Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Materials for

Photoinduced cycloaddition of biomass derivatives to high-performance spiro-fuel

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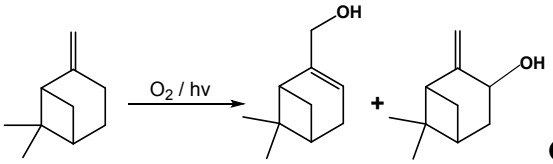
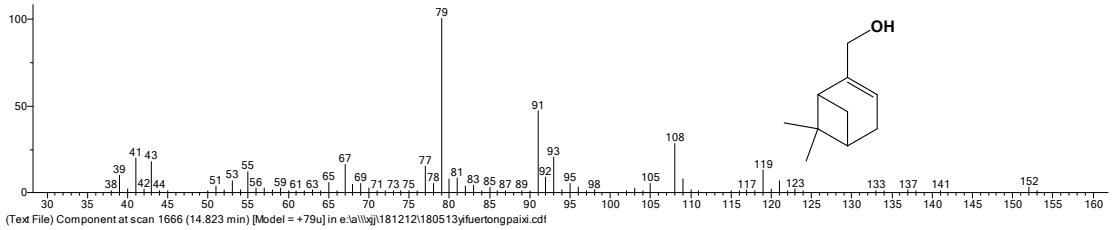
[1]These authors contributed equally (J. Xie and L. Pan)

Scheme S1 Results of the blank test with pure β-pinene.



Conversion: 4.8 %

Figure S1 Mass spectrum of oxidation products of β-pinene.



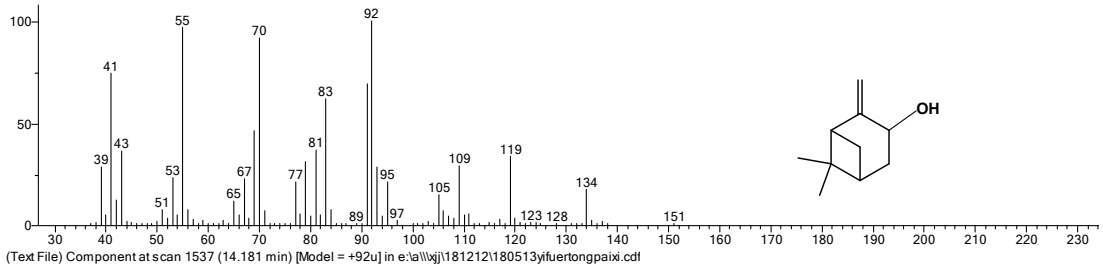


Figure S2 Mass spectrum of isophorone self-adduct.

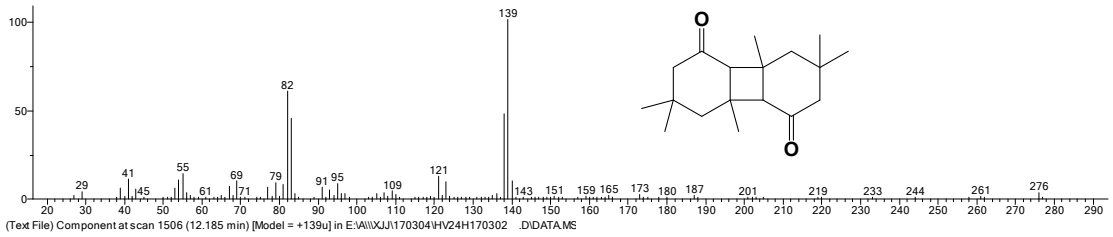
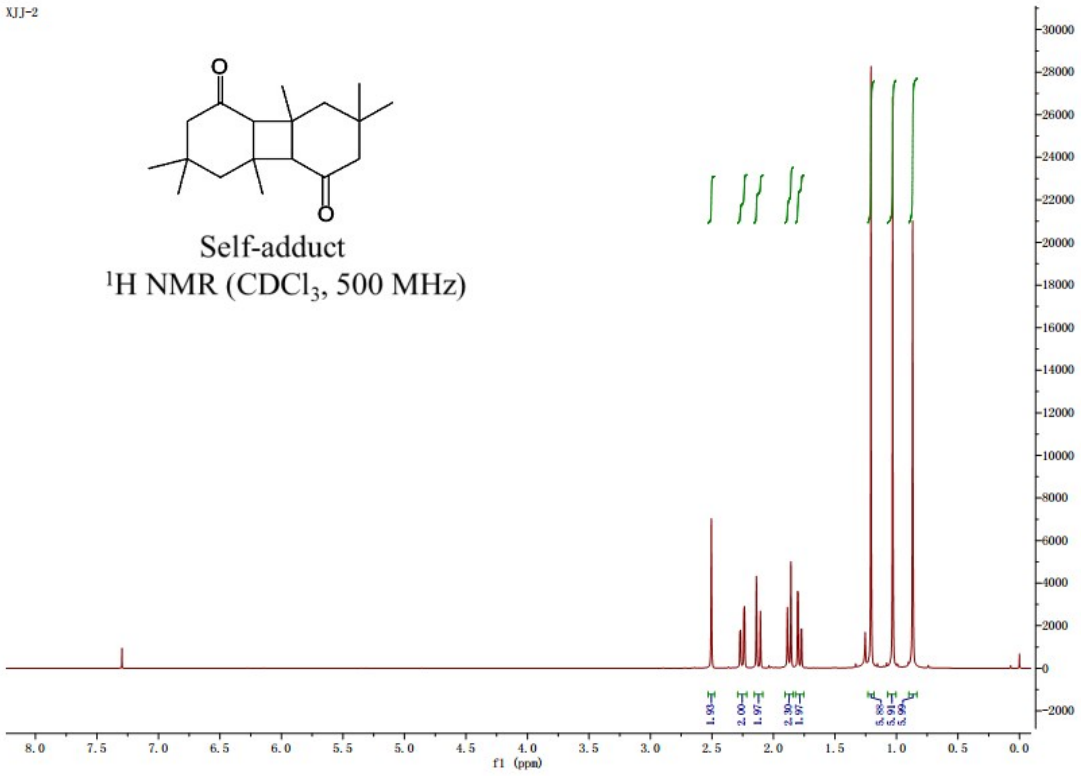


Figure S3 ^{1}H and ^{13}C NMR spectra of isophorone self-adduct (One of the isomers obtained by multiple recrystallization with CH_2Cl_2).



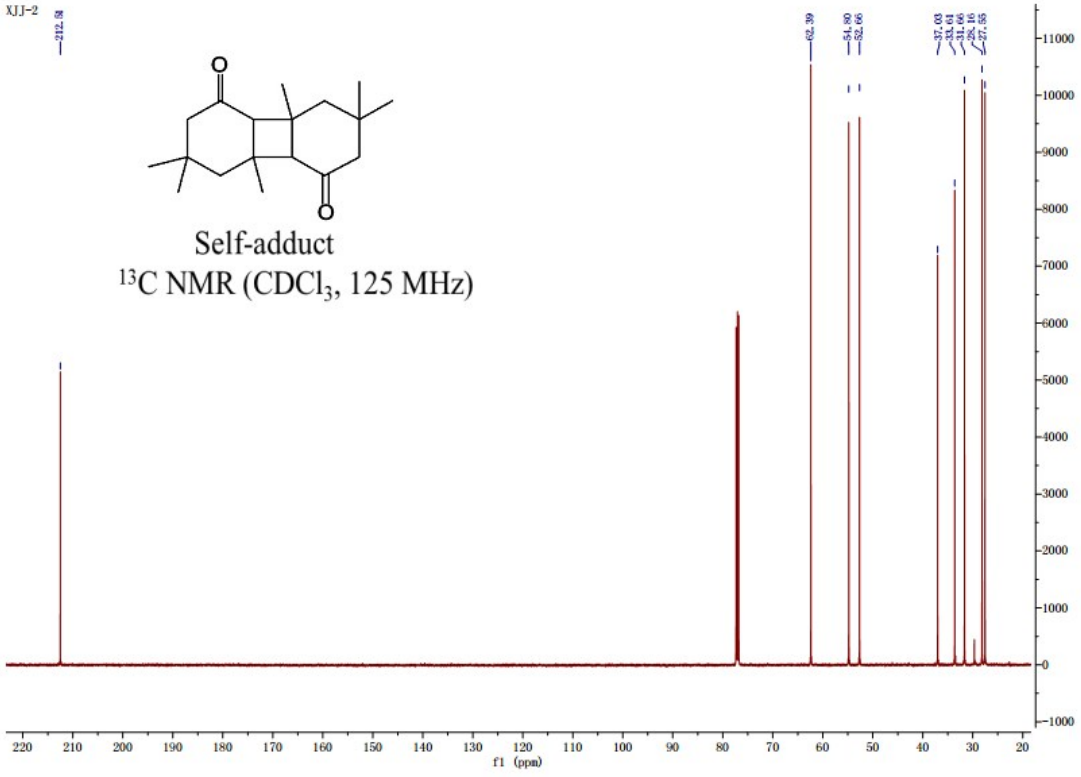


Figure S4 Mass spectrum of isophorone photoisomerized product.

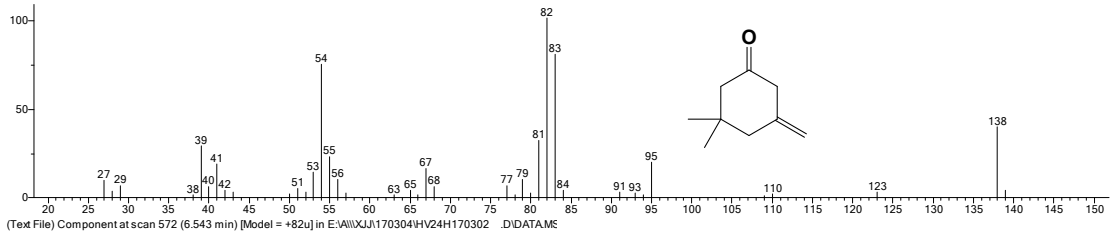


Figure S5 Mass spectrum of isophorone and β-pinene co-adduct.

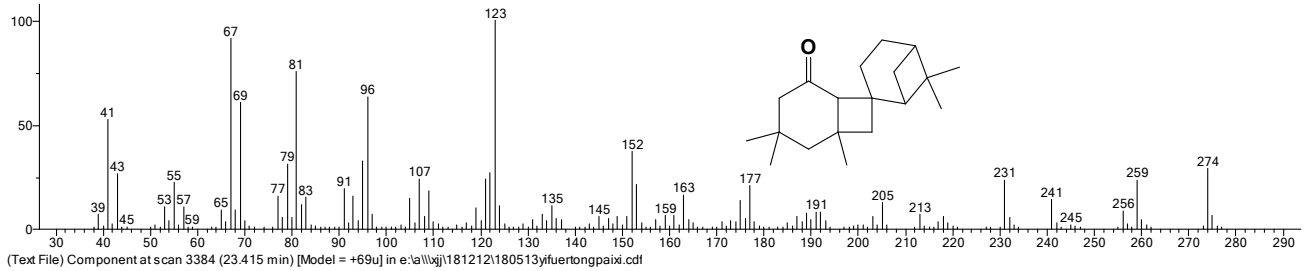
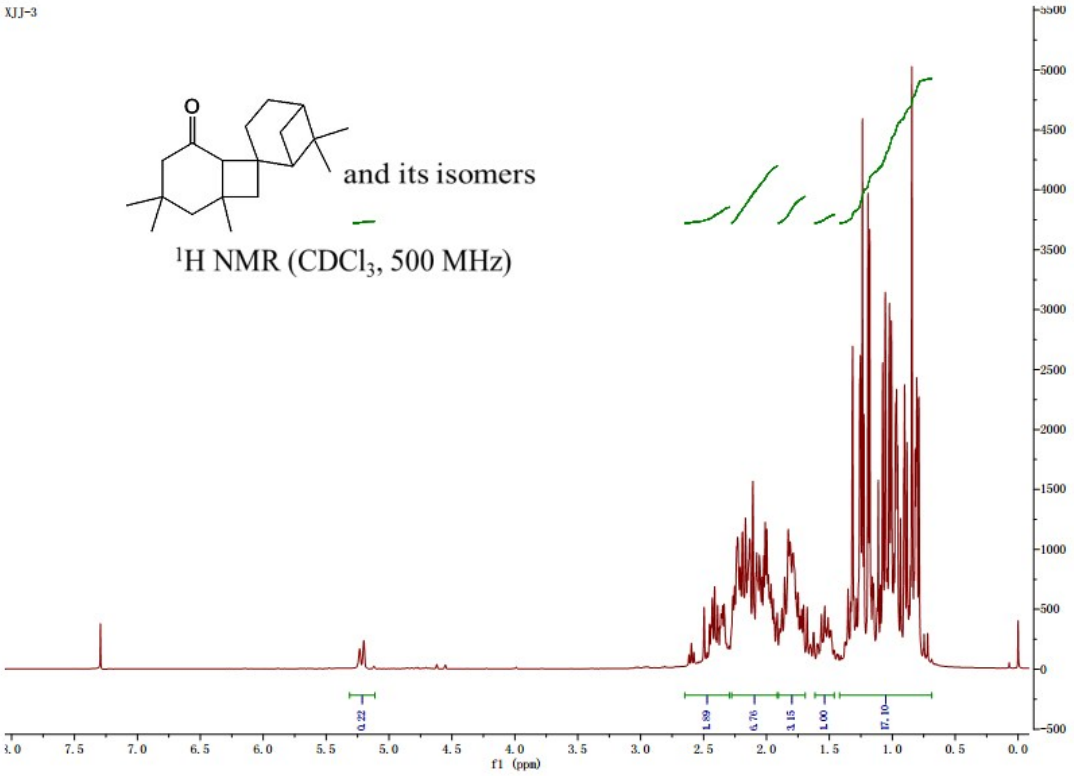


Figure S6 ^{1}H and ^{13}C NMR spectra of isophorone and β-pinene co-adduct.



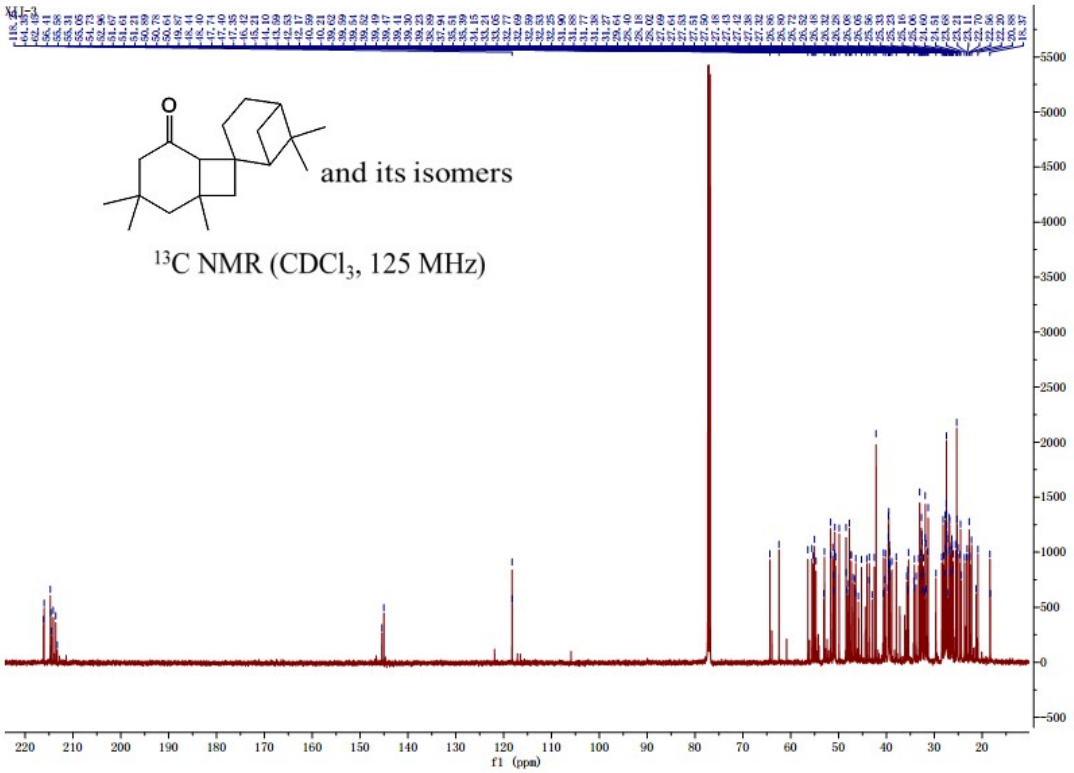


Figure S7 GC spectra of isophorone and β-pinene reaction solution.

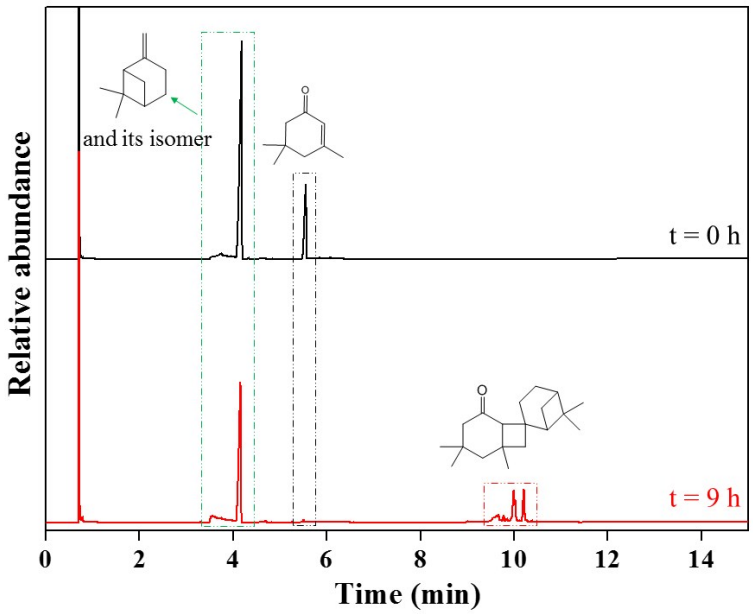


Figure S8 Mass spectra of isophorone and n-hexene co-adduct.

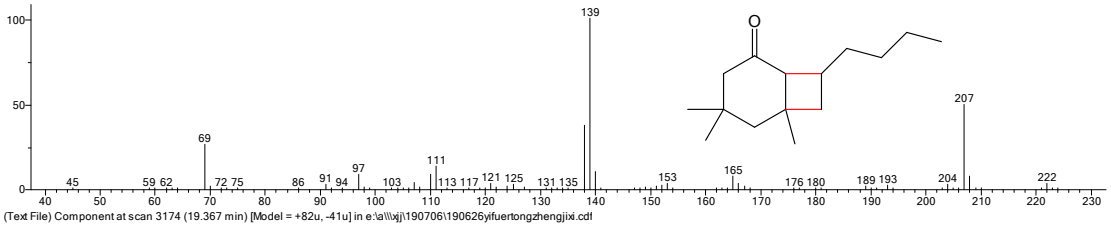


Figure S9 GC spectra of isophorone and n-hexene reaction solution.

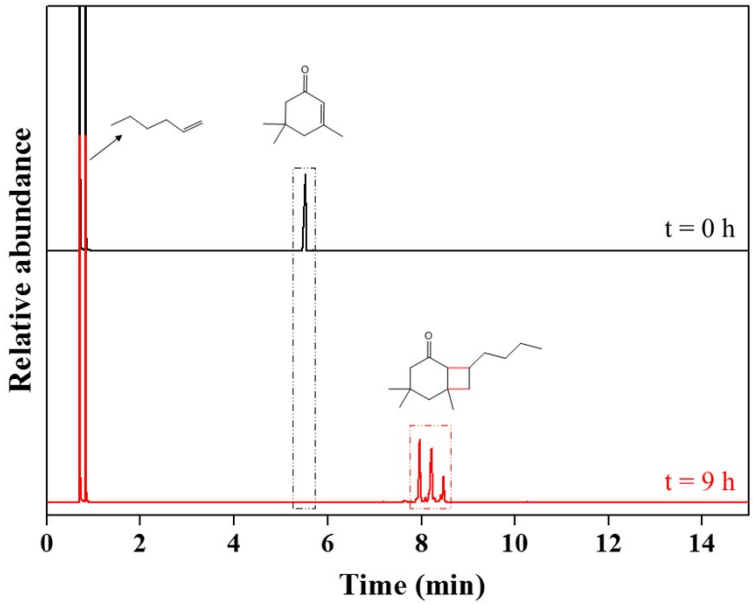


Figure S10 Mass spectra of isophorone and α-pinene co-adduct.

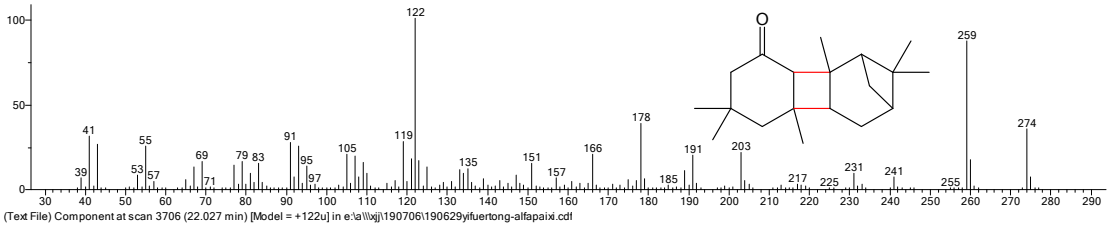


Figure S11 GC spectra of isophorone and α-pinene reaction solution.

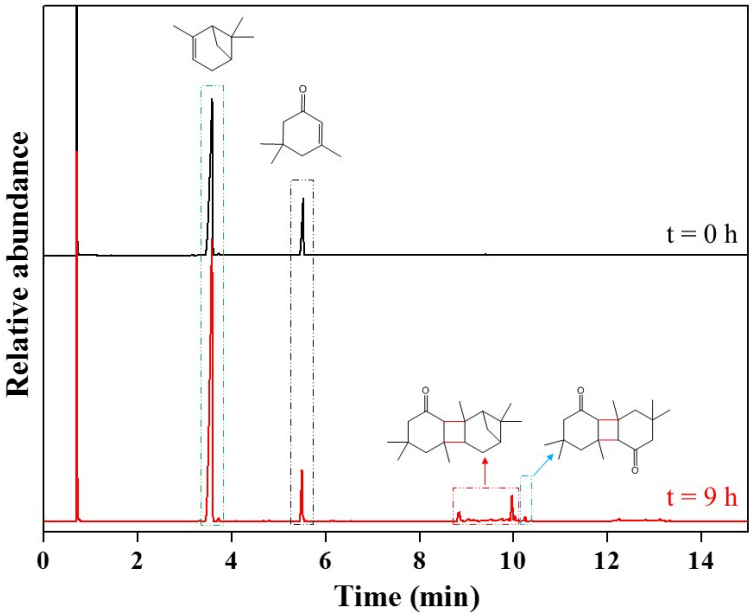


Figure S12 Mass spectra of isophorone and camphene co-adduct.

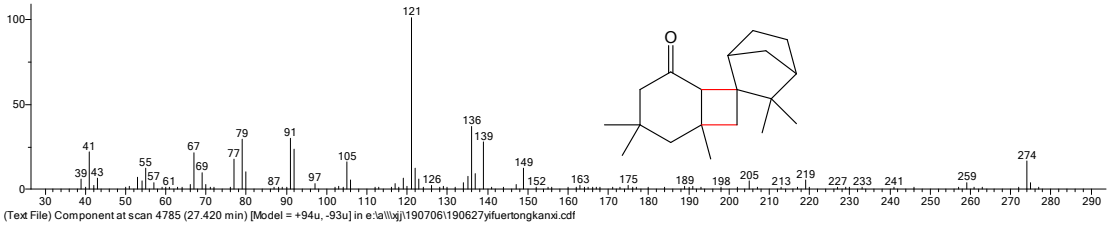


Figure S13 GC spectra of isophorone and camphene reaction solution.

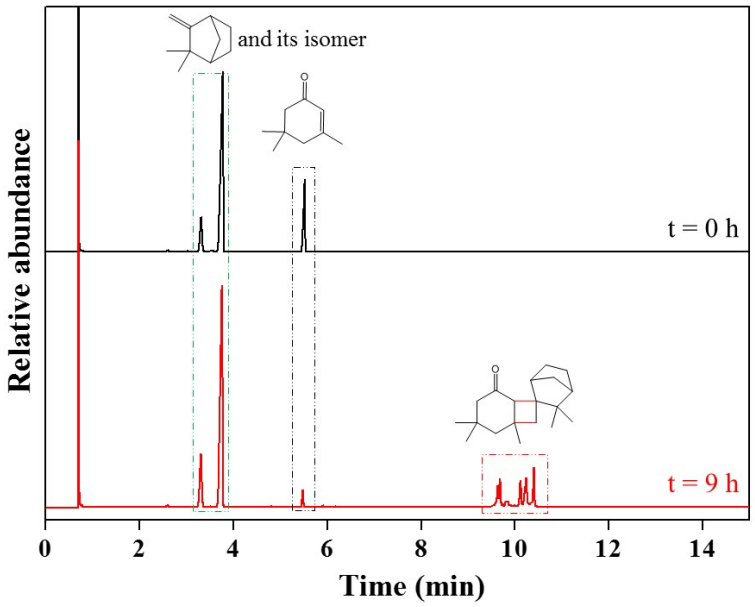
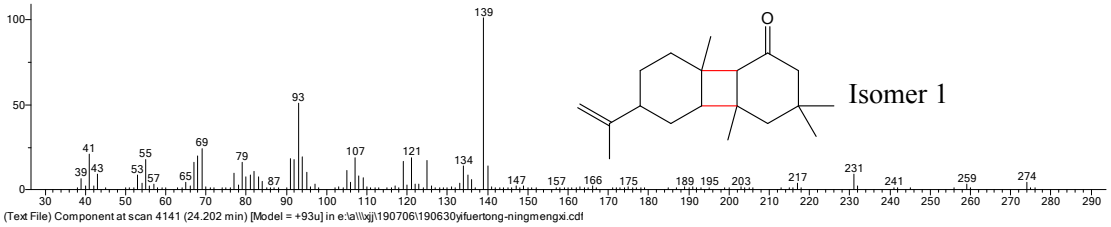


Figure S14 Mass spectra of isophorone and cinene co-adduct.



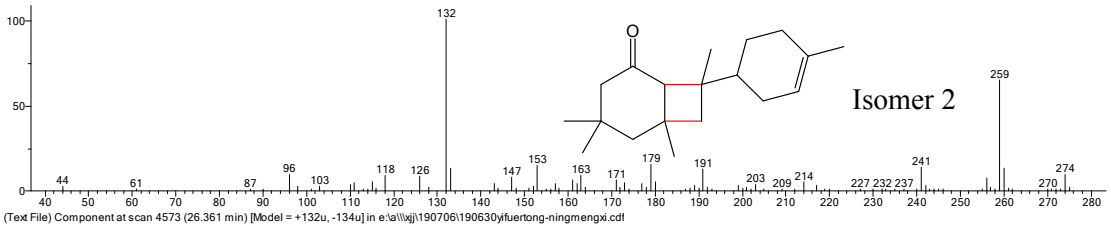


Figure S15 GC spectra of isophorone and cinene reaction solution.

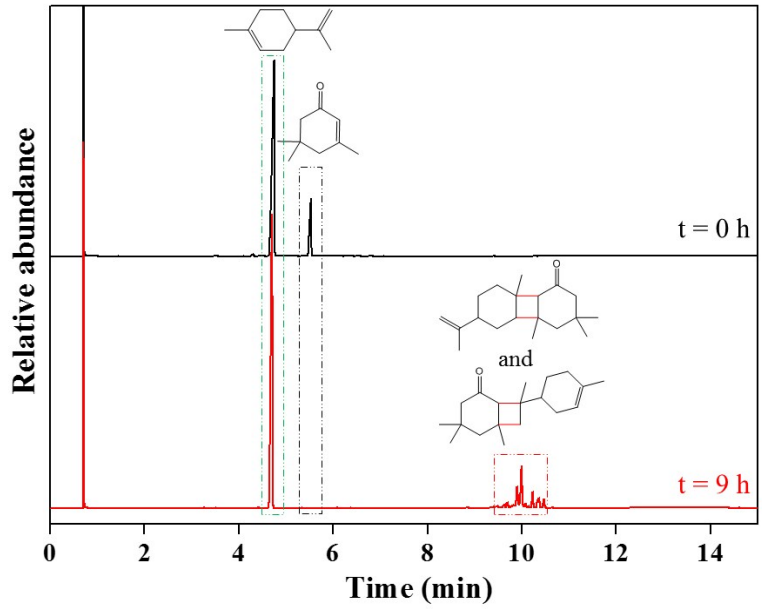


Figure S16 Mass spectra of isophorone and 2-methoxy-4-vinylphenol co-adduct.

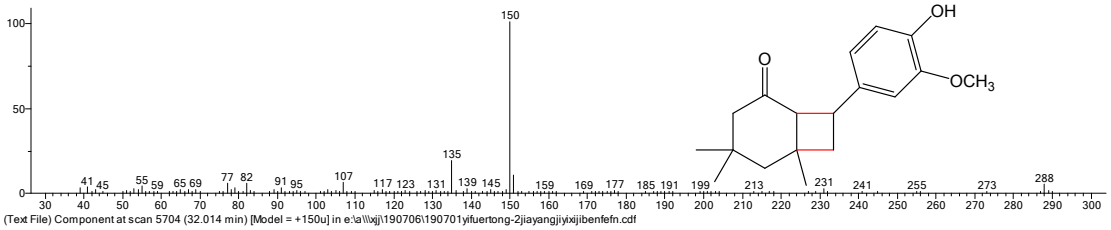


Figure S17 Mass spectra of 2-methoxy-4-vinylphenol self-adduct.

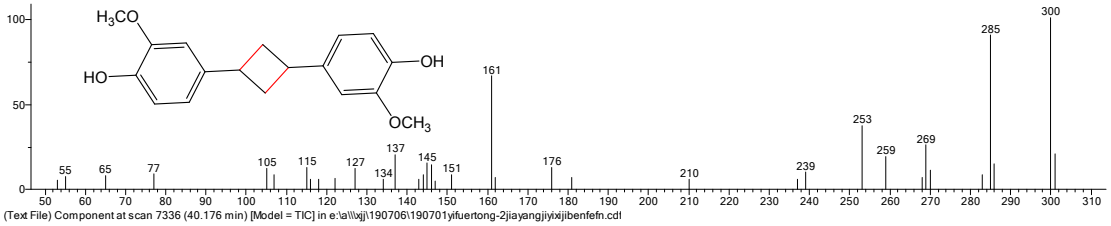


Figure S18 GC spectra of isophorone and 2-methoxy-4-vinylphenol reaction solution.

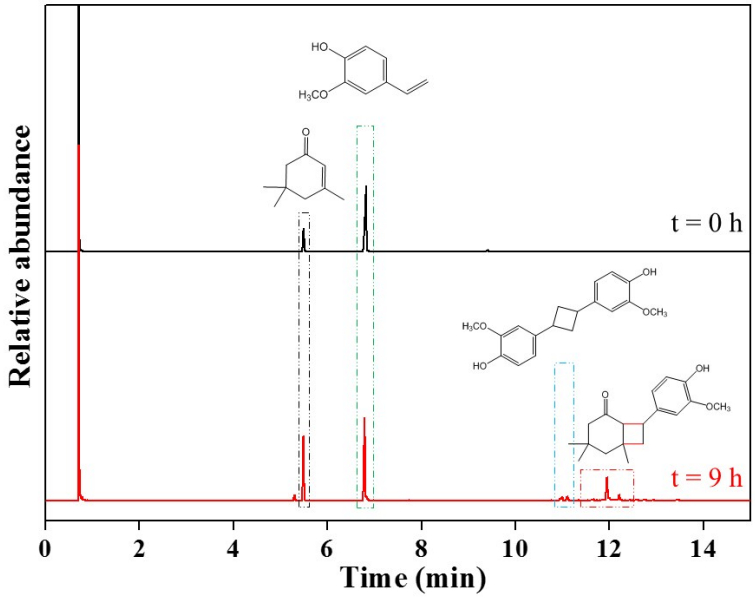


Figure S19 Mass spectra of 2-cyclopentenone and β-pinene co-adduct.

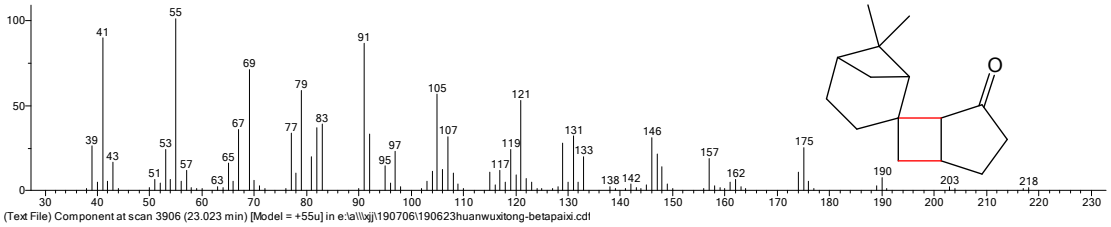


Figure S20 Mass spectra of 2-cyclopentenone self-adduct.

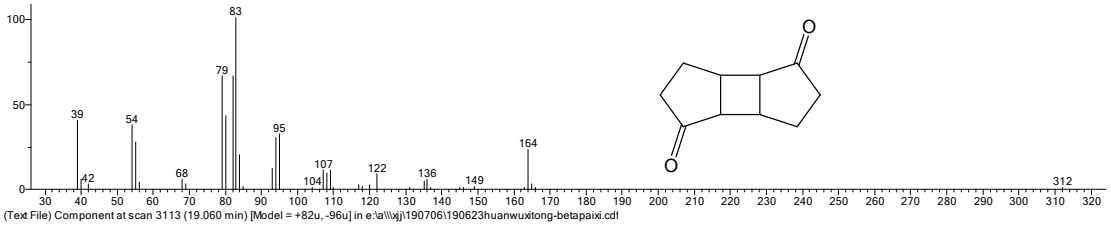


Figure S21 GC spectra of 2-cyclopentenone and β-pinene reaction solution.

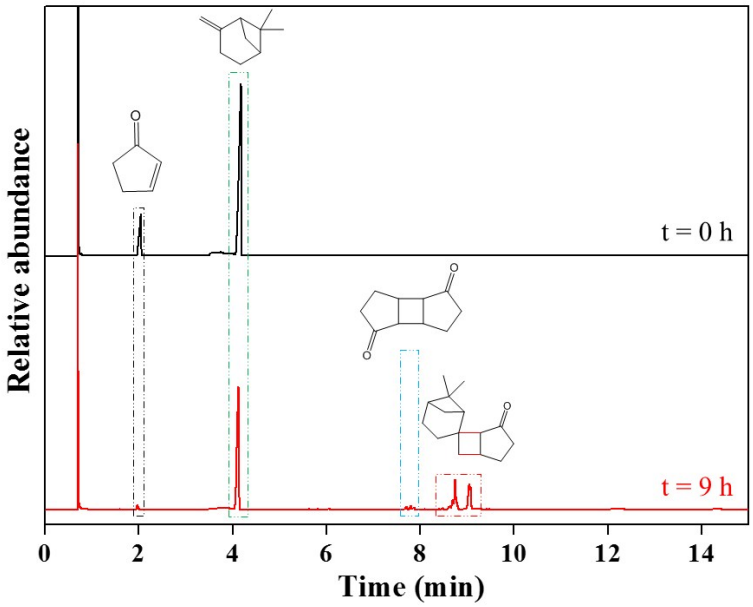


Figure S22 Mass spectra of 3-methyl-2-cyclopenten-1-one and β-pinene co-adduct.

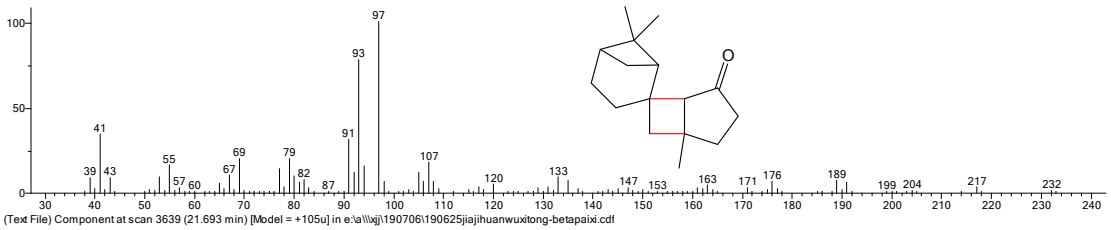


Figure S23 GC spectra of 3-methyl-2-cyclopenten-1-one and β-pinene reaction solution.

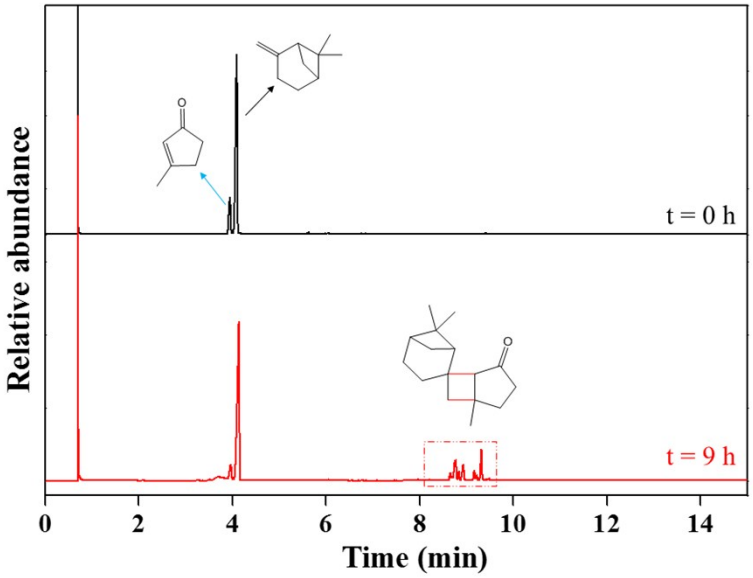


Figure S24 Mass spectra of carvone and β-pinene co-adduct.

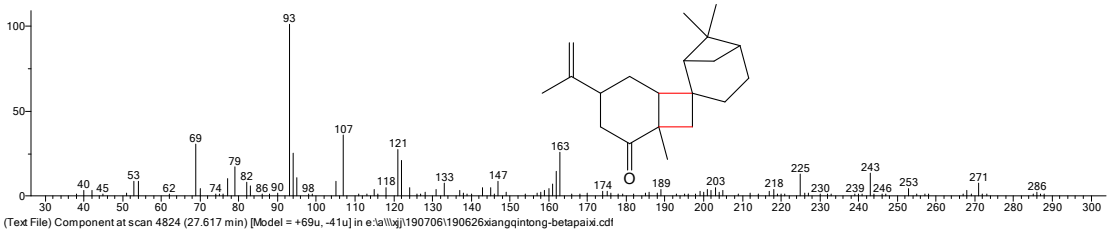


Figure S25 GC spectra of carvone and β-pinene reaction solution.

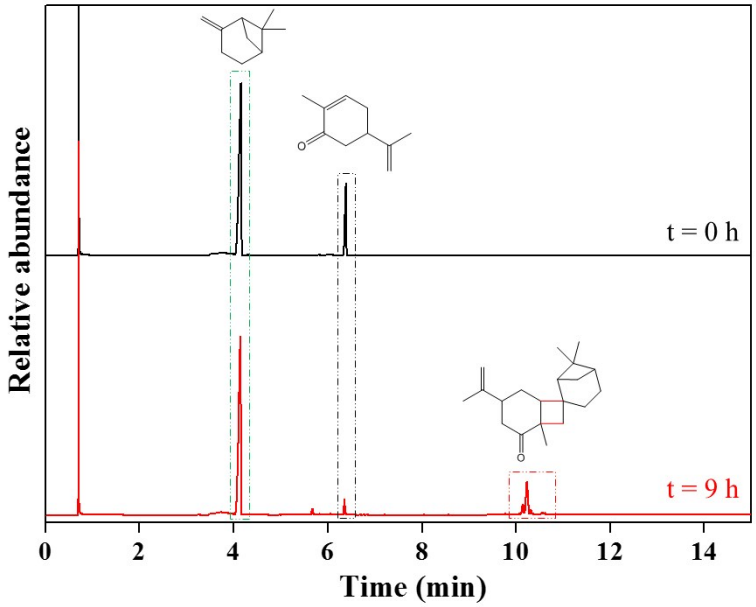


Figure S26 Mass spectra of coumarin and β-pinene co-adduct.

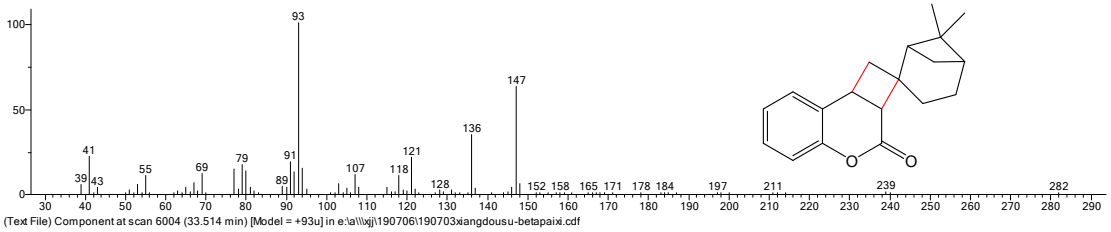


Figure S27 Mass spectra of coumarin self-adduct.

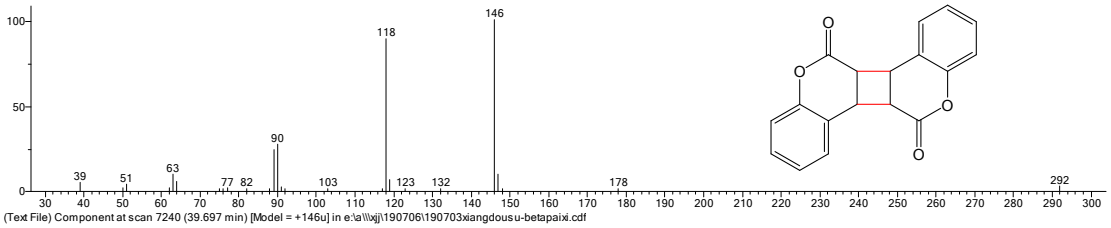


Figure S28 GC spectra of coumarin and β-pinene reaction solution.

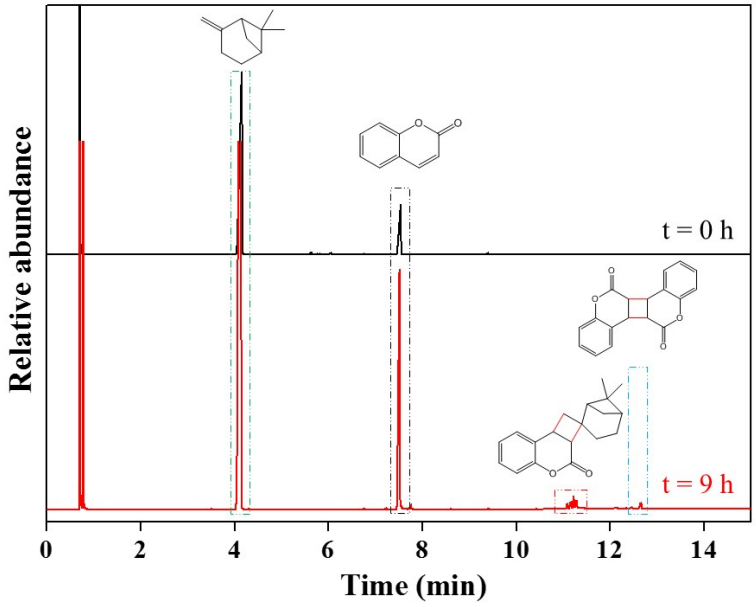


Figure S29 Mass spectra of cinnamic aldehyde and β-pinene co-adduct.

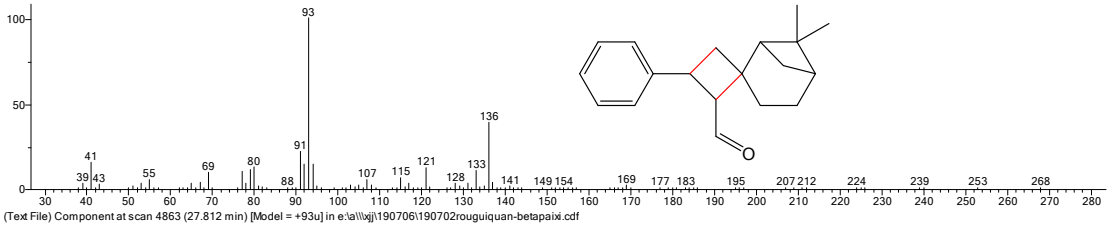


Figure S30 GC spectra of cinnamic aldehyde and β-pinene reaction solution.

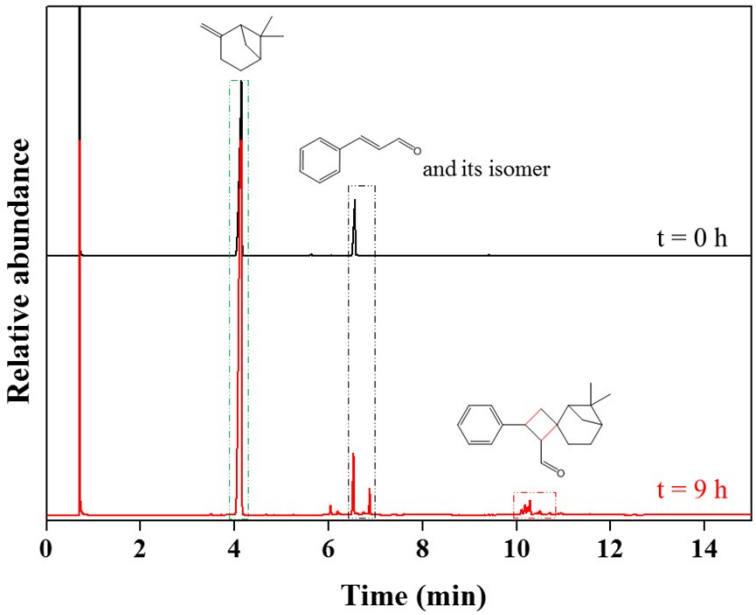


Figure S31 Mass spectra of isophorone and 2-methylfuran co-adduct.

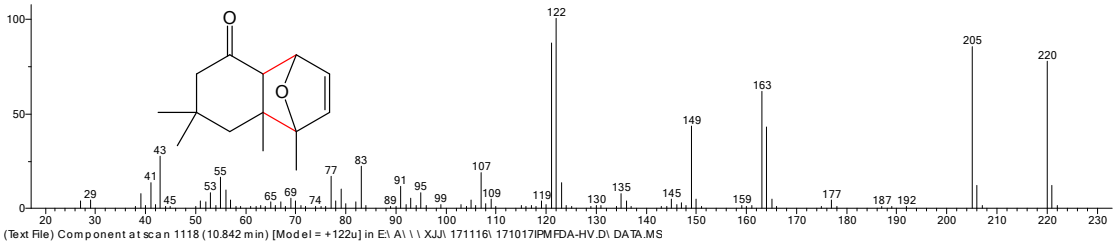


Figure S32 GC spectra of isophorone and 2-methylfuran reaction solution.

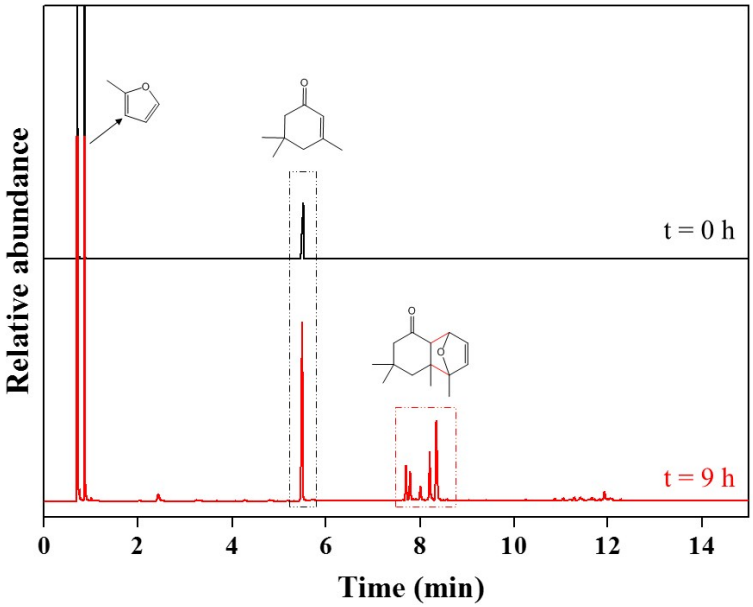


Figure S33 Mass spectra of isophorone and 2,5-dimethylfuran co-adduct.

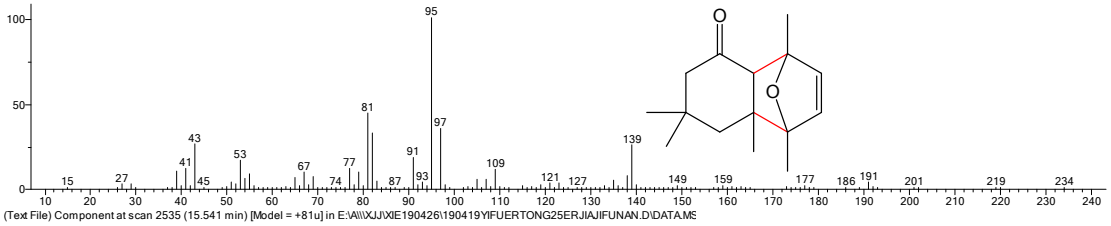


Figure S34 GC spectra of isophorone and 2,5-dimethylfuran reaction solution.

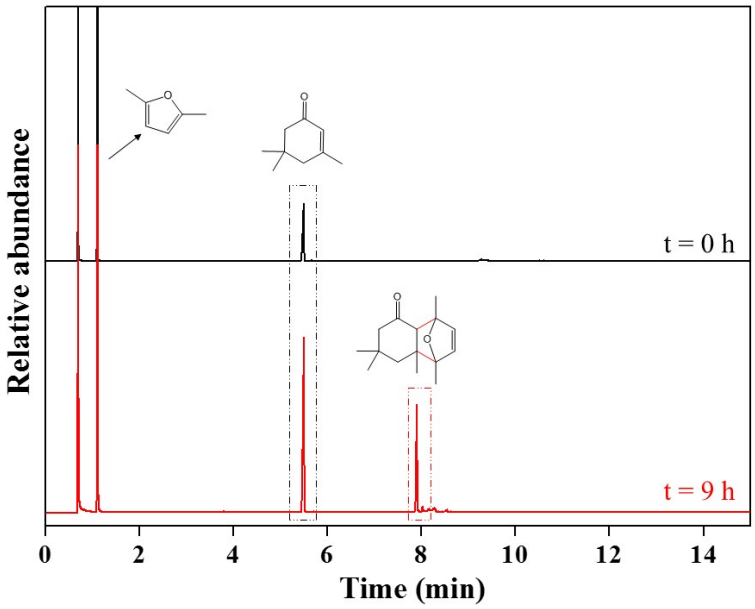


Figure S35 Mass spectrum of the obtained spiro-fuel derived from isophorone and β-pinene.

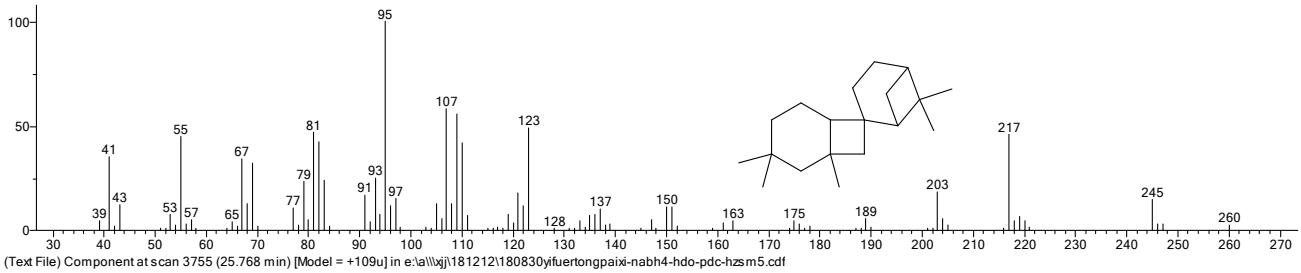


Figure S36. GC spectra of the HDO solution and obtained spiro-fuel after vacuum distillation.

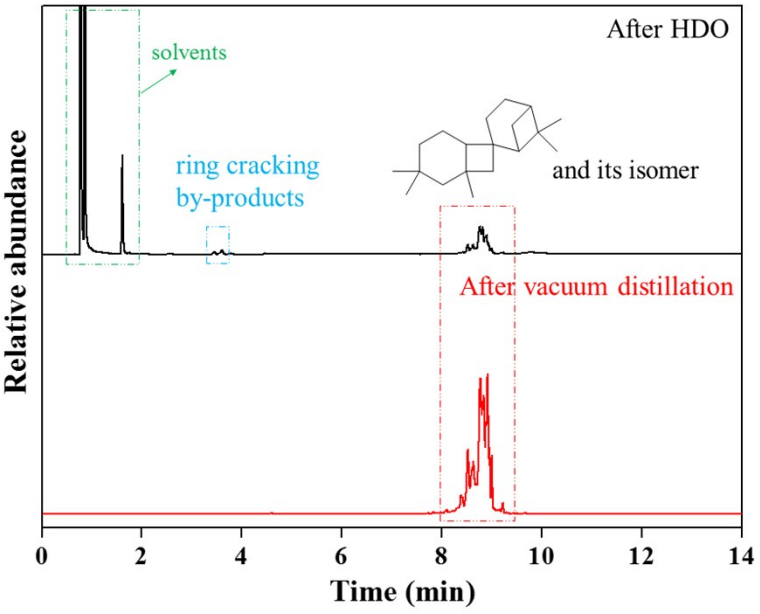
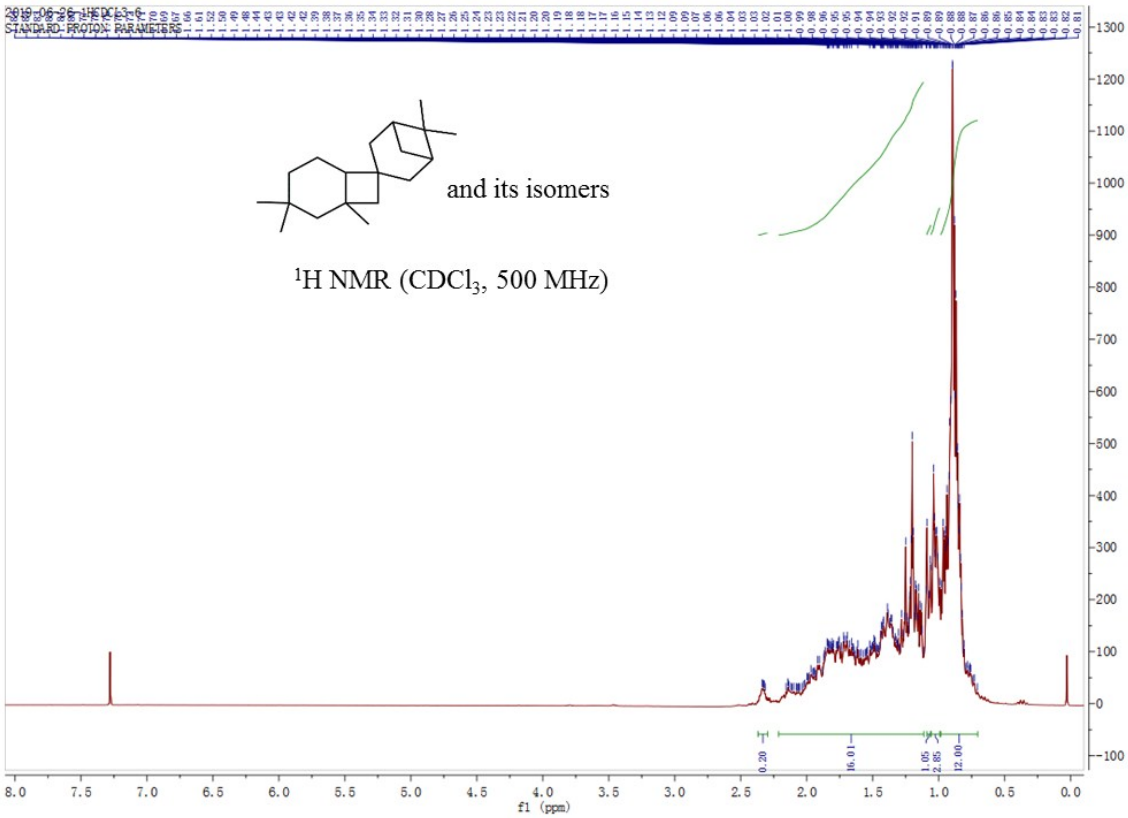


Figure S37. ^{1}H and ^{13}C NMR spectra of the obtained spiro-fuel derived from isophorone and β-pinene.



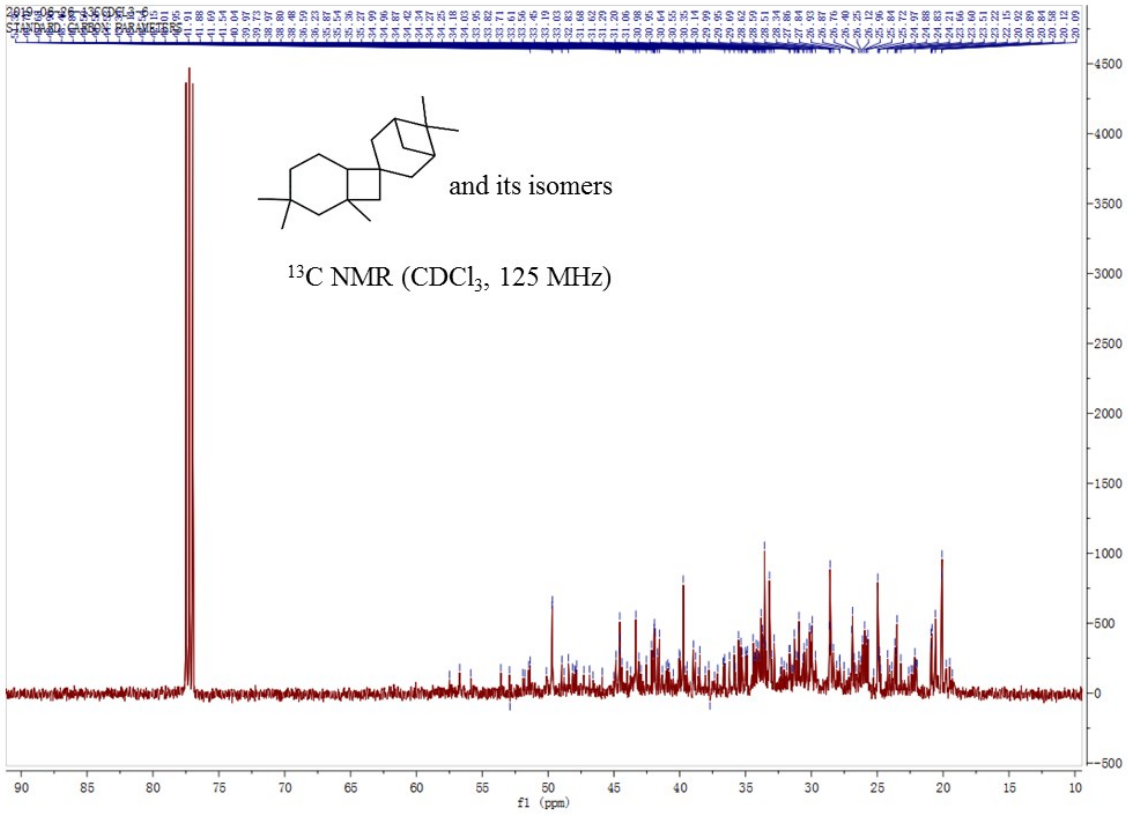
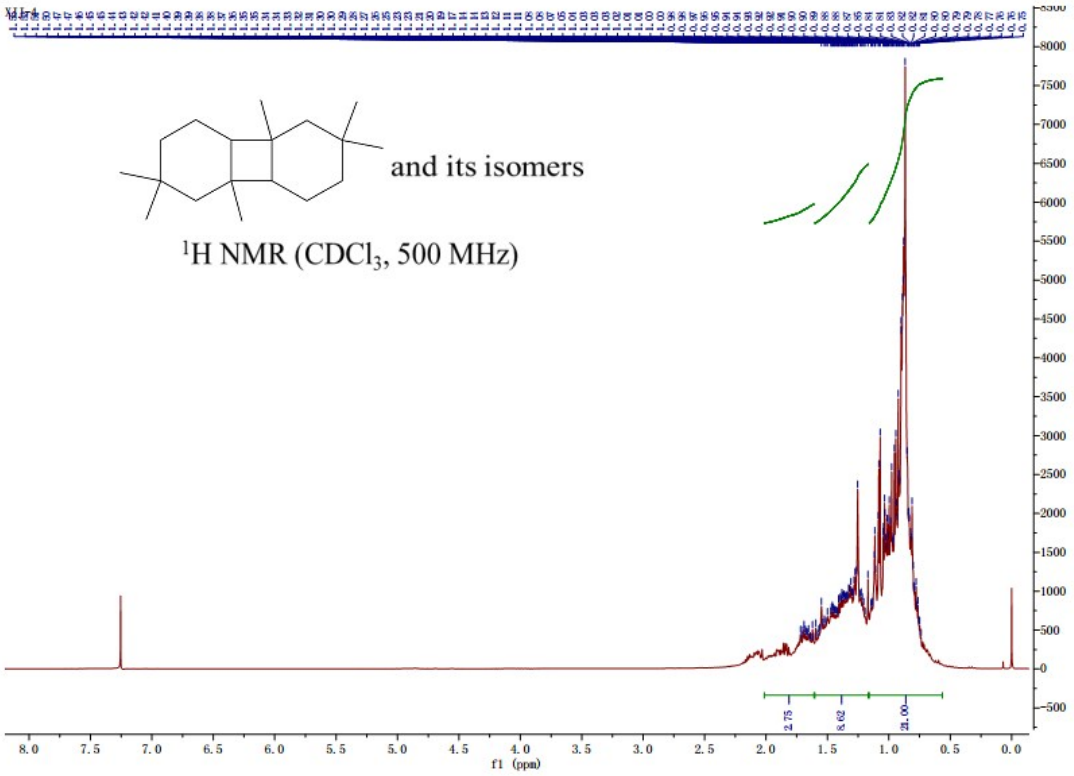


Figure S38. ^{1}H and ^{13}C NMR spectra of the obtained fuel derived from isophorone self-adduct.



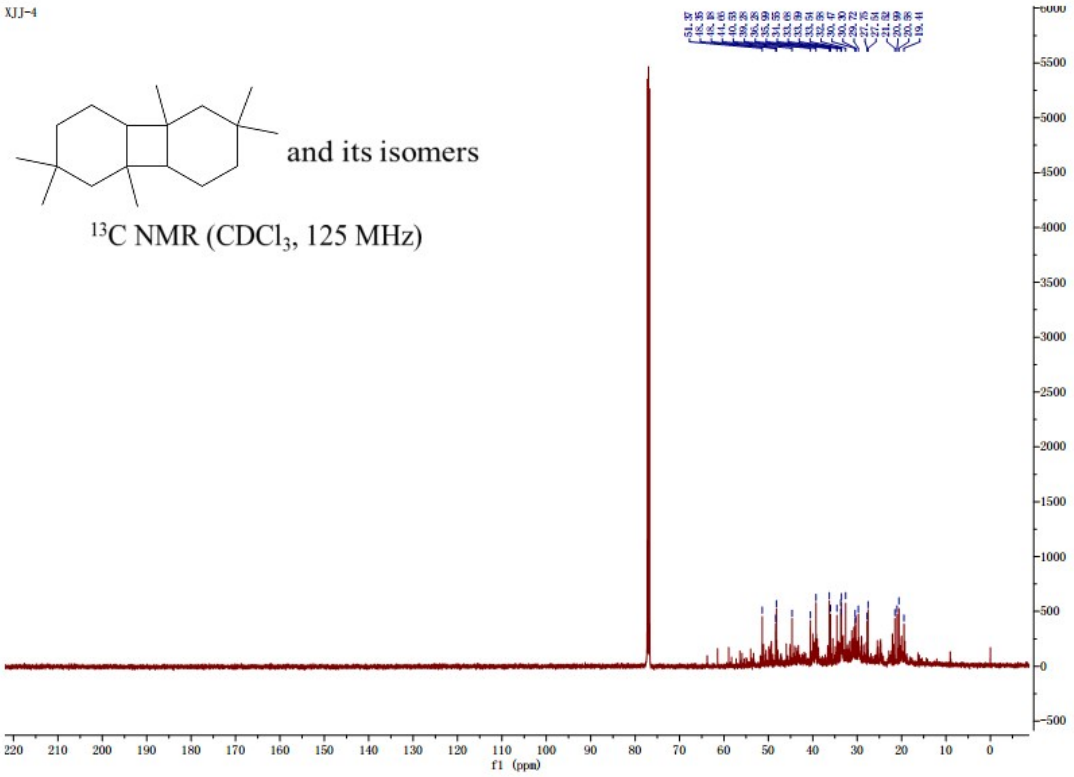


Figure S39 Mass spectrum of the obtained fuel derived from isophorone self-adduct.

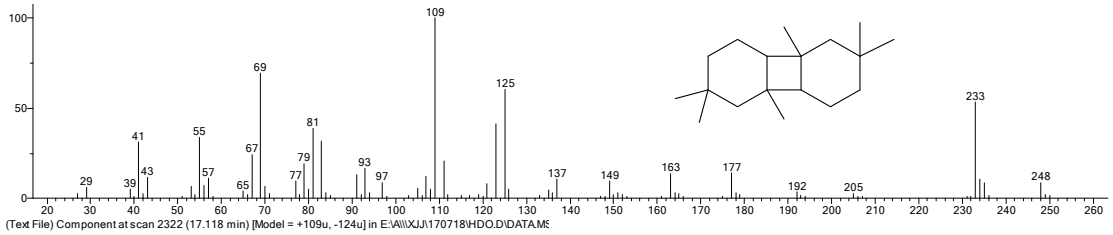
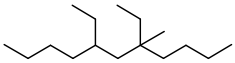
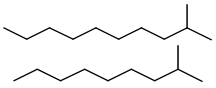
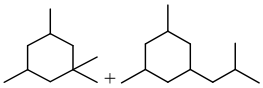
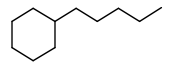
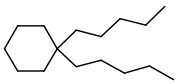
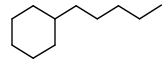
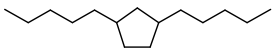
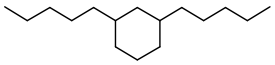
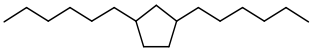
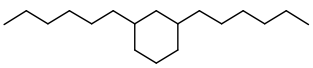
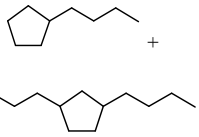
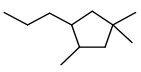
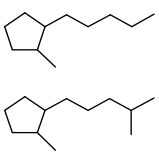
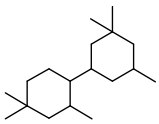
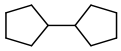
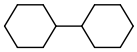
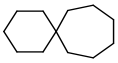
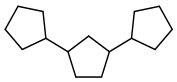
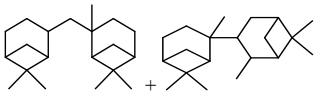
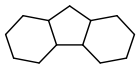


Table S1 Properties of some reported biofuels.

Feedstock	Main component structure	Density/kg·m^{-3} (20°C)	Freezing point/°C	Reference
Biobutanol		0.78	-78	Energy Environ. Sci., 2010, 3, 352.
Furfural and methyl isobutyl ketone		- -	-49.7 -74.9	ChemSusChem, 2013, 6, 1149.
Diacetone alcohol		0.83	-56.7	Green Chem., 2016, 18, 5751.
2-Methylfuran and cyclohexanone	 	0.804 0.825	< -60.0 -26.4	Chem. Eng. Sci., 2015, 138, 239.
Aromatic oxygenates and furfural alcohols		0.804	< -80	Fuel Process. Technol., 2017, 163, 45.
Cyclic ketones and furanic aldehydes	   	0.815 0.822 0.819 0.826	-24.6 -21.7 -14.3 -9.5	Fuel Process. Technol., 2016, 148, 361.
Cyclopentanone and butanal		0.82	-94.0	Ind. Eng. Chem. Res., 2015, 54, 11825.
Mesityl oxide and 2-methylfuran		0.82	-56 ~ -54	Sci. Rep., 2016, 6, 32379.
5-Hydroxymethyl-furfural and ketones		0.81 0.81	-25 -46	ChemSusChem, 2017, 10, 711.

Isophorone		0.858	-51.0	Sci. Rep., 2017, 7, 6111.
Cyclic ketones		0.867	-38.0	Green Chem., 2015, 17, 4473.
		0.887	1.2	
Cyclic ketones		0.870	-76	Chem. Commun., 2017, 53, 10303.
		0.893	-51	
Cyclopentanone		0.91	-	AIChE J., 2016, 62, 2754.
Pinenes		0.938	< -30	Energy Fuels, 2010, 24, 267.
Phenols and benzyl ether or benzyl alcohol		0.959	-15	Chem. Eng. Sci., 2017, 158, 64.