

SUPPLEMENTARY MATERIAL

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TABLE S1

The first six excitation energy (eV) of sesquiterpenes at the CIS/6-31G(d,p) level

Species	E_{t1}	E_{t2}	E_{t3}	E_{t4}	E_{t5}	E_{t6}
Longicyclene	10.51	10.69	11.03	11.14	11.28	11.37
4-Aromadendrene	7.28	8.72	9.42	9.70	9.97	10.13
10-Aromadendrene	7.98	9.35	9.67	9.82	10.03	10.18
α -Patchoulene	7.53	9.09	9.31	9.66	9.90	10.41
β -Patchoulene	7.34	9.27	9.28	9.48	10.15	10.28
α -Cedrene	7.66	9.23	9.49	9.75	10.45	10.49
β -Cedrene	7.99	9.21	9.73	9.88	10.11	10.78
α -Cubebene	7.33	9.28	9.53	9.78	9.91	10.01
β -Cubebene	7.71	9.21	9.59	9.72	9.77	10.14
Longifolene	7.79	8.75	9.55	9.74	9.99	10.62
Alloisolongifolene	7.98	9.27	9.79	9.93	10.15	10.68
α -Panasinanene	7.73	9.16	9.41	9.54	10.11	10.30
β -Panasinsanene	7.88	9.12	9.62	9.88	10.17	10.65
Sativene	7.87	8.77	9.64	9.83	10.08	10.75
Clovene	7.90	9.42	9.61	9.72	10.55	10.66
α -Copaene	7.39	9.03	9.41	9.523	10.34	10.54
Thujepsene	7.44	9.02	9.40	9.52	10.03	10.32
α -cis-Bergamotene	7.40	7.97	9.05	9.40	9.42	9.52
Sesquicarene	7.95	7.99	9.38	9.39	9.70	9.77
β -Selinene	8.09	8.17	9.25	9.44	9.83	9.84
β -Caryophyllene	7.70	7.89	9.17	9.33	9.44	9.53
Isocaryophyllene	7.33	7.76	8.92	9.12	9.29	9.37
Guaiadiene	7.27	8.24	8.65	9.27	9.37	9.51
α -Cadinene	7.64	7.83	9.28	9.28	9.46	9.54
β -Cadinene	7.68	8.04	9.28	9.39	9.50	9.61
α -Humulene	7.22	7.79	7.83	8.52	8.96	9.14
Bisabolene	7.47	7.94	8.08	9.07	9.10	9.26
α -Zingiberene	5.60	7.91	8.41	8.65	8.74	8.87

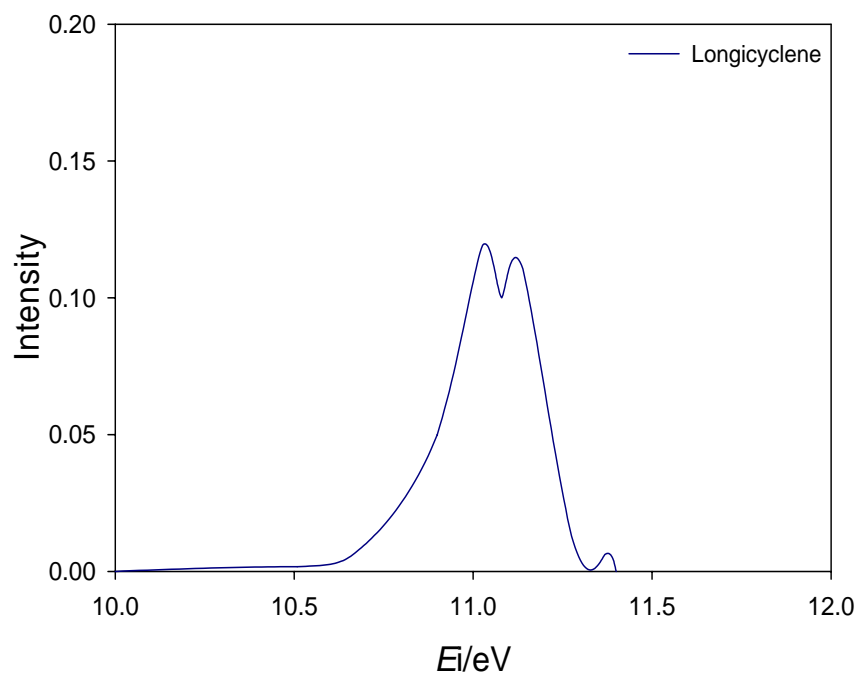


FIGURE S1. Calculated UV-Vis spectrum of longicyclene at the CIS/6-31G (d,p) level.

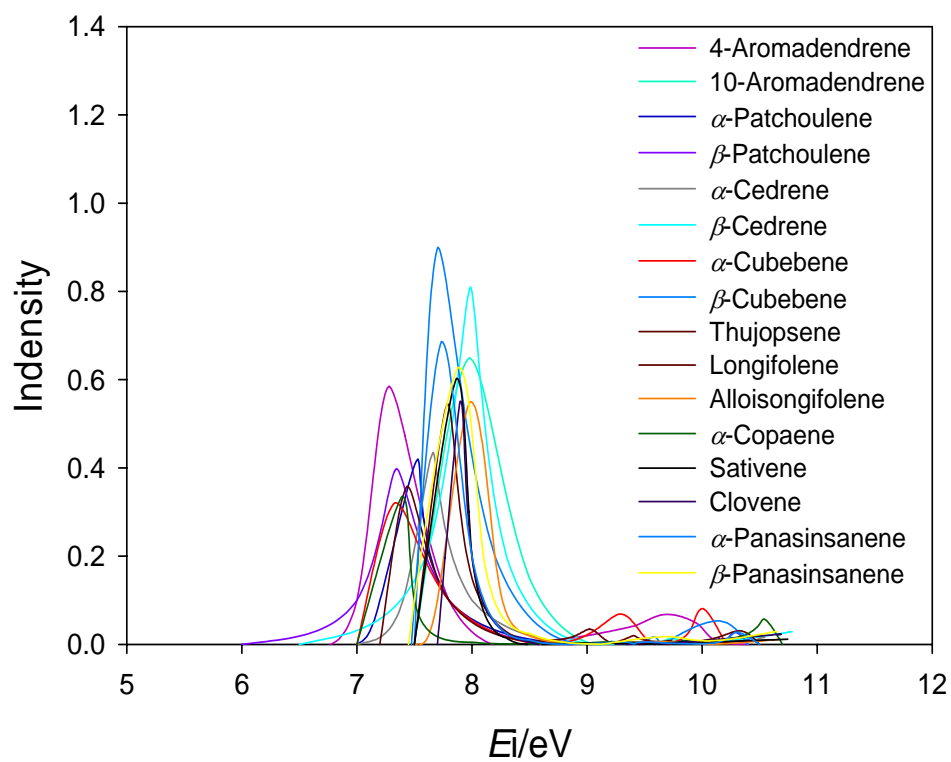


FIGURE S2. Calculated UV-Vis spectra of unsaturated sesquiterpenes with one double bond at the CIS/6-31G (d,p) level.

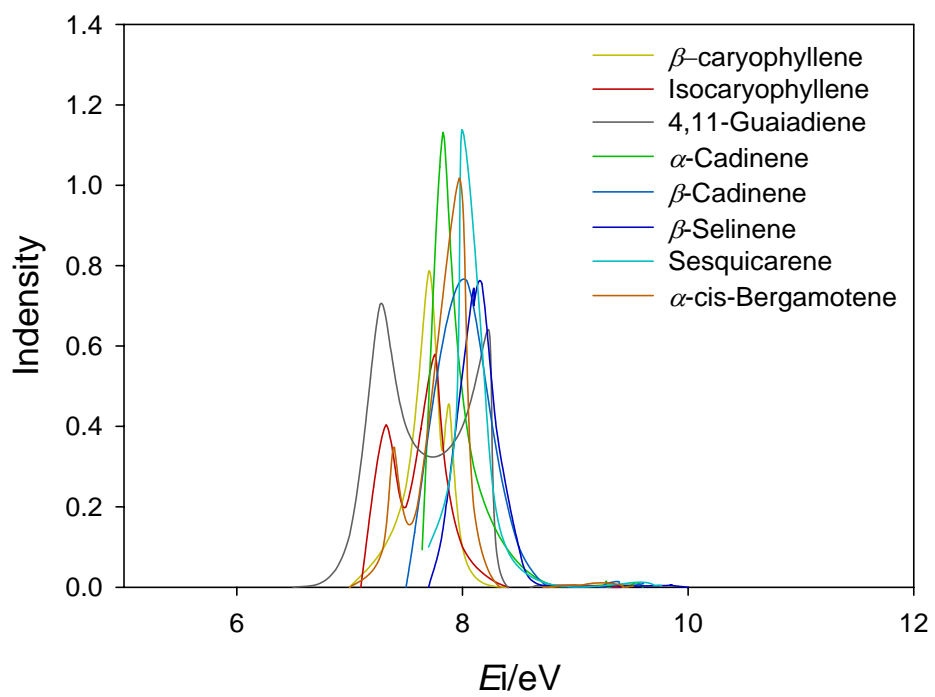


FIGURE S3. Calculated UV-Vis spectra of unsaturated sesquiterpenes with two double bonds at the CIS/6-31G (d,p) level.

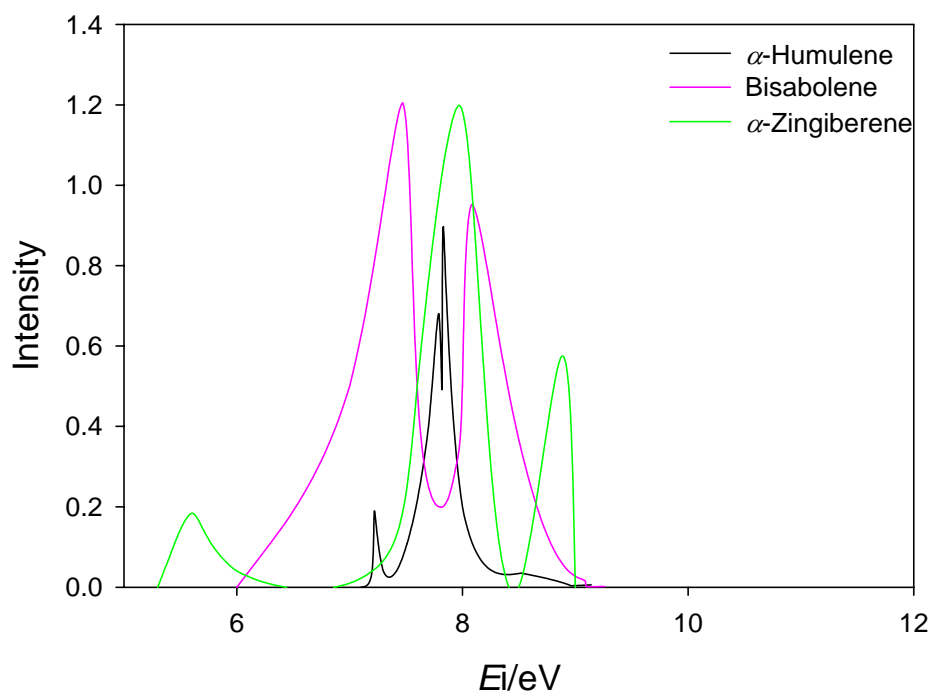


FIGURE S4. Calculated UV-Vis spectra of unsaturated sesquiterpenes with three double bonds at the CIS/6-31G (d,p) level.