Equations:

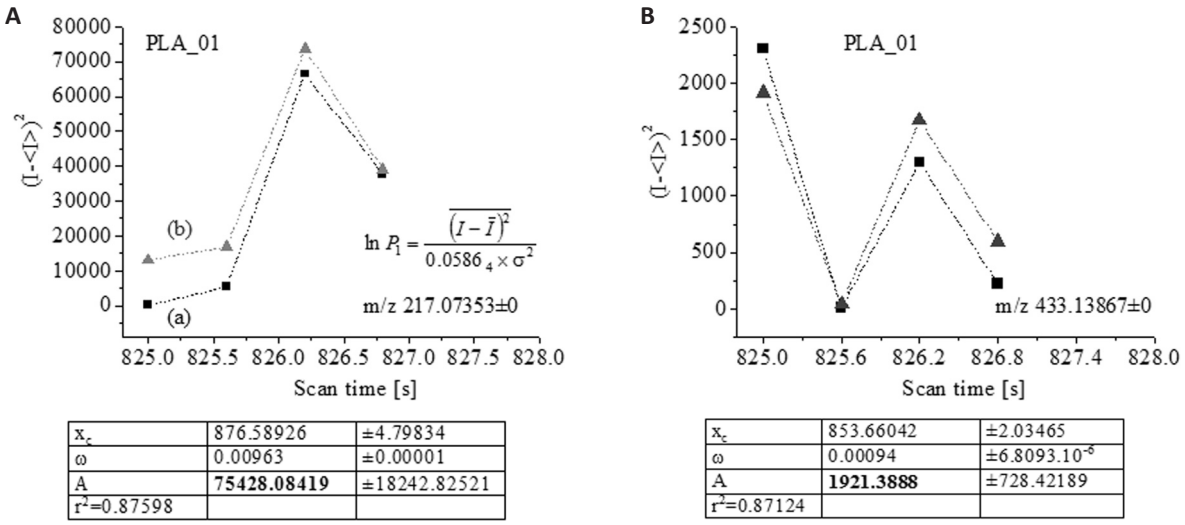
$$x - \bar{x} = \left(\sqrt{-2 \times \sigma^2 \times \ln P_1}\right) \times \sin(2 \times \pi \times P_2) \quad (S1)$$

$$(x - \bar{x})^2 = (-2 \times \sigma^2 \times \ln P_1) \times \sin^2(2 \times \pi \times P_2) \quad (S2)$$

$$\sigma^2 = \overline{x^2} - (\bar{x})^2 \quad \text{or} \quad \sigma^2 = \overline{(x - \bar{x})^2} \quad (S3)$$

$$\ln P_1 = \frac{\overline{(I - I)^2}}{0.0586_4 \times \sigma^2} \quad (S4)$$

$$\frac{A}{2 \times \sigma'^2} = \frac{1}{5.8639.10^{-2}} \times \frac{(x - \bar{x})^2}{\overline{x^2} - (\bar{x})^2} \quad (S5)$$



x_c	876.58926	±4.79834
ω	0.00963	±0.00001
A	**75428.08419**	±18242.82521
r^2=0.87598		

x_c	853.66042	±2.03465
ω	0.00094	±6.8093.10^{-6}
A	**1921.3888**	±728.42189
r^2=0.87124		

Figure S1. Functional relationship (I-<I>)2=*f*(t) of measurable variable intensity (I (arb.units)) with respect to span of scan time (t (s)) (A) and curve-fitted pattern by means of SineSqr fitting function (B) of data on mass spectrometric ions at m/z 217 and 433 of PLA of sample PLA_01; chemometrics.

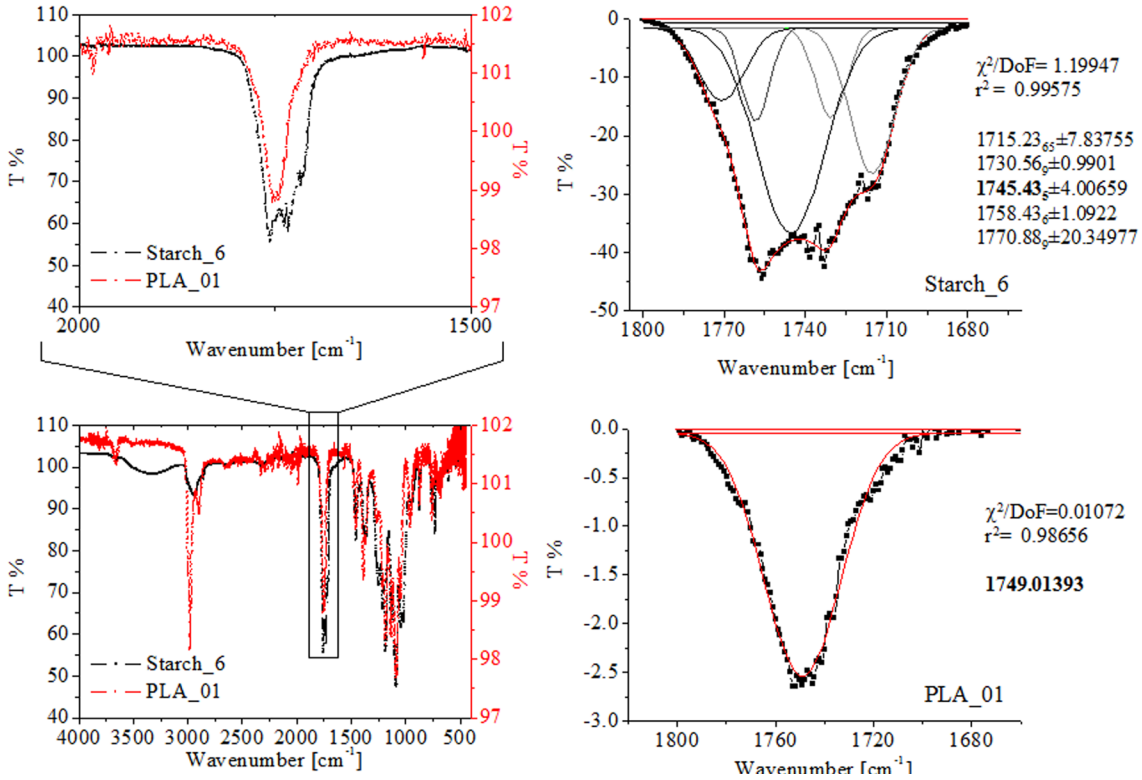


Figure S2. FT-IR spectrum of samples Starch_6 and PLA_01; curve fitted spectrometric patterns using Gauss function; chemometrics; optimisation of curve-fitting procedure for data processing of FT-IR spectra has been described [56].

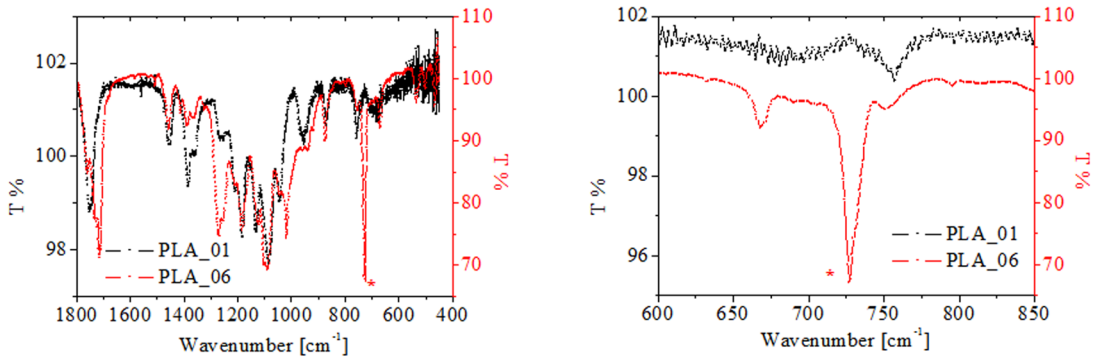


Figure S3. FT-IR spectrum of samples PLA_01 and PLA_06.

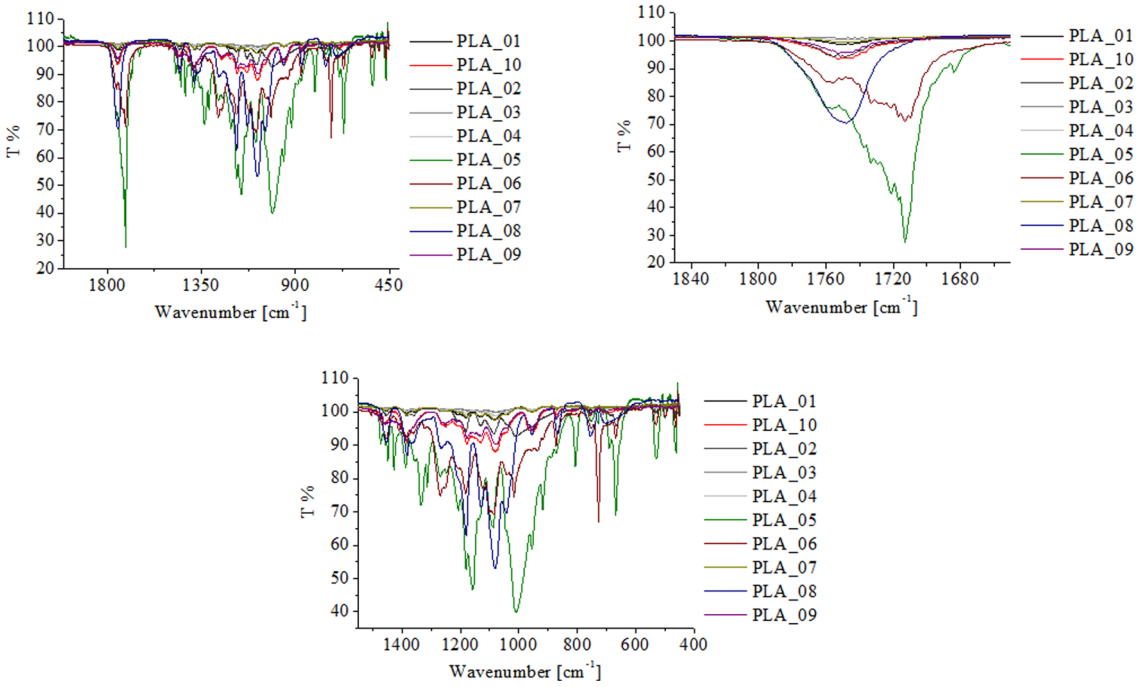


Figure S4. FT-IR spectra of biopolymer samples PLA_01-PLA_10 within different regions of the electromagnetic spectrum: Transmission (T, %) vs. wavenumber (cm^{-1}); the experimental datasheets can be downloaded free of charge, herein[44].

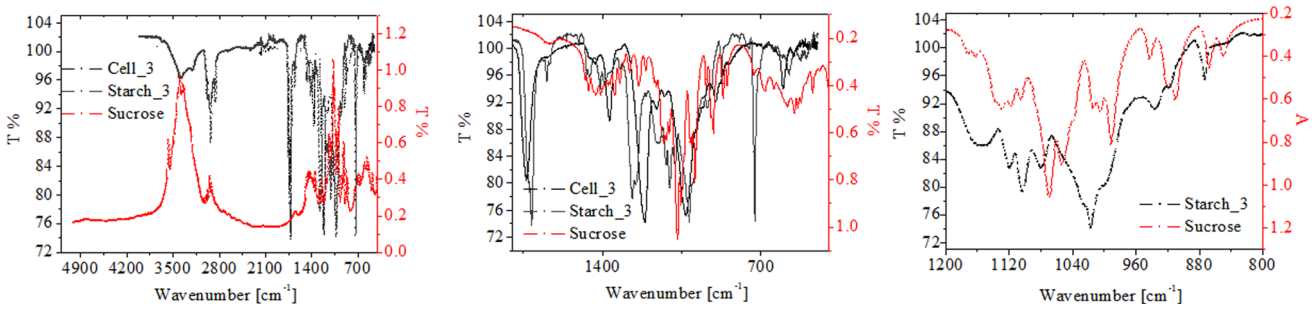


Figure S5. FT-IR spectra of biopolymer samples Cell_3 and Strach_3 within different regions of the electromagnetic spectrum: Transmission (T, %) vs. wavenumber (cm^{-1}); the experimental datasheets can be downloaded free of charge, herein[44]; standard FT-IR spectrum of sucrose within 5000-500cm^{-1}: Absorption vs. wavenumber(cm^{-1}).

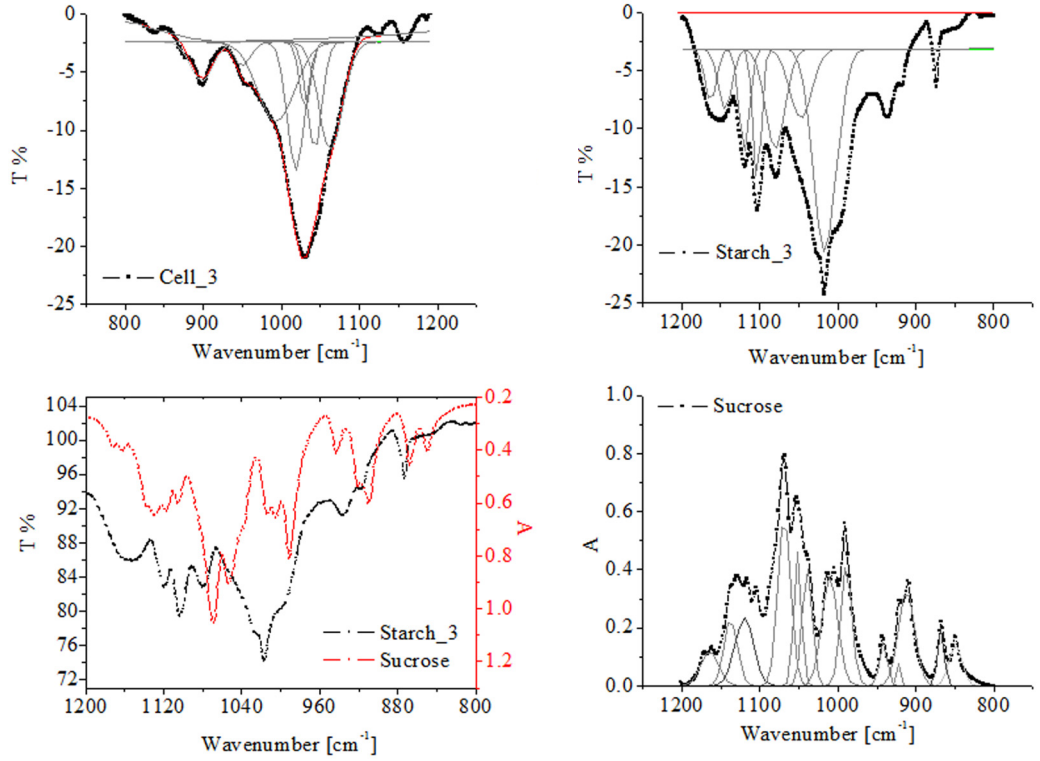


Figure S6. FT-IR spectra of biopolymer samples Cell_3 and Strach_3 within different regions of the electromagnetic spectrum: Transmission (T, %) vs. wavenumber (cm^{-1}); the experimental datasheets can be downloaded free of charge, herein[44]; standard FT-IR spectrum of sucrose within 1200-800cm^{-1}: Absorption vs. wavenumber (cm^{-1}); curve-fitted IR-spectroscopic pattern via Gauss function.

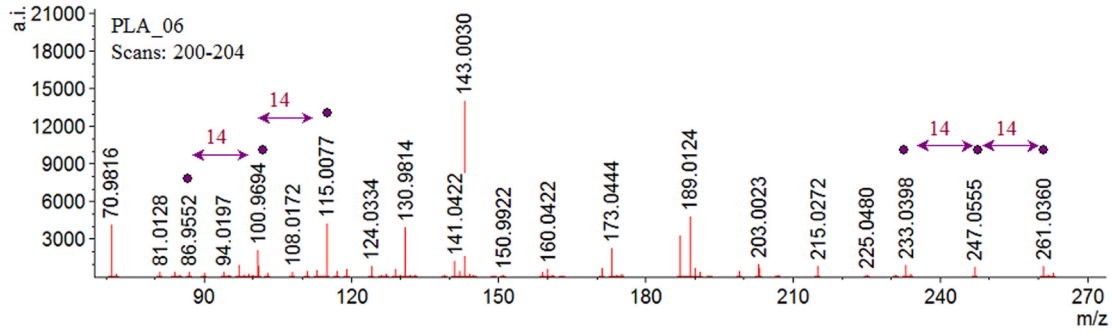
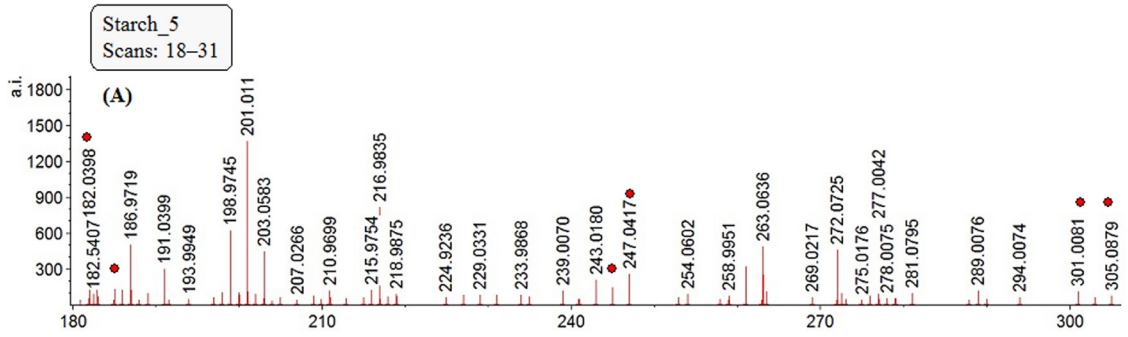
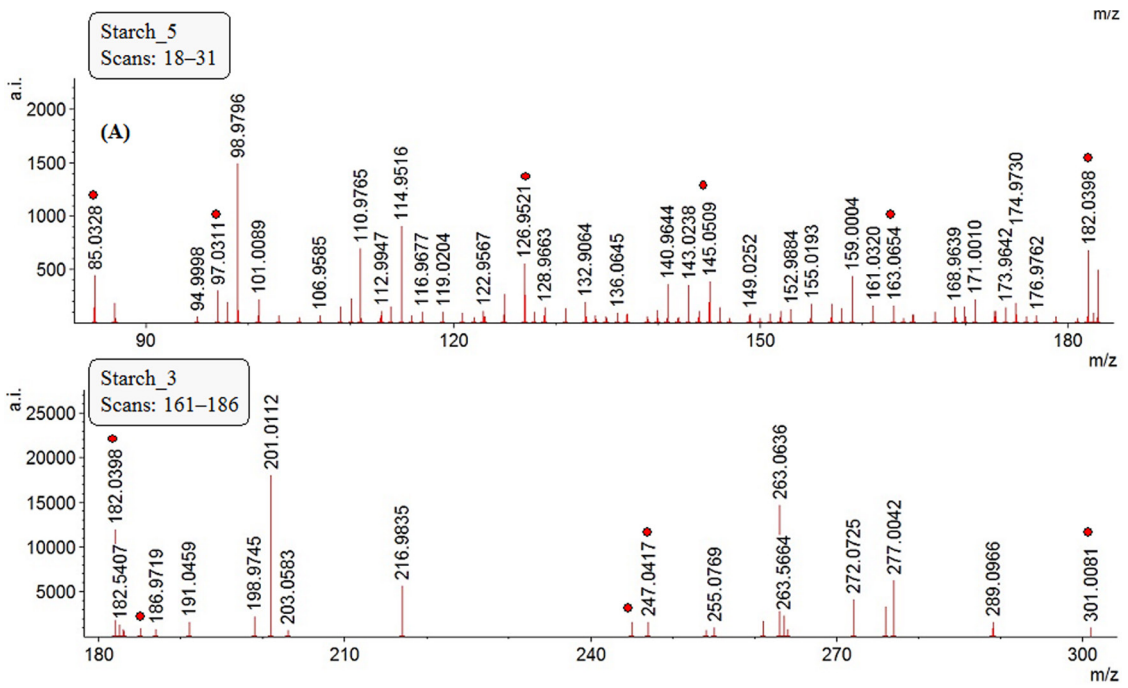
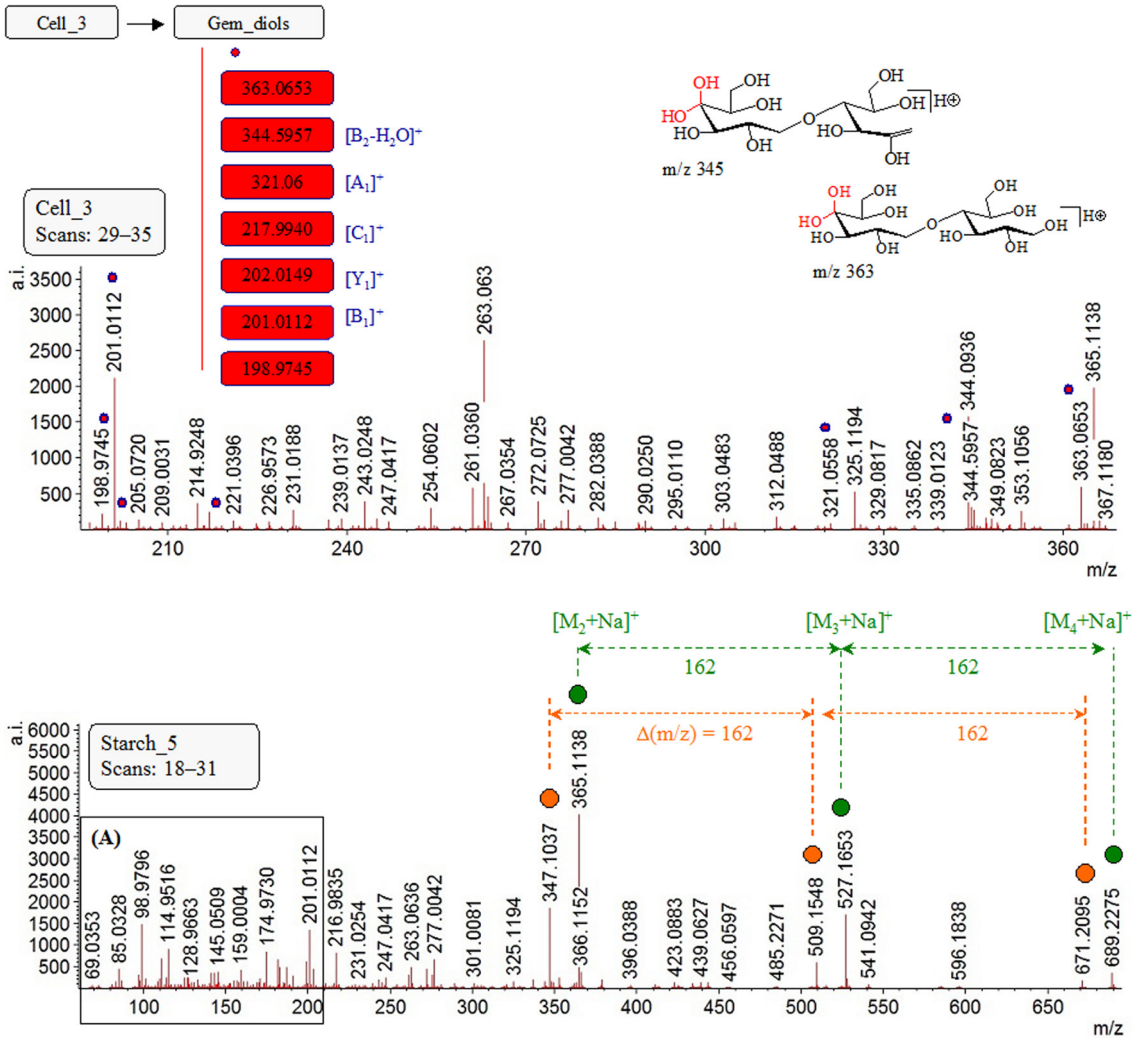


Figure S7. Mass spectrum of biopolymer sample PLA_06 within scan numbers 200-204 or RT =4.74-4.78mins; the experimental datasheets can be downloaded free of charge, herein[44].

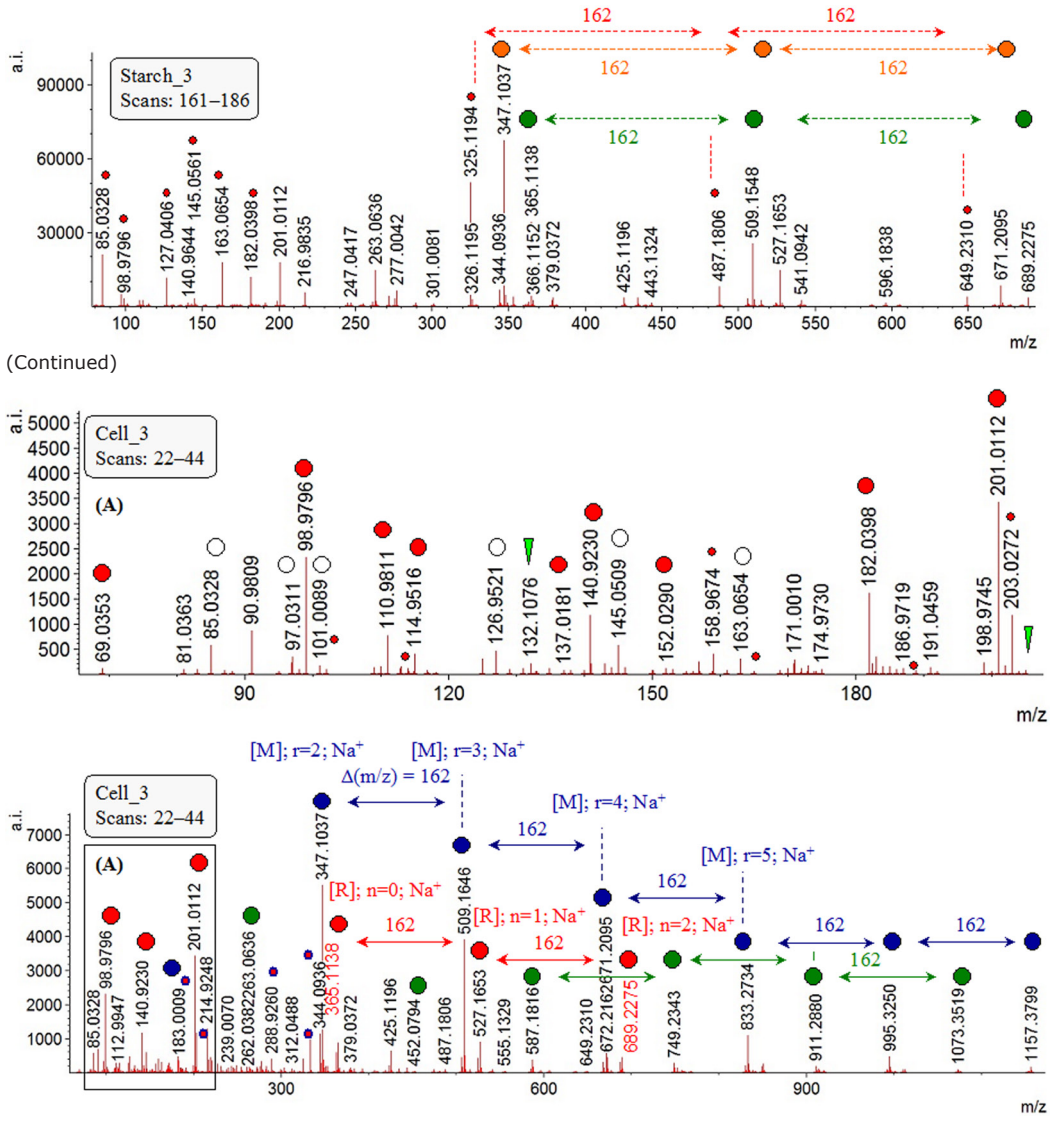



Starch_5
Scans: 18–31
(A)
a.i.
m/z
Starch_3
Scans: 161–186

(Continued)


Cell_3
Gem_diols
363.0653
344.5957
[B2-H2O]+
321.06
[A1]+
217.9940
[C1]+
202.0149
[Y1]+
201.0112
[B1]+
198.9745
m/z 345
m/z 363
Cell_3
Scans: 29–35
a.i.
m/z

[M2+Na]+
[M3+Na]+
[M4+Na]+
162
162
Δ(m/z) = 162
162
Starch_5
Scans: 18–31
(A)
a.i.
m/z



(Continued)

Figure S8. Mass spectra of biopolymer samples Starch_3, Starch_5, and Cell_3 within scan numbers 18-31, 161-186, and 22-44 as well as RT =1.65-1.89 , 1.75-2.01, 1.72-1.86, and 1.73-1.79mins; chemical diagrams of analytes.

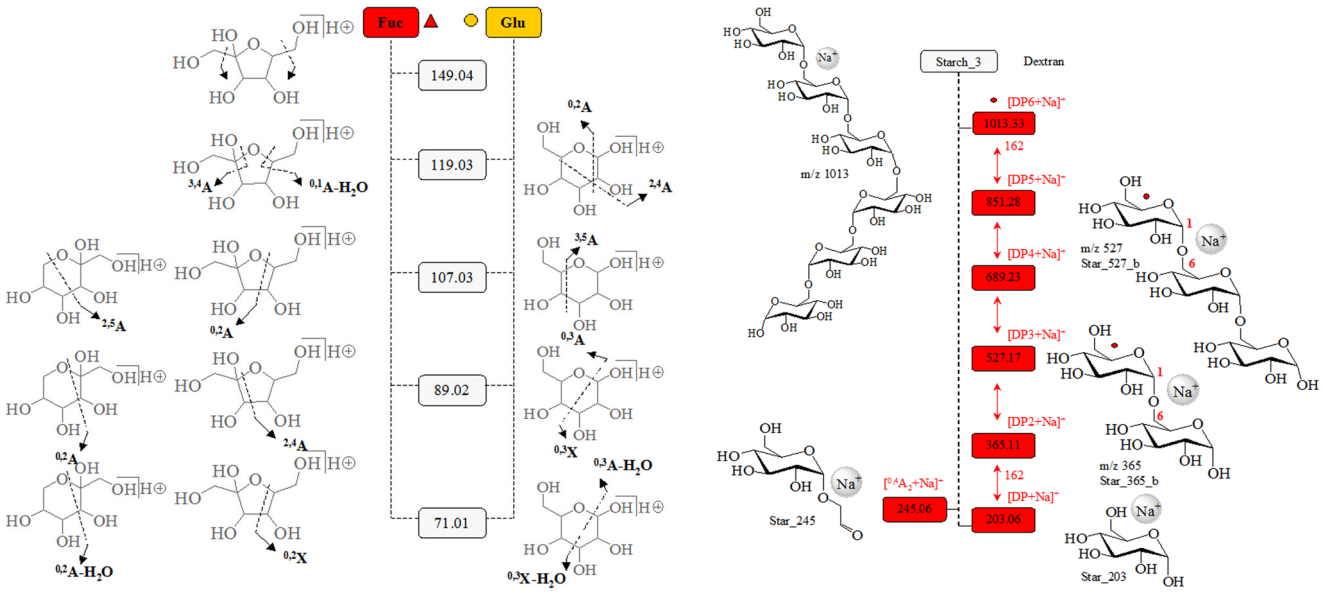


Figure S9. Chemical diagrams of product ions of cellulose within low m/z values [29,S1]; product ions of glucose and fructose and proposed structures of ions of Starch_3 biopolymer assigned to dextran fragment ions.

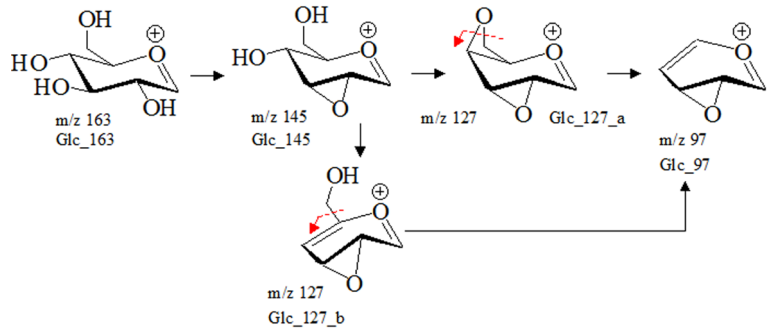


Figure S10. Fragmentation scheme of carbohydrate monomers; thus, producing product ions within low m/z values[63].

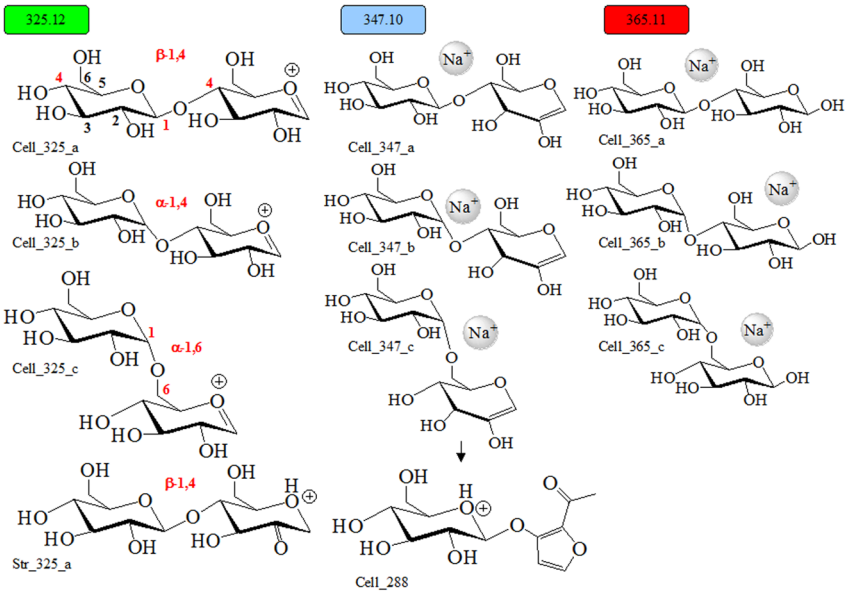


Figure S11. Chemical diagrams of carbohydrate ions at m/z 325, 347, and 365 depending on glycoside type bond and protomer.

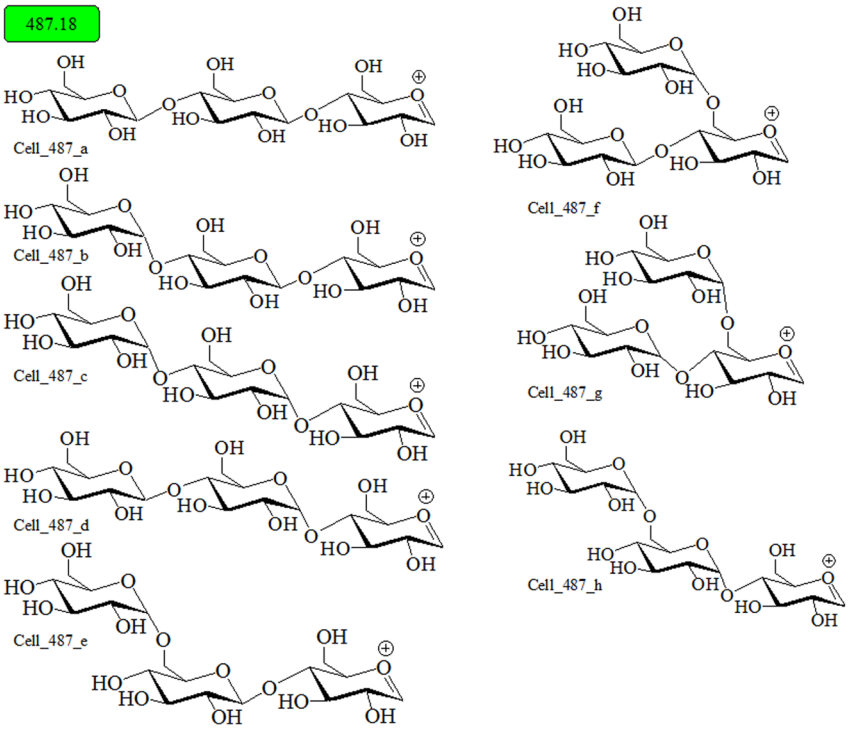


Figure S12. Chemical diagrams of carbohydrate ions at m/z 487 depending on protomer.

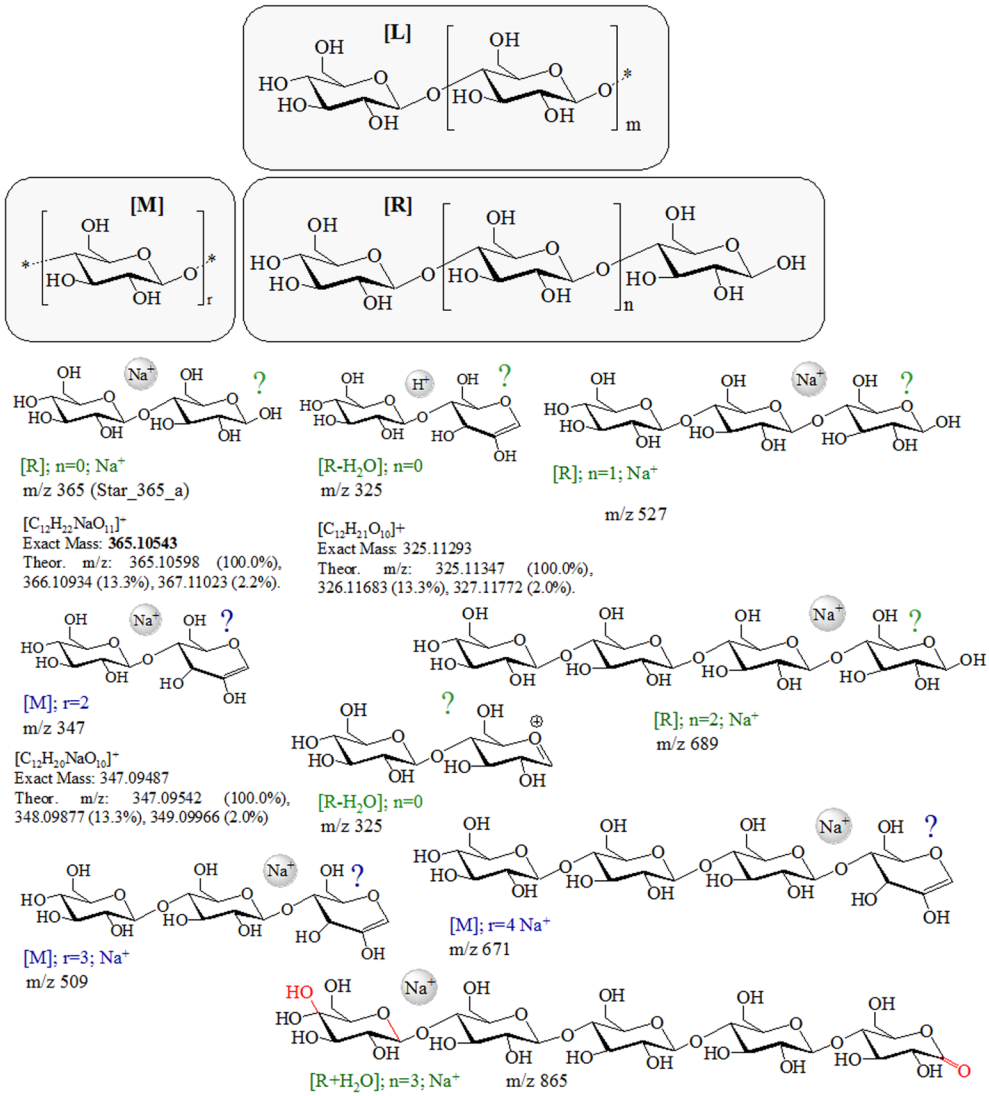


Figure S13. Common chemical diagrams of dimers and oligomers of type [L], [R], and [M] carbohydrates according to[57].

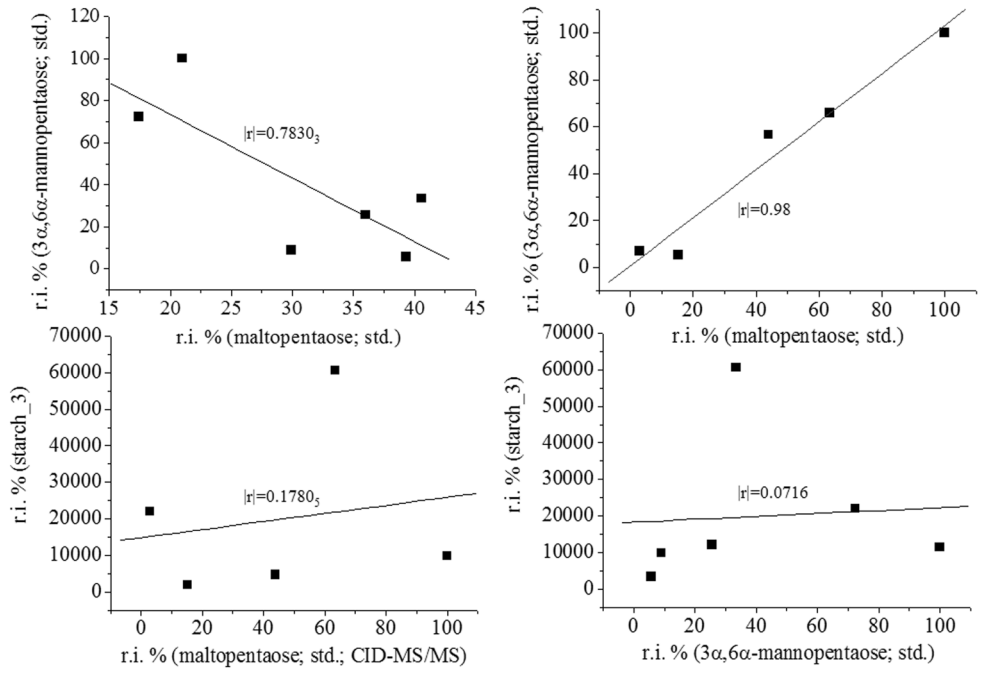


Figure S14. Functional linear relationship between intensity data on common characteristic product mass spectrometric ions of carbohydrate standard samples according to Spina E et al.[S2]; chemometrics.

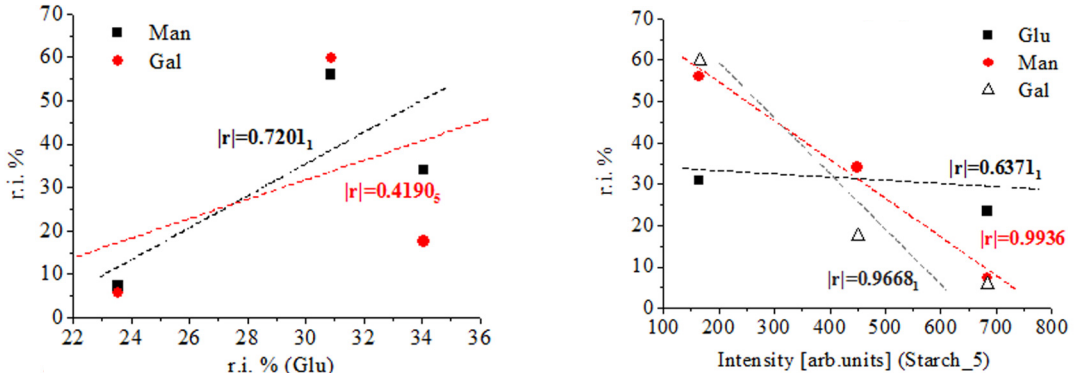


Figure S15. Correlative analysis of intensity parameters of product ions of glucose, mannose, and galactose at m/z 182, 163, and 85 according to[63]; correlation with experimental results from the standard samples of glucose, mannose, and galactose and sample Starch_5 within scan number 18-31; chemometrics.

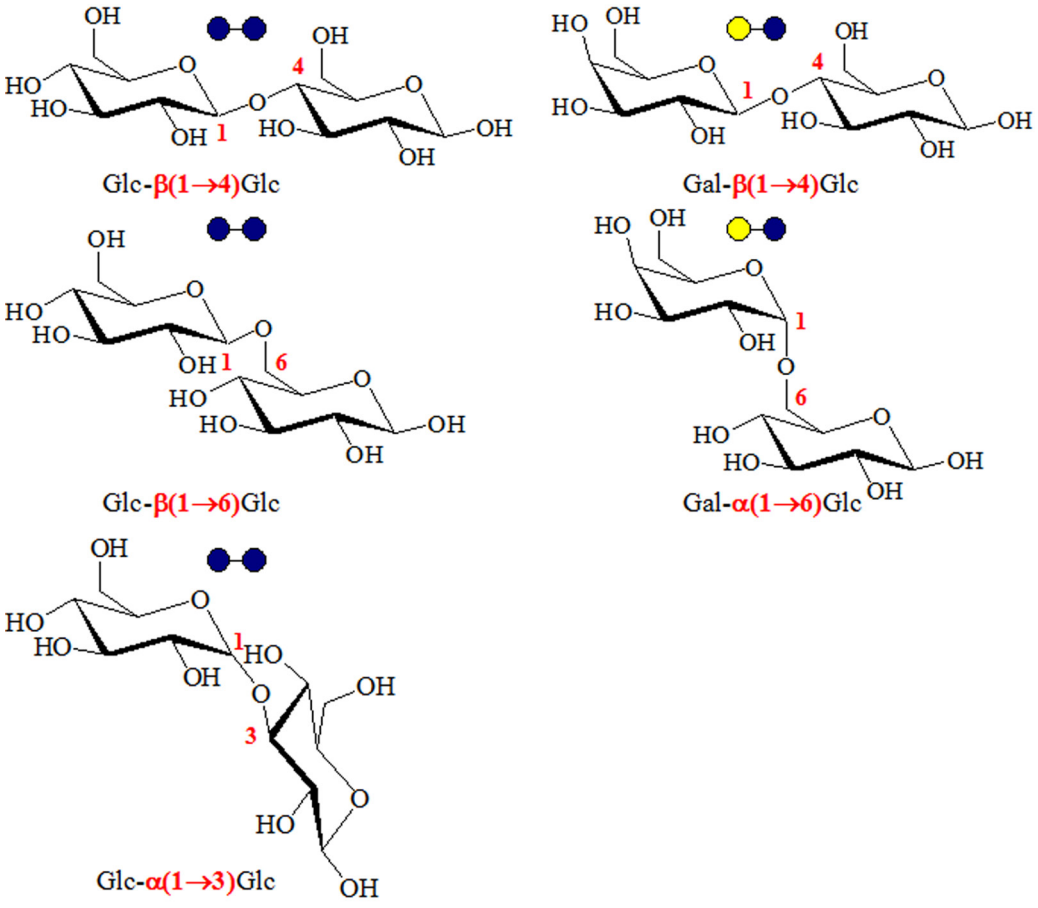


Figure S16. Chemical diagrams of carbodihydrates depending on the type of glycoside bond.

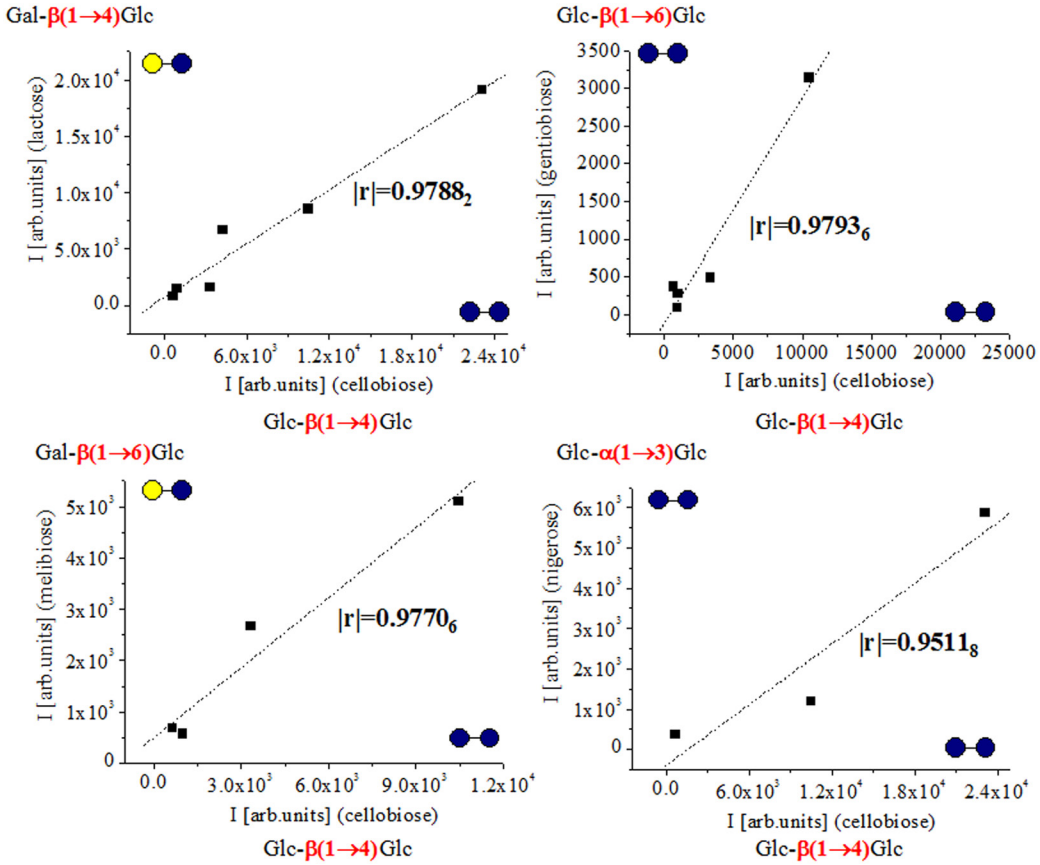


Figure S17. Correlative analysis of intensity data on common characteristic mass spectrometric peaks of ions of carbodihydrates depending on the type of the glycoside bond according to Zhan L et al.[S3]; chemometrics.

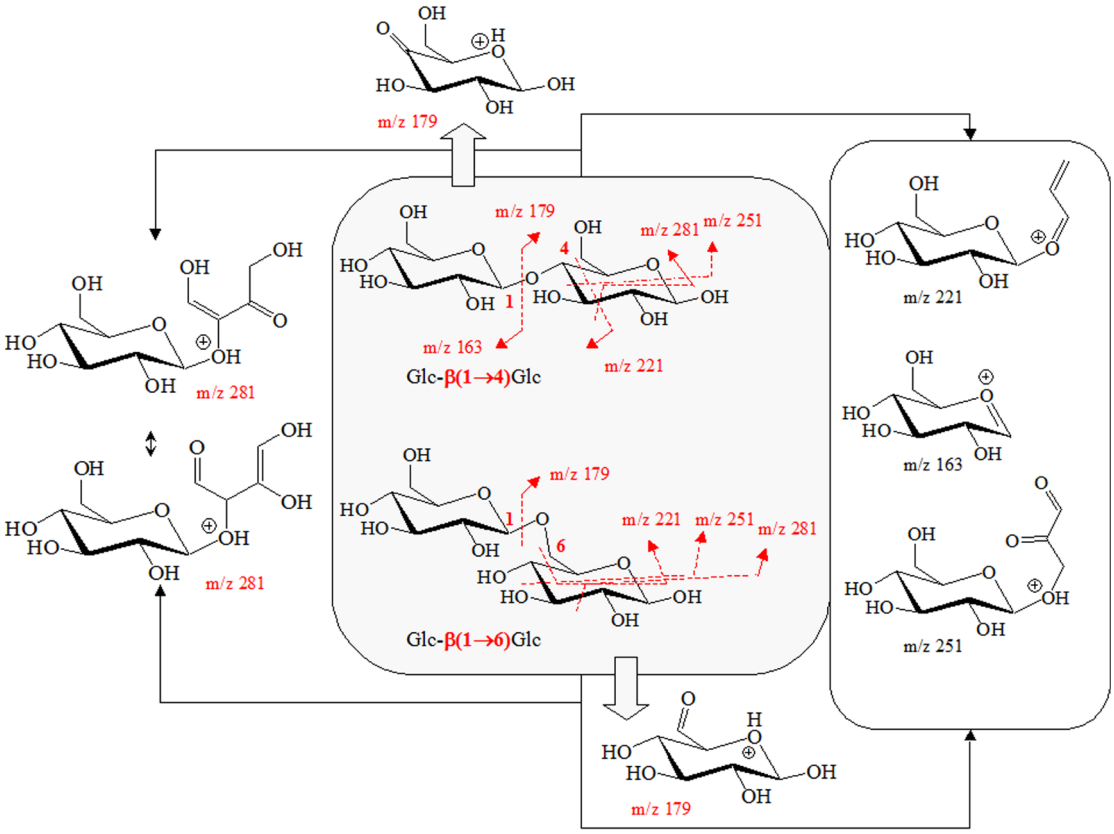


Figure S18. Mass spectrometric fragmentation paths of cellobiose and gentiobiose depending on the type of glycoside linkage of the monomeric sub-units of carbodihydrates according to Polfer N et al[S4].

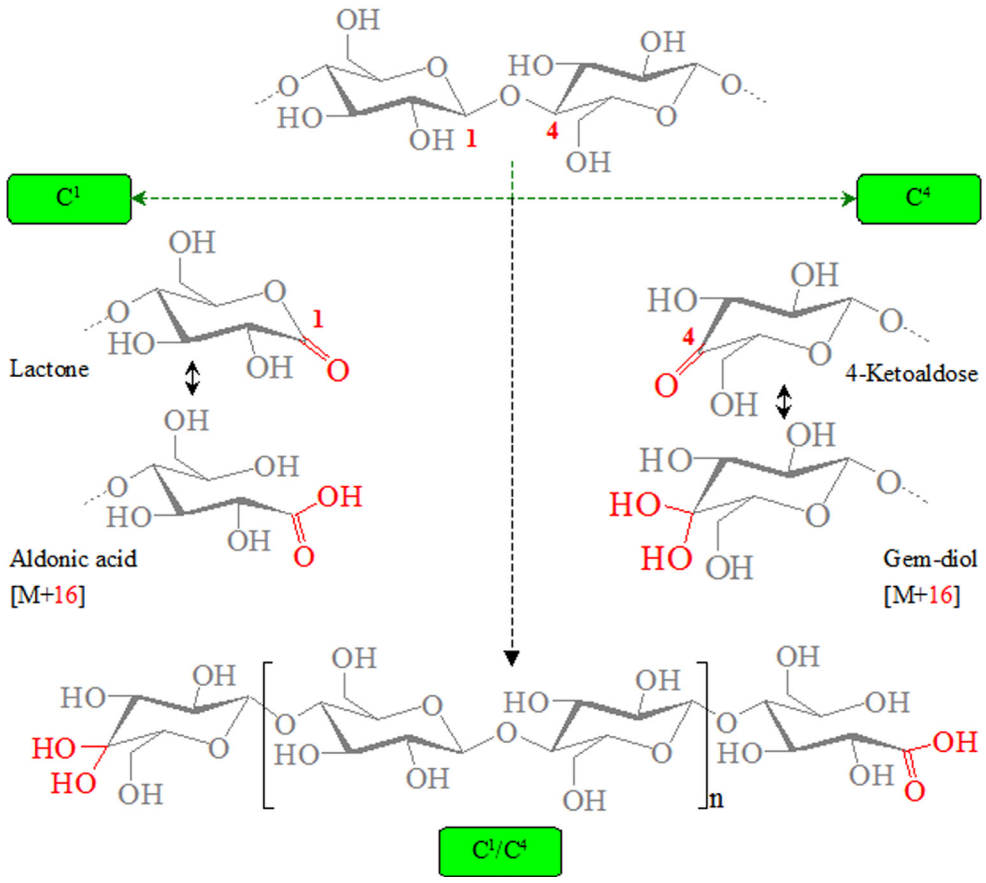


Figure S19. Chemical diagrams of C^{1-} and C^{4-} products of oxidation of carbohydrates adapted from Silva C et al[S5].

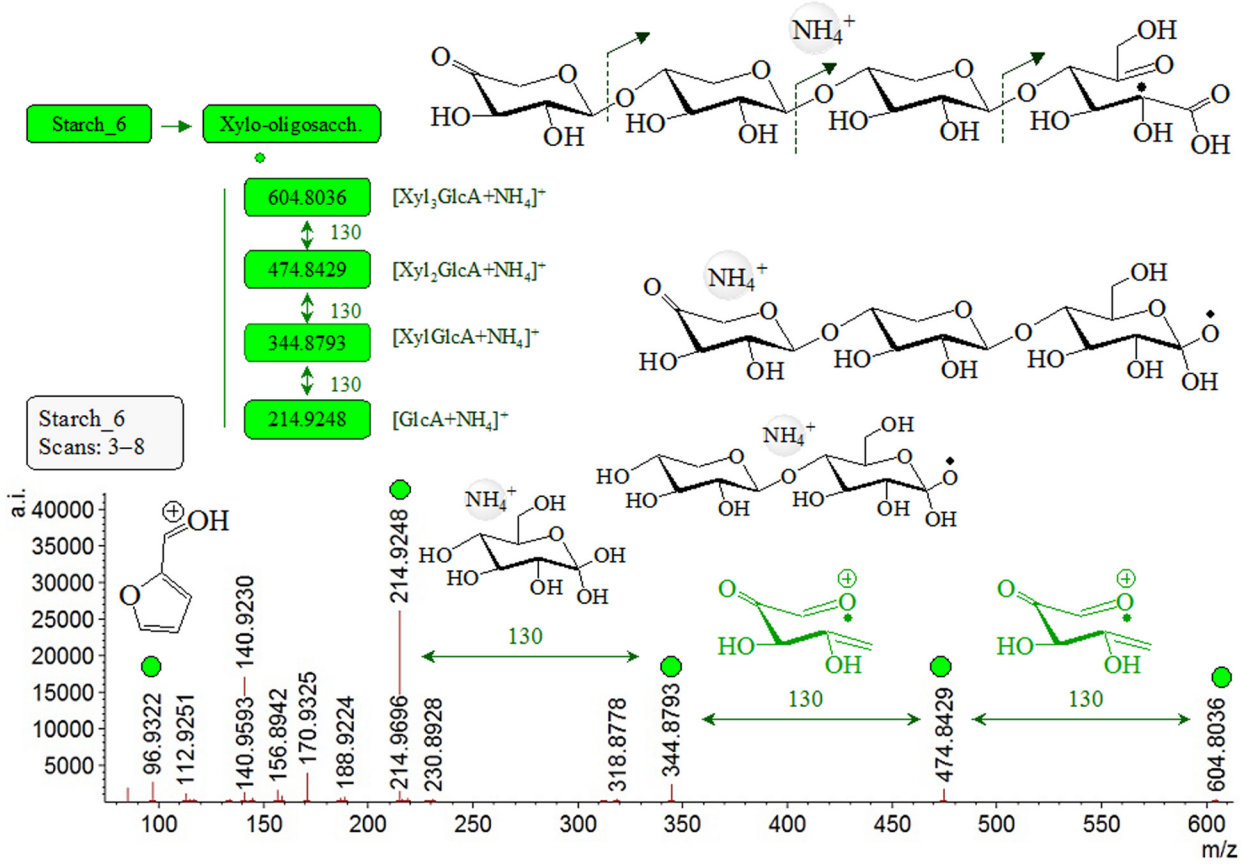


Figure S20. Mass spectrum of Starch_3 biopolymer of film, containing corn starch and polyethylene used in agricultural sector within scan numbers 3-8 (RT=1.55-1.61mins); chemical diagrams of analyte product ions.

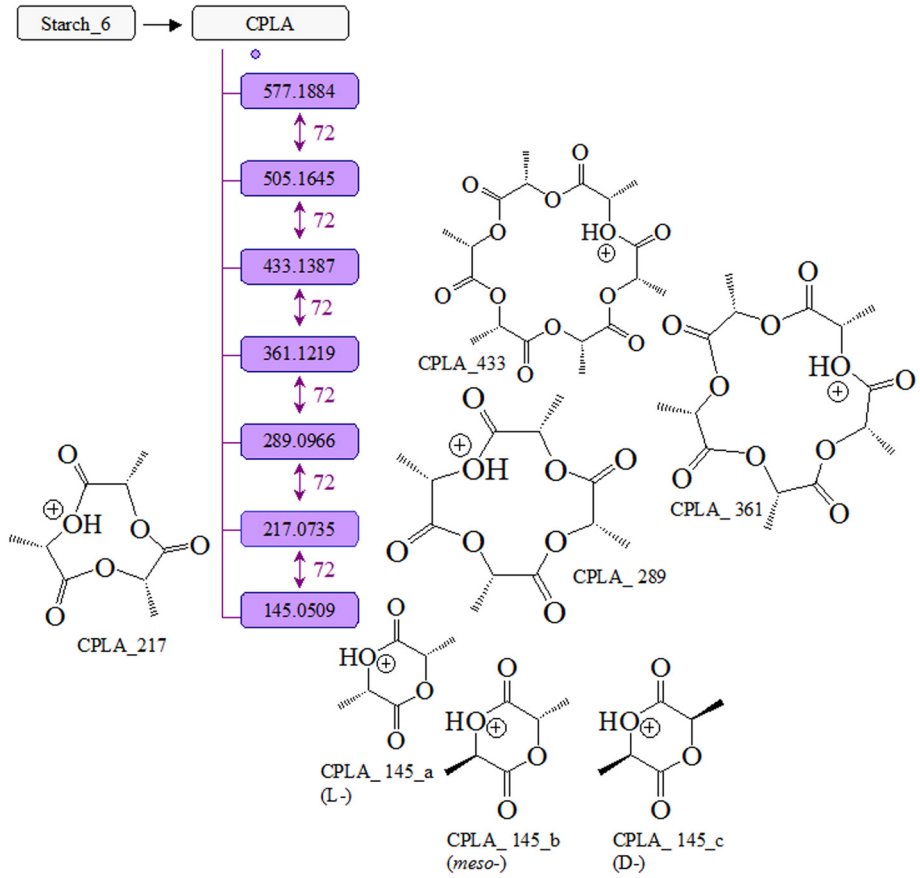


Figure S21. Chemical diagrams of cyclic product ions of *poly* (lactic acid) observed in Starch_6 sample.

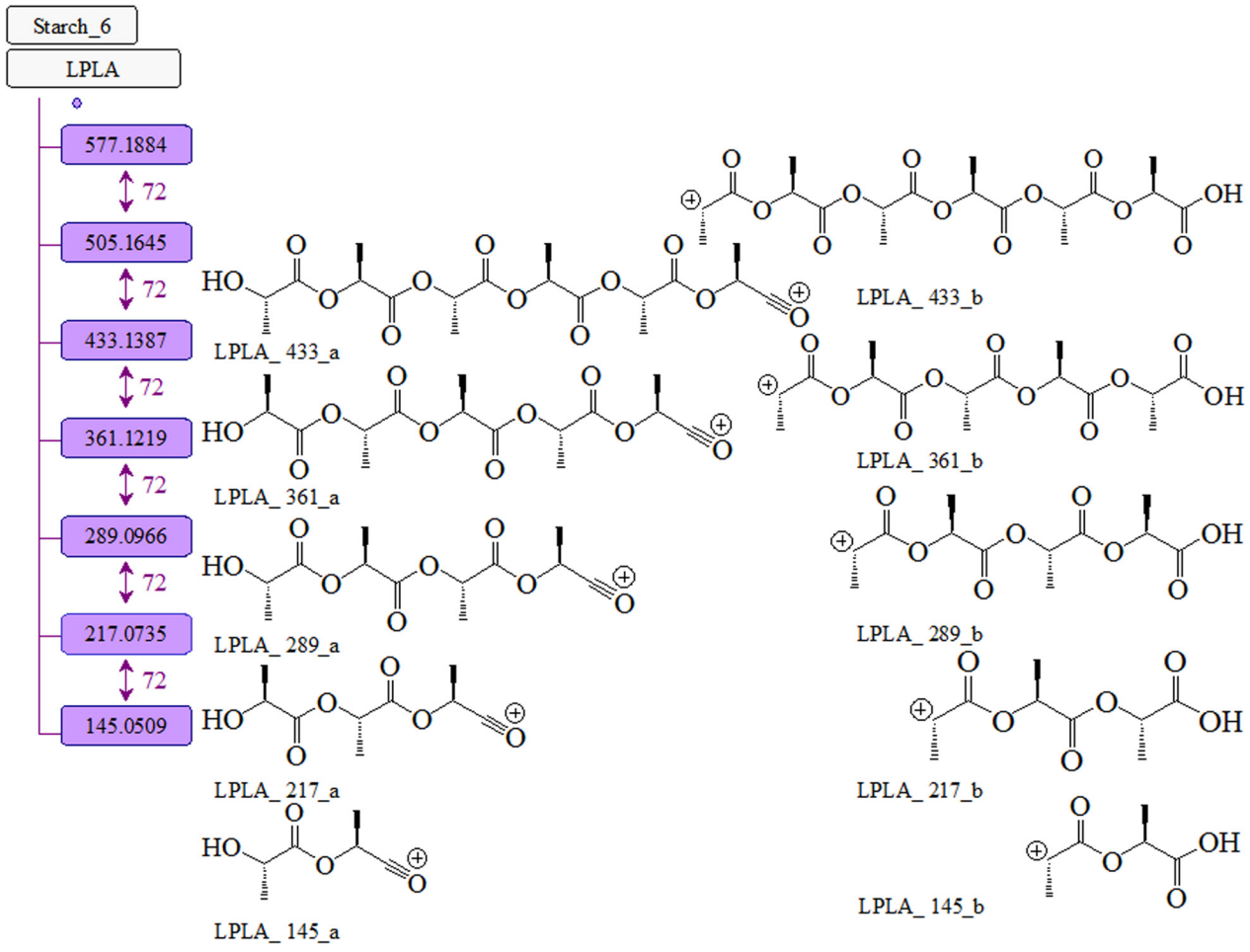


Figure S22. Chemical diagrams of linear product ions of PLA of Starch_6 sample.

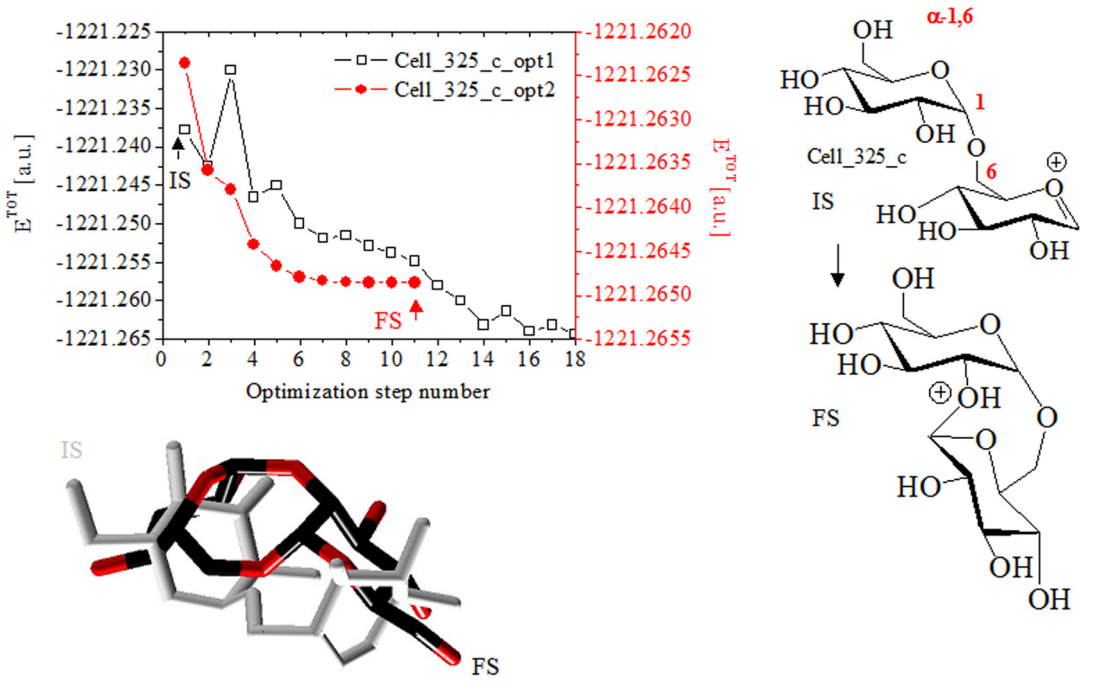


Figure S23. Theoretical M062X/SDD optimisation of carbohydrate product ion Cell$_{_325_c}$ at m/z 325: Total energy (E^{TOT} [a.u.]) with respect to optimisation step umber; chemical diagrams of species; optimised 3D molecular geometry of the ion.

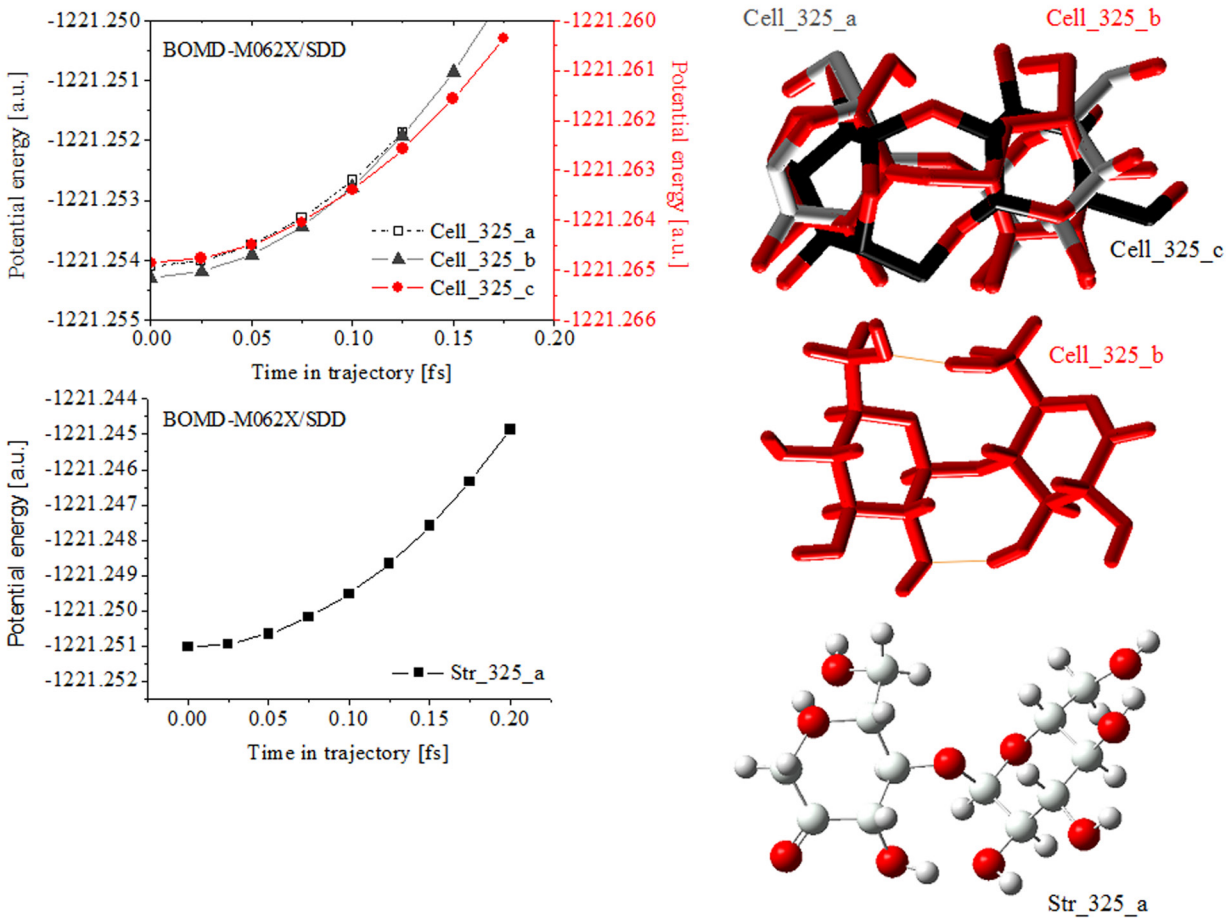


Figure S24. BOMD-DFT data on carbohydrate product ions at m/z 325: Potential energy ([a.u.]) vs. time in trajectory [fs].

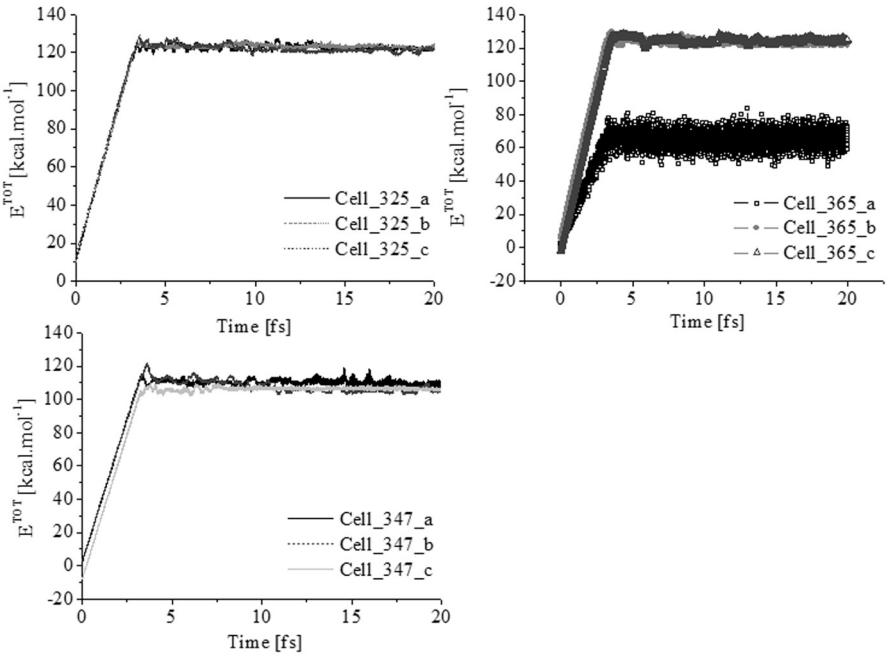


Figure S25. MM2/MD data on carbohydrate product ions at m/z 365 and 347: Total energy (E^{TOT} [kcal.mol^{-1}]) vs. time [fs].

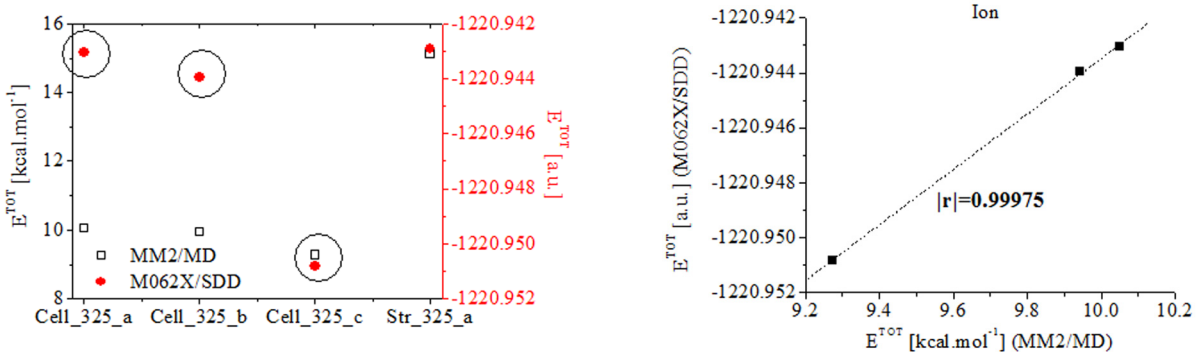


Figure S26. Correlative analysis between total energy values (E^{TOT} [units]) depending on theoretical method; chemometrics.

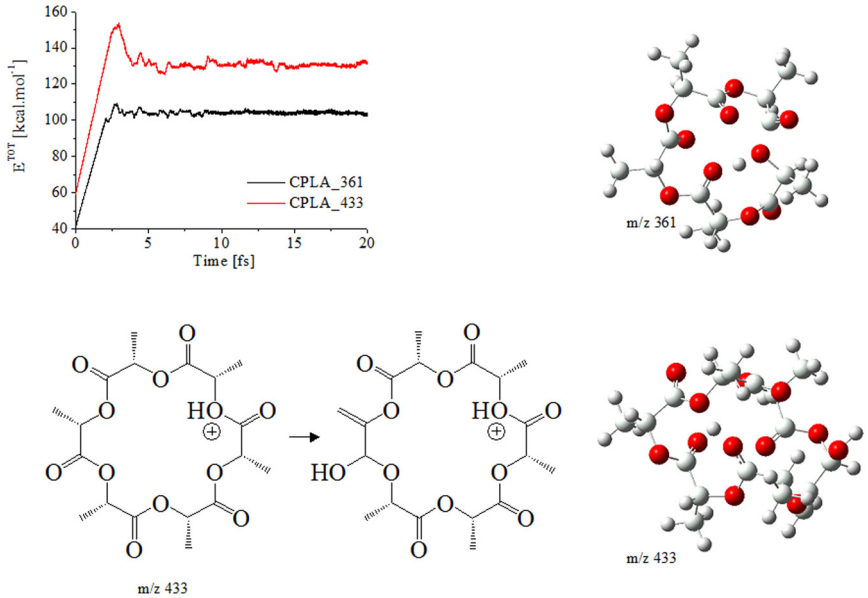


Figure S27. MM2/MD data on *poly* (lactic acid) product ions at m/z 433 and 316: Total energy (E^{TOT} (kcal.mol^{-1})) vs. time (fs); chemical diagrams of ions; optimised 3D molecular geometry of species.

Table S1. Plant-based Polymer Products According to Work[33]

Sample/ Plastic Type	Plastic Product	Colour, Printing Ink	Material Information from Producer/Distributor/vendor
Cell_1	Tea bag wrapping	Transparent, black ink	Regenerated cellulose (> 90%); natural resources according to ASTM D6866; 100% compostable industrially and at ambient temperature and in sea water, fragrance and aroma barrier
Cell_2	Chocolate wrapping	Transparent	Wood pulp
Cell_3	Cigarette filter	White	Unbleached cellulose, biodegradable; degrade environmentally friendly and naturally
Cell_4	Pellet	Grey	Based on cellulose acetate, cellulose blend, composed with a high content of natural resources, excellent heat resistance, does not contain harmful plasticizers, certified BPA-free, e.g., screw into disposable cutlery, tend to degrade when long dwell times and high temperatures are experienced
Cell_6	Bag for foodstuff	Transparent, white and red ink	Cellulose made of wood, to at least 90% made renewable resources, other ingredients: water glycerine, varnishes

Table S2. ANOVA Test Data on Experimental Measurable Variables of Ions at m/z 347, 509, and 671 of Carbohydrates of Samples Starch_5 and Starch_3 within RT =1.75-2.01 and 1.72-1.86mins (See Data on Figure S8.)

m/z 347					
Dataset	N	Mean	sd(yEr±)	se(yEr±)	
Data11_5	24	347.14364	0.05809	0.01186	
Data11_3	12	347.10841	0.01643	0.00474	
H_0:		The means of all selected datasheets are equal			
H_1:		The means of one or more selected datasheets are different			
Source	DoF	Sum of squares	Mean square	F value	P value
Model	1	0.00993051729	0.00993051729	4.19012	0.04845
Error	34	0.0805795231	0.00236998597		
At the 0.01 level, the population means are not significantly different					
Means Comparison using Bonferroni Test					
Datasheet	Mean	Difference between means	Simultaneous confidence intervals		Significant at 0.01 level
			Lower limit	Upper limit	
Data11_5	347.14364				
Data11_3	347.10841	0.03523	-0.01173	0.08219	No
m/z 509					
Dataset	N	Mean	sd(yEr±)	se(yEr±)	
Data11_5	17	509.16982	0.02999	0.00727	
Data11_3	12	509.16707	0.02884	0.00833	
H_0:		The means of all selected datasheets are equal			
H_1:		The means of one or more selected datasheets are different			
Source	DoF	Sum of squares	Mean square	F value	P value
Model	1	$5.3262909.10^{-5}$	$5.3262909.10^{-5}$	0.06109	0.80664
Error	27	0.0235389299	$8.7181221.10^{-4}$		
At the 0.01 level, the population means are not significantly different					
Means Comparison using Bonferroni Test					
Datasheet	Mean	Difference between means	Simultaneous confidence intervals		Significant at 0.01 level
			Lower limit	Upper limit	
Data11_5	509.16982				
Data11_3	509.16707	0.00275	-0.02809	0.0336	No
m/z 671					
Dataset	N	Mean	sd(yEr±)	se(yEr±)	
Data11_5	12	671.22271	0.06501	0.01877	
Data11_3	12	671.20953	0	0	
H_0:		The means of all selected datasheets are equal			
H_1:		The means of one or more selected datasheets are different			

Source	DoF	Sum of squares	Mean square	F value	P value
Model	1	0.00104119304	0.00104119304	0.49275	0.49006
Error	22	0.0464867782	0.00211303537		
At the 0.01 level, the population means are not significantly different					
Means Comparison using Bonferroni Test					
Datasheet	Mean	Difference between means	Simultaneous confidence intervals		Significant at 0.01 level
			Lower limit	Upper limit	
Data11_5	671.22271				
Data11_3	671.20953	0.01317	-0.03972	0.06607	No

Table S3. ANOVA Test Data on Experimental Measurable Variables of Ion at m/z 145 of PLA and Carbohydrate (See Data on Tables S4 and Tables S5.)

Datasheet	**N**	**Mean**	**sd(yEr±)**	**se(yEr±)**	
Data11_A	10	145.05614	6.74949.10-6	2.13437.10-6	
Data11_B	8	145.05089	3.53553.10-6	1.25.10-6	
H0:	The means of all selected datasheets are equal				
H1:	The means of one or more selected datasheets are different				
Source	DoF	Sum of squares	Mean square	F value	P value
Model	1	1.2241835.10-4	1.224183.10-4	3.93707.106	0
Error	16	4.97500.10-10	3.109375.10-11		
At the 0.01 level, the population means are significantly different					
Means Comparison using Bonferroni Test					
Datasheet	Mean	Difference between means	Simultaneous confidence intervals		Significant at 0.01 level
			Lower limit	Upper limit	
Data11_A	145.05614				
Data11_B	145.05089	0.00525	0.00524	0.00526	Yes

Table S4. Data on Experimental Mass Spectrometric Measurands (m/z) and Intensity (I) of Peaks [arb. units] Starch_3 (Sample Starch_3.raw of Film of 100% Corn Starch) Within Scan Number 156-168 Scan (RT= 1.73-1.83mins); Descriptive Statistics; Parameters of Equation (2)

Scan	**m/z**	**I [arb.units]**	**m/z**	**I [arb.units]**	**m/z**	**I [arb.units]**
159	145.05614	50521	163.06538	27558	325.11935	64276
160	145.05614	69647	163.06538	39089	325.11935	103174
161	145.05614	75052.0827	163.06538	44223.0983	325.11935	125941.239
162	145.05614	78183.0827	163.06538	47787.0983	325.11935	140337.239
164	145.05614	74774	163.06538	46113	325.11935	130775
165	145.05614	74158	163.06538	43006	325.11935	126738
166	145.05614	73709.0827	163.06538	40919.0983	325.11935	120010.239
167	145.05614	66188	163.06538	37195	325.11935	112508
168	145.05614	62010	163.06538	33542	325.11935	99467
Mean	145.05614	-	163.06538	-	325.11935	-
sd(yEr±)	0	-	0	-	0	-
sd(yEr±)	0	-	0	-	0	-
<I>	-	69360.2498	-	39936.9217	-	113691.858
<I>2	-	4.81.109	-	1.59.109	-	1.29.1010
<I2>	-	4.88.109	-	1.63.109	-	1.34.1010
<I2>-<I>2	-	6.67.107	-	3.68.107	-	4.58.108
D"SD	-	1.76.10-9	-	9.70.10-10	-	1.21.10-8

Table S5. Data on Experimental Mass Spectrometric Measurands (m/z) and Intensity (I) of Peaks [arb. units] PLA_01 (Sample PLA_01 of Single-use Drinking Cup of Pure PLA of Fermented Corn Starch) Within Scan Number 1000-1003 Scan (RT =13.75-13.78mins); Descriptive Statistics; Parameters of Equation (2)

Scan	m/z	I [arb.units]	m/z	I [arb.units]	m/z	I [arb.units]
1000	145.0509	482.91734	217.0735	894.8547	289.0967	608.79206
1001	145.0509	446.91734	217.0735	977.8547	289.0892	469.79207
1002	145.0509	544.91734	217.0735	646.8547	289.1041	373.79205
1003	145.0509	485.91734	217.0735	1098.8547	289.0967	484.79206
Mean	145.0509	-	217.0735	-	289.0967	-
sd(yEr±)	0	-	0	-	0.00605	-
sd(yEr±)	0	-	0	-	0.00303	-
<I>	-	490.16734	-	904.6047	-	484.29206
<I>2	-	24,0264.02	-	818,309.66	-	234,538.8
<I2>	-	241,498.71	-	845,716.86	-	241,519.05
<I2>-<I>2	-	1,234.6907	-	27,407.191	-	6,980.2508
<(I-<I>)2>	-	-	-	27,407.188	-	-
lnP1	-	-	-	17.053204	-	-
D"SD	-	3.26.10-14	-	7.23.10-13	-	1.84.10-13
Scan	m/z	I [arb.units]	m/z	I [arb.units]	-	-
1000	361.122	374.72942	433.1387	615.66678	-	-
1001	361.122	372.72942	433.1387	660.66678	-	-
1002	361.122	490.72942	433.1387	699.66678	-	-
1003	-	-	433.1387	678.66678	-	-
Mean	361.122	-	433.1387	-	-	-
sd(yEr±)	0	-	0	-	-	-
sd(yEr±)	0	-	0	-	-	-
<I>	-	412.72942	-	663.66678	-	-
<I>2	-	170,345.57	-	440,453.6	-	-
<I2>	-	173,388.24	-	441,412.1	-	-
<I2>-<I>2	-	3,042.6667	-	958.50127	-	-
<(I-<I>)2>	-	-	-	958.5	-	-
lnP1	-	-	-	17.0532	-	-
D"SD	-	8.03.10-14	-	2.53.10-14	-	-

Table S6. Thermochemistry (M062X/SDD) of Observable Mass Spectrometric Ions of Carbohydrates in Ground and Transition States in Gas-phase, Depending on theoretical Level of Computations and Ionic Structures; Theoretical Intensity (I^{Theor}_{SD}) Data on Equations (3) and (4)

	m/z 325		m/z 325		m/z 325	
	Cell_325_a		Cell_325_b		Cell_325_c	
	M062X/SDD		M062X/SDD		M062X/SDD	
	GS	TS	GS	TS	GS	TS
EZPVE	225.58893	224.62656	224.96437	225.4301	227.42277	226.54144
Ecorr	0.380776	0.378839	0.379974	0.380060	0.383087	0.381209
Hcorr	0.381720	0.379783	0.380919	0.381005	0.384031	0.382153
Gcorr	0.311045	0.310014	0.308131	0.309086	0.314035	0.313568
e0	0.359499	0.357965	0.358504	0.359246	0.362421	0.361017
E	-1,220.87333	-1,220.841	-1,220.871	-1,220.87	-1,220.882	-1,220.846
H	-1,220.87238	-1,220.84	-1,220.870	-1,220.86	-1,220.881	-1,220.845
G	-1,220.94306	-1,220.91	-1,220.942	-1,220.94	-1,220.951	-1,220.914
DQC	307,010.6549		321.5287		0.39885	
ITh.SD	2.8463.10-6		9.2111.10-8		3.2442.10-9	

	m/z 325	m/z 163	m/z 145			
	Str_325_a	Str_163	Str_145			
	M062X/SDD	M062X/SDD	M062X/SDD			
	GS	TS	GS	TS	GS	TS
EZPVE	224.96437	224.64420	114.66254	114.07964	96.58851	95.73501
Ecorr	0.379974	0.378831	0.193773	0.192831	0.163079	0.161639
Hcorr	0.380919	0.379775	0.194717	0.193775	0.164024	0.162583
Gcorr	0.308131	0.308493	0.146744	0.145357	0.119572	0.117804
e0	0.358504	0.357993	0.182726	0.181797	0.153924	0.152563
E	-1,220.87107	-1,220.864	-610.55932	-610.556	-534.1905	-534.1761
H	-1,220.87012	-1,220.863	-610.55837	-610.555	-534.1896	-534.1752
G	-1,220.94291	-1,220.935	-610.6063	-610.6035	-534.234	-534.2199
DQC	0.0849		1,382.4836		1,078.854	
ITh.SD	1.4975.10-9		1.9099.10-7		1.6872.10-7	

Notes: EZPVE -zero-point vibration energy [kcal/mol]; ε0 -zero-point correction (Hartree/partice); Ecorr-thermal correction to energy (Hartree/partice); Hcorr-thermal correction to enthalpy [Hartree/partice]; Gcorr-thermal correction to free energy (Hartree/partice); E-sum of electronic and thermal energies (Hartree/partice); H-sum of electronic and thermal enthalpies (Hartree/partice); G - sum of electronic and thermal free energies (Hartree/partice).

Table S7. Atomic Co-ordinates of Mass Spectrometric Species in Ground and Transition States Used to Compute the data on Table S6 and Table S8

	Str_145 (GS)				**Str_145 (TS)**		
	x	**y**	**z**		**x**	**y**	**z**
C	0.046961	1.237751	-0.469549	C	0.10779	1.22732	-0.46123
C	-1.161031	0.815954	-0.041824	C	-1.08315	0.8456	-0.085
C	1.16595	0.297933	-0.822653	C	1.26107	0.25315	-0.78
O	-2.137193	1.698511	0.308466	O	-2.1317	1.75409	0.35914
C	-1.516273	-0.632542	0.039295	C	-1.46122	-0.63152	0.03044
C	2.519357	0.636789	-0.118874	C	2.57442	0.63779	-0.12771
O	0.879456	-1.059328	-0.262995	O	0.93452	-1.05833	-0.27183
C	-0.466123	-1.642961	-0.394094	C	-0.41107	-1.64195	-0.40294
O	2.453838	-0.204396	1.079024	O	2.5089	-0.20339	1.07018
O	-2.644729	-0.988281	0.393958	O	-2.58967	-0.98727	0.38511
H	0.232108	2.301741	-0.578512	H	0.2872	2.30266	-0.58734
H	1.304652	0.177181	-1.899359	H	1.35971	0.1782	-1.90791
H	-2.988406	1.274413	0.555598	H	-2.93368	1.27525	0.54683
H	2.564592	1.691208	0.151852	H	2.61963	1.69222	0.14299
H	3.37768	0.345028	-0.724683	H	3.43275	0.34604	-0.73352
H	1.512554	-1.056727	0.642956	H	1.56762	-1.05577	0.63415
H	-0.491918	-2.536227	0.230949	H	-0.43685	-2.53522	0.2221
H	-0.597107	-1.923446	-1.442468	H	-0.54205	-1.92243	-1.45132
H	3.141817	-0.122753	1.762228	H	3.19687	-0.12175	1.75338
		Str_163 (GS)				Str_163 (TS)	
	x	y	z		x	y	z
C	0.323887	1.162807	0.071122	C	0.33867	1.1592	0.09496
C	1.40542	0.273799	-0.577548	C	1.42822	0.2889	-0.57776
C	-1.106233	0.65286	-0.126297	C	-1.07542	0.63321	-0.08642
O	0.506659	2.444947	-0.544201	O	0.49561	2.47215	-0.5006
C	2.407138	-0.286889	0.418493	C	2.41924	-0.28515	0.43431
O	0.818004	-0.978366	-1.22176	O	0.83011	-0.97663	-1.20594
O	-1.899176	1.381025	0.811846	O	-1.88707	1.38276	0.82767
C	-1.165396	-0.863743	0.176375	C	-1.15329	-0.86201	0.1922

C	-0.246026	-1.530923	-0.796795	C	-0.23392	-1.52919	-0.78097
O	-2.480246	-1.36174	-0.066272	O	-2.46814	-1.36	-0.05045
O	1.591049	-1.077224	1.321549	O	1.60315	-1.07549	1.33737
H	0.488513	1.206495	1.155863	H	0.50063	1.20823	1.1717
H	1.871515	0.799191	-1.410083	H	1.88364	0.80095	-1.39429
H	-1.432379	0.83293	-1.160488	H	-1.42026	0.83466	-1.14463
H	-0.005357	3.145984	-0.092177	H	0.00669	3.14779	-0.0763
H	3.160314	-0.903199	-0.080539	H	3.17242	-0.90146	-0.06472
H	2.891856	0.554497	0.925676	H	2.90396	0.55623	0.9415
H	-2.849326	1.4005	0.582661	H	-2.83722	1.40223	0.59848
H	-0.789945	-1.026044	1.198137	H	-0.77784	-1.02431	1.21396
H	-0.521993	-2.470242	-1.2786	H	-0.50989	-2.46851	-1.26278
H	-2.911426	-1.770662	0.707911	H	-2.89932	-1.76893	0.72373
H	2.095173	-1.486066	2.050238	H	2.10728	-1.48433	2.06606
	Cell_325_a (GS)				Cell_325_a (TS)		
	x	y	z		x	y	z
C	0.80268	-0.4892	1.34132	C	0.83535	-0.49285	1.35843
O	1.23229	0.81076	0.86764	O	1.28369	0.85539	0.82218
C	1.12875	-1.52761	0.26623	C	1.20645	-1.57694	0.32879
C	2.64218	0.93449	0.50594	C	2.5908	1.02979	0.59099
C	-3.94702	0.70869	-0.58633	C	-3.92275	0.72141	-0.58954
O	-3.40122	1.55034	0.18819	O	-3.37639	1.56286	0.18482
C	2.81098	2.35456	0.00168	C	2.83585	2.36601	-0.00471
C	3.02631	-0.13872	-0.52944	C	3.05045	-0.12724	-0.53625
O	4.46238	-0.15725	-0.68862	O	4.48644	-0.14605	-0.69618
O	0.66574	-2.81312	0.72023	O	0.69004	-2.80145	0.71424
C	2.63054	-1.50944	0.01605	C	2.65475	-1.49801	0.00924
O	2.87053	-2.57434	-0.9195	O	2.89405	-2.56282	-0.92659
O	1.9088	2.53036	-1.13319	O	1.93313	2.54209	-1.13911
C	-3.35728	-0.62872	-0.88931	C	-3.33339	-0.61606	-0.893
C	-2.05808	1.35005	0.91928	C	-2.03292	1.36223	0.9152
C	-1.21053	2.55501	0.52039	C	-1.18536	2.56709	0.51605
C	-1.42702	0.01453	0.51179	C	-1.40231	0.02664	0.50721
O	-0.59026	-0.38103	1.6217	O	-0.56505	-0.36922	1.61665
O	-4.46379	-1.48792	-1.14641	O	-4.4402	-1.47503	-1.14966
C	-2.44702	-1.09308	0.25269	C	-2.42265	-1.08074	0.24848
O	-1.83474	-2.27722	-0.25778	O	-1.81084	-2.26493	-0.26246
O	-0.8059	2.38796	-0.84363	O	-0.78145	2.40014	-0.8482
H	1.26746	-0.75031	2.2976	H	1.29305	-0.73886	2.29188
H	0.62553	-1.2751	-0.67822	H	0.64978	-1.2634	-0.68334
H	3.27341	0.79505	1.39613	H	3.2987	0.80631	1.38954
H	-4.90928	0.99382	-1.01446	H	-4.88516	1.00677	-1.01715
H	3.85244	2.51367	-0.29787	H	3.87718	2.52485	-0.30473
H	2.54924	3.06256	0.79414	H	2.57466	3.07407	0.78791
H	2.50869	0.05199	-1.47853	H	2.53238	0.06368	-1.48506
H	4.76777	0.24229	-1.52389	H	4.79148	0.25355	-1.53155
H	1.17058	-3.52693	0.27234	H	1.19448	-3.51532	0.26601
H	3.18238	-1.68999	0.95211	H	3.20712	-1.67878	0.94496
H	3.82405	-2.68384	-1.1066	H	3.84745	-2.67246	-1.11419
H	2.16913	3.27126	-1.71252	H	2.19331	3.28301	-1.71846

H	-2.71212	-0.50789	-1.78157	H	-2.68866	-0.49523	-1.78556
H	-2.35618	1.3648	1.97007	H	-2.33049	1.37689	1.96614
H	-0.35993	2.58368	1.21022	H	-0.33441	2.59551	1.20545
H	-1.80509	3.46713	0.6256	H	-1.77969	3.47929	0.62168
H	-0.83783	0.18495	-0.39483	H	-0.81354	0.19707	-0.39968
H	-4.16208	-2.40585	-1.3103	H	-4.13873	-2.39299	-1.31382
H	-3.0314	-1.29669	1.16157	H	-3.00661	-1.28437	1.15763
H	-1.11769	-2.65746	0.31696	H	-1.09359	-2.64536	0.31186
H	0.18336	2.37119	-0.94876	H	0.20777	2.38321	-0.95383
		Cell_325_b (GS)				Cell_325_b (TS)	
	x	y	z		x	y	z
C	0.75595	-0.179392	-1.048368	C	0.77448	-0.17149	-1.0444
O	1.765306	0.802306	-1.256844	O	1.79324	0.83439	-1.28417
C	1.40784	-1.526935	-0.728926	C	1.44927	-1.54193	-0.70206
C	2.728506	0.983423	-0.161453	C	2.70504	1.04096	-0.12314
C	-4.03987	0.197224	1.134758	C	-4.02517	0.21277	1.12727
O	-3.222443	1.083988	1.545271	O	-3.20774	1.09953	1.53779
C	3.74467	1.974925	-0.717012	C	3.75937	1.99047	-0.72449
C	3.383409	-0.35622	0.230041	C	3.39811	-0.34067	0.22256
O	4.107705	-0.254443	1.468135	O	4.12241	-0.2389	1.46065
O	0.391355	-2.527409	-0.488977	O	0.40606	-2.51187	-0.49646
C	2.296202	-1.386721	0.494799	C	2.31091	-1.37118	0.48732
O	2.823699	-2.707717	0.725874	O	2.8384	-2.69217	0.71839
O	4.829277	2.015386	0.251604	O	4.84398	2.03093	0.24412
C	-3.747121	-0.667994	-0.034347	C	-3.73242	-0.65245	-0.04183
C	-1.972236	1.490086	0.768028	C	-1.95753	1.50563	0.76054
C	-2.403141	2.762708	0.058007	C	-2.38844	2.77825	0.05052
C	-1.495046	0.389876	-0.205094	C	-1.48034	0.40542	-0.21258
O	-0.089462	0.227199	0.065211	O	-0.07476	0.24274	0.05773
O	-4.538629	-1.838457	0.122165	O	-4.52393	-1.82291	0.11468
C	-2.231266	-0.945216	-0.035077	C	-2.21656	-0.92967	-0.04256
O	-2.007208	-1.811503	-1.140232	O	-1.99251	-1.79596	-1.14772
O	-3.482379	2.320454	-0.80181	O	-3.46768	2.336	-0.8093
H	0.169372	-0.219166	-1.970938	H	0.1841	-0.20364	-1.97839
H	2.018475	-1.82404	-1.590201	H	2.03319	-1.80851	-1.59766
H	2.2177	1.391371	0.719912	H	2.23228	1.40701	0.71261
H	-4.932091	0.042604	1.743135	H	-4.91739	0.05815	1.73565
H	3.287287	2.961278	-0.841951	H	3.302	2.97683	-0.84944
H	4.101157	1.612919	-1.688266	H	4.11584	1.62845	-1.69574
H	4.036777	-0.699481	-0.587232	H	4.05147	-0.68392	-0.59472
H	4.750606	0.48827	1.41171	H	4.76531	0.50381	1.40422
H	0.809771	-3.31713	-0.082725	H	0.82446	-3.3016	-0.09021
H	1.706718	-1.053244	1.359343	H	1.72142	-1.0377	1.35186
H	3.511204	-2.691929	1.422714	H	3.52591	-2.67639	1.41523
H	5.516947	2.669576	0.030846	H	5.53165	2.68512	0.02336
H	-3.984867	-0.107401	-0.956124	H	-3.97016	-0.09186	-0.96361
H	-1.233122	1.659185	1.54992	H	-1.21842	1.67473	1.54243
H	-1.546781	3.143637	-0.510896	H	-1.53208	3.15918	-0.51838
H	-2.741881	3.51875	0.772379	H	-2.72718	3.53429	0.76489
H	-1.656833	0.722504	-1.239801	H	-1.64213	0.73805	-1.24729

H	-4.28464	-2.513463	-0.542287	H	-4.26994	-2.49792	-0.54977
H	-1.918187	-1.41138	0.911597	H	-1.90348	-1.39584	0.90411
H	-1.136282	-2.295906	-1.023599	H	-1.12158	-2.28036	-1.03109
H	-3.876476	3.030029	-1.342853	H	-3.86177	3.04557	-1.35034
	Cell_325_c (GS)				Cell_325_c (TS)		
	x	y	z		x	y	z
C	0.905723	-0.941333	1.084908	C	0.9234	-0.96751	1.09584
O	2.263611	-1.344994	0.887578	O	2.29961	-1.32372	0.83471
C	0.941468	0.577029	1.245508	C	1.00619	0.50493	1.30318
C	2.951594	-0.771427	-0.279347	C	2.88451	-0.69902	-0.20114
C	-1.848856	0.707703	1.279506	C	-1.83741	0.69879	1.27073
O	-1.934093	-0.634925	1.554979	O	-1.92347	-0.64396	1.54535
C	4.360927	-1.34794	-0.216487	C	4.36965	-1.36055	-0.23127
C	2.953267	0.771472	-0.191031	C	2.96365	0.75994	-0.20332
O	3.369548	1.399687	-1.410383	O	3.37952	1.38861	-1.42256
O	-0.379776	1.23929	1.48032	O	-0.36777	1.2291	1.47082
C	1.513099	1.224461	-0.00345	C	1.52399	1.21385	-0.01434
O	1.348897	2.636502	0.239775	O	1.36104	2.62585	0.22994
O	5.136161	-0.578845	-1.178231	O	5.14479	-0.59142	-1.19307
C	-2.250113	1.153913	-0.114738	C	-2.23936	1.14626	-0.12291
C	-2.216632	-1.64836	0.501143	C	-2.20757	-1.65646	0.49103
C	-0.8882	-2.329345	0.179779	C	-0.8799	-2.33824	0.16822
C	-2.917101	-1.08838	-0.760479	C	-2.90855	-1.09508	-0.76969
O	-3.96368	-2.035072	-1.044686	O	-3.95606	-2.04078	-1.05377
O	-2.484007	2.55773	0.015012	O	-2.47209	2.55017	0.00797
C	-3.456108	0.325839	-0.543138	C	-3.44631	0.3194	-0.55098
O	-3.899902	0.91336	-1.78029	O	-3.89057	0.90811	-1.78741
O	0.085907	-1.270206	-0.045368	O	0.09486	-1.27969	-0.05692
H	0.567436	-1.451062	1.988917	H	0.57775	-1.46251	1.97702
H	1.528939	0.836622	2.128701	H	1.54148	0.82466	2.11811
H	2.438744	-1.073373	-1.200309	H	2.44709	-1.08358	-1.21303
H	-2.346884	1.288831	2.056652	H	-2.33443	1.27976	2.04864
H	4.348759	-2.411446	-0.471728	H	4.35641	-2.42388	-0.48725
H	4.759705	-1.219952	0.796105	H	4.76935	-1.2336	0.78112
H	3.572381	1.091519	0.66147	H	3.58366	1.07894	0.64893
H	4.236929	1.026163	-1.690433	H	4.24641	1.01461	-1.70352
H	-0.28378	2.209861	1.238632	H	-0.27117	2.19974	1.22969
H	0.951909	0.925031	-0.897934	H	0.96188	0.91542	-0.90859
H	1.828842	3.183639	-0.414587	H	1.84093	3.17306	-0.42441
H	6.02959	-0.937558	-1.329488	H	6.03783	-0.95072	-1.34524
H	-1.439328	0.957287	-0.832152	H	-1.42926	0.9495	-0.84106
H	-2.917579	-2.337069	0.975385	H	-2.90869	-2.34496	0.96532
H	-0.966042	-2.919785	-0.73493	H	-0.95887	-2.92799	-0.74684
H	-0.560586	-2.978054	0.997627	H	-0.55218	-2.98776	0.98537
H	-2.205445	-1.028268	-1.597015	H	-2.19747	-1.03494	-1.60671
H	-4.187991	-2.083808	-1.993837	H	-4.18111	-2.0887	-2.00278
H	-2.886978	2.927429	-0.797583	H	-2.87538	2.92073	-0.80408
H	-4.24864	0.328432	0.218071	H	-4.23828	0.32208	0.21081
H	-4.855721	0.80356	-1.944244	H	-4.8466	0.79915	-1.95072

	Str_325_a (GS)				Str_325_a (TS)		
	x	y	z		x	y	z
C	0.6561	-0.41229	-0.99712	C	0.67926	-0.39263	-0.98147
O	1.58362	0.6278	-1.29588	O	1.61524	0.66922	-1.3084
C	1.40022	-1.6848	-0.58948	C	1.444	-1.68575	-0.55322
C	2.57526	0.94277	-0.25752	C	2.56063	1.0071	-0.21096
C	-4.37449	0.16558	0.91704	C	-4.35477	0.19212	0.92237
O	-3.51275	1.36929	0.78118	O	-3.49303	1.39582	0.78652
C	3.52208	1.92659	-0.93632	C	3.5418	1.95313	-0.93098
C	3.31396	-0.31897	0.22968	C	3.33368	-0.29243	0.23502
O	4.04427	-0.06532	1.44272	O	4.06399	-0.03879	1.44806
O	0.4487	-2.71599	-0.24818	O	0.46842	-2.68946	-0.24284
C	2.30152	-1.39406	0.5971	C	2.32125	-1.36753	0.60244
O	2.92529	-2.6535	0.91202	O	2.94501	-2.62696	0.91736
O	4.6327	2.1092	-0.01583	O	4.65242	2.13573	-0.0105
C	-3.84393	-0.97886	0.03505	C	-3.82421	-0.95232	0.04039
C	-2.02519	1.24737	0.84062	C	-2.00547	1.27391	0.84596
C	-1.56133	2.66116	0.43135	C	-1.54161	2.68769	0.43669
C	-1.5983	0.17324	-0.15664	C	-1.57858	0.19978	-0.1513
O	-0.19472	0.01105	0.10707	O	-0.17499	0.03759	0.11241
O	-4.64357	-1.68627	-0.56641	O	-4.62385	-1.65974	-0.56108
C	-2.32814	-1.17327	0.03447	C	-2.30842	-1.14674	0.03981
O	-1.95591	-2.04638	-1.01369	O	-1.93619	-2.01985	-1.00835
O	-2.66328	3.09618	-0.43303	O	-2.64356	3.12271	-0.42769
H	0.05458	-0.56149	-1.89747	H	0.07432	-0.53497	-1.89211
H	2.01172	-2.01086	-1.44014	H	2.03144	-1.98434	-1.43478
H	2.07662	1.40204	0.60639	H	2.09625	1.42865	0.61186
H	-5.37782	0.4583	0.60729	H	-5.3581	0.48484	0.61263
H	-4.36382	-0.09509	1.97805	H	-4.3441	-0.06856	1.98339
H	-3.66329	2.17746	0.11528	H	-3.64357	2.204	0.12062
H	3.0133	2.87546	-1.13536	H	3.03303	2.902	-1.13002
H	3.86355	1.49302	-1.88354	H	3.88326	1.51954	-1.87819
H	3.97891	-0.68815	-0.56658	H	3.99862	-0.6616	-0.56124
H	4.65854	0.69	1.30494	H	4.67826	0.71653	1.31027
H	0.91807	-3.46294	0.18128	H	0.93778	-3.43641	0.18662
H	1.7059	-1.03634	1.44793	H	1.72562	-1.00981	1.45327
H	3.61451	-2.54098	1.59805	H	3.63423	-2.51445	1.60339
H	5.30286	2.73743	-0.34195	H	5.32258	2.76396	-0.33661
H	-1.74454	0.98435	1.86178	H	-1.72482	1.01088	1.86712
H	-0.6201	2.59101	-0.11871	H	-0.60038	2.61754	-0.11337
H	-1.4719	3.33338	1.28587	H	-1.45218	3.35992	1.29121
H	-1.77097	0.51827	-1.18871	H	-1.75125	0.5448	-1.18337
H	-2.03923	-1.5585	1.02944	H	-2.01951	-1.53196	1.03478
H	-1.11994	-2.54331	-0.78812	H	-1.10022	-2.51677	-0.78278
H	-2.56838	3.94175	-0.90477	H	-2.54866	3.96828	-0.89943

Table S8. Vibration Modes (M062X/SDD) of Mass Spectrometric Species in Ground and Transition States, Obtained Using Corresponding Atomic Co-ordinates Shown in Table S7.

Str_325_a (TS)				Str_325_a (GS)			
Freq.	-26.2702	23.0387	35.5875	Freq.	31.7761	34.9679	49.9572
Freq.	58.8882	66.3387	89.5306	Freq.	58.7286	70.1371	90.1714
Freq.	105.4099	110.259	123.7155	Freq.	109.9225	119.1085	142.0753
Freq.	148.388	185.8284	200.1498	Freq.	149.6546	188.6169	201.0179
Freq.	212.4454	244.6678	254.3646	Freq.	216.0369	246.5977	262.5756
Freq.	276.4418	297.0406	302.4679	Freq.	278.8896	299.6104	304.915
Freq.	318.8315	327.8564	339.4855	Freq.	315.5736	330.8911	339.1072
Freq.	343.0016	347.9289	377.5662	Freq.	347.4105	357.1803	377.9563
Freq.	380.4265	415.5485	420.6735	Freq.	381.0172	418.5827	422.8373
Freq.	434.9387	442.0063	462.1495	Freq.	437.4351	445.9208	448.9918
Freq.	479.888	518.014	529.0505	Freq.	485.6988	521.3508	529.6483
Freq.	552.8254	559.3759	584.215	Freq.	546.0681	559.3074	582.3062
Freq.	598.9131	631.593	635.944	Freq.	599.0522	635.4129	636.4959
Freq.	645.9777	701.2565	761.905	Freq.	642.2301	701.5885	768.3764
Freq.	848.2728	862.6041	869.9479	Freq.	850.7974	869.5476	885.5578
Freq.	885.9521	921.4479	939.6311	Freq.	921.8054	931.6919	942.0446
Freq.	942.1216	952.0281	993.8327	Freq.	951.0684	990.0065	994.5976
Freq.	1,003.971	1,016.303	1,030.184	Freq.	1,004.971	1029.7849	1040.536
Freq.	1,041.434	1,046.336	1,063.300	Freq.	1,043.054	1,065.1952	1,077.551
Freq.	1,073.052	1,074.566	1,096.844	Freq.	1,095.034	1,108.8263	1,128.811
Freq.	1,103.760	1,123.337	1,138.575	Freq.	1,137.188	1,142.1646	1,146.370
Freq.	1,147.714	1,150.602	1,153.989	Freq.	1,150.755	1,155.6267	1,164.831
Freq.	1,166.523	1,168.232	1,178.096	Freq.	1,169.882	1,175.6583	1,194.292
Freq.	1,187.545	1,200.064	1,203.140	Freq.	1,202.375	1,226.7167	1,247.014
Freq.	1,243.830	1,247.051	1,252.549	Freq.	1,251.890	1,257.8692	1,265.500
Freq.	1,272.623	1,274.611	1,280.093	Freq.	1,273.092	1,280.7552	1,284.667
Freq.	1,284.100	1,285.000	1,293.716	Freq.	1,289.873	1,303.6502	1,324.438
Freq.	1,303.913	1,337.991	1,341.991	Freq.	1,341.369	1,348.7433	1,360.760
Freq.	1,365.643	1,370.565	1,374.244	Freq.	1,367.786	1,370.4836	1,389.074
Freq.	1,390.923	1,398.181	1,402.117	Freq.	1,395.699	1,400.3922	1,424.388
Freq.	1,429.647	1,438.974	1,446.708	Freq.	1,428.751	1,442.8534	1,447.680
Freq.	1,454.056	1,466.943	1,472.925	Freq.	1,453.767	1,467.1037	1,472.355
Freq.	1,475.099	1,499.312	1,514.838	Freq.	1,478.671	1,487.7623	1,499.303
Freq.	1,548.132	1,549.453	1,792.690	Freq.	1,548.675	1,550.1918	1,792.808
Freq.	2,588.410	3,030.002	3,077.877	Freq.	2,588.642	3,029.9232	3,071.827
Freq.	3,080.678	3,090.786	3,096.876	Freq.	3,080.262	3,096.585	3,105.570
Freq.	3,109.861	3,117.858	3,134.513	Freq.	3,110.013	3,124.0581	3,134.598
Freq.	3,142.094	3,161.994	3,198.415	Freq.	3,142.019	3,162.0236	3,175.750
Freq.	3,212.913	3,231.964	3,344.838	Freq.	3,198.674	3,213.0949	3,231.879
Freq.	3,686.712	3,727.411	3,757.532	Freq.	3,339.221	3,687.4849	3,728.332
Freq.	3,769.766	3,809.583	3,835.532	Freq.	3,769.839	3,810.3445	3,835.398
Str_145 (GS)				Str_145 (TS)			
Freq.	70.1494	88.038	173.9863	Freq.	-530.9048	40.8385	101.3718
Freq.	224.3448	307.8254	335.8745	Freq.	151.1661	215.1589	288.521
Freq.	347.2926	356.1119	395.5457	Freq.	336.1343	359.3932	373.4555
Freq.	425.4095	512.4143	533.2074	Freq.	385.5276	427.4832	522.7878
Freq.	560.8048	653.5576	678.4455	Freq.	543.9188	617.8768	682.0327

Freq.	727.727	763.3002	850.795	Freq.	714.5783	750.2704	851.6068
Freq.	894.7522	926.5932	987.9574	Freq.	924.9161	950.0447	982.5764
Freq.	1,027.442	1043.463	1,066.666	Freq.	1,024.635	1,030.0954	1,050.097
Freq.	1,097.400	1119.657	1,163.856	Freq.	1,087.975	1,103.8753	1,112.502
Freq.	1,190.774	1213.788	1,252.778	Freq.	1,155.205	1,211.051	1,225.276
Freq.	1,269.005	1299.489	1,325.019	Freq.	1,260.971	1,285.1303	1,334.287
Freq.	1,374.731	1399.017	1,401.032	Freq.	1,372.372	1,389.1888	1,434.763
Freq.	1,426.250	1491.804	1,507.179	Freq.	1,470.866	1,491.519	1,516.562
Freq.	1,551.791	1751.736	1,781.782	Freq.	1,557.930	1,746.4733	1,917.222
Freq.	2,282.945	3136.288	3,160.989	Freq.	2,324.416	2,764.9536	3,136.494
Freq.	3,171.211	3232.656	3,240.940	Freq.	3,141.866	3,162.9124	3,231.269
Freq.	3,244.005	3680.256	3,846.553	Freq.	3,241.267	3,851.5569	4,115.217

Table S9. Thermochemistry (M062X/SDD) of Observable Mass Spectrometric Ions of PLA in Ground and Transition States in Gas-phase, Depending on Theoretical Level of Computations and Ionic Structures; Theoretical Intensity (I^{Theor}_{SD}) Data on Equations (3) and (4)

	m/z 145		**m/z 145**		**m/z 145**	
	CPLA_145_a		**CPLA_145_b**		**CPLA_145_c**	
	M062X/SDD		**M062X/SDD**		**M062X/SDD**	
	GS	**TS**	**GS**	**TS**	**GS**	**TS**
EZPVE	95.19585	94.37331	95.42336	94.50907	95.25603	94.60863
Ecorr	0.162034	0.160319	0.162274	0.160381	0.162003	0.160677
Hcorr	0.162978	0.161264	0.163218	0.161325	0.162947	0.161621
Gcorr	0.115746	0.114839	0.116599	0.115546	0.116451	0.115733
ε0	0.151704	0.150393	0.152067	0.150610	0.151800	0.150768
E	-534.176319	-534.16572	-534.17881	-534.1668	-534.1806	-534.1704
H	-534.175375	-534.16478	-534.17786	-534.1658	-534.1797	-534.1695
G	-534.222608	-534.21120	-534.22448	-534.2116	-534.2262	-534.2154
DQC	308.7478		302.46515		518.30159	
ITh.SD	9.026205.10-8		8.9339.10-8		1.1695.10-7	
	m/z 361		m/z 433		m/z 289	
	CPLA_361		CPLA_433		CPLA_289	
	*		*		M062X/SDD	
	GS	TS	GS	TS	GS	TS
EZPVE	248.69738	248.61934	295.65467	295.3645		
Ecorr	0.421415	0.420279	0.501650	0.500608		
Hcorr	0.422359	0.421223	0.502594	0.501553		
Gcorr	0.340564	0.343618	0.410787	0.410581		
ε0	0.396325	0.396200	0.471156	0.470693		
E	-1,318.47003	-1,318.468	-1,582.029	-1,582.03		
H	-1,318.46909	-1,318.467	-1,582.028	-1,582.03		
G	-1,318.5509	-1,318.545	-1,582.12	-1,582.12		
DQC	0.028467		275.6071			
ITh.SD	8.66717.10-10		8.2448.10-8			

Notes: EZPVE-zero-point vibration energy (kcal/mol); ε0-zero-point correction (Hartree/partice); Ecorr-thermal correction to energy (Hartree/partice); Hcorr-thermal correction to enthalpy (Hartree/partice); Gcorr-thermal correction to free energy (Hartree/partice); E-sum of electronic and thermal energies (Hartree/partice); H-sum of electronic and thermal enthalpies (Hartree/partice); G-sum of electronic and thermal free energies (Hartree/partice).
* M062X/STO-3g

Table S10. Atomic Co-ordinates of Mass Spectrometric Species in Ground and Transition States used to Compute the Data on Table S9 and Table S11

	PLA_145_a (GS)				PLA_145_a (GS)		
	x	y	z		x	y	z
C	1.6101	-0.423727	-0.244064	C	-1.58966	0.4286	-0.1818
O	0.309333	-1.321542	-0.289973	O	-0.27661	1.35778	-0.2684
C	1.175529	1.016962	-0.0955	C	-1.12527	-1.04191	-0.00348
O	2.621315	-1.036317	-0.284186	O	-2.64873	1.09834	-0.18521
C	1.038589	1.386171	1.388559	C	-1.02305	-1.37142	1.43594
O	-0.045976	1.238721	-0.842691	O	0.06151	-1.22397	-0.79532
C	-1.226434	0.610332	-0.462561	C	1.24197	-0.59558	-0.41519
O	-2.283746	1.198044	-0.39288	O	2.29928	-1.18329	-0.34551
C	-1.166279	-0.913857	-0.291874	C	1.18181	0.92862	-0.24451
C	-1.853743	-1.421471	0.962707	C	1.86928	1.43623	1.01008
H	0.499048	-2.289876	-0.331272	H	-0.48353	2.30478	-0.28392
H	1.927791	1.637054	-0.585877	H	-1.91216	-1.62227	-0.53843
H	0.68828	2.419154	1.44615	H	-0.67274	-2.40441	1.49356
H	2.004096	1.31555	1.896486	H	-1.98856	-1.30079	1.94385
H	0.319372	0.742452	1.907452	H	-0.30384	-0.7277	1.95484
H	-1.566544	-1.366133	-1.204751	H	1.5821	1.38088	-1.15738
H	-2.892468	-1.076425	0.933949	H	2.908	1.09118	0.98132
H	-1.390463	-1.025801	1.870095	H	1.406	1.04056	1.91746
H	-1.863105	-2.513691	1.002019	H	1.87864	2.52845	1.04939
	PLA_145_b (GS)				PLA_145_b (GS)		
	x	y	z		x	y	z
C	-1.49381	0.695322	-0.280447	C	-1.4754	0.69439	-0.22445
O	-0.090414	1.29869	0.055747	O	-0.05878	1.33152	0.06793
C	-1.358464	-0.812631	-0.252991	C	-1.30795	-0.84569	-0.16495
O	-2.3528	1.489117	-0.467676	O	-2.38593	1.5497	-0.37213
C	-1.608613	-1.373277	1.154647	C	-1.59549	-1.36359	1.19463
O	-0.074311	-1.200032	-0.806982	O	-0.06118	-1.19034	-0.76702
C	1.130149	-0.80538	-0.247401	C	1.14327	-0.79569	-0.20744
O	2.148722	-1.439515	-0.417335	O	2.16184	-1.42982	-0.37737
C	1.128842	0.514871	0.541575	C	1.14196	0.52457	0.58154
C	2.373608	1.347363	0.291128	C	2.38673	1.35705	0.33109
H	-0.013263	2.282391	0.004268	H	-0.00012	2.29232	0.04422
H	-2.091972	-1.21087	-0.955852	H	-2.07868	-1.20114	-0.91571
H	-1.464908	-2.455119	1.112943	H	-1.4518	-2.44544	1.15294
H	-2.636761	-1.172094	1.467638	H	-2.62364	-1.16239	1.50758
H	-0.929421	-0.958415	1.905849	H	-0.91631	-0.94874	1.94584
H	0.95231	0.336914	1.605774	H	0.96541	0.34662	1.64574
H	2.489512	1.58441	-0.769821	H	2.50263	1.5941	-0.72986
H	3.24008	0.748445	0.587247	H	3.25321	0.75814	0.62721
H	2.374568	2.260649	0.892849	H	2.38769	2.27034	0.93281
	PLA_145_c (GS)				PLA_145_c (TS)		
	x	y	z		x	y	z
C	-1.244181	0.936286	-0.034349	C	-1.23312	0.93625	-0.00255
O	0.27531	1.318589	-0.053595	O	0.29863	1.34991	-0.06247
C	-1.320708	-0.504547	0.437866	C	-1.27984	-0.5344	0.49943
O	-1.990235	1.789316	-0.375592	O	-2.02707	1.84642	-0.30706

C	-2.666396	-1.12644	0.085	C	-2.66026	-1.1166	0.10192
O	-0.282625	-1.267493	-0.241734	O	-0.27649	-1.25765	-0.22482
C	1.06443	-0.984721	-0.060027	C	1.07056	-0.97488	-0.04311
O	1.928063	-1.7824	-0.350647	O	1.9342	-1.77256	-0.33373
C	1.383272	0.416663	0.491271	C	1.38941	0.42651	0.50818
C	2.726743	0.945646	0.029274	C	2.73288	0.95549	0.04619
H	0.522101	2.208376	-0.404347	H	0.5283	2.21845	-0.38752
H	-1.154383	-0.511011	1.524548	H	-1.14819	-0.50121	1.54174
H	-2.81639	-1.122035	-0.996433	H	-2.81023	-1.11218	-0.97951
H	-2.669148	-2.160093	0.433649	H	-2.66304	-2.15026	0.45056
H	-3.48216	-0.583123	0.568699	H	-3.47602	-0.57327	0.58562
H	1.267572	0.452525	1.578893	H	1.27369	0.46238	1.59581
H	2.938898	1.93056	0.454076	H	2.94503	1.9404	0.47099
H	2.793203	0.97046	-1.061785	H	2.79933	0.9803	-1.04487
H	3.497245	0.252923	0.381034	H	3.50338	0.26277	0.39795

Table S11. Vibration Modes (M062X/SDD) of Mass Spectrometric Species in Ground and Transition States, Obtained Using Corresponding Atomic Co-ordinates Shown in Table S10

CPLA_145_a (GS)				**CPLA_145_a (GS)**			
Freq.	47.1189	67.6807	106.5524	Freq.	-205.592	42.0415	70.3259
Freq.	205.4716	224.0436	228.7075	Freq.	153.8893	222.2723	237.1756
Freq.	266.5313	303.6356	367.6351	Freq.	263.8073	272.8065	286.8025
Freq.	375.386	413.3008	464.4635	Freq.	366.1552	410.0902	433.3524
Freq.	526.9157	542.365	564.8478	Freq.	452.6157	516.0665	549.9181
Freq.	618.3046	681.7797	722.6457	Freq.	615.357	713.4441	741.524
Freq.	781.9339	831.4824	893.9222	Freq.	776.4308	823.3506	904.901
Freq.	982.315	1,022.321	1,085.75	Freq.	976.414	1,026.889	1,095.027
Freq.	1,105.2478	1,137.787	1,149.16	Freq.	1,124.112	1,146.910	1,180.113
Freq.	1,185.0333	1,229.838	1,315.09	Freq.	1,209.637	1,239.040	1,265.056
Freq.	1,331.9096	1,342.322	1,378.73	Freq.	1,347.245	1,398.671	1,403.912
Freq.	1,418.2104	1,451.510	1,457.39	Freq.	1,422.541	1,457.635	1,472.025
Freq.	1,507.8584	1,515.579	1,517.76	Freq.	1,508.009	1,516.278	1,517.143
Freq.	1,521.8554	1,827.000	1,989.05	Freq.	1,523.151	1,584.049	1,826.420
Freq.	3,077.4185	3,083.870	3,155.22	Freq.	2,992.791	3,074.423	3,084.711
Freq.	3,173.1997	3,183.728	3,190.39	Freq.	3,151.008	3,170.115	3,186.212
Freq.	3,193.9263	3,199.100	3,627.11	Freq.	3,192.771	3,193.331	3,877.112
CPLA_145_b (GS)				CPLA_145_b (TS)			
Freq.	55.6591	89.5295	127.2564	Freq.	-356.0893	51.1094	100.5904
Freq.	204.8607	227.3888	245.2698	Freq.	155.2145	228.5986	246.3471
Freq.	266.8809	309.4923	354.7688	Freq.	260.5933	273.708	303.6425
Freq.	389.6729	414.5031	450.045	Freq.	373.8704	398.7914	442.4012
Freq.	479.6321	549.2846	572.8571	Freq.	459.1666	511.5624	558.2699
Freq.	653.4013	686.3315	735.2884	Freq.	650.3413	726.4353	749.2917
Freq.	772.3694	823.2604	902.3319	Freq.	773.6482	802.9953	910.6661
Freq.	982.4858	1,025.975	1,096.94	Freq.	984.55	1,025.397	1,107.399
Freq.	1,116.1305	1,135.605	1,142.76	Freq.	1,128.047	1,135.119	1,162.800
Freq.	1,189.001	1,222.190	1,315.15	Freq.	1,205.585	1,243.132	1,267.091
Freq.	1,334.5293	1,351.046	1,386.69	Freq.	1,325.014	1,386.448	1,431.535
Freq.	1,405.0321	1,455.236	1,461.33	Freq.	1,456.600	1,461.757	1,472.356
Freq.	1,513.1518	1,516.213	1,518.64	Freq.	1,512.610	1,516.078	1,519.144
Freq.	1,523.612	1,825.141	1,975.77	Freq.	1,529.551	1,567.285	1,826.569

Freq.	3,089.3376	3,090.952	3,162.05	Freq.	2,796.636	3,085.289	3,090.377
Freq.	3,185.6614	3,194.882	3,197.75	Freq.	3,164.373	3,181.763	3,193.391
Freq.	3,198.8862	3,202.42	3,624.91	Freq.	3,194.454	3,198.383	3,964.068
CPLA_145_c (TS)					CPLA_145_c (TS)		
Freq.	58.2637	106.7824	130.9675	Freq.	-507.5359	60.3652	107.966
Freq.	209.4044	232.376	243.126	Freq.	167.0873	198.7095	234.6247
Freq.	269.8463	298.9328	344.7835	Freq.	250.0159	282.864	317.8806
Freq.	365.5842	402.6893	459.7494	Freq.	364.8075	376.6299	393.7908
Freq.	484.8054	554.0917	595.5472	Freq.	474.5654	516.4975	582.9721
Freq.	616.0008	652.3982	743.1151	Freq.	614.3587	650.0821	746.5671
Freq.	780.2779	826.0346	920.3034	Freq.	772.1703	807.2959	895.1715
Freq.	986.2138	1,036.900	1,081.20	Freq.	959.6426	1,022.474	1,053.979
Freq.	1,119.9996	1,137.567	1,170.82	Freq.	1,095.354	1,117.986	1,124.029
Freq.	1,174.4358	1,209.693	1,311.18	Freq.	1,149.915	1,190.055	1,220.478
Freq.	1,336.1228	1,338.589	1,360.26	Freq.	1,230.483	1,251.029	1,324.948
Freq.	1,401.7348	1,460.804	1,464.17	Freq.	1,387.310	1,454.585	1,461.464
Freq.	1,508.6039	1,512.396	1,518.68	Freq.	1,507.529	1,512.787	1,519.175
Freq.	1,522.6984	1,831.520	1,990.56	Freq.	1,519.460	1,616.871	1,831.716
Freq.	3,085.6374	3,086.208	3,104.53	Freq.	3,086.976	3,105.219	3,156.040
Freq.	3,155.2807	3,187.184	3,196.67	Freq.	3,186.826	3,198.383	3,214.480
Freq.	3,211.3645	3,217.744	3,618.65	Freq.	3,217.654	3,566.616	4,081.802

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