

Supporting Information:

Absolute Configuration Assignment of Norcamphor-Derived Furyl Hydroperoxide Using Density Functional Theory Calculations of Optical Rotation and Vibrational Circular Dichroism

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Norcamphor-derived furyl <i>exo</i> -hydroperoxide.....	2
Norcamphor-derived furyl <i>endo</i> -hydroperoxide.....	15

norcamphor-derived furyl *exo*-hydroperoxide

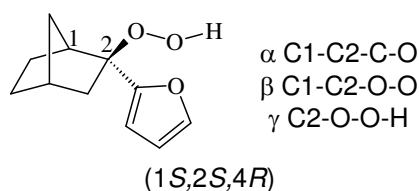


Table S1. Monte-Carlo MMFF94 conformer search using Spartan 02 (stable with respect to variation of the initial temperature up to 20000K and method, i.e. from Monte-Carlo to Systematic).

Conformer	ΔE	α	β	γ	H---O
1	0.00	48.3	174.5	103.6	3.179
2	0.25	39.3	-52.1	-86.9	2.525
3	0.47	-116.4	169.4	98.4	3.407
4	0.50	-153.7	-61.6	-106.1	3.454
5	1.72	-93.6	172.7	-118.3	4.570
6	2.23	-86.5	-47.4	119.4	5.108
7	2.66	35.8	168.7	-131.9	4.634
8	3.11	21.5	-61.0	114.4	3.969
9	5.10	-102.1	60.8	119.3	4.924
10	5.63	-99.0	49.0	-120.4	5.200
11	6.22	41.0	74.4	126.7	4.757

ΔE in kcal/mol. Dihedral angles (α , β , γ) are in degrees. H---O is the distance in Å from H of hydroperoxide to O of furyl group.

Table S2. B3LYP/6-31G** geometry optimization and free energy calculation of the conformers in Table S1 using Gaussian 03.

Conformer ^a	E^b	α	β	γ	H---O	G^c	ΔE (kcal/mol)	ΔG (kcal/mol)
4→ a	-653.162712540	-144.7	-62.7	-85.9	3.485	-652.965397	0.065756	0.000000
3→ b	-653.162817329	-98.3	169.2	80.6	3.490	-652.965228	0.000000	0.106049
1→ c	-653.161892048	42.7	169.3	85.6	3.255	-652.965154	0.580623	0.152485
2→ d	-653.161747347	62.6	-53.9	-76.6	2.176	-652.964450	0.671424	0.594252
5→ e	-653.159966986	-90.6	171.1	-120.5	4.687	-652.963021	1.788617	1.490963
7→ f	-653.159122354	49.8	172.9	-125.9	4.425	-652.962685	2.318632	1.701806
6→ g	-653.159053697	-86.1	-61.3	109.9	5.012	-652.962538	2.361715	1.794050
8→ h	-653.159263588	34.4	-68.6	107.7	3.705	-652.962296	2.230006	1.945907
9→ i	-653.154994029	-105.7	56.1	117.7	4.953	-652.958119	4.909195	4.567015
11→ j	-653.154876328	47.3	61.2	120.7	4.718	-652.958014	4.983054	4.632903
10→ k	-653.154819778	-103.7	57.3	-102.8	5.167	-652.957718	5.018540	4.818646

^a $n \rightarrow \alpha$ means that MMFF94 conformer n becomes conformer α after B3LYP/6-31G** reoptimization.

^b B3LYP/6-31G** electronic energy in Hartree per particle.

^c Sum of electronic and thermal Gibbs energies in Hartree per particle ($T=298.15K$).

Table S3. TDDFT/B3LYP optical rotations at 589.3nm computed adopting the polarizability consistent Sadlej basis set of GIAO using Gaussian 03. Molecular geometries have been optimized at B3LYP/6-31G**, see Table S2.^a

Conformer	ΔE (kcal/mol)	ΔG (kcal/mol)	%P(ΔE) ^b	%P(ΔG) ^c	$[\alpha]_{D,i}$	$[\alpha]_{D,i} \times$ %P(ΔE)/100	$[\alpha]_{D,i} \times$ %P(ΔG)/100
a	0.07	0.00	33.10	31.25	-63.43	-21.00	-19.82
b	0.00	0.11	36.99	26.13	24.03	8.89	6.28
c	0.58	0.15	13.88	24.16	131.41	18.24	31.74
d	0.67	0.59	11.91	11.46	4.58	0.55	0.52
e	1.79	1.49	1.81	2.52	-118.64	-2.14	-2.99
f	2.32	1.70	0.74	1.77	-17.67	-0.13	-0.31
g	2.36	1.79	0.69	1.51	122.26	0.84	1.85
h	2.23	1.95	0.86	1.17	100.98	0.87	1.18
i	4.91	4.57	0.01	0.01	TOT ^d →	6.11	18.45
j	4.98	4.63	0.01	0.01			
k	5.02	4.82	0.01	0.01			

^a Optical rotations have been calculated for those conformations having ΔG less than 2 kcal/mol only, as higher free energy conformations have negligible populations and can be neglected.

^b Percentage populations obtained from ΔE values using Boltzmann statistics at T=298.15K.

^c Percentage populations obtained from ΔG values using Boltzmann statistics at T=298.15K.

^d Predicted optical rotations from energy and free energy based populations.

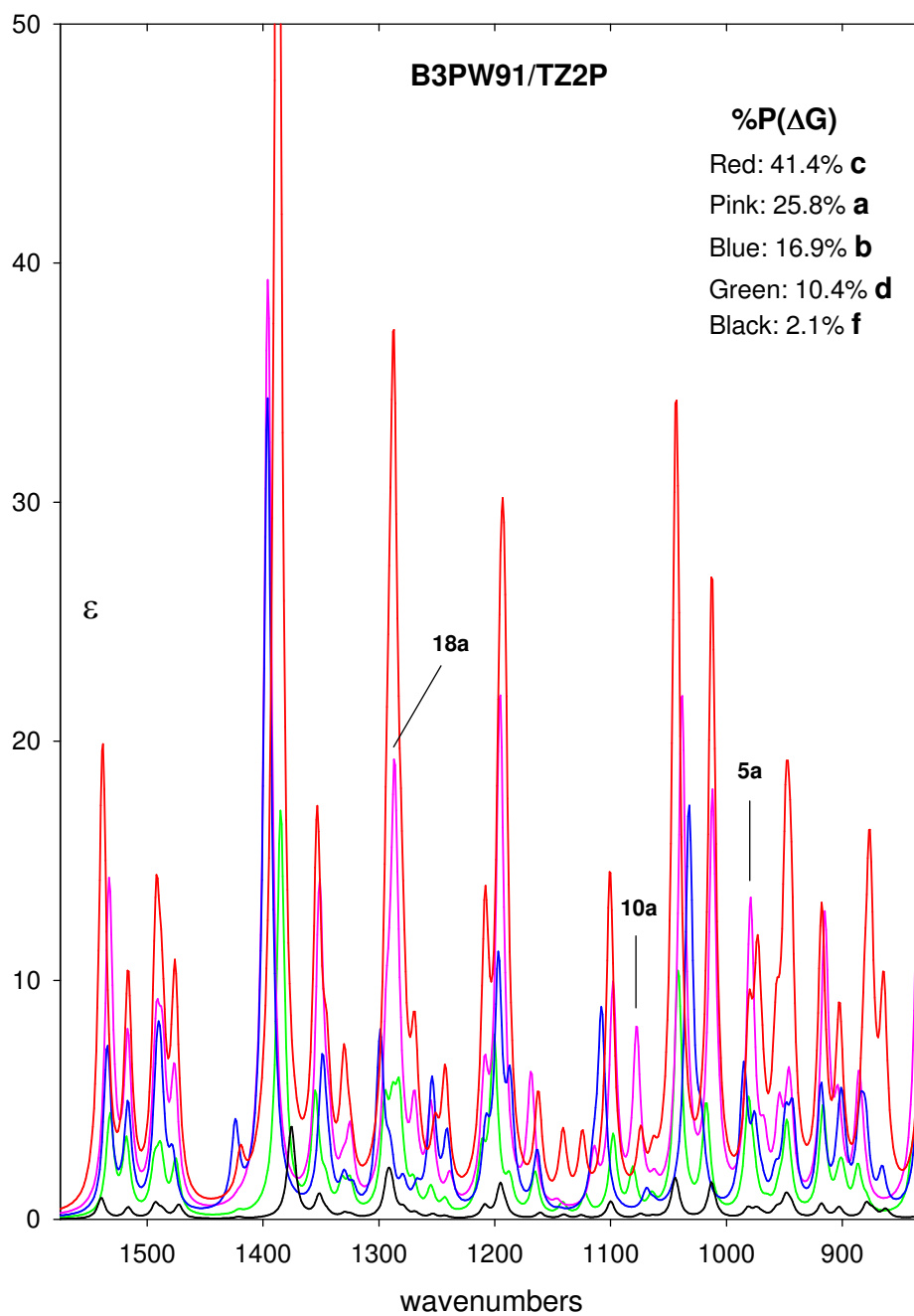


Figure S1. Calculated IR spectra of the five most populated B3PW91/TZ2P conformers of *exo*-**3**. Bands **5a**, **10a** and **18a** are evident in the experimental IR spectrum of **3**.

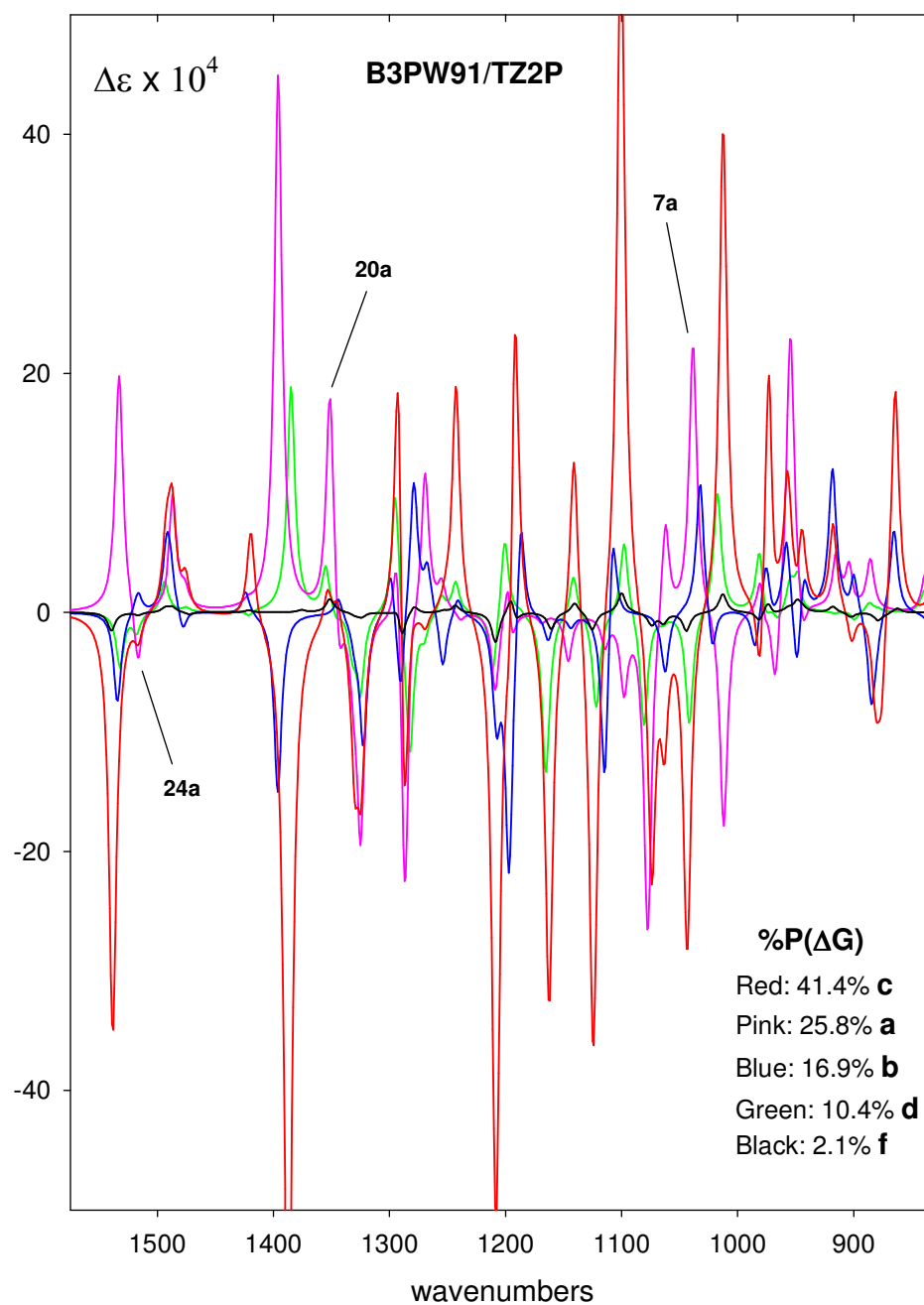


Figure S2. Calculated VCD spectra of the five most populated B3PW91/TZ2P conformers of *exo*-**3**. Bands **7a**, **20a** and **24a** are evident in the experimental VCD spectrum of (+)-**3**.

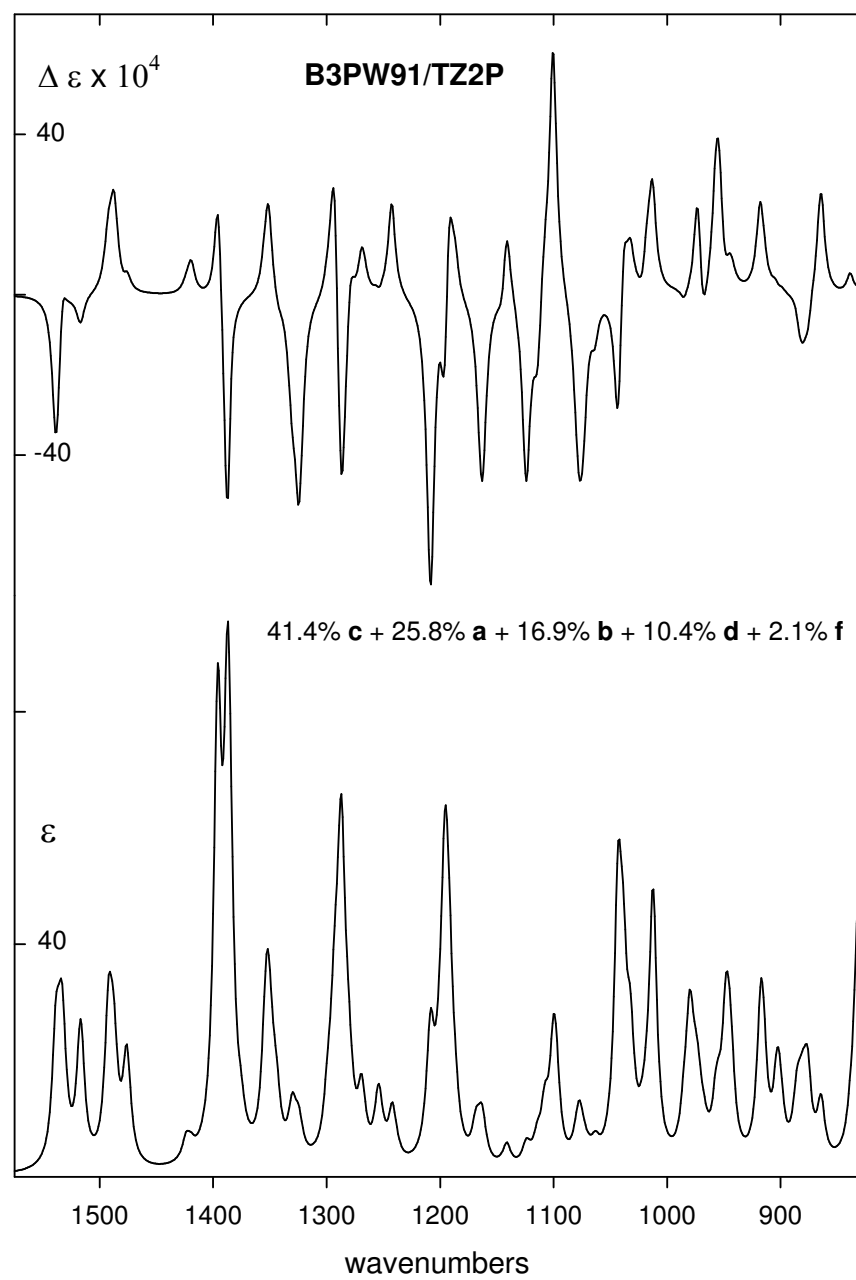


Figure S3. B3PW91/TZ2P conformationally-averaged IR and VCD spectra of *exo-3*.

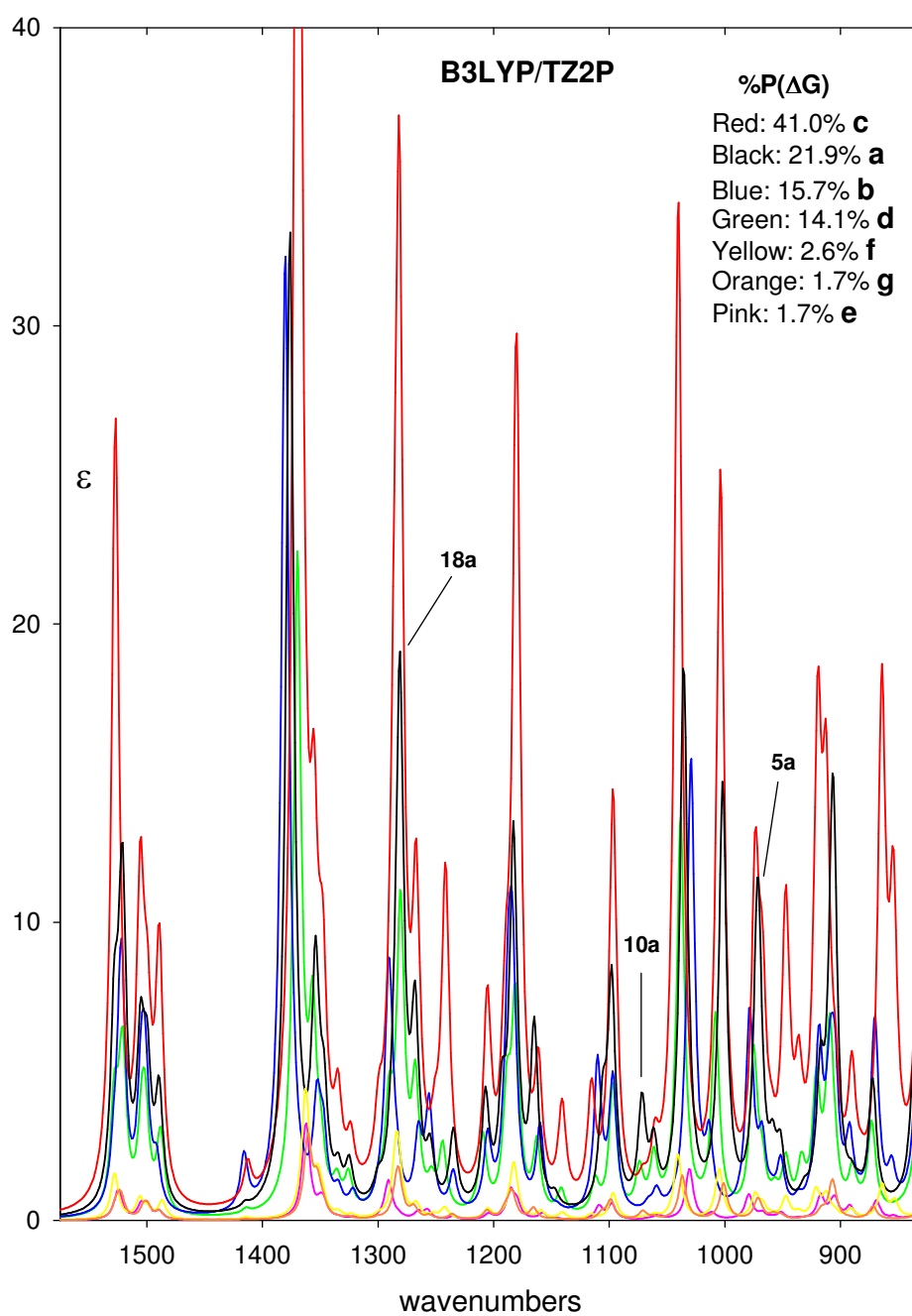


Figure S4. Calculated IR spectra of the seven most populated B3LYP/TZ2P conformers of *exo*-**3**. Bands **5a**, **10a** and **18a** are evident in the experimental IR spectrum of **3**.

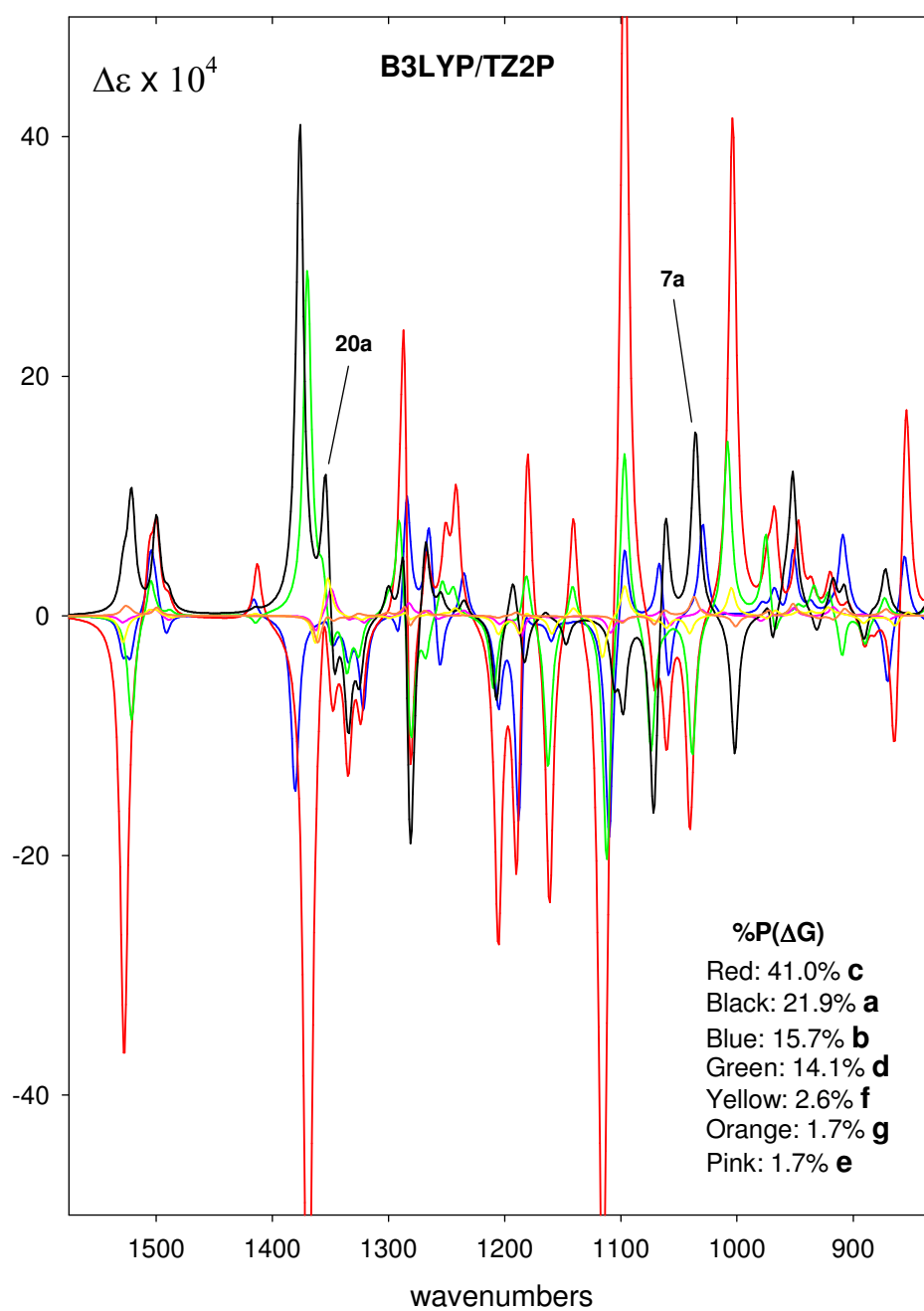


Figure S5. Calculated VCD spectra of the seven most populated B3LYP/TZ2P conformers of *exo*-**3**. Bands **7a** and **20a** are evident in the experimental VCD spectrum of (+)-**3**.

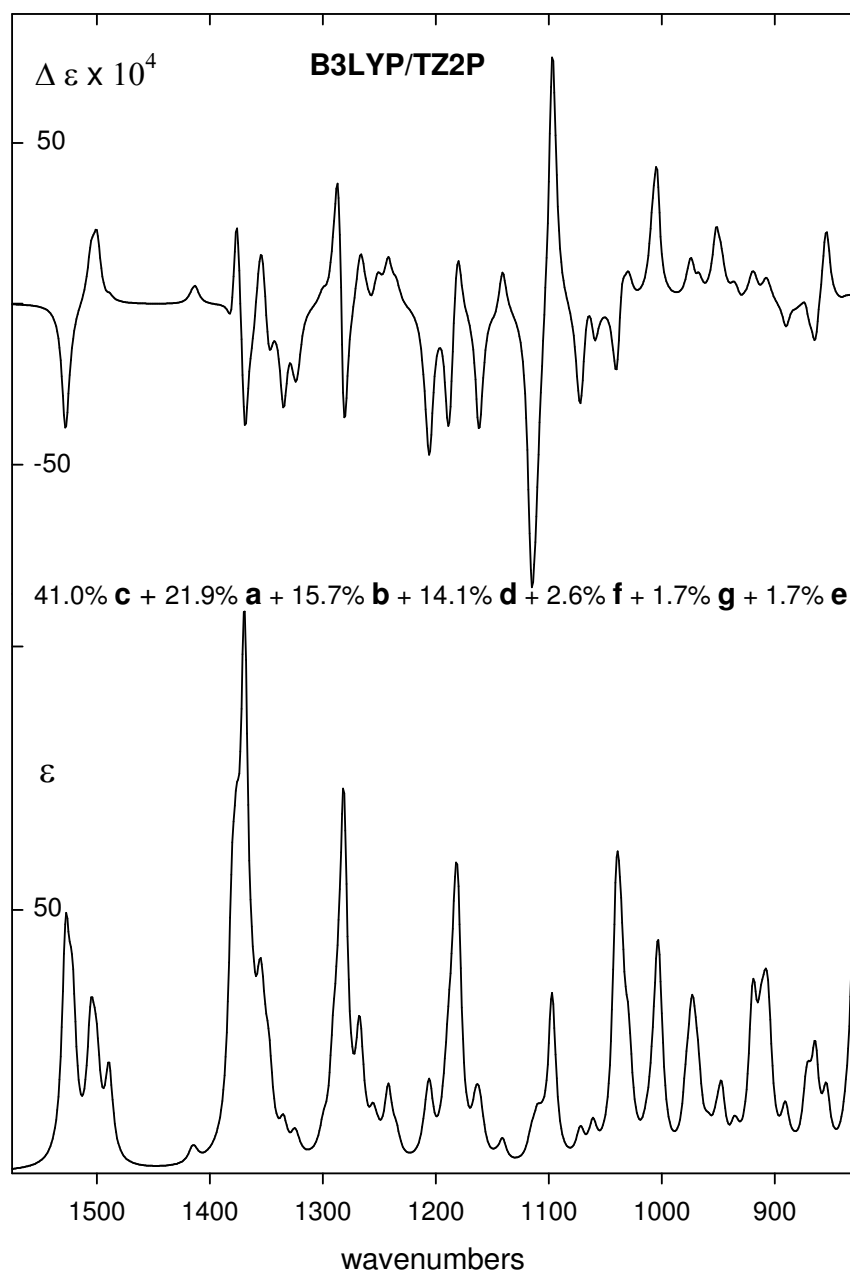


Figure S6. B3LYP/TZ2P conformationally-averaged IR and VCD spectra of *exo-3*.

Cartesian coordinates (in Å) for conformers **a-h** of *exo-3*.

Conformer	B3PW91/TZ2P	B3LYP/TZ2P
a	H 0.946094 0.948175 1.779295	H 0.957212 0.948434 1.779926
	C 1.205563 0.307231 0.940233	C 1.212636 0.307443 0.941644
	C 2.201394 -1.753281 0.117076	C 2.211586 -1.760815 0.112937
	C 1.009681 -0.195609 -1.413616	C 1.006191 -0.198778 -1.421218
	C 2.376001 -0.528631 -0.792901	C 2.380396 -0.531807 -0.802726
	C 0.219574 0.441093 -0.238281	C 0.215877 0.437974 -0.236358
	C 1.368983 -1.182376 1.298215	C 1.386264 -1.186209 1.306293
	H 3.169008 -2.123754 0.459488	H 3.180396 -2.132010 0.446922
	H 1.096578 0.545529 -2.209592	H 1.090262 0.540419 -2.217272
	H 3.171286 -0.629731 -1.530365	H 3.171656 -0.632794 -1.542604
	H 0.413705 -1.689564 1.424031	H 0.437378 -1.698259 1.445342
	H 1.699500 -2.576901 -0.392755	H 1.703671 -2.582491 -0.391359
	H 0.503499 -1.067111 -1.824248	H 0.499620 -1.070117 -1.827947
	H 1.910051 -1.273713 2.240849	H 1.939376 -1.269455 2.241208
	C 2.538157 0.599213 0.234580	C 2.547127 0.601562 0.226903
	H 3.398100 0.459926 0.891747	H 3.408967 0.463387 0.879759
	H 2.578733 1.593082 -0.208144	H 2.586480 1.593825 -0.215782
	C -3.062852 -0.951946 -0.649030	C -3.080334 -0.949275 -0.650165
	C -3.198630 -0.699397 0.674414	C -3.207457 -0.711323 0.677488
	H -4.072640 -0.884948 1.275948	H -4.076985 -0.902321 1.281384
	C -1.951812 -0.148860 1.096681	C -1.955479 -0.165380 1.102105
	H -1.682082 0.168615 2.089894	H -1.685080 0.141585 2.096828
	C -1.145702 -0.110766 0.001142	C -1.151674 -0.113356 0.005288
	O -1.827006 -0.599691 -1.075708	O -1.840523 -0.591675 -1.080116
	H -3.718760 -1.367860 -1.393872	H -3.738913 -1.355468 -1.395651
	O 0.095465 1.827257 -0.654675	O 0.092272 1.833221 -0.655495
	O -0.441314 2.614019 0.418550	O -0.436418 2.632584 0.433558
	H -1.392358 2.505545 0.281309	H -1.387490 2.582007 0.262533
b	H 0.932651 0.279321 2.137168	H 0.936290 0.271825 2.141392
	C 1.196813 -0.034012 1.128387	C 1.197970 -0.040340 1.133126
	C 2.093032 -1.713231 -0.375674	C 2.089310 -1.726719 -0.381412
	C 1.037789 0.369003 -1.249227	C 1.040370 0.373756 -1.253163
	C 2.362319 -0.255251 -0.782112	C 2.365822 -0.263021 -0.785680
	C 0.234234 0.553818 0.065124	C 0.231968 0.555680 0.066636
	C 1.274782 -1.557968 0.935770	C 1.272594 -1.570924 0.939067
	H 3.027440 -2.246848 -0.194762	H 3.020480 -2.264951 -0.205340
	H 1.185836 1.352309 -1.692779	H 1.196516 1.356324 -1.691718
	H 3.173422 -0.135889 -1.499414	H 3.176510 -0.146201 -1.501893
	H 0.293532 -2.028392 0.885434	H 0.292523 -2.040410 0.890624
	H 1.548118 -2.259248 -1.146493	H 1.538372 -2.266485 -1.150522
	H 0.514922 -0.250741 -1.975004	H 0.515073 -0.239326 -1.980651
	H 1.799021 -2.001341 1.783076	H 1.799824 -2.014135 1.782958
	C 2.558992 0.417037 0.583228	C 2.567490 0.407235 0.586587
	H 3.393035 0.000448 1.150907	H 3.398813 -0.014379 1.152177
	H 2.663174 1.499642 0.528361	H 2.678033 1.487899 0.534964
	C -2.781309 -1.311724 -0.604319	C -2.789703 -1.320722 -0.604825
	C -3.266480 -0.634877 0.462391	C -3.276197 -0.638942 0.458824
	H -4.256743 -0.719966 0.877663	H -4.265102 -0.723844 0.873853

	C -2.203446 0.203852 0.913892 H -2.211255 0.879650 1.752925 C -1.147510 -0.025149 0.085954 O -1.496168 -0.948682 -0.850168 H -3.199039 -2.046500 -1.269937 O 0.123865 1.935850 0.444013 O -0.568750 2.658417 -0.585836 H -1.490994 2.443890 -0.381702	C -2.213927 0.207421 0.909198 H -2.227817 0.885481 1.744431 C -1.154464 -0.019464 0.084817 O -1.499227 -0.953341 -0.851637 H -3.203659 -2.058532 -1.266763 O 0.128840 1.944071 0.454993 O -0.550162 2.690966 -0.588234 H -1.478876 2.529419 -0.363538
c	H -0.813719 -0.142506 -2.111001 C -1.136664 -0.262510 -1.079154 C -2.142137 -1.634546 0.652669 C -1.115343 0.573407 1.188462 C -2.417534 -0.126880 0.766464 C -0.234659 0.510062 -0.086286 C -1.241901 -1.724696 -0.610047 H -3.070810 -2.190685 0.515310 H -1.280632 1.619689 1.439521 H -3.267677 0.124152 1.399679 H -0.269848 -2.171230 -0.405023 H -1.654010 -2.031142 1.544059 H -0.651444 0.094254 2.049672 H -1.713806 -2.322293 -1.390677 C -2.523782 0.280915 -0.708511 H -3.327237 -0.233205 -1.239043 H -2.619334 1.354811 -0.860869 C 3.026853 -0.860806 -0.641176 C 3.127825 -0.872454 0.708618 H 3.975149 -1.203153 1.285482 C 1.888889 -0.359488 1.198284 H 1.611069 -0.217492 2.228554 C 1.121900 -0.077518 0.111623 O 1.819863 -0.379934 -1.023247 H 3.693422 -1.149270 -1.435332 O -0.102675 1.809705 -0.704248 O 0.510356 2.720401 0.221184 H 1.447853 2.593793 0.024474	H -0.815869 -0.133428 -2.113371 C -1.139679 -0.258397 -1.083970 C -2.151646 -1.642406 0.647795 C -1.120360 0.573866 1.196393 C -2.426498 -0.128750 0.768230 C -0.232349 0.510327 -0.081451 C -1.251837 -1.729608 -0.624085 H -3.080147 -2.196574 0.511676 H -1.287966 1.618007 1.448357 H -3.276249 0.119332 1.400887 H -0.283932 -2.184155 -0.425492 H -1.660338 -2.041891 1.534593 H -0.659323 0.093930 2.056941 H -1.730888 -2.316517 -1.406699 C -2.532053 0.286929 -0.710760 H -3.334616 -0.223822 -1.243347 H -2.627864 1.359905 -0.858848 C 3.039692 -0.861701 -0.642815 C 3.131205 -0.892892 0.707880 H 3.972446 -1.234309 1.284874 C 1.888625 -0.381559 1.200552 H 1.608608 -0.255239 2.230691 C 1.125963 -0.079138 0.116034 O 1.830716 -0.368715 -1.025531 H 3.708402 -1.139936 -1.436578 O -0.099572 1.818217 -0.700924 O 0.522267 2.737885 0.234553 H 1.454074 2.655579 -0.011282
d	H -0.772338 0.798647 -1.823897 C -1.111495 0.229931 -0.962533 C -2.160250 -1.770338 -0.061817 C -1.135152 -0.064502 1.435370 C -2.432030 -0.476772 0.720019 C -0.237902 0.471704 0.285304 C -1.223913 -1.288031 -1.203635 H -3.088570 -2.183002 -0.460091 H -1.309091 0.746296 2.144488 H -3.292308 -0.529564 1.386317 H -0.256578 -1.788014 -1.194216 H -1.702588 -2.540431 0.560845 H -0.670878 -0.890738 1.971321 H -1.668559 -1.471256 -2.182423 C -2.506008 0.557145 -0.411271	H -0.773435 0.828791 -1.810722 C -1.112949 0.245512 -0.961390 C -2.163830 -1.778354 -0.091384 C -1.141394 -0.086706 1.442428 C -2.440079 -0.492525 0.713508 C -0.236295 0.465089 0.296358 C -1.228289 -1.273250 -1.233599 H -3.090160 -2.188795 -0.492983 H -1.319672 0.713542 2.160062 H -3.300708 -0.557760 1.376113 H -0.263148 -1.774437 -1.238916 H -1.700619 -2.554090 0.517896 H -0.680242 -0.918436 1.969565 H -1.679153 -1.435370 -2.211823 C -2.514102 0.563905 -0.404725

	H -3.299802 0.346749 -1.129864 H -2.598138 1.584417 -0.061861 C 3.013249 -0.647951 -0.757233 C 3.171008 -0.994225 0.542470 H 4.044965 -1.442128 0.984913 C 1.947317 -0.652688 1.189706 H 1.708498 -0.782349 2.231722 C 1.131351 -0.122730 0.238906 O 1.785479 -0.113490 -0.960150 H 3.647650 -0.716448 -1.623781 O -0.153333 1.885638 0.594520 O 0.505700 2.580556 -0.476289 H 1.417920 2.596946 -0.159837	H -3.305752 0.365196 -1.127161 H -2.608890 1.583730 -0.039189 C 3.034089 -0.621040 -0.758565 C 3.173531 -1.023470 0.527444 H 4.038932 -1.493037 0.960822 C 1.940813 -0.704857 1.177302 H 1.692445 -0.880618 2.208713 C 1.134965 -0.130119 0.243401 O 1.804790 -0.071123 -0.952852 H 3.677284 -0.653794 -1.618654 O -0.149243 1.883118 0.628005 O 0.497287 2.606066 -0.452500 H 1.411694 2.635487 -0.139606
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f	H -0.799789 -0.084985 -2.115195 C -1.122609 -0.243383 -1.088680 C -2.099922 -1.685419 0.600941 C -1.116337 0.524124 1.202013 C -2.405548 -0.187163 0.759463 C -0.231333 0.516191 -0.071637 C -1.202244 -1.720414 -0.666402 H -3.018100 -2.255486 0.450864 H -1.308442 1.556947 1.491314 H -3.260375 0.026891 1.400252	H -0.805850 -0.104768 -2.115533 C -1.128760 -0.252583 -1.089095 C -2.117153 -1.680379 0.620048 C -1.119520 0.541090 1.204119 C -2.415936 -0.173165 0.765664 C -0.229328 0.513469 -0.073731 C -1.219548 -1.732505 -0.655249 H -3.037533 -2.246456 0.477998 H -1.307950 1.576471 1.480271 H -3.268946 0.050107 1.403488

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g	H 0.953315 0.887078 1.800062 C 1.200230 0.267806 0.939851 C 2.164806 -1.791963 0.078416 C 0.983413 -0.193755 -1.418265 C 2.349255 -0.555419 -0.812908 C 0.208588 0.441226 -0.229678 C 1.346291 -1.230020 1.272629 H 3.129479 -2.180563 0.408942 H 1.073579 0.552056 -2.209407 H 3.139206 -0.654196 -1.556374 H 0.384065 -1.723727 1.393020 H 1.648820 -2.599990 -0.441767 H 0.460328 -1.053622 -1.831919 H 1.890743 -1.344098 2.210940 C 2.535579 0.551464 0.233983 H 3.397085 0.386572 0.883154 H 2.596145 1.549430 -0.198941 C -3.099267 -0.865624 -0.661669 C -3.202183 -0.711288 0.679862 H -4.066999 -0.926167 1.284900 C -1.940349 -0.208860 1.113411 H -1.653774 0.049998 2.118418 C -1.160899 -0.096595 0.006691 O -1.868021 -0.498982 -1.088499 H -3.777608 -1.214709 -1.420528 O 0.118105 1.831357 -0.635056 O -0.472039 2.605208 0.428452 H 0.288480 3.129445 0.706387	H 0.964011 0.897066 1.797113 C 1.208879 0.274167 0.941110 C 2.179876 -1.793539 0.078841 C 0.984452 -0.195397 -1.426026 C 2.357791 -0.554066 -0.820561 C 0.206759 0.437913 -0.228966 C 1.369222 -1.226312 1.284962 H 3.145847 -2.182263 0.400987 H 1.071831 0.549239 -2.216579 H 3.144621 -0.653268 -1.565377 H 0.415244 -1.727694 1.422691 H 1.657684 -2.600532 -0.434104 H 0.463464 -1.055876 -1.837343 H 1.928261 -1.327529 2.214702 C 2.545571 0.561347 0.225718 H 3.409130 0.401868 0.871421 H 2.601960 1.557004 -0.209263 C -3.112029 -0.871688 -0.661579 C -3.209590 -0.722750 0.681558 H -4.071247 -0.939126 1.288151 C -1.943530 -0.221854 1.116250 H -1.657555 0.031462 2.121352 C -1.163631 -0.103471 0.009931 O -1.875967 -0.502313 -1.091372 H -3.791222 -1.216382 -1.419370 O 0.106625 1.835360 -0.638126 O -0.490728 2.614363 0.439994 H 0.255911 3.180642 0.674214
h	H -0.768809 0.781303 -1.826838 C -1.104478 0.219633 -0.957865 C -2.133984 -1.793027 -0.064207 C -1.125752 -0.080322 1.437111 C -2.418089 -0.504592 0.721075	H -0.771871 0.784327 -1.826567 C -1.108609 0.222227 -0.960469 C -2.148373 -1.795071 -0.063171 C -1.132412 -0.076073 1.445574 C -2.429628 -0.500275 0.725040

C -0.231781	0.469215	0.290539	C -0.230688	0.467550	0.292447
C -1.203078	-1.298759	-1.204657	C -1.217031	-1.301041	-1.212819
H -3.057931	-2.214978	-0.462923	H -3.073116	-2.215825	-0.457739
H -1.307773	0.725178	2.150224	H -1.314399	0.730506	2.155189
H -3.278659	-0.566973	1.386088	H -3.289658	-0.560411	1.388827
H -0.230159	-1.786762	-1.196757	H -0.248792	-1.794921	-1.212326
H -1.667265	-2.558741	0.556710	H -1.679851	-2.559450	0.555890
H -0.652263	-0.903313	1.969567	H -0.663126	-0.897999	1.980530
H -1.646707	-1.483069	-2.183805	H -1.668380	-1.478552	-2.188266
C -2.504277	0.530806	-0.408496	C -2.513080	0.539171	-0.409085
H -3.296126	0.313469	-1.127213	H -3.304462	0.324234	-1.127151
H -2.614114	1.554004	-0.049873	H -2.620999	1.561577	-0.052154
C 3.016197	-0.629752	-0.764404	C 3.024918	-0.643314	-0.764855
C 3.185478	-0.966608	0.536464	C 3.192851	-0.973707	0.538471
H 4.067640	-1.400106	0.976873	H 4.073094	-1.405521	0.981048
C 1.963049	-0.631980	1.188825	C 1.968423	-0.634113	1.192394
H 1.733525	-0.750618	2.234201	H 1.741571	-0.749340	2.237275
C 1.140471	-0.113175	0.238738	C 1.143023	-0.118052	0.242515
O 1.782496	-0.110550	-0.963603	O 1.785982	-0.121564	-0.966324
H 3.647205	-0.695401	-1.633523	H 3.654203	-0.713325	-1.632855
O -0.166891	1.881564	0.610854	O -0.157883	1.888614	0.612133
O 0.594064	2.573317	-0.396073	O 0.615904	2.580569	-0.407880
H -0.108460	3.022720	-0.880893	H -0.082605	3.069933	-0.861393

norcamphor-derived furyl *endo*-hydroperoxide

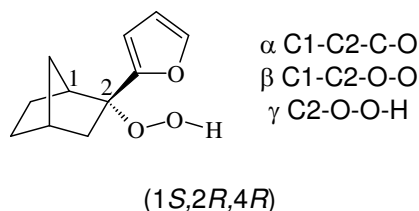


Table S4. Monte-Carlo MMFF94 conformer search using Spartan 02.

Conformer	ΔE^a	α	β	γ	H---O ^b
1	0.00	175.8	61.8	102.4	2.987
2	0.26	-4.9	55.4	97.4	3.309
3	0.64	172.3	-160.9	-82.6	2.182
4	0.85	-47.0	-172.9	-104.9	3.287
5	1.16	106.0	-168.1	-99.7	3.560
6	1.94	16.5	61.5	-121.8	4.525
7	2.15	79.9	-170.1	118.2	4.729
8	2.71	-1.2	-160.4	125.6	5.028
9	2.88	158.6	55.8	-138.8	4.550
10	5.17	4.3	-100.7	130.9	5.183
11	5.26	1.3	-99.9	-122.7	4.963
12	5.35	86.8	-97.2	-113.0	4.702
13	6.60	160.5	-92.0	141.8	4.673

^a In kcal/mol.

^b H---O is the distance in Å from H of hydroperoxide to O of furyl group.

Table S5. B3LYP/6-31G** geometry-optimization and free energy calculation of the conformers in Table S4 using Gaussian 03.

Conformer ^a	E^b	α	β	γ	H---O	G^c	ΔE (kcal/mol)	ΔG (kcal/mol)
1→ a	-653.162057926	146.6	59.9	86.7	3.454	-652.964966	0.000000	0.000000
2→ b	-653.161513412	17.3	60.3	82.4	3.462	-652.963996	0.341688	0.608684
4→ c	-653.160437135	-45.8	-171.8	-88.3	3.236	-652.963993	1.017062	0.610567
5→ d	-653.161366687	95.3	-171.6	-80.7	3.482	-652.963779	0.433759	0.744854
9→ e	-653.158810935	157.2	65.2	-115.4	4.524	-652.962549	2.037518	1.516691
6→ f	-653.158621308	44.8	62.4	-117.2	4.806	-652.962092	2.156511	1.803462
7→ g	-653.158571129	84.6	-173.6	118.4	4.689	-652.961555	2.187998	2.140435
8→ h	-653.157695085	-55.0	-176.5	123.4	4.355	-652.961381	2.737724	2.249622
3→ i	-653.159126436	176.9	-163.4	-76.1	2.180	-652.961290	1.839538	2.306725
12→ j	-653.154797506	156.4	-80.4	-114.0	4.064	-652.957574	4.555983	4.638551
13→ k	-653.153175681	154.7	-80.7	129.5	4.785	-652.956511	5.573694	5.305593
11→ l	-653.153670987	-47.6	-77.2	-117.4	4.704	-652.956458	5.262884	5.338851
10→ m	-653.152033482	19.7	-84.6	124.9	5.223	-652.955691	6.290434	5.820151

^a $n \rightarrow \alpha$ means that MMFF94 conformer n becomes conformer α after B3LYP/6-31G** reoptimization.

^b B3LYP/6-31G** electronic energy in Hartree per particle.

^c Sum of electronic and thermal Gibbs energies in Hartree per particle ($T=298.15K$).

Table S6. TDDFT/B3LYP optical rotations at 589.3nm computed adopting the polarizability consistent Sadlej basis set of GIAO using Gaussian 03. Molecular geometries have been optimized at B3LYP/6-31G**, see Table S5.^a

Conformer	ΔE (kcal/mol)	ΔG (kcal/mol)	%P(ΔE) ^b	%P(ΔG) ^c	$[\alpha]_{D,i}$	$[\alpha]_{D,i} \times$ %P(ΔE)/100	$[\alpha]_{D,i} \times$ %P(ΔG)/100
a	0.00	0.00	42.36	45.57	135.31	57.32	61.66
b	0.34	0.61	23.79	16.31	36.09	8.59	5.89
c	1.02	0.61	7.61	16.26	-80.01	-6.09	-13.01
d	0.43	0.74	20.37	12.96	44.72	9.11	5.80
e	2.04	1.52	1.36	3.52	-12.16	-0.17	-0.43
f	2.16	1.80	1.11	2.17	-97.14	-1.08	-2.11
g	2.19	2.14	1.05	1.23	195.55	2.06	2.40
h	2.74	2.25	0.42	1.02	55.04	0.23	0.56
i	1.84	2.31	1.90	0.93	-43.59	-0.83	-0.40
j	4.56	4.64	0.02	0.02	TOT ^d →	69.14	60.36
k	5.57	5.31	0.00	0.01			
l	5.26	5.34	0.01	0.01			
m	6.29	5.82	0.00	0.00			

^a Optical rotations have been calculated for those conformations having ΔG less than or close to 2 kcal/mol only, as higher free energy conformations have negligible populations and can be neglected.

^b Percentage populations obtained from ΔE values using Boltzmann statistics at T=298.15K.

^c Percentage populations obtained from ΔG values using Boltzmann statistics at T=298.15K.

^d Predicted optical rotations from energy and free energy based populations.

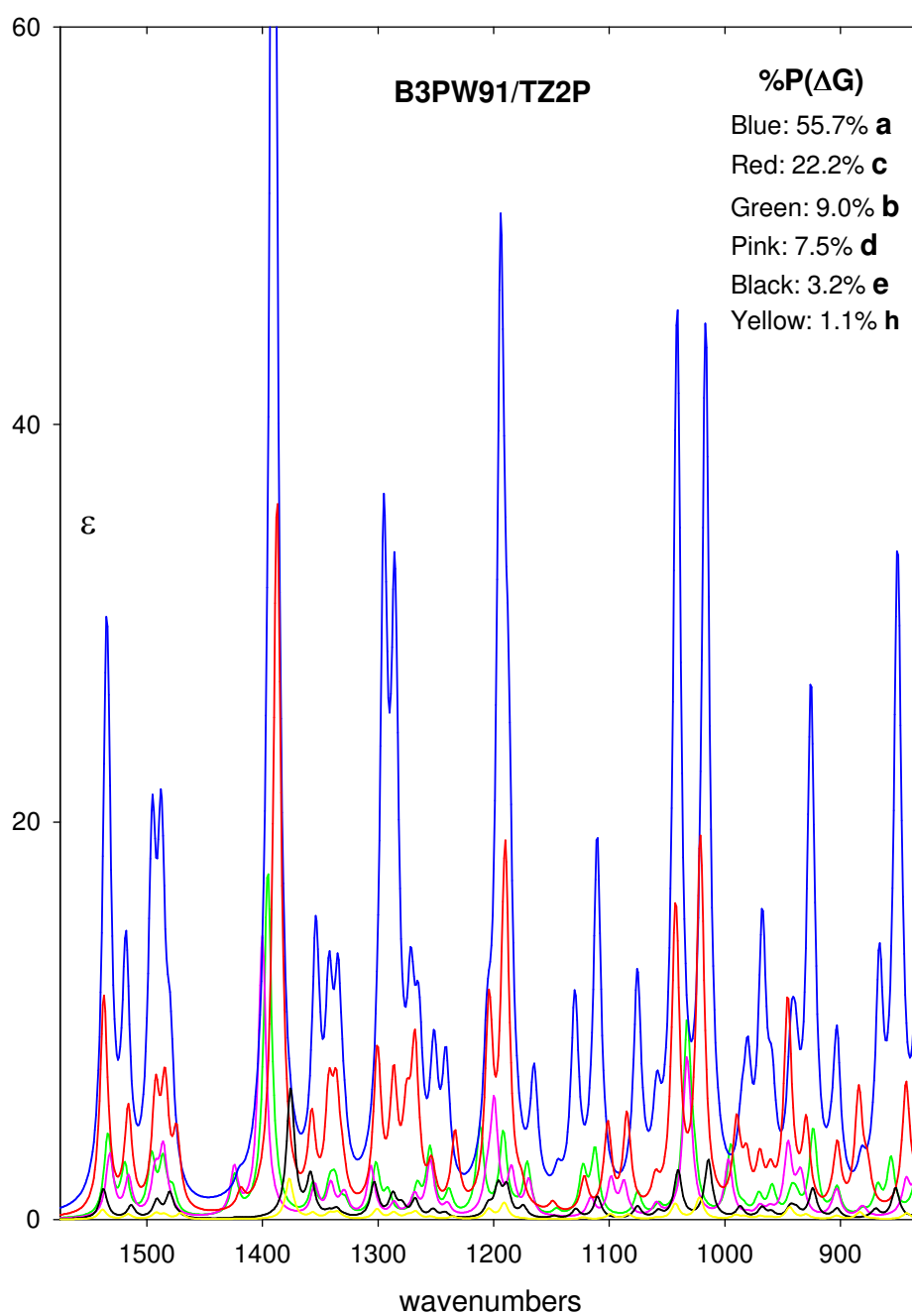


Figure S7. Calculated IR spectra of the six most populated B3PW91/TZ2P conformers of *endo-3*.

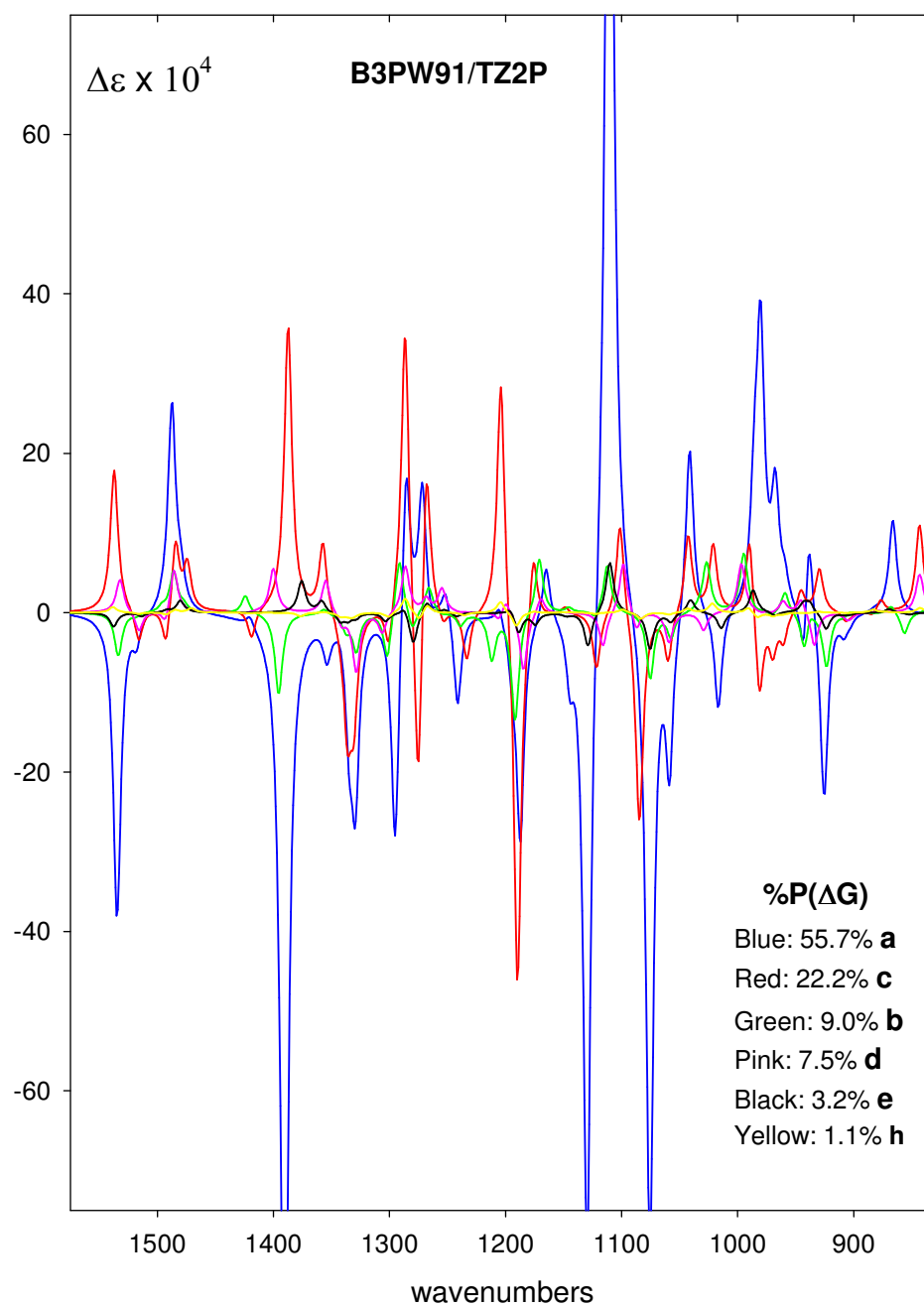


Figure S8. Calculated VCD spectra of the six most populated B3PW91/TZ2P conformers of *endo-3*.

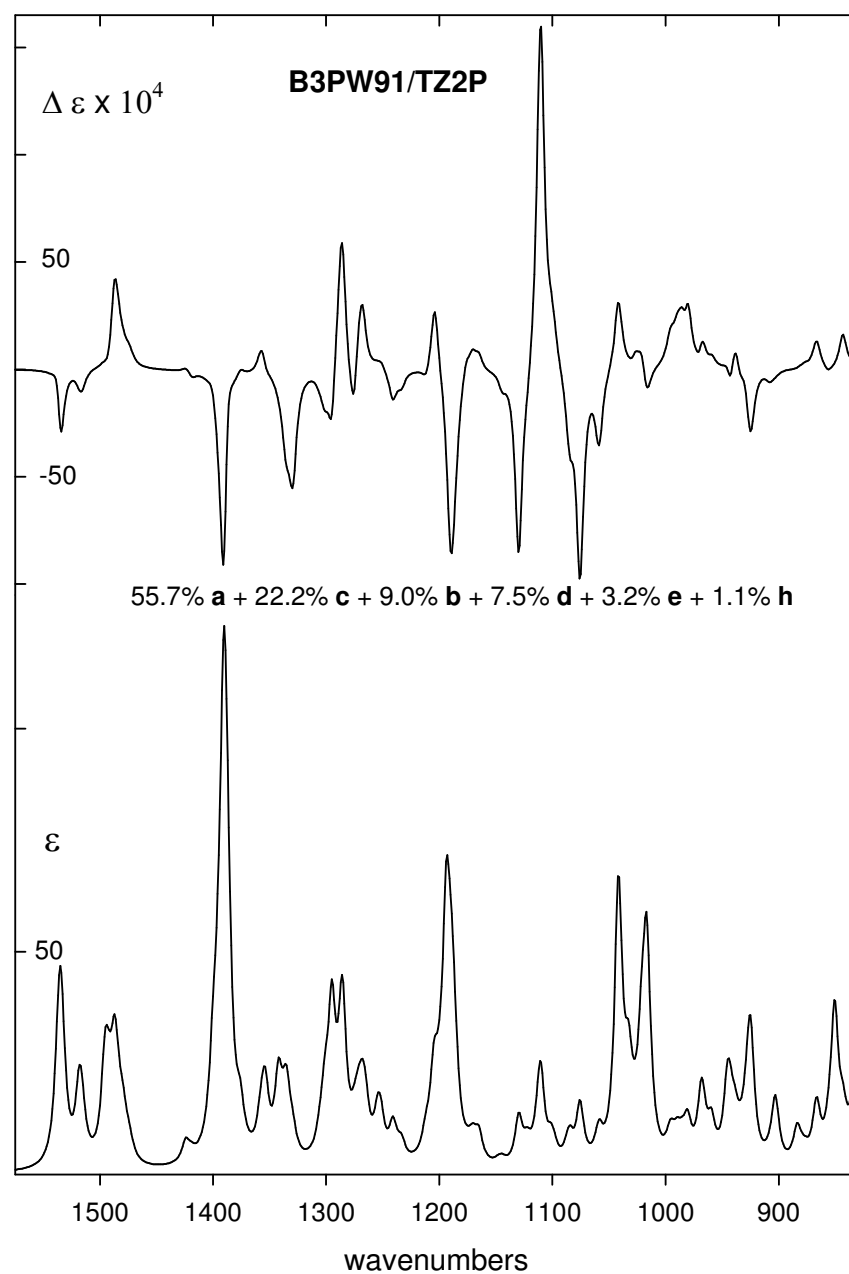


Figure S9. B3PW91/TZ2P conformationally-averaged IR and VCD spectra of *endo*-**3**.

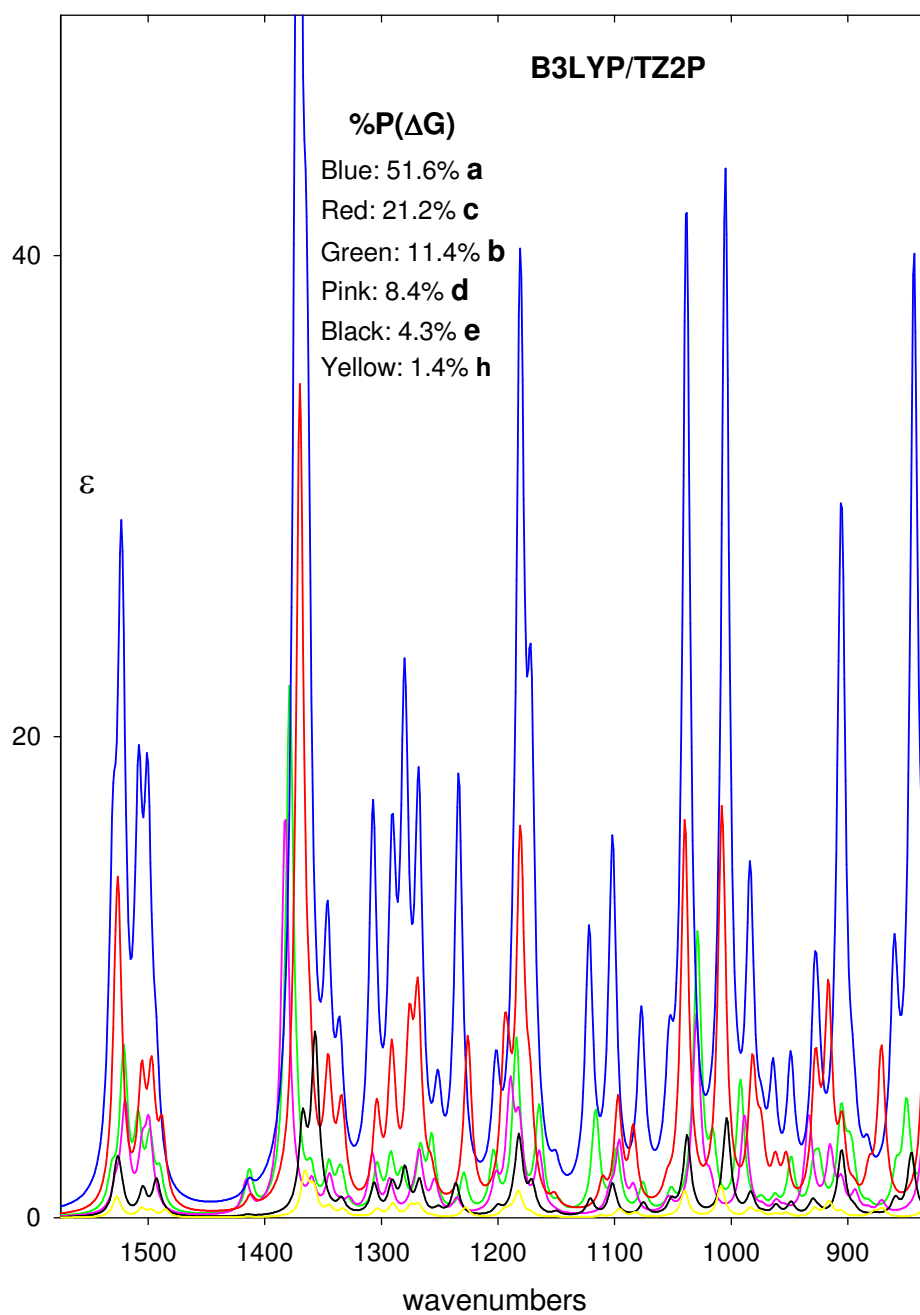


Figure S10. Calculated IR spectra of the six most populated B3LYP/TZ2P conformers of *endo*-**3**.

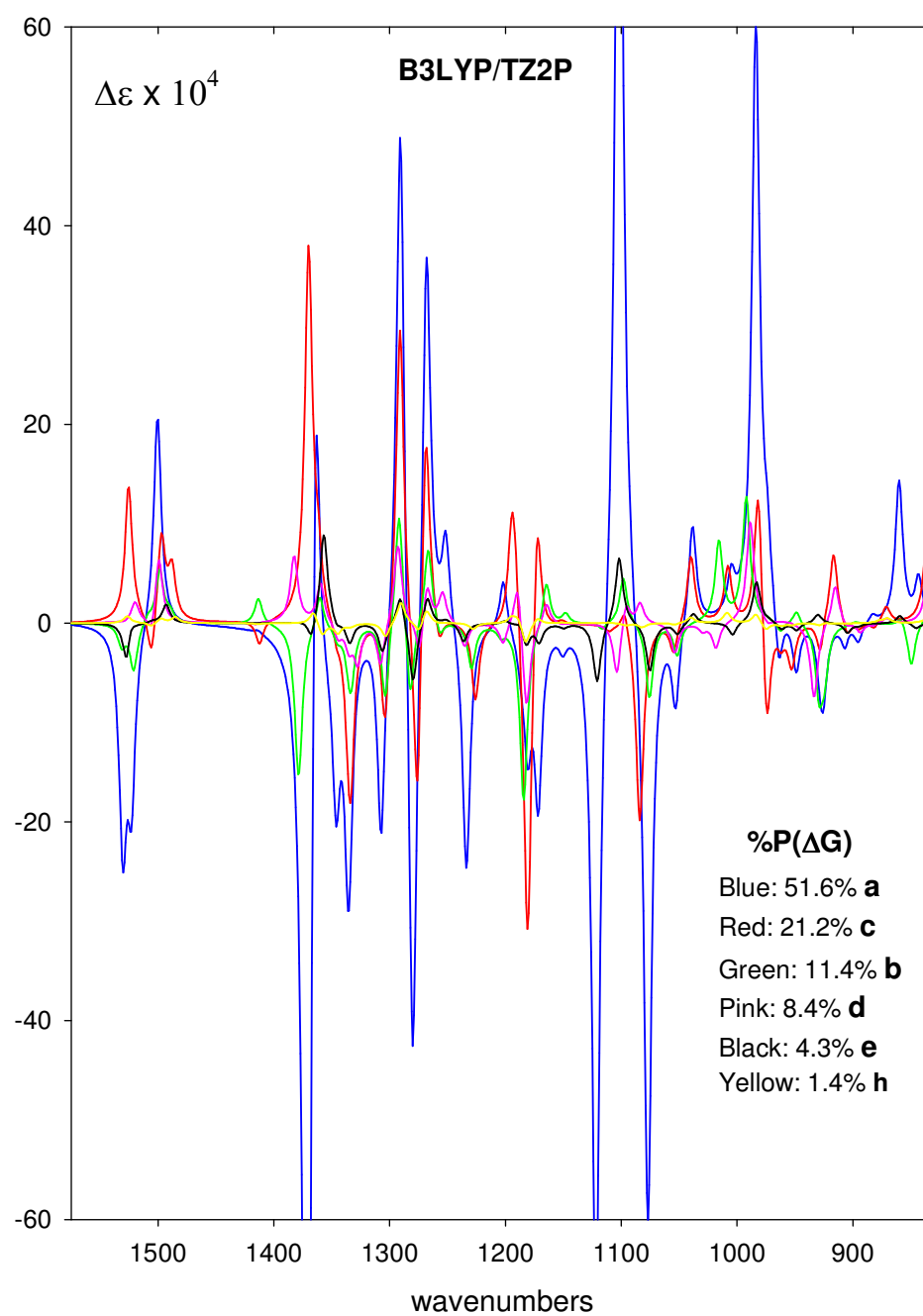


Figure S11. Calculated VCD spectra of the six most populated B3LYP/TZ2P conformers of *endo*-**3**.

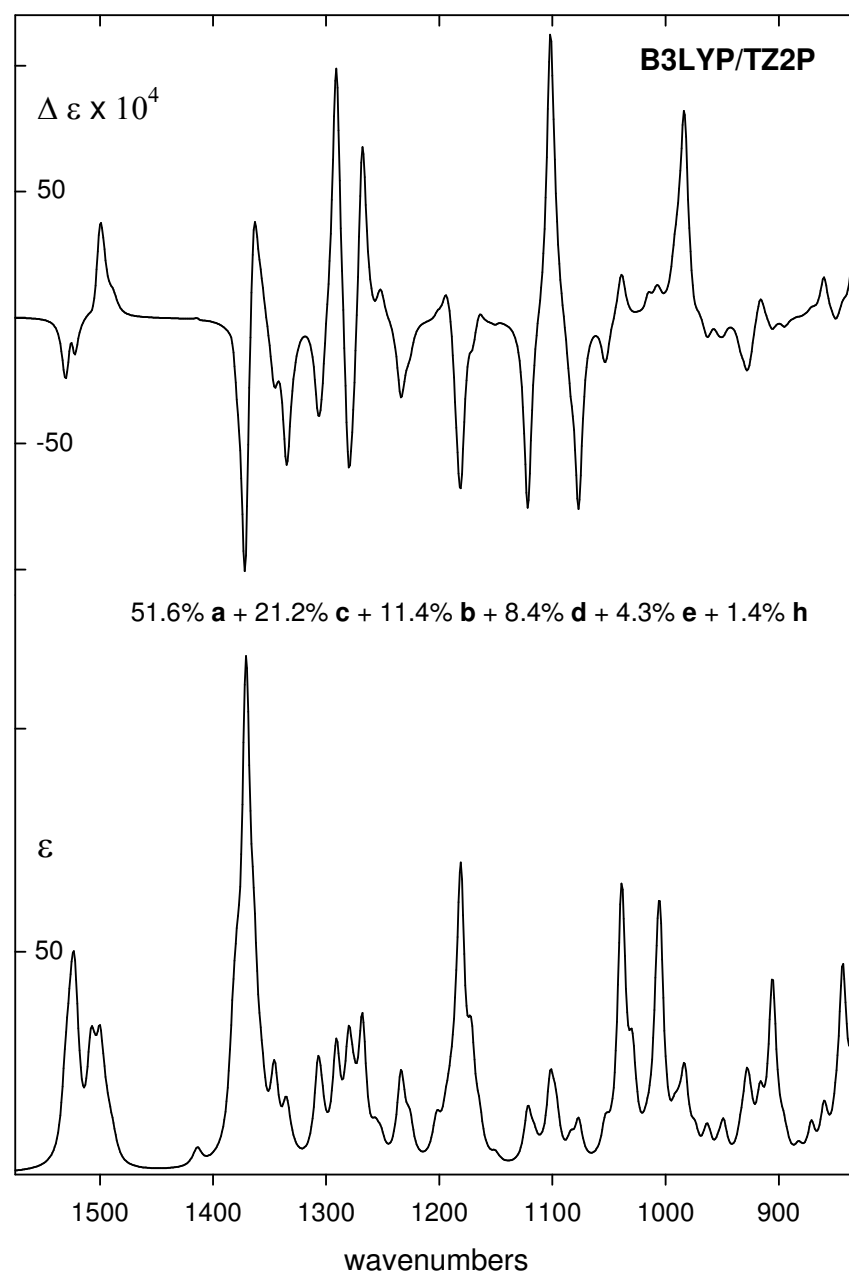


Figure S12. B3LYP/TZ2P conformationally-averaged IR and VCD spectra of *endo-3*.

Cartesian coordinates (in Å) for conformers **a-h** of *endo-3*.

Conformer	B3PW91/TZ2P	B3LYP/TZ2P
a	C -2.015882 -1.386805 -0.365840	C -2.025281 -1.387989 -0.383903
	C -2.440496 0.756912 0.668803	C -2.448489 0.753854 0.678666
	C -0.175261 0.190471 -0.252547	C -0.170673 0.186701 -0.246286
	C -1.075816 0.136569 1.003365	C -1.080881 0.122595 1.010182
	C -0.833668 -0.862298 -1.192245	C -0.830852 -0.861488 -1.202380
	C -3.085783 -0.287011 -0.282268	C -3.095010 -0.279856 -0.293758
	H -2.348127 1.741658 0.218447	H -2.353777 1.743098 0.242657
	H -0.126802 -1.654144 -1.432408	H -0.126638 -1.654104 -1.441492
	H -4.015235 -0.680683 0.132661	H -4.027764 -0.673893 0.109914
	H -2.390997 -2.348431 -0.714473	H -2.403429 -2.342993 -0.743306
	H -3.020937 0.865277 1.586093	H -3.031268 0.848566 1.594535
	H -0.611408 0.556176 1.892027	H -0.618853 0.529773 1.904014
	H -1.138923 -0.392194 -2.127616	H -1.127750 -0.385233 -2.135665
	H -3.316648 0.130233 -1.263035	H -3.316263 0.150920 -1.269436
	C -1.422226 -1.360144 1.049756	C -1.437010 -1.378857 1.040503
	H -2.146489 -1.596614 1.831226	H -2.166047 -1.618417 1.814804
	H -0.551362 -2.007281 1.166441	H -0.572518 -2.032150 1.156225
	C 1.258821 -0.098788 0.060978	C 1.266434 -0.100495 0.065053
	C 2.035723 0.087540 1.162096	C 2.042061 0.058320 1.171566
	H 1.706837 0.461602 2.116503	H 1.712140 0.407602 2.133264
	C 3.359337 -0.311968 0.807969	C 3.371169 -0.328633 0.809858
	H 4.236298 -0.306967 1.433315	H 4.244194 -0.336250 1.438344
	C 3.293630 -0.708073 -0.484845	C 3.313282 -0.691683 -0.493612
	H 4.021074 -1.090525 -1.179601	H 4.043105 -1.052776 -1.194729
	O 2.029987 -0.584985 -0.955382	O 2.044855 -0.560222 -0.966823
	O -0.259315 1.429745 -0.981487	O -0.260933 1.437365 -0.972084
	O 0.132290 2.511488 -0.119731	O 0.122322 2.529412 -0.093064
	H 1.088758 2.533478 -0.258105	H 1.066409 2.608602 -0.288697
b	C 2.061462 -1.130263 0.819175	C 2.061077 -1.145567 0.818220
	C 2.370940 0.475772 -0.962298	C 2.380634 0.474570 -0.962087
	C 0.178766 0.292649 0.233168	C 0.174196 0.291176 0.235523
	C 1.008399 -0.233847 -0.963436	C 1.009197 -0.231881 -0.966918
	C 0.900604 -0.357479 1.456781	C 0.897331 -0.370460 1.462207
	C 3.089423 -0.124355 0.276492	C 3.098253 -0.137397 0.280163
	H 2.276083 1.557322 -0.916161	H 2.292394 1.554892 -0.910587
	H 0.218202 -1.024799 1.982624	H 0.213874 -1.038702 1.982528
	H 4.013913 -0.630168 -0.006639	H 4.019503 -0.645604 -0.004384
	H 2.483473 -1.889971 1.476404	H 2.479177 -1.909551 1.470864
	H 2.902205 0.228981 -1.882588	H 2.910882 0.228251 -1.881620
	H 0.479909 -0.181902 -1.911179	H 0.482707 -0.173585 -1.913595
	H 1.222726 0.415271 2.156384	H 1.221440 0.396100 2.165514
	H 3.346282 0.634042 1.016987	H 3.356454 0.616087 1.023313
	C 1.399959 -1.637090 -0.469346	C 1.397693 -1.644987 -0.479302
	H 2.094101 -2.135286 -1.148517	H 2.091049 -2.140190 -1.159411
	H 0.548857 -2.294296 -0.290263	H 0.545840 -2.300597 -0.306904
	C -1.285633 -0.032672 0.157331	C -1.294293 -0.027306 0.156615
	C -2.351837 0.460960 0.844618	C -2.362686 0.464165 0.842439
	H -2.311953 1.207371 1.620674	H -2.325941 1.210374 1.616807

	C -3.506021 -0.218068 0.348947 H -4.528871 -0.085569 0.659569 C -3.058384 -1.072798 -0.599602 H -3.540993 -1.786109 -1.244309 O -1.710720 -0.968373 -0.732120 O 0.289609 1.701596 0.458814 O -0.191557 2.400596 -0.702807 H -1.148662 2.377708 -0.555064	C -3.519518 -0.217044 0.345723 H -4.540557 -0.083388 0.657107 C -3.074194 -1.073367 -0.603294 H -3.555991 -1.785796 -1.246830 O -1.720191 -0.968764 -0.736211 O 0.295947 1.705469 0.473485 O -0.160962 2.427127 -0.703260 H -1.115324 2.469641 -0.540645
c	C 2.096109 -0.810412 1.007346 C 2.369500 0.042554 -1.238527 C 0.187623 0.312663 0.011167 C 1.000406 -0.596733 -0.950337 C 0.963269 0.170721 1.349159 C 3.119371 -0.091397 0.113883 H 2.289594 1.071103 -1.579736 H 0.327869 -0.229763 2.137547 H 4.027818 -0.686315 0.006118 H 2.531909 -1.291333 1.882416 H 2.868920 -0.528812 -2.022624 H 0.440560 -0.872621 -1.840522 H 1.320809 1.145173 1.677277 H 3.408886 0.875546 0.526783 C 1.392751 -1.734931 0.003255 H 2.060605 -2.457633 -0.468730 H 0.537484 -2.263928 0.426248 C -1.244024 -0.115230 0.100397 C -2.093274 -0.413726 1.119550 H -1.856504 -0.416979 2.169369 C -3.358587 -0.713834 0.531321 H -4.266614 -0.996192 1.037148 C -3.189900 -0.573368 -0.804182 H -3.844854 -0.692656 -1.649795 O -1.915972 -0.210448 -1.085732 O 0.252960 1.639200 -0.536322 O -0.342782 2.560163 0.391263 H -1.259596 2.575251 0.086640	C 2.109705 -0.808450 1.010594 C 2.376851 0.044896 -1.246480 C 0.184548 0.307696 0.014146 C 1.005044 -0.601609 -0.952591 C 0.968013 0.170940 1.355785 C 3.132746 -0.083797 0.110992 H 2.293354 1.071333 -1.588313 H 0.338591 -0.231200 2.146174 H 4.042090 -0.674947 0.002805 H 2.548877 -1.285751 1.884345 H 2.876479 -0.526458 -2.028698 H 0.445497 -0.880716 -1.840088 H 1.322549 1.146116 1.680375 H 3.417944 0.884497 0.520344 C 1.407839 -1.741764 0.004452 H 2.079288 -2.458872 -0.468036 H 0.559191 -2.277624 0.428201 C -1.249573 -0.120414 0.103523 C -2.100686 -0.421076 1.120910 H -1.865191 -0.427638 2.169433 C -3.369820 -0.719236 0.531269 H -4.275710 -1.001311 1.038205 C -3.204747 -0.576350 -0.804984 H -3.859625 -0.693067 -1.648907 O -1.924806 -0.212571 -1.088281 O 0.250504 1.641224 -0.537665 O -0.354137 2.573807 0.396962 H -1.255346 2.630938 0.050336
d	C -2.023023 -1.033456 -0.817822 C -2.446733 0.323812 1.137229 C -0.193229 0.344895 -0.011599 C -1.055058 -0.332145 1.091760 C -0.884498 -0.131918 -1.318223 C -3.111160 -0.154116 -0.181303 H -2.396749 1.406288 1.219510 H -0.190556 -0.687764 -1.945862 H -4.013402 -0.734675 0.018642 H -2.395806 -1.721624 -1.575588 H -2.986138 -0.050687 2.008688 H -0.545695 -0.372278 2.052578 H -1.231777 0.730429 -1.884872 H -3.393697 0.675543 -0.830140 C -1.374019 -1.674958 0.417935	C -2.023740 -1.036467 -0.827836 C -2.455996 0.306912 1.146814 C -0.189538 0.346377 -0.008143 C -1.055242 -0.343963 1.094504 C -0.885207 -0.121898 -1.323553 C -3.121085 -0.165167 -0.181649 H -2.412435 1.387503 1.237285 H -0.191576 -0.667624 -1.957642 H -4.018876 -0.751862 0.013546 H -2.392700 -1.719229 -1.590472 H -2.992604 -0.078459 2.013678 H -0.547067 -0.389894 2.054016 H -1.238728 0.743203 -1.879249 H -3.407150 0.668292 -0.821876 C -1.370185 -1.688283 0.407543

	H -2.064276 -2.278170 1.010179 H -0.491356 -2.271673 0.185001 C 1.258360 -0.026239 0.107919 C 2.239043 0.454038 0.921638 H 2.119205 1.221965 1.667886 C 3.426627 -0.270249 0.602515 H 4.402475 -0.157881 1.044594 C 3.083349 -1.138114 -0.377310 H 3.624976 -1.882979 -0.933347 O 1.769895 -0.998939 -0.692942 O -0.288248 1.755022 0.207881 O 0.362262 2.442497 -0.872214 H 1.293572 2.365567 -0.615508	H -2.057751 -2.297950 0.993935 H -0.486913 -2.279926 0.170799 C 1.266107 -0.021728 0.108599 C 2.248414 0.446637 0.927620 H 2.131910 1.207031 1.679946 C 3.438058 -0.278822 0.603000 H 4.411441 -0.171202 1.048377 C 3.097368 -1.138153 -0.385997 H 3.637876 -1.877547 -0.947224 O 1.778631 -0.993396 -0.703889 O -0.294387 1.761745 0.224708 O 0.340841 2.473713 -0.869173 H 1.270174 2.458497 -0.593687
e	C -1.974570 -1.370202 -0.505578 C -2.453922 0.653145 0.721784 C -0.166141 0.232748 -0.232451 C -1.072889 0.038120 1.005683 C -0.812223 -0.729987 -1.276719 C -3.078759 -0.320035 -0.314871 H -2.396509 1.671243 0.339589 H -0.087385 -1.472131 -1.605741 H -3.988837 -0.779141 0.074734 H -2.322054 -2.304198 -0.945686 H -3.038287 0.681421 1.642284 H -0.623078 0.380907 1.934722 H -1.137474 -0.170667 -2.154592 H -3.336900 0.176445 -1.250654 C -1.386250 -1.463548 0.909137 H -2.108985 -1.790297 1.659064 H -0.499619 -2.095318 0.970582 C 1.264052 -0.088678 0.056972 C 1.996284 -0.200691 1.195474 H 1.636091 -0.078607 2.202311 C 3.333736 -0.497335 0.796951 H 4.189183 -0.651801 1.432905 C 3.316821 -0.541641 -0.555849 H 4.072227 -0.723869 -1.300193 O 2.068735 -0.300559 -1.022492 O -0.266710 1.532692 -0.836496 O 0.249731 2.515238 0.082165 H -0.569255 2.905663 0.412058	C -1.990400 -1.372026 -0.505467 C -2.461895 0.663015 0.725528 C -0.163808 0.224547 -0.229401 C -1.079017 0.037868 1.011433 C -0.814397 -0.743223 -1.277249 C -3.091159 -0.308299 -0.320301 H -2.398645 1.681110 0.349583 H -0.094486 -1.492375 -1.596417 H -4.006449 -0.759479 0.062701 H -2.343985 -2.302938 -0.944094 H -3.047134 0.688157 1.644091 H -0.629855 0.378848 1.939466 H -1.130194 -0.187790 -2.159254 H -3.337840 0.191110 -1.256147 C -1.405708 -1.467803 0.916992 H -2.133080 -1.785915 1.664306 H -0.527324 -2.107950 0.983688 C 1.269748 -0.093314 0.061069 C 2.006677 -0.196398 1.197994 H 1.649822 -0.067997 2.203697 C 3.347595 -0.493125 0.798318 H 4.202200 -0.640449 1.434812 C 3.331478 -0.547384 -0.554716 H 4.085315 -0.732497 -1.297567 O 2.076596 -0.311604 -1.023602 O -0.261525 1.527639 -0.845737 O 0.257064 2.525932 0.081592 H -0.560116 2.979284 0.327912
f	C 1.996422 -1.203337 0.785224 C 2.387981 0.467330 -0.914234 C 0.157757 0.297827 0.230433 C 1.001708 -0.198192 -0.973568 C 0.840272 -0.433019 1.433473 C 3.062528 -0.202366 0.314261 H 2.350704 1.551193 -0.815319 H 0.128467 -1.108713 1.906811 H 3.981158 -0.716804 0.028245 H 2.385260 -2.004285 1.413102	C 1.999421 -1.226360 0.760341 C 2.400539 0.486854 -0.908401 C 0.154368 0.293062 0.233162 C 1.007218 -0.176526 -0.984323 C 0.836408 -0.469522 1.426141 C 3.072364 -0.211920 0.313929 H 2.364985 1.566958 -0.790827 H 0.124499 -1.156427 1.879698 H 3.990601 -0.720601 0.021264 H 2.385772 -2.040607 1.370172

	H 2.932013 0.245708 -1.833380 H 0.492048 -0.093695 -1.928418 H 1.161648 0.293416 2.181196 H 3.319138 0.518119 1.091561 C 1.356294 -1.631514 -0.541672 H 2.058624 -2.107331 -1.228832 H 0.489188 -2.277627 -0.417166 C -1.310472 0.013626 0.120283 C -2.397061 0.650581 0.624334 H -2.383771 1.566151 1.189335 C -3.534881 -0.115526 0.228907 H -4.570057 0.092235 0.442736 C -3.057292 -1.161818 -0.483194 H -3.519044 -1.995212 -0.982722 O -1.701064 -1.098669 -0.560821 O 0.317349 1.686948 0.524318 O -0.178073 2.463823 -0.585866 H 0.649387 2.718478 -1.013669	H 2.945629 0.279665 -1.828794 H 0.500532 -0.048672 -1.936194 H 1.155312 0.237880 2.190842 H 3.325166 0.491644 1.106127 C 1.362025 -1.625785 -0.583774 H 2.067584 -2.083142 -1.278114 H 0.497092 -2.275389 -0.479126 C -1.317464 0.016367 0.112778 C -2.411920 0.702119 0.529235 H -2.405841 1.662659 1.010439 C -3.550401 -0.089496 0.173288 H -4.586499 0.145978 0.342379 C -3.068597 -1.199787 -0.431433 H -3.525616 -2.069183 -0.866227 O -1.703608 -1.155170 -0.479549 O 0.315215 1.680302 0.564407 O -0.163723 2.496930 -0.547310 H 0.673948 2.838706 -0.887677
g	C -1.984018 -1.047188 -0.834071 C -2.425804 0.237796 1.165909 C -0.178251 0.357781 -0.004608 C -1.016165 -0.374967 1.086356 C -0.871312 -0.105942 -1.317664 C -3.087607 -0.212441 -0.163929 H -2.409505 1.317213 1.291717 H -0.165887 -0.626962 -1.961993 H -3.975706 -0.818722 0.022094 H -2.346937 -1.722916 -1.607724 H -2.946804 -0.185460 2.026205 H -0.494833 -0.428515 2.039678 H -1.253100 0.751485 -1.871876 H -3.395580 0.629866 -0.785383 C -1.308766 -1.705863 0.378139 H -1.981029 -2.339965 0.958729 H -0.415045 -2.273984 0.121649 C 1.279277 0.010918 0.087975 C 2.291093 0.550029 0.815123 H 2.215153 1.411443 1.455716 C 3.454139 -0.225295 0.530852 H 4.447982 -0.082912 0.921398 C 3.065583 -1.181516 -0.344495 H 3.576694 -1.986534 -0.842522 O 1.742973 -1.051473 -0.627294 O -0.320292 1.751682 0.268518 O 0.356471 2.501986 -0.762328 H -0.397635 2.918534 -1.196397	C -1.993898 -1.039897 -0.846860 C -2.433163 0.229061 1.175914 C -0.174878 0.355748 -0.001615 C -1.019427 -0.388668 1.087380 C -0.872767 -0.095613 -1.324487 C -3.098749 -0.204310 -0.165747 H -2.415280 1.305396 1.314452 H -0.170157 -0.614410 -1.971358 H -3.988859 -0.807686 0.012434 H -2.359698 -1.705565 -1.626022 H -2.954477 -0.204593 2.029204 H -0.498867 -0.453691 2.038746 H -1.249632 0.767849 -1.869512 H -3.400334 0.646627 -0.776194 C -1.319487 -1.716771 0.363367 H -1.994582 -2.351913 0.937172 H -0.430481 -2.287012 0.102189 C 1.286624 0.012423 0.086374 C 2.312035 0.576400 0.775204 H 2.249483 1.462750 1.379722 C 3.471933 -0.216232 0.506769 H 4.469608 -0.059457 0.877784 C 3.071235 -1.208242 -0.322739 H 3.572809 -2.033401 -0.793201 O 1.738752 -1.085991 -0.593819 O -0.319085 1.753646 0.285538 O 0.354855 2.523356 -0.756232 H -0.402448 2.983619 -1.140675
h	C 2.077016 -0.853596 0.988494 C 2.365069 0.046389 -1.237628 C 0.181984 0.318412 0.017311 C 0.986596 -0.578648 -0.964723 C 0.957807 0.135522 1.351213	C 2.092828 -0.844842 0.995961 C 2.372060 0.043409 -1.246719 C 0.179580 0.312460 0.018919 C 0.991893 -0.589321 -0.963846 C 0.962951 0.142327 1.357449

C 3.111892 -0.130025 0.112117	C 3.125653 -0.118289 0.108954
H 2.300876 1.082900 -1.558139	H 2.302528 1.075752 -1.574384
H 0.317615 -0.267714 2.133750	H 0.329400 -0.261154 2.143326
H 4.010879 -0.736555 -0.008758	H 4.027098 -0.719448 -0.009011
H 2.504934 -1.360960 1.852491	H 2.525693 -1.343122 1.861134
H 2.857932 -0.513589 -2.033905	H 2.865663 -0.520862 -2.037760
H 0.422175 -0.824115 -1.860624	H 0.427641 -0.844099 -1.855383
H 1.339991 1.092558 1.706078	H 1.337762 1.103690 1.703350
H 3.418987 0.821733 0.548267	H 3.426037 0.838279 0.535946
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H 2.021192 -2.464522 -0.524789	H 2.043293 -2.467909 -0.510819
H 0.498071 -2.269520 0.370933	H 0.523685 -2.282355 0.386099
C -1.249495 -0.107565 0.099460	C -1.255138 -0.111933 0.102289
C -2.083432 -0.469003 1.109897	C -2.092599 -0.468047 1.112374
H -1.838883 -0.527181 2.156238	H -1.850198 -0.521918 2.157896
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H -4.257085 -1.047332 1.017858	H -4.268102 -1.043835 1.021395
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H -3.864332 -0.588337 -1.651425	H -3.877074 -0.599323 -1.650464
O -1.929355 -0.141796 -1.081444	O -1.936911 -0.151146 -1.084739
O 0.261286 1.649052 -0.510552	O 0.256872 1.647587 -0.518979
O -0.450048 2.539032 0.373541	O -0.461914 2.549312 0.374537
H 0.278823 3.078163 0.702407	H 0.259316 3.134377 0.639274