Plantacare 2000, a Biosurfactant for an Eco-friendly Palladium Catalyzed Cyanation of Aromatic Bromides

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Supporting Information

GENERAL METHODS

All reagents were used as purchased from commercial suppliers without further purification. Flash column chromatography was performed trough Biotage® Isolera automated flash chromatography system using Biotage® Snap Ultra Column 25g size, Merck aluminum backed plates pre-coated with silica gel 60 (UV254) were used for analytical thin-layer chromatography and were visualized by staining with a solution of $KMnO_4$. Reactions carried out under MW dielectric heating were performed with a Discover microwave oven equipped with the 10 mL vial for reaction. ^1H NMR and ^{13}C NMR spectra were recorded on 400 MHz and 600 MHz Brucker Advance NMR spectrometers. Deuterated chloroform and methanol were used as the solvents and chemical shift values (δ) are reported in parts per million (ppm) referring to the residual signals of the deuterated solvent (δ 7.26 for ^1H and δ 77.6 for ^{13}C in $CDCl_3$, δ 3.34 for ^1H and δ 49.00 for ^{13}C in CD_3OD, δ 2.50 for ^1H and δ 40.00 for ^{13}C in $(CD_3)_2SO$). Data are represented as follows: chemical shift, multiplicity (s=singlet, d=doublet, dd=doublet of doublets, dt=doublet of triplets, t=triplet, q=quartet, m=multiplet or multiple resonances, bs=broad singlet), coupling constant (*J*) in Hertz and the integration in ppm. Mass spectrometry data were collected on Varian Saturn 2000 GC/MS spectrometer with ion trap detector and equipped with 30 m OV-101 capillary column, splitting injector at 240 °C using the following method: 40 °C - 3 min, 40-200 °C 10 °C/min – 17 min, 200-240 °C 20 °C/min – 5 min. Metal analyses of Pd and Fe content were carried out using an Agilent MP-AES 4210 instrument.

Table S1 List of the most commonly used cyanation agents in descending order of toxicity (LD50). The comparison is purely indicative, as the LD_{50} values determined on different organisms are not directly comparable.

Compound	LD50 (mg/kg)[a]	Organism	Reference/source
$K_4(Fe(CN)_6$	6400	Rat (oral)	https://pubchem.ncbi.nlm.nih.gov/#tab/sidsrcname=ChemIDplus&query=13943-58-3&input_type=text
$HCONH_2$	5577	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/sigma/f9037?userType=undefined
CuSCN	5000	Rat (oral)	https://www.sigmaaldrich.cn/IT/en/sds/aldrich/298212?userType=undefined
DMF/ NH_4I	3010 (DMF), No data for NH_4I	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/sial/227056?userType=anonymous
Ethyl cyanoacetate	2000	Rat (oral)	https://www.fishersci.com/store/msds?partNumber=AC118280010&countryCode=US&language=en
DMF/$(NH_4)_2CO_3$	1800 $(NH_4)_2CO_3$, 3010 (DMF)	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/SIGALD/379999?userType=undefined
Bu_4NCN	1000	Rat (oral)	https://datasheets.scbt.com/sc-237015.pdf
Tosyl cyanide	1000	unknown	https://www.fishersci.com/store/msds?partNumber=AC455820050&productDescription=P-TOLUENESULFONYL+CYANID+5GR&vendorId=VN00032119&countryCode=US&language=en
KSCN	854	Rat (oral)	https://www.carlroth.com/medias/SDB-9899-IT-IT.pdf?context=bWFzdGVyfHNlY3VyaXR5RGF0YXNoZWV0c3wyNTU3MzN8YXBwbGljYXRpb24vcGRmfGFEVTRMMmd3Wmk4NU1UYzNOVFE1TWpBNU5qTXdMMU5FUWw4NU9EazVYMGxVWDBsVUxuQmtaZ3xjMjQ5ZTlhM2ZjMjM5OWFiYTI4ZGNiZDI0MTY4MGRjMzdhYmRiNDNjNjRkNDMwNDllNGE2NWI2NjYwNTZhNzUz
$PPh_3(SCN)_2$	750	Rat (oral)	https://www.fishersci.com/store/msds?partNumber=AC140420250&productDescription=TRIPHENYLPHOSPHINE%2C+99%25+25GR&vendorId=VN00032119&countryCode=US&language=en
MeCN	617	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/sial/271004?userType=undefined
DMF/NH_3	350 NH_3 ,3010 (DMF)	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/aldrich/294993?userType=undefined
BnCN	270	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/aldrich/b19401?userType=undefined
Diammino-maleonitrile	187	Oral rat	https://www.fishersci.com/store/msds?partNumber=AC172700250&countryCode=US&language=en
Benzylthio-cyanate	100	unknown	https://www.tcichemicals.com/BE/en/sds/T0198_EU_6N.pdf
Acetone Cyanohydrine	15.8	Rat (oral)	https://www.fishersci.com/store/msds?partNumber=AC102380050&productDescription=ACETONE+CYANOHYDRIN%2C+99%25+5GR&vendorId=VN00032119&countryCode=US&language=en
$CNCH_2CN$	14	Rat (oral)	https://www.fishersci.com/store/msds?partNumber=AC125275000&countryCode=US&language=en
DDQ	13	Mouse (Intravenous)	https://www.sigmaaldrich.com/IT/en/sds/aldrich/d60400?userType=anonymous
Zn(CN)2	8.35	Rat (Oral)	https://www.sigmaaldrich.com/IT/en/sds/aldrich/256498?userType=anonymous
KCN	7.49	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/sigald/11813?userType=undefined
NaCN	5.733	Rat (oral)	https://www.sigmaaldrich.com/IT/en/sds/SIGALD/205222?userType=undefined
TMSCN	5.1	Unknown (oral)	https://www.sigmaaldrich.com/IT/en/sds/aldrich/212849?userType=anonymous
CuCN	5.1	Unknown	https://www.sigmaaldrich.com/IT/en/sds/sigald/216305?userType=anonymous
$CNCH_2CO_2Et$	nd		
1-Cyano benzotriazole	nd		
1-Cyano benzimidazole	nd		
1-Cyano imidazole	nd		
Aryl(cyano)iodonium triflates	nd		
N-Cyano-N-phenyl-*p*-toluenesulfonamide	nd	Unknown (oral)	https://www.combi-blocks.com/msds/OT-2253.pdf

Table S2 Solvents employed in metal catalyzed cyanation of aryl halides using $K_4(Fe(CN)_6$ as cyanide source

Solvent	Classification[1]	Flash point (°C)[b]	
Toluene	Problematic	4.4	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_lang=it&p_card_id=0078&p_version=2#:~:text=Flash%20point%3A%204°C%20c.c.
NMP (N-methylpyrrolidinone)	Hazardous	91	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=0513&p_version=1&p_lang=en
1,4-Dioxane	Hazardous	12	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_lang=en&p_card_id=0041&p_version=1
DMF	Hazardous	58	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=0457&p_version=1&p_lang=it
DMA (dimethylacetamide)	Hazardous	63	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=0259&p_version=1
MeCN	Problematic	2	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_lang=it&p_card_id=0088&p_version=2#:~:text=Flash%20point%3A%202°C%20c.c
EtOH	Reccomended	12.8	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=44&p_version=1&p_lang=en
i-PrOH	Reccomended	12	https://chemicalsafety.ilo.org/dyn/icsc/showcard.display?p_card_id=554&p_version=1&
Water	Reccomended	-	

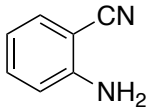
General procedure for the cyanation reactions

Method A (convectional heating). A 10 mL MW tube was filled with Na_2CO_3 (0.122 mmol), $K_4[Fe(CN)_6]$-$3H_2O$ (0.170 mmol) and a solution of PL-2000 (1.5 wt% in H_2O, 2 mL) and capped with a screw cap. The reaction mixture was stirred for 15 minutes, and aryl bromide (1 mmol) was added. Then [Pd(dppf)Cl_2]-CH_2Cl_2 (269 mg, 0.098 mmol) was added. The solution was stirred at 80 °C for 16 h. After cooling, the mixture was filtered under vacuum and the solid was washed with EtOAc (5 mL) to obtain a residual solid and the organic phase. The aqueous mixture was extracted with EtOAc (5 mL). The two phases were separated, and the organic phase was washed with H_2O (5 mL), dried over anhydrous Na_2SO_4, filtered, evaporated under reduced pressure and analysed by GC/MS or 1H-NMR to obtain the desired product. If necessary, the crude product was purified by chromatography on silica gel with EtOAc in petroleum ether or MeOH and DCM as eluent. The yields refer to the isolated products.

Method B (MW heating). A 10 mL MW tube was filled with Na_2CO_3 (0.122 mmol), $K_4[Fe(CN)_6]$-$3H_2O$ (0.170 mmol) and a solution of PL-2000 (1.5 wt% in H_2O, 2 mL). The mixture was stirred for 15 min and aryl bromide (1 mmol) was added. Then [Pd(dppf)Cl_2]-CH_2Cl_2 (269 mg, 0.098 mmol) was added. After stirring at rt for 5 min, the tube was submitted to MW dielectric heating at 120 °C for 1.5 h with cooling at a fixed power of 300 watts. After irradiation, the mixture was cooled to room temperature and the mixture was treated for method A.

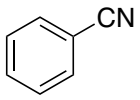
Table S3 MW optimization

Pd Catalyst/Ligand, base	Surfactant	Conditions	**2** [%][a]
[Pd(dppf)Cl_2]·CH_2Cl_2 (9.8 mol%), $K_4[Fe(CN)_6]$ (17 mol%), Na_2CO_3 (12 mol%)	PL-2000 1.5 wt%	MW 80 °C, 45 min	20
[Pd(dppf)Cl_2]·CH_2Cl_2 (9.8 mol%), $K_4[Fe(CN)_6]$ (17 mol%), Na_2CO_3 (12 mol%)	PL-2000 1.5 wt%	MW 80 °C, 1.5 h	50
[Pd(dppf)Cl_2]·CH_2Cl_2 (9.8 mol%), $K_4[Fe(CN)_6]$ (17 mol%), Na_2CO_3 (12 mol%)	PL-2000 1.5 wt%	MW 100 °C, 1.5 h	55
[Pd(dppf)Cl_2]·CH_2Cl_2 (9.8 mol%), $K_4[Fe(CN)_6]$ (17 mol%), Na_2CO_3 (12 mol%)	PL-2000 1.5 wt%	MW 140 °C, 1.5 h	64
[Pd(dppf)Cl_2]·CH_2Cl_2 (9.8 mol%), $K_4[Fe(CN)_6]$ (17 mol%), Na_2CO_3 (12 mol%)	PL-2000 1.5 wt%	MW 160 °C, 1.5 h	63



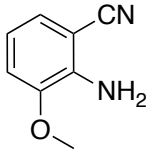
2 **2-Aminobenzonitrile**

Purification: 20% EtOAc in petroleum ether. **Yield:** 96%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (dd, *J*= 1.6, 8.04, 1H), 7.35-7.31 (m, 1H), 6.76-6.72 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 149.55, 133.99, 132.35, 118.00, 117.58, 115.13, 96.05.[1]



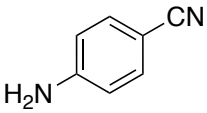
3 **Benzonitrile**

Purification: 5% EtOAc in petroleum ether. **Yield:** 90%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (m, 1H), 7.57 (m, 1H), 7.44 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 132.77, 132.11, 129.11, 118.83, 112.40[2]



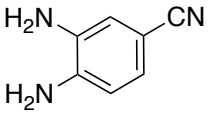
4 **2-Amino-3-methoxybenzonitrile**

Purification: 10-20% EtOAc in petroleum ether. **Yield:** 84%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.05 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.73 (dd, *J* = 8.1, 1.3 Hz, 1H), 6.60 (t, *J* = 8.1 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.65, 140.91, 123.31, 117.58, 117.44, 113.49, 95.32, 55.75.[3]



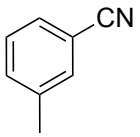
5 **4-Aminobenzonitrile**

Purification: 20-25% EtOAc in petroleum ether. **Yield:** 87%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (m, 2H), 6.64 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 150.54, 133.77, 120.23, 114.42, 99.93.[4]



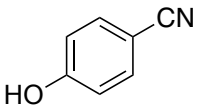
6 **3,4-Diaminobenzonitrile**

Purification: 20% MeOH in DCM. **Yield:** 94%. **^{1}H NMR** (600 MHz, DMSO) δ 6.79 (dd, *J*= 2.04, 8.1, 1H), 6.75 (d, *J*= 1.98, 1H), 6.53 (d, *J*= 7.98, 1H).**^{13}C NMR** 151 MHz, DMSO) δ 140.68, 135.21, 122.88, 121.56, 116.20, 113.68, 97.33.[5]



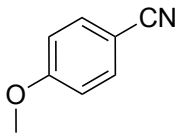
7 **3-Methylbenzonitrile**

Purification: 5% EtOAc in petroleum ether. **Yield:** 45%. **^{1}H NMR** (600 MHz, DMSO) δ 7.55 (d, *J*= 2.04, 8.1, 2H), 7.28 (d, *J*= 1.98, 2H), 2.4 (s, 3H).**^{13}C NMR** 151 MHz, DMSO) δ 162.87, 134.40, 119.21, 114.77, 103.93 , 21.3.[6]



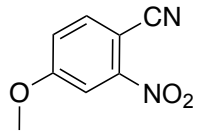
8 **4-Hydroxybenzonitrile**

Purification: 5% MeOH in DCM. **Yield:** 48%. **^{1}H NMR** (400 MHz, DMSO) δ 7.55 (d, *J*= 2.04, 2H), 7.28 (d, *J*= 1.98, 2H).**^{13}C NMR** 151 MHz, DMSO) δ 161.8, 133.84, 119.08, 115.97, 101.68.[7]



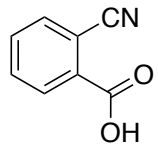
9 **4-Methoxybenzonitrile**

Purification: 5-10% MeOH in DCM. **Yield:** 65%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.56 (d, *J* = 14.4 Hz, 2H), 6.92 (d, *J* = 14.4 Hz, 2H), 3.84 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 162.87, 133.73, 119.21, 114.77, 103.93, 55.54.[8]



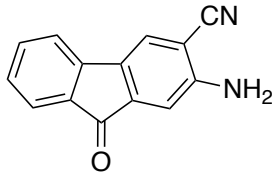
10 **4-Methoxy-2-nitrobenzonitrile**

Purification: 10% EtOAc in petroleum ether. **Yield:** 67%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.76 – 7.68 (m, 2H), 7.21 (dd, *J* = 8.6, 2.8 Hz, 1H), 3.92 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 163.25, 150.20, 136.64, 119.96, 115.27, 111.17, 99.40, 56.59. [9]



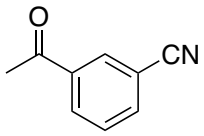
11 **2-Cyanobenzoic acid**

Purification: 10% MeOH in DCM. **Yield:** 46%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.82-7.79 (m, 1H), 7.63-7.48 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.85, 134.62, 133.94, 133.51, 132.34, 128.87, 117.37, 112.32.[10]



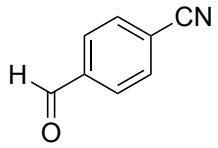
12 **2-Amino-9-oxo-9*H*-fluorene-3-carbonitrile**

Purification: 30% EtOAc in petroleum ether. **Yield:** 30%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 – 7.82 (m, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 42.8 Hz, 4H), 7.05 (s, 1H). **^{13}C NMR** (101 MHz, DMSO) δ 192.99, 153.76, 136.40, 133.33, 128.22, 125.25, 124.59, 120.77, 111.73, 96.01.



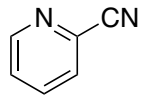
13 **3-Acetylbenzonitrile**

Purification: 20% EtOAc in petroleum ether. **Yield:** 60%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 (m, 1H), 7.86 (d, *J*= 9.12, 1H), 7.77 (d, *J*= 7.68, 1H), 7.67 (t, *J*= 7.62, 15.24, 1H), 2.7 (s, 3H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.13, 139.83, 135.28, 132.64, 132.50, 129.91, 118.10, 111.00, 27.84.[11]



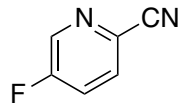
14 **4-Formylbenzonitrile**

Purification: 20% EtOAc in petroleum ether. **Yield:** 42%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.06-8.00 (m, 2H), 7.90-7.86 (m, 2H.**^{13}C NMR** (151 MHz, $CDCl_3$) δ 190.76, 138.70, 132.97, 129.96, 117.80, 117.61.



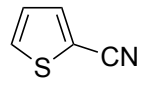
15 **Picolinonitrile**

Purification: 20% EtOAc in petroleum ether. **Yield:** 93%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.7 (d, *J*= 4.84, 1H), 7.83 (td, *J*= 1.5, 7.72, 1H), 7.68 (m, 1H), 7.51 (ddd, *J*= 1.3, 1.7, 4.8, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.13, 137.01, 134.01, 128.52, 126.91, 117.15.[12]



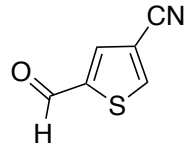
16 **2-Cyano-5-fluoropyridine**

Purification: 5% MeOH in DCM. **Yield:** 95%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.40 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.59 – 7.51 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 159.8 (d, 1*J* = 257 Hz), 151.54, 137.33, 137.16, 123.82, 123.70, 122.17, 122.14, 114.43.



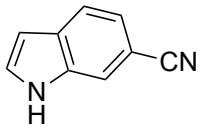
17 **Thiophene-2-carbonitrile**

Purification: 20% AcOEt in PE. **Yield:** 56%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.70-7.62 (m, 2H), 7.04-7.03 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 137.52, 132.66, 127.83, 124.40, 123.79, 114.36



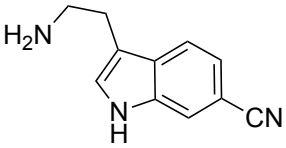
18 **5-Formylthiophene-3-carbonitrile**

Purification: 20-50% EtOAc in petroleum ether. **Yield:** 90%. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.20 (s, 1H), 7.87 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 181.64, 145.22, 142.49, 136.24, 113.66, 112.19.[13]



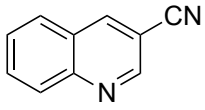
19 **1*H*-Indole-5-carbonitrile**

Purification: 5% EtOAc in petroleum ether. **Yield:** 94%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.48-7.41 (m, 2H), 7.35 (t, *J*= 3.32, 1H), 6.64 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.45, 127.65, 126.40 (2C), 124.90, 120.78, 111.96, 103.48, 102.89.[14]



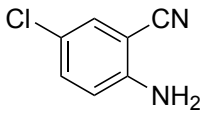
20 **3-(2-Aminoethyl)-1*H*-indole-6-carbonitrile**

Purification: 5% MeOH in Ethyl Acetate. **Yield:** 90%.**^{1}H NMR** (600 MHz, MeOD) δ 8.04 (s, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.29 (s, 1H), 2.97 (s, 2H). **^{13}C NMR** (151 MHz, MeOD) δ 138.60, 127.31, 124.95, 123.90, 123.76, 120.58, 113.31, 112.09, 100.86, 41.58, 27.35.[15]



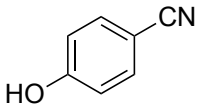
21 **Quinoline-3-carbonitrile**

Purification: 5% MeOH in DCM. **Yield:** 68%.**^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.2 Hz, 1H), 8.56 (d, *J* = 2.2 Hz, 1H), 8.20 (d, *J* = 8.9 Hz, 1H), 7.95–7.89 (m, 2H), 7.75–7.69 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 149.75, 148.81, 141.48, 132.79, 129.88, 128.51, 128.27, 126.21, 117.11, 106.60.[16]



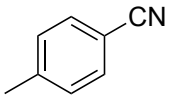
22 **2-Amino-5-chlorobenzonitrile**

Purification: 100% DCM. **Yield:** 67%.**^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.31 – 7.28 (m, 1H), 6.72-6.70 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 148.35, 134.38, 131.28, 122.33, 116.60, 116.50, 96.89.



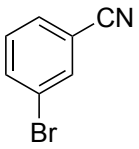
23 **4-Hydroxybenzonitrile**

Purification: 15-20% MeOH in DCM. **Yield:** 50%.**^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.59– 7.56 (m, 2H), 6.97 – 6.94 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 160.11, 134.39 (2 C), 119.31 (2 C), 116.47, 103.17.



24 **4-Methylbenzonitrile**

Purification: 5-20% AcOEt in PE. **Yield:** 69%.**^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.62 – 7.60 (m, 2H), 6.98 – 6.96 (m, 2H), 3.87 (s, 3H) . **^{13}C NMR** (151 MHz, $CDCl_3$) δ 162.83, 134.04, 119.34, 114.75, 103.92, 22.67



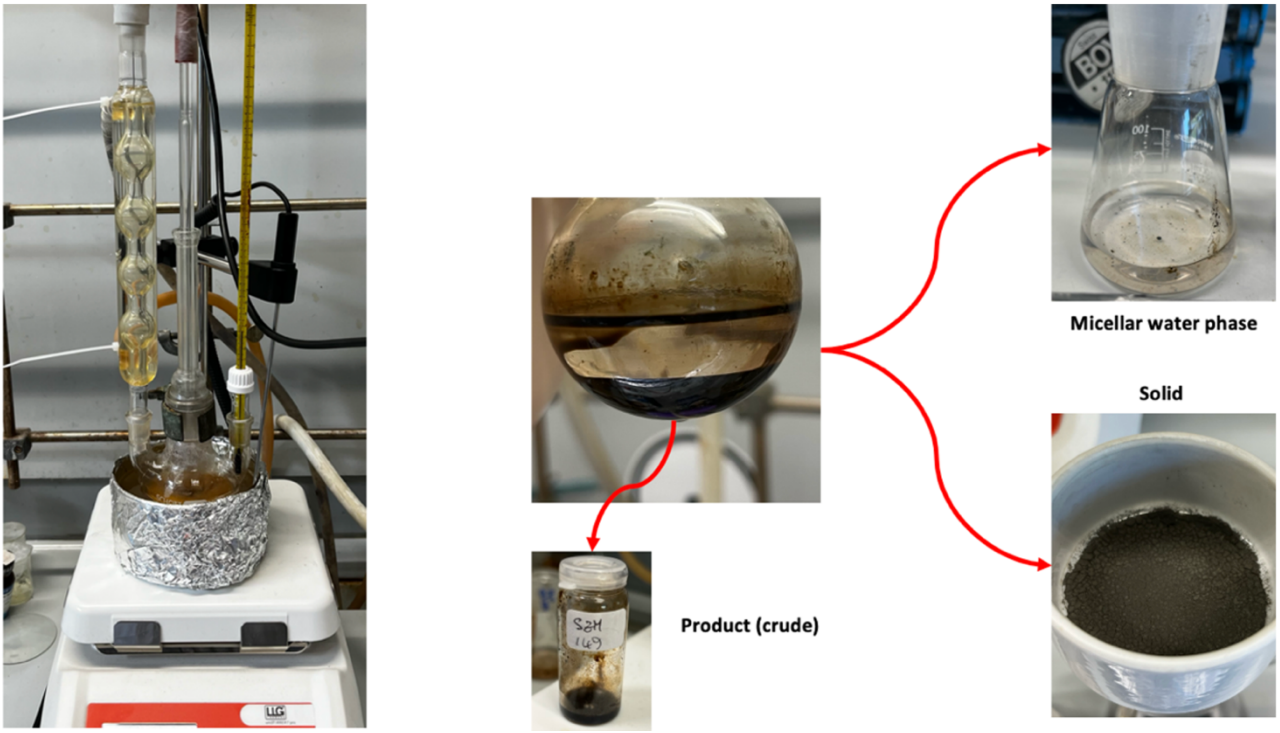
25 **3-Bromobenzonitrile**

Purification: 5% MeOH in DCM. **Yield:** 70%.**^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.81 – 7.77 (m, 2H), 7.76 – 7.75 (m, 1H), 7.39 (t, *J* = 8.5 Hz, 1H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 136.2, 134.79, 130.78, 130.68, 122.39, 117.39, 114.17.

WORK-UP AND RECYCLE

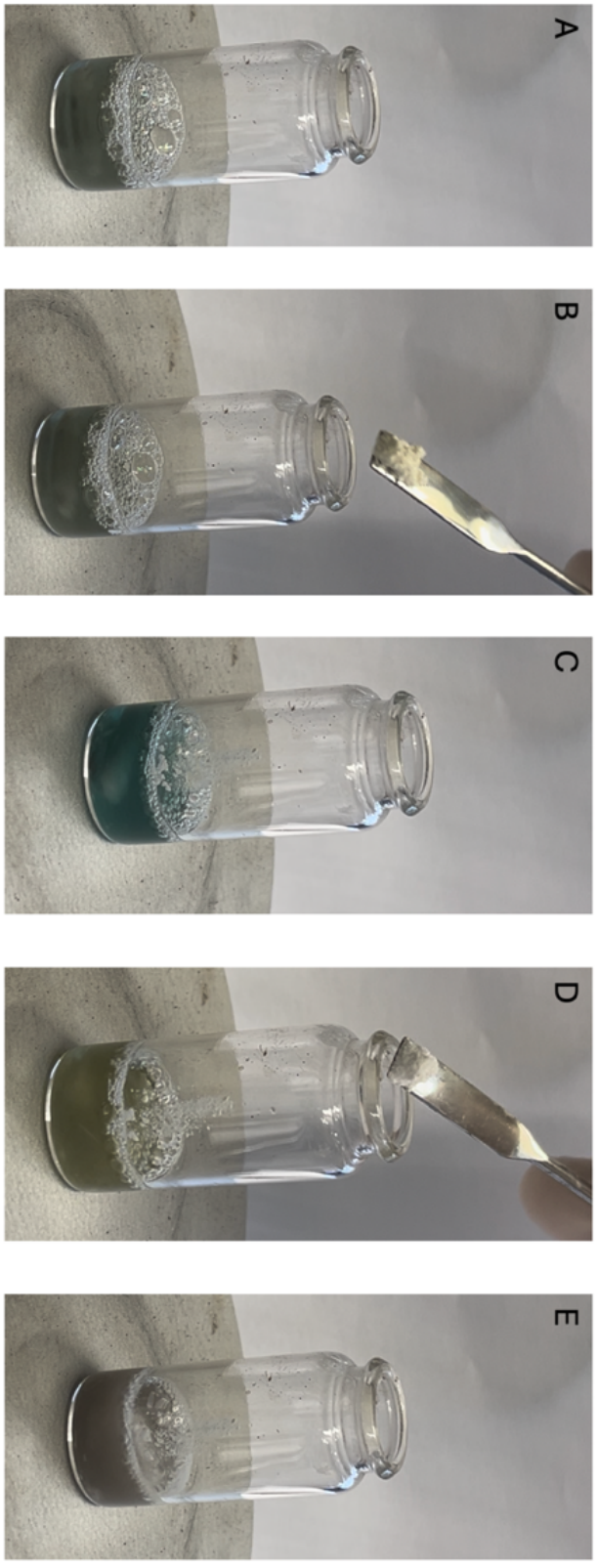
To evaluate the scalability and recycling of catalyst and water containing the surfactant, cyanation of o-bromoaniline was carried out at a larger scale (5 mmol) using $Pd(dppf)_2Cl_2$ (9.8 mol%), $K_4[Fe(CN)_6]$ (19 mol%), Na_2CO_3 (12 mol%) under heating (80 °C) for 16 h. The desired product was obtained in 93% isolated yield. After heating, stirring was stopped to perform phase separation of the remaining solid (brown colour), water and organic phase (Figure S1). The aqueous phase was collected with a Pasteur pipette and used for the second cycle of the reaction, while the organic phase and solid were collected with 50 mL EtOAc. After filtration, the brown solid was collected. The desired product dissolved in the organic solvent was concentrated under vacuum to obtain the final oily product. The recovered solid was used together with the water phase in another cyanation reaction.

Figure S1. Workup and recovery



The second cycle of cyanation was carried adding the recovered solid (containing the Pd catalyst and iron species) to the water phase, Na_2CO_3, $K_4[Fe(CN)_6]$ and the SM.

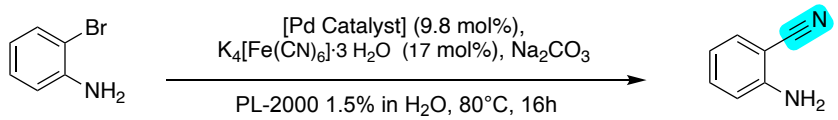
Figure S2. A) Recovered micellar water phase; B) Addition of $K_4[Fe(CN)_6]$; C) Color change with formation of other Iron species; D) Addition of Na_2CO_3 ; E) Final micellar water phase color.



MP-AES ANALYSIS

A known amount of the different phases was digested in aqua regia and stirred for 1 h at room temperature. The acid mixture was diluted with deionized water and analyzed with MP-AES instrument to determine the metal content.

Table S4 MP-AES analysis results



1 **2**

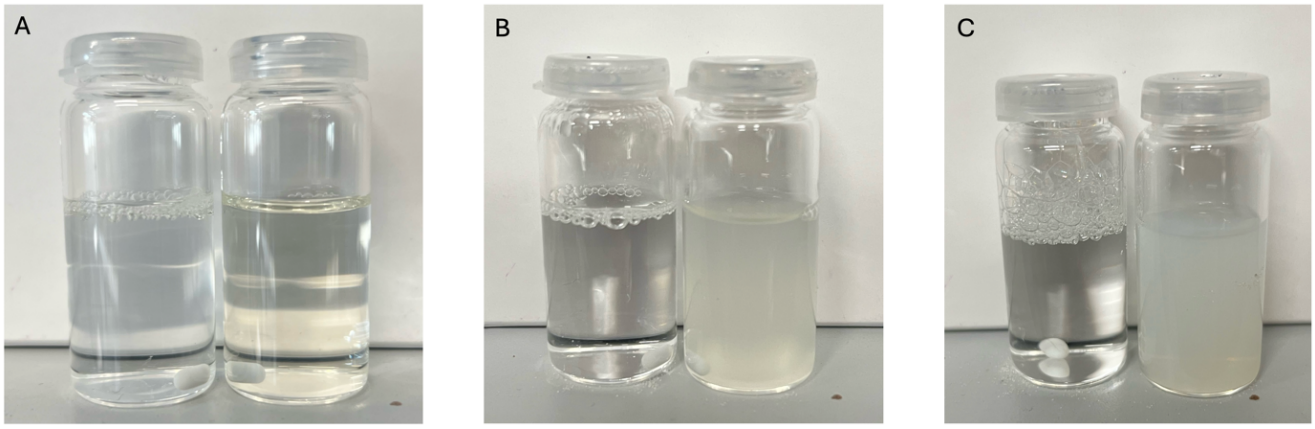
I CYCLE			
Phase	Pd (ppm)	Fe(ppm)	
Water phase	11.20	15.60	Low levels of Pd and Fe remain dissolved. Fe likely originates from slight dissociation of ferrocyanide or leaching from solid phases. Pd may be present as leached species or minor catalyst degradation.
Solid	42142.86	150357.14	Major accumulation of Fe**,** likely as Fe(III) species or iron cyanide complexes (possibly Prussian Blue-like materials). High Pd presence suggests catalyst precipitation or adsorption onto solids.
Organic Phase	4304.40	2342.79	Significant Pd remains in the organic phase, consistent with its solubility in organic solvents. Some Fe partitions here, possibly due to interactions with phosphine ligands.

II CYCLE (RECYCLE)			
Water phase	38.46	853.85	Increase in Fe**,** likely due to further decomposition or leaching of iron species into the aqueous phase. Higher Pd suggests more catalyst loss into water.
Solid	19393.94	166363.64	Lower Pd content than Cycle 1**,** possibly due to redissolution or catalyst loss. Fe remains dominant, even increasing, suggesting continued precipitation of Fe species.
Organic Phase	619.55	2098.60	Large Pd decrease**,** suggesting substantial catalyst loss or deactivation. Fe concentration is stable, possibly due to minor solubility of iron-cyanide species in the organic phase.

PL-2000 STABILITY STUDIES

This comparison highlights the different thermal stabilities and properties of two surfactants (TPGS-750-M and PL-2000).

Figure S3 TEMPERATURE EFFECTS ON SULFACTANTS



The solutions of PL-2000 (Left) and TPGS-750-M (Right) are both 1.5 wt% in water, and their behavior is observed at three temperatures: 21°C, 75°C, and 100°C.

A) **At 21°C**: Both solutions are likely clear.
B) **At 75°C**: The TPGS-750-M solution becomes cloudy, indicating a cloud point effect, where the surfactant begins to aggregate and precipitate out of the solution.
C) **At 100°C**: TPGS-750-M has fully cloud colour and separated from the solution is formed an oil phase at the bottom of the vial.

DLS ANALYSIS

All the samples were diluted in water (3 drops in 1 mL of water) after manually shacked in order to dissolve the deposit at the bottom of the vessel. Water used for this analysis is double distilled and previously filtered with PES 0.22 nm syringe filter devices. Concentration of each sample is checked to be in range for DLS. Samples were prepared just before analysis then are placed in plastic cuvettes with 4 optical windows, as required by this technique for size distribution analysis, whereas disposable folded capillary cells were used for Zeta-potential analysis.

For the Analysis each sample was left to acclimatize for 120 seconds at 25 °C, then undergo 3 sets of measurements, each one composed by 10 runs.

For Zeta potential analysis a single measurement is performed, composed of 10-100 runs, freely selected by the instrument software, to maximize the signal.

Results are obtained from a recording of 3 measurements (red, green and blu lines) and reported in the graph "Intensity vs diameter (nm)". Please notice the logarithmic scale of the x axis.

The intensity graph is useful for the correct size determination of the nanoparticles, but when multiples populations are present, looking also at the volume graph can be the best choice, since it gives a clearer idea on the amount of each population.

The instrument automatically extrapolates the mean diameter and the polydispersity index (PDI), which is a number between 0 (no polydisperse particles having the same size) and 1 (highly polydisperse sample). When the sample is not conforming to the optimal criteria for DLS analysis the red line: "refer to quality report" appears. In case of these analysis large aggregates that tend to deposit are responsible for this.

Table S5 Samples analized

Sample	Description
A	Aqueous solution after separation
B	H_2O, PL-2000 (1.5%), heated at 80°C for 16 h
C	H_2O, PL-2000 (1.5%), rt
D	Crude reaction mixture after heating
E	Reaction mixture before heating

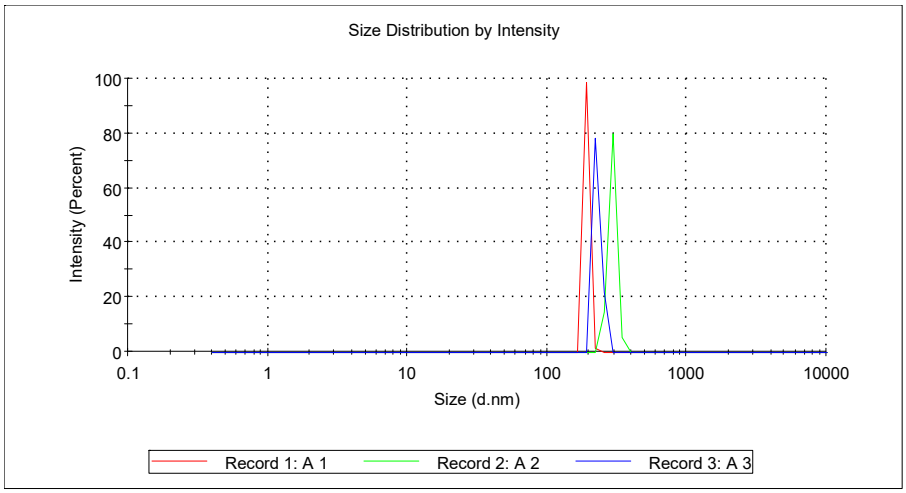
Figure S4 Results of DLS analysis and final report in Table

Sample A

Results

			Size (d.n...	% Intensity:	St Dev (d.n...
Z-Average (d.nm):	1650	**Peak 1:**	227,8	100,0	14,39
PdI:	1,000	**Peak 2:**	0,000	0,0	0,000
Intercept:	1,13	**Peak 3:**	0,000	0,0	0,000

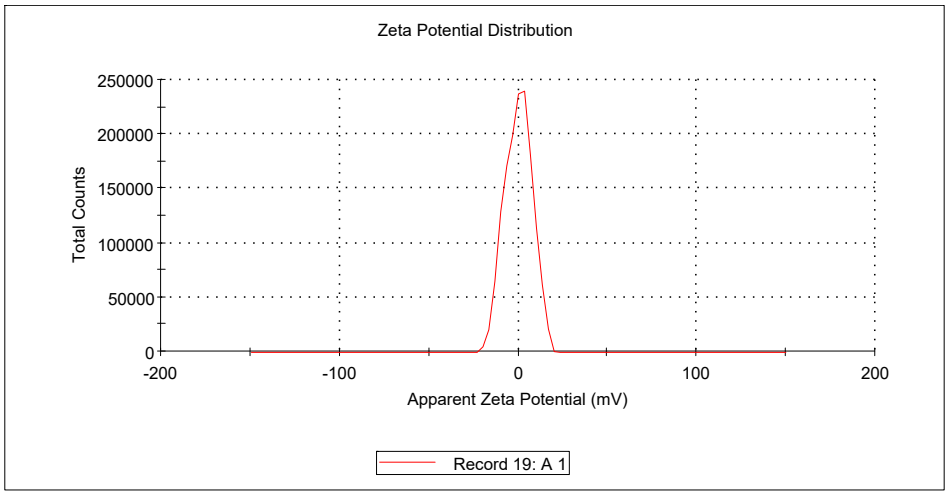
Result quality Refer to quality report



Results

			Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV):	0,164	**Peak 1:**	0,164	100,0	7,48
Zeta Deviation (mV):	7,48	**Peak 2:**	0,00	0,0	0,00
Conductivity (mS/cm):	3,82	**Peak 3:**	0,00	0,0	0,00

Result quality Good

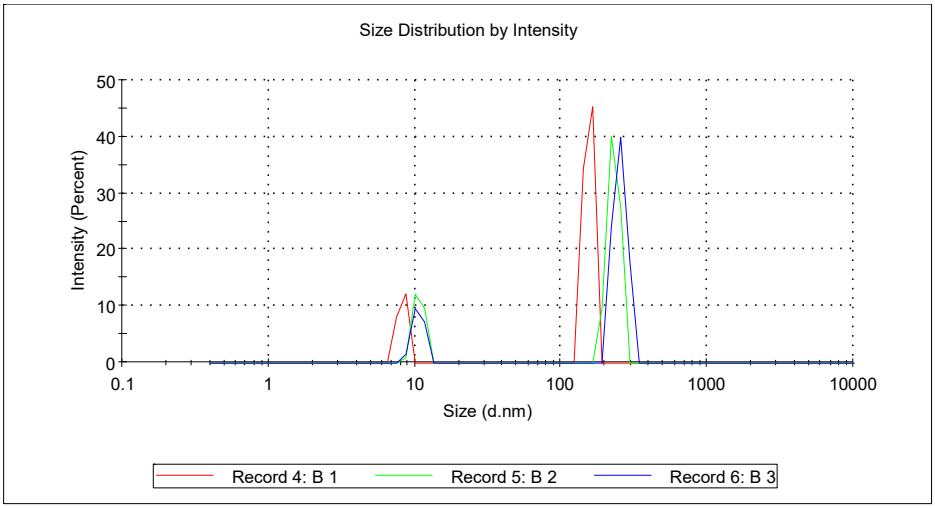


Sample B

Results

			Size (d.n...	% Intensity:	St Dev (d.n...
Z-Average (d.nm):	636,1	**Peak 1:**	253,5	81,5	26,59
PdI:	0,604	**Peak 2:**	10,61	18,5	0,9494
Intercept:	0,987	**Peak 3:**	0,000	0,0	0,000

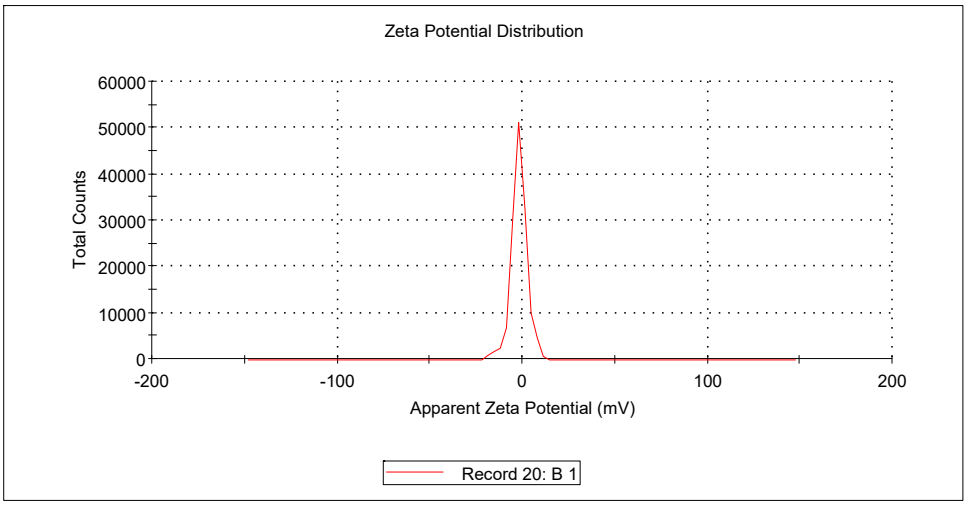
Result quality **Refer to quality report**



Results

			Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV):	-1,88	**Peak 1:**	-1,88	100,0	4,51
Zeta Deviation (mV):	4,51	**Peak 2:**	0,00	0,0	0,00
Conductivity (mS/cm):	0,0606	**Peak 3:**	0,00	0,0	0,00

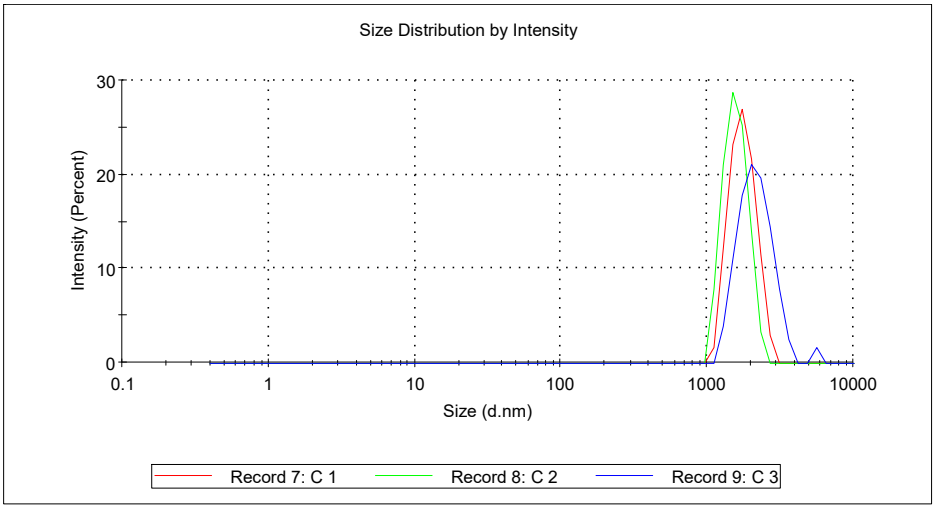
Result quality **See result quality report**



Sample C

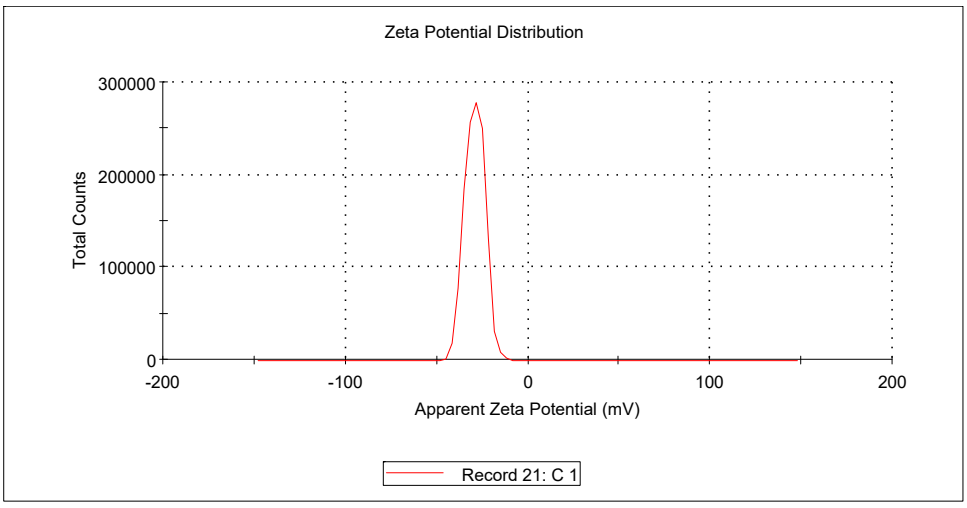
Results

			Size (d.n...	% Intensity:	St Dev (d.n...
Z-Average (d.nm):	2485	**Peak 1:**	2147	98,3	535,5
PdI:	0,266	**Peak 2:**	5560	1,7	0,000
Intercept:	0,913	**Peak 3:**	0,000	0,0	0,000
Result quality	Refer to quality report				



Results

			Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV):	-29,1	**Peak 1:**	-29,1	100,0	5,36
Zeta Deviation (mV):	5,36	**Peak 2:**	0,00	0,0	0,00
Conductivity (mS/cm):	0,762	**Peak 3:**	0,00	0,0	0,00
Result quality	Good				

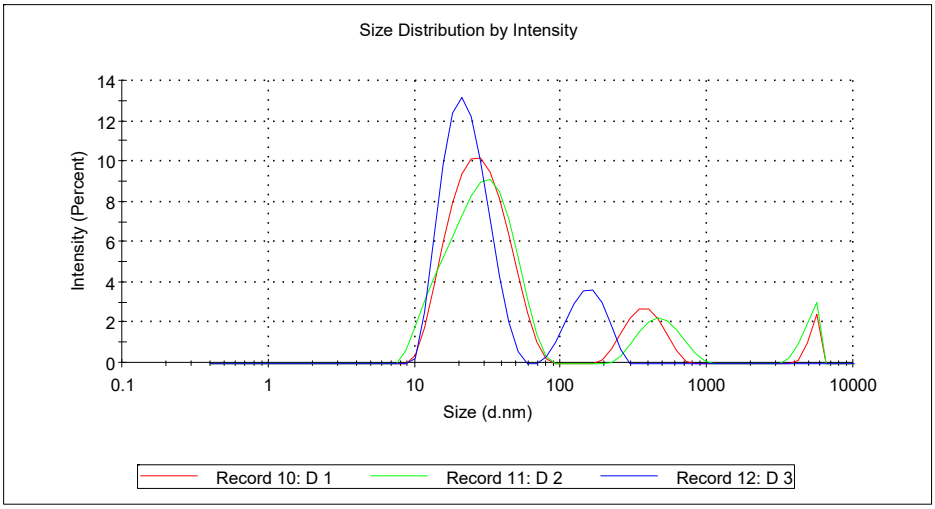


Sample D

Results

			Size (d.n...	% Intensity:	St Dev (d.n...
Z-Average (d.nm):	100,7	**Peak 1:**	23,16	80,8	7,920
PdI:	0,172	**Peak 2:**	155,0	19,2	42,06
Intercept:	0,880	**Peak 3:**	0,000	0,0	0,000

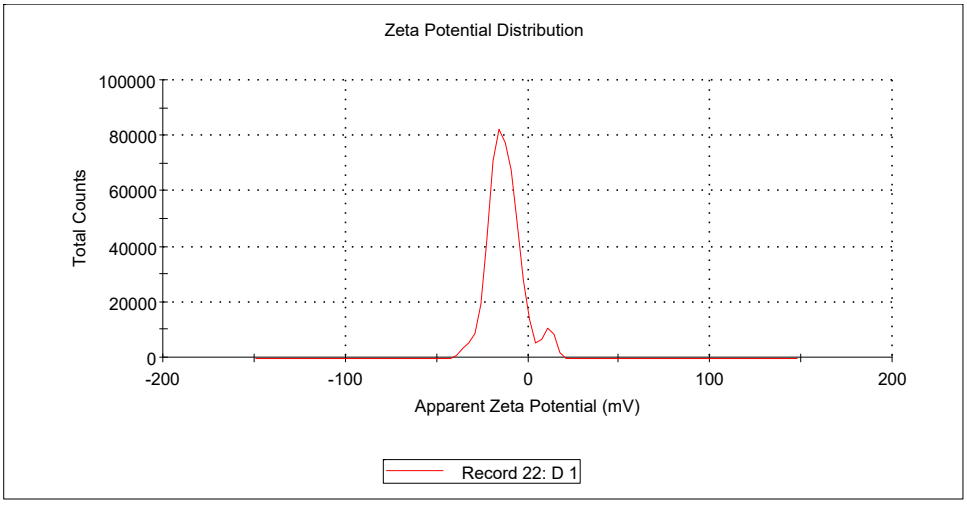
Result quality **Refer to quality report**



Results

			Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV):	-12,5	**Peak 1:**	-14,0	93,3	7,66
Zeta Deviation (mV):	9,52	**Peak 2:**	10,3	6,7	3,85
Conductivity (mS/cm):	0,0381	**Peak 3:**	0,00	0,0	0,00

Result quality **See result quality report**

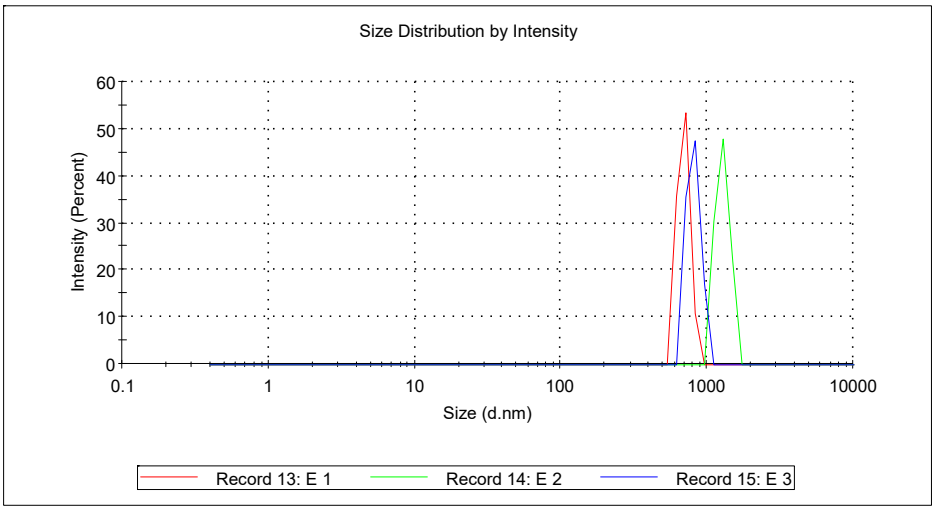


Sample E

Results

			Size (d.n...	% Intensity:	St Dev (d.n...
Z-Average (d.nm):	2107	**Peak 1:**	807,3	100,0	84,22
PdI:	0,661	**Peak 2:**	0,000	0,0	0,000
Intercept:	0,823	**Peak 3:**	0,000	0,0	0,000

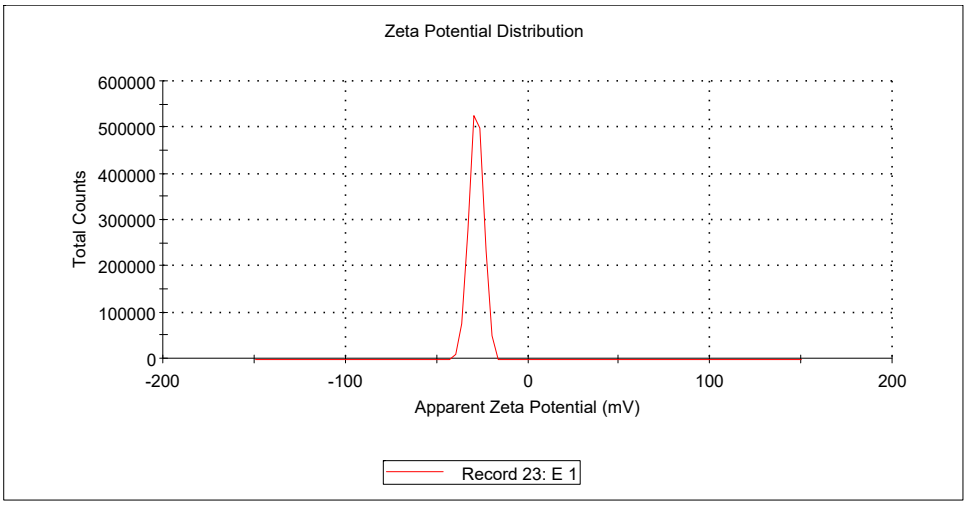
Result quality Refer to quality report



Results

			Mean (mV)	Area (%)	St Dev (mV)
Zeta Potential (mV):	-28,4	**Peak 1:**	-28,4	100,0	3,92
Zeta Deviation (mV):	3,92	**Peak 2:**	0,00	0,0	0,00
Conductivity (mS/cm):	1,78	**Peak 3:**	0,00	0,0	0,00

Result quality Good



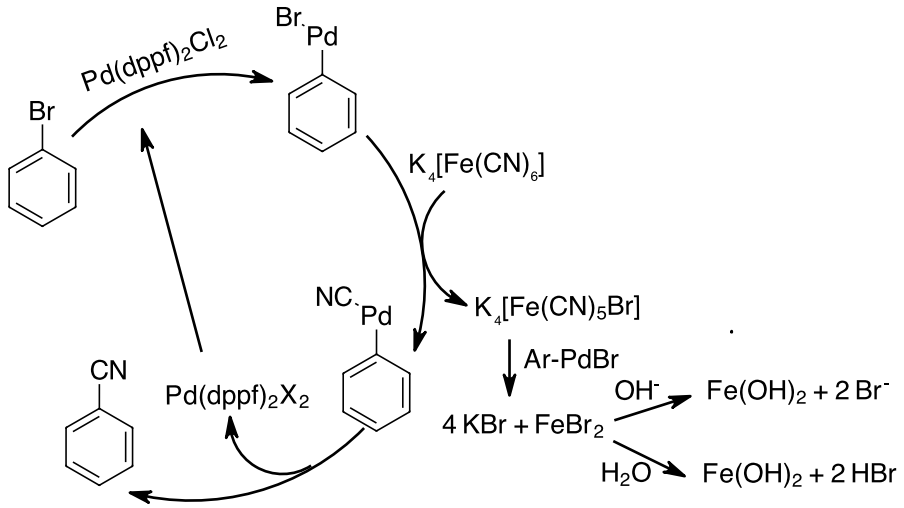


Figure S5 Proposed mechanism for cyanation of aryl bromides in water using $K_4[Fe(CN)_6]$ including the nature of Fe containing byproducts

GREEN METRICS

$$AE = \left(\frac{Molecular\ weight\ of\ final\ product}{Sum\ of\ molecular\ weight\ of\ all\ reactants}\right)$$

$$1/SF = 1/1 + \left(\frac{AE\ *\ (sum\ of\ reagents\ in\ excess)}{expected\ product\ mass\ at\ 100\%\ yield}\right)$$

$$RME = \frac{Mass\ of\ product}{Total\ mass\ of\ reactants}$$

$$MRP = \frac{Total\ mass\ of\ recovered\ reaction\ and\ postreaction\ solvents\ + mass\ of\ recovered\ catalyst\ and\ ligands}{Total\ mass\ of\ used\ reaction\ and\ postreaction\ solvents + mass\ of\ used\ catalyst\ and\ ligand}$$

$$E - factor = \frac{total\ mass\ of\ waste}{mass\ of\ final\ product}$$

	Method A	Method B	Method C	Method D
Yield	0.96	0.78	0.84	0.88
AE	0.1987517	0.14625994	0.1987517	0.18418796
RME	0.4651824	0.17451733	0.29103984	0.33327328
MRP	0.29742499	0.38517602	0	0
1/SF	0.99832049	0.99876351	0.99832049	0.99844336
E-factor	141.189572	35.4208175	232.383405	609.596309

Method A: proposed method

Atom Economy = [118.14 (Prod) / (172.02 (SM) + 422.39 ($K_4[Fe(CN)_6]$) = 0.198

1/SF = 1/(1+(0.1897 (AE)/118.14 (Product 100% yield) = 0.998

RME = 113.4144 (product) / 71.81 ($K_4[Fe(CN)_6]$) + 172.02 (SM) = 0.4652

MRP = 5 mL (H_2O)+80.02 (Cat.) / 5 mL (H_2O) + 10 mL (AcOEt) + 2 mL (H_2O) + 80.0268 (Cat) = 0.297

E-Factor = 1000 (Sodium Sulphate) + 5 mL (H_2O) + 10 mL (AcOEt) + 12.93 (Base) / 113.414 (prod.) = 141.2

Table S6 Materials for Green Metrics calculations of Method A

REAGENT	**g**	**mmol**	**MW**
Bromoaniline	0.172	1	172.02
$Pd(dppf)Cl_2 \cdot CH_2Cl_2$*Recovered	0.080	0.098	816.64
Na_2CO_3	0.013	0.122	105.989
$K_4[Fe(CN)_6] \cdot 3H_2O$	0.072	0.170	422.39
H_2O *Recovered	2		
AcOEt	10		
H_20	5		
Sodium Sulfate	1		
Pl2000 *Recovered	0.03		
product	0.113	0.96	118.14

Table S8 Materials for Green Metrics calculations of Method B

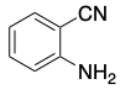
REAGENT	**g**	**mmol**	**MW**
Bromoaniline	0.172	1	172.02
Catalyst *Recovered	0.004	0.005	948.34
DCM	4		
$Zn(CN)_2$	0.356	0.56	635.72
H_2O *Recovered	2		
Surfactant *Recovered	0.04		
THF	0.200		
AcOEt	2		
H_20	2		
Sodium Sulfate	1		
PMHS *Recovered	0.064	1	222.5
product	0.092	0.78	118.14

Table S7 Materials for Green Metrics calculations of Method C

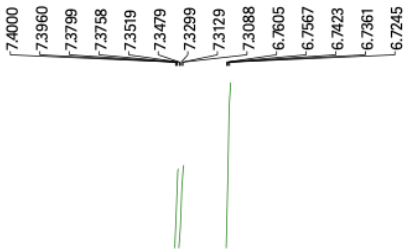
REAGENT	**g**	**mmol**	**MW**
Bromoaniline	0.172	1	172.02
$Pd(PPh_3)_4$	0.023	0.02	1155.57
DBU	0.038	0.25	152.24
$K_4[Fe(CN)_6]\cdot 3H_2O$	0.168	0.4	422.39
H_2O	1.5		
t-BuOH	1.5		
MeOH	10		
DCM	10		
product	0.099	0.84	118.14

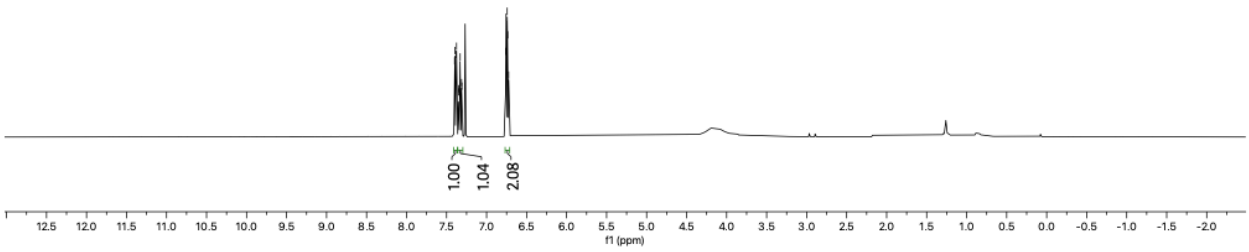
Table S8 Materials for Green Metrics calculations of Method D

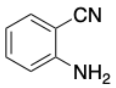
REAGENT	**g**	**mmol**	**MW**
Bromoaniline	0.219	1	219.02
NaF	0.042	1	41.98
TBAB	0.322	1	322.37
$K_4[Fe(CN)_6]\cdot 3H_2O$	0.0929	0.22	422.39
H_2O	2		
$Pd(OAc)_2$	11.23	0.05	422.39
product	0.104	0.88	118.14


CN
NH2

2

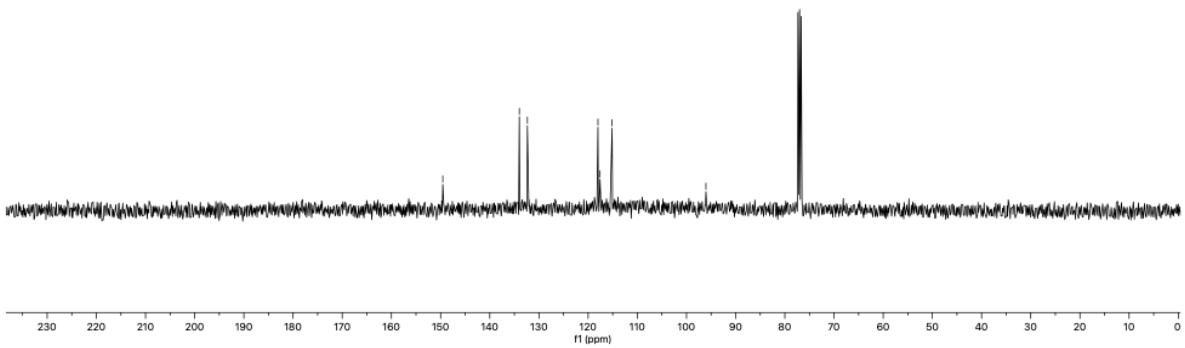

7.4000
7.3960
7.3799
7.3758
7.3519
7.3479
7.3299
7.3129
7.3088
6.7605
6.7567
6.7423
6.7361
6.7245

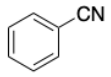

1.00
1.04
2.08
f1 (ppm)


CN
NH2

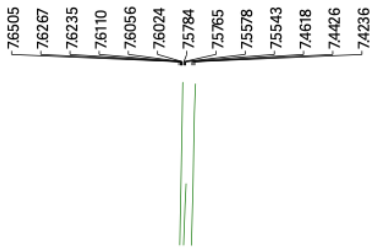
2

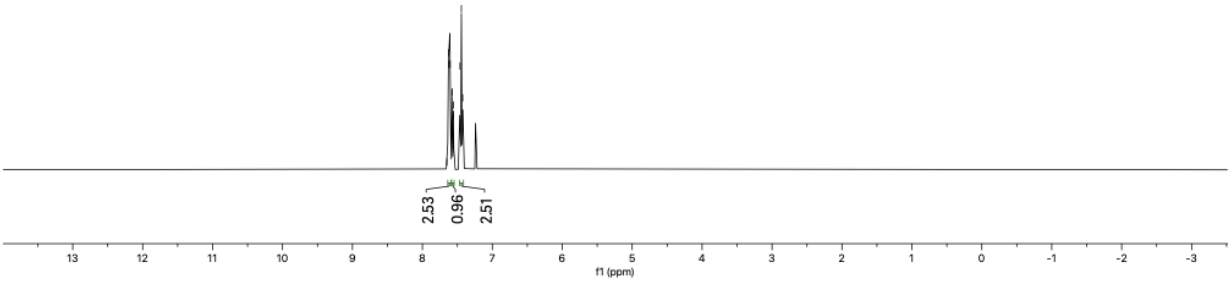

149.5519
133.9886
132.3481
118.0025
117.5796
115.1261
96.0485

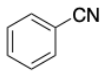

f1 (ppm)


CN

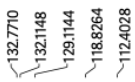
3

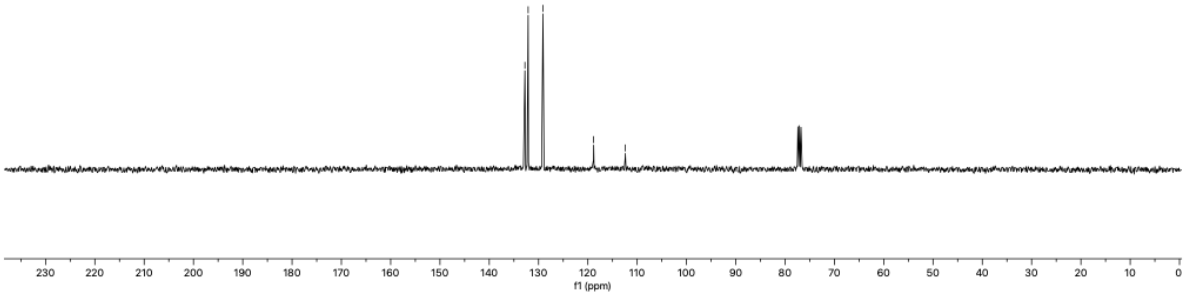

7.6505
7.6267
7.6235
7.6110
7.6056
7.6024
7.5784
7.5765
7.5578
7.5543
7.4618
7.4426
7.4236

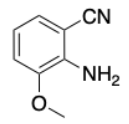

2.53
0.96
2.51
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


CN

3

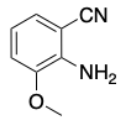

132.7710
132.1148
129.1144
118.8264
112.4028


230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
NH2
O

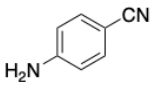
4

0.74
0.83
0.61
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


CN
NH2
O

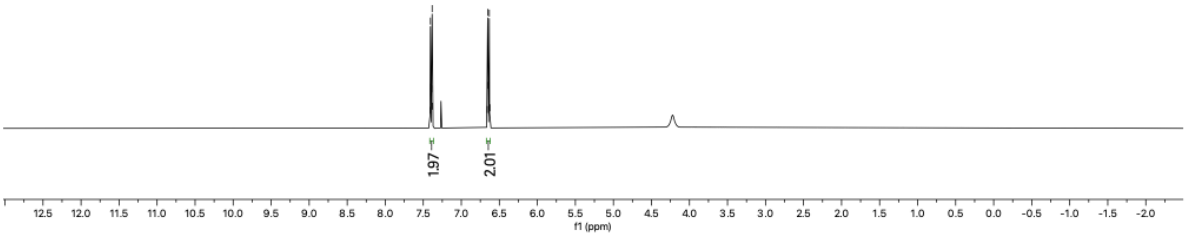
4

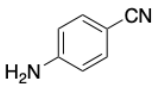
146.6492
140.9083
123.3081
117.6818
117.4426
113.4932
86.3179
65.7541
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CN
H2N

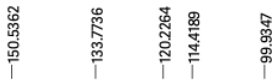
5

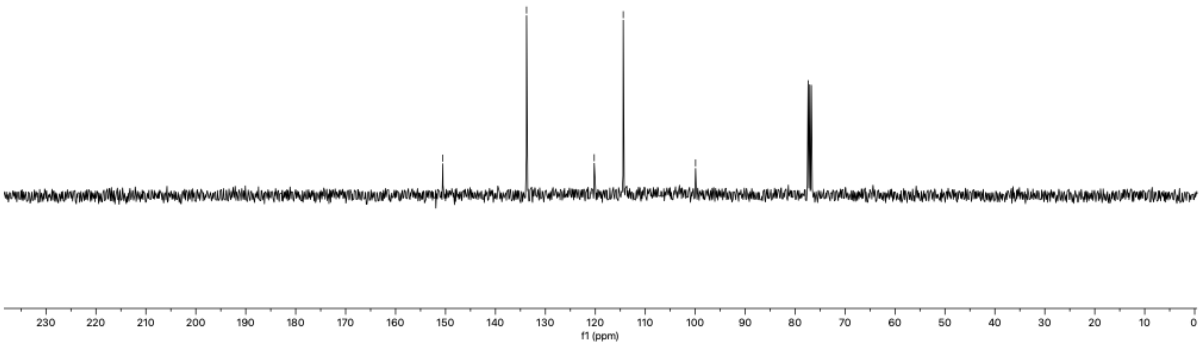

7.4118
7.4056
7.4004
7.3888
7.3836
7.3777
6.6594
6.6532
6.6480
6.6364
6.6312
6.6253

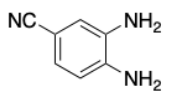

1.97
2.01
f1 (ppm)


CN
H2N

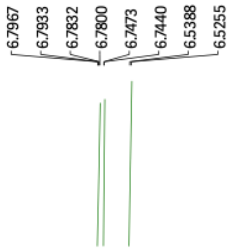
5

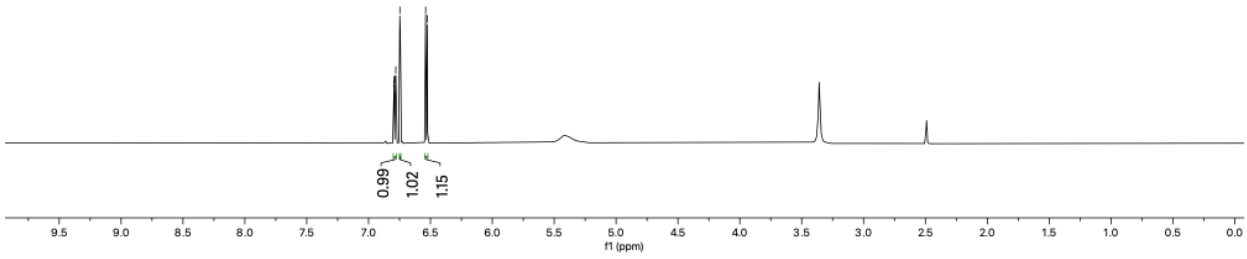

150.5362
133.7736
120.2264
114.4189
99.9347

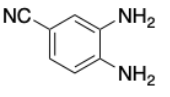

f1 (ppm)


NC
NH2
NH2

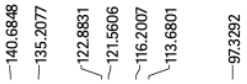
6

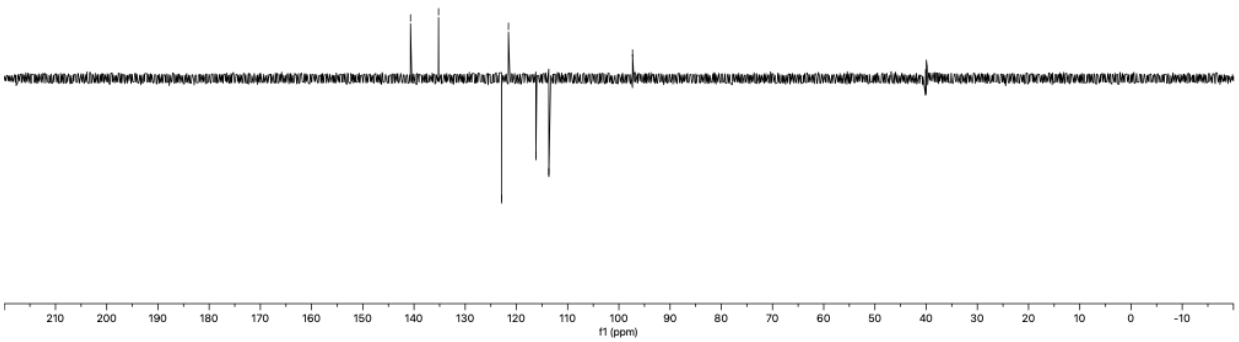

6.7967
6.7933
6.7832
6.7800
6.7473
6.7440
6.5388
6.5255

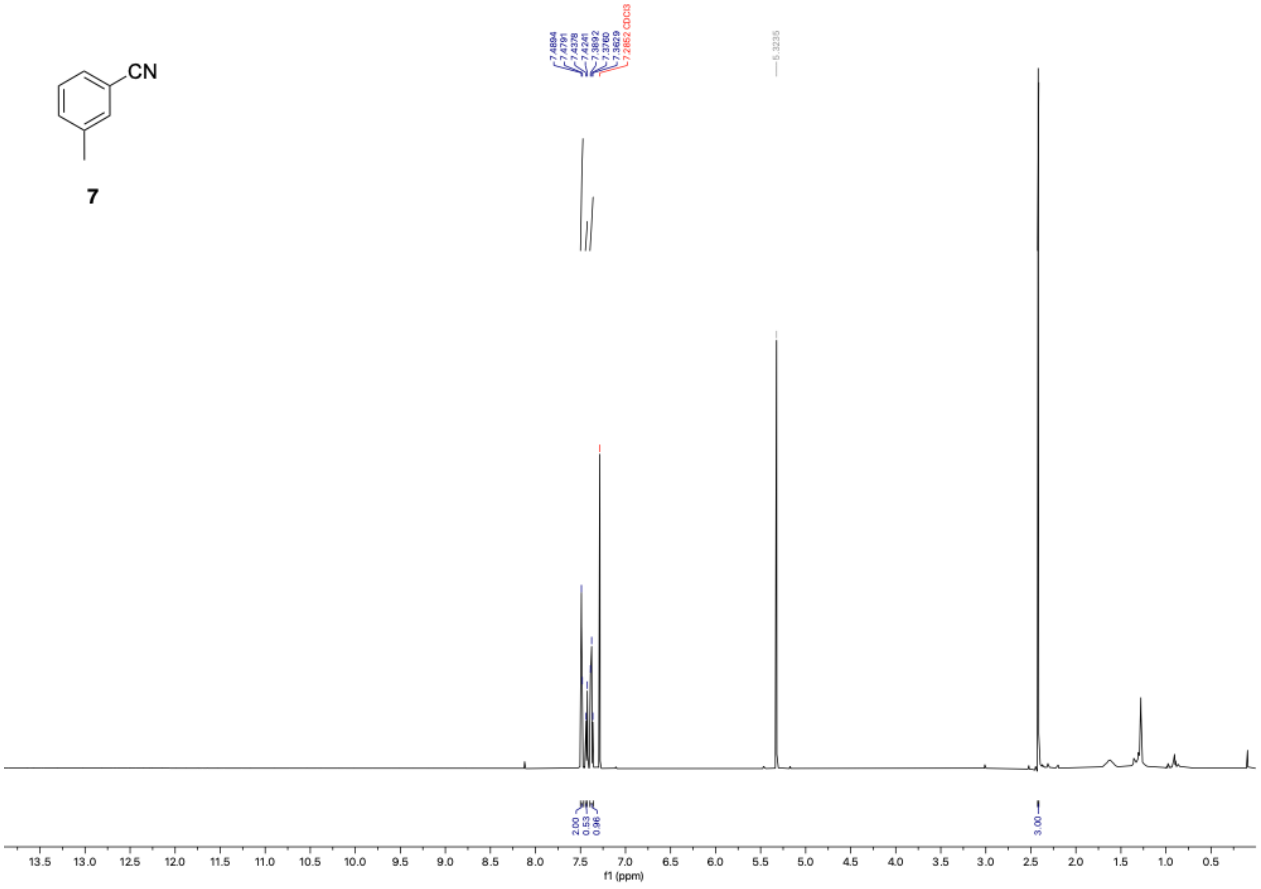

0.99
1.02
1.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

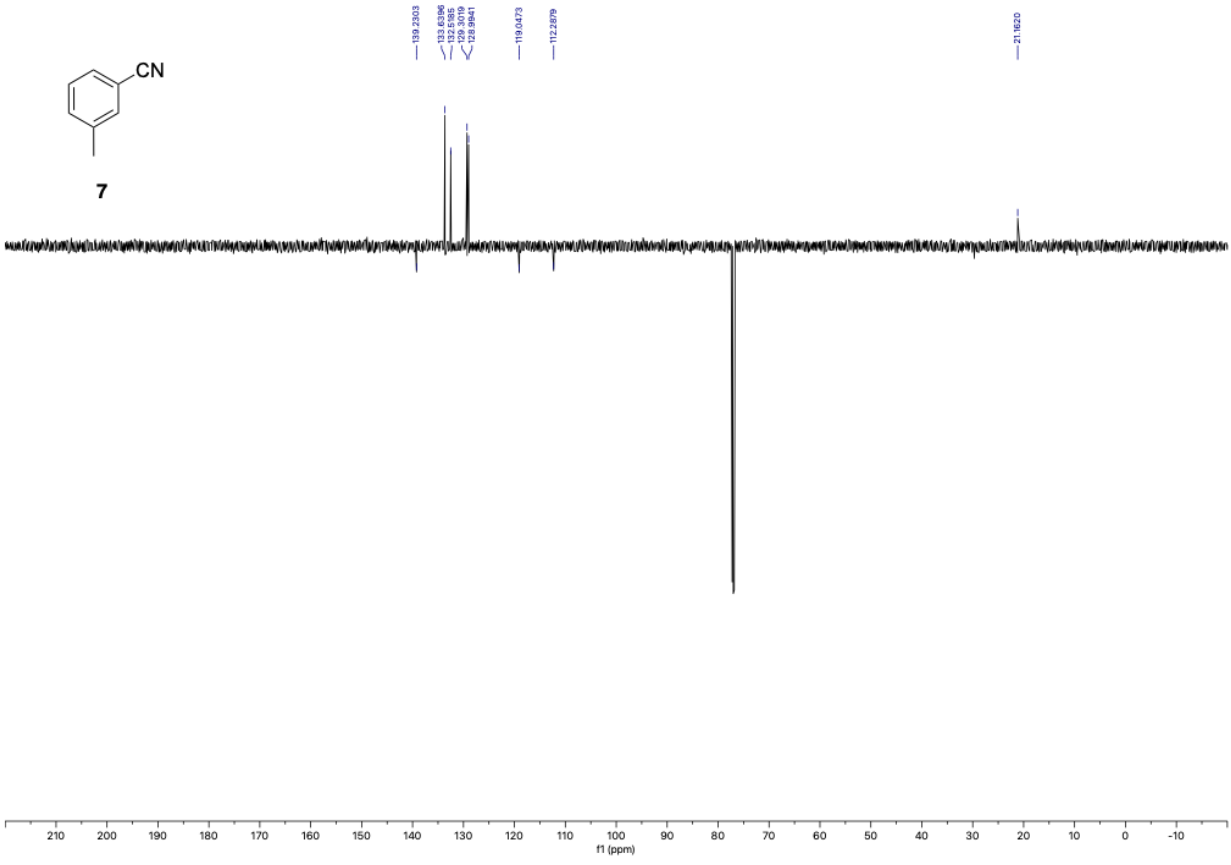

NC
NH2
NH2

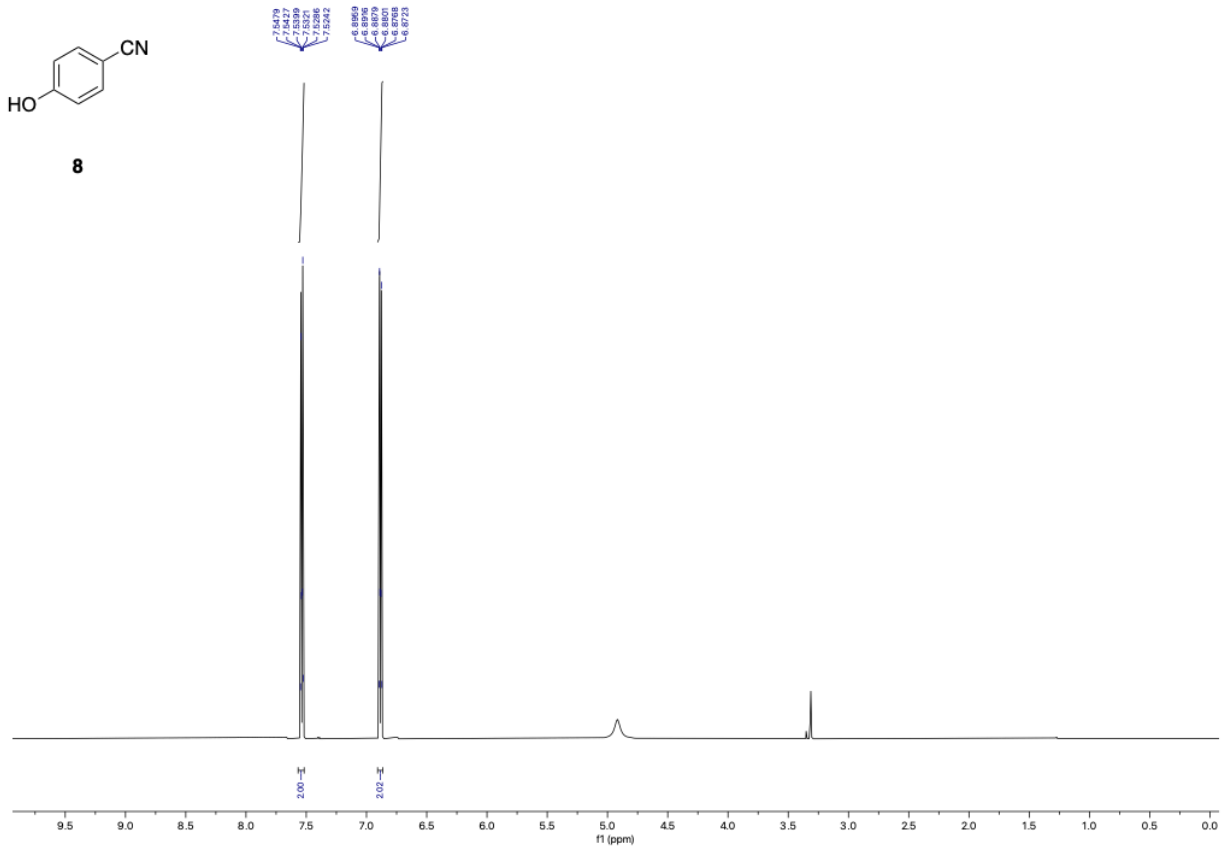
6

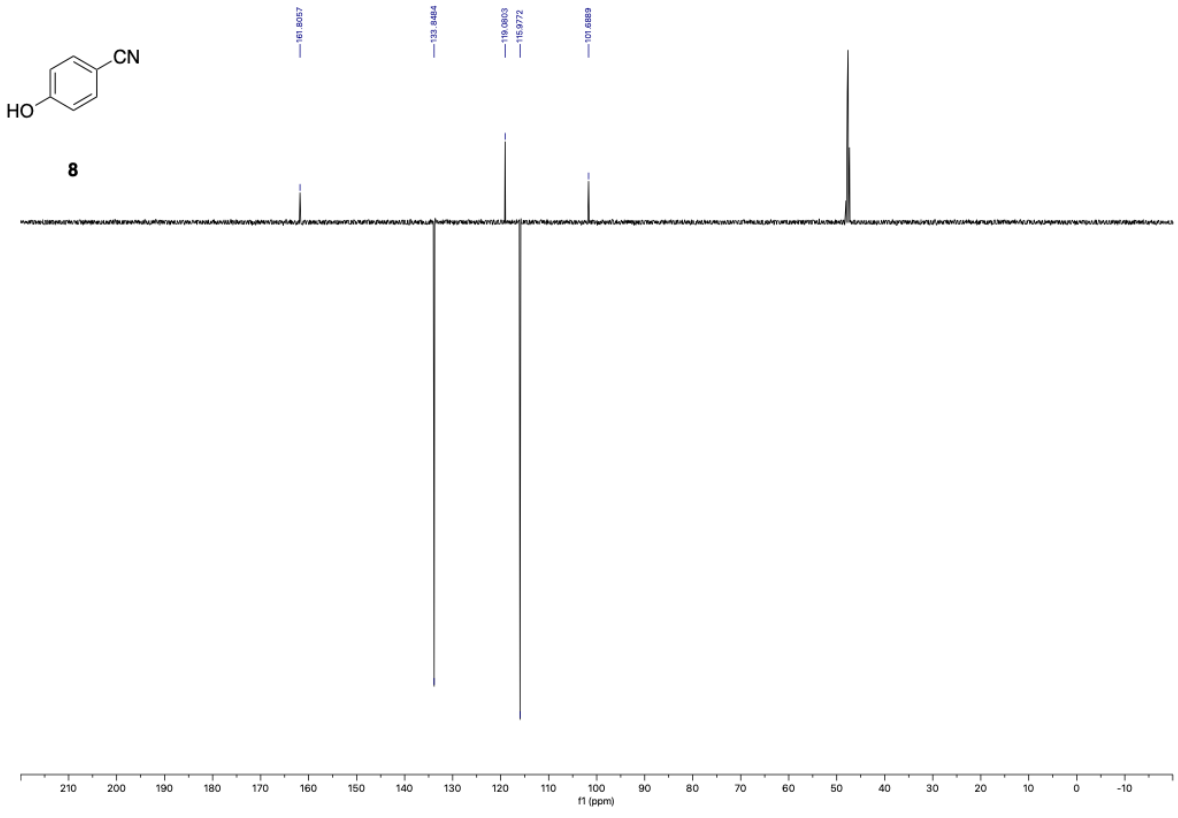

140.6848
135.2077
122.8831
121.5606
116.2007
113.6801
97.3292

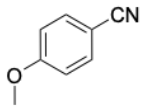

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CN
7
7.4694
7.4596
7.4378
7.4241
7.3892
7.3765
7.3629
7.2652 CDCl3
5.3235
2.00
0.53
0.96
3.00
f1 (ppm)


CN
7
139.2303
133.6396
132.5165
129.1059
128.3941
119.0473
112.2879
21.1620
f1 (ppm)

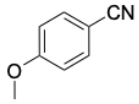

CN
HO
8
7.5479
7.5427
7.5399
7.5321
7.5295
7.5242
6.8959
6.8896
6.8879
6.8835
6.8768
6.8723
2.00
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


CN
HO
8
161.8057
133.8484
119.0803
115.9772
101.6889
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CN
O

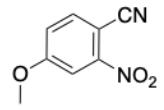
9

7.5761
7.5521
7.2680 CDCl3
6.9480
6.9297
3.8434
2.00
2.10
3.63
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


CN
O

9

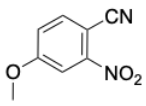
162.8719
133.7312
119.2158
114.7755
103.9348
55.5490
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CN
O
NO2

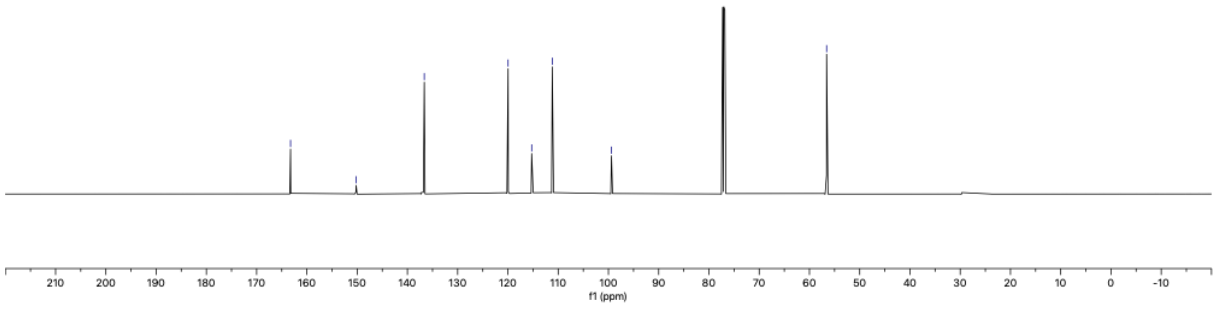
10

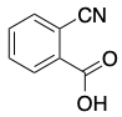
7.7466
7.7322
7.7241
7.7098
7.2232
7.2189
7.2088
7.2044
7.1868 CDCl3
3.9961
1.95
1.01
3.00
f1 (ppm)


163.2529
150.1993
136.6401
119.9632
115.2737
111.1668
99.3905
56.5858


CN
O
NO2

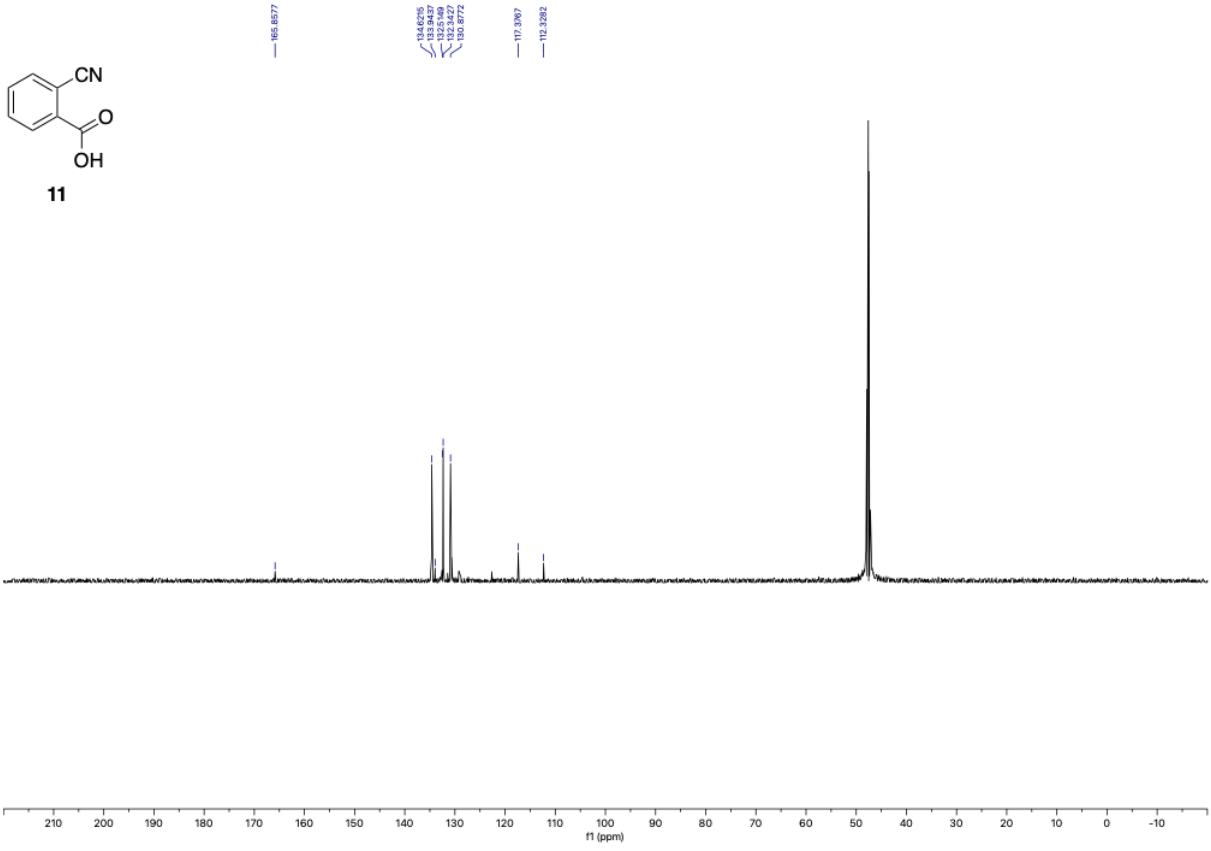
10


f1 (ppm)

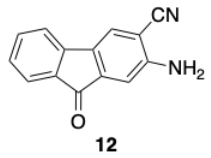

CN
O
OH

11

1.08
0.87
2.01
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

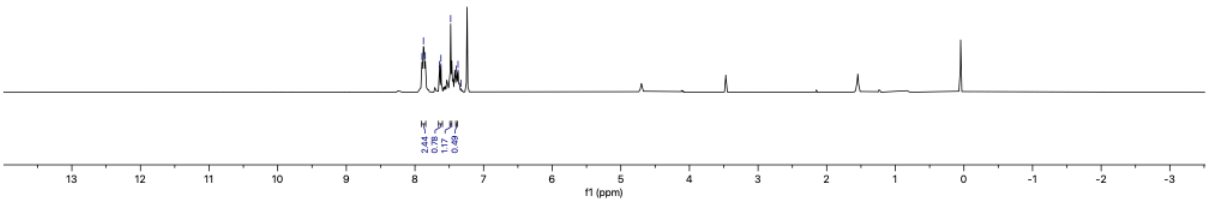

165.8577
134.6275
133.9437
133.5149
132.3427
130.8772
117.3767
112.3282
CN
O
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

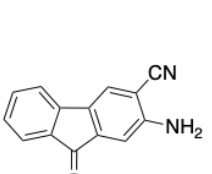
11


CN
NH2
O

12

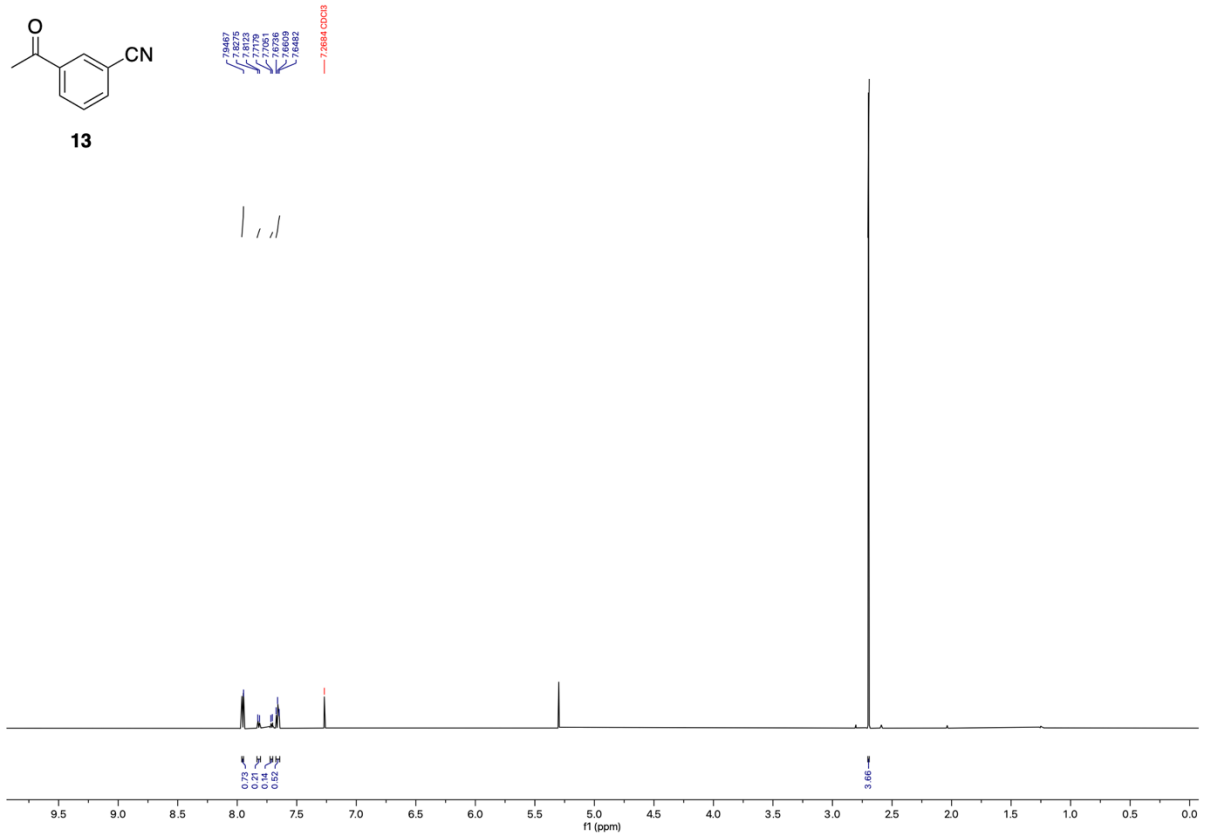

7.8972
7.8761
7.8464
7.8414
7.6211
7.4795
7.3980
7.3725
7.3287

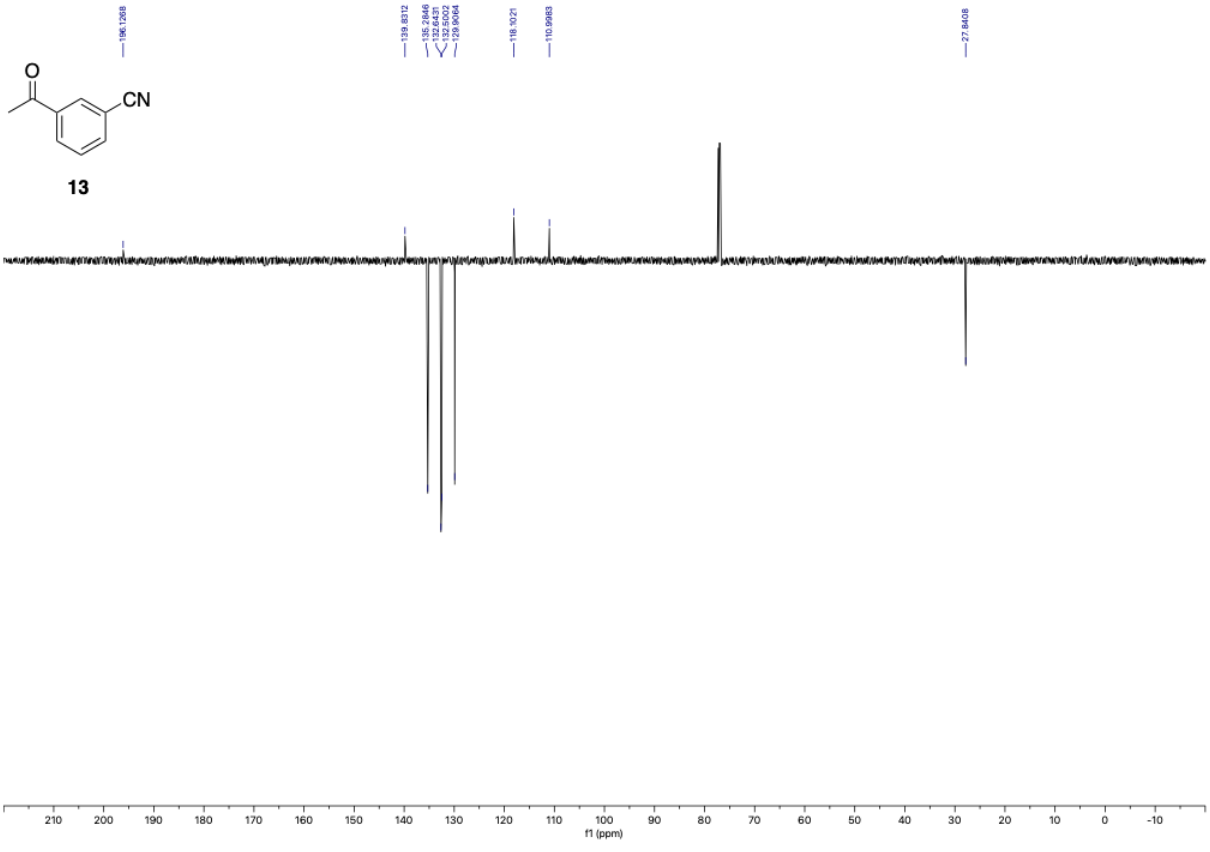

2.44
2.78
1.17
0.49
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


CN
NH2
O

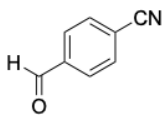
12

192.9897
153.7589
136.4002
133.3288
128.2994
125.2640
124.5865
120.7714
111.7320
96.0066
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
CN
13
7.8467
7.8275
7.8123
7.7179
7.7091
7.6736
7.6609
7.6482
7.2684 CDCl3
0.73
0.21
0.44
0.52
3.66
f1 (ppm)

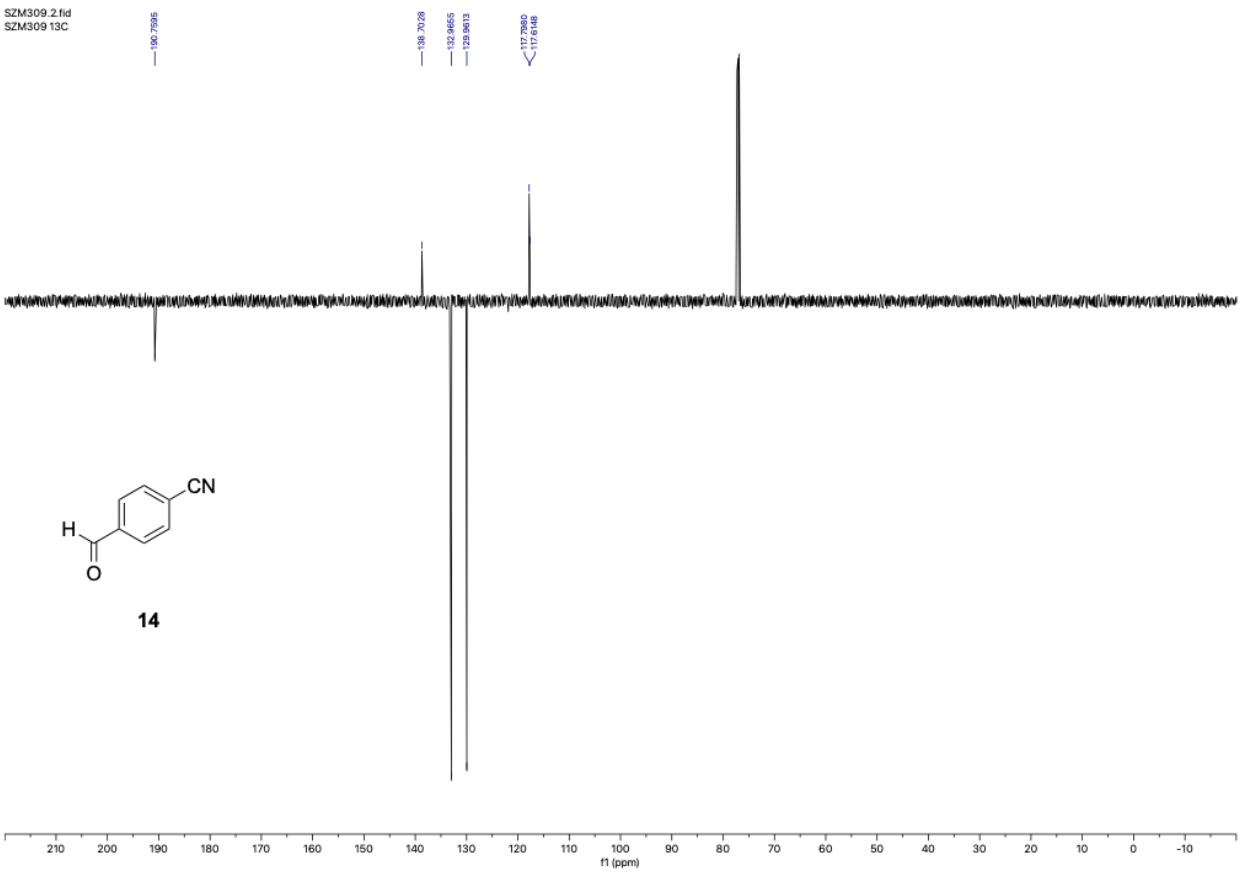

196.1268
139.8372
135.2846
132.6431
129.9064
118.1021
110.9983
27.8408
O
CN
13
f1 (ppm)

SZM309.1.fid
SZM309

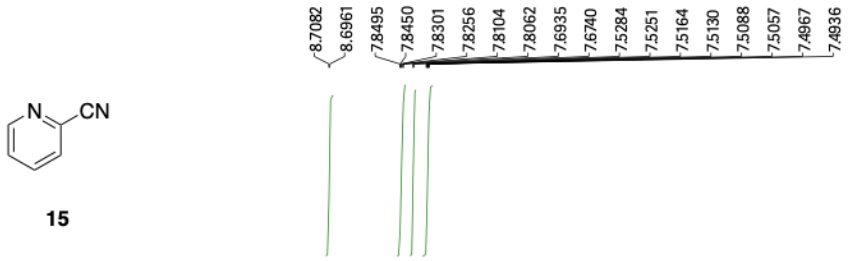


14

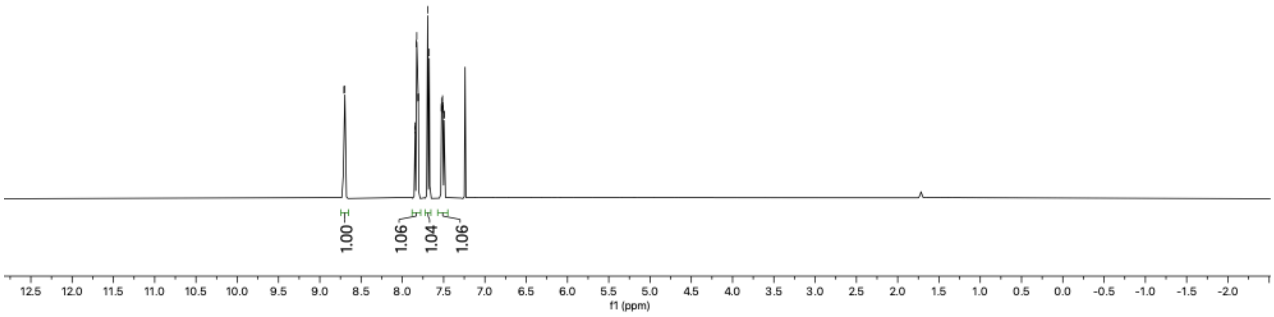
SZM309.2.fid
SZM309 13C



14

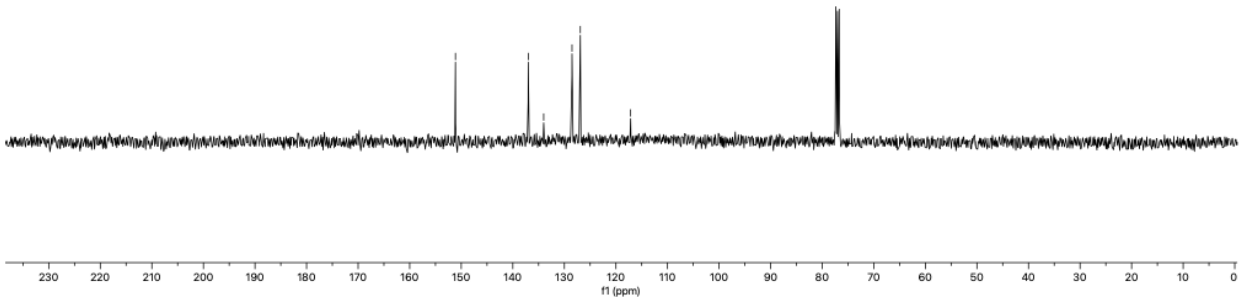

8.7082
8.6961
7.8495
7.8450
7.8301
7.8256
7.8104
7.8062
7.6935
7.6740
7.5284
7.5251
7.5164
7.5130
7.5088
7.5057
7.4967
7.4936
N
CN

15

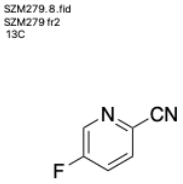

1.00
1.06
1.04
1.06
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


151.1268
137.0109
134.0142
128.5202
126.9052
117.1531
N
CN

15

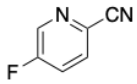

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

SZM279.8.fid
SZM279 fr2
13C



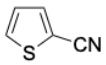
16

SZM279.1.fid
SZM279 fr1 1H



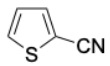
16

SZM300.1.fid
SZM300

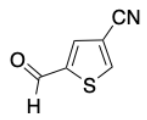


17

SZM300.2.fid
SZM300 13C

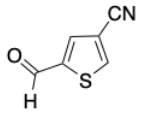


17


CN
O
S
H

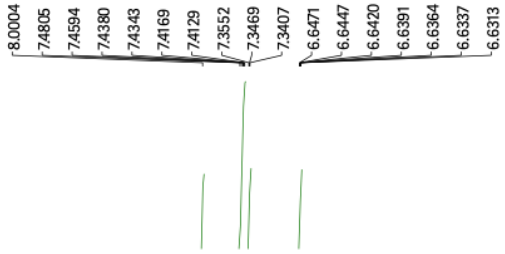
18

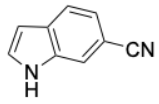
9.9426
8.2592
7.9322
7.2536 CDCl3
1.00
1.17
1.19
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


CN
O
S
H

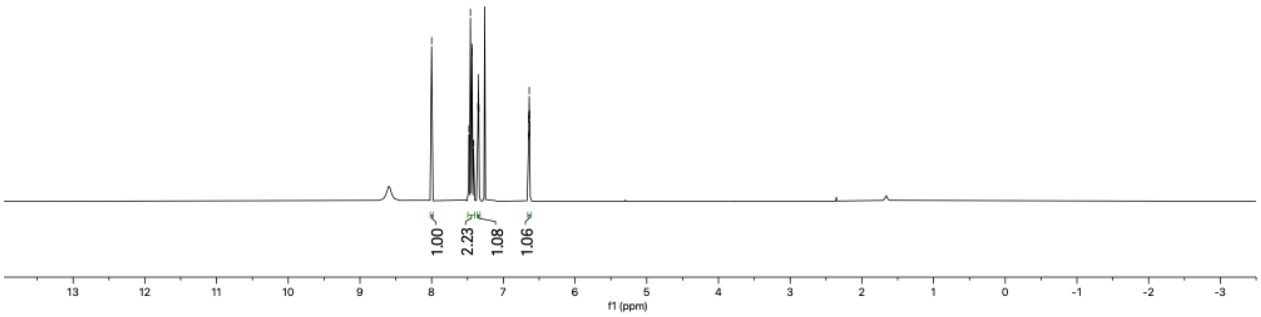
18

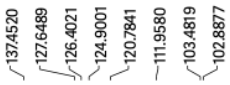
181.6444
145.2204
142.4910
136.2371
113.6617
112.1926
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

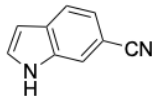

8.0004
7.4805
7.4594
7.4380
7.4343
7.4169
7.4129
7.3552
7.3469
7.3407
6.6471
6.6447
6.6420
6.6391
6.6364
6.6337
6.6313


CN
N
H

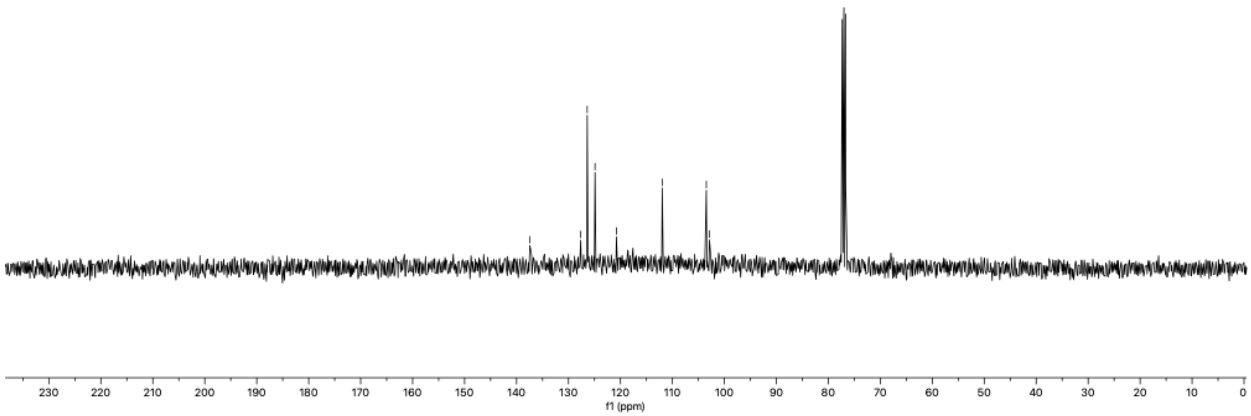
19

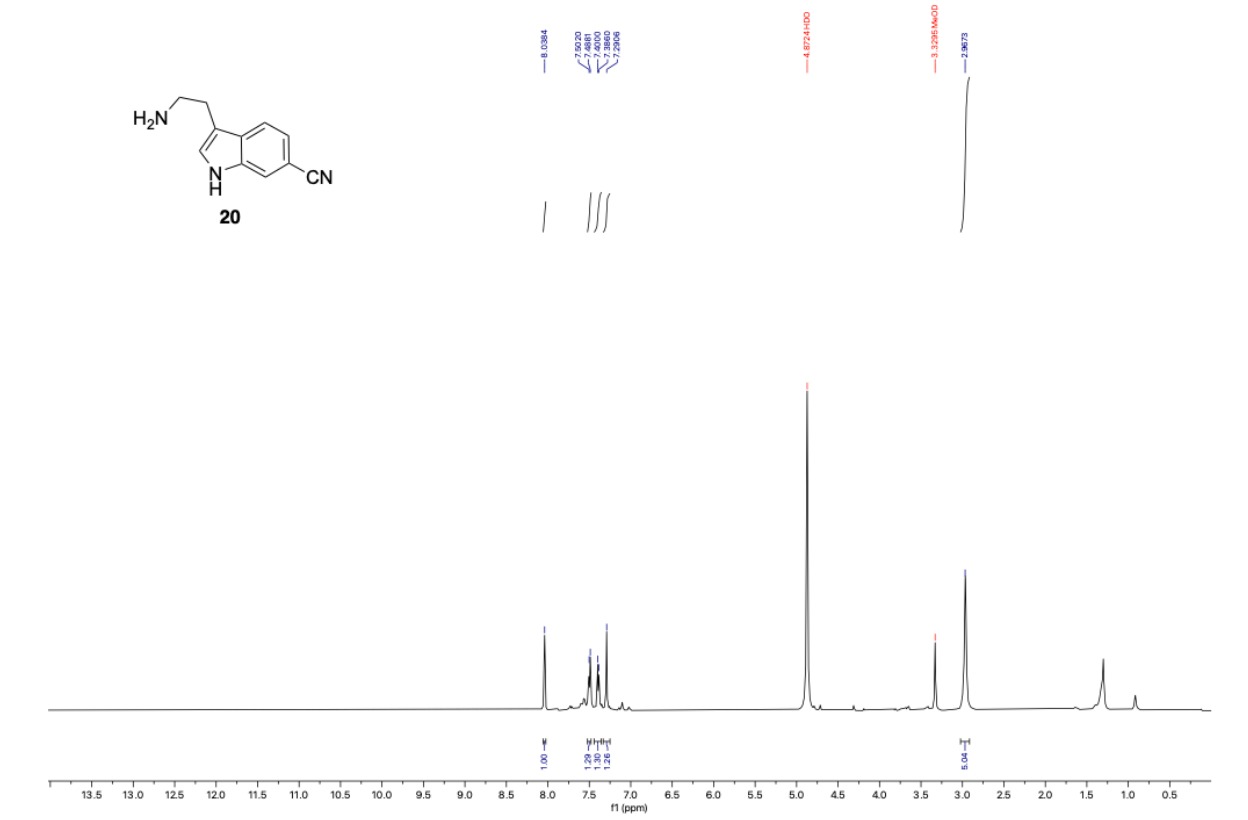

1.00
2.23
1.08
1.06
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

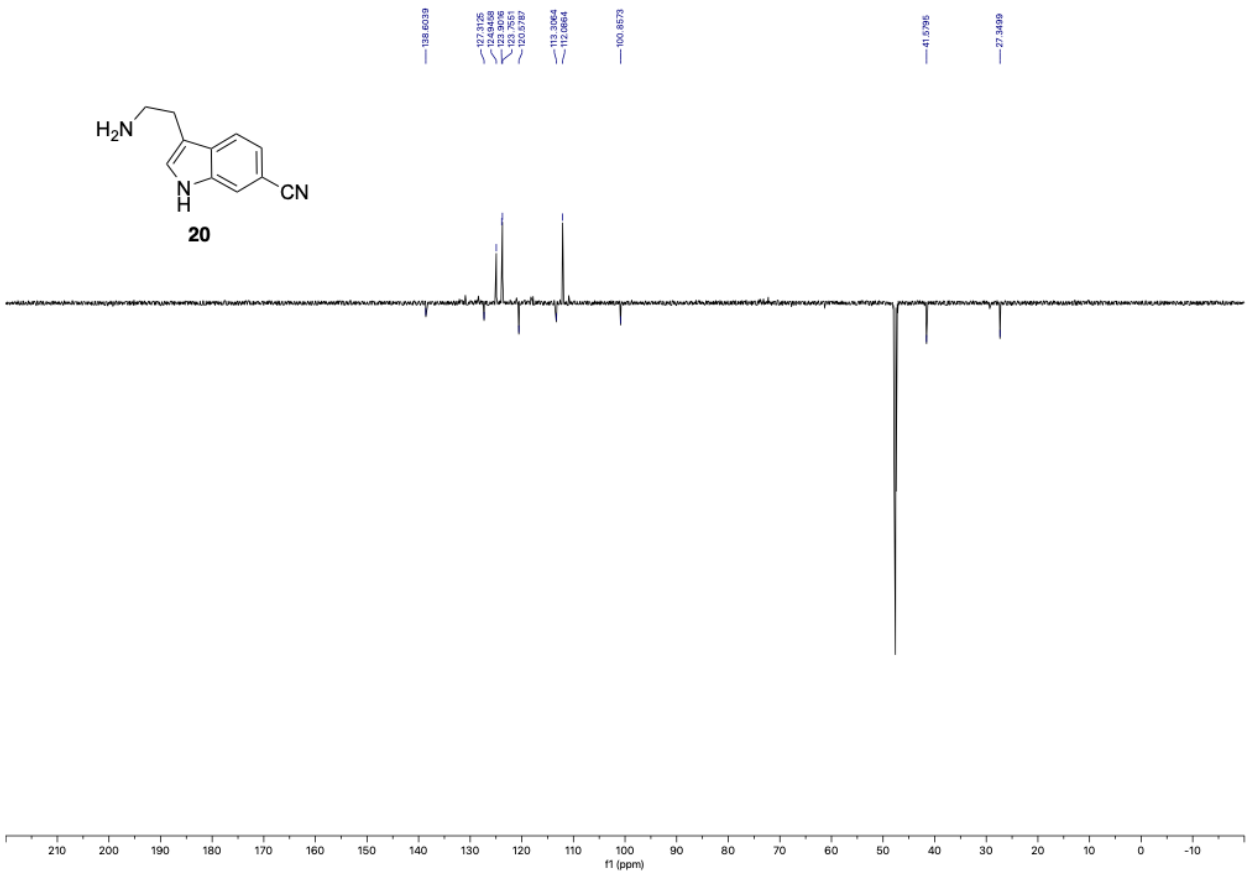

137.4520
127.6489
126.4021
124.9001
120.7841
111.9580
103.4819
102.8877

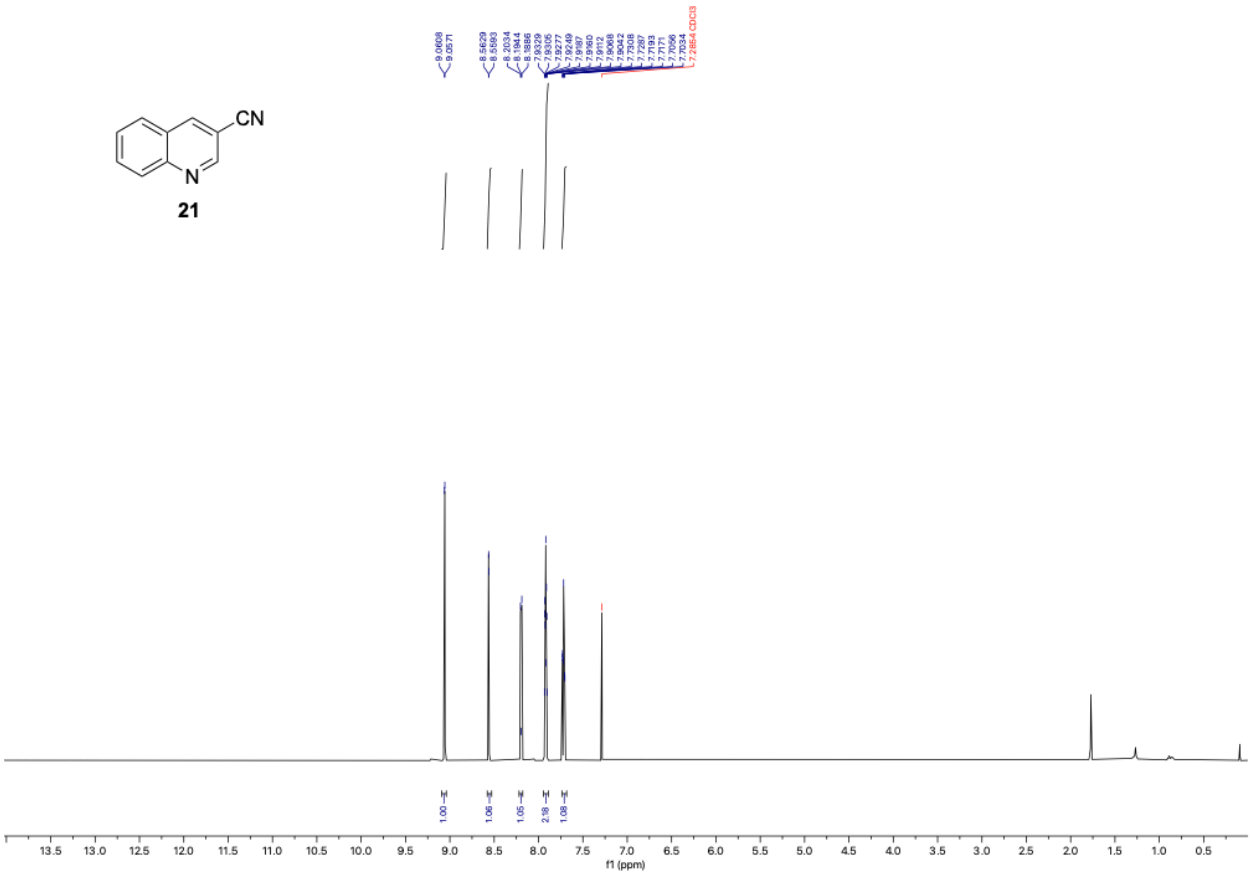

CN
N
H

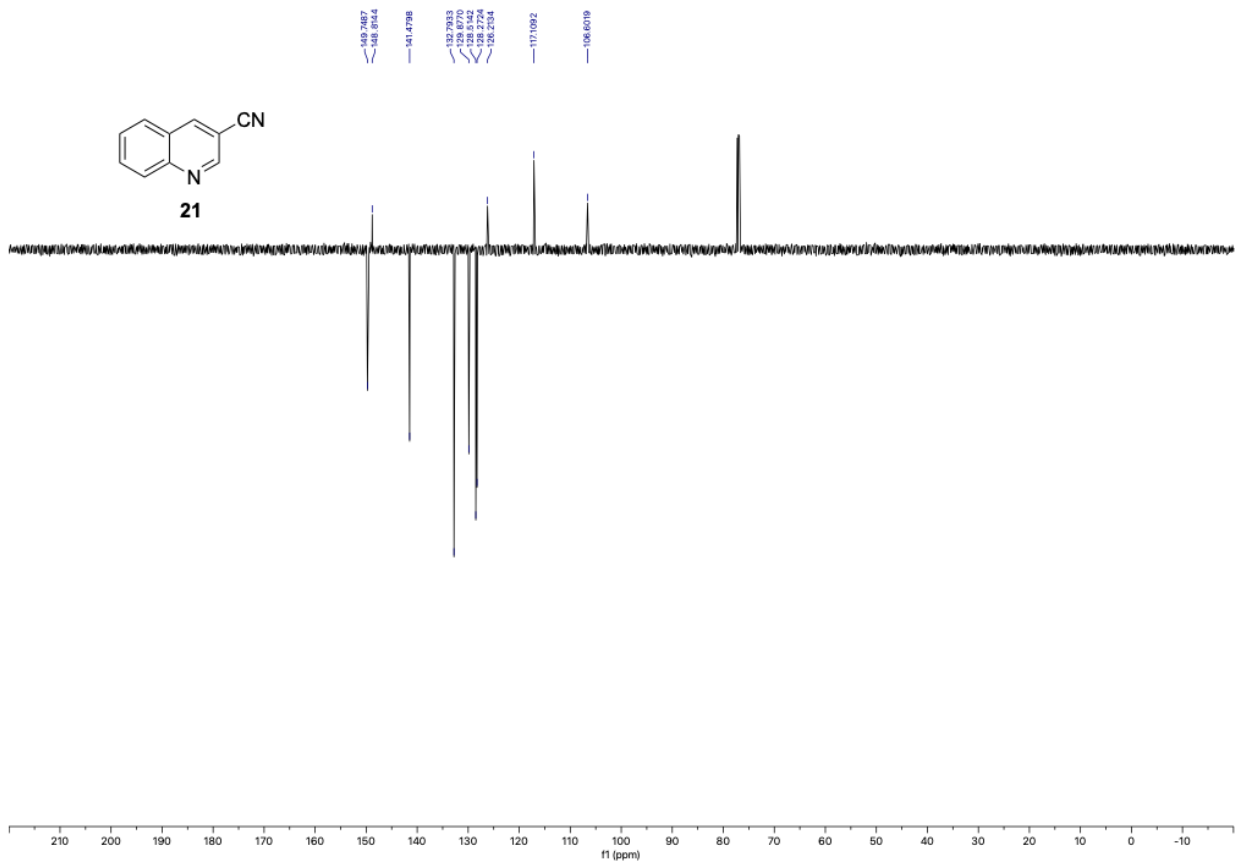
19


230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

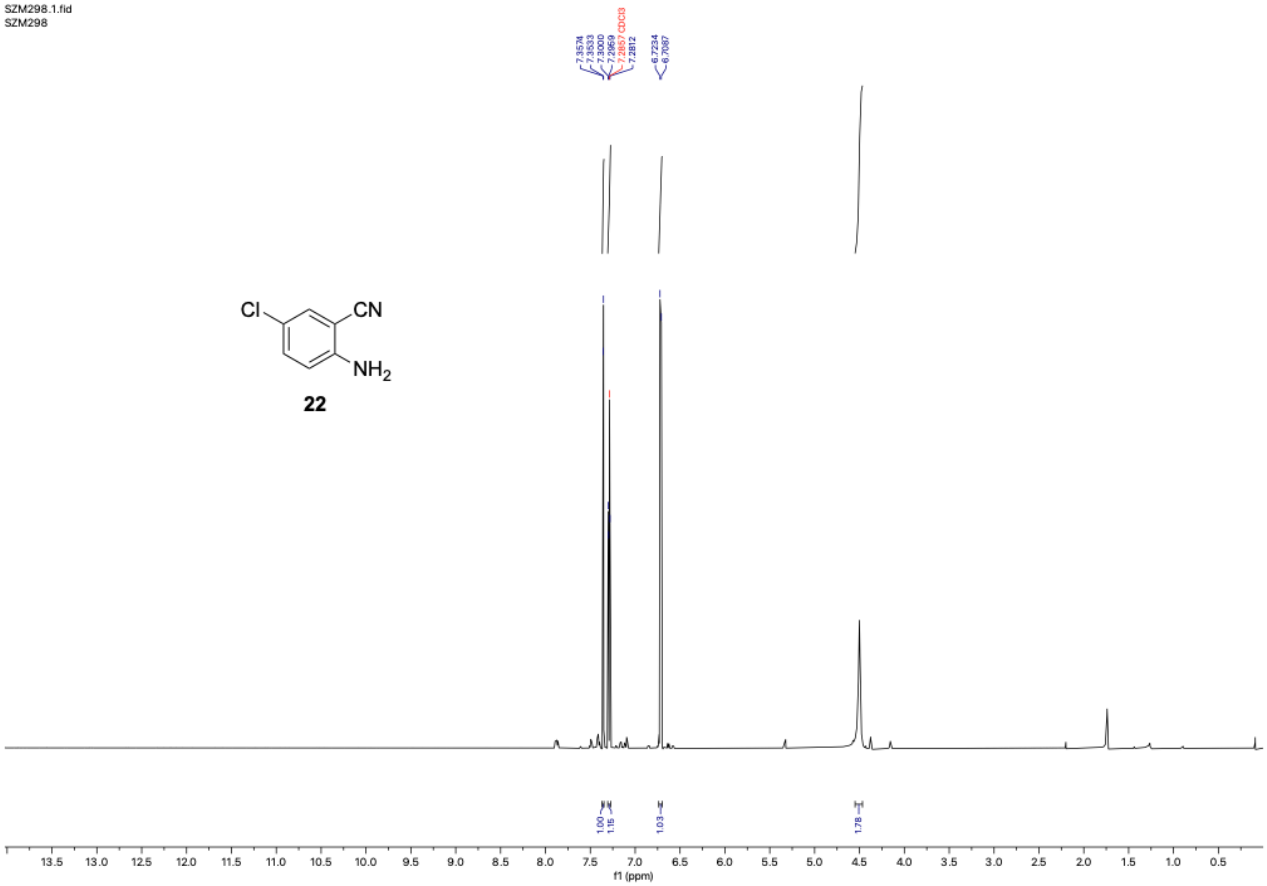

20
8.0384
7.5920
7.4881
7.3660
7.3560
7.2906
4.8724 HDO
3.3295 MeOD
2.9673
1.00
1.29
1.30
1.26
5.04
f1 (ppm)


20
138.6039
127.3125
124.9458
123.9966
123.7535
120.5787
113.3064
112.0864
100.8573
41.5795
27.3499
f1 (ppm)


CN
N
21
9.0608
9.0571
8.5629
8.5583
8.4004
8.3944
8.3886
7.9329
7.9305
7.9277
7.9249
7.9197
7.9160
7.9112
7.9068
7.9042
7.7299
7.7287
7.7193
7.7171
7.7066
7.7034
7.2854 CDCl3
1.00
1.06
1.05
2.19
1.08
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

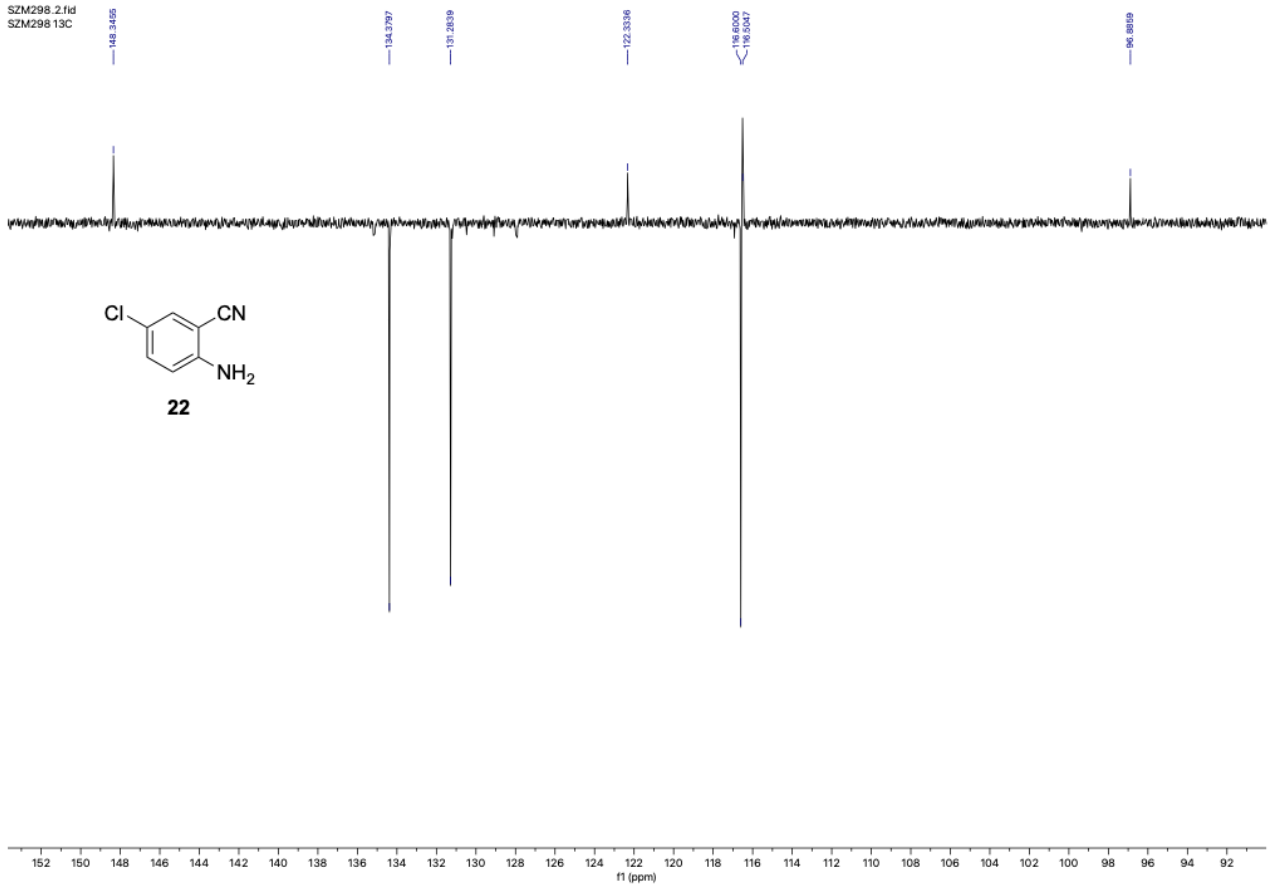

149.7487
148.8144
141.4798
132.7933
129.8770
128.5142
128.2724
126.2104
117.1092
106.6019
CN
N
21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

SZM298.1.fid
SZM298



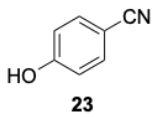
22

SZM298.2.fid
SZM298 13C

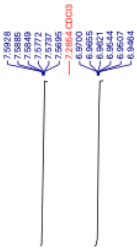


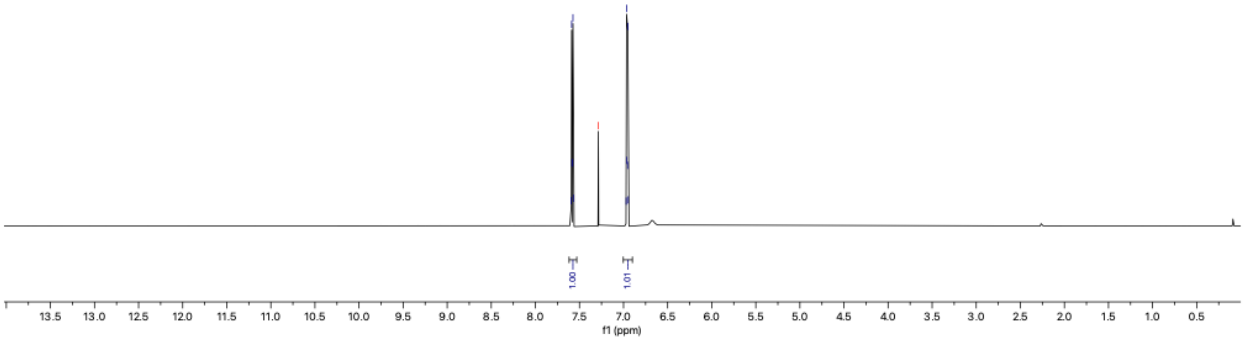
22

SZM308.1.fid
SZM308

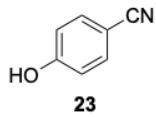


23

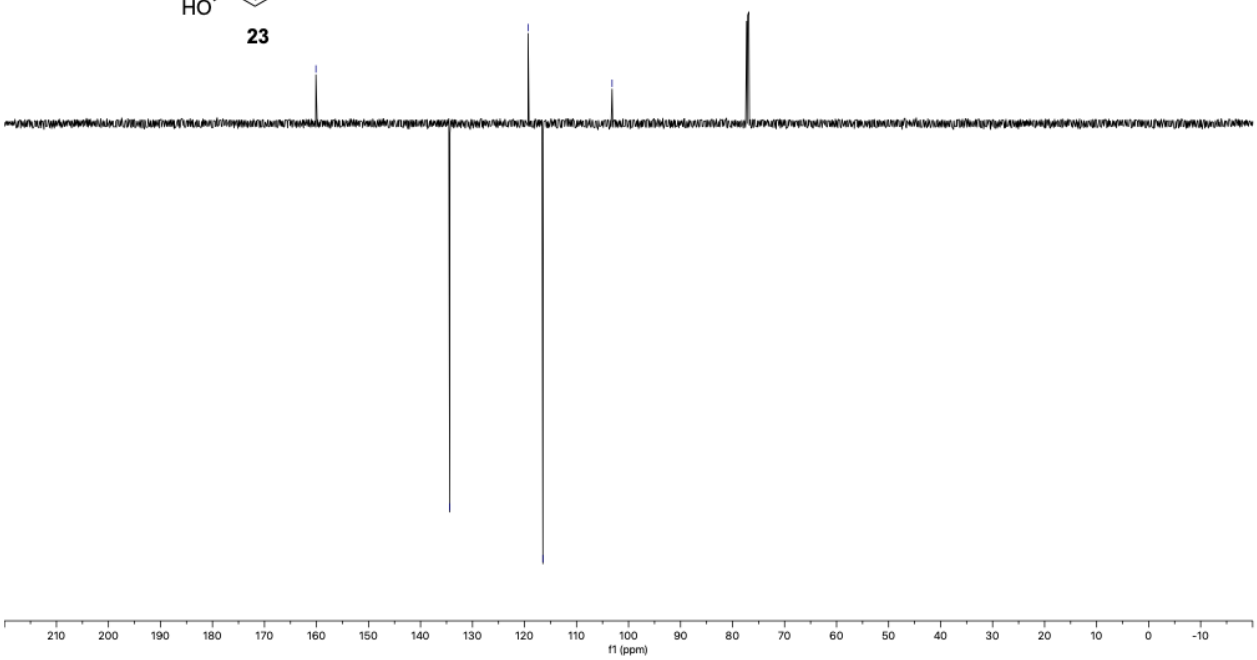


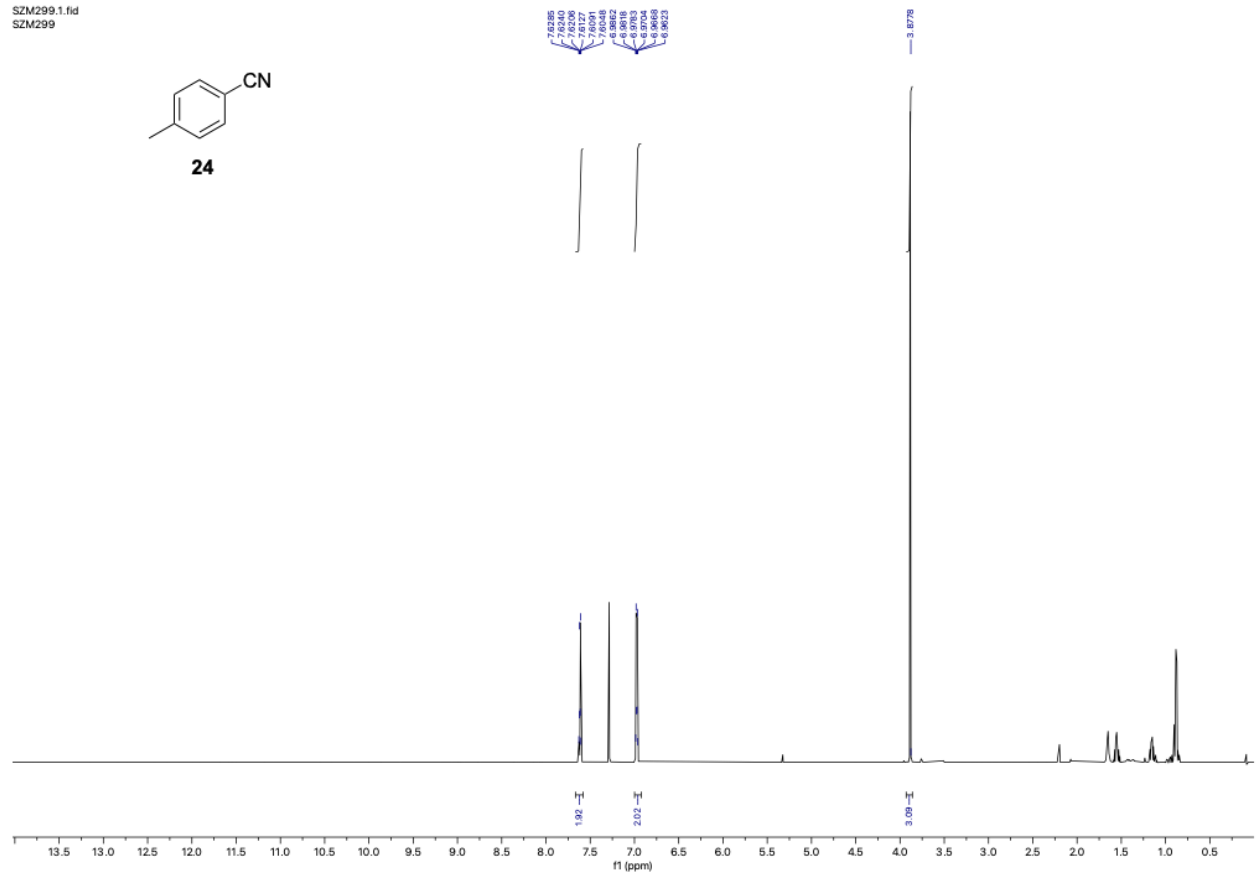


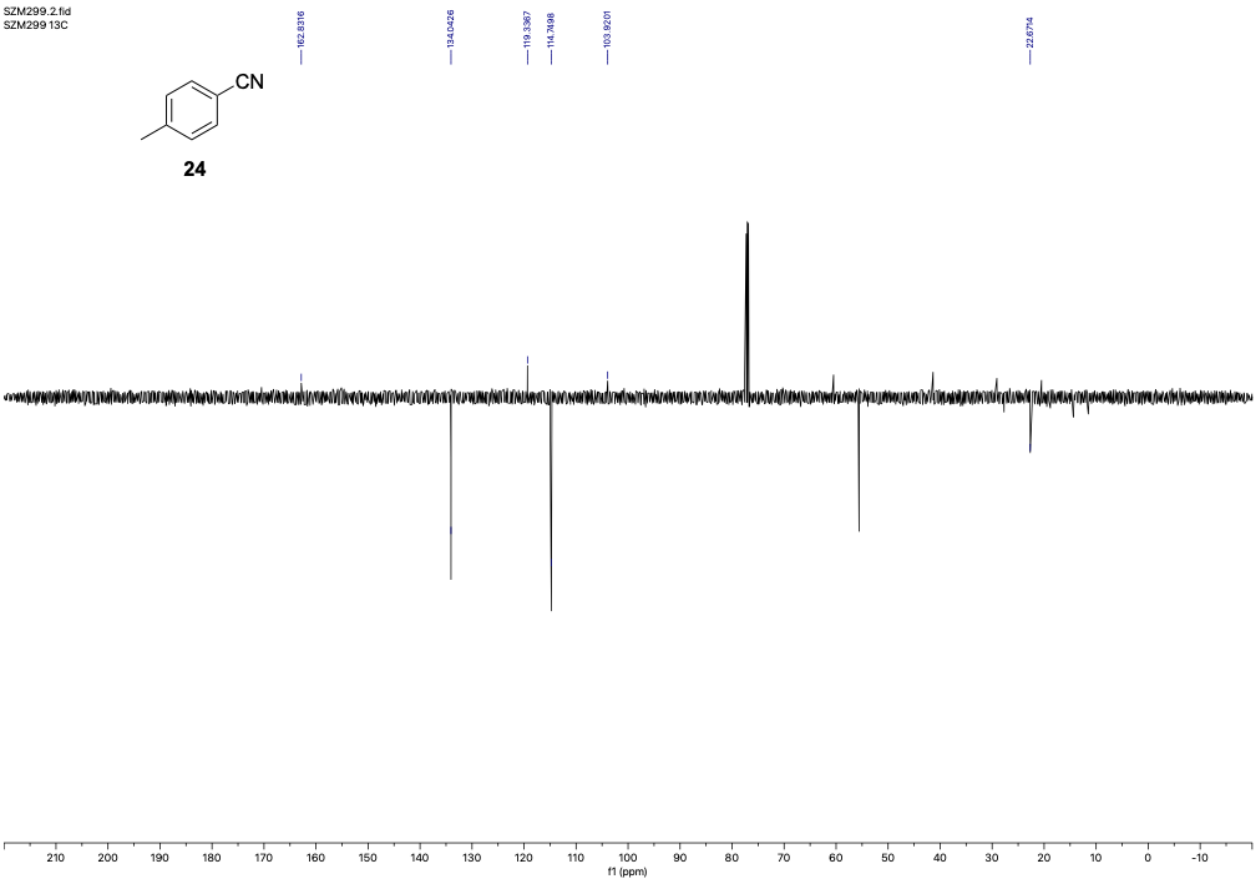
SZM308.2.fid
SZM308 13C



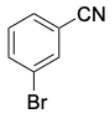
23




SZM299.1.fid
SZM299
CN
24
7.76285
7.76240
7.76206
7.76177
7.76091
7.76048
6.98662
6.98618
6.97783
6.97704
6.96658
6.96623
3.8778
1.92
2.02
3.09
f1 (ppm)

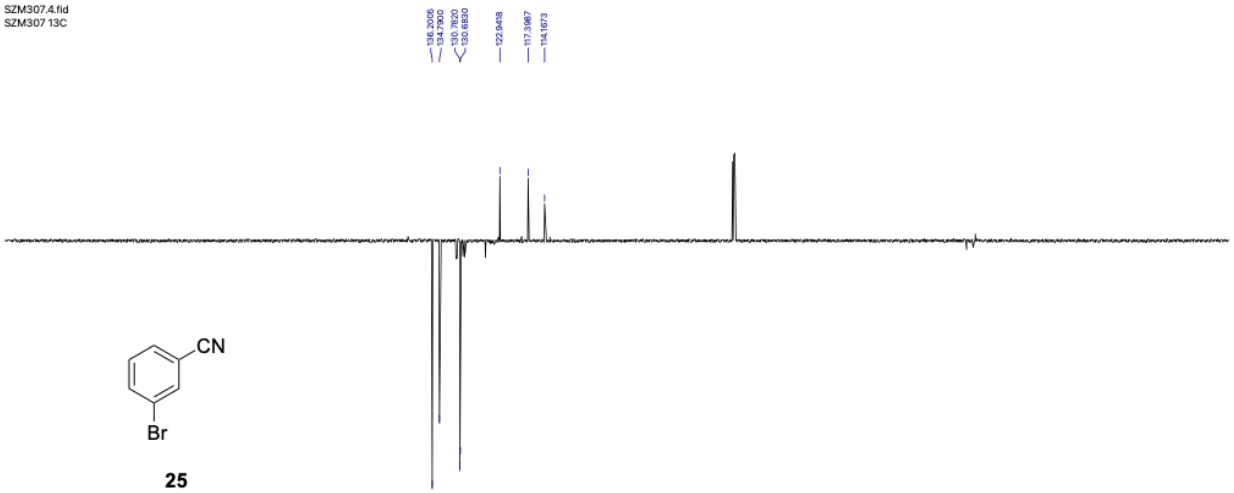

SZM299.2.fid
SZM299 13C
CN
24
162.8316
134.0426
119.3367
114.7498
103.9201
22.6794
f1 (ppm)

SZM307.3.fid
SZM307 coda



25

SZM307.4.fid
SZM307 13C



25

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