Electronic supplementary Information

A waste-minimized protocol for the electrochemical reductive amination and its environmental assessment.

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1. General Remarks

General Remarks: Unless otherwise stated, all chemicals were purchased and used without any further purification. GLC analyses were performed by using Hewlett-Packard HP 5890 SERIES II equipped with a capillary column DB-5MS (30 m, 0.32 mm), a flame ionization detector (FID), and helium or nitrogen as gas carrier. GC-EIMS analyses were carried out by using a Hewlett-Packard HP 6890 N Network GC system/5975 mass selective detector equipped with an electron impact ionizer at 70 eV. Melting points were measured on a Büchi 510 apparatus. NMR spectra were recorded on a Bruker DRXADVANCE 400 MHz (^{1}H at 400 MHz, ^{13}C at 100.6 MHz and ^{19}F at 376.4 MHz) in $CDCl_3$, d6-DMSO, Methanol-d6. Chemical shifts are reported in ppm (δ), coupling constant (J) in Hertz, and multiplicity are reported as follows: s=singlet, bs=broad singlet, d=doublet, dd=double doublet, td=double triplet, t=triplet, m=multiplet. Elemental analysis (EA) was conducted on Elementar UNICUBE® elemental analyzer. Electrodes were polished using polishing pad and Al_2O_3 powder. The experimental apparatus consists of a reactor, a common laboratory plate used for magnetic stirring and a programmable DC power supply AXIOMET (AX-3003P). The reactor was built by adapting an aluminium electrode and a graphite electrode (surface inside the vial of 4.5 cm x 0.5 cm; electrode distance 0.6 cm) to a common vial cap. The system was then sealed externally with silicone. The reaction is carried out by adapting the aluminium electrode to the anode and the graphite electrode to the cathode.

2. General Procedures

General procedure A: In a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), aldehyde **1a-n** (3 mmol), amine **2a-k** (3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3a-w** (91-73% yield).

General procedure B: In a 8 mL vial equipped with a cap and a magnetic stirrer add ketone **1j-m** (3 mmol) and amine **2a** (3 mmol). Let the mixture stir at 90°C for 5 hours. After this time, let the reaction mixture cool to room temperature, then equip the vial with a two electrodes system (aluminium anode and graphite cathode). Add tetraethylammonium bromide (627.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile: water (84% w/w acetonitrile), then electrolyze the resulting mixture in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the crude product. The crude product is further purified by adding HCl (aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate:petroleum ether (1:9) in order to obtain hydrochloride salt product **3q-t** (62-51% yield) as white crystal.

General procedure gram-scale synthesis: In a 50mL flask equipped with a magnetic stirrer, an ice-bath and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (15 mmol), aldehyde **1c** (30 mmol), amine **2a** (30 mmol) and 30 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 1.5 A under stirring at room temperature until 3 F/ mol of current were passed (ca. 100 minutes). After reaction completion, the mixture was distilled using a simple distillation apparatus. The acetonitrile : water azeotrope was recovered at 82%. The residue was then diluted in 100 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process. The obtained mixture was then distilled and ethyl acetate was recovered at 85%, giving the product **3c** as a yellow oil (78% yield).

3. E-factor calculations

E-factor N-benzylbutan-1-amine (3a)

E-factor (without solvent recovery) = [0.31836g(**1a**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.41631g(product **3a**)] / [0.41631g(product **3a**)] = **29.34**

E-factor (within solvent recovery) = [0.31836g(**1a**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.41631g(product **3a**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.41631g(product **3a**)] = **6.11**

E-factor N-(4-fluorobenzyl)butan-1-amine (3b)

E-factor (without solvent recovery) = [0.37233g(**1b**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.49482g(product **3b**)] / [0.49482g(product **3b**)] = **24.63**

E-factor (within solvent recovery) = [0.37233g(**1b**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.49482g(product **3b**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.49482g(product **3b**)] = **5.09**

E-factor N-(4-chlorobenzyl)butan-1-amine (3c)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.51603g(product **3c**)] / [0.51603g(product **3c**)] = **23.68**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.51603g(product **3c**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.51603g(product **3c**)] = **4.94**

E-factor N-(3-fluorobenzyl)butan-1-amine (3d)

E-factor (without solvent recovery) = [0.37233g(**1d**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.42957g(product **3d**)] / [0.42957g(product **3d**)] = **28.53**

E-factor (within solvent recovery) = [0.37233g(**1d**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.42957g(product **3d**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.42957g(product **3d**)] = **6.02**

E-factor N-(3-methoxybenzyl)butan-1-amine (3e)

E-factor (without solvent recovery) = [0.40845g(**1e**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.43491g(product **3e**)] / [0.43491g(product **3e**)] = **28.25**

E-factor (within solvent recovery) = [0.40845g(**1e**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.43491g(product **3e**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.43491g(product **3e**)] = **6.02**

E-factor N-(4-propoxybenzyl)butan-1-amine (3f)

E-factor (without solvent recovery) = [0.4926g(**1f**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50466g(product **3f**)] / [0.50466g(product **3f**)] = **24.37**

E-factor (within solvent recovery) = [0.4926g(**1f**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50466g(product **3f**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.50466g(product **3f**)] = **5.21**

E-factor N-(2-methylbenzyl)butan-1-amine (3g)

E-factor (without solvent recovery) = [0.36045g(**1g**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.38826g(product **3g**)] / [0.38826g(product **3g**)] = **31.62**

E-factor (within solvent recovery) = [0.36045g(**1g**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.38826g(product **3g**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.38826g(product **3g**)] = **6.74**

E-factor N-(naphthalen-2-ylmethyl)butan-1-amine (3h)

E-factor (without solvent recovery) = [0.46854g(**1h**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.49278g(product **3h**)] / [0.49278g(product **3h**)] = **24.92**

E-factor (within solvent recovery) = [0.46854g(**1h**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.49278g(product **3h**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.49278g(product **3h**)] = **5.32**

E-factor N-(4-chlorobenzyl)hexan-1-amine (3i)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.30357g(**2b**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.54861g(product **3i**)] / [0.54861g(product **3i**)] = **22.36**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.30357g(**2b**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.54861g(product **3i**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.54861g(product **3i**)] = **4.74**

E-factor N-(4-chlorobenzyl)pentan-1-amine (3j)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.26151g(**2c**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50181g(product **3j**)] / [0.50181g(product **3j**)] = **24.46**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.26151g(**2c**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50181g(product **3j**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.50181g(product **3j**)] = **5.19**

E-factor N-(4-chlorobenzyl)octan-1-amine (3k)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.38775g(**2d**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.62436g(product **3k**)] / [0.62436g(product **3k**)] = **19.67**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.38775g(**2d**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.62436g(product **3k**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.62436g(product **3k**)] = **4.18**

E-factor N-(4-chlorobenzyl)-2,4,4-trimethylpentan-2-amine (3l)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.38775g(**2e**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.63198g(product **3l**)] / [0.63198g(product **3l**)] = **19.42**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.38775g(**2e**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.63198g(product **3l**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.63198g(product **3l**)] = **4.12**

E-factor N-(4-chlorobenzyl)propan-2-amine (3m)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.17733g(**2f**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.46287g(product **3m**)] / [0.46287g(product **3m**)] = **26.42**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.17733g(**2f**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.46287g(product **3m**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.46287g(product **3m**)] = **5.53**

E-factor N-(4-chlorobenzyl)cyclohexan-1-amine (3n)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.29754g(**2g**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.59067g(product **3n**)] / [0.59067g(product **3n**)] = **20.70**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.29754g(**2g**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.59067g(product **3n**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.59067g(product **3n**)] = **4.32**

E-factor N-(4-chlorobenzyl)cyclopentan-1-amine (3o)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.25545g(**2h**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50961g(product **3o**)] / [0.50961g(product **3o**)] = **24.06**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.25545(**2h**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.50961g(product **3o**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.50961g(product **3o**)] = **5.09**

E-factor N-benzyl-1-(4-chlorophenyl)methanamine (3p)

E-factor (without solvent recovery) = [0.42171g(**1c**) + 0.32148g(**2i**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.59784g(product **3p**)] / [0.59784g(product **3p**)] = **20.48**

E-factor (within solvent recovery) = [0.42171g(**1c**) + 0.32148g(**2i**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.59784g(product **3p**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.59784g(product **3p**)] = **4.30**

E-factor N-(1-phenylethyl)butan-1-amine (3q)

E-factor (without solvent recovery) = [0.36045g(**1i**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.32976g(product **3q**)] / [0.32976g(product **3q**)] = **37.42**

E-factor (within solvent recovery) = [0.36045g(**1i**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.32976g(product **3q**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.32976g(product **3q**)] = **8.11**

E-factor N-(1-(p-tolyl)ethyl)butan-1-amine (3r)

E-factor (without solvent recovery) = [0.40254g(**1j**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.33291g(product **3r**)] / [0.33291g(product **3r**)] = **37.19**

E-factor (within solvent recovery) = [0.40254g(**1j**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.33291g(product **3r**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.33291g(product **3r**)] = **8.15**

E-factor N-(1-(4-chlorophenyl)ethyl)butan-1-amine (3s)

E-factor (without solvent recovery) = [0.46377g(**1k**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.32244g(product **3s**)] / [0.32244g(product **3s**)] = **38.62**

E-factor (within solvent recovery) = [0.46377g(**1k**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.32244g(product **3s**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.32244g(product **3s**)] = **8.64**

E-factor N-(1-(naphthalen-1-yl)ethyl)butan-1-amine (3t)

E-factor (without solvent recovery) = [0.51063g(**1l**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.36150g(product **3t**)] / [0.36150g(product **3t**)] = **34.47**

E-factor (within solvent recovery) = [0.51063g(**1l**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.36150g(product **3t**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.36150g(product **3t**)] = **7.73**

E-factor N-butylfurfurylamine (3u)

E-factor (without solvent recovery) = [0.28827g(**1m**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.34017g(product **3u**)] / [0.34017g(product **3u**)] = **36.04**

E-factor (within solvent recovery) = [0.28827g(**1m**) + 0.21942g(**2a**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.34017g(product **3u**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.34017g(product **3u**)] = **7.62**

E-factor clobenzorex (3v)

E-factor (without solvent recovery) = [0.42171g(**1n**) + 0.40563g(**2j**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.69320g(product **3v**)] / [0.69320g(product **3v**)] = **17.64**

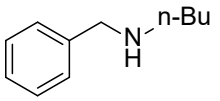
E-factor (without solvent recovery) = [0.42171g(**1n**) + 0.40563g(**2j**) + 0.63048g(TEABr) + 2.442g(azeotrope) + 9.02g(ethyl acetate) – 0.69320g(product **3v**) – 2.002g(azeotrope recovered) – 7.667g(ethyl acetate recovered)] / [0.69320g(product **3v**)] = **3.69**

E-factor gram-scale synthesis (3c)

E-factor (without solvent recovery) = [4.2171g(**1c**) + 2.1942g(**2a**) + 3.1524g(TEABr) + 24.42g(azeotrope) + 90.20g(ethyl acetate) – 4.6263g(product **3c**)] / [4.6263g(product **3c**)] = **25.83**

E-factor (within solvent recovery) = [4.2171g(**1c**) + 2.1942g(**2a**) + 3.1524g(TEABr) + 24.42g(azeotrope) + 90.20g(ethyl acetate) – 4.6263g(product **3c**) – 20.024g(azeotrope recovered) – 76.67g(ethyl acetate recovered)] / [4.6263g(product **3c**)] = **4.95**

4. E-factor table



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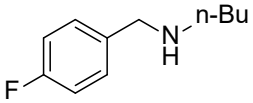

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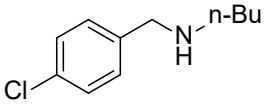

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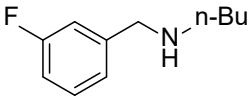

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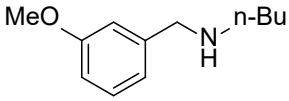

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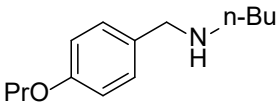

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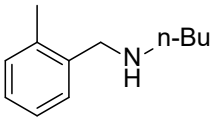

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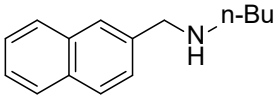

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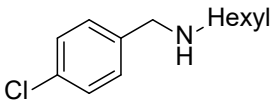

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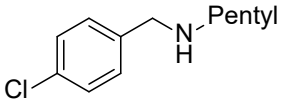

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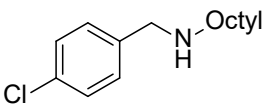

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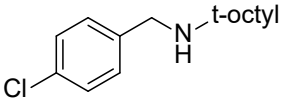
4.18



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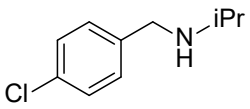
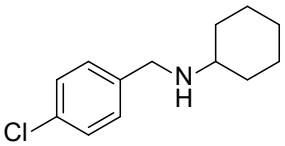
4.12



3m
5.53



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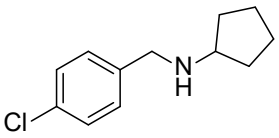
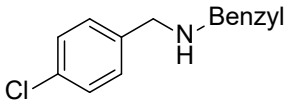
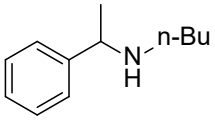
4.32



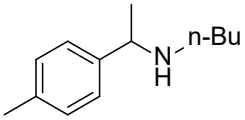
3o
5.09



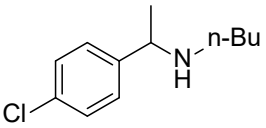
3p
4.30



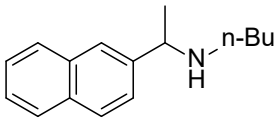
3q
8.11



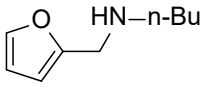
3r
8.15



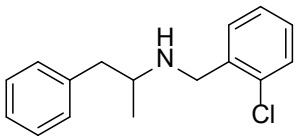
3s
8.64



3t
7.73



3u
7.62



3v
3.69

5. Ecoscale data

Org. Biomol. Chem., 2020, **18**, 5832 (Electrochemical)

Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		Benzaldehyde	C7H6O	106.12404	1.05	100%	0.050476	0.053	0.499415589	Infinity
2		p-Toluidine	C7H9N	107.15516		100%	0	0.064	0.597264751	Infinity
3		Tetrabutylammonium hydrogen sulfate	C16H35N . H2S	339.53408		100%	0	0.169	0.497740904	Infinity
4		DMSO	C2H6OS	78.12904	1.1	100%	5	5.5	70.39635966	Infinity
5		Water	H2O	18.01528	1	100%	10	10	555.0843506	Infinity
6		Ethyl acetate	C4H8O2	88.10632	0.902	100%	5	4.51	51.18815540	Infinity

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Reductive Amination Product	C14H15N	197.28	0.097	0.491686942	0	0

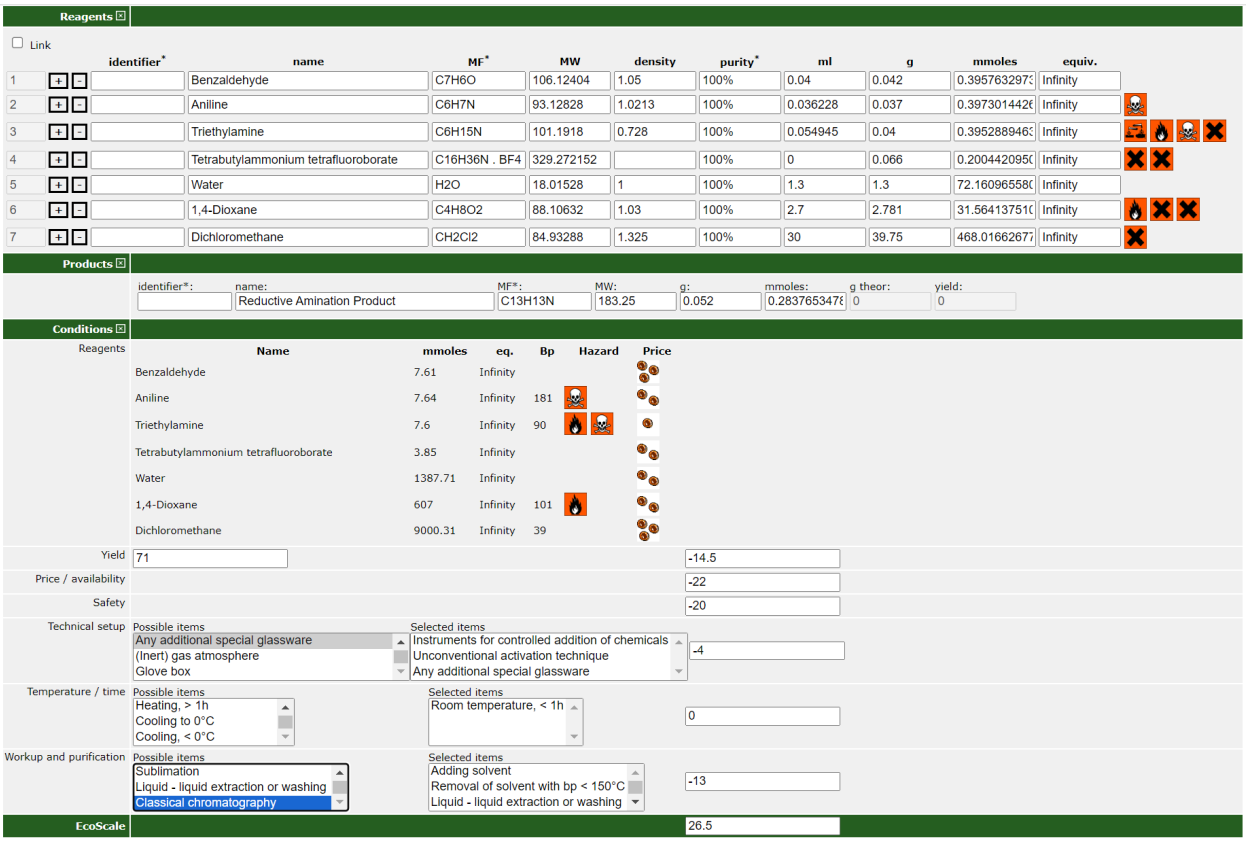
Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
Benzaldehyde	5.14	Infinity	179		
p-Toluidine	6.15	Infinity	200		
Tetrabutylammonium hydrogen sulfate	5.13	Infinity			
DMSO	725.73	Infinity	189		
Water	5722.51	Infinity			
Ethyl acetate	527.71	Infinity	75		

Yield	98		-1
Price / availability			-19
Safety			-15
Technical setup	Possible items: Pressure equipment, > 1 atm; Any additional special glassware; (Inert) gas atmosphere	Selected items: Unconventional activation technique; Any additional special glassware	-3
Temperature / time	Possible items: Heating, > 1h; Cooling to 0°C; Cooling, < 0°C	Selected items: Room temperature, < 24h	-1
Workup and purification	Possible items: Sublimation; Liquid - liquid extraction or washing; Classical chromatography	Selected items: Removal of solvent with bp < 150°C; Liquid - liquid extraction or washing; Classical chromatography	-13
EcoScale			48

Org.Lett. 2023, **25**, 432 (Electrochemical)



Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		Benzaldehyde	C7H6O	106.12404	1.05	100%	0.04	0.042	0.395763297	Infinity
2		Aniline	C6H7N	93.12828	1.0213	100%	0.036228	0.037	0.397301442	Infinity
3		Triethylamine	C6H15N	101.1918	0.728	100%	0.054945	0.04	0.395288946	Infinity
4		Tetrabutylammonium tetrafluoroborate	C16H36N . BF4	329.272152		100%	0	0.066	0.200442095	Infinity
5		Water	H2O	18.01528	1	100%	1.3	1.3	72.16096558	Infinity
6		1,4-Dioxane	C4H8O2	88.10632	1.03	100%	2.7	2.781	31.56413751	Infinity
7		Dichloromethane	CH2Cl2	84.93288	1.325	100%	30	39.75	468.0166267	Infinity

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Reductive Amination Product	C13H13N	183.25	0.052	0.283765347	0	0

Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
Benzaldehyde	7.61	Infinity			
Aniline	7.64	Infinity	181		
Triethylamine	7.6	Infinity	90		
Tetrabutylammonium tetrafluoroborate	3.85	Infinity			
Water	1387.71	Infinity			
1,4-Dioxane	607	Infinity	101		
Dichloromethane	9000.31	Infinity	39		

Yield	71	-14.5
Price / availability		-22
Safety		-20

Technical setup

Possible items: Any additional special glassware; (Inert) gas atmosphere; Glove box

Selected items: Instruments for controlled addition of chemicals; Unconventional activation technique; Any additional special glassware

-4

Temperature / time

Possible items: Heating, > 1h; Cooling to 0°C; Cooling, < 0°C

Selected items: Room temperature, < 1h

0

Workup and purification

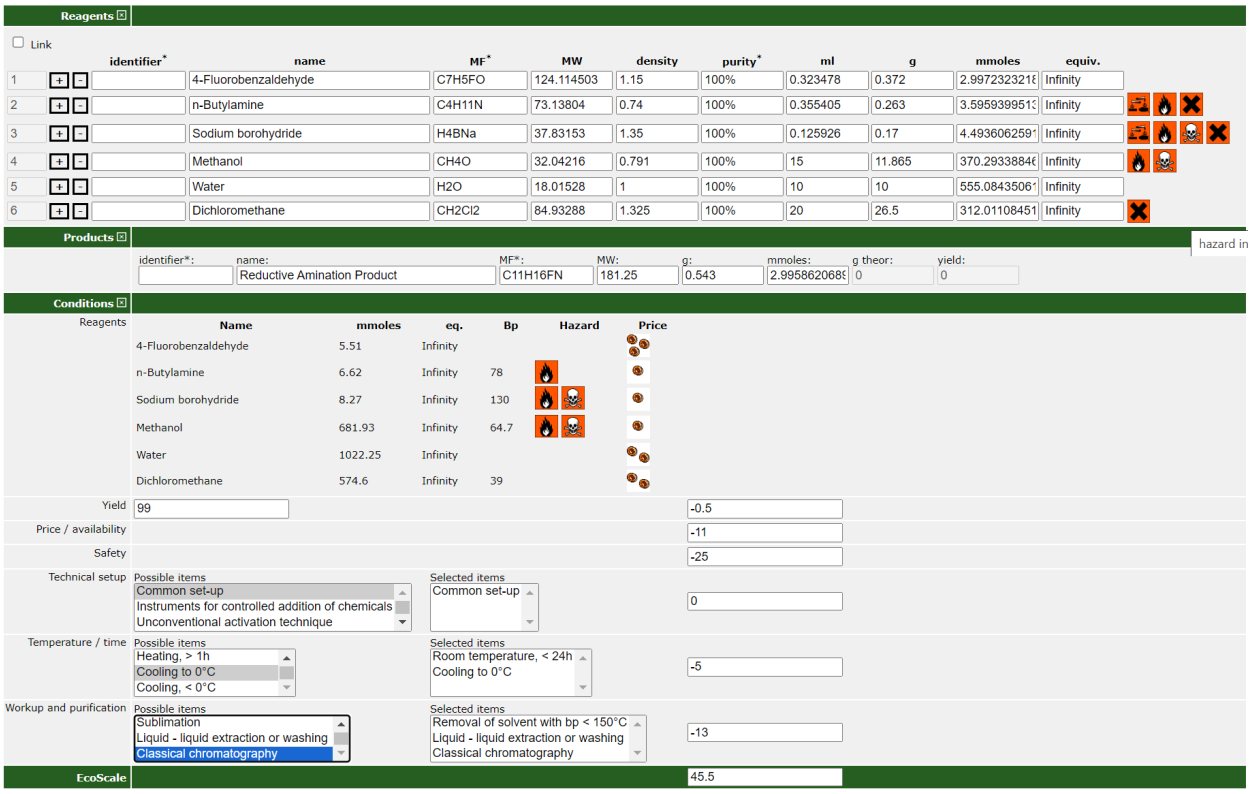
Possible items: Sublimation; Liquid - liquid extraction or washing; Classical chromatography

Selected items: Adding solvent; Removal of solvent with bp < 150°C; Liquid - liquid extraction or washing

-13

EcoScale 26.5

J. Org. Chem. 2019, **84**, 1421 (with NaBH4)



Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		4-Fluorobenzaldehyde	C7H5FO	124.114503	1.15	100%	0.323478	0.372	2.997232321	Infinity
2		n-Butylamine	C4H11N	73.13804	0.74	100%	0.355405	0.263	3.595939951	Infinity
3		Sodium borohydride	H4BNa	37.83153	1.35	100%	0.125926	0.17	4.493606259	Infinity
4		Methanol	CH4O	32.04216	0.791	100%	15	11.865	370.2933884	Infinity
5		Water	H2O	18.01528	1	100%	10	10	555.0843506	Infinity
6		Dichloromethane	CH2Cl2	84.93288	1.325	100%	20	26.5	312.01108451	Infinity

Products

hazard in

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Reductive Amination Product	C11H16FN	181.25	0.543	2.995862068	0	0

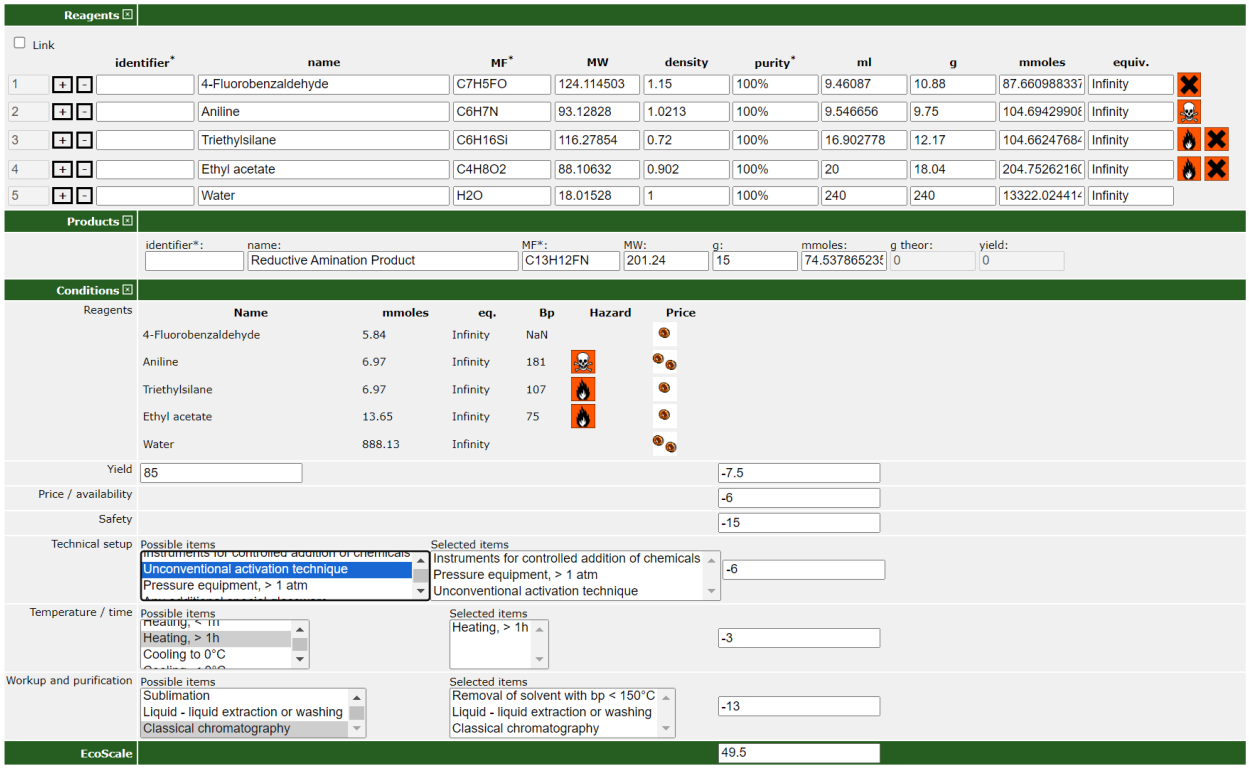
Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
4-Fluorobenzaldehyde	5.51	Infinity			
n-Butylamine	6.62	Infinity	78		
Sodium borohydride	8.27	Infinity	130		
Methanol	681.93	Infinity	64.7		
Water	1022.25	Infinity			
Dichloromethane	574.6	Infinity	39		

Yield	99	-0.5
Price / availability		-11
Safety		-25
Technical setup	Possible items: Common set-up; Instruments for controlled addition of chemicals; Unconventional activation technique — Selected items: Common set-up	0
Temperature / time	Possible items: Heating, > 1h; Cooling to 0°C; Cooling, < 0°C — Selected items: Room temperature, < 24h; Cooling to 0°C	-5
Workup and purification	Possible items: Sublimation; Liquid - liquid extraction or washing; Classical chromatography — Selected items: Removal of solvent with bp < 150°C; Liquid - liquid extraction or washing; Classical chromatography	-13
EcoScale		45.5

Green Chem., 2021, **23**, 5625 (in flow with Et3SiH)



Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		4-Fluorobenzaldehyde	C7H5FO	124.114503	1.15	100%	9.46087	10.88	87.660983337	Infinity
2		Aniline	C6H7N	93.12828	1.0213	100%	9.546656	9.75	104.69429908	Infinity
3		Triethylsilane	C6H16Si	116.27854	0.72	100%	16.902778	12.17	104.66247684	Infinity
4		Ethyl acetate	C4H8O2	88.10632	0.902	100%	20	18.04	204.75262160	Infinity
5		Water	H2O	18.01528	1	100%	240	240	13322.024414	Infinity

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Reductive Amination Product	C13H12FN	201.24	15	74.537865235	0	0

Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
4-Fluorobenzaldehyde	5.84	Infinity	NaN		
Aniline	6.97	Infinity	181		
Triethylsilane	6.97	Infinity	107		
Ethyl acetate	13.65	Infinity	75		
Water	888.13	Infinity			

Yield: 85 → -7.5

Price / availability → -6

Safety → -15

Technical setup

Possible items: Unconventional activation technique; Pressure equipment, > 1 atm

Selected items: Instruments for controlled addition of chemicals; Pressure equipment, > 1 atm; Unconventional activation technique → -6

Temperature / time

Possible items: Heating, > 1h; Cooling to 0°C

Selected items: Heating, > 1h → -3

Workup and purification

Possible items: Sublimation; Liquid - liquid extraction or washing; Classical chromatography

Selected items: Removal of solvent with bp < 150°C; Liquid - liquid extraction or washing; Classical chromatography → -13

EcoScale → 49.5

This work (Electrochemical)

Reagents

Link

	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1		4-Fluorobenzaldehyde	C7H5FO	124.114503	1.15	100%	3.23777	3.723435	30	Infinity
2		n-Butylamine	C4H11N	73.13804	0.74	100%	2.965055	2.194141	30	Infinity
3		Tetraethylammonium bromide	C8H20BrN	210.1575		100%	0	3.15	14.98875843	Infinity
4		Acetonitrile	CH3CN	41.05252	0.781	100%	32.151088	25.11	611.6555086	Infinity
5		Water	H2O	18.01528	1	100%	4.89	4.89	271.4362474	Infinity
6		Ethyl acetate	C4H8O2	88.10632	0.902	100%	100	90.2	1023.763108	Infinity

Products

identifier*:	name:	MF*:	MW:	g:	mmoles:	g theor:	yield:
	Reductive Amination Product	C11H16FN	181.25	4.24	23.39310344	0	0

Conditions

Reagents

Name	mmoles	eq.	Bp	Hazard	Price
4-Fluorobenzaldehyde	7.07	Infinity			
n-Butylamine	7.07	Infinity	78		
Tetraethylammonium bromide	3.53	Infinity			
Acetonitrile	144.25	Infinity	81		
Water	64.01	Infinity			
Ethyl acetate	241.45	Infinity	75		

Yield	78		-11
Price / availability			-5
Safety			-20
Technical setup	Possible items: Any additional special glassware; (Inert) gas atmosphere; Glove box	Selected items: Unconventional activation technique; Any additional special glassware	-3
Temperature / time	Possible items: Heating, > 1h; Cooling to 0°C; Cooling, < 0°C	Selected items: Room temperature, < 24h	-1
Workup and purification	Possible items: Cooling to room temperature; Adding solvent; Simple filtration	Selected items: Simple filtration; Removal of solvent with bp < 150°C; Liquid - liquid extraction or washing	-6
EcoScale			54

6. LCA data and charts

Goal and scope definition

The main aim of the herein presented LCA analysis is to assess the potential environmental impact associated to two different reducing agent ($NaBH_4$ and triethylsilane) and three organic electrolytes (tetraethylammonium bromide, tetrabutylammonium hydrogen sulfate, tetrabutylammonium tetrafluoroborate). To give further insight about the electrochemical method developed, Aluminium used as electrode was assessed as well.

The functional unit was defined as 1 g of the desired target product. At the same time, the system boundary was determined based on a cradle-to-gate approach, considering the emissions and resource exploitation for both the extraction and manufacturing of all materials and energy and the respective process's emissions to water, air, and soil. Moreover, it was assumed that all the processes analysed were performed at one location. The environmental effects caused by transport to provide raw materials, and the impacts of chemical factories have been included.[1]

Inventory analysis

While setting up the LCA analysis, new inventories for different materials had to be created to be included in the model. Given the presence of many data gaps in the literature procedures taken as reference, some assumptions were adopted to construct the dataset.

Generally, for the inventories' construction, a retrosynthetic approach was used, and when not possible because of missing database data or too uncertain secondary data, similar compounds were adopted (e.g., triethylamine instead of t-butylamine, $CaCl_2$ instead of $MgSO_4$ or $NaSO_4$, $NaHCO_3$ instead of Na_2CO_3).

The energy utilized in the procedures under investigation for heating, stirring, evaporating, and pumping is not measured or documented. For these reasons, thermodynamics assumptions considering a proportional watt (W) absorption per hour of heating plates (for T> 25 °C procedures such as reactions and distillations or stirring), heating bath (fixed temperature of 50 °C) and vacuum pump were considered.

When using secondary data to create inventories, if the isolated product yield is missing, a 100% value is assumed. General assumptions were made regarding process energy (0.0002 MJ per g of the compound) and electricity consumption (0.000333 KWh per g of the compound) for all unavailable compounds that had to be specifically modeled.[2]

Moreover, when solvent or additive amounts for solutions preparation or purification steps were missing, the volumes were considered based on our expertise.

The emissions to air during the synthetic processes (0.20% volatile input materials) and air (CO_2), water (river), and sludge emissions after wastewater treatment were calculated as well; No emissions to the soil were determined since no agricultural destination of the digested sludge was considered. In this wastewater treatment, 65.80% of the organic compounds were retained in the sludge, 24.50% were oxidized and emitted to air in the form of CO_2, and the remaining 9.70% were released into the river.[3,4]

Impact assessment

The impact assessment was modelled with SimaPro v9.6.0.1 software, using ReCiPe 20165 Midpoint (H) and Endpoint (H) and. Precisely, 18 impact categories were considered when ReCiPe 2016 method was used (Global warming; Stratospheric ozone depletion; Human carcinogenic; Human non-carcinogenic toxicity; Fine particulate matter; Ionizing radiation; Ozone formation, Human health; Terrestrial acidification; Freshwater eutrophication; Marine eutrophication; Freshwater ecotoxicity; Water consumption; Land use; Fossil resource scarcity; Mineral resource scarcity; Ozone formation, terrestrial ecosystems; Terrestrial ecotoxicity; Marine ecotoxicity).[5]

Midpoint impact categories and endpoint damage areas (Human health, Ecosystems, and Resources) were analysed from a hierarchical perspective over a 100-year period. Long-term emissions, which affect scenarios beyond 100 years, were excluded due to their high uncertainties and their relationship to heavy metal toxicity. Therefore, they are not particularly relevant in organic chemical processing. The results are presented and analysed in midpoints, and the results are weighted and normalized in endpoint damage areas to compare our approach against others by a single indicator as a benchmark of the global environmental impact. In this process, midpoint characterization results are converted to intermediate units to be weighted and normalized to represent, in millipoints (mPts), the relative impact of the results according to their severity in a global context.

Inventories

Inventories for the synthesis processes

Table S1. Synthesis of tetrabutylammonium hydrogen sulfate (patent US3816533)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
tetrabutylammonium hydroxide	1.070153	-	-	-	-
H_2SO_4	0.404499	0.000809	-	-	-
H_2O	1.605229	0.00321	-	1.602018542	-
H_2O (reaction side product)	0.0742356	-	-	0.0742356	-
Chemical factory	4xE-13 p	-	-	-	-
Electricity	0.338257 KWh	-	-	-	-

Table S2. Synthesis of tetrabutylammonium tetrafluoroborate (patent US3816533)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Tetrabutylammonium hydroxide	0.788046	-	-	-	-
H_2O[a] (x TBAH 40%)	1.182069	0.002364	-	1.179704862	-
HBF_4	0.26665	0.000533	-	-	-
H_20[b]	0.26665	0.000533	-	0.2661167	-
Chemical factory	4xE-13 p	-	-	-	-
Electricity	0.389592 KWh	-	-	-	-

[a]Amount calculated to obtain a 40% v/v tetrabutylammonium hydroxide solution; [b]Amount calculated to obtain a 50% v/v HBF_4 solution;

Table S3. Synthesis of triethylsilane (patent CN102050833)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Ethylmagnesium bromide	5.601156 g	-	-	1.339407[b]	1.339407[b]
Trichlorosilane	1.456075 g	0.002912	0.077673[a]	0.030752	0.208607
Diethyl ether	11.703123 g	0.023406	0.023406	2.867264	7.700652
Chemical factory	4xE-13 p	-	-	-	-
Electricity	1.843875 KWh	-	-	-	-

[a]As trichlorosilane; [b] 50% of the unreacted material

Table S4. Synthesis of tetraethylammonium bromide (patent FR3095437 A1)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Bromoethane	0.89848 g	0.00179696	0.08204315	0.03248239	0.22034446
Triethylamine	0.523364 g	0.001046728	-	-	-
Acetonitrile	1.1231 g	0.0022462	0.2751595	0.1089407	0.7389998
Chemical factory	4xE-13 p	-	-	-	-
Electricity	0.198922 KWh	-	-	-	-

Inventories for the needed compounds in the synthesis processes

Table S5. Synthesis of trichlorosilane (directly taken from: *Sustainable Production and Consumption* 2023, **41**, 156–166)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Silicon	0.25	-	-	-	0.1
Air compressed	0.00045 m3	-	-	-	-
H_2O	6.136363	-	-	-	-
Hydrochloric acid	1.670454	-	-	-	-
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Table S6. Synthesis of HBr (patent 6036936)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
H_2	0.012501	-	-	-	-
Br_2	0.987742	-	-	-	-
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Table S7. Synthesis of Bromoethane (DOI: 10.15227/orgsyn.001.0003)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
HBr	0.886025	0.000286	0.035146[b]	0.013914	0.094392
EtOH	0.445152	0.00089	0.005688	0.002252	0.015276
H_2SO_4	0.890305	-	-	0.890305[c]	-
H_2O[a]	0.961351	0.001922	-	0.959429	-
H_2O (reaction side product)	0.16524	-	-	0.16524	-
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]From HBr; [b]As HBr; [c]As sodium sulfate

Table S8. Synthesis of ethylmagnesium bromide (patent CN102050833)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Bromoethane	0.963105	0.001926	-	-	-
Magnesium	0.214692	0.000429	-	-	-
Diethyl ether	2.564267	0.005128	0.628245	0.248733	1.687287
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Table S9. Synthesis of 1-bromobutane (DOI: 10.15227/orgsyn.001.0003)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Water	1.160512	0.002321	-	1.158191	-
HBr	0.76923	0.00153846	0.043813595[b]	0.017346607	0.117670
H_2SO_4	0.993589	0.001987	0.243429[c]	0.096378133	0.653781562
1-butanol	0.56923	0.001138	-	-	-
Na_2CO_3[a]	0.032051	-	-	0.016025[d]	0.016025[d]
$Cacl_2$	0.01282	-	-	0.00641[d]	0.00641[d]
water (reaction side product)	0.131325	-	-	0.131325	-
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a] $NaHCO_3$ used; [b]as HBr; [c]as H_2SO_4; [d]50% of the material

Table S10. Synthesis of tetrabutylammonium bromide (patent FR3095437 A1)

Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
1-Bromobutane	0.72599	0.001452	0.073734465	0.029192829	0.198029706
Triethylamine	0.341194	0.000682	-	-	-
Acetonitrile	0.722525	0.001445	0.177018625	0.070084925	0.47542145
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Table S11. Synthesis of tetrabutylammonium hydroxide (patent FR3095437 A1)

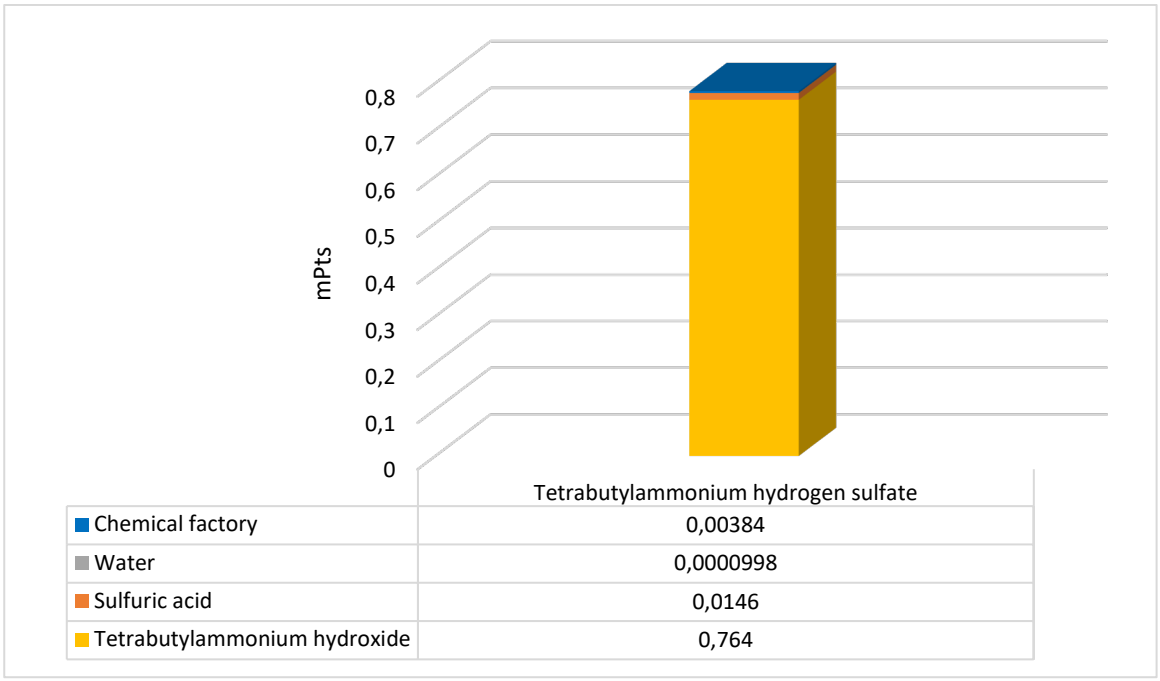
Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Tetrabutylammonium bromide	1.242373	-	-	-	-
Potassium hydroxide	0.621186	-	-	0.202472[a]	0.202472[a]
Methanol	3.105932	0.006212	0.76095334	0.301275404	2.043703256
H_2O	2.795339	0.005591		2.789748	-
KBr (reaction side product)	0.458652	-	-	0.229326[a]	0.229326[a]
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]50% of the unreacted material or produced side product

Table S12. Synthesis of tetrafluoroboric acid (DOI: 10.1055/b-0035-111176)

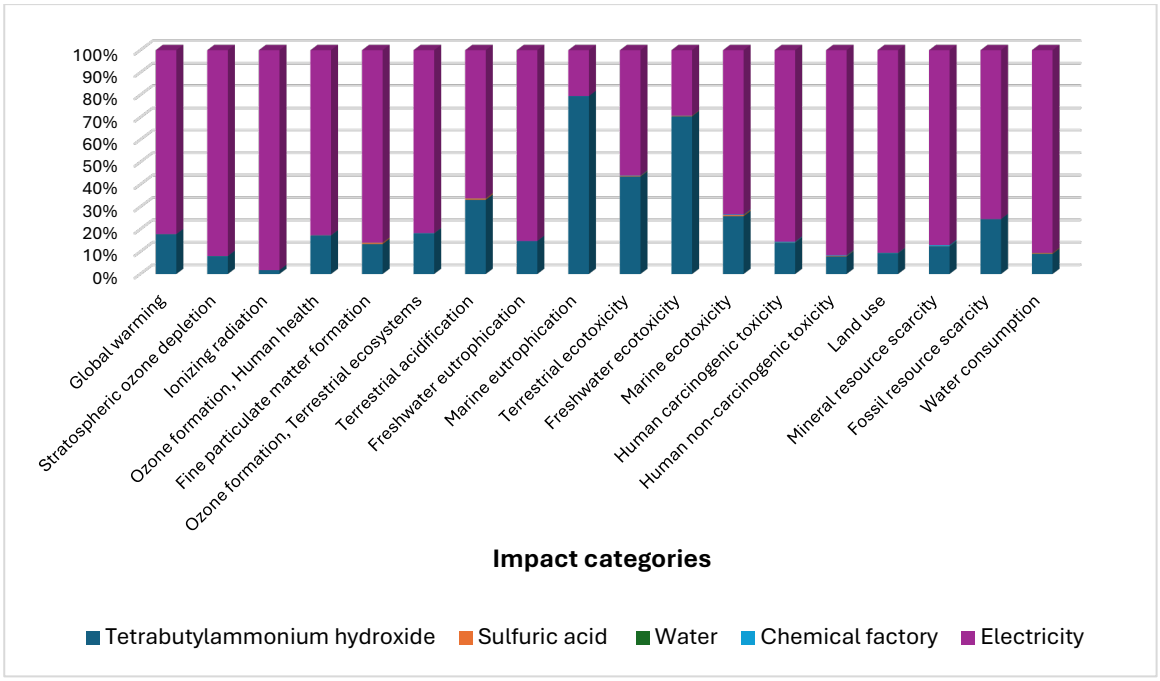
Inputs	Quantity for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Sludge to landfill
Boric acid	0.704226	0.001408	-	-	-
Hydrofluoric acid	0.905434	0.001811	-	-	-
H_2O	0.603623	0.001207	-	0.602415754	-
Transport lorry (16-32 ton)	1xE-4 tKm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Heat from steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Endpoint and Midpoint characterization

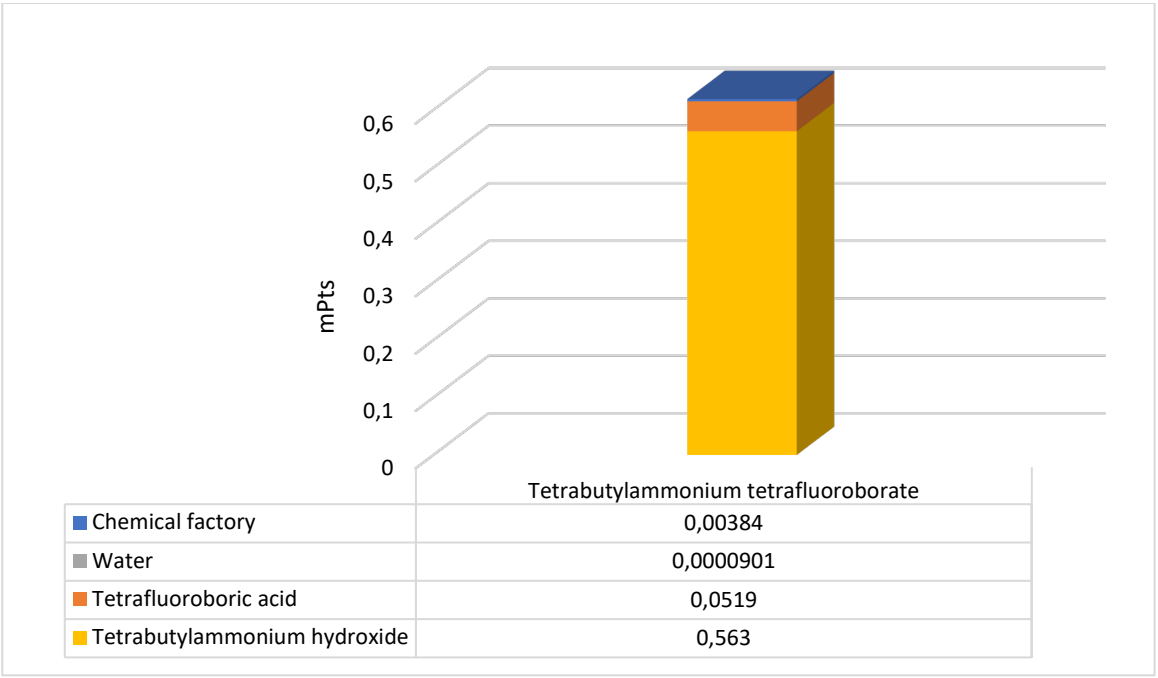


Chemical factory	0,00384
Water	0,0000998
Sulfuric acid	0,0146
Tetrabutylammonium hydroxide	0,764

Scheme S1. Endpoint characterization for tetrabutylammonium hydrogen sulfate detailing the single score portion due the other components

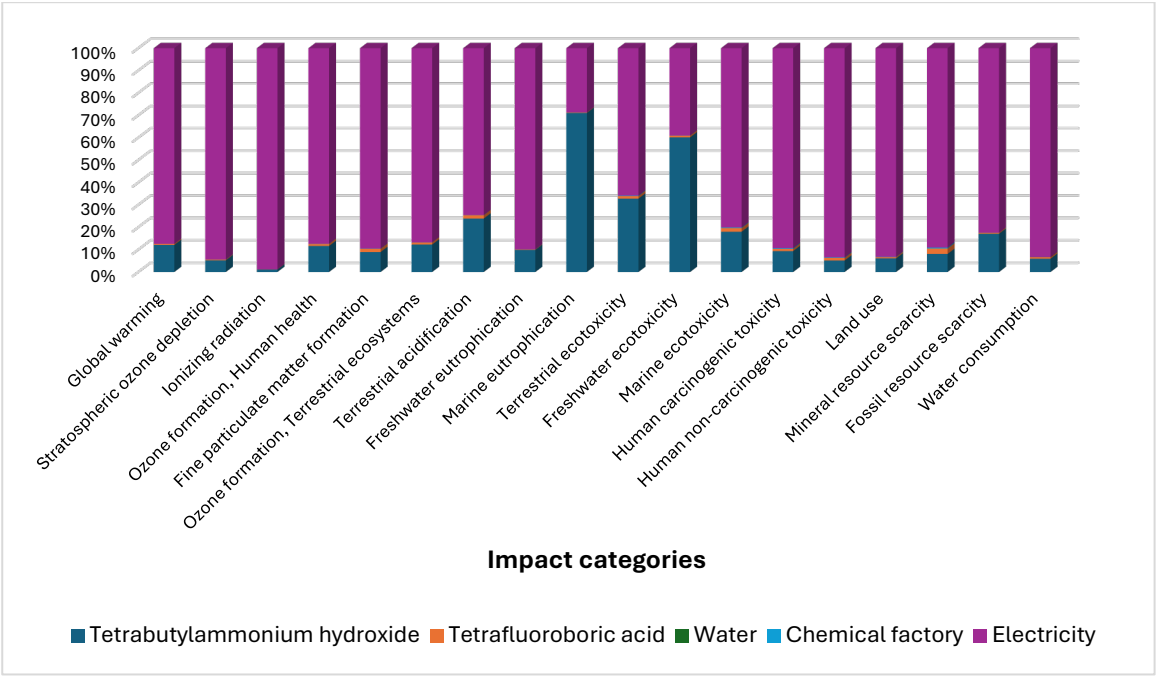


Scheme S2. Midpoint characterization to impact categories for the synthesis of tetrabutylammonium hydrogen sulfate

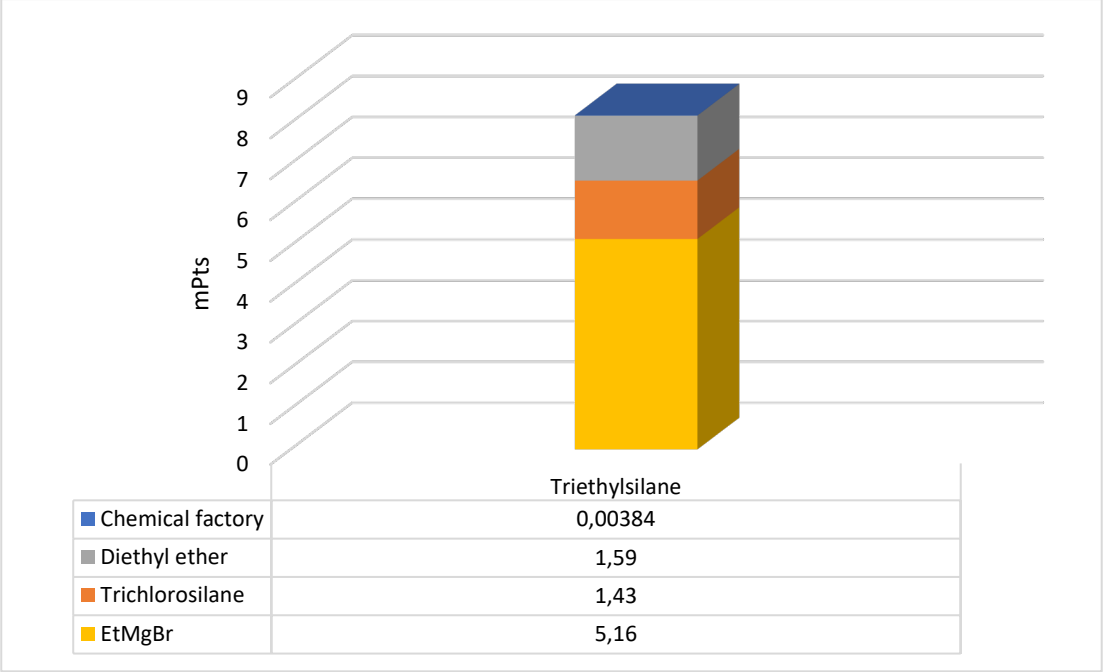


Chemical factory	0,00384
Water	0,0000901
Tetrafluoroboric acid	0,0519
Tetrabutylammonium hydroxide	0,563

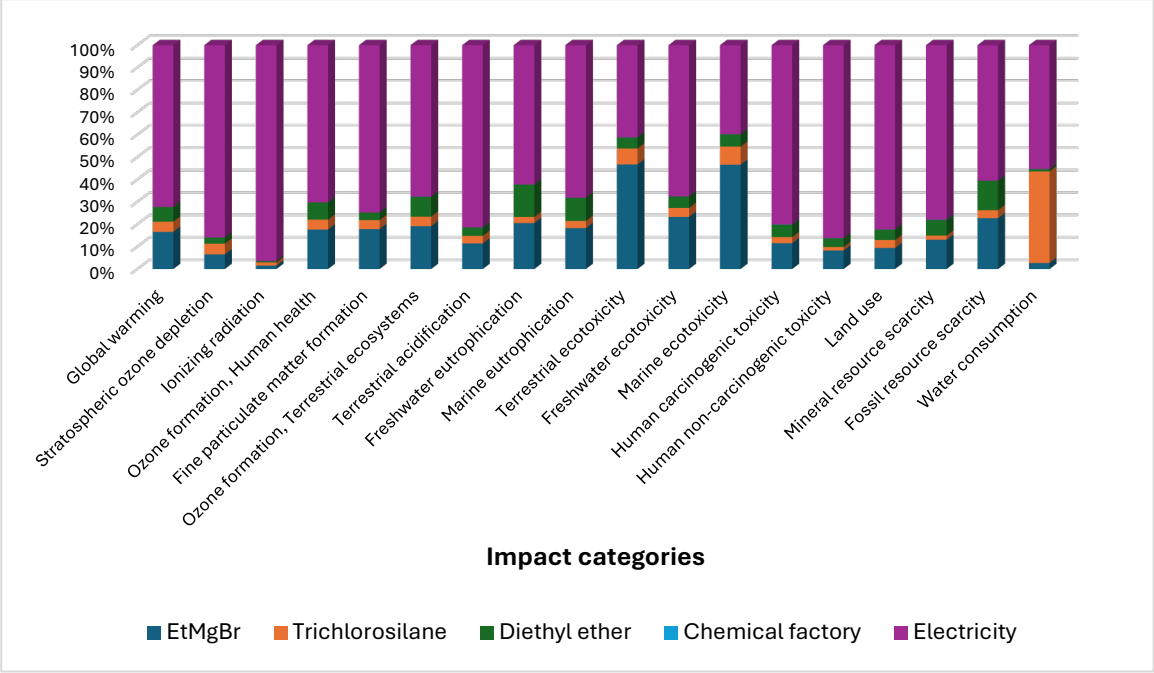
Scheme S3. Endpoint characterization for tetrabutylammonium tetrafluoroborate detailing the single score portion due the other components



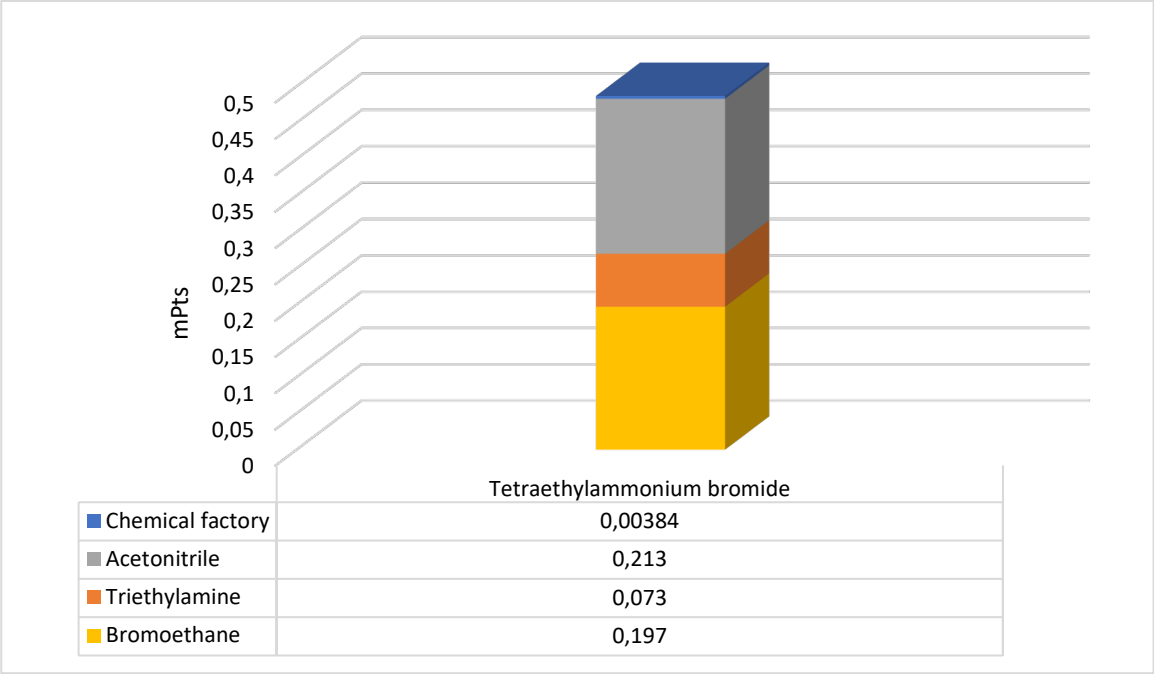
Scheme S4. Midpoint characterization to impact categories for the synthesis of tetrabutylammonium tetrafluoroborate



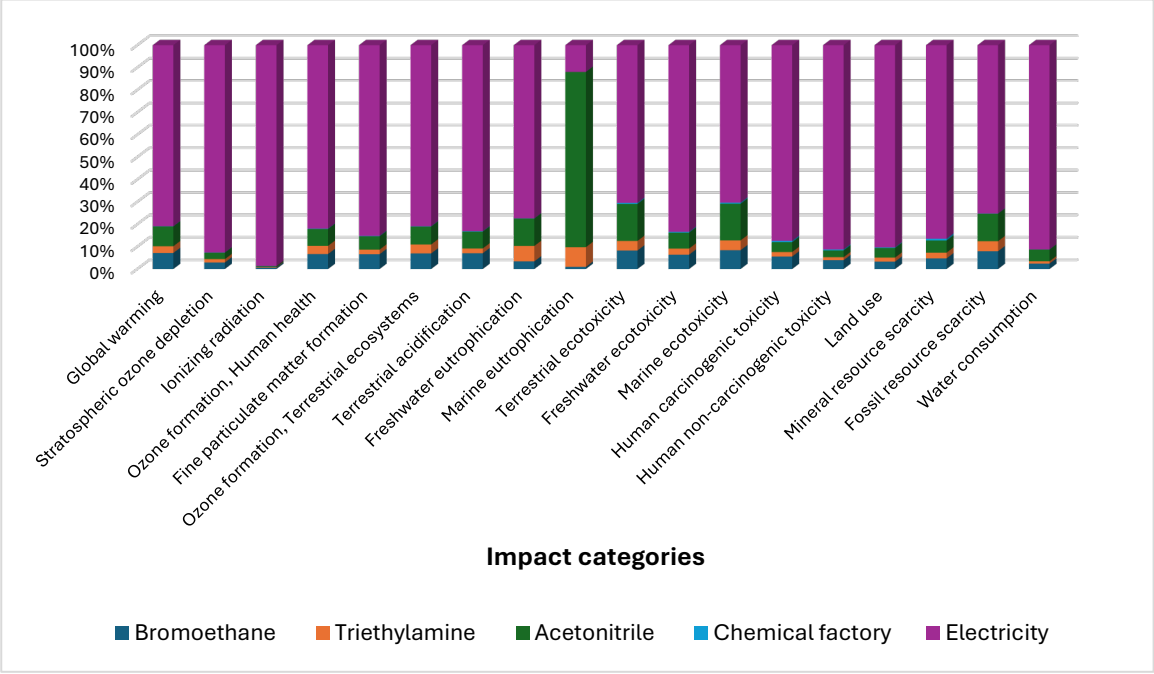
Scheme S5. Endpoint characterization for triethylsilane detailing the single score portion due the other components



Scheme S6. Midpoint characterization to impact categories for the synthesis of triethylsilane



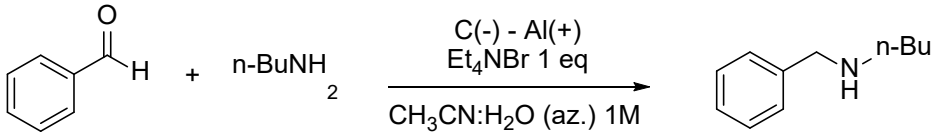
Scheme S7. Endpoint characterization for tetraethylammonium bromide detailing the single score portion due the other components



Scheme S8. Midpoint characterization to impact categories for the synthesis of tetraetylammonium bromide

7. Characterization Data

Chem. Name	N-benzylbutan-1-amine (**3a**)
Lit. Ref.	N. Shankaraiah, N. Markandeya, V. Srinivasulu, K. Sreekanth, Ch. S. Reddy, L. S. Santos and A. Kamal, *J. Org. Chem.*, 2011, **76**, 7017–7026.



1a **2a** **3a**

MW: 163.26

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (630.48 mg, 3 mmol), benzaldehyde **1a** (318.36 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3a** as a yellow oil (416.3 mg, 85% yield).

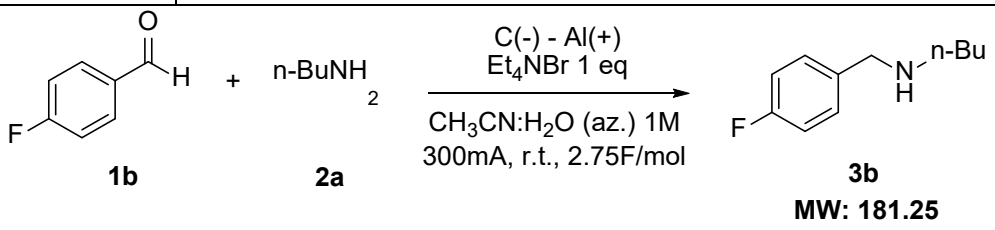
Elemental analysis: Calc: C: 80.92; H: 10.50; N: 8.58; Found: C: 80.90; H: 10.51; N: 8.59

Mol. Formula	$C_{11}H_{17}N$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.21-7.38	5	m	
	3.81	2	s	
	2.65	2	t	7.2
	1.53	2	p	7.2
	1.37	2	h	7.3
	0.94	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 140.5, 128.4, 128.1, 126.9, 54.1, 49.2, 32.2, 20.5, 14.1.

GC-EIMS (m/z, %): 163(6), 120(81), 118(11), 92(14), 91(100), 65(12).

Chem. Name	N-(4-fluorobenzyl)butan-1-amine (**3b**)
Lit. Ref.	L.-Y. Fu, J. Ying, X. Qi, J.-B. Peng and X.-F. Wu, *J. Org. Chem.*, 2019, **84**, 1421–1429.



1b **2a** **3b**

MW: 181.25

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (630.48 mg, 3 mmol), 4-fluorobenzaldehyde **1b** (372.33 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3b** as a yellow oil (494.8mg, 91% yield).

Elemental analysis: Calc: C: 72.89; H: 8.90; F: 10.48; N: 7.73; Found: C: 72.88; H: 8.92; F: 10.48; N: 7.72

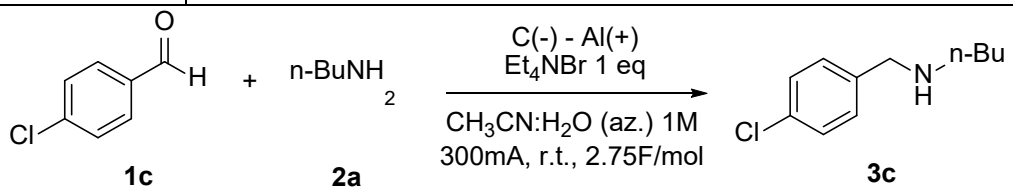
Mol. Formula	$C_{11}H_{16}FN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.31	2	dd	8.4, 5.5
	7.02	2	t	8.6
	3.78	2	s	
	2.64	2	t	7.2
	1.79	2	s (broad)	
	1.52	2	p	7.1
	1.38	2	p	7.4
	0.93	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 161.9 (J_{C-F}=244.5Hz), 136.0 (J_{C-F}=3.1Hz), 129.7 (J_{C-F}=8.0Hz), 115.1 (J_{C-F}=21.2Hz), 53.2, 49.1, 32.1, 20.5, 14.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ: - 116.1

GC-EIMS (m/z, %): 181(7), 136(69), 109(100).

Chem. Name	N-(4-chlorobenzyl)butan-1-amine (**3c**)
Lit. Ref.	W. Liao, Y. Chen, Y. Liu, H. Duan, J. L. Petersen and X. Shi, *Chem. Comm.*, 2009, 6436.



1c **2a** **3c**

MW: 197.71

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (630.48 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3d** as a yellow oil (516.0mg, 87% yield).

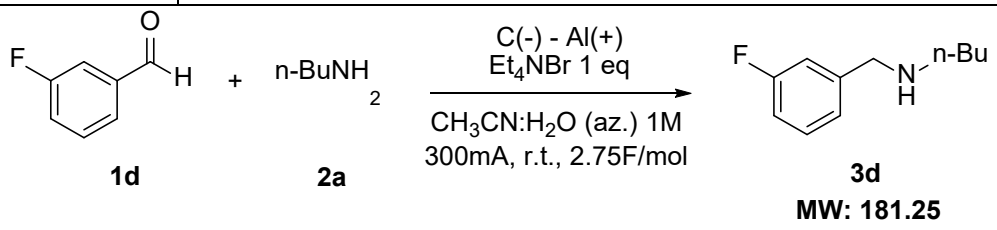
Elemental analysis: Calc: C: 66.83; H: 8.16; Cl: 17.93; N: 7.08; Found: C: 66.82; H: 8.19; Cl: 17.92; N: 7.07

Mol. Formula	$C_{11}H_{16}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.28	4	m	
	3.75	2	s	
	2.61	2	t	7.2
	1.50	2	p	7.1
	1.36	2	h	7.2
	0.92	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 139.1, 132.5, 129.4, 128.4, 53.3, 49.1, 32.2, 20.5, 14.0.

GC-EIMS (m/z, %): 197(6), 156(16), 154(53), 127(32), 125(100), 89(11).

Chem. Name	N-(3-fluorobenzyl)butan-1-amine (**3d**)
Lit. Ref.	



1d **2a** **3d**

MW: 181.25

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 3-fluorobenzaldehyde **1d** (372.33 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3d** as a yellow oil (429.6mg, 79% yield).

Elemental analysis: Calc: C: 72.89; H: 8.90; F: 10.48; N: 7.73; Found: C: 72.88; H: 8.93; F: 10.46; N: 7.72

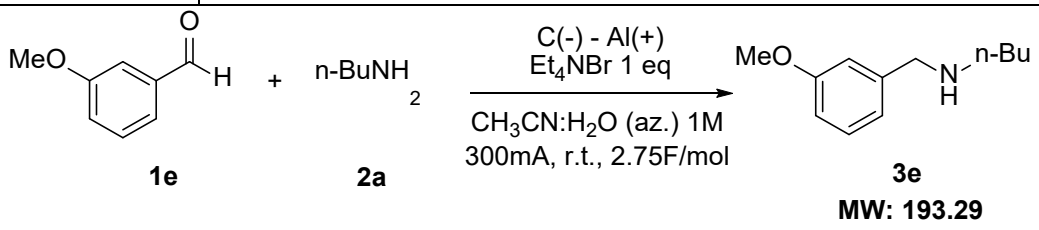
Mol. Formula	$C_{11}H_{16}FN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.26	1	m	
	7.07	2	m	
	6.93	1	m	
	3.77	2	s	
	2.61	2	t	7.2
	1.50	2	p	7.1
	1.37	2	h	7.2
	0.92	3	t	7.4

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 163.0 (J_{C-F}=245.4Hz), 143.3 (J_{C-F}=6.8Hz), 129.7 (J_{C-F}=8.2Hz), 123.5 (J_{C-F}=2.8Hz), 114.8 (J_{C-F}=21.2Hz), 113.6 (J_{C-F}=21.1Hz), 53.5, 49.1, 32.2, 20.4, 14.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ: - 113.6

GC-EIMS (m/z, %): 181(5), 136(66), 109(100).

Chem. Name	N-(3-methoxybenzyl)butan-1-amine (**3e**)
Lit. Ref.	



1e **2a** **3e**

MW: 193.29

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 3-methoxybenzaldehyde **1e** (408.45 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3e** as a yellow oil (434.9mg, 75% yield).

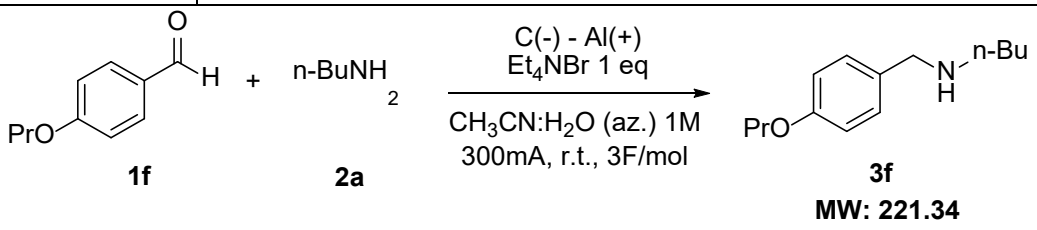
Elemental analysis: Calc: C: 74.57; H: 9.91; N: 7.25; Found: C: 74.56; H: 9.91; N: 7.24

Mol. Formula	$C_{12}H_{19}NO$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.20	1	t	8.0
	6.87	2	m	
	6.76	1	dd	8.2, 2.6
	3.76	3	s	
	3.73	2	s	
	2.59	2	t	
	1.88	1, broad		
	1.47	2	m	
	1.33	2	h	7.2
	0.90	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 159.7, 142.2, 129.3, 120.4, 113.5, 112.4, 55.1, 54.0, 49.1, 32.2, 20.5, 14.0.

GC-EIMS (m/z, %): 193(11), 150(20), 121(100), 78(12).

Chem. Name	N-(4-propoxybenzyl)butan-1-amine (**3f**)
Lit. Ref.	



1f **2a** **3f**

MW: 221.34

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-propoxybenzaldehyde **1f** (492.60 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 3 F/mol of current were passed (ca. 50 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3f** as a yellow oil (504.7mg, 76% yield).

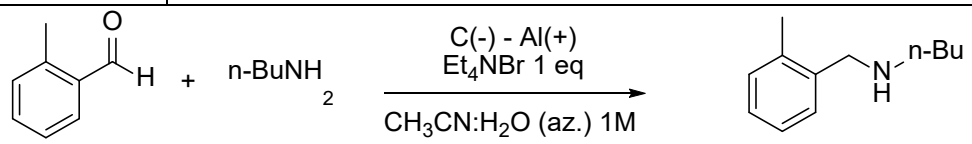
Elemental analysis: Calc: C: 75.97; H: 10.47; N: 6.33; Found: C: 75.97; H: 10.48; N: 6.32

Mol. Formula	$C_{14}H_{23}NO$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.23	2	d	8.1
	6.87	2	d	8.1
	3.92	2	t	6.5
	3.72	2	s	
	2.62	2	t	7.2
	1.82	2	h	7.2
	1.50	2	p	7.3
	1.36	2	h	7.3
	1.05	3	t	7.4
	0.93	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 158.2, 132.4, 129.3, 114.4, 69.5, 53.5, 49.1, 32.2, 22.6, 20.5, 14.0, 10.5.

GC-EIMS (m/z, %): 221(8), 178(17), 149(100), 121(35).

Chem. Name	N-(2-methylbenzyl)butan-1-amine (**3g**)
Lit. Ref.	J. L. Jeffrey, E. S. Bartlett and R. Sarpong, *Angew. Chem.*, 2013, **125**, 2250–2253.



1g **2a** **3g**

MW: 177.29

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 2-methylbenzaldehyde **1g** (360.45 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 3 F/mol of current were passed (ca. 50 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3g** as a yellow oil (388.3mg, 73% yield).

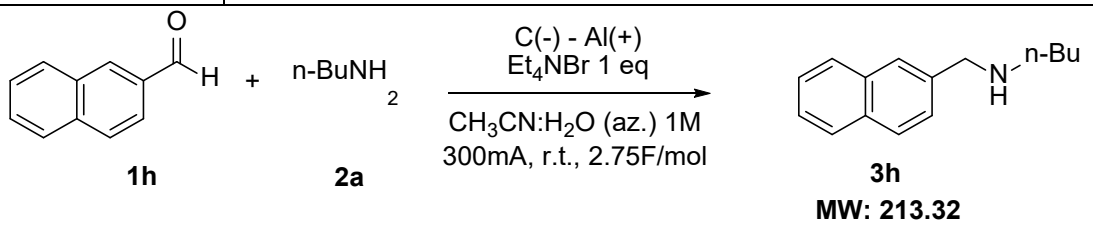
Elemental analysis: Calc: C: 81.30; H: 10.80; N: 7.90; Found: C: 81.29; H: 10.81; N: 7.90

Mol. Formula	$C_{12}H_{19}N$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.30	1	m	
	7.17	3	m	
	3.77	2	s	
	2.68	2	t	7.1
	2.36	3	s	
	1.53	2	p	7.1
	1.38	2	h	7.3
	0.94	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ:138.6, 136.2, 130.2, 128.3, 126.9, 125.9, 51.7, 49.6, 32.3, 20.6, 19.0, 14.1.

GC-EIMS (m/z, %): 177(14), 134(26), 105(100), 104(12).

Chem. Name	N-(Naphthalen-2-ylmethyl)butan-1-amine (**3h**)
Lit. Ref.	L.-Y. Fu, J. Ying, X. Qi, J.-B. Peng and X.-F. Wu, *J. Org. Chem.*, 2019, **84**, 1421–1429.



1h **2a** **3h**

MW: 213.32

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 2-naphthaldehyde **1h** (468.54 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 3 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3h** as a yellow oil (492.8mg, 77% yield).

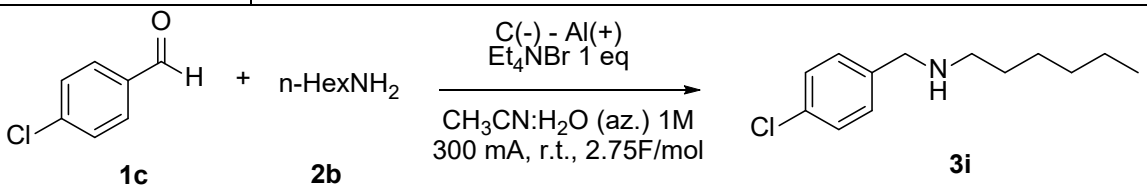
Elemental analysis: Calc: C: 84.46; H: 8.98; N: 6.57; Found: C: 84.45; H: 8.97; Br: 35.32; N: 6.58

Mol. Formula	$C_{15}H_{19}N$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.84	3	m	
	7.78	1	s	
	7.48	3	m	
	3.96	2	s	
	2.68	2	t	7.2
	1.55	2	p	7.2
	1.40	2	h	7.3
	0.96	3	t	7.3

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 138.2, 133.5, 132.7, 128.1, 127.8, 127.7, 126.7, 126.4, 126.0, 125.5, 54.2, 49.2, 32.3, 20.6, 14.1.

GC-EIMS (m/z, %): 213(19), 170(79), 141(100).

Chem. Name	N-(4-chlorobenzyl)hexan-1-amine (**3i**)
Lit. Ref.	C. Guyon, E. Da Silva, R. Lafon, E. Métay and M. Lemaire, *RSC Advances*, 2015, **5**, 2292–2298.



1c **2b** **3i**

MW: 225.76

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), hexylamine **2b** (303.57 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3i** as a yellow oil (548.6mg, 81% yield).

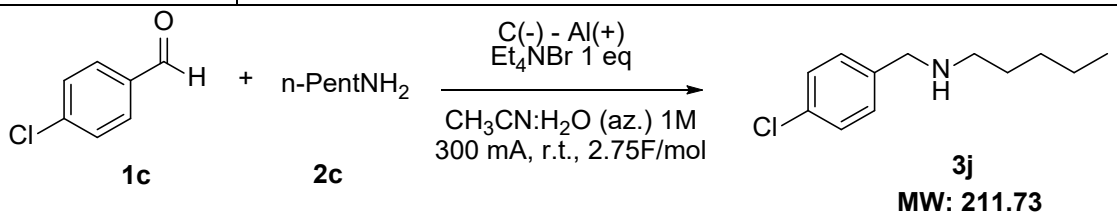
Elemental analysis: Calc: C: 69.16; H: 8.93; Cl: 15.70; N: 6.20; Found: C: 69.16; H: 8.94; Cl: 15.71; N: 6.18

Mol. Formula	$C_{13}H_{20}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, DMSO-d^6)	δ value:	No. H	Mult	J value/Hz
	7.33	4	m	
	3.65	2	s	
	2.44	2	t	7.1
	1.40	2	p	6.8
	1.25	6	m	
	0.85	3	t	6.8

^{13}C NMR (100.6 Hz, DMSO-d^6) δ: 140.7, 131.3, 130.1, 128.4, 52.7, 49.1, 31.8, 30.0, 27.0, 22.6, 14.4.

GC-EIMS (m/z, %): 225(5), 156(23), 154(73), 127(34), 125(100).

Chem. Name	N-(4-chlorobenzyl)pentan-1-amine (**3j**)
Lit. Ref.	



1c **2c** **3j**

MW: 211.73

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), pentylamine **2c** (261.48 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3j** as a yellow oil (501.8mg, 79% yield).

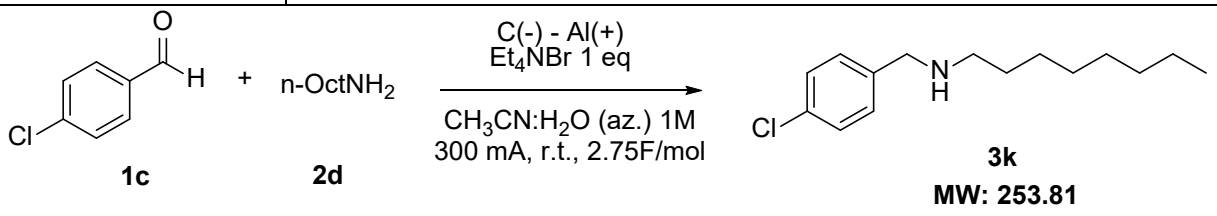
Elemental analysis: Calc: C: 68.07; H: 8.57; Cl: 16.74; N: 6.62; Found: C: 68.05; H: 8.58; Cl: 16.74; N: 6.63

Mol. Formula	$C_{12}H_{18}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.33	4	m	
	3.65	2	s	
	2.44	2	t	7.1
	1.41	2	p	7.2
	1.25	4	m	
	0.84	3	m	

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 140.7, 131.4, 130.0, 128.4, 52.7, 49.1, 29.7, 29.6, 22.6, 14.4.

GC-EIMS (m/z, %): 211(4), 156(19), 154(63), 127(28), 125(100).

Chem. Name	N-(4-chlorobenzyl)octan-1-amine (**3k**)
Lit. Ref.	



1c **2d** **3k**

MW: 253.81

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), octylamine **2a** (387.72 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3k** as a yellow oil (624.4mg, 82% yield).

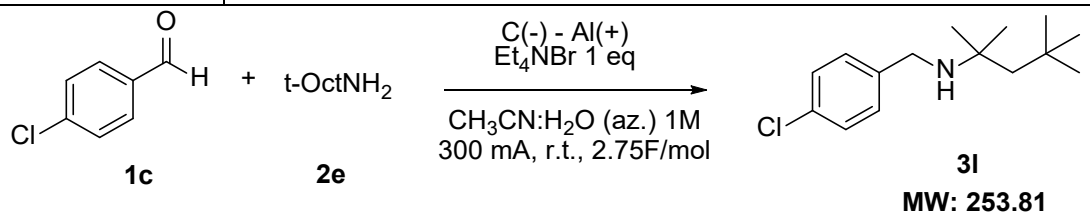
Elemental analysis: Calc: C: 70.98; H: 9.53; Cl: 13.97; N: 5.52; Found: C: 70.97; H: 9.53; Cl: 13.98; N: 5.53

Mol. Formula	$C_{15}H_{24}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.29	4	m	
	3.76	2	s	
	2.61	2	t	7.2
	1.51	2	p	7.1
	1.29	10	m	
	0.90	3	t	6.6

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 139.1, 132.5, 129.4, 128.4, 53.3, 49.5, 31.8, 30.1, 29.5, 29.3, 27.3, 22.7, 14.1.

GC-EIMS (m/z, %): 253(7), 156(21), 154(64), 127(26), 125(100).

Chem. Name	N-(4-chlorobenzy)tert-octanamine (**3l**)
Lit. Ref.	



1c **2e** **3l**

MW: 253.81

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), tert-octanamine **2e** (387.72 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3l** as a yellow oil (616.7mg, 83% yield).

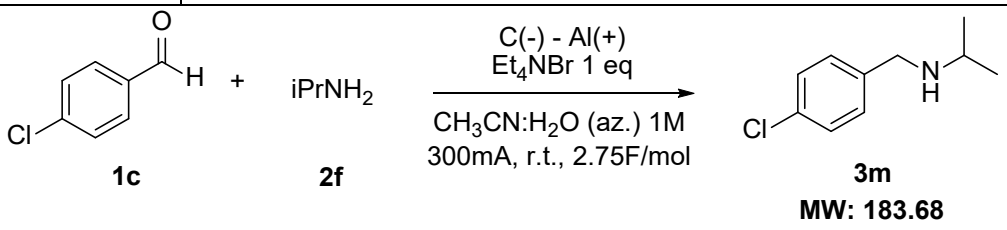
Elemental analysis: Calc: C: 70.98; H: 9.53; Cl: 13.97; N: 5.52; Found: C: 70.98; H: 9.53; Cl: 13.99; N: 5.51

Mol. Formula	$C_{15}H_{24}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.29	4	m	
	3.71	2	s	
	1.50	2	s	
	1.22	6	s	
	1.06	9	s	

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 140.0, 132.3, 129.5, 128.4, 54.7, 53.1, 45.9, 31.8, 30.9, 29.0.

GC-EIMS (m/z, %): 253(7), 182(42), 125(100).

Chem. Name	N-(4-chlorobenzyl)propan-2-amine (**3m**)
Lit. Ref.	D. Kim, B. Kang and S. H. Hong, *Org. Chem. Front.*, 2016, **3**, 475–479.



1c **2f** **3m**

MW: 183.68

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), isopropylamine **2f** (177.33 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton and concentrated under reduced pressure, giving the product **3m** as a yellow oil (462.9mg, 84% yield).

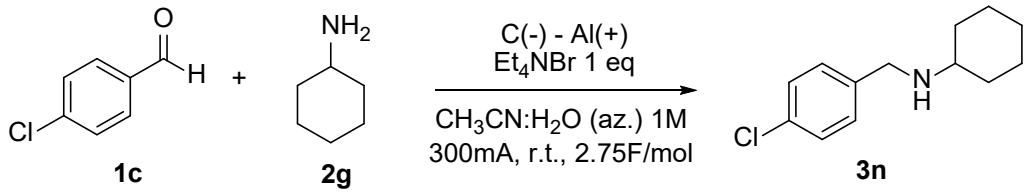
Elemental analysis: Calc: C: 65.39; H: 7.68; Cl: 19.30; N: 7.63; Found: C: 65.40; H: 7.69; Cl: 19.32; N: 7.61

Mol. Formula	$C_{10}H_{14}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, DMSO-d^6)	δ value:	No. H	Mult	J value/Hz
	7.31	4	m	
	3.64	2	s	
	2.64	1	hept	6.3
	0.96	6	d	6.2

^{13}C NMR (100.6 Hz, DMSO-d^6) δ: 141.0, 131.3, 130.1, 128.4, 50.1, 47.7, 23.2.

GC-EIMS (m/z, %): 183(8), 170(19), 168(65), 127(31), 125(100).

Chem. Name	N-(4-chlorobenzyl)cyclohexan-1-amine (**3n**)
Lit. Ref.	V. Ehmke, E. Winkler, D. W. Banner, W. Haap, W. B. Schweizer, M. Rottmann, M. Kaiser, C. Freymond, T. Schirmeister and F. Diederich, *ChemMedChem*, 2013, **8**, 967–975.



1c **2g** **3n**

MW: 223.74

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), cyclohexylamine **2g** (297.54 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton and concentrated under reduced pressure, giving the product **3n** as a yellow oil (590.7mg, 88% yield).

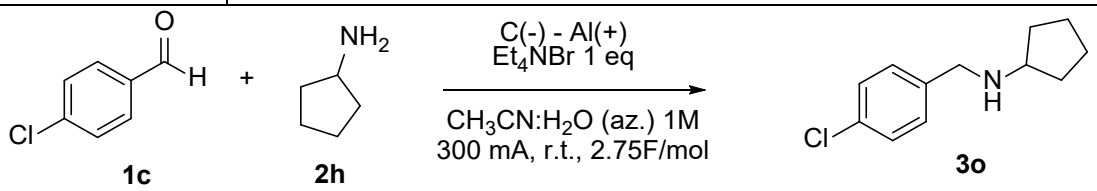
Elemental analysis: Calc: C: 69.79; H: 8.11; Cl: 15.84; N: 6.26; Found: C: 69.77; H: 8.12; Cl: 15.82; N: 6.25

Mol. Formula	$C_{13}H_{18}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.27	4	m	
	3.79	2	s	
	2.47	1	tt	10.2, 3.6
	1.91	2	m	
	1.74	2	m	
	1.20	6	m	

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 139.6, 132.4, 129.4, 128.5, 56.2, 50.3, 33.6, 26.2, 25.0.

GC-EIMS (m/z, %): 223(35), 182(23), 180(71), 127(29), 125(100).

Chem. Name	N-(4-chlorobenzyl)cyclopentan-1-amine (**3o**)
Lit. Ref.	



1c **2h** **3o**

MW: 209.72

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), cyclopentylamine **2h** (255.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3o** as a yellow oil (509.6mg, 81% yield).

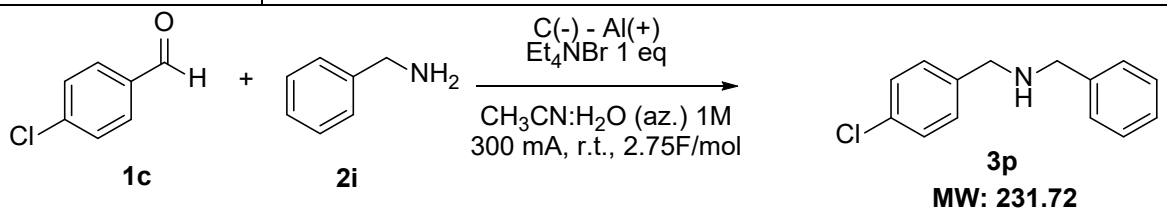
Elemental analysis: Calc: C: 68.73; H: 7.69; Cl:16.90; N: 6.68; Found: C: 68.74; H: 7.69; Cl: 16.91; N: 6.66

Mol. Formula	$C_{12}H_{16}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.27	4	m	
	3.73	2	s	
	3.09	1	p	6.6
	1.84	2	m	
	1.70	2	m	
	1.54	2	m	
	1.36	2	m	

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 139.3, 132.5, 129.5, 128.4, 59.2, 52.0, 33.2, 24.1.

GC-EIMS (m/z, %): 209(27), 182(26), 180(82), 166(14), 127(31), 125(100).

Chem. Name	N-benzyl-1-(4-chlorophenyl)methanamine (**3p**)
Lit. Ref.	S. Das, B. Join, K. Junge and M. Beller, *Chem. Comm.*, 2012, **48**, 2683.



1c **2i** **3p**

MW: 231.72

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 4-chlorobenzaldehyde **1c** (421.71 mg, 3 mmol), benzylamine **2i** (321.48 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted with 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the product **3p** as a yellow oil (597.8mg, 86% yield).

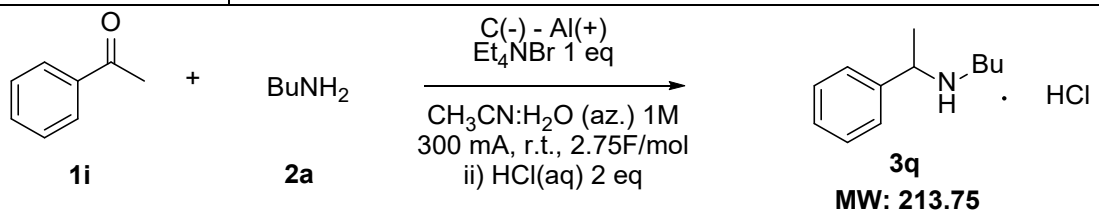
Elemental analysis: Calc: C: 56.25; H: 4.20; N: 14.58; Found: C: 56.27; H: 4.19; N: 14.57

Mol. Formula	C_9H_8FNO	**m.p.**	177-179°C	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.35	9	m	
	3.81	4	d	8.9

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 140.2, 138.9, 132.6, 129.5, 128.5, 128.4, 128.2, 127.1, 53.1, 52.4.

GC-EIMS (m/z, %): 231(42), 230(27), 142(27), 140(87), 127(29), 125(79), 106(36), 92(35), 91(100).

Chem. Name	N-(1-phenylethyl)butan-1-amine (**3q**)
Lit. Ref.	



1i **2a** **3q**

MW: 213.75

Method:

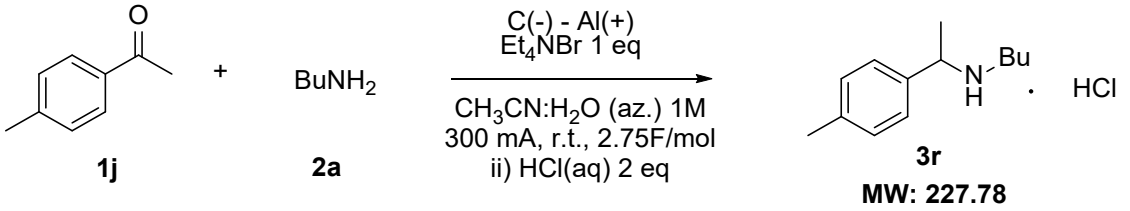
Prepared according to general procedure B: In a 8 mL vial equipped with a cap and a magnetic stirrer add acetophenone **1i** (360.45 mg, 3 mmol) and butylamine **2a** (219.42 mg, 3 mmol). Let the mixture stir at 90°C for 5 hours. After this time, let the reaction mixture cool to room temperature, then equip the vial with a two electrodes system (aluminium anode and graphite cathode). Add tetraethylammonium bromide (627.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile), then electrolyze the resulting mixture in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the crude product. The crude product is further purified by adding HCl(aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate : petroleum ether (1 : 9) in order to obtain hydrochloride salt product **3q** (397.6mg, 62% yield) as white crystal.

Elemental analysis: Calc: C: 67.43; H: 9.43; Cl: 16.58; N: 6.55; Found: C: 67.42; H: 9.44; Cl: 16.58; N: 6.55

Mol. Formula	$C_{12}H_{20}ClN$	**m.p.**	142-144°C	
^{1}H NMR (400 MHz, MeOH-d^4)	δ value:	No. H	Mult	J value/Hz
	7.51	5	m	
	4.40	1	q	6.9
	2.96	1	m	
	2.74	1	m	
	1.70	5	m	
	1.38	2	h	7.5
	0.95	3	t	7.4

^{13}C NMR (100.6 Hz, MeOH-d^4) δ: 136.4, 129.3, 129.1, 127.3, 58.3, 45.5, 27.8, 19.4, 18.3, 12.4.

Chem. Name	N-(1-(p-tolyl)ethyl)butan-1-amine (**3r**)
Lit. Ref.	



1j **2a** **3r**

MW: 227.78

Method:

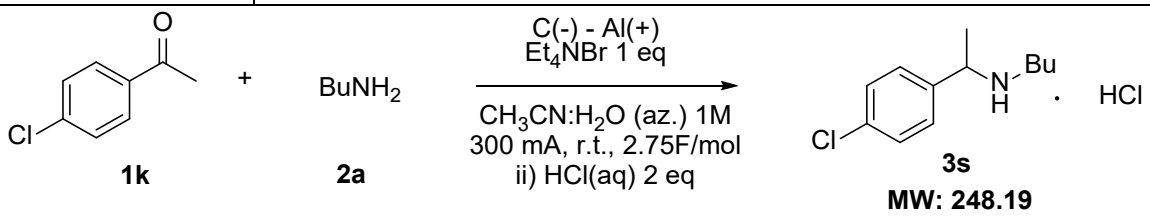
Prepared according to general procedure B: In a 8 mL vial equipped with a cap and a magnetic stirrer add 4-methylacetophenone **1j** (402.54 mg, 3 mmol) and butylamine **2a** (219.42 mg, 3 mmol). Let the mixture stir at 90°C for 5 hours. After this time, let the reaction mixture cool to room temperature, then equip the vial with a two electrodes system (aluminium anode and graphite cathode). Add tetraethylammonium bromide (627.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile), then electrolyze the resulting mixture in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the crude product. The crude product is further purified by adding HCl(aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate : petroleum ether (1 : 9) in order to obtain hydrochloride salt product **3r** (396.3mg, 58% yield) as white crystal.

Elemental analysis: Calc: C: 68.55; H: 9.74; Cl: 15.56; N: 6.15; Found: C: 68.53; H: 9.75; Cl: 15.56; N: 6.16

Mol. Formula	$C_{13}H_{22}ClN$	**m.p.**	150-152°C	
^{1}H NMR (400 MHz, MeOH-d^4)	δ value:	No. H	Mult	J value/Hz
	7.35	4	m	
	4.33	1	m	
	2.92	1	ddd	12.5, 10.1, 5.8
	2.73	1	ddd	12.3, 10.0, 6.0
	2.39	3	s	
	1.66	5	m	
	1.38	2	h	7.4
	0.95	3	t	7.4

^{13}C NMR (100.6 Hz, MeOH-d^4) δ: 139.5, 133.3, 129.7, 127.3, 58.0, 45.3, 27.8, 19.8, 19.5, 18.3, 12.5.

Chem. Name	N-(1-(4-chlorophenyl)ethyl)butan-1-amine (**3s**)
Lit. Ref.	



1k **2a** **3s**

MW: 248.19

Method:

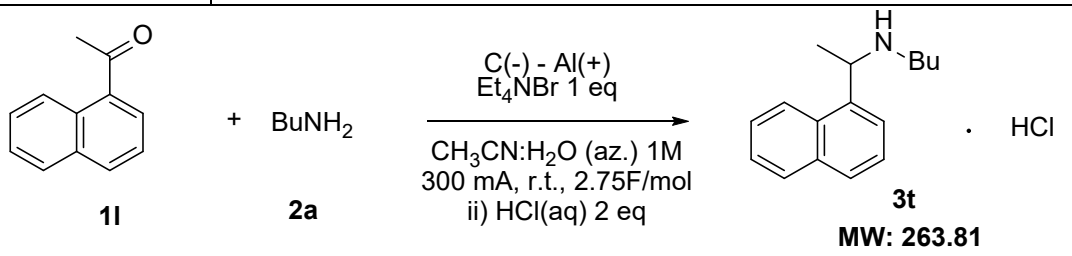
Prepared according to general procedure B: In a 8 mL vial equipped with a cap and a magnetic stirrer add 4-chloroacetophenone **1k** (463.77 mg, 3 mmol) and butylamine **2a** (219.42 mg, 3 mmol). Let the mixture stir at 90°C for 5 hours. After this time, let the reaction mixture cool to room temperature, then equip the vial with a two electrodes system (aluminium anode and graphite cathode). Add tetraethylammonium bromide (627.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile), then electrolyze the resulting mixture in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the crude product. The crude product is further purified by adding HCl(aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate : petroleum ether (1 : 9) in order to obtain hydrochloride salt product **3s** (379.7 mg, 51% yield) as white crystal.

Elemental analysis: Calc: C: 58.07; H: 7.72; Cl: 28.57; N: 5.64; Found: C: 58.06; H: 7.72; Cl: 28.57; N: 5.65

Mol. Formula	$C_{12}H_{19}Cl_2N$	**m.p.**	163-165°C	
^{1}H NMR (400 MHz, $CDCl_3$)	δ value:	No. H	Mult	J value/Hz
	7.54	4	m	
	4.43	1	m	
	2.97	1	ddd	12.2, 10.1, 5.9
	2.76	1	m	
	1.69	5	m	
	1.39	2	h	7.5
	0.96	3	t	7.6

^{13}C NMR (100.6 Hz, $CDCl_3$) δ: 135.2, 135.1, 129.3, 129.2, 57.6, 45.6, 27.9, 19.5, 18.3, 12.6.

Chem. Name	N-(1-(naphthalen-1-yl)ethyl)butan-1-amine (**3t**)
Lit. Ref.	



1l **2a** **3t**

MW: 263.81

Method:

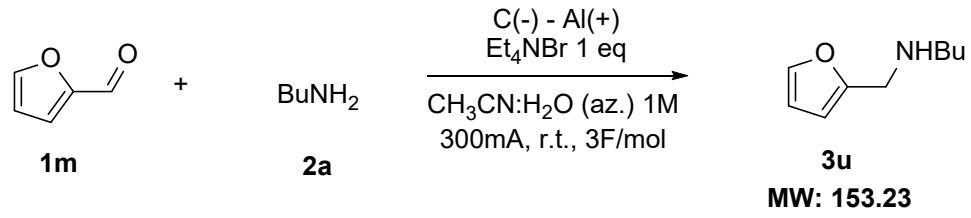
Prepared according to general procedure B: In a 8 mL vial equipped with a cap and a magnetic stirrer add 1-acetonaphthone **1l** (510.63 mg, 3 mmol) and butylamine **2a** (219.42 mg, 3 mmol). Let the mixture stir at 90°C for 5 hours. After this time, let the reaction mixture cool to room temperature, then equip the vial with a two electrodes system (aluminium anode and graphite cathode). Add tetraethylammonium bromide (627.45 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile), then electrolyze the resulting mixture in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of current were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton using compressed air to speed up the process and concentrated under reduced pressure, giving the crude product. The crude product is further purified by adding HCl(aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate : petroleum ether (1 : 9) in order to obtain hydrochloride salt product **3t** (419.5 mg, 53% yield) as white crystal.

Elemental analysis: Calc: C: 72.85; H: 8.41; Cl: 13.44; N: 5.31; Found: C: 72.83; H: 8.42; Cl: 13.46; N: 5.30

Mol. Formula	$C_{16}H_{22}ClN$	**m.p.**	177-179°C	
^{1}H NMR (400 MHz, MeOH-d^4)	δ value:	No. H	Mult	J value/Hz
	8.23	1	d	8.6
	7.99	2	d	8.2
	7.82	1	d	7.2
	7.63	3	m	
	5.40	1	q	6.7
	3.09	1	m	
	2.86	1	m	
	1.82	3	d	6.7
	1.70	2	m	
	1.36	2	h	7.4
	0.92	3	t	7.3

^{13}C NMR (100.6 Hz, MeOH-d^4) δ: 134.1, 133.0, 130.7, 129.5, 129.0, 127.1, 126.2, 125.2, 123.5, 121.7, 52.8, 45.9, 28.0, 19.5, 18.8, 12.4.

Chem. Name	N-butylfurfurylamine (**3u**)
Lit. Ref.	P. Galletti, A. Montecavalli, F. Moretti, A. Pasteris, C. Samorì and E. Tagliavini, *New J. Chem.*, 2009, **33**, 1859.



1m **2a** **3u**

MW: 153.23

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), furfural **1m** (288.27 mg, 3 mmol), butylamine **2a** (219.42 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 3 F/mol of c urrent were passed (ca. 50 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton and concentrated under reduced pressure, giving the product **3u** as a yellow oil (340.2 mg, 74% yield).

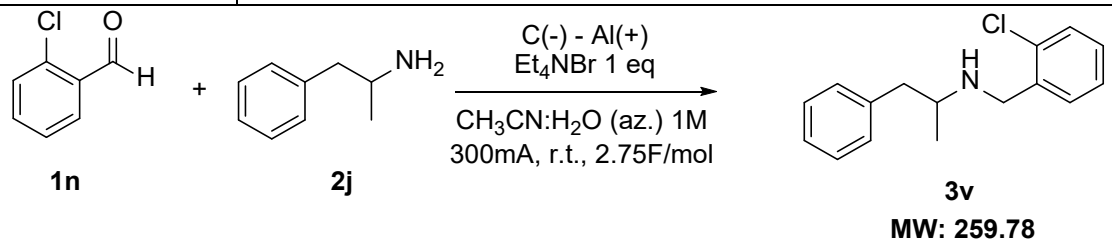
Elemental analysis: Calc: C: 70.55; H: 9.87; N: 9.14; Found: C: 70.54; H: 9.86; N: 9.15

Mol. Formula	$C_9H_{15}NO$	**m.p.**	oil	
^{1}H NMR (400 MHz, DMSO-d^6)	δ value:	No. H	Mult	J value/Hz
	7.34	1	m	
	6.30	1	m	
	6.16	1	d	3.3
	3.77	2	s	
	2.60	2	t	7.2
	1.47	2	p	7.1
	1.33	2	h	7.1
	0.90	3	t	7.3

^{13}C NMR (100.6 Hz, DMSO-d^6) δ: 154.0, 141.7, 110.1, 106.7, 48.8, 46.2, 32.1, 20.4, 14.0.

GC-EIMS (m/z, %): 153(5), 110(37), 81(100).

Chem. Name	Clobenzorex (**3v**)
Lit. Ref.	



1n **2j** **3v**

MW: 259.78

Method:

Prepared according to general procedure A: in a 8mL vial equipped with a magnetic stirrer and a two electrodes system (aluminium anode and graphite cathode) tetraethylammonium bromide (627.45 mg, 3 mmol), 2-chlorobenzaldehyde **1n** (421.71 mg, 3 mmol), 1-phenylpropan-2-amine **2j** (405.63 mg, 3 mmol) and 3 mL of azeotropic mixture of acetonitrile : water (84% w/w acetonitrile) were consecutively added and the resulting mixture was electrolyzed in CCE at 300 mA under stirring at room temperature until 2.75 F/mol of c urrent were passed (ca. 45 minutes). After reaction completion the mixture was concentrated under reduced pressure. The residue was diluted in 10 mL of ethyl acetate, then it was filtered on cotton and concentrated under reduced pressure, giving the product **3v** as a yellow oil. The hydrochloride salt is obtained by adding HCl(aq.) (2 eq.). Remove water under reduced pressure, then add a mixture of ethyl acetate : petroleum ether (1 : 9) in order to obtain hydrochloride salt product **3v** (693.2 mg, 78% yield) as white crystal.

Elemental analysis: Calc: C: 73.98; H: 6.98; Cl: 13.65; N: 5.39; Found: C: 73.99; H: 6.98; Cl: 13.66; N: 5.37

Mol. Formula	$C_{16}H_{18}ClN$	**m.p.**	oil	
^{1}H NMR (400 MHz, MeOH-d^4)	δ value:	No. H	Mult	J value/Hz
	7.78	1	dd	7.1, 2.1
	7.56	1	dd	7.5, 1.6
	7.47	2	m	
	7.35	5	m	
	4.50	2	s	
	3.69	1	m	
	3.42	1	dd	13.1, 4.0
	2.85	1	dd	13.1, 10.4
	1.36	3	d	6.3

^{13}C NMR (100.6 Hz, MeOH-d^4) δ: 136.1, 134.5, 132.2, 131.2, 129.8, 129.4, 129.1, 128.6, 127.7, 127.0, 56.4, 45.6, 38.7, 14.7.

GC-EIMS (m/z, %): 170(21), 168(78), 127(30), 125(100), 91(29), 89(26).

8. References

1 J. Osorio-Tejada, F. Ferlin, L. Vaccaro and V. Hessel, *Green Chem.,* 2022, **24**, 325–337.

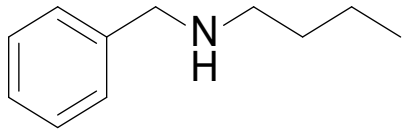
2 G. Wernet, S. Hellweg and K. Hungerbühler, *Int. J. Life Cycle Assess*., 2012, **17**, 720–728.

3 R. Hischier, S. Hellweg, C. Capello and A. Primas, *Int. J. Life Cycle Assess.,* 2005, **10**, 59–67.

4 D. G, Ecoinvent Rep. No. 13. Dübend. Swiss Cent. Life Cycle Invent.

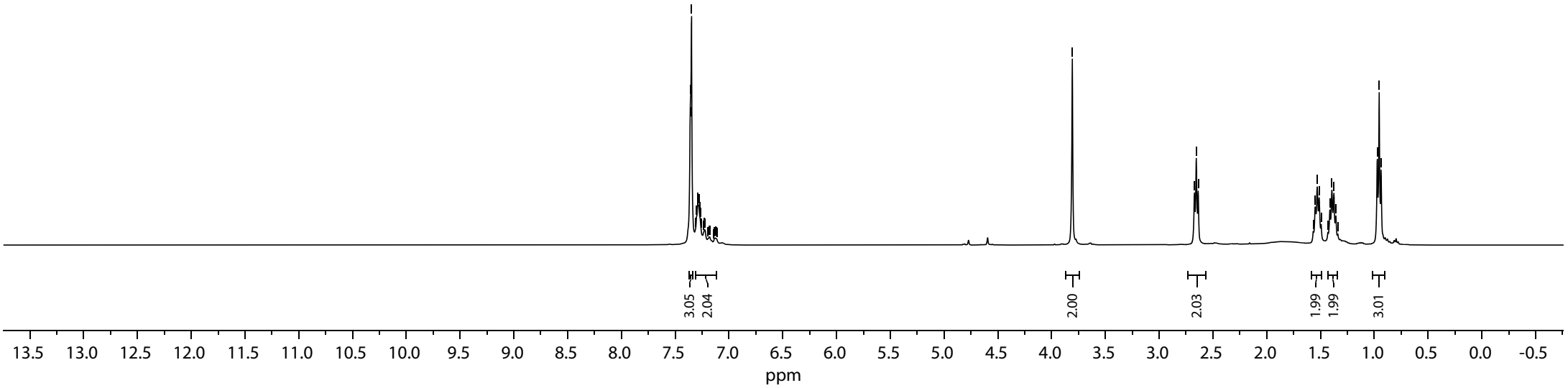
5 M. A. J. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander and R. van Zelm, *Int. J. Life Cycle Assess.,* 2017, **22**, 138–147.

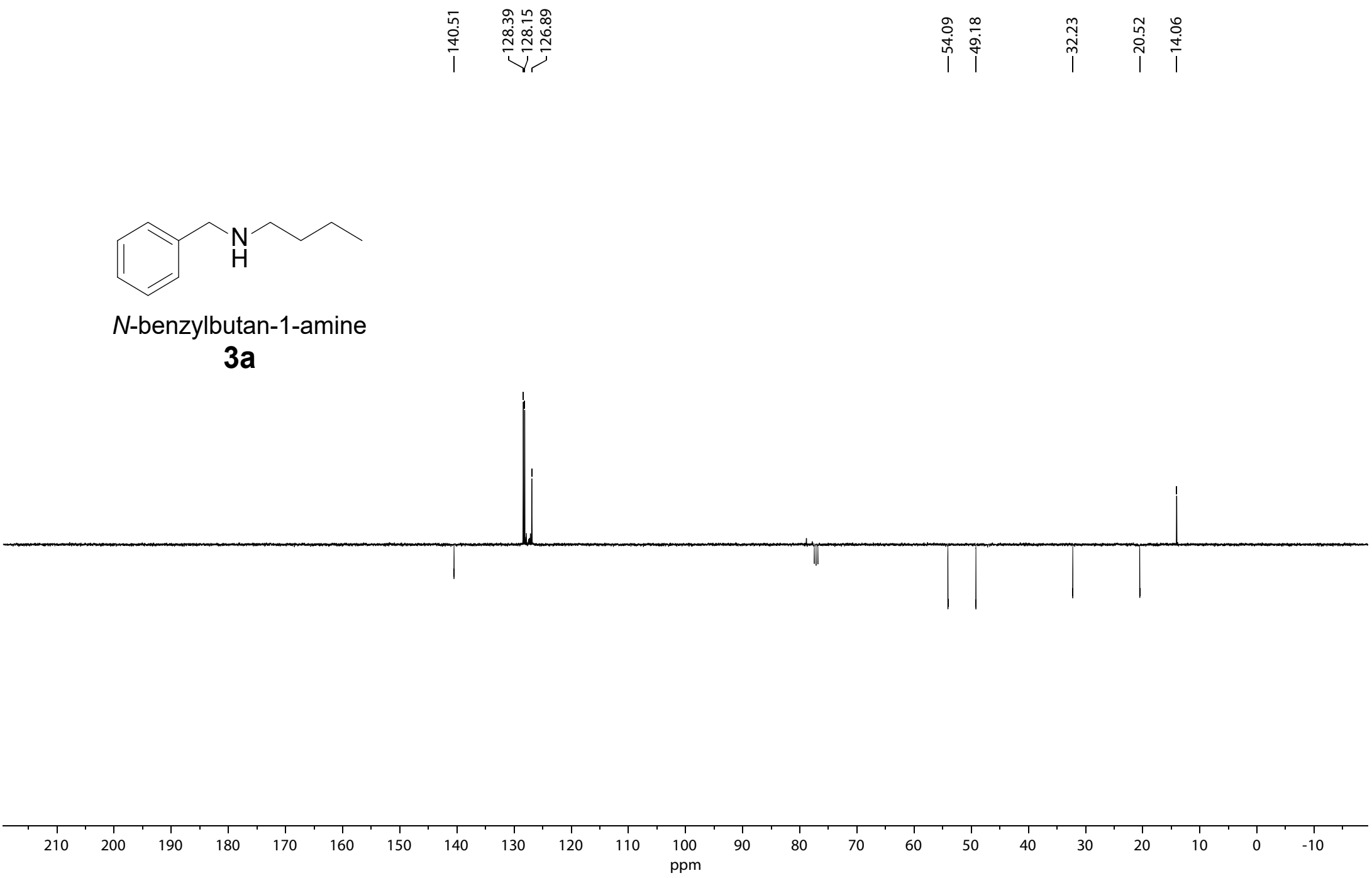
9. Copies of the NMR spectra



N-benzylbutan-1-amine

3a




140.51
128.39
128.15
126.89
54.09
49.18
32.23
20.52
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N
H
N-benzylbutan-1-amine
3a
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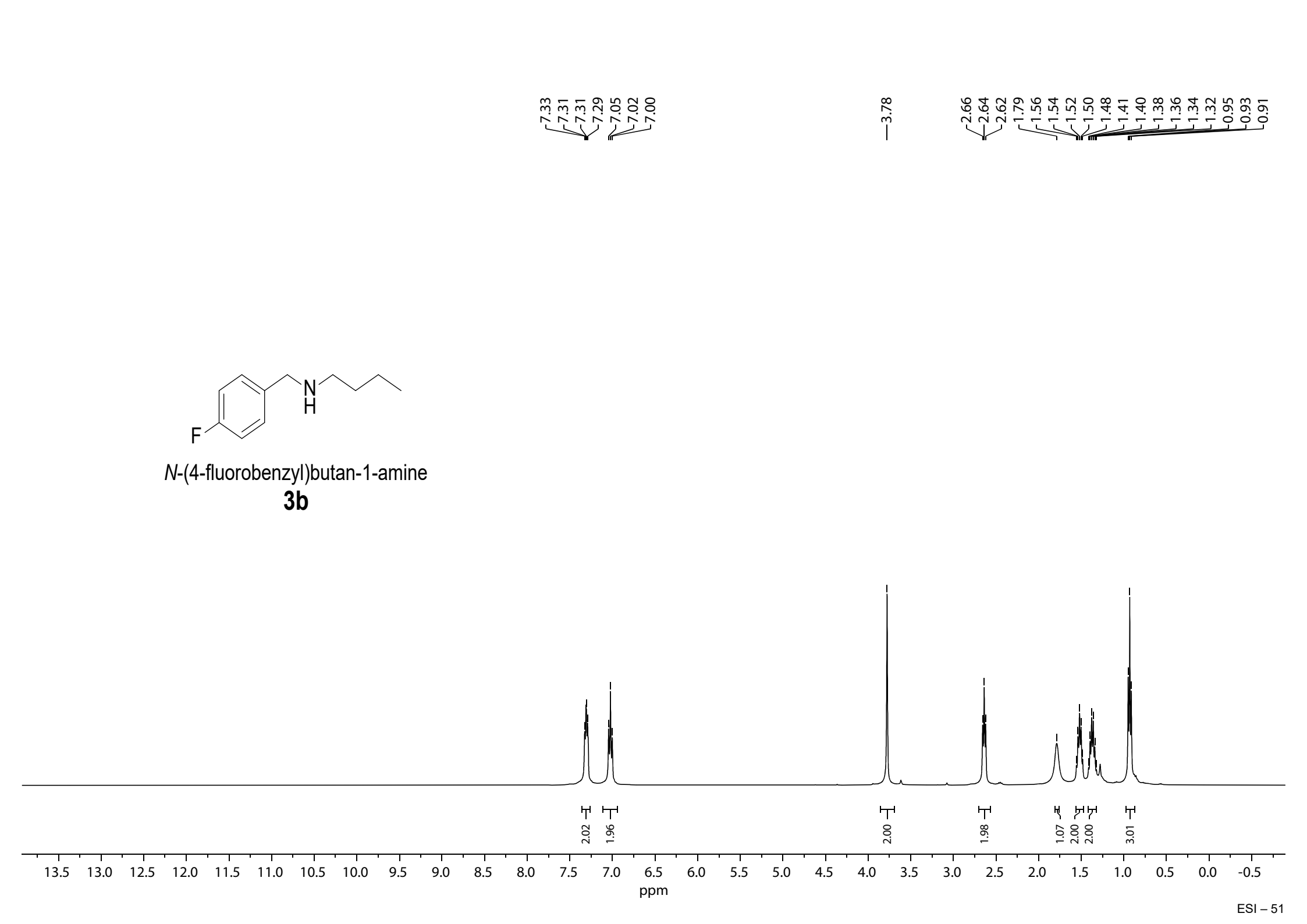
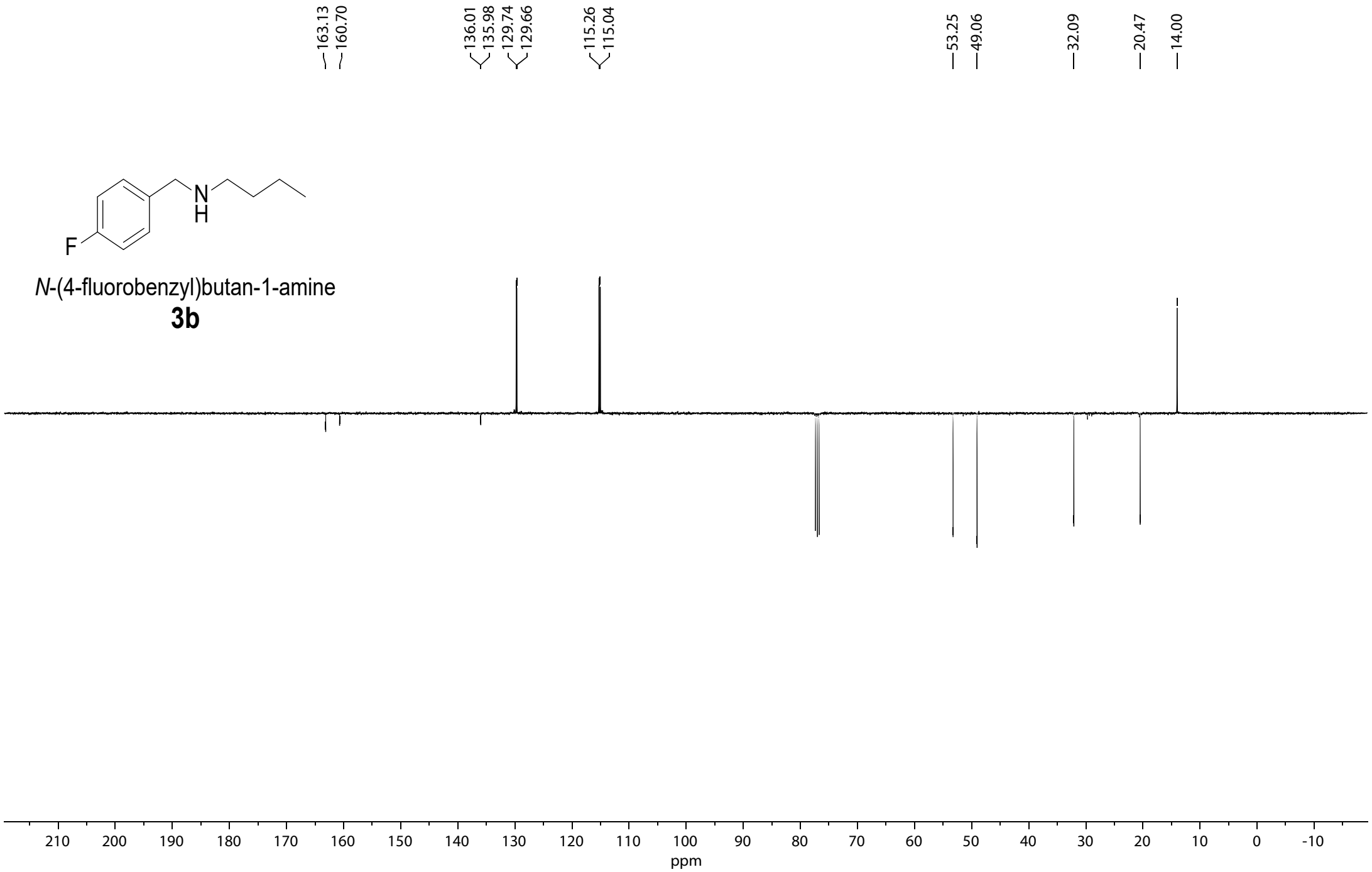
ppm



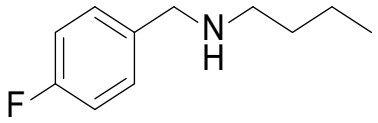
N-(4-fluorobenzyl)butan-1-amine

3b



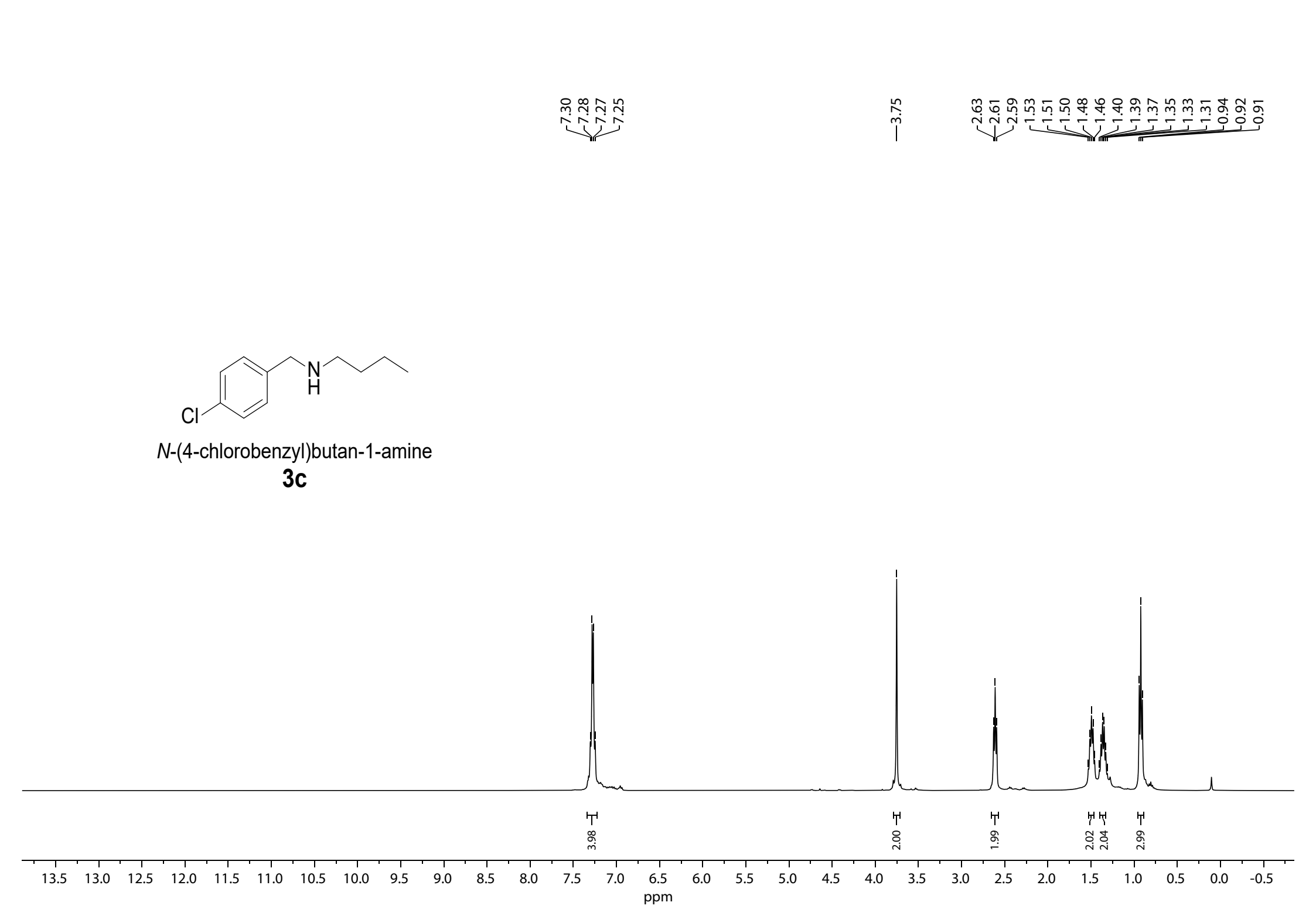
N-(4-fluorobenzyl)butan-1-amine

3b



N-(4-fluorobenzyl)butan-1-amine

3b



N-(4-chlorobenzyl)butan-1-amine

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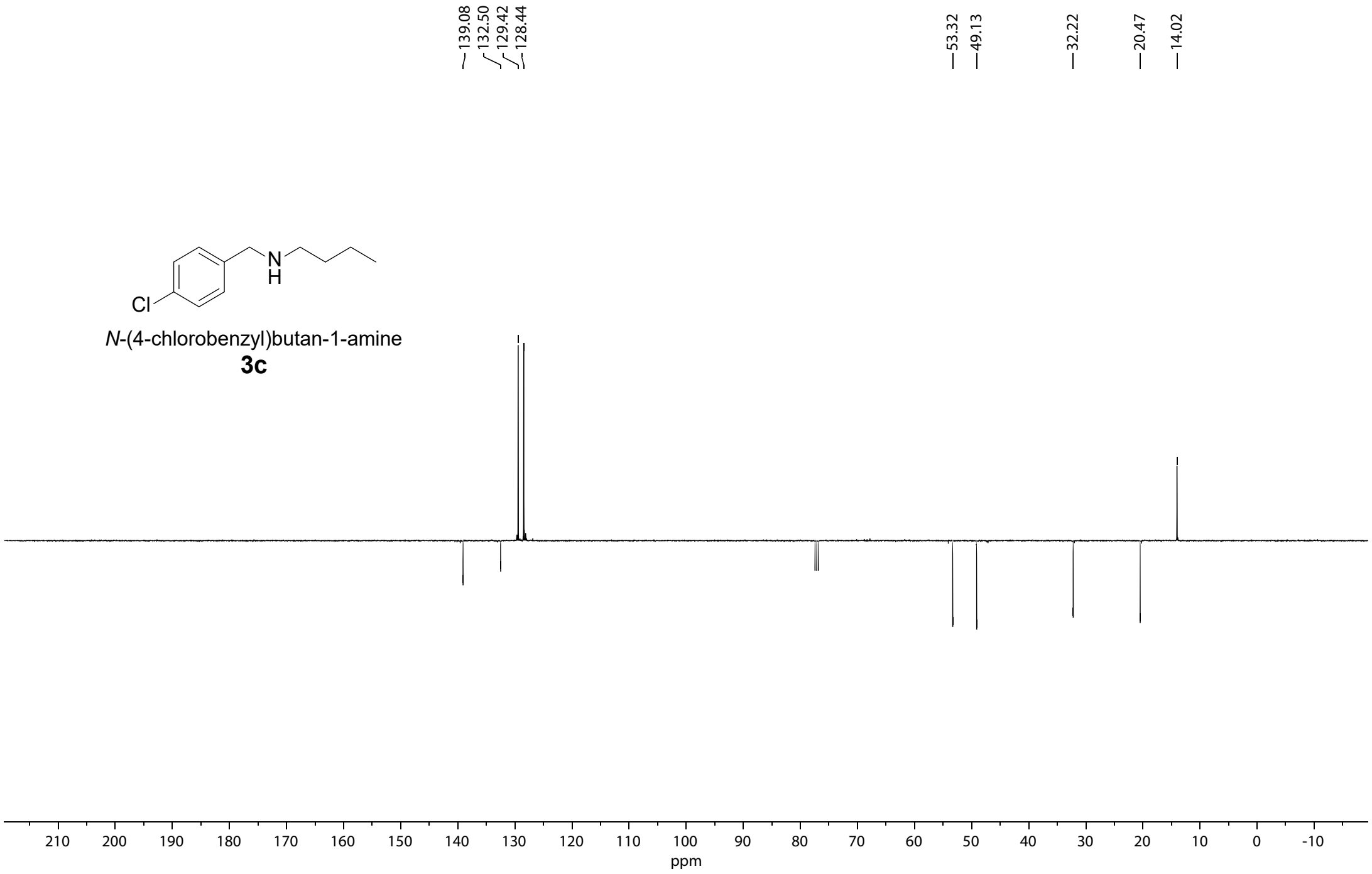
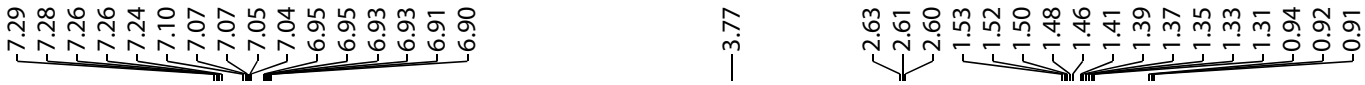
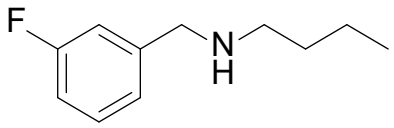


N-(4-chlorobenzyl)butan-1-amine

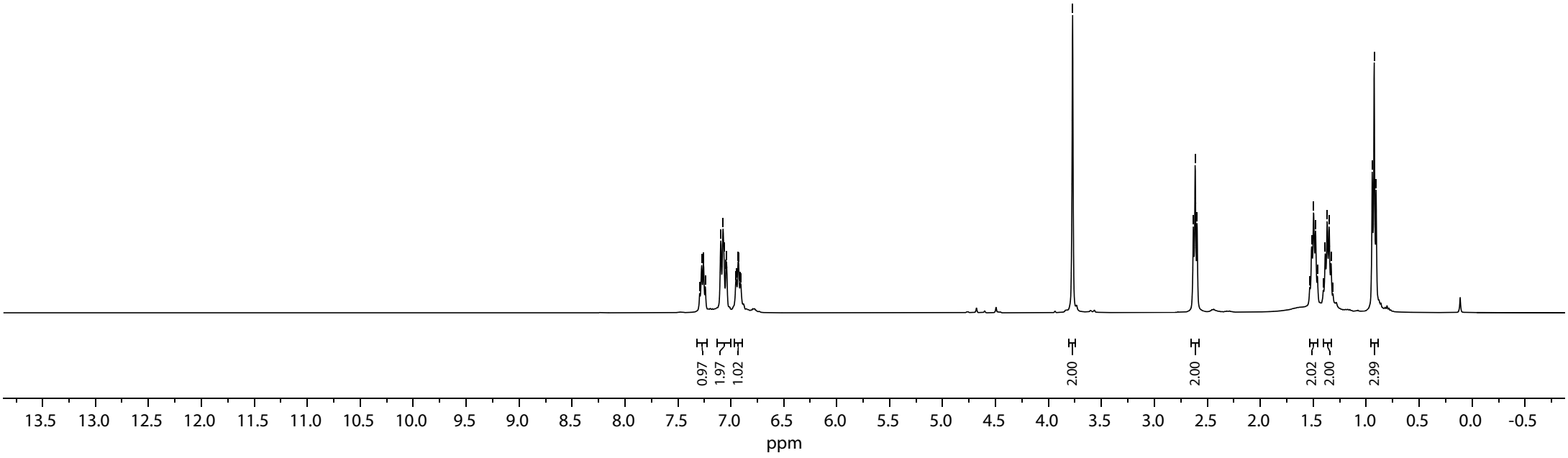
3c

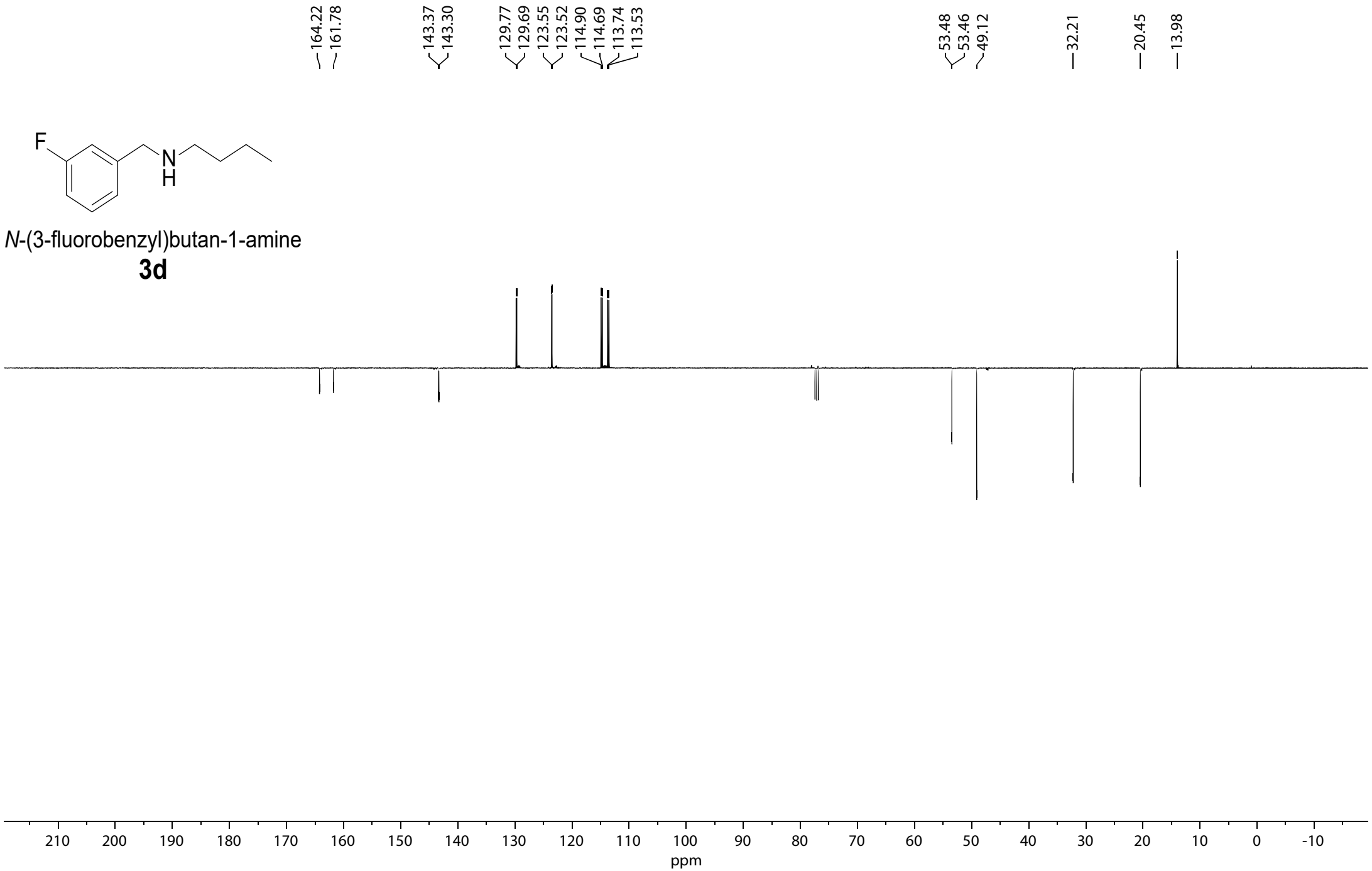




N-(3-fluorobenzyl)butan-1-amine

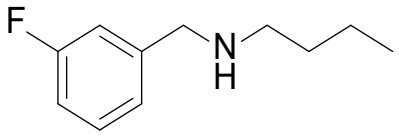
3d





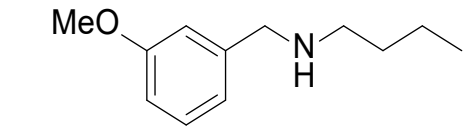
N-(3-fluorobenzyl)butan-1-amine

3d



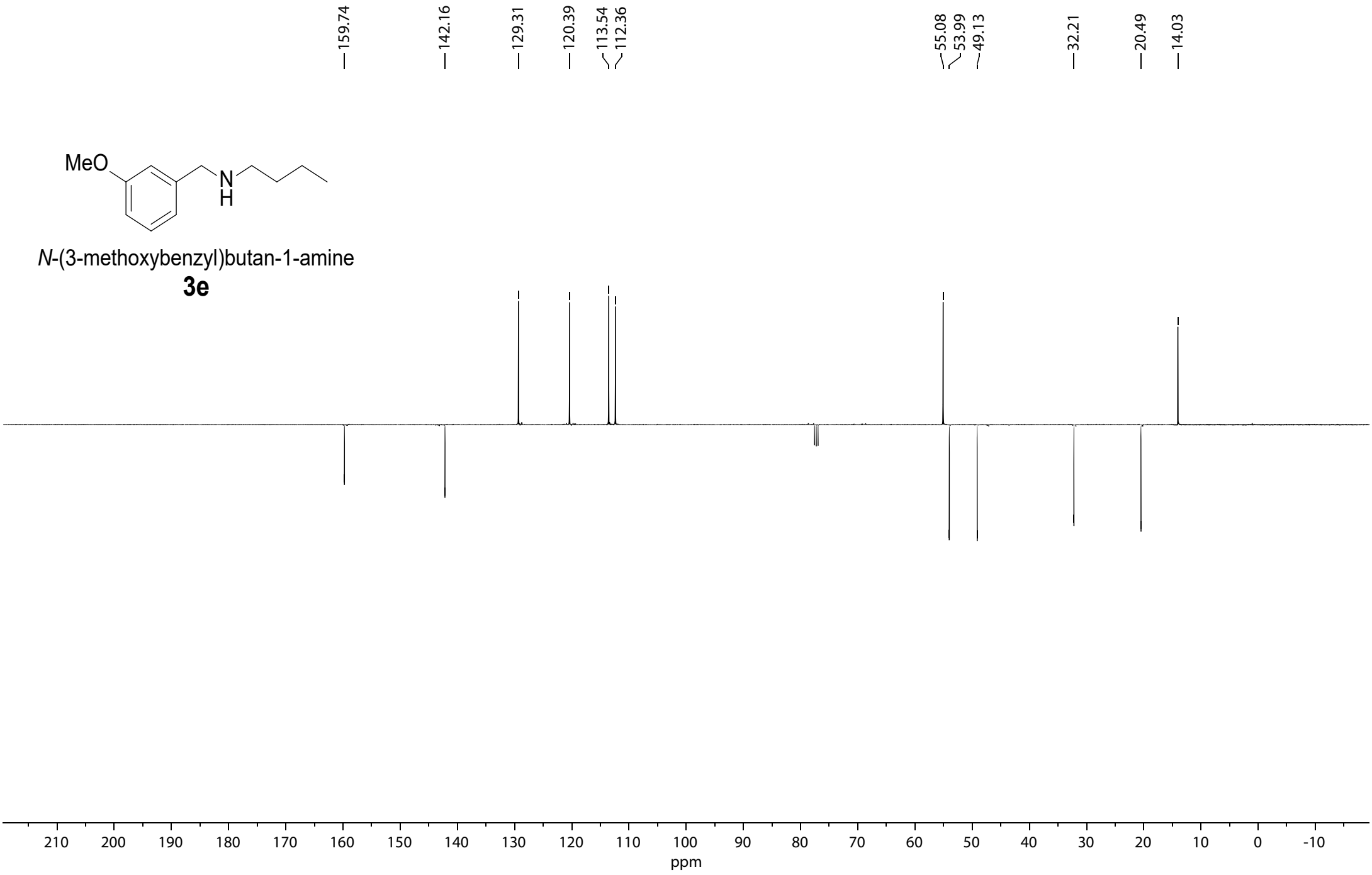
N-(3-fluorobenzyl)butan-1-amine

3d



N-(3-methoxybenzyl)butan-1-amine

3e



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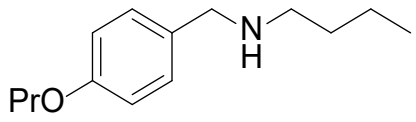

N-(4-propoxybenzyl)butan-1-amine

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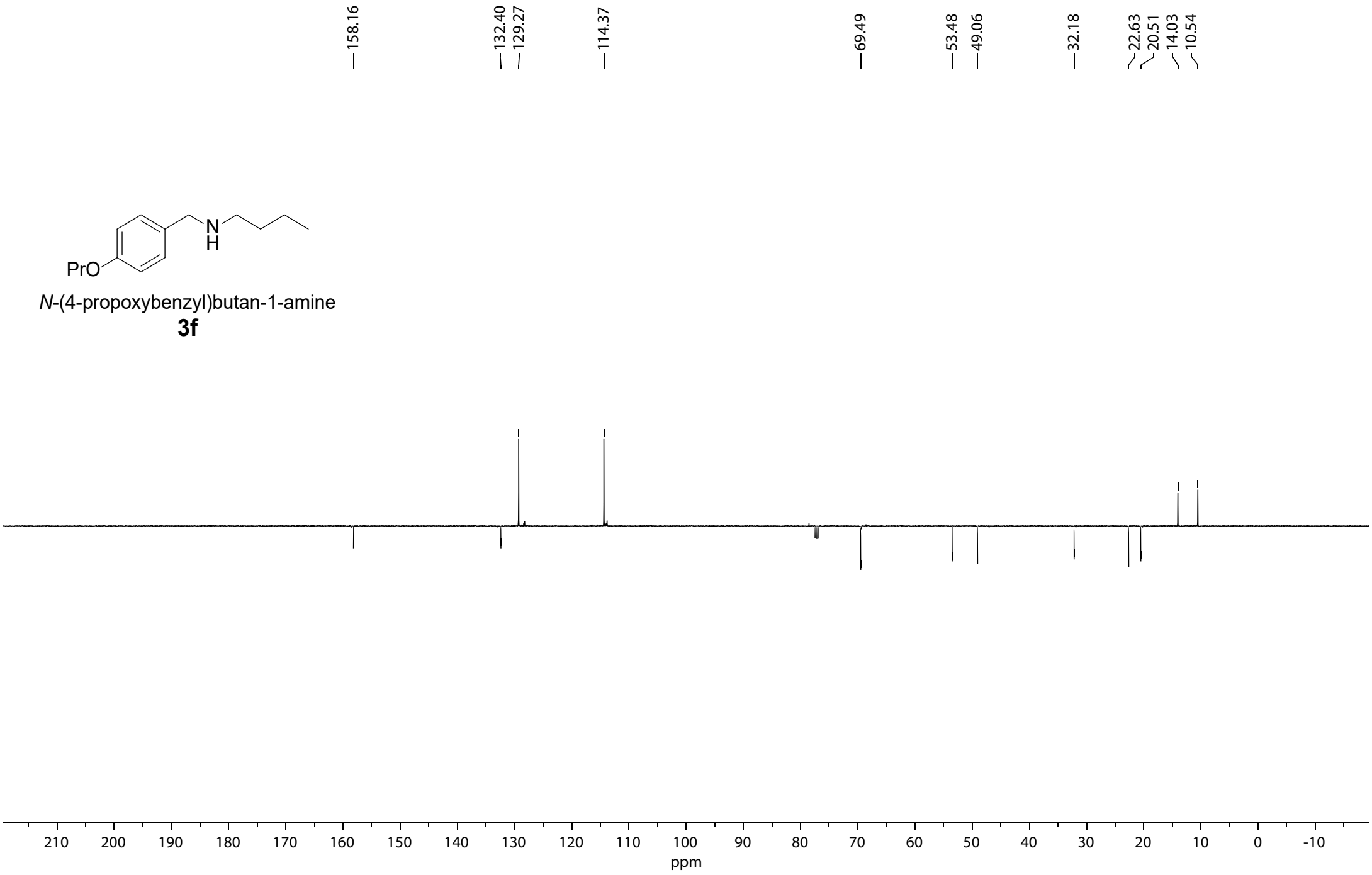

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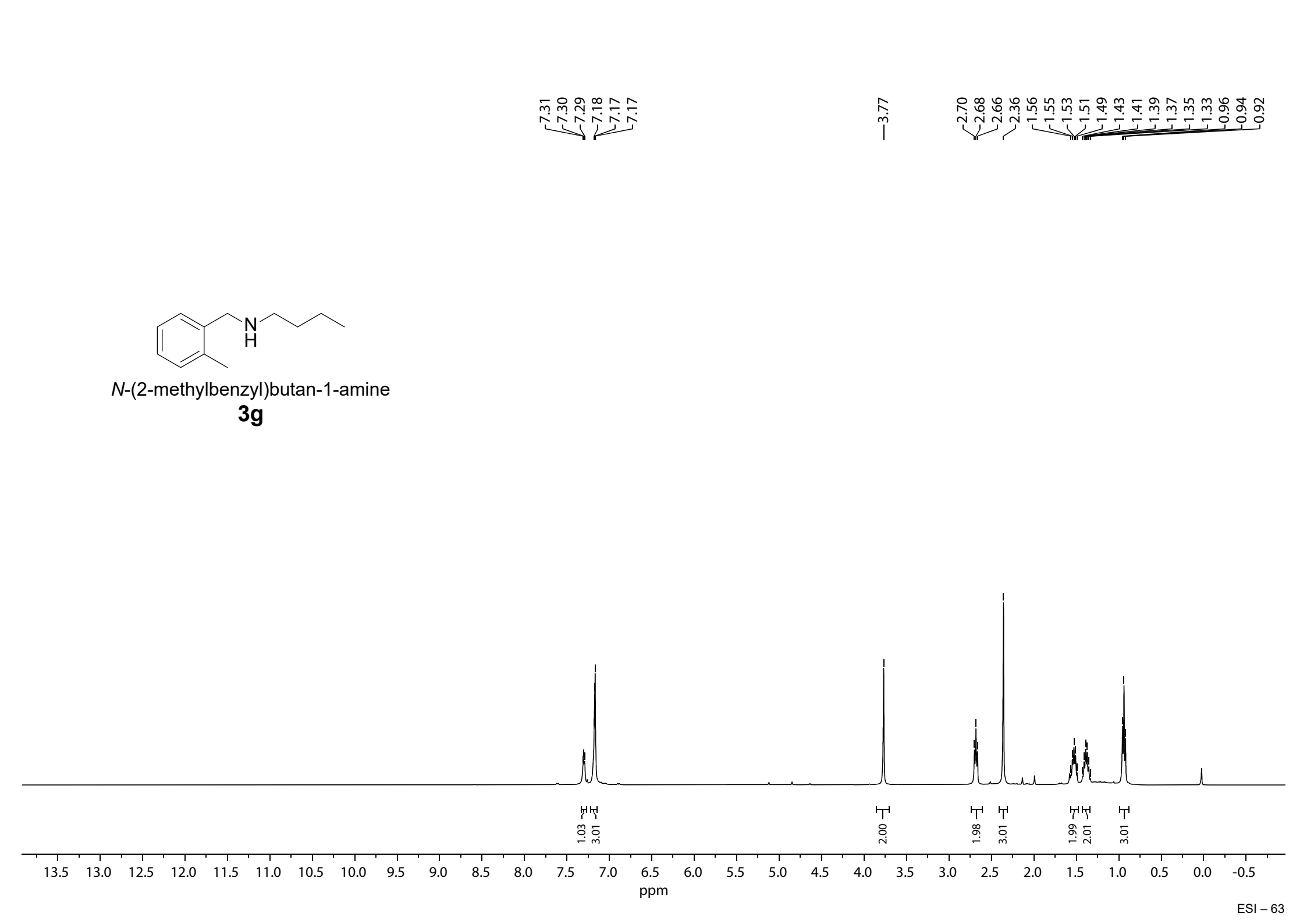

N-(2-methylbenzyl)butan-1-amine

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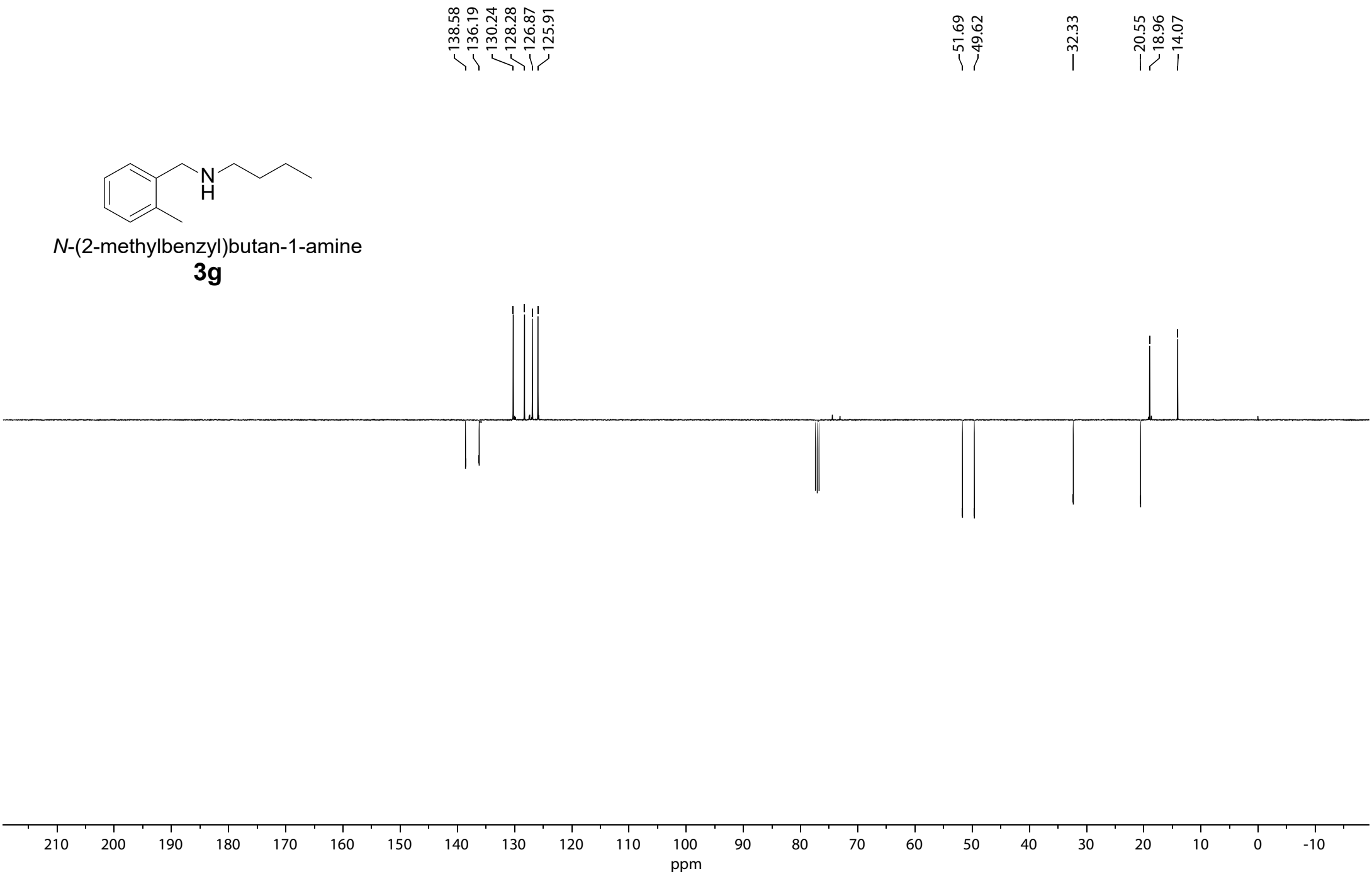

N-(2-methylbenzyl)butan-1-amine

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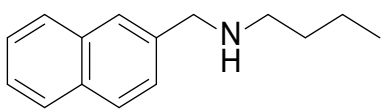

N-(naphthalen-2-ylmethyl)butan-1-amine

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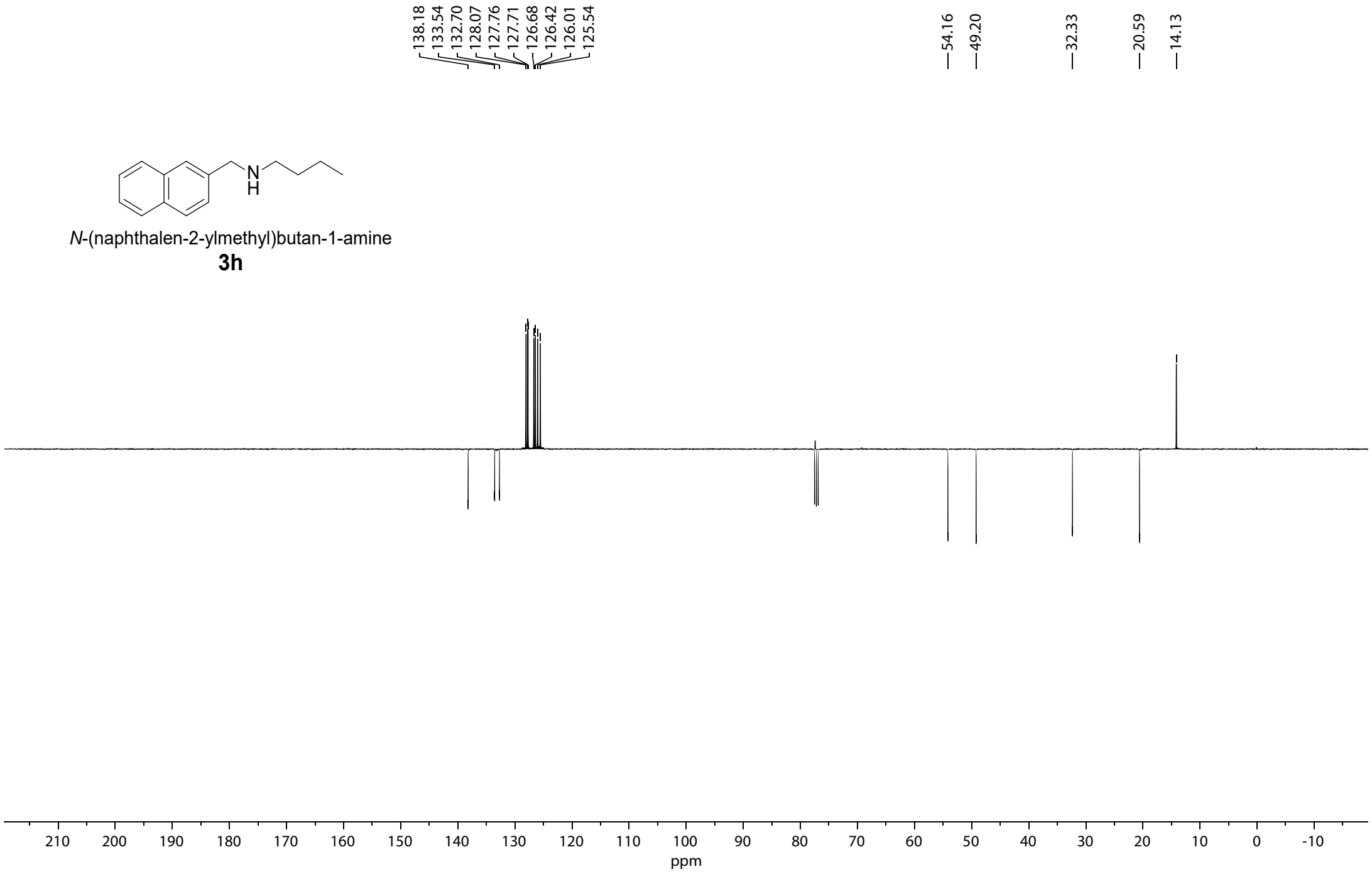
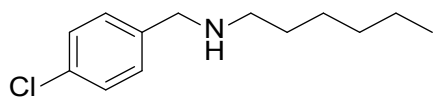


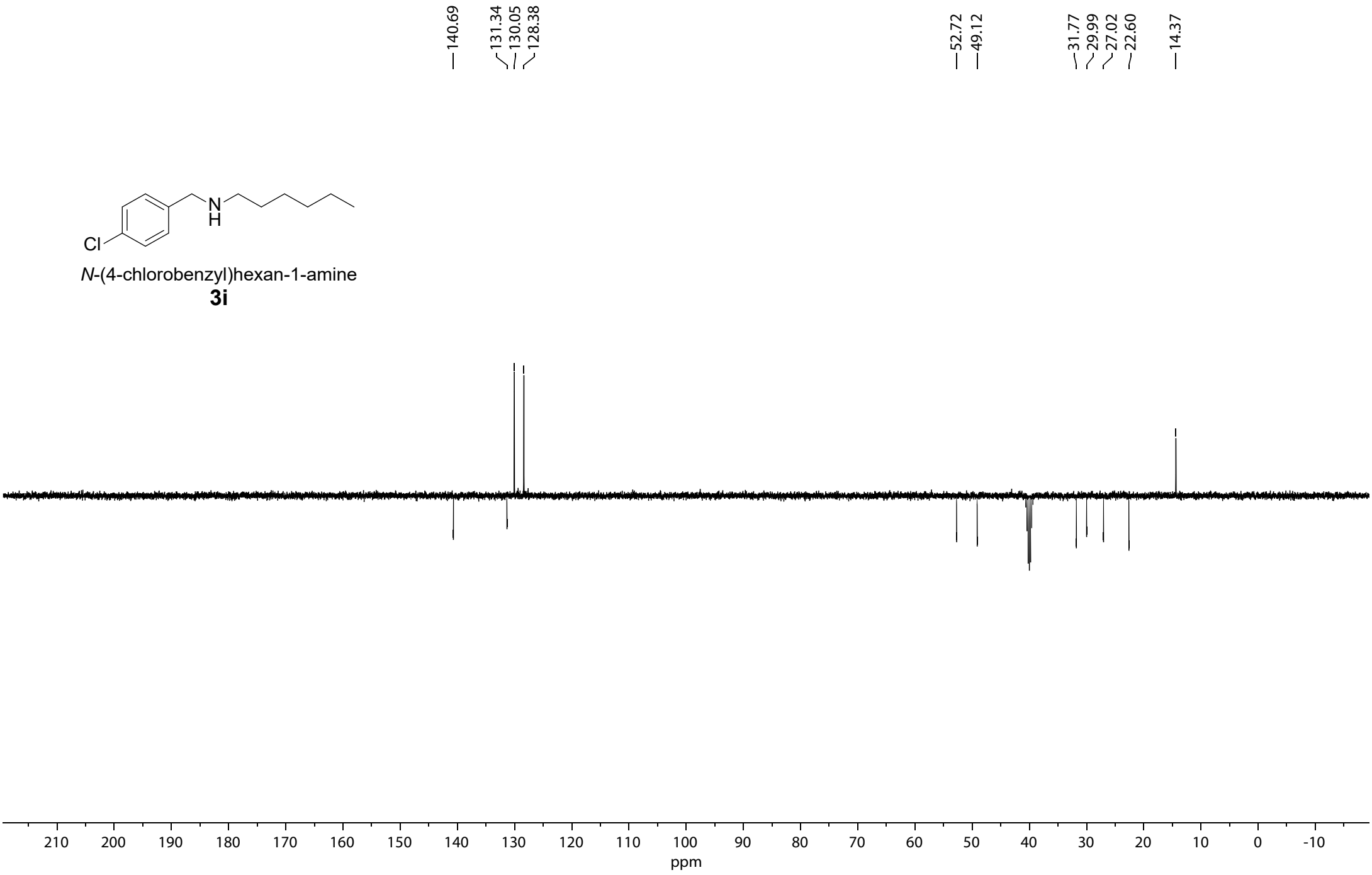
N-(naphthalen-2-ylmethyl)butan-1-amine

3h



N-(4-chlorobenzyl)hexan-1-amine

3i



N-(4-chlorobenzyl)hexan-1-amine

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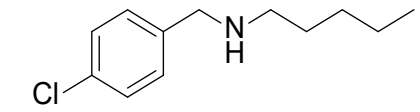

N-(4-chlorobenzyl)pentan-1-amine

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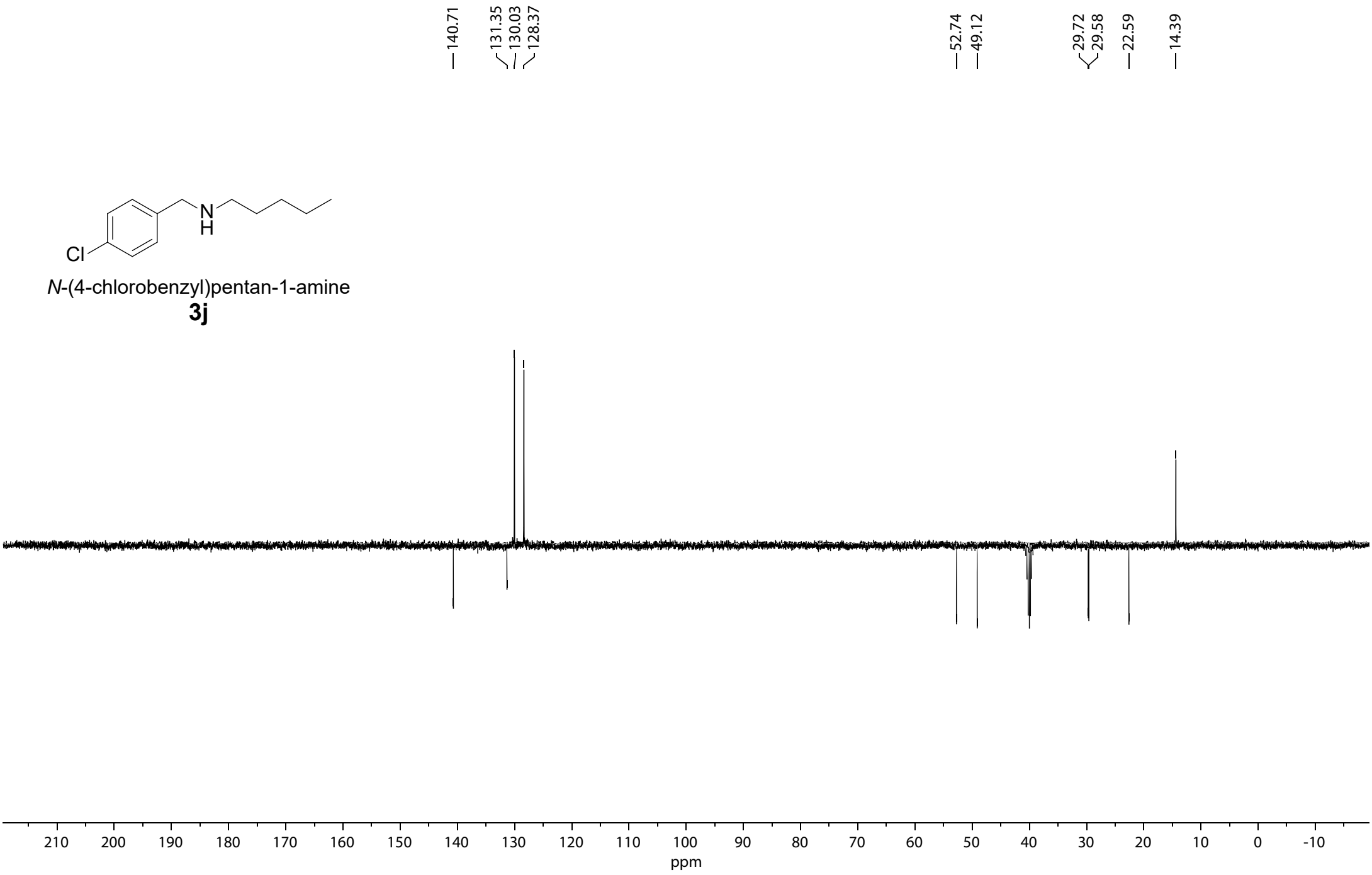

N-(4-chlorobenzyl)pentan-1-amine

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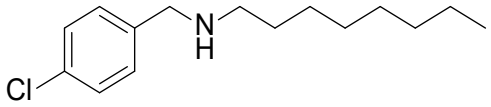

N-(4-chlorobenzyl)octan-1-amine

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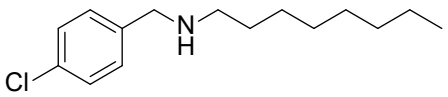

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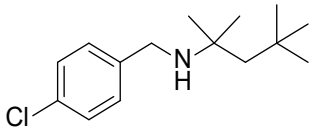
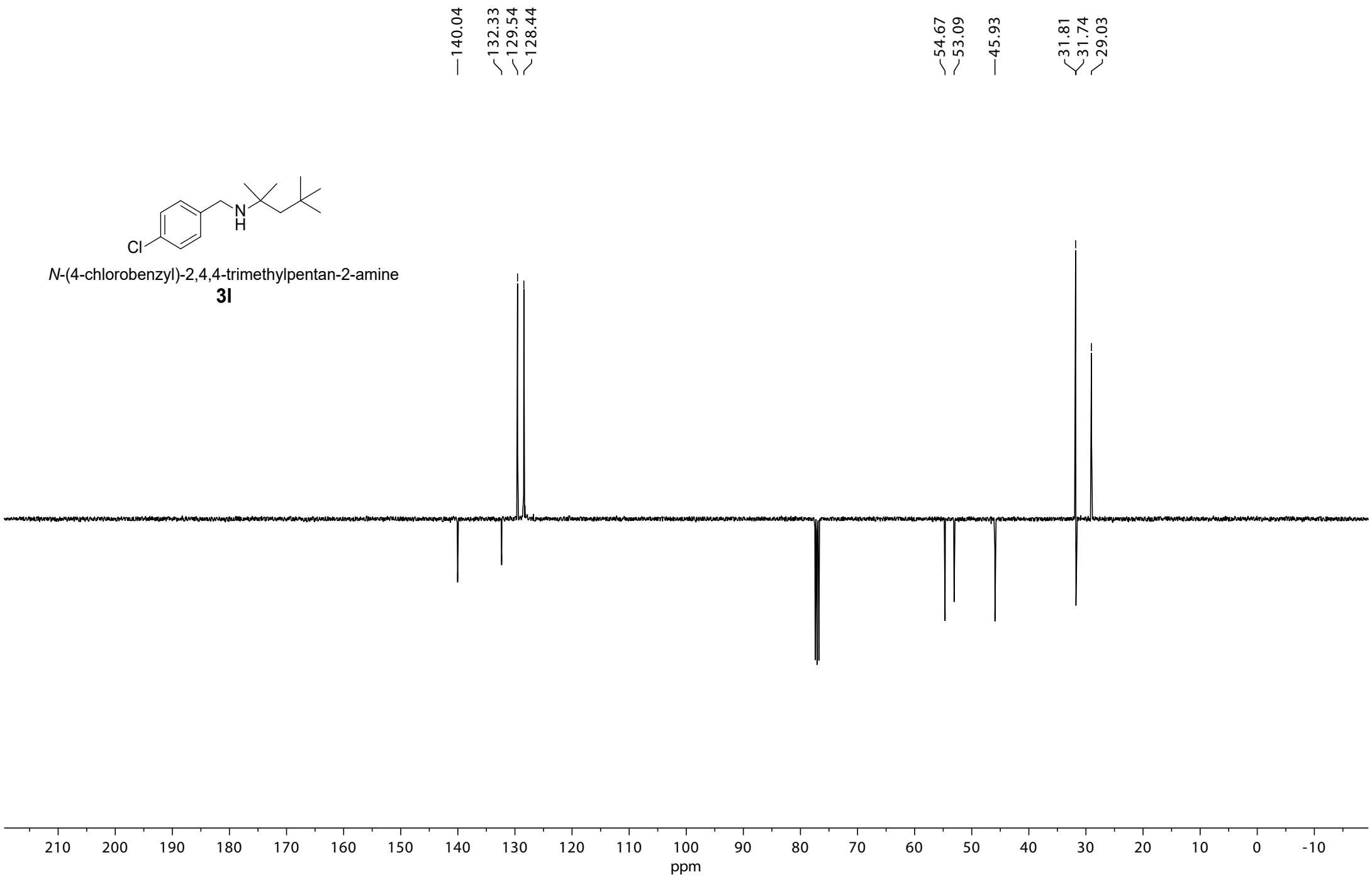


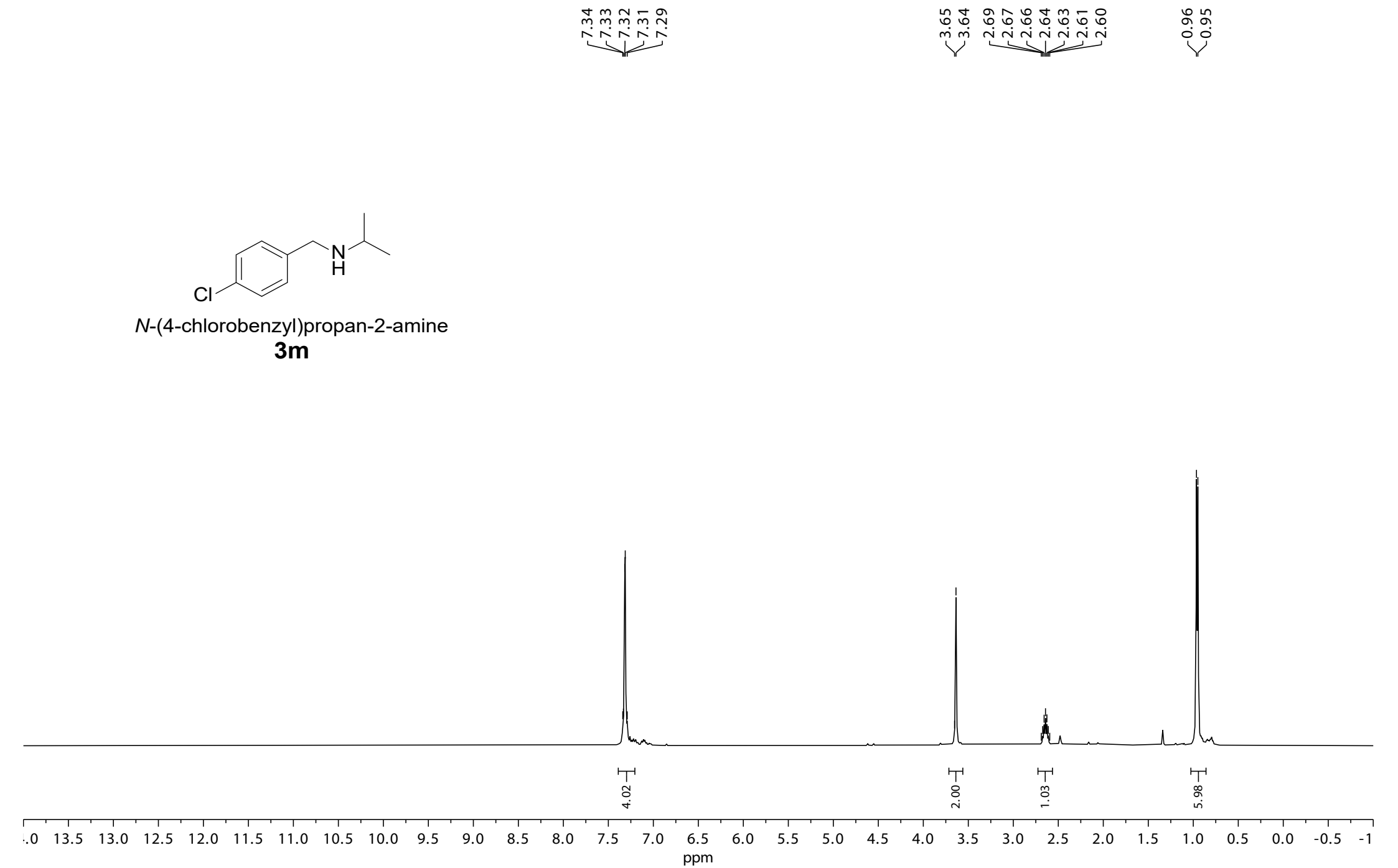
N-(4-chlorobenzyl)-2,4,4-trimethylpentan-2-amine

3l



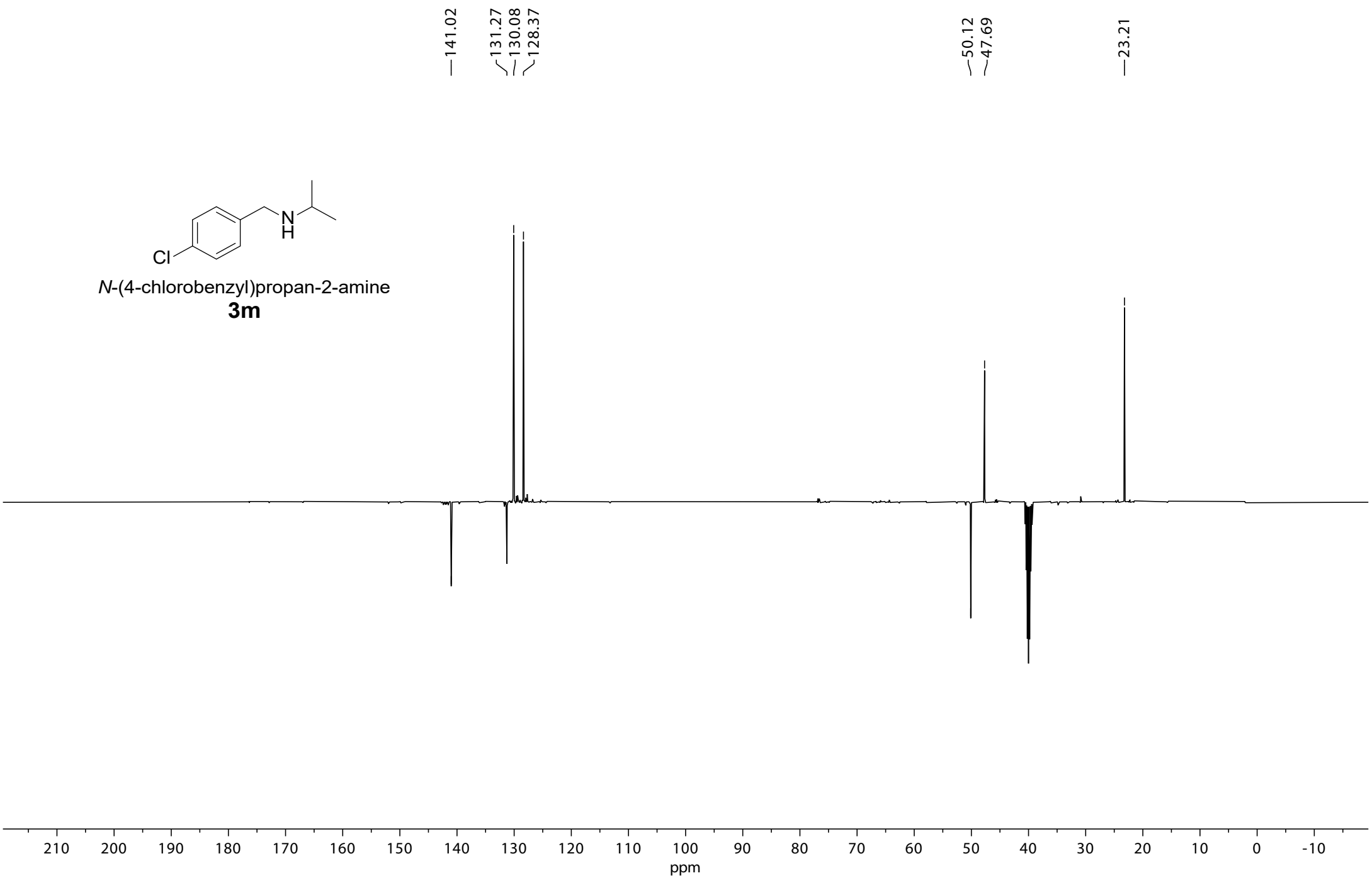
N-(4-chlorobenzyl)-2,4,4-trimethylpentan-2-amine

3l



N-(4-chlorobenzyl)propan-2-amine

3m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Cl
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N-(4-chlorobenzyl)propan-2-amine
3m
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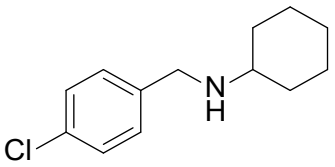
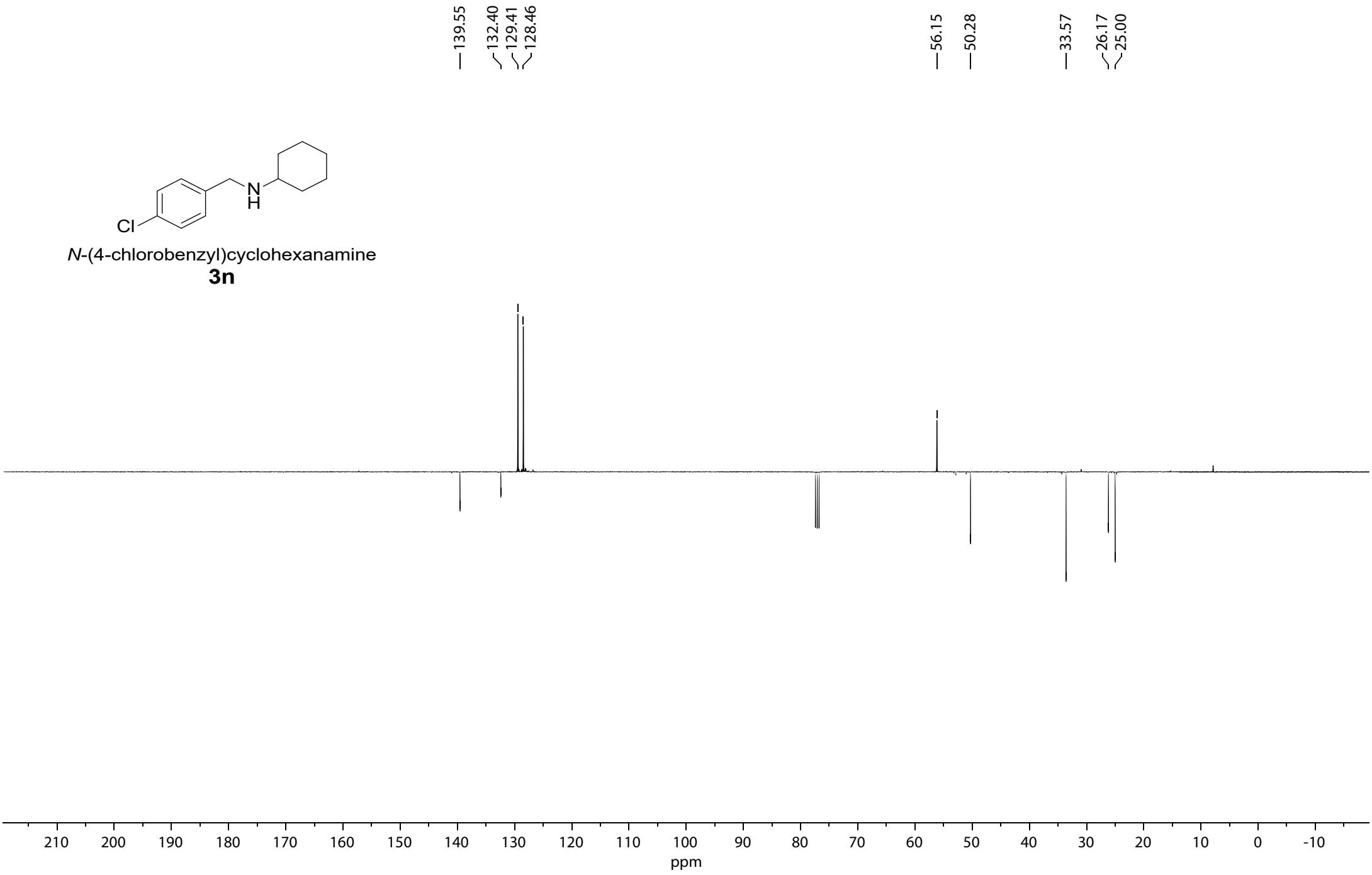
ppm



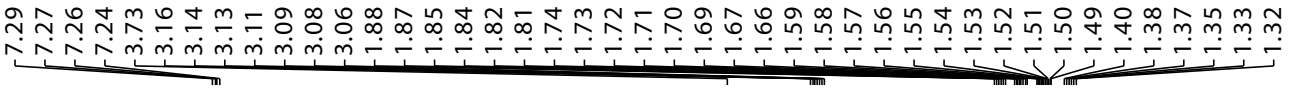
N-(4-chlorobenzyl)cyclohexanamine

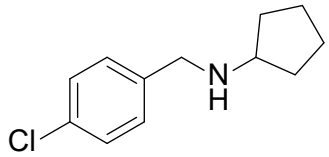
3n



N-(4-chlorobenzyl)cyclohexanamine

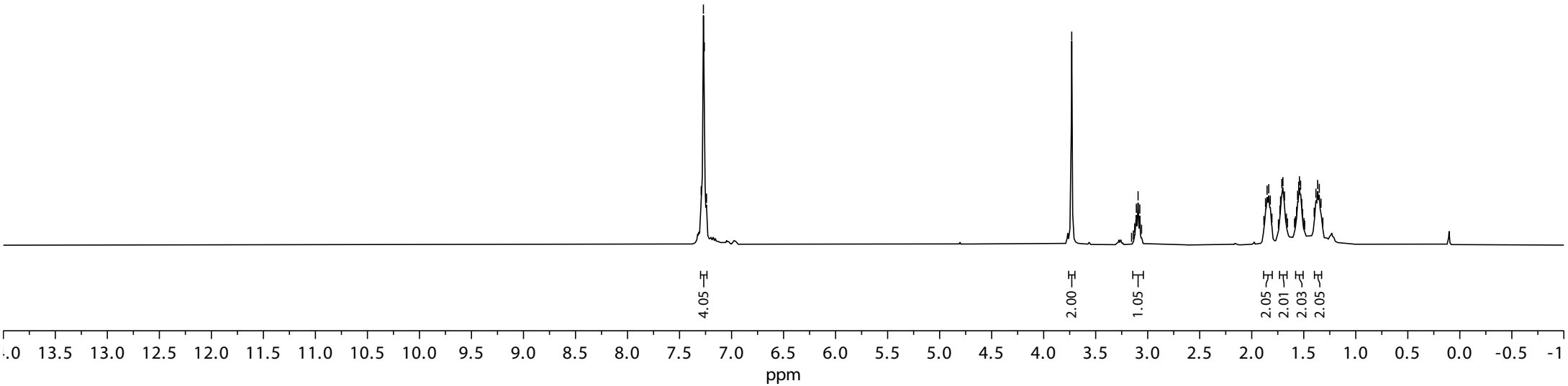
3n

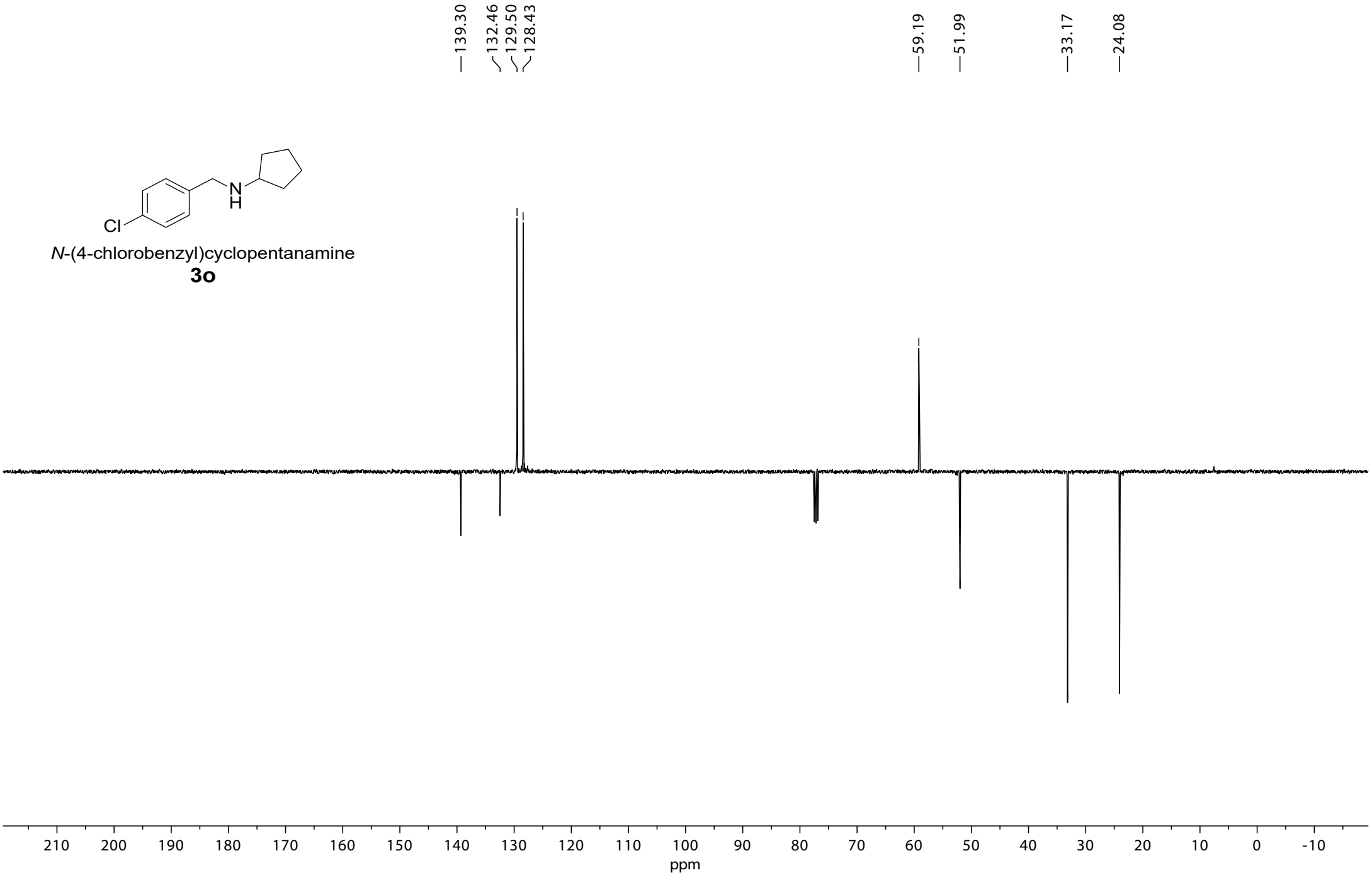




N-(4-chlorobenzyl)cyclopentanamine

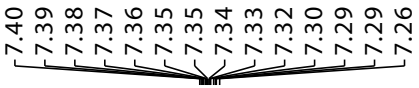
3o

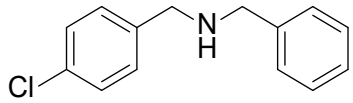




N-(4-chlorobenzyl)cyclopentanamine

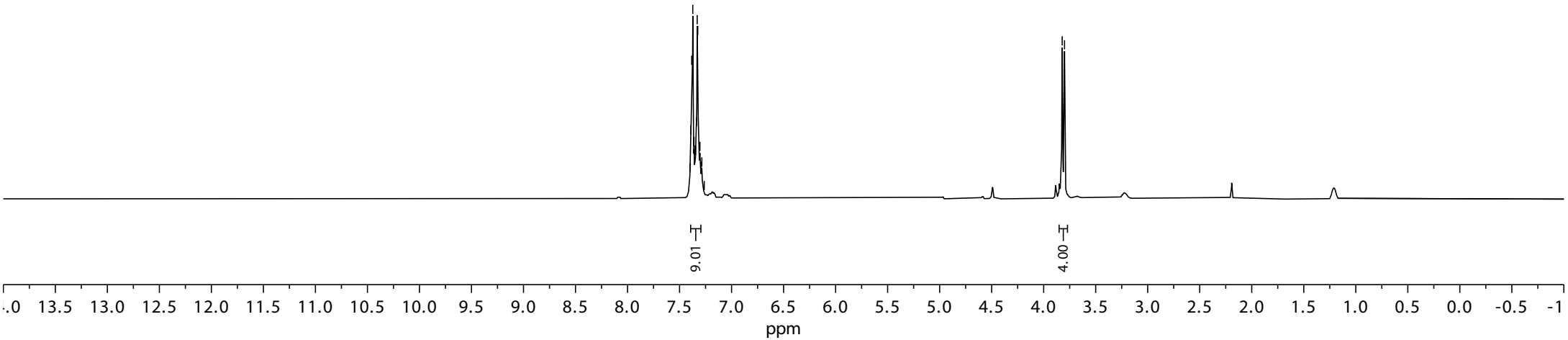
3o

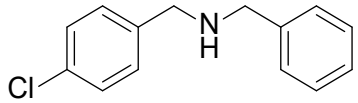




N-benzyl-1-(4-chlorophenyl)methanamine

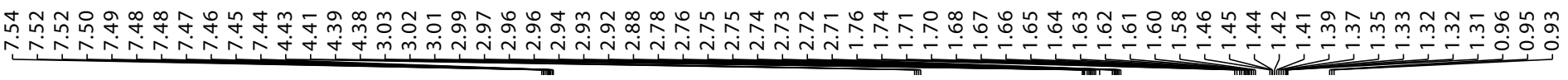
3p

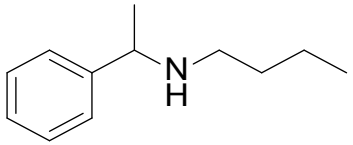




N-benzyl-1-(4-chlorophenyl)methanamine

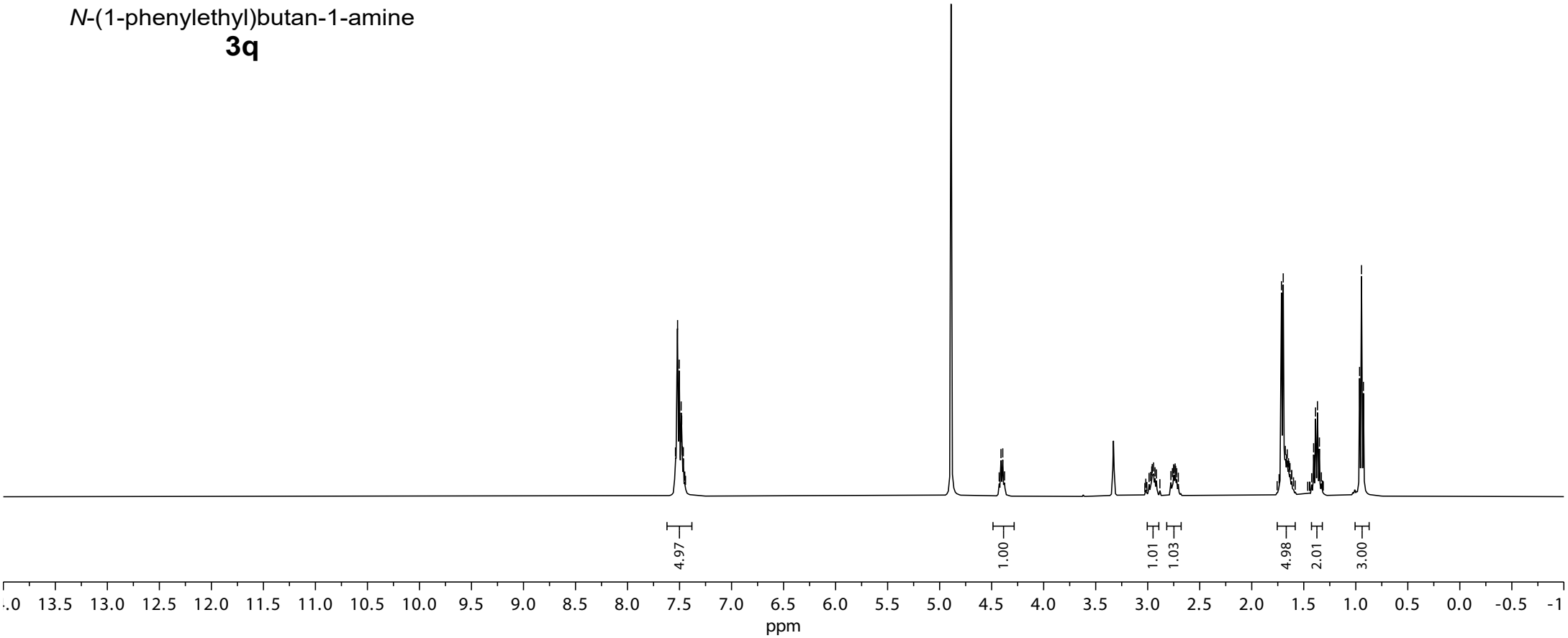
3p

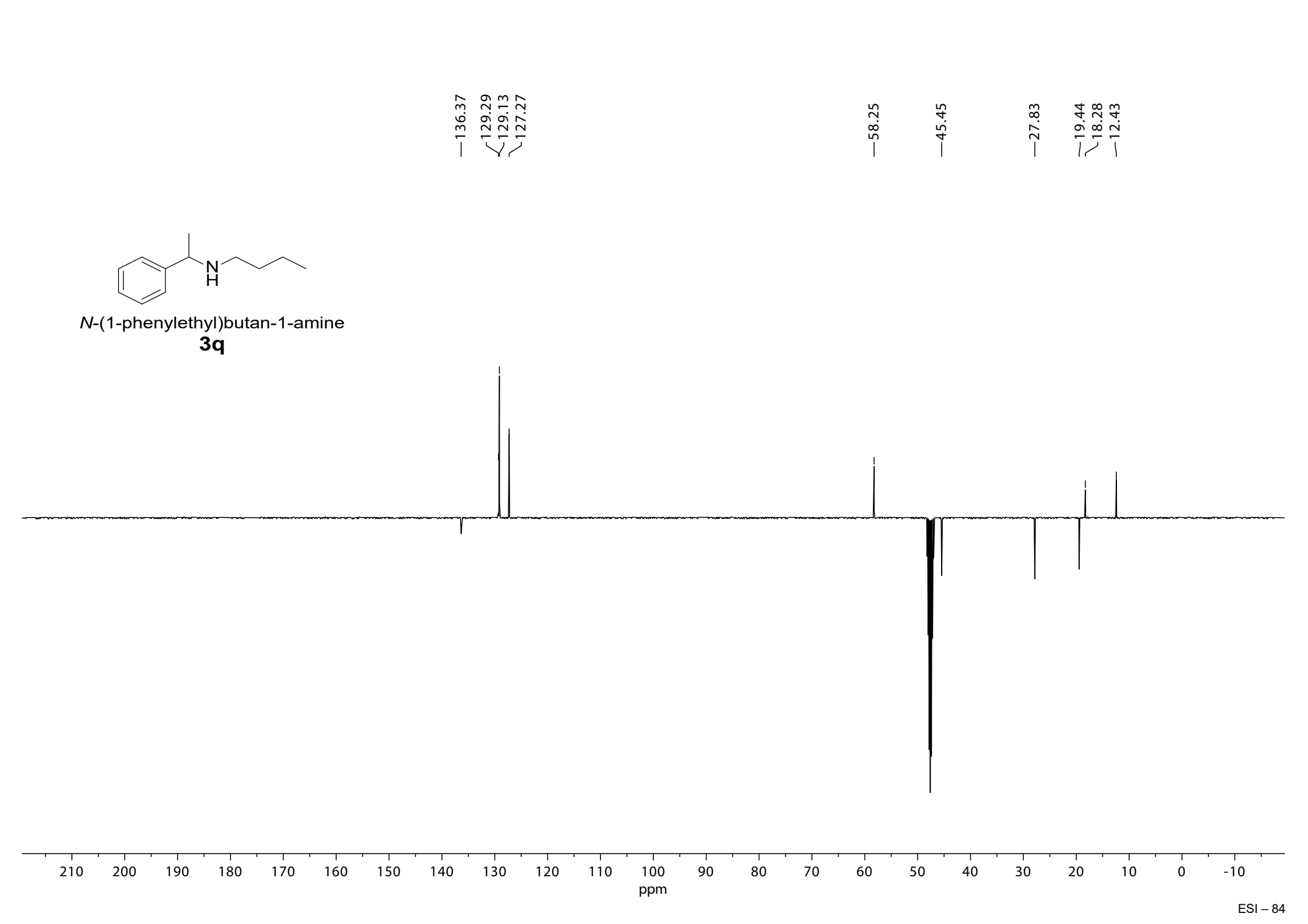




N-(1-phenylethyl)butan-1-amine

3q




136.37
129.29
129.13
127.27
58.25
45.45
27.83
19.44
18.28
12.43
N
H
N-(1-phenylethyl)butan-1-amine
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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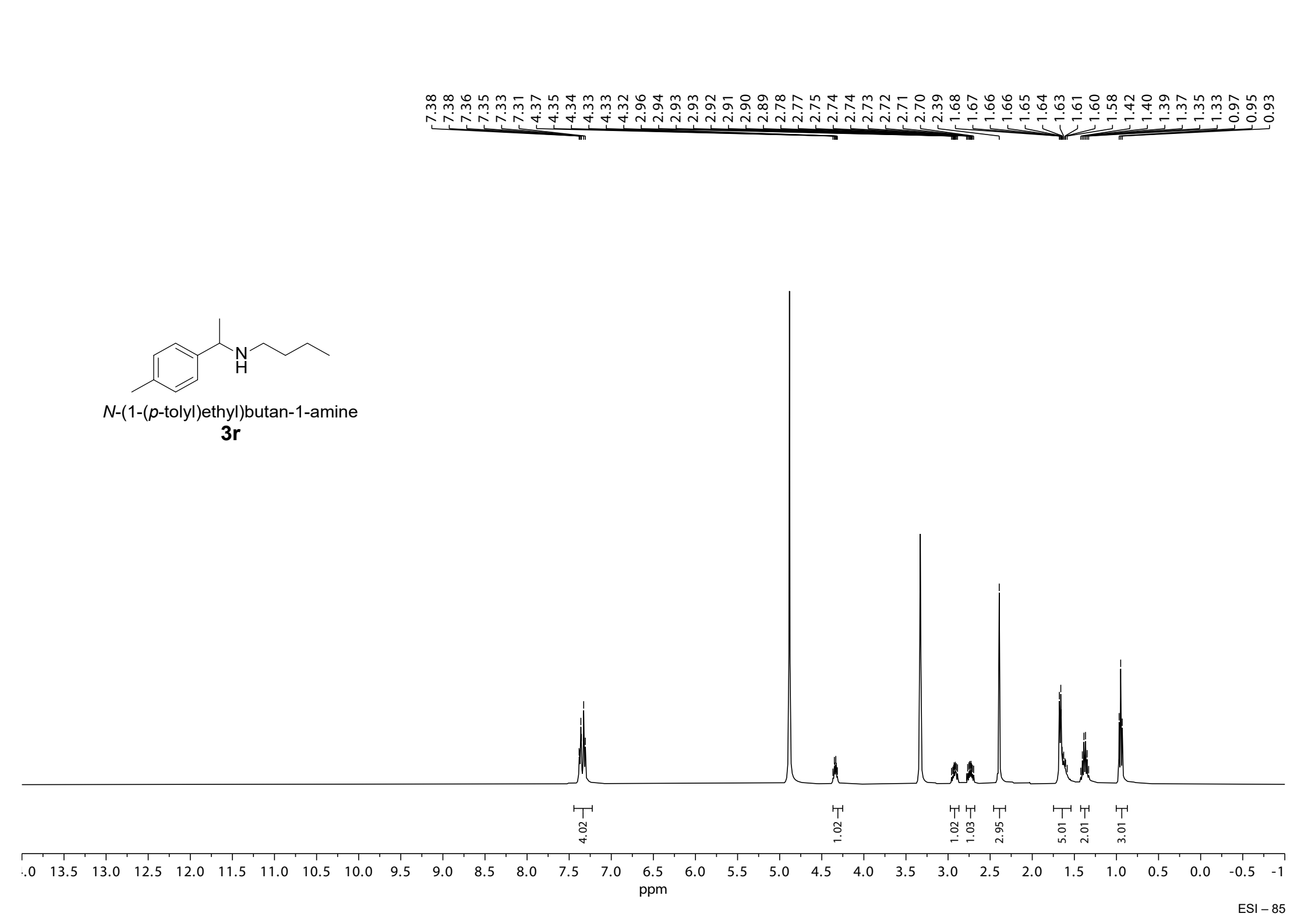
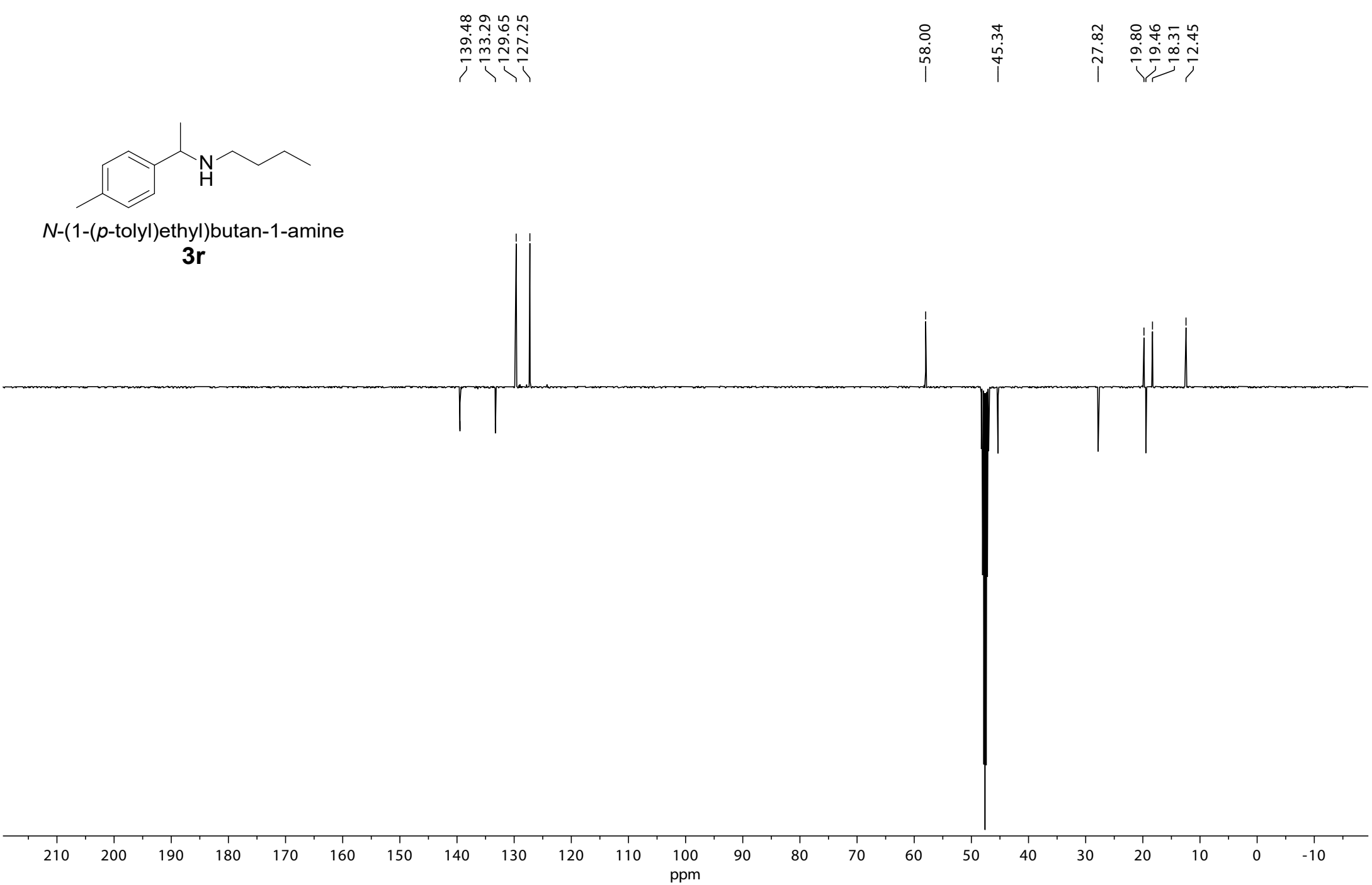
-10
ppm



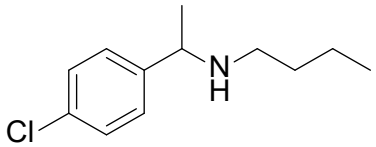
N-(1-(*p*-tolyl)ethyl)butan-1-amine

3r



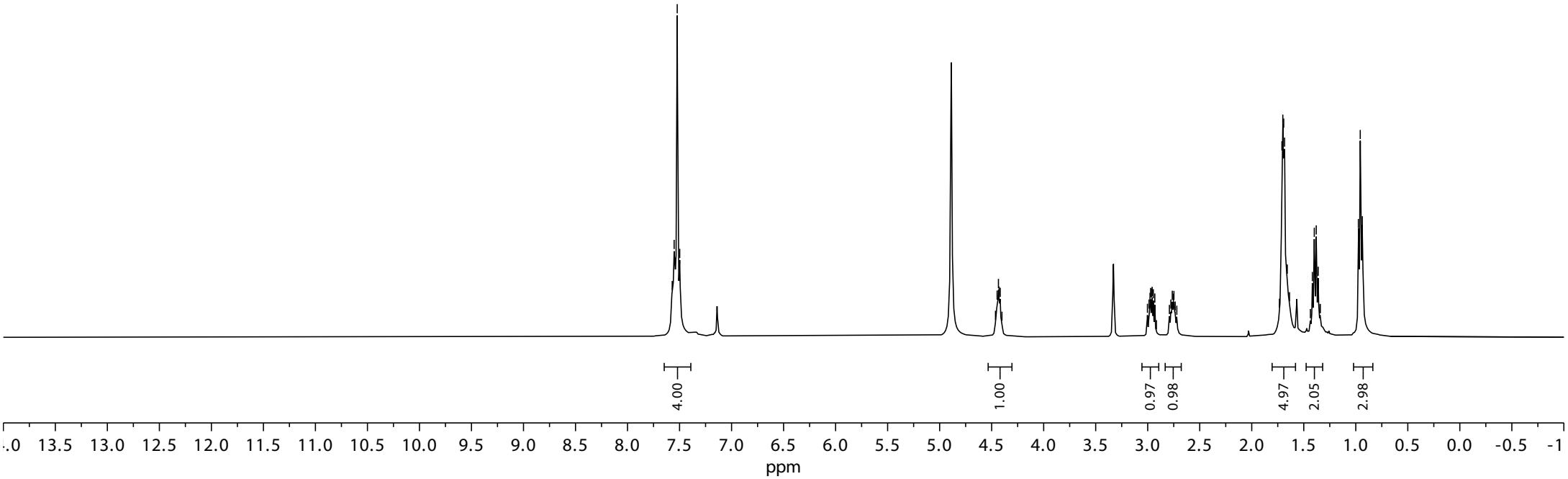
N-(1-(*p*-tolyl)ethyl)butan-1-amine

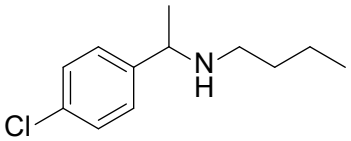
3r



N-(1-(4-chlorophenyl)ethyl)butan-1-amine

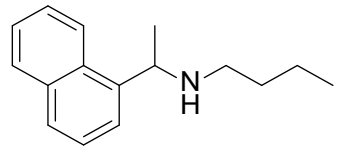
3s





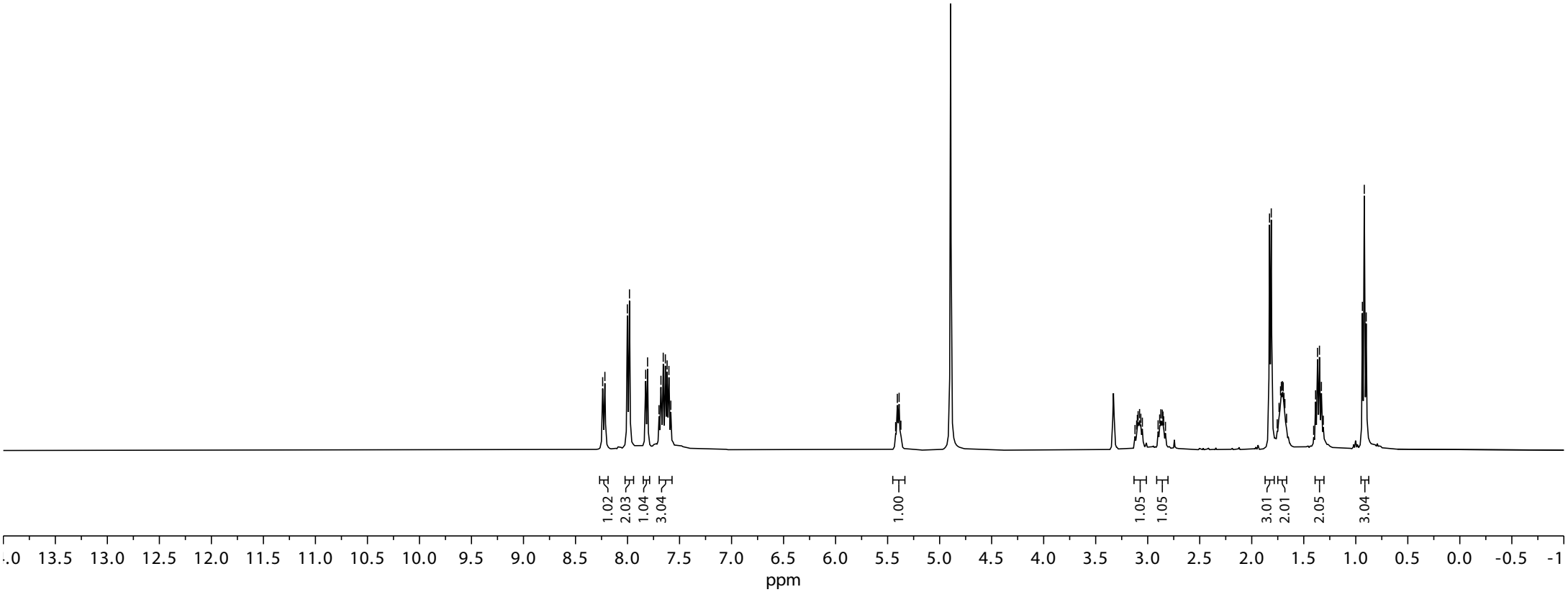
N-(1-(4-chlorophenyl)ethyl)butan-1-amine

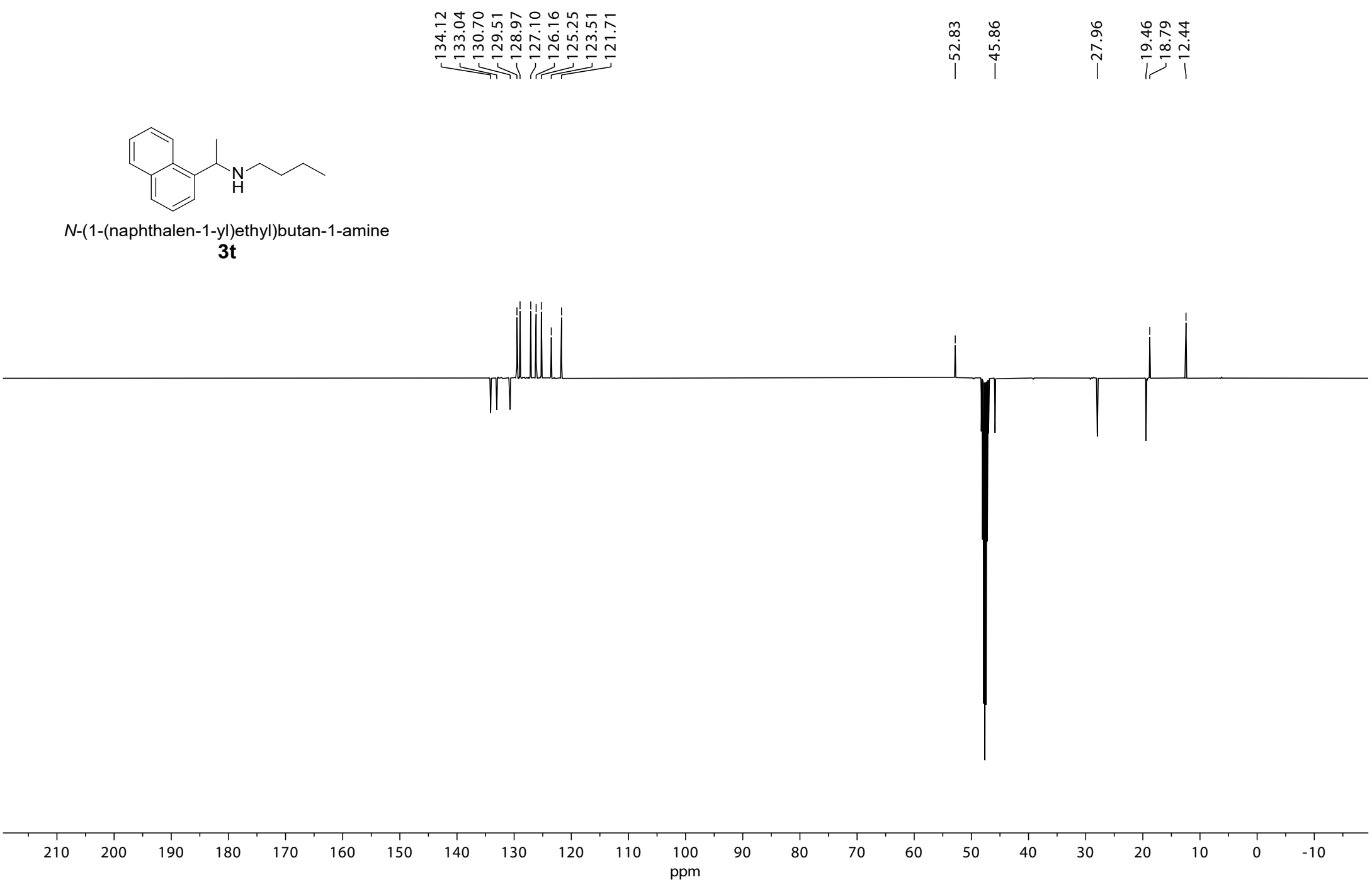
3s



N-(1-(naphthalen-1-yl)ethyl)butan-1-amine

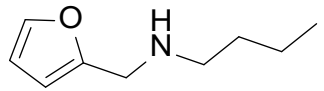
3t





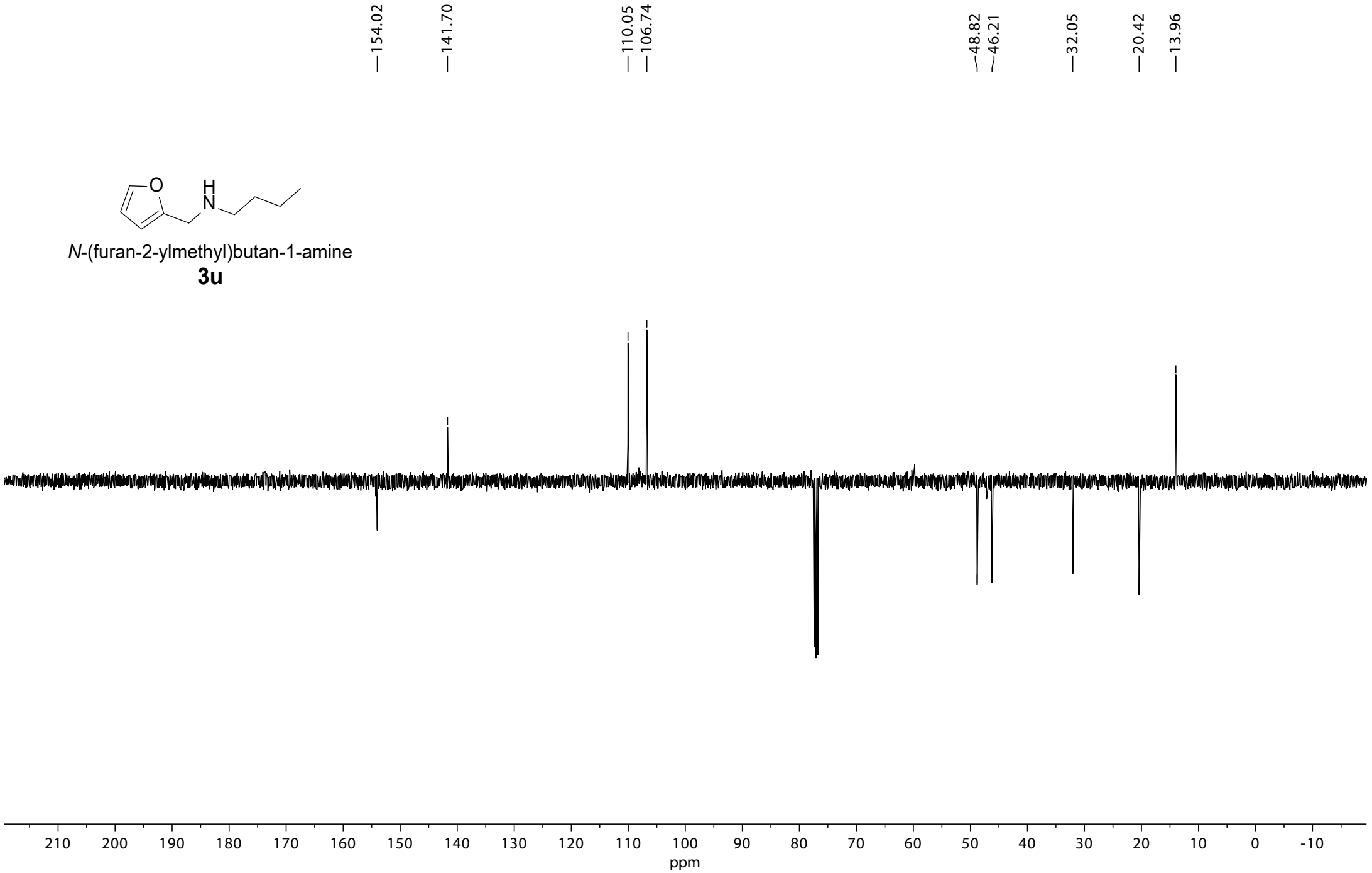
N-(1-(naphthalen-1-yl)ethyl)butan-1-amine

3t



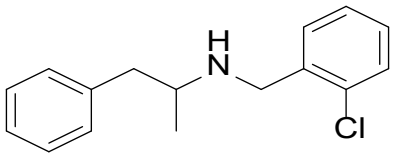
N-(furan-2-ylmethyl)butan-1-amine

3u



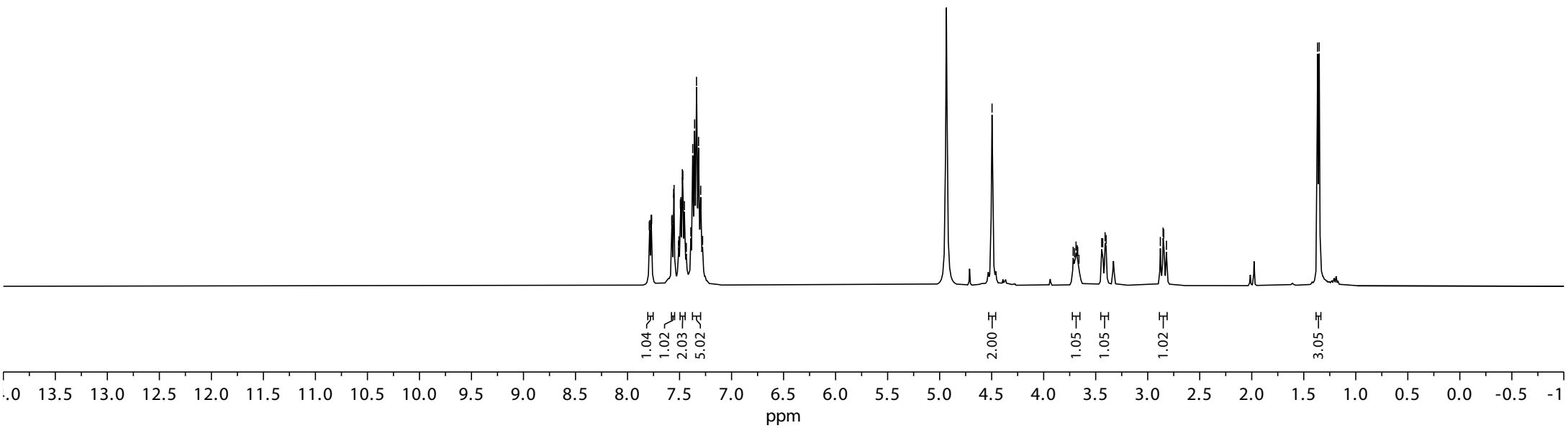
N-(furan-2-ylmethyl)butan-1-amine

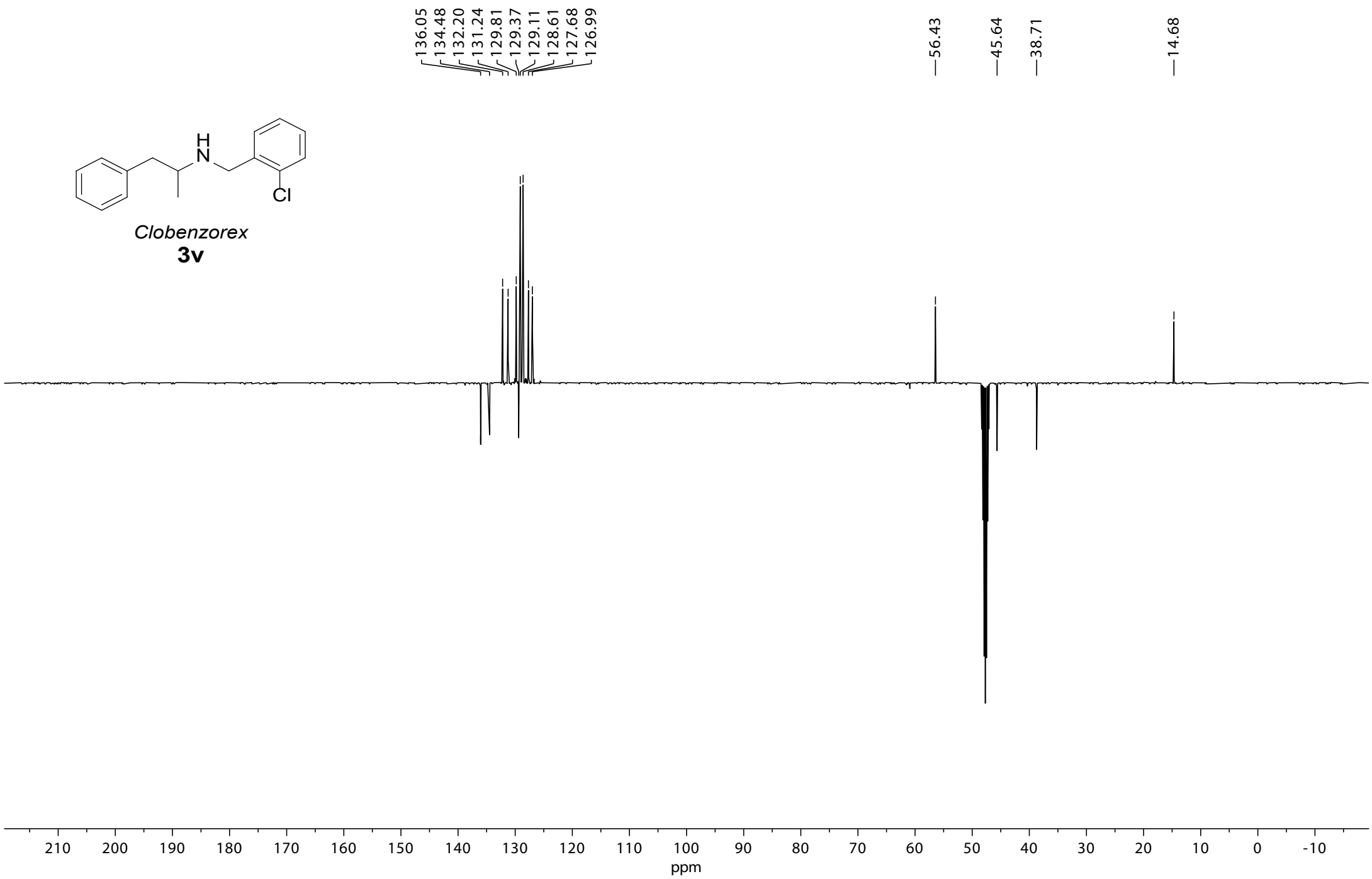
3u



Clobenzorex

3v




136.05
134.48
132.20
131.24
129.81
129.37
129.11
128.61
127.68
126.99
56.43
45.64
38.71
14.68
H
N
Cl
Clobenzorex
3v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm