Supporting of

Temperature Effects on Optical Properties and Chemical Composition of Secondary Organic Aerosol Derived from n-Dodecane

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Calculation Method of RI Values

The extinction coefficients (α_{ext}) of the particles with CRDS can be calculated with Equation (1):

$$\alpha_{ext} = \frac{L}{cl}\left(\frac{1}{\tau} - \frac{1}{\tau_0}\right) \quad (1)$$

where L is the distance of the two mirrors in the cavity, l is the length of the cavity that filled with aerosol particles, c is the speed of the light, τ_0 is the ring down time of the CRDS when it is filled with zero air, and τ is the ting down time of the CRDS when it is filled with aerosol particles

For the homogeneous spherical particles, the α_{ext} can be calculated with Equation (2):

$$\alpha_{ext} = N\sigma_{ext} = \frac{1}{4}N\pi D^2 Q_{ext} \quad (2)$$

where N is the concentration of the spherical particles, σ_{ext} is the extinction cross section, D is the particle diameter, and Q_{ext} is the extinction efficiency.

Q_{ext} is the ratio of Beer's law extinction cross section to the geometric area of the spherical particles, it is dimensionless, and can be expressed with Equation (3):

$$Q_{ext} = \frac{4\alpha_{ext}}{N\pi D^2} \quad (3)$$

For the polydisperse SOA particles formed in the smog chamber, they follow log-normal distribution and the geometric standard deviation is always smaller than 1.5, the Q_{ext} with a surface mean diameter D_s can be expressed with Equation (4) (with the assumption that the aerosol particles during each size bin are homogeneous spherical particles) (Nakayama et al., 2010):

$$Q_{ext}(D_s) = \frac{\alpha_{ext}}{\int N(D_p)\frac{1}{4}\pi D_p^2 dD_p} \quad (4)$$

where D_p is the geometrical diameter of the particle, dD_p is the size bin of the particles, and $N(D_p)$ is the number concentration of the particles in dD_p with D_p per unit volume.

For the particles with D_p in each size bin dD_p, the surface area $S(D_p)$ can be expressed by Equation (5):

$$S(D_P) = N(D_p)\pi D_p^2 \quad (5)$$

So the Equation (4) can also be expressed with Eauqtion (6):

$$Q_{ext}(D_s) = \frac{\alpha_{ext}}{\int \frac{1}{4}S(D_p)dD_p} = \frac{4\alpha_{ext}}{S_{tot}} \quad (6)$$

where S_{tot} is the total surface area of the particles, and the values can be obtained with SMPS.

While the extinction efficiency can also be calculated with Mie-Lorenz theory, Equation (7):

$$Q_{ext}(D_s) = \int f(D_p)Q_{ext}(D_p)dD_p \quad (7)$$

where $f(D_p)$ is the normalized surface area weighted size distribution function.

Then the measured extinction efficiency ($Q_{ext,mea}$) is compared to calculated extinction efficiency ($Q_{ext,cal}$). And the best-fit RI value is determined by minimizing the following reduced merit function (χ_r), Equation (8):

$$\chi_r = \frac{1}{N}\sum_{i=1}^{N}(Q_{ext,mea} - Q_{ext,cal}(n,k))_i^2 \quad (8)$$

where N is the number of diameters to be calculated.

The QSPR can be expressed with Equation (9):

$$RI_{predicted} = 0.031717(\mu) + 0.0006087(\alpha) - 3.0227\left(\frac{\rho_m}{M}\right) + 1.38709 \quad (9)$$

where μ is the unsaturation of the molecular formula, α is the polarizability of the molecular formula, ρ_m is the mass density (g/cm^3), and M is the molar mass (g/mol).

The mass density of the compound is estimated by AIM model, the detailes of which can be referred to Girolami (1994)

μ is calculated through the conventional approach, which is used in many organic chemistry texts, Equation (10)

$$\mu = (\#C + 1) - 0.5(\#H - \#N) \quad (10)$$

where #C,#H, and #N are the number of the C, H, and N respectively.

α is calculated based on the molecular formula of the compound, it can be expressed by Equation (11):

$$\alpha = 1.51(\#C) + 0.17(\#H) + 0.57(\#O) + 1.05(\#N) + 2.99(\#S) + 2.48(\#P) + 0.22(\#F) + 2.16(\#Cl) + 3.29(\#Br) + 5.45(\#I) + 0.32 \quad (11)$$

where # is the number of the atoms of each element in the molecular formula.

Calculation Method of Average Elemental Composition and Ratios

Due to the complexity of chemical composition in secondary organic aerosol particles, it is common to express the bulk composition as averaged elemental ratios. The average elemental composition and ratios (C, H, O, H/C, O/C) can be estimated from the identified molecular formulas(Bateman et al., 2012):

$$< \mathrm{Y} >= \frac{\sum_i x_i Y_i}{\sum_i x_i} \quad (12)$$

$$< \mathrm{Y/Z} >= \frac{\sum_i x_i Y_i}{\sum_i x_i Z_i} \quad (13)$$

where Y=C, H, O, Y/Z=H/C, O/C. x_i is the peak abundance of elemental composition.

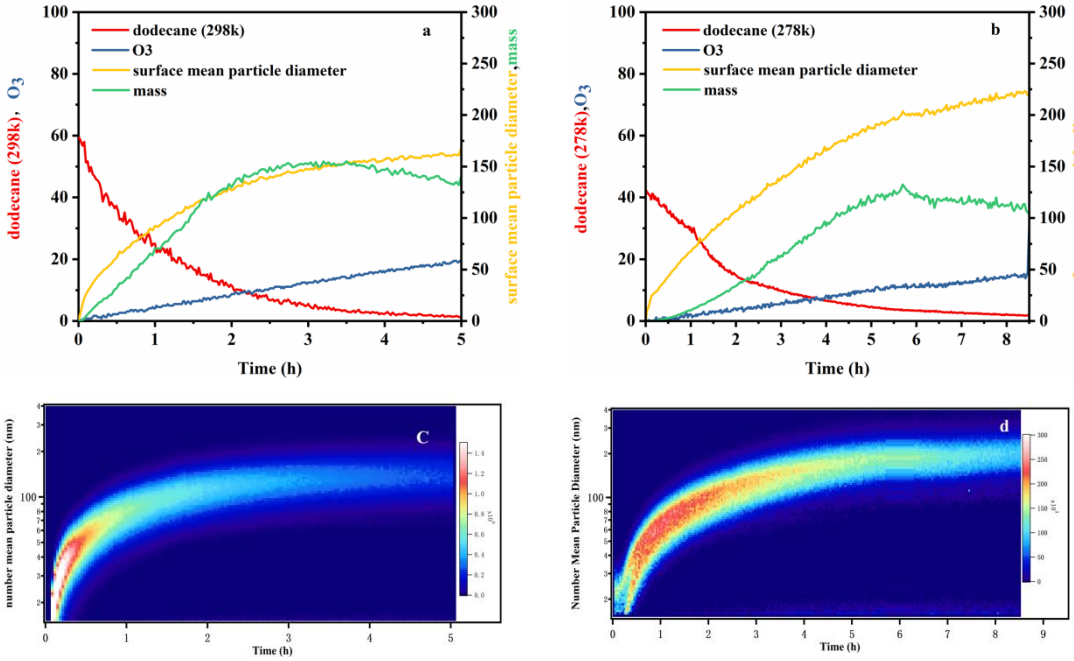


Figure S1. Reaction profiles of *n*-dodecane photo-oxidation experiments at two different temperature conditions, (a) time-dependent concentration of dodecane, O_3, surface mean particle diameter and aerosol mass (the density used in the system is 1.1 g/cm^3, measured with our CPMA and SMPS) at 25 ˚C; (b) time-dependent concentration of dodecane, O_3, surface mean particle diameter and aerosol mass (the density used in the system is 1.1 g/cm^3, measured with our CPMA and SMPS) at 5 ˚C; (c) number size distribution of formed aerosol particles at 25 ˚C; (d) number size distribution of formed aerosol particles at 5 ˚C.

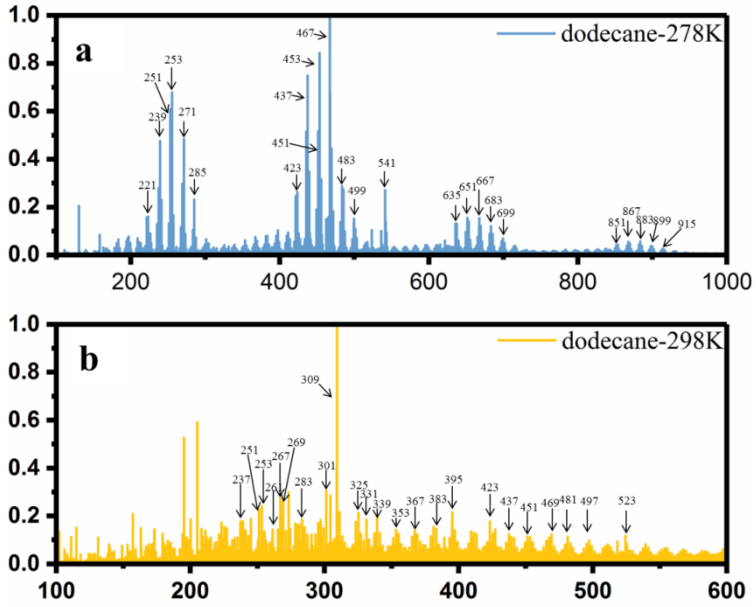
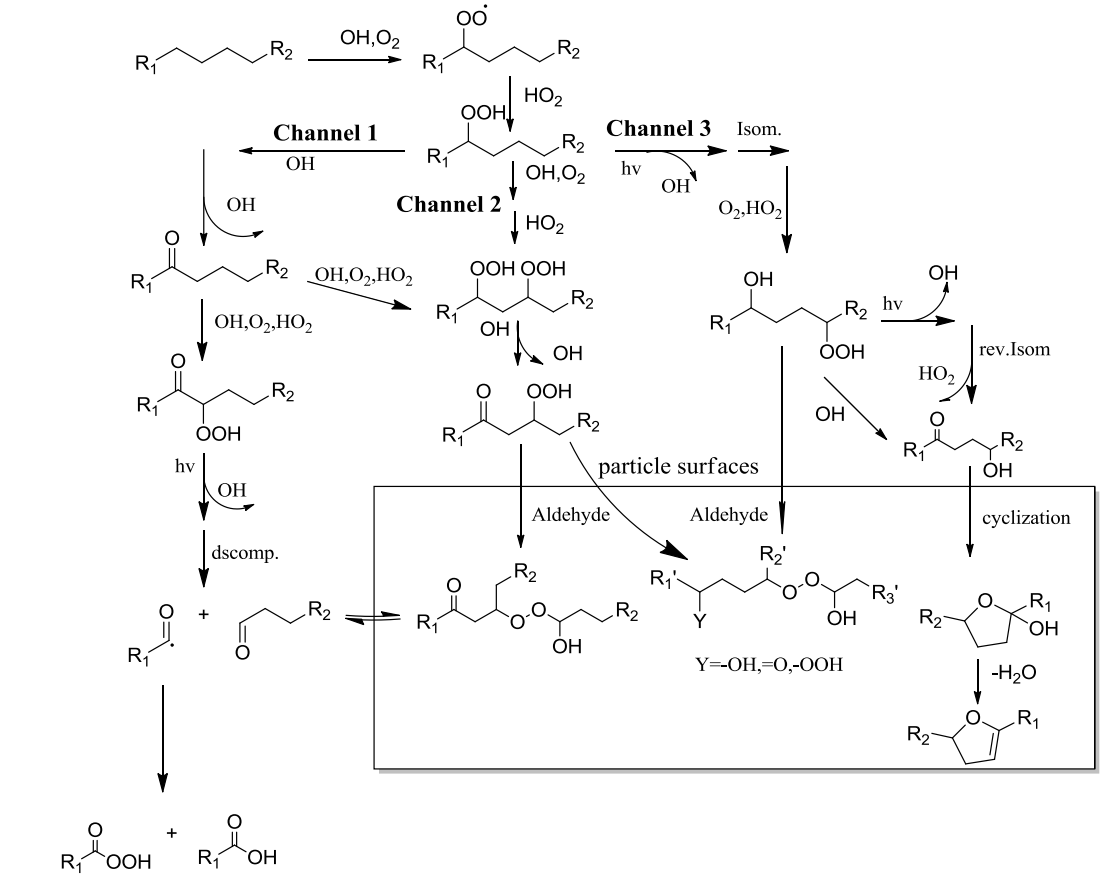


Figure S2. Mass specra of *n*-dodecane SOA obtained by ESI-TOF-MS in positive ion mode. (a) low temperature condition; (b) room temperature condition.



Low Temperature, Particle Surface

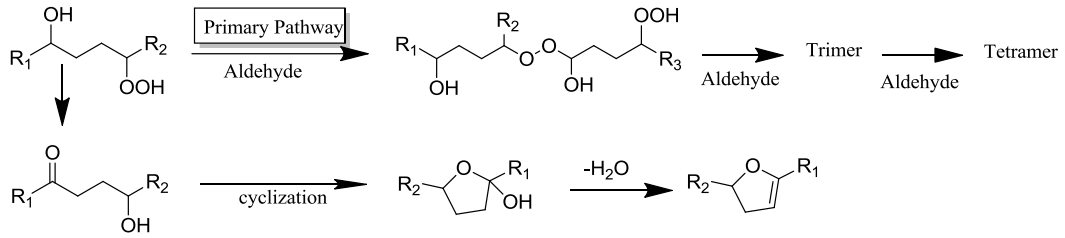
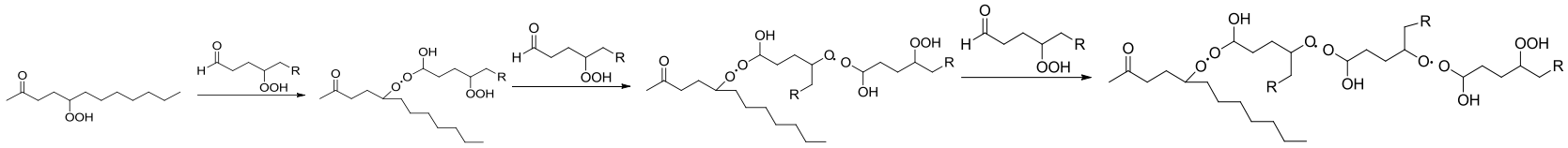
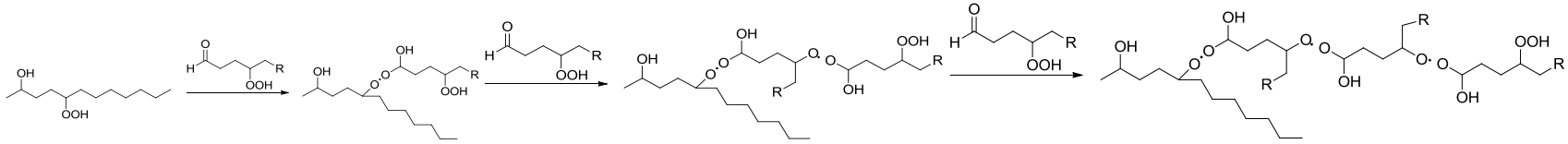


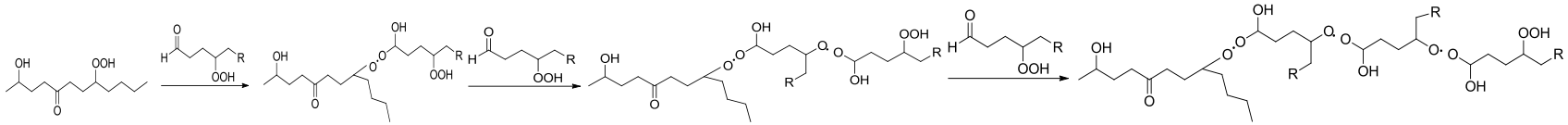
Figure S3. The proposed reaction mechanism of long-chain alkanes under low-NOx condition (Fahnestock et al., 2015;Yee et al., 2013, 2012).



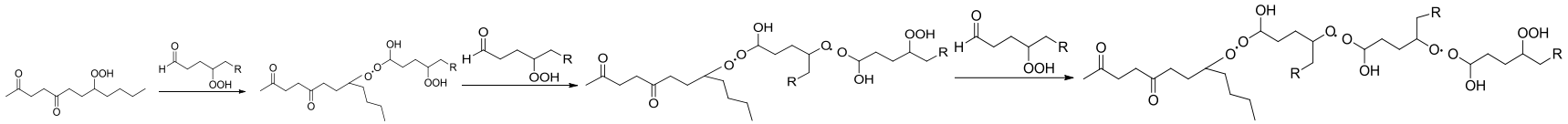
$C_{12}H_{24}O_3$ $C_{10}H_{20}O_3$ $C_{22}H_{44}O_6$ $C_{32}H_{64}O_9$ $C_{42}H_{84}O_{12}$



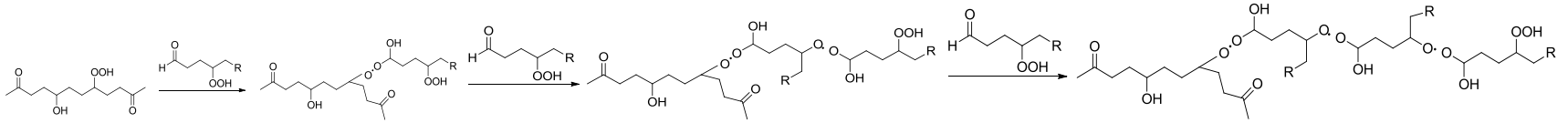
$C_{12}H_{26}O_3$ $C_{22}H_{46}O_6$ $C_{32}H_{46}O_9$ $C_{42}H_{86}O_{12}$



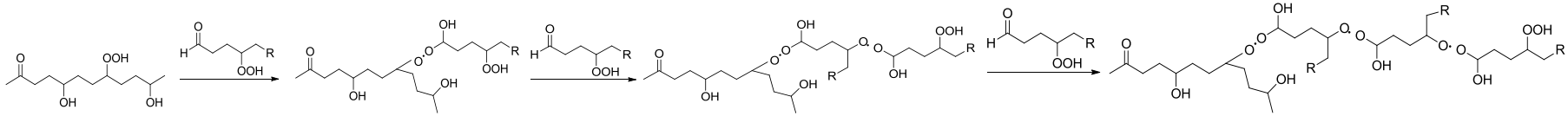
$C_{12}H_{24}O_4$ $C_{22}H_{44}O_7$ $C_{32}H_{64}O_{10}$ $C_{42}H_{84}O_{13}$



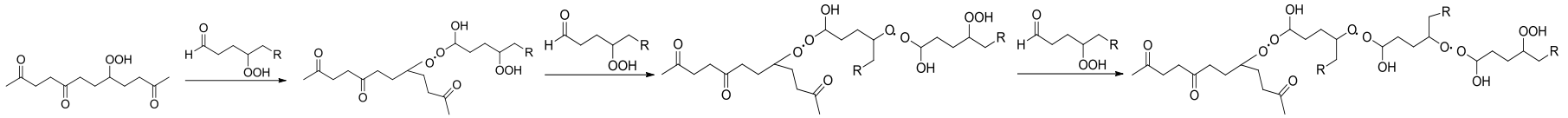
$C_{12}H_{22}O_4$ $C_{22}H_{42}O_7$ $C_{32}H_{62}O_{10}$ $C_{42}H_{82}O_{13}$



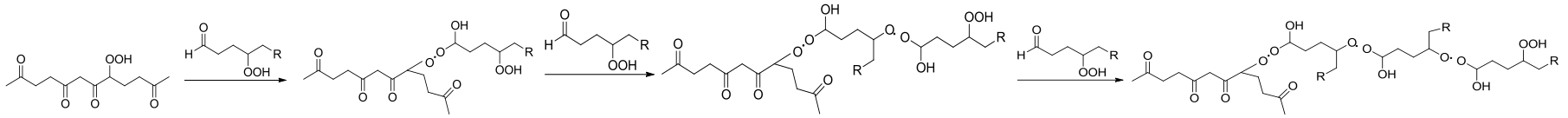
$C_{12}H_{22}O_5$ $C_{22}H_{42}O_8$ $C_{32}H_{62}O_{11}$ $C_{42}H_{82}O_{14}$



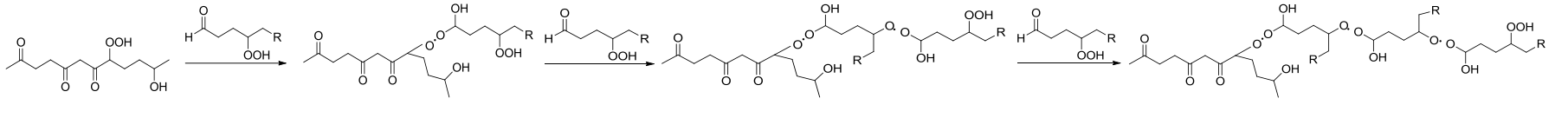
$C_{12}H_{24}O_5$ $C_{22}H_{44}O_8$ $C_{32}H_{64}O_{11}$ $C_{42}H_{84}O_{14}$



$C_{12}H_{20}O_5$ $C_{22}H_{40}O_8$ $C_{32}H_{60}O_{11}$ $C_{42}H_{80}O_{14}$



$C_{12}H_{18}O_6$ $C_{22}H_{38}O_9$ $C_{32}H_{58}O_{12}$ $C_{42}H_{78}O_{15}$



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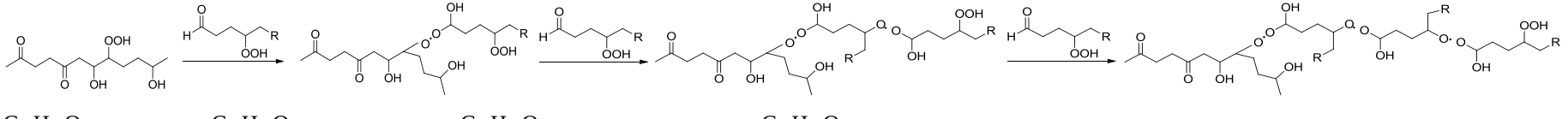
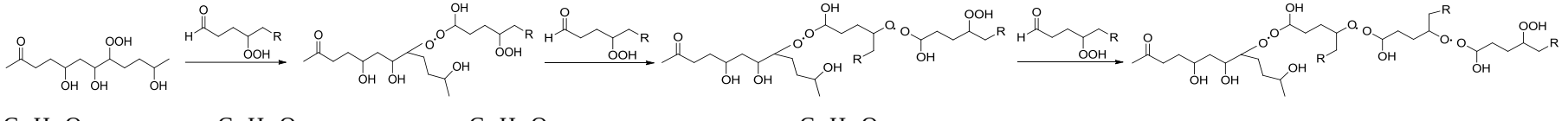
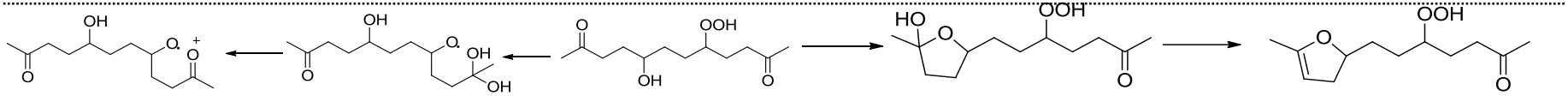


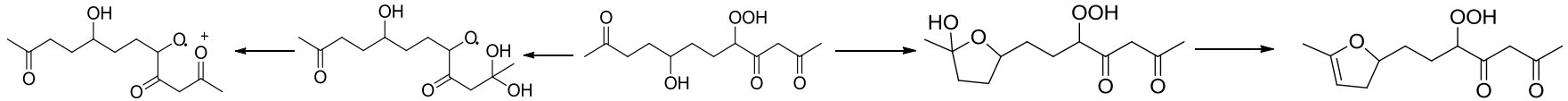
$C_{12}H_{22}O_6$ $C_{22}H_{42}O_9$ $C_{32}H_{62}O_{12}$ $C_{42}H_{82}O_{15}$



$C_{12}H_{24}O_6$ $C_{22}H_{44}O_9$ $C_{32}H_{64}O_{12}$ $C_{42}H_{84}O_{15}$



$C_{12}H_{21}O_4$ $C_{12}H_{22}O_5$ $C_{12}H_{22}O_5$ $C_{12}H_{22}O_5$ $C_{12}H_{20}O_4$



$C_{12}H_{19}O_5$ $C_{12}H_{20}O_6$ $C_{12}H_{20}O_6$ $C_{12}H_{20}O_6$ $C_{12}H_{18}O_5$

Figure S4. Scheme for forming 11 types of PHA oligomers from reaction of an aldehyde of carbon length 10, with various hydroperoxy compounds and scheme for forming two types of furan derivatives with two kind of hydroperoxy compounds.

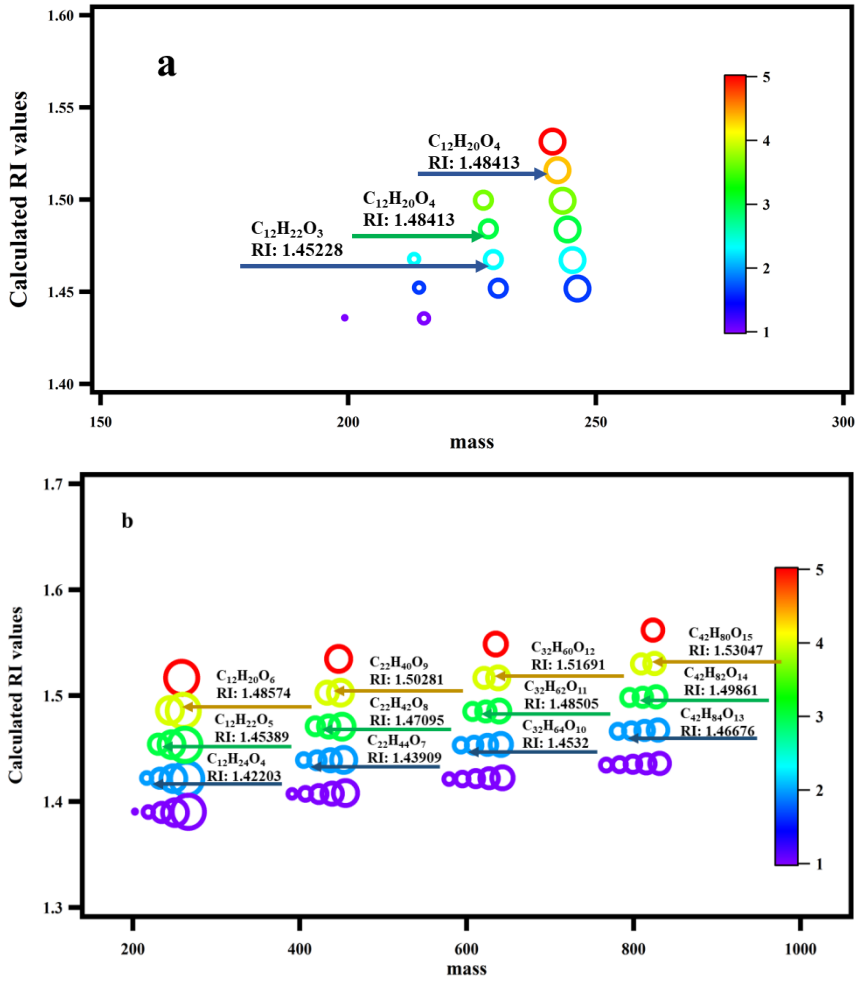


Figure S5. Calculated RI values of the surrogate system: (a) furan derivatives via intramolecular reaction (b) the oligomers via the formation of peroxy-hemiacetal. The color map refers to the unsaturation of the molecular formula. The size of the circle refers to the O/C ratio.

Table S1. The calculated RI values for identified molecules under two temperature conditions. (Dod-R refers to the room temperature condition; Dod-L refers to the low temperature condition)

Condition	Molecular Formula	Molecular Weight	M+H	M+Na	Polarizability	Unsaturation	Predicted RI_{cal}
Dod-R	$C_{10}H_{12}O_3$	180	181.08		19.17	5	1.541
Dod-R	$C_{10}H_{14}O_3$	182	183.10		19.51	4	1.510
Dod-R	$C_{10}H_{16}O_3$	184	185.117		19.85	3	1.479
Dod-R	$C_{10}H_{20}O_2$	172		195.13	19.96	1	1.415
Dod-R	$C_8H_{14}O_4$	174		197.07	17.06	2	1.445
Dod-R	$C_{12}H_{22}O_2$	198	199.17		23.32	2	1.452
Dod-R	$C_{10}H_{16}O_4$	200	201.11		20.42	3	1.479
Dod-R	$C_8H_{12}O_6$	204	205.17		17.86	3	1.476
Dod-R	$C_{11}H_{12}O_4$	208	209.08		21.25	6	1.575
Dod-R	$C_{10}H_{20}O_3$	188		211.13	20.53	1	1.418
Dod-R	$C_8H_{14}O_5$	190		213.07	17.63	2	1.444
Dod-R	$C_{11}H_{18}O_4$	214	215.12		22.27	3	1.481
Dod-R	$C_{10}H_{16}O_5$	216	217.11		20.99	3	1.481
Dod-R	$C_{12}H_{20}O_2$	196		219.13	22.98	3	1.483
Dod-R	$C_{12}H_{22}O_2$	198		221.15	23.32	2	1.452
Dod-R	$C_{10}H_{16}O_4$	200		223.09	20.42	3	1.479
Dod-R	$C_{10}H_{18}O_4$	224	225.11		20.76	2	1.450
Dod-R	$C_{12}H_{18}O_4$	226	227.13		23.78	4	1.516
Dod-R	$C_{10}H_{12}O_6$	228	229.07		20.88	5	1.543
Dod-R	$C_{11}H_{14}O_4$	210		233.08	21.59	5	1.545
Dod-R	$C_{12}H_{20}O_3$	212		235.12	23.55	3	1.484
Dod-R	$C_{12}H_{22}O_3$	214		237.14	23.89	2	1.447
Dod-R	$C_{12}H_{24}O_3$	216		239.16	24.23	1	1.422
Dod-R	$C_{10}H_{18}O_5$	218		241.10	21.33	2	1.449
Dod-R	$C_{10}H_{20}O_5$	220		243.12	21.67	1	1.419
Dod-R	$C_9H_{18}O_6$	222		245.10	20.39	1	1.417
Dod-R	$C_{11}H_{18}O_6$	246	247.11		23.41	3	1.483
Dod-R	$C_{12}H_{18}O_4$	226		249.11	23.78	4	1.516
Dod-R	$C_{11}H_{22}O_6$	250	251.15		24.09	1	1.422
Dod-R	$C_{10}H_{20}O_7$	252	253.13		22.81	2	1.420
Dod-R	$C_{11}H_{20}O_5$	232		255.12	23.18	2	1.452
Dod-R	$C_{11}H_{22}O_5$	234		257.13	23.52	1	1.422

Dod-R	$C_{10}H_{20}O_6$	236		259.11	22.24	1	1.419
Dod-R	$C_{12}H_{20}O_6$	260	261.13		25.26	3	1.483
Dod-R	$C_{11}H_{20}O_7$	264	265.13		24.32	2	1.453
Dod-R	$C_{12}H_{2O}O_5$	244		267.12	24.12	3	1.484
Dod-R	$C_{12}H_{22}O_5$	246		269.14	25.03	2	1.454
Dod-R	$C_{12}H_{24}O_5$	248		271.15	23.37	1	1.424
Dod-R	$C_{14}H_{24}O_5$	272	273.16		28.39	3	1.489
Dod-R	$C_{13}H_{22}O_6$	274	275.14		27.11	3	1.487
Dod-R	$C_{15}H_{26}O_3$	254		277.17	29.1	3	1.490
Dod-R	$C_{16}H_{22}O_4$	278	279.15		30.5	6	1.586
Dod-R	$C_{12}H_{24}O_7$	280	281.16		26.51	1	1.425
Dod-R	$C_{12}H_{20}O_6$	260		283.12	25.26	3	1.486
Dod-R	$C_{12}H_{22}O_6$	262		285.13	25.6	2	1.456
Dod-R	$C_{16}H_{30}O_4$	286	287.22		31.86	2	1.461
Dod-R	$C_{14}H_{24}O_6$	288	289.16		28.96	3	1.489
Dod-R	$C_{15}H_{24}O_4$	268		291.16	29.33	4	1.522
Dod-R	$C_{16}H_{30}O_3$	270		293.20	31.29	2	1.459
Dod-R	$C_{15}H_{28}O_4$	272		295.18	30.01	2	1.459
Dod-R	$C_{14}H_{26}O_5$	274		297.16	28.73	2	1.457
Dod-R	$C_{15}H_{22}O_6$	298	299.15		30.13	5	1.553
Dod-R	$C_{12}H_{22}O_7$	278		301.13	30.47	4	1.523
Dod-R	$C_{14}H_{22}O_7$	302	303.14		29.19	4	1.521
Dod-R	$C_{14}H_{24}O_7$	304	305.16		29.53	3	1.491
Dod-R	$C_{16}H_{28}O_4$	284		307.18	31.52	3	1.491
Dod-R	$C_{16}H_{30}O_4$	286		309.20	31.86	2	1.461
Dod-R	$C_{15}H_{28}O_5$	288		311.18	30.58	2	1.459
Dod-R	$C_{14}H_{26}O_6$	290		313.16	29.3	2	1.457
Dod-R	$C_{16}H_{26}O_6$	314	315.18		32.32	4	1.525
Dod-R	$C_{16}H_{28}O_6$	316	317.19		32.66	3	1.492
Dod-R	$C_{16}H_{30}O_6$	318	319.21		33	2	1.462
Dod-R	$C_{16}H_{26}O_5$	298		321.17	31.75	4	1.523
Dod-R	$C_{15}H_{26}O_6$	302		325.16	30.81	3	1.491
Dod-R	$C_{15}H_{28}O_6$	304		327.18	31.15	2	1.460
Dod-R	$C_{15}H_{30}O_6$	306		329.19	31.49	1	1.428
Dod-R	$C_{17}H_{30}O_6$	330	331.21		34.51	3	1.495
Dod-R	$C_{17}H_{30}O_5$	314		337.19	33.94	3	1.494

Dod-R	$C_{16}H_{28}O_6$	316		339.18	32.66	3	1.493
Dod-R	$C_{15}H_{26}O_7$	318		341.15	31.38	3	1.492
Dod-R	$C_{17}H_{26}O_7$	342	343.17		34.4	5	1.558
Dod-R	$C_{16}H_{28}O_8$	348	349.18		33.8	3	1.494
Dod-R	$C_{17}H_{28}O_6$	328		351.18	34.17	4	1.526
Dod-R	$C_{17}H_{30}O_6$	330		353.19	34.51	3	1.495
Dod-R	$C_{16}H_{28}O_7$	332		355.17	33.23	3	1.494
Dod-R	$C_{16}H_{30}O_7$	334		357.19	33.57	2	1.462
Dod-R	$C_{19}H_{32}O_5$	340		363.21	37.3	4	1.528
Dod-R	$C_{18}H_{30}O_6$	342		365.19	36.02	4	1.528
Dod-R	$C_{18}H_{32}O_6$	344		367.21	36.36	3	1.496
Dod-R	$C_{17}H_{30}O_7$	346		369.18	35.08	3	1.495
Dod-R	$C_{16}H_{28}O_8$	348		371.17	33.8	3	1.494
Dod-R	$C_{19}H_{32}O_6$	356		379.21	37.87	4	1.529
Dod-R	$C_{19}H_{34}O_6$	358		381.22	38.21	3	1.497
Dod-R	$C_{18}H_{32}O_7$	360		383.20	36.93	3	1.497
Dod-R	$C_{20}H_{36}O_7$	388	389.25		40.63	3	1.500
Dod-R	$C_{20}H_{34}O_6$	370		393.22	39.72	4	1.531
Dod-R	$C_{18}H_{28}O_8$	372		395.17	32.82	5	1.560
Dod-R	$C_{19}H_{34}O_7$	374		397.22	38.78	3	1.498
Dod-R	$C_{18}H_{32}O_8$	376		399.20	37.5	3	1.497
Dod-R	$C_{21}H_{36}O_6$	388		407.24	41.57	4	1.532
Dod-R	$C_{20}H_{34}O_7$	386		409.22	40.29	4	1.531
Dod-R	$C_{20}H_{36}O_7$	388		411.23	40.63	3	1.500
Dod-R	$C_{20}H_{38}O_7$	390		413.26	40.97	2	1.468
Dod-R	$C_{21}H_{42}O_8$	422	423.30		43.73	1	1.439
Dod-R	$C_{21}H_{38}O_7$	424		425.25	42.48	3	1.501
Dod-R	$C_{20}H_{36}O_8$	404		427.23	41.2	3	1.50
Dod-R	$C_{22}H_{36}O_8$	428	429.25		44.22	5	1.565
Dod-R	$C_{23}H_{40}O_6$	416		435.27	45.27	4	1.535
Dod-R	$C_{22}H_{38}O_7$	414		437.25	43.99	4	1.534
Dod-R	$C_{21}H_{36}O_8$	416		439.23	42.71	4	1.532
Dod-R	$C_{21}H_{38}O_8$	418		441.24	43.05	3	1.501
Dod-R	$C_{24}H_{42}O_6$	426		449.28	47.12	4	1.536
Dod-R	$C_{22}H_{42}O_9$	450	451.29		45.81	2	1.472
Dod-R	$C_{22}H_{38}O_8$	430		453.25	44.56	4	1.534

Dod-R	$C_{22}H_{42}O_{10}$	466	467.29		46.38	2	1.471
Dod-R	$C_{22}H_{38}O_{9}$	446		469.24	45.13	4	1.534
Dod-R	$C_{22}H_{40}O_{9}$	448		471.26	45.47	3	1.502
Dod-R	$C_{24}H_{40}O_{8}$	456		479.26	47.92	5	1.568
Dod-R	$C_{22}H_{40}O_{11}$	480	481.26		46.61	3	1.504
Dod-R	$C_{23}H_{40}O_{9}$	460		483.26	46.98	4	1.536
Dod-R	$C_{22}H_{42}O_{11}$	494	495.28		46.95	2	1.472
Dod-R	$C_{24}H_{42}O_{9}$	474		497.27	48.83	4	1.537
Dod-R	$C_{22}H_{42}O_{12}$	498	499.27		47.52	2	1.473
Dod-R	$C_{25}H_{42}O_{9}$	486		509.27	50.34	5	1.570
Dod-R	$C_{23}H_{42}O_{12}$	510	511.27		49.03	3	1.506
Dod-R	$C_{24}H_{42}O_{10}$	490		513.26	49.4	4	1.538
Dod-R	$C_{24}H_{42}O_{12}$	522	523.28		50.54	4	1.539
Dod-R	$C_{24}H_{42}O_{11}$	506		529.26	49.97	4	1.538
Dod-R	$C_{28}H_{50}O_{8}$	514		537.34	55.66	4	1.542
Dod-R	$C_{26}H_{46}O_{10}$	518		541.29	53.1	4	1.540
Dod-R	$C_{27}H_{48}O_{10}$	532		555.31	54.95	4	1.540
Dod-R	$C_{28}H_{52}O_{11}$	542		565.35	57.71	3	1.511
Dod-R	$C_{27}H_{50}O_{13}$	582	583.33		57	3	1.511
Dod-L	$C_{12}H_{22}O$	182	183.17		22.75	2	1.451
Dod-L	$C_{12}H_{20}O_{2}$	196	197.15		22.98	3	1.483
Dod-L	$C_{12}H_{22}O_{2}$	198	199.17		23.32	2	1.452
Dod-L	$C_{10}H_{16}O_{3}$	184		207.10	19.85	3	1.479
Dod-L	$C_{10}H_{18}O_{3}$	186		209.11	20.19	2	1.447
Dod-L	$C_{10}H_{20}O_{3}$	188		211.13	20.53	1	1.415
Dod-L	$C_{11}H_{16}O_{4}$	212	213.11		21.93	4	1.514
Dod-L	$C_{12}H_{2O}O_{3}$	212		235.13	23.55	3	1.484
Dod-L	$C_{12}H_{22}O_{3}$	214		237.14	23.89	2	1.452
Dod-L	$C_{12}H_{24}O_{3}$	216		239.16	24.43	1	1.420
Dod-L	$C_{14}H_{24}O_{3}$	240	241.18		27.25	3	1.488
Dod-L	$C_{11}H_{22}O_{6}$	250	251.15		24.09	1	1.422
Dod-L	$C_{10}H_{20}O_{7}$	252	253.13		22.81	2	1.420
Dod-L	$C_{12}H_{24}O_{4}$	232		255.15	24.8	1	1.422
Dod-L	$C_{12}H_{16}O_{6}$	256	257.10		24.58	5	1.548
Dod-L	$C_{11}H_{22}O_{7}$	266	267.14		24.66	1	1.423

Dod-L	$C_{12}H_{22}O_5$	246		269.14	25.03	2	1.454
Dod-L	$C_{12}H_{24}O_5$	248		271.15	25.37	1	1.422
Dod-L	$C_{14}H_{24}O_5$	272	273.17		28.39	3	1.489
Dod-L	$C_{13}H_{22}O_5$	258		281.13	26.54	3	1.488
Dod-L	$C_{11}H_{22}O_8$	282	283.14		24.66	1	1.421
Dod-L	$C_{12}H_{22}O_6$	262		285.13	25.6	2	1.454
Dod-L	$C_{12}H_{24}O_6$	264		287.14	25.94	1	1.421
Dod-L	$C_{14}H_{26}O_5$	274		297.16	28.73	2	1.457
Dod-L	$C_{13}H_{24}O_6$	276		299.15	27.45	2	1.455
Dod-L	$C_{16}H_{22}O_4$	278		301.14	30.5	6	1.586
Dod-L	$C_{14}H_{22}O_7$	302	303.14		29.19	4	1.521
Dod-L	$C_{16}H_{30}O_4$	286		309.20	31.86	2	1.461
Dod-L	$C_{15}H_{30}O_7$	322	323.21		32.06	1	1.428
Dod-L	$C_{16}H_{30}O_5$	302		325.20	32.43	2	1.461
Dod-L	$C_{16}H_{32}O_5$	304		327.21	32.77	1	1.428
Dod-L	$C_{18}H_{34}O_4$	314		337.23	35.56	2	1.464
Dod-L	$C_{17}H_{32}O_5$	316		339.21	34.28	2	1.462
Dod-L	$C_{17}H_{34}O_5$	318		341.23	34.62	1	1.430
Dod-L	$C_{19}H_{36}O_4$	328		351.25	37.41	2	1.465
Dod-L	$C_{18}H_{34}O_5$	330		353.23	36.13	2	1.464
Dod-L	$C_{17}H_{32}O_6$	332		355.21	34.85	2	1.462
Dod-L	$C_{19}H_{34}O_5$	342		365.23	37.64	3	1.497
Dod-L	$C_{19}H_{36}O_5$	344		367.25	37.98	2	1.465
Dod-L	$C_{18}H_{34}O_6$	346		369.22	36.7	2	1.464
Dod-L	$C_{20}H_{38}O_5$	358		381.26	39.83	2	1.467
Dod-L	$C_{19}H_{36}O_6$	360		383.24	38.55	2	1.465
Dod-L	$C_{21}H_{40}O_5$	372		395.27	41.68	2	1.468
Dod-L	$C_{20}H_{38}O_6$	374		397.25	40.4	2	1.468
Dod-L	$C_{23}H_{36}O_6$	408	409.26		44.59	6	1.598
Dod-L	$C_{21}H_{40}O_6$	388		411.27	42.25	2	1.469
Dod-L	$C_{22}H_{36}O_7$	412	413.26		43.65	5	1.565
Dod-L	$C_{21}H_{40}O_8$	420	421.28		43.39	2	1.470
Dod-L	$C_{21}H_{42}O_8$	422	423.30		43.73	1	1.439
Dod-L	$C_{22}H_{42}O_8$	424	435.30		45.24	2	1.471
Dod-L	$C_{22}H_{38}O_7$	414		437.25	43.99	4	1.534
Dod-L	$C_{21}H_{42}O_9$	438	439.29		44.3	1	1.439

Dod-L	$C_{22}H_{40}O_9$	448	449.27		45.47	3	1.503
Dod-L	$C_{22}H_{42}O_9$	450	451.29		45.81	2	1.472
Dod-L	$C_{24}H_{46}O_6$	430		453.32	47.8	2	1.474
Dod-L	$C_{24}H_{48}O_6$	432		455.33	48.14	1	1.443
Dod-L	$C_{22}H_{40}O_{10}$	464	465.27		46.04	3	1.504
Dod-L	$C_{22}H_{42}O_{10}$	466	467.29		46.38	2	1.472
Dod-L	$C_{22}H_{44}O_{10}$	468	469.30		46.72	1	1.440
Dod-L	$C_{24}H_{48}O_7$	448		471.33	48.71	1	1.443
Dod-L	$C_{22}H_{40}O_{11}$	480	481.26		46.61	3	1.504
Dod-L	$C_{22}H_{42}O_{11}$	482	483.28		46.95	2	1.472
Dod-L	$C_{22}H_{44}O_{11}$	484	485.30		47.29	1	1.441
Dod-L	$C_{21}H_{42}O_{12}$	486	487.27		46.01	1	1.441
Dod-L	$C_{22}H_{40}O_{12}$	496	497.26		47.18	3	1.505
Dod-L	$C_{24}H_{44}O_9$	476		499.28	49.17	3	1.506
Dod-L	$C_{22}H_{44}O_{12}$	500	501.29		47.86	1	1.442
Dod-L	$C_{24}H_{42}O_{12}$	522	523.28		50.54	4	1.539
Dod-L	$C_{22}H_{36}O_{15}$	540	541.21		48.21	5	1.570
Dod-L	$C_{30}H_{56}O_7$	528		551.39	59.13	3	1.513
Dod-L	$C_{31}H_{54}O_8$	554	555.38		60.87	5	1.577
Dod-L	$C_{29}H_{56}O_{10}$	564	565.40		59.33	2	1.481
Dod-L	$C_{30}H_{56}O_8$	544		567.38	59.7	3	1.513
Dod-L	$C_{31}H_{52}O_9$	568	569.37		61.1	6	1.609
Dod-L	$C_{30}H_{58}O_{10}$	578	579.41		61.18	2	1.482
Dod-L	$C_{32}H_{54}O_9$	582	583.38		62.95	6	1.610
Dod-L	$C_{34}H_{58}O_8$	594	595.42		66.08	6	1.613
Dod-L	$C_{31}H_{58}O_9$	574		597.40	62.12	3	1.514
Dod-L	$C_{34}H_{56}O_7$	576		599.39	65.17	7	1.517
Dod-L	$C_{33}H_{62}O_8$	586		609.43	65.25	3	1.516
Dod-L	$C_{32}H_{60}O_9$	588		611.41	63.97	3	1.484
Dod-L	$C_{32}H_{62}O_6$	590		613.44	62.6	2	1.513
Dod-L	$C_{33}H_{62}O_{11}$	634	635.44		66.96	3	1.519
Dod-L	$C_{33}H_{64}O_{11}$	636	637.45		67.3	2	1.487
Dod-L	$C_{34}H_{64}O_{11}$	648	649.45		68.81	3	1.520
Dod-L	$C_{36}H_{68}O_8$	628		651.48	70.8	3	1.521
Dod-L	$C_{33}H_{64}O_{12}$	652	653.45		67.87	2	1.487
Dod-L	$C_{35}H_{68}O_{11}$	664	665.45		71	2	1.489

Dod-L	$C_{34}H_{66}O_{12}$	666	667.46		69.72	2	1.488
Dod-L	$C_{34}H_{68}O_{12}$	668	669.48		70.06	1	1.457
Dod-L	$C_{34}H_{64}O_{13}$	680	681.44		69.95	3	1.520
Dod-L	$C_{36}H_{68}O_{10}$	660		683.47	71.94	3	1.522
Dod-L	$C_{34}H_{68}O_{13}$	684	685.47		70.63	1	1.457
Dod-L	$C_{34}H_{64}O_{14}$	696	697.44		70.52	3	1.521
Dod-L	$C_{34}H_{66}O_{14}$	698	699.45		70.86	2	1.489
Dod-L	$C_{38}H_{68}O_{11}$	700	701.48		75.53	5	1.588
Dod-L	$C_{36}H_{64}O_{12}$	688		711.43	72.4	5	1.585
Dod-L	$C_{36}H_{66}O_{12}$	690		713.44	72.74	4	1.554
Dod-L	$C_{36}H_{68}O_{12}$	692		715.46	73.08	3	1.521
Dod-L	$C_{38}H_{68}O_{12}$	716	717.47		76.1	5	1.588
Dod-L	$C_{35}H_{66}O_{15}$	726	727.45		72.94	3	1.522
Dod-L	$C_{35}H_{68}O_{15}$	728	729.46		73.28	2	1.491
Dod-L	$C_{38}H_{66}O_{13}$	730	731.46		76.33	6	1.619
Dod-L	$C_{38}H_{72}O_{13}$	736	737.50		71.65	3	1.525
Dod-L	$C_{40}H_{76}O_{10}$	716		739.53	79.34	3	1.526
Dod-L	$C_{39}H_{76}O_{13}$	752	753.53		79.54	2	1.494
Dod-L	$C_{40}H_{78}O_{13}$	766	767.55		81.39	2	1.495
Dod-L	$C_{41}H_{80}O_{14}$	796	797.56		83.81	2	1.497
Dod-L	$C_{42}H_{82}O_{14}$	810	811.58		85.66	2	1.498
Dod-L	$C_{43}H_{84}O_{14}$	824	825.59		87.51	2	1.500
Dod-L	$C_{50}H_{92}O_{9}$	814		837.68	96.59	5	1.601
Dod-L	$C_{48}H_{92}O_{10}$	828		851.65	94.14	3	1.536
Dod-L	$C_{44}H_{84}O_{15}$	852	853.59		89.59	3	1.533
Dod-L	$C_{45}H_{84}O_{15}$	864	865.59		91.1	4	1.566
Dod-L	$C_{48}H_{92}O_{11}$	844		867.65	94.71	3	1.536
Dod-L	$C_{45}H_{88}O_{15}$	868	869.62		91.78	2	1.502
Dod-L	$C_{48}H_{90}O_{12}$	858		881.63	94.94	4	1.569
Dod-L	$C_{46}H_{90}O_{15}$	882	883.64		93.63	2	1.503
Dod-L	$C_{46}H_{92}O_{15}$	884	885.65		93.97	1	1.472
Dod-L	$C_{46}H_{88}O_{16}$	896	897.62		93.86	3	1.536
Dod-L	$C_{46}H_{90}O_{16}$	898	899.63		94.2	2	1.504
Dod-L	$C_{46}H_{88}O_{17}$	913	913.61		94.43	3	1.536
Dod-L	$C_{46}H_{90}O_{17}$	914	915.62		94.77	2	1.504

Table S2. The calculated RI values for the surrogate system: oligomers (11 types of PHA) and furan derivatives.

Molecular Formula	Molecular Weight	Polarizability	Unsaturation	Predicted RI
$C_{12}H_{26}O_3$	218.32	24.57	0	1.39017
$C_{12}H_{24}O_3$	216.31	24.23	1	1.42236
$C_{12}H_{22}O_4$	230.29	24.46	2	1.45422
$C_{12}H_{24}O_4$	232.31	24.8	1	1.42203
$C_{12}H_{22}O_5$	246.29	25.03	2	1.45389
$C_{12}H_{24}O_5$	248.3	25.37	1	1.42174
$C_{12}H_{20}O_5$	244.27	24.69	3	1.48607
$C_{12}H_{18}O_6$	258.26	24.92	4	1.51681
$C_{12}H_{20}O_6$	260.27	25.26	3	1.48574
$C_{12}H_{24}O_6$	264.3	25.94	1	1.4215
$C_{12}H_{22}O_6$	262.29	25.6	2	1.4536
$C_{22}H_{44}O_6$	404.56	44.44	1	1.43921
$C_{22}H_{46}O_6$	406.58	44.78	0	1.40724
$C_{22}H_{42}O_7$	418.54	44.67	2	1.47106
$C_{22}H_{44}O_7$	420.56	45.01	1	1.43909
$C_{22}H_{42}O_8$	434.54	45.24	2	1.47095
$C_{22}H_{44}O_8$	436.56	45.58	1	1.43899
$C_{22}H_{40}O_8$	432.53	44.9	3	1.50292
$C_{22}H_{38}O_9$	446.51	45.13	4	1.53478
$C_{22}H_{40}O_9$	448.53	45.47	3	1.50281
$C_{22}H_{44}O_9$	452.56	46.15	1	1.43948
$C_{22}H_{42}O_9$	450.54	45.81	2	1.47085
$C_{32}H_{64}O_9$	592.82	64.65	1	1.45319
$C_{32}H_{66}O_9$	594.83	64.99	0	1.42134
$C_{32}H_{62}O_{10}$	606.8	64.88	2	1.48505
$C_{32}H_{64}O_{10}$	608.82	65.22	1	1.4532
$C_{32}H_{62}O_{11}$	622.8	65.45	2	1.48505
$C_{32}H_{64}O_{11}$	624.81	65.79	1	1.45361
$C_{32}H_{60}O_{11}$	620.78	65.11	3	1.5169
$C_{32}H_{58}O_{12}$	634.77	65.34	4	1.54876
$C_{32}H_{60}O_{12}$	637.78	65.68	3	1.51691
$C_{32}H_{64}O_{12}$	640.81	66.36	1	1.45403
$C_{32}H_{62}O_{12}$	638.8	66.02	2	1.48547
$C_{42}H_{84}O_{12}$	781.07	84.86	1	1.46637

$C_{42}H_{86}O_{12}$	783.09	85.2	0	1.4349
$C_{42}H_{82}O_{13}$	795.05	85.09	2	1.49823
$C_{42}H_{84}O_{13}$	797.07	85.43	1	1.46676
$C_{42}H_{82}O_{14}$	811.05	85.66	2	1.49861
$C_{42}H_{84}O_{14}$	813.07	86	1	1.46715
$C_{42}H_{80}O_{14}$	809.04	85.32	3	1.53008
$C_{42}H_{78}O_{15}$	823.02	85.55	4	1.56194
$C_{42}H_{80}O_{15}$	825.04	85.89	3	1.53047
$C_{42}H_{84}O_{15}$	829.07	86.57	1	1.46753
$C_{42}H_{82}O_{15}$	827.05	86.23	2	1.499
$C_{12}H_{23}O_2$	199.3	23.49	1.5	1.43592
$C_{12}H_{21}O_3$	213.28	23.72	2.5	1.46778
$C_{12}H_{23}O_3$	215.3	24.06	1.5	1.43562
$C_{12}H_{22}O_3$	214.29	23.89	2	1.45228
$C_{12}H_{21}O_4$	229.28	24.29	2.5	1.46748
$C_{12}H_{20}O_4$	228.27	24.12	3	1.48413
$C_{12}H_{22}O_4$	230.29	24.46	2	1.45198
$C_{12}H_{19}O_4$	227.27	23.95	3.5	1.49964
$C_{12}H_{17}O_5$	241.25	24.18	4.5	1.5315
$C_{12}H_{19}O_5$	243.27	24.52	3.5	1.49934
$C_{12}H_{18}O_5$	242.26	24.35	4	1.51599
$C_{12}H_{22}O_5$	246.29	25.03	2	1.45173
$C_{12}H_{21}O_5$	245.28	24.86	2.5	1.46723
$C_{12}H_{20}O_5$	244.27	24.69	3	1.48384

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