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One-pot protocol for the fluorosulfonation and Suzuki coupling of phenols and bromophenols, streamlined access to biaryls and terphenyls

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Contents

Materials, Methods and Experimental Procedure

General remarks

All commercially available reagents (from Acros, Aldrich, Fluka) were used without further purification. The SO_2F_2 is commercially available from Wuhan newradar special gas co. LTD. NMR spectra were recorded on a Brucker Advance II 400 spectrometer using TMS as internal standard (400 MHz for ^1H NMR). All reactions were carried out under air atmosphere.The isolated yields of products were obtained by short chromatography on a silica gel (200-300 mesh) column using petroleum ether (60-90 °C), unless otherwise noted.

General procedure for the cross-coupling reaction of phenols and arylboronic acids

A mixture of phenols (0.5 mmol), Et_3N (1.5 mmol) was added to a reaction flask (25 mL), before SO_2F_2 was introduced into the mixture by slowly bubbling from a balloon, and the mixtures was stirred in EtOH/H_2O (2 mL/2 mL) at 25 ^oC for 4 hours. And then arylboronic acid (0.6 mmol), 1 mol% $Pd(OAc)_2$, Et_3N (1.5 mmol) was added to the mixture for anthor 10 hours at 25 ^oC. Subsequently, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layers were concentrated in vacuo and the product was isolated by short chromatography.

General procedure for the preperation of biphenylsulfonyl fluorides

Route A: A mixture of 4-bromophenol (0.5 mmol), arylboronic acids (0.6 mmol), 1 mol% $Pd(OAc)_2$, K_2CO_3 (1.0 mmol) EtOH/H_2O (2 mL/2 mL) were added to a reaction flask (25 mL), and the mixture was allowed to stir at room temperature for 2 hours, before a mixture of Et_3N (1.5 mmol) and SO_2F_2 by slowly bubbling from a balloon was added to the mixture for 4 hours at room temperature. Subsequently, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layers were concentrated in vacuo and the product was isolated by short chromatography.

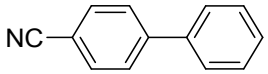
Route B: A mixture of 4-bromophenol (0.5 mmol), Et_3N (1.5 mmol) EtOH/H_2O (2 mL/2 mL) was added to a reaction flask (25 mL), before SO_2F_2 was introduced into the mixture by slowly bubbling from a balloon, and the mixture was allowed to stir at room temperature for 4 hours, then arylboronic acid (0.6 mmol), 1 mol% $Pd(OAc)_2$, K_2CO_3 (1.5 mmol) added to the mixture for 2 hours at room temperature. Subsequently, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layers were concentrated in vacuo and the product was isolated by short chromatography.

General procedure for the preperation of terphenyls

A mixture of bromopheno (0.5 mmol), arylboronic acids (0.6 mmol), 1 mol% $Pd(OAc)_2$, K_2CO_3 (1.0 mmol) EtOH/H_2O (2 mL/2 mL) were added to a reaction flask (25 mL), and the mixture was allowed to stir at room temperature for 2 hours, before a mixture of Et_3N (1.5 mmol) and SO_2F_2 by slowly bubbling from a balloon was added to the mixture for 4 hours at room temperature.Then, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layers were concentrated in vacuo and the product was isolated by short chromatography. Subsequently, the product of biphenylsulfonyl fluoride,arylboronic acid(1.2 equiv), $Pd(OAc)_2$ (1 mol%), Et_3N (2.0 equiv), EtOH/H_2O (2 mL/2 mL), was added to a reaction flask (25 mL), and the mixtures was stirred at 80 ^oC for 12 hours. Then, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 15 mL). Finally the combined organic layers were concentrated in vacuo and the product was isolated by short chromatography.

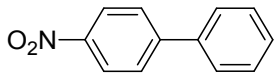
Characterization Data

[2a]: Biphenyl-4-carbonitrile[1]



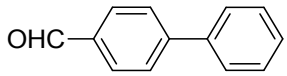
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.7 Hz, 2H), 7.69 (d, J = 8.5 Hz, 2H), 7.59 (d, J = 8.1 Hz, 2H), 7.49 (t, J = 7.4 Hz, 2H), 7.46 – 7.39 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 139.1, 132.5, 129.0, 128.6, 127.7, 127.2, 118.9, 110.8.

[2b]: 4-Nitro-1,1'-biphenyl.[2]



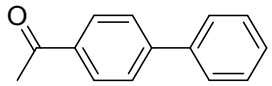
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.9 Hz, 2H), 7.74 (d, J = 9.0 Hz, 2H), 7.63 (d, J = 7.6 Hz, 2H), 7.58 – 7.36 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 138.7, 129.1, 128.8, 127.7, 127.3, 124.0.

[2c]: 4-Formyl-biphenyl.[3]



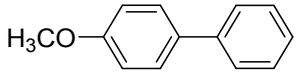
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 7.95 (d, J = 7.5 Hz, 2H), 7.75 (d, J = 7.7 Hz, 2H), 7.64 (d, J = 7.1 Hz, 2H), 7.48 (t, J = 7.1 Hz, 2H), 7.43 (d, J = 6.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.9, 147.1, 139.7, 135.1, 130.2, 129.0, 128.4, 127.6, 127.3.

[2d]: 1-(Biphenyl-4-yl)ethanone. [3]



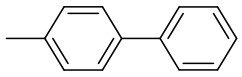
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.6 Hz, 2H), 7.69 (d, J = 8.6 Hz, 2H), 7.63 (d, J = 7.6 Hz, 2H), 7.48 (t, J = 7.4 Hz, 2H), 7.40 (t, J = 7.3 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 145.7, 139.8, 135.8, 128.9, 128.9, 128.2, 127.2, 127.2, 26.6.

[2e]: 4-Methoxybiphenyl. [3]



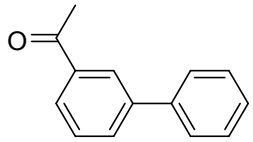
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (t, J = 8.2 Hz, 4H), 7.42 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 8.5 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 140.8, 133.7, 128.7, 128.1, 126.7, 126.6, 114.1, 55.3.

[2f]: 4-Methylbiphenyl.[4]



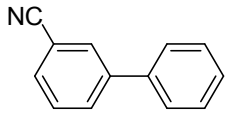
Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 7.6 Hz, 2H), 7.49 (d, J = 7.9 Hz, 2H), 7.42 (t, J = 7.2 Hz, 2H), 7.31 (t, J = 6.8 Hz, 1H), 7.24 (d, J = 7.4 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 138.3, 137.0, 129.4, 128.7, 127.1, 126.9, 126.9, 21.1.

[2g]: 1-(Biphenyl-3-yl)ethanone.[5]



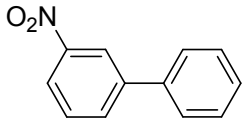
Colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.93 (d, J = 8.9 Hz, 1H), 7.79 (d, J = 8.7 Hz, 1H), 7.62 (d, J = 8.1 Hz, 2H), 7.54 (t, J = 8.0 Hz, 1H), 7.47 (t, J = 6.8 Hz, 2H), 7.39 (t, J = 7.9 Hz, 1H), 2.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.1, 141.1, 140.1, 137.6, 131.7, 129.0, 128.9, 127.8, 127.1, 126.9, 26.7.

[2h]: Biphenyl-3-carbonitrile.[6]



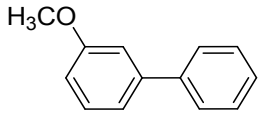
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.80 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 7.7 Hz, 1H), 7.54 (dt, J = 10.0, 4.9 Hz, 3H), 7.47 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 138.8, 131.4, 130.6, 129.5, 129.0, 128.3, 127.0, 118.8, 112.8.

[2i]: 3-Nitro-biphenyl.[7]



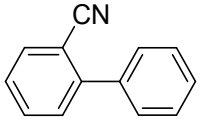
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.20 (d, J = 9.4 Hz, 1H), 7.92 (d, J = 7.7 Hz, 1H), 7.62 (t, J = 9.0 Hz, 3H), 7.50 (t, J = 7.4 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8, 138.6, 133.0, 129.7, 129.1, 128.5, 127.1, 122.0, 121.9.

[2j]: 3-Methoxy-biphenyl.[5]



Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.1 Hz, 2H), 7.48 (t, J = 7.7 Hz, 2H), 7.44 – 7.35 (m, 2H), 7.24 (d, J = 6.8 Hz, 1H), 7.19 (s, 1H), 6.95 (d, J = 8.2 Hz, 1H), 3.89 (s, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 142.8, 141.1, 129.8, 128.8, 127.4, 127.2, 119.7, 112.9, 112.7, 55.3.

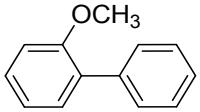
[2k]: 2-Cyano-biphenyl.[3]



Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.5 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H),

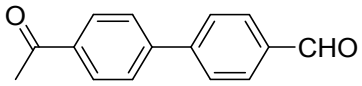
7.56 (d, J = 7.2 Hz, 2H), 7.53 – 7.39 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 138.1, 133.7, 132.8, 130.0, 128.7, 128.7, 127.5, 118.7, 111.2.

[2l]: 2-Methoxy-biphenyl.[3]



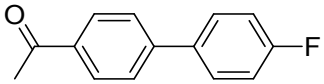
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 7.3 Hz, 2H), 7.38 (t, J = 7.1 Hz, 2H), 7.29 (t, J = 8.1 Hz, 3H), 7.01 (t, J = 7.3 Hz, 1H), 6.95 (d, J = 8.1 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 138.5, 130.8, 130.7, 129.5, 128.6, 127.9, 126.9, 120.8, 111.2, 55.5.

[2m]: 4-Formyl-4'-acetyl-biphenyl.[8]



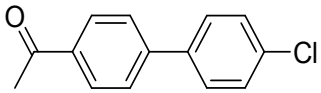
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 8.08 (d, J = 7.7 Hz, 2H), 7.99 (d, J = 7.2 Hz, 2H), 7.80 (d, J = 7.4 Hz, 2H), 7.74 (d, J = 7.7 Hz, 2H), 2.67 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 197.6, 191.8, 145.7, 144.1, 136.7, 135.8, 130.3, 129.0, 127.9, 127.6, 26.8.

[2n]: 4-Fluorine-4'-acetyl-biphenyl.[1]



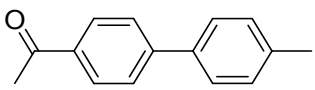
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 7.96 (d, J = 8.4 Hz, 2H), 7.72 (d, J = 8.2 Hz, 2H), 7.65 – 7.56 (m, 2H), 7.18 (t, J = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.8, 146.1, 135.1, 130.3, 129.0 128.9, 127.5, 116.0, 115.8.

[2o]: 4-Chlorine-4'-acetyl-biphenyl.[9]



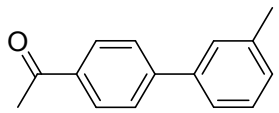
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.7 Hz, 2H), 7.65 (d, J = 7.7 Hz, 2H), 7.56 (d, J = 7.8 Hz, 2H), 7.44 (d, J = 7.8 Hz, 2H), 2.64 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 197.7, 144.4, 138.3, 136.0, 134.4, 129.1, 129.0, 128.5, 127.1, 26.7.

[2p]: 4-methyl-4'-acetyl-biphenyl.[10]



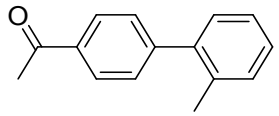
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 7.94 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.1 Hz, 2H), 7.55 (d, J = 7.9 Hz, 2H), 7.29 (d, J = 7.8 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.9, 147.1, 138.5, 136.7, 134.9, 130.2, 129.7, 127.3, 127.1, 21.18.

[2q]: 3-Methyl-4'-acetyl-biphenyl.[11]



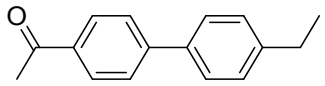
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.8 Hz, 2H), 7.68 (d, J = 7.7 Hz, 2H), 7.46 – 7.33 (m, 3H), 7.23 (s, 1H), 2.64 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 145.9, 139.8, 138.6, 135.7, 129.0, 128.8, 128.0, 127.2, 124.4, 26.7, 21.5.

[2r]: 2-Methyl-4'-acetyl-biphenyl.[12]



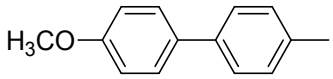
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.7 Hz, 2H), 7.41 (d, J = 7.7 Hz, 2H), 7.24 (d, J = 22.8 Hz, 4H), 2.63 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.9, 146.9, 140.7, 135.5, 135.1, 130.6, 129.5, 128.2, 127.9, 126.0, 26.7, 20.4.

[2s]: 4-Ethyl-4'-acetyl-biphenyl.[13]



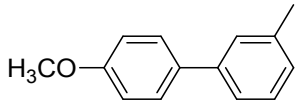
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.9 Hz, 2H), 7.68 (d, J = 7.9 Hz, 2H), 7.56 (d, J = 7.6 Hz, 2H), 7.31 (d, J = 7.6 Hz, 2H), 2.71 (d, J = 7.5 Hz, 2H), 2.64 (s, 3H), 1.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 145.7, 144.6, 137.2, 135.5, 128.9, 128.5, 127.2, 127.00, 28.6, 26.7, 15.6.

[2t]: 4-Methoxy-4'-methylbiphenyl.[3]



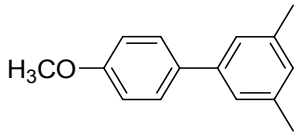
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.6 Hz, 2H), 7.44 (d, J = 7.7 Hz, 2H), 7.22 (d, J = 7.5 Hz, 2H), 6.96 (d, J = 8.4 Hz, 2H), 3.84 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 137.9, 136.3, 133.7, 129.4, 127.9, 126.5, 114.1, 55.3, 21.0.

[2u]: 4'-Methoxy-3-methylbiphenyl. [3]



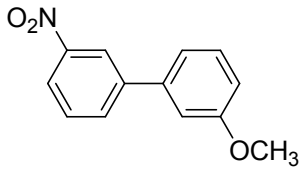
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8.8 Hz, 2H), 7.35 (d, J = 8.8 Hz, 2H), 7.30 (t, J = 7.4 Hz, 1H), 7.12 (d, J = 7.2 Hz, 1H), 6.97 (dd, J = 9.3, 2.5 Hz, 2H), 3.84 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 140.7, 138.2, 133.8, 128.6, 128.1, 127.5, 127.4, 123.8, 114.1, 55.3, 21.5

[2v]: 4'-Methoxy-3,5-dimethyl-biphenyl.[14]



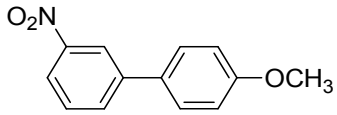
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.9 Hz, 2H), 7.17 (s, 2H), 6.95 (d, J = 4.3 Hz, 3H), 3.83 (s, 3H), 2.36 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 140.8, 138.2, 134.0, 128.3, 128.2, 124.7, 114.1, 55.3, 21.4.

[2x]: 3-Methoxy-3'-nitro-biphenyl.[15]



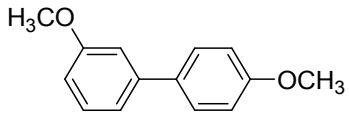
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.19 (s, 1H), 7.90 (s, 1H), 7.60 (s, 1H), 7.41 (s, 1H), 7.21 (s, 1H), 7.14 (s, 1H), 6.99 (s, 1H), 3.89 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 148.6, 142.7, 140.1, 133.1, 130.2, 129.7, 122.2, 113.8, 55.4.

[2y]: 4-Methoxy-3'-nitro-biphenyl.[16]



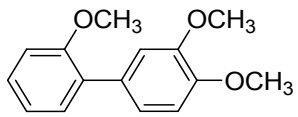
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 8.16 (s, 1H), 7.87 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 7.7 Hz, 3H), 7.02 (d, J = 8.2 Hz, 2H), 3.87 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 148.7, 142.4, 132.5, 131.0, 129.6, 128.2, 121.4, 114.5, 55.4.

[2z]: 3,4'-Dimethoxy-biphenyl.[16]



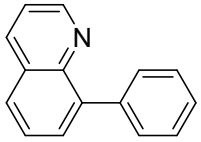
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.0 Hz, 2H), 7.31 (s, 1H), 7.11 (d, J = 22.3 Hz, 2H), 6.95 (d, J = 7.2 Hz, 2H), 6.85 (s, 1H), 3.81 (d, J = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 159.3, 142.4, 133.6, 129.8, 128.2, 119.3, 114.2, 112.5, 112.0, 55.3.

[2aa]: 2, 3',4'-Trimethoxy-biphenyl.[17]



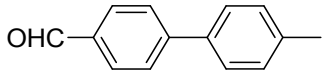
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 7.1 Hz, 2H), 7.08 (d, J = 9.3 Hz, 2H), 6.98 (d, J = 15.2 Hz, 2H), 6.91 (s, 1H), 3.89 (s, 6H), 3.79 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 148.3, 148.1, 131.2, 130.7, 130.4, 128.3, 121.8, 120.8, 113.0, 111.2, 110.8,

[2ab]: 8-phenylquinoline.[18]



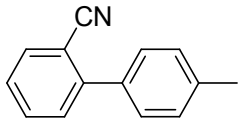
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.17 (s, 1H), 7.77 (s, 1H), 7.70 (t, J = 7.5 Hz, 3H), 7.57 (s, 1H), 7.48 (d, J = 7.7 Hz, 2H), 7.38 (d, J = 4.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 146.0, 140.9, 139.6, 136.3, 130.6, 130.4, 128.8, 128.0, 127.6, 127.4, 126.3, 121.0.

[2ae]: 4'-methyl-[1,1'-biphenyl]-4-carbaldehyde.[19]



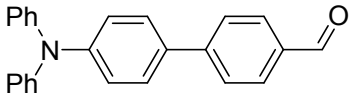
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 7.94 (d, J = 7.5 Hz, 2H), 7.74 (d, J = 7.6 Hz, 2H), 7.55 (d, J = 7.4 Hz, 2H), 7.29 (d, J = 7.4 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.0, 147.1, 138.5, 136.7, 134.9, 134.8, 130.3, 129.7, 127.4, 127.2, 21.2.

[2af]: 4'-methyl-[1,1'-biphenyl]-2-carbonitrile[4]



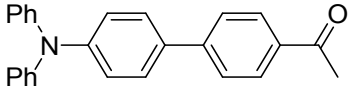
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.62 (t, J = 7.6 Hz, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 7.41 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 7.6 Hz, 2H), 2.42 (s, 3H,).^{13}C NMR (101 MHz, $CDCl_3$) δ145.5, 138.7, 136.2, 132.5, 129.8, 127.4, 127.0, 119.0, 110.5, 21.1.

[2ag]: 4'-(diphenylamino)-[1,1'-biphenyl]-4-carbaldehyde[20]



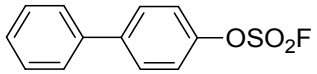
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.92 (d, J = 7.2 Hz, 2H), 7.73 (d, J = 7.9 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.29 (t, J = 7.8 Hz, 4H), 7.14 (s, 6H), 7.07 (t, J = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.8, 148.4, 147.3, 134.6, 132.7, 130.3, 129.3, 128.0, 126.8, 124.8, 123.4, 123.0.

[2ai]: 1-(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)ethanone[20]



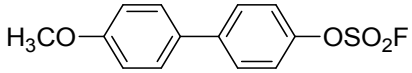
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 6.4 Hz, 2H), 7.65 (d, J = 6.5 Hz, 2H), 7.51 (d, J = 6.6 Hz, 2H), 7.36 – 7.26 (m, J = 6.4 Hz, 4H), 7.14 (d, J = 8.6 Hz, 6H), 7.06 (t, J = 6.8 Hz, 2H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.3, 135.2, 133.0, 129.3, 128.9, 127.9, 126.4, 124.7, 123.3, 123.2, 26.6.

[3e] Biphenyl-4-yl fluorosulfate.[21]



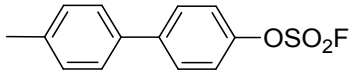
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.5 Hz, 2H), 7.47 (d, J = 7.7 Hz, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.33 (d, J = 8.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 141.9, 139.2, 128.6, 128.0, 127.17, 127.0, 121.1.

[3f] 4'-Methoxybiphenyl-4-yl fluorosulfate.[22]



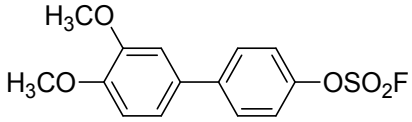
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 7.4 Hz, 2H), 7.41 (d, J = 7.4 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 6.91 (d, J = 7.4 Hz, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 148.7, 141.4, 131.5, 128.3, 126.8, 120.9, 114.2, 55.2.

[3g] 4'-Methylbiphenyl-4-yl fluorosulfate. [22]



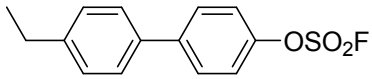
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.7 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.5 Hz, 2H), 7.18 (d, J = 7.9 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 141.8, 138.0, 136.3, 129.6, 128.7, 127.22, 127.0, 121.0, 21.1.

[3h] 3',4'-Dimethoxybiphenyl-4-yl fluorosulfate. [22]



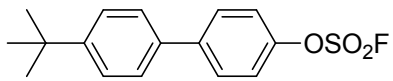
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 6.4 Hz, 2H), 7.38 (d, J = 6.7 Hz, 2H), 7.08 (d, J = 19.1 Hz, 2H), 6.96 (s, 1H), 3.93 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 149.2, 149.0, 141.8, 132.1, 128.6, 121.1, 119.6, 111.5, 110.3, 55.9.

[3i] 4-ethylbiphenylsulfonyl fluoride.



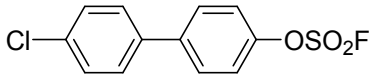
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.9 Hz, 2H), 7.48 (d, J = 7.4 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 7.4 Hz, 2H), 2.71 (q, J = 7.3 Hz, 2H), 1.28 (t,J = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 144.4, 141.9, 136.6, 128.8, 128.5, 127.1, 121.1, 28.5, 15.5. HRMS (ESI-TOF) m/z: $[M-H]^+$ Calcd for $C_{14}H_{13}FO_3S$ 279.0491; Found 279.0510.

[3j] 4-tert-butylbiphenylsulfonyl fluoride.



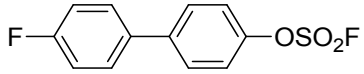
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.0 Hz, 2H), 7.50 (s, 4H), 7.39 (d, J = 8.0 Hz, 2H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 149.1, 141.8, 136.3, 128.8, 126.8, 125.9, 121.1, 34.6, 31.3. HRMS (ESI-TOF) m/z: $[M-H]^+$ Calcd for $C_{16}H_{17}FO_3S$ 307.0804; Found 307.0829

[3k] 4'-chloro-[1,1'-biphenyl]-4-yl sulfurofluoridate.



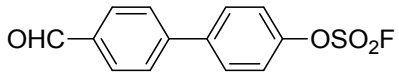
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.9 Hz, 2H), 7.49 (d, J = 7.8 Hz, 2H), 7.46 – 7.39 (m, 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ 149.8, 140.7, 137.6, 134.3, 121.3. HRMS (ESI-TOF) m/z: $[M-H]^+$ Calcd for $C_{12}H_8ClFO_3S$ 284.9788; Found 284.9792.

[3l] 4'-Fluorobiphenyl-4-yl fluorosulfate.[23]



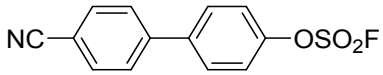
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 8.2 Hz, 3H), 7.39 (dd, J = 8.0, 5.9 Hz, 2H), 7.29 (s, 1H), 7.00 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 160.5, 148.2, 139.8, 132.4, 127.8, 120.2, 114.9.

[3m] 4'-Formylbiphenyl-4-yl fluorosulfate. [22]



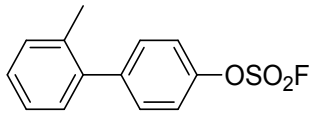
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.90 (d, J = 7.8 Hz, 2H), 7.64 (d, J = 8.5 Hz, 4H), 7.38 (d, J = 8.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.7, 150.0, 145.0, 140.4, 135.7, 130.4, 129.3, 127.8, 121.5.

[3n] 4'-Cyanobiphenyl-4-yl fluorosulfate.[24]



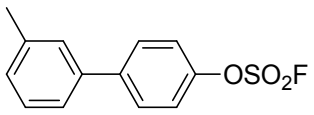
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.1 Hz, 2H), 7.60 (t, J = 7.6 Hz, 4H), 7.40 (d, J = 8.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.07, 143.54, 139.87, 133.50, 132.77, 129.23, 127.83, 121.61, 118.49, 111.87.

[3o] 2'-Methylbiphenyl-4-yl fluorosulfate. [22]



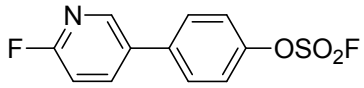
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (q, J = 8.7 Hz, 4H), 7.32 – 7.23 (m, 3H), 7.19 (d, J = 7.2 Hz, 1H), 2.26 (s, 3H), 1.55 (s, 3H), 0.00 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.0, 142.7, 139.9, 135.3, 131.2, 130.6, 129.7, 128.0, 126.0, 120.6, 20.4.

[3p] 3'-Methylbiphenyl-4-yl fluorosulfate. [22]



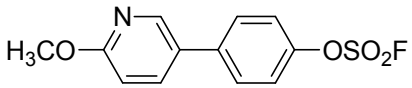
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.6 Hz, 2H), 7.26 (s, 1H), 7.25 – 7.20 (m, 4H), 7.09 (s, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 142.1, 139.2, 138.7, 129.0, 128.9, 128.89, 128.0, 124.3, 121.1, 21.5.

[3q] 4-(naphthalen-2-yl)phenyl sulfurofluoridate.



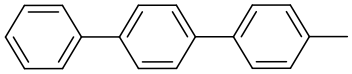
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.96 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.9 Hz, 2H), 7.45 (t, J = 11.5 Hz, 2H), 7.05 (d, J = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 162.4, 150.0, 146.1, 139.9, 137.7, 129.2, 121.9, 109.9. HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{11}H_7F_2NO_3S$ 309.9752; Found 309.9748

[3r] 4-(6-methoxypyridin-3-yl)phenyl sulfurofluoridate.



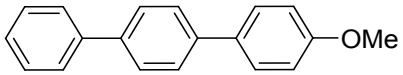
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 8.1 Hz, 2H), 6.84 (d, J = 8.5 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.0, 149.2, 145.1, 138.7, 137.3, 128.5, 128.1, 121.4, 111.1, 53.6. HRMS (ESI-TOF) m/z: $[M-H]^+$ Calcd for $C_{12}H_{10}FNO_4S$ 282.0236; Found 282.0242

[4d] 4-Methyl-p-terpheny.[25]



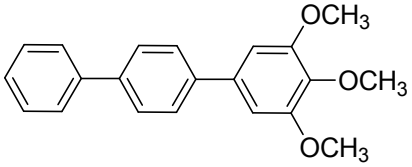
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.60 (m, 6H), 7.55 (d, J = 7.9 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 7.4 Hz, 1H), 7.31 – 7.23 (m, 2H), 2.42 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.7, 140.0, 139.8, 137.7, 137.1, 129.5, 128.7, 127.4, 127.2, 127.0, 126.8, 21.14.

[4e] 4-Methoxy-p-terpheny.[26]



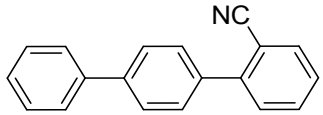
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.5 Hz, 6H), 7.59 (d, J = 7.1 Hz, 2H), 7.46 (d, J = 13.9 Hz, 2H), 7.36 (t, J = 7.2 Hz, 1H), 7.00 (d, J = 7.1 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 140.7, 139.7, 139.4, 133.2, 128.7, 128.0, 127.4, 127.2, 127.0, 126.9, 114.2, 55.3.

[4f] 3,4,5,-Trimethoxy-p-terpheny.[27]



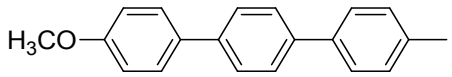
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.59 (m, 6H), 7.47 (t, J = 6.9 Hz, 2H), 7.43 – 7.34 (m, 1H), 6.83 (s, 2H), 3.95 (s, 3H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.5, 140.6, 140.2, 137.7, 136.7, 128.8, 127.4, 127.44, 127.3, 127.0, 104.3, 60.9, 56.2.

[4g] 2-Cyano-*p*-terphenyl.[28]



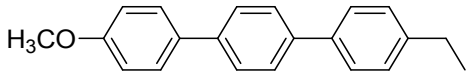
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ (d, J = 7.7 Hz, 1H), 7.72 (d, J = 8.1 Hz, 2H), 7.66 (t, J = 8.2 Hz, 5H), 7.57 (d, J = 7.8 Hz, 1H), 7.46 (q, J = 7.7 Hz, 3H), 7.38 (t, J = 7.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 141.5, 140.3, 136.9, 133.8, 132.8, 130.0, 129.1, 128.8, 127.6, 127.5, 127.4, 127.1, 118.8, 111.1.

[4h] 4-**Methoxy-4''-Methyl-p-terphenyl.[29]**



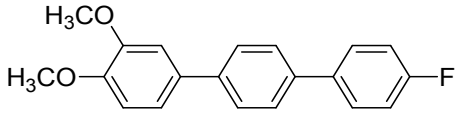
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.59 (m, 4H), 7.56 (dd, J = 15.3, 8.3 Hz, 4H), 7.26 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.6 Hz, 2H), 3.86 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 139.4, 137.8, 137.0, 133.2, 129.4, 128.0, 127.2, 126.9, 126.7, 114.2, 55.3, 21.1.

[4i] 4-ethyl-4''-methoxy-1,1':4',1''-terphenyl.[28]



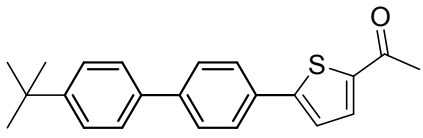
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.60 (m, 4H), 7.57 (dd, J = 8.2, 5.5 Hz, 4H), 7.29 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.7 Hz, 2H), 3.86 (s, 3H), 2.70 (q, J = 7.5 Hz, 2H), 1.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 143.3, 139.3, 138.0, 133.2, 128.3, 128.0, 127.2, 126.9, 126.8, 114.2, 55.3, 28.5, 15.6.

[4j] 4''-fluoro-3,4-dimethoxy-1,1':4',1''-terphenyl.[22]



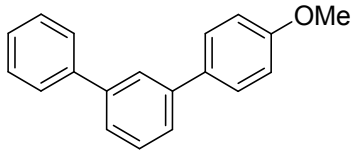
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ7.69 – 7.51 (m, 6H), 7.19 (dd, J = 8.3, 2.1 Hz, 1H), 7.17 – 7.10 (m, 3H), 6.97 (d, J = 8.3 Hz, 1H), 3.97 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2, 148.7, 139.9, 138.7, 133.6, 128.5, 128.5, 127.3, 127.2, 119.3, 115.8, 115.5, 111.5, 110.3, 56.0, 55.9.

[4k] 1-(5-(4'-(tert-butyl)-[1,1'-biphenyl]-4-yl)thiophen-2-yl)ethanone.



Yellow solid, ^{1}H NMR (400 MHz, cdcl$_3$) δ 7.65 (d, J = 3.9 Hz, 1H), 7.59 (d, J = 8.3 Hz, 2H), 7.44 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 3.9 Hz, 1H), 2.56 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 190.6, 152.9, 152.4, 142.6, 133.5, 130.5, 126.0, 126.0, 123.4, 34.76, 31.1, 26.5.
HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{22}OS$ 335.1470; Found 335.1478

[4l] 4-Methoxy-*m*-terpheny.[30]



White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.64 (d, J = 7.7 Hz, 2H), 7.58 (d, J = 8.5 Hz, 2H), 7.49 (dt, J = 24.4, 7.5 Hz, 5H), 7.36 (t, J = 7.3 Hz, 1H), 7.00 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 141.7, 141.3, 141.2, 133.6, 129.1, 128.7, 128.2,

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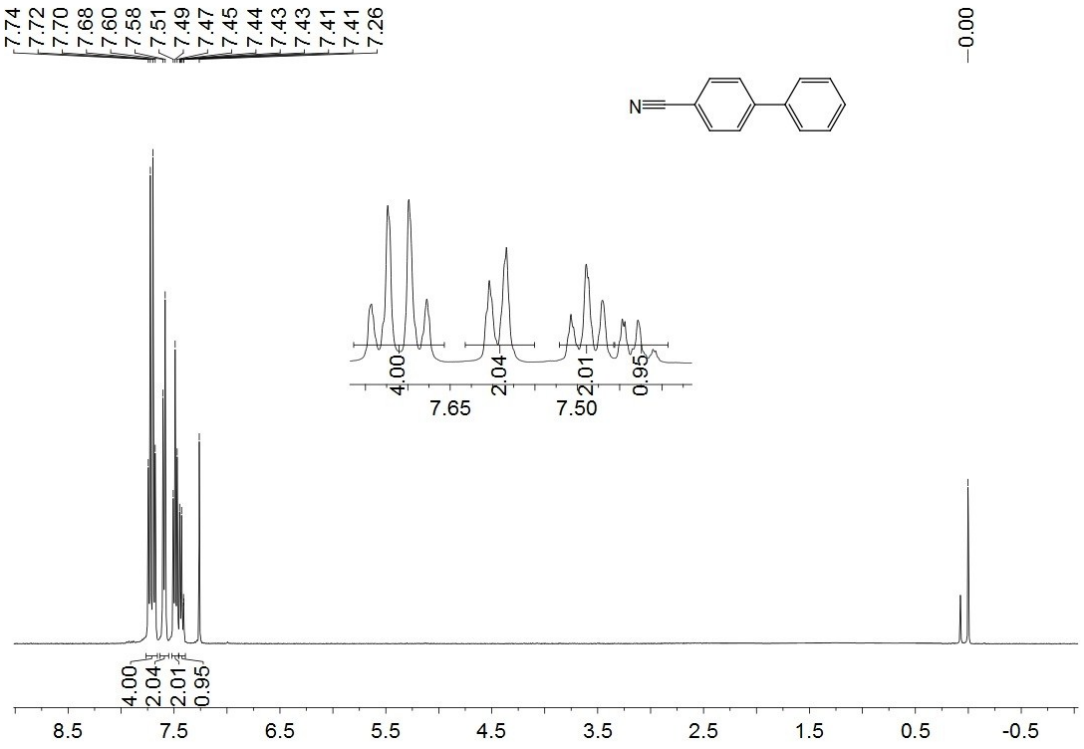
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7.44
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7.43
7.41
7.41
7.26
0.00
N
4.00
2.04
2.01
0.95
7.65
7.50
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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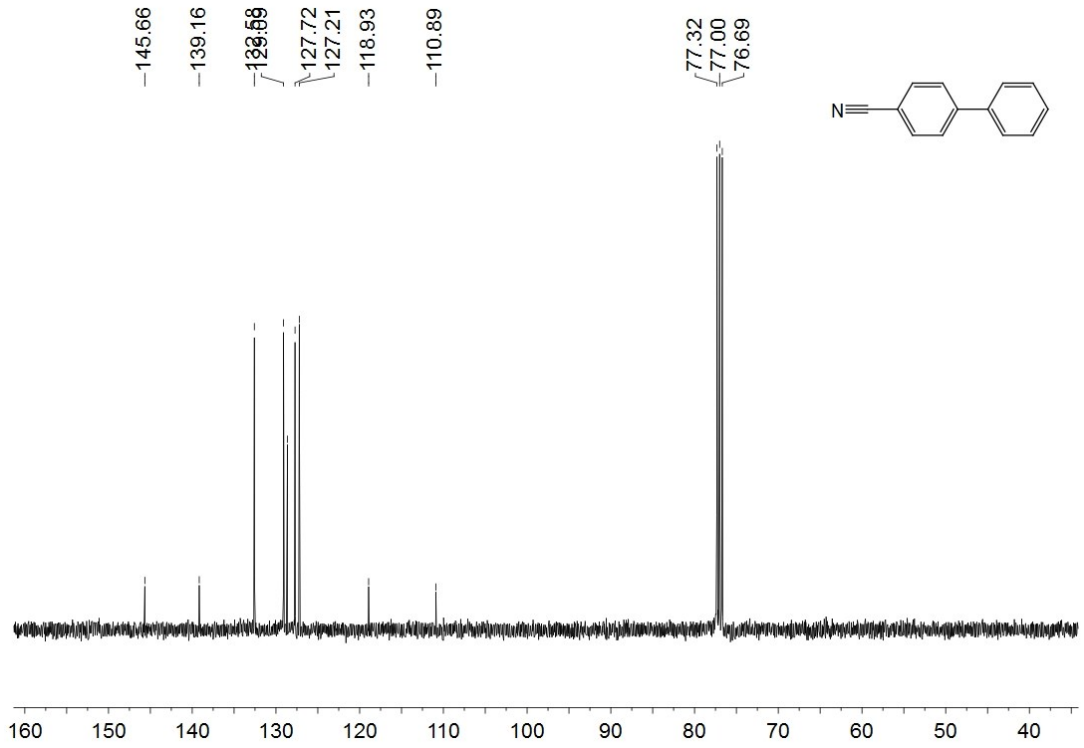
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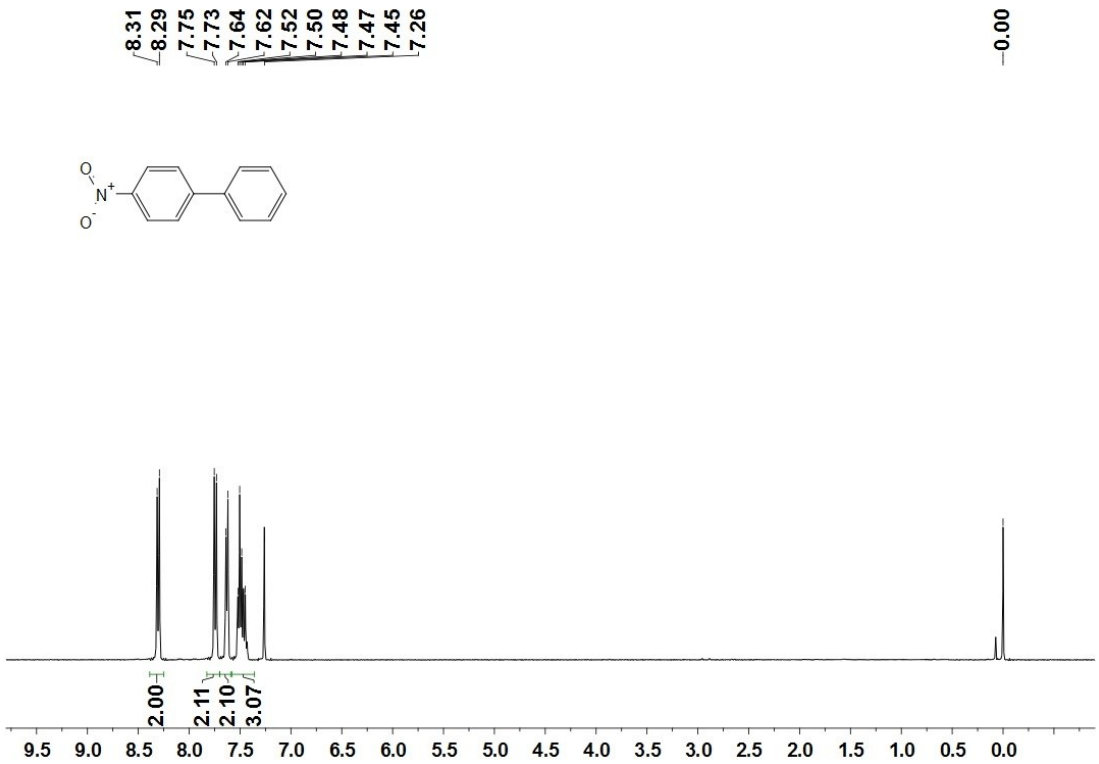
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7.47
7.45
7.26
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2.00
2.11
2.10
3.07
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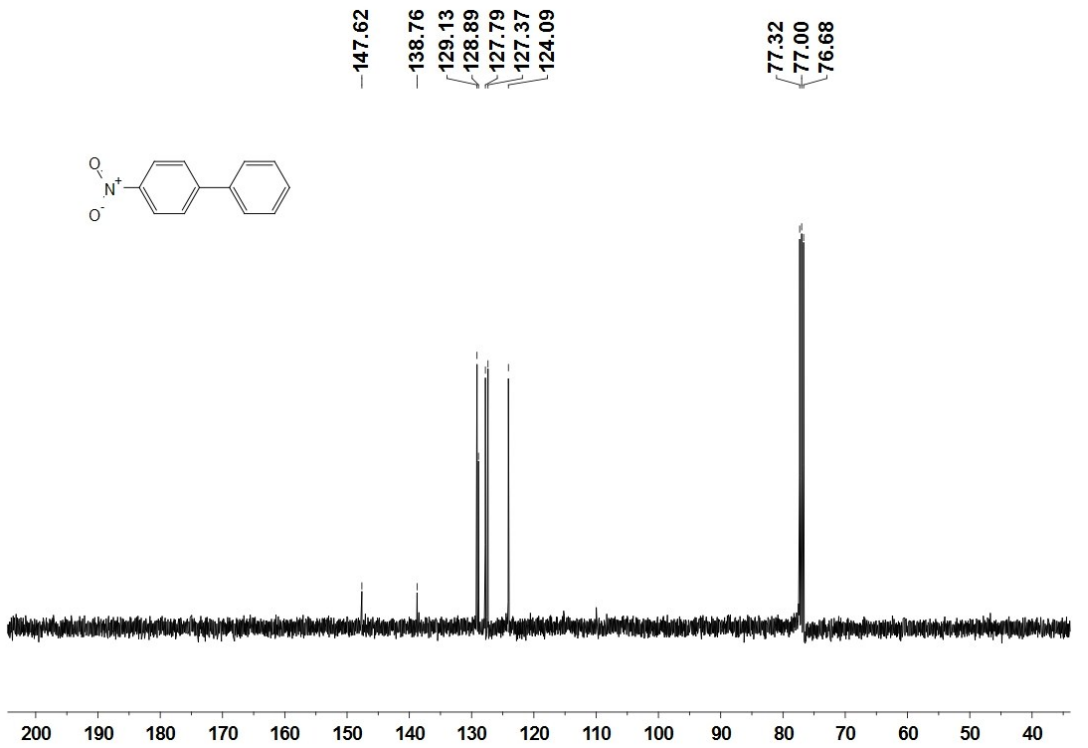
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76.68
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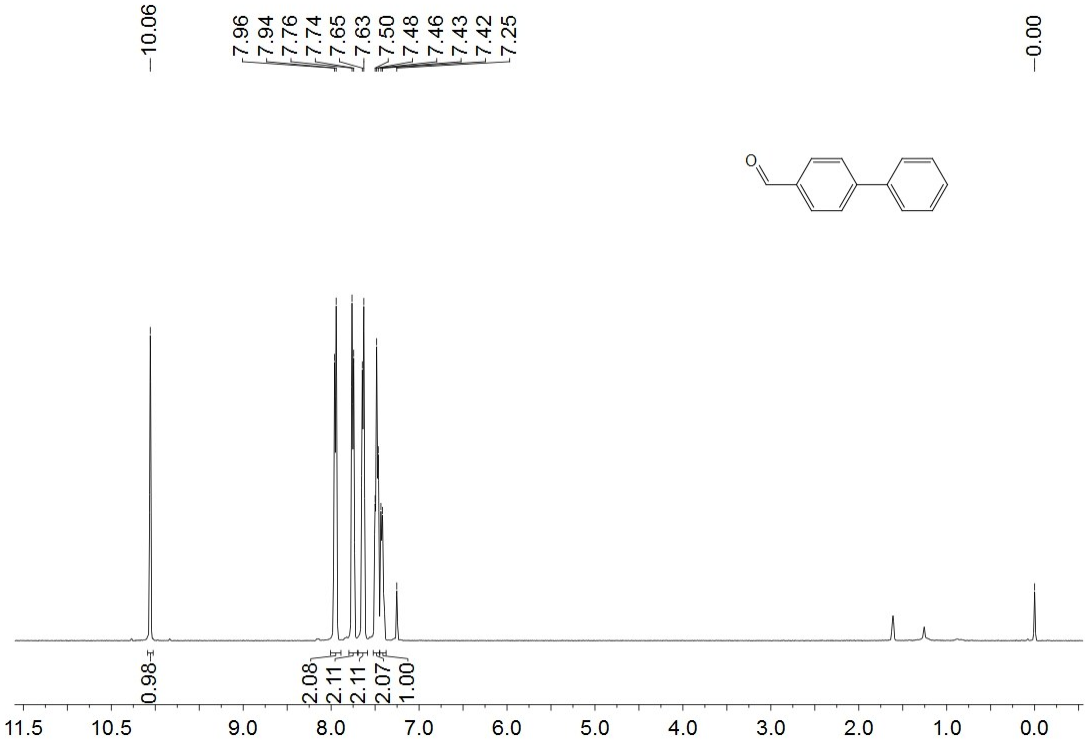
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7.42
7.25
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O
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2.08
2.11
2.11
2.07
1.00
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6.0
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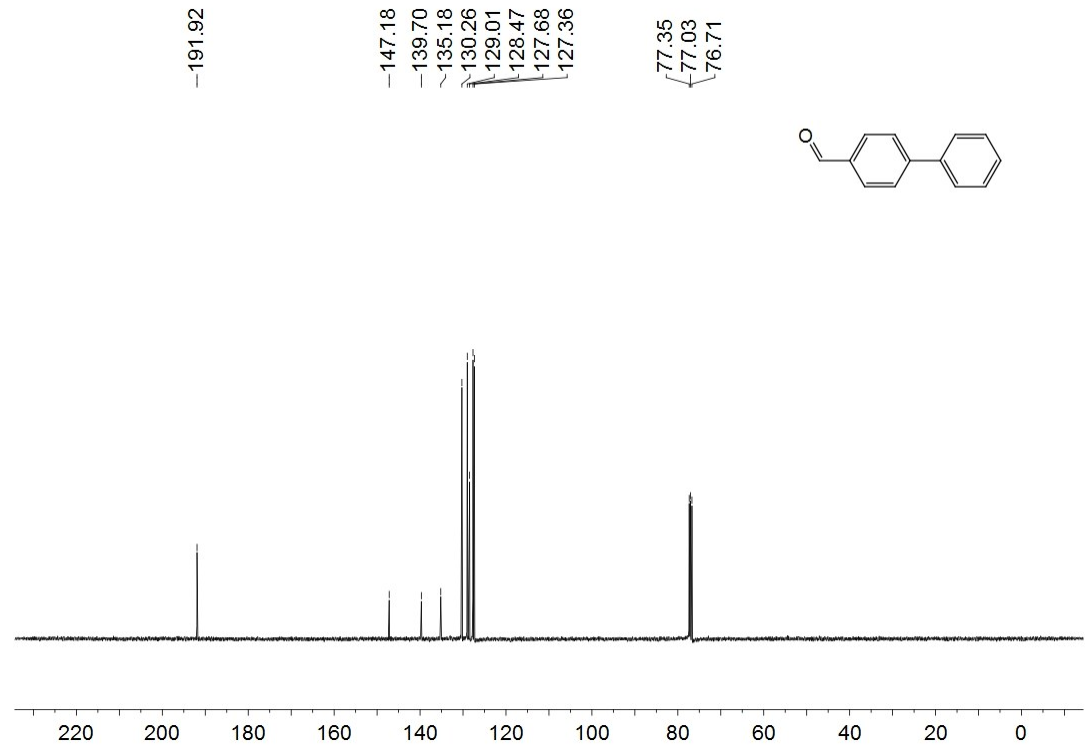
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140
120
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80
60
40
20
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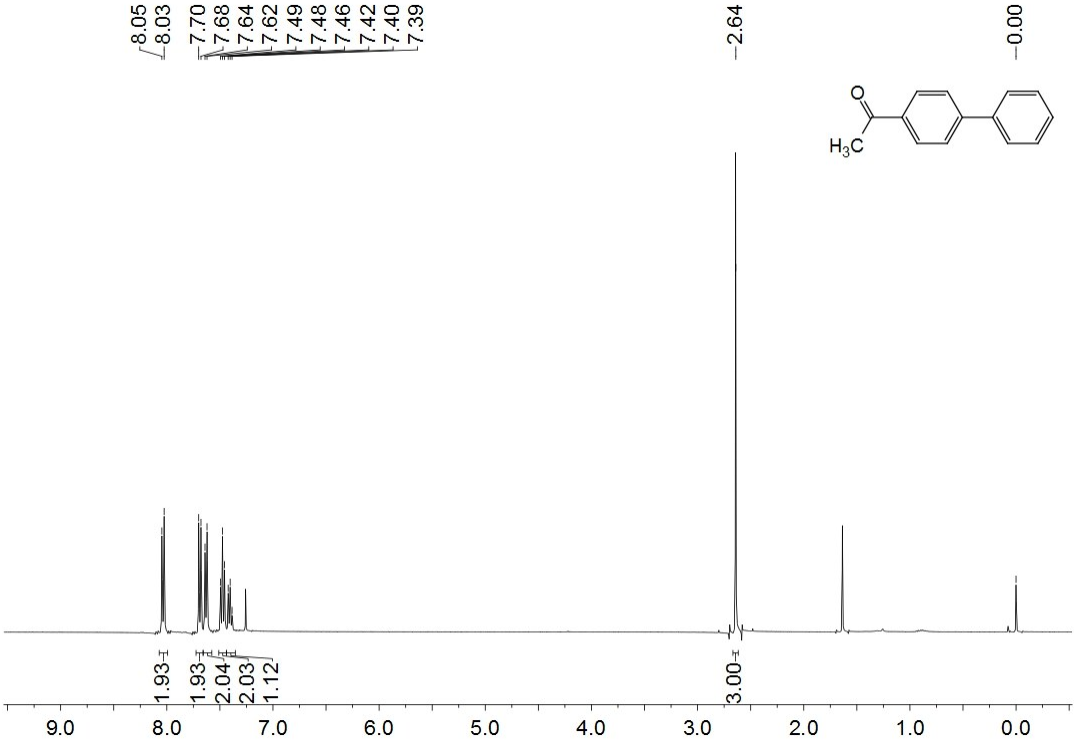
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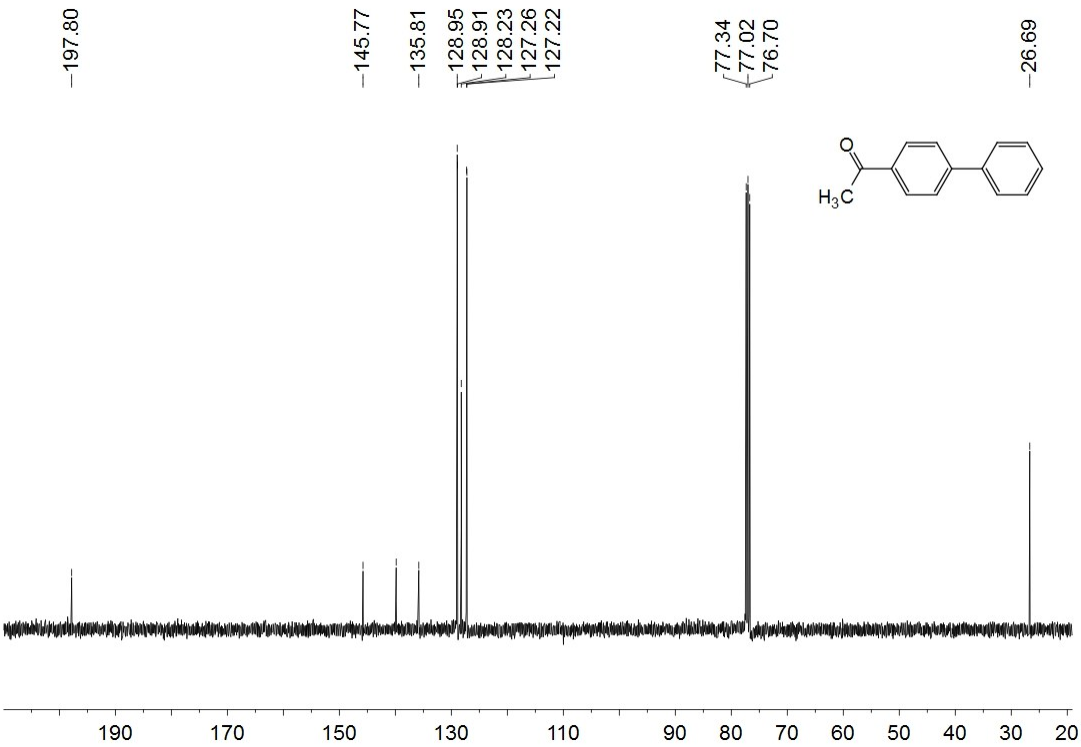
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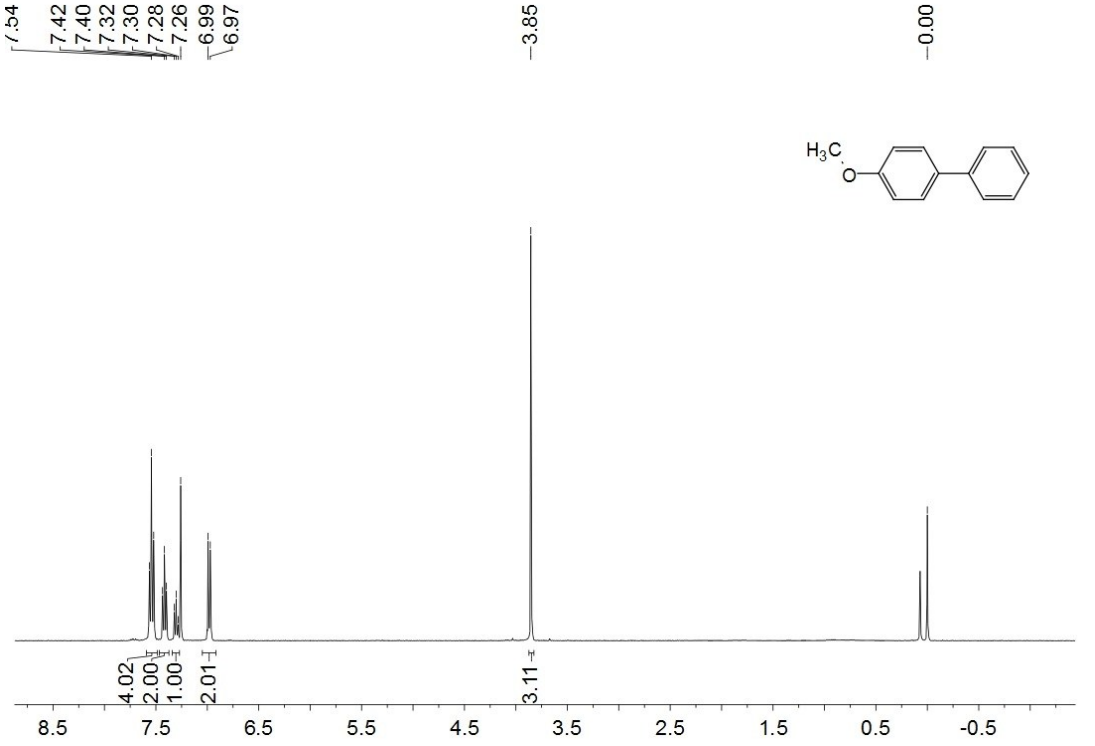
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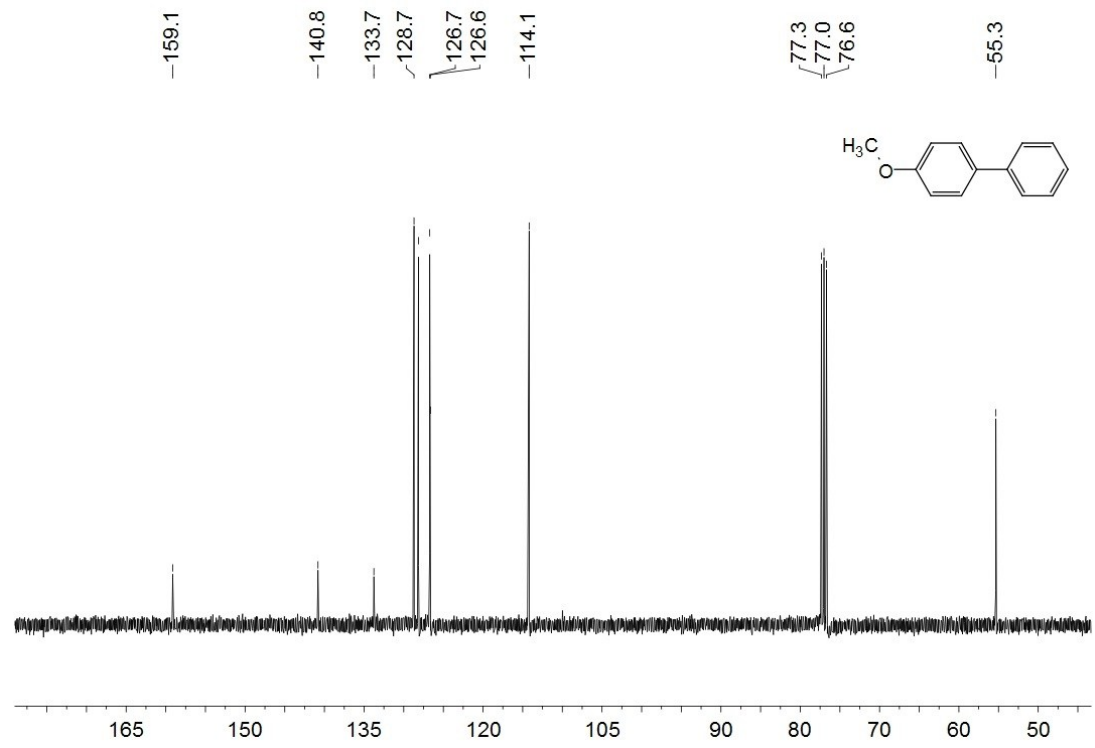
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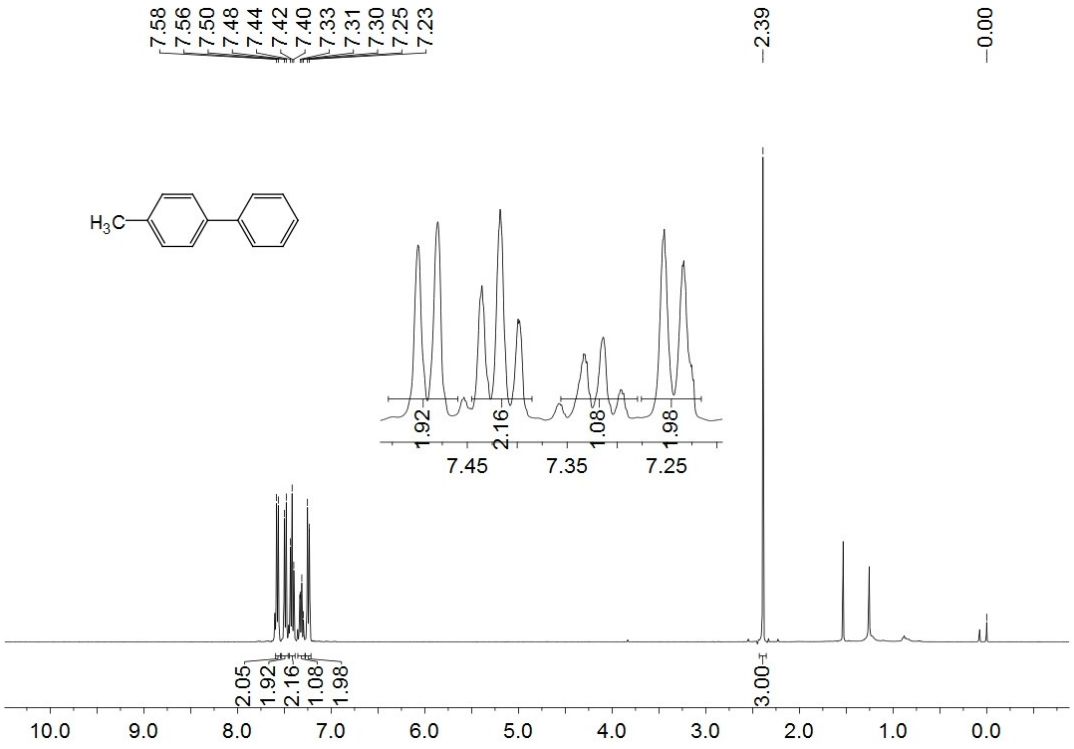
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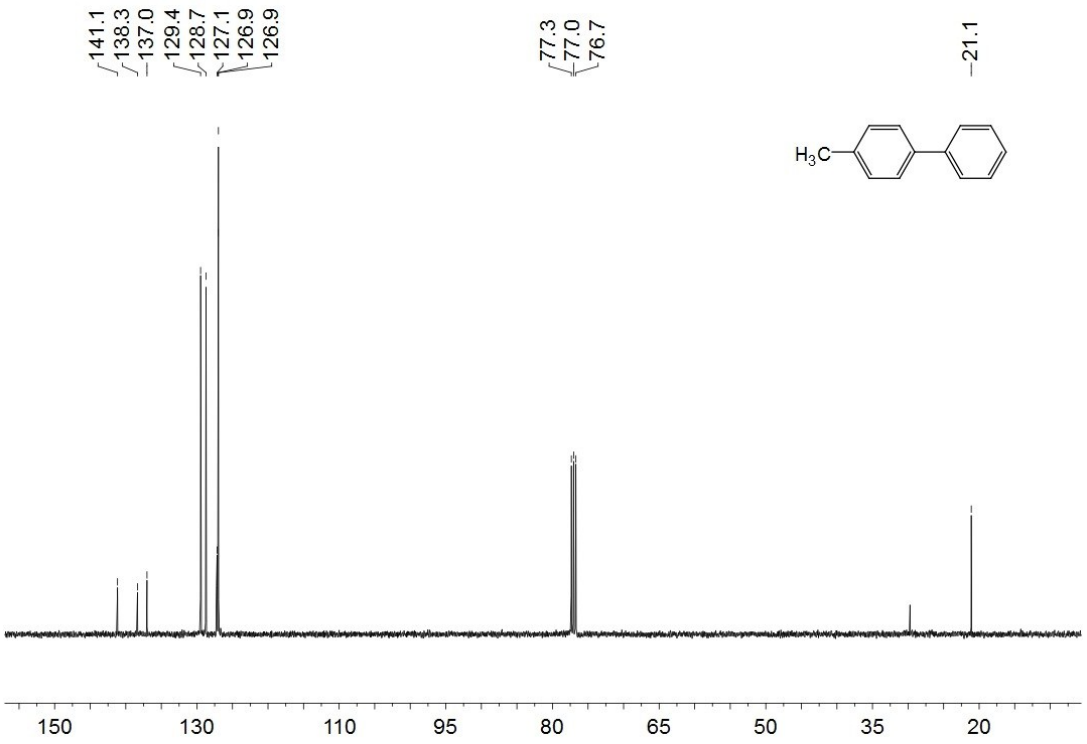
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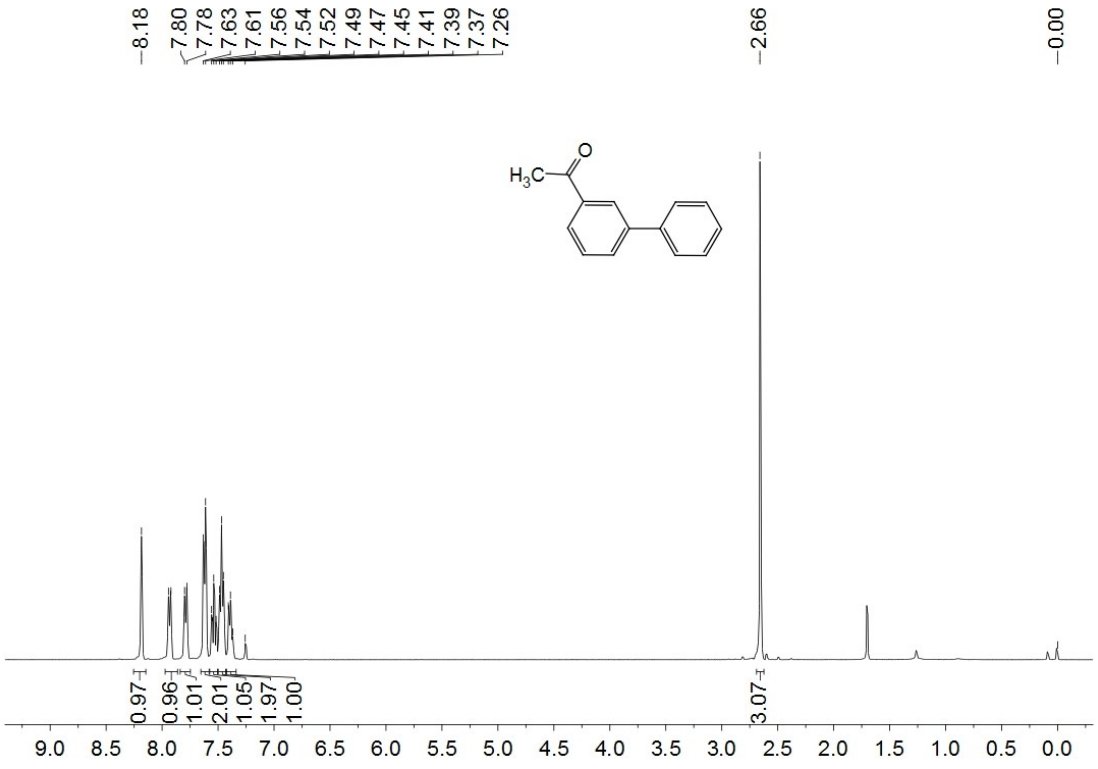
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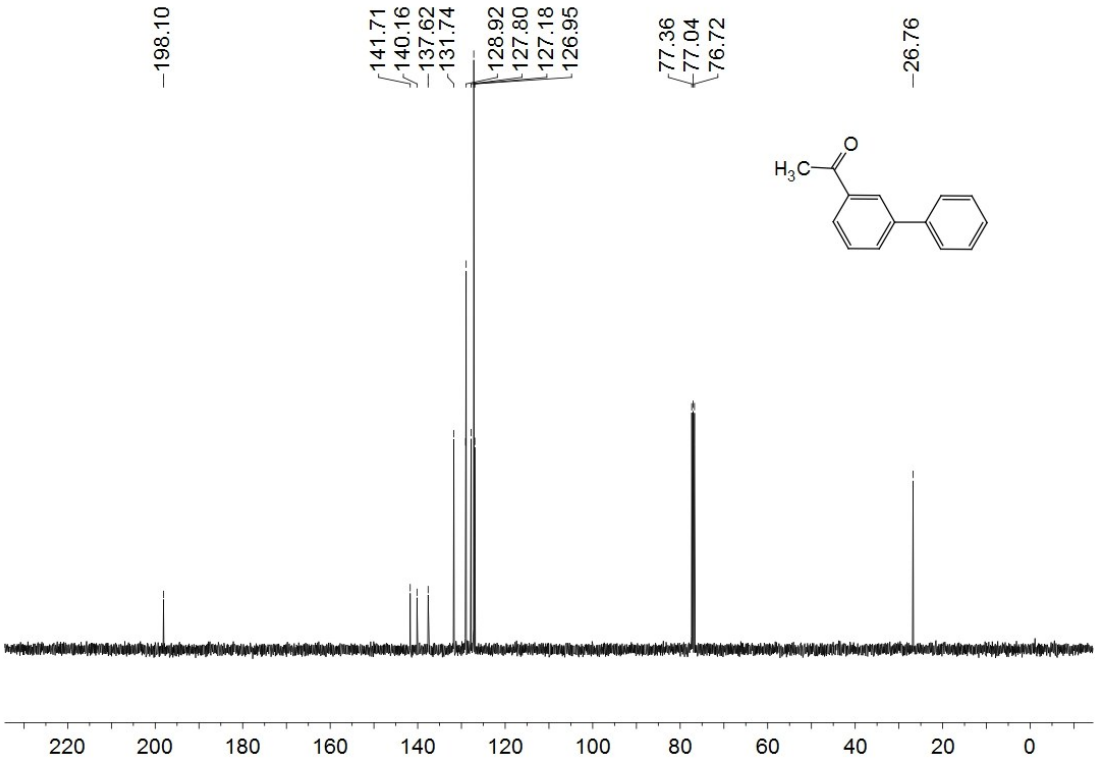
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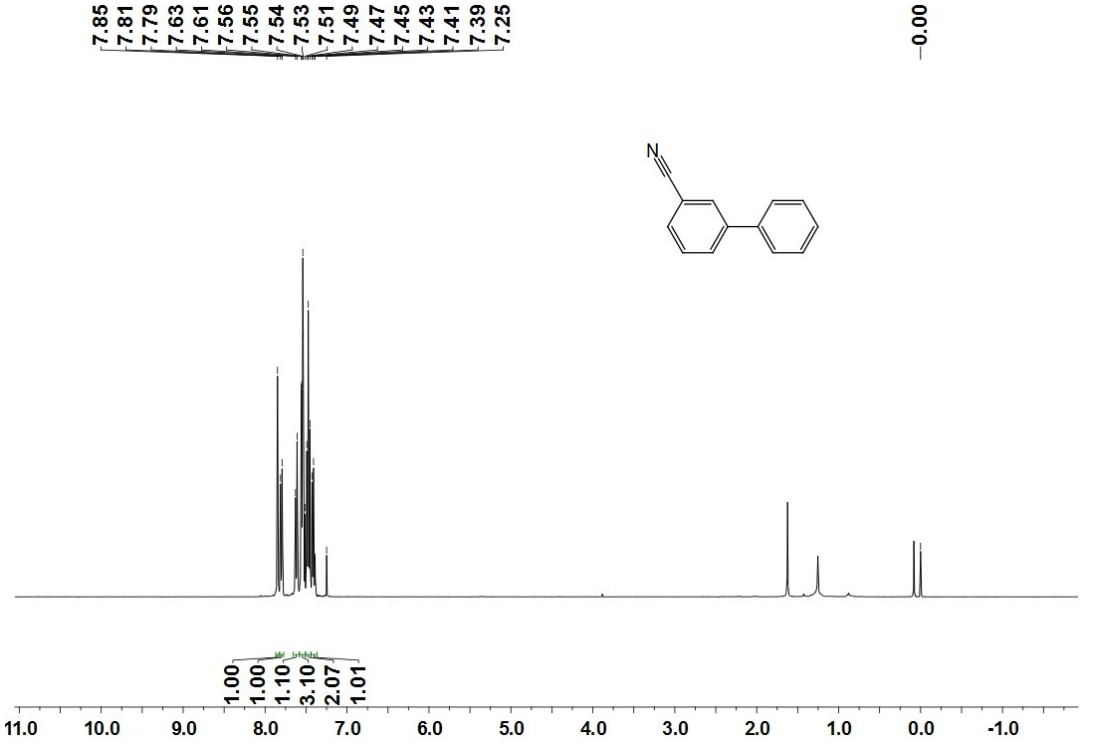
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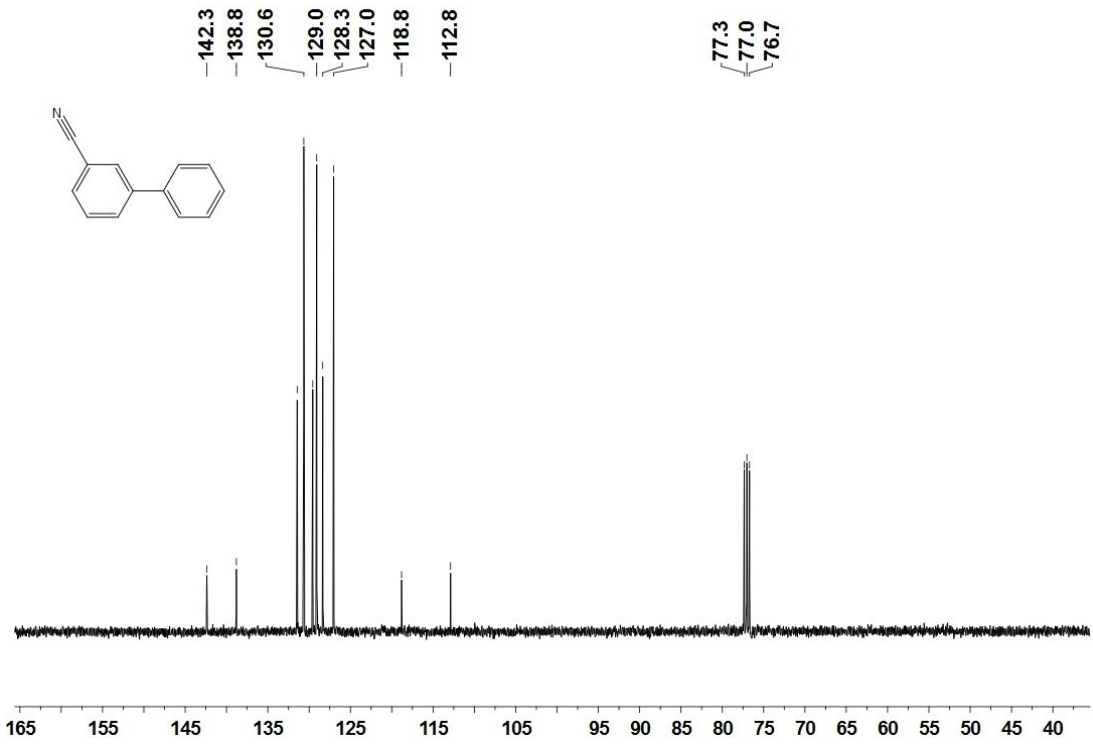
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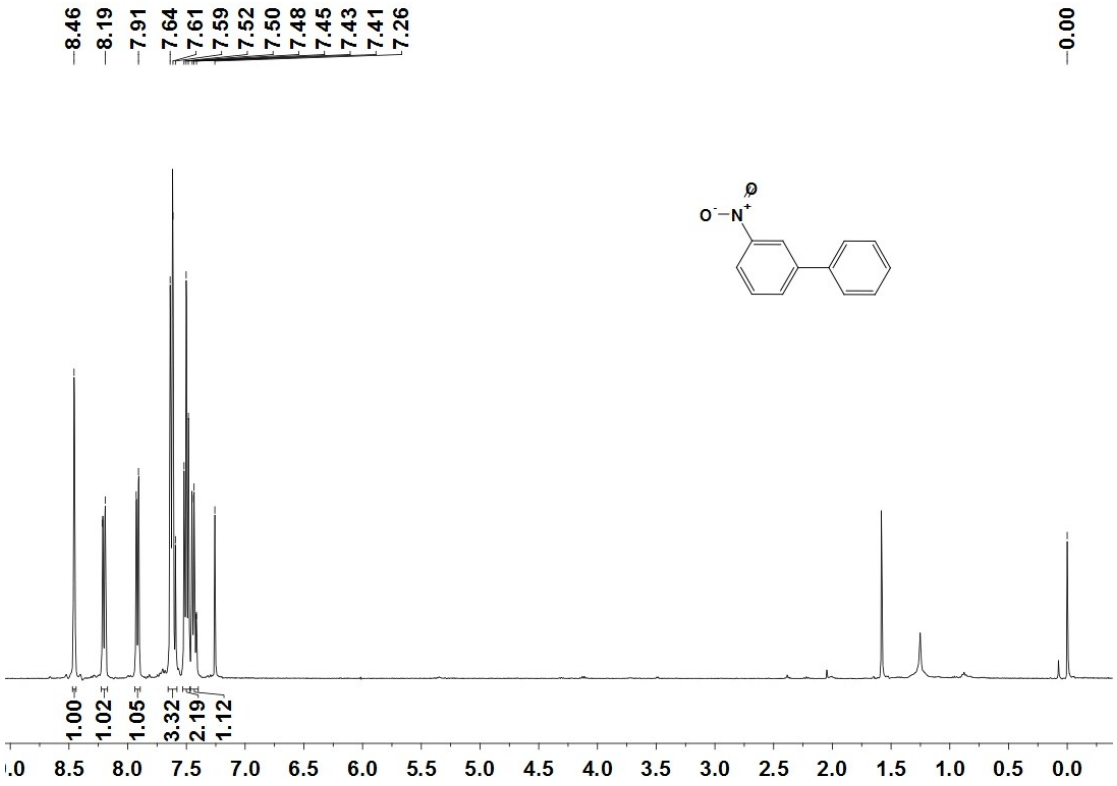
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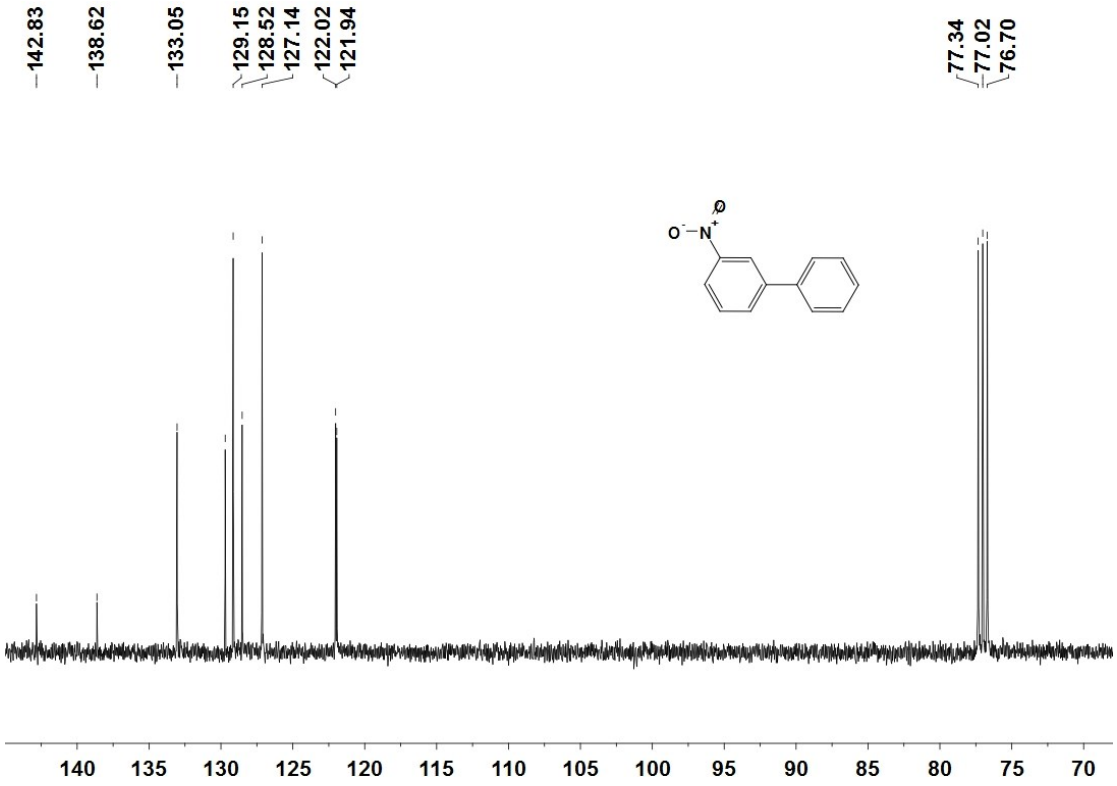
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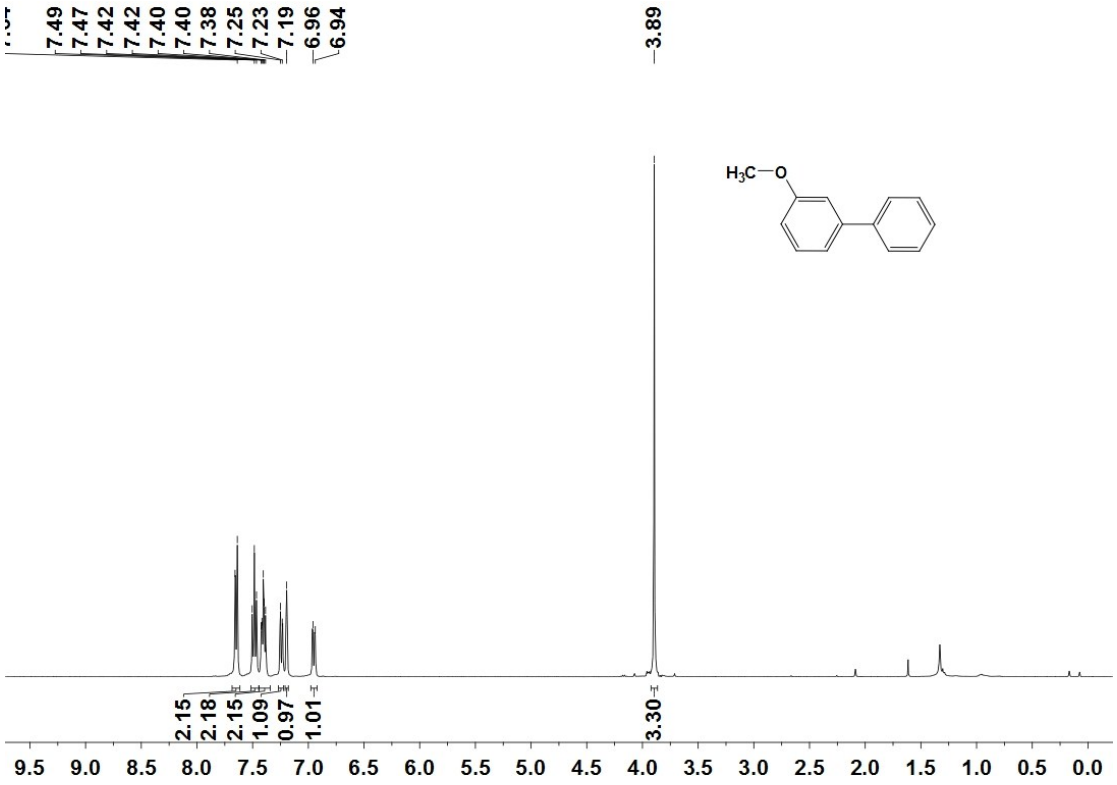
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H3C—O
2.15
2.18
2.15
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1.01
3.30
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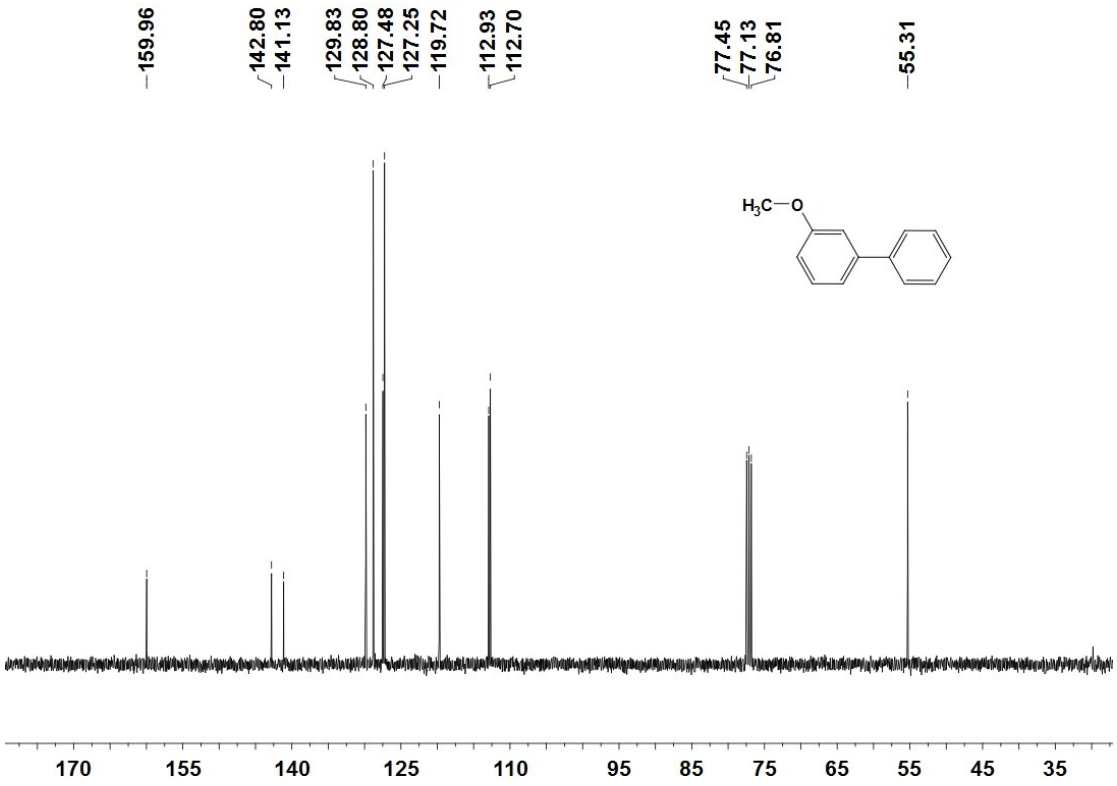
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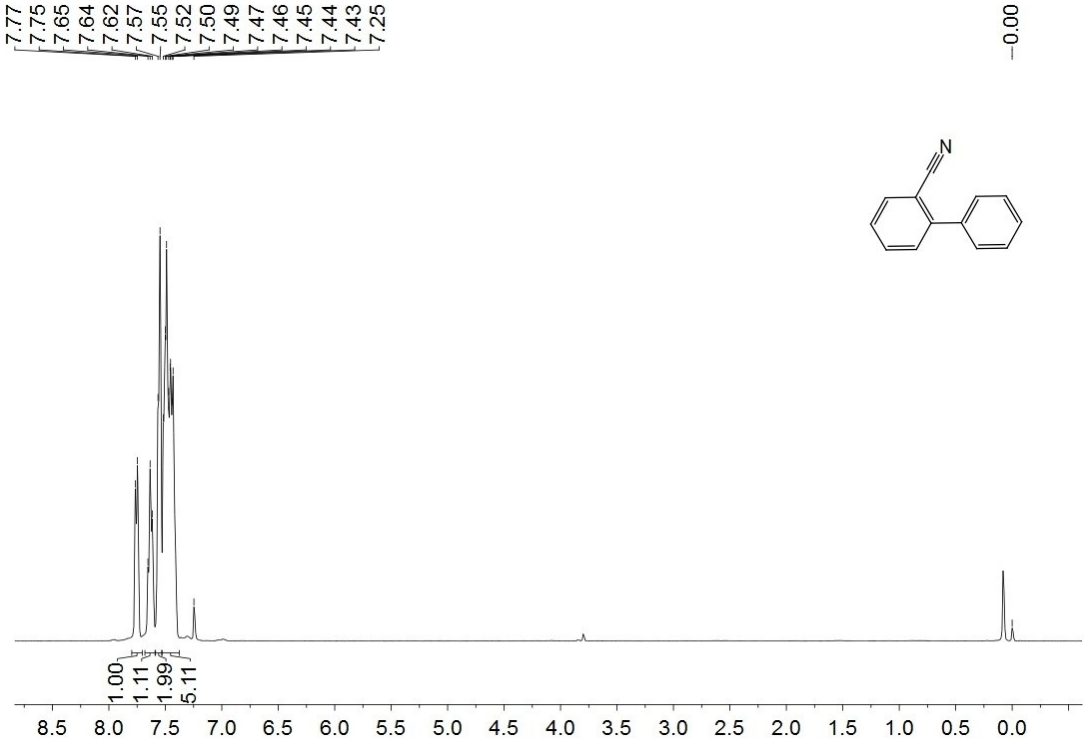
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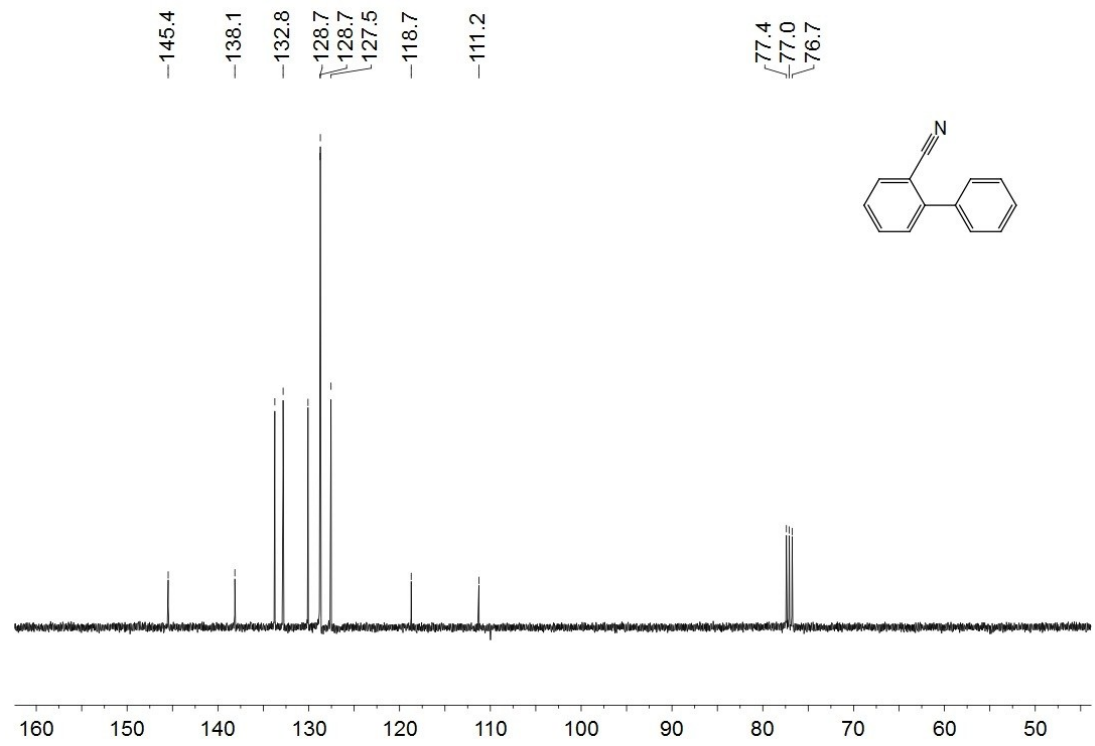
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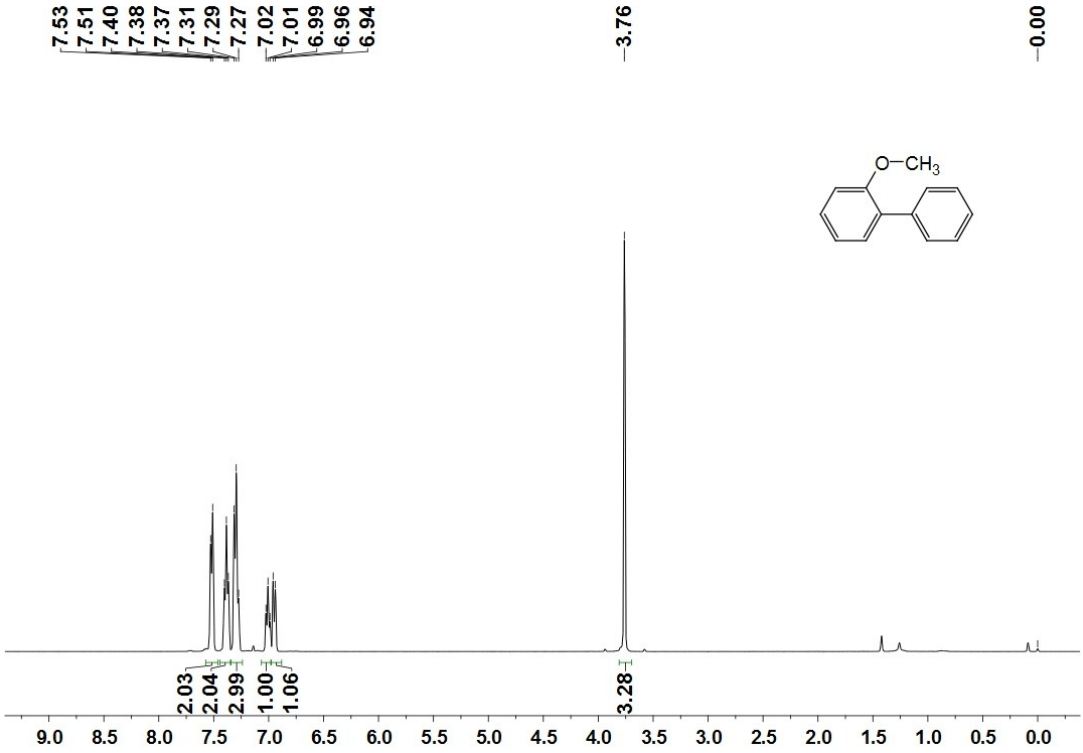
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6.94
3.76
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O—CH3
2.03
2.04
2.99
1.00
1.06
3.28
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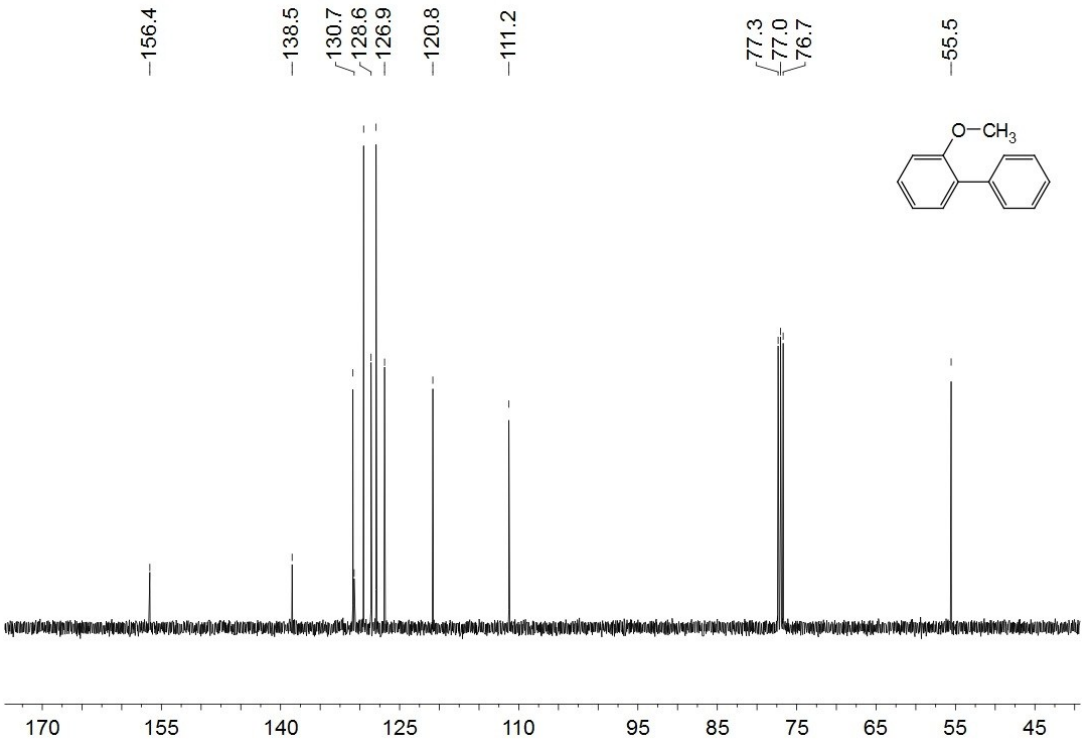
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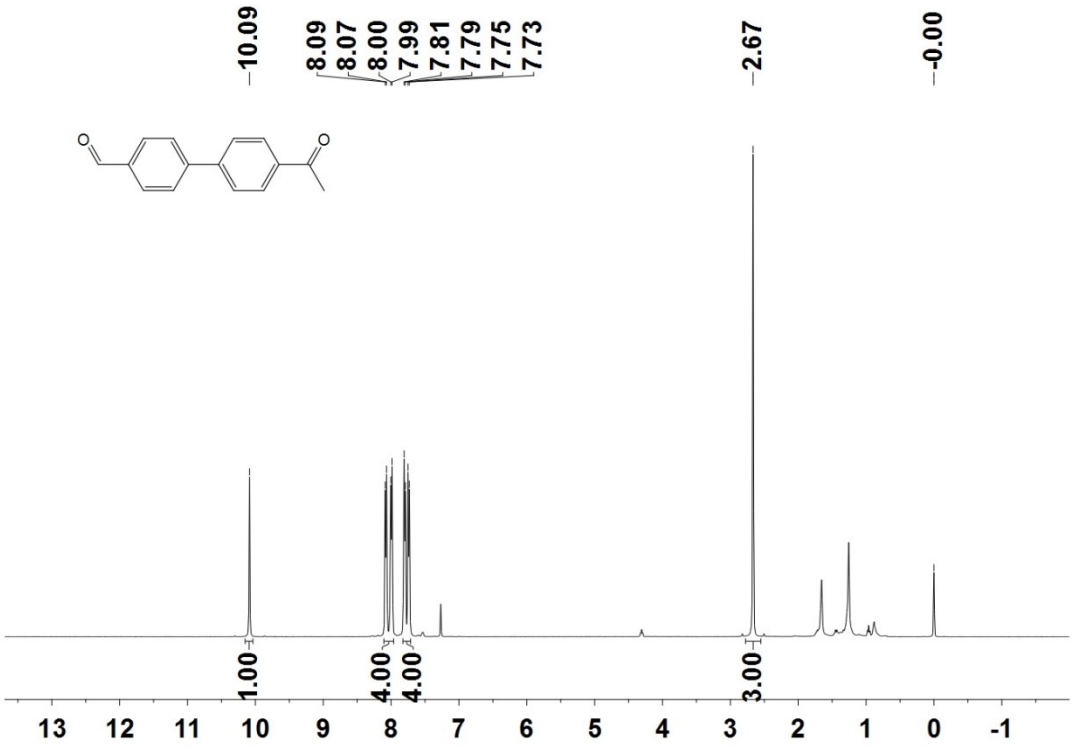
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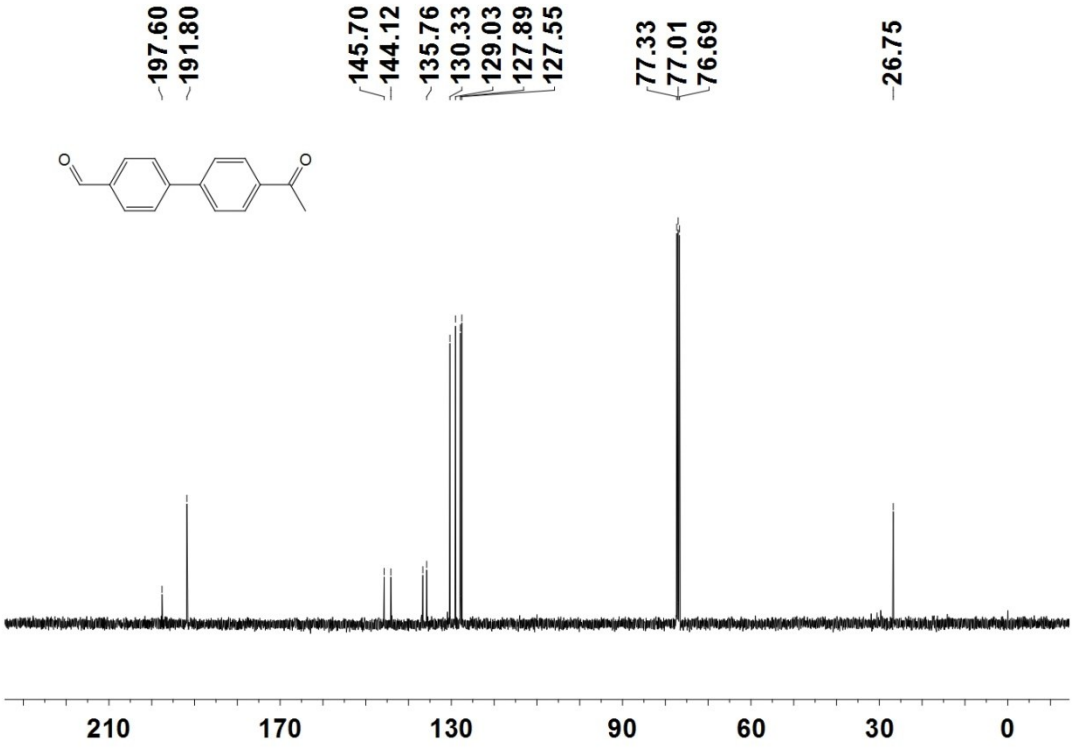
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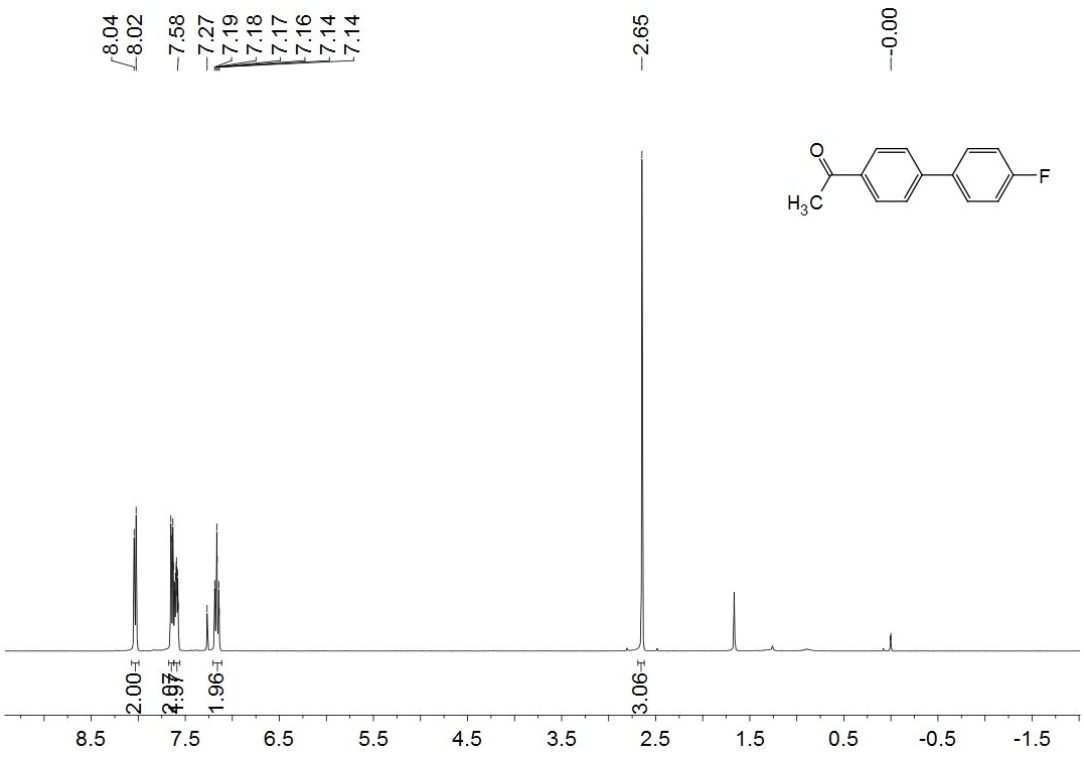
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H3C
F
2.00
2.07
1.96
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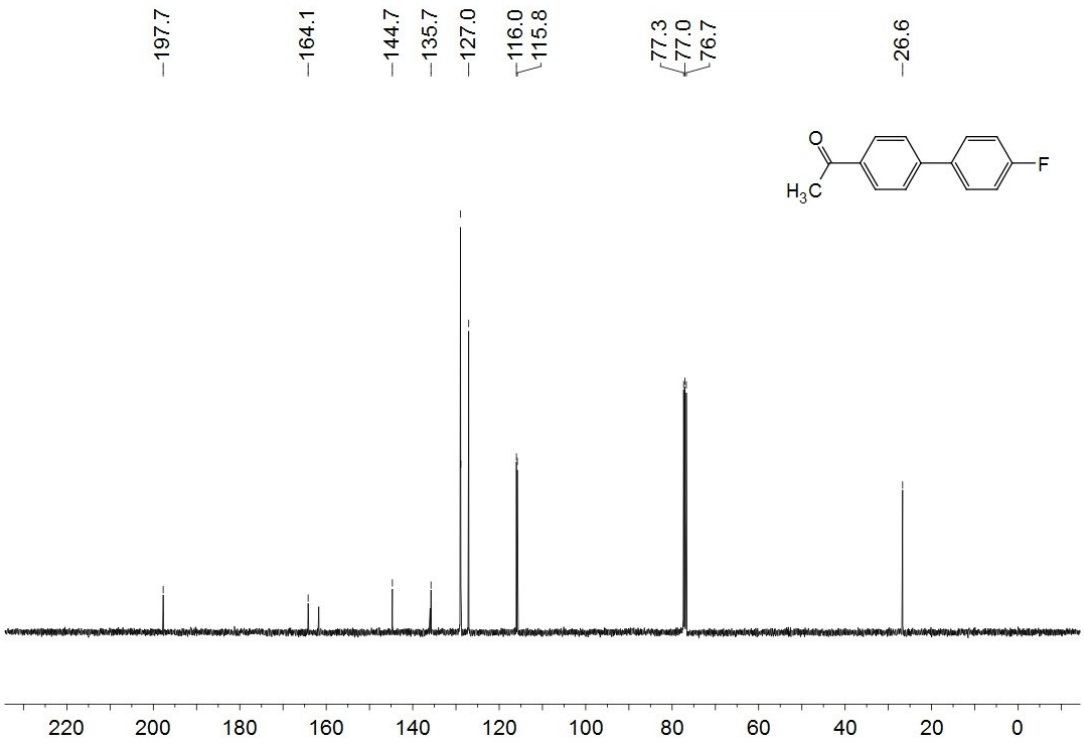
-1.5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F
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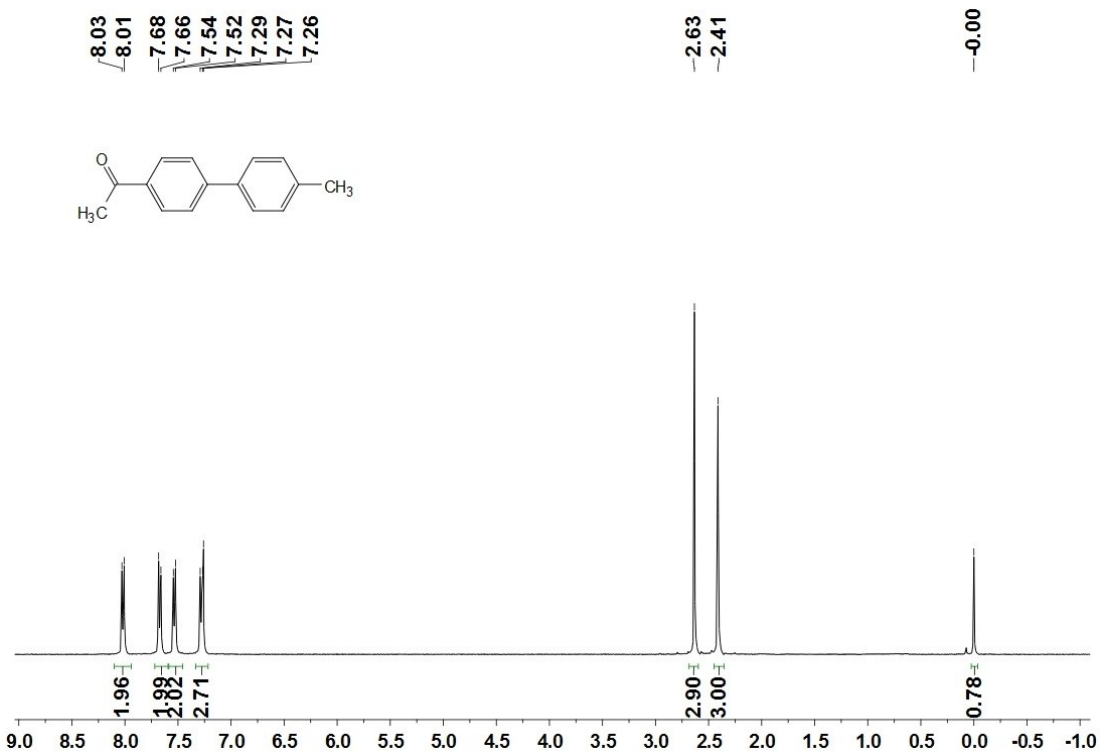
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2.41
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H3C
CH3
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1.99
2.02
2.71
2.90
3.00
0.78
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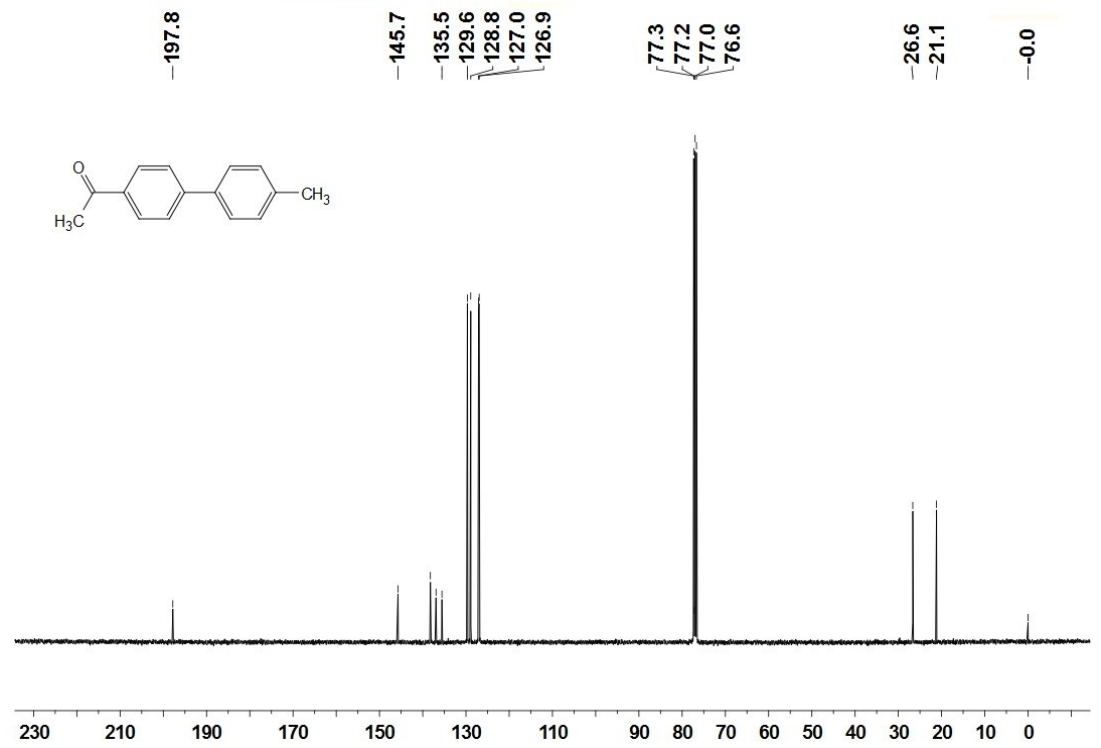
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CH3
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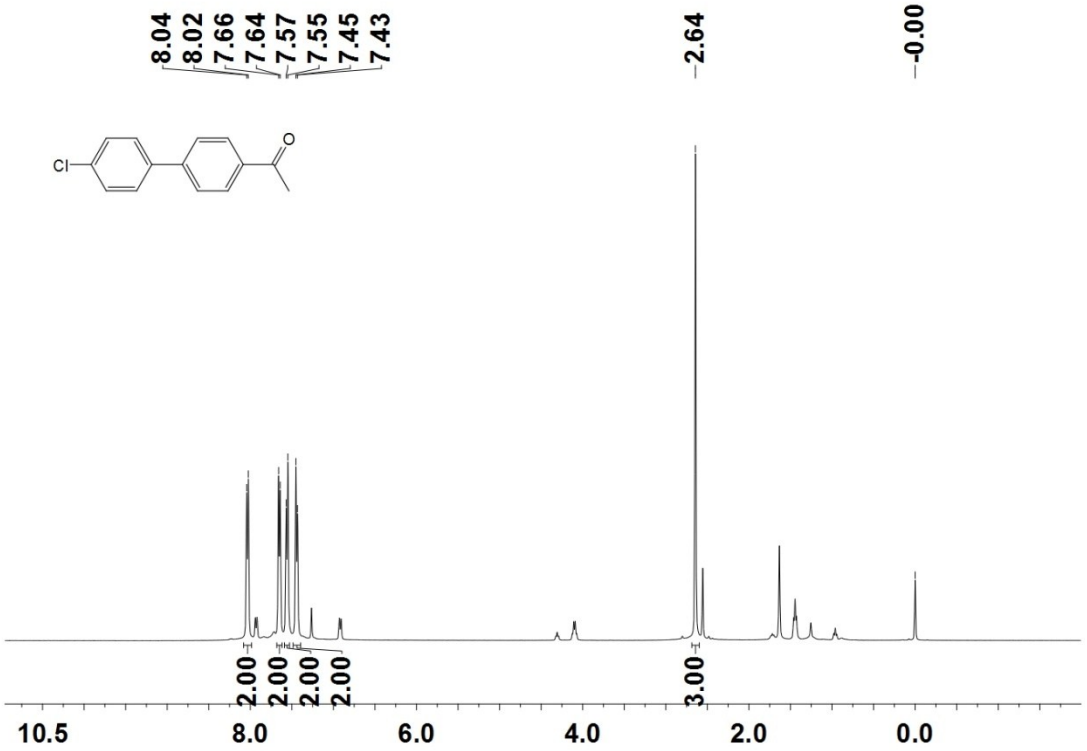
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2.00
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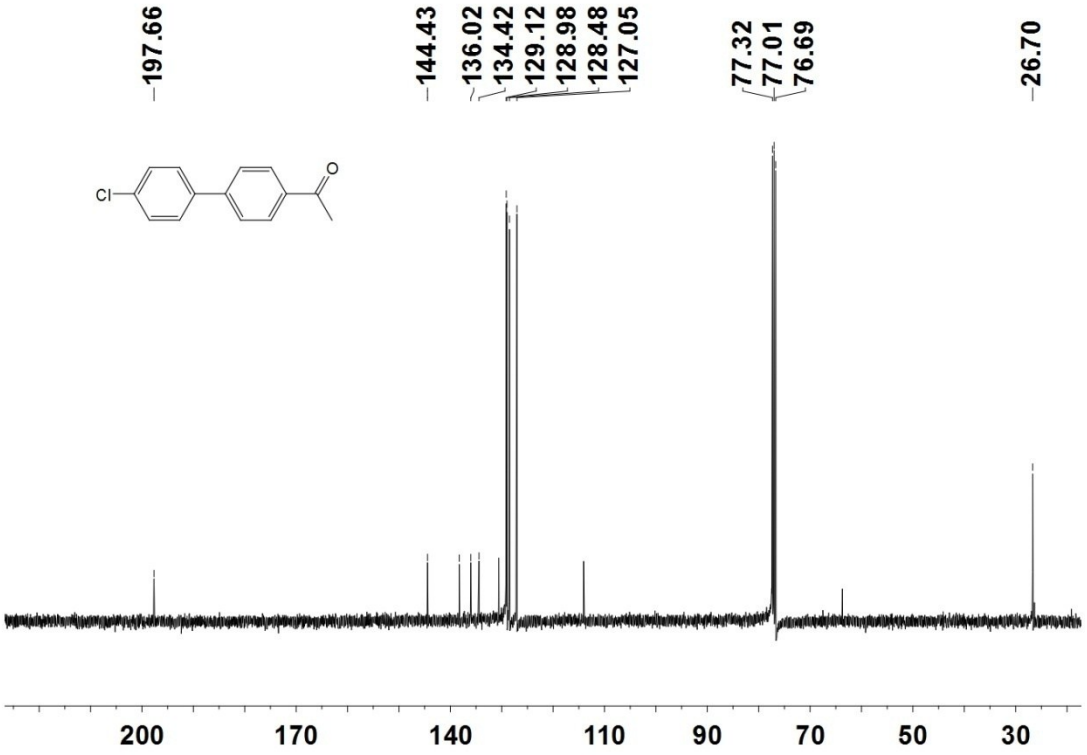
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50
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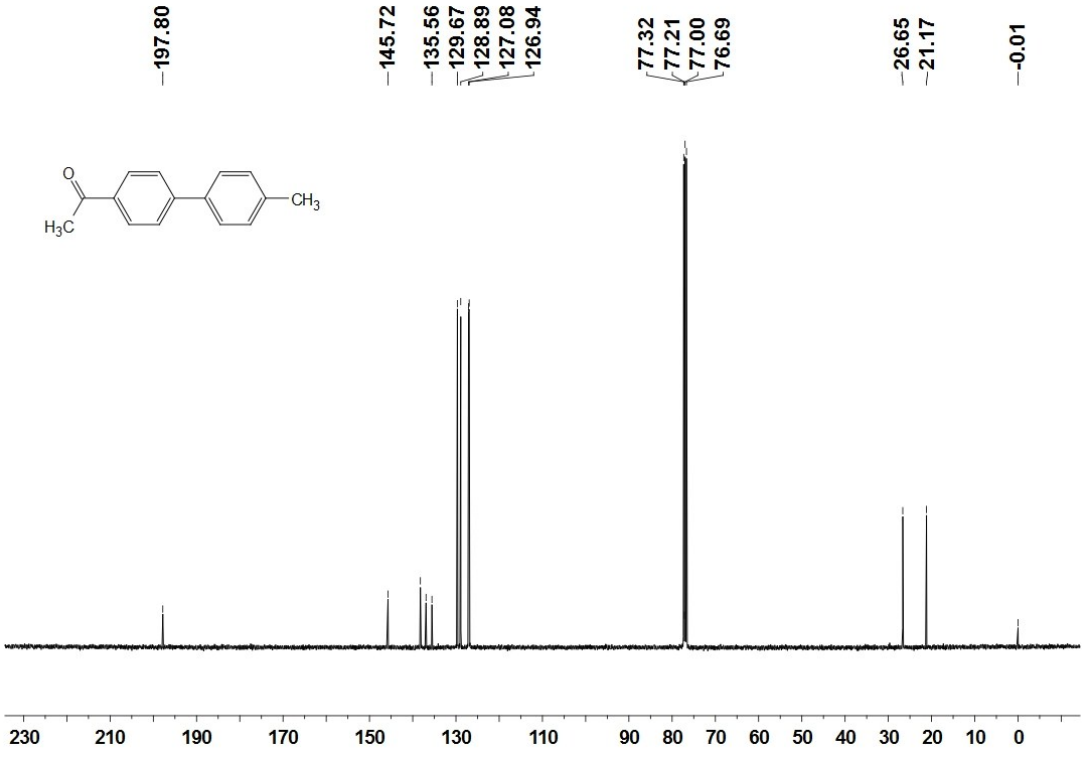
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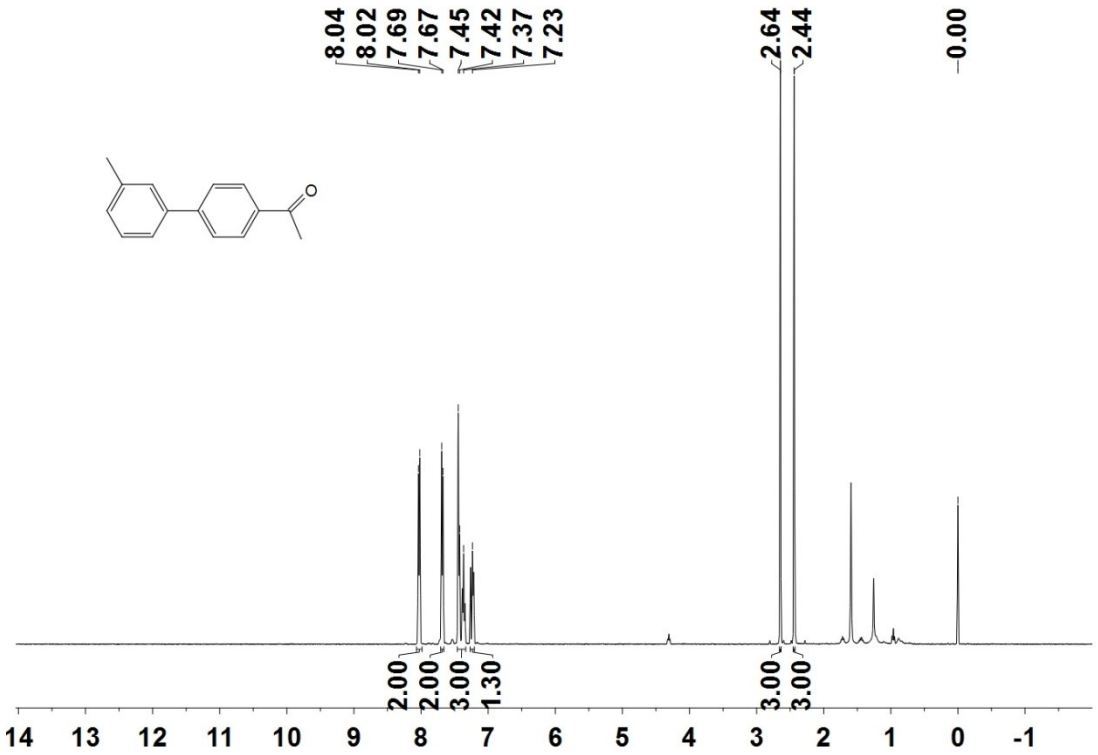
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1.30
3.00
3.00
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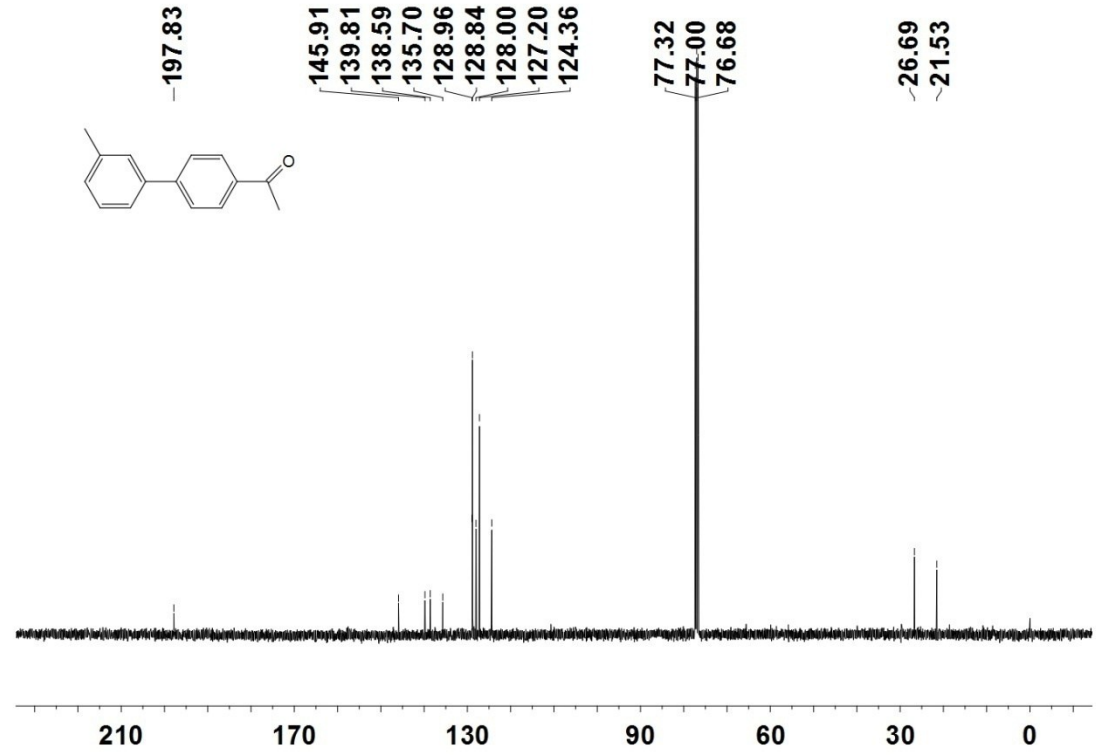
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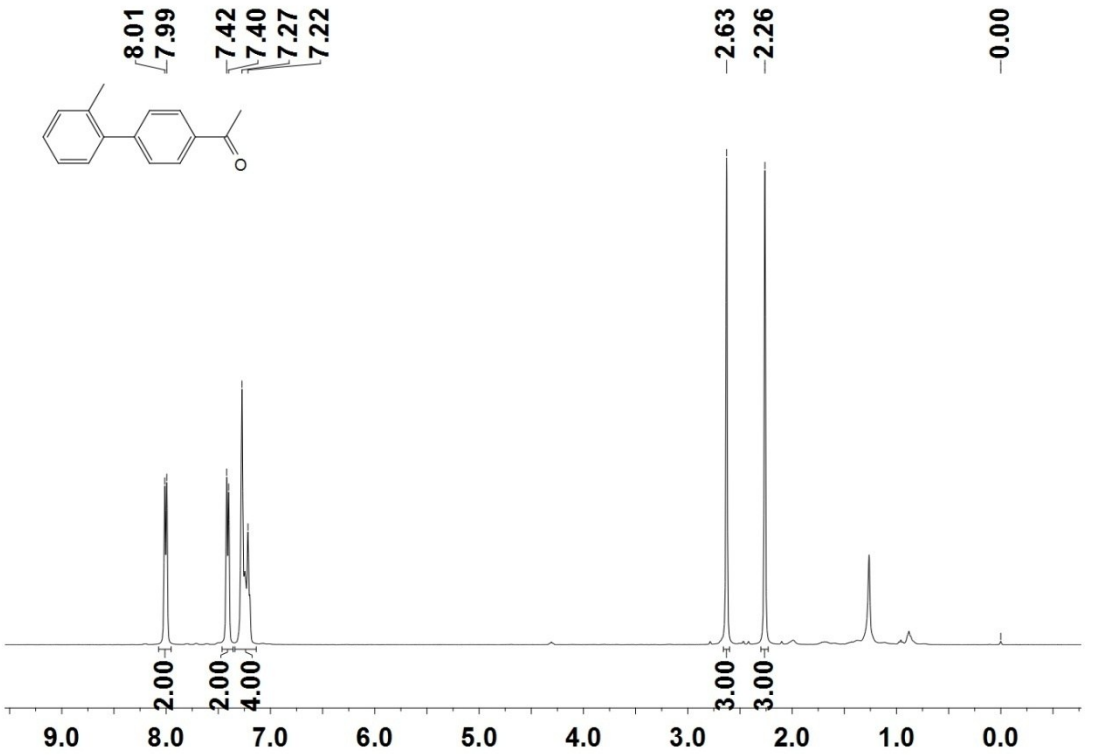
3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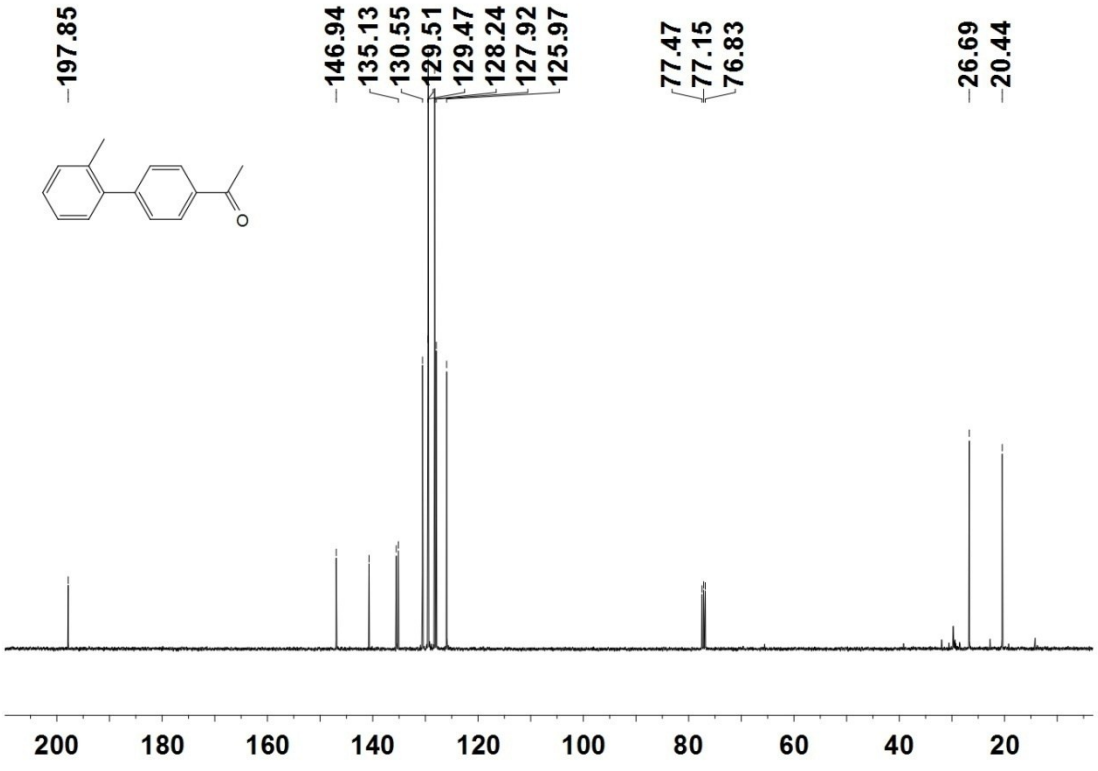
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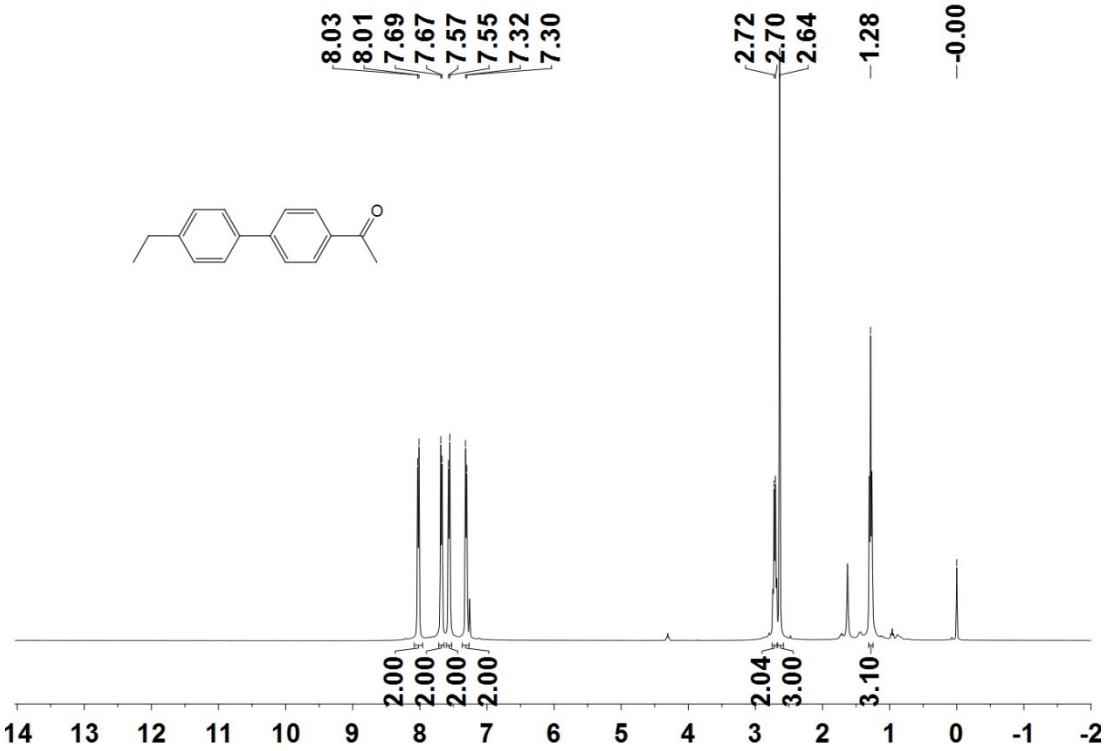
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3.10
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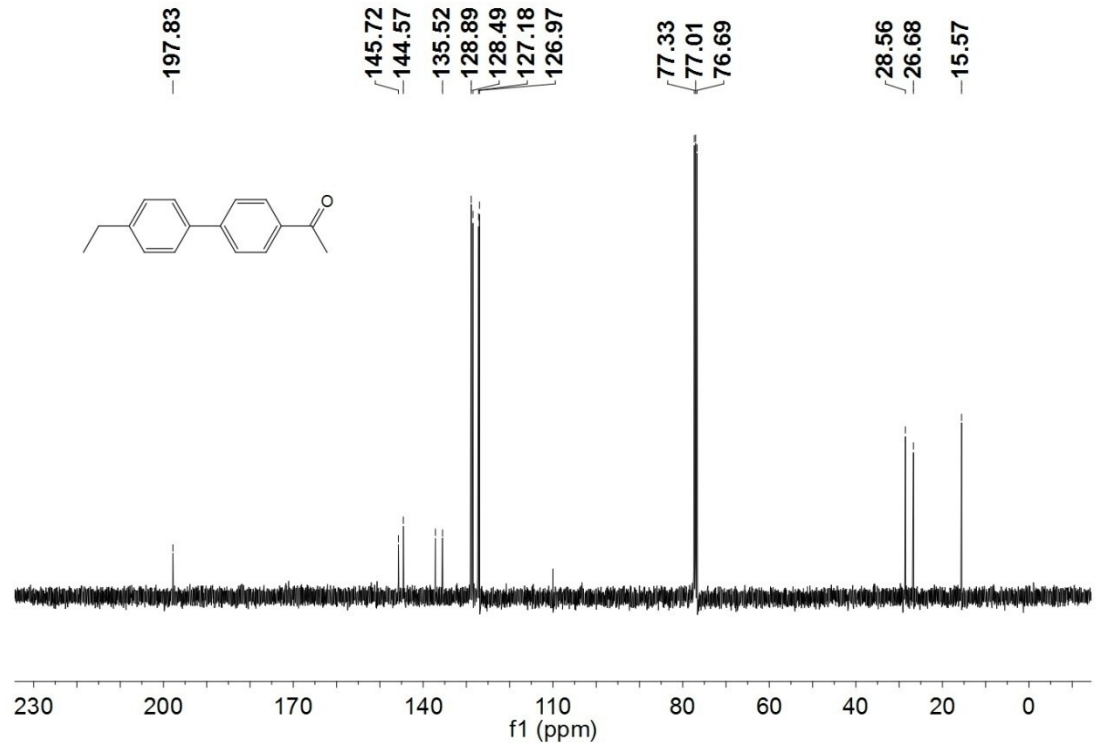
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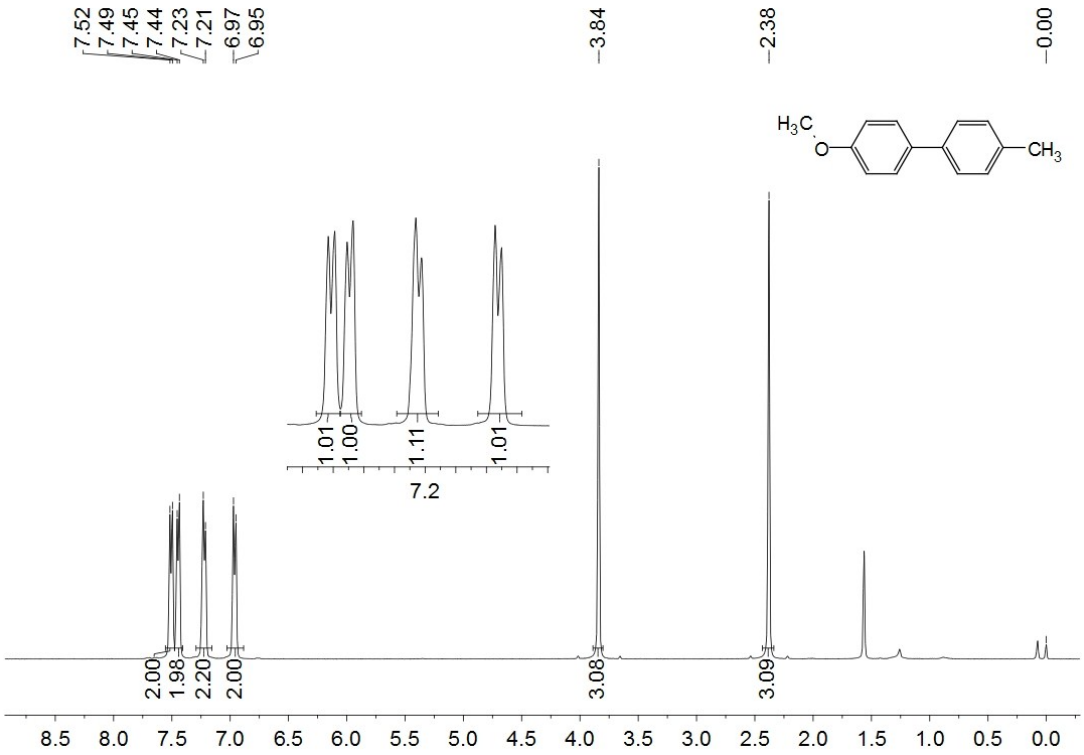
f1 (ppm)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2.00
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2.20
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3.08
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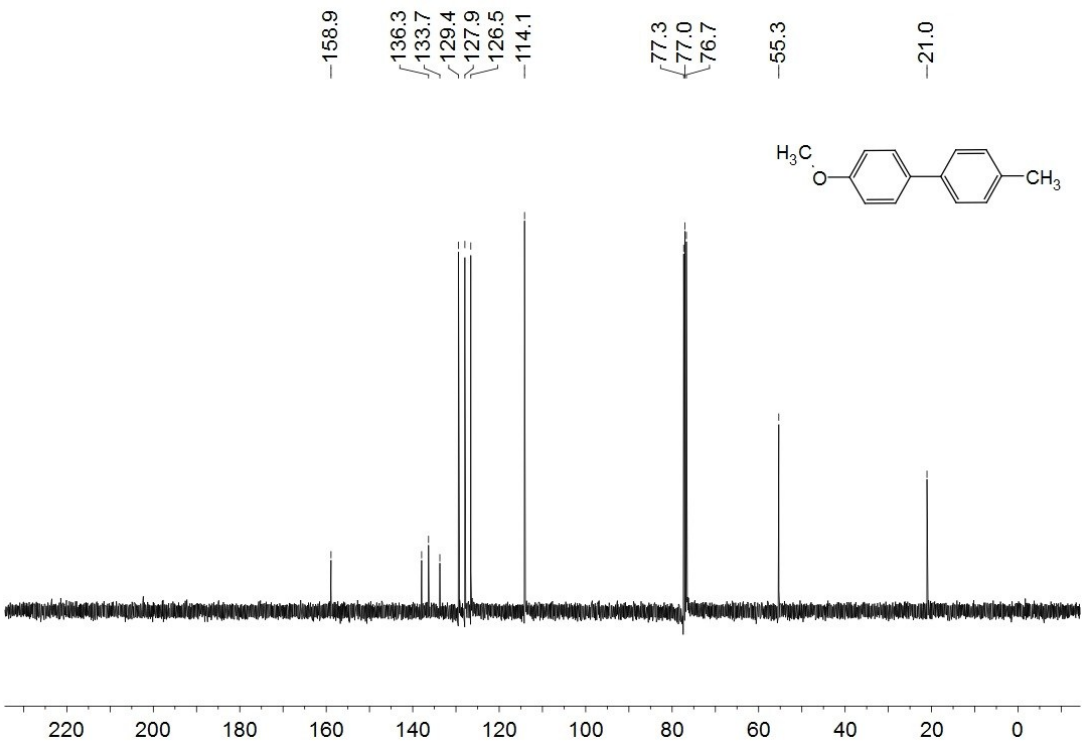
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O
CH3
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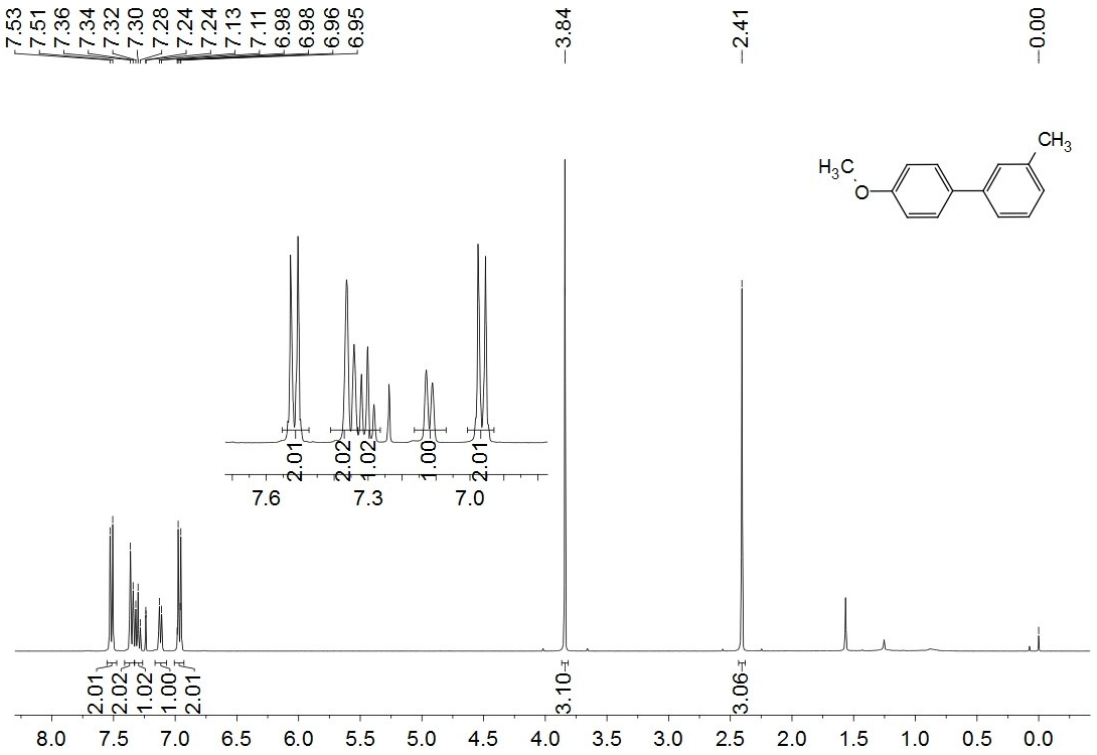
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H3C
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1.02
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2.02
1.02
1.00
2.01
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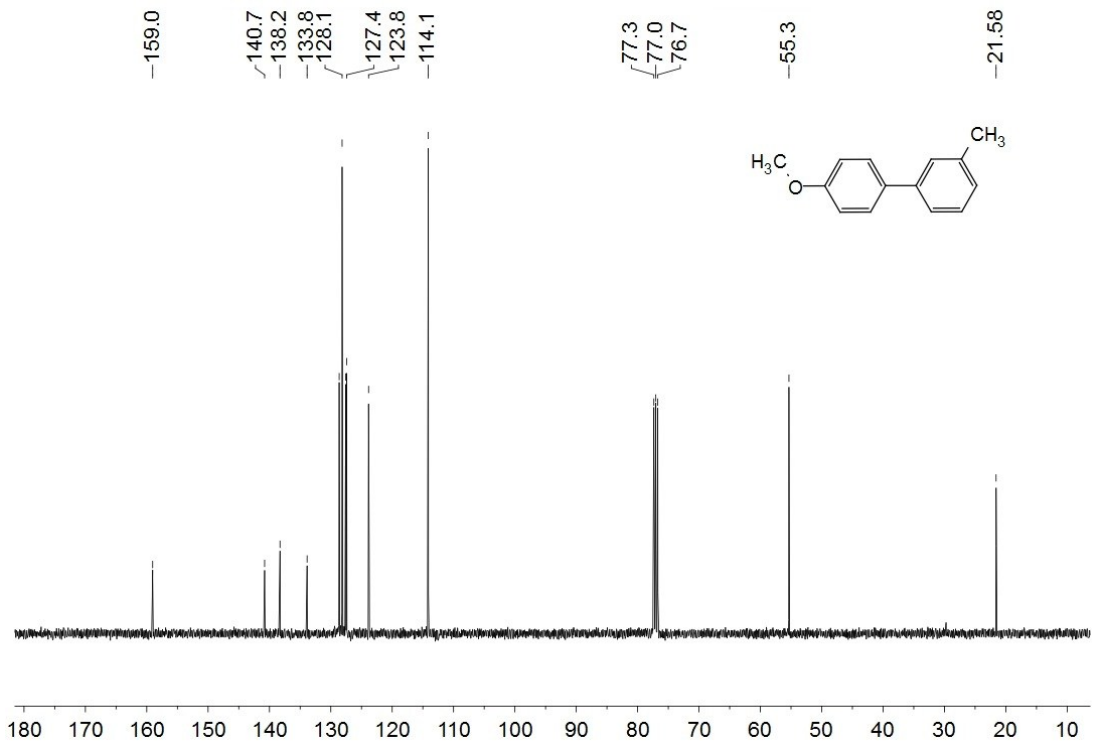
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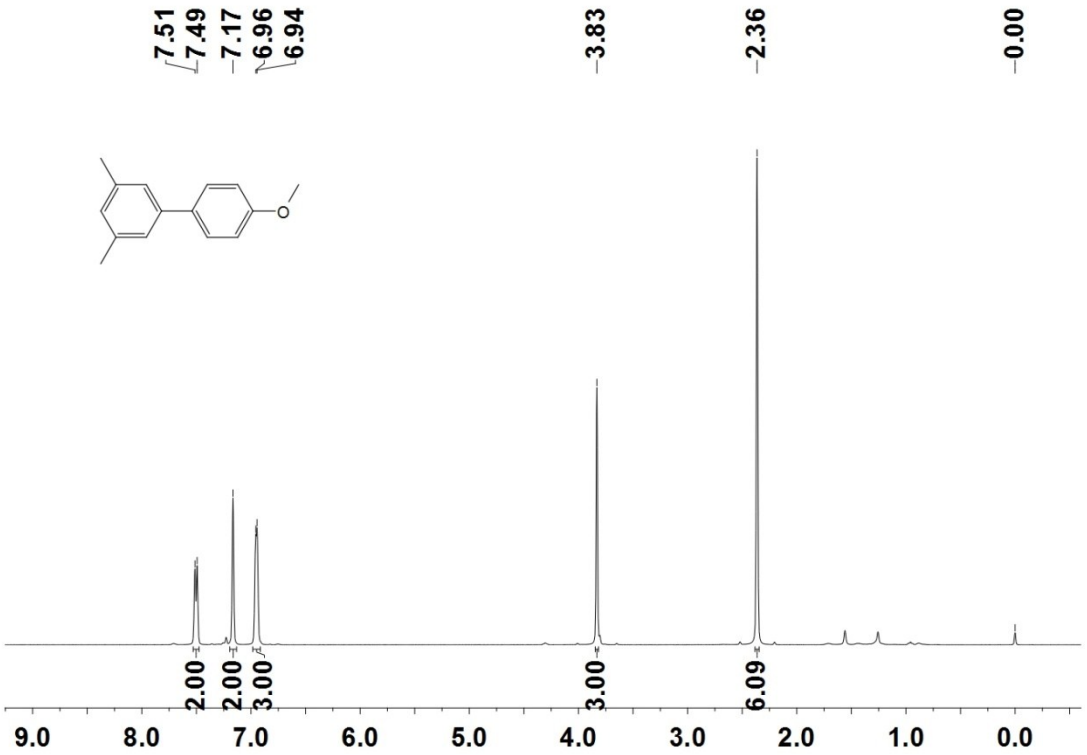
10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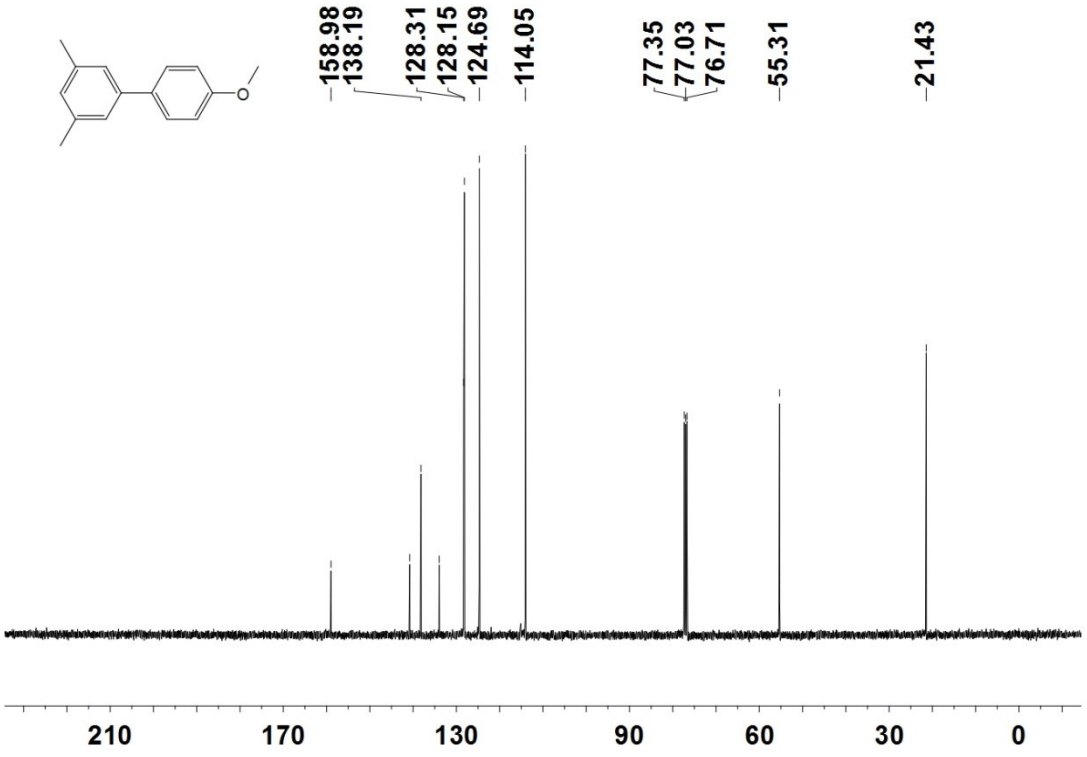
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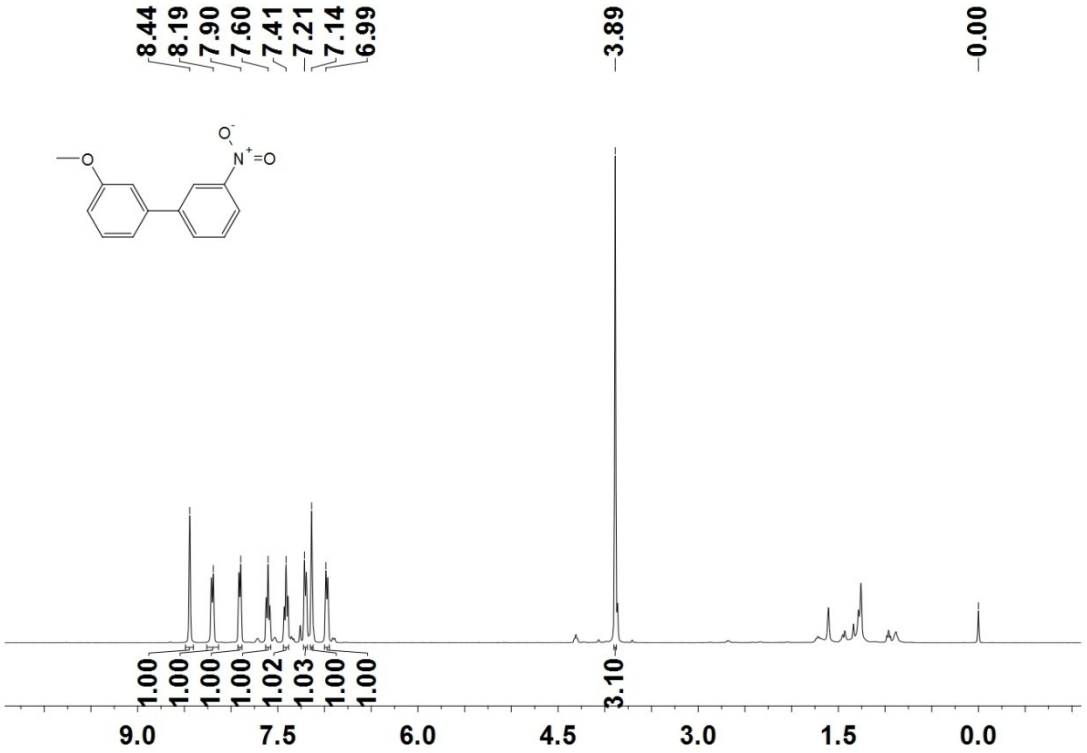
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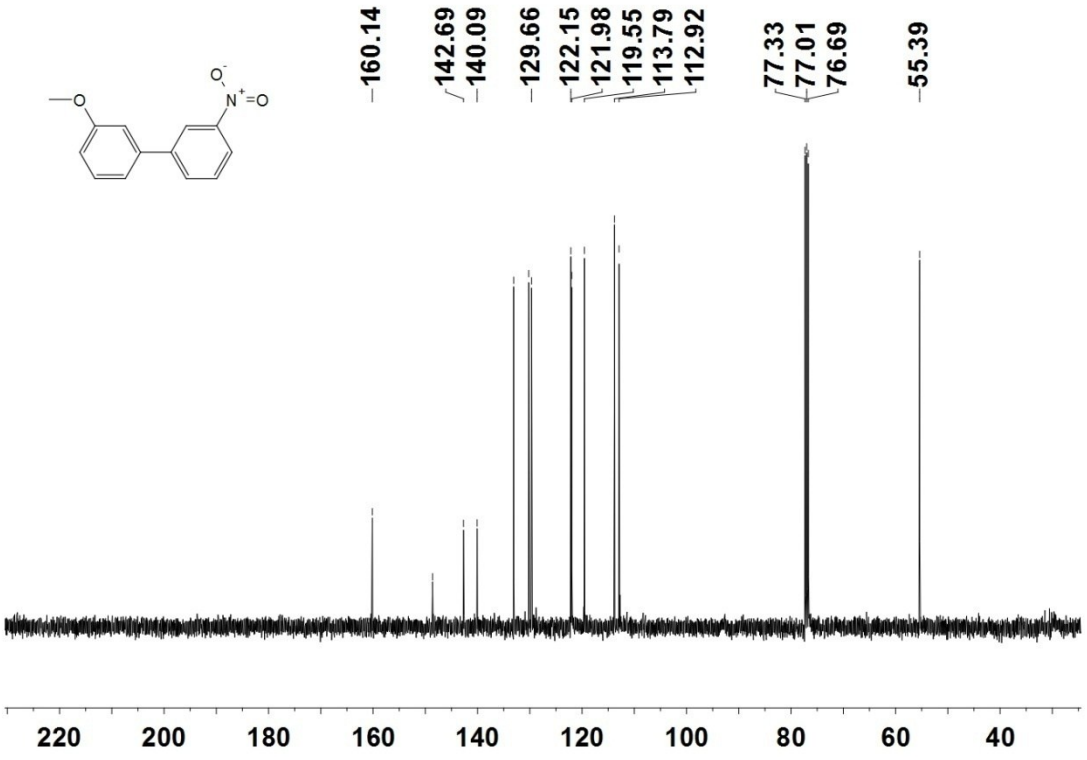
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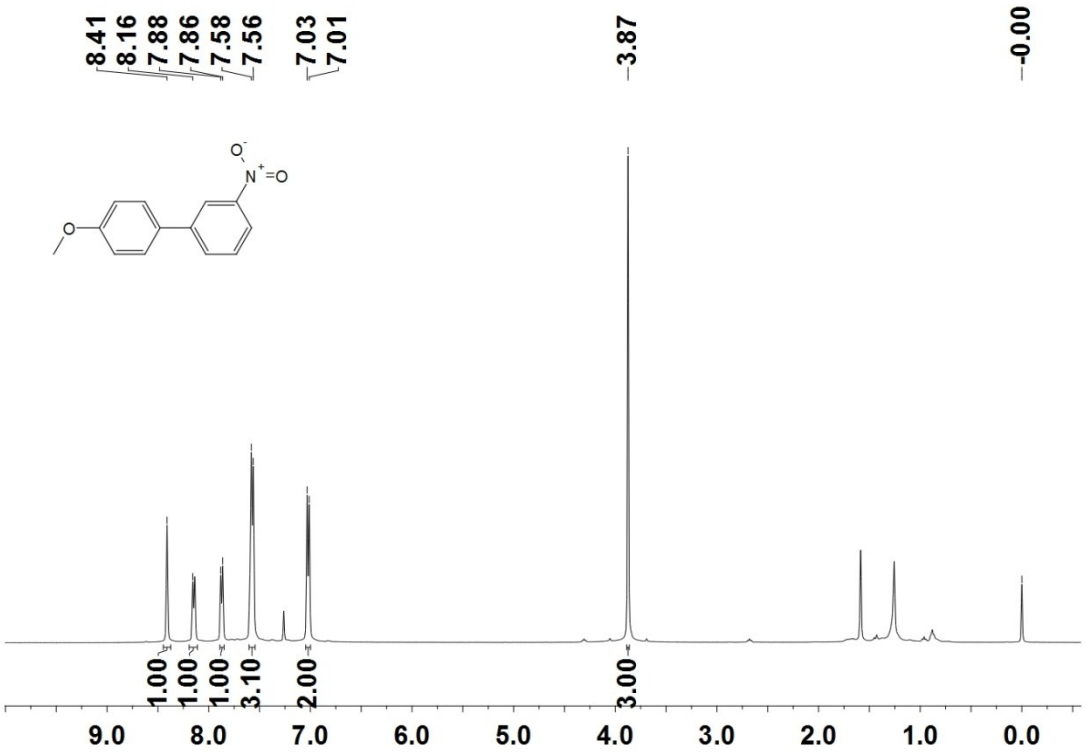
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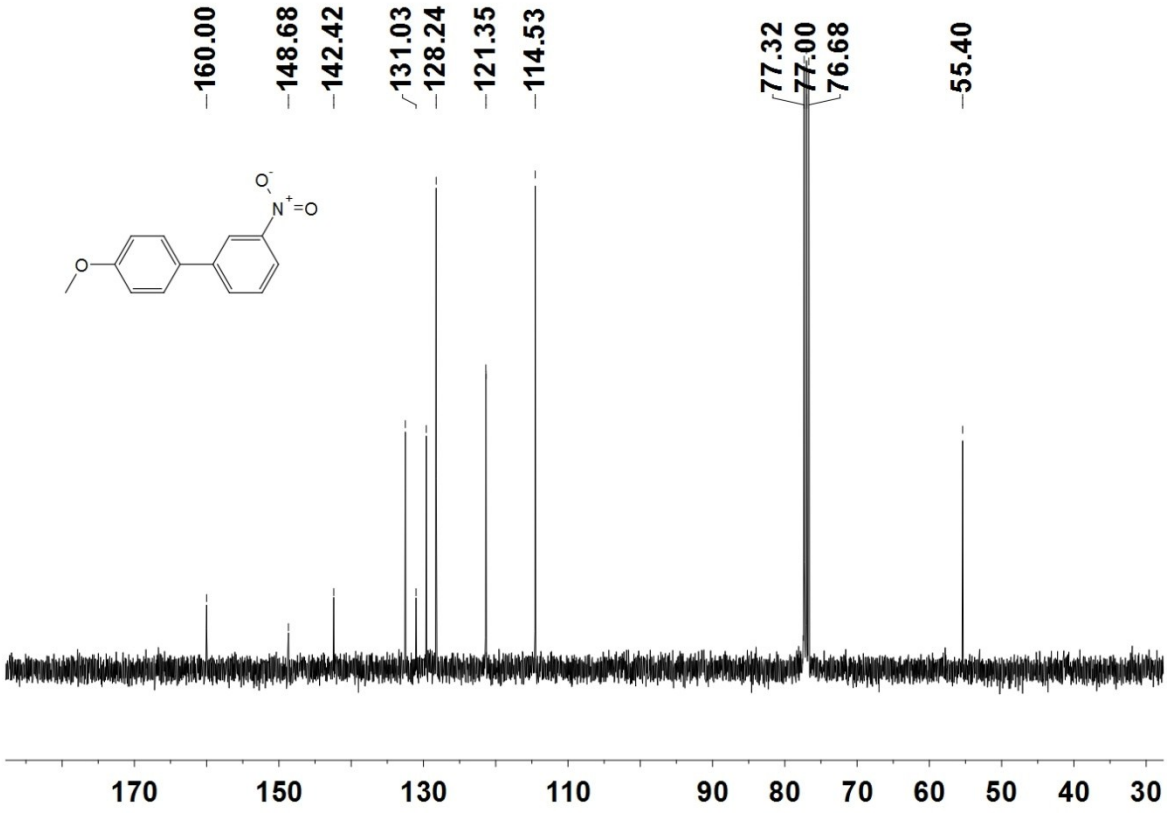
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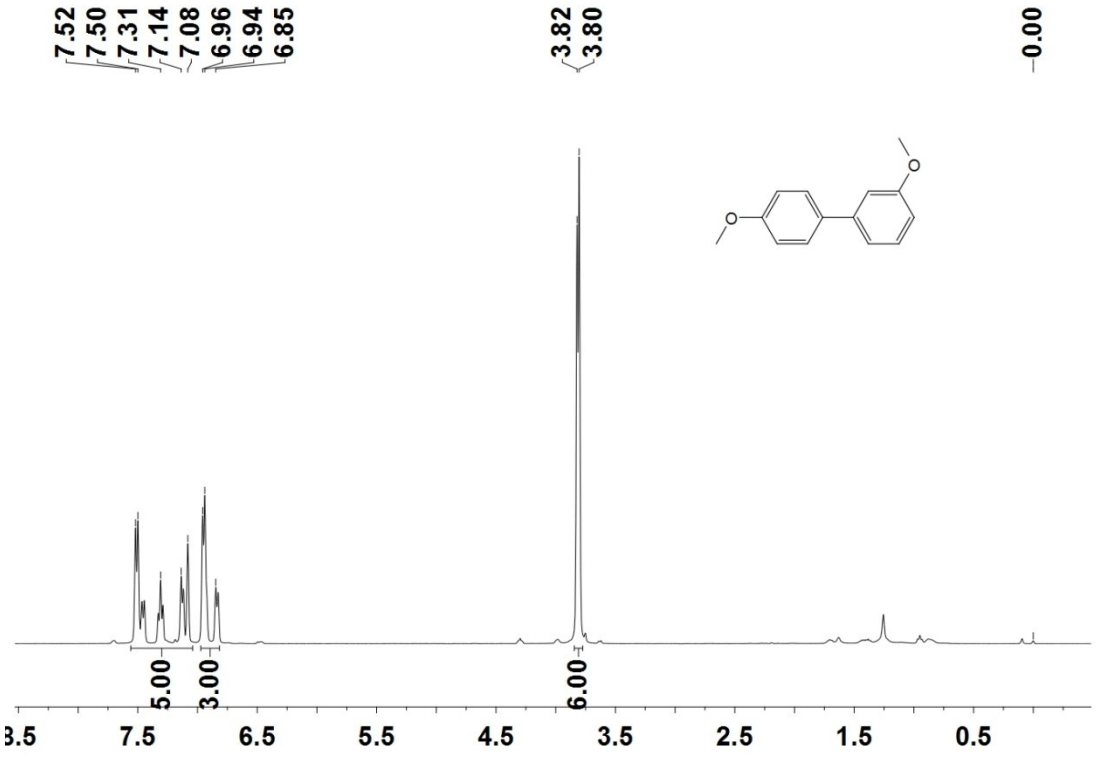
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7.50
7.31
7.14
7.08
6.96
6.94
6.85
3.82
3.80
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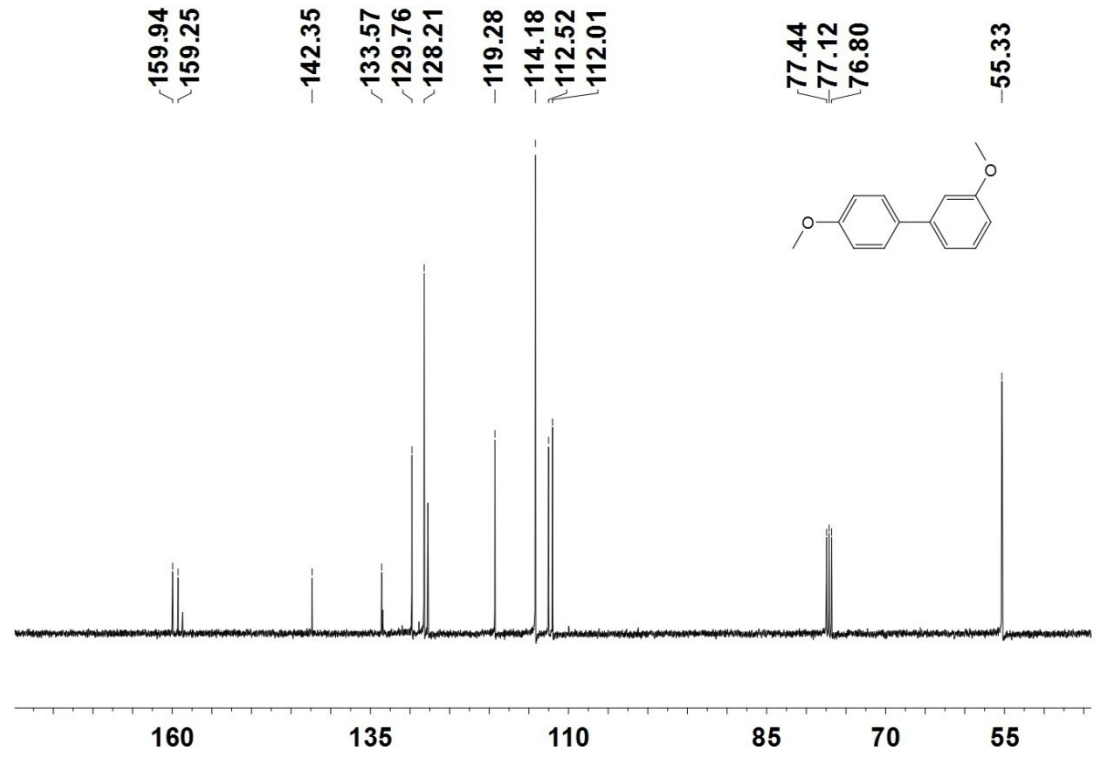
5.00
3.00
6.00
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5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142.35
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129.76
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112.52
112.01
77.44
77.12
76.80
55.33
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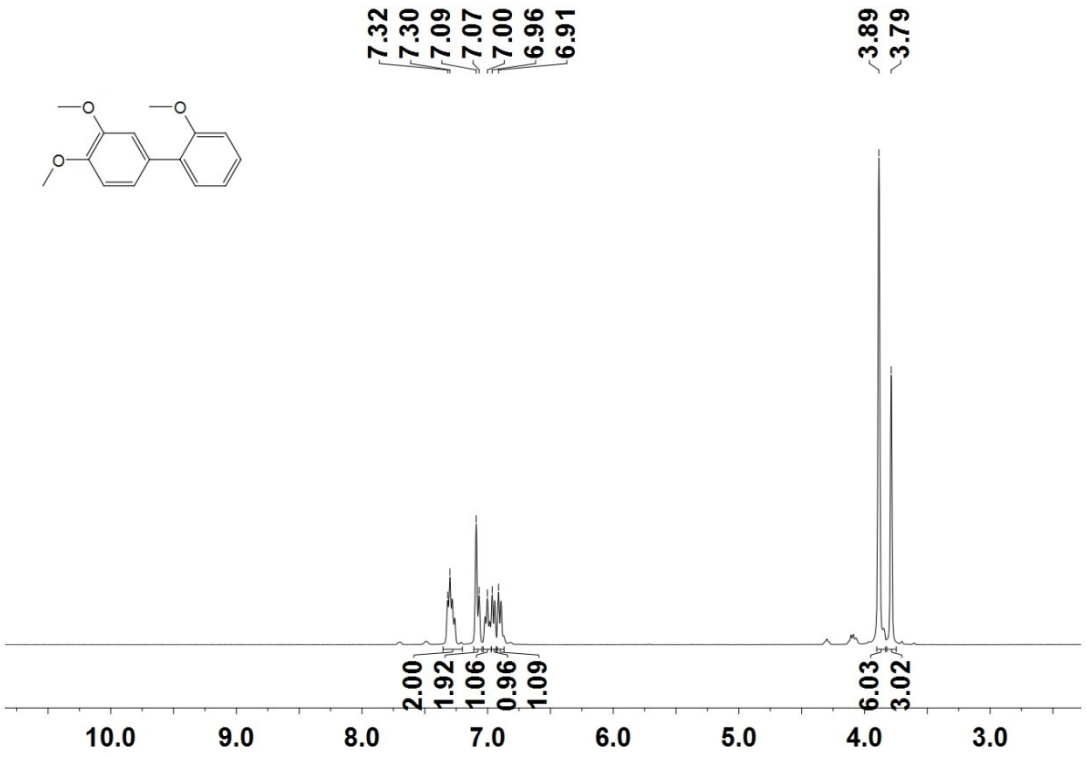
110
85
70
55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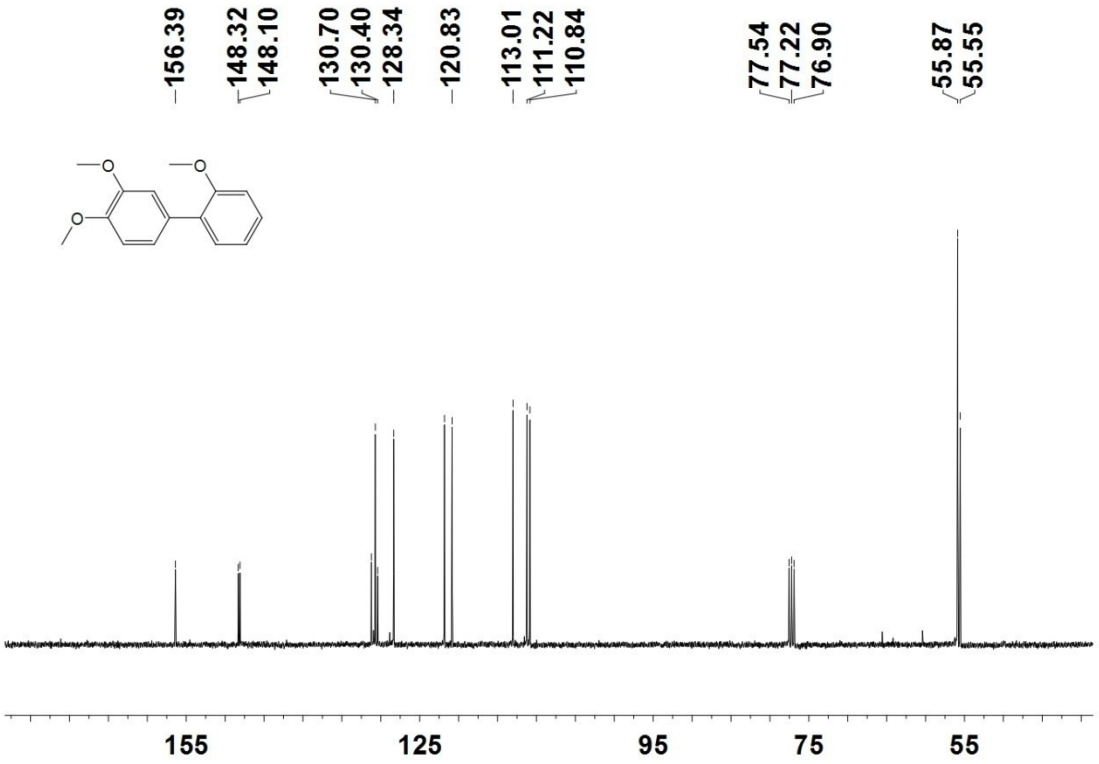
7.30
7.09
7.07
7.00
6.96
6.91
3.89
3.79
2.00
1.92
1.06
0.96
1.09
6.03
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0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128.34
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113.01
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110.84
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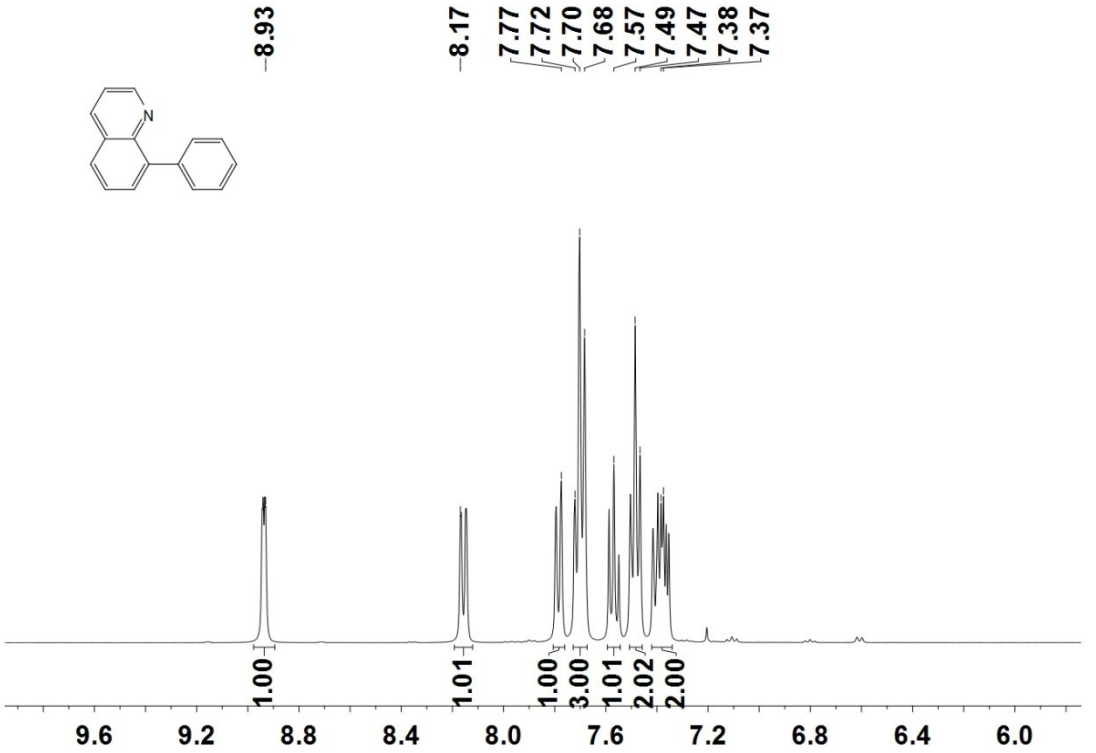
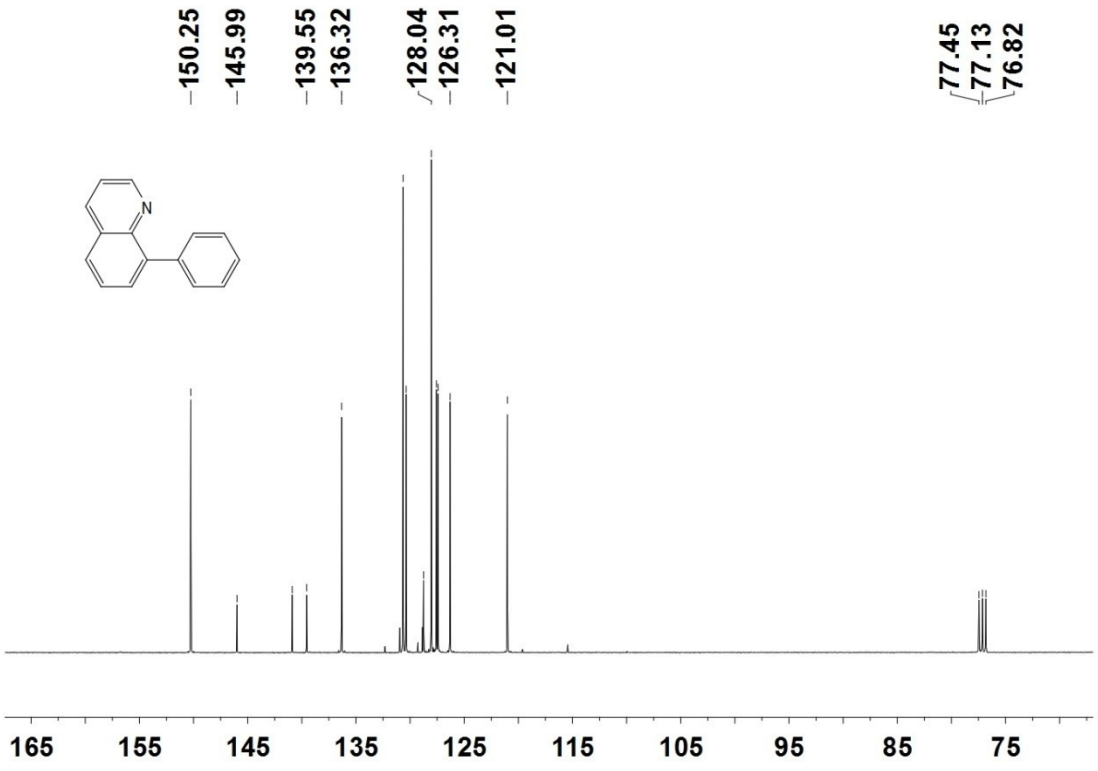
77.22
76.90
55.87
55.55
155
125
95
75
55


8.93
8.17
7.77
7.72
7.70
7.68
7.57
7.49
7.47
7.38
7.37
N
1.00
1.01
1.00
3.00
1.01
2.02
2.00
9.6
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0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145.99
139.55
136.32
128.04
126.31
121.01
77.45
77.13
76.82
N
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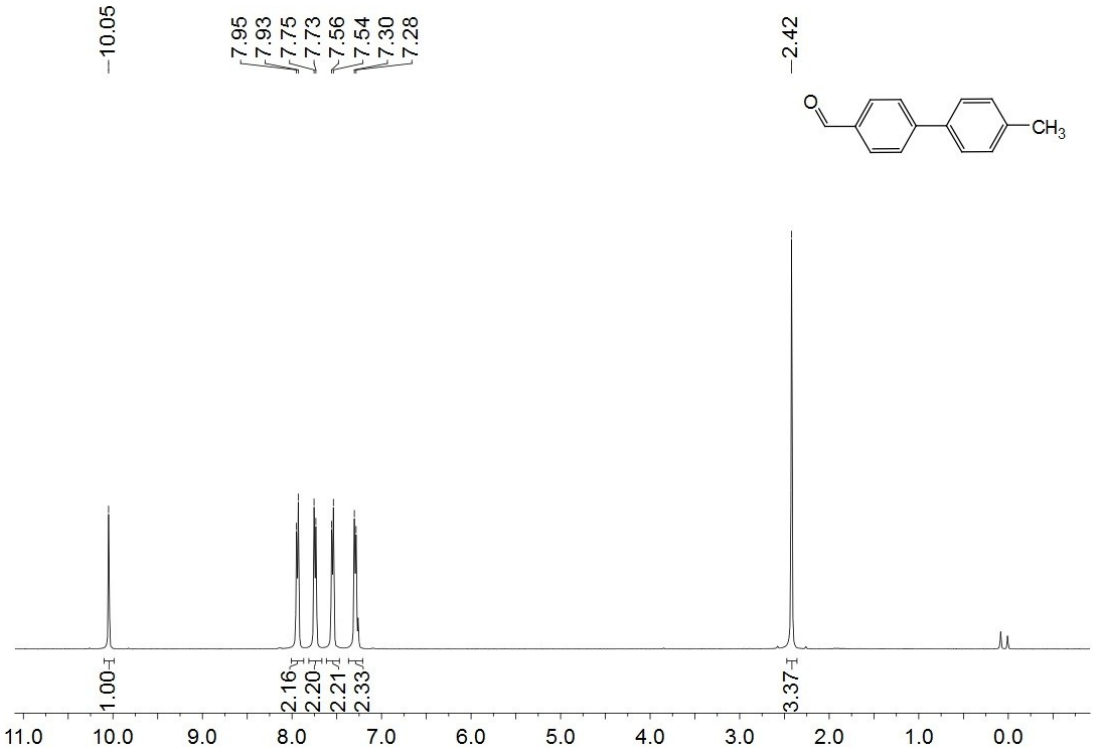
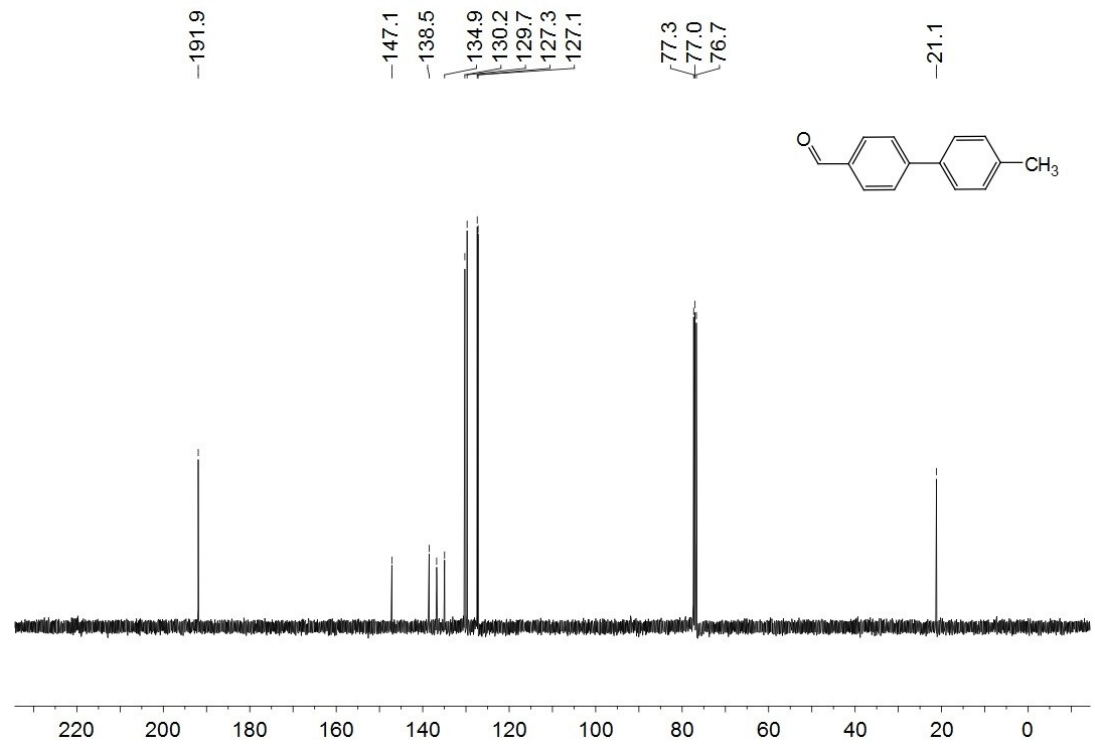
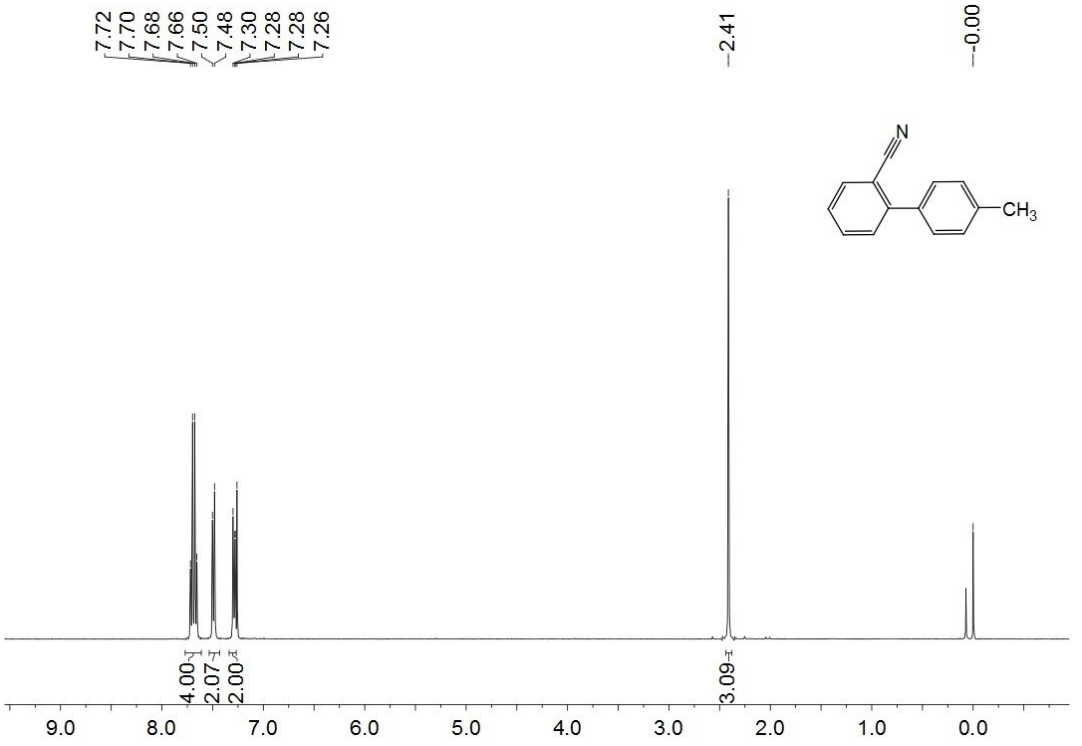
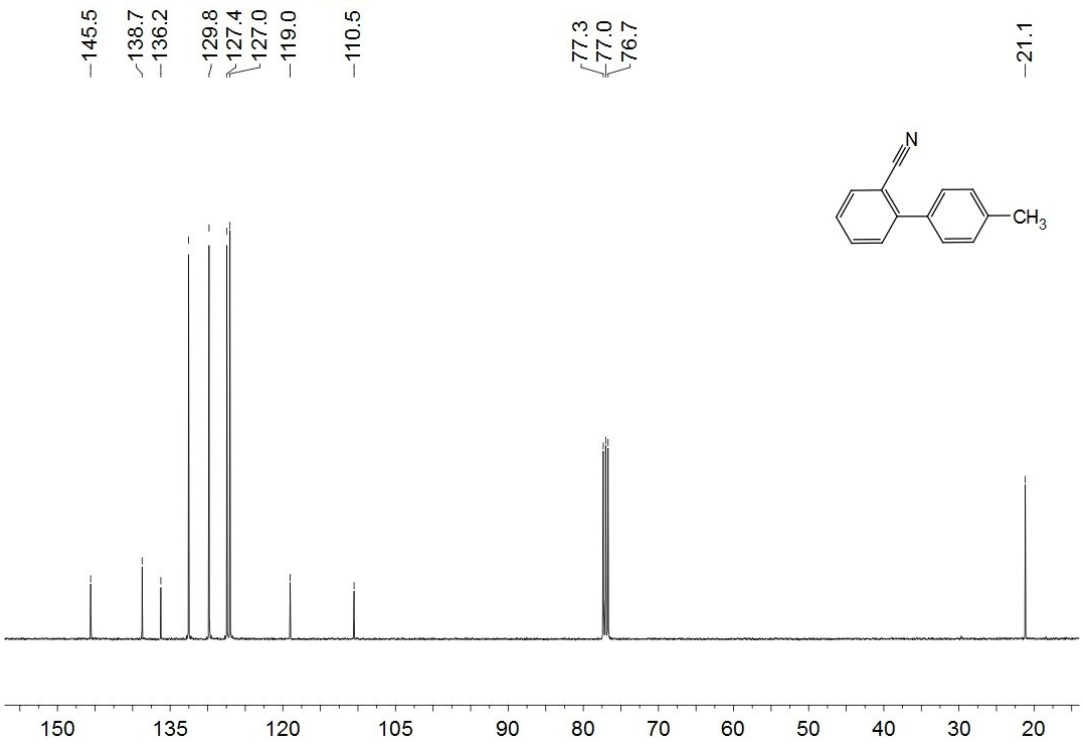
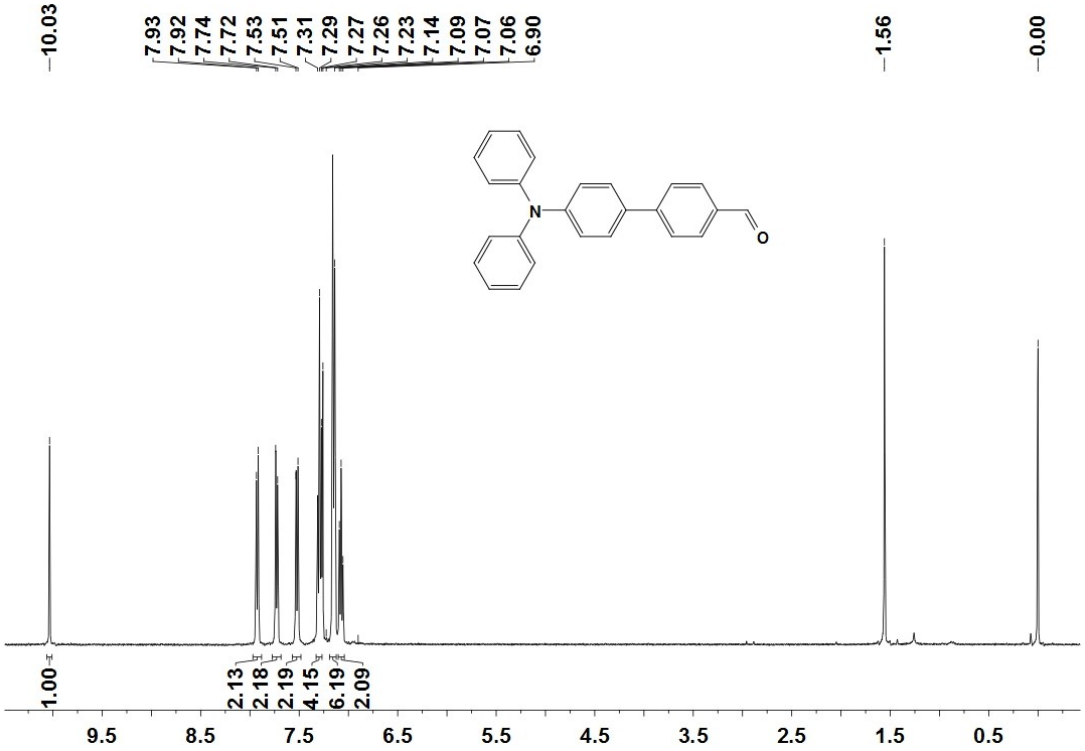
155
145
135
125
115
105
95
85
75

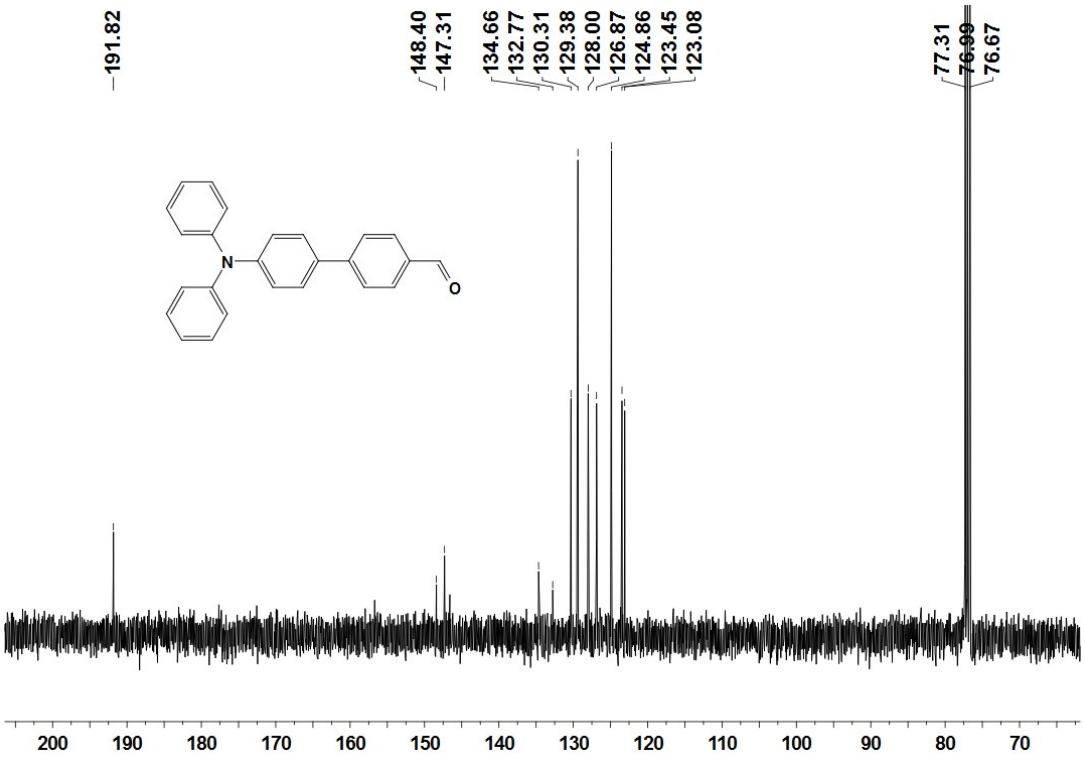

10.05
7.95
7.93
7.75
7.73
7.56
7.54
7.30
7.28
2.42
O
CH3
1.00
2.16
2.20
2.21
2.33
3.37
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


191.9
147.1
138.5
134.9
130.2
129.7
127.3
127.1
77.3
77.0
76.7
21.1
O
CH3
220
200
180
160
140
120
100
80
60
40
20
0


7.72
7.70
7.68
7.66
7.50
7.48
7.30
7.28
7.28
7.26
2.41
0.00
N
CH3
4.00
2.07
2.00
3.09
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


145.5
138.7
136.2
129.8
127.4
127.0
119.0
110.5
77.3
77.0
76.7
21.1
N
CH3
150
135
120
105
90
80
70
60
50
40
30
20


10.03
7.93
7.92
7.74
7.72
7.53
7.51
7.31
7.29
7.27
7.26
7.23
7.14
7.09
7.07
7.06
6.90
1.56
0.00
N
O
1.00
2.13
2.18
2.19
4.15
6.19
2.09
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5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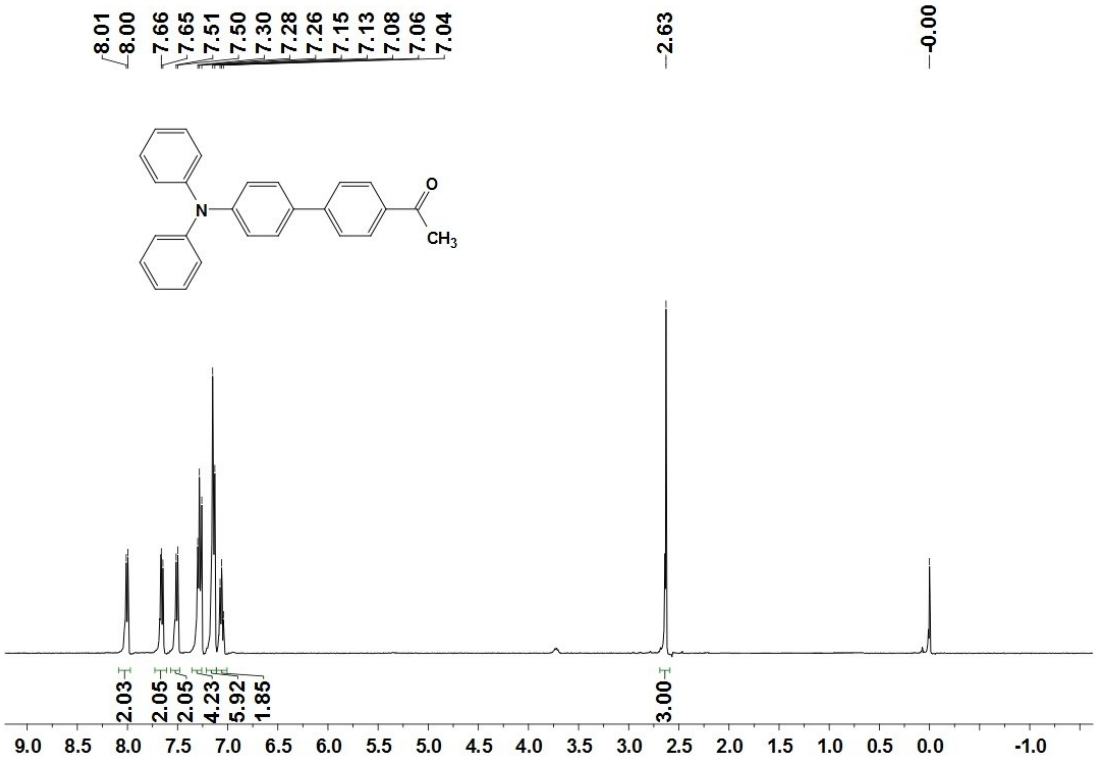
130.31
129.38
128.00
126.87
124.86
123.45
123.08
77.31
76.99
76.67
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70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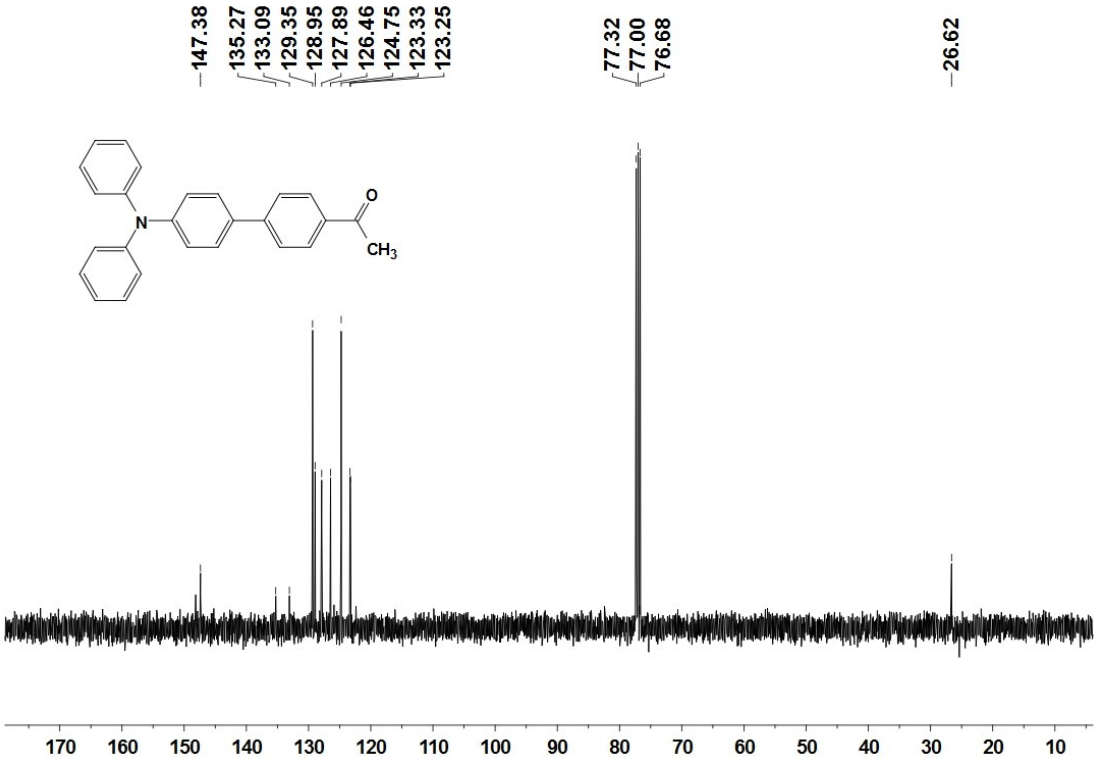
8.00
7.66
7.65
7.51
7.50
7.30
7.28
7.26
7.15
7.13
7.08
7.06
7.04
2.63
0.00
O
N
CH3
2.03
2.05
2.05
4.23
5.92
1.85
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0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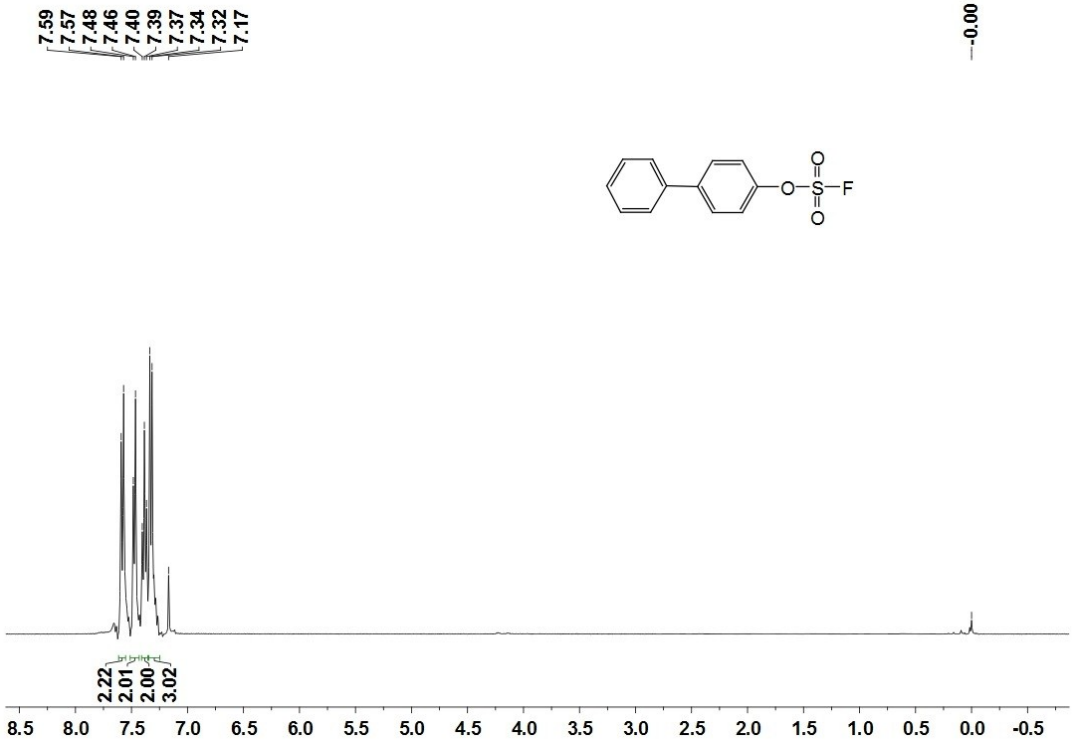
133.09
129.35
128.95
127.89
126.46
124.75
123.33
123.25
77.32
77.00
76.68
26.62
O
N
CH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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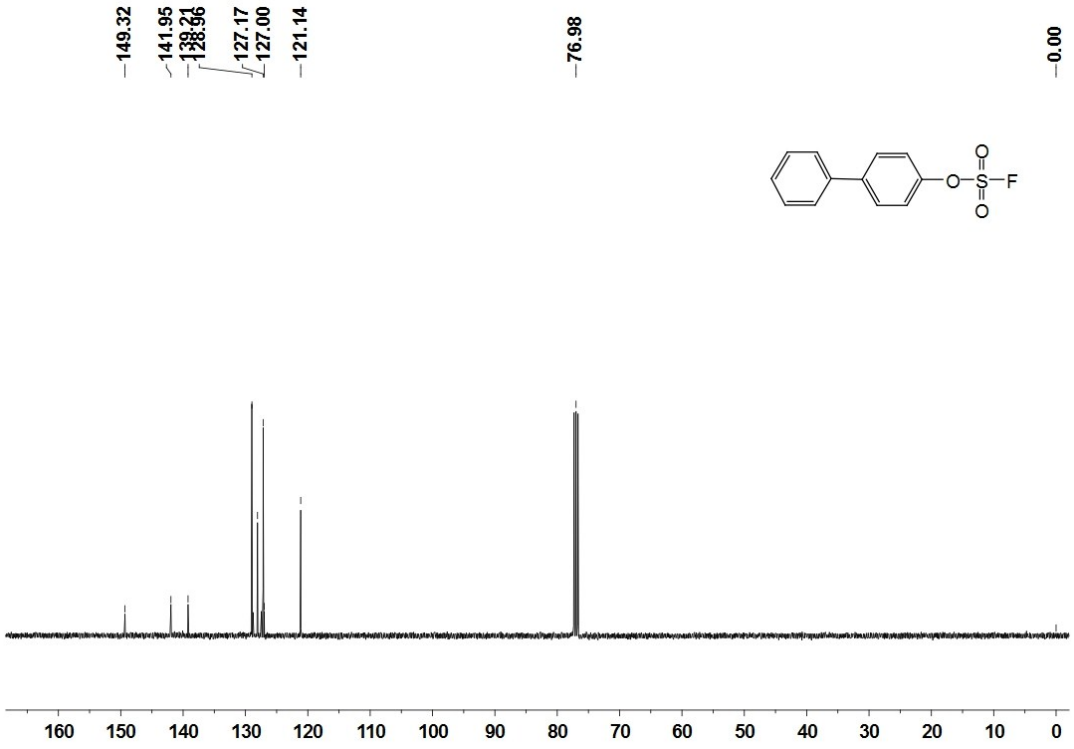
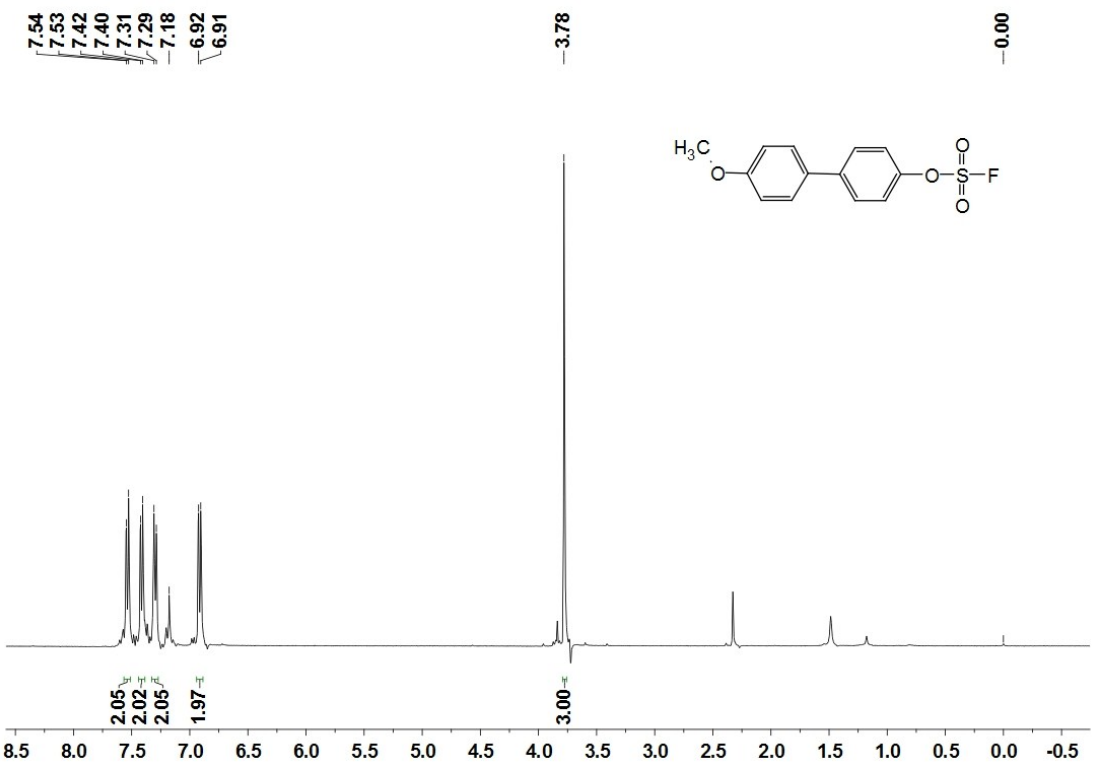
7.57
7.48
7.46
7.40
7.39
7.37
7.34
7.32
7.17
0.00
O
O
S
F
O
2.22
2.01
2.00
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


149.32
141.95
139.21
128.96
127.17
127.00
121.14
76.98
0.00
O
O
S
F
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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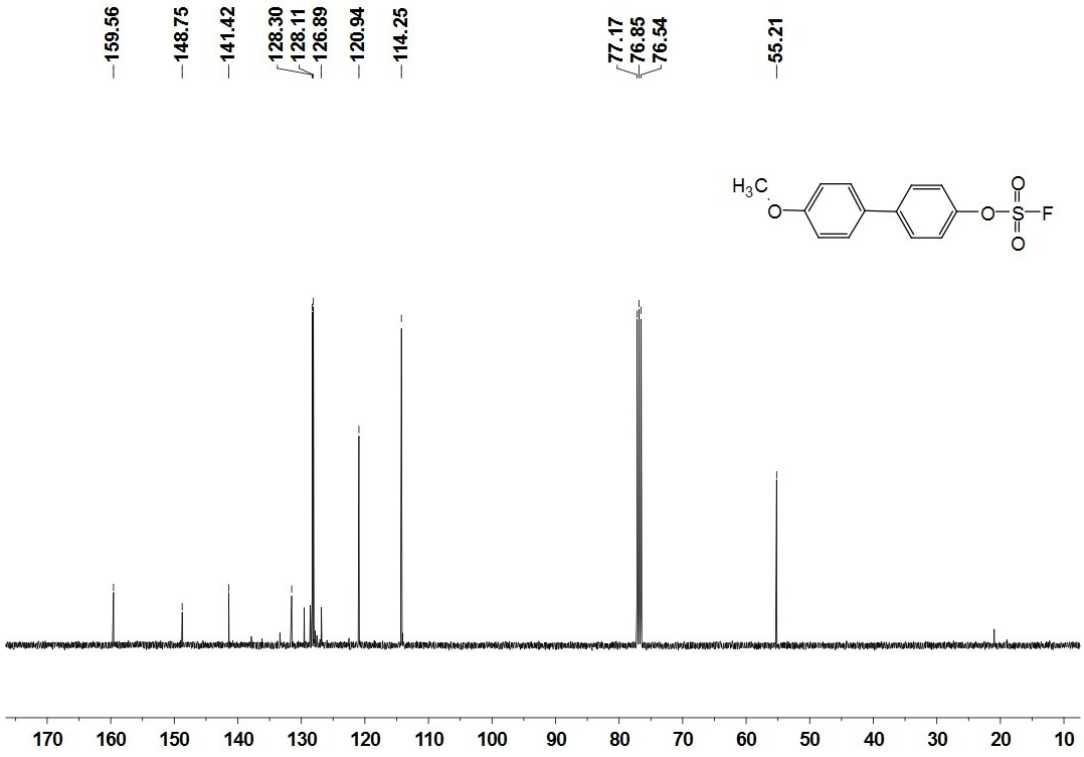
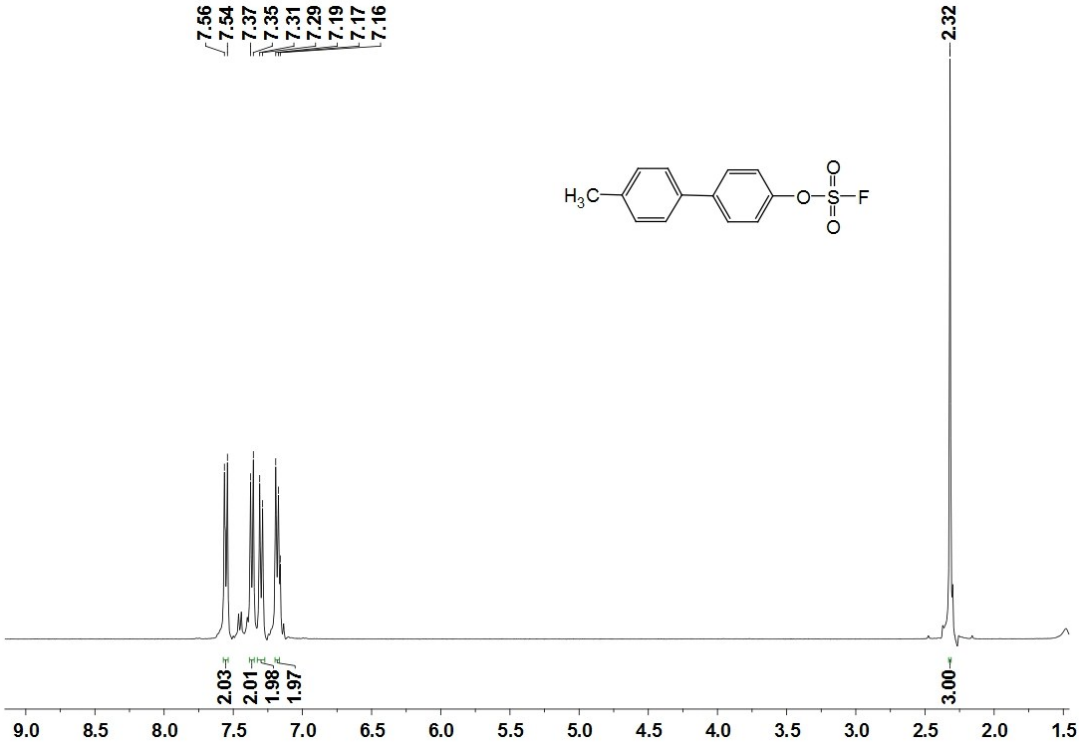
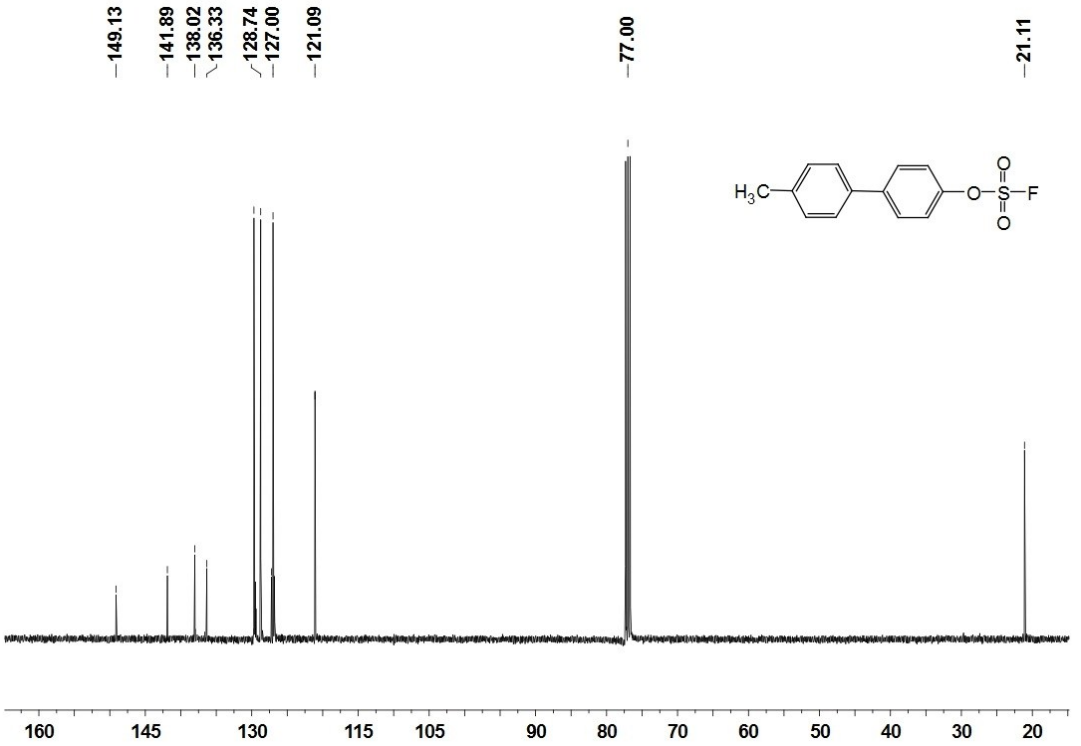
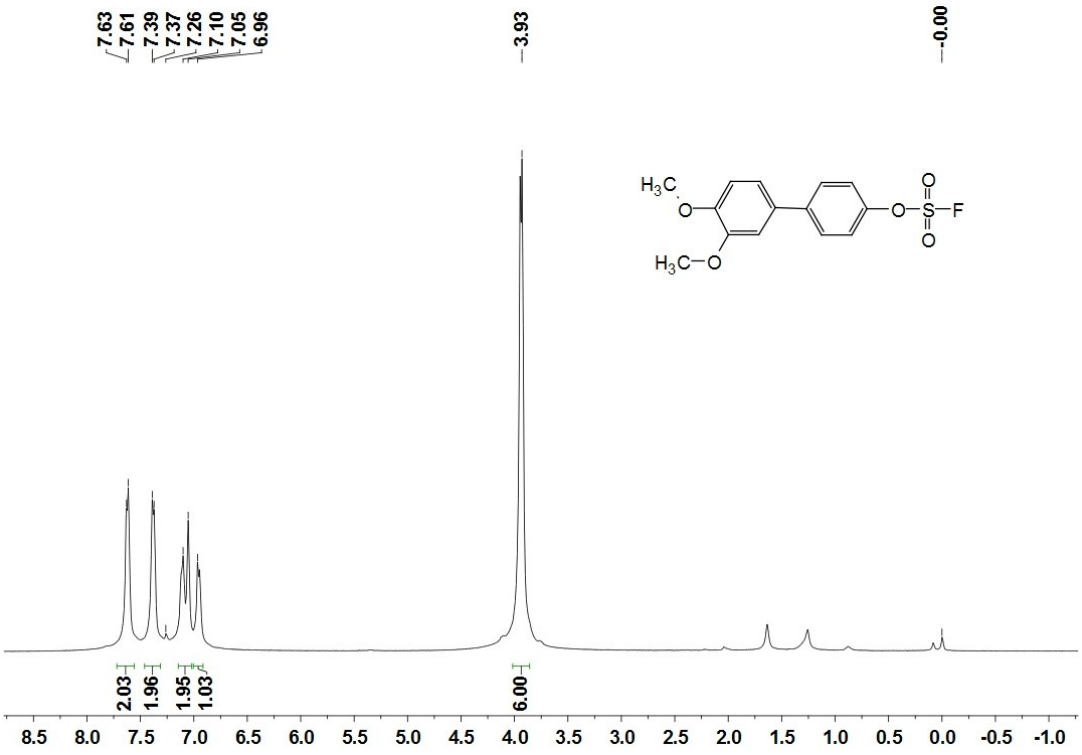
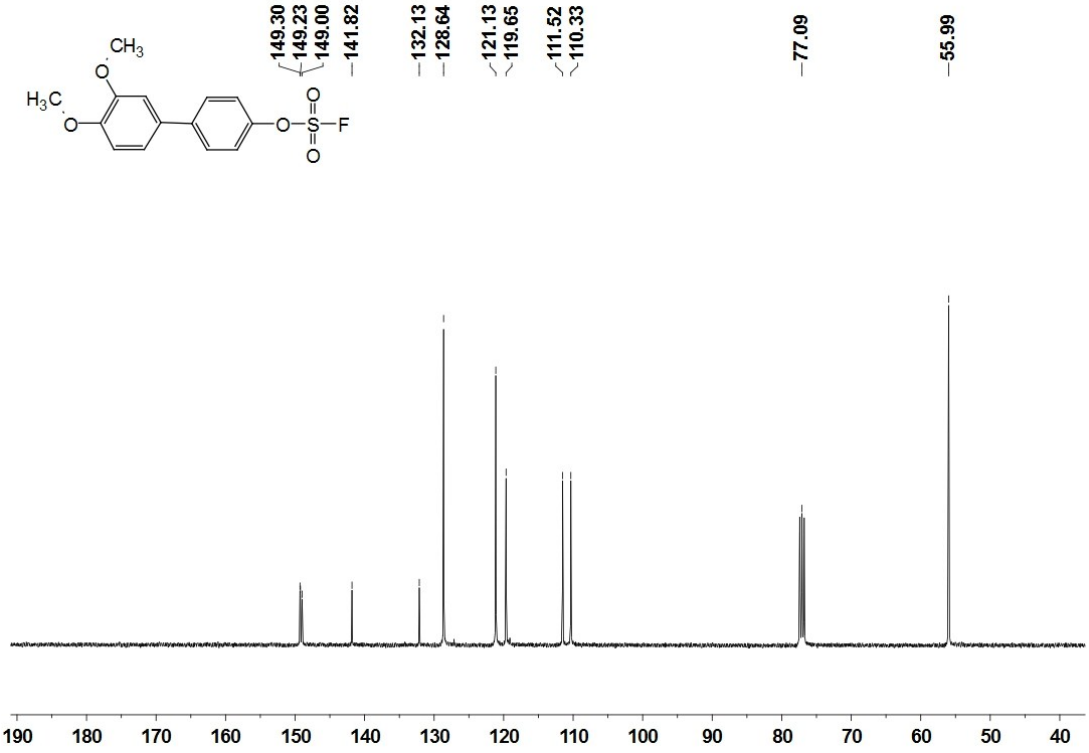
7.42
7.40
7.31
7.29
7.18
6.92
6.91
3.78
0.00
2.05
2.02
2.05
1.97
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


159.56
148.75
141.42
128.30
128.11
126.89
120.94
114.25
77.17
76.85
76.54
55.21
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


7.56
7.54
7.37
7.35
7.31
7.29
7.19
7.17
7.16
2.32
H3C
O
S
F
2.03
2.01
1.98
1.97
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5


149.13
141.89
138.02
136.33
128.74
127.00
121.09
77.00
21.11
H3C
O
S
F
160
145
130
115
105
90
80
70
60
50
40
30
20


7.63
7.61
7.39
7.37
7.26
7.10
7.05
6.96
3.93
0.00
2.03
1.96
1.95
1.03
6.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0


149.30
149.23
149.00
141.82
132.13
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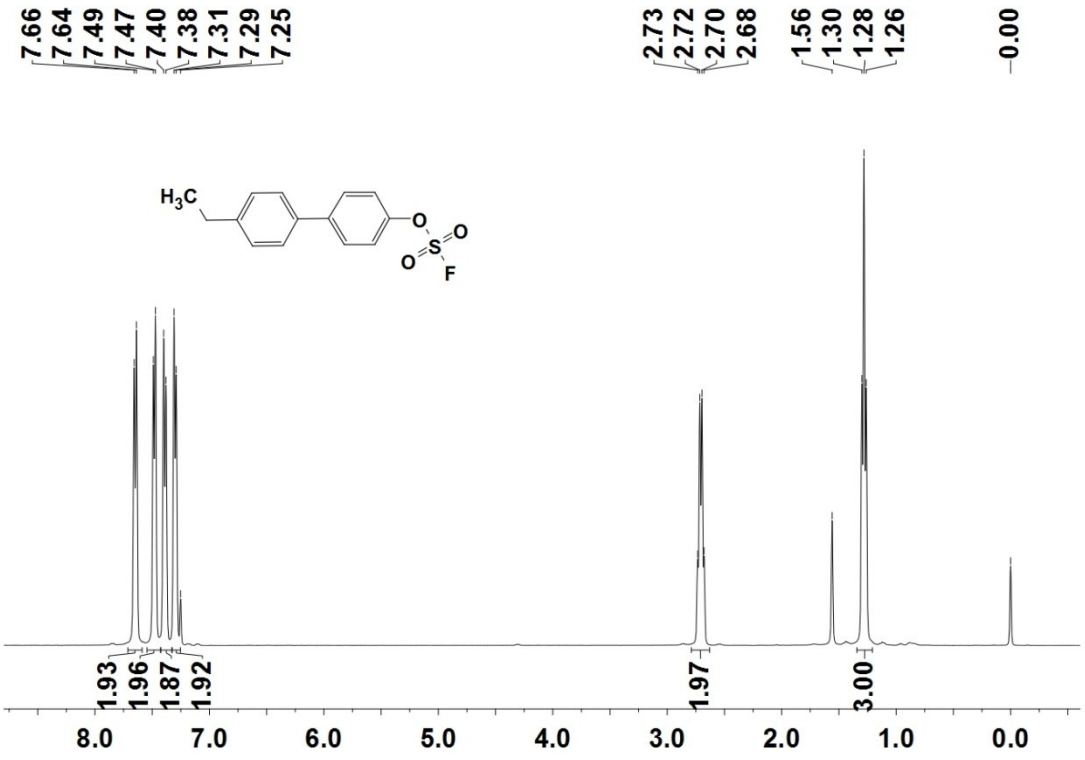
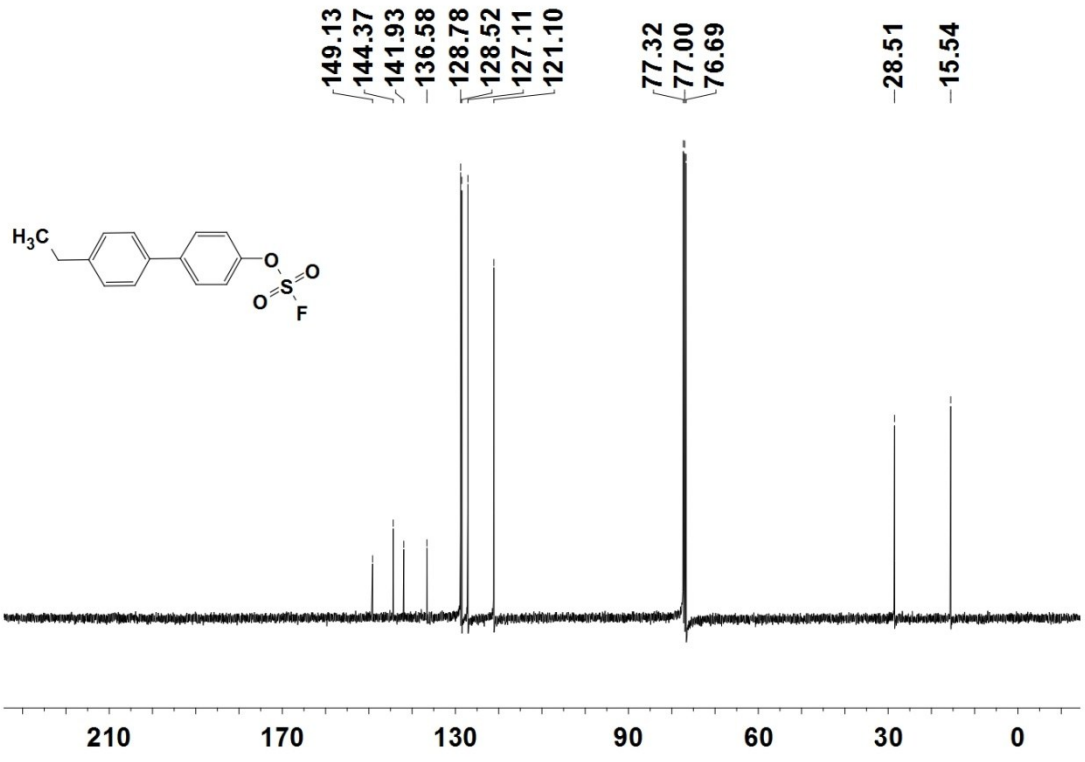
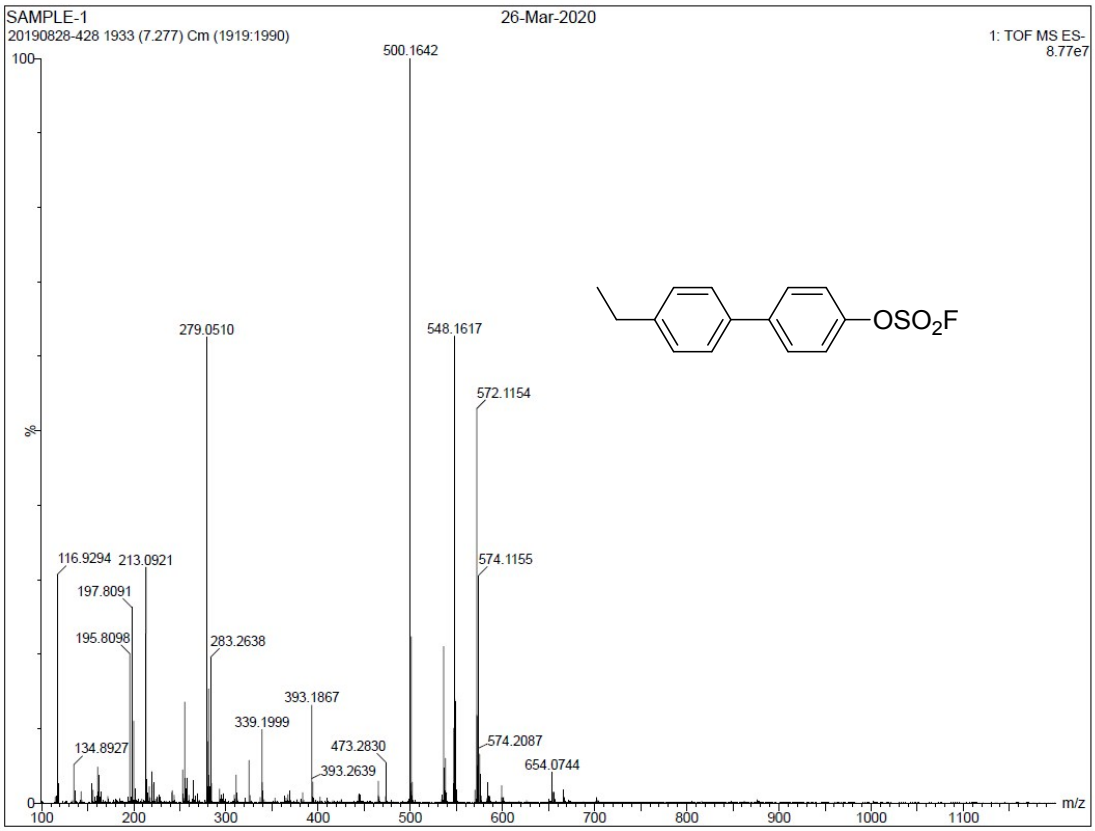
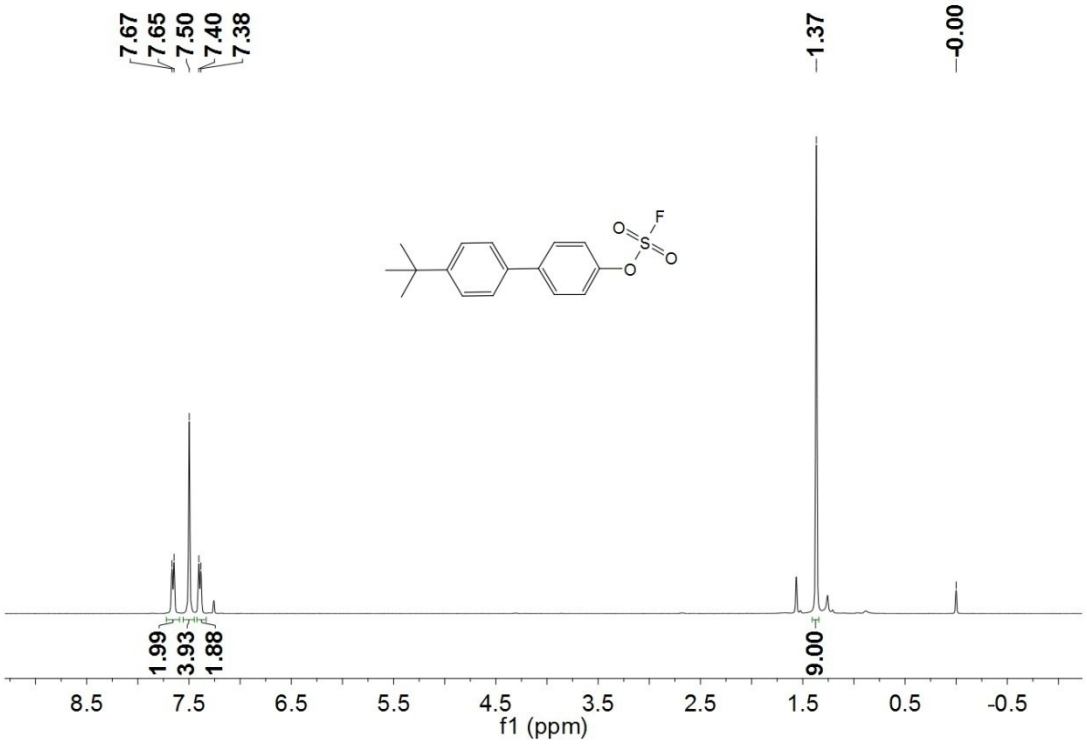
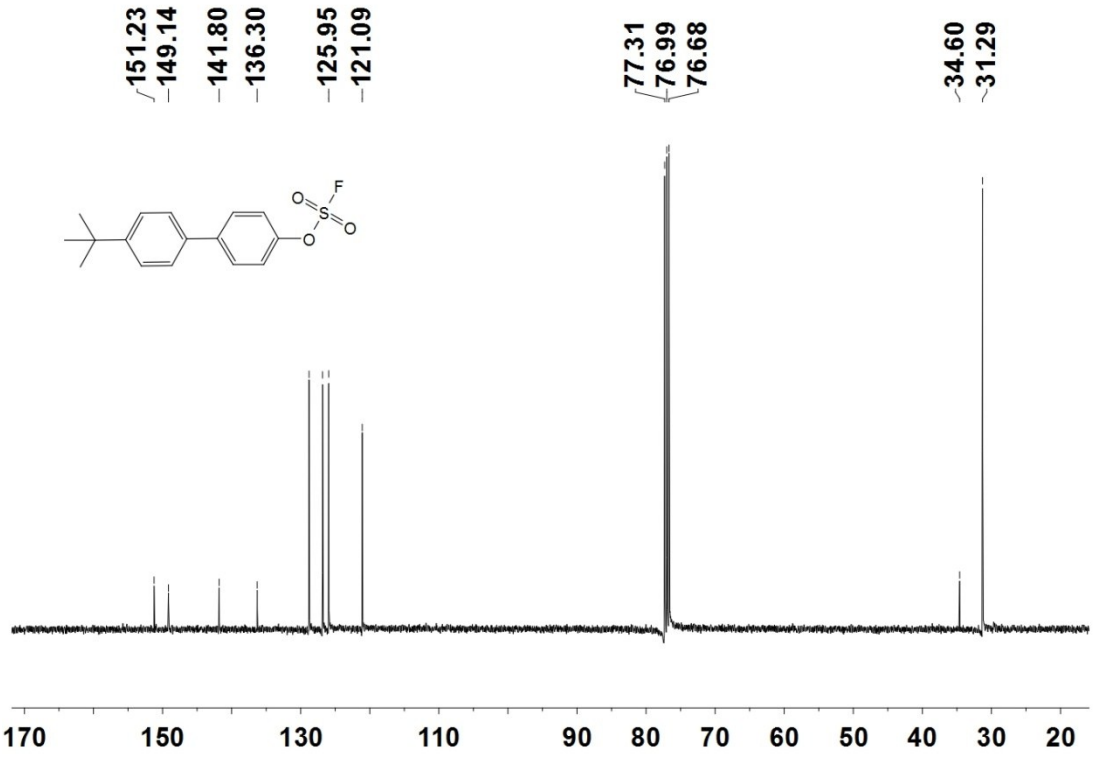
121.13
119.65
111.52
110.33
77.09
55.99
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40

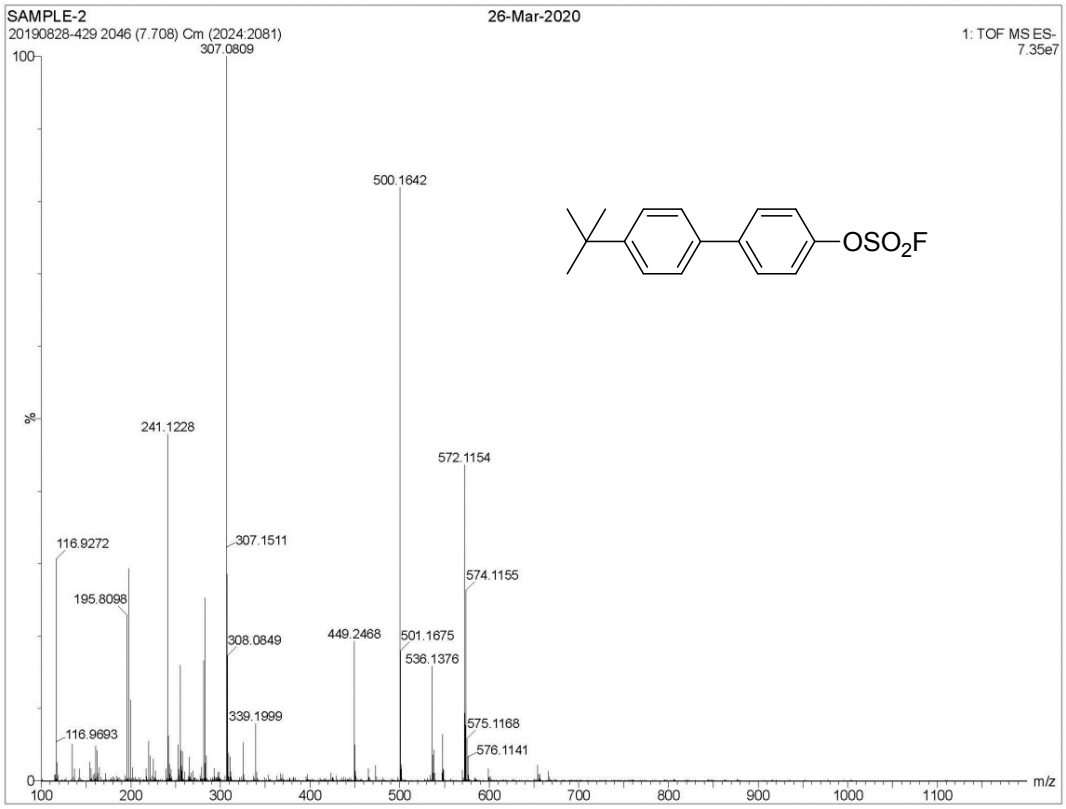

7.66
7.64
7.49
7.47
7.40
7.38
7.31
7.29
7.25
2.73
2.72
2.70
2.68
1.56
1.30
1.28
1.26
0.00
H3C
O
S
O
O
F
1.93
1.96
1.87
1.92
1.97
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

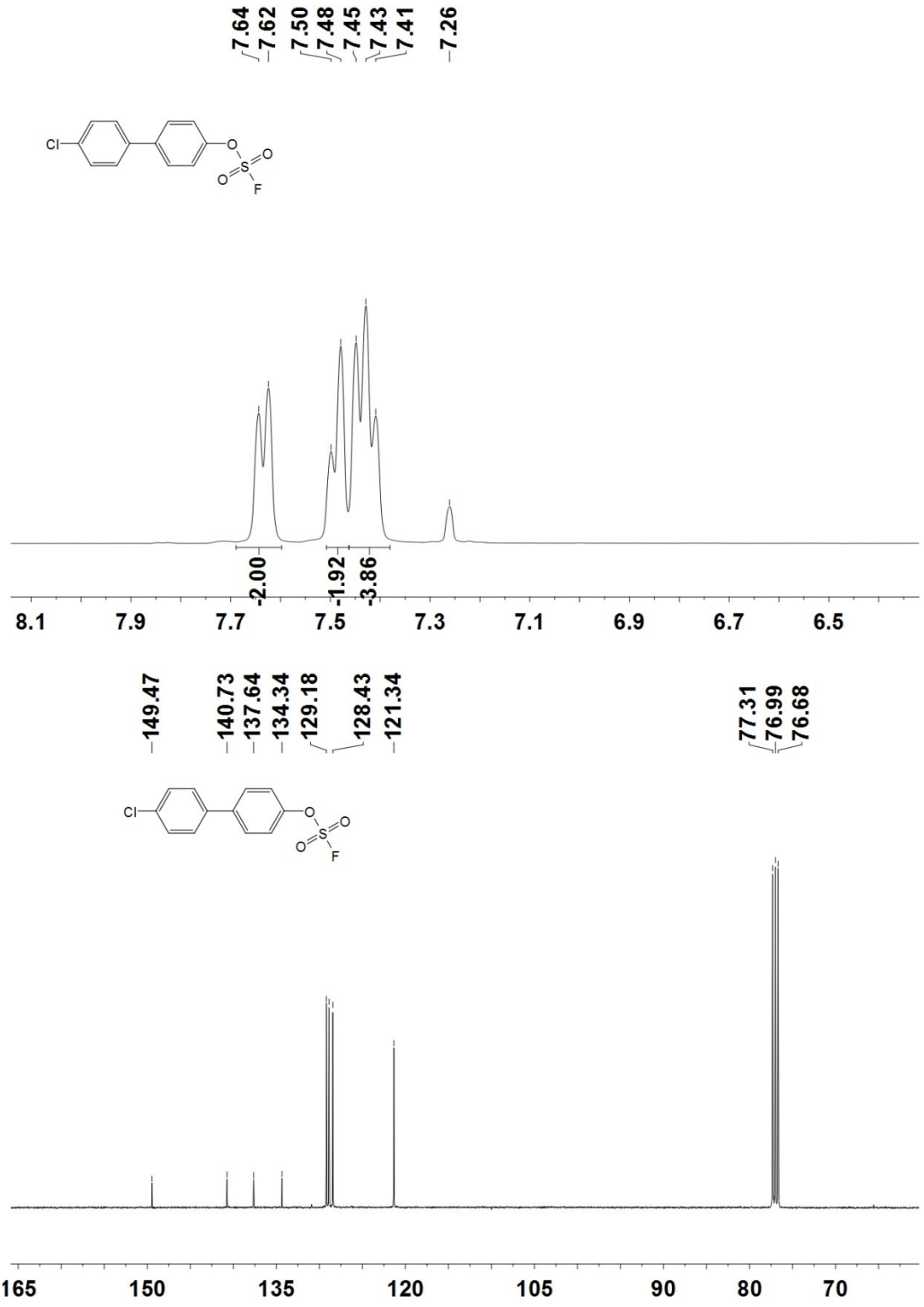

149.13
144.37
141.93
136.58
128.78
128.52
127.11
121.10
77.32
77.00
76.69
28.51
15.54
H3C
O
S
O
O
F
210
170
130
90
60
30
0

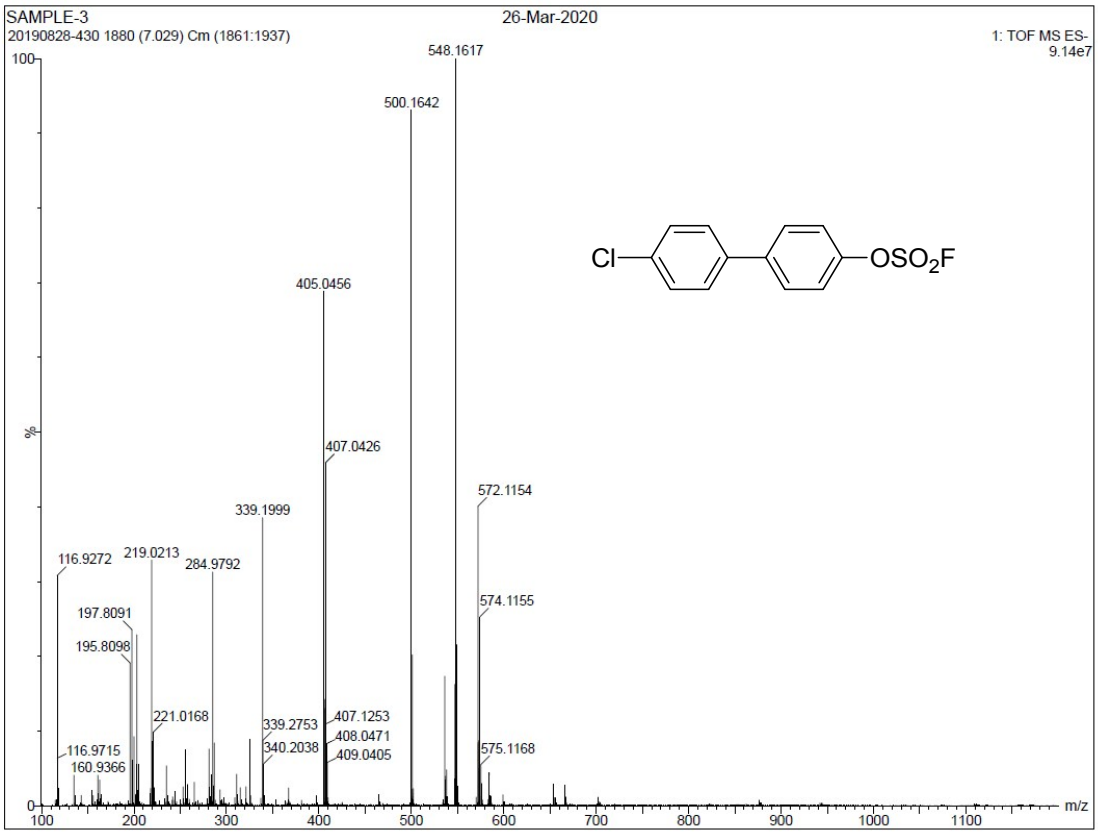

SAMPLE-1
26-Mar-2020
20190828-428 1933 (7.277) Cm (1919:1990)
1: TOF MS ES-
8.77e7
100
%
0
500.1642
279.0510
548.1617
572.1154
574.1155
116.9294
213.0921
197.8091
195.8098
283.2638
393.1867
339.1999
473.2830
574.2087
134.8927
393.2639
654.0744
OSO2F
100
200
300
400
500
600
700
800
900
1000
1100
m/z

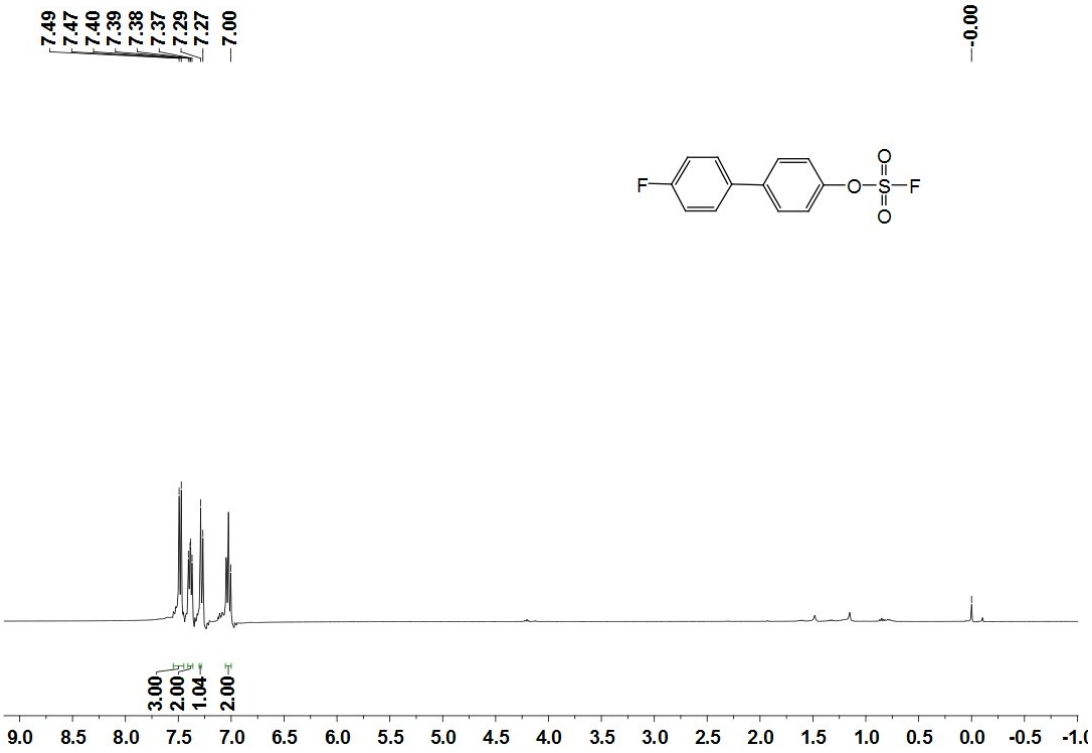

7.67
7.65
7.50
7.40
7.38
1.37
0.00
1.99
3.93
1.88
9.00
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


151.23
149.14
141.80
136.30
125.95
121.09
77.31
76.99
76.68
34.60
31.29
170
150
130
110
90
80
70
60
50
40
30
20


SAMPLE-2
20190828-429 2046 (7.708) Cm (2024:2081)
26-Mar-2020
1: TOF MS ES-
7.35e7
100
%
0
307.0809
500.1642
241.1228
572.1154
116.9272
307.1511
574.1155
195.8098
449.2468
501.1675
308.0849
536.1376
339.1999
575.1168
116.9693
576.1141
OSO2F
100
200
300
400
500
600
700
800
900
1000
1100
m/z


7.64
7.62
7.50
7.48
7.45
7.43
7.41
7.26
Cl
O
S
O
O
F
2.00
1.92
3.86
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
6.5
149.47
140.73
137.64
134.34
129.18
128.43
121.34
77.31
76.99
76.68
165
150
135
120
105
90
80
70


SAMPLE-3
26-Mar-2020
20190828-430 1880 (7.029) Cm (1861:1937)
1: TOF MS ES-
9.14e7
100
%
0
548.1617
500.1642
405.0456
407.0426
572.1154
339.1999
116.9272
219.0213
284.9792
574.1155
197.8091
195.8098
221.0168
339.2753
407.1253
408.0471
340.2038
409.0405
116.9715
160.9366
575.1168
Cl
OSO2F
100
200
300
400
500
600
700
800
900
1000
1100
m/z


7.49
7.47
7.40
7.39
7.38
7.37
7.29
7.27
7.00
-0.00
F
O
S
F
O
O
3.00
2.00
1.04
2.00
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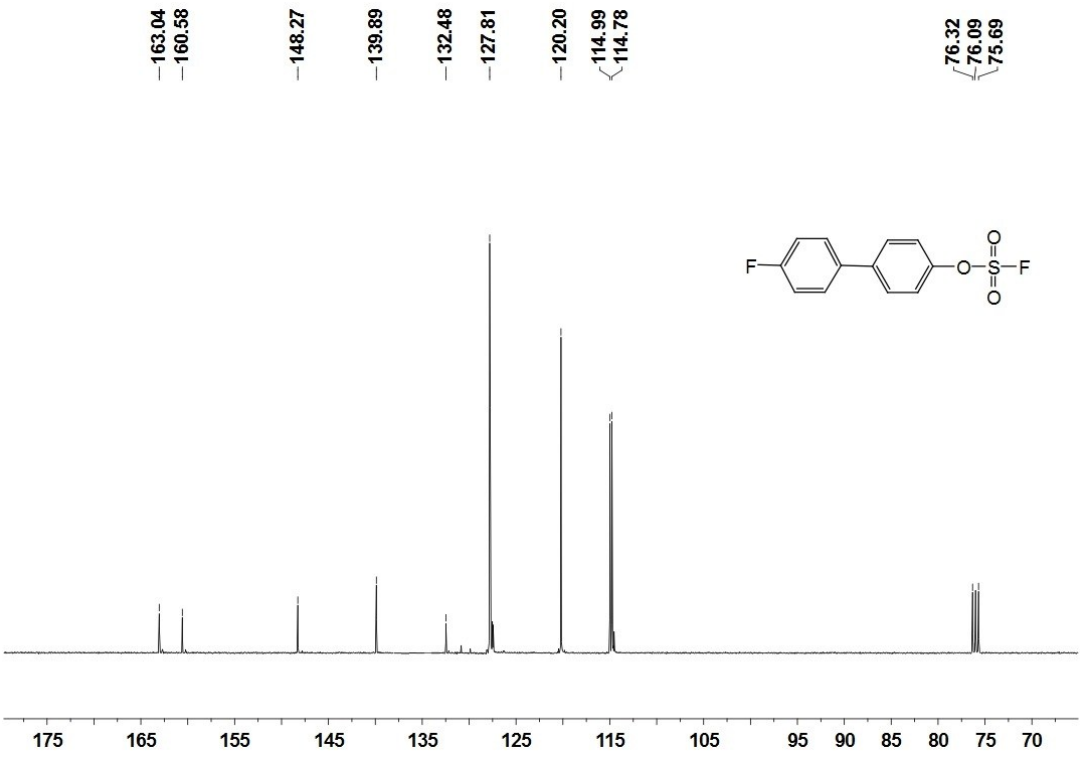
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75.69
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F
O
O
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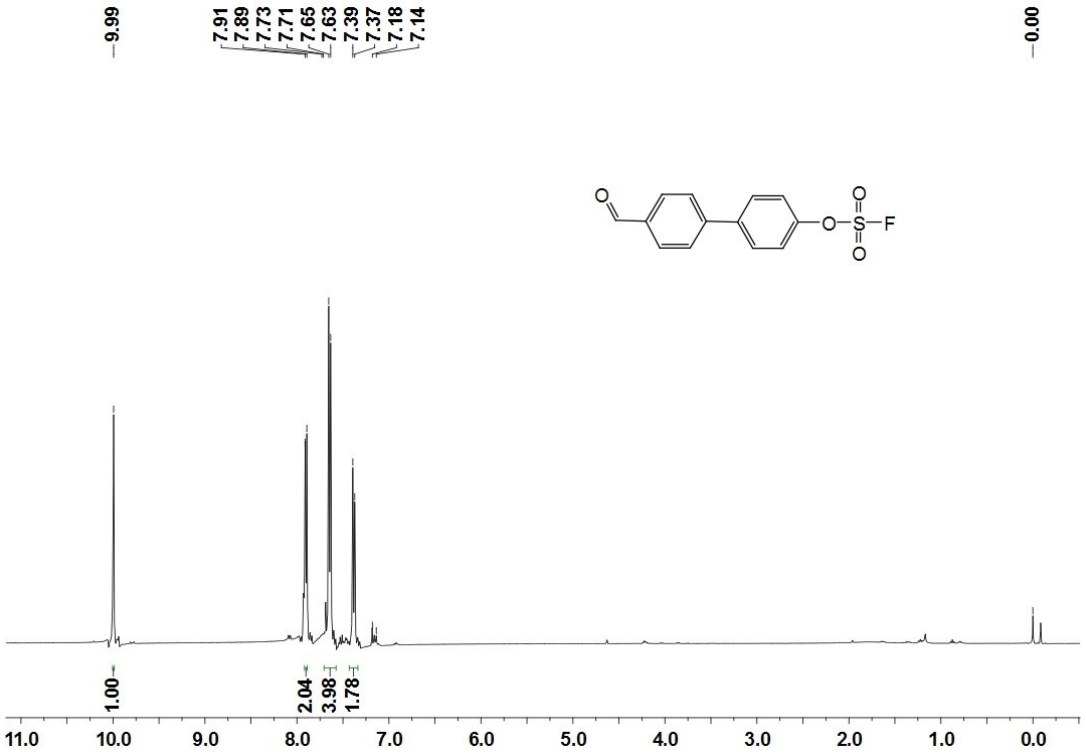
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7.14
0.00
O
O
S
F
O
1.00
2.04
3.98
1.78
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6.0
5.0
4.0
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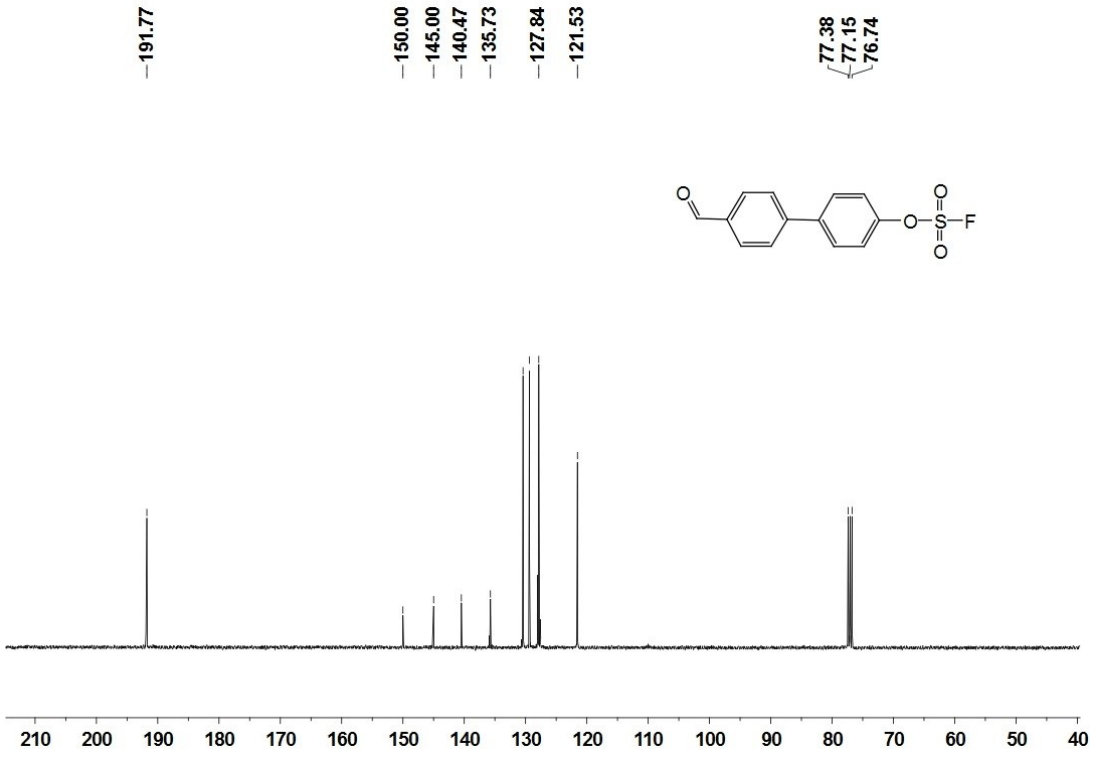
2.0
1.0
0.0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77.38
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76.74
O
O
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50
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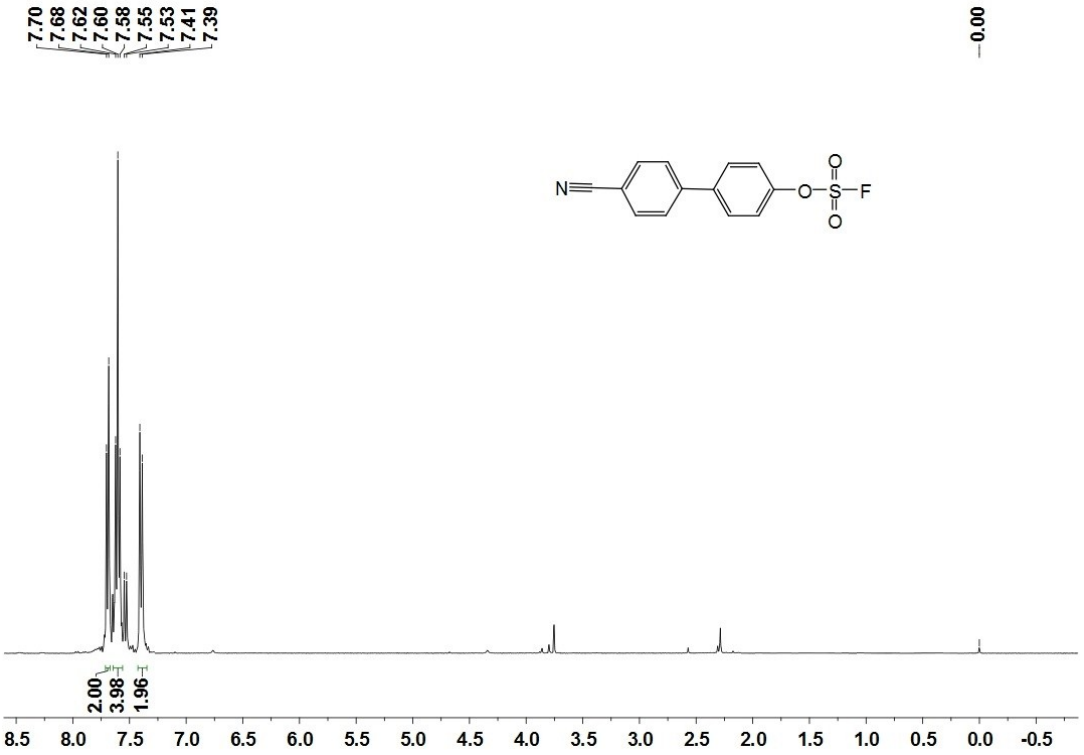
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N
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S
F
2.00
3.98
1.96
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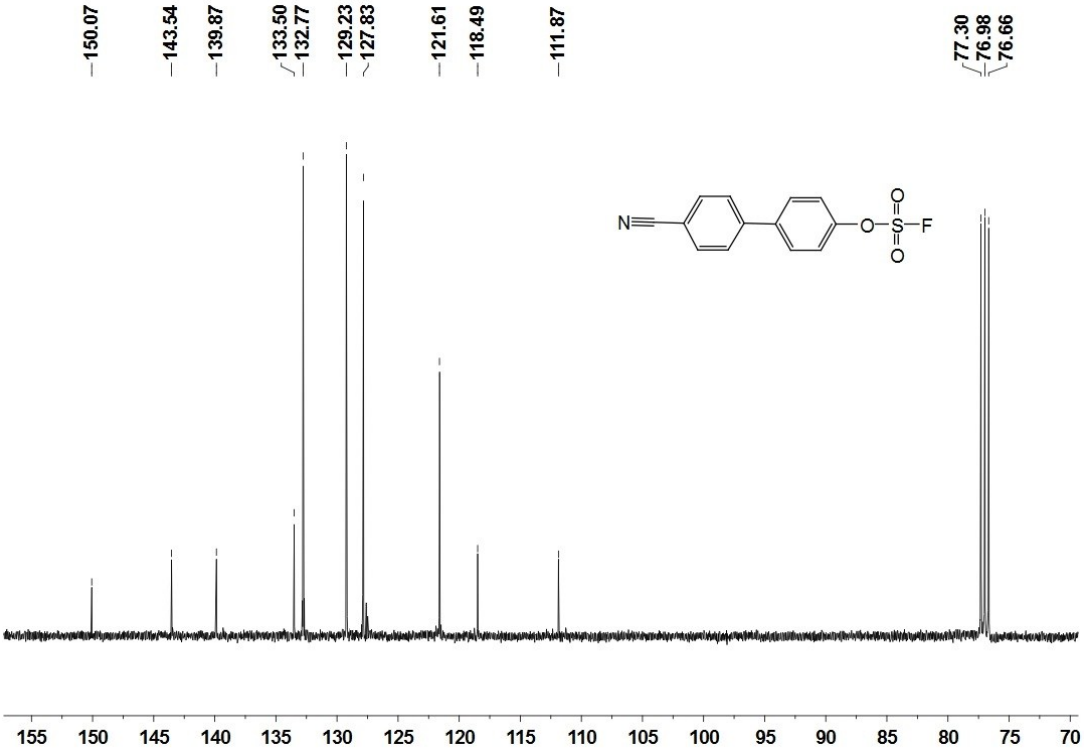
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76.66
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S
F
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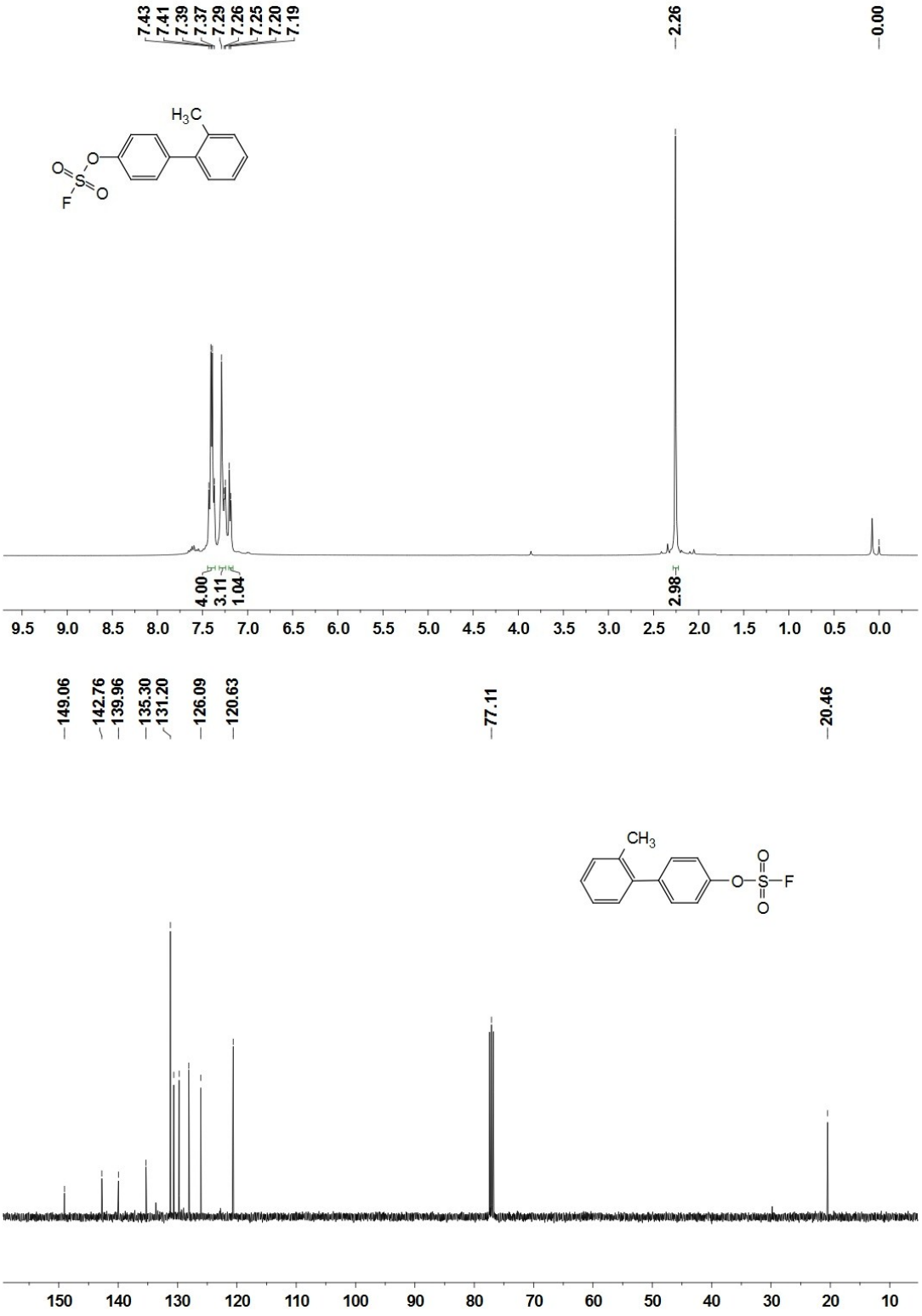
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2.26
0.00
H3C
O
S
O
F
O
4.00
3.11
1.04
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
149.06
142.76
139.96
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CH3
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S
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O
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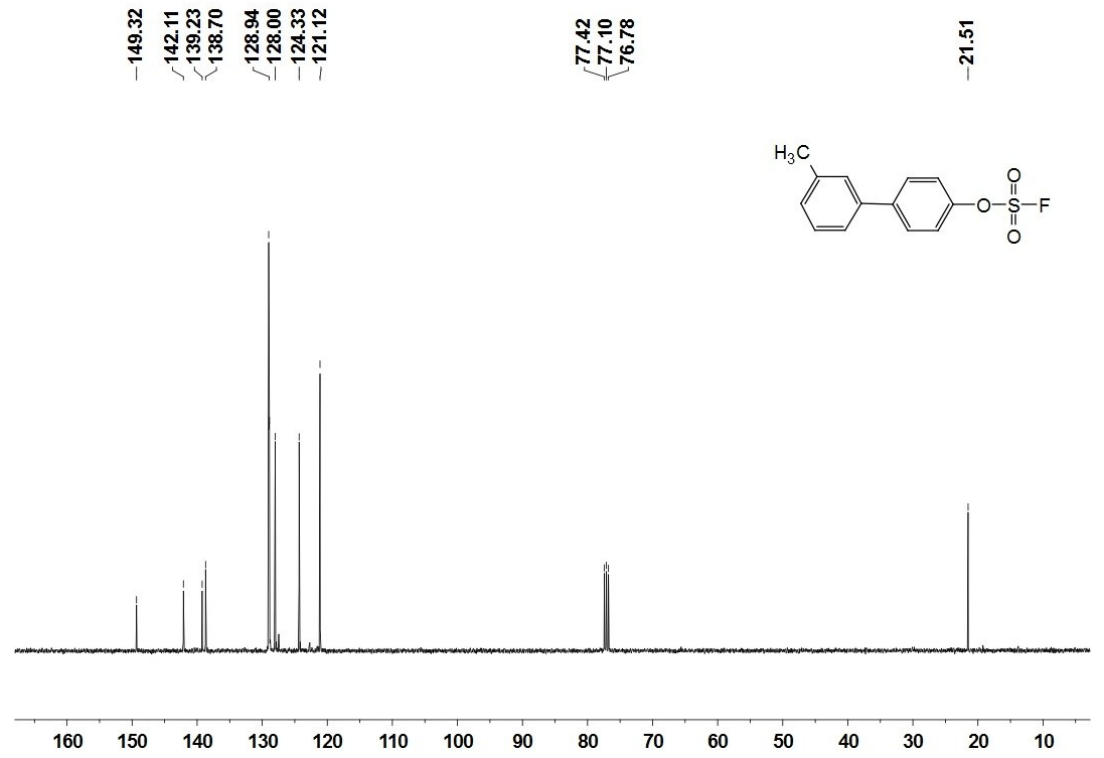
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124.33
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76.78
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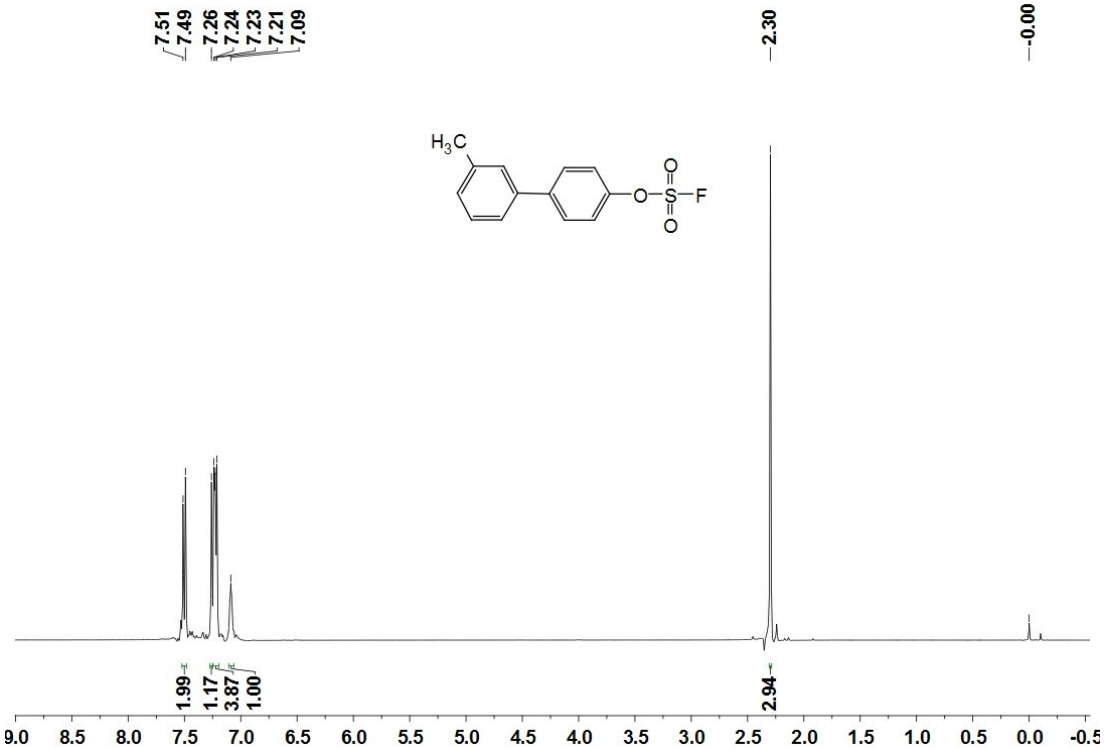
O
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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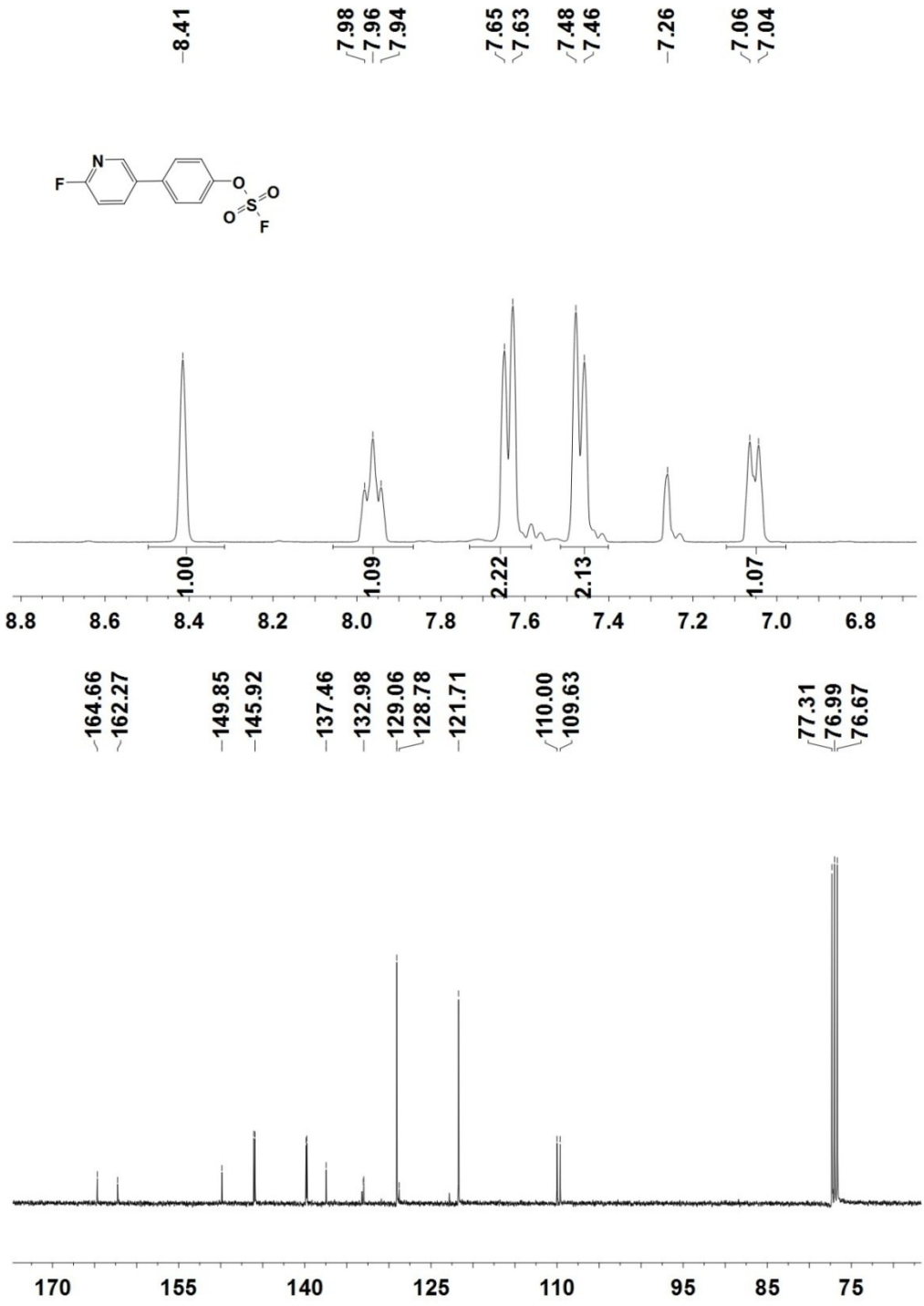
7.21
7.09
2.30
-0.00
H3C
O
S
F
O
O
1.99
1.17
3.87
1.00
2.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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7.46
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7.06
7.04
N
F
O
O
S
O
O
F
1.00
1.09
2.22
2.13
1.07
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
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162.27
149.85
145.92
137.46
132.98
129.06
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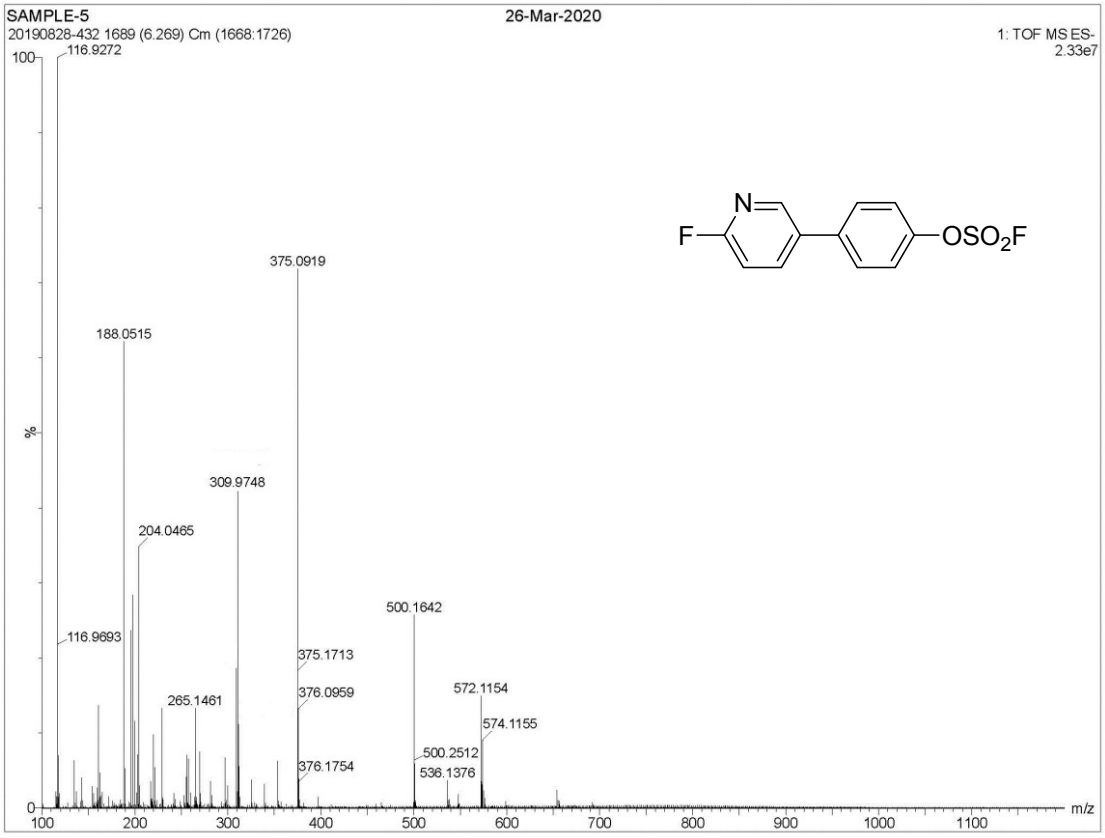
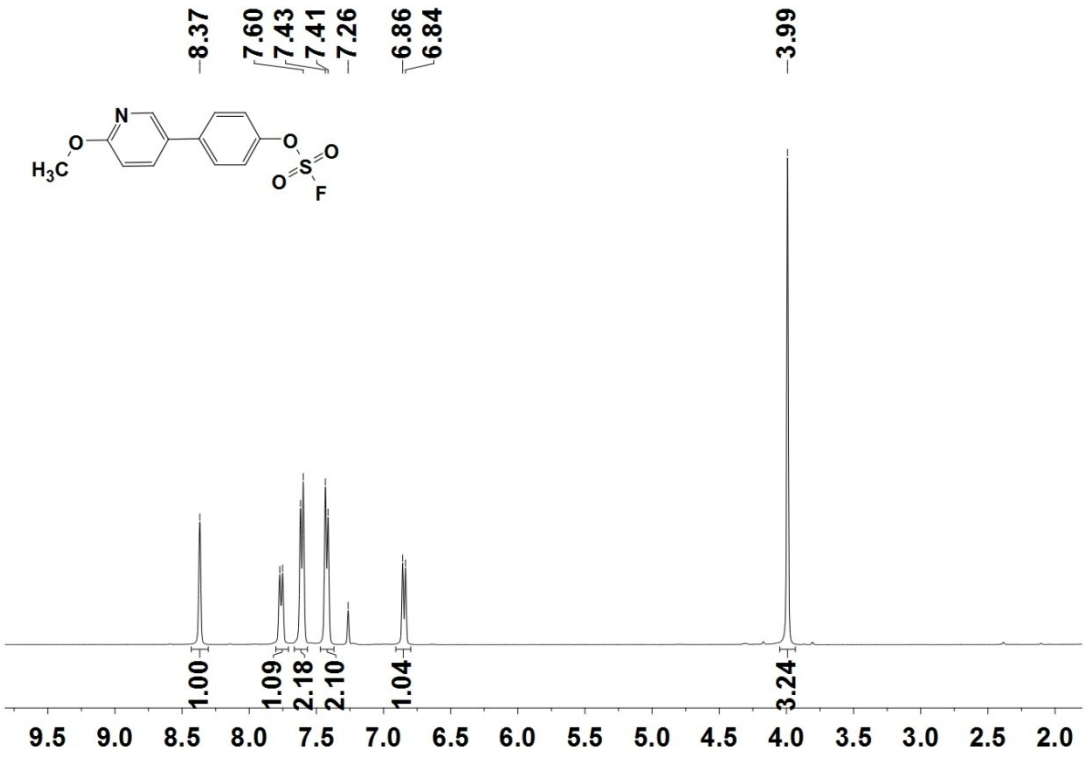
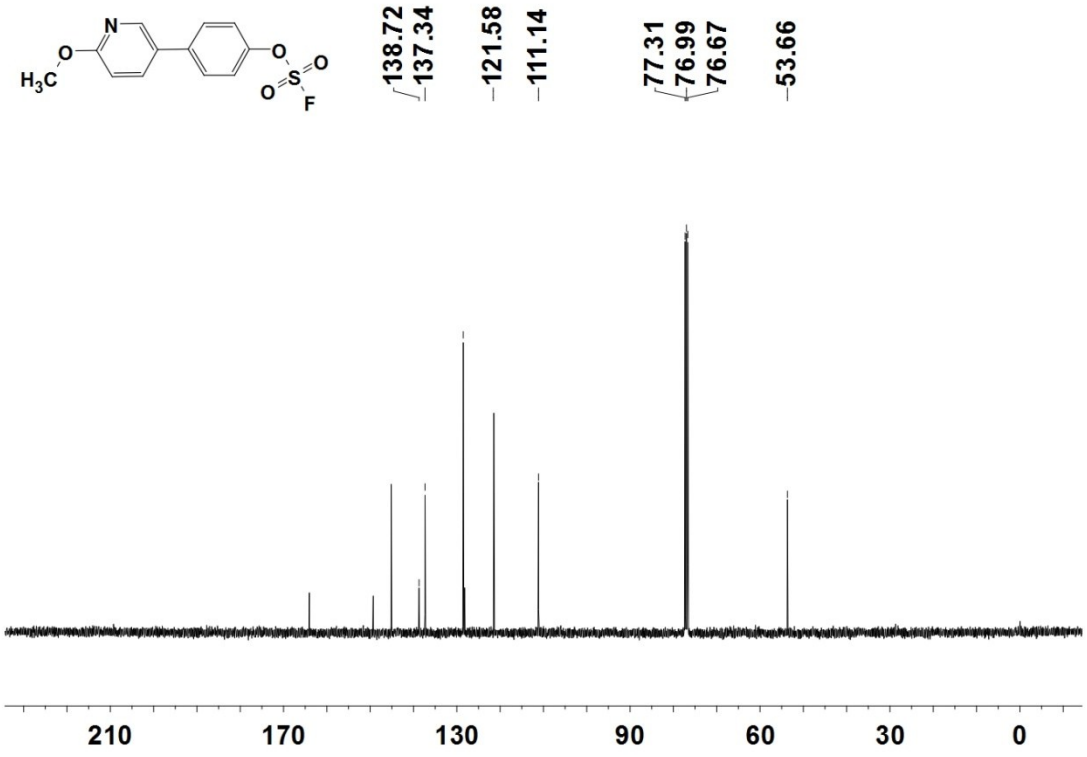
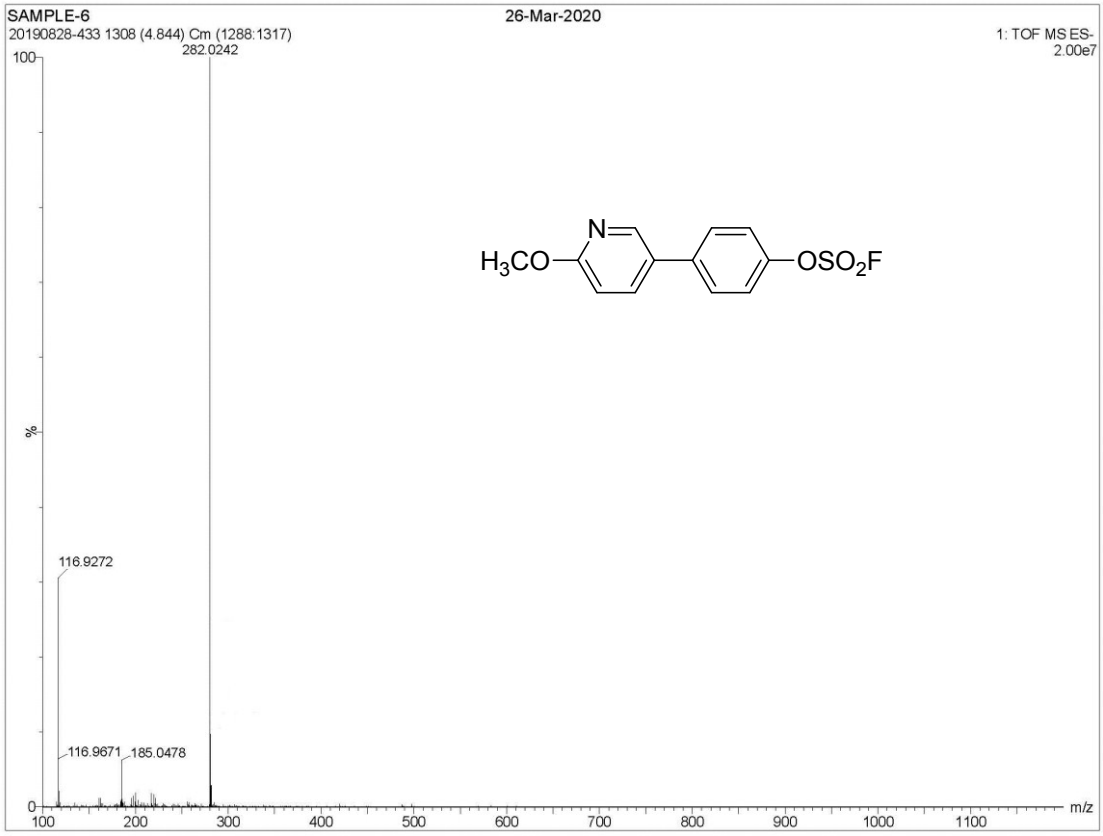
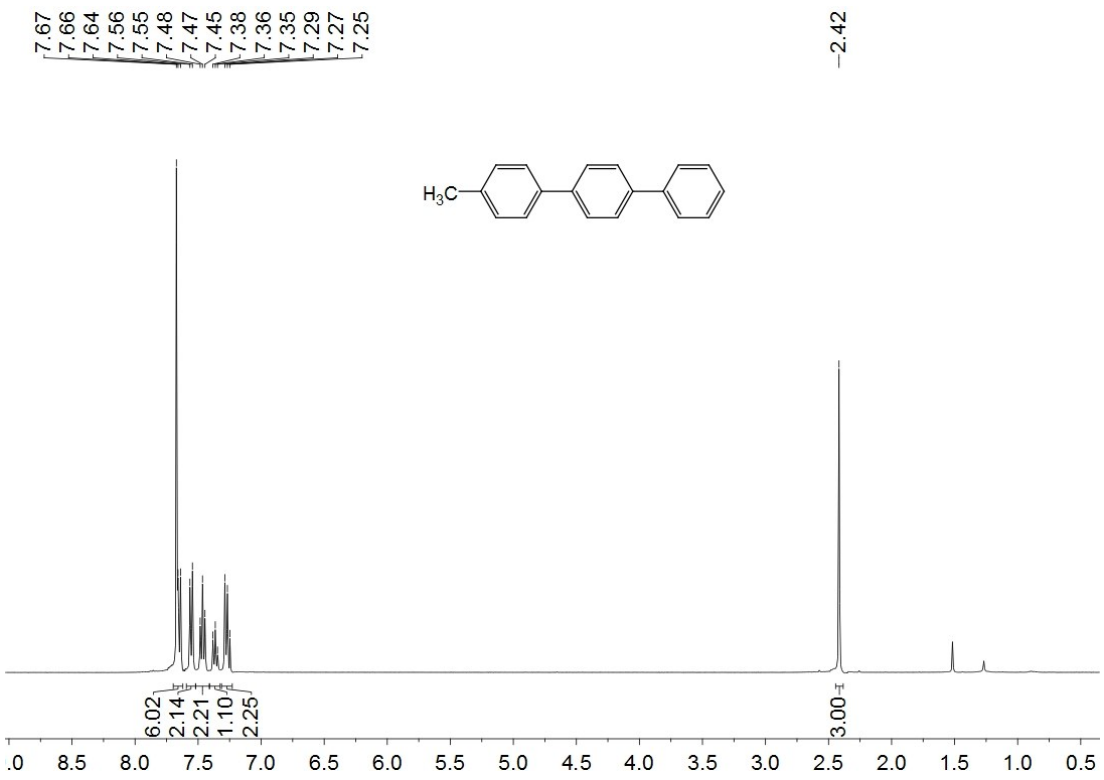
140
125
110
95
85
75


SAMPLE-5
26-Mar-2020
20190828-432 1689 (6.269) Cm (1668:1726)
1: TOF MS ES-
2.33e7
100
%
0
116.9272
375.0919
188.0515
309.9748
204.0465
500.1642
116.9693
375.1713
376.0959
572.1154
265.1461
574.1155
500.2512
376.1754
536.1376
100
200
300
400
500
600
700
800
900
1000
1100
m/z
N
F
OSO2F


8.37
7.60
7.43
7.41
7.26
6.86
6.84
3.99
1.00
1.09
2.18
2.10
1.04
3.24
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0


138.72
137.34
121.58
111.14
77.31
76.99
76.67
53.66
210
170
130
90
60
30
0


SAMPLE-6
26-Mar-2020
20190828-433 1308 (4.844) Cm (1288:1317)
1: TOF MS ES-
2.00e7
282.0242
100
%
116.9272
116.9671
185.0478
0
100
200
300
400
500
600
700
800
900
1000
1100
m/z
N
H3CO
OSO2F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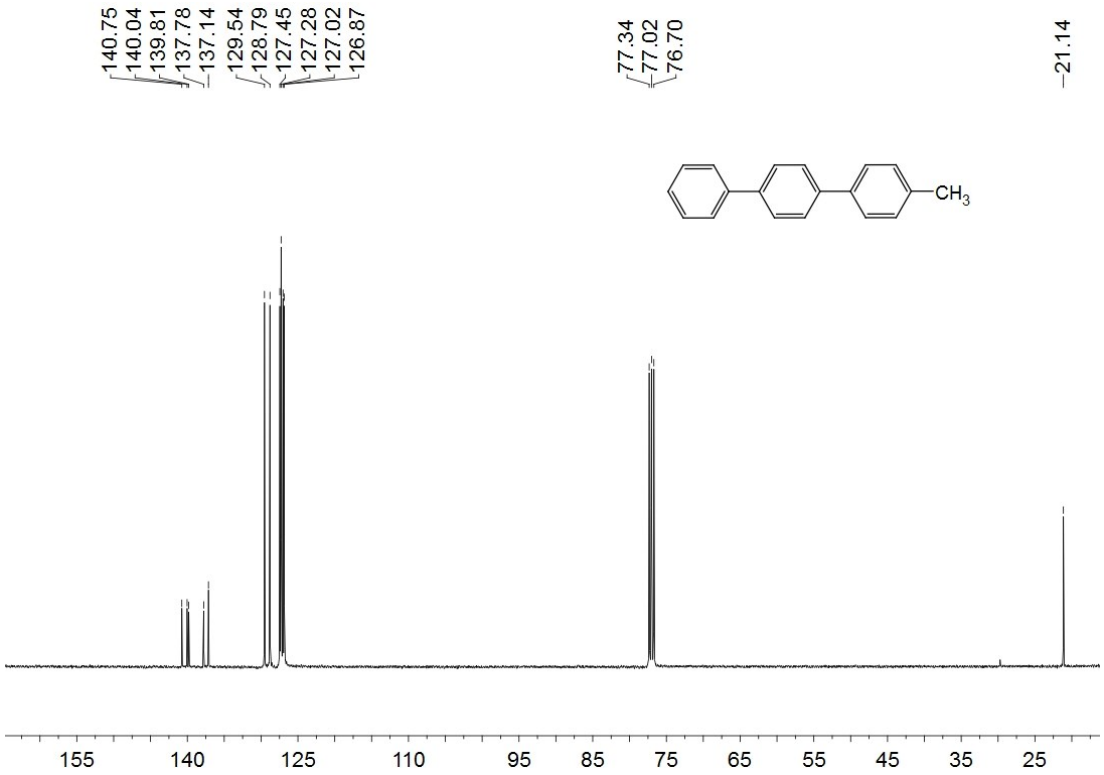
7.64
7.56
7.55
7.48
7.47
7.45
7.38
7.36
7.35
7.29
7.27
7.25
2.42
H3C
6.02
2.14
2.21
1.10
2.25
3.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5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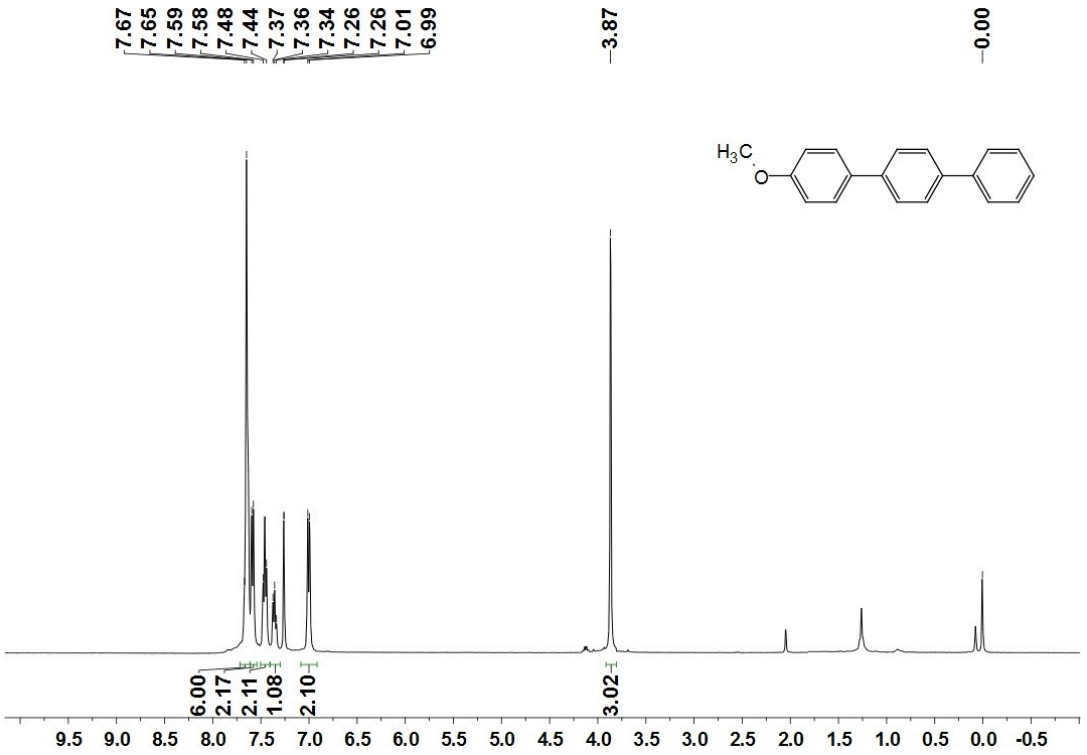
140.04
139.81
137.78
137.14
129.54
128.79
127.45
127.28
127.02
126.87
77.34
77.02
76.70
21.14
CH3
155 140 125 110 95 85 75 65 55 45 35 25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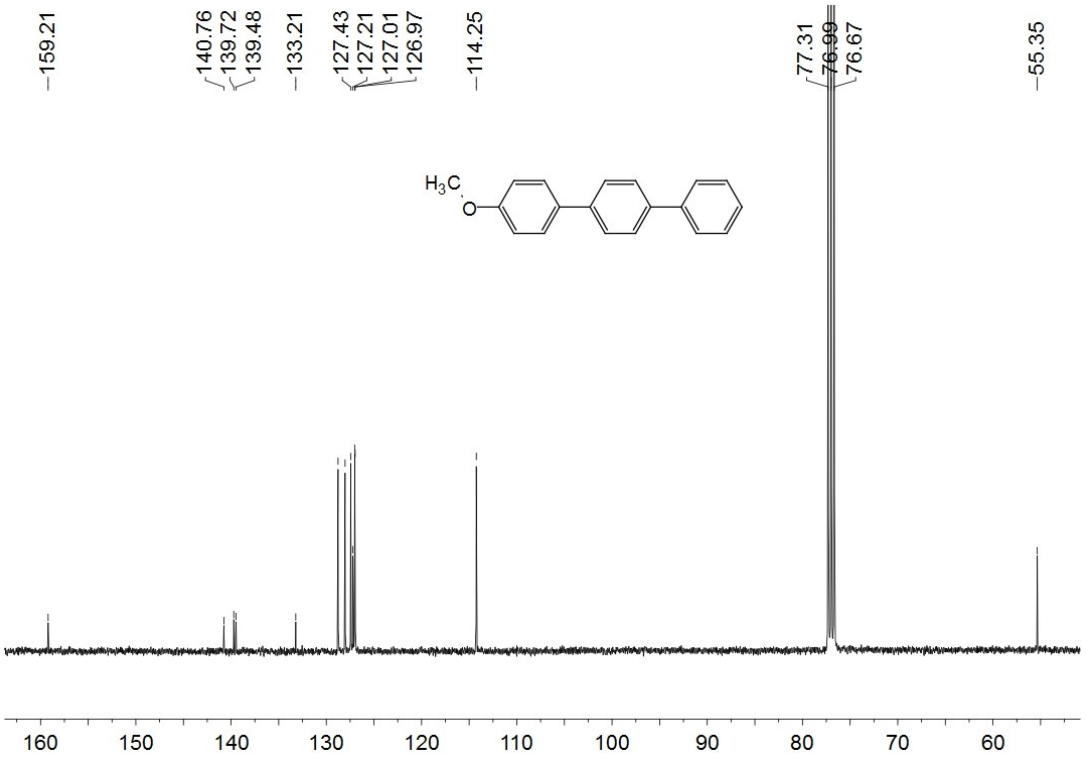
7.59
7.58
7.48
7.44
7.37
7.36
7.34
7.26
7.26
7.01
6.99
3.87
0.00
H3C
O
6.00
2.17
2.11
1.08
2.10
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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139.72
139.48
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127.43
127.21
127.01
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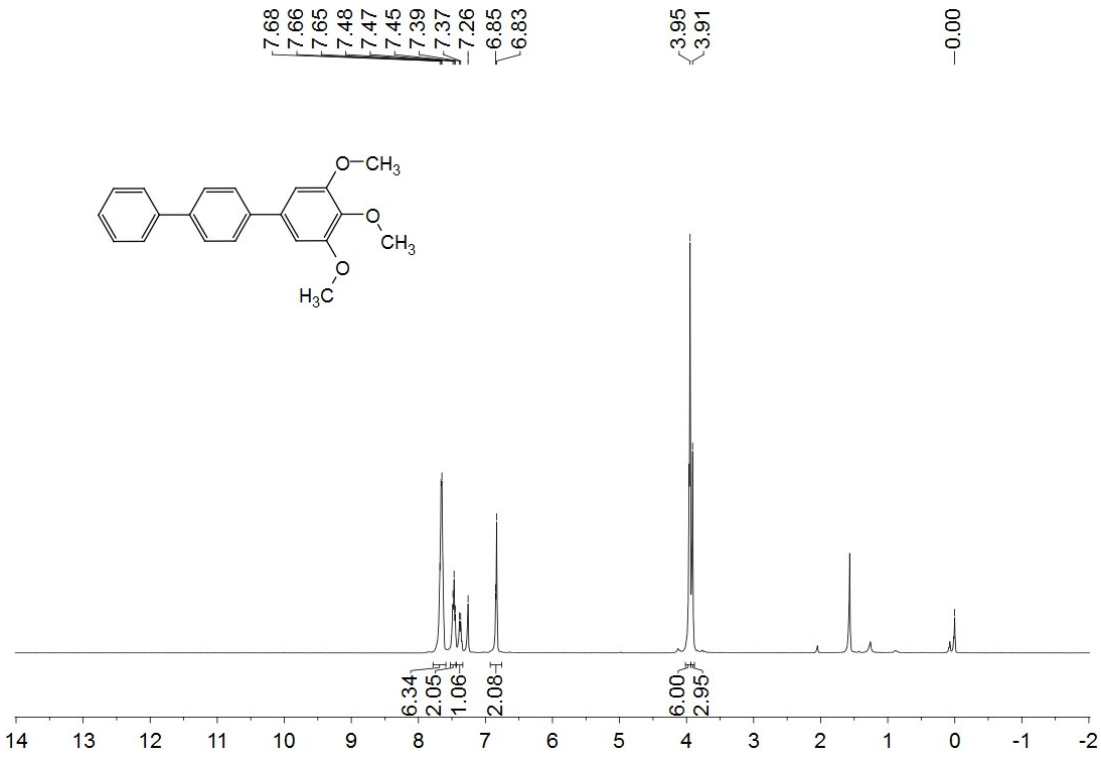
114.25
77.31
76.99
76.67
55.35
H3C
O
160 150 140 130 120 110 100 90 80 70 60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7.65
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7.37
7.26
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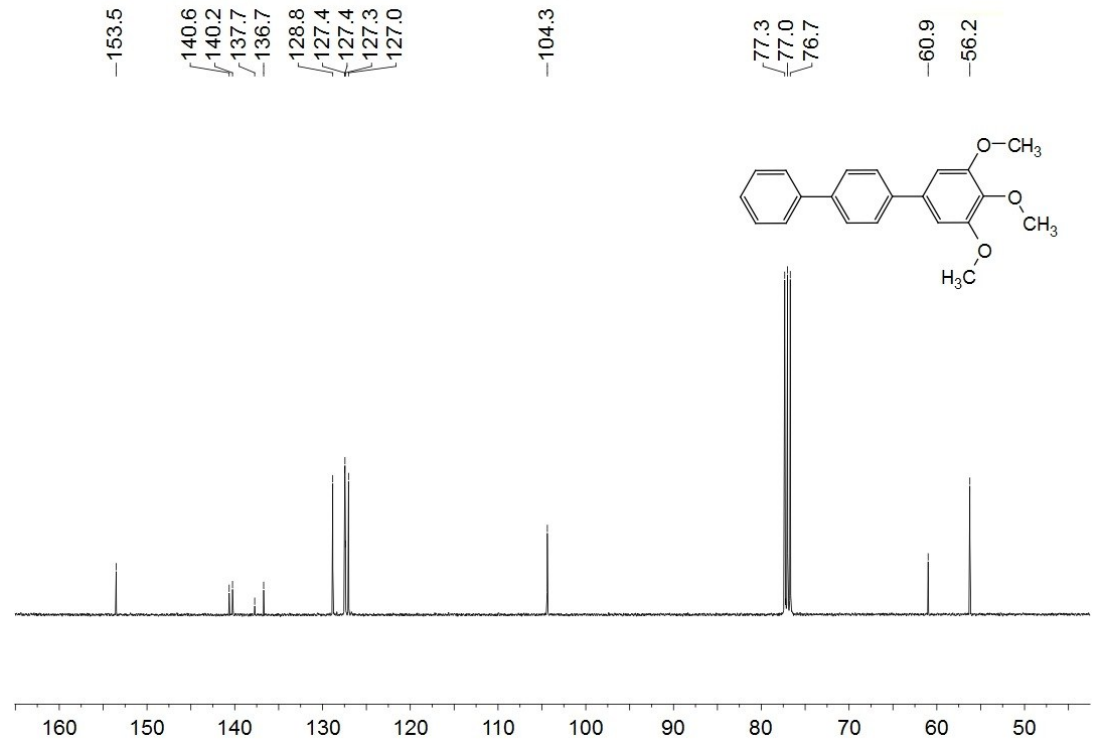
6.83
3.95
3.91
0.00
O—CH3
O
CH3
O
H3C
6.34
2.05
1.06
2.08
6.00
2.95
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2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127.4
127.3
127.0
104.3
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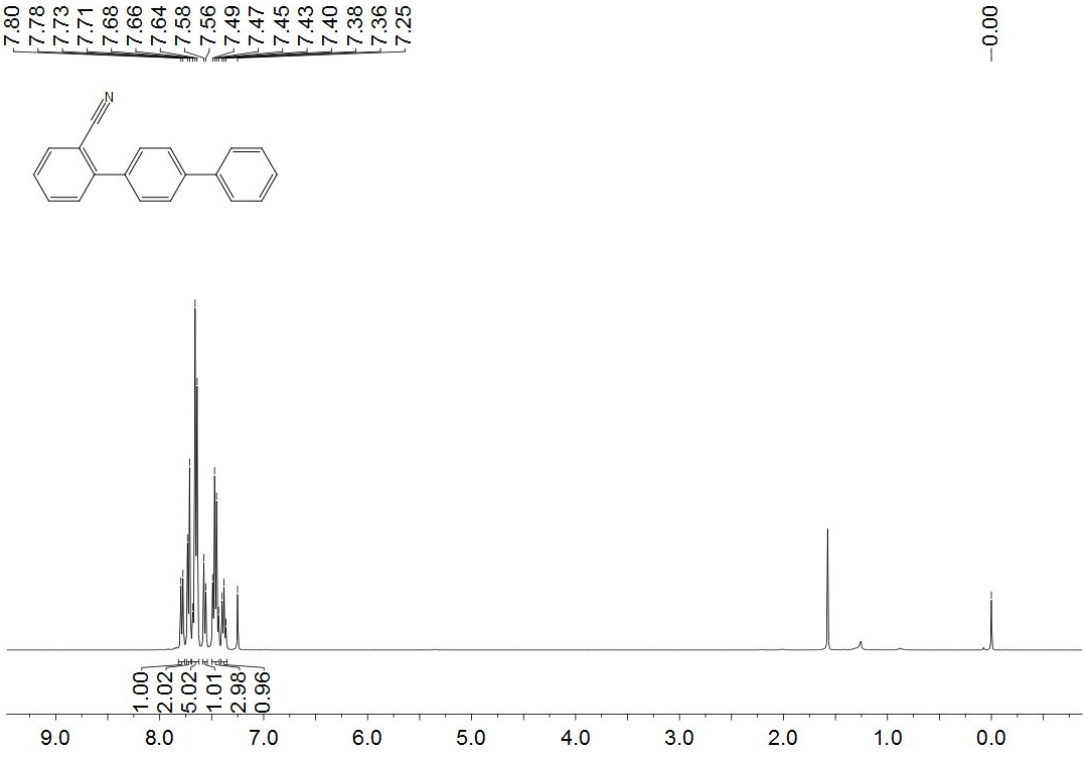
60.9
56.2
O—CH3
O
CH3
O
H3C
160 150 140 130 120 110 100 90 80 70 60 50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7.45
7.43
7.40
7.38
7.36
7.25
0.00
N
1.00
2.02
5.02
1.01
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8.0
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6.0
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4.0
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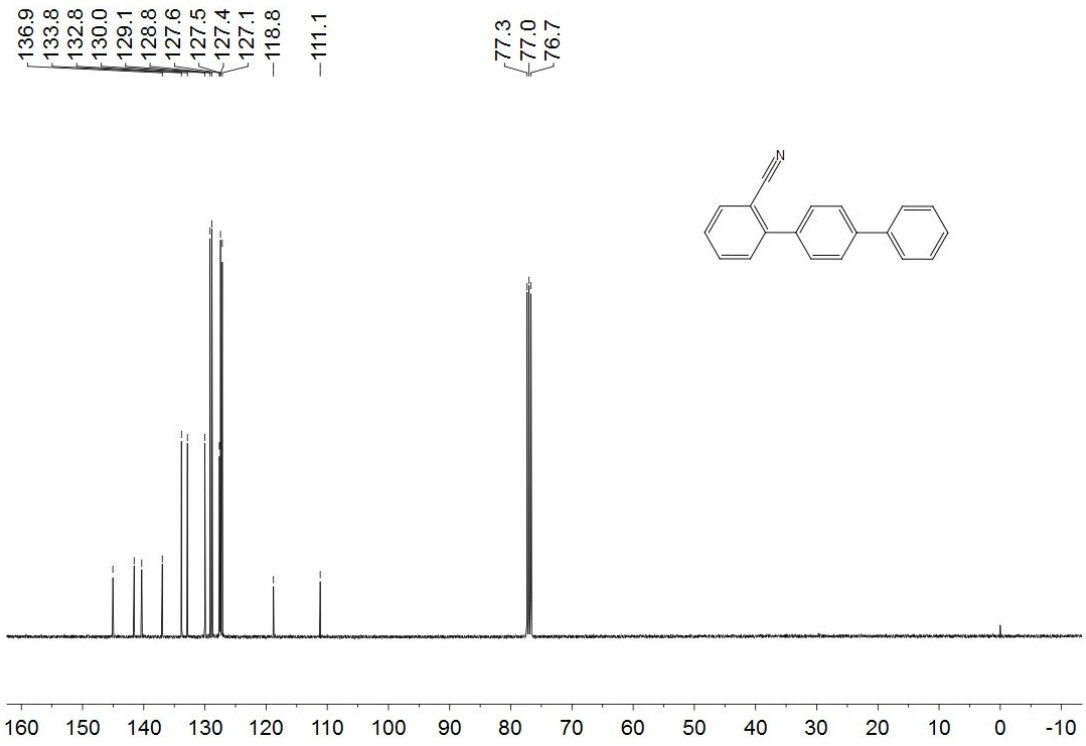
2.0
1.0
0.0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127.5
127.4
127.1
118.8
111.1
77.3
77.0
76.7
N
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140
130
120
110
100
90
80
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60
50
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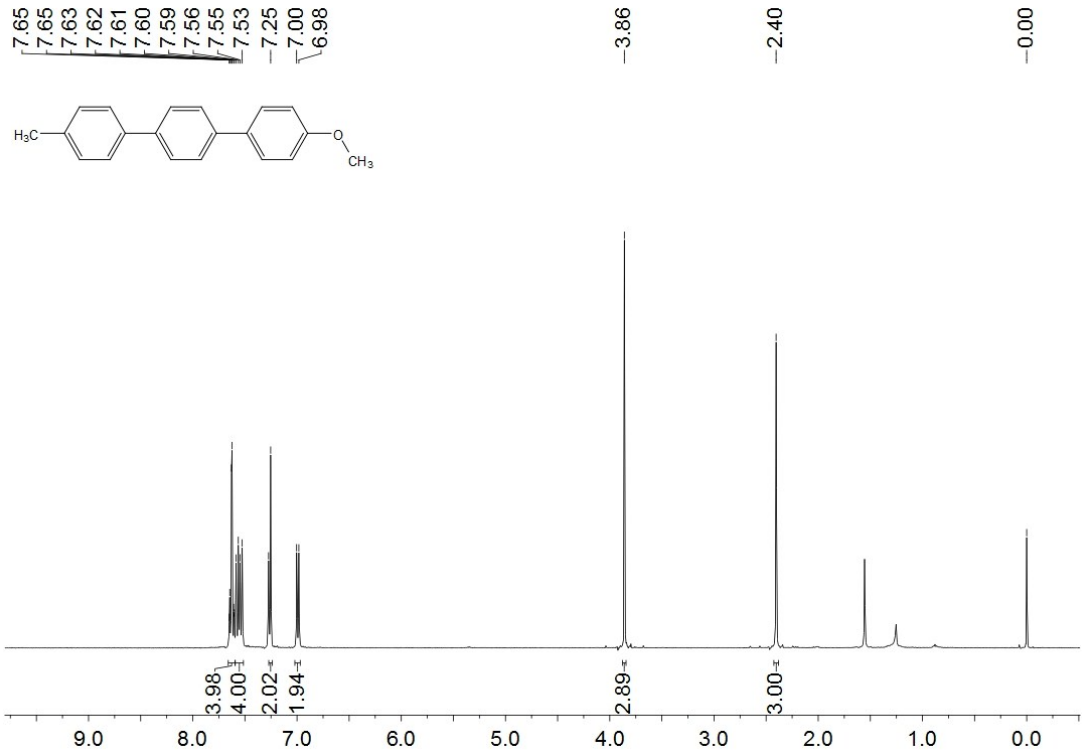
20
10
0
-10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3.86
2.40
0.00
H3C
O
CH3
3.98
4.00
2.02
1.94
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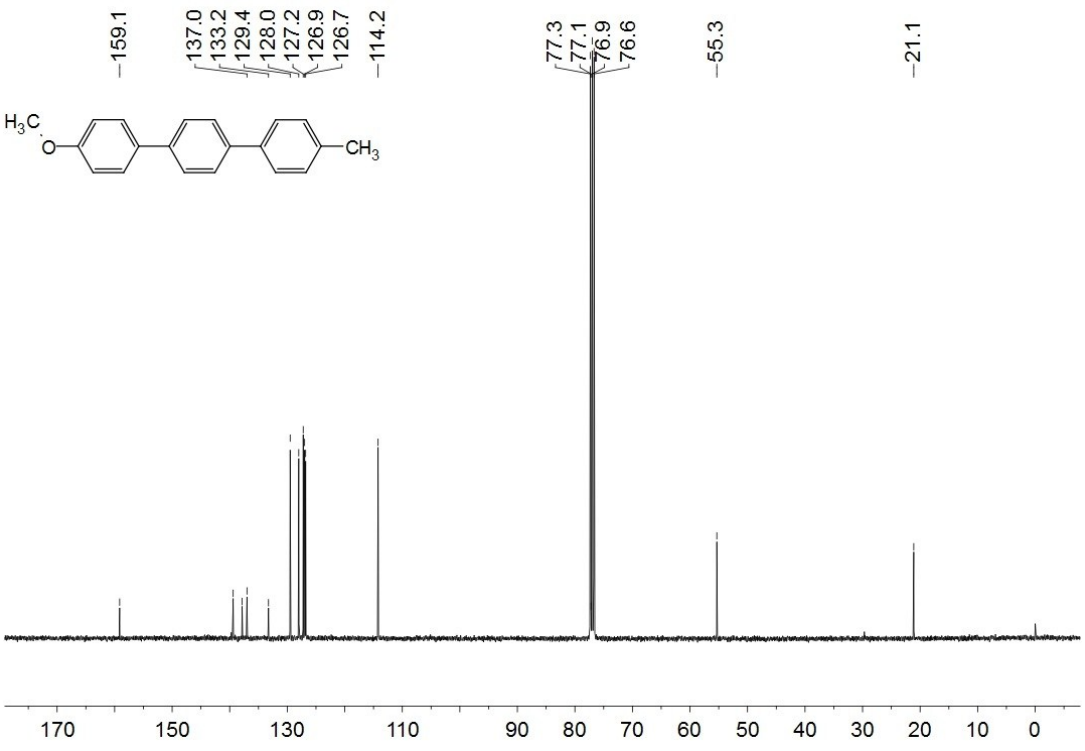
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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76.9
76.6
55.3
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H3C
O
CH3
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130
110
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70
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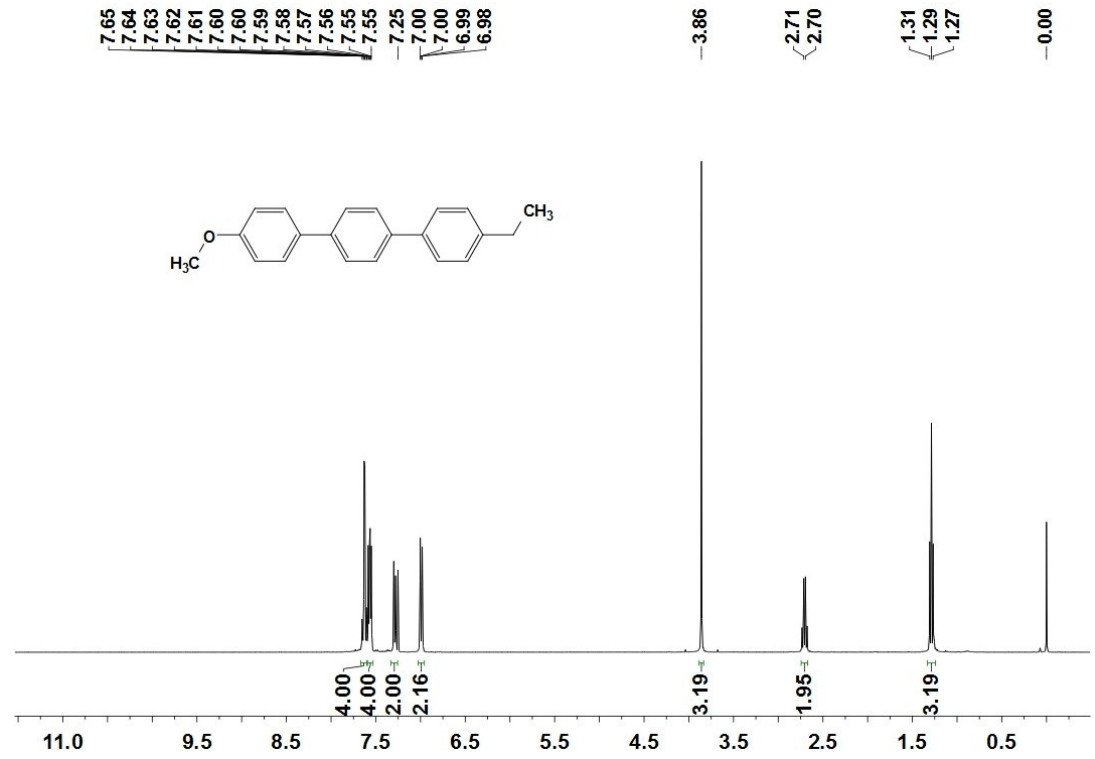
10
0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7.63
7.62
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7.59
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7.56
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7.55
7.25
7.00
7.00
6.99
6.98
3.86
2.71
2.70
1.31
1.29
1.27
0.00
CH3
O
H3C
4.00
4.00
2.00
2.16
3.19
1.95
3.19
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6.5
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4.5
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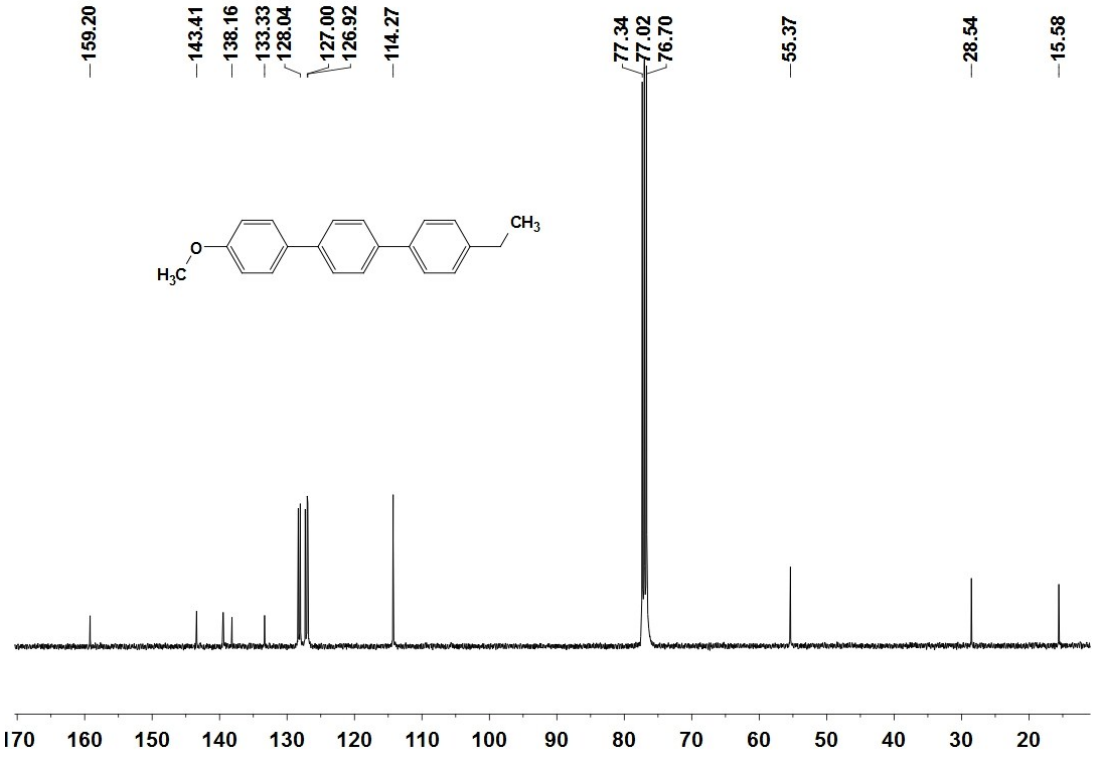
2.5
1.5
0.5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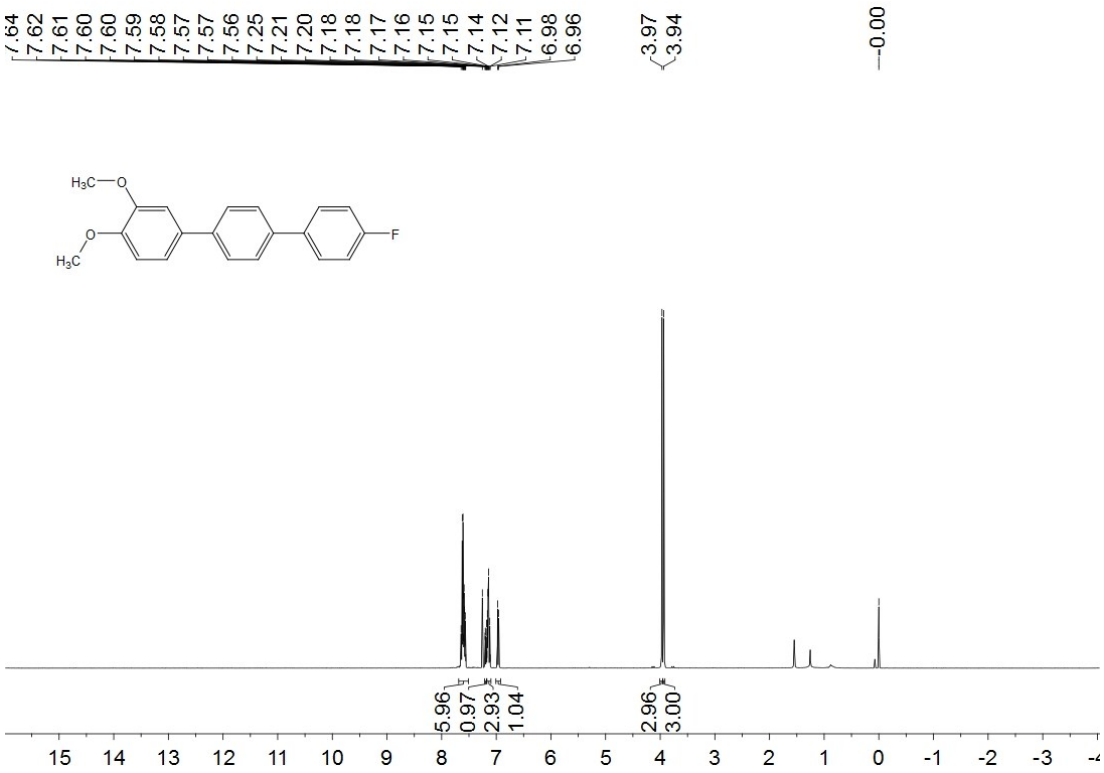
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7.18
7.18
7.17
7.16
7.15
7.15
7.14
7.12
7.11
6.98
6.96
3.97
3.94
0.00
H3C—O
O
H3C
F
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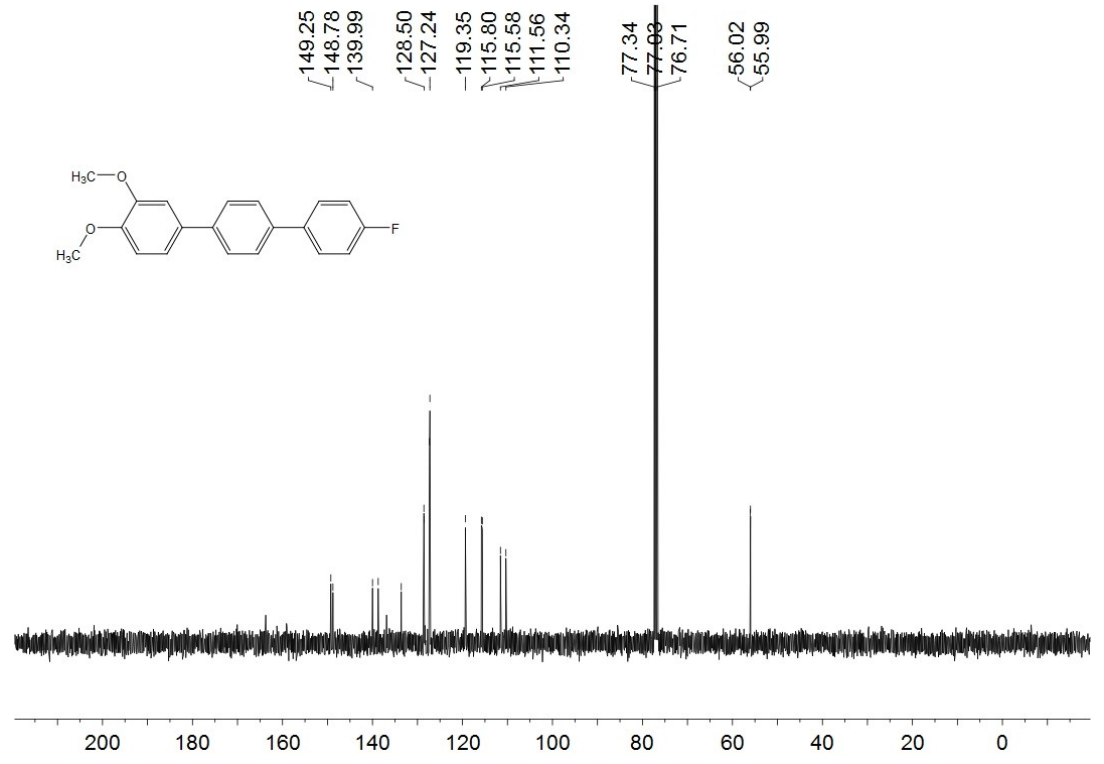
0.97
2.93
1.04
2.96
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3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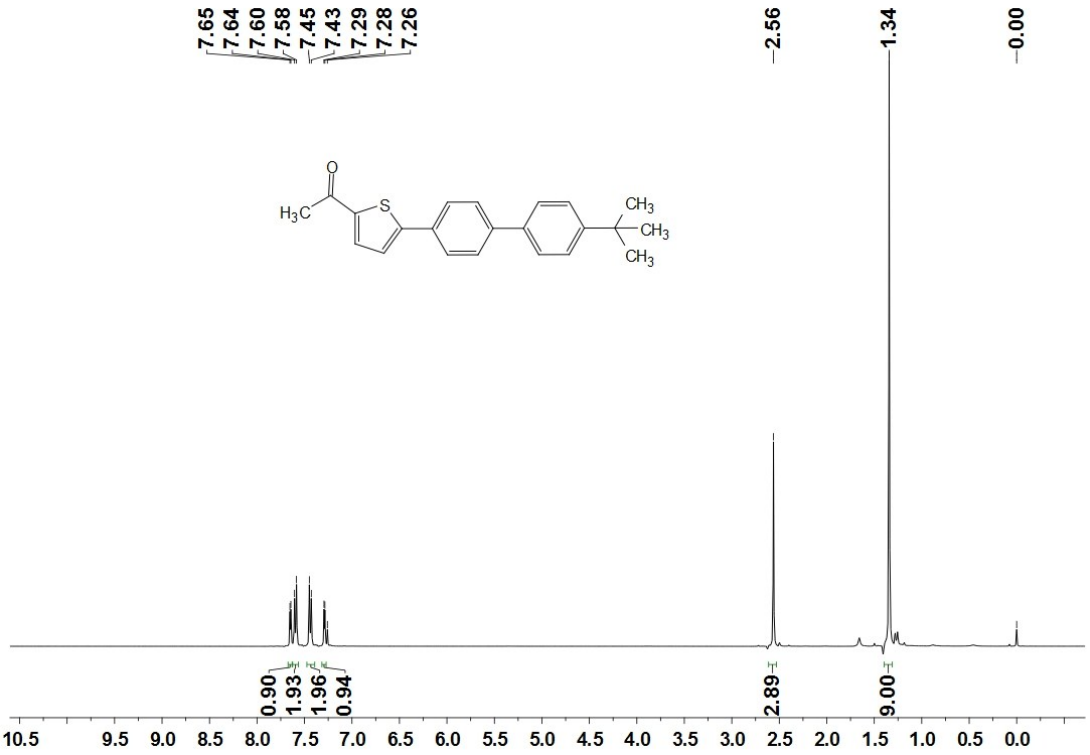
76.71
56.02
55.99
H3C—O
O
H3C
F
200 180 160 140 120 100 80 60 40 20 0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0.94
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2.0
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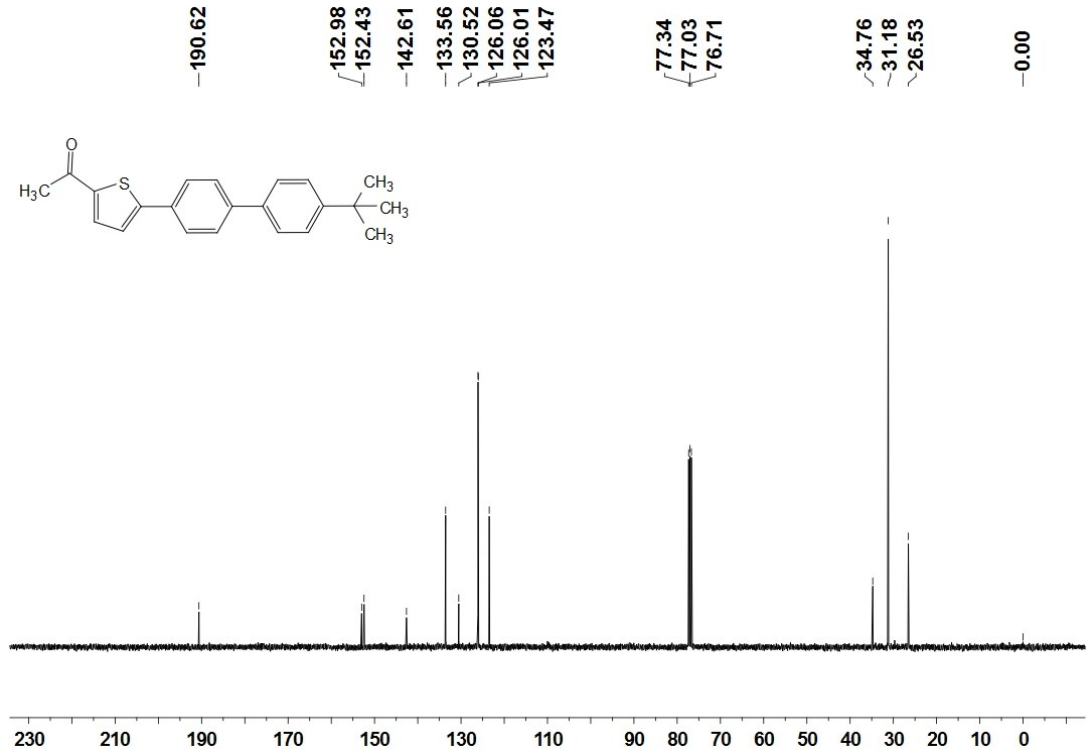
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90
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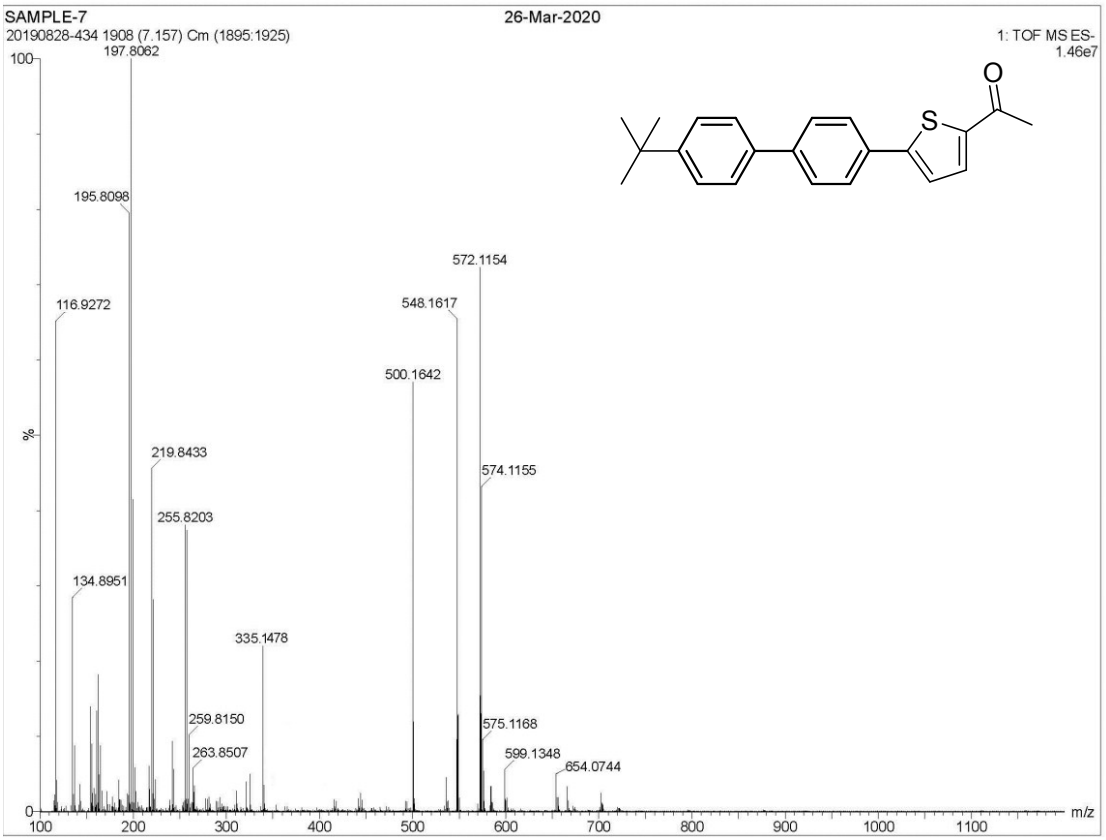
SAMPLE-7
26-Mar-2020
20190828-434 1908 (7.157) Cm (1895:1925)
1: TOF MS ES-
1.46e7
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%
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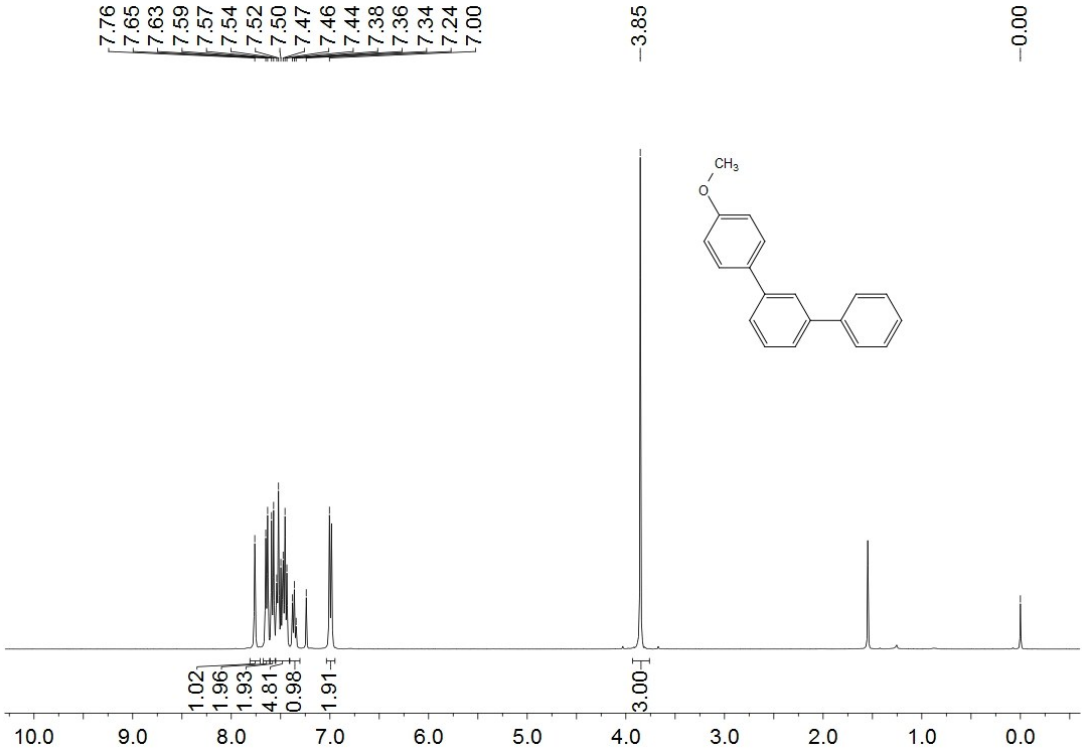
195.8098
116.9272
572.1154
548.1617
500.1642
219.8433
574.1155
255.8203
134.8951
335.1478
259.8150
575.1168
263.8507
599.1348
654.0744
O
S
100
200
300
400
500
600
700
800
900
1000
1100
m/z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7.65
7.63
7.59
7.57
7.54
7.52
7.50
7.47
7.46
7.44
7.38
7.36
7.34
7.24
7.00
3.85
0.00
CH3
O
1.02
1.96
1.93
4.81
0.98
1.91
3.00
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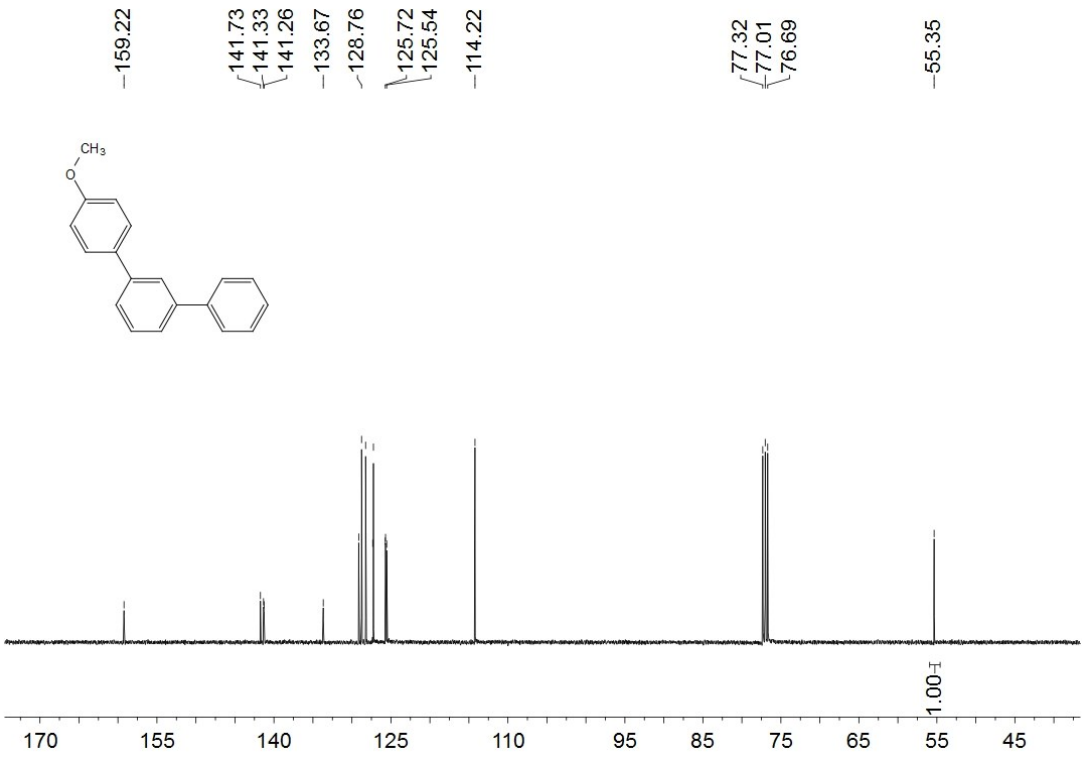
159.22
141.73
141.33
141.26
133.67
128.76
125.72
125.54
114.22
77.32
77.01
76.69
55.35
CH3
O
1.00
170
155
140
125
110
95
85
75
65
55
45