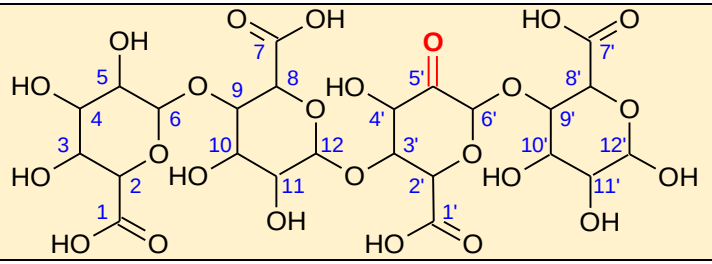
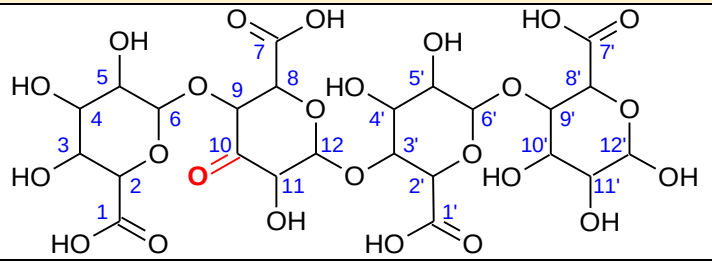
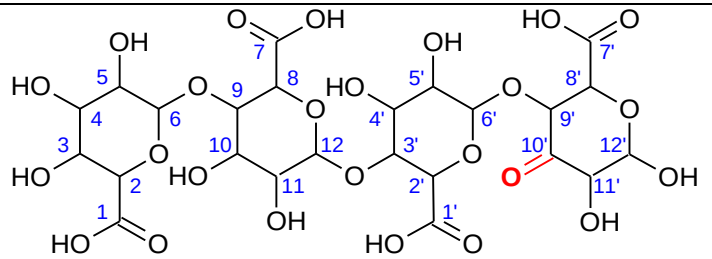
12	C_5H	3	C_5-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		1.5
13	$C_{4'}H$	5	$C_{4'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		2.5
14	$C_{5'}H$	8	$C_{5'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		4.0
15	$C_{10}H$	4	C_{10}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		2.0

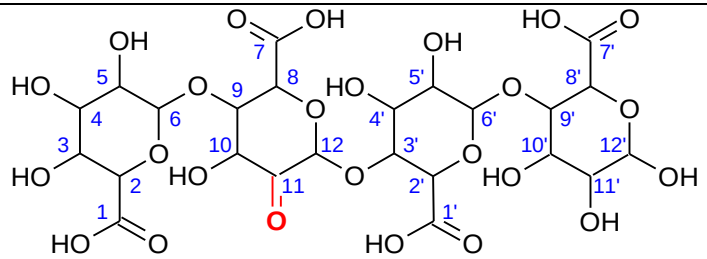
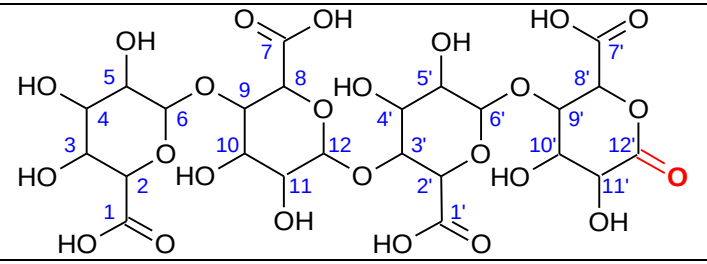
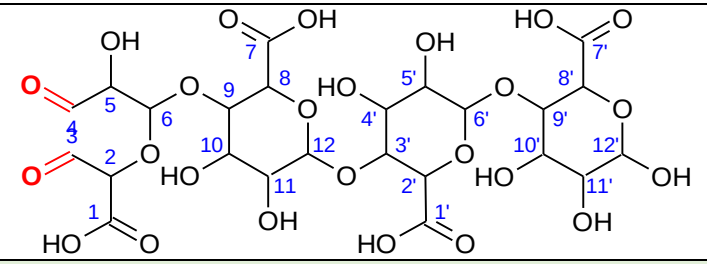
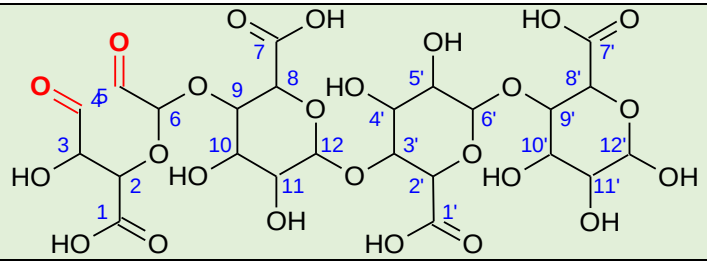
16	$C_{10'}H$	7	$C_{10'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		3.5
17	$C_{11}H$	2	C_{11}-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		1.0
18	$C_{11'}H$	4	$C_{11'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		2.0
19	$C_{12'}H$	7	$C_{12'}$-OH is formed geminal diol $C_{24}H_{34}O_{26}$ (738 Da)		3.5

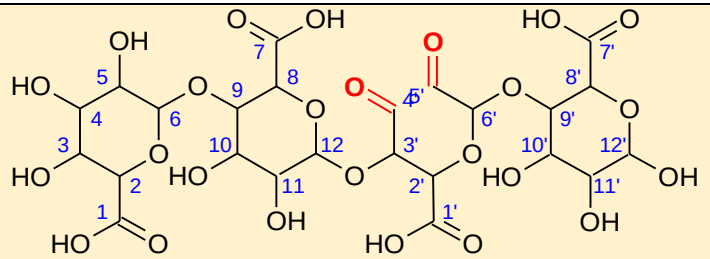
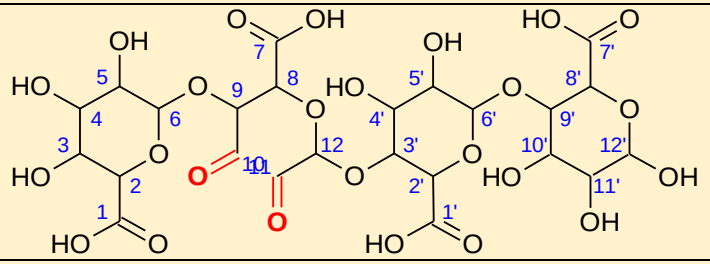
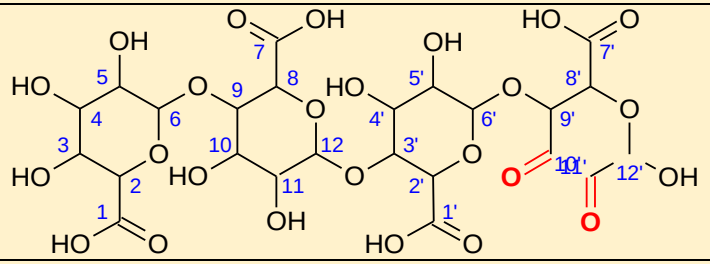
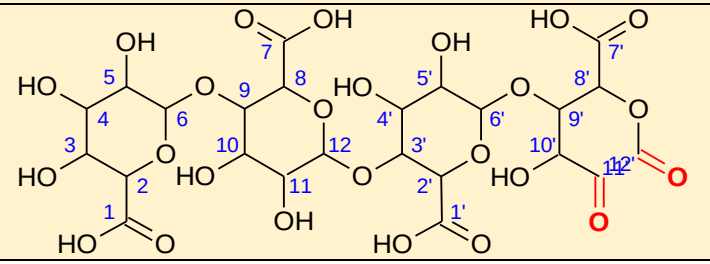
20	C_1OH	1	C_1O-OH is formed peroxyacid $C_{24}H_{34}O_{26}$ (738 Da)		0.5
21	C_3OH	8	C_3O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		4.0
22	C_4OH	9	C_4O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		4.5
23	C_5OH	2	C_5O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		1.0

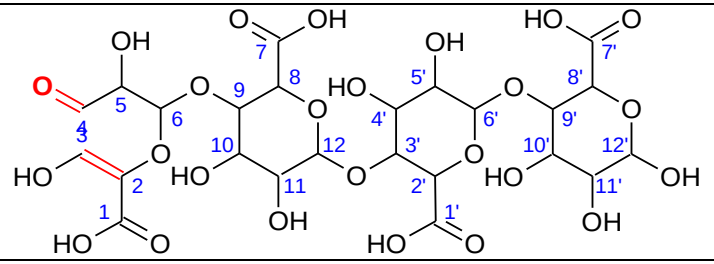
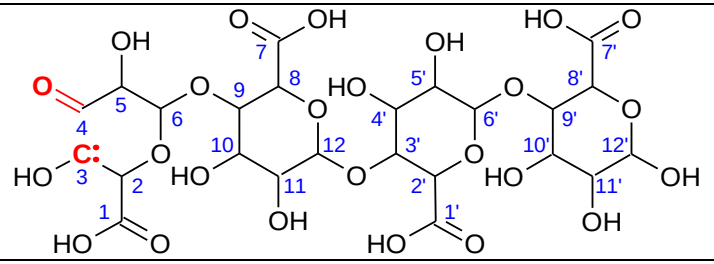
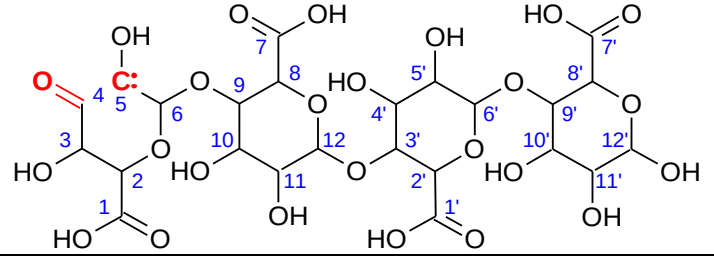
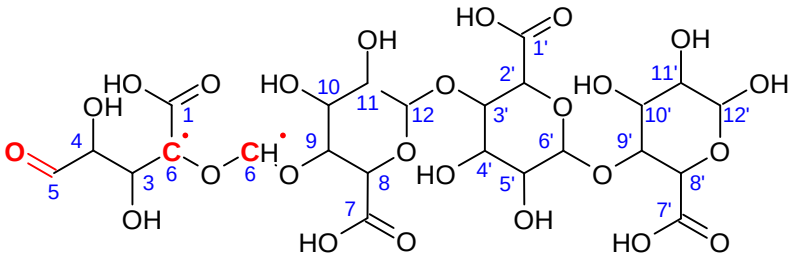
24	C_7OH	1	C_7O-OH is formed peroxyacid $C_{24}H_{34}O_{26}$ (738 Da)		0.5
25	$C_{10}OH$	1	C_{10}O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		0.5
26	$C_{10'}OH$	2	$C_{10'}$O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		1.0
27	$C_{11'}OH$	2	$C_{11'}$O-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		1.0

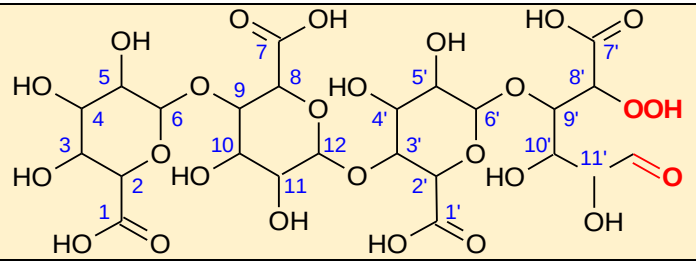
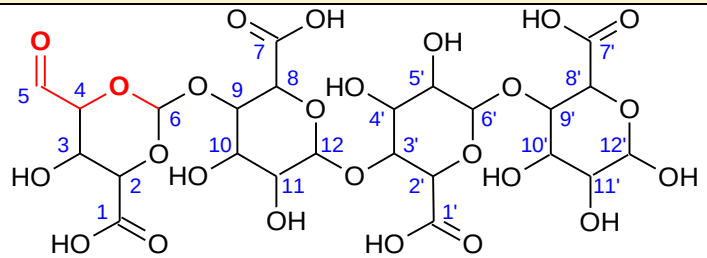
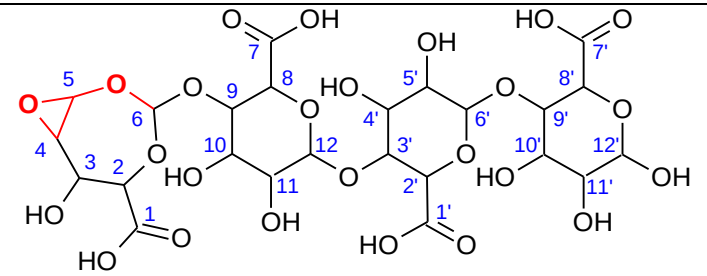
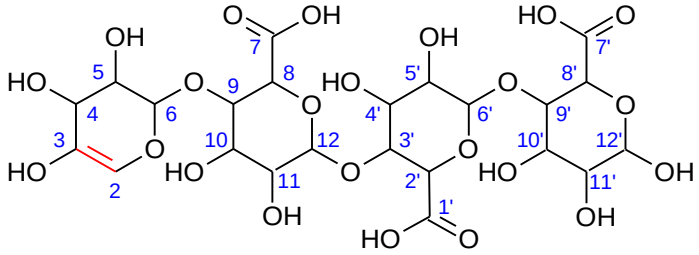
28	$C_{12'}OH$	1	$C_{12'}O$-OH is formed hydroperoxide $C_{24}H_{34}O_{26}$ (738 Da)		0.5
29	C_3H and C_3OH	1	H_2O and C_3=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
30	C_4H and C_4OH	1	H_2O and C_4=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
31	$C_{4'}H$ and $C_{4'}OH$	1	H_2O and $C_{4'}$=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5

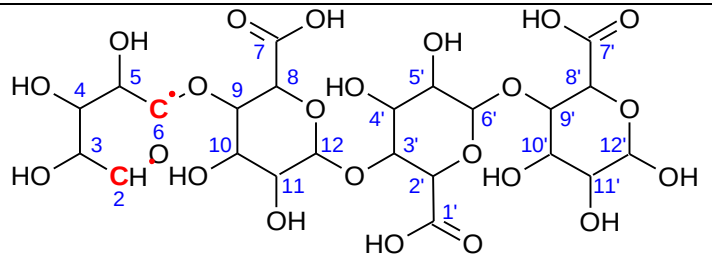
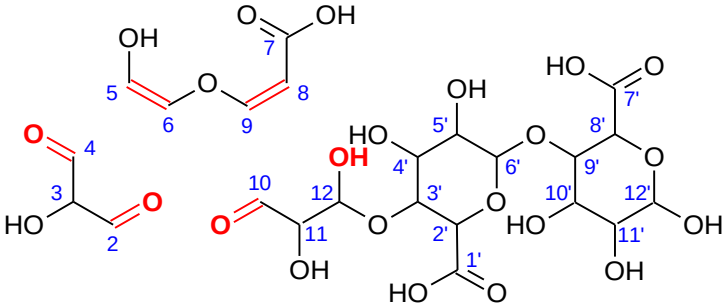
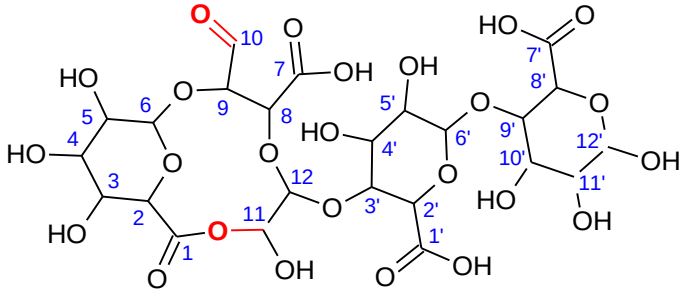
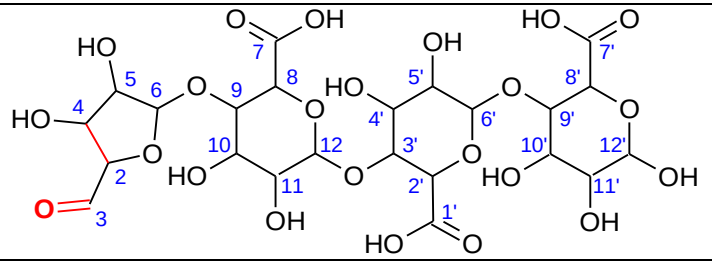
32	C_5H and C_5OH	1	H_2O and C_5=O is ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
33	$C_{5'}H$ and $C_{5'}OH$	3	H_2O and $C_{5'}$=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.5
34	$C_{10}H$ and $C_{10}OH$	1	H_2O and C_{10}=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
35	$C_{10'}H$ and $C_{10'}OH$	1	H_2O and $C_{10'}$=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5

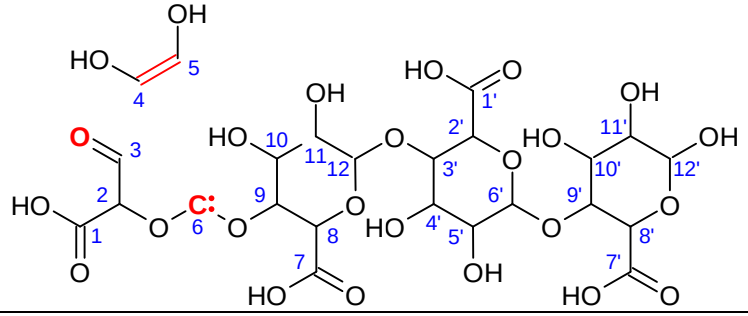
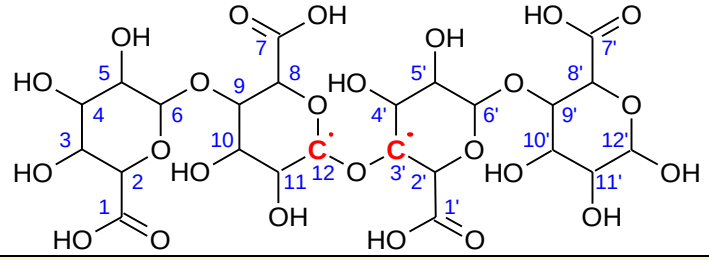
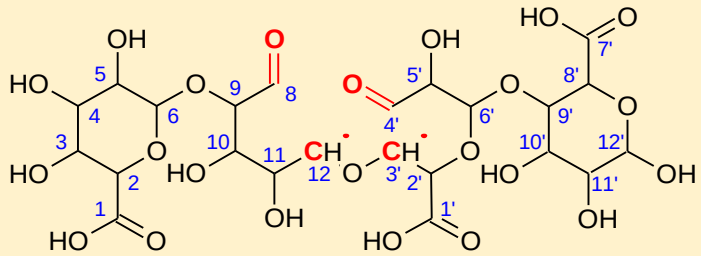
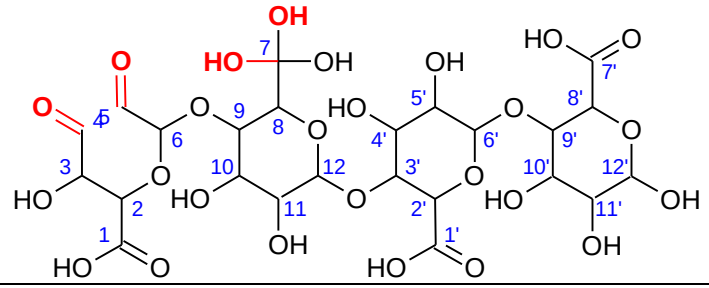
36	$C_{11}H$ and $C_{11}OH$	1	H_2O and C_{11}=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
37	$C_{12'}H$ and $C_{12'}OH$	2	H_2O and $C_{12'}$=O is formed ketone group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.0
38	C_3OH and C_4OH	2	C_3-C_4 bond is broken, H_2O, C_3=O and C_4=O are formed 2 aldehyde groups, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.0
39	C_4OH and C_5OH	8	C_4-C_5 bond is broken, H_2O, C_4=O and C_5=O are formed 2 aldehyde groups, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		4.0

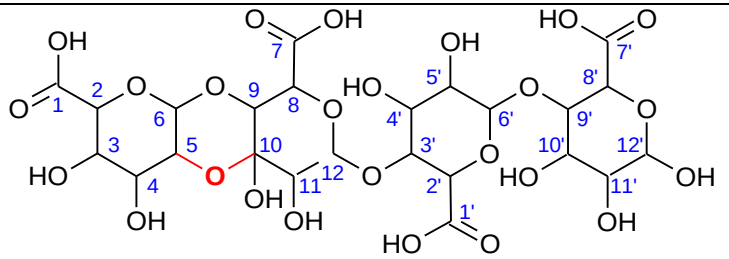
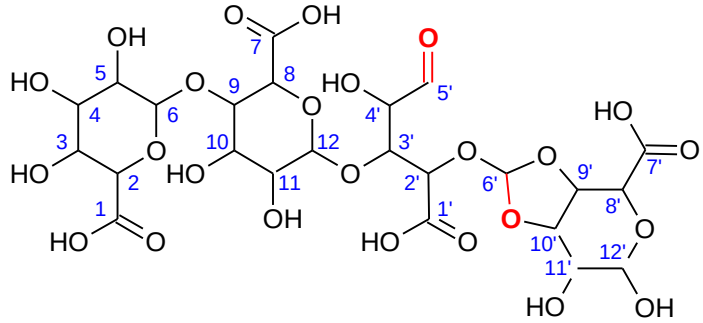
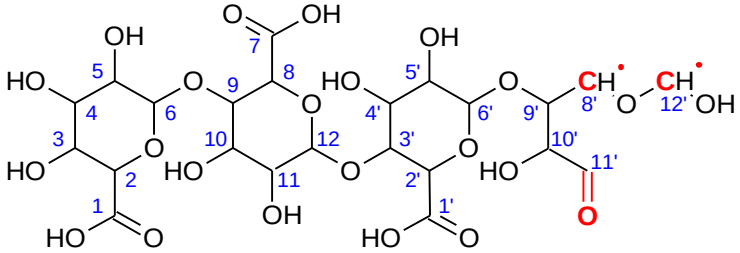
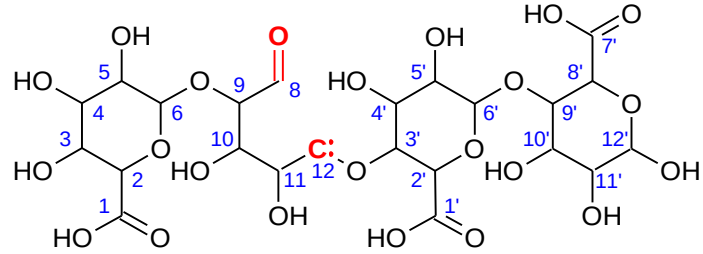
40	$C_{4'}H$ and $C_{5'}OH$	3	$C_{4'}$-$C_{5'}$ bond is broken, H_2O, $C_{4'}$=O and $C_{5'}$=O are formed 2 aldehyde groups, ring 3 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.5
41	$C_{10}OH$ and $C_{11}OH$	3	C_{10}-C_{11} bond is broken, H_2O, C_{10}=O and C_{11}=O are formed 2 aldehyde groups, ring 2 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.5
42	$C_{10'}H$ and $C_{11'}OH$	3	$C_{10'}$-$C_{11'}$ bond is broken, H_2O, $C_{10'}$=O and $C_{11'}$=O are formed 2 aldehyde groups, ring 4 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		1.5
43	$C_{11'}H$ and $C_{12'}OH$	5	$C_{11'}$-$C_{12'}$ bond is broken, H_2O, $C_{11'}$=O and $C_{12'}$=O are formed 2 aldehyde groups, ring 4 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		2.5

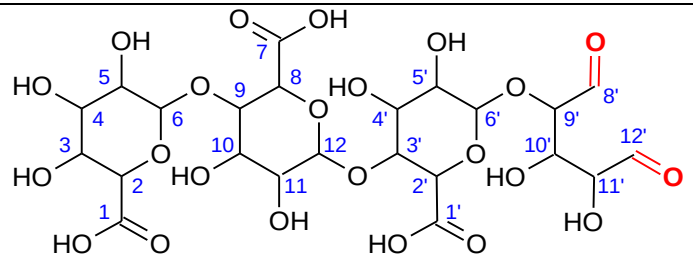
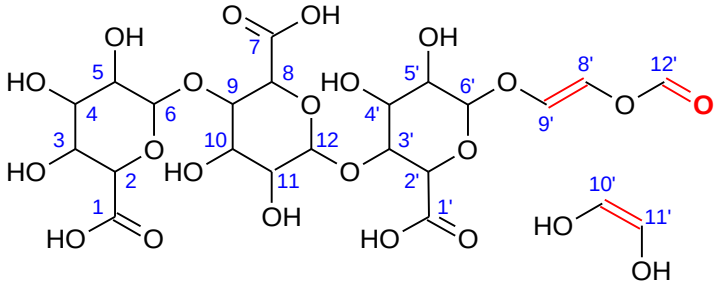
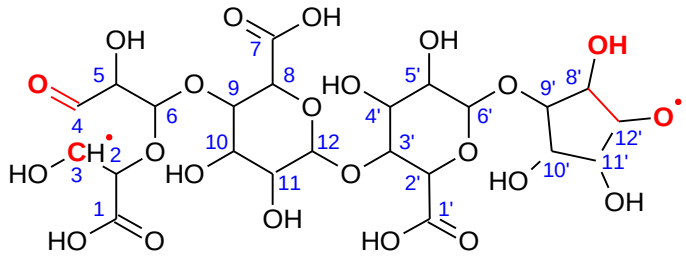
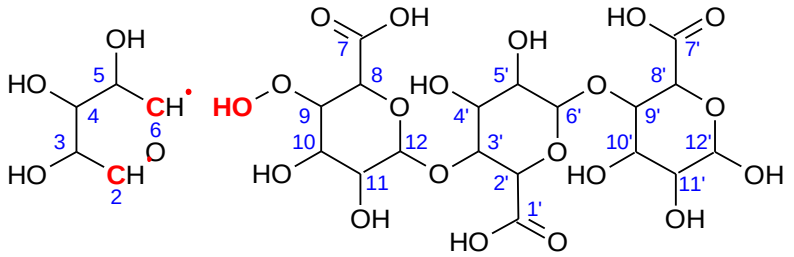
44	C_2H and C_4OH	1	H_2O is formed, C_3-C_4 bond is broken, C_2=C_3 is formed aldehyde group, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
45	C_3H and C_4OH	1	H_2O is formed, C_3-C_4 bond is broken aldehyde and carbene C_2-(:C_3)-O formation, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
46	C_4OH and C_5H	1	H_2O is formed, C_4-C_5 bond is broken aldehyde and carbene C_6-(:C_5)-O formation, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
47	C_2H and C_5OH	1	H_2O is formed, C_5-C_6 bond is broken, C_5=O, $^{\bullet}C_2$ and $^{\bullet}C_6$ are formed aldehyde group, ring 1 opening $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5

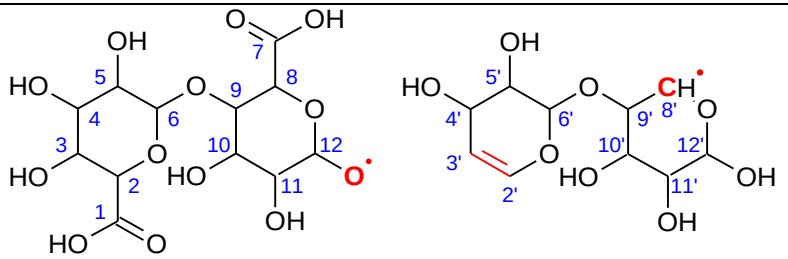
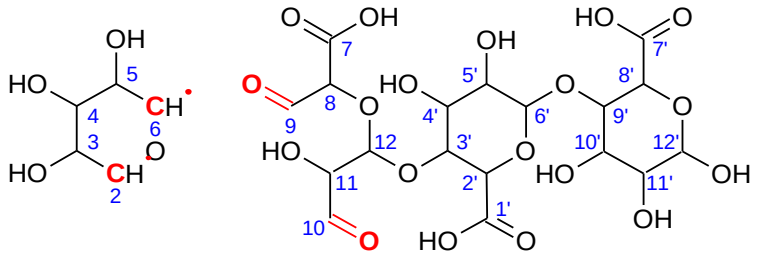
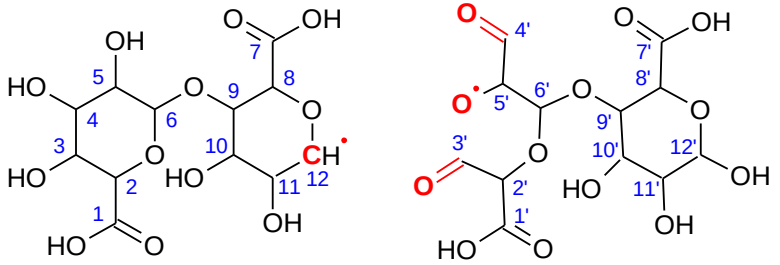
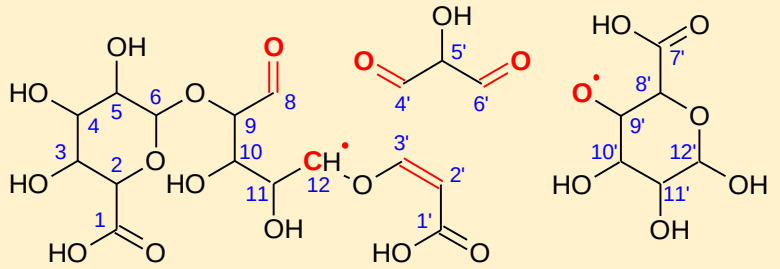
48	$C_{12'}OH$	3	$C_{8'}O$-$C_{12'}$ bond is broken, $C_{8'}O$-OH is formed aldehyde and hydroperoxide groups, ring 4 opening $C_{24}H_{34}O_{26}$ (738 Da)		1.5
49	C_5OH and later on C_4OH	1	C_5-C_6 bond is broken, ring 1 opening, H_2O is formed, C_4O-C_6 is formed aldehyde and ether group $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
50	C_5OH and later on C_4OH	1	C_5-C_6 bond is broken (aldehyde formation), ring 1 opening, C_5O-C_6 and C_4O-C_5 are formed $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
51	C_1OH and C_2H	2	H_2O formation and CO_2 liberation, carbene C_3=C_2 formation $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		1.0

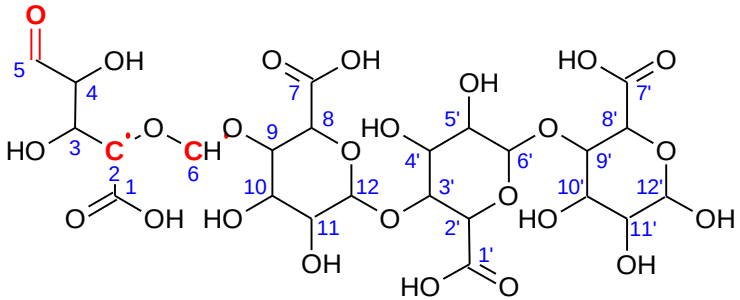
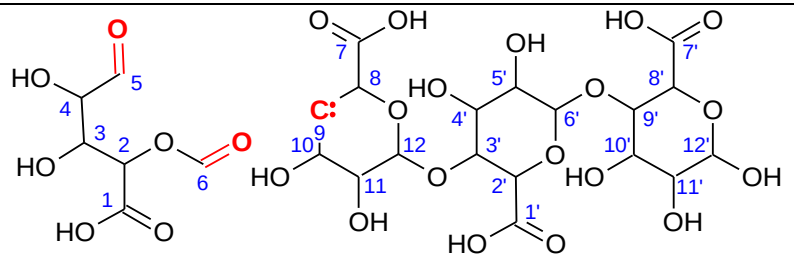
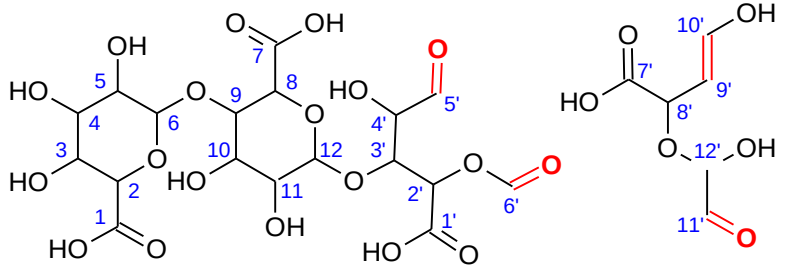
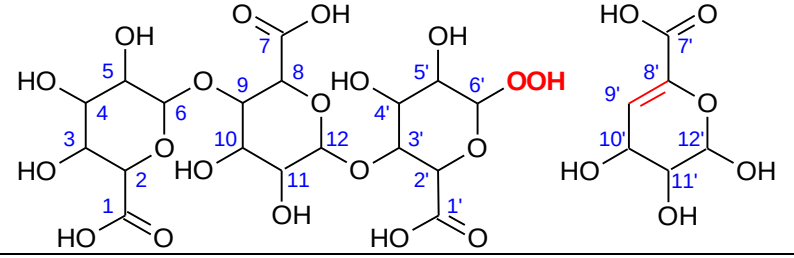
52	C_1OH and C_6H	1	CO_2 liberation, H_2O formation, $^{\bullet}C_2$ and $^{\bullet}C_6$ formation $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5
53	C_1OH and later on $C_{10}OH$	2	H-abs. from C_1OH: CO_2 liberation, C_2O-C_6 bond breaking, ring 1 opening (aldehyde) H-abs. from $C_{10}OH$: H_2O formation, C_9-C_{10} bond breaking, ring 2 opening (aldehyde form.), C_5=C_6 and C_8=C_9 formation, C_4-C_5 and C_8-OC_{12} bonds breaking, H-transfer from C_4OH to $C_{12}O^{\bullet}$ (aldehyde form.) $C_{15}H_{22}O_{16}$ (458 Da) + $C_5H_6O_4$ (130 Da) + $C_3H_4O_3$ (88 Da) + H_2O (18 Da) + CO_2 (44 Da)		1.0
54	C_1OH and $C_{10}OH$	1	H_2O formation, C_{10}-C_{11} bond breaking (ring 2 opening and aldehyde formation), C_1O-C_{11} bond formation (larger ring) $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
55	C_1OH and C_3OH	1	H_2O formation, CO_2 liberation, C_3-C_4 bond breaking and C_2-C_4 bond formation (aldehyde and small ring formation) $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5

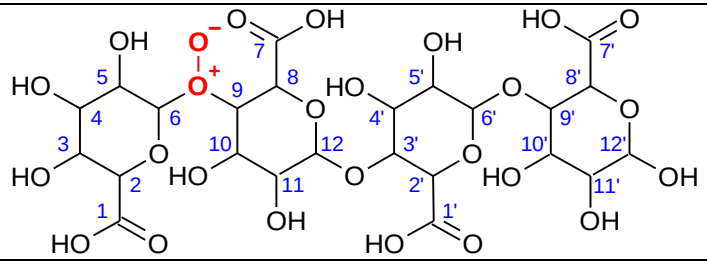
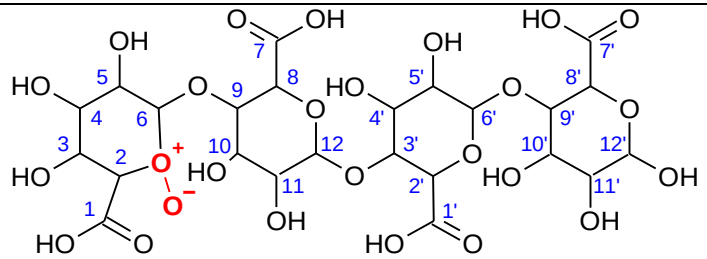
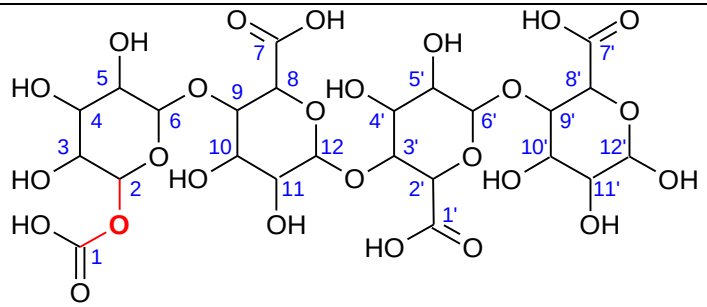
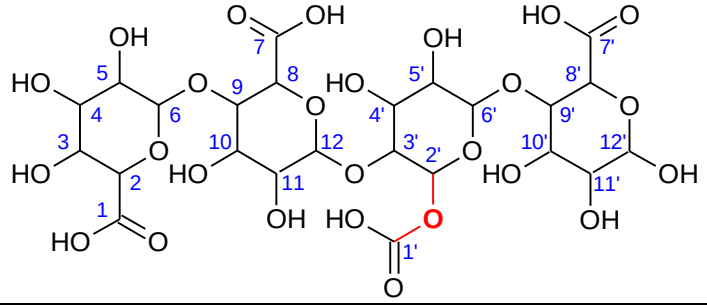
56	C_3OH and later on C_6H	1	H-abs. from C_3OH: C_3-C_4 bond breaking (aldehyde formation), C_4=C_5 double bond formation, C_5-C_6 bond breaking, H-abs. from C_6H: H_2O formation, 1,2-ethenediol formation, O-(:C_6)-O formation $C_{22}H_{28}O_{23}$ (660 Da) + $C_2H_4O_2$ (60 Da) + H_2O (18 Da)		0.5
57	$C_{3'}H$ and $C_{12}H$	1	H_2O formation, 2 C radicals formation $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
58	C_7OH and later on $C_{4'}OH$	5	H-abs. from $C_{4'}OH$: $C_{3'}$-$C_{4'}$ bond breaking (aldehyde formation and ring 3 opening) H-abs. from C_7OH: CO_2 liberation, H_2O formation, C_8O-C_{12} bond breaking (ring 2 opening and aldehyde formation), $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		2.5
59	C_5OH and later on C_4OH	1	C_7OH bond formation, H-abstraction from C_4OH by C_7O, C_4-C_5 bond breaking, (ring 1 opening, aldehyde and triol formation) $C_{24}H_{34}O_{26}$ (738 Da)		0.5

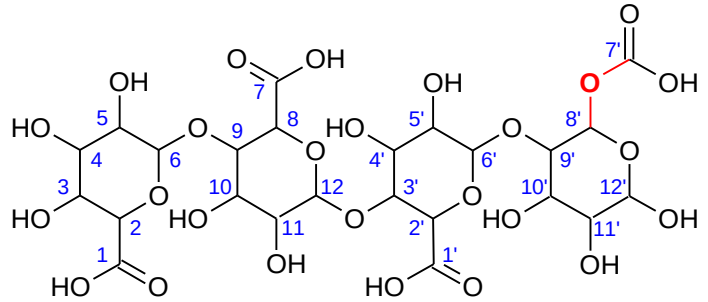
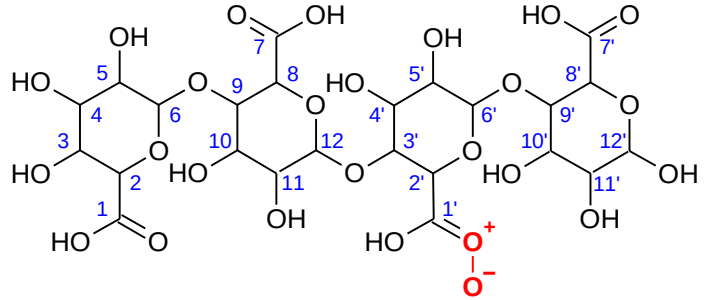
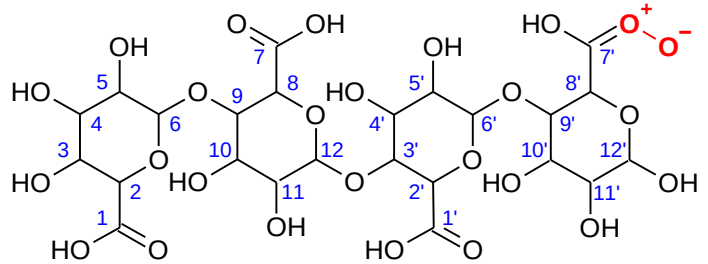
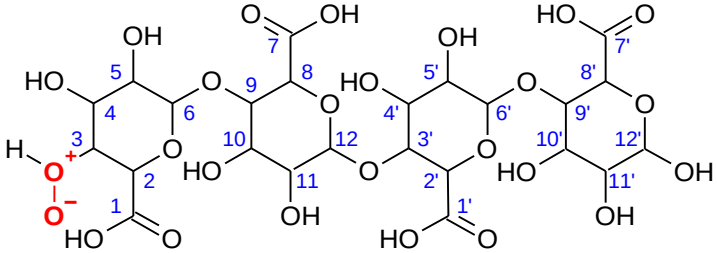
60	C_5OH and $C_{10}H$	1	H_2O formation, C_5-O-C_{10} formation (extra ring formation) $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
61	$C_{5'}OH$ and $C_{10'}OH$	1	H_2O formation, $C_{5'}$-$C_{6'}$ bond breaking (ring 3 opening, aldehyde formation), $C_{6'}$-O-$C_{10'}$ formation (small ring formation) $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
62	$C_{7'}OH$ and $C_{11'}OH$	2	H_2O formation, CO_2 liberation, $C_{11'}$-$C_{12'}$ bond breaking (ring 4 opening and aldehyde formation), $^{\bullet}C_{8'}$ and $^{\bullet}C_{12'}$ formation $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		1.0
63	C_7OH and later on $C_{12}H$	2	CO_2 liberation, C_8O-C_{12} bond breaking (ring 2 opening and aldehyde formation), H_2O formation, :C_{12} formation $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		1.0

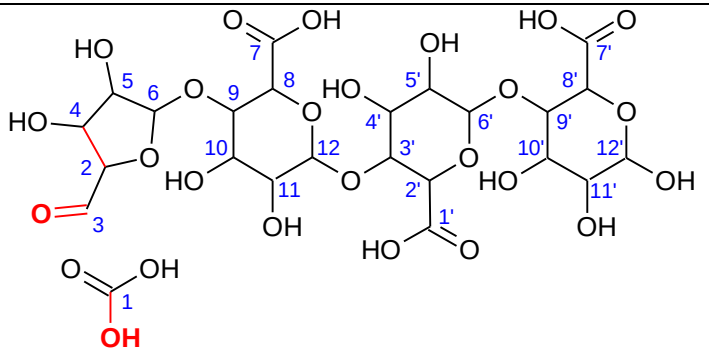
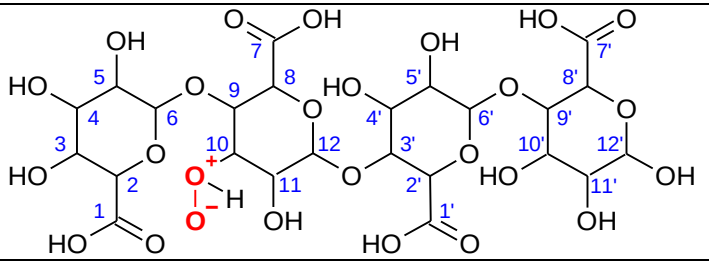
64	$C_{7'}OH$ and $C_{12'}OH$	1	H_2O formation, CO_2 liberation, $C_{8'}O$-$C_{12'}$ bond breaking (ring 4 opening and aldehyde formation) $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5
65	$C_{12'}OH$ and later on $C_{7'}OH$	1	$C_{11'}$-$C_{12'}$ bond breaking (ring 4 opening and aldehyde formation), H_2O formation, CO_2 liberation, $C_{8'}$=$C_{9'}$ double bond formation and $C_{9'}$=$C_{10'}$ breaking (1,2-ethenediol formation) $C_{21}H_{28}O_{21}$ (616 Da) + $C_2H_4O_2$ (60 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5
66	C_4OH and later on $C_{12'}OH$	1	C_3-C_4 bond breaking (ring 1 opening and aldehyde formation), H_2O formation, $C_{8'}O$-$C_{12'}$ bond breaking (ring 4 opening and aldehyde formation), H-transfer from $C_{7'}OH$ to $C_{8'}O$ (CO_2 liberation), $C_{8'}$-$C_{12'}$ bond formation, $^{\bullet}C_3$ formation $C_{23}H_{32}O_{23}$ (676 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5
67	C_7OH and later on C_1OH	2	Binding to C_6-O(=**O**)-C_9, H-abstraction from C_7OH (hydroperoxyl group formation), C_6-OC_9 glycosidic bond cleavage, H-transfer from C_1OH to $C_7O^{\bullet}$ (CO_2 liberation), $^{\bullet}C_2$ and $^{\bullet}C_6$ formation $C_{18}H_{26}O_{20}$ (562 Da) + $C_5H_8O_4$ (132 Da) + CO_2 (44 Da)		1.0

68	$C_{1'}OH$ and $C_{7'}OH$	1	H_2O formation, 2 CO_2 liberation, $C_{2'}=C_{3'}$ double bond formation, $C_{12}O$-$C_{3'}$ glycosidic bond cleavage, $C_{12}O^{\bullet}$ and $^{\bullet}C_{8'}$ formation $C_{12}H_{17}O_{13}$ (369 Da) + $C_{10}H_{15}O_8$ (263 Da) + H_2O (18 Da) + $2CO_2$ (2·44 Da)		0.5
69	$C_{10}OH$ and later on C_1OH	1	C_9-C_{10} bond breaking (ring 2 opening and aldehyde formation), C_6-OC_9 glycosidic bond cleavage, H-abstraction from C_1OH (H_2O formation and CO_2 liberation), $^{\bullet}C_2$ and $^{\bullet}C_6$ formation $C_{18}H_{24}O_{19}$ (544 Da) + $C_5H_8O_4$ (132 Da) + H_2O (18 Da) + CO_2 (44 Da)		0.5
70	$C_{4'}OH$ and later on $C_{5'}OH$	1	$C_{3'}$-$C_{4'}$ bond breaking (ring 3 opening and aldehyde formation), H-abstraction from $C_{5'}OH$ (H_2O formation), C_{12}-$OC_{3'}$ glycosidic bond cleavage (aldehyde formation) $C_{12}H_{15}O_{13}$ (367 Da) + $C_{12}H_{17}O_{12}$ (353 Da) + H_2O (18 Da)		0.5
71	$C_{4'}OH$ and C_7OH	4	H-abs. from $C_{4'}OH$: $C_{3'}$-$C_{4'}$ bond breaking (ring 3 opening and aldehyde formation), H-abs. from C_7OH: CO_2 liberation, H_2O formation, C_8O-C_{12} bond breaking (ring 2 opening and aldehyde formation), $C_{2'}=C_{3'}$ bond formation, $C_{2'}$-$OC_{6'}$ and $C_{6'}$-$OC_{9'}$ bonds breaking, glycosidic bond cleavage $C_{14}H_{19}O_{13}$ (395 Da) + $C_6H_9O_7$ (193 Da) + $C_3H_4O_3$ (88 Da) + H_2O (18 Da) + CO_2 (44 Da)		2.0

72	C_5OH and C_2H	1	H_2O formation, C_5-C_6 bond breaking (ring 1 opening and aldehyde formation), $^{\bullet}C_2$ and $^{\bullet}C_6$ formation $C_{24}H_{32}O_{25}$ (720 Da) + H_2O (18 Da)		0.5
73	C_5OH and later on C_9H	1	C_5-C_6 bond breaking (ring 1 opening and aldehyde formation), H-abstraction from C_9H (H_2O formation), C_6O-C_9 glycosidic bond cleavage $C_{18}H_{24}O_{18}$ (528 Da) + $C_6H_8O_7$ (192 Da) + H_2O (18 Da)		0.5
74	$C_{5'}OH$ and later on $C_{11'}OH$	1	$C_{5'}$-$C_{6'}$ bond breaking (ring 3 opening and aldehyde formation), H-abstraction from $C_{11'}OH$ (H_2O formation), $C_{6'}O$-$C_{9'}$ bond breaking, $C_{9'}$=$C_{10'}$ double bond formation and $C_{10'}$-$C_{11'}$ bond breaking (glycosidic bond cleavage, ring 4 opening and aldehyde formation) $C_{18}H_{24}O_{19}$ (544 Da) + $C_6H_8O_6$ (176 Da) + H_2O (18 Da)		0.5
75	$C_{8'}H$	1	$C_{6'}O$-$C_{9'}$ glycosidic bond cleavage, $C_{8'}$=$C_{9'}$ formation, $C_{6'}O$-OH formation $C_{18}H_{26}O_{20}$ (562 Da) + $C_6H_8O_6$ (176 Da)		0.5

No.	Binding of O atom	Number of events	Description	Structure	%
76	C_6-**O**-C_9	1	Binding at C_6-**O**-C_9 $C_{24}H_{34}O_{26}$ (738 Da)		0.5
77	C_2-**O**-C_6	1	Binding at C_2-**O**-C_6 $C_{24}H_{34}O_{26}$ (738 Da)		0.5
78	**C_1-C_2**	1	C_1-C_2 breaking, C_1-**O**-C_2 formation $C_{24}H_{34}O_{26}$ (738 Da)		0.5
79	**$C_{1'}$-$C_{2'}$**	1	$C_{1'}$-$C_{2'}$ breaking, $C_{1'}$-**O**-$C_{2'}$ formation $C_{24}H_{34}O_{26}$ (738 Da)		0.5

80	**$C_{7'}$-$C_{8'}$**	1	$C_{7'}$-$C_{8'}$ breaking, $C_{7'}$-**O**-$C_{8'}$ formation $C_{24}H_{34}O_{26}$ (738 Da)		0.5
81	$C_{1'}$**O**	2	$C_{1'}$O-**O** formation $C_{24}H_{34}O_{26}$ (738 Da)		1.0
82	$C_{7'}$**O**	3	$C_{7'}$O-**O** formation $C_{24}H_{34}O_{26}$ (738 Da)		1.5
83	C_3**O**H	2	C_3O(-**O**)H formation $C_{24}H_{34}O_{26}$ (738 Da)		1.0

84	C_3**O**H	1	C_3O-**O**-C_1 formation, H-transfer from C_3OH to C_1O (diol formation), C_1-C_2 and C_1O-OC_3 bonds breaking (H_2CO_3 formation), C_3-C_4 bond breaking and C_2-C_4 bond formation (aldehyde and small ring formation) $C_{23}H_{32}O_{23}$ (676 Da) + CH_2O_3 (62 Da)		0.5
85	C_{10}**O**H	1	$C_{10}O$(-**O**)H formation $C_{24}H_{34}O_{26}$ (738 Da)		0.5
Total		**200**			**100**