

Electronic Supplementary Information

DMSO/I₂ mediated C–C bond cleavage of α -ketoaldehydes followed by C–O bond formation: A metal-free approach for one-pot esterification

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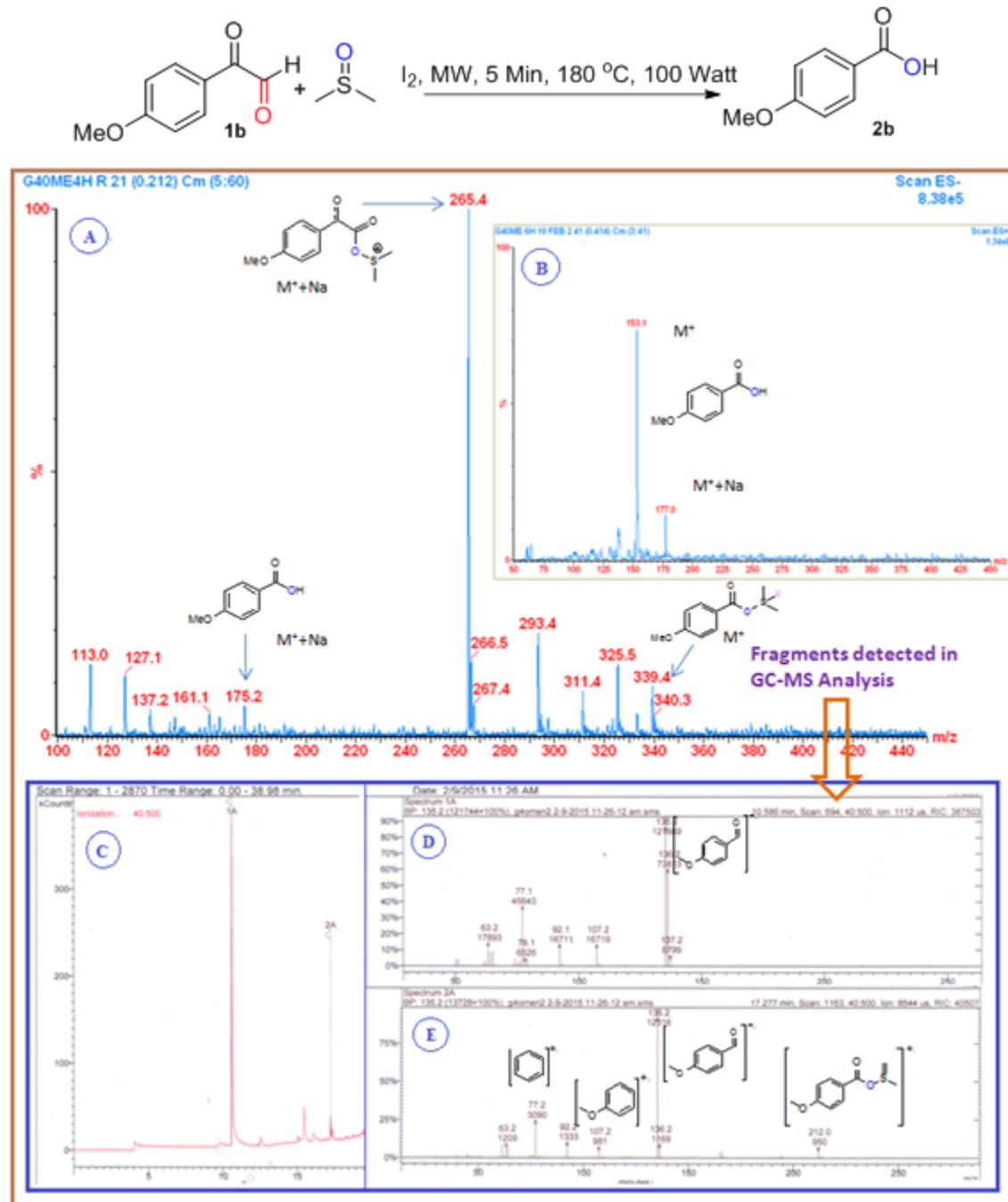
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1.0. Example for formation of carboxylic acid product : Figure showing ESI-MS and GC-MS mass peaks of intermediates and product



2.0. Analytical data:

Benzoic acid (2a)^{1a,b}: ¹H NMR (400 MHz, MeOD): δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H). ¹³C NMR (101 MHz, MeOD): δ 170.1, 134.1, 131.8, 130.8, 129.50. (+) ESI-MS: 145.1 (M⁺ + Na).

2-Bromobenzoic acid (2b)^{1a}: ¹H NMR (400 MHz, MeOD) δ 7.70-7.67 (m, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.33-7.25 (m, 2H). ¹³C NMR (126 MHz, MeOD) δ 169.6, 135.3, 134.5, 133.6, 132.1, 128.4, 122.0. (-) ESI-MS: 199.2 (M⁺ -1).

4-Bromobenzoic acid (2c)^{1a,b,d}: ¹H NMR (400 MHz, MeOD) δ 7.82 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H). ¹³C NMR (126 MHz, MeOD) δ 168.8, 132.8, 132.5, 131.1, 128.8; (-) ESI-MS: 199.2 (M⁺ -1).

3-Nitrobenzoic acid (2d)^{1a}: ¹H NMR (400 MHz, MeOD) δ 8.65 (d, *J* = 1.7 Hz, 1H), 8.36 – 8.31 (m, 1H), 8.26 (d, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H). ¹³C NMR (126 MHz, MeOD) δ 165.9, 148.2, 135.0, 132.4, 129.6, 126.8, 123.8. (-) ESI-MS: 166.1 (M⁺ -1).

3-bromo-4-fluorobenzoic acid (2e)^{1e}: ¹H NMR (400 MHz, CDCl₃): δ 8.34 (m, 1H), 8.07 (m, 1H), 7.23 (m, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -98.11 (td, *J* = 7.2, 5.2 Hz). ¹³C NMR (101 MHz, CDCl₃): δ 170.2, 162.7 (d, *J* = 256.2 Hz), 136.1 (d, *J* = 1.7 Hz), 131.5 (d, *J* = 8.8 Hz), 126.7 (d, *J* = 3.5 Hz), 116.7 (d, *J* = 23.1 Hz), 109.5 (d, *J* = 21.8 Hz); (-) ESI-MS: 216.8 (M⁺ -1).

2,4-dichlorobenzoic acid (2f)^{1b}: ¹H NMR (400 MHz, CDCl₃) δ 7.99 (d, *J* = 8.5 Hz, 1H), 7.53 (d, *J* = 1.9 Hz, 1H), 7.35 (dd, *J* = 8.5, 2.0 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 169.2, 139.5, 136.0, 133.5, 131.4, 127.1. (-) ESI-MS: 189.2 (M⁺ -1).

4-Chlorobenzoic acid (2g)^{1b,d}: ¹H NMR (400 MHz, MeOD) δ 7.89 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 8.6 Hz, 2H). ¹³C NMR (101 MHz, MeOD) δ 168.7, 140.2, 132.3, 129.7. (-) ESI-MS: 155.2 (M⁺ -1)

3-Bromo-4-methoxybenzoic acid (2h)^{1c}: ¹H NMR (400 MHz, MeOD) δ 8.05 (d, *J* = 2.1 Hz, 1H), 7.90 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 1H), 3.85 (s, 3H). ¹³C NMR (126 MHz, MeOD): δ 168.4, 161.0, 135.7, 132.0, 125.4, 112.5, 112.1, 57.0; (-) ESI-MS: 228.9 (M⁺ -1).

3,4-Dimethylbenzoic acid (2i)^{1d}: ¹H NMR (400 MHz, CDCl₃) δ 7.93 – 7.81 (m, 2H), 7.28 – 7.18 (m, 1H), 2.33 (d, *J* = 4.5 Hz, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 172.7, 143.3, 136.8, 131.2, 129.8, 127.8, 126.9, 20.1, 19.67; (-) ESI-MS: 148.8 (M⁺ -1).

4-Fluorobenzoic acid (2j)^{1d}: ¹H NMR (400 MHz, CDCl₃) δ 8.16 – 8.13 (m, 2H), 7.15 (t, *J* = 8.0 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 168.7, 168.4, 165.9, 138.5, 133.4, 128.4, 116.5; (-) ESI-MS: 139.0 (M⁺ -1).

4-Nitrobenzoic acid (2k)^{1a,b}: ¹H NMR (400 MHz, MeOD) δ 8.23 (d, *J* = 8.8 Hz, 2H), 8.13 (d, *J* = 8.8 Hz, 2H). ¹³C NMR (126 MHz, MeOD) δ 167.6, 151.9, 137.6, 131.9, 124.5. (-) ESI-MS: 166.2 (M⁺ -1).

4-Methylbenzoic acid (2l)^{1a,b}: ¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 8.1 Hz, 2H), 7.27 (t, *J* = 8.1 Hz, 2H), 2.46 (s, 3H). ¹³C NMR (101 MHz, MeOD) δ 170.0, 145.0, 130.8, 130.1, 129.1, 21.6; (+) ESI-MS: 137.4 (M⁺ + 1).

4-Phenylbenzoic acid (2m)^{1d}: ¹H NMR (500 MHz, MeOD) δ 7.99 (dt, *J* = 8.4, 1.8 Hz, 2H), 7.65 – 7.60 (m, 2H), 7.59 – 7.55 (m, 2H), 7.38–7.35 (m, 2H), 7.31 – 7.26 (m, 1H). ¹³C NMR (126 MHz, MeOD) δ 169.7, 147.0, 141.2, 131.3, 130.6, 130.0, 129.2, 128.2, 128.0. (-) ESI-MS: 197.3 (M⁺ -1).

3,4,5-Trimethoxybenzoic acid (2n)^{1e}: ¹H NMR (400 MHz, CDCl₃) δ 7.38 (s, 2H), 3.94 (s, 3H), 3.93 (s, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 171.4, 152.9, 142.9, 124.1, 107.3, 60.9, 56.2. (-) ESI-MS: 211.2 (M⁺ -1).

4-methoxybenzoic acid (2o)^{1a,b}: ¹H NMR (500 MHz, MeOD) δ 7.87 (d, *J* = 8.9 Hz, 2H), 6.87 (d, *J* = 8.9 Hz, 2H), 3.75 (s, 3H). ¹³C NMR (126 MHz, MeOD): δ 169.8, 165.0, 132.8, 124.0, 114.6, 55.9. (-) ESI-MS: 151.2(M⁺-1)

4-methoxy-2-methylbenzoic acid (2p)^{1c}: ¹H NMR (400 MHz, DMSO-d₆) δ 7.84 (d, *J*=8.3Hz, 1H), 6.84 (s,1H), 6.82 (s, 1H), 3.79 (s, 3H), 2.52 (s, 3H).¹³CMR (126MHz, DMSO-d₆) δ 168.0, 161.7, 142.1, 132.7, 122.0, 116.6, 111.1, 55.2, 21.8, (+) ESI-MS: 163.3 (M⁺+1).

4-(tert-butyl)benzoic acid^{1a} (2q): ¹H NMR (400 MHz, CDCl₃): δ 8.04 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 1.35 (s, 9H). ¹³C NMR (126 MHz, CDCl₃): δ 172.4, 150.2, 130.1, 129.1, 125.6, 40.6, 31.3. (-) ESI-MS: 177.2 (M⁺ -1).

4-bromo-3-chlorobenzoic acid¹¹ (2r): ¹H NMR (400 MHz, CDCl₃): δ 7.99-7.96 (t, 1H), 7.65-7.62 (m, 1H), 7.42-7.41 (d, *J* = 4 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃): δ 167.4, 136.5, 134.9, 134.0, 133.7, 133.5, 121.1. (-) ESI-MS: 232.9 (M⁺ -1).

3-chlorobenzoic acid^{1b} (2s): ¹H NMR (400 MHz, CDCl₃): δ 8.09 (s, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 1H). ¹³C NMR (101 MHz, MeOD): δ 168.4, 135.5, 133.9, 131.2, 130.5, 129.0.

Nicotinic acid^{1g} (3a): ¹H NMR (400 MHz, MeOD) δ 9.02 (s, 1H), 8.64 (d, *J* = 3.6 Hz, 1H), 8.32 (dt, *J* = 7.9, 1.8 Hz, 1H), 7.48 (dd, *J* = 7.7, 5.1 Hz, 1H); ¹³C NMR (101 MHz, MeOD) δ 167.7, 153.6, 151.2, 139.3, 128.7, 125.3. (+) ESI-MS: 124.2 (M⁺ +1).

5-methylthiophene-2-carboxylic acid^{1h} (3b): ¹H NMR (500 MHz, CDCl₃) δ 7.71 (d, *J* = 2.6 Hz, 1H), 6.81 (s, 1H), 2.55 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 147.7, 133.4, 128.0, 124.6, 13.7. (+) ESI-MS: 143.1 (M⁺ +1).

4-Phenoxybenzoic acid^{1c} (3c): ¹H NMR (400 MHz, CDCl₃): δ 8.08 (d, *J* = 8.8 Hz, 2H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H). ¹³C NMR (126 MHz, MeOD): δ 169.3, 163.4, 157.09, 133.0, 131.2, 126.1, 125.7, 121.2, 118.2.

Benzofuran-2carboxylic acid^{1c} (3d): ¹H NMR (500 MHz, MeOD): δ 7.72 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 4.2 Hz, 2H), 7.48 – 7.44 (m, 1H), 7.31 (t, *J* = 7.5 Hz, 1H). ¹³C NMR (126 MHz, MeOD): δ 161.0, 155.7, 146.0, 127.3, 127.1, 123.5, 122.6, 113.4, 111.5. ESI-MS: 163.2 (M⁺+H).

2-Furaic acid^{1j} (3e): ¹H NMR (500 MHz, CDCl₃): δ 10.92 (s, 1H), 7.65 (d, *J* = 21.1 Hz, 1H), 7.34 (dd, *J* = 22.5, 3.4 Hz, 1H), 6.59 – 6.54 (m, 1H). ¹³C NMR (126 MHz, CDCl₃): δ 163.8, 147.5, 143.8, 120.2, 112.3. (+) ESI-MS: 113.2 (M⁺ +1).

Methyl benzoate^{2a} (4a): ¹H NMR (400 MHz, CDCl₃) δ 8.09 – 7.99 (m, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 2H), 3.99 (s, 3H); GC-MS:136.1 (M⁺).

Methyl 4-methoxybenzoate^{2a} (4b): ¹H NMR (400 MHz, CDCl₃ + CD₃OD) δ 8.00 (d, *J* = 8.7 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H), 3.86 (s, 3H).

Methyl 2-fluorobenzoate^{2b} (4c): ¹H NMR (400 MHz, CDCl₃) δ 7.94 (td, *J* = 7.6, 1.8 Hz, 1H), 7.55 – 7.46 (m, 1H), 7.24 – 7.07 (m, 2H), 3.93 (s, 3H); GC-MS:154.0 (M⁺).

Methyl 4-aminobenzoate^{2a} (4d): ¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 8.6 Hz, 2H), 6.62 (d, *J* = 8.6 Hz, 2H), 4.15 (s, 2H), 3.84 (s, 3H); GC-MS:151.1 (M⁺). ¹³C NMR (126 MHz, CDCl₃): δ 167.28, 151.02, 131.61, 119.52, 113.79, 51.64.

Methyl 5-methylthiophene-2-carboxylate^{2c} (4e): ¹H NMR (400 MHz, CDCl₃) δ 7.61 (d, *J* = 3.7 Hz, 1H), 6.76 (dd, *J* = 3.7, 0.9 Hz, 1H), 3.86 (s, 3H), 2.52 (s, 3H).

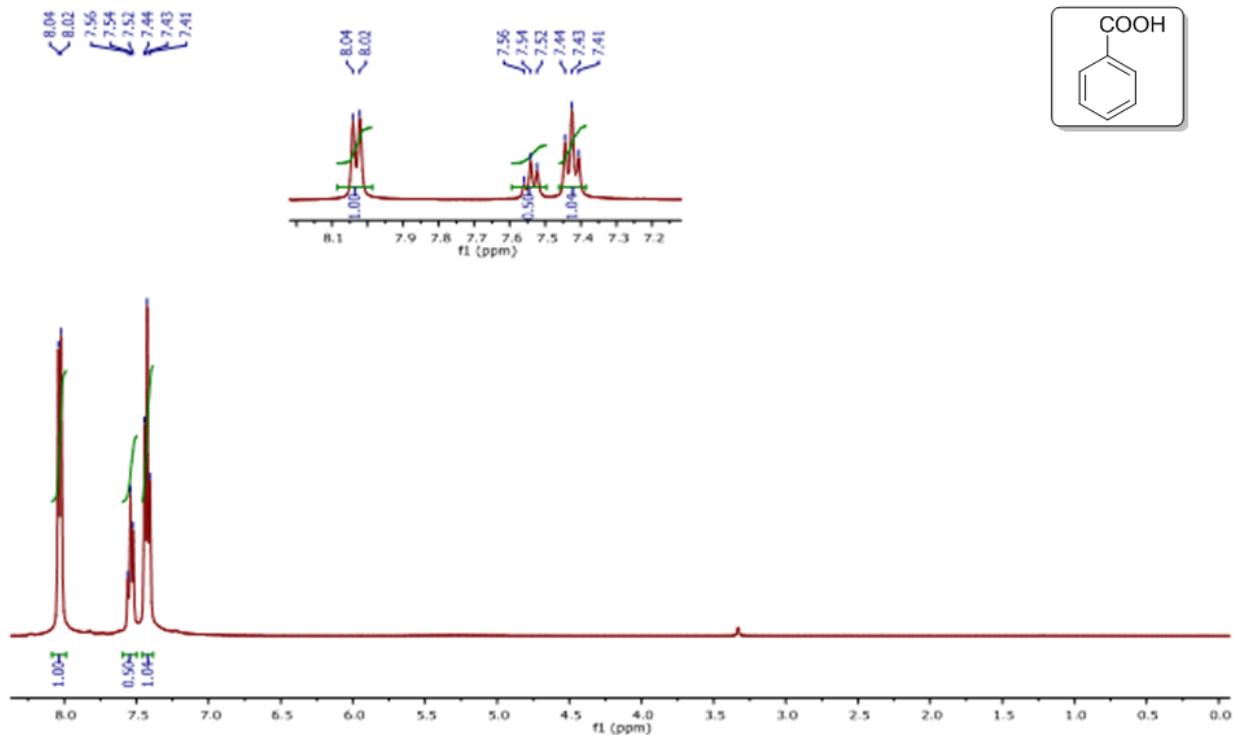
Ethyl benzofuran-2-carboxylate^{2d} (4f): ¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 7.9 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.52 (s, 1H), 7.46 – 7.39 (m, 1H), 7.29 (dd, *J* = 13.2, 6.0 Hz, 1H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H).

Dihydro β -Ionic Acid ^{2e}(5a): ¹H NMR (400 MHz, CDCl₃): δ 2.43 – 2.39 (m, 2H), 2.37 – 2.34 (m, 2H), 1.93–1.89 (t, J = 6.2 Hz, 2H), 1.61 (s, 3H), 1.61 – 1.55 (m, 2H), 1.44 – 1.41 (m, 2H), 1.00 (s, 6H). ¹³C NMR (101 MHz, CDCl₃): δ 180.3, 135.4, 128.5, 39.7, 34.9, 34.7, 32.7, 28.3, 23.5, 19.65, 19.4. HRMS (+ESI, *m/z*) calc for C₁₂H₂₀O₂ (M⁺) 196.1458, found (M+H⁺) 197.1530

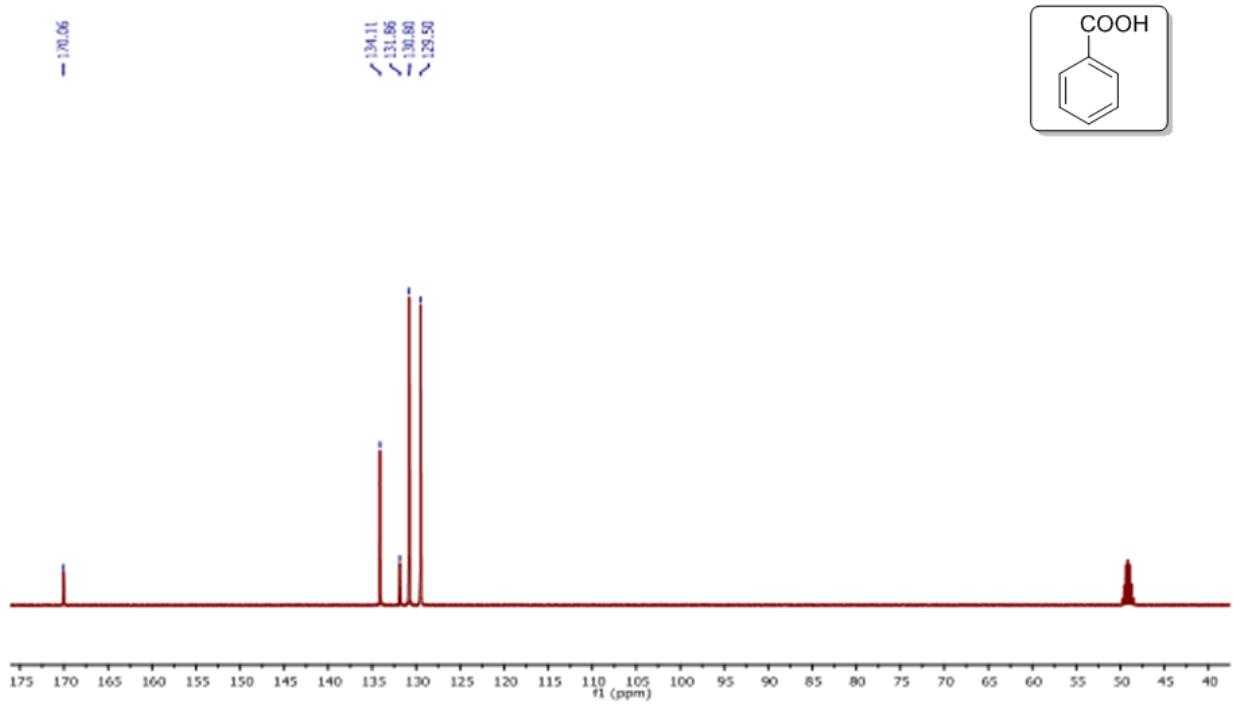
2.0. Scanned Spectra

Benzoic Acid (2a):

^1H NMR

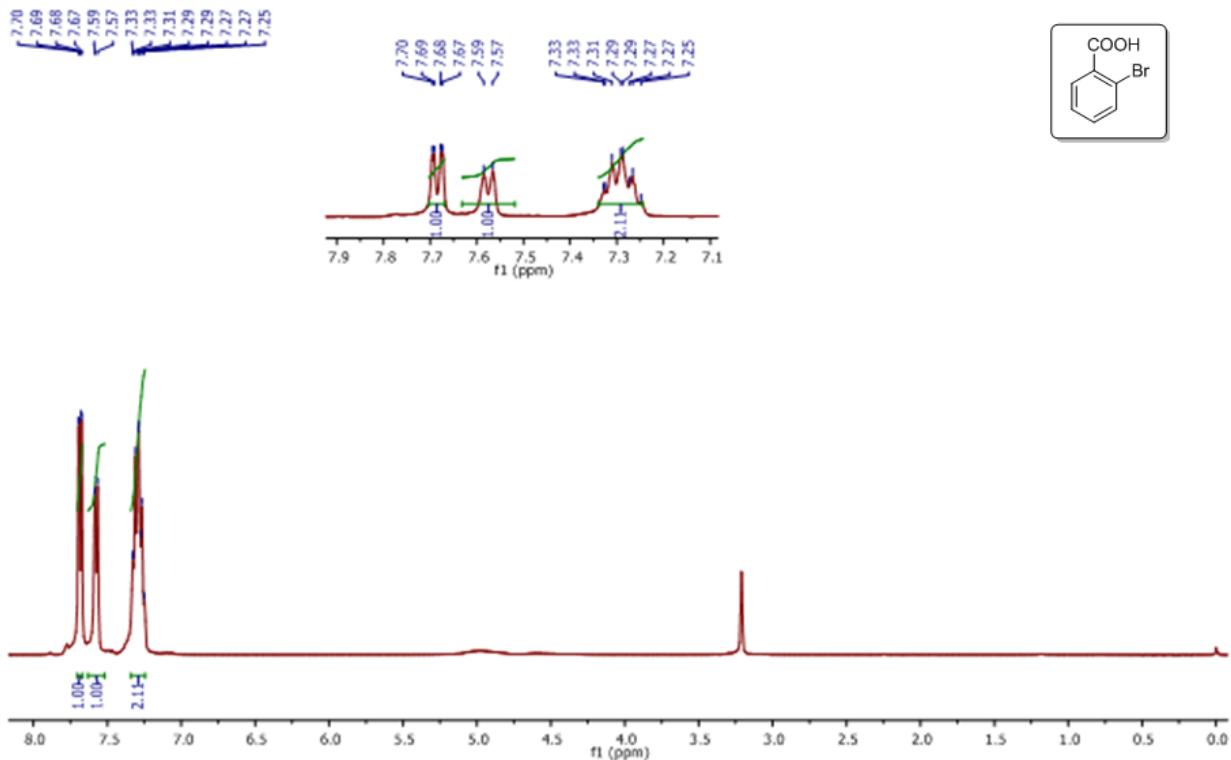


^{13}C NMR

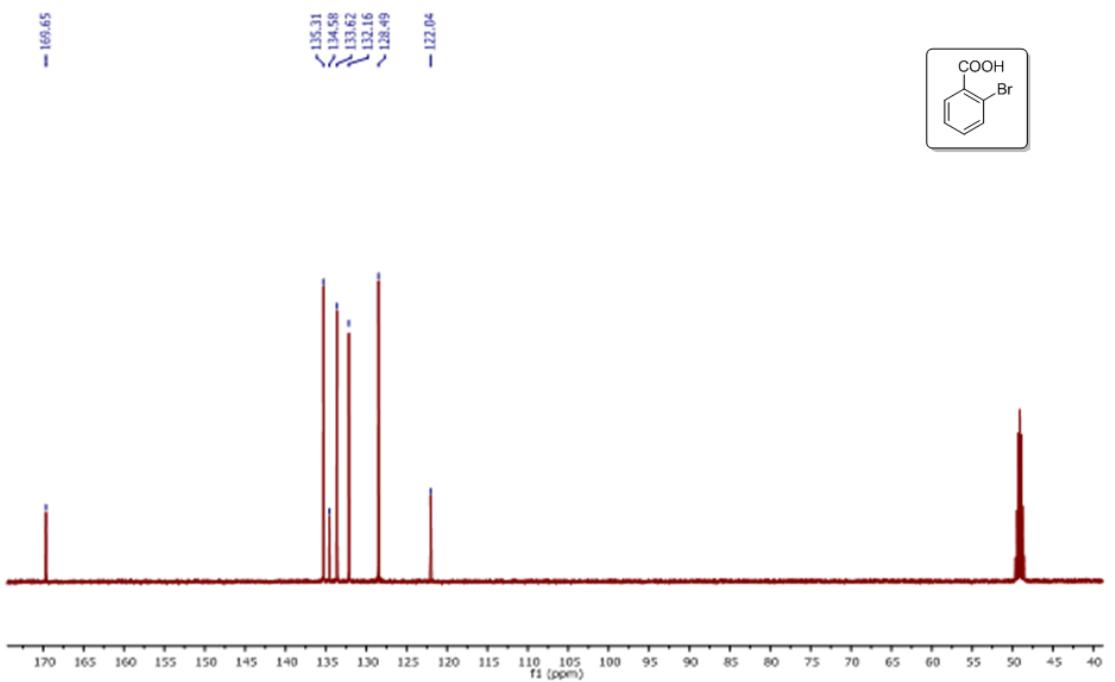


2-Bromobenzoic acid (2b):

¹H NMR

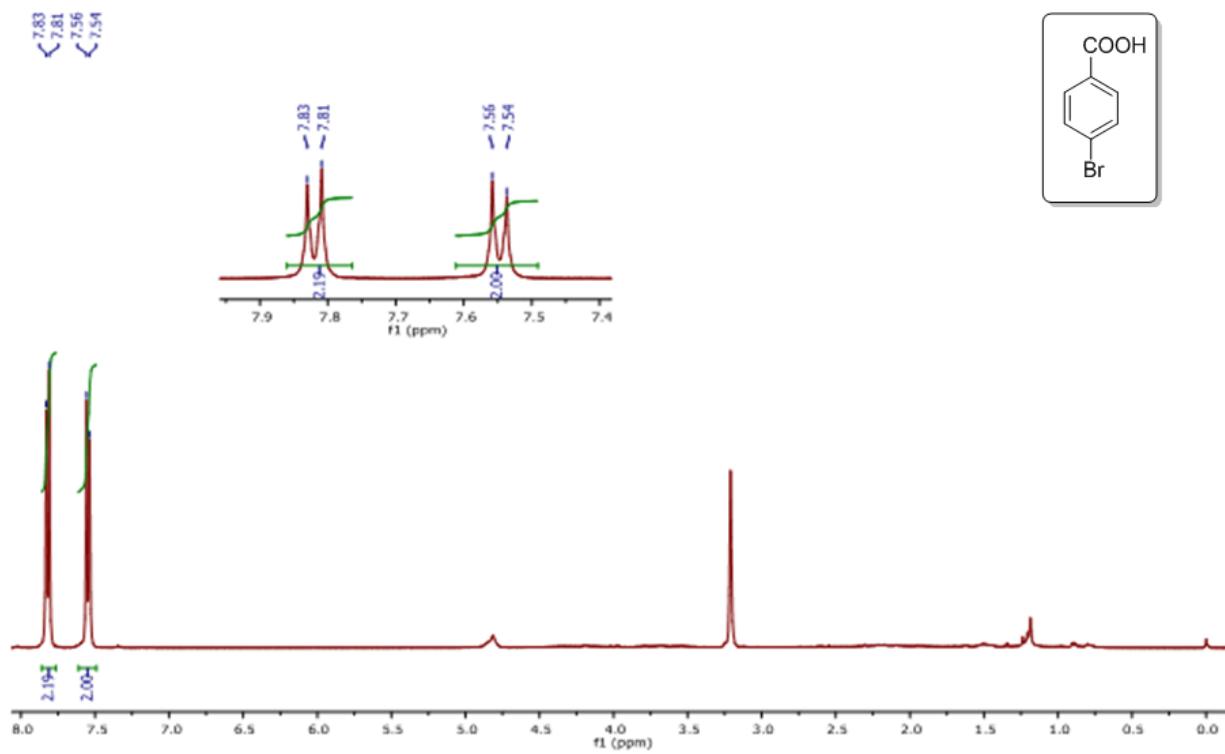


¹³C NMR

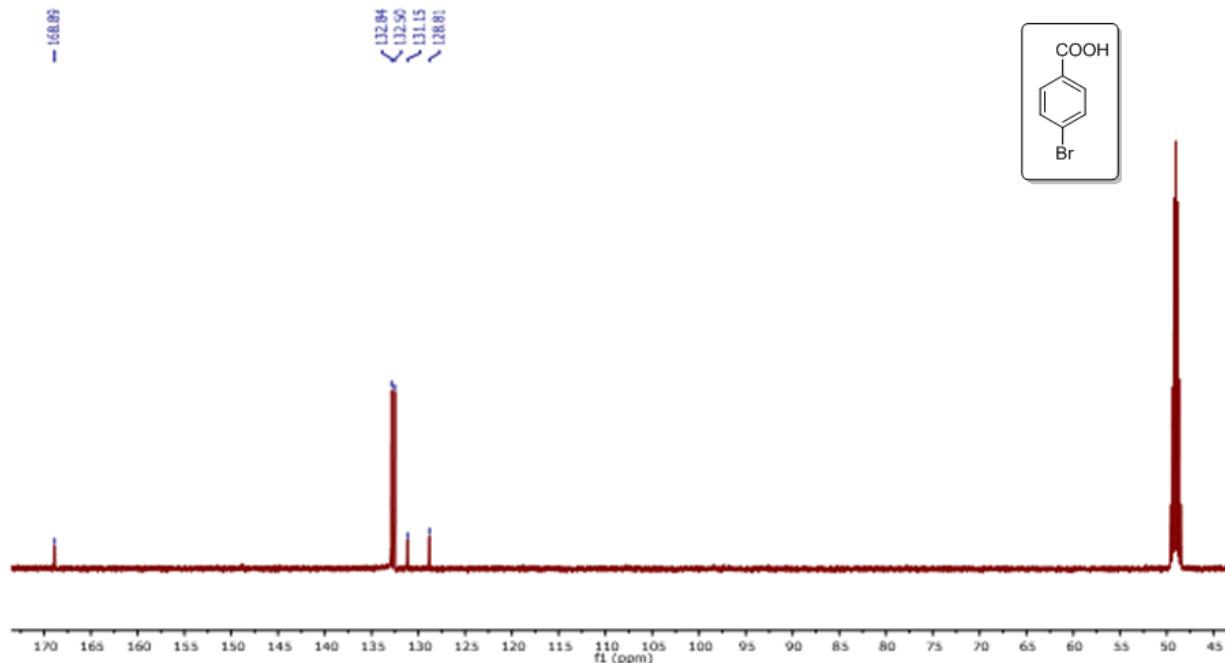


4-Bromobenzoic acid (2c):

^1H NMR

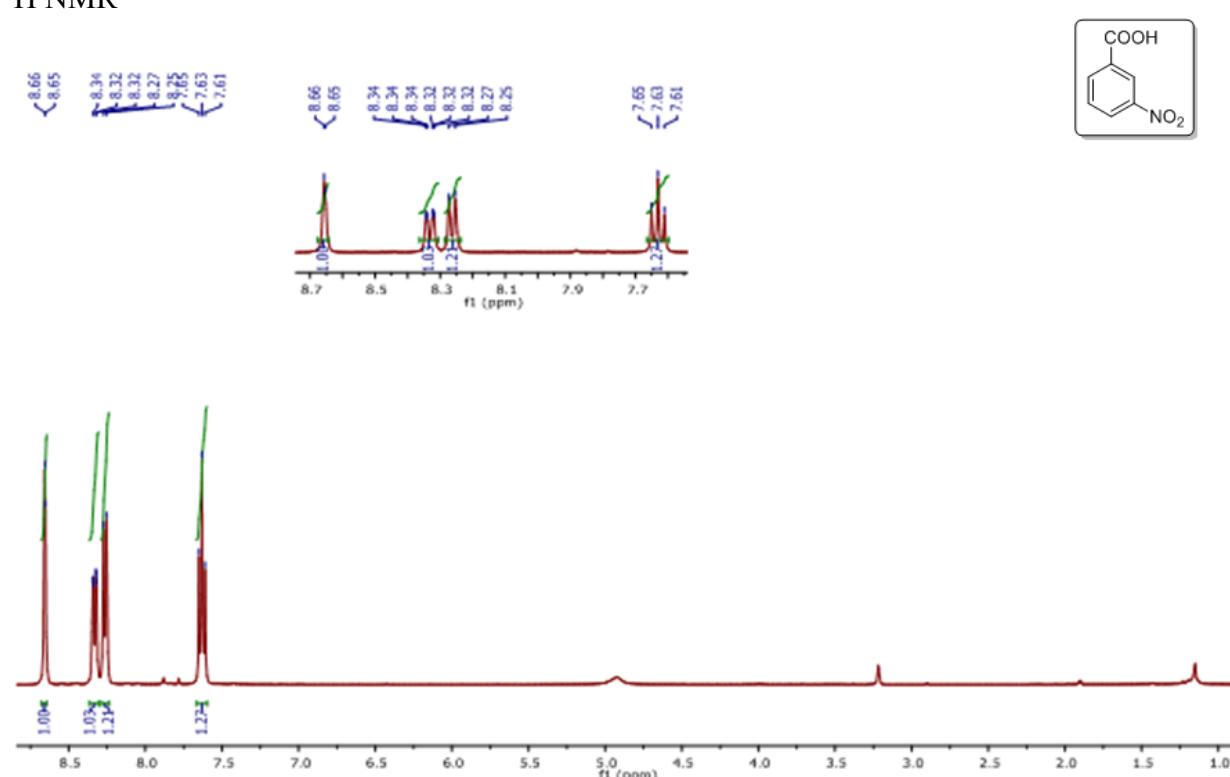


^{13}C NMR

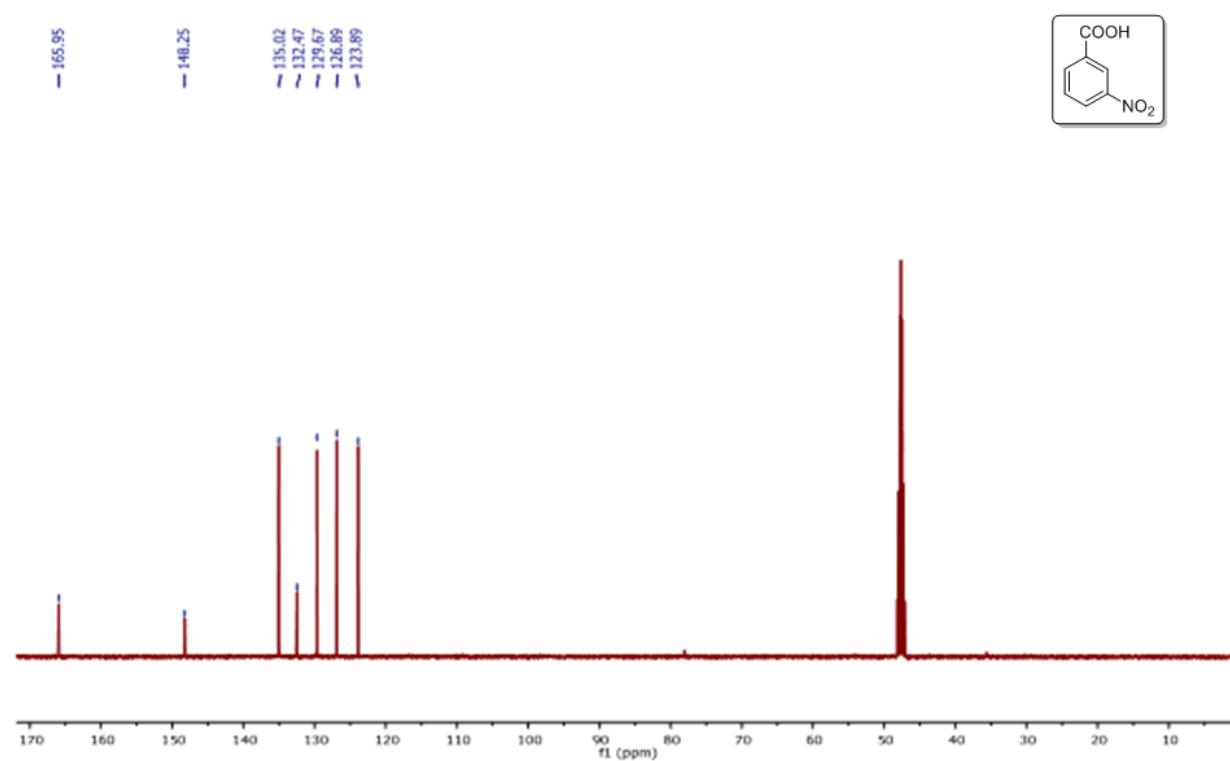


3-Nitrobenzoic acid (2d):

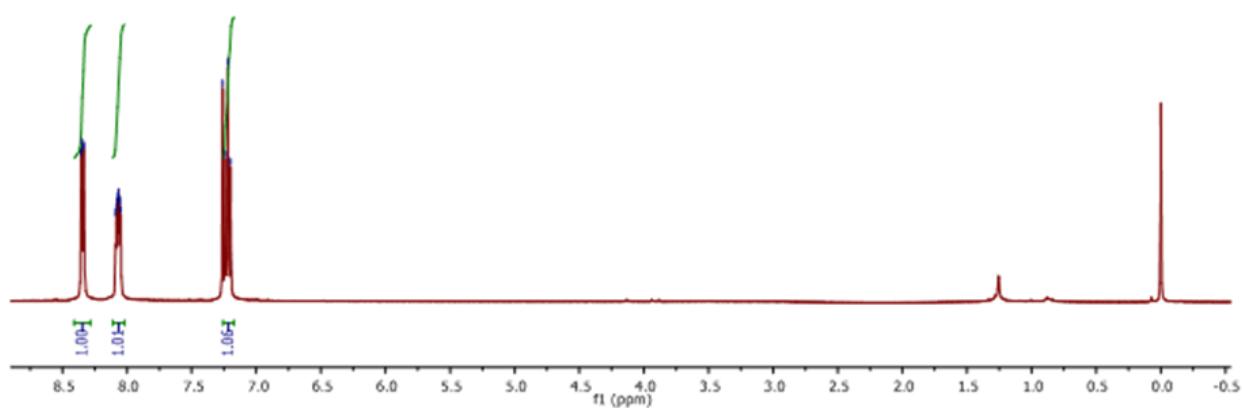
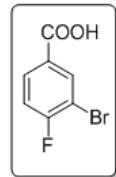
¹H NMR



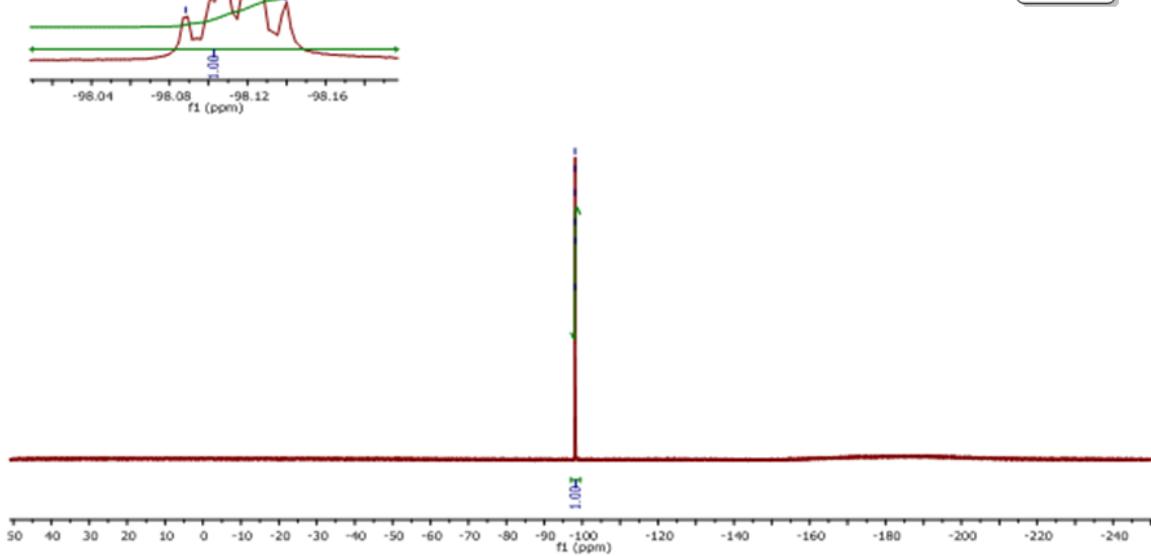
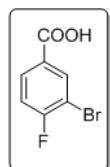
¹³C NMR



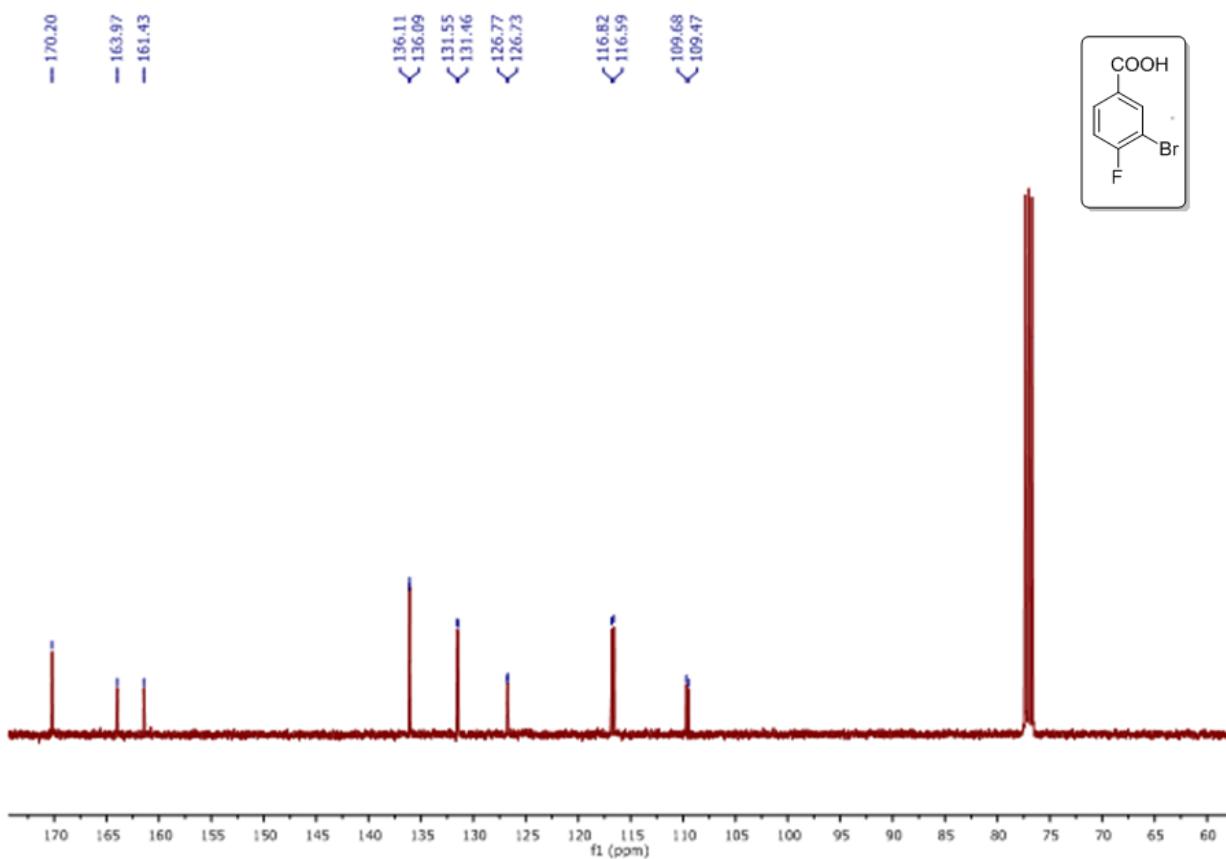
3-bromo,4-Fluorobenzoic acid (2e):
¹H NMR



¹⁹F NMR

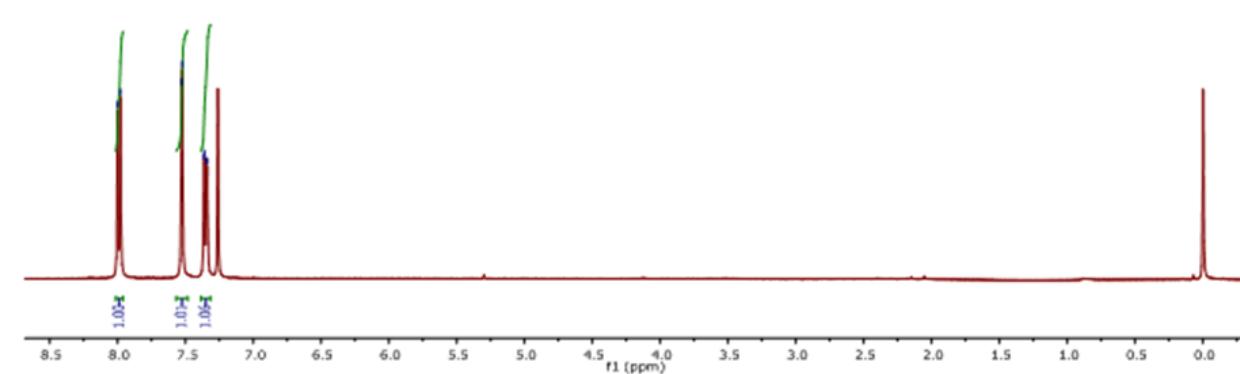
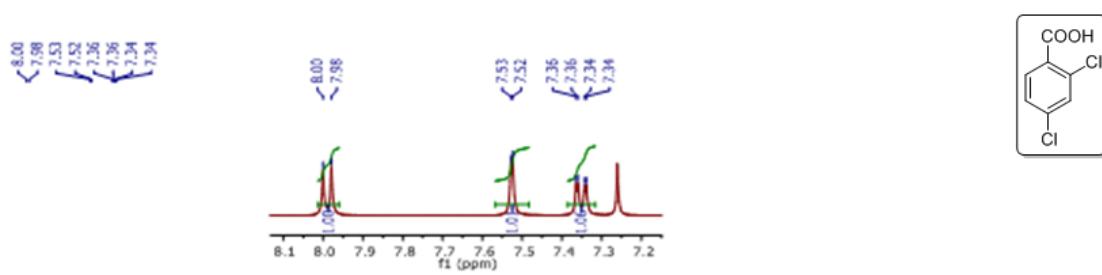


¹³C NMR

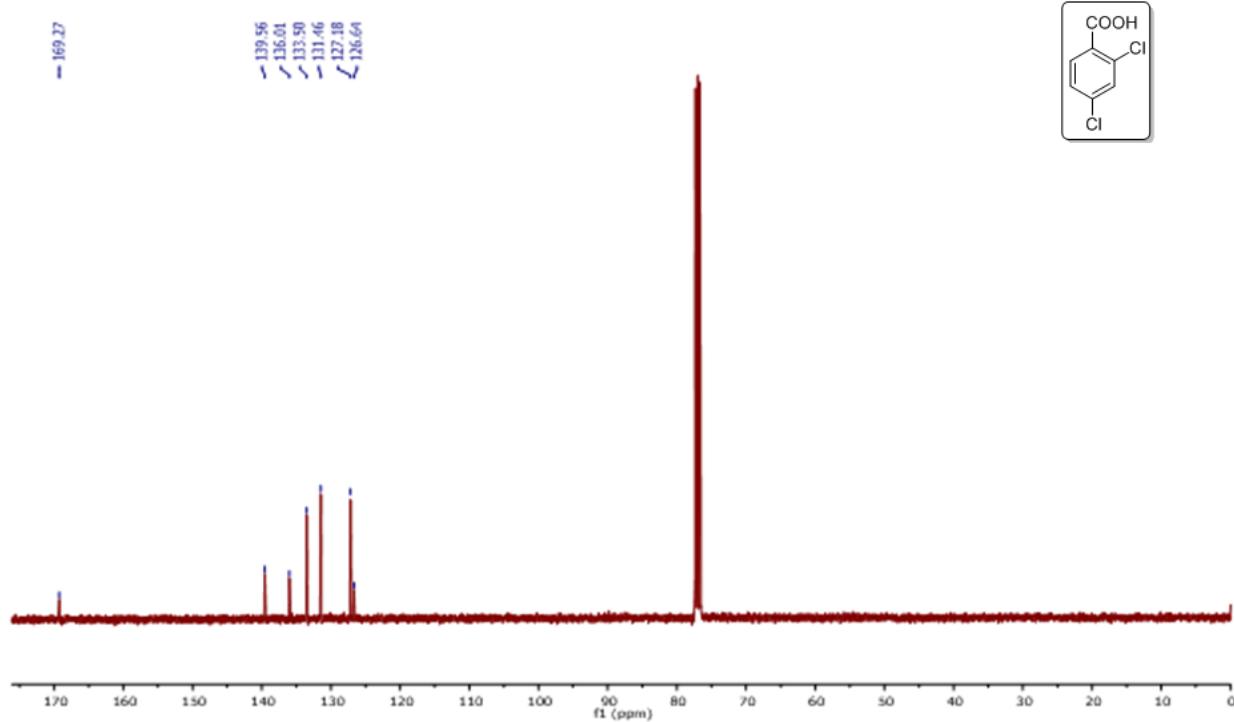


2,4-dichloro benzoic acid (2f):

¹H NMR

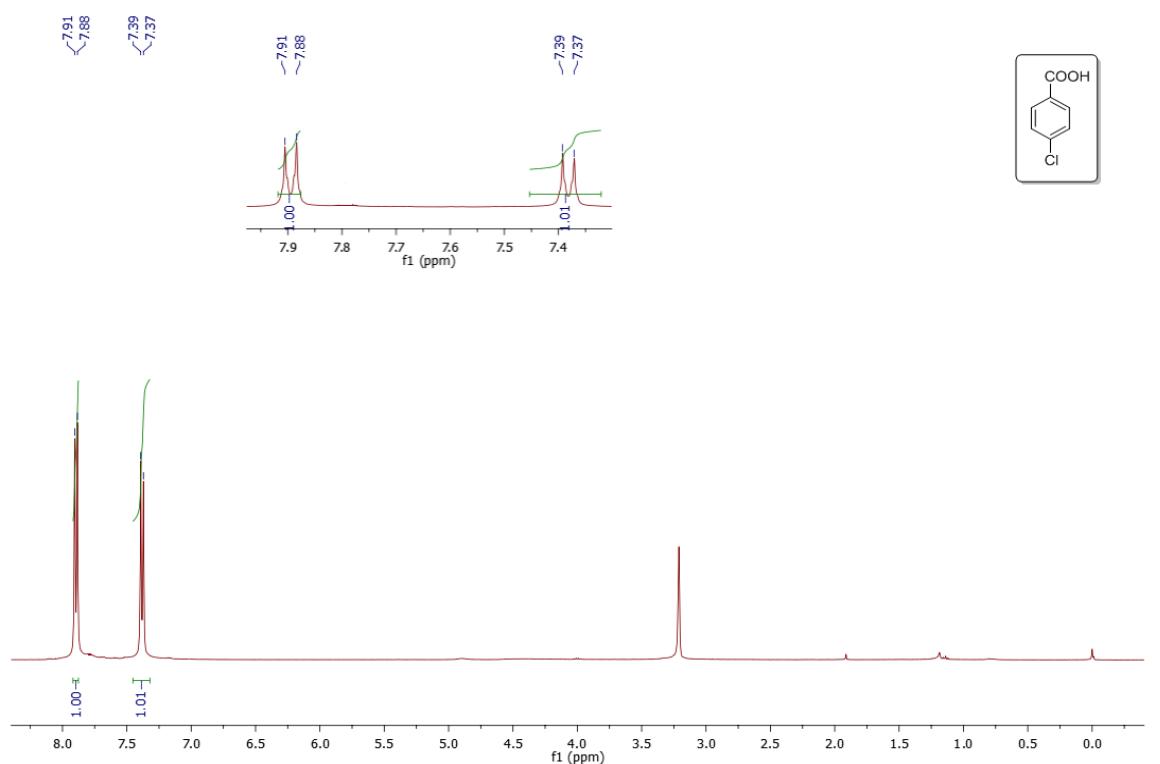


¹³C NMR

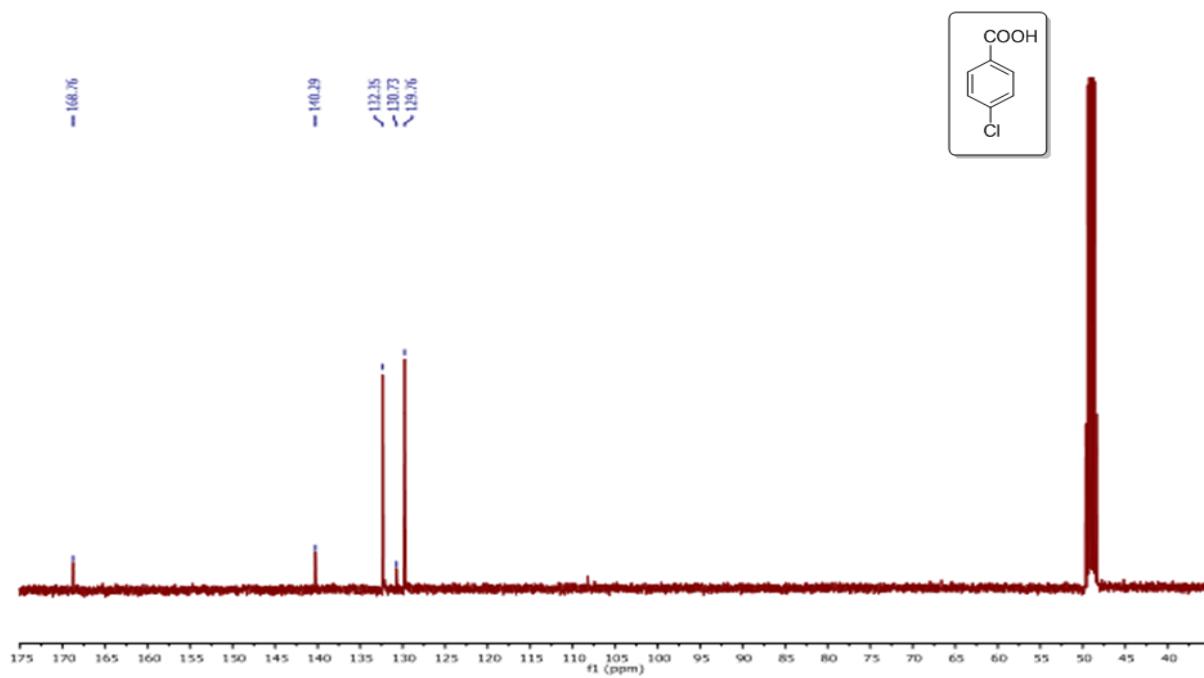


4-Chloro benzoic acid (2g):

¹H NMR

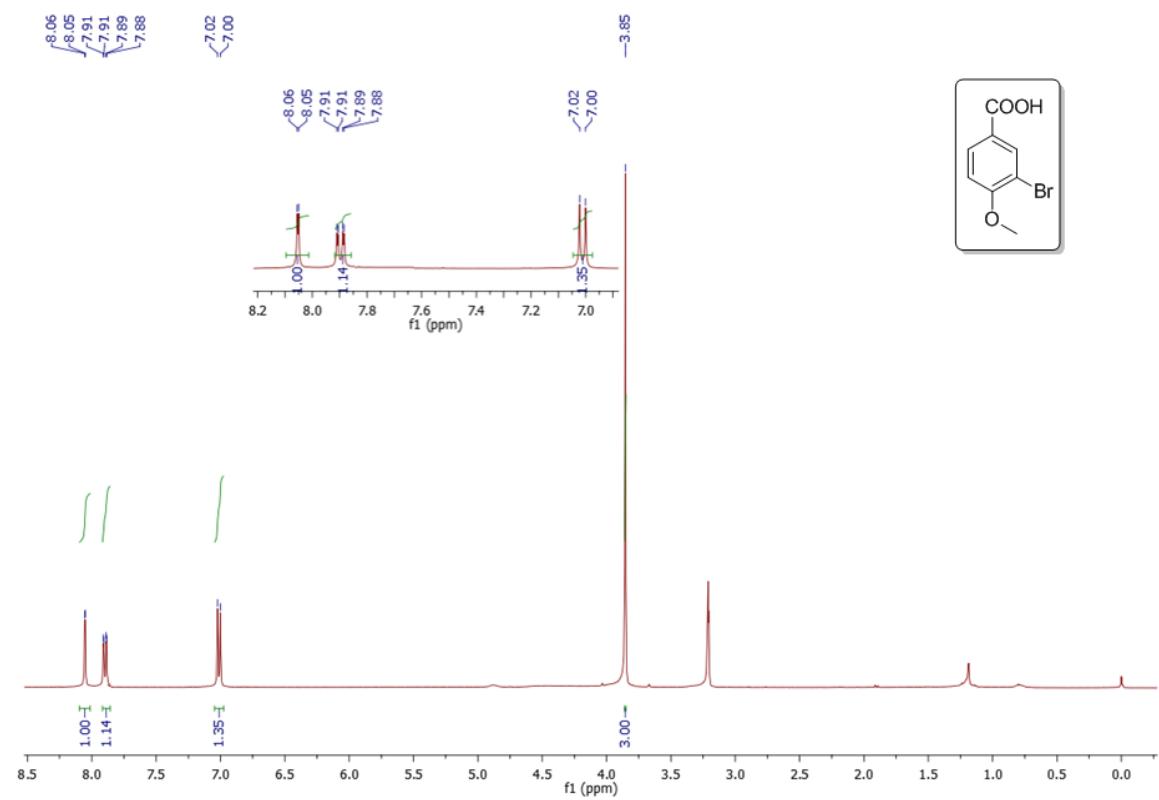


¹³C NMR

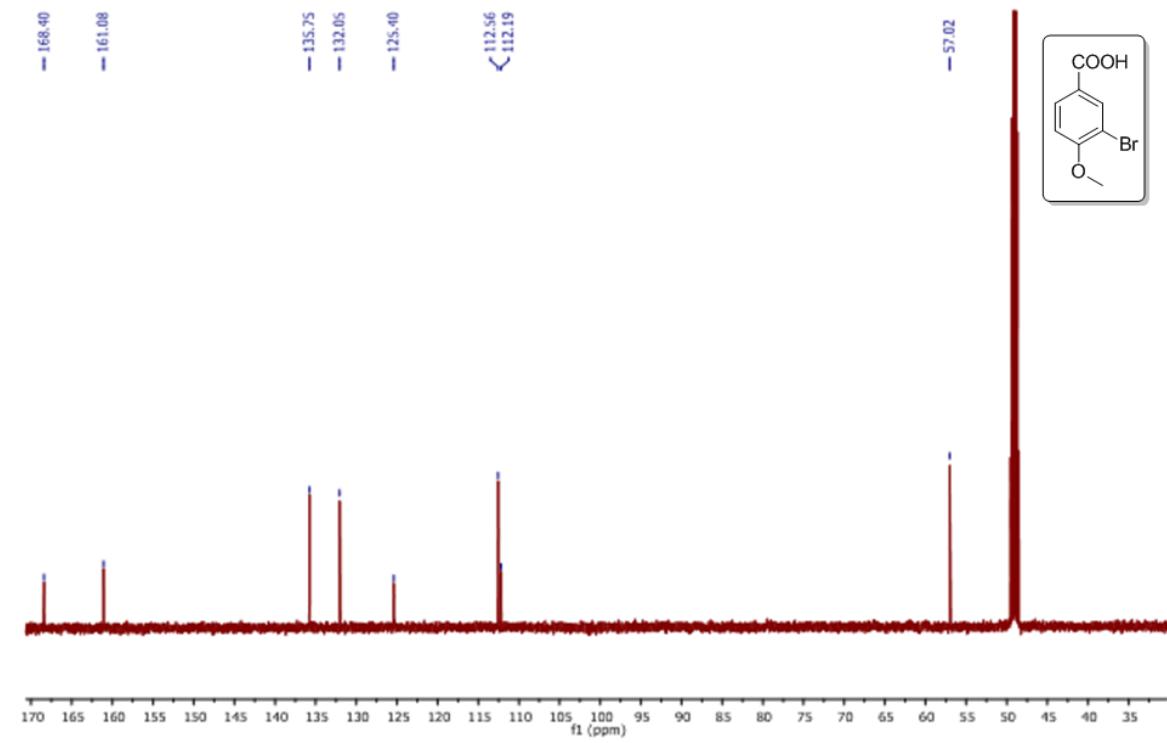


3-Bromo,4-methoxy benzoic acid (2h):

¹H NMR

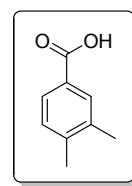
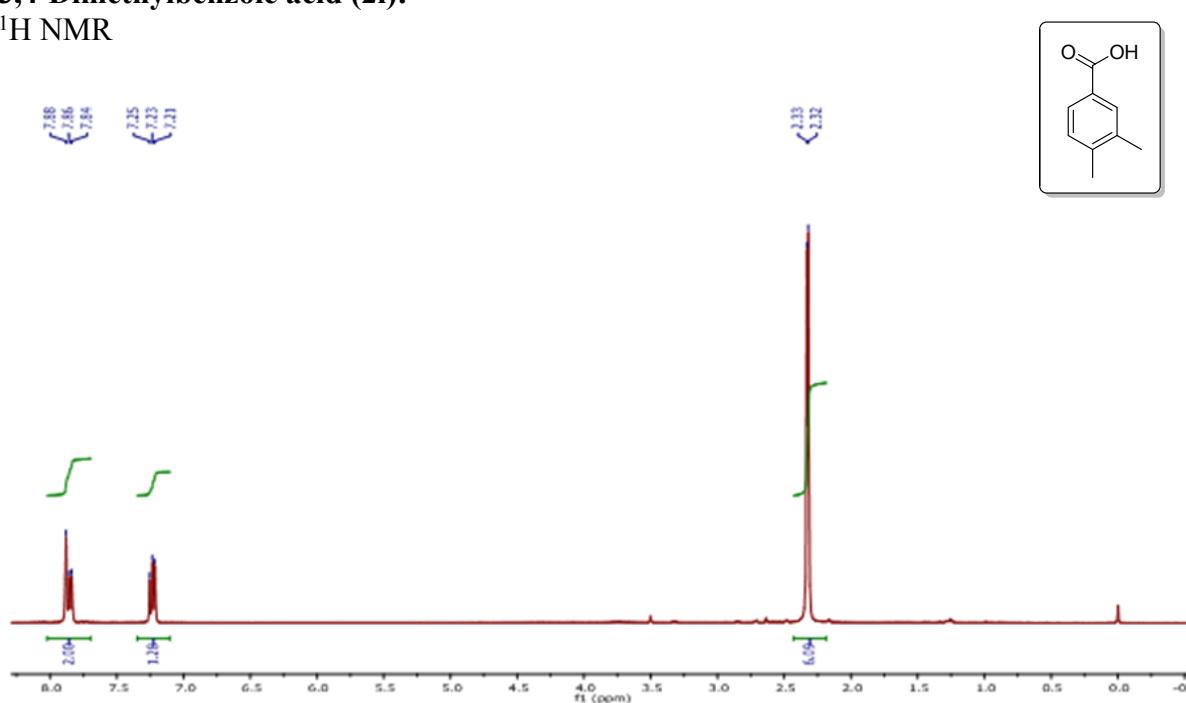


¹³C NMR

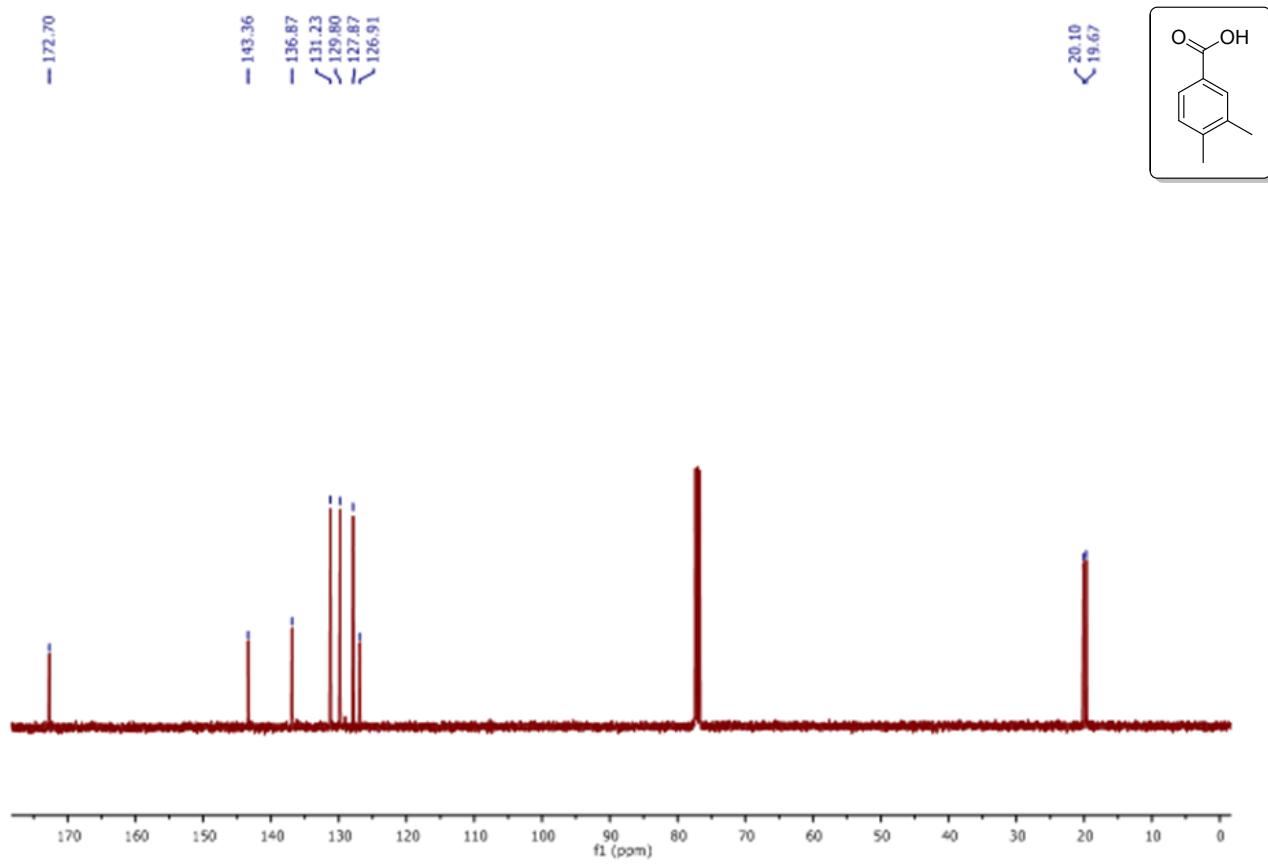


3,4-Dimethylbenzoic acid (2i):

¹H NMR

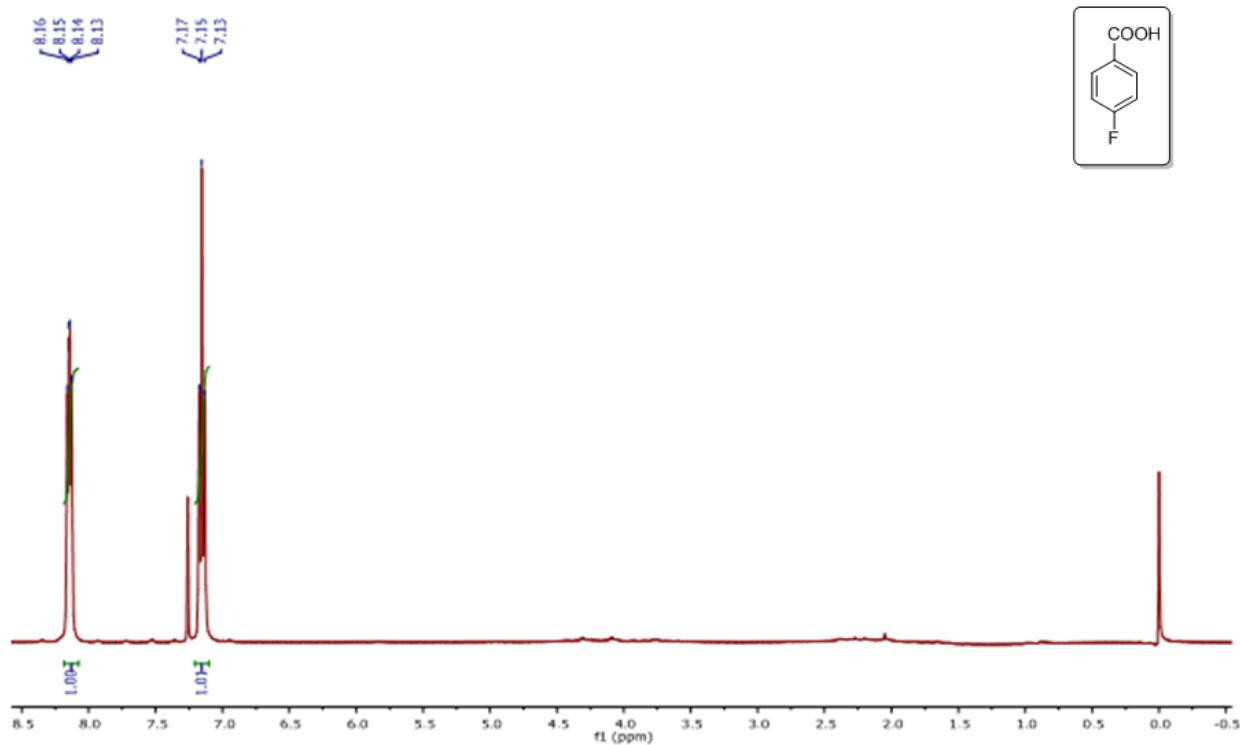


¹³C NMR

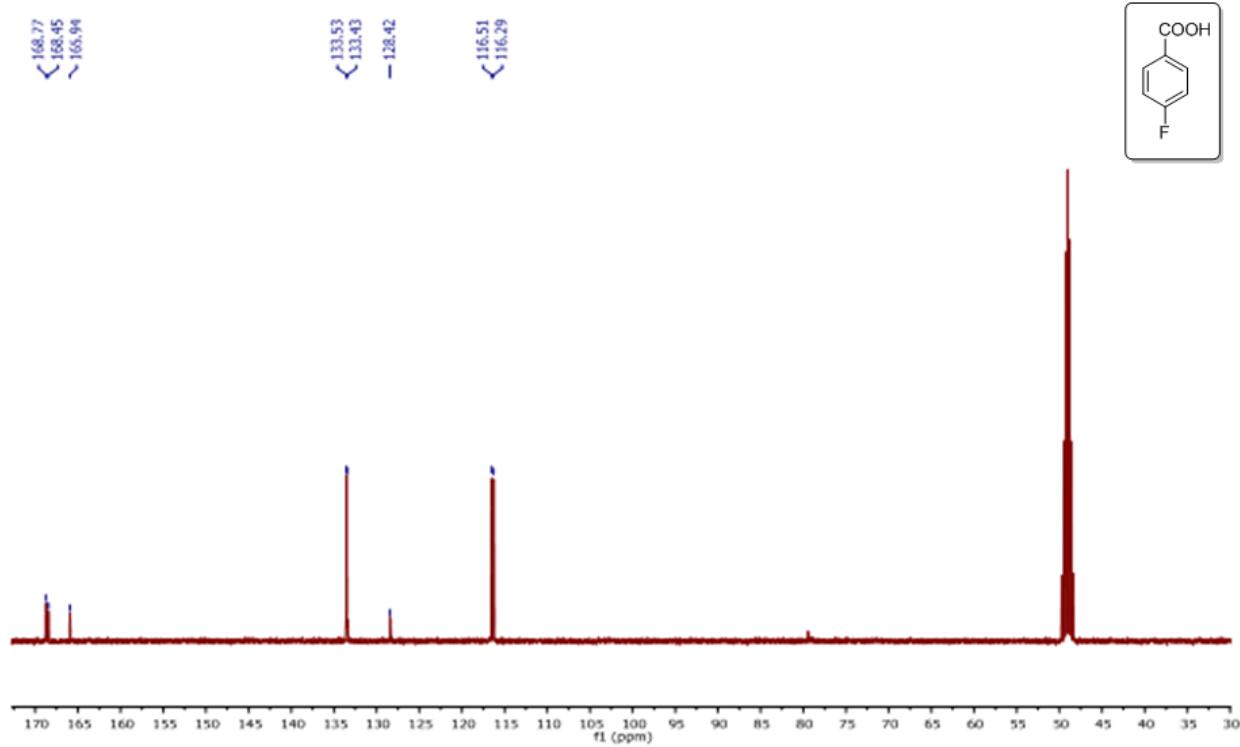


4-Fluorobenzoic acid (2j):

¹H NMR

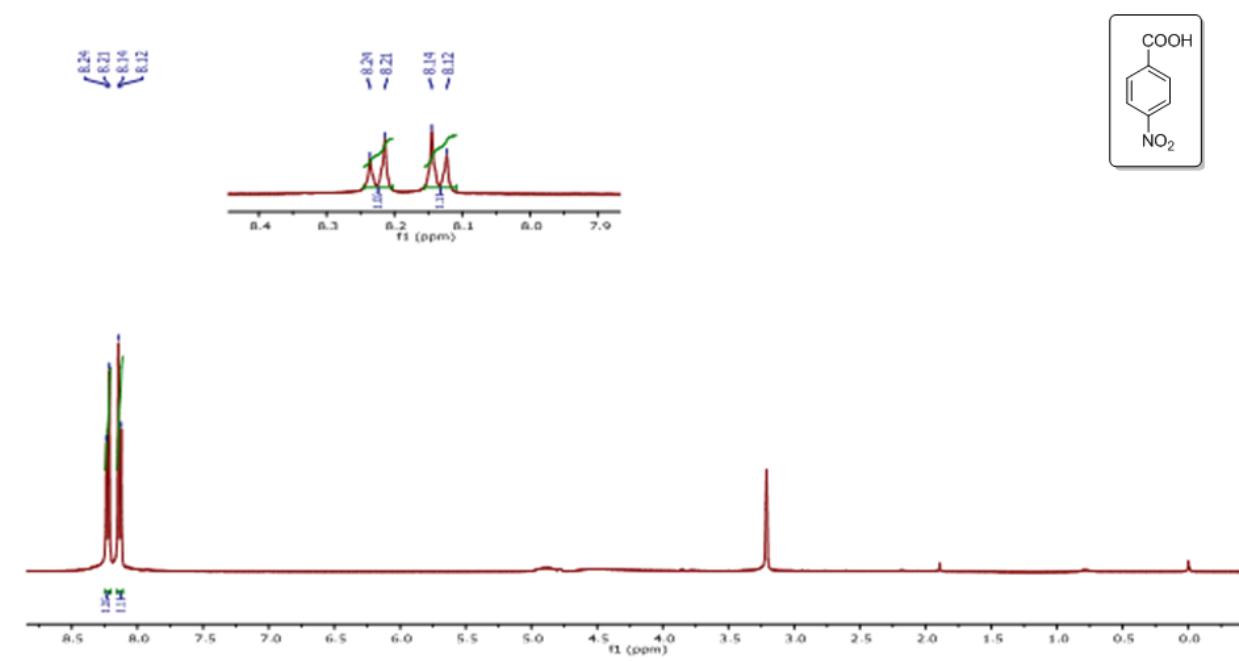


¹³C NMR

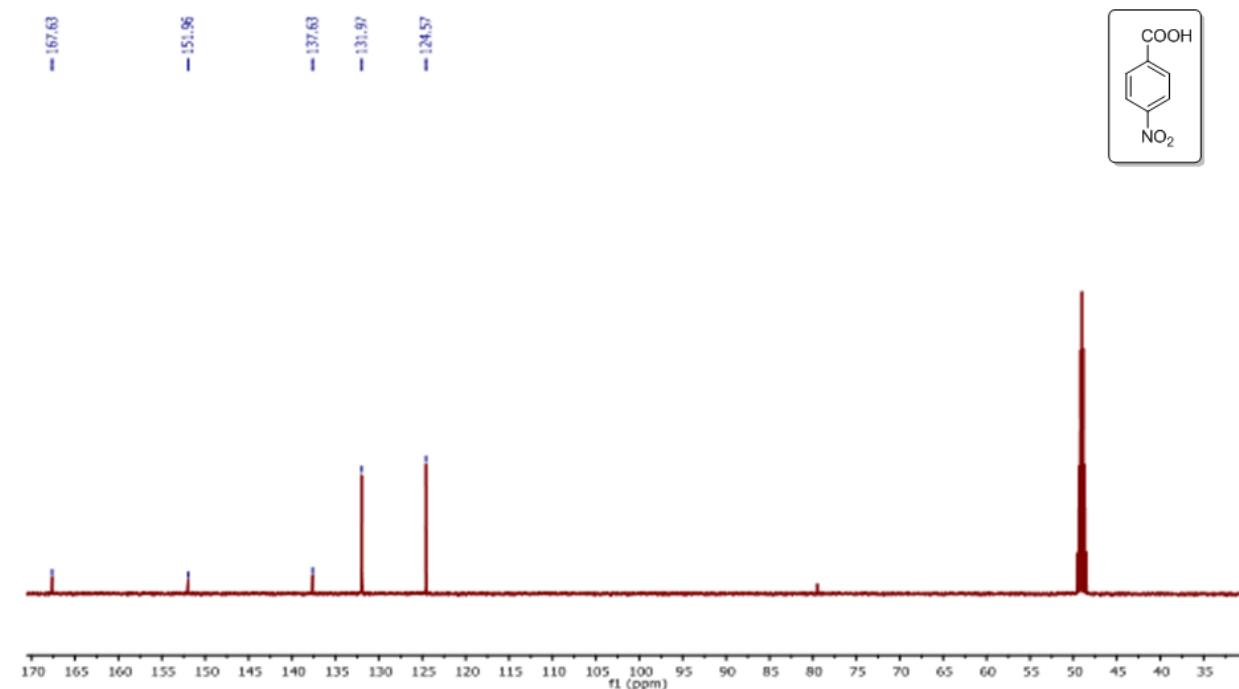


4-Nitro benzoic acid (2k):

¹H NMR

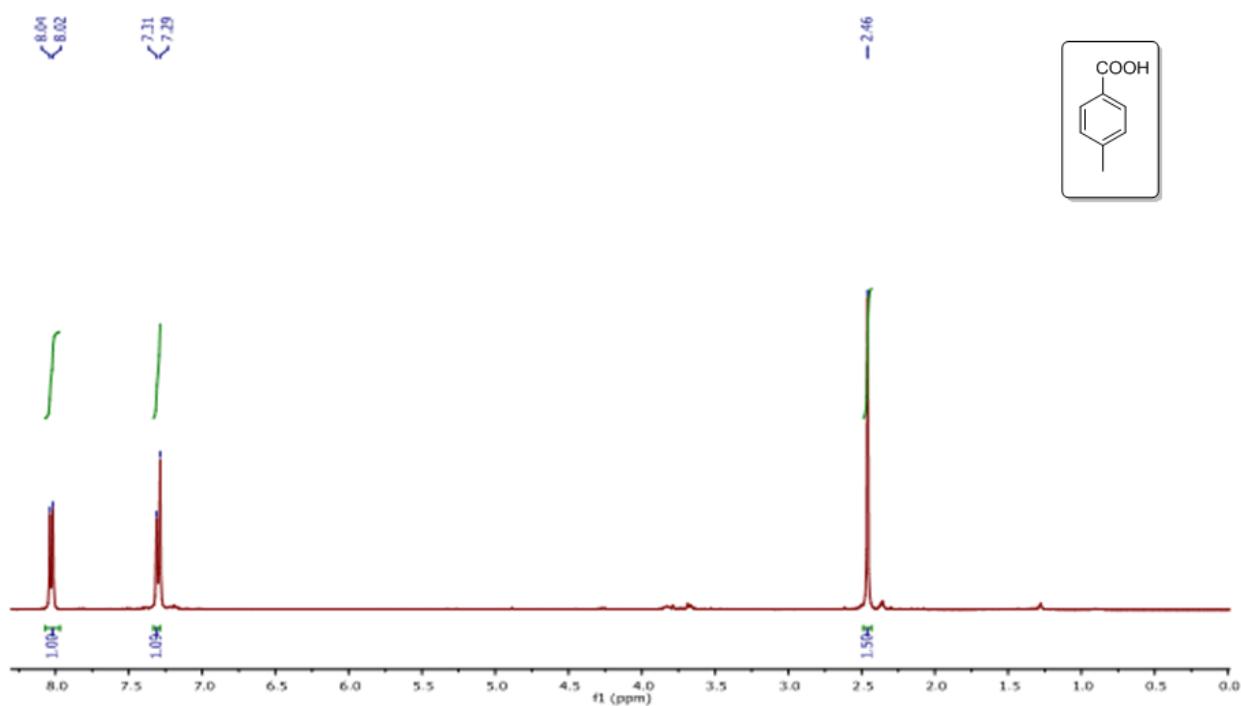


¹³C NMR

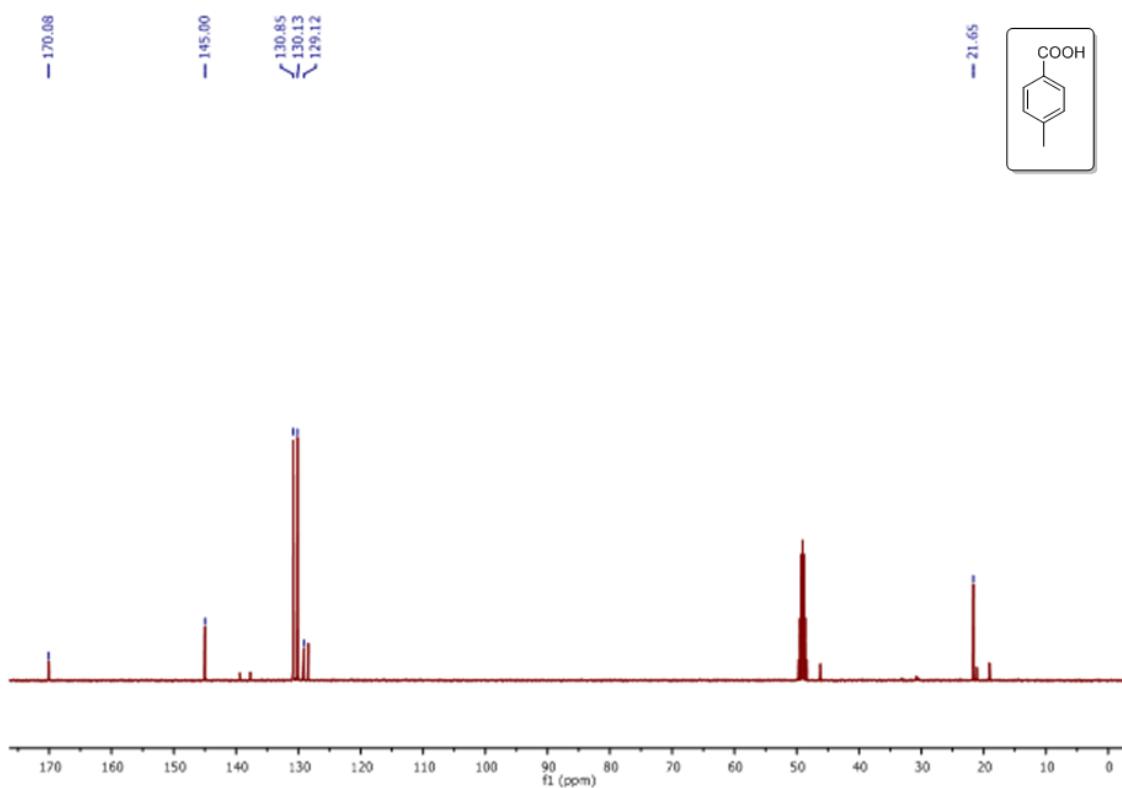


4-Methyl benzoic acid (2l):

¹H NMR

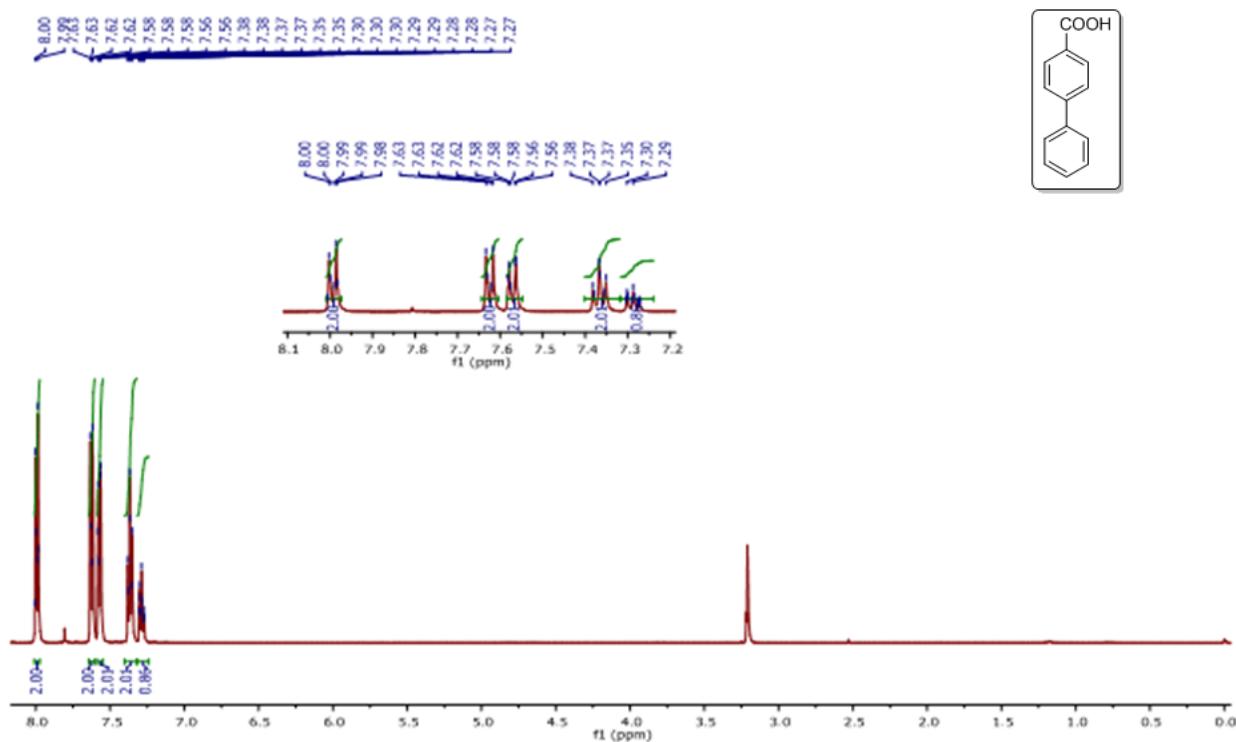


¹³C NMR

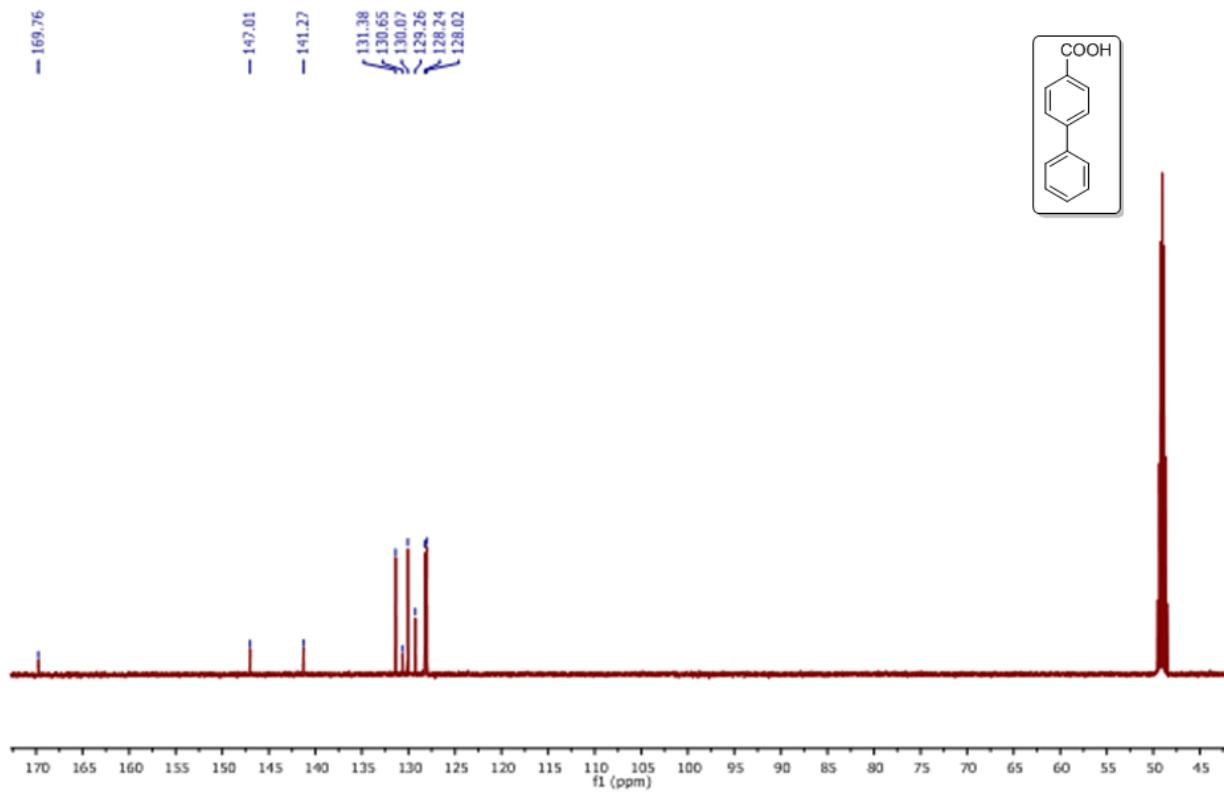


4-Phenyl Benzoic acid (2m):

¹H NMR

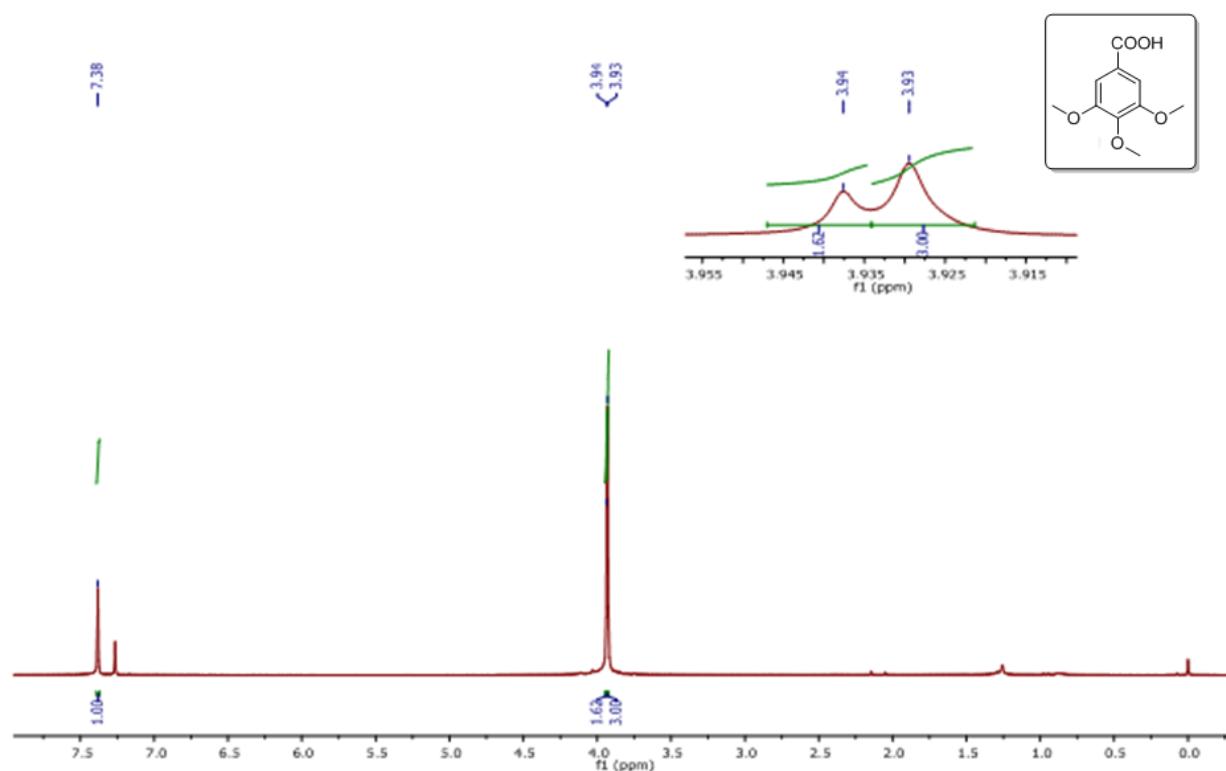


¹³C NMR

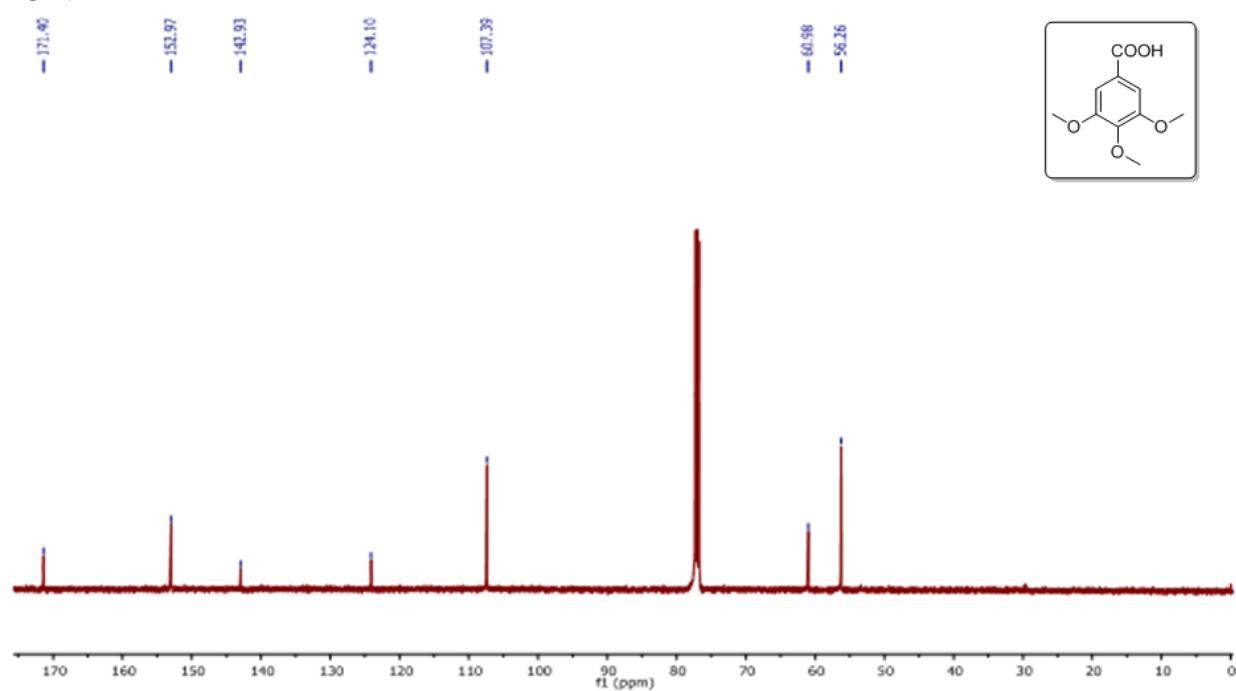


3,4,5 Trimethoxybenzoic acid (2n):

¹H NMR

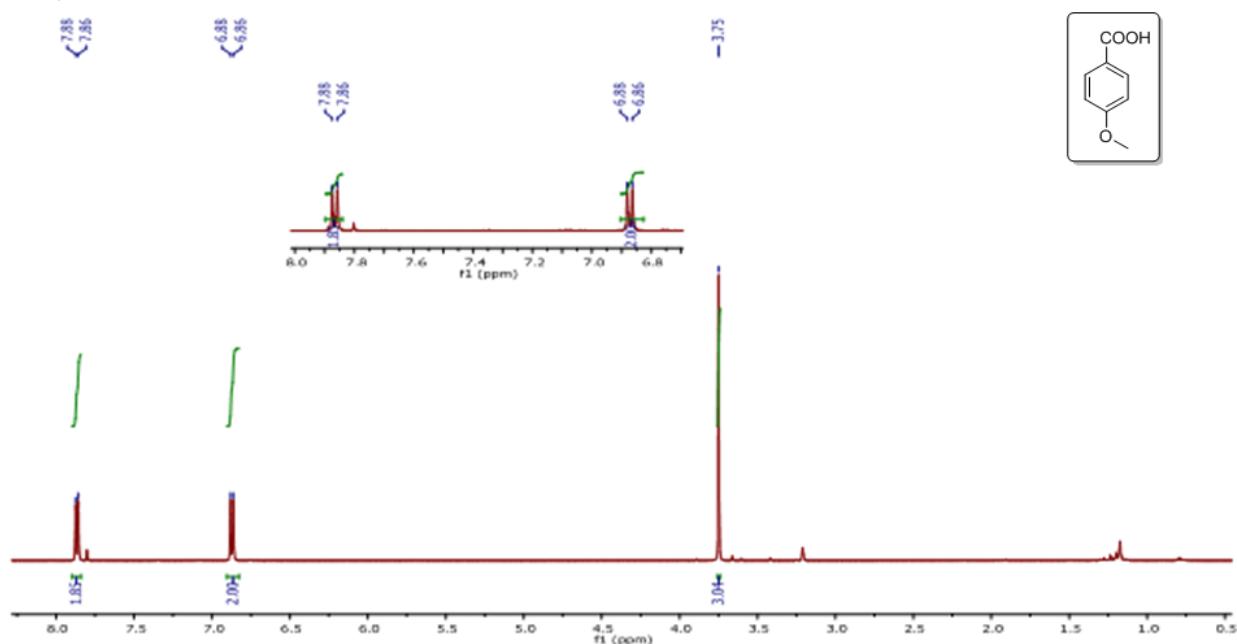


¹³C NMR

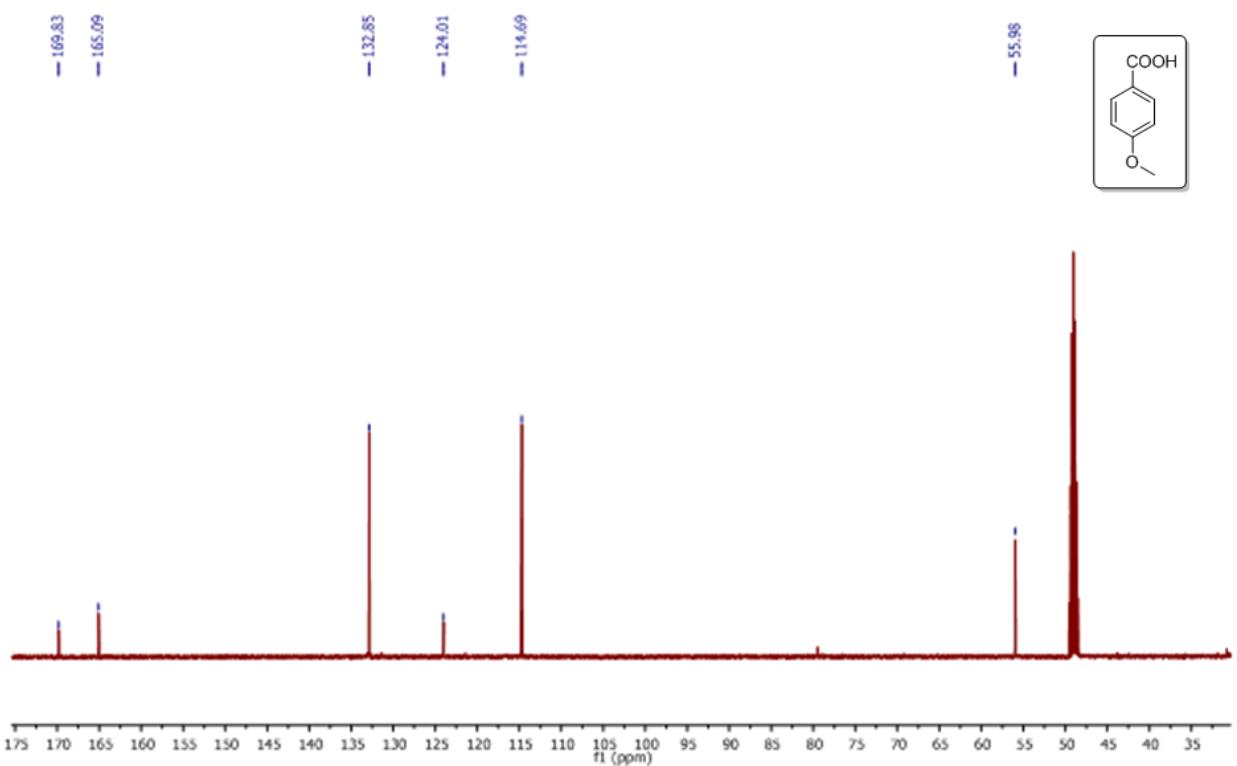


4-methoxybenzoic acid (2o):

¹H NMR

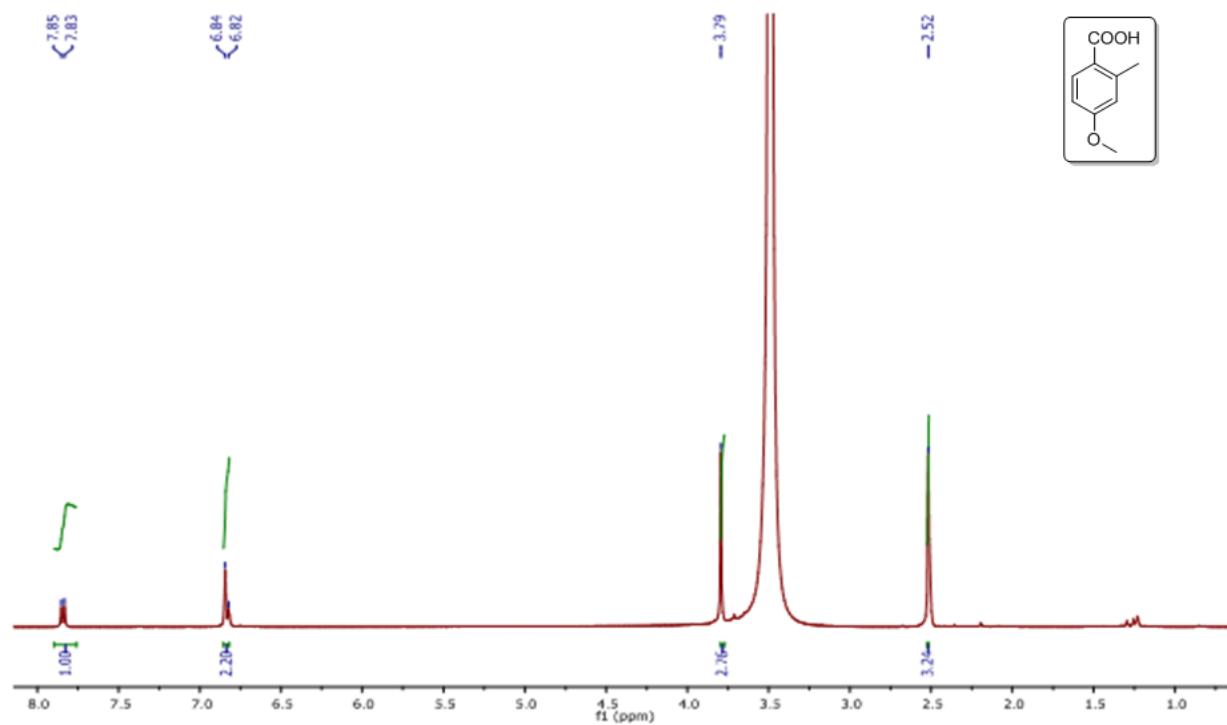


¹³C NMR

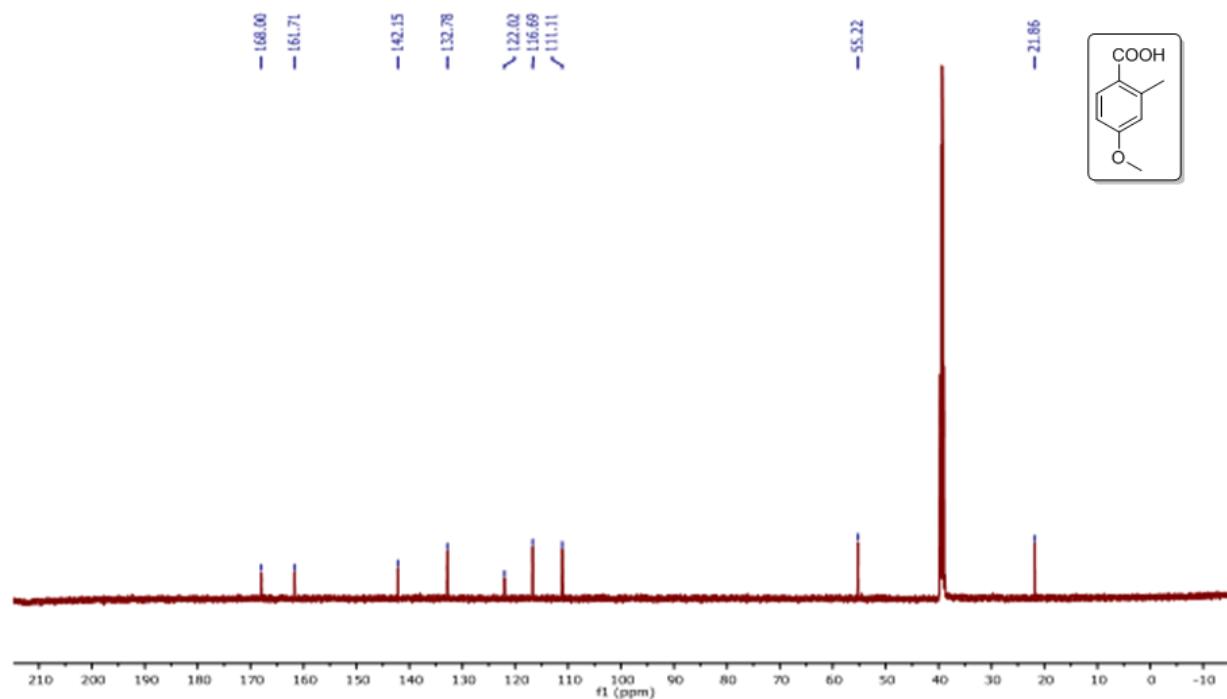


4-methoxy-2-methylbenzoic acid (2p):

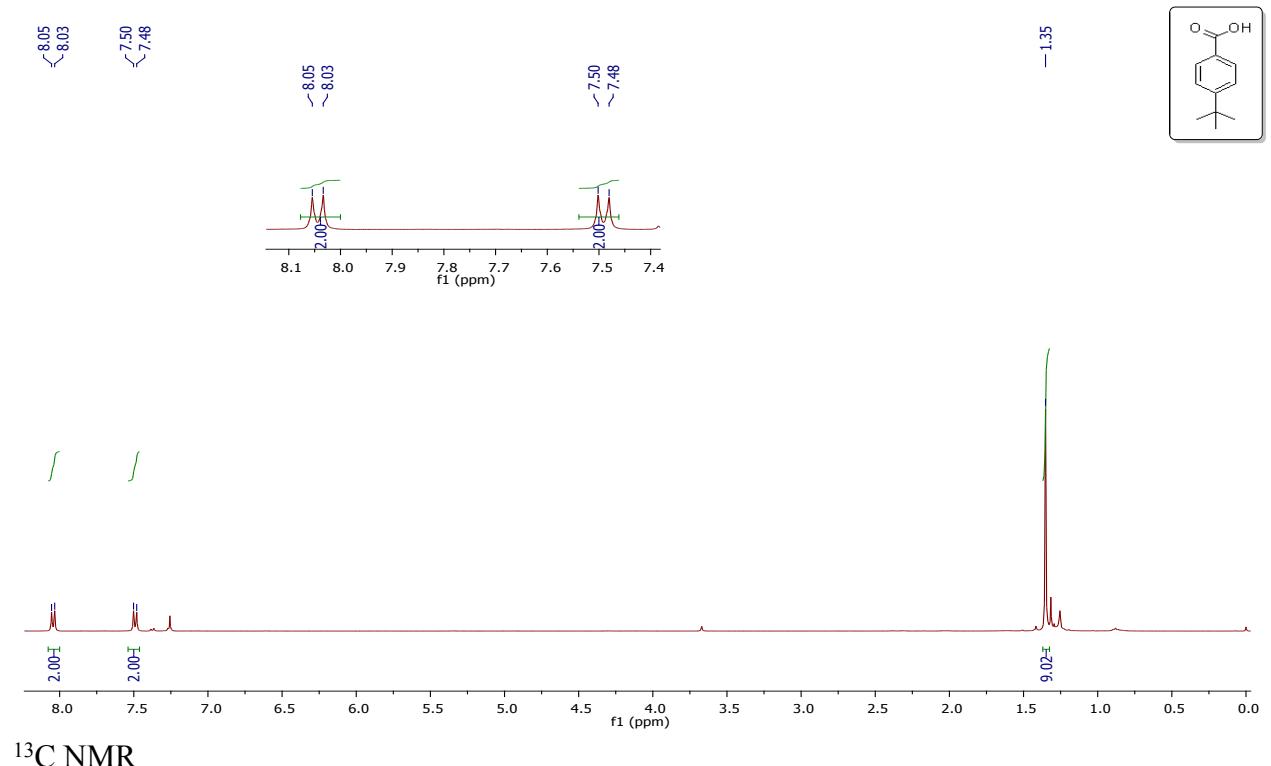
¹H NMR



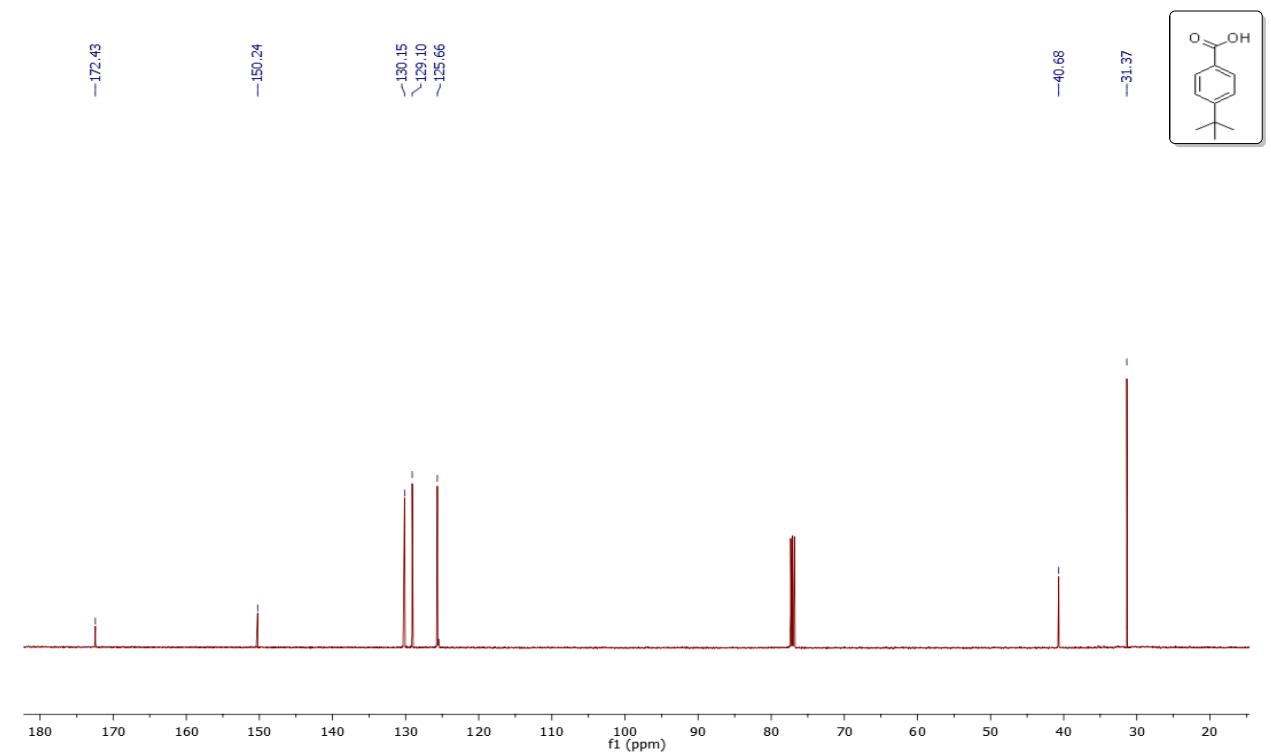
¹³C NMR



4-(tert-butyl)benzoic acid (2q):
 ^1H NMR

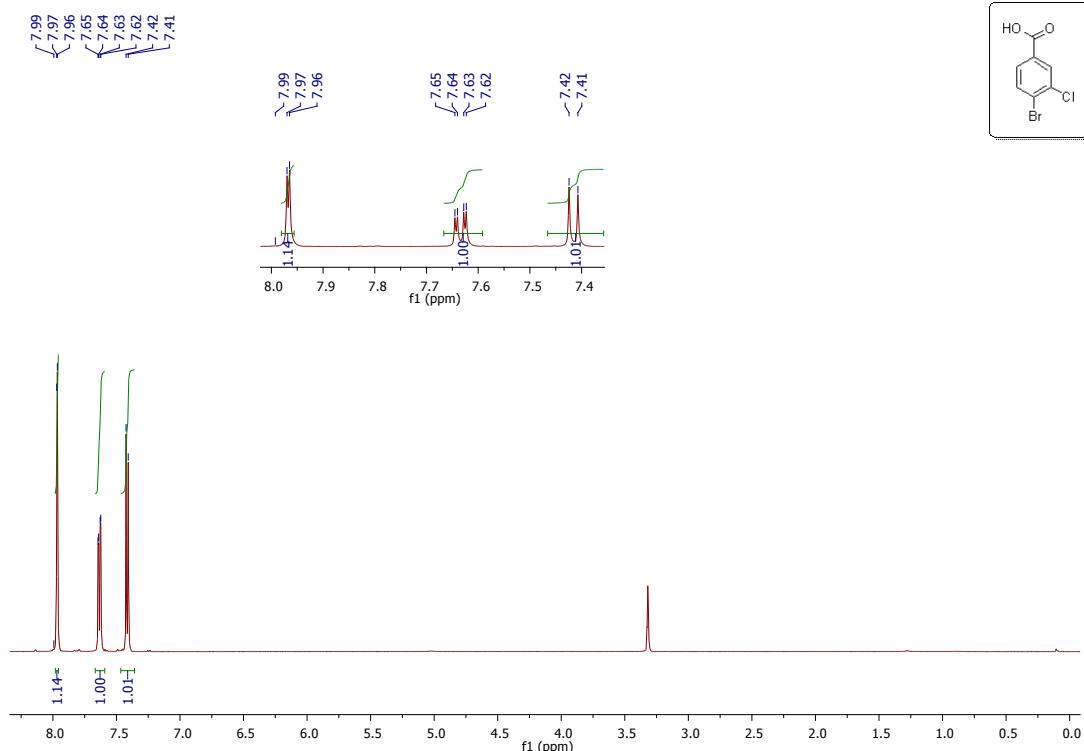


^{13}C NMR

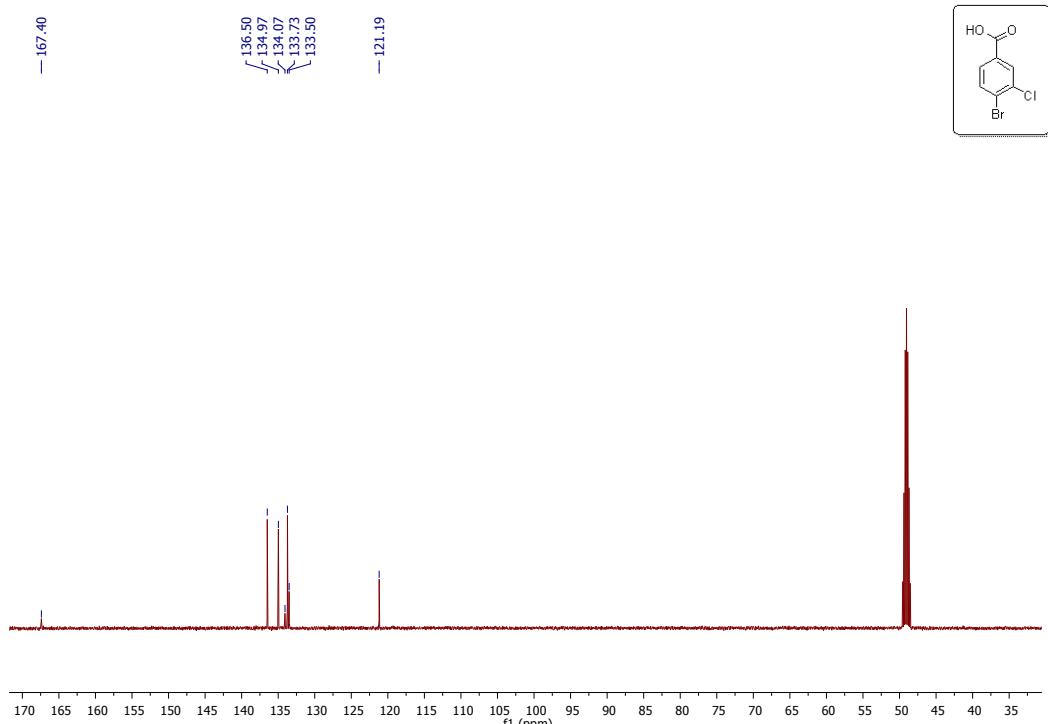


4-bromo-3-chlorobenzoic acid (2r):

¹H NMR:

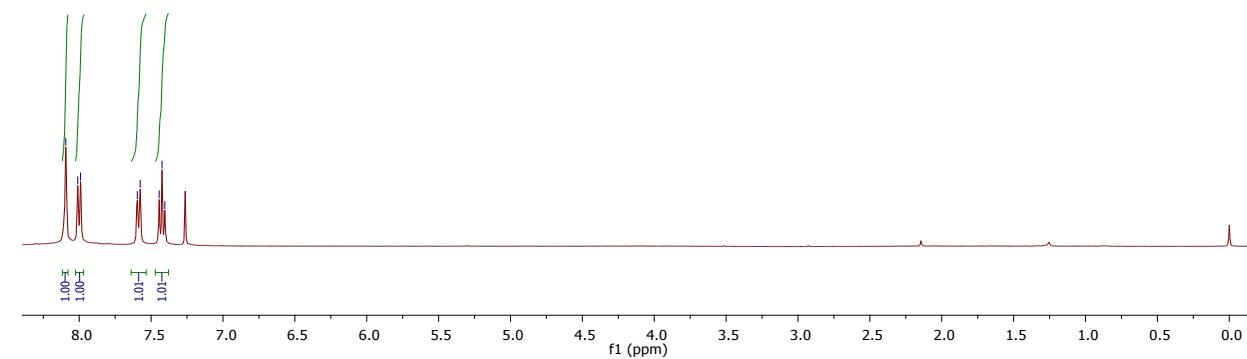
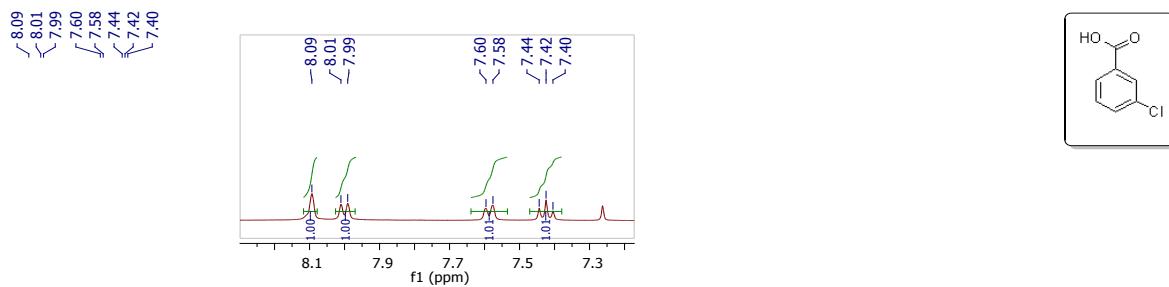


¹³C NMR:

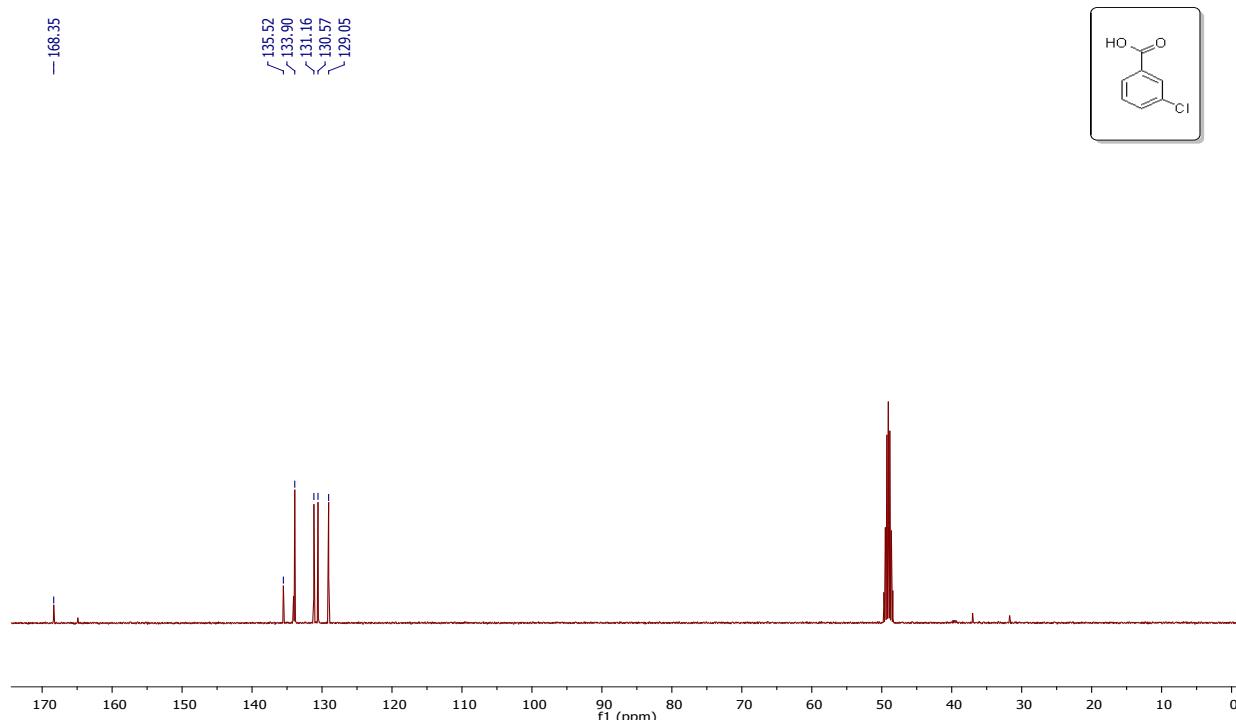


3-Chlorobenzoic acid (2s):

¹H NMR

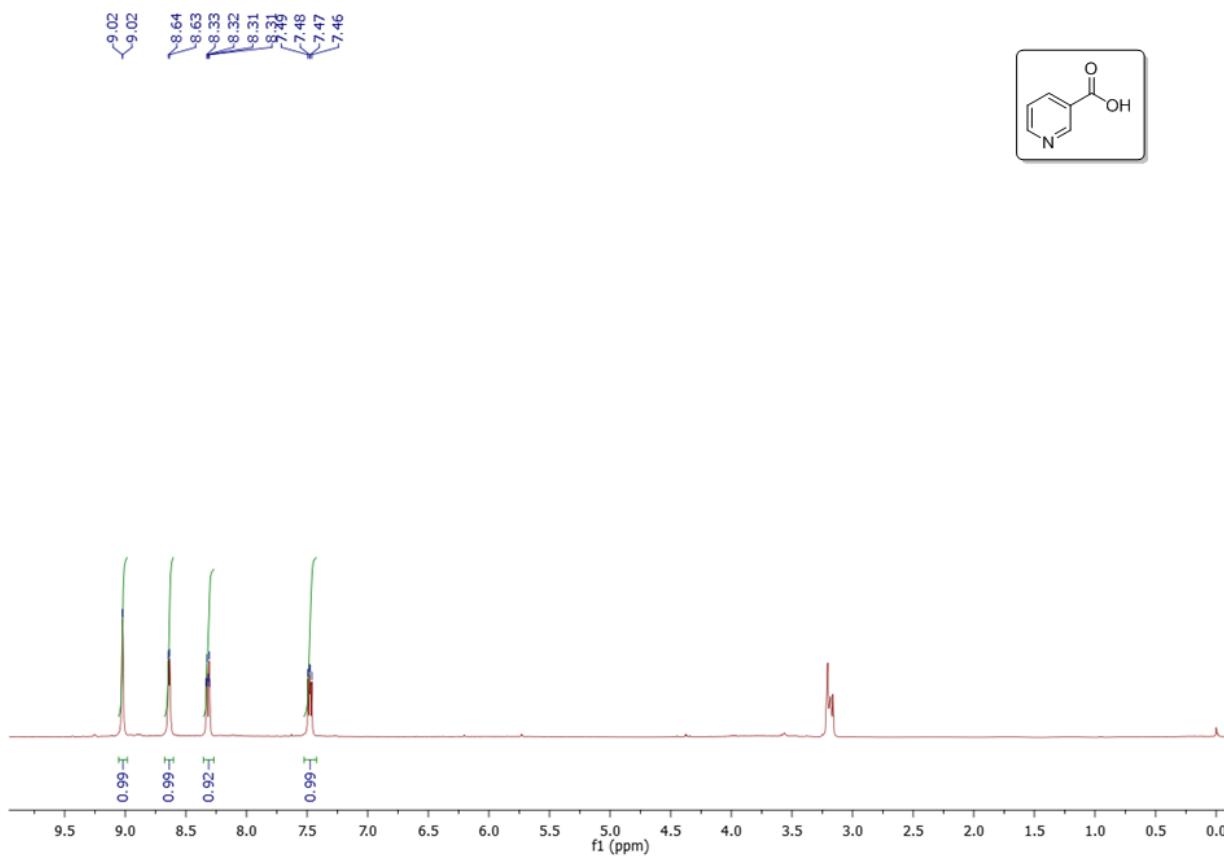


¹³C NMR

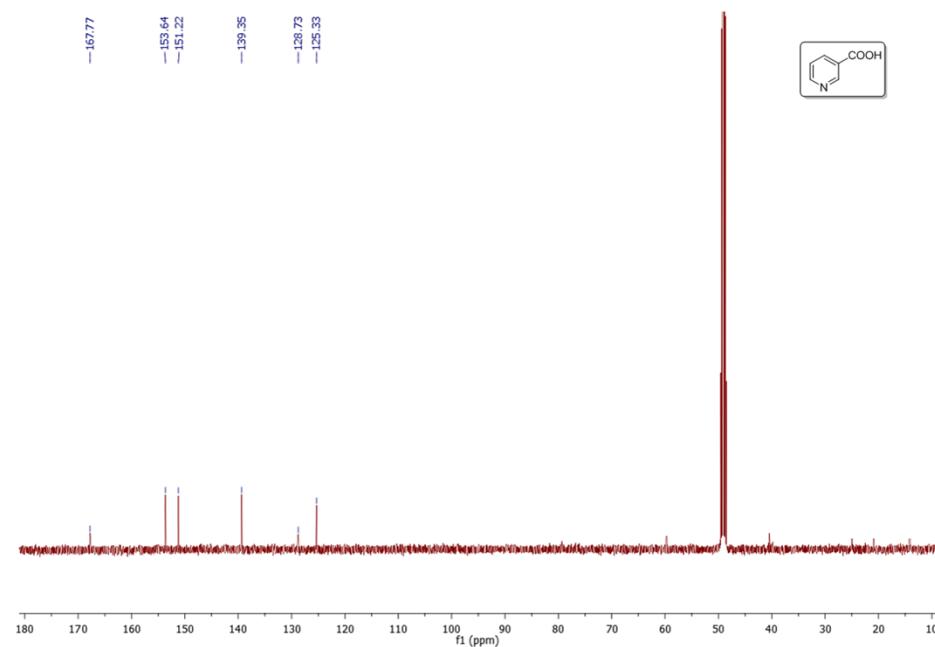


Nicotinic acid (3a):

¹H NMR

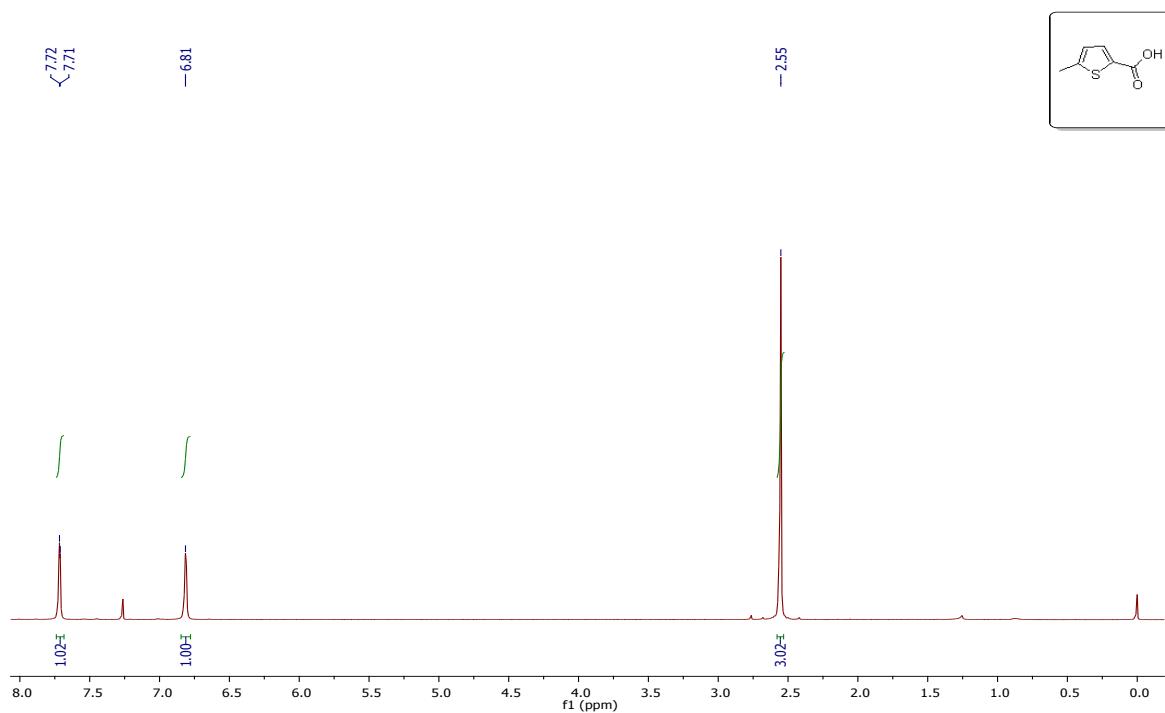


¹³C NMR

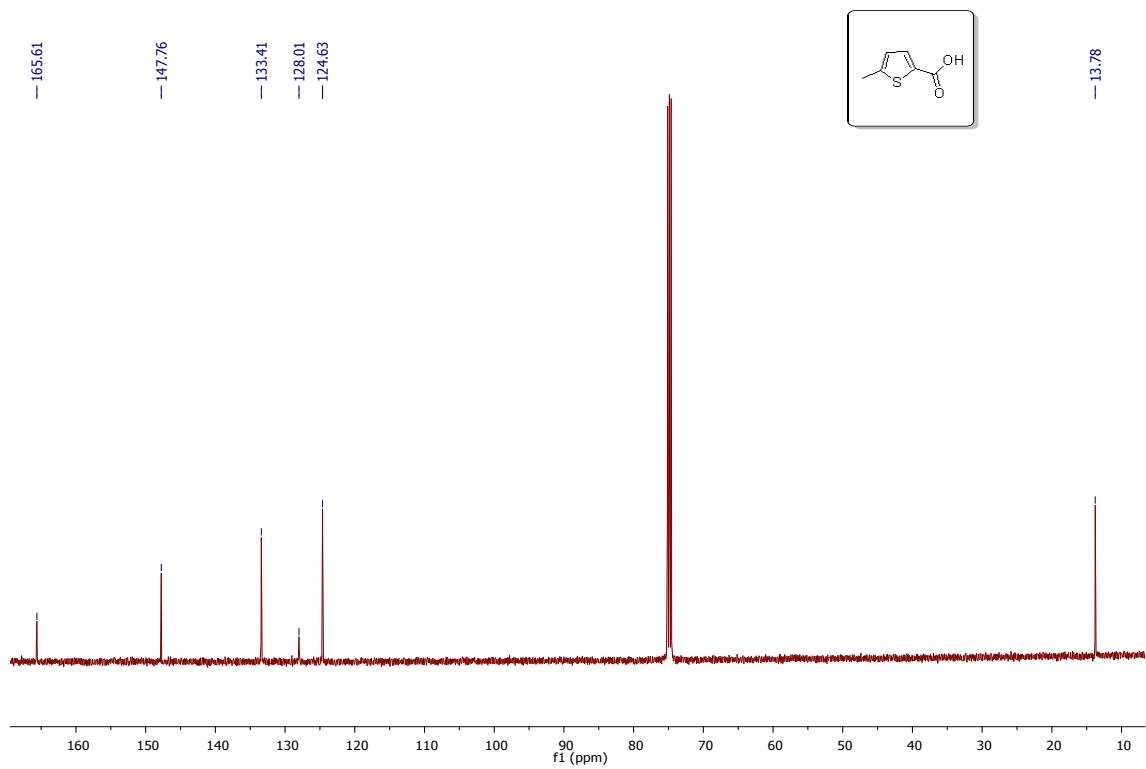


5-methylthiophene-2-carboxylic acid (3b):

¹H NMR

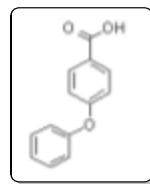
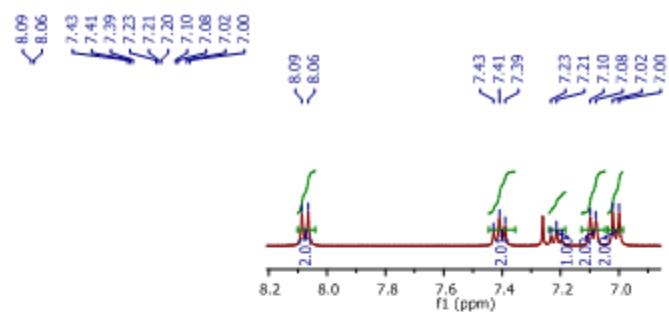


¹³C NMR

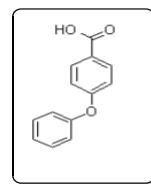
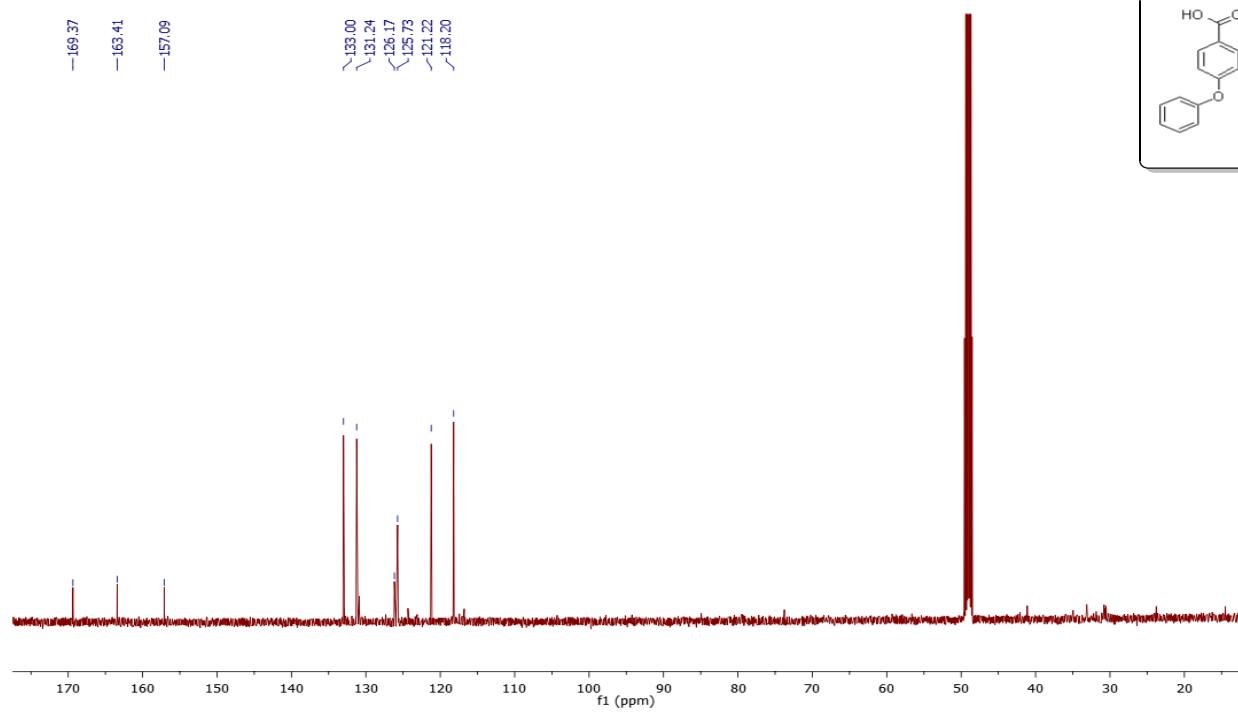


4-Phenoxybenzoic acid (3c):

¹H NMR

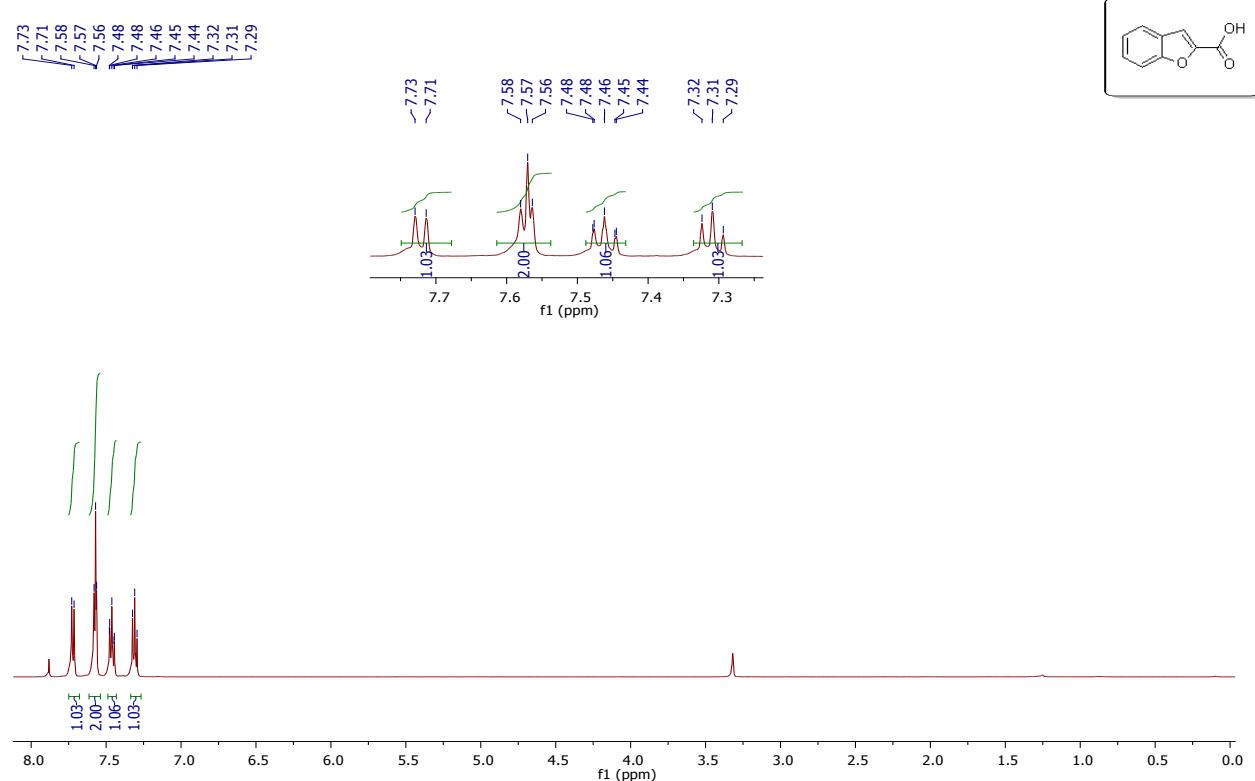


¹³C NMR

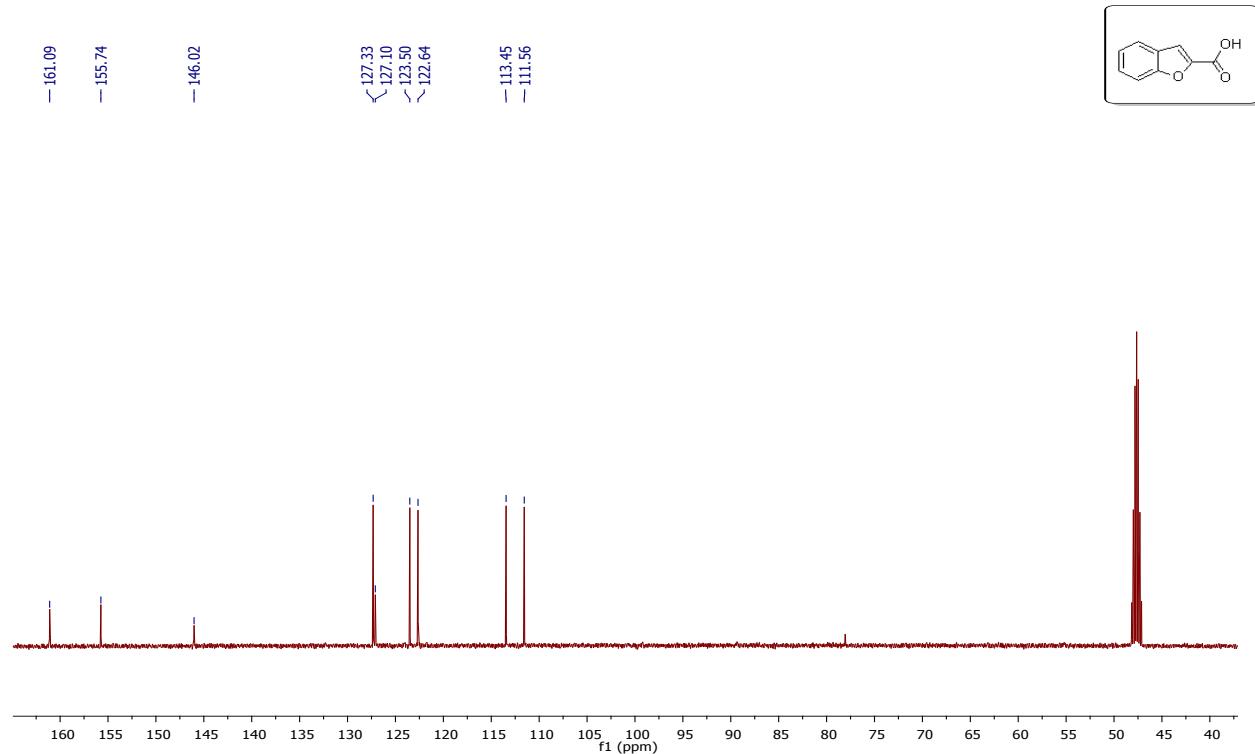


Benzofuran-2-carboxylic acid (3d):

¹H NMR

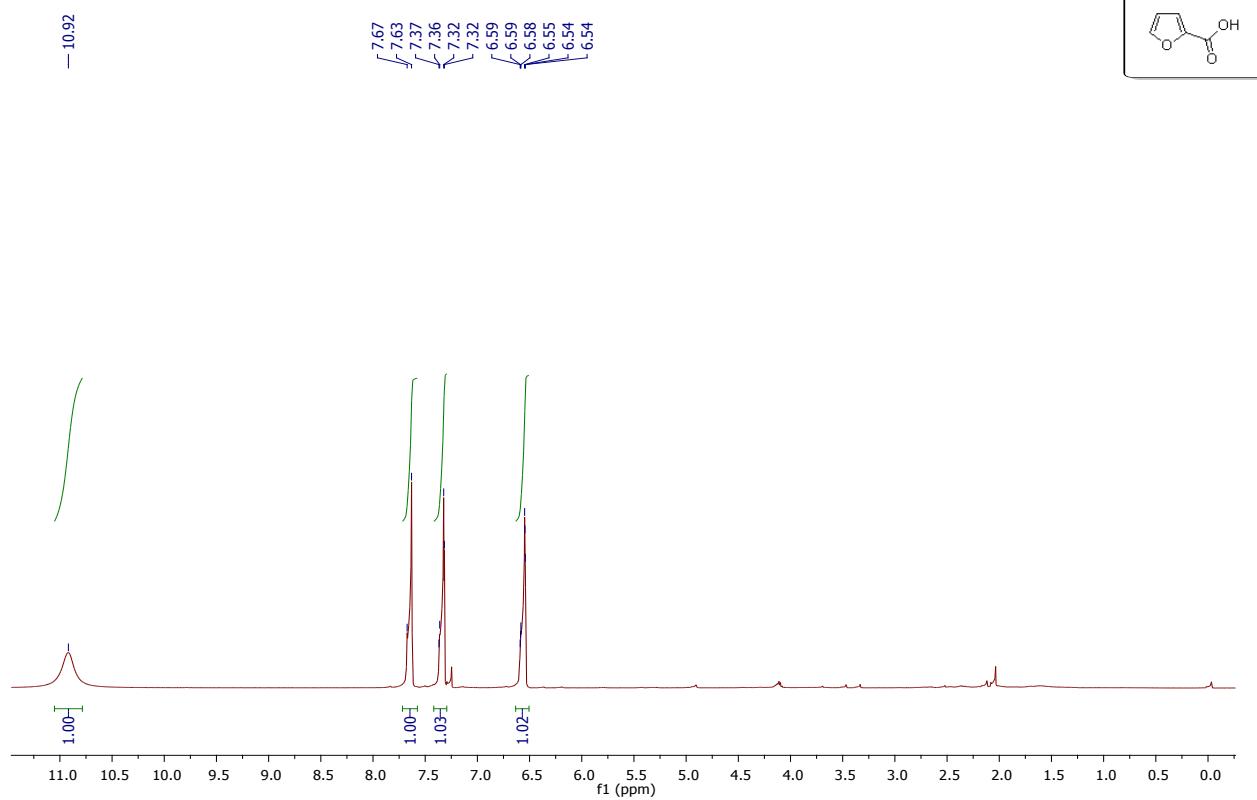


¹³C NMR

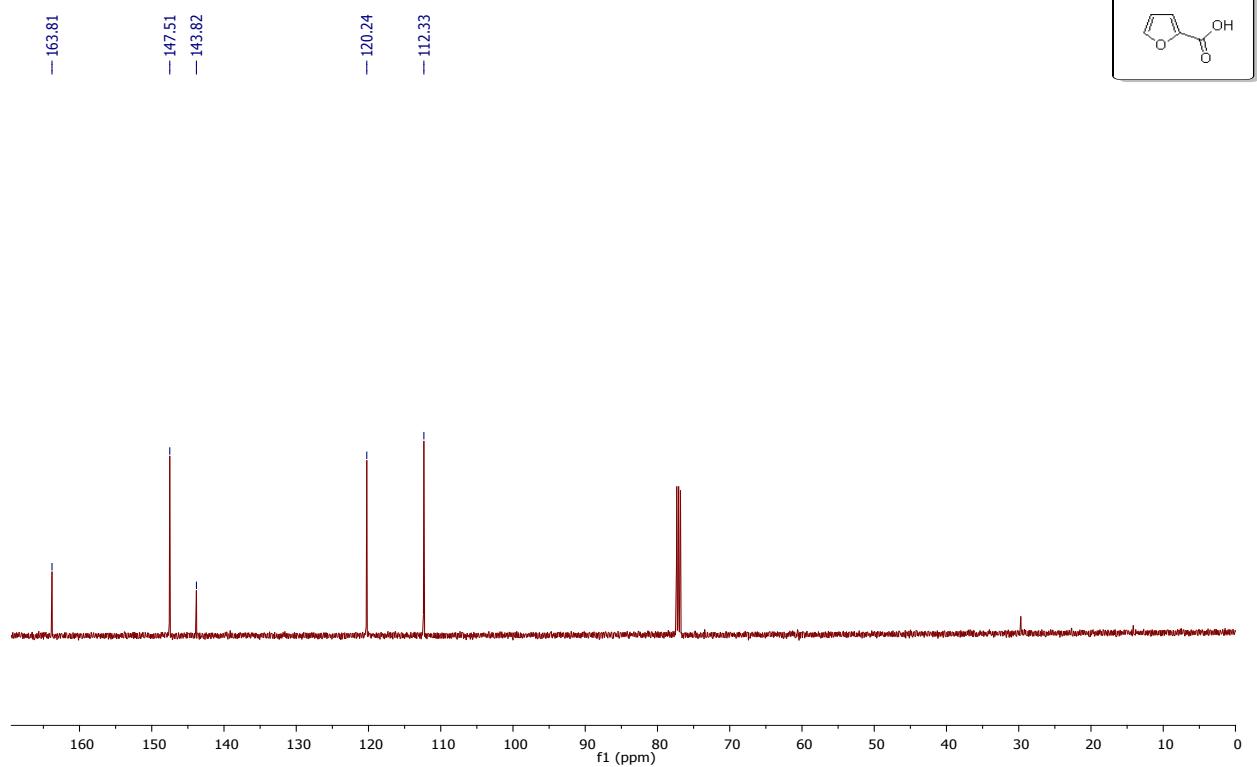


2-Furaic acid (3e):

^1H NMR

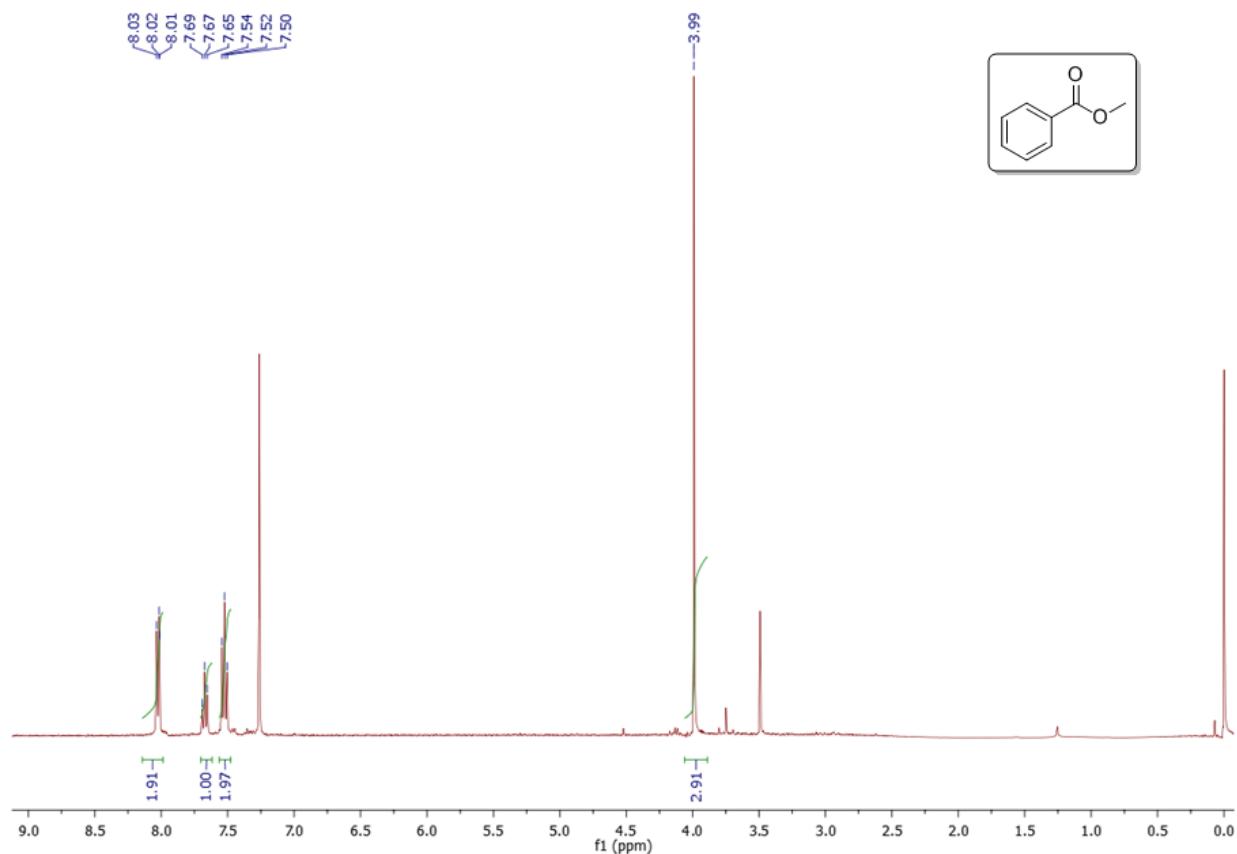


^{13}C NMR



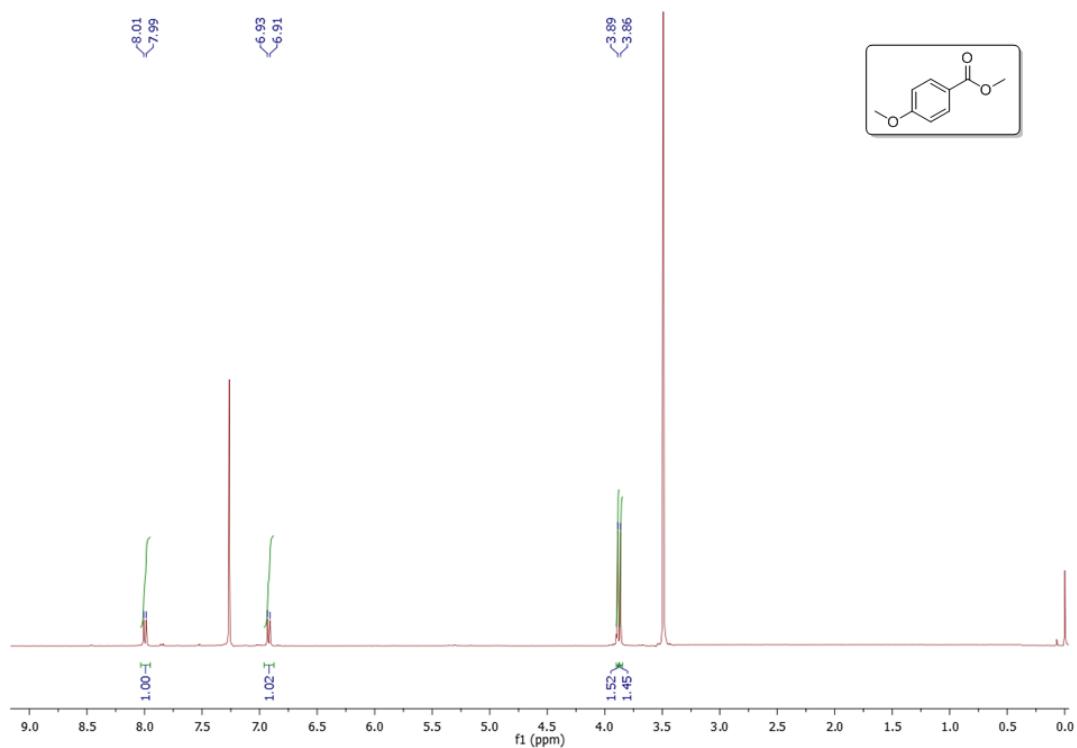
Methyl benzoate (4a):

^1H NMR



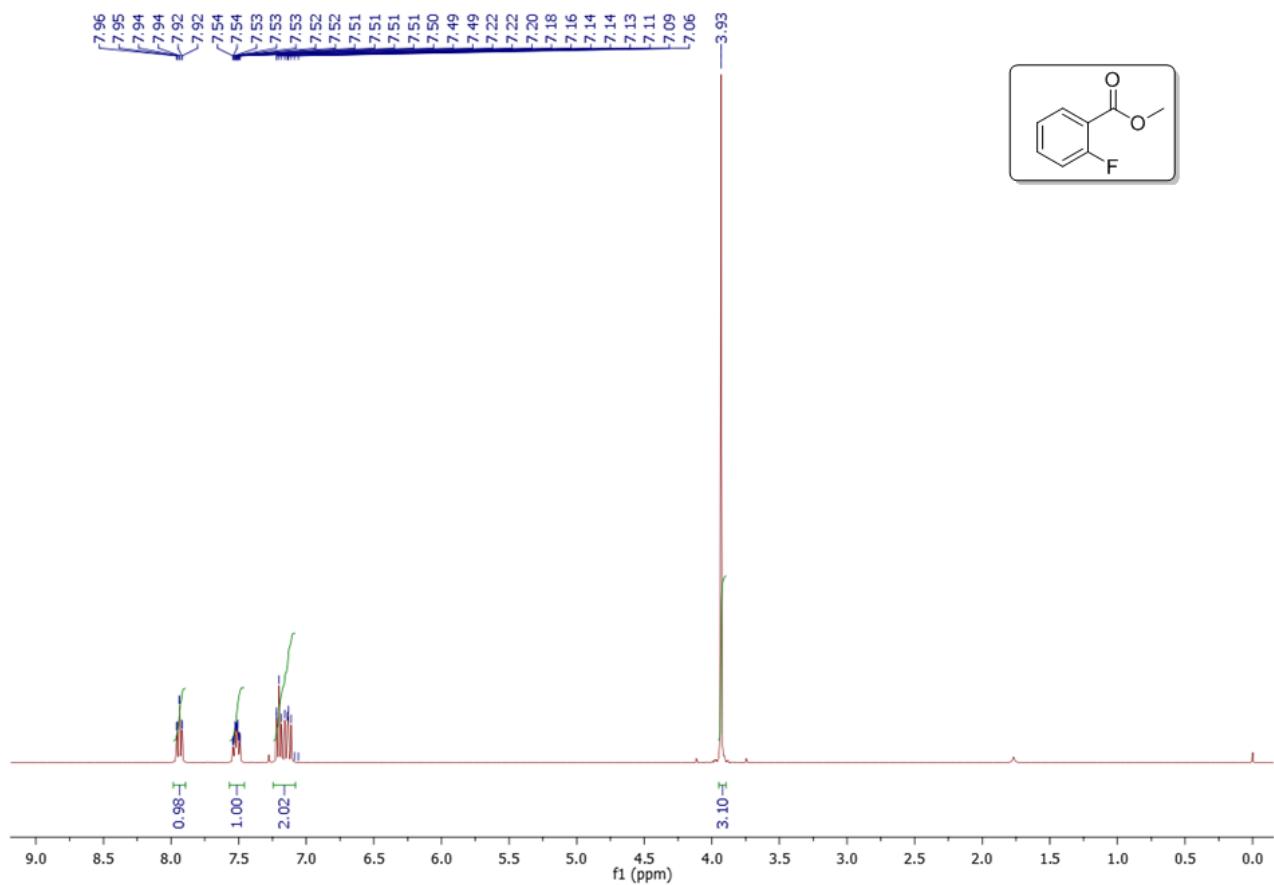
Methyl 4-methoxybenzoate (4b):

^1H NMR



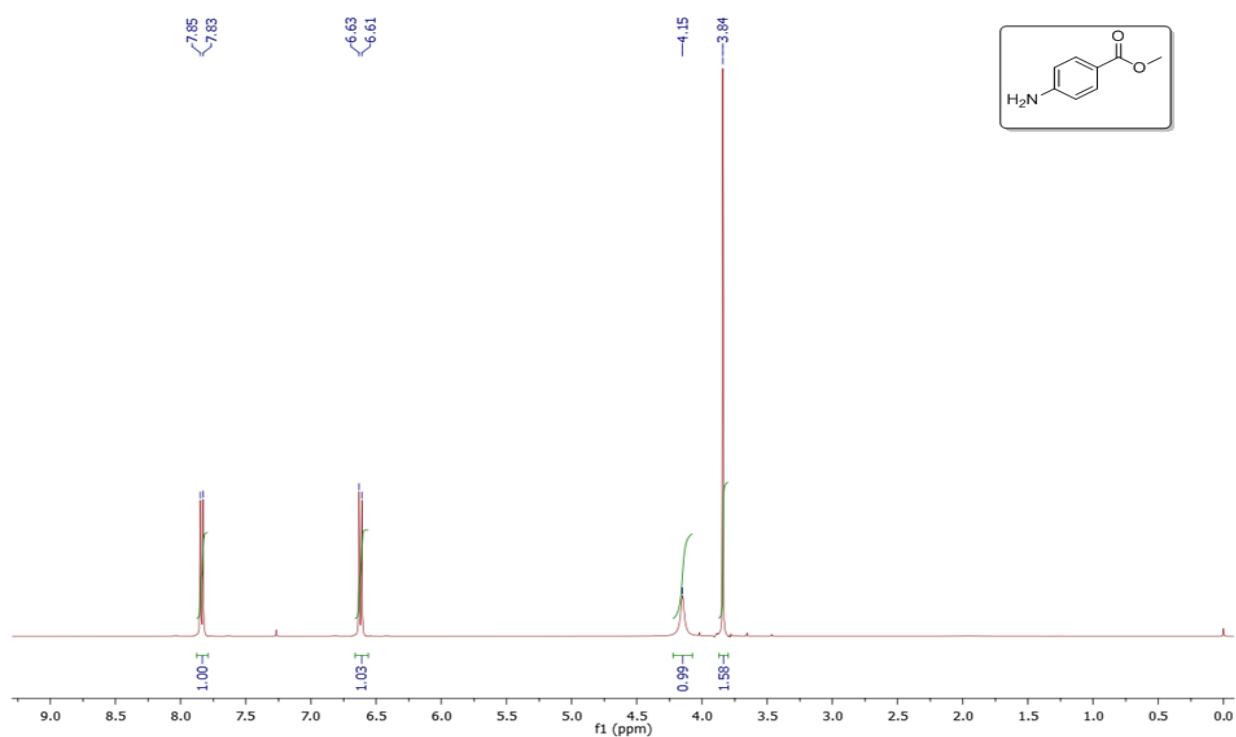
Methyl 2-fluorobenzoate (4c):

¹H NMR

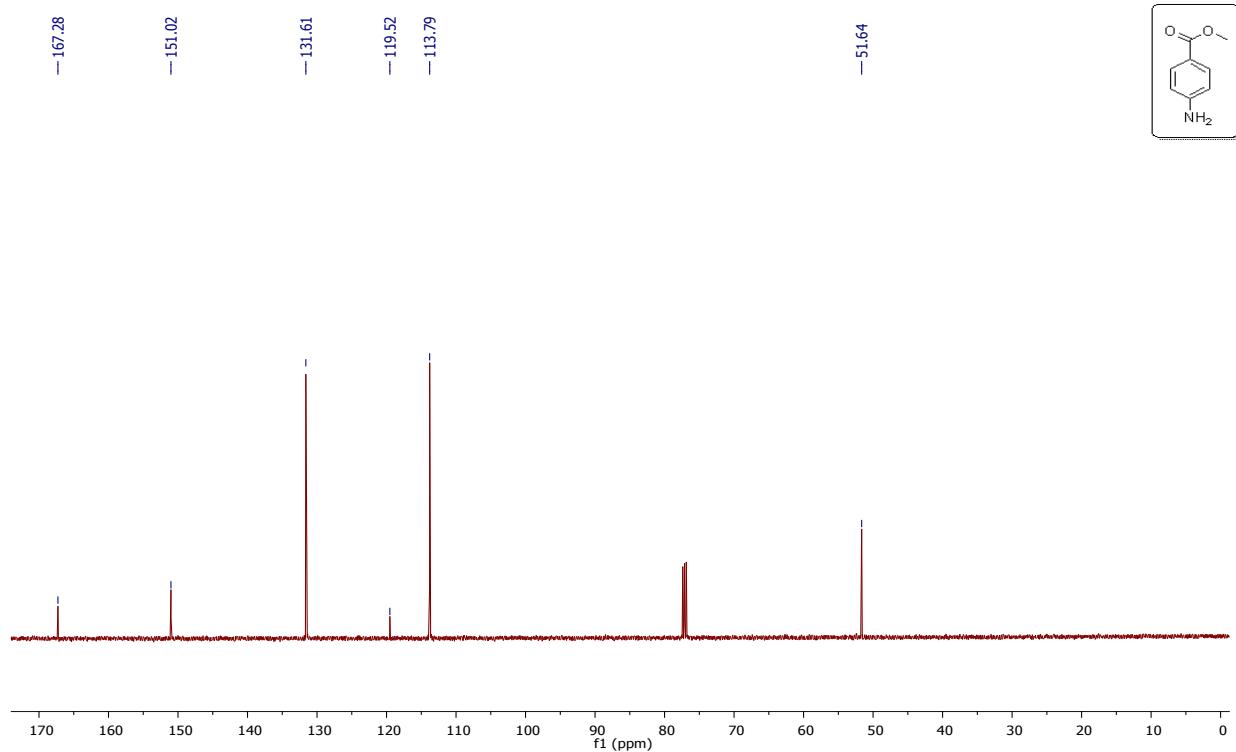


Methyl 4-aminobenzoate (4d):

¹H NMR

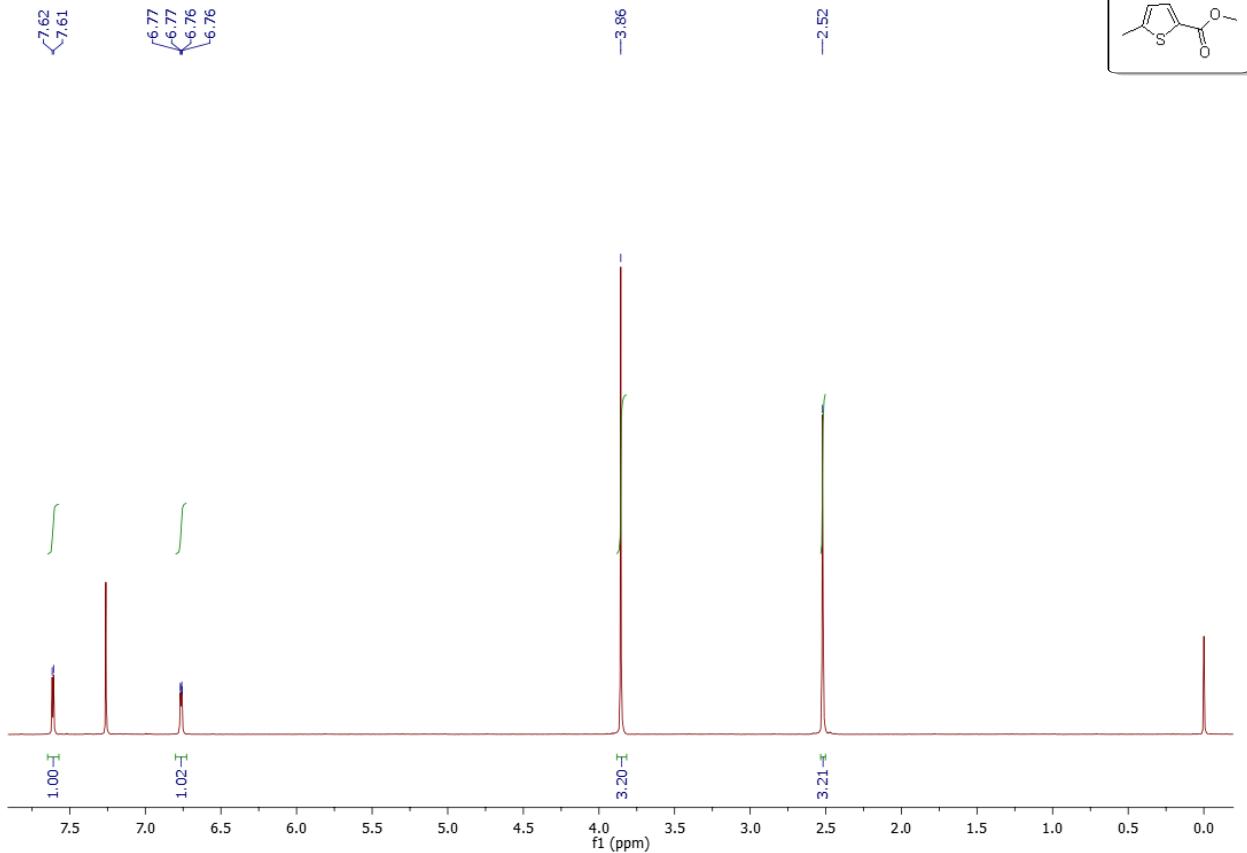


¹³C NMR



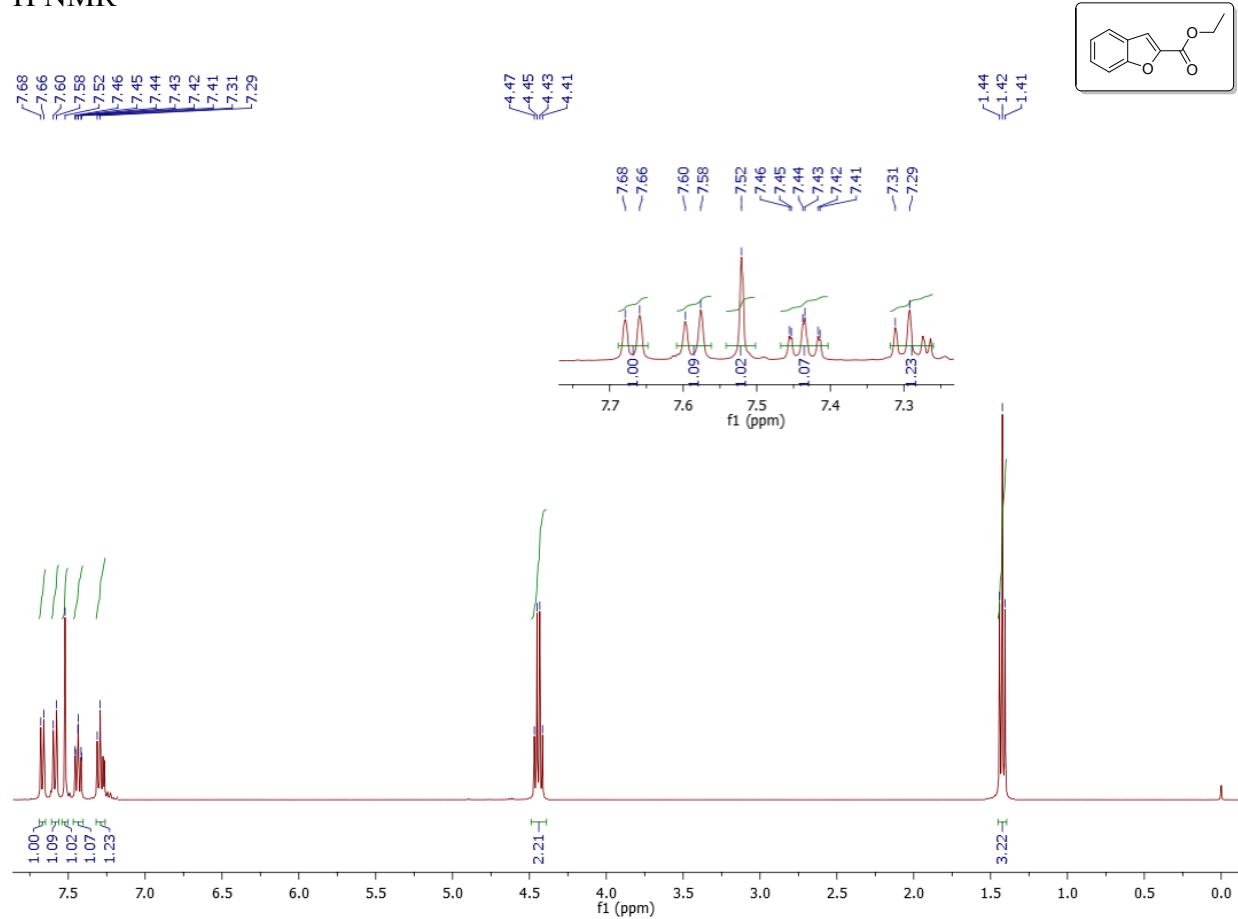
Methyl 5-methylthiophene-2-carboxylate (4e):

^1H NMR



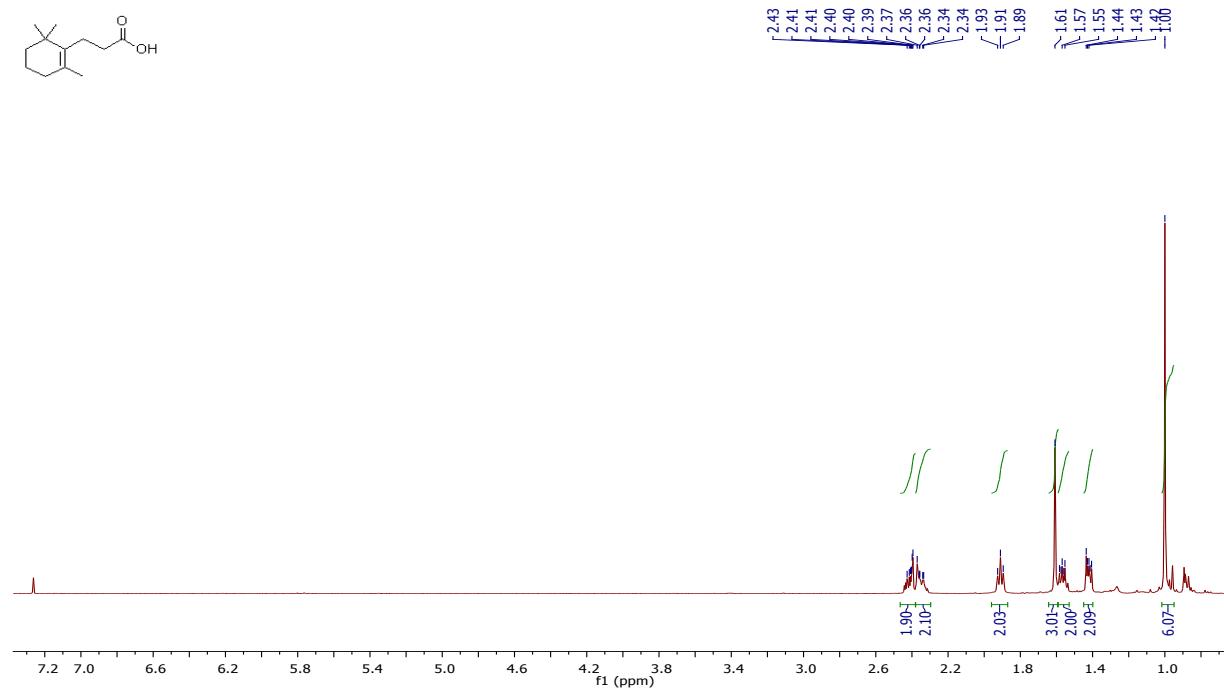
Ethyl benzofuran-2-carboxylate (4f):

¹H NMR

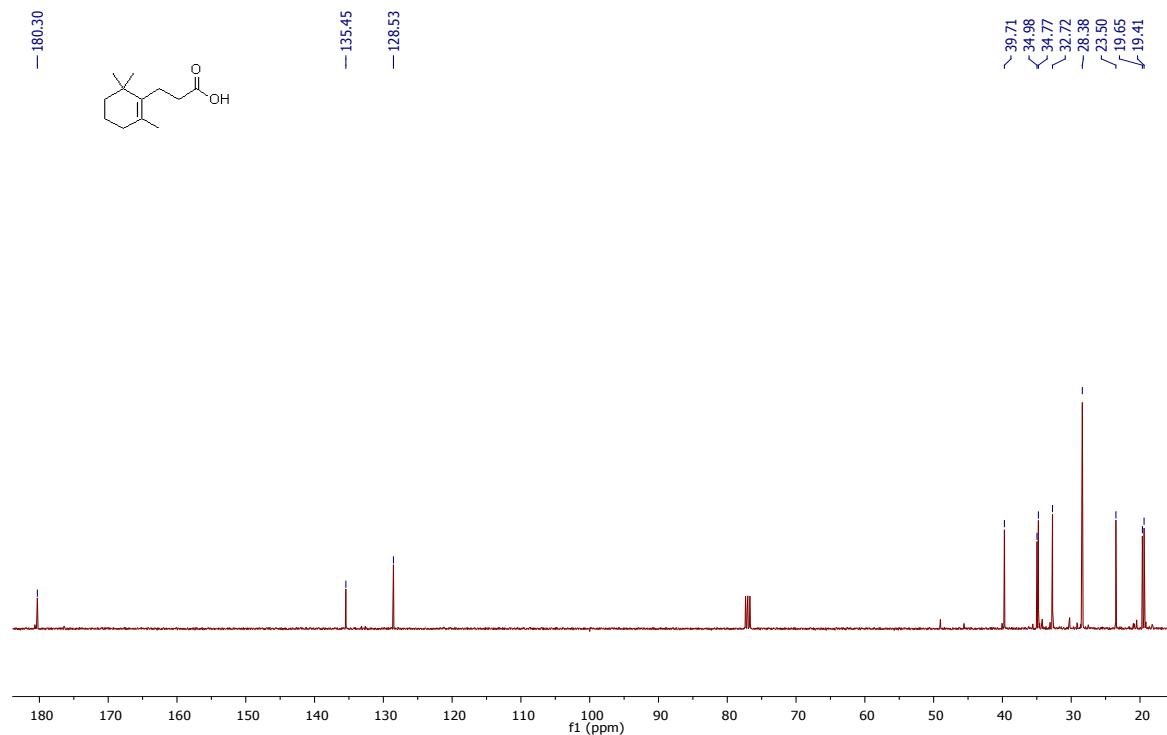


Dihydro β -Ionic Acid (5a):

^1H NMR



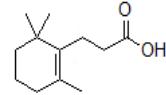
^{13}C NMR



HRMS

Qualitative Compound Report

Data File	L6-INT.d	Sample Name	L6-INT
Sample Type	Sample	Position	Vial 22
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_MS_25072012.m	Acquired Time	9/5/2012 5:43:31 PM
IRM Calibration Status	Success	DA Method	as.m
Comment			

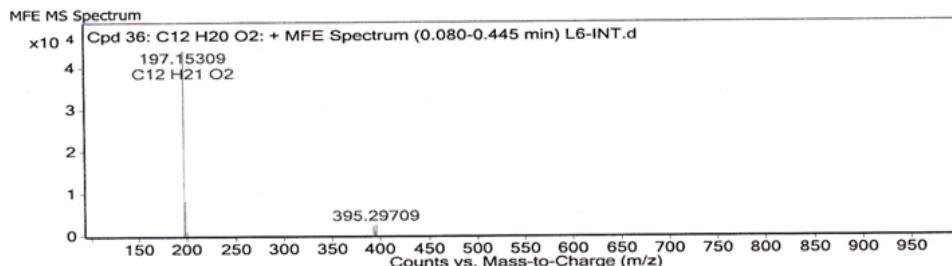


Sample Group Info.

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 36: C12 H20 O2	0.221	196.14582	C12 H20 O2	C12 H20 O2	2.6	C12 H20 O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 36: C12 H20 O2	197.15309	0.221	Find by Molecular Feature	196.14582



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
197.15309	1	43989.6	C12 H21 O2	(M+H)+
198.15685	1	8227.4	C12 H21 O2	(M+H)+
199.16182	1	921.6	C12 H21 O2	(M+H)+
393.29273	1	2343.5		(2M+H)+
394.3047	1	920.7		(2M+H)+
395.29709	1	2393.4		(2M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	197.15309	197.15361	2.59	100	100	82.78	87.32
2	198.15685	198.15702	0.83	18.7	13.3	15.48	11.61
3	199.16182	199.15957	-11.26	2.1	1.22	1.73	1.07

References

1. (a) T. M. Shaikh and F. -E. Hong, *Adv. Synth. Cat.*, 2011, **353**, 1491-1496. (b) T. M. Shaikh and S. Arumugam, *Eur. J. Org. Chem.*, 2008, **29**, 4877–4880. (c) T. H. Nguyen, N. T. T. Chau, A. S. Castanet, K. P. P. Nguyen and J. Mortier, *J. Org. Chem.*, 2007, **72**, 3419-3429. (d) K. Nemoto, H. Yoshida, N. Egusa, N. Morohashi and T. Hattori, *J. Org. Chem.*, 2010, **75**, 7855–7862. (e) C. M. Yang and Y. T. Chung, *Tetrahedron Lett.*, 2014, **55**, 5548-5550. (f) S. Kumar, S. K. Dixit and S. K. Awasthi, *Tetrahedron Lett.*, 2014, **55**, 3802–3804. (g) C. Boersch, E. Merkul and T. J. J. Müller, *Angew. Chem., Int. Ed.*, 2011, **50**, 10448 –10452. (h) B. Pieber, T. Glasnov and C. O. Kappe, *RSC Adv.*, 2014, **4**, 13430-13433.(i) H. -S. Li, G. Liu, *J.Org. Chem.*, 2014, **79**, 509-516.(j) Zheng, R.; Zhou, Q.; Gu, H.; Jiang, H., Wu, J.; Jin, Z.; Han, D.; Dai, G.; Chen, R. *Tetrahedron Letters* 2014, **55**, 5671-5880. (k) Q. Jiang, A. Zhao, B. Xu, J. Jia, X. Liu, and C. Guo, *J. Org. Chem.*, 2014, **79**, 2709–2715. (l) C. D. Gabbott, B. M. Heron, A. C. Instone, P. N. Horton, M. B. Hursthouse, *Tetrahedron.*, 2005, **61**, 463-471.
2. (a) Q. Jiang, A. Zhao, B. Xu, J. Jia, X. Liu, and C. Guo, *J. Org. Chem.*, 2014, **79**, 2709–2715. (b) X. -F. Bai, F. Ye, L. -S. Zheng, G. -Q. Lai, C. -G. Xia, L. -W. Xu, *Chem. Commun.* 2012, **48**, 8592-8594. (c) H. Jia, G. Dai, J. Weng, Z. Zhang, Q. Wang, F. Zhou, L. Jiao, Y. Cui, Y. Ren, S. Fan, J. Zhou, W. Qing, Y. Gu, J. Wang, Y. Sai, W. Su, *Journal of Medicinal Chemistry* 2014, **57**, 7577-7589.(d) X. Lei, C.-H. Jiang, X. Wen, Q.-L. Xu, H. Sun, *RSC Advances* 2015, **5**, 14953-14957. (e) R.A.Vishwakarma, S.D. Sawant, P.P. Singh, A.H. Dar, P.R.Sharma, A.K .Saxena, A..Nargotra, K.A. Arvind, M. Ramesh, A.K .Qazi, A. Hussain, C. Nuyan, US 20150051173 A1, 2015.