

Supporting Information

Photoinduced Oxidative Activation of Electron-rich Arene: Alkenylation with H₂ Evolution under External-oxidant-free Conditions

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General Information

Unless otherwise stated, analytical grade solvents and commercially available reagents were used without further purification. 9-Mesityl-10-methylacridinium perchlorate ($\text{Acr}^+-\text{Mes ClO}_4^-$) is purchased from Tokyo Chemical Industry (TCI). The substituted styrene derivatives were prepared following references.¹ All manipulations were carried out by using standard schlenk techniques. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200–300 mesh silica gel in petroleum ether (bp. 60–90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum ether to the ethyl acetate. All new compounds were characterized by ^1H NMR, ^{13}C NMR and HRMS. The known compounds were characterized by ^1H NMR and ^{13}C NMR. The ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. The chemical shifts (δ) were given in part per million relative to internal tetramethyl silane (TMS, 0 ppm for ^1H), CDCl_3 (77.0 ppm for ^{13}C). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion + Hydrogen (M+H). IR spectra were recorded on a Mettler Toledo React IR 15 spectrometer using a diamond comb. GC-MS data was measured with a Shimadzu GC-MS-QP2010. Hydrogen gas content was analyzed by gas chromatography (7890-II, Tianmei, China, TCD, argon as a carrier gas and 5 Å molecular sieve column, a thermal conductivity detector). The source of the blue LEDs is the LED lights made by ourselves. The power of each blue light is 3W. There is 3.0 cm distance between the reactor and LEDs. The photographs of this photochemical setup were show below.

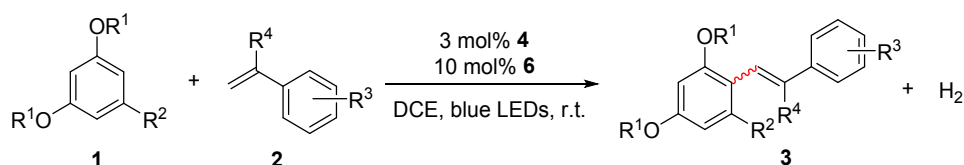


Experimental Procedures

1. Preparation of $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}^2$:

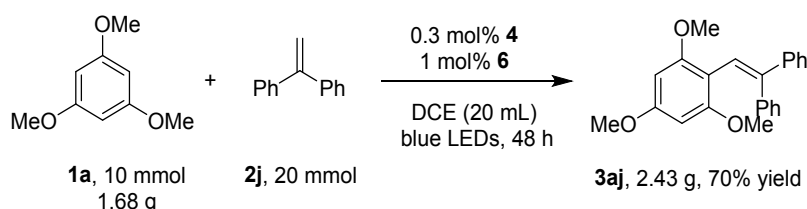
A 500 mg (1.48 mmol) sample of $[\text{Co}(\text{dmgH})(\text{dmgH}_2)\text{Cl}_2]$ was suspended in 50 mL of methanol. 4-(Dimethylamino)pyridine (361 mg, 2.96 mmol, 2 equiv) was then added to the flask, after 6 h, the green suspension change to a brown precipitate. The suspension was filtered and the precipitate washed with water (10 mL), ethanol (10 mL), and diethyl ether (10 mL) respectively to give $[\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}]$.

2. General procedure for external-oxidant-free oxidative cross-coupling of electron-rich arenes and styrenes:



A schlenk tube equipped with a stir bar was loaded with 9-mesityl-10-methylacridinium perchlorate **4** (0.006 mmol, 3 mol %), $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}$ **6** (0.02 mmol, 10 mol %), arene **1** (0.2 mmol) and styrenes **2** (0.4 mmol) in degassed dry DCE (4 mL) under N₂ atmosphere. The solution was then stirred at room temperature under the irradiation of 12W blue LED for 24 h. After completion of the reaction, the products were determined by TLC and GC-MS. Then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 50:1) to afford corresponding products **3**.

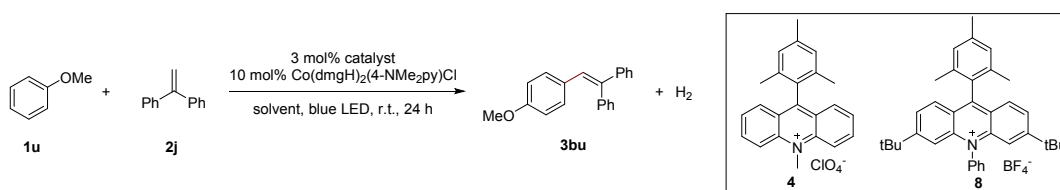
3. Gram scale synthesis:



A 100 mL schlenk flask equipped with a stir bar was loaded with 9-mesityl-10-methylacridinium perchlorate **4** (12 mg, 0.03 mmol, 0.3 mol %), $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}$ **6** (45 mg, 0.1 mmol, 1 mol %), 1,3,5-trimethoxybenzene **1a** (1.68 g, 10 mmol) and 1,1-diphenylethylene **2j** (3.6 g, 20 mmol) in

degassed dry DCE (20 mL) under N₂ atmosphere. The solution then stirred at room temperature under the irradiation of 30W blue LED for 48 h. After completion of the reaction, the product was determined by TLC and GC-MS. Then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 50:1) to afford corresponding stilbene derivatives **3aj** in 70% yield (2.43 g).

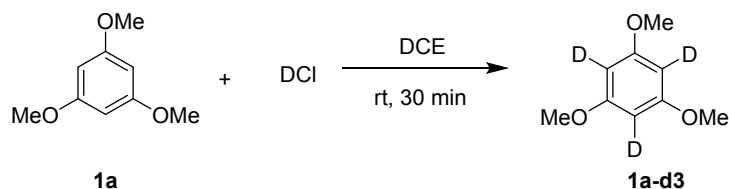
4. Condition optimization of the alkenylation of anisole:



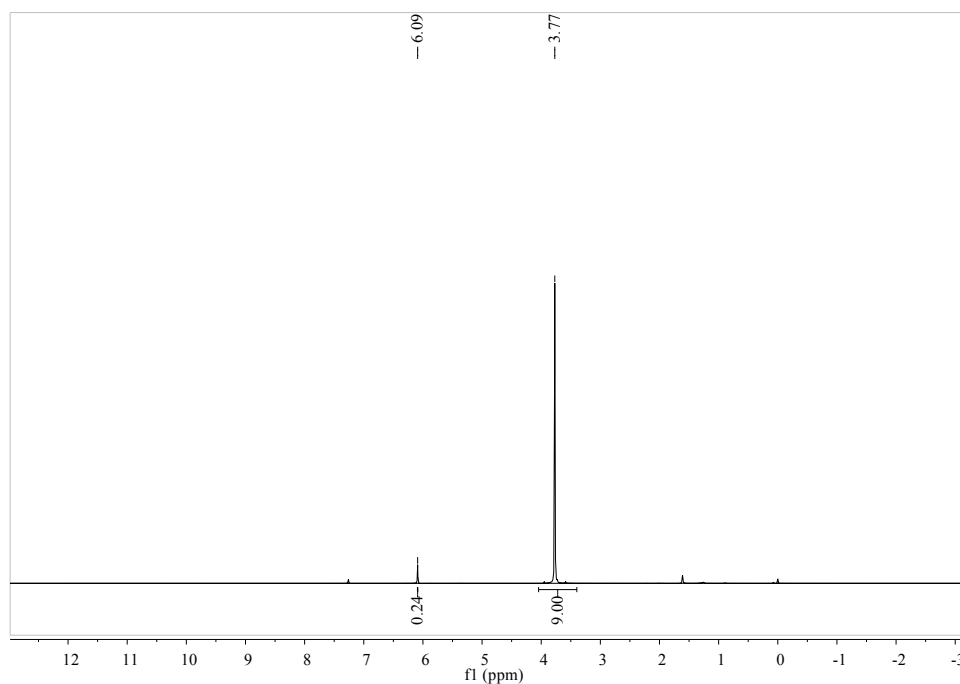
entry	catalyst	solvent	yield(%)
1	4	DCE	n.d.
2	4	DCE/HFIP	trace
3	8	DCE/HFIP	5
4	8	CHCl ₃ /HFIP	15

5. Kinetic isotope effect (KIE) experiment:

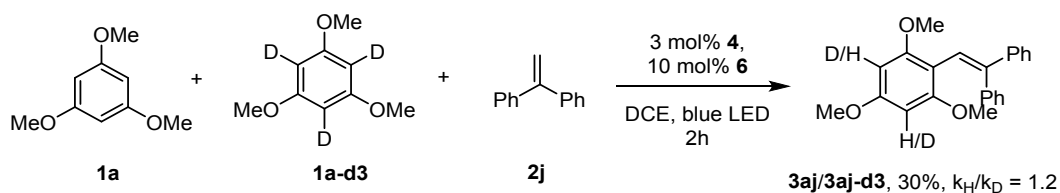
Synthesis of 1,3,5-trimethoxybenzene-d₃.



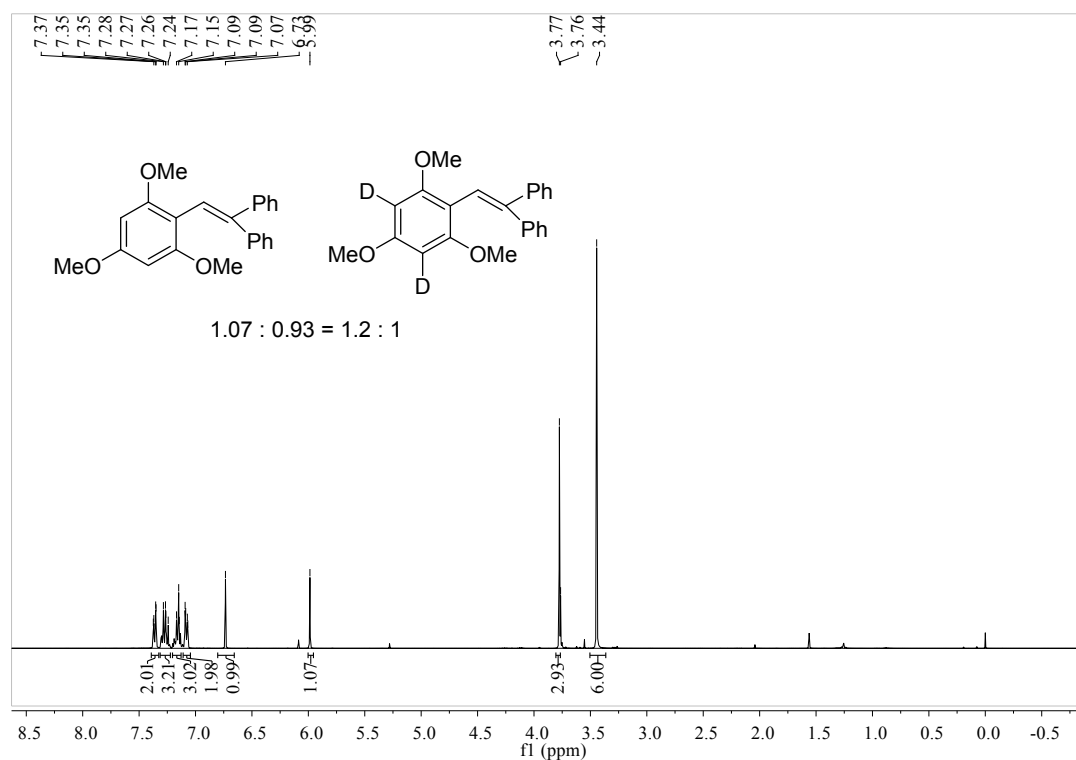
In an oven dried schlenk tube equipped with a stir-bar, 1,3,5-trimethoxybenzene (2.0 mmol) was added. The reaction tube was allowed to be vacuumed and purged with nitrogen for three times. Then, 1,2-dichloroethane (2 mL) and deuterium chloride solution (1 mL, 35 wt. % in D₂O, 99 atom % D (Aldrich)) was added by syringe under nitrogen. Finally, the schlenk tube was allowed to stir at room temperature for 30 min. After completion of the reaction, the reaction mixture was extracted with dichloromethane (3 x 5 mL). The organic layers were combined and dried over sodium sulfate. The desired product (92 atom % D) was obtained after removing the solvent. ¹H NMR spectra for the product was shown as follow:



Procedure for KIE measurement.



A schlenk tube equipped with a stir bar was loaded with 9-mesityl-10-methylacridinium perchlorate **4** (0.006 mmol, 3 mol %), $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}$ **6** (0.02 mmol, 10 mol %), 1,3,5-trimethoxybenzene **1a** (0.1 mmol), 1,3,5-trimethoxybenzene-d3 **1a-d3** (0.1 mmol), and 1,1-diphenylene **2j** (0.4 mmol) in degassed dry DCE (4 mL) under N_2 atmosphere. The solution then stirred at room temperature under the irradiation of 12W blue LED for 2 h. After then, the products was determined by TLC and GC-MS. Then the pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 50:1) to afford corresponding stilbene derivatives **3aj/3aj-d3** in 30% yield. ^1H NMR spectra for the isolated product was shown as follow, which indicate that the ratio of **3aj:3aj-d3** is 1.2:1.



6. Kinetic studies by using Operando-IR.

General procedure of in-situ IR experiments

General procedure: In a self-prepared three-necked micro reactor with a magnetic stirrer, $\text{Acr}^+\text{-Mes ClO}_4^-$ (12.0 mg, 0.03 mmol), $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}$ (45 mg, 0.1 mmol) and 1,3,5-trimethoxybenzene **1a** (168 mg, 1 mmol) were added. The reactor was allowed to be vacuumed and purged with nitrogen for three times. Then 10 mL degassed DCE was added via a syringe. After complete dissolution of catalysts, the alkene (2 mmol) was added. The mixture was allowed to stir at 40 °C and recorded by React IR. 5 mins later, a 30 W blue LED lamp was turned on. The course of the reaction could be observed from the characteristic IR band of olefin. After 4 hours, the reaction was stopped. The yield of corresponding product was detected by GC-FID using naphthalene as the internal standard.

According to operation of aforementioned general procedure of Operando-IR, the olefination of **1a** with 1,1-diphenylene **2j** was monitored by React IR 15. Absorption peak of the **1a** at 1150 cm^{-1} was found. And with the decrease in absorption of this peak, a new peak at 1025 cm^{-1} belonged to the product **3aj** can be observed through in-situ IR. After 4 hours, 0.5 mmol of **3aj** was afforded. The reaction was recorded by React IR as shown in Fig. S1. The 2D spectroscopy was also shown.

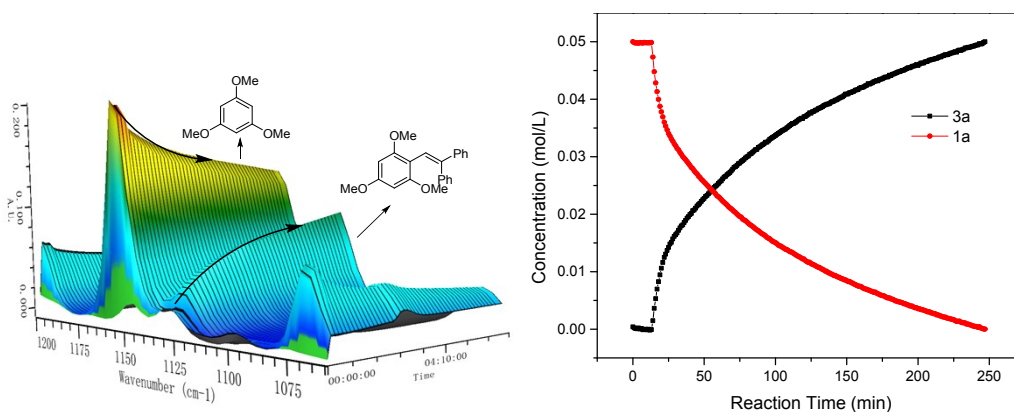


Figure S1. Kinetic plots of olefination of **1a** with 1,1-diphenylene.

Kinetic studies

Reaction order for 1a. The reaction order with respect to **1a** was determined by studying the initial rate of reaction with different concentration of **1a**. Using the above mentioned general procedure, **1a** (0.5 ~ 2 mmol), $\text{Acr}^+\text{-Mes ClO}_4^-$ (12.0 mg, 0.03 mmol), $\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{Py})\text{Cl}$ (45 mg, 0.1 mmol) and 1,1-diphenylene **2j** (2 mmol) were added. Product yield from the corresponding reaction was monitored by GC-FID using naphthalene as the internal standard. Finally, the profiles of relative concentrations vs time for product **3aj** could be obtained to analyse the initial rate of reaction. A plot of initial rate ($\Delta[\mathbf{3aj}]/\Delta t$) versus $[\mathbf{1a}]$ gave a straight line ($R^2 = 0.99422$), indicative of a first order with respect to $[\mathbf{1a}]$.

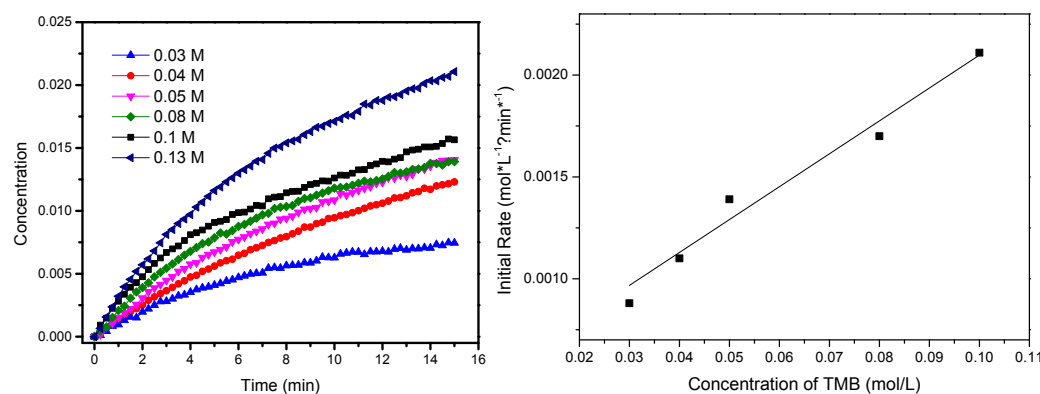


Figure S2. First order kinetic experiment dependence on $[\mathbf{1a}]$.

Reaction orders for alkene, photosensitizer and cobalt complex. The reaction orders with respect to alkene, photosensitizer, and cobalt complex were also determined by the same method. From Figure S3-S5, the initial rate of reaction was changeless when using different concentrations of alkene and cobalt complex. Therefore, these results indicated a zero order reaction dependence on $[\text{Co}(\text{dmgH})_2(4\text{-NMe}_2\text{py})\text{Cl}]$ and $[\mathbf{2j}]$. When the concentration of photosensitizer is low, the initial

rate constant is linearly related to the concentration of photosensitizer. The reaction rate is saturated in high concentration of photosensitizer. This may be due to the limited number of photons of the used LED lamp.

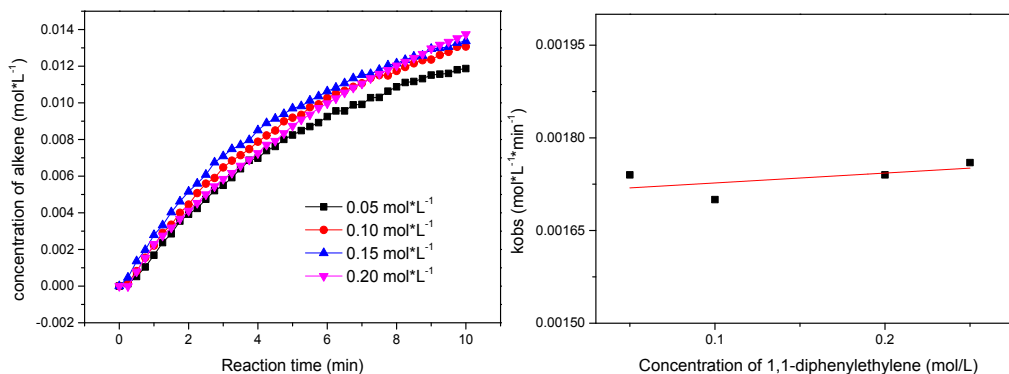


Figure S3. The profiles of relative initial rate vs time in different [2j].

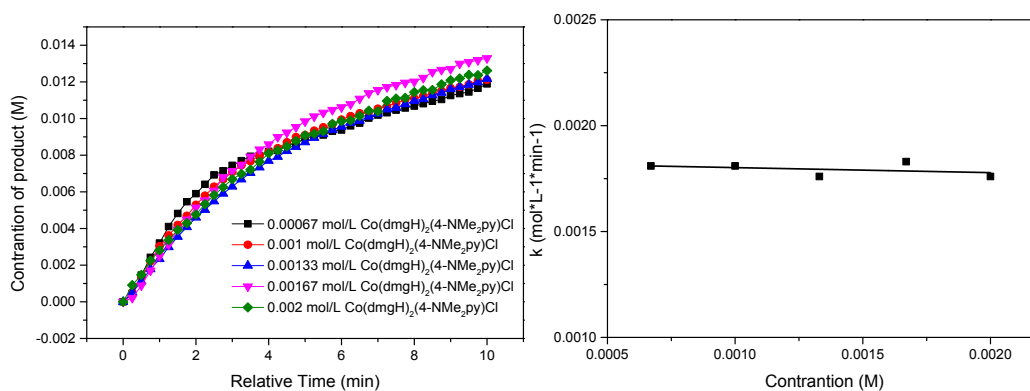


Figure S4. The profiles of relative initial rate vs time in different [Co(dmgh)₂(4-NMe₂py)Cl].

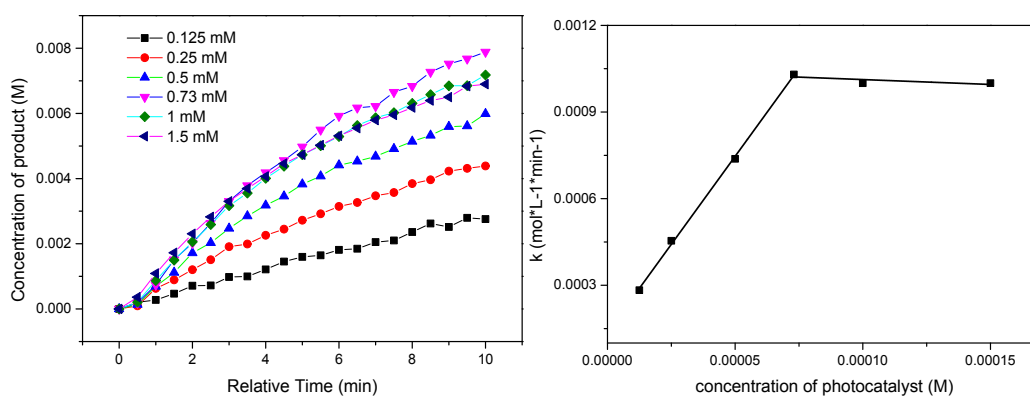


Figure S5. The profiles of relative initial rate vs time in different [Acr⁺-Mes ClO₄⁻].

7. Emission quenching experiments for Acr⁺-Mes ClO₄⁻.

Emission intensities were recorded using a HITACHI F-4500 Fluorescence Spectrometer. All $\text{Acr}^+\text{-Mes ClO}_4^-$ solutions were excited at 450 nm and the emission intensity at 512 nm was observed. DCE was degassed with a stream of N_2 for 30 min and then moved to glove box. All the solutions were prepared in the glove box. In a typical experiment, the emission spectrum of a 5×10^{-4} M solution of $\text{Acr}^+\text{-Mes ClO}_4^-$ in DCE was collected. Then, appropriate amount of quencher was added to the measured solution and the emission spectrum of the sample was collected.

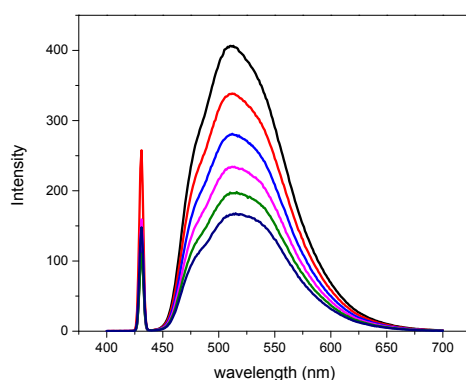


Figure S6. $\text{Acr}^+\text{-Mes ClO}_4^-$ emission quenching by 1,3,5-trimethoxybenzene.

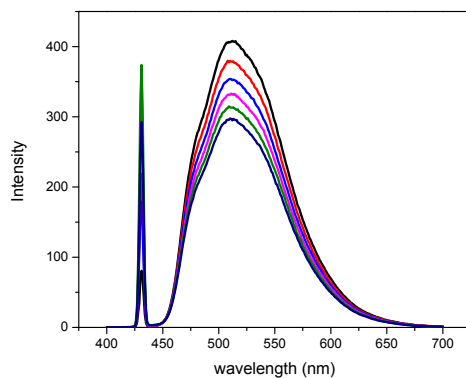


Figure S7. $\text{Acr}^+\text{-Mes ClO}_4^-$ emission quenching by styrene.

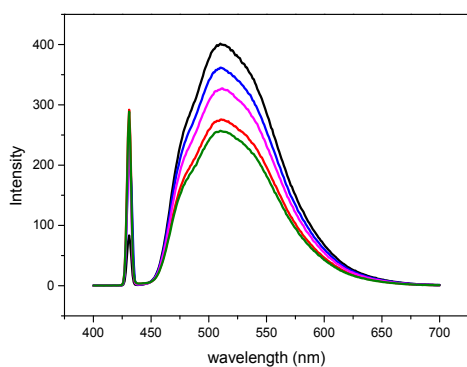


Figure S8. Acr⁺-Mes ClO₄⁻ emission quenching by 1,1-diphenylethene.

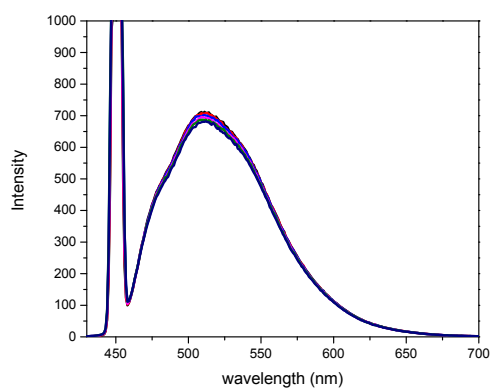


Figure S9. Acr⁺-Mes ClO₄⁻ emission quenching by 4-cyanostyrene.

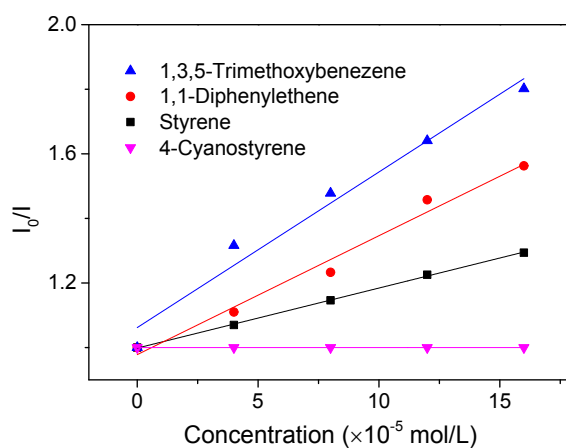
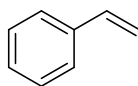
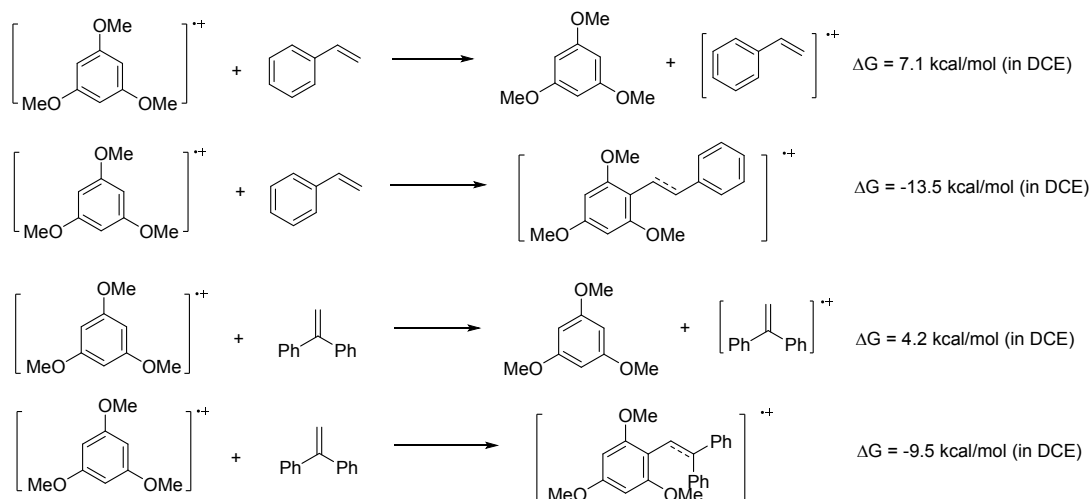


Figure S10. Stern-Volmer emission quenching studies of Acr⁺-Mes ClO₄⁻ by 1,3,5-trimethoxybenzene, styrene, 1,1-diphenylethene and 4-cyanostyrene.

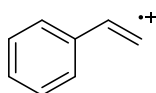
8. General Computational Calculation Details

DFT calculations were performed using the M06-2X levels of theory³ with the Gaussian09 program⁴. The 6-311+G(d,p) basis set was used for the C, H and O. Frequency calculations at the same level of theory have been performed to identify all of the stationary points as minima (zero imaginary frequencies) and to provide free energies at 298.15 K. The solvation energies were calculated with SMD model⁵. Solvation effect was taken into consideration during geometry optimization with dichloroethane as the solvent.



Thermal correction to Gibbs Free Energy=	0.102753		
Sum of electronic and thermal Free Energies=	-309.490807		
C	-1.77871400	-1.03990900	-0.00000600
C	-0.40771500	-1.28153300	0.00000000
C	0.51005000	-0.22572000	0.00000600
C	0.01737800	1.08621000	0.00000600
C	-1.34984600	1.32862100	0.00000000
C	-2.25458100	0.26688900	-0.00000700
H	-2.47276500	-1.87270600	-0.00001100
H	-0.03861100	-2.30218600	0.00000100
H	0.70494300	1.92426400	0.00001300
H	-1.71381000	2.34987300	0.00000000

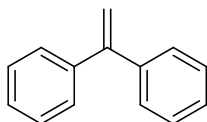
H	-3.32112800	0.46029700	-0.00001200
C	1.95307900	-0.53794400	0.00001100
H	2.18948900	-1.59978100	0.00003000
C	2.95568800	0.34100700	-0.00000800
H	2.79499600	1.41398700	-0.00003100
H	3.98485000	0.00052200	-0.00000500



Thermal correction to Gibbs Free Energy= 0.102833

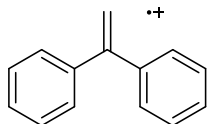
Sum of electronic and thermal Free Energies= -309.255993

C	-1.77527200	-1.04569800	0.00000000
C	-0.42958400	-1.30967200	0.00000200
C	0.51803900	-0.23920700	0.00000100
C	0.04101900	1.11033900	-0.00000200
C	-1.30633400	1.35994200	-0.00000400
C	-2.21718700	0.28838500	-0.00000300
H	-2.49644100	-1.85303900	0.00000100
H	-0.06171600	-2.32927100	0.00000500
H	0.74127500	1.93533800	-0.00000200
H	-1.67508100	2.37740900	-0.00000600
H	-3.28094900	0.49652200	-0.00000500
C	1.89354400	-0.57052300	0.00000300
H	2.14406100	-1.62707500	0.00000500
C	2.92739800	0.33986300	0.00000200
H	2.76730700	1.41065300	-0.00000100
H	3.95181000	-0.01111000	0.00000300



Thermal correction to Gibbs Free Energy=			0.177691
Sum of electronic and thermal Free Energies=			-540.439138
C	0.00000000	2.50736400	-0.00000700
H	0.92472200	3.07029600	-0.06643300
H	-0.92472300	3.07029600	0.06641600
C	0.00000000	1.16932800	-0.00000300
C	1.27539500	0.39991000	-0.04174000
C	1.38498800	-0.74509400	-0.83962600
C	2.39013300	0.81372600	0.69459900
C	2.58588700	-1.44122900	-0.91996800
H	0.52687000	-1.08390700	-1.41061600
C	3.58976300	0.11201100	0.62078400
H	2.31031900	1.68149400	1.34030700
C	3.69261900	-1.01551400	-0.18902600
H	2.65605900	-2.31882100	-1.55273700
H	4.44214900	0.44096700	1.20461800
H	4.62652500	-1.56300400	-0.24531400
C	-1.27539500	0.39991000	0.04173700
C	-1.38499000	-0.74508500	0.83963600
C	-2.39013100	0.81372000	-0.69460800
C	-2.58588900	-1.44121900	0.91998100
H	-0.52687400	-1.08389200	1.41063000
C	-3.58976100	0.11200600	-0.62079000
H	-2.31031400	1.68148100	-1.34032500
C	-3.69261900	-1.01551100	0.18903200
H	-2.65606400	-2.31880500	1.55275900

H	-4.44214500	0.44095500	-1.20463000
H	-4.62652500	-1.56300000	0.24532300

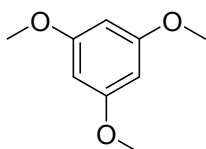


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Sum of electronic and thermal Free Energies= -540.208888

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H	0.92604900	3.06115500	-0.00730300
H	-0.92604900	3.06115300	0.00732100
C	0.00000100	1.10582800	0.00000000
C	1.26100100	0.38751000	-0.03828300
C	1.34335900	-0.85205500	-0.71269700
C	2.42323900	0.92189900	0.56229000
C	2.54653200	-1.53106700	-0.77815000
H	0.47035100	-1.24335400	-1.22174100
C	3.61311600	0.22250000	0.51369700
H	2.37396200	1.85806900	1.10517700
C	3.67864900	-1.00076900	-0.15951700
H	2.60972300	-2.46824000	-1.31714500
H	4.49505500	0.62262100	0.99842200
H	4.61938500	-1.53706300	-0.20784500
C	-1.26100000	0.38751000	0.03828200
C	-1.34336100	-0.85205000	0.71270200
C	-2.42323600	0.92189600	-0.56229900
C	-2.54653600	-1.53106100	0.77815600
H	-0.47035400	-1.24334700	1.22175100
C	-3.61311400	0.22249800	-0.51370500

H	-2.37395700	1.85806300	-1.10519200
C	-3.67865000	-1.00076700	0.15951700
H	-2.60972800	-2.46823000	1.31715700
H	-4.49505000	0.62261600	-0.99843600
H	-4.61938600	-1.53705900	0.20784600

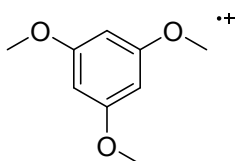


Thermal correction to Gibbs Free Energy= 0.159348

Sum of electronic and thermal Free Energies= -575.593010

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C	0.85084900	-1.09294500	0.00006500
C	-0.51792500	-1.30555400	0.00003600
C	-1.37204800	-0.18986000	-0.00005400
C	-0.87247400	1.10204100	-0.00008200
C	0.52092900	1.28363500	-0.00011400
H	2.46468000	0.31831100	0.00001200
H	-0.95862400	-2.29251600	0.00009600
H	-1.50764300	1.97651000	-0.00009600
O	1.76718900	-2.09133900	0.00011200
O	-2.69482200	-0.48458100	0.00003600
O	0.92813900	2.57630300	-0.00010800
C	2.32530100	2.83066400	-0.00004900
H	2.43316900	3.91363400	-0.00008300
H	2.79975100	2.41781900	0.89461700
H	2.79985000	2.41776000	-0.89463500
C	-3.61572600	0.59637600	-0.00003500
H	-4.60651400	0.14624200	0.00012500

H	-3.49652900	1.21472200	0.89402700
H	-3.49672400	1.21450000	-0.89426800
C	1.29065800	-3.42904400	0.00016000
H	0.69621300	-3.63462800	-0.89448200
H	2.17563400	-4.06262900	0.00026400
H	0.69606500	-3.63456200	0.89471200

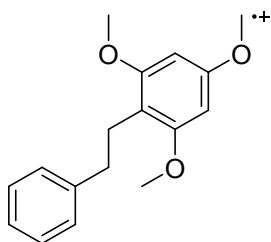


Thermal correction to Gibbs Free Energy= 0.161502

Sum of electronic and thermal Free Energies= -575.369515

C	-1.24413500	0.24176800	-0.00001400
C	-0.90131000	-1.09166900	-0.00000300
C	0.47523400	-1.49726500	-0.00002000
C	1.51458300	-0.52487500	-0.00005100
C	1.19148000	0.80512000	-0.00009600
C	-0.18887000	1.17918600	-0.00006800
H	-2.27445100	0.56318400	-0.00001500
H	0.71920800	-2.55303600	-0.00000300
H	1.92855900	1.59632400	-0.00012500
O	-1.74912100	-2.10210300	0.00001500
O	2.74415800	-1.03206400	-0.00002900
O	-0.38165600	2.47085200	-0.00010400
C	-1.71418900	3.01634400	0.00015500
H	-1.57922400	4.09368100	0.00025300
H	-2.24380400	2.70013500	-0.89920800
H	-2.24352700	2.69992600	0.89960600
C	3.83984500	-0.11273200	-0.00002000

H	4.73778900	-0.72475800	0.00000800
H	3.81262000	0.51035200	-0.89741500
H	3.81258300	0.51038100	0.89735300
C	-3.15352700	-1.81565600	0.00012400
H	-3.42137400	-1.25444800	-0.89738000
H	-3.64888400	-2.78220400	0.00022300
H	-3.42122100	-1.25434900	0.89761100

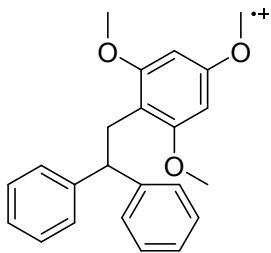


Thermal correction to Gibbs Free Energy= 0.290104

Sum of electronic and thermal Free Energies= -884.881809

C	2.81460900	-1.04799600	-0.03585600
C	3.40072300	0.22345700	0.12766800
C	2.65457400	1.43270500	0.03755200
C	1.31306300	1.36736000	-0.22039000
C	0.66589700	0.09804900	-0.41500900
C	1.46254700	-1.10225100	-0.29197900
H	3.40886000	-1.94531200	0.04105800
H	3.18123300	2.36562900	0.18251000
O	0.50131200	2.41770100	-0.32046000
O	4.67426300	0.39741600	0.37871900
O	0.77030800	-2.21734700	-0.45062800
C	1.45266500	-3.47338500	-0.36077000
H	1.91127500	-3.58350600	0.62399700
H	0.68758300	-4.23130400	-0.50450900
H	2.20719600	-3.54686300	-1.14678200

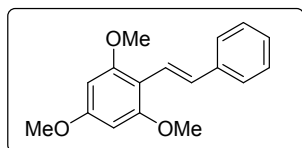
C	1.07152800	3.71907100	-0.16110500
H	1.83036900	3.89619900	-0.92675600
H	0.24892900	4.41829700	-0.28462000
H	1.50534000	3.82524000	0.83588900
C	5.55355300	-0.73312600	0.51020400
H	5.55587500	-1.31484200	-0.41216700
H	6.53732500	-0.30804000	0.68743200
H	5.24869900	-1.34609000	1.35952400
C	-0.79179600	0.02293400	-0.66189600
H	-1.03572500	-0.88248500	-1.21698800
H	-1.11477100	0.89645400	-1.22948100
C	-1.55478200	0.00264700	0.69615700
H	-1.22271000	-0.85962600	1.27888300
H	-1.30737000	0.90873400	1.25420300
C	-3.03933900	-0.07389600	0.45396400
C	-3.69598300	-1.30532100	0.44864800
C	-3.77290800	1.08476900	0.18789200
C	-5.06173000	-1.37914700	0.18734100
H	-3.13345600	-2.21059900	0.65646100
C	-5.13757200	1.01408000	-0.07452100
H	-3.26848500	2.04666900	0.19187900
C	-5.78527500	-0.21924600	-0.07602300
H	-5.56104300	-2.34151800	0.19164700
H	-5.69612800	1.92135500	-0.27582600
H	-6.84871500	-0.27477100	-0.27866300



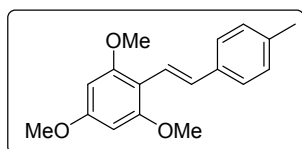
Thermal correction to Gibbs Free Energy=			0.367010
Sum of electronic and thermal Free Energies=			-1115.823738
C	-2.98210900	0.23610800	-0.78559900
C	-3.41606300	-0.83943700	0.01287900
C	-2.56740300	-1.92613100	0.37167500
C	-1.26517700	-1.91459000	-0.04399800
C	-0.75240900	-0.81560200	-0.81902600
C	-1.67164800	0.23078400	-1.21194900
H	-3.65798700	1.03096100	-1.06072100
H	-2.99048900	-2.72013400	0.97127100
O	-0.36518700	-2.85925200	0.22398900
O	-4.63576000	-0.93928800	0.47974500
O	-1.13177100	1.15646900	-1.98177700
C	-1.89112700	2.32904100	-2.29183100
H	-2.20445900	2.82565600	-1.37075600
H	-1.21966700	2.97082600	-2.85638200
H	-2.75869200	2.06776800	-2.90191700
C	-0.78218600	-3.97936900	1.00903400
H	-1.58590000	-4.51903200	0.50325200
H	0.09366000	-4.61615300	1.10078800
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C	-5.60442000	0.08856800	0.20983300
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H	-6.50605200	-0.22744100	0.72663800

H	-5.25616200	1.04257300	0.60746400
C	0.70515900	-0.71394600	-1.08250100
H	0.90785700	0.00854100	-1.87158100
H	1.08732000	-1.69175800	-1.37976900
C	1.43898700	-0.27578900	0.23397800
H	1.20581800	-1.03437000	0.98629200
C	2.94644700	-0.32943200	0.01831300
C	3.77774400	0.78875300	0.07516800
C	3.52770300	-1.58042800	-0.22454600
C	5.15322500	0.66189800	-0.12208300
H	3.36568800	1.76720200	0.28771800
C	4.89671800	-1.70900900	-0.41855200
H	2.89840900	-2.46582400	-0.24732600
C	5.71700300	-0.58234300	-0.37377000
H	5.78195300	1.54397800	-0.07401000
H	5.32629000	-2.68824500	-0.59820600
H	6.78590200	-0.67858900	-0.52602700
C	0.88252200	1.04354700	0.73146200
C	0.27312600	1.10777700	1.98499900
C	0.89908800	2.19326300	-0.06512800
C	-0.30031600	2.29351800	2.44168300
H	0.24740400	0.21921700	2.60876000
C	0.32770000	3.37773500	0.38590300
H	1.35369300	2.15917000	-1.05026800
C	-0.27537600	3.43108900	1.64171400
H	-0.76619200	2.32531900	3.42012800
H	0.34859100	4.25987900	-0.24465500
H	-0.71980000	4.35516400	1.99383200

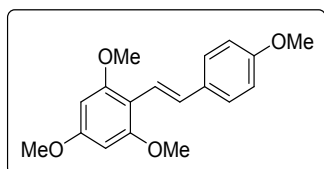
Characterization of Products



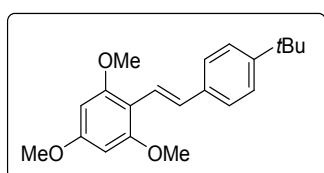
(*E*)-1,3,5-Trimethoxy-2-styrylbenzene (**3aa**), 37.8 mg, 70% yield, yellow oil. Only the data of *E*-isomer was shown here. ^1H NMR (400 MHz, CDCl_3) δ 7.54 (d, $J = 7.3$ Hz, 2H), 7.49 (d, $J = 16.8$ Hz, 1H), 7.42 (d, $J = 16.6$ Hz, 1H), 7.34 (t, $J = 7.7$ Hz, 2H), 7.21 (t, $J = 7.3$ Hz, 1H), 6.19 (s, 2H), 3.90 (s, 6H), 3.85 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 160.2, 159.5, 139.7, 129.9, 128.4, 126.5, 126.1, 119.8, 108.1, 90.8, 55.8, 55.3; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{19}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 271.1329 found 271.1321.



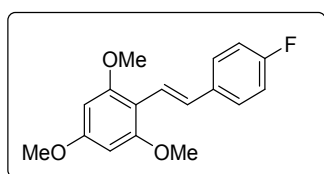
(*E*)-1,3,5-Trimethoxy-2-(4-methylstyryl)benzene (**3ab**), 34.6 mg, 61% yield, white solid. Only the data of *E*-isomer was shown here. ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, $J = 17.1$ Hz, 2H), 7.39 (s, 1H), 7.34 (d, $J = 16.6$ Hz, 1H), 7.12 (d, $J = 8.0$ Hz, 2H), 6.15 (s, 2H), 3.86 (s, 6H), 3.81 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.0, 159.3, 136.8, 136.2, 129.8, 129.1, 126.0, 118.8, 108.2, 90.7, 55.7, 55.2, 21.2; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{21}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 285.1485 found 285.1488.



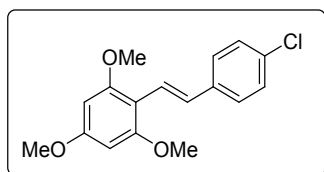
(*E*)-1,3,5-Trimethoxy-2-(4-methoxystyryl)benzene (**3ac**), 31.8 mg, 53% yield, white solid. Only the data of *E*-isomer was shown here. ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.34 (m, 3H), 7.24 (d, $J = 9.6$ Hz, 1H), 6.86 (d, $J = 8.7$ Hz, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.8, 159.2, 158.5, 132.4, 129.5, 127.2, 117.8, 113.8, 108.3, 90.8, 55.7, 55.3, 55.3; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{21}\text{O}_4^+$, $[\text{M}+\text{H}]^+$, 301.1434 found 301.1424.



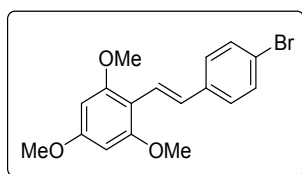
Only the data of *E*-isomer was shown here. (*E*)-2-(4-(Tert-butyl)styryl)-1,3,5-trimethoxybenzene (**3ad**), 41.7 mg, 64% yield, white solid. ¹H NMR (400 MHz, CDCl₃) δ 7.48 (s, 1H), 7.45 (d, *J* = 7.7 Hz, 2H), 7.38 (d, *J* = 2.7 Hz, 2H), 7.35 (d, *J* = 5.6 Hz, 1H), 6.18 (s, 2H), 3.89 (s, 6H), 3.85 (s, 3H), 1.35 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 160.0, 159.4, 149.5, 137.0, 129.9, 125.9, 125.4, 119.2, 108.4, 90.9, 55.8, 55.3, 34.5, 31.4; HRMS (ESI) calcd for C₂₁H₂₇O₃⁺, [M+H]⁺, 327.1955 found 327.1951.



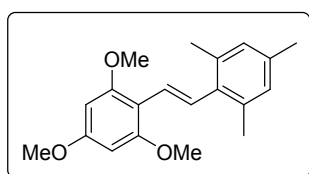
(*Z*, *E*)-2-(4-Fluorostyryl)-1,3,5-trimethoxybenzene (**3ae**), 37.4 mg, 65% yield, white solid. A mixture of *Z*/*E* isomers was isolated (*Z*/*E* = 1: 13 ratio determined based on GC). ¹H NMR (400 MHz, CDCl₃) of *E*-isomer: δ 7.50 – 7.37 (m, 3H), 7.29 (d, *J* = 16.6 Hz, 1H), 7.04 – 6.95 (m, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) mixture of *Z*/*E* isomers: δ 163.0 (*J*_{CF} = 245.2 Hz), 160.2, 159.4, 158.3, 135.8, 135.7, 129.8, 129.4, 129.3, 128.6, 127.5, 127.4, 119.6, 119.5, 115.20 (*J*_{C-F} = 21.5 Hz), 114.4 (d, *J* = 21.2 Hz), 107.9, 90.7, 55.7, 55.3; ¹⁹F NMR (377 MHz, CDCl₃) mixture of *Z*/*E* isomers: δ -115.57, -116.25; HRMS (ESI) calcd for C₁₇H₁₈FO₃⁺, [M+H]⁺, 289.1234 found 289.1227.



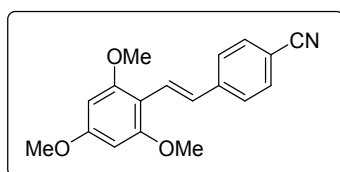
(*E*)-2-(4-Chlorostyryl)-1,3,5-trimethoxybenzene (**3af**), 31.6 mg, 52% yield, white solid. Only the data of *E*-isomer was shown here. ¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 4.6 Hz, 2H), 7.29 – 7.23 (m, 2H), 6.16 (s, 2H), 3.88 (s, 6H), 3.83 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 160.4, 159.6, 138.2, 131.9, 128.5, 128.5, 127.3, 120.5, 107.8, 90.7, 55.8, 55.4; HRMS (ESI) calcd for C₁₇H₁₈ClO₃⁺, [M+H]⁺, 305.0939 found 305.0938.



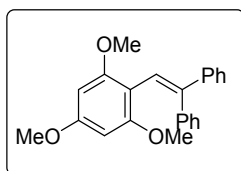
(*E*)-2-(4-Bromostyryl)-1,3,5-trimethoxybenzene (**3ag**), 36.3 mg, 52% yield, white solid. Only the data of *E*-isomer was shown here. ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.44 (m, 2H), 7.42 (s, 2H), 7.42 – 7.36 (m, 2H), 6.20 (s, 2H), 3.91 (s, 6H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.5, 159.6, 138.7, 131.5, 128.5, 127.7, 120.6, 120.0, 107.7, 90.7, 55.8, 55.4; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{18}\text{BrO}_3^+$, $[\text{M}+\text{H}]^+$, 349.0434 found 349.0427.



(*E*)-1,3,5-Trimethoxy-2-(2,4,6-trimethylstyryl)benzene (**3ah**), 58.0 mg, 93% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.36 (d, $J = 17.0$ Hz, 1H), 6.92 (s, 2H), 6.81 (d, $J = 17.0$ Hz, 1H), 6.21 (s, 2H), 3.87 (s, 6H), 3.87 (s, 3H), 2.40 (s, 6H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.0, 159.3, 136.4, 135.9, 135.4, 128.8, 128.6, 124.4, 108.7, 91.0, 55.9, 55.4, 21.2, 21.0; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{25}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 313.1798 found 313.1794.



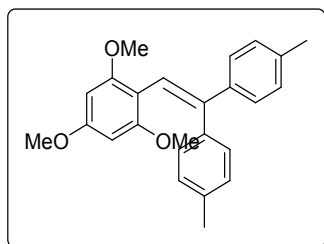
(*Z, E*)-4-(2,4,6-trimethoxystyryl)benzonitrile (**3ai**), 43% yield, 25.4 mg, white solid. A mixture of *Z/E* isomers was isolated (*Z/E* = 1: 6 ratio determined based on ^1H NMR and GC). ^1H NMR (400 MHz, CDCl_3) of *E*-isomer δ 7.45 (d, $J = 8.4$ Hz, 2H), 7.30 – 7.23 (m, 2H), 6.63 – 6.55 (m, 2H), 6.10 (s, 2H), 3.84 (s, 3H), 3.58 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) of *E*-isomer δ 161.7, 158.5, 144.3, 131.7, 129.2, 128.5, 124.7, 119.6, 109.7, 107.1, 90.8, 55.6, 55.6; ; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{25}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 296.1281 found 296.1289.



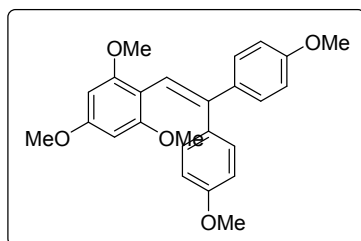
(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)dibenzene (**3aj**), 68.5 mg, 99% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.43 – 7.40 (m, 2H), 7.37 – 7.28 (m, 3H), 7.25 – 7.17 (m, 3H), 7.17 – 7.09 (m, 2H), 6.79 (s, 1H), 6.04 (s, 2H), 3.83 (s, 3H), 3.50 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.6,

158.4, 143.9, 143.5, 142.5, 129.5, 128.4, 127.9, 127.4, 127.0, 126.5, 119.8, 109.0, 90.3, 55.3, 55.2;

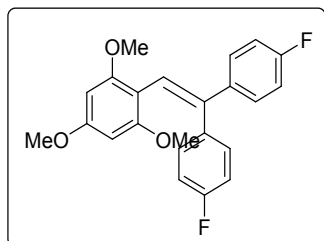
HRMS (ESI) calcd for $C_{23}H_{22}O_3^+$, $[M+H]^+$, 347.1642 found 347.1635.



4,4'-(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)bis(methylbenzene) (**3ak**), 67.3 mg, 89% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, $J = 8.1$ Hz, 2H), 7.09 (d, $J = 8.0$ Hz, 2H), 6.96 (s, 4H), 6.65 (s, 1H), 5.99 (s, 2H), 3.78 (s, 3H), 3.45 (s, 6H), 2.34 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 158.3, 143.3, 141.2, 139.5, 136.6, 135.8, 129.3, 128.5, 128.2, 128.0, 118.6, 109.3, 90.4, 55.2, 55.1, 21.2, 21.1; HRMS (ESI) calcd for $C_{25}H_{17}O_3^+$, $[M+H]^+$, 375.1955 found 375.1946.

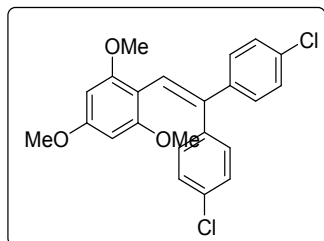


4,4'-(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)bis(methoxybenzene) (**3al**), 80.4 mg, 99% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.25 (m, 2H), 7.03 – 6.93 (m, 2H), 6.86 – 6.75 (m, 2H), 6.74 – 6.63 (m, 2H), 6.58 (s, 1H), 6.00 (s, 2H), 3.81 (s, 3H), 3.78 (s, 3H), 3.76 (s, 3H), 3.48 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 158.8, 158.2, 158.1, 142.6, 136.7, 135.1, 130.5, 129.4, 117.4, 113.1, 112.7, 109.4, 90.3, 55.2, 55.2, 55.2, 55.1; HRMS (ESI) calcd for $C_{25}H_{27}O_5^+$, $[M+H]^+$, 407.1853 found 407.1826.

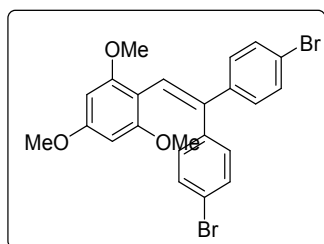


4,4'-(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)bis(fluorobenzene) (**3am**), 71.0 mg, 93% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.10 – 7.00 (m, 2H), 6.99 – 6.94 (m, 2H), 6.90 – 6.81 (m, 2H), 6.65 (s, 1H), 6.00 (s, 2H), 3.78 (s, 3H), 3.49 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1 ($J_{C-F} = 63.5$ Hz), 160.71, 160.67 ($J_{C-F} = 62.7$ Hz), 158.2, 141.4, 139.7 ($J_{C-F} = 62.7$ Hz),

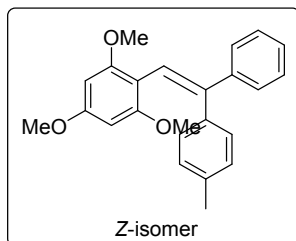
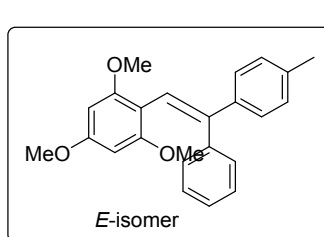
138.2 ($J_{C-F} = 3.3$ Hz), 130.9 ($J_{C-F} = 7.8$ Hz), 129.7 ($J_{C-F} = 7.9$ Hz), 119.8, 114.7 ($J_{C-F} = 21.3$ Hz), 114.3 ($J_{C-F} = 21.1$ Hz), 108.4, 90.2, 55.2, 55.1; ^{19}F NMR (377 MHz, CDCl_3) δ -115.72, -115.92; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{21}\text{F}_2\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 383.1453 found 383.1444.



4,4'-(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)bis(chlorobenzene) (**3an**), 77.1 mg, 93% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.25 (s, 4H), 7.15 (d, $J = 8.5$ Hz, 2H), 7.00 (d, $J = 8.5$ Hz, 2H), 6.71 (s, 1H), 5.99 (s, 2H), 3.78 (s, 3H), 3.48 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.9, 158.1, 141.8, 140.9, 140.5, 132.9, 132.1, 130.6, 129.4, 128.0, 127.7, 120.8, 108.1, 90.2, 55.2, 55.0; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{21}\text{Cl}_2\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 415.0862 found 415.0852.

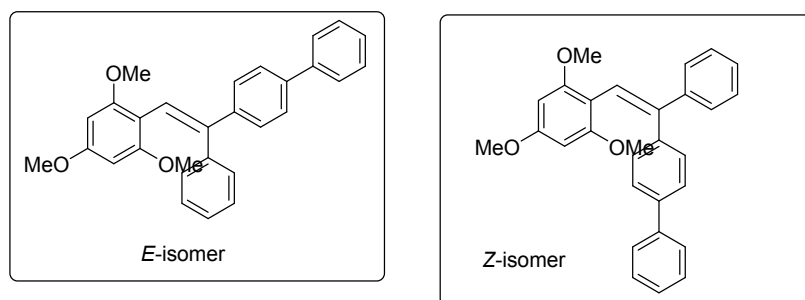


4,4'-(2-(2,4,6-Trimethoxyphenyl)ethene-1,1-diyl)bis(bromobenzene) (**3ao**), 75.3 mg, 75% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.40 (d, $J = 8.5$ Hz, 2H), 7.30 (d, $J = 8.4$ Hz, 2H), 7.19 (d, $J = 8.5$ Hz, 2H), 6.94 (d, $J = 8.4$ Hz, 2H), 6.72 (s, 1H), 5.99 (s, 2H), 3.79 (s, 3H), 3.48 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.0, 158.2, 142.2, 141.0, 140.9, 131.0, 131.0, 130.7, 129.8, 121.2, 120.9, 120.4, 108.1, 90.3, 55.2, 55.1; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{21}\text{Br}_2\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 502.9852 found 502.9810.

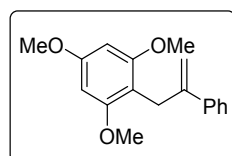


(*Z*, *E*)-1,3,5-Trimethoxy-2-(2-phenyl-2-(*p*-tolyl)vinyl)benzene (**3ap**), 71.3 mg, 99% yield, white solid. A mixture of *E/Z* isomers was isolated (53:47 ratio determined based on GC and ^1H NMR). ^1H NMR (400 MHz, CDCl_3) of *E*-isomer δ 7.36 – 7.29 (m, 3H), 7.24 – 7.18 (m, 2H), 7.17 – 7.11 (m, 2H), 7.02 (s, 2H), 6.75 (s, 1H), 6.03 (s, 2H), 3.82 (s, 3H), 3.49 (s, 6H), 2.40 (s, 3H); ^1H NMR (400 MHz, CDCl_3)

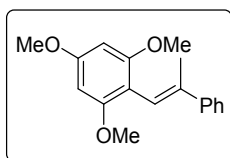
of *Z*-isomer: ^1H NMR (400 MHz, CDCl_3) δ 7.46 – 7.37 (m, 2H), 7.36 – 7.26 (m, 2H), 7.24 – 7.17 (m, 1H), 7.17 – 7.11 (m, 2H), 7.02 (s, 2H), 6.74 (s, 1H), 6.05 (s, 2H), 3.83 (s, 3H), 3.51 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) mixture of *Z/E* isomers: δ 160.4, 158.3, 158.3, 144.0, 143.4, 143.2, 142.5, 141.0, 139.4, 136.6, 135.8, 129.4, 129.3, 128.5, 128.3, 128.2, 128.0, 127.8, 127.3, 126.9, 126.3, 119.3, 119.0, 109.2, 109.0, 90.3, 90.3, 55.2, 55.1, 55.1, 21.2, 21.1; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{25}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 361.1798 found 361.1789.



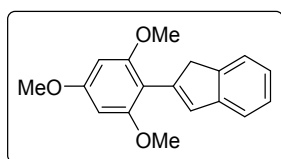
(*Z,E*)-4-(1-Phenyl-2-(2,4,6-trimethoxyphenyl)vinyl)-1,1'-biphenyl (**3aq**), 83.6 mg, 99% yield, white solid. A mixture of *E/Z* isomers was isolated (59:41 ratio determined based on GC and ^1H NMR). ^1H NMR (400 MHz, CDCl_3) of *E*-isomer: δ 7.65 – 7.56 (m, 2H), 7.56 – 7.51 (m, 1H), 7.50 – 7.38 (m, 5H), 7.36 – 7.26 (m, 2H), 7.25 – 7.04 (m, 4H), 6.81 (s, 1H), 6.00 (s, 2H), 3.77 (s, 3H), 3.46 (s, 6H); ^1H NMR (400 MHz, CDCl_3) of *Z*-isomer: δ 7.65 – 7.56 (m, 2H), 7.56 – 7.51 (m, 1H), 7.50 – 7.38 (m, 5H), 7.36 – 7.26 (m, 2H), 7.25 – 7.04 (m, 4H), 6.77 (s, 1H), 6.00 (s, 2H), 3.77 (s, 3H), 3.46 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) mixture of *Z/E* isomers δ ^{13}C NMR (101 MHz, CDCl_3) δ 160.61, 160.59, 158.3, 143.8, 142.90, 142.85, 142.3, 141.6, 141.0, 140.9, 139.6, 138.9, 129.8, 129.4, 128.7, 128.6, 128.4, 127.9, 127.4, 127.1, 127.0, 126.9, 126.8, 126.5, 126.4, 125.9, 120.0, 119.9, 108.9, 90.3, 90.3, 55.2, 55.1; HRMS (ESI) calcd for $\text{C}_{29}\text{H}_{27}\text{O}_3^+$, $[\text{M}+\text{H}]^+$, 423.1955 found 423.1943.



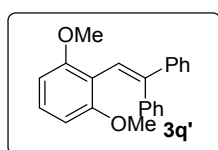
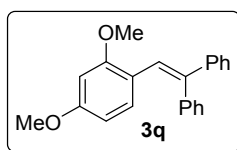
1,3,5-Trimethoxy-2-(2-phenylallyl)benzene (**3ar**), 27.3 mg, 48% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 7.3$ Hz, 2H), 7.33 (t, $J = 7.5$ Hz, 2H), 7.26 (t, $J = 7.3$ Hz, 1H), 6.17 (s, 2H), 5.22 (d, $J = 1.2$ Hz, 1H), 4.60 (d, $J = 1.5$ Hz, 1H), 3.83 (s, 3H), 3.76 (s, 6H), 3.71 (s, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.7, 159.1, 147.0, 142.3, 128.0, 127.1, 126.1, 110.8, 108.8, 90.6, 55.8, 55.3, 27.9.



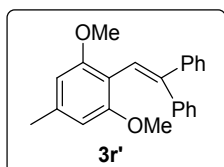
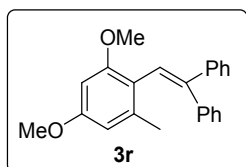
(E)-1,3,5-Trimethoxy-2-(2-phenylprop-1-en-1-yl)benzene (**3as**), 26.7 mg, 47%, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.63 – 7.55 (m, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 4.0 Hz, 1H), 6.61 (d, J = 1.0 Hz, 1H), 6.18 (s, 2H), 3.84 (s, 3H), 3.80 (s, 6H), 1.96 (d, J = 1.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.4, 158.5, 143.2, 138.1, 128.0, 126.7, 125.9, 118.6, 108.7, 90.5, 55.7, 55.3, 17.9.



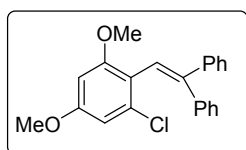
2-(2,4,6-Trimethoxyphenyl)-1H-indene (**3at**), 19.2 mg, 34 %, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, J = 7.3 Hz, 1H), 7.38 (d, J = 7.5 Hz, 1H), 7.24 (dd, J = 8.1, 6.6 Hz, 1H), 7.13 (td, J = 7.4, 1.1 Hz, 1H), 7.01 (s, 1H), 6.20 (s, 2H), 3.85 (s, 3H), 3.83 (s, 2H), 3.79 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.3, 158.9, 145.5, 143.9, 140.0, 131.5, 125.9, 123.8, 123.1, 120.5, 108.4, 90.9, 55.8, 55.3, 42.4.



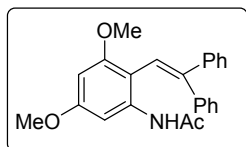
(2-(2,4-Dimethoxyphenyl)ethene-1,1-diyl)dibenzene **3ba** and (2-(2,6-dimethoxyphenyl)ethene-1,1-diyl)dibenzene **3ba'**, 27.2 mg, 43% yield, yellow solid. A mixture of regioisomers was isolated (**3ba**: **3ba'** = 85:15 ratio determined based on GC). ^1H NMR (400 MHz, CDCl_3) of **3ba** δ 7.34 – 7.22 (m, 8H), 7.22 – 7.16 (m, 2H), 7.10 – 7.02 (m, 1H), 6.67 (d, J = 8.6 Hz, 1H), 6.41 (d, J = 2.5 Hz, 1H), 6.14 (dd, J = 8.6, 2.4 Hz, 1H), 3.79 (d, J = 4.6 Hz, 3H), 3.74 (s, 3H); ^1H NMR (400 MHz, CDCl_3) of **3ba'** δ 7.85 – 7.75 (m, 3H), 7.63 – 7.56 (m, 2H), 7.43 – 7.34 (m, 4H), 7.17 – 7.10 (m, 3H), 6.79 (s, 1H), 6.39 (s, 1H), 3.47 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) mixture of isomers: ^{13}C NMR (101 MHz, CDCl_3) δ 159.8, 158.8, 157.6, 144.5, 143.9, 143.5, 142.0, 140.9, 140.7, 137.5, 132.4, 130.7, 130.6, 130.0, 129.4, 128.3, 128.2, 128.0, 127.9, 127.7, 127.3, 127.1, 127.0, 126.9, 126.6, 122.7, 119.8, 119.4, 103.9, 103.5, 97.9, 55.4, 55.2, 55.1; HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{21}\text{O}_2^+$, $[\text{M}+\text{H}]^+$, 317.1536 found 317.1535.



(2-(2,4-Dimethoxy-6-methylphenyl)ethene-1,1-diyl)dibenzene **3bb** and (2-(2,6-dimethoxy-4-methylphenyl)ethene-1,1-diyl)dibenzene **3bb'**, 35.0 mg, 53% yield, yellow solid. A mixture of regioisomers was isolated (**3bb**: **3bb'** = 78:22 ratio determined based on GC and ^1H NMR). ^1H NMR (400 MHz, CDCl_3) of **3bb**: δ 7.39 – 7.35 (m, 2H), 7.33 – 7.26 (m, 3H), 7.16 – 7.12 (m, 3H), 7.06 – 6.98 (m, 2H), 6.74 (s, 1H), 6.21 (s, 2H), 3.75 (s, 3H), 3.54 (s, 3H), 1.98 (s, 3H); ^1H NMR (400 MHz, CDCl_3) of **3bb'**: δ 7.86 – 7.77 (m, 3H), 7.66 – 7.56 (m, 1H), 7.48 (t, $J = 7.6$ Hz, 3H), 7.34 – 7.33 (m, 1H), 7.11 – 7.05 (m, 2H), 6.77 (s, 1H), 6.22 (s, 2H), 3.45 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.36, 158.31, 157.42, 144.27, 143.98, 143.80, 143.59, 142.35, 141.24, 138.64, 138.11, 137.59, 132.47, 130.11, 129.86, 129.48, 128.39, 128.36, 128.31, 128.02, 127.87, 127.60, 127.37, 127.26, 127.06, 126.78, 126.49, 123.69, 120.03, 119.57, 113.04, 106.07, 104.52, 95.74, 55.19, 55.13, 22.21, 20.67; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{23}\text{O}_2^+$, $[\text{M}+\text{H}]^+$, 331.1693 found 331.1697.

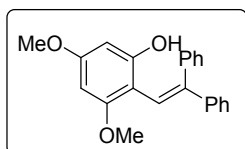


(2-(2-Chloro-4,6-dimethoxyphenyl)ethene-1,1-diyl)dibenzene (**3bc**), 52.5 mg, 75% yield, yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.35 (m, 2H), 7.34 – 7.27 (m, 3H), 7.21 – 7.11 (m, 3H), 7.05 (dd, $J = 6.6, 3.1$ Hz, 2H), 6.68 (s, 1H), 6.48 (d, $J = 2.3$ Hz, 1H), 6.16 (d, $J = 2.3$ Hz, 1H), 3.74 (s, 3H), 3.35 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.6, 158.1, 145.6, 142.9, 141.2, 135.1, 130.0, 129.6, 128.3, 128.0, 127.5, 127.4, 126.9, 120.9, 119.3, 105.4, 97.3, 55.4, 55.1; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{23}\text{O}_2^+$, $[\text{M}+\text{H}]^+$, 331.1693 found 331.1697.

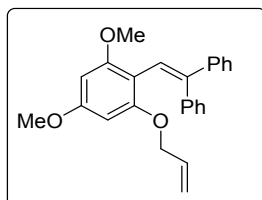


N-(2-(2,2-Diphenylvinyl)-3,5-dimethoxyphenyl)acetamide (**3bd**), 32.1 mg, 43% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.31 (m, 6H), 7.25 – 7.19 (m, 3H), 7.17 – 7.10 (m, 2H), 7.07 (s, 1H), 6.73 (s, 1H), 6.25 (d, $J = 1.9$ Hz, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz,

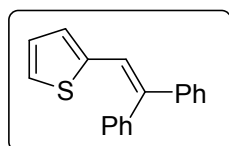
CDCl₃) δ 167.9, 160.3, 159.0, 144.6, 142.8, 139.6, 135.2, 129.6, 128.5, 128.4, 128.3, 128.2, 127.9, 121.3, 109.6, 97.5, 94.8, 55.6, 55.4, 24.9; HRMS (ESI) calcd for C₂₄H₂₄NO₃⁺, [M+H]⁺, 373.1678 found 373.1673.



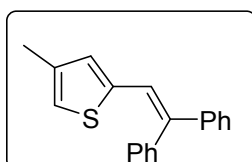
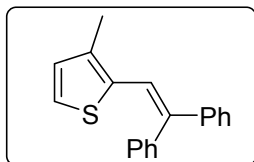
2-(2-(2,2-Diphenylvinyl)-3,5-dimethoxyphenyl)ethane-1,1-diol (**3be**), 38.5 mg, 58% yield, white solid. ¹H NMR (400 MHz, CDCl₃) δ 7.44 – 7.34 (m, 5H), 7.34 – 7.28 (m, 3H), 7.28 – 7.21 (m, 2H), 6.81 (s, 1H), 6.11 (d, *J* = 2.3 Hz, 1H), 5.97 (d, *J* = 2.3 Hz, 1H), 5.11 (s, 1H), 3.79 (s, 3H), 3.77 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 160.9, 159.5, 153.1, 143.7, 142.8, 139.3, 129.7, 128.6, 128.3, 128.3, 128.1, 127.7, 120.6, 106.5, 92.9, 91.2, 55.6, 55.2; HRMS (ESI) calcd for C₂₂H₂₁O₃⁺, [M+H]⁺, 333.1485 found 333.1486.



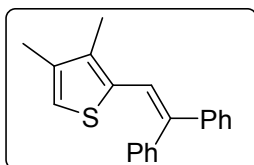
(2-(2-(Allyloxy)-4,6-dimethoxyphenyl)ethene-1,1-diyl)dibenzene (**3bf**), 46.9 mg, 63% yield, white solid. ¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.34 (m, 2H), 7.31 – 7.22 (m, 3H), 7.20 – 7.12 (m, 3H), 7.11 – 7.02 (m, 2H), 6.72 (s, 1H), 6.01 – 5.97 (m, 2H), 5.86 – 5.73 (m, 1H), 5.23 (ddd, *J* = 17.3, 3.1, 1.5 Hz, 1H), 5.14 (dd, *J* = 10.5, 1.5 Hz, 1H), 4.25 (dt, *J* = 5.1, 1.5 Hz, 2H), 3.76 (s, 3H), 3.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 160.3, 158.4, 157.4, 143.9, 143.6, 142.2, 133.7, 129.6, 128.3, 127.8, 127.3, 126.9, 126.4, 119.9, 116.8, 109.5, 91.6, 90.5, 69.1, 55.2, 55.1; HRMS (ESI) calcd for C₂₅H₂₅O₃⁺, [M+H]⁺, 373.1798 found 373.1789.



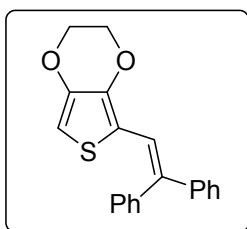
2-(2-(2,2-Diphenylvinyl)thiophene)ethene-1,1-diyl)dibenzene (**3bg**), 23.6 mg, 45% yield, colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.52 – 7.41 (m, 3H), 7.37 – 7.21 (m, 8H), 7.03 (d, *J* = 5.0 Hz, 1H), 6.96 – 6.90 (m, 1H), 6.89 – 6.84 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 141.7, 141.3, 139.7, 139.4, 130.3, 129.3, 128.9, 128.3, 128.0, 127.3, 126.7, 126.3, 126.2, 120.8. HRMS (ESI) calcd for C₁₈H₁₅S⁺, [M+H]⁺, 263.0889 found 263.0843.



2-(2,2-Diphenylvinyl)-3-methylthiophene **3bh** and 2-(2,2-diphenylvinyl)-4-methylthiophene **3bh'**, 39.2 mg, 71% yield, yellow solid. A mixture of regioisomers was isolated (**3bh**: **3bh'** = 2:1 ratio determined based on ^1H NMR). ^1H NMR (400 MHz, CDCl_3) of **3bh** δ 7.48 – 7.40 (m, 3H), 7.37 – 7.19 (m, 8H), 6.93 (d, $J = 5.1$ Hz, 1H), 6.72 (d, $J = 5.1$ Hz, 1H), 2.33 (s, 3H); ^1H NMR (400 MHz, CDCl_3) of **3bh'** δ 7.52 – 7.39 (m, 3H), 7.35 – 7.19 (m, 8H), 6.73 (s, 1H), 6.61 (s, 1H), 2.13 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) of mixture ^{13}C NMR (101 MHz, CDCl_3) δ 142.5, 141.9, 141.1, 139.5, 139.5, 139.4, 139.3, 137.6, 136.7, 134.8, 131.5, 130.7, 130.4, 129.3, 129.2, 129.2, 128.4, 128.1, 127.3, 127.0, 126.8, 125.0, 122.1, 121.0, 119.4, 15.5, 14.6. HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{17}\text{S}^+$, $[\text{M}+\text{H}]^+$, 277.1045 found 277.1004.



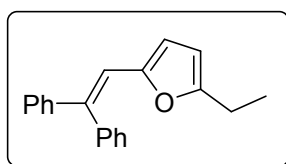
2-(2,2-Diphenylvinyl)-3,4-dimethylthiophene (**3bi**), 44.7 mg, 77% yield, colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.48 – 7.39 (m, 3H), 7.34 – 7.22 (m, 8H), 6.64 (s, 1H), 2.21 (s, 3H), 2.09 (d, $J = 0.7$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.5, 139.7, 139.2, 137.2, 136.8, 134.9, 130.7, 129.0, 128.2, 127.9, 127.2, 126.9, 121.2, 120.0, 15.0, 13.0. HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{19}\text{S}^+$, $[\text{M}+\text{H}]^+$, 291.1202 found 291.1205.



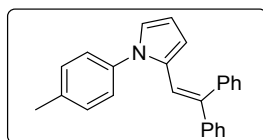
5-(2,2-Diphenylvinyl)-2,3-dihydrothieno[3,4-b][1,4]dioxine (**3bj**), 51.2 mg, 80% yield, colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.51 – 7.40 (m, 3H), 7.37 – 7.24 (m, 7H), 7.24 – 7.18 (m, 1H), 6.06 (s, 1H), 4.25 (dd, $J = 7.4, 3.6$ Hz, 2H), 4.18 (dd, $J = 7.4, 3.5$ Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 141.8,

141.0, 140.6, 139.3, 137.3, 130.6, 129.2, 128.2, 128.0, 127.0, 126.6, 116.2, 116.0, 100.3, 64.8, 64.6.

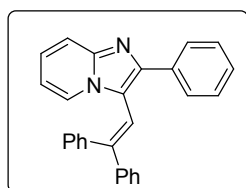
HRMS (ESI) calcd for $C_{20}H_{17}O_2S^+$, $[M+H]^+$, 321.0944 found 321.0951.



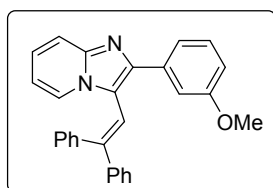
2-(2,2-Diphenylvinyl)-5-ethylfuran (**3bk**), 31.8 mg, 58% yield, colorless oil. 1H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.35 (m, 3H), 7.34 – 7.16 (m, 7H), 6.93 (s, 1H), 5.80 (d, $J = 2.7$ Hz, 1H), 5.38 (d, $J = 3.0$ Hz, 1H), 2.54 (d, $J = 7.5$ Hz, 2H), 1.13 (t, $J = 7.6$ Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 151.4, 141.8, 140.5, 138.4, 129.6, 128.8, 128.2, 127.4, 127.1, 126.7, 116.2, 110.1, 106.2, 21.4, 12.0; HRMS (EI) calcd for $C_{20}H_{18}O$, $[M]^+$, 274.1358 found 274.1351.



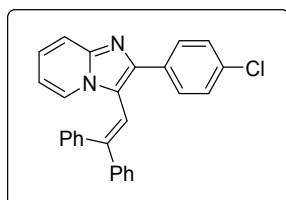
2-(2,2-Diphenylvinyl)-1-(p-tolyl)-1H-pyrrole (**3bl**), 52.3 mg, 78% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.37 (m, 3H), 7.32 – 7.24 (m, 6H), 7.23 – 7.14 (m, 5H), 6.76 (dd, $J = 2.6, 1.7$ Hz, 1H), 6.72 (s, 1H), 6.13 – 5.93 (m, 1H), 5.39 (dd, $J = 3.8, 1.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 141.1, 138.1, 137.2, 137.1, 131.1, 130.0, 129.8, 129.0, 128.2, 127.4, 126.8, 126.8, 126.2, 122.9, 116.9, 110.7, 109.2, 21.1; HRMS (ESI) calcd for $C_{25}H_{22}N^+$, $[M+H]^+$, 333.1485 found 333.1486.



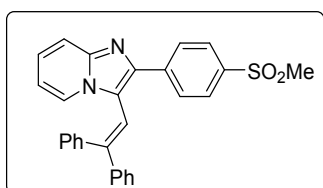
3-(2,2-Diphenylvinyl)-2-phenylimidazo[1,2-a]pyridine (**3bm**), 72.2 mg, 97% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, $J = 7.4$ Hz, 2H), 7.57 (d, $J = 9.0$ Hz, 1H), 7.52 (d, $J = 6.9$ Hz, 1H), 7.47 – 7.43 (m, 2H), 7.42 – 7.35 (m, 5H), 7.30 (t, $J = 7.3$ Hz, 1H), 7.16 – 6.99 (m, 7H), 6.45 (t, $J = 6.7$ Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.2, 144.7, 144.6, 142.3, 139.7, 134.6, 129.1, 128.6, 128.4, 128.3, 128.3, 128.0, 128.0, 127.7, 124.4, 124.1, 118.7, 117.0, 115.0, 111.4; HRMS (ESI) calcd for $C_{27}H_{21}N_2^+$, $[M+H]^+$, 373.1699 found 373.1690.



3-(2,2-Diphenylvinyl)-2-(3-methoxyphenyl)imidazo[1,2-a]pyridine (**3bn**), 71.6 mg, 89% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.61 – 7.53 (m, 2H), 7.53 – 7.47 (m, 2H), 7.43 (dd, J = 6.7, 3.1 Hz, 2H), 7.40 – 7.34 (m, 3H), 7.27 (t, J = 8.2 Hz, 1H), 7.14 – 6.98 (m, 7H), 6.90 – 6.82 (m, 1H), 6.46 (td, J = 6.8, 1.1 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.9, 160.3, 159.0, 144.6, 142.8, 139.6, 135.2, 129.6, 128.5, 128.4, 128.3, 128.2, 127.9, 121.3, 109.6, 97.5, 94.8, 55.6, 55.4, 24.9; HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{23}\text{N}_2\text{O}^+$, $[\text{M}+\text{H}]^+$, 403.1805 found 403.1800.

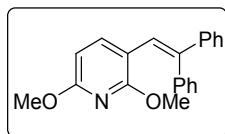


2-(4-Chlorophenyl)-3-(2,2-diphenylvinyl)imidazo[1,2-a]pyridine (**3bo**), 64.9 mg, 80% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, J = 8.3 Hz, 2H), 7.56 (t, J = 7.7 Hz, 2H), 7.47 – 7.36 (m, 5H), 7.32 (d, J = 8.3 Hz, 2H), 7.13 – 7.02 (m, 4H), 7.00 – 6.91 (m, 3H), 6.49 (t, J = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 146.97, 144.70, 143.11, 142.05, 139.43, 133.45, 133.04, 129.14, 129.05, 128.54, 128.42, 128.31, 128.27, 128.00, 124.64, 123.99, 118.91, 117.00, 114.31, 111.65; HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{20}\text{ClN}_2^+$, $[\text{M}+\text{H}]^+$, 407.1310 found 407.1303.

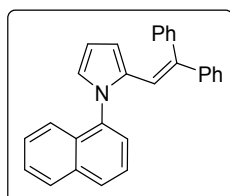


3-(2,2-Diphenylvinyl)-2-(4-(methylsulfonyl)phenyl)imidazo[1,2-a]pyridine (**3bp**), 45.9 mg, 51% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, J = 8.6 Hz, 2H), 7.89 (d, J = 8.6 Hz, 2H), 7.71 (d, J = 6.9 Hz, 1H), 7.60 (d, J = 9.1 Hz, 1H), 7.48 – 7.35 (m, 5H), 7.18 – 7.14 (m, 1H), 7.11 – 7.06 (m, 1H), 7.04 – 7.01 (m, 2H), 6.97 (s, 1H), 6.95 – 6.85 (m, 2H), 6.61 (td, J = 6.8, 1.0 Hz, 1H), 3.05 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 148.4, 144.9, 141.8, 141.6, 140.1, 139.1, 138.8, 129.1, 128.7, 128.5,

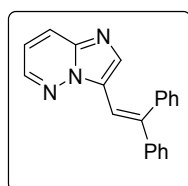
128.5, 128.4, 128.2, 128.1, 127.4, 125.2, 124.0, 120.3, 117.3, 113.4, 112.2, 44.5; HRMS (ESI) calcd for $C_{28}H_{23}N_2O_2S^+$, $[M+H]^+$, 451.1475 found 451.1466.



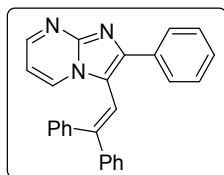
3-(2,2-Diphenylvinyl)-2,6-dimethoxypyridine (**3bq**), 52.6 mg, 83% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.22 (m, 8H), 7.20 (d, $J = 2.0$ Hz, 1H), 7.18 (d, $J = 1.6$ Hz, 1H), 7.01 (s, 1H), 6.87 (d, $J = 8.3$ Hz, 1H), 5.96 (d, $J = 8.3$ Hz, 1H), 3.95 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6, 160.6, 143.5, 141.3, 140.6, 140.5, 130.4, 128.5, 128.0, 127.6, 127.2, 127.2, 121.4, 112.0, 100.3, 53.5, 53.4; HRMS (ESI) calcd for $C_{21}H_{20}NO_2^+$, $[M+H]^+$, 318.1489 found 318.1496.



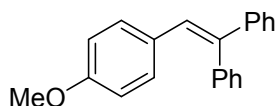
2-(2,2-Diphenylvinyl)-1-(naphthalen-1-yl)-1H-pyrrole (**3br**), 66.8 mg, 90% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, $J = 7.8$ Hz, 2H), 7.65 – 7.37 (m, 8H), 7.35 – 7.26 (m, 2H), 7.13 – 7.03 (m, 3H), 7.02 – 6.87 (m, 2H), 6.84 – 6.77 (m, 1H), 6.39 (s, 1H), 6.20 – 6.10 (m, 1H), 5.45 (d, $J = 2.8$ Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5, 141.1, 138.0, 136.2, 134.1, 132.8, 131.4, 129.9, 129.0, 128.8, 128.0, 128.0, 127.4, 127.3, 126.7, 126.6, 126.5, 125.8, 125.2, 124.3, 123.4, 116.5, 109.8, 109.1; HRMS (ESI) calcd for $C_{28}H_{22}N^+$, $[M+H]^+$, 372.1747 found 372.1751.



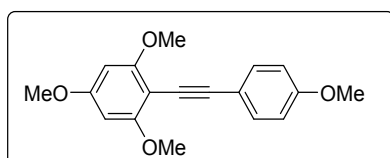
3-(2,2-Diphenylvinyl)imidazo[1,2-b]pyridazine (**3bs**), 42.8 mg, 72% yield, white solid. 1H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, $J = 3.2$ Hz, 1H), 7.88 (d, $J = 9.0$ Hz, 1H), 7.65 (s, 1H), 7.53 – 7.41 (m, 5H), 7.39 – 7.24 (m, 5H), 7.00 (dd, $J = 9.1, 4.4$ Hz, 1H), 6.66 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 142.2, 141.4, 140.5, 138.7, 133.6, 129.4, 129.3, 128.3, 128.1, 127.7, 127.2, 127.0, 125.6, 116.2, 111.8; HRMS (ESI) calcd for $C_{20}H_{16}N_3^+$, $[M+H]^+$, 298.1339 found 298.1334.



3-(2,2-Diphenylvinyl)-2-phenylimidazo[1,2-a]pyrimidine (**3bt**), 53.7 mg, 72% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 8.40 (dd, $J = 4.1, 2.0$ Hz, 1H), 8.12 (dd, $J = 5.2, 3.3$ Hz, 2H), 7.72 (dd, $J = 6.9, 2.0$ Hz, 1H), 7.55 – 7.33 (m, 8H), 7.24 – 7.10 (m, 5H), 7.05 (s, 1H), 6.49 (dd, $J = 6.9, 4.1$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 149.2, 147.7, 146.5, 146.2, 141.8, 139.4, 133.9, 131.4, 129.0, 128.7, 128.7, 128.6, 128.4, 128.4, 128.3, 128.3, 117.0, 114.3, 107.6; HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{20}\text{N}_3^+$, $[\text{M}+\text{H}]^+$, 374.1652 found 374.1649.



(2-(4-Methoxyphenyl)ethene-1,1-diyl)dibenzene (**3bu**)⁶, 8.6 mg, 15% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.18 (m, 10H), 6.95 (d, $J = 8.7$ Hz, 2H), 6.91 (s, 1H), 6.67 (d, $J = 8.8$ Hz, 2H), 3.74 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.3, 143.5, 140.6, 140.5, 130.8, 130.4, 130.0, 128.7, 128.1, 127.6, 127.4, 127.2, 127.2, 113.4, 55.1.



1,3,5-Trimethoxy-2-((4-methoxyphenyl)ethynyl)benzene (**10**)⁷, 20.2 mg, 34% yield, white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.56 – 7.46 (m, 2H), 6.85 (d, $J = 8.9$ Hz, 2H), 6.12 (s, 2H), 3.89 (s, 6H), 3.84 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.0, 161.3, 159.1, 133.0, 116.4, 113.7, 96.2, 94.6, 90.4, 80.3, 56.1, 55.4, 55.2.

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NMR spectra

