Supporting Information

4-(3-Aminopropyl)-benzene-1,2-diol: An Improved Material-Independent Surface-Coating Reagent Compared to Dopamine

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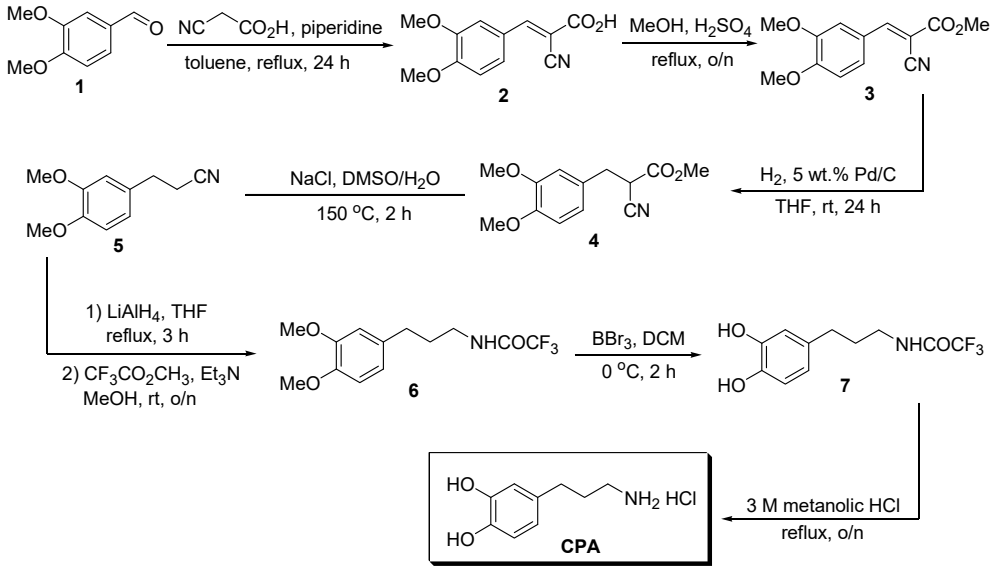


Scheme S1. Synthesis of CPA·HCl from 3,4-dimethoxybenzaldehyde.

Computational Details. The DMol3 package[1,2] was used for obtaining the ground structures and Kohn-Sham orbitals of CPA and DA. Geometry optimization was performed with the B3LYP functional[3,4] and the triple numerical plus polarization (TNP) set,[5] and the optimized structures were subjected to frequency calculation with the same level of theory to confirm the true local minimum. Because the reaction was performed under alkaline conditions, we calculated the deprotonated DA and CPA.

Table S1. Cartesian Coordinates of Calculated Structures

DA
Charge: -1, spin multiplicity: 1

1	H	1.994408	-1.166261	-0.301654
2	C	1.063444	-0.632814	-0.184355
3	C	1.116982	0.811116	-0.034042
4	C	2.445650	1.518289	-0.089549
5	C	-0.048819	1.497474	0.154686
6	H	-0.042153	2.574132	0.276646
7	C	-1.350336	0.862310	0.160249
8	O	-2.403692	1.490430	0.277546
9	C	-1.384180	-0.672073	0.003631
10	C	-0.103649	-1.328909	-0.185477
11	H	-0.118191	-2.407656	-0.282841
12	O	-2.449774	-1.285025	0.058091
13	C	3.651750	0.613932	0.167889
14	H	2.471172	2.323151	0.650755

15	H	2.583300	2.010442	-1.059600
16	H	3.376039	-0.056710	1.026749
17	N	4.815381	1.384910	0.370659
18	H	3.714664	-0.108724	-0.684379
19	H	5.565858	0.747845	0.642957

CPA
Charge: -1, spin multiplicity: 1

1	H	1.895307	-1.575663	-0.311685
2	C	1.046538	-0.908069	-0.216138
3	C	1.319808	0.511092	-0.107595
4	C	2.738696	0.956336	-0.197962
5	C	0.281213	1.394174	0.001308
6	H	0.466694	2.458850	0.080232
7	C	-1.102663	0.980940	0.025114
8	O	-2.044310	1.773527	0.122752
9	C	-1.373302	-0.532691	-0.067018
10	C	-0.212788	-1.406753	-0.181428
11	H	-0.411468	-2.469796	-0.234712
12	O	-2.519642	-0.977489	-0.037549
13	C	3.215269	1.034774	-1.667101
14	H	3.397175	0.267077	0.338891
15	H	2.856024	1.941861	0.259286
16	H	3.193944	0.050693	-2.135761
17	C	4.683112	1.597943	-1.773687
18	H	2.539358	1.678515	-2.234710
19	H	5.303946	0.956722	-1.128974
20	H	4.639086	2.592401	-1.279759
21	N	5.190029	1.595903	-3.091054
22	H	4.766674	2.384513	-3.582408

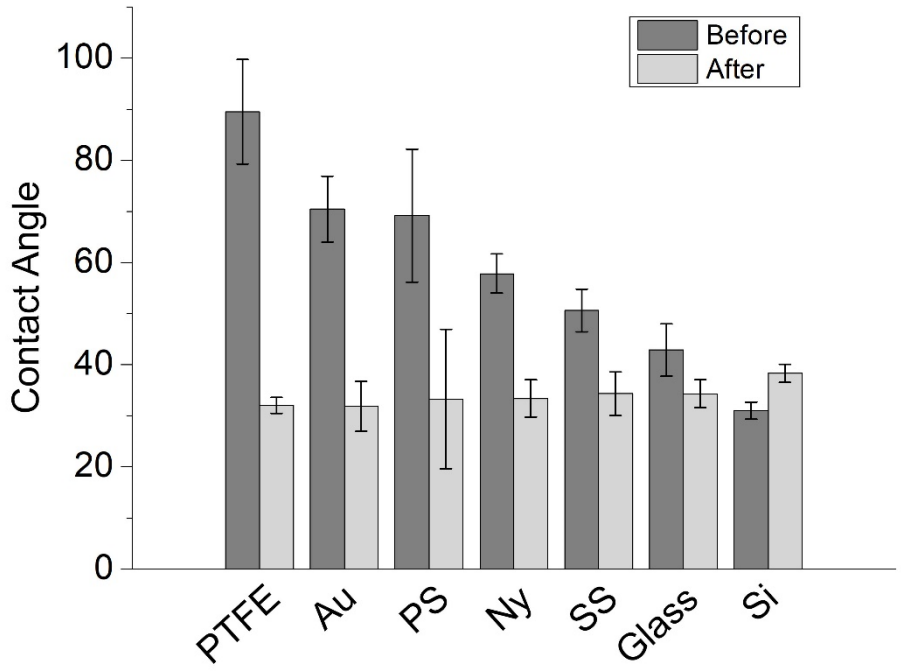


Figure S1. Static water contact angles of solid substrates before and after pCPA coating.

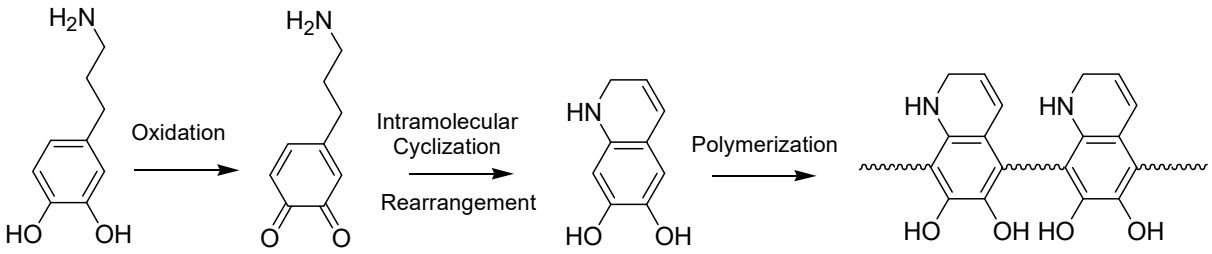


Figure S2. Suggested mechanism of the oxidative polymerization of CPA.

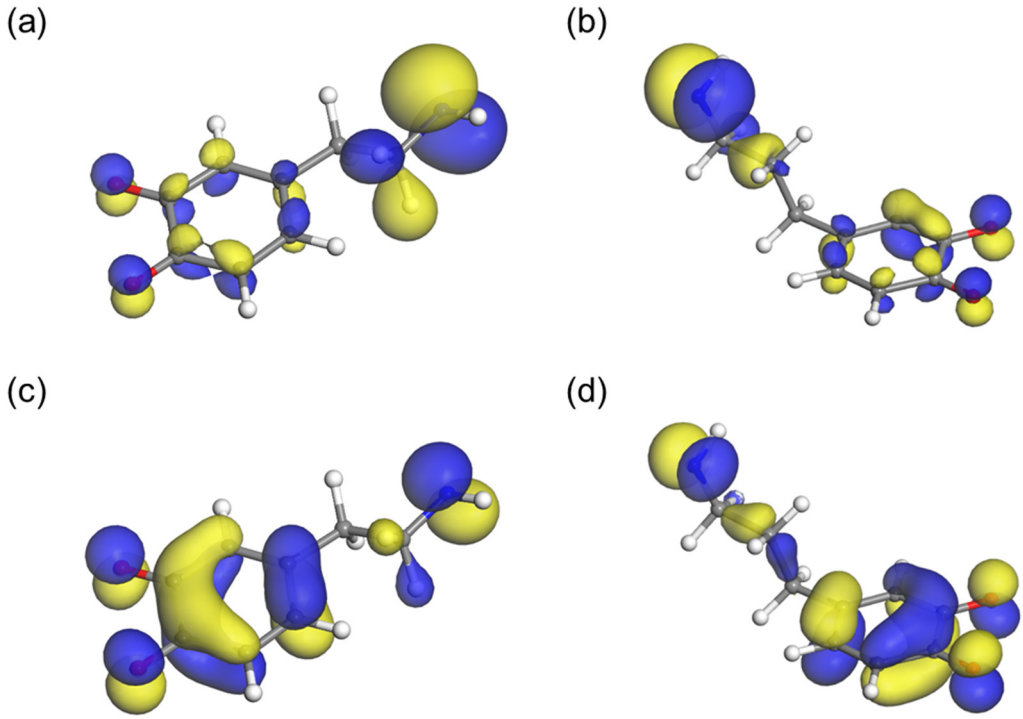


Figure S3. Kohn-Sham orbitals of the optimized structures. HOMO of (a) DA and (b) CPA, LUMO of (c) DA and (d) CPA.

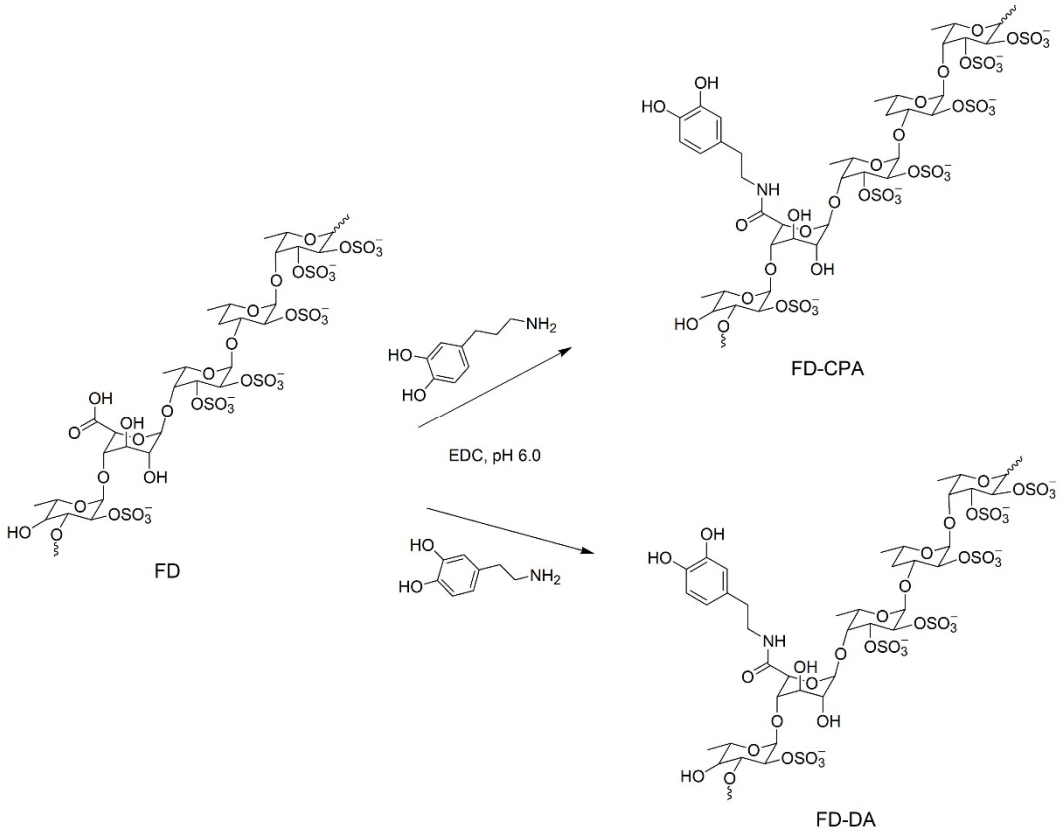


Figure S4. Schematic illustration of the syntheses of FD-DA and FD-CPA.

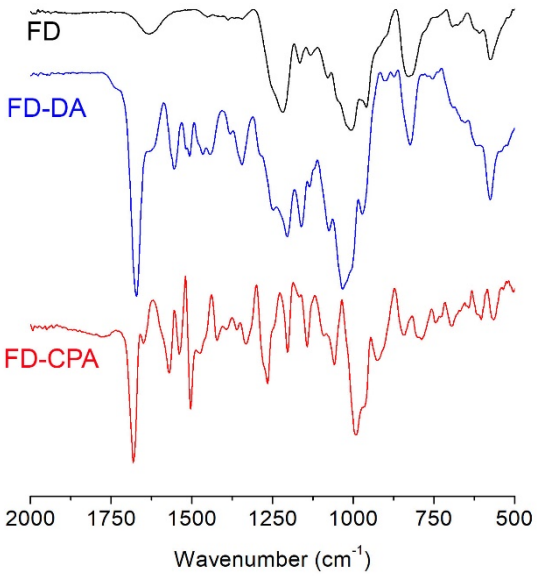


Figure S5. FT-IR spectra of FD, FD-DA, and FD-CPA.

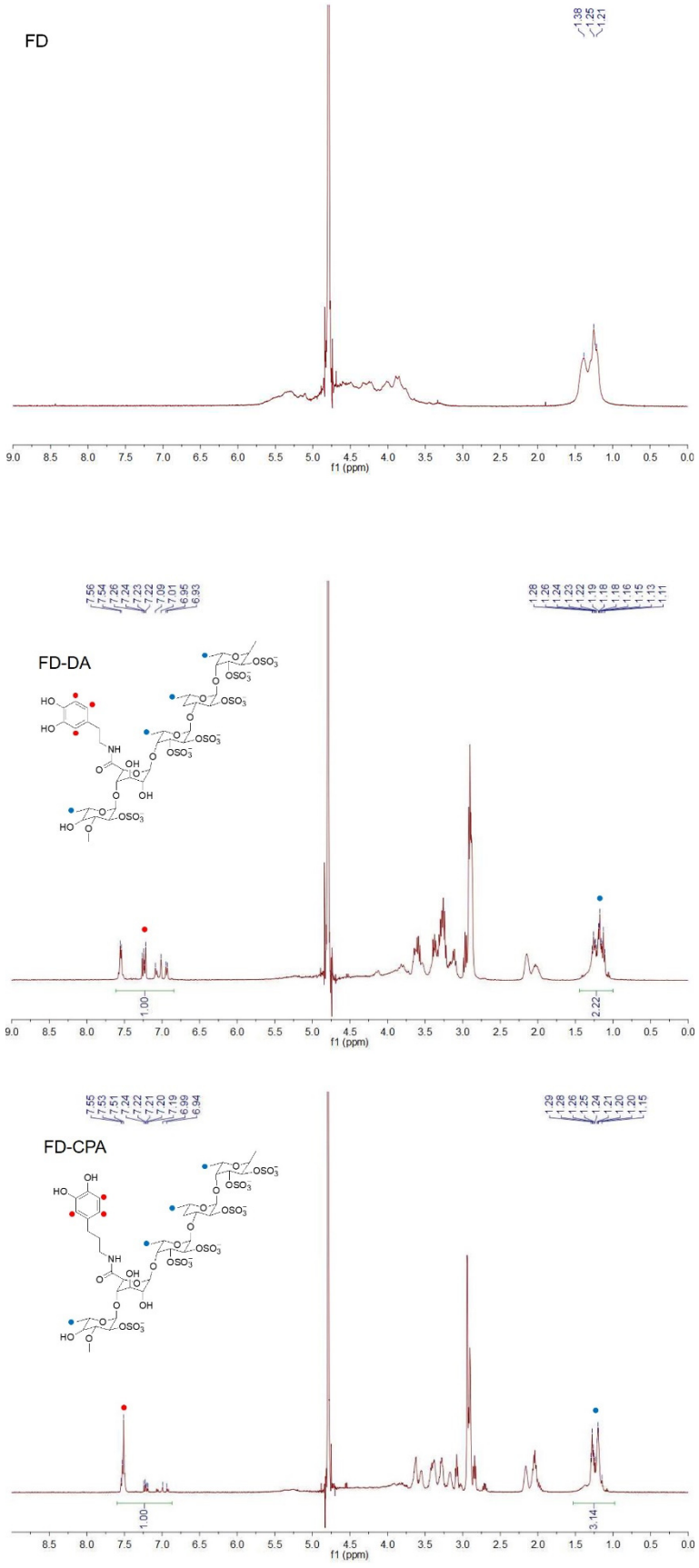
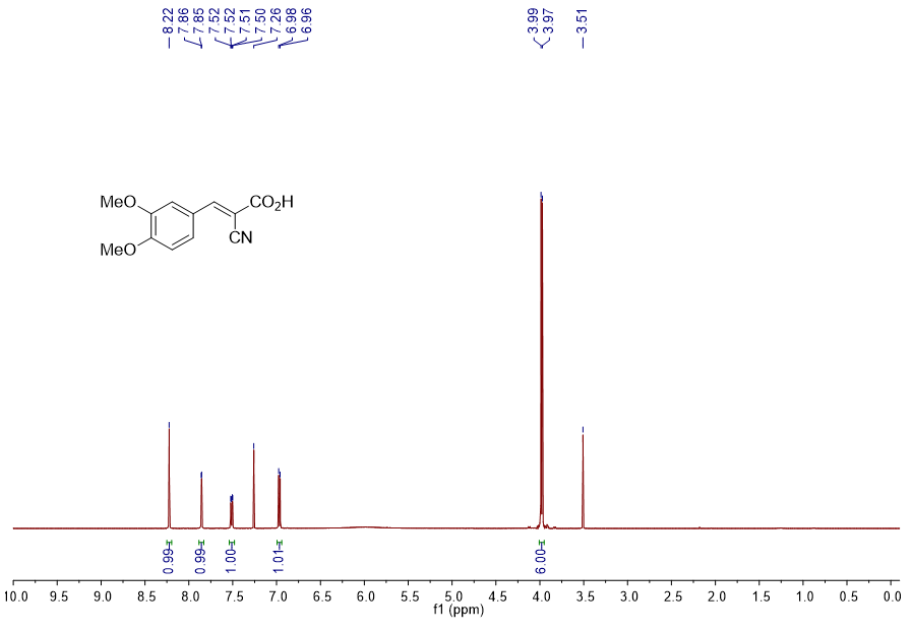
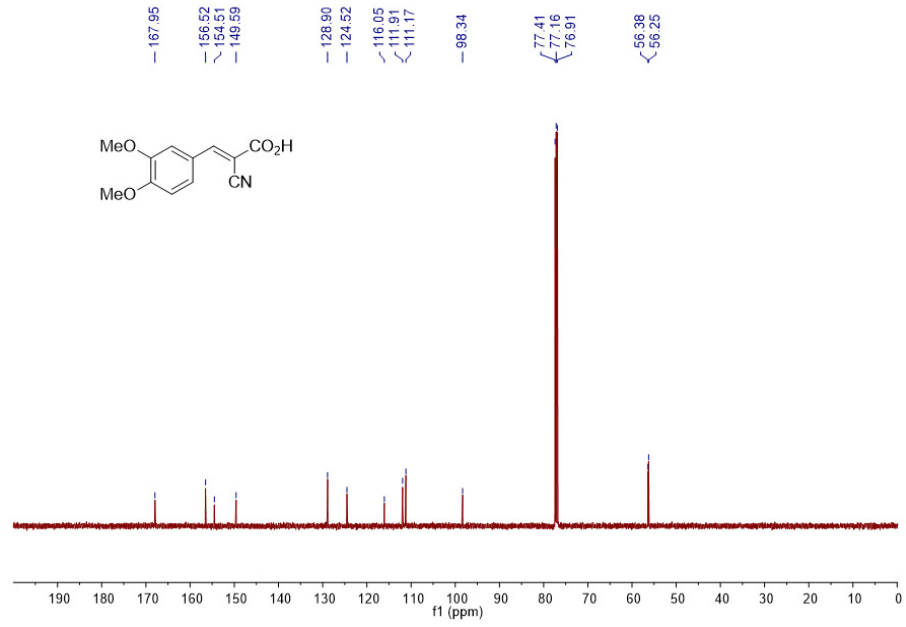


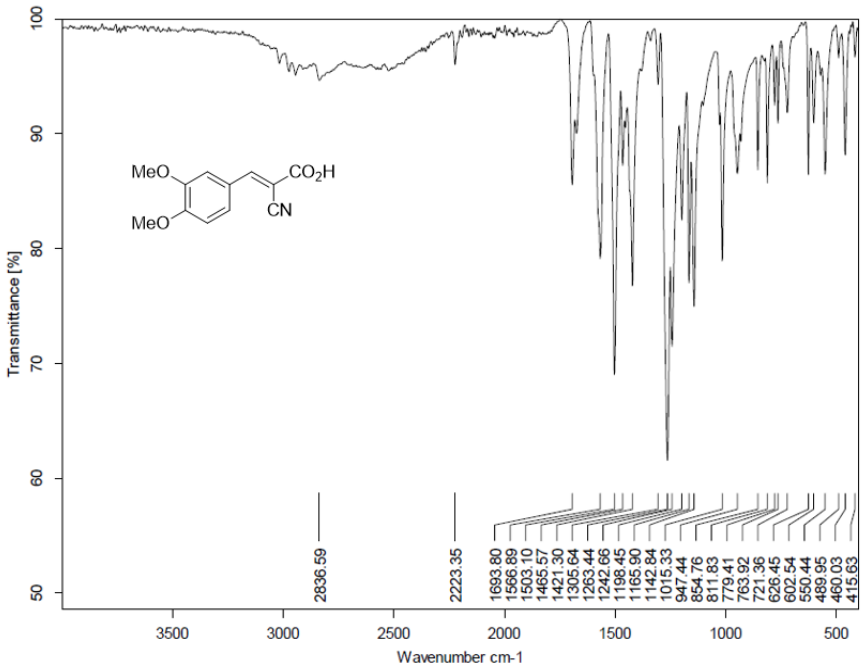
Figure S6. ^{1}H NMR spectra of FD, FD-DA, and FD-CPA.

[Appendix: ^{1}H NMR, ^{13}C NMR, FT-IR]

2-Cyano-3-(3,4-dimethoxyphenyl)acrylic acid (**2**)






Transmittance [%]
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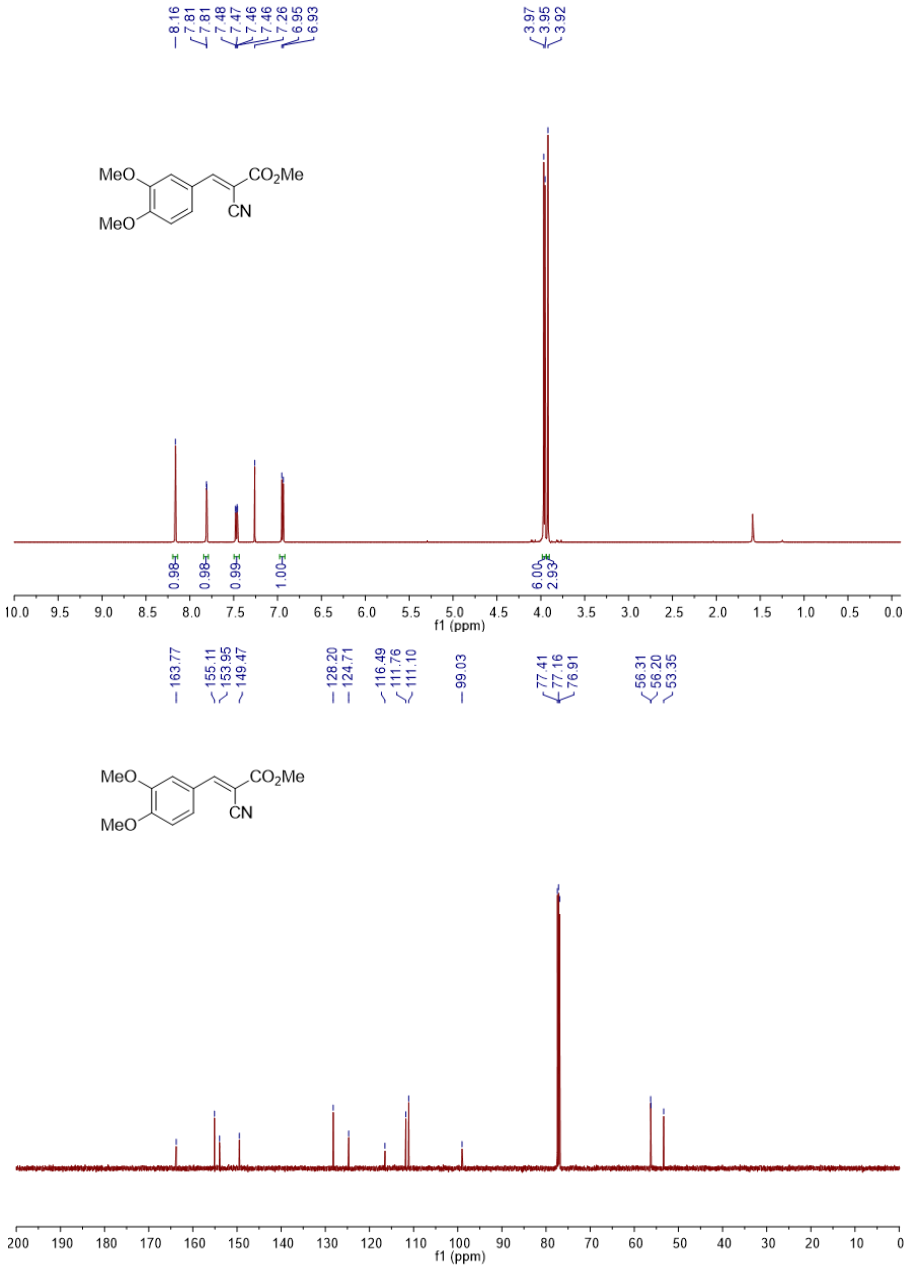
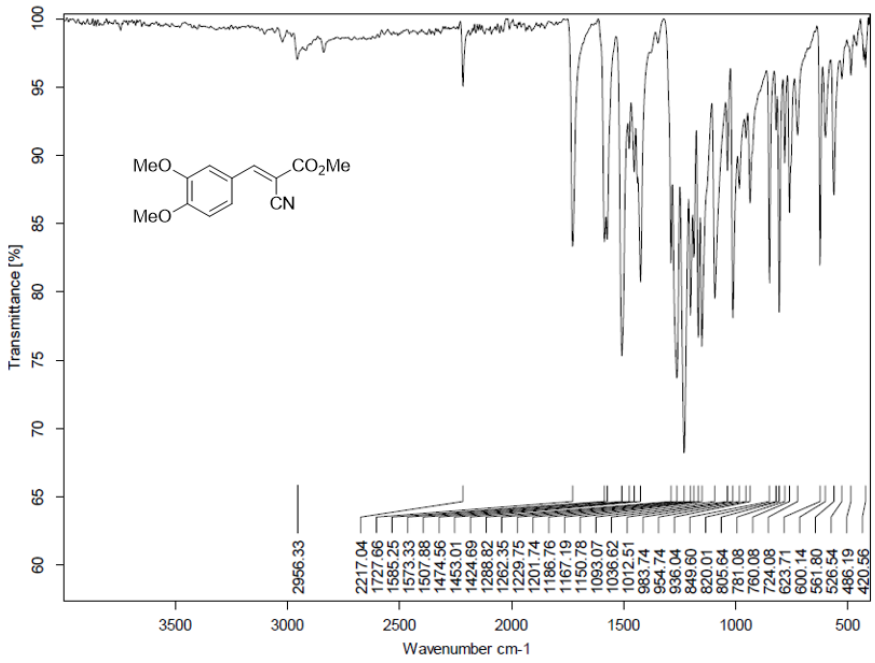
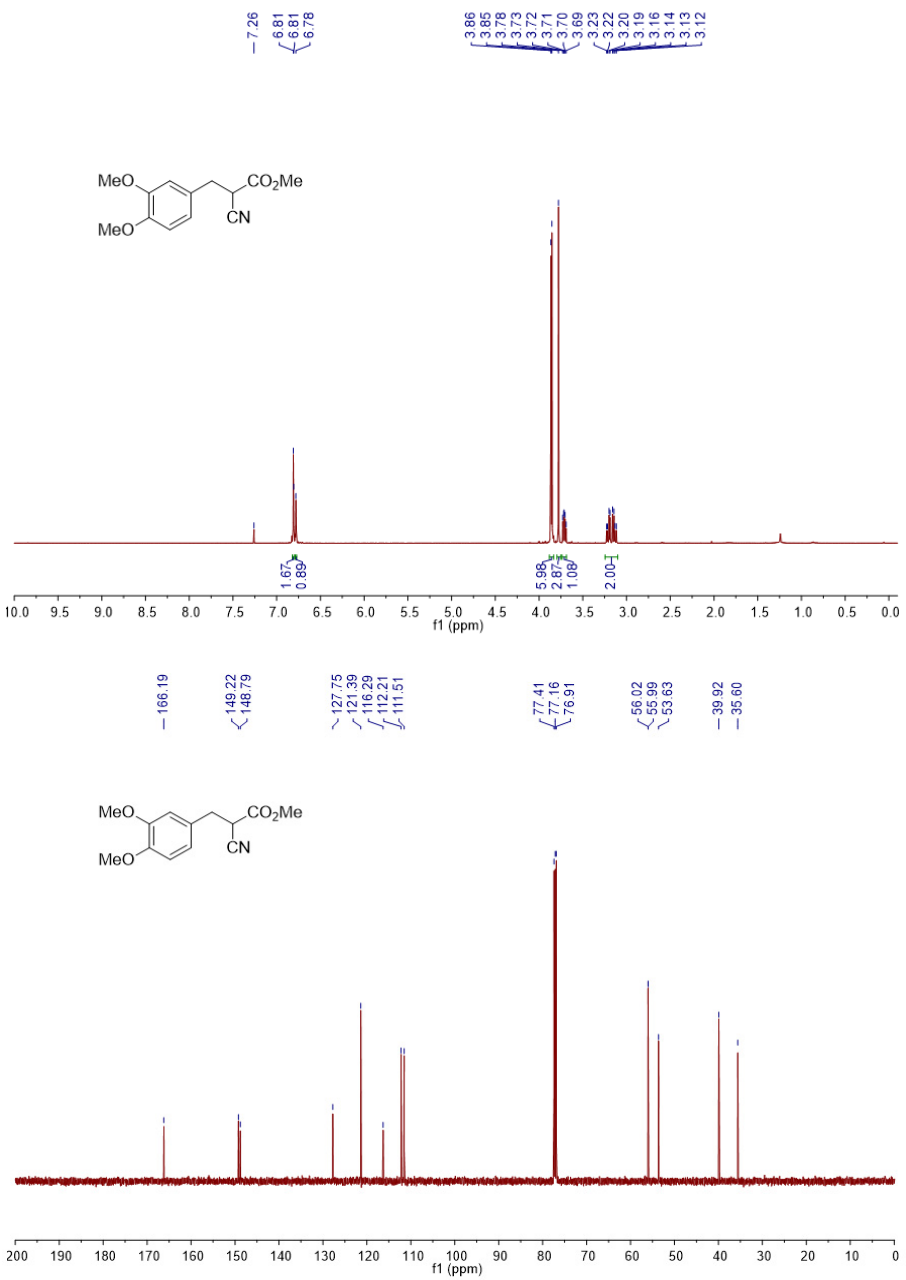
90
80
70
60
50
MeO
MeO
CO2H
CN
2836.59
2223.35
1693.80
1586.89
1503.10
1465.57
1421.30
1305.64
1263.44
1242.66
1198.45
1165.90
1142.84
1015.33
947.44
854.76
811.83
779.41
763.92
721.36
626.45
602.54
550.44
489.95
460.03
415.63
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

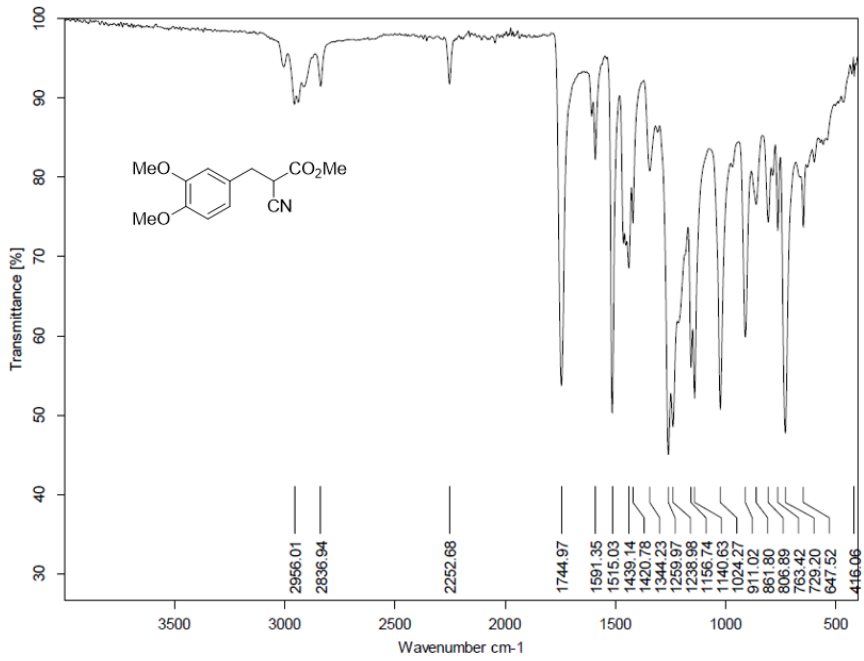
Methyl 2-cyano-3-(3,4-dimethoxyphenyl)acrylate (**3**)




Transmittance [%]
100
95
90
85
80
75
70
65
60
MeO
MeO
CO2Me
CN
2956.33
2217.04
1727.66
1585.25
1573.33
1507.88
1474.56
1453.01
1424.69
1288.82
1262.35
1229.75
1201.74
1186.76
1167.19
1150.78
1093.07
1036.62
1012.51
983.74
954.74
936.04
849.60
820.01
805.64
781.08
760.08
724.08
623.71
600.14
561.80
526.54
496.19
420.56
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Methyl 2-cyano-3-(3,4-dimethoxyphenyl)propanoate (**4**)




Transmittance [%]
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70
60
50
40
30
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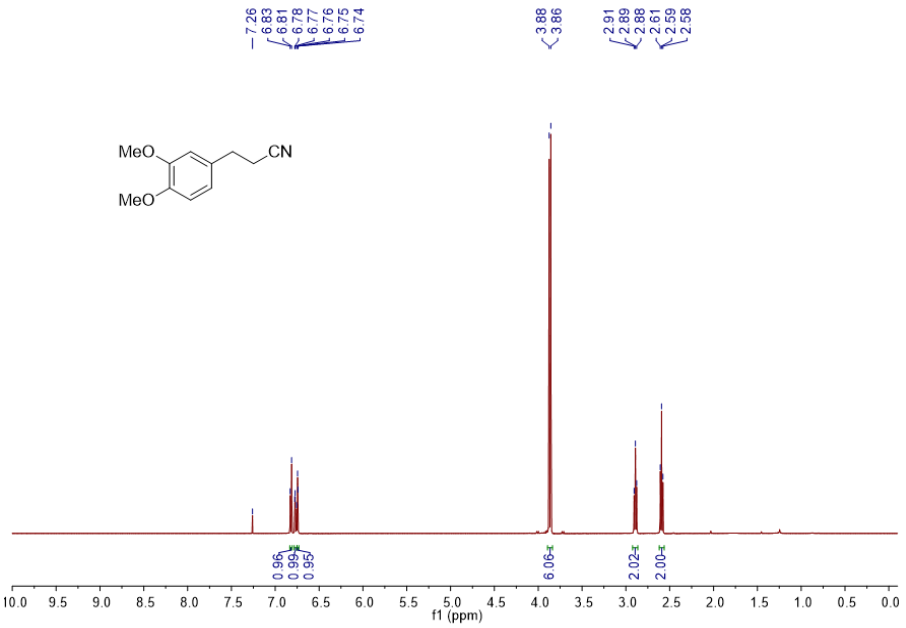
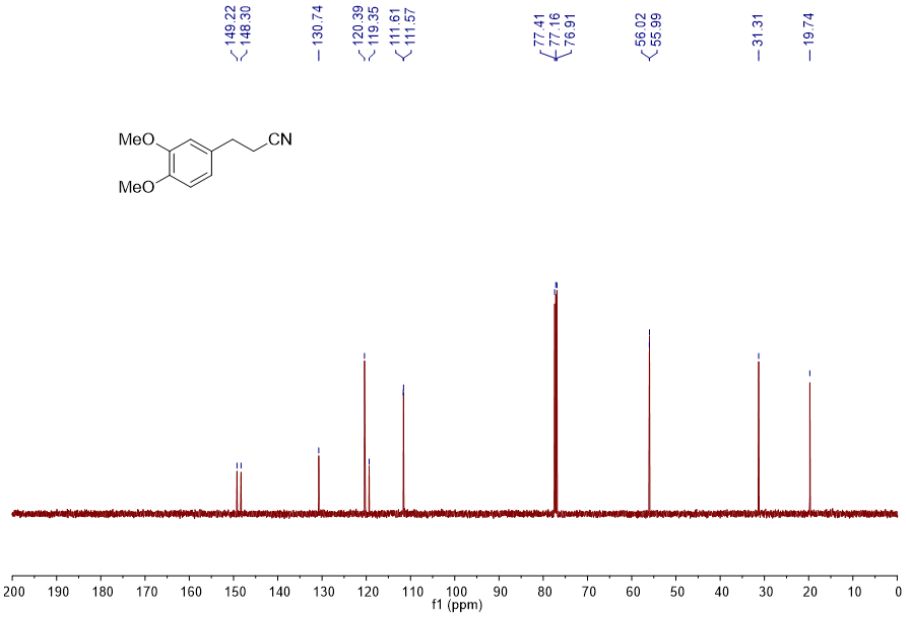
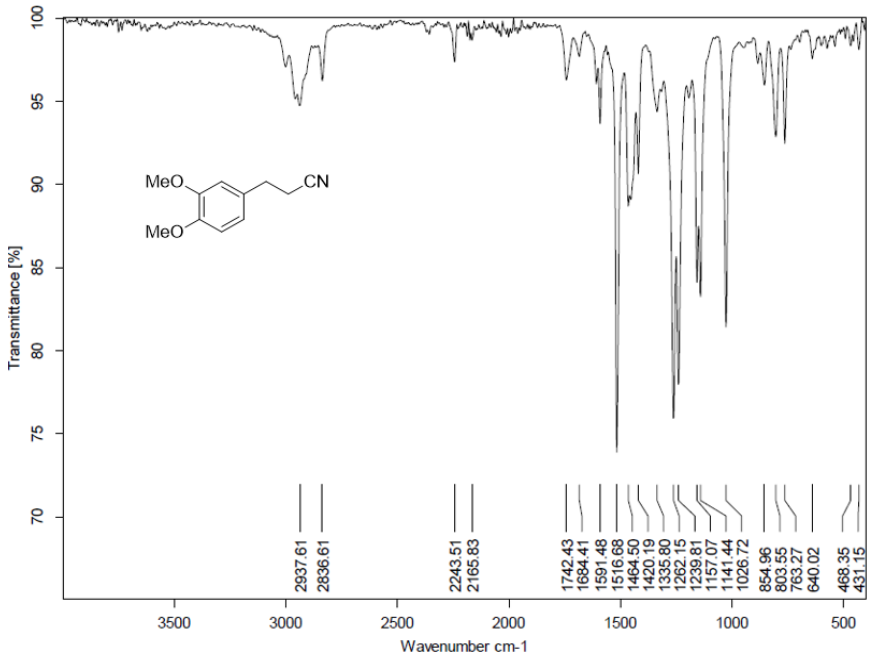
MeO
CO2Me
CN
2956.01
2836.94
2252.68
1744.97
1591.35
1515.03
1439.14
1420.78
1344.23
1259.97
1238.98
1156.74
1140.63
1024.27
911.02
861.80
806.89
763.42
729.20
647.52
416.06
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

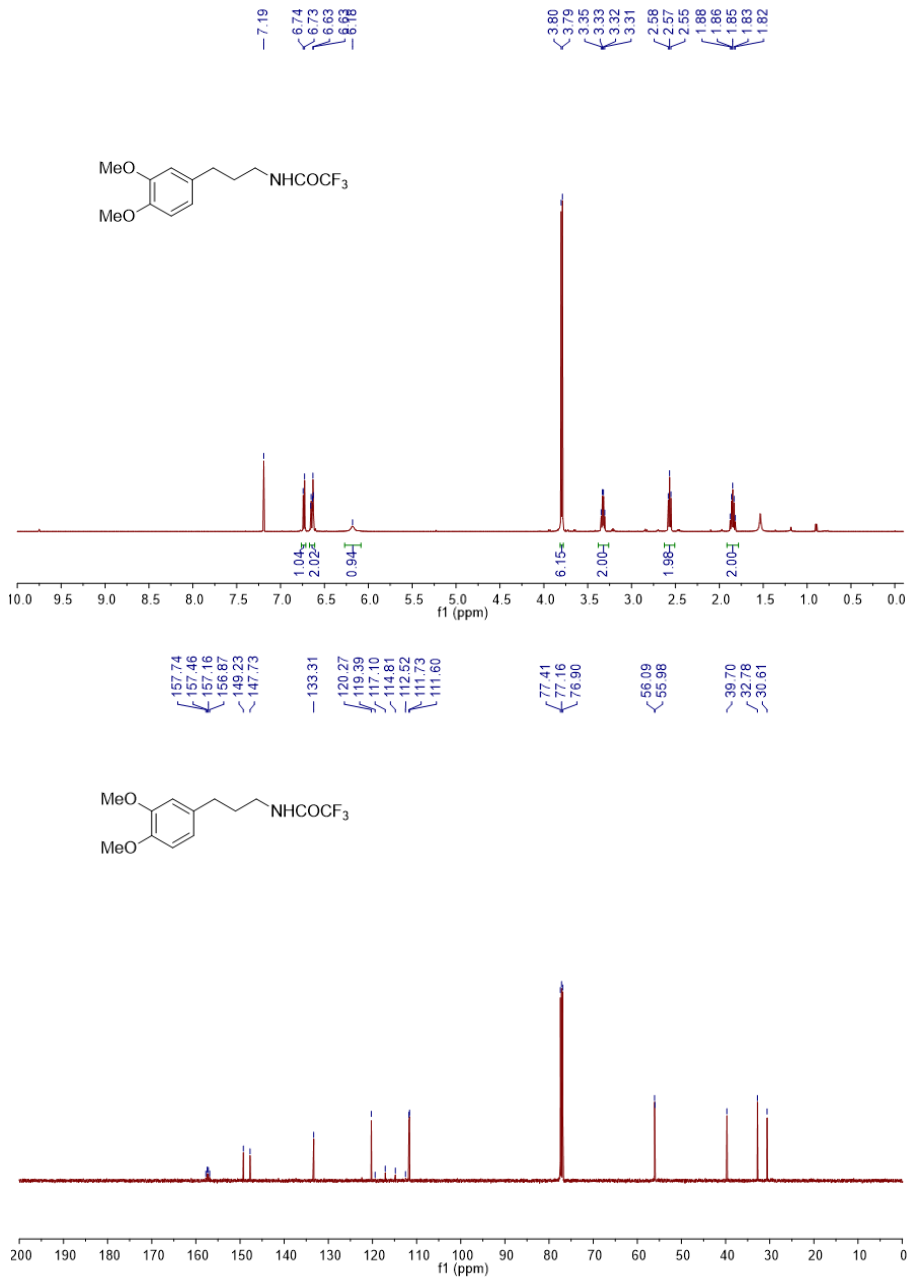
3-(3,4-Dimethoxyphenyl)propanenitrile (**5**)

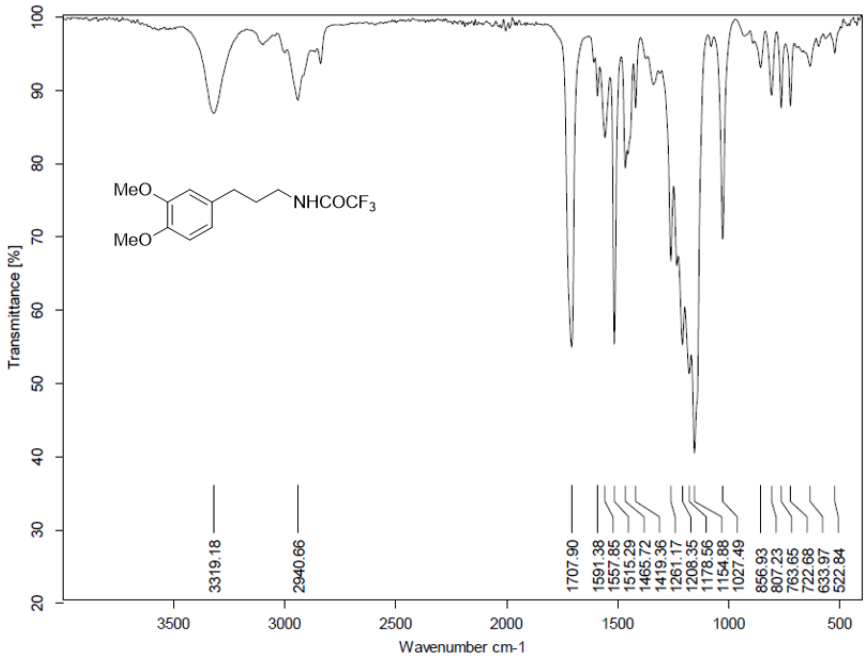





Transmittance [%]
100
95
90
85
80
75
70
MeO
MeO
CN
2937.61
2836.61
2243.51
2165.83
1742.43
1684.41
1591.48
1516.68
1464.50
1420.19
1335.80
1262.15
1239.81
1157.07
1141.44
1026.72
854.96
803.55
763.27
640.02
468.35
431.15
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

N-TFA 3-(3,4-dimethoxyphenyl)propanamine (**6**)




Transmittance [%]
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90
80
70
60
50
40
30
20
MeO
MeO
NHCOCF3
3319.18
2940.66
1707.90
1591.38
1557.85
1515.29
1465.72
1419.36
1261.17
1208.35
1178.56
1154.88
1027.49
856.93
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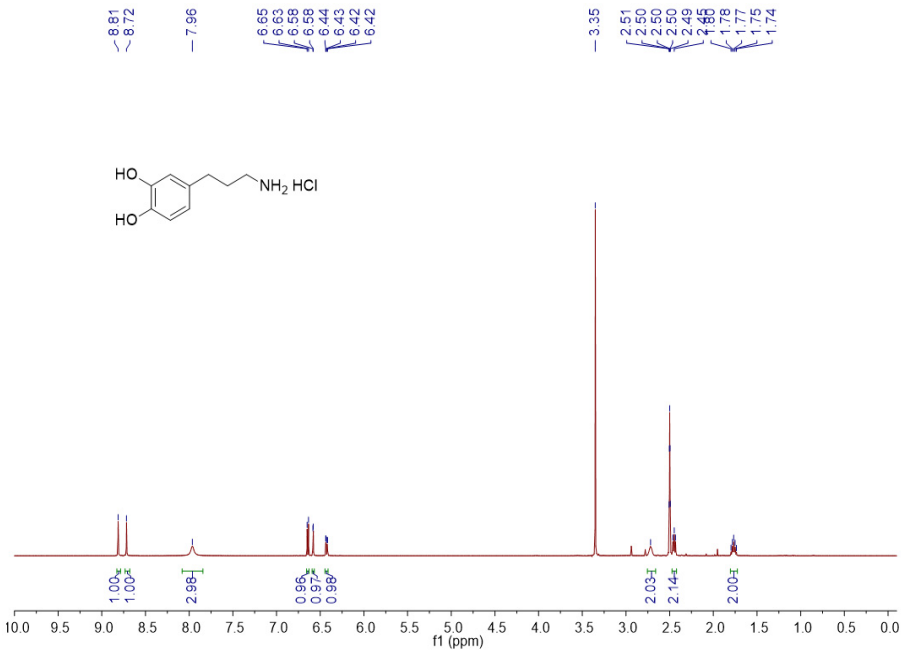
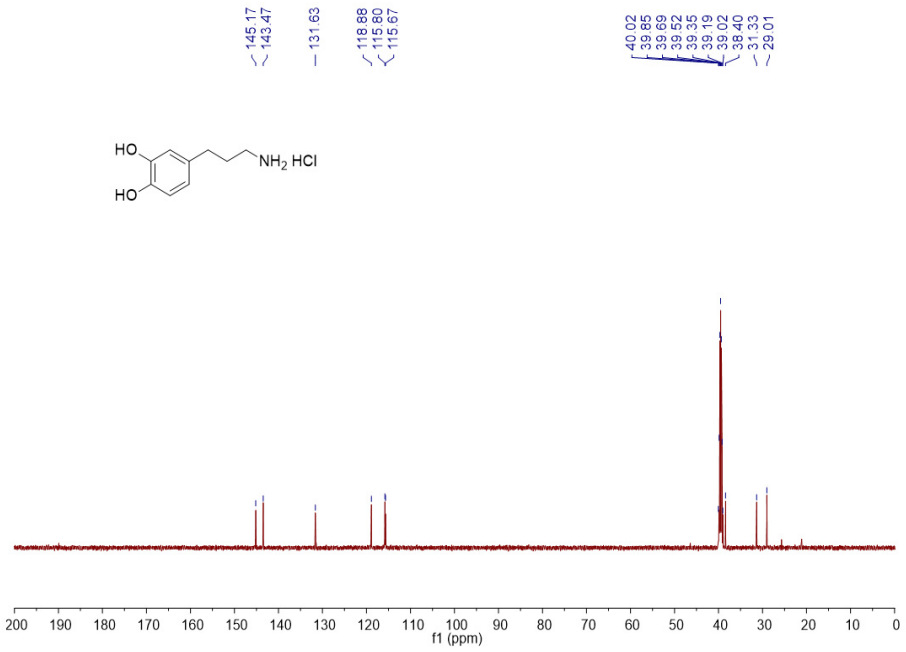
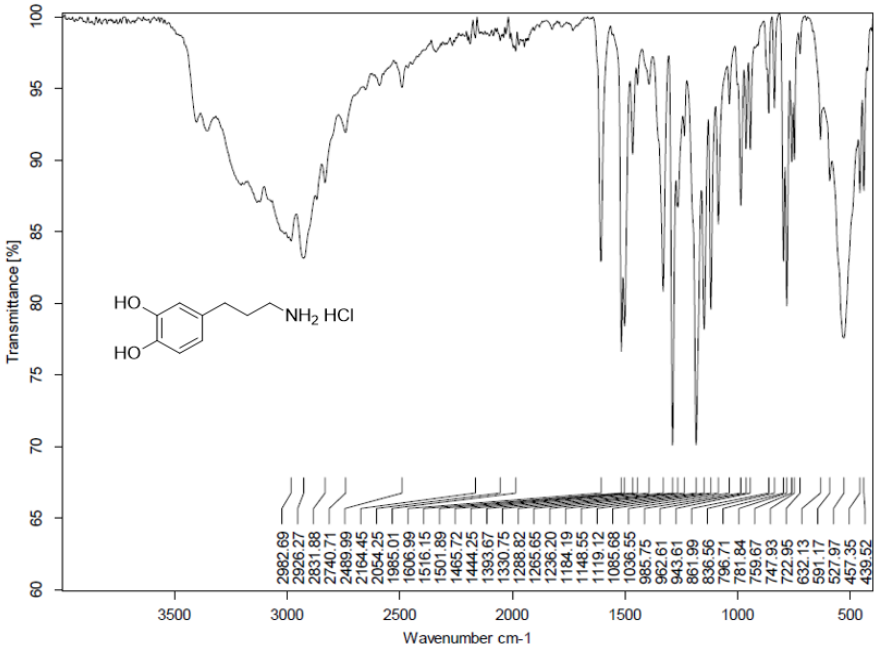
763.65
722.68
633.97
522.84
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

CPA·HCl


8.81
8.72
7.96
6.65
6.63
6.58
6.58
6.44
6.43
6.42
6.42
3.35
2.51
2.50
2.50
2.50
2.49
1.78
1.77
1.75
1.74
HO
HO
NH2 HCl
1.00
1.00
2.98
0.95
0.97
0.98
2.03
2.14
2.00
f1 (ppm)


145.17
143.47
131.63
118.88
115.80
115.67
40.02
39.85
39.69
39.52
39.35
39.19
39.02
38.40
31.33
29.01
HO
HO
NH2 HCl
f1 (ppm)



References

(1) Delley, B. *J. Chem. Phys.* **1990**, 92, 508.
(2) Delley, B. *J. Chem. Phys.* **2000**, 113, 7756.
(3) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648.
(4) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785.
(5) Delley, B. *J. Phys. Chem. A* **2006**, 110, 13632.