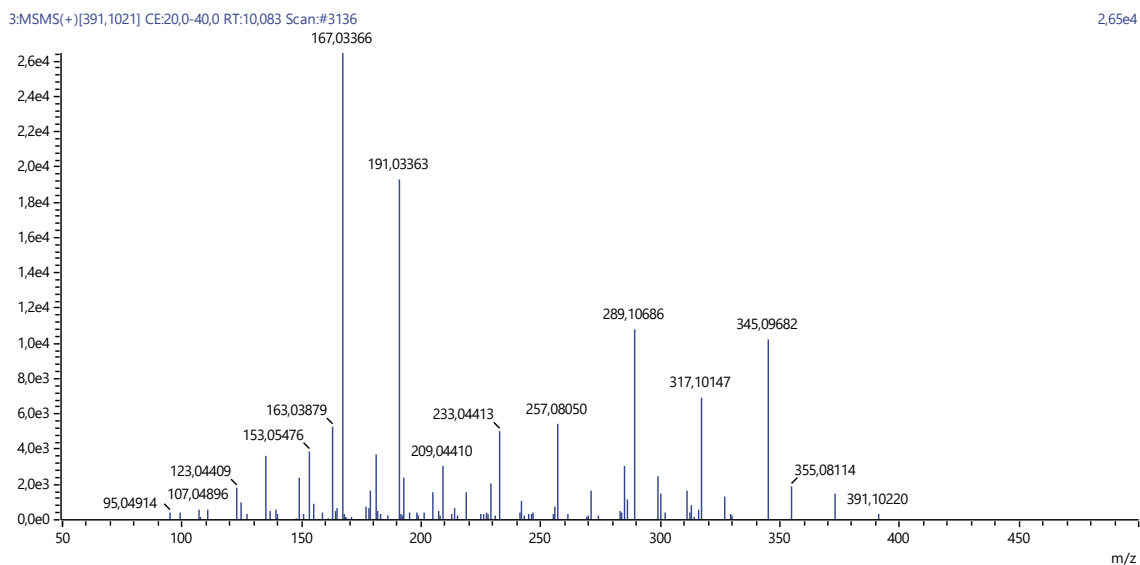


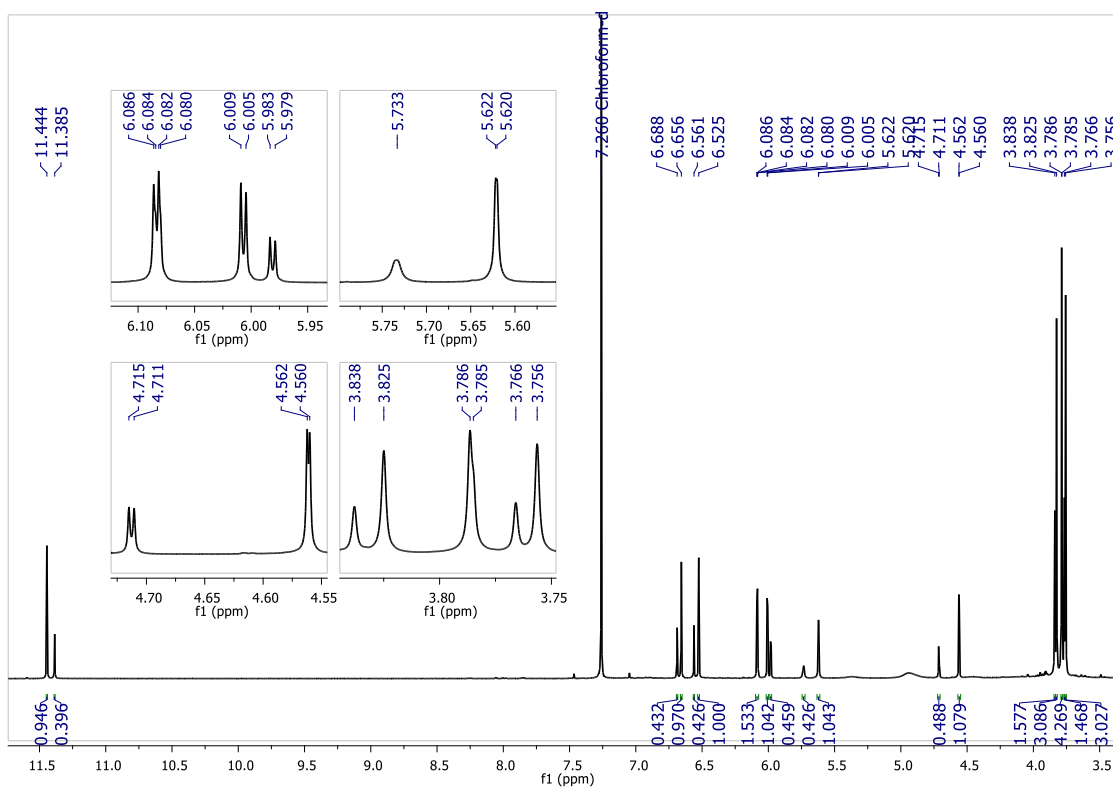
# Supporting Information

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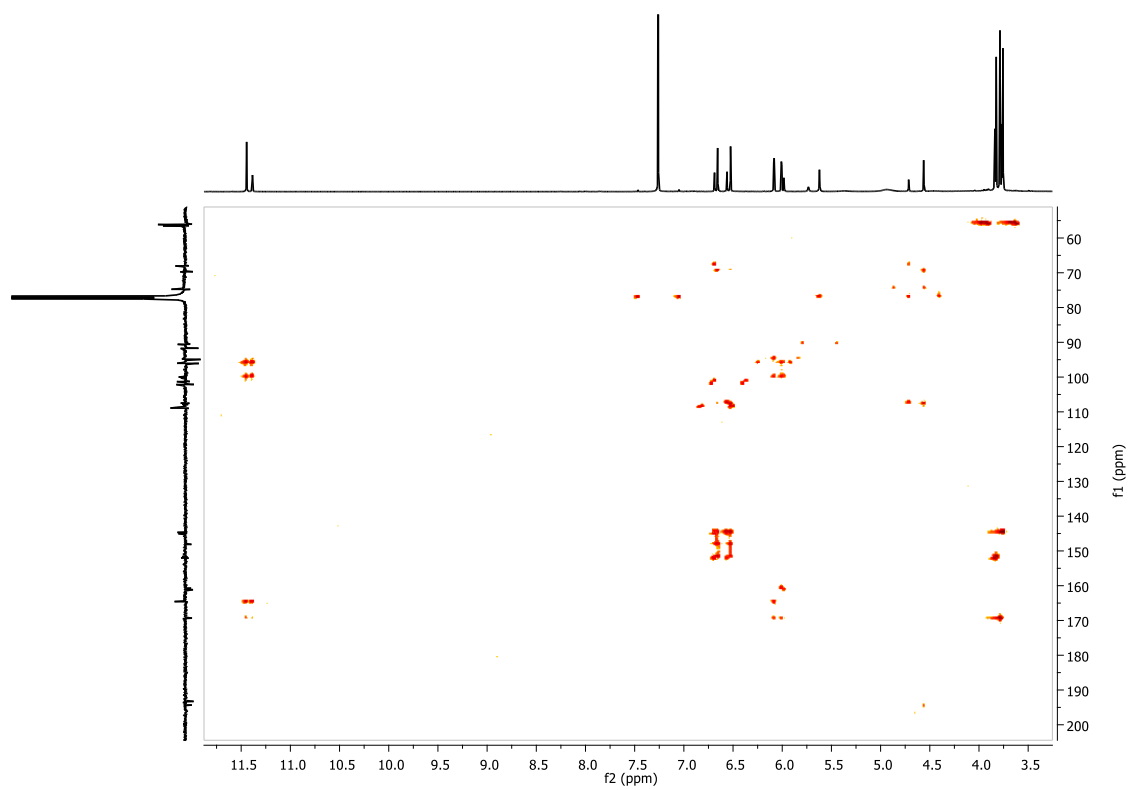
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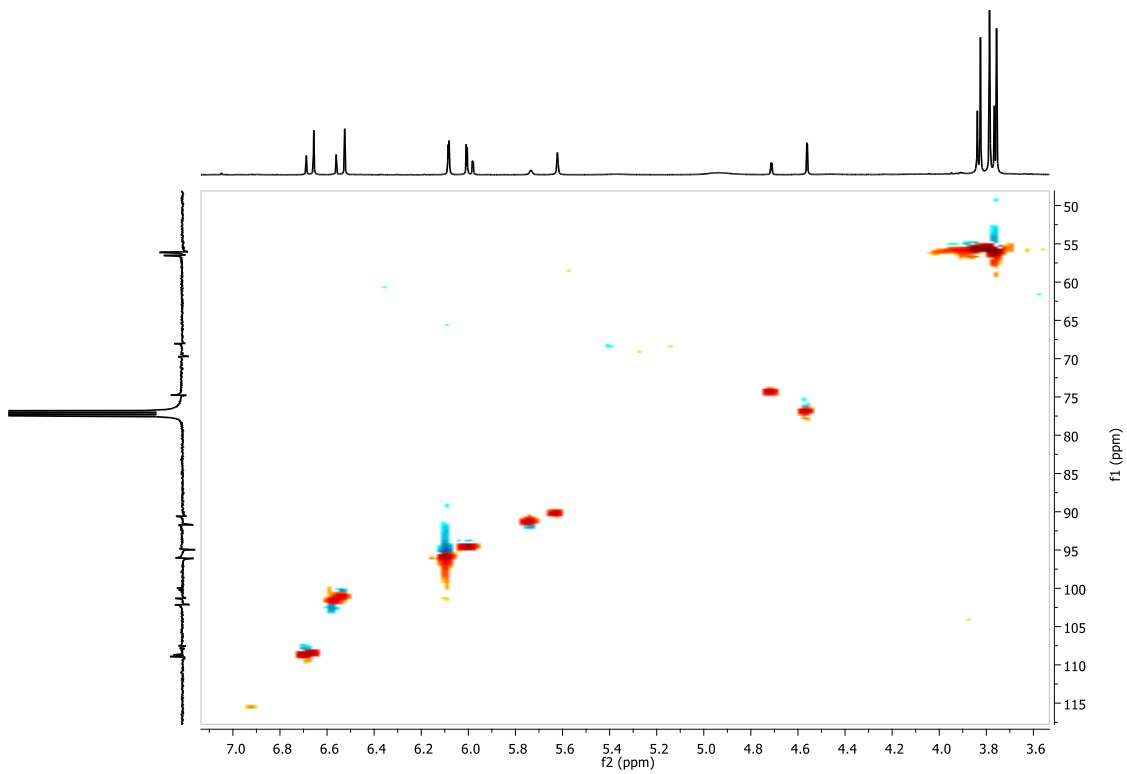
**Figure S1.** Mass spectrum ( $MS^2$ ) of the  $m/z$  391.1021 ion, obtained in positive ion mode using ESI



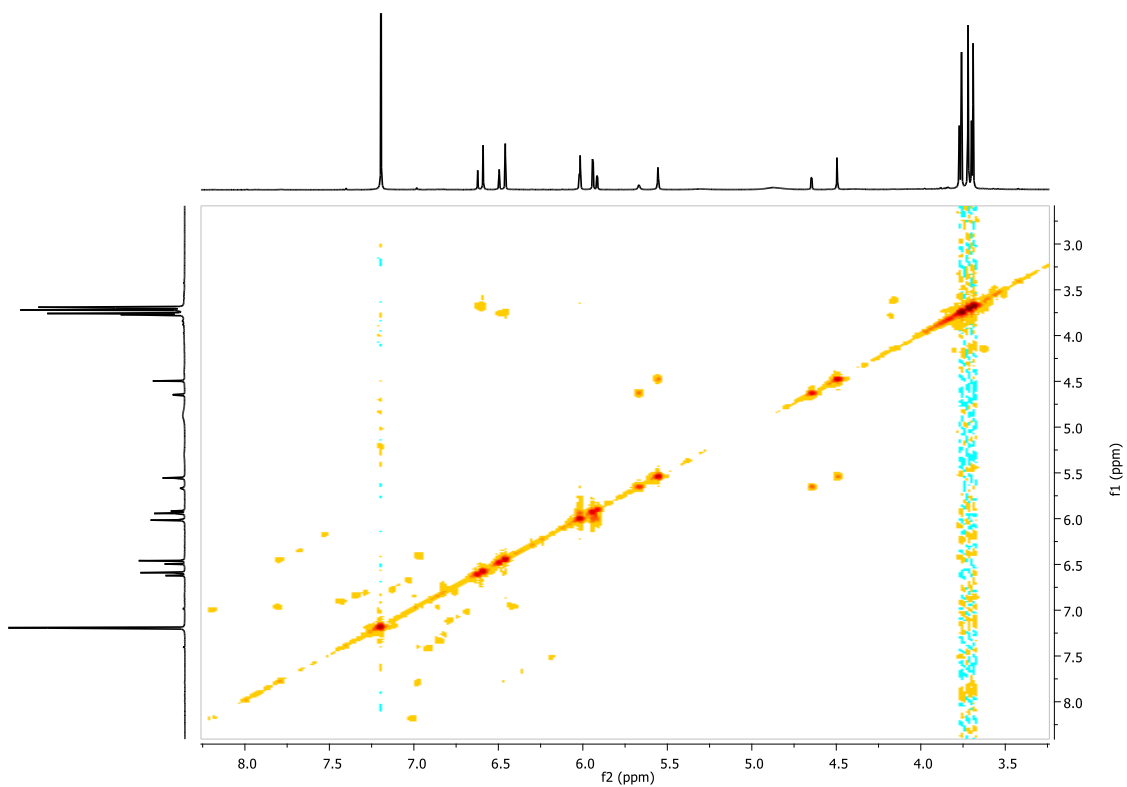
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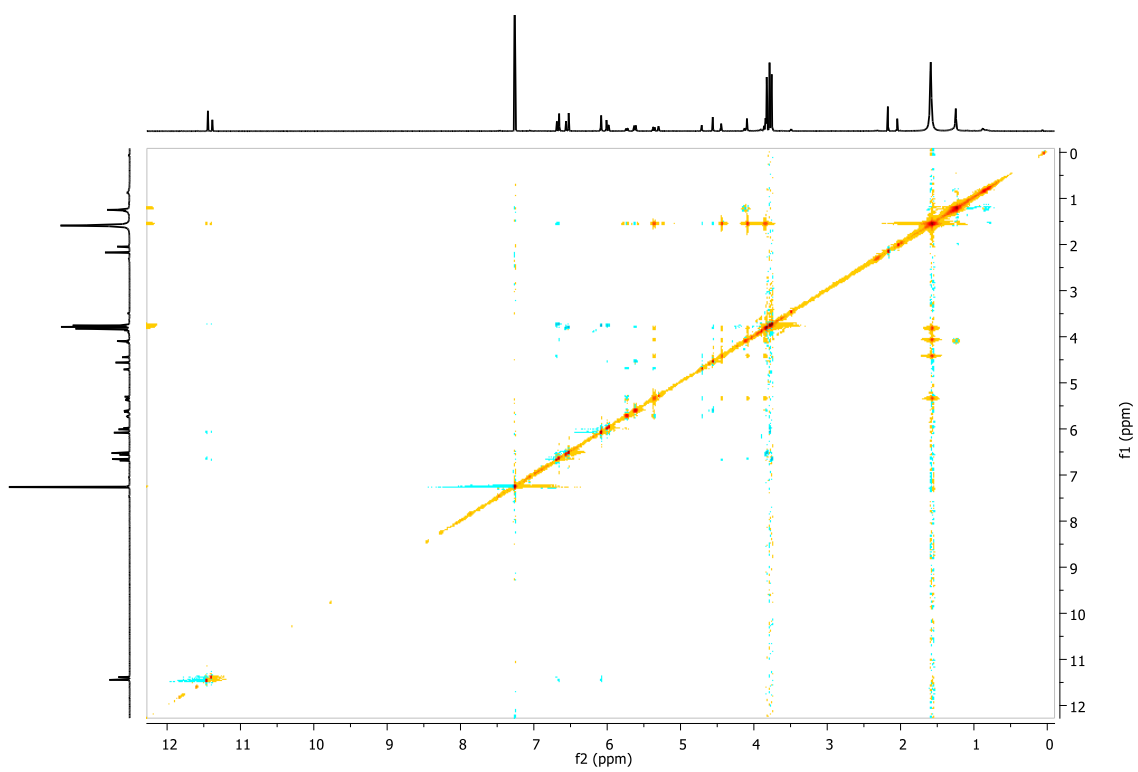
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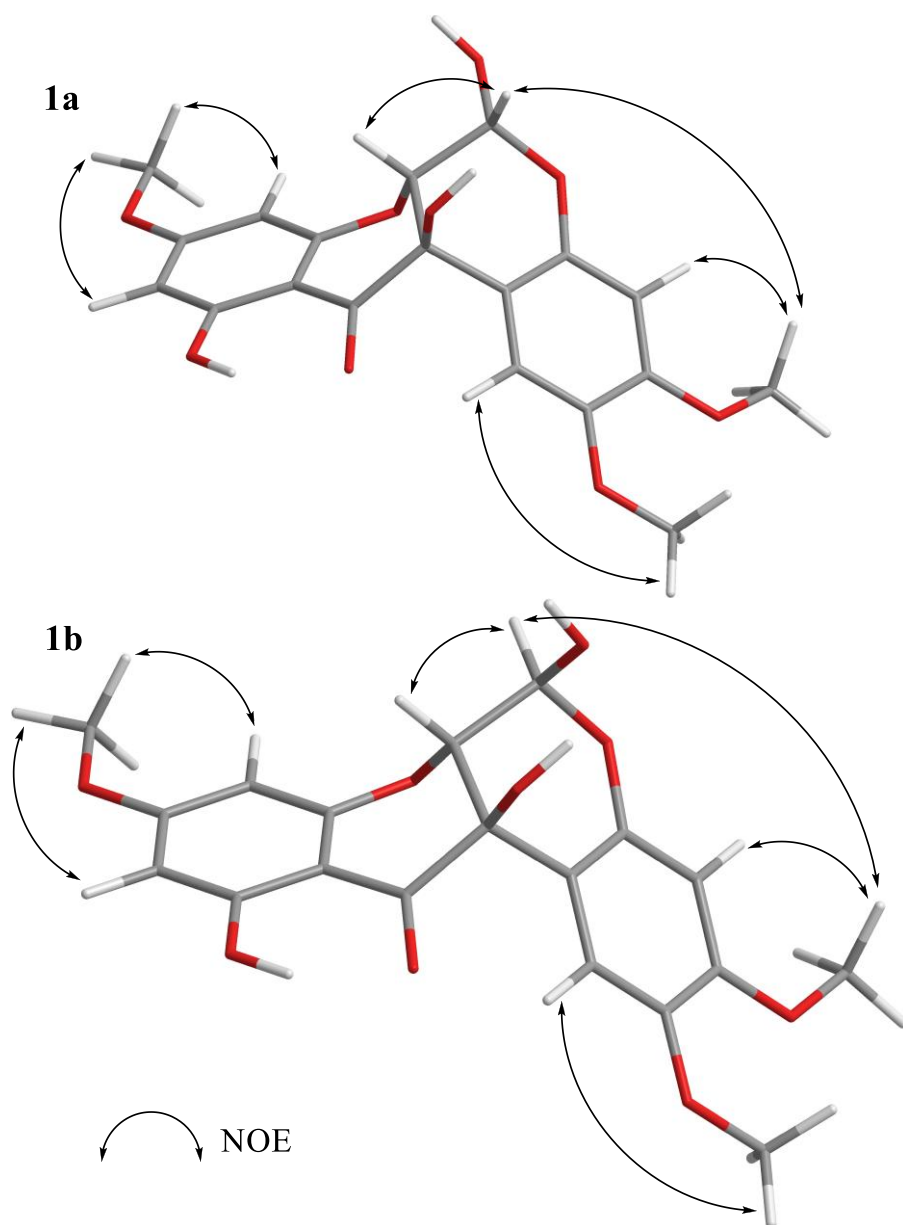
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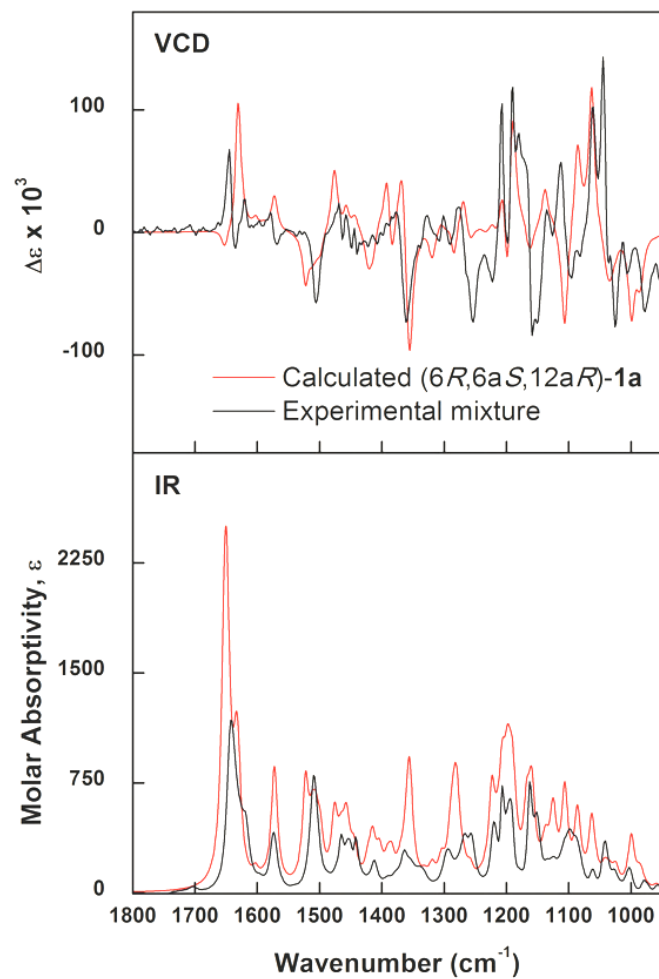
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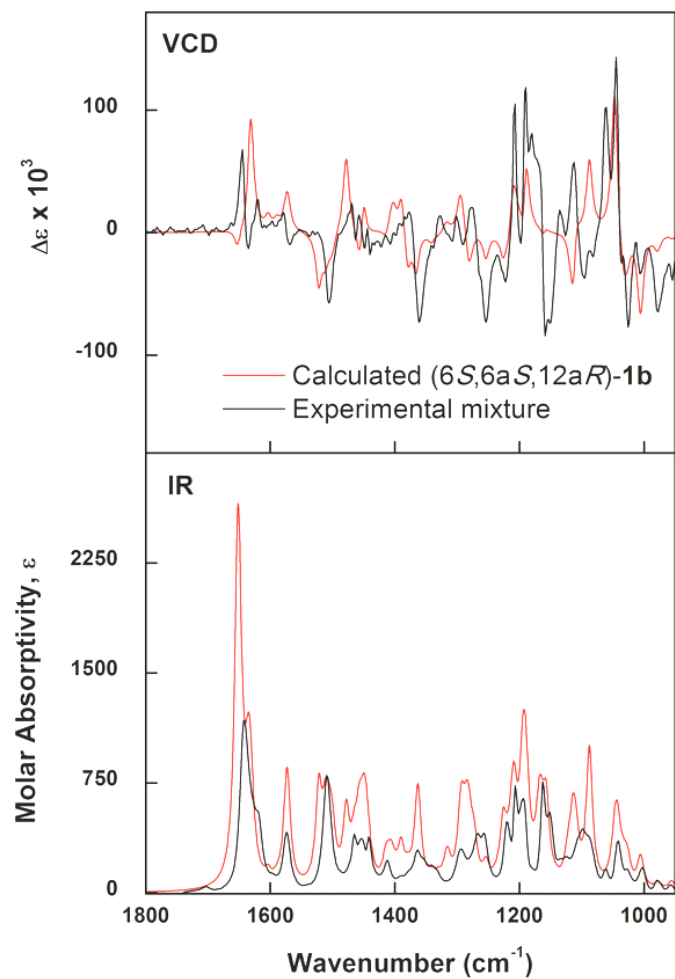
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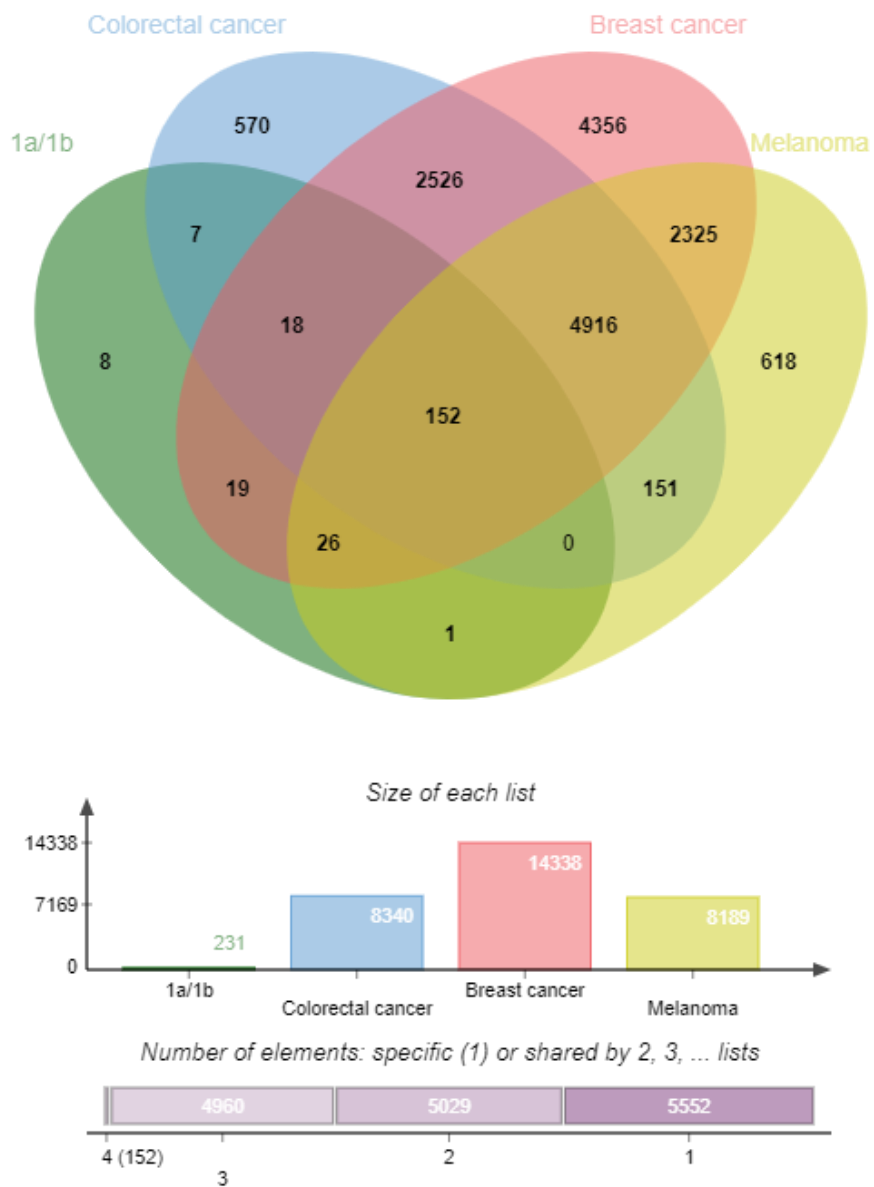
**Figure S7.** Long-distance correlations observed through the 2D NOESY experiment for **1a** and **1b**.



**Figure S8.** Comparison between experimental IR and VCD spectra for the mixture **1a+1b** (black trace) with calculated B3PW91/PCM(CHCl<sub>3</sub>)/6-311G(d,p) data for individual (6R,6aS,12aR)-**1a**.

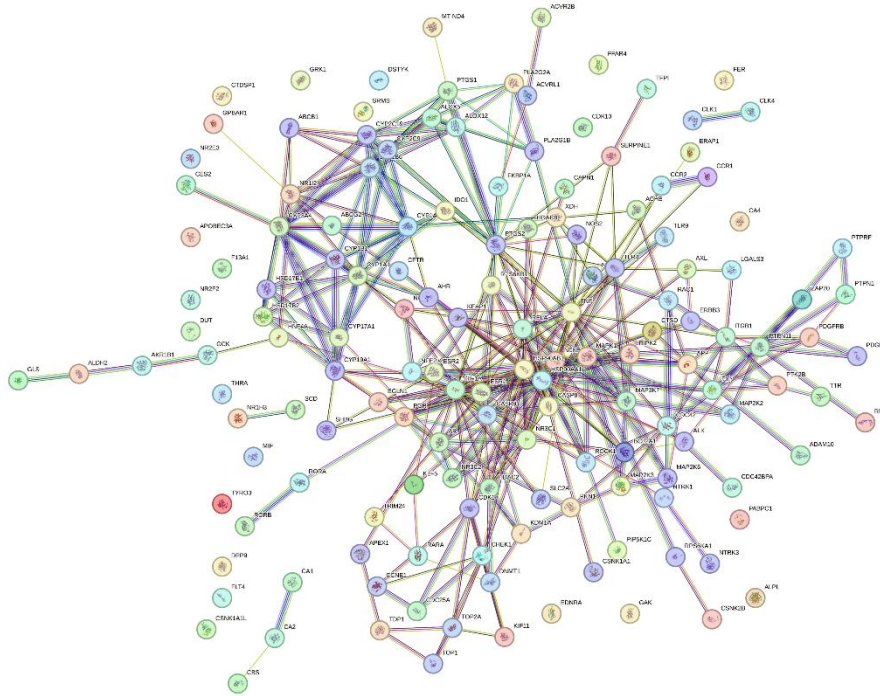


**Figure S9.** Comparison between experimental IR and VCD spectra for the mixture **1a+1b** (black trace) with calculated B3PW91/PCM(CHCl<sub>3</sub>)/6-311G(d,p) data for individual (6S,6aS,12aR)-**1b**.

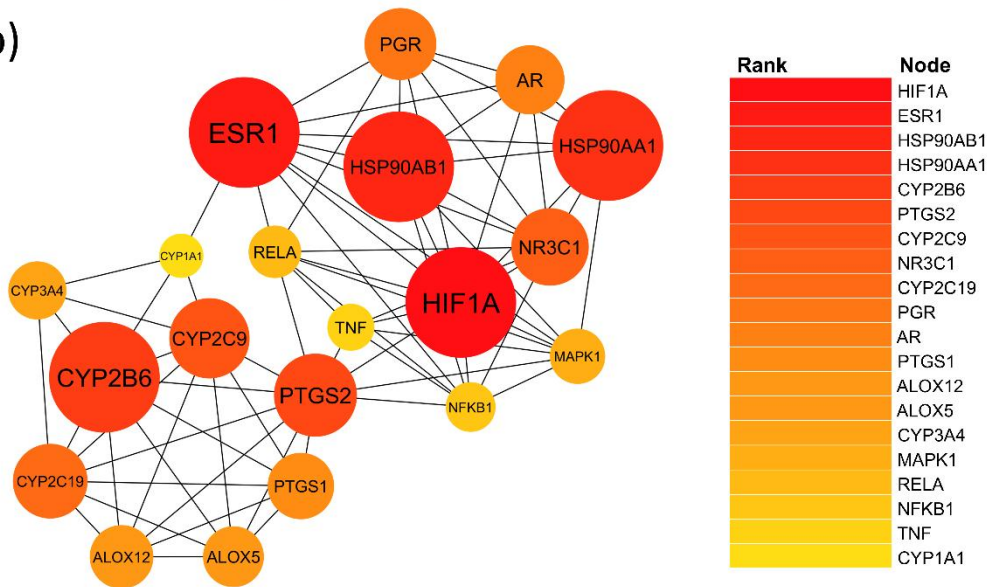


**Figure S10.** Venn diagram of potential targets for cancer treatment using mixture of **1a** and **1b**.

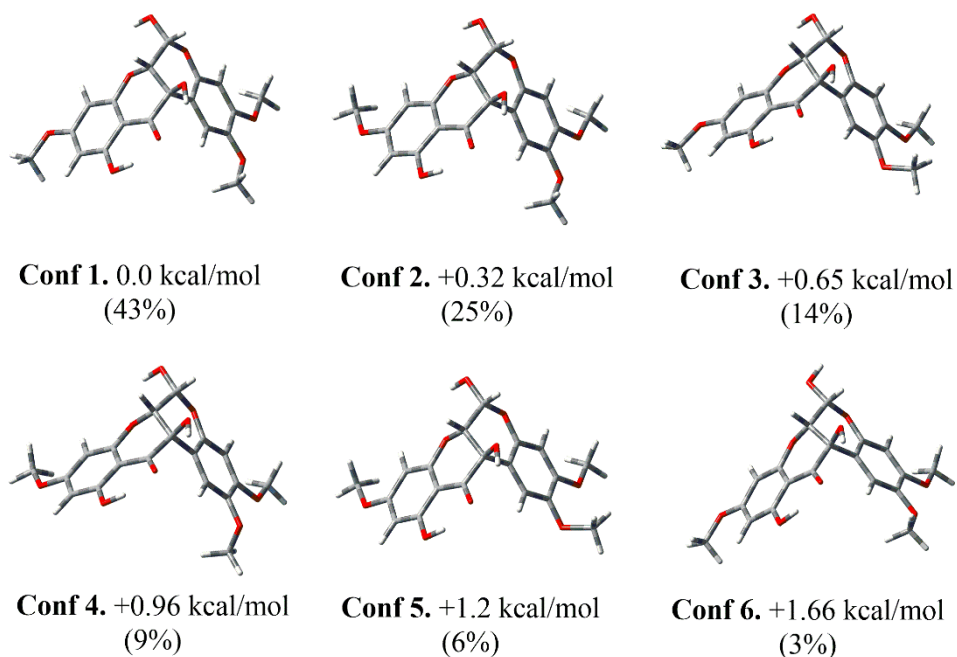
(a)



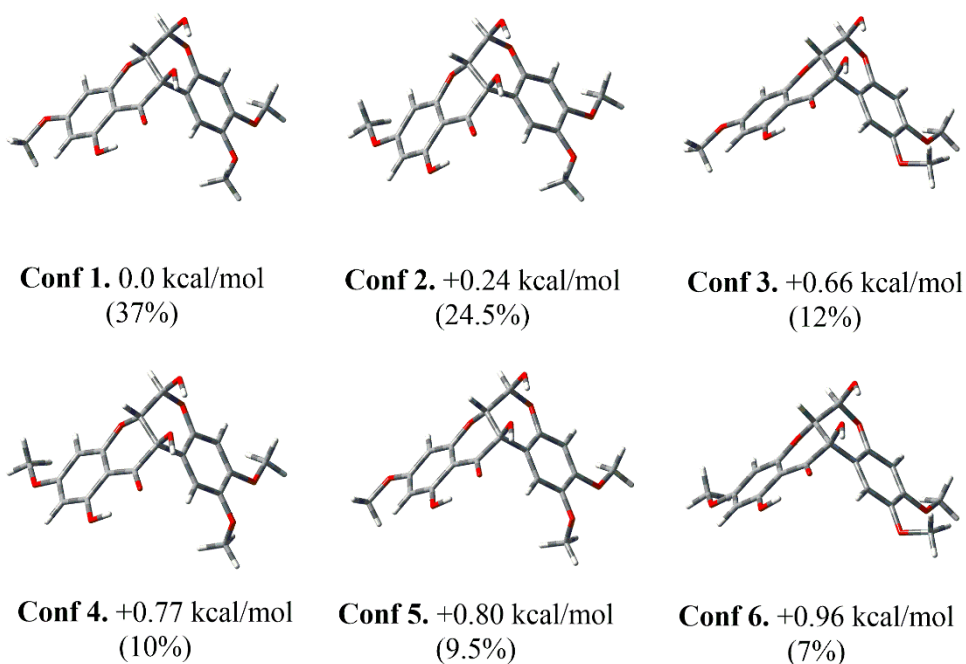
(b)



**Figure S11.** PPI network for cancer treatment using the mixture of **1a** and **1b**. (A) PPI network analysis. (B) Top 20 nodes are the likely key proteins in the interaction.



**Figure S12.** Optimized structures, relative energies ( $\Delta G_{298K}$ ), and Boltzmann populations (%) of the lowest-energy conformers identified for (6R,6aS,12aR)-**1a** at the B3PW91/PCM(CHCl<sub>3</sub>)/6-311G(d,p) level. Referenced to  $G = -885647.1515$  kcal/mol.



**Figure S13.** Optimized structures, relative energies ( $\Delta G_{298K}$ ), and Boltzmann populations (%) of the lowest-energy conformers identified for (6S,6aS,12aR)-**1b** at the B3PW91/PCM(CHCl<sub>3</sub>)/6-311G(d,p) level. Referenced to  $G = -885648.0501$  kcal/mol.

**Table S1.** Functions of potential target genes based on KEGG pathway analysis.

Term	Number of pathway gene	P-Value
Pathways in cancer	RET, ITGB1, ALK, HDAC2, HSP90AB1, ROCK1, FLT4, SLC2A1, KEAP1, PTGS2, HIF1a, RELA, CASP9, CDC42, EDNRA, CASP8, MAPK1, RAC1, PDGFRB, NTRK1, EGLN1, NQO1, PDGFRA, HSP90AA1, MAP2K2, NOS2, ESR1, ESR2, NFKB1, AR, RPS6KB1, CCNE1, RARA, NFE2L2	1.25E-12
Yersinia infection	MAP2K3, ITGB1, MAP2K2, ROCK1, TNF, RELA, NFKB1, CDC42, ZAP70, RPS6KA1, PTK2B, MAPK1, PIP5K1C, PKN1, RAC1, MAP3K7, TLR4, MAP2K6	1.83E-11
Chemical carcinogenesis - receptor activation	HSP90AA1, MAP2K2, HSP90AB1, AHR, CYP3A4, ESR1, CDC25A, RELA, ESR2, NFKB1, AR, KLF5, CYP2B6, RPS6KB1, CYP1a2, RPS6KA1, CYP1a1, CYP1b1, MAPK1, PGR	3.88E-10
PD-L1 expression and PD-1 checkpoint pathway in cancer	MAP2K3, ALK, MAP2K2, PTPN11, HIF1a, RELA, NFKB1, ZAP70, RPS6KB1, CSNK2B, TLR9, MAPK1, TLR4, MAP2K6	6.65E-10
Lipid and atherosclerosis	MAP2K3, HSP90AA1, HSP90AB1, TNF, RELA, NFKB1, CDC42, CASP9, CYP2C9, CASP8, CYP2B6, CYP1a1, MAPK1, RAC1, MAP3K7, TLR4, NOX1, MAP2K6, NFE2L2	3.02E-09
Central carbon metabolism in cancer	NTRK1, PDGFRB, RET, PDGFRA, LDHB, MAP2K2, NTRK3, SLC2A1, MAPK1, HIF1a, GSK, GLS	6.81E-09
Toxoplasmosis	MAP2K3, ITGB1, NOS2, TNF, RELA, NFKB1, CASP9, CASP8, ALOX5, MAPK1, MAP3K7, TLR4, MAP2K6	9.74E-08
Human immunodeficiency virus 1 infection	MAP2K3, MAP2K2, TNF, RELA, NFKB1, CASP9, CASP8, RPS6KB1, CHEK1, CDK1, PTK2B, MAPK1, RAC1, MAP3K7, TLR4, APOBEC3A, MAP2K6	1.05E-07
Chemical carcinogenesis - reactive oxygen species	NQO1, PTPN11, MT-ND4, MAP2K2, KEAP1, PTPN11, AHR, HIF1a, RELA, NFKB1, CYP1a2, CYP1a1, CYP1b1, MAPK1, RAC1, NOX1, NFE2L2	2.53E-07
Toll-like receptor signaling pathway	MAP2K3, MAP2K2, CASP8, TLR9, MAPK1, RAC1, TNF, MAP3K7, TLR4, RELA, NFKB1, MAP2K6	6.29E-07
HIF-1 signaling pathway	EGLN1, LDHB, MAP2K2, RPS6KB1, NOS2, SERPINE1, SLC2A1, MAPK1, HIF1a, TLR4, RELA, NFKB1	6.29E-07
Salmonella infection	MAP2K3, HSP90AA1, MAP2K2, HSP90AB1, RIPK2, TNF, RELA, NFKB1, CDC42, CASP8, TLR9, MAPK1, PKN1, RAC1, MAP3K7, TLR4, MAP2K6	9.82E-07
Fluid shear stress and atherosclerosis	NQO1, HSP90AA1, HSP90AB1, KEAP1, TNF, ACVR2B, RELA, NFKB1, RAC1, MAP3K7, NOX1, MAP2K6, NFE2L2	1.21E-06
Prostate cancer	PDGFRB, CASP9, PDGFRA, AR, HSP90AA1, MAP2K2, HSP90AB1, CCNE1, MAPK1, RELA, NFKB1	1.88E-06
Arachidonic acid metabolism	CYP2C9, CYP2B6, PLA2G1b, ALOX5, PLA2G2A, ALOX12, CYP2C19, PTGS2, PTGS1	4.02E-06
Hepatitis B	MAP2K3, MAP2K2, TNF, RELA, NFKB1, CASP9, CASP8, CCNE1, PTK2B, MAPK1, MAP3K7, TLR4, MAP2K6	5.59E-06
Human cytomegalovirus infection	CCR1, PDGFRA, MAP2K2, ROCK1, PTGS2, TNF, RELA, NFKB1, CASP9, CASP8, RPS6KB1, PTK2B, MAPK1, RAC1, MAP2K6	6.82E-06
PI3K-Akt signaling pathway	PDGFRB, ITGB1, NTRK1, RET, PDGFRA, HSP90AA1, MAP2K2, HSP90AB1, FLT4, RELA, NFKB1, CASP9, ERBB3, RPS6KB1, CCNE1, MAPK1, PKN1, RAC1, TLR4	7.03E-06
Adherens junction	CDC42, PTPN11, FER, ROCK1, CSNK2B, MAPK1, FYN, RAC1, MAP3K7, PTPRF	9.73E-06
MAPK signaling pathway	MAP2K3, PDGFRB, NTRK1, RET, PDGFRA, MAP2K2, FLT4, TNF, RELA, NFKB1, CDC42, ERBB3, RPS6KA1, MAPK1, RAC1, MAP3K7, MAP2K6	9.92E-06