

Electronic Supplementary Information for:

Chitosan-azo dye bioplastics reversibly resoluble and recoverable under visible light irradiation

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1. Supplementary Figures

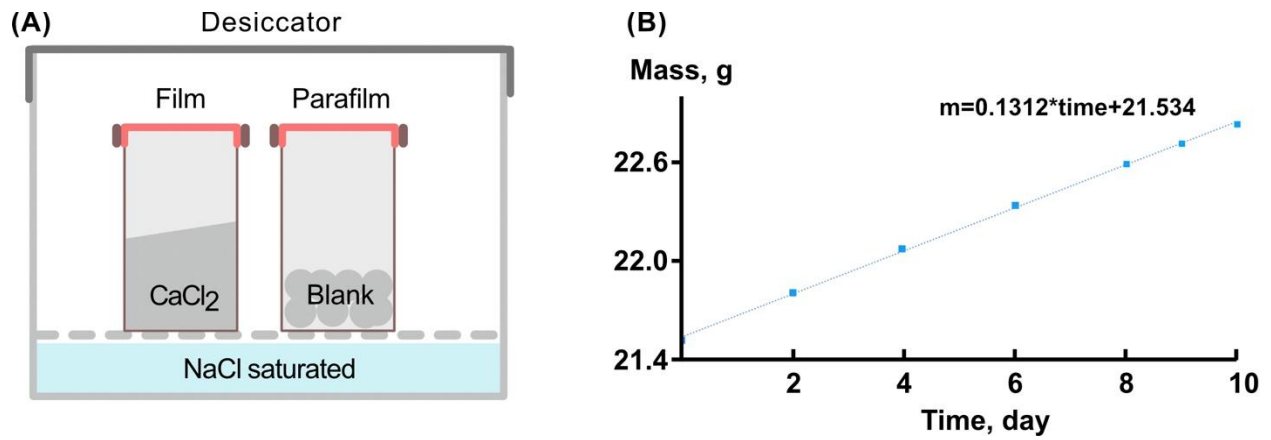
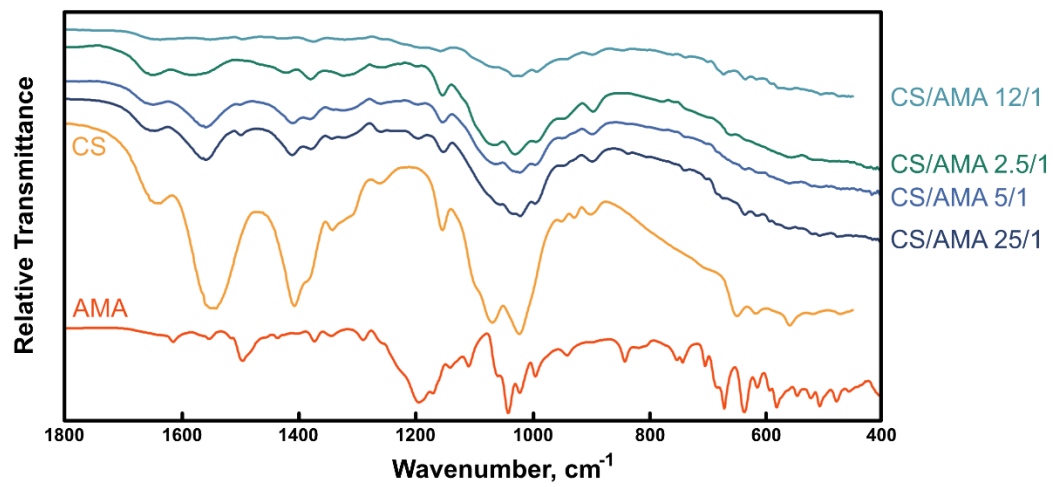
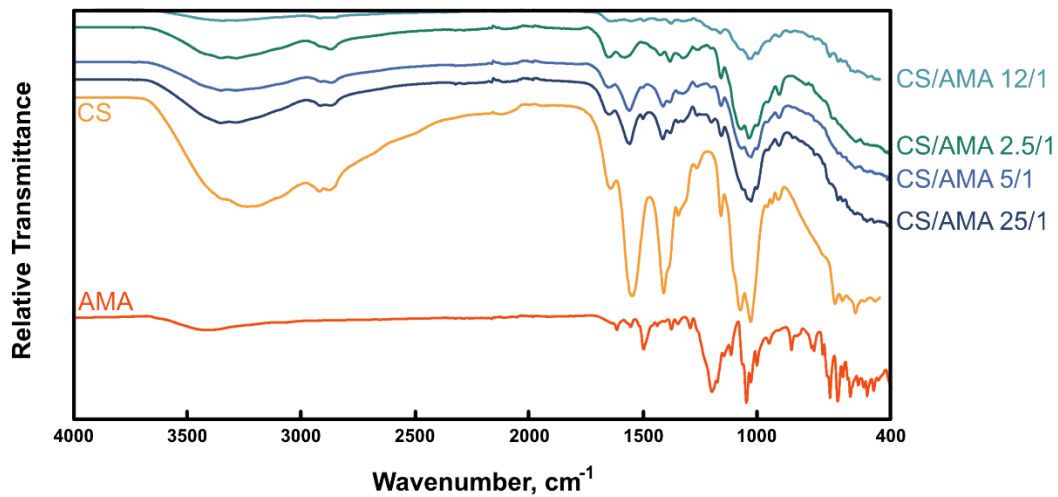


Figure S1. (A) Setup for determination of water vapour permeability of polymer films. (B) An example determination of water vapour transmission rate through a CS-AMA (ratio 5/1 mass) film.

(A)



(B)

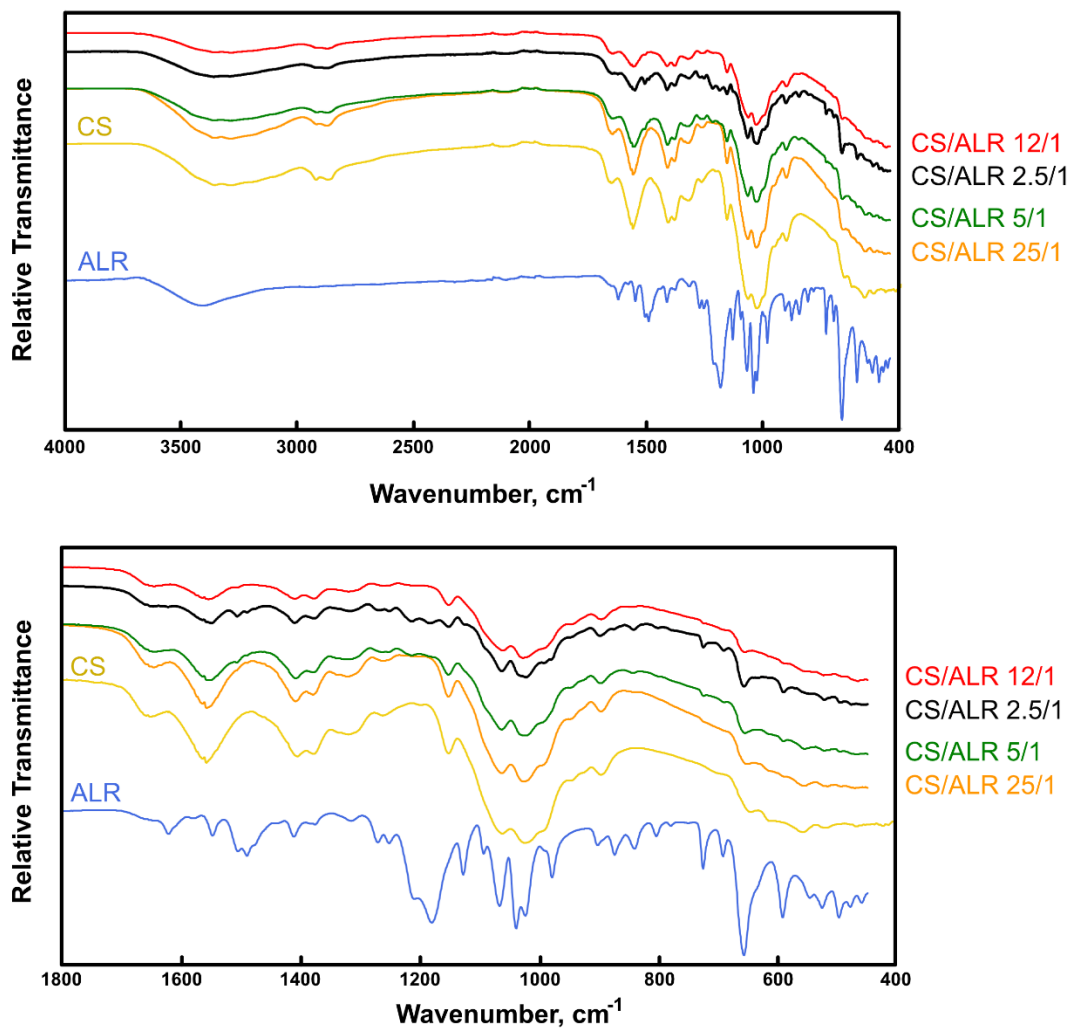


Figure S2. (A) FTIR spectra of CS-AMA thick films with different mass ratios of CS/AMA. (B) FTIR spectra of CS-ALR thick films with different mass ratios of CS/ALR.

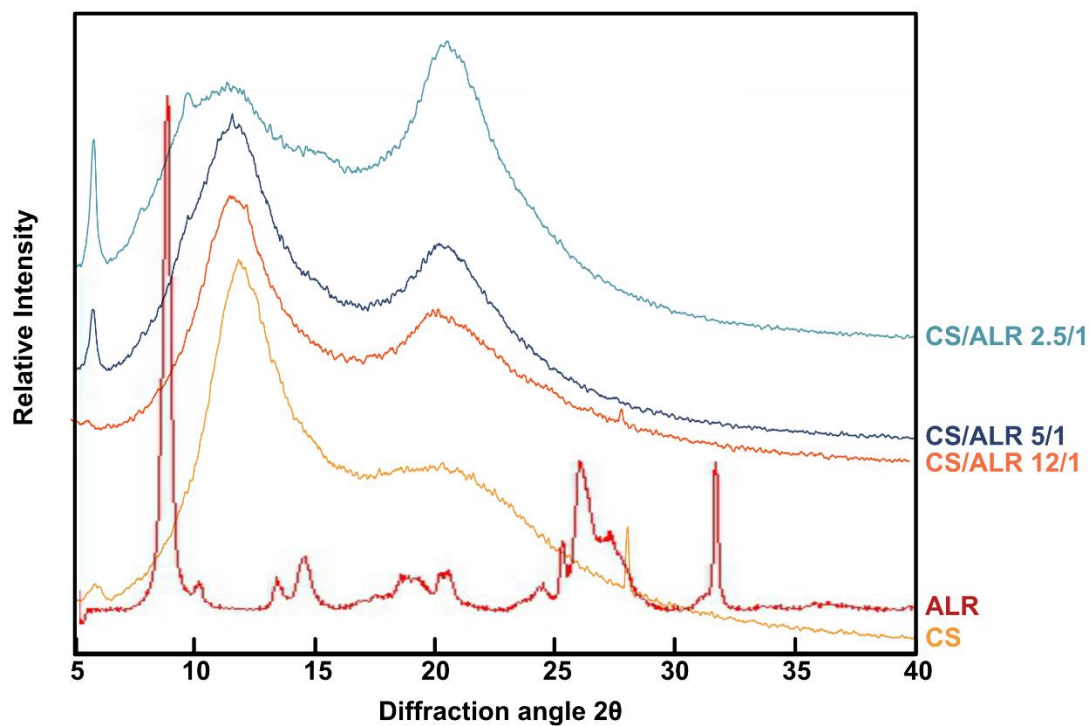


Figure S3. XRD spectra of CS, ALR, and their films with different mass ratios.

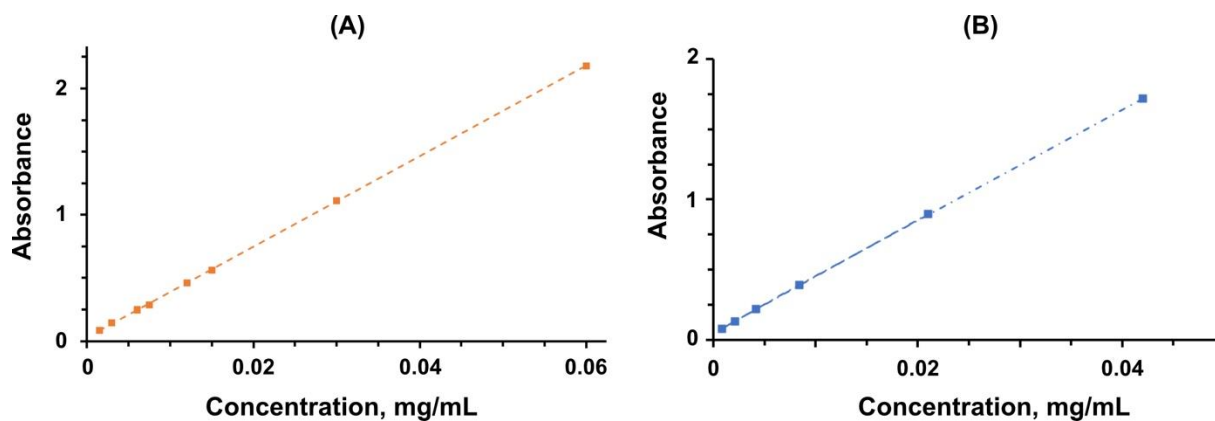


Figure S4. (A) Calibration curve for AMA in water solution for 522 nm irradiation with trend line equation $A = 35.83c + 0.0306$. (B) Calibration curve for ALR in water for 500 nm irradiation with trend line equation $A = 39.79c + 0.0516$.

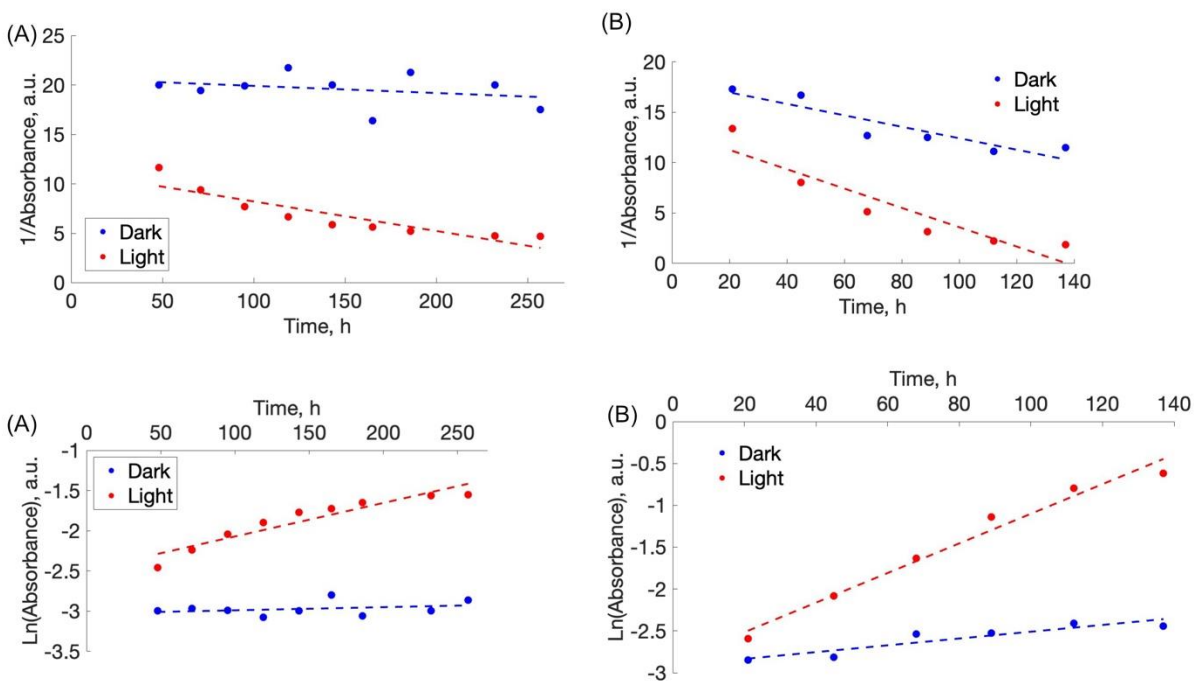


Figure S5. (A) Change with time of the absorbance maxima of AMA in solution during disassembly of the free-standing thick film CS-AMA. (B) Change with time of the absorbance maxima of ALR in solution during disassembly of the free-standing thick film CS-ALR, both plotted as 1/A and Ln(A) for comparison.

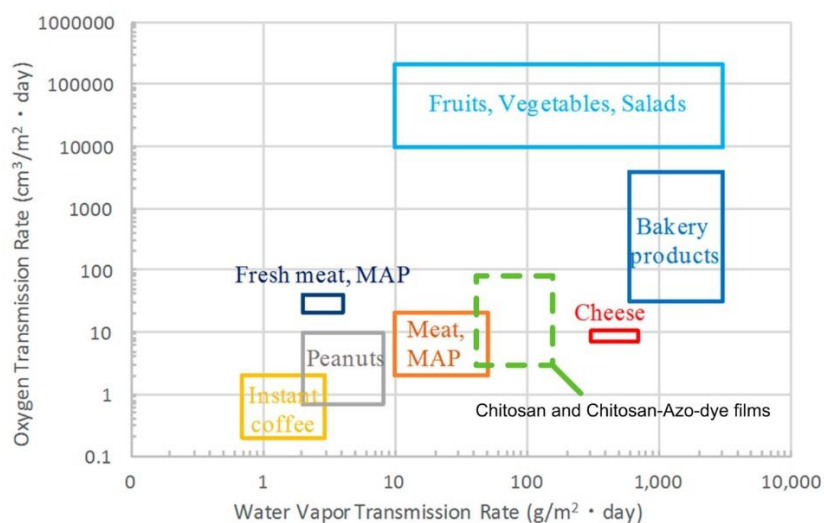


Figure S6. Packaging requirements of barrier films for selected food products. MAP is modified atmosphere packaging. Source: J. Wang et al. *ACS Sustainable Chem. Eng.* **2018**, *6*, 49–70. The green insert represents the range comparison of these variables measured from our materials in our study.

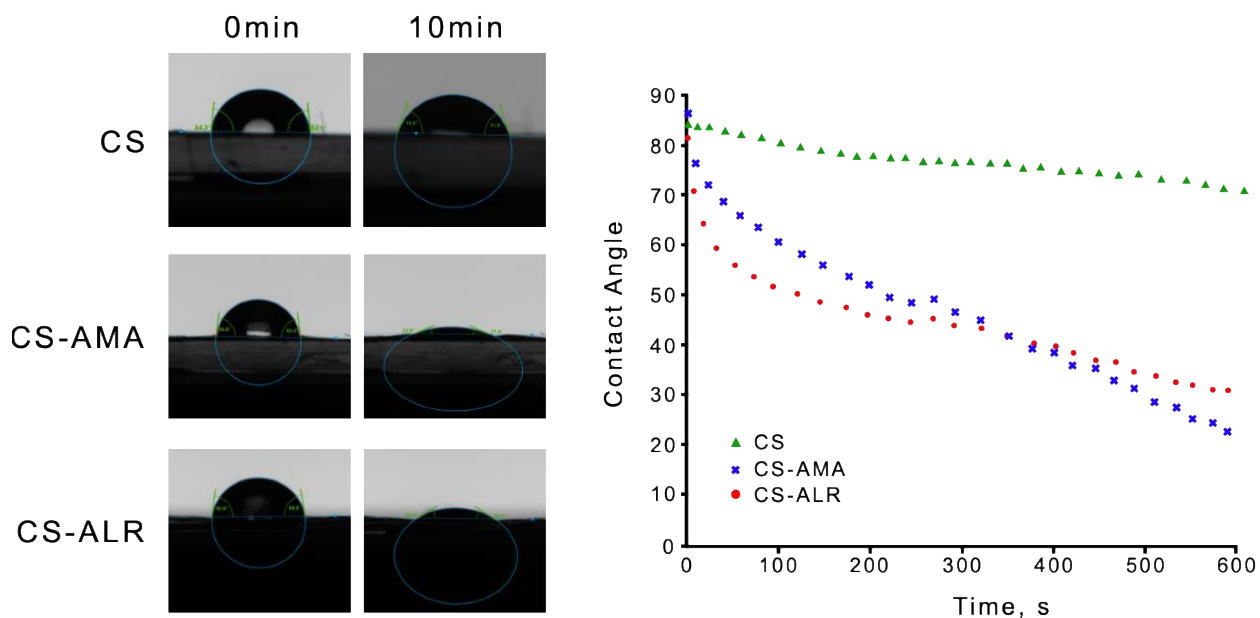


Figure S7. Left: Measurement of contact angle between water drop and surface of free-standing films of CS, CS-AMA (mass ratio 1/0.125), and CS-ALR (mass ratio 1/0.125). The fitting method used was “Ellipse-Target-1”. Right: Change of the angle with time.

2. Materials and Characterization Methods

2.1 Materials

Allura red (dye content 80%), amaranth (dye content 85-95%), chitosan of low molecular weight (50,000–190,000 Da), and parafilm, were purchased from Sigma Aldrich. Dyes were recrystallized prior to use. Calcium chloride (97%), sodium chloride, sodium hydroxide (0.1N water solution), activated charcoal, glacial acetic acid, 90% ethanol, and 37% hydrochloric acid, were purchased from ThermoFisher and were used without additional purification. Powdered calcium chloride for water permeability measurements was dried in an oven until a constant weight was achieved, for 3 hours at 110 °C. Glacial acetic acid and hydrochloric acid were diluted with distilled water to 1% by mass concentrations.

2.2 UV-Vis spectroscopy

UV-Vis spectroscopy was performed in transmittance mode using a Varian Cary 300 Bio UV-Visible Spectrophotometer from Agilent Technologies. The centrifuged sample aliquot was placed in a 1 cm quartz cuvette. Prior to the measurement, the UV-Vis spectrum of a distilled water or 1% water solution of acetic acid was measured as a background reference. All measurements were conducted at room temperature 21–23°C.

2.3 Density measurements

Samples were cut into strips 30 x 10 mm from the centre of a peeled film with uniform thickness. Linear dimensions of the films were measured with an electronic calliper to approx. 0.001 mm (Mitutoyo 293 340-30) with 0.0001 mm accuracy. The volume of a rectangular film sample was determined as width × length × thickness, in mm³. The density was measured by dividing mass of a film sample by its volume. Additionally, the density was measured in triplicate gravimetrically *via* buoyancy methods in 90% ethanol using laboratory balances.

2.4 X-ray diffraction (XRD) analysis

Samples were cut into strips 2 × 5 cm from the centre of peeled films, of uniform thickness. XRD of films was performed using a Bruker D8 Advance X-ray diffractometer with a powder specimen holder and a round silicon wafer as a support, CuK α radiation of 1.54178 Å, and a LYNXEYE linear position sensitive detector (Bruker AXS, Madison, WI), 2 θ = 5°–40°, over step intervals of 0.02° and a 0.200 scanning speed.

2.5 FTIR measurements

The infrared (IR) spectra of the films were acquired on a Spectrum II instrument from Perkin Elmer over a total range of 4000 to 400 cm⁻¹ at the best resolution 0.5 cm⁻¹, including a single bounce diamond attenuated total reflectance (ATR) accessory. The IR spectra were recorded in transmittance mode, averaged over 10 scans.

2.6 Water permeability measurements

Water vapour transmission rates (WVTR) were measured using the experimental setup shown in Fig. S1. The thickness of films varied from 20 to 800 μm and were cut into 4 × 4 cm squares. Samples of film were placed between holders with an exposed area 0.001 m² and mounted on the top of 15 mL vial with 15–20 g of calcium chloride dehydrated at 100°C for 1 day. The initial total mass of the film, holders, and vial containing calcium chloride was recorded. For a reference blank, a thick piece of parafilm (Sigma Aldrich) was used, that was mounted in a similar way as the studied films. The parafilm has an extremely low water vapour transmission rate,²³ and the calcium chloride mass change of this blank was measured as close to zero. The vial with the studied film and blank was placed at room temperature in a desiccator above a saturated sodium chloride solution. At specific time intervals the vials were taken from the desiccator and weighed, and the change of mass was plotted *vs* time. WVTR was calculated from the slope of the linear plot, normalized by exposed area, as g/day·m² (Fig. S1B).

2.7 Swelling tests

Dry samples were cut into 30 × 10 mm strips from the centre of peeled film which had the most uniform thickness. The initial mass m_0 was recorded and the film strips were submerged into 10 mL distilled water for 24 h at room temperature, after which the films were gently dried with compressed air and weighed (m_f). The swelling percentage was calculated as $((m_f - m_0)/m_0) \times 100\%$. The measurements were performed in triplicate.

2.8 Mechanical properties

Tensile stress, strain, and Young's modulus of the films were measured by an Instron Mini 44 tensile tester with a 500 N load cell. Sample films 5 × 2 cm were tightened in the instrument grips while the crosshead speed was set to the rate of 5 mm/min. Measurements were conducted at temperatures between 22–25°C and at a relative ambient humidity 30–40%. Additionally, CS films were tested at temperature 22–25°C in a wet state, where the sample was submerged into distilled water for 5 min and then gently dried with compressed air. All measurements were performed in triplicate.

2.9 Contact angle measurements

The contact angles of the surface of the films were determined using an optical contact angle goniometer (Model OCA 20, Dataphysics, USA). The sessile drop method was employed, whereby a droplet of water was placed on the sample mounted on a stage, and the image of the drop taken by a high-resolution camera. Images were recorded immediately ($t \approx 0$ s) and over time ($t = 5$ and 10 min) to allow the drop to equilibrate. The contact angle was then determined using the SCA20 software. The measurements were performed in triplicates.

2.10 Data analysis

All experimental measurements, unless stated otherwise, were performed in triplicate, and the numerical results are reported as a mean of the 3 ± standard deviation. The plots are presented with error bars representing 1 standard deviation.

2.11 Determination of degree of deacetylation (DDA) of chitosan by FTIR

The values of the degree of deacetylation (DD, %) were calculated from the degree of acetylation (DA, %) as $DD = 100\% - DA$. The DA values were calculated from the following equation proposed by (R. Czechowska-Biskup, D. Jarosińska, B. Rokita, Piotr Ulański and J. M. Rosiak, *Progress on Chemistry and Application of Chitin and its Derivatives*, 2012, 17, 5–20). The results of the calculations were found to agree very closely to the results of obtained by titration methods.

$$DA, \% = \frac{A_{1655}}{A_{3450}} \times 100/1.33$$

Where A_{1655} and A_{3450} are values of absorbance from baselines 1655 cm^{-1} (C=O band) and 3450 cm^{-1} (OH band) to maximum, respectively.

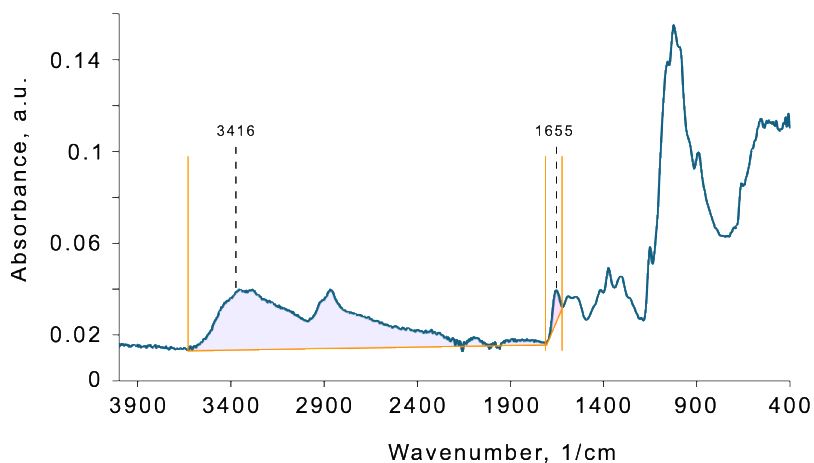


Figure S8. FTIR spectrum of CS, Sigma Aldrich. References bands and corresponding baselines.

3. Additional Computational Data

Table S1. Absolute energies E for all AMA structures discussed in the text, calculated at the B3LYP-D3BJ/ma-def2-TZVP level.

Structure	E, Hartree	
	<i>cis</i>	<i>trans</i>
1a	-2824.93661703	-2824.97290785
1b	-2824.93084777	-2824.96796543
1c	-2824.93423872	-2824.97944680
1d	-2824.93121114	-2824.97596179
2a	-2824.98159498	-2824.95863723
2b	-2824.97704046	-2824.95571980

Table S2. Absolute Gibb's free energies G at 298.15 K for all AMA structures discussed in the text, calculated at the B3LYP-D3BJ/ma-def2-TZVP level.

Structure	G, Hartree	
	<i>cis</i>	<i>trans</i>
1a	-2824.69595674	-2824.73177110
1b	-2824.69028573	-2824.72695454
1c	-2824.69476204	-2824.73858877
1d	-2824.69104446	-2824.73501896
2a	-2824.74116951	-2824.71843039
2b	-2824.73680214	-2824.71523528

4. xyz Coordinates of Structures

Coordinates of all structures are given in units of Angström (Å).

cis-1a

C	2.54453725536494	0.85424459199804	-0.19634219919546
C	2.82450214637420	-0.52455968140773	-0.19063583920160
C	1.81980332239799	-1.45632009861673	-0.05321053930149
C	0.46850553463337	-1.06143774593547	0.07209667350423
C	0.18676366821436	0.33739503762534	0.08281109790295
C	1.24516816442284	1.26772817578570	-0.03875152190163
C	-1.15880742251236	0.78826706824716	0.12954367326269
C	-2.23021558565218	-0.06206901096457	0.06672490908145
C	-1.96781769131871	-1.44834603079409	-0.01218112383597
C	-0.65107480901855	-1.95958003499529	0.06714821937902
H	3.85179437433654	-0.84716688506962	-0.29669691762472
H	2.07832359958388	-2.50342212040443	-0.06386959051704
H	1.02482474651252	2.32729251581494	-0.04453391363918
H	-1.35891060748944	1.85078741334600	0.17303565335240
N	-0.64935956892524	-3.33702139560267	-0.16548598193523
N	0.12313394181295	-4.24396835651035	0.23543986638755
C	1.00886203968925	-4.19033591897534	1.32606337013987
C	0.79227076076804	-3.44373089973311	2.46835828024068
C	2.03384709892125	-5.19555235450551	1.33655286983066
C	1.48312165141309	-3.73531190096604	3.65672053091064
C	2.42741018716201	-4.73181911207405	3.72076391688866
C	2.76012288271666	-5.45838970411170	2.53806437223818
H	0.03638015630375	-2.67085393230223	2.46898650527910
H	1.25924931588966	-3.18606237066862	4.56053282105591
C	2.33951701671410	-5.93426340419511	0.17038567590375
C	3.32954955172116	-6.88441114712097	0.17674070376040
C	4.05596806891542	-7.13808381945285	1.35668566102972

C	3.77603973340471	-6.44763046129532	2.50869459882035
H	1.77001965931871	-5.72953165750901	-0.72527939789959
H	3.55535938904224	-7.43693877940164	-0.72904325955941
H	4.33395579462066	-6.63241850251899	3.41380735984526
H	4.84346661247030	-7.88382162984191	1.35571684219431
S	3.16328611549347	-5.15200993090534	5.32795186284201
S	-3.92184530531034	0.60905835355693	0.02513736165963
S	3.87774008929703	2.03771323128353	-0.50188874163091
O	-2.98180223598013	-2.31493774018529	-0.15456592177435
H	-2.53926439542798	-3.17686401155025	-0.30862552635665
O	2.75512046468046	-6.54472949593578	5.54144031331427
O	2.57387613082372	-4.20800342041976	6.27360240697026
O	4.60818026080016	-4.99715972613032	5.14440050830681
O	3.29839256968302	3.35203944272528	-0.21618458238438
O	4.95178525394879	1.64186507897000	0.41089061330834
O	4.21220792274255	1.83373795204735	-1.91636305449171
O	-4.60961108724834	-0.02470111269808	1.14806475538331
O	-3.72947144478619	2.05200132701995	0.18658927967600
O	-4.43859532652440	0.22879220437810	-1.28948259121915

cis-1b

C	1.04677857353067	-2.94429000189615	4.03686506097100
C	0.81865304695687	-4.32963045538011	3.92771420925952
C	-0.41554290974492	-4.82436811659323	3.57424311858071
C	-1.50025818448582	-3.95909945751891	3.30244706061308
C	-1.27447808019618	-2.55557275779820	3.43431185034378
C	0.00423345709021	-2.08195292498292	3.81386954237286
C	-2.30548648969461	-1.63875388517074	3.10554877441853
C	-3.50246170294325	-2.02812465445647	2.56548022408645
C	-3.71221869930663	-3.40839778793092	2.35581561299036
C	-2.76967452609840	-4.37187726478303	2.77870846056944
H	1.63789561250947	-5.00908728111601	4.12234627440903
H	-0.54278716251128	-5.89142366761549	3.49072071052356
H	0.17570537620784	-1.01628719630429	3.89174519146227
H	-2.13596323613476	-0.57946363002575	3.24702770579432
N	-3.17022246587413	-5.64982886076342	2.37146648053186
N	-2.98731367244153	-6.78277578374762	2.87365912004702
C	-2.52655816617547	-7.12280961355733	4.17100650968141
C	-3.07375573090673	-6.60837672052864	5.39147566995713
C	-1.69457390305586	-8.22469370393817	4.22182833129325
C	-2.73719021570866	-7.26117357416220	6.62828334659440
C	-1.87552569434493	-8.39697825669435	6.62173195354926
C	-1.34705852634491	-8.83454290759184	5.43190886599763
H	-1.33000694180424	-8.62951478530217	3.28524314563395
H	-0.69489736299315	-9.69630499157888	5.44631797178023
C	-4.00007643369560	-5.53803856685951	5.42168212181160
C	-4.53110669416958	-5.09035326598438	6.60298245357438
C	-4.17017573345281	-5.70218761345682	7.81815645243936
C	-3.30555178943781	-6.76483789174014	7.82943025794295
H	-4.29130566139245	-5.05323399835081	4.50544232008384
H	-5.22146045596569	-4.25573784826831	6.59270946349300

H	-4.58183167525408	-5.33360155345411	8.75093565682697
H	-3.03124311029541	-7.24421580838815	8.75645490223927
S	-4.74856162273965	-0.78089885732917	2.11672640755653
S	2.71448237965116	-2.33864094187103	4.38529591426571
S	-1.55346209903063	-9.38563389648788	8.11468632186015
O	-4.13402769949262	0.48893264425819	2.51051935363389
O	-4.92372194182976	-0.92505438044044	0.67180500774431
O	-5.92819125810469	-1.13539157954818	2.90456238415114
O	2.57880270286989	-0.88496922581407	4.50271881458630
O	3.10897698124443	-3.00672420989371	5.62653042996876
O	3.49632381697375	-2.76824686206712	3.21958027363936
O	-0.62240759050128	-10.42680126346982	7.67727789511838
O	-0.99179740634679	-8.45701073305753	9.09553440218976
O	-2.87695921599895	-9.89720660023129	8.48617988334147
O	-4.84565081753995	-3.83208242260803	1.76995164666104
H	-4.69973707102096	-4.79081684550067	1.62807244541057

cis-1c

C	-6.43618982289527	-1.58853731289427	2.58829098830876
C	-6.57353501553868	-2.99035366449562	2.65028669588490
C	-5.46937598645383	-3.80484736317881	2.72042417288346
C	-4.16368728530816	-3.26242201185147	2.71356014765661
C	-4.02165323838997	-1.85317377306452	2.64680851607751
C	-5.17929630114649	-1.03688219287143	2.59369666394415
C	-2.71447178921255	-1.30622308985647	2.58921002509124
C	-1.59026433946171	-2.08564900508915	2.62749593366500
C	-1.71709479730414	-3.49609480022329	2.77263773301342
C	-2.98891101654689	-4.08808870450775	2.78115090654790
H	-7.56937708898840	-3.41399806350327	2.64994557622413
H	-5.58634767865003	-4.87894610815979	2.77430961455004
H	-5.07416022047815	0.03933751056927	2.54914442581328
H	-2.58300812961840	-0.23663567150310	2.49554921322477
N	-3.22051514246048	-5.44753742788978	2.49890523417081
N	-2.63905055699910	-6.45469258560906	2.95520040746405
C	-1.84904442220808	-6.52117409056987	4.13293321657366
C	-0.86275164757357	-7.56208894258445	4.17310347463396
C	-2.16825644688985	-5.85077928074334	5.29825778916701
C	-0.26197987276101	-7.92106309892306	5.41892219121903
C	-0.68140560700783	-7.25391523344315	6.60868897149049
C	-1.59246598668686	-6.22877088114150	6.52378457925814
H	-2.91152175352544	-5.06492246294371	5.27579252180660
H	-1.88557741661767	-5.72867124410262	7.43618643166111
C	-0.47288236815015	-8.23950267755336	2.99437608048223
C	0.47979771916074	-9.22527657781257	3.03413715005848
C	1.08281457387147	-9.57542285336314	4.25837886808508
C	0.72018552180522	-8.94422613062550	5.42088798264366
H	-0.94492495268442	-7.95775739030715	2.06368201370282
H	0.77339508195597	-9.73071511932016	2.12066454646829

H	1.84216823219369	-10.34926135498144	4.28297423124556
H	1.18548135318072	-9.20288419895224	6.35954006720870
S	0.03901779690441	-1.27972791270432	2.44199250689144
S	-7.92756402862459	-0.57403317678205	2.47567618898909
S	-0.09818783204712	-7.78337943105318	8.24735154034213
O	-0.29000331910569	0.14433927320481	2.32977509000081
O	0.78168124234271	-1.61792450636494	3.65130560224305
O	0.58368743423878	-1.85151493464581	1.21085404429292
O	-7.46613522058471	0.81287145406927	2.55664317791540
O	-8.51357486196717	-0.93082519070145	1.17794177880545
O	-8.74907514733006	-0.99945352683451	3.61443043236546
O	-0.73653029022111	-6.86877303257937	9.18961115197501
O	-0.56635522458879	-9.16928137544268	8.34744081080119
O	1.36061176744343	-7.66908754370845	8.19221333342304
O	-0.57926105136045	-4.22161385012673	2.77801883443763
H	-0.69570486371023	-5.03854044483458	3.28145913729242

cis-1d

C	-5.70699693621395	-1.27688800114968	1.00335010587422
C	-5.92580793569515	-2.65077050232726	0.77743304533192
C	-5.05160372931422	-3.59384752917037	1.26195385498269
C	-3.90032286273555	-3.21348461990025	1.98969252148905
C	-3.67451131178271	-1.83211792314951	2.21242985794757
C	-4.59905693463474	-0.88252563613674	1.71151367158463
C	-2.49537917627993	-1.44219581936589	2.89715513153219
C	-1.59290816126325	-2.34842254797216	3.38035699897561
C	-1.84721514136381	-3.74398267441241	3.23765709440129
C	-2.97153802273826	-4.17471857309337	2.51916929454261
H	-6.79779122990567	-2.95096528495233	0.21111009124112
H	-5.23143083255993	-4.64502120442953	1.08008520536095
H	-4.42722381836106	0.17273070937883	1.87937205757447
H	-2.27731031175783	-0.39177233132522	3.03555798906146
N	-3.11778441921290	-5.46697657874867	1.97946252916952
N	-2.94523024955626	-6.57125541173767	2.53170090570336
C	-2.81847085567203	-6.84204611456721	3.92875847302429
C	-3.83475468094686	-6.52017806104181	4.88786823059090
C	-1.80052880658536	-7.70336356663695	4.28932942957145
C	-3.77275523137605	-7.12690086976490	6.18874794826706
C	-2.71119342082525	-8.02742953330458	6.50283446001687
C	-1.73302929189507	-8.26741706820081	5.57160901665617
H	-1.06580154519475	-7.97187146844965	3.53955752085108
H	-0.93195501599073	-8.94494851865648	5.83070277203633
C	-4.93040121778472	-5.67995534850714	4.57748803541949
C	-5.89981575744639	-5.41013415356427	5.50770950446441
C	-5.82467645159095	-5.97863294721597	6.79336984944084
C	-4.79502746338447	-6.82081339407409	7.12262540732588
H	-5.00265231911570	-5.23204031790688	3.60013789399083
H	-6.71688188717180	-4.74757081809206	5.24939936981018

H	-6.58772757040636	-5.74967290805040	7.52858798179842
H	-4.73366574566172	-7.26170530202474	8.10567749386105
S	-0.05647141938630	-1.72288219993800	4.14628206839258
S	-6.89738113304789	-0.08859077366429	0.34332441233616
S	-2.66812678861635	-8.97946691534706	8.05391247232224
O	-0.20404054195107	-0.26604272950767	4.07616295399426
O	-0.05468520529420	-2.24843160368780	5.50688148249416
O	1.00724871241531	-2.24217509084468	3.28699905078325
O	-6.34923102139828	1.23242056652336	0.65547238462229
O	-6.95255912824594	-0.38749366896372	-1.09263849554554
O	-8.14918899272886	-0.39630303564074	1.04369676243716
O	-1.43054870176744	-9.75620707875394	7.97750307206326
O	-2.68660269855660	-7.99014964929985	9.13154486991271
O	-3.88330991618365	-9.79727293158348	7.99139277952669
O	-0.90301582890142	-4.58681814528870	3.69900879889589
H	-1.27681900191372	-5.45106242545305	3.92291364586684

trans-1a

C	2.53355291042644	0.61310716851333	0.37173619011279
C	2.75149918732816	-0.77213923135671	0.45420893308609
C	1.71623322586821	-1.67240087104055	0.31744177480002
C	0.39185827111722	-1.23110574106027	0.09247184717927
C	0.17039869281647	0.17540718475338	0.01878210666899
C	1.25575353362850	1.07035990202512	0.15760215553315
C	-1.14489212928331	0.67457052496954	-0.18524861057404
C	-2.24183283781273	-0.13208806086209	-0.31257569268918
C	-2.04419434324354	-1.53229977126611	-0.24959797435100
C	-0.75456136723025	-2.09247277518432	-0.05349699680655
H	3.75846551122369	-1.12962036691634	0.62662090632766
H	1.90740812908873	-2.72954594131960	0.38435769850737
H	1.08021446857777	2.13654450775132	0.09622855776760
H	-1.29933120501708	1.74445702791094	-0.23999088640024
N	-0.81812864190256	-3.46837970602317	-0.01946958355056
N	0.22533659821731	-4.17753149961879	0.05332614053909
C	0.00563605402745	-5.56207128562874	0.16346622708699
C	-1.14213492616934	-6.12091444377071	0.68940110256763
C	1.08092694506193	-6.42230225803881	-0.23207096846920
C	-1.27255942890137	-7.51135643118481	0.82644830329428
C	-0.26915279429095	-8.37067940599774	0.44626020044210
C	0.93833416532017	-7.84108176139337	-0.09808496664594
H	-1.93615901416545	-5.46640774093119	1.02254884670794
H	-2.17237290090923	-7.93613445220197	1.24959532967743
C	2.28149151457026	-5.89638276017101	-0.76780254522378
C	3.30232011334484	-6.72631657056318	-1.15420076963207
C	3.16400708240134	-8.12323951810616	-1.02706425941480
C	2.01455803279907	-8.66696127730964	-0.51372051035652
H	2.37214354863389	-4.82404470604581	-0.86249406088310
H	4.21663453635677	-6.30524280021220	-1.55681852273632

H	1.90657387581649	-9.73593242787775	-0.41435272151535
H	3.97408358914680	-8.77489283657975	-1.33586546309842
S	-0.51718418341073	-10.15551527747652	0.67075232078368
S	-3.88627767709172	0.61047634322549	-0.55609375898219
S	3.92892185313385	1.74473879224522	0.56801375312805
O	-3.09039441975007	-2.35156756187267	-0.38455386172140
H	-2.70475634532556	-3.25001159465833	-0.30691343693738
O	0.57542487849063	-10.57579407387080	1.55264278815193
O	-1.84511301134004	-10.27891525723474	1.27085026681692
O	-0.41984847038770	-10.71717483345903	-0.67960165131285
O	3.37951445347081	3.08005167125568	0.32595714785803
O	4.38326893417662	1.52726703361137	1.94524458198248
O	4.90070573992769	1.30670818732989	-0.43893321151059
O	-4.34910273110112	0.08364965765726	-1.83794898186220
O	-3.61670630019500	2.05019388310935	-0.57168012487149
O	-4.66732311744340	0.16943135487510	0.59769238052567

trans-1b

C	0.07697001183858	-1.91743692672435	2.37326455423800
C	0.18411341955336	-3.31751371167454	2.41349259320514
C	-0.92009594339466	-4.11856227124288	2.61461479125318
C	-2.20567010361874	-3.55594647095272	2.78834755019263
C	-2.31473008601520	-2.13503850522148	2.73647370377016
C	-1.16204839224524	-1.34410752147887	2.52766677865886
C	-3.58495871518994	-1.51773029822652	2.89544412387747
C	-4.73930204662235	-2.22057428823828	3.10262926701385
C	-4.65428029783569	-3.63328074018772	3.15767662392313
C	-3.41641295665262	-4.30769983631311	3.00162272010715
H	1.15936536604228	-3.76596675075214	2.27499613870947
H	-0.81296980772535	-5.18937306988475	2.64401540832911
H	-1.25535249450591	-0.26666884591745	2.48407480730947
H	-3.65493486362182	-0.43842202895498	2.85499582406375
N	-3.59287895859656	-5.67572963666779	3.06917807214483
N	-2.61203133829631	-6.46985393538946	3.03405547102854
C	-2.90405128576220	-7.84753306926557	3.07444139701797
C	-4.03249483809883	-8.50587013148233	2.47297963231900
C	-1.94878036422664	-8.61455513684142	3.71303622484395
C	-4.16611979541670	-9.92954787102925	2.62759520557414
C	-3.17894483324124	-10.66167537682323	3.35264528888041
C	-2.09262590930312	-9.99962986502200	3.86825136079666
H	-1.08605660905896	-8.10376249088609	4.12235789772548
H	-1.34729473765755	-10.57356824578789	4.40072746234989
C	-4.98684728408338	-7.82336405773895	1.67747572159013
C	-6.04191212702787	-8.48562079101732	1.10339975671040
C	-6.19889113277210	-9.87054093698463	1.29736111684721
C	-5.28057575879560	-10.57431788323243	2.03155065099735
H	-4.87556218796692	-6.76348000142796	1.51980532420461
H	-6.75409641959061	-7.93440061175857	0.50058334277143

H	-7.04217489744500	-10.38725801636159	0.85264443319828
H	-5.38305502809962	-11.63998000716620	2.16414486193454
S	-6.31273663502826	-1.32785544476393	3.30928213622545
S	1.56618486288528	-0.91711218029307	2.15169912974631
S	-3.28818325415057	-12.46061402464090	3.58799906304478
O	-5.93405990420410	0.07982222310237	3.16286242017875
O	-7.16927451835404	-1.82207047826035	2.23346132125620
O	-6.76427532494292	-1.67947057926512	4.65398156789850
O	1.08528963554149	0.43803872230401	1.87532334573960
O	2.28132972569803	-1.04539414366682	3.42580821997980
O	2.26740914396480	-1.54465229502627	1.02715726734100
O	-2.11521112659379	-12.80549116000290	4.39147305063631
O	-4.56374170409928	-12.67343566459571	4.27697383843930
O	-3.26168434708646	-13.01460002841212	2.23109179976013
O	-5.76381032177027	-4.34919603606164	3.36408618435942
H	-5.46057581642729	-5.28086957976491	3.37206254980813

trans-1c

C	-6.50865225440250	-1.46547787408170	2.09186244371876
C	-6.75385577985493	-2.84897789046129	1.99167521917593
C	-5.76516443468286	-3.76754912053342	2.25840597417210
C	-4.47247360354174	-3.35036781912535	2.64261527043193
C	-4.22257467091604	-1.95791639947504	2.74335066498111
C	-5.25922651178456	-1.03504222847875	2.46378324221179
C	-2.92581922196329	-1.51711422289865	3.12438135743882
C	-1.89371254907441	-2.37136522108998	3.40058183267658
C	-2.11779086699980	-3.77189030160035	3.30336193456727
C	-3.39772774329811	-4.27050077282782	2.93202791650066
H	-7.74242600458424	-3.17993369799569	1.70082748610885
H	-5.96469854189441	-4.82635176560756	2.17469164048195
H	-5.06855544656035	0.02720365891926	2.54431766600739
H	-2.72963886314494	-0.45544570726095	3.20212718141625
N	-3.69805341896023	-5.60561517087447	2.83819715203274
N	-2.77000932820445	-6.45627837032039	3.04278704081762
C	-3.14144621147118	-7.81085442990629	3.01095505422217
C	-2.09449457008254	-8.77982849261518	2.87721855665056
C	-4.44547045623412	-8.24153718706889	3.15104131850128
C	-2.42101572916005	-10.17548060191933	2.89628988442298
C	-3.78216922137218	-10.57172663102802	3.04833665523803
C	-4.75646644365128	-9.60881391613415	3.16608692848390
H	-5.22465025364106	-7.50109755801321	3.26673691749478
H	-5.78061918646578	-9.93385057477516	3.28646598996345
C	-0.74111490899957	-8.39525382204163	2.71262322376061
C	0.24968623355985	-9.33419952720504	2.58312615217227
C	-0.06837276850079	-10.70645936294543	2.60907489060849
C	-1.36776499267118	-11.11646692680539	2.76001687400617
H	-0.49464013458768	-7.34452996469393	2.68266925497009
H	1.27853396638279	-9.01577323151284	2.46003446039234

H	0.71937378095089	-11.44473511589623	2.50645174938232
H	-1.61648023669340	-12.16622328915743	2.77440500122605
S	-0.27456059431862	-1.68715690634292	3.88332860412593
S	-7.84289392657212	-0.30691655314038	1.71304198991145
S	-4.27002141131523	-12.31995078515042	3.11193167722028
O	-0.48320983228788	-0.23753999339809	3.83426748804562
O	-0.03974454099534	-2.20177494173423	5.23058768534548
O	0.65881732346640	-2.18124527163259	2.87356678545416
O	-7.30162338249780	1.02068610922830	2.01008779296214
O	-8.12671365849832	-0.53038748632751	0.29136773877096
O	-8.94323772248140	-0.71499865722047	2.59283984110133
O	-5.72378672924478	-12.30035542523567	3.26712936719776
O	-3.81475472716650	-12.88180798207145	1.83684119763617
O	-3.55432542745211	-12.86040146316168	4.27126005231299
O	-1.12813779662211	-4.61095302469294	3.56598002158900
H	-1.50496720150996	-5.53421408368947	3.43723282409139

trans-1d

C	-6.61426338542043	-1.49139401462052	2.36212648981654
C	-6.83764995531844	-2.88015233816944	2.28484375199629
C	-5.80521187051336	-3.77554501977126	2.43842195634029
C	-4.48705460803026	-3.32889837875115	2.68072741521955
C	-4.25879920826385	-1.93087498209724	2.75222560493409
C	-5.34112747407866	-1.03229871439213	2.59097995976232
C	-2.93704988774491	-1.46112417644728	2.98120406418516
C	-1.86185095910010	-2.29296060215342	3.13416513154637
C	-2.06577784641828	-3.69919051690873	3.07020796588817
C	-3.36861367066646	-4.22348292248807	2.85340901069222
H	-7.84338934749891	-3.23399373624930	2.09873856829966
H	-5.99123249667254	-4.83743532068251	2.36481968386661
H	-5.16665372599617	0.03425476368315	2.64793459151515
H	-2.75609809284373	-0.39537676880755	3.03620011561839
N	-3.65839624032772	-5.56699231956750	2.80652191897221
N	-2.70088578162347	-6.39757324573023	2.92700123215023
C	-2.97065701810698	-7.77600150007587	2.90295223178537
C	-4.22054466224272	-8.43739621393327	3.17544454120497
C	-1.85921821402945	-8.54895714327692	2.61780102400214
C	-4.27365942959104	-9.87290270500534	3.08513934183311
C	-3.10187198370100	-10.61254388196648	2.74166028167941
C	-1.92303942874929	-9.94400865908006	2.52599912446823
H	-0.92194756026017	-8.03554966717232	2.44201808638579
H	-1.04261952628141	-10.52007561301980	2.27891169227699
C	-5.39242196819829	-7.74625795393761	3.57273322793312
C	-6.55959161410771	-8.41684109801553	3.84015814247107
C	-6.61875776235541	-9.81640797464286	3.71953839424150
C	-5.50316268440374	-10.52526451545405	3.35685946278032
H	-5.35566972507356	-6.67387063441506	3.65254820115294
H	-7.43736849967150	-7.85784398780914	4.14323550460525

H	-7.54685716264631	-10.33944707336341	3.92193915281299
H	-5.53699893690445	-11.60053253310751	3.27804179779169
S	-0.21107511744205	-1.57177540876668	3.41093996780825
S	-8.00943195307229	-0.36519338058920	2.14342643726032
S	-3.10318829874826	-12.42482872046098	2.59569458022967
O	-0.45956523716835	-0.12747132943108	3.41450872929537
O	0.21573184366548	-2.09717236782532	4.70588802693848
O	0.59034848227416	-2.02654710596280	2.27649225049967
O	-7.45411936779107	0.97817810683489	2.31758909521312
O	-8.49163478031749	-0.64053701606511	0.78560779088912
O	-8.96403552620470	-0.75617979803220	3.18635898968184
O	-1.73130750748364	-12.77028575010695	2.22342876622016
O	-3.49638874252615	-12.90562803458204	3.92306542022440
O	-4.09248470887483	-12.71508512890270	1.55483570760408
O	-1.03310339647072	-4.51533719934951	3.22057391289744
H	-1.39633496299963	-5.44799741933171	3.13765265700984

cis-2a

C	-6.57979618175602	-1.39138888488788	2.42451687654638
C	-6.88581069314423	-2.75706045866508	2.37814535617122
C	-5.88993902319062	-3.70909553607848	2.48706858579877
C	-4.54690026219665	-3.33488076468566	2.64583628843656
C	-4.23502468091335	-1.96029448311914	2.68870729644634
C	-5.26228984326955	-1.00564920425742	2.57594979413214
C	-2.86326809656265	-1.54931555140865	2.84598785063844
C	-1.82103820294238	-2.40449022681336	2.96351859445489
C	-2.05501382164805	-3.84303912039193	2.94026648965237
C	-3.45989808570204	-4.30463640441157	2.76960600158836
H	-7.91762409578949	-3.05606506047141	2.24795252434857
H	-6.13618743657195	-4.76131346096930	2.45080866487190
H	-5.02318908725327	0.04949167758782	2.60245571185887
H	-2.64488019001712	-0.48854295995233	2.87276439519425
N	-3.79495665511937	-5.58021705459691	2.72587908462833
N	-2.86918840260710	-6.50108475338227	2.84855536010552
C	-3.16618419718588	-7.85948480180349	2.79114838109804
C	-2.11401292249109	-8.79593350683118	3.05826053874145
C	-4.42955466411110	-8.31991385771524	2.48762064492488
C	-2.40136370068394	-10.19943414737626	2.99475254457226
C	-3.72078382999950	-10.63440353607471	2.67441283837331
C	-4.69489270866933	-9.69703343494470	2.43295499345232
H	-5.21195465961381	-7.60218180061377	2.28771865313713
H	-5.68867999064287	-10.04668271152660	2.18998887484066
C	-0.79973964654862	-8.37967026418159	3.38750077606639
C	0.18978542326138	-9.29583677360200	3.63910868287655
C	-0.08926236667424	-10.67396498705540	3.57318415222493
C	-1.34967911086407	-11.11337024558993	3.26073563833722
H	-0.55453960804084	-7.32842737833196	3.45216547948316
H	1.18587616179778	-8.95070471802480	3.88985222267025

H	0.69667644304911	-11.39405423092860	3.77235451027324
H	-1.56813607889299	-12.16864314921868	3.20896599759600
S	-0.13740815959504	-1.73889826752739	3.14282766942193
S	-7.91632852433006	-0.17839351251323	2.31371910879389
S	-4.15440462520989	-12.39398110697938	2.58419657575186
O	-0.33565505933707	-0.28558774461145	3.14220172585298
O	0.34421709118036	-2.26242037728563	4.41894840004892
O	0.58263378062276	-2.23084982333222	1.96978238637818
O	-7.25226547864236	1.11378106465575	2.13473830255283
O	-8.70895244956834	-0.60979286535195	1.15792570102538
O	-8.62947814671742	-0.30919232298986	3.58853899785014
O	-5.56651349853904	-12.41394563063827	2.20415384042087
O	-3.25714680792436	-12.95238836281178	1.56780031537850
O	-3.89250026860288	-12.91138287688942	3.93081793661608
O	-1.13676050653960	-4.67666260410493	3.05638029907347
H	-1.91324332880301	-6.12922489629744	2.96691793529409

cis-2b

C	-6.62182491586067	-1.38454392960346	2.57789716610932
C	-6.90416622028439	-2.75559874184950	2.54585773414246
C	-5.88875138501960	-3.68878980052810	2.63163851888893
C	-4.54771910059977	-3.29171454233419	2.75482353390214
C	-4.26029676697282	-1.91092332267076	2.77716370204163
C	-5.30754959662478	-0.97539577409756	2.68857187727117
C	-2.89175663118383	-1.47432931338382	2.88270157762032
C	-1.83037532230882	-2.31017134877854	2.95887304734051
C	-2.03817775870017	-3.75398073112678	2.94593298550870
C	-3.43988702542432	-4.23903577446988	2.85494771887936
H	-7.93299663839509	-3.07438651722483	2.44168763257234
H	-6.12306442254841	-4.74311574049654	2.59331538539553
H	-5.08609730109910	0.08385275137684	2.70001700627767
H	-2.69191977551259	-0.40967963242036	2.89736124626948
N	-3.76030980104188	-5.52183933637203	2.86307018069449
N	-2.82125668434383	-6.43021830190701	2.94683405812713
C	-3.00890879750960	-7.81312908888618	2.95915018147613
C	-4.26194537256160	-8.50609210286072	3.06116129341801
C	-1.83923425514843	-8.55006567243640	2.88114099675383
C	-4.25054879658597	-9.94647969813784	3.05472180598986
C	-3.01752449582562	-10.65606947104007	2.96511256080478
C	-1.84441153735735	-9.94856277190079	2.88595142084690
H	-0.89670892944132	-8.01965970302997	2.80896601860919
H	-0.91566615272152	-10.49756752818531	2.82193941775544
C	-5.50866212557773	-7.84240463697995	3.18455495996126
C	-6.68370880872956	-8.54438382258375	3.28005424032003
C	-6.67421585722691	-9.95031984919081	3.25440410334778
C	-5.48957772789193	-10.63083935205320	3.14755812516399
H	-5.51655903881929	-6.76702945233960	3.19924550973436
H	-7.61960859730800	-8.00590516145366	3.37427918285453

H	-7.60617791723621	-10.50051435976234	3.32311668138486
H	-5.47513188066240	-11.70937616032556	3.13328829065280
S	-0.15377762788891	-1.61328563198386	3.06677299222196
S	-7.98273079934152	-0.19750052196663	2.49336111794734
S	-2.93455668550345	-12.47031872308100	2.96675709008679
O	-0.37792516155018	-0.16358548014407	3.07181560086886
O	0.38919690739534	-2.12444308424707	4.32336309114571
O	0.52658338751760	-2.09456221693145	1.86590941781519
O	-7.34656342016864	1.10598829055692	2.29652788832707
O	-8.79233753517000	-0.64685348998666	1.35617468259316
O	-8.66658613597453	-0.33760537450932	3.78329535537114
O	-1.50894055475331	-12.77721716860797	2.84645152265988
O	-3.52210347160460	-12.86990477082840	4.24875655858582
O	-3.73130451993671	-12.88678703208711	1.80904403825098
O	-1.10056332938231	-4.57133728557607	3.00986379513461
H	-1.85952099911521	-6.04518189255462	2.98124450487655

trans-2a

C	2.54617641123048	0.38162102806283	0.13075396393104
C	2.66245054597629	-0.87407830166102	0.72179939583708
C	1.55286516758629	-1.69713649458111	0.84967733257794
C	0.28449323535066	-1.29176799993174	0.40073288842345
C	0.15736069047809	0.01487387117821	-0.12307384431185
C	1.29349009101836	0.81989593411686	-0.27256799076471
C	-1.15750128011309	0.54024067541201	-0.44156545312450
C	-2.31319659917097	-0.07514277055391	-0.12842131934253
C	-2.28424271724142	-1.39664279961886	0.53957908106366
C	-0.93747212394832	-2.09925542541790	0.50537657319155
H	3.62624031137741	-1.19296756014283	1.09546258217905
H	1.67233741396775	-2.63474719714427	1.37593679438877
H	1.19729844436959	1.81672902557886	-0.68273241328321
H	-1.21428094949481	1.51865390070809	-0.90319970677985
N	-1.03890691554335	-3.39444539886972	0.49145243890692
N	0.03175754501183	-4.16576168373442	0.32744564254685
C	-0.07606541183390	-5.55262639886413	0.22481695309853
C	-1.27624166331411	-6.19896401225452	0.42277834526546
C	1.10470505658313	-6.31589358357887	-0.05505174695783
C	-1.35108457367175	-7.60017533500881	0.35526720705619
C	-0.25111433944678	-8.37795054865891	0.09228324976588
C	1.00748938832321	-7.74588689027288	-0.12402963916368
H	-2.15555670556094	-5.60767023907123	0.63389944981096
H	-2.29839558355060	-8.09581415284121	0.51603538641340
C	2.37042880288048	-5.71145491501068	-0.26073476815196
C	3.48762079561809	-6.46197011080032	-0.52639966159453
C	3.39070818844830	-7.86392599159130	-0.59794344031045
C	2.18489326725431	-8.48652533782833	-0.40245921216498
H	2.48636279196440	-4.63650159099574	-0.21427424080674
H	4.44016867145390	-5.96942342821384	-0.68145323544601

H	2.10681328331312	-9.56139929189886	-0.45386388793730
H	4.27421204530582	-8.45590803554049	-0.80881400306695
S	-0.43819491618440	-10.18129348974646	0.03259342675947
S	-3.88776843634226	0.77003319287061	-0.46840432980901
S	4.02440395389012	1.40420289735841	-0.08102103380220
O	-3.24836328759161	-1.91951686287732	1.06056492215301
O	0.48250037713109	-10.69035232732169	1.05488132557130
O	-1.84898075861582	-10.42360940570849	0.33219064577270
O	-0.04524064630437	-10.55497635299144	-1.32993601807661
O	3.52381849198520	2.73859838808209	-0.40991830258440
O	4.71082030198908	1.32043251225871	1.21109773363700
O	4.75308230445796	0.75230220944090	-1.17248970887468
O	-4.66038328087737	-0.18052432773744	-1.26304911201551
O	-3.48504923060714	1.96750024349877	-1.21405730744005
O	-4.44551909649384	1.06326264889312	0.85022258965861
H	0.90178420694192	-3.73418995699071	0.05292578480070

trans-2b

C	0.07428052998766	-2.06041626974446	3.18981896076351
C	-0.00747727551319	-3.35353887842366	3.69903644092478
C	-1.17936691979815	-4.08715045769958	3.57580647772784
C	-2.31716192297100	-3.55330264253170	2.94614720943486
C	-2.25121432161744	-2.21209580691175	2.49920561132369
C	-1.05237542899802	-1.49766453925358	2.60776780307935
C	-3.44309083941463	-1.55748069496168	1.99416615332742
C	-4.67881166479489	-2.08991791585098	2.04365555800330
C	-4.86973820186738	-3.44808458843298	2.59699408433151
C	-3.59614621219489	-4.25281250197186	2.78760868083677
H	0.84892553951526	-3.77138394789131	4.21098430527236
H	-1.21906970679027	-5.05764925741923	4.05140409094414
H	-1.00481610851371	-0.47309151904110	2.26252148132332
H	-3.34179928492659	-0.55046903773618	1.60772239110541
N	-3.80969336000463	-5.53423400777067	2.72043405391603
N	-2.82329369033582	-6.41580811238604	2.75258928361781
C	-2.97395904673710	-7.80118061674431	2.61623519542833
C	-4.18206901849589	-8.53061878298907	2.87523462085653
C	-1.82495715684282	-8.49396604758443	2.28374755424577
C	-4.14069232502310	-9.96809245080430	2.78713509497078
C	-2.92677319733242	-10.63579409900160	2.44849075305665
C	-1.80158121259161	-9.89179354255511	2.20368743710336
H	-0.91600306488825	-7.93631048443975	2.08218708219696
H	-0.88867714223467	-10.40864281813606	1.94357399269414
C	-5.40481811214633	-7.90452806559581	3.23252535605878
C	-6.52803397945642	-8.64842215724770	3.49241268368066
C	-6.49067677698803	-10.05143864004559	3.40189088974413
C	-5.32966220381679	-10.69261455350952	3.05743155550555
H	-5.45143246964565	-6.82830725216188	3.27326640839139
H	-7.44819291951572	-8.14118012064497	3.75764133261988

H	-7.38490909942457	-10.63177112598320	3.60248115910361
H	-5.29614448714988	-11.76835293603673	2.98453568030646
S	-6.09689870205611	-1.09670067410900	1.48576961699415
S	1.63186855709836	-1.14654143411894	3.31107758550935
S	-2.80388257231211	-12.44427912119812	2.34251339338228
O	-5.48096929294177	0.12290269210177	0.95111680296737
O	-6.74939156435872	-1.91553517067565	0.46752126478826
O	-6.89068941454210	-0.86923437388327	2.69135692521946
O	1.26595430386747	0.25679966677349	3.12036851602390
O	2.13436492765891	-1.46095912150253	4.65123741123362
O	2.45532611847070	-1.70016666400709	2.23276218259546
O	-1.41507996017448	-12.70072640732132	1.95741685772400
O	-3.14374500235485	-12.92254320530841	3.68605167323602
O	-3.78258462216231	-12.83404238316583	1.32344413602862
O	-5.95320637113591	-3.92915485294972	2.86772671069966
H	-1.87124050252985	-6.08264159212810	2.65004066170257