

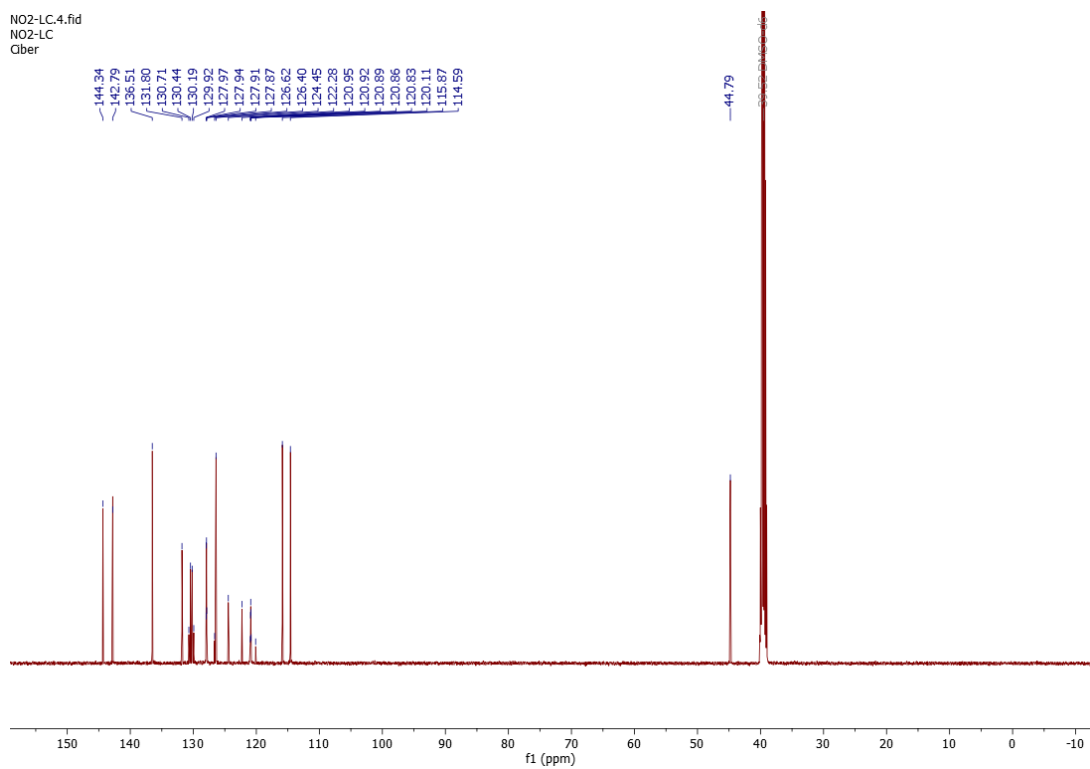
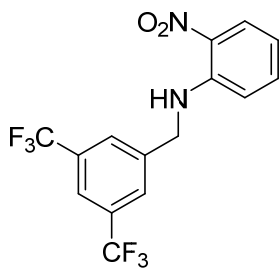
SUPPORTING INFORMATION

Synthesis of *N*¹-(3,5-bis(trifluoromethyl)benzyl)benzene-1,2-diamine and *N,N*-bis(2-nitrophenyl)-3,5-bis(trifluoromethyl)aniline

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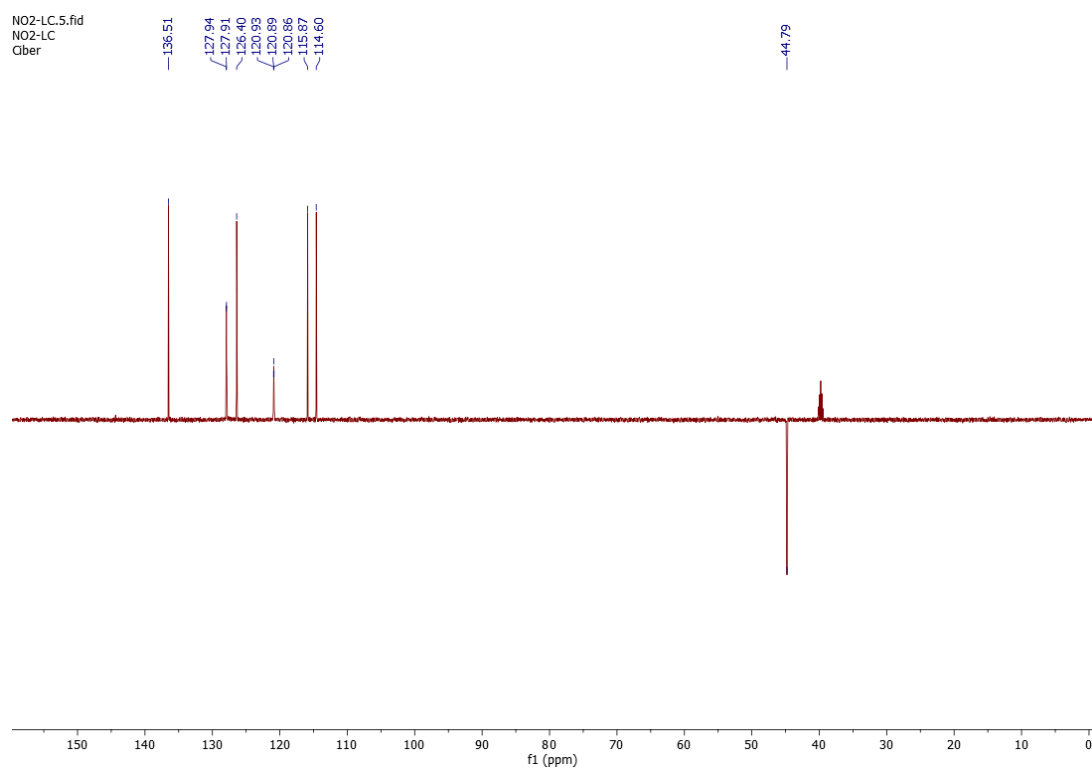
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***N*-(3,5-Bis(trifluoromethyl)benzyl)-2-nitroaniline (3)**



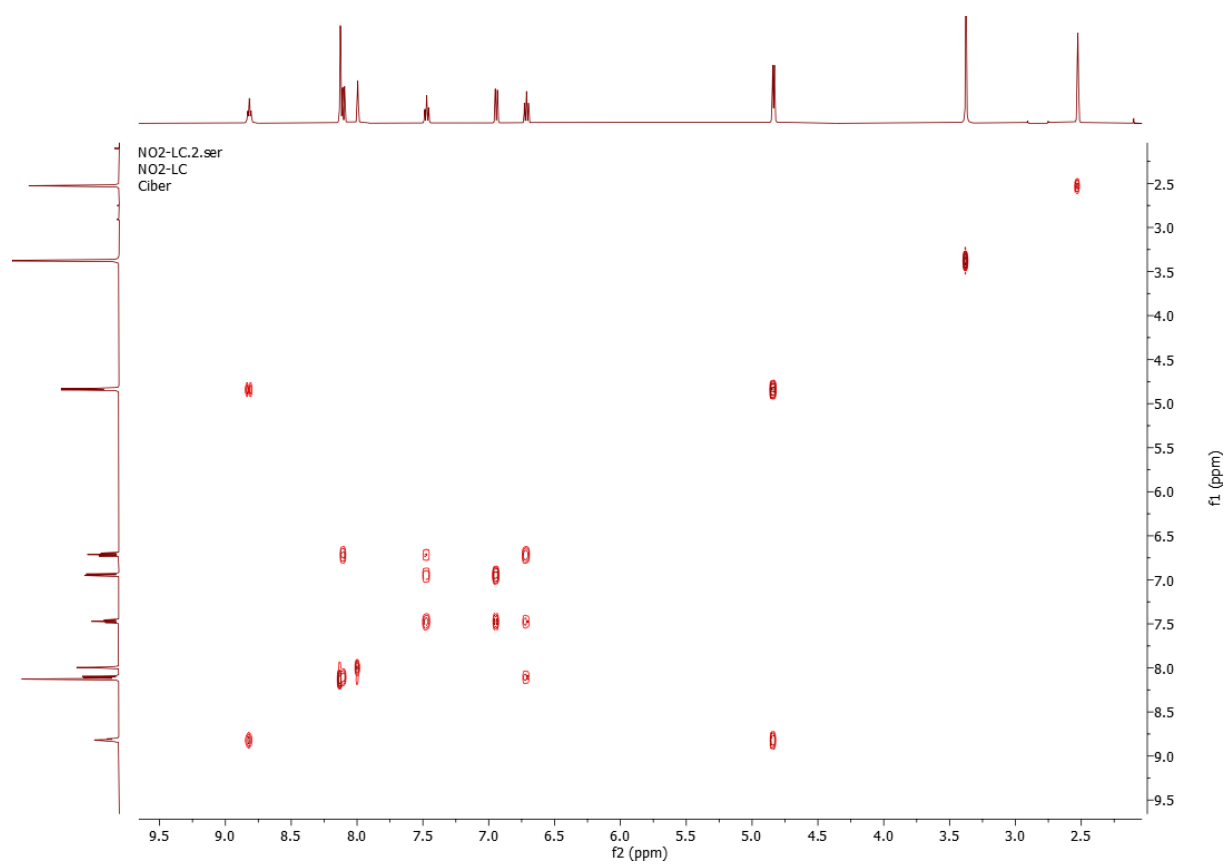
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NO2-LC
Ciber

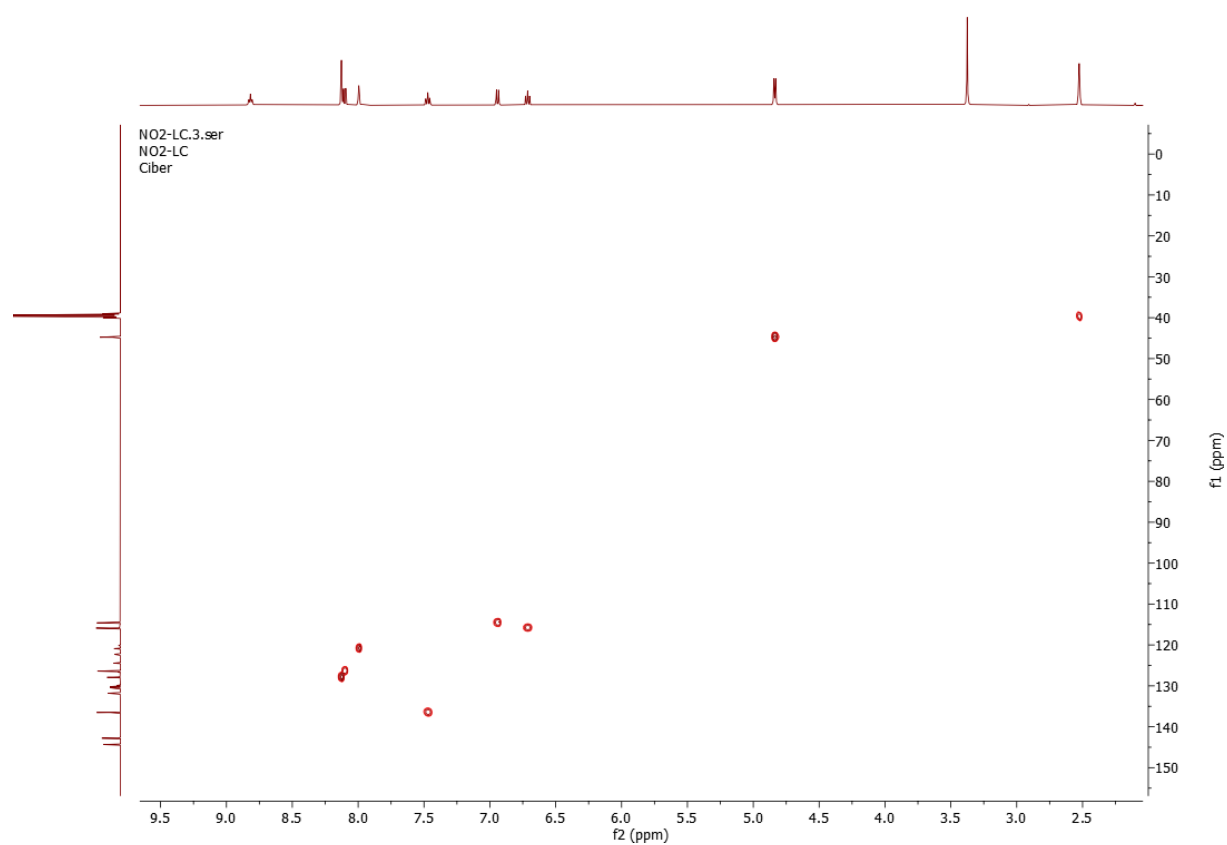


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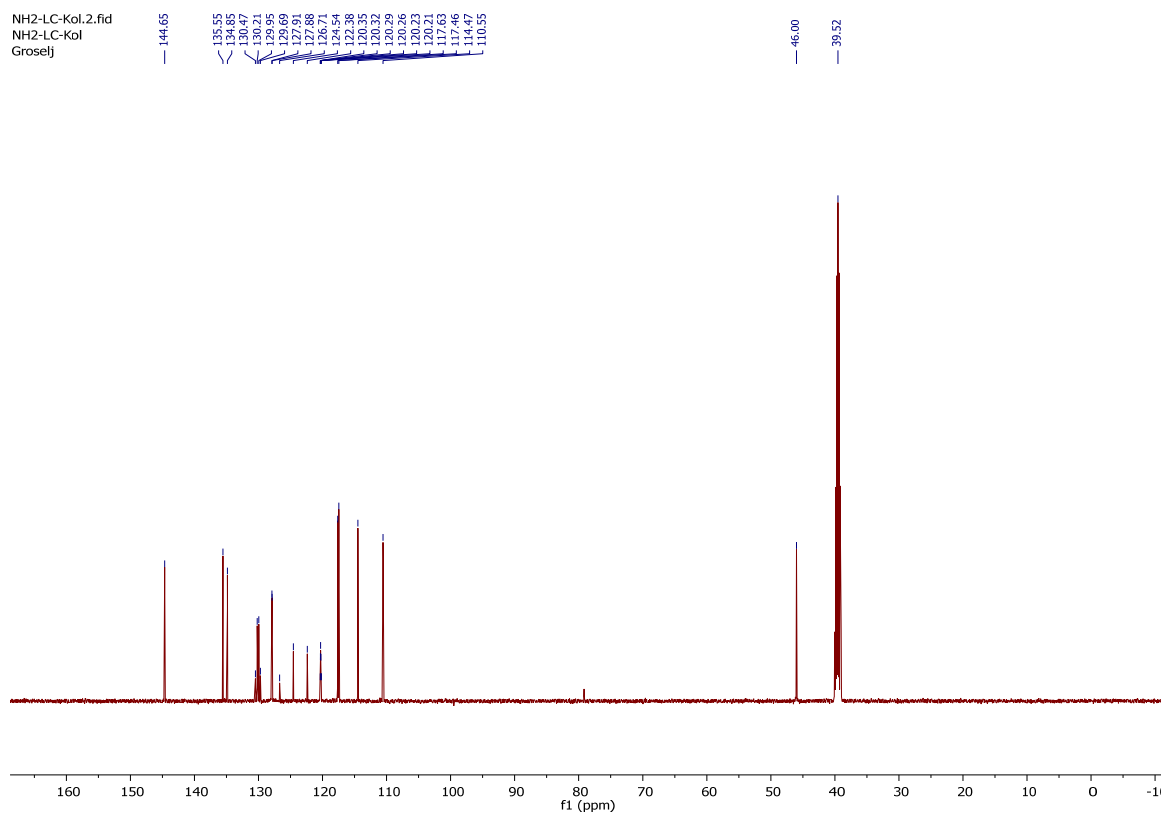
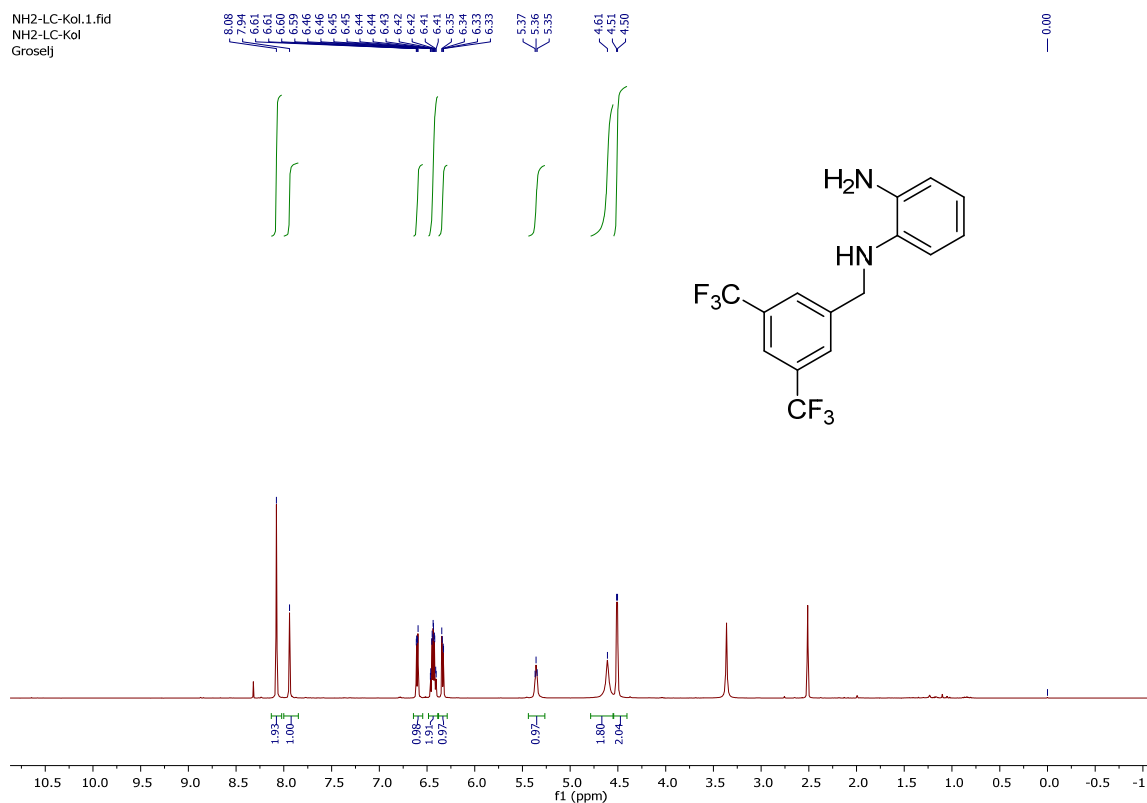
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HSQC

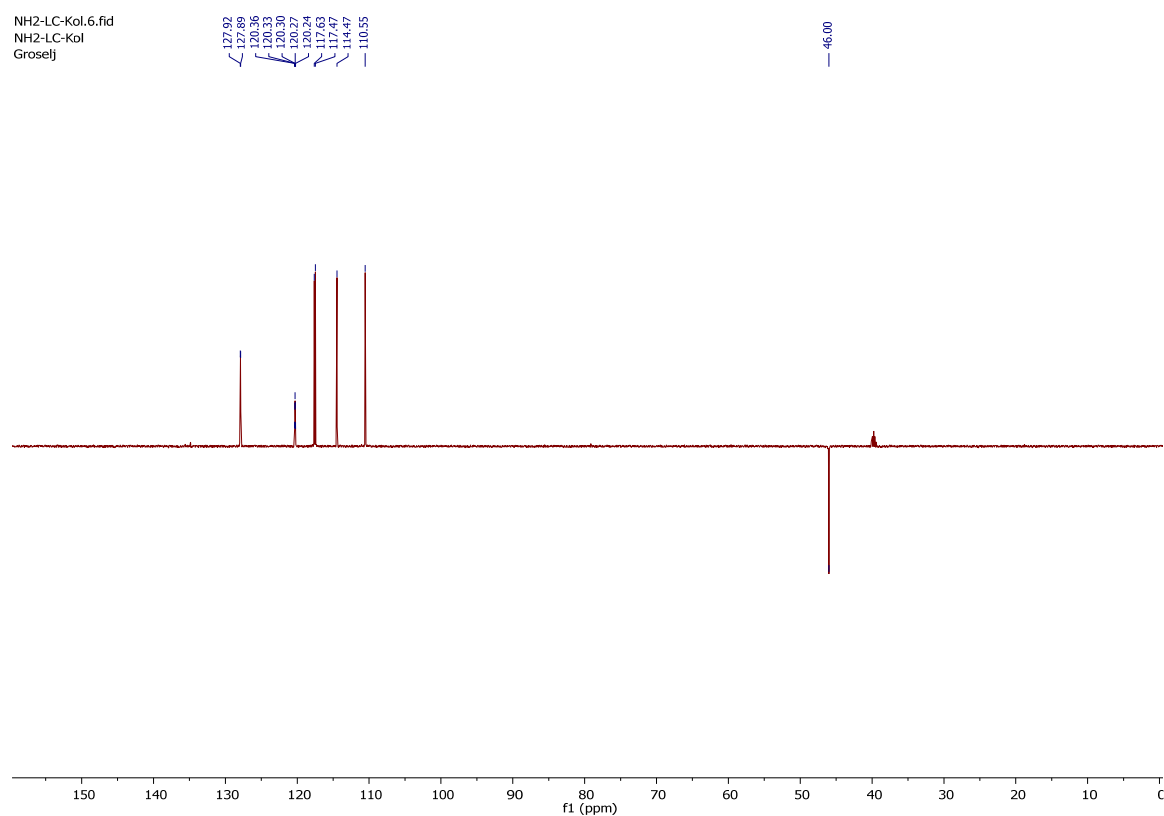


***N*¹-(3,5-Bis(trifluoromethyl)benzyl)benzene-1,2-diamine (4a)**

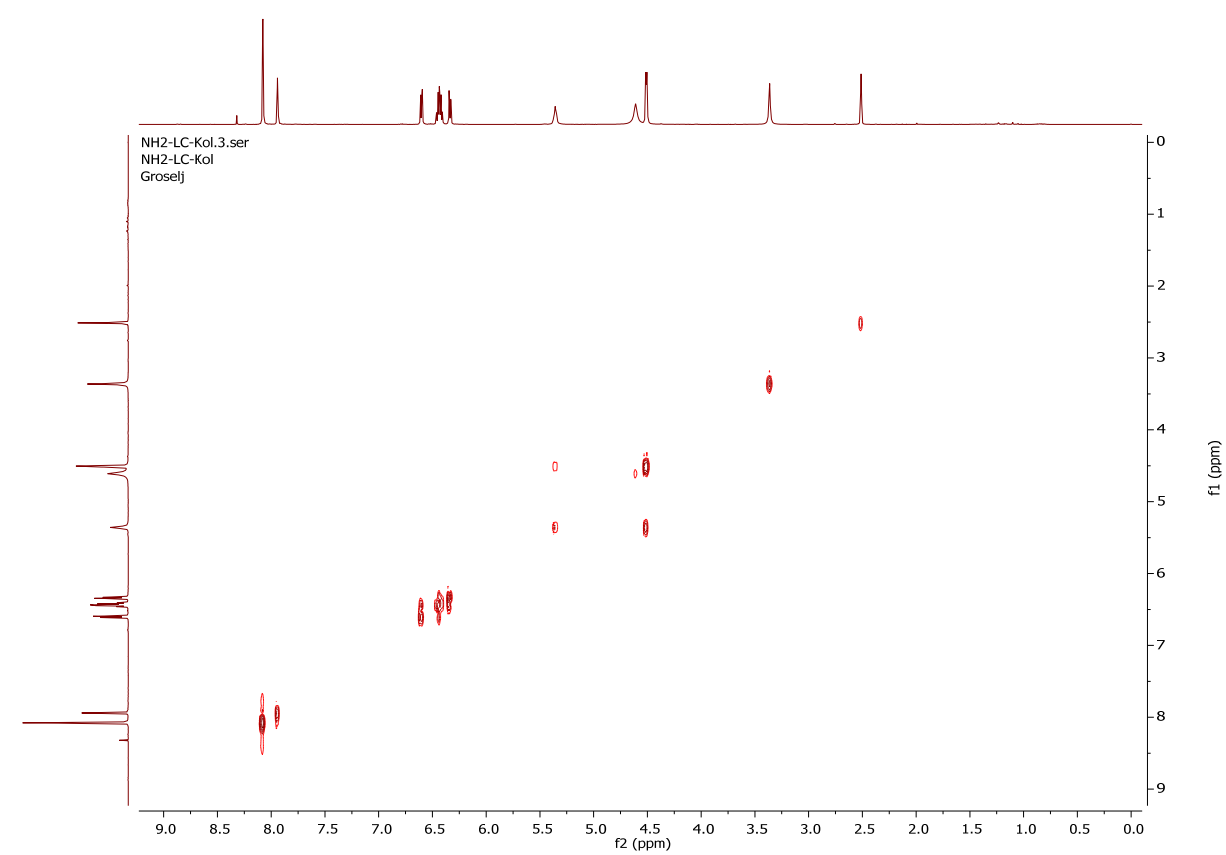


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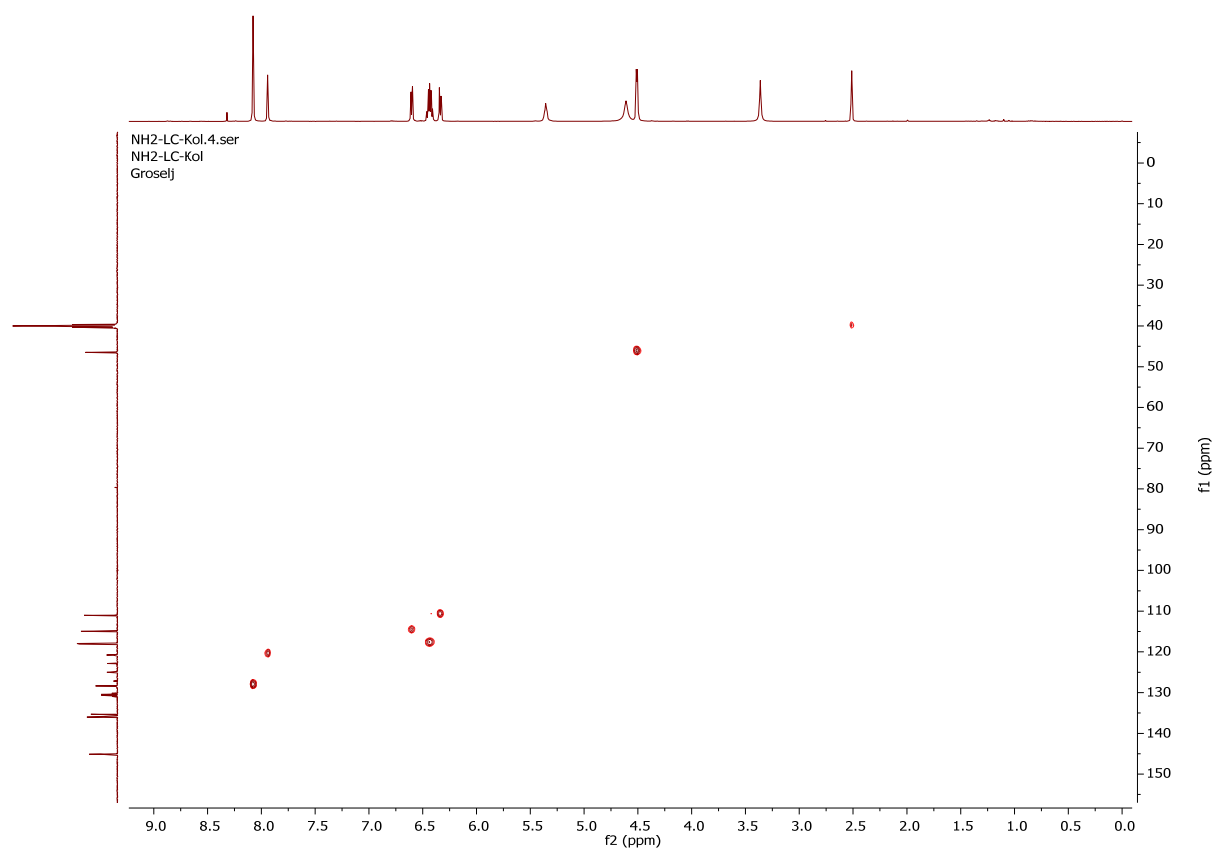
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NH2-LC-Kol
Groselj



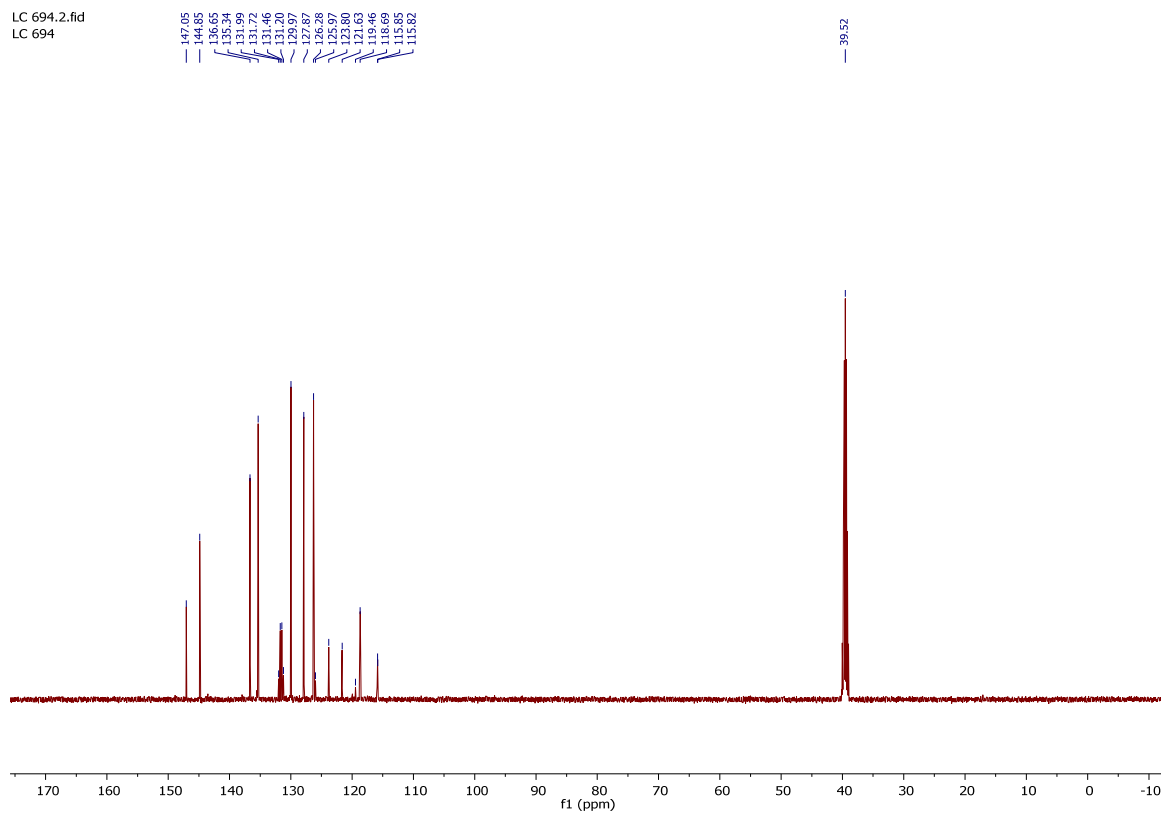
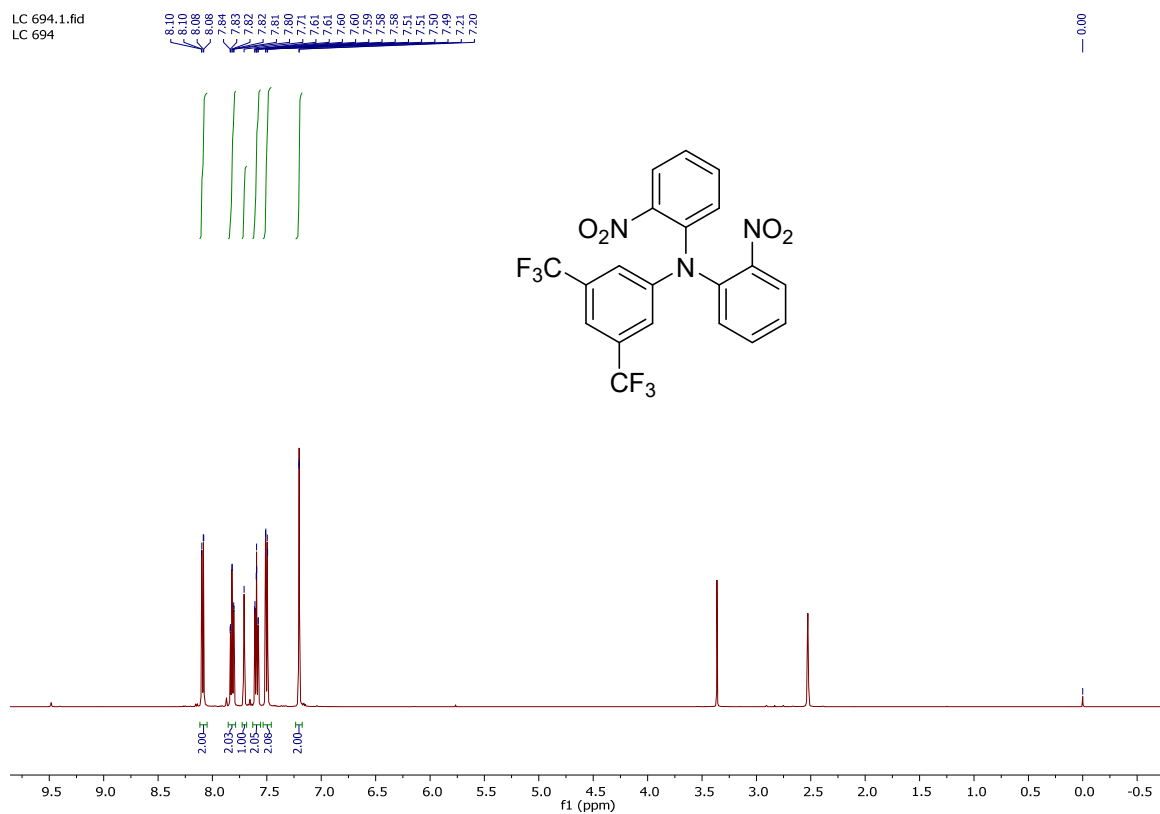
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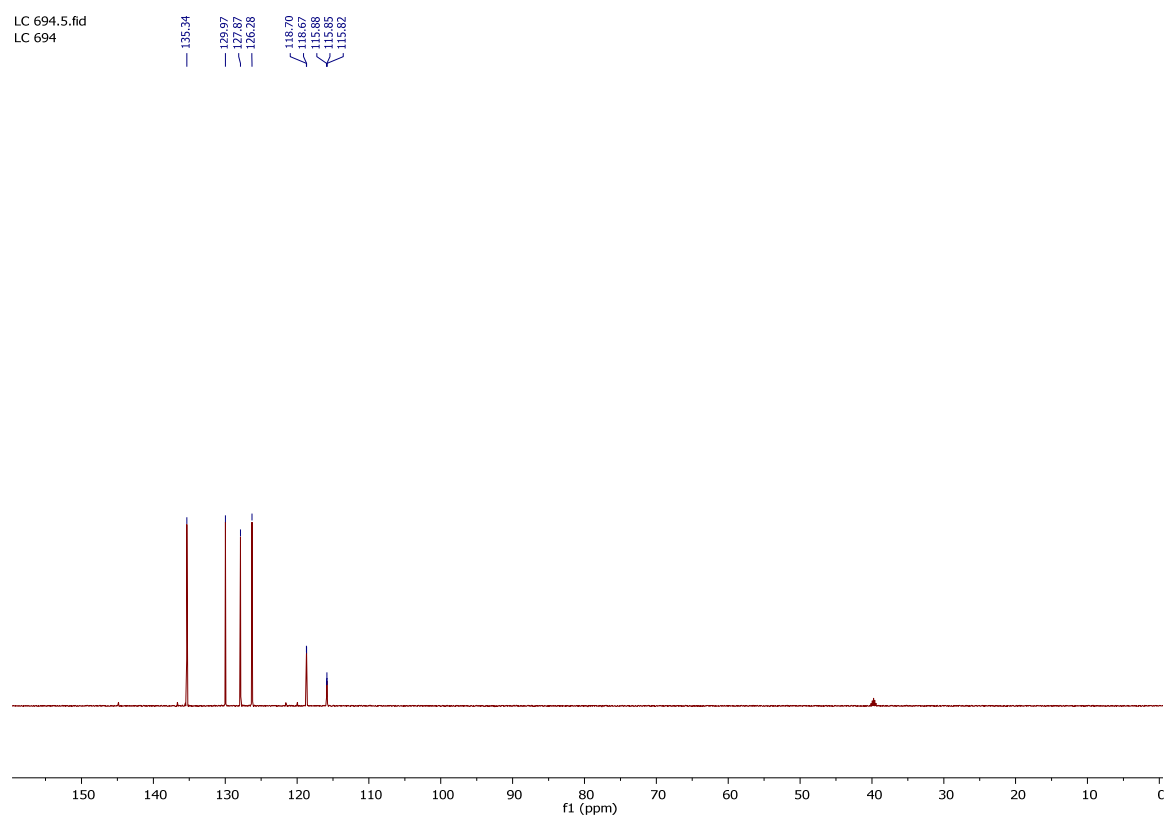


N,N-Bis(2-nitrophenyl)-3,5-bis(trifluoromethyl)aniline (7)



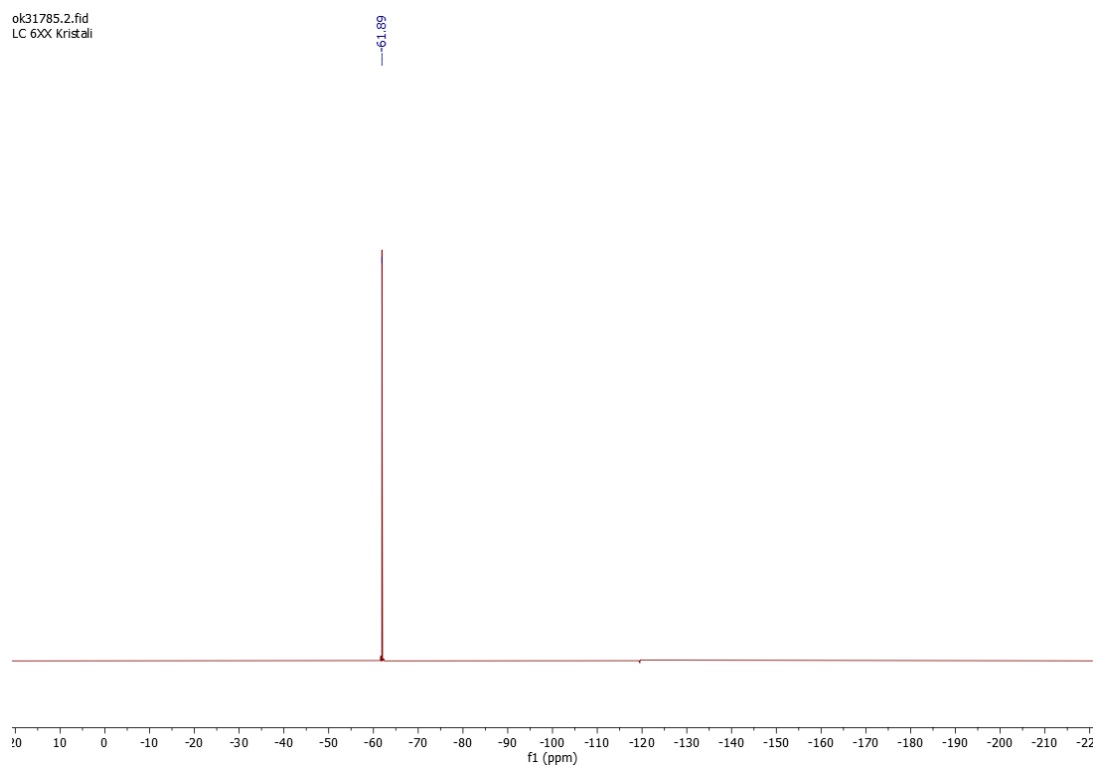
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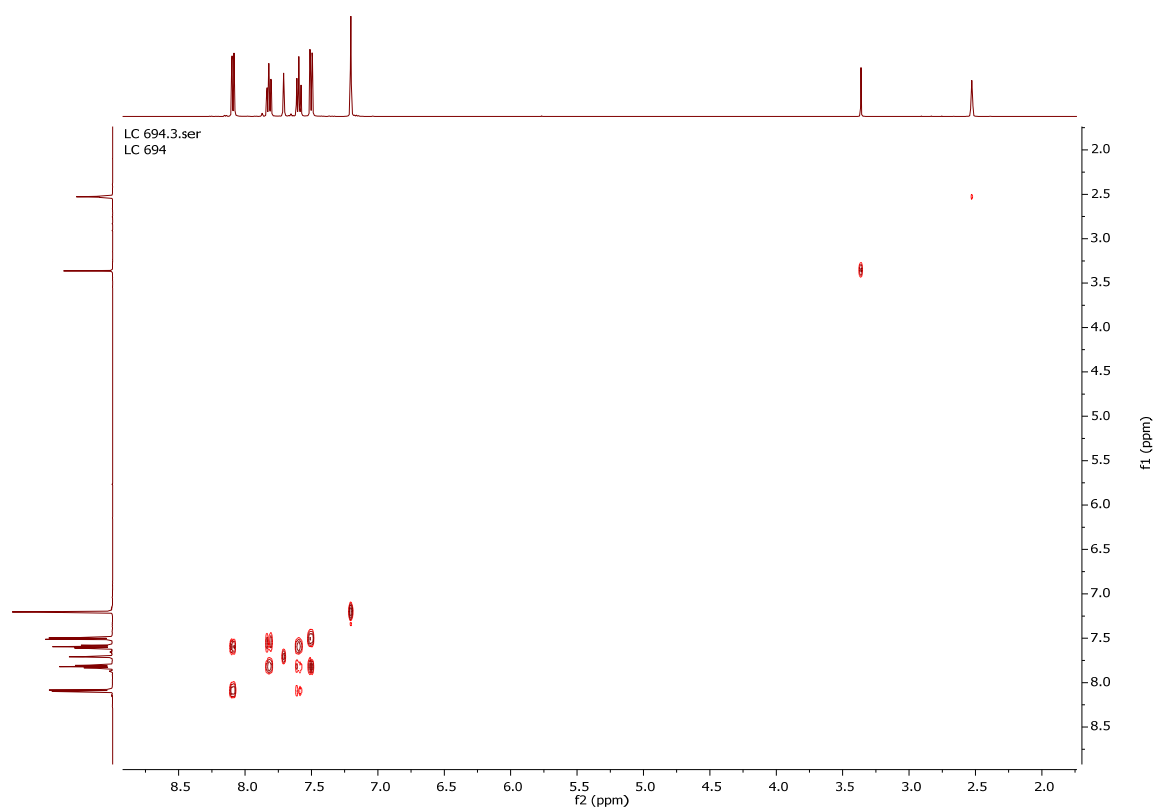


^{19}F -NMR

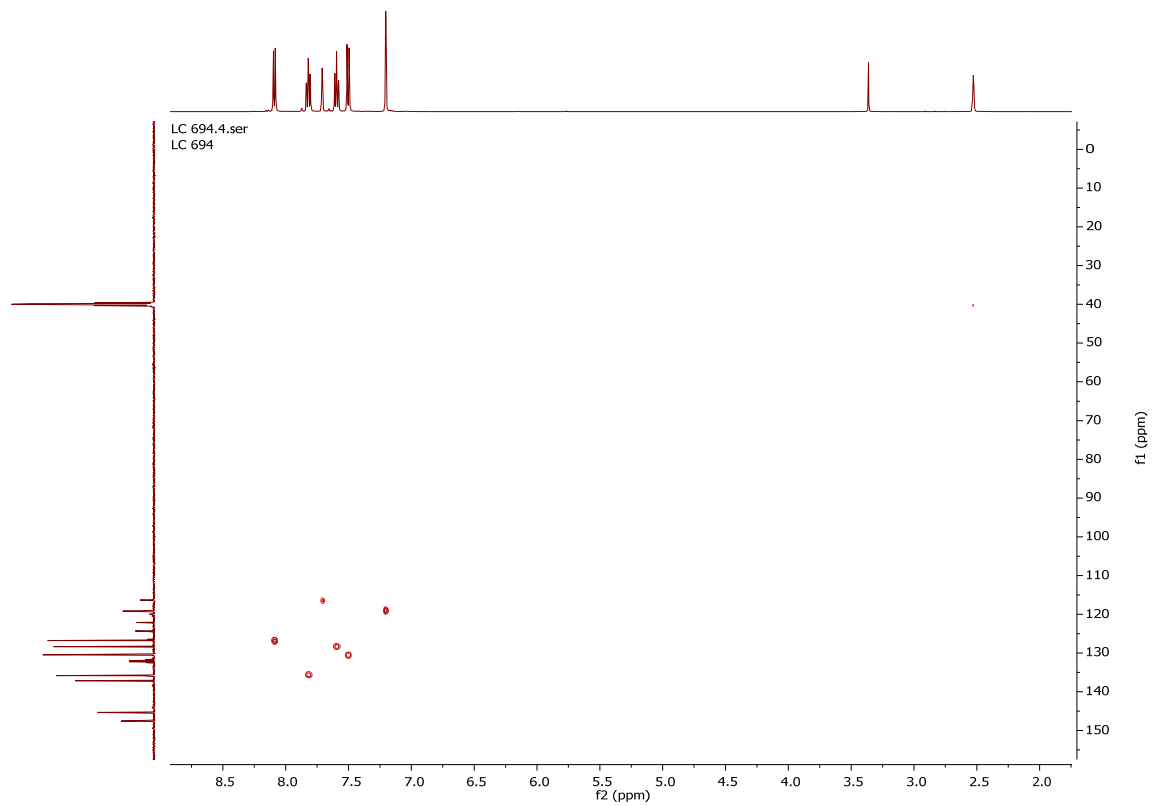
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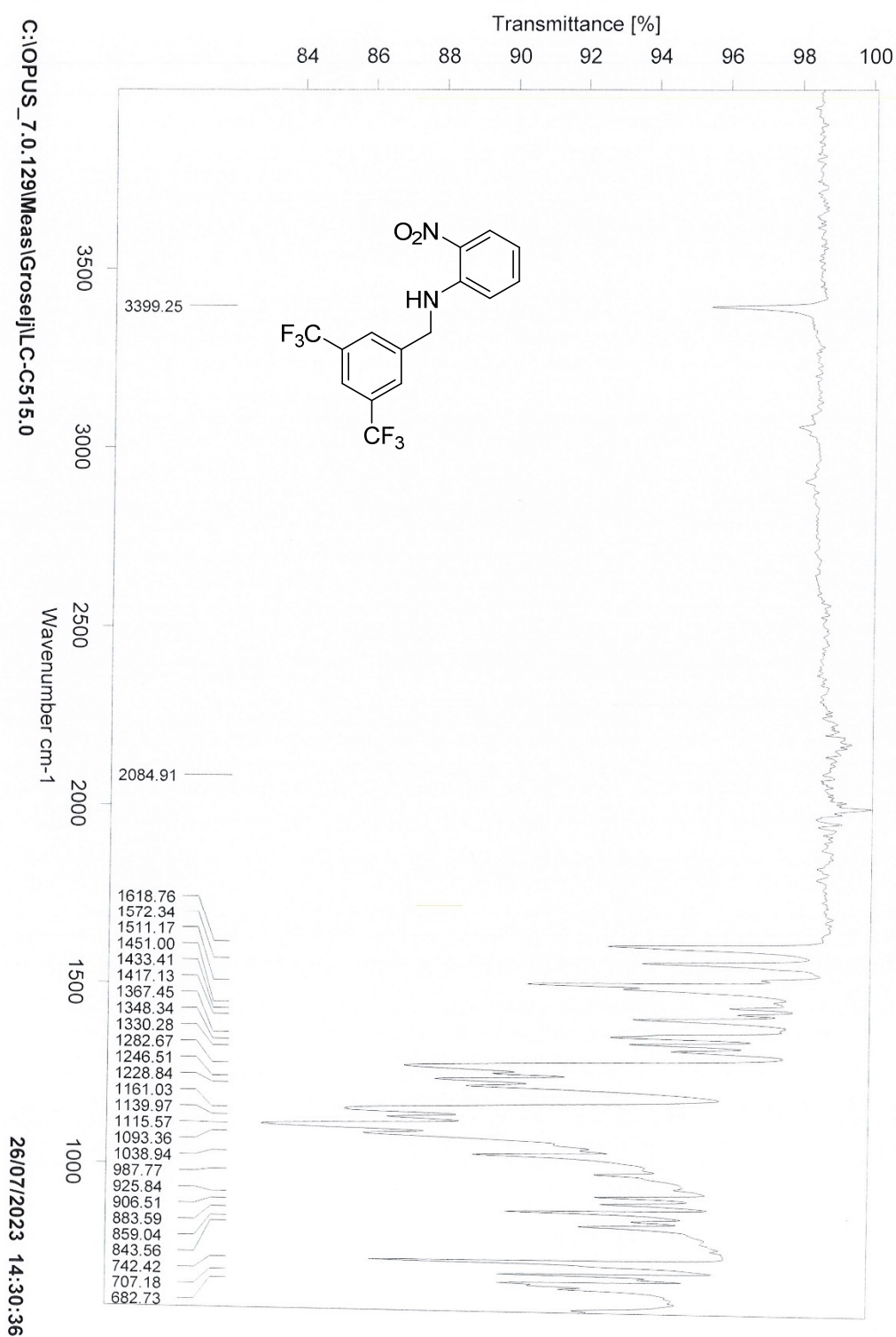


HSQC

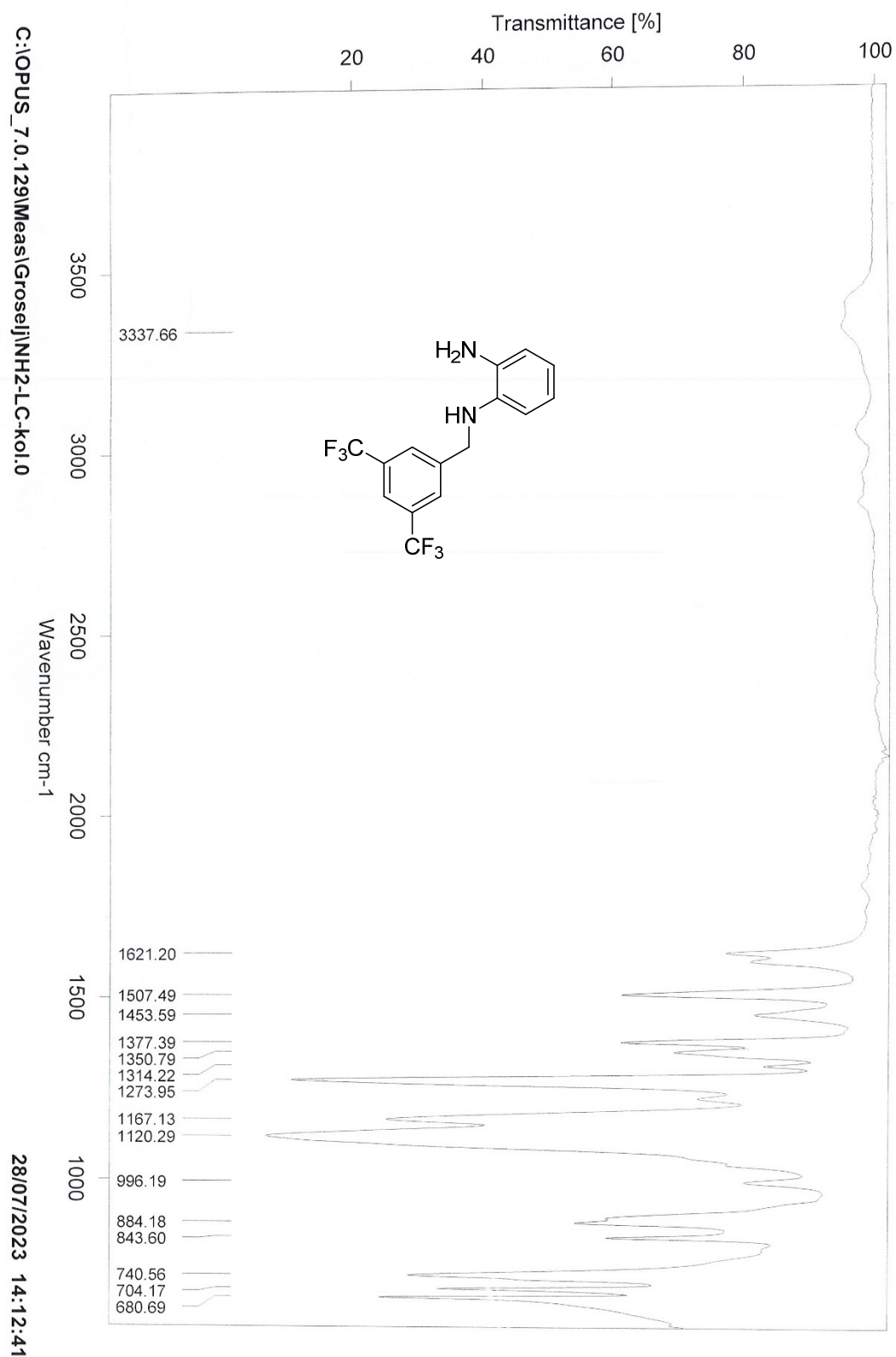


2. IR spectra

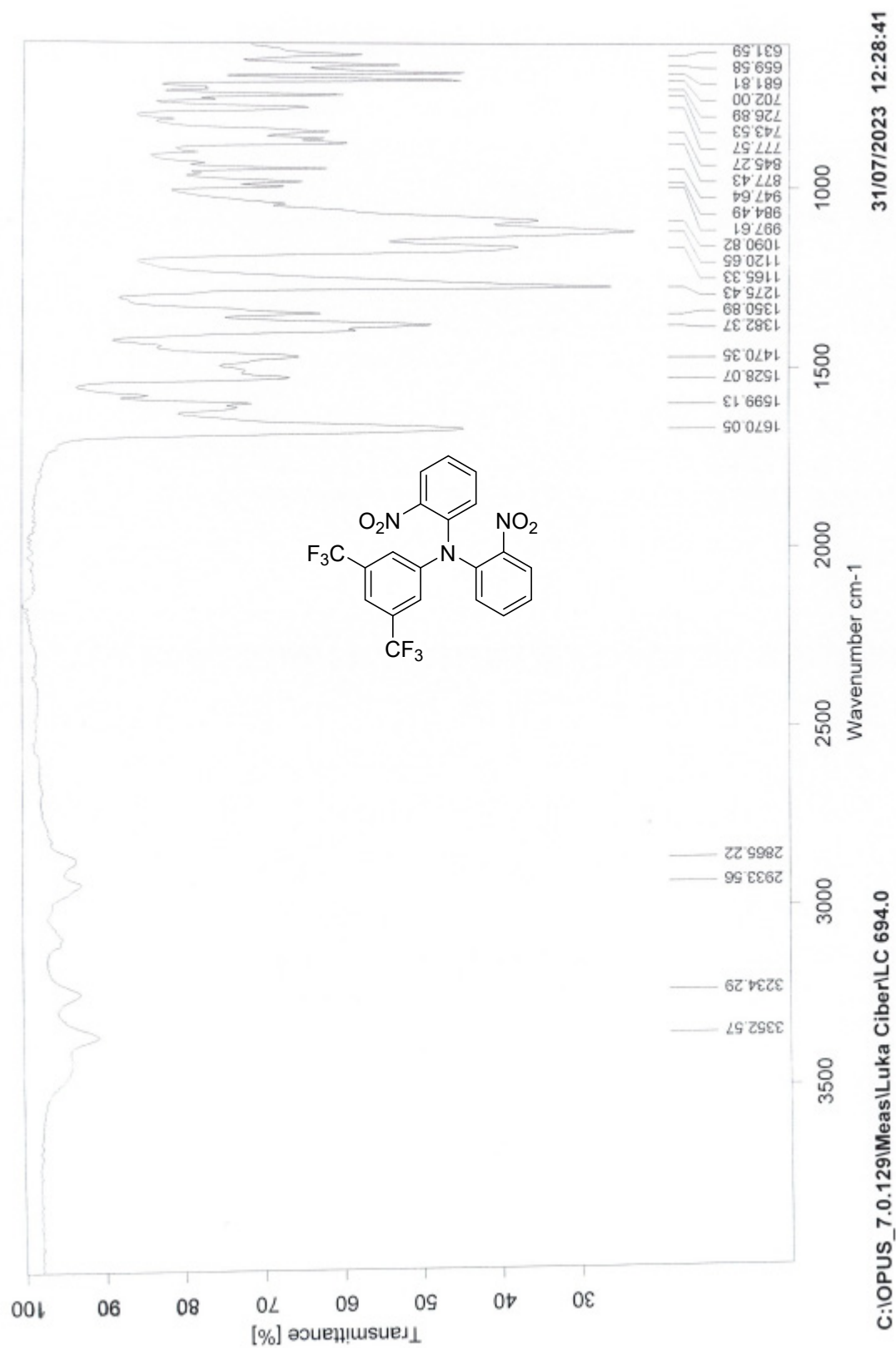
N-(3,5-Bis(trifluoromethyl)benzyl)-2-nitroaniline (3)



***N*¹-(3,5-Bis(trifluoromethyl)benzyl)benzene-1,2-diamine (4a)**

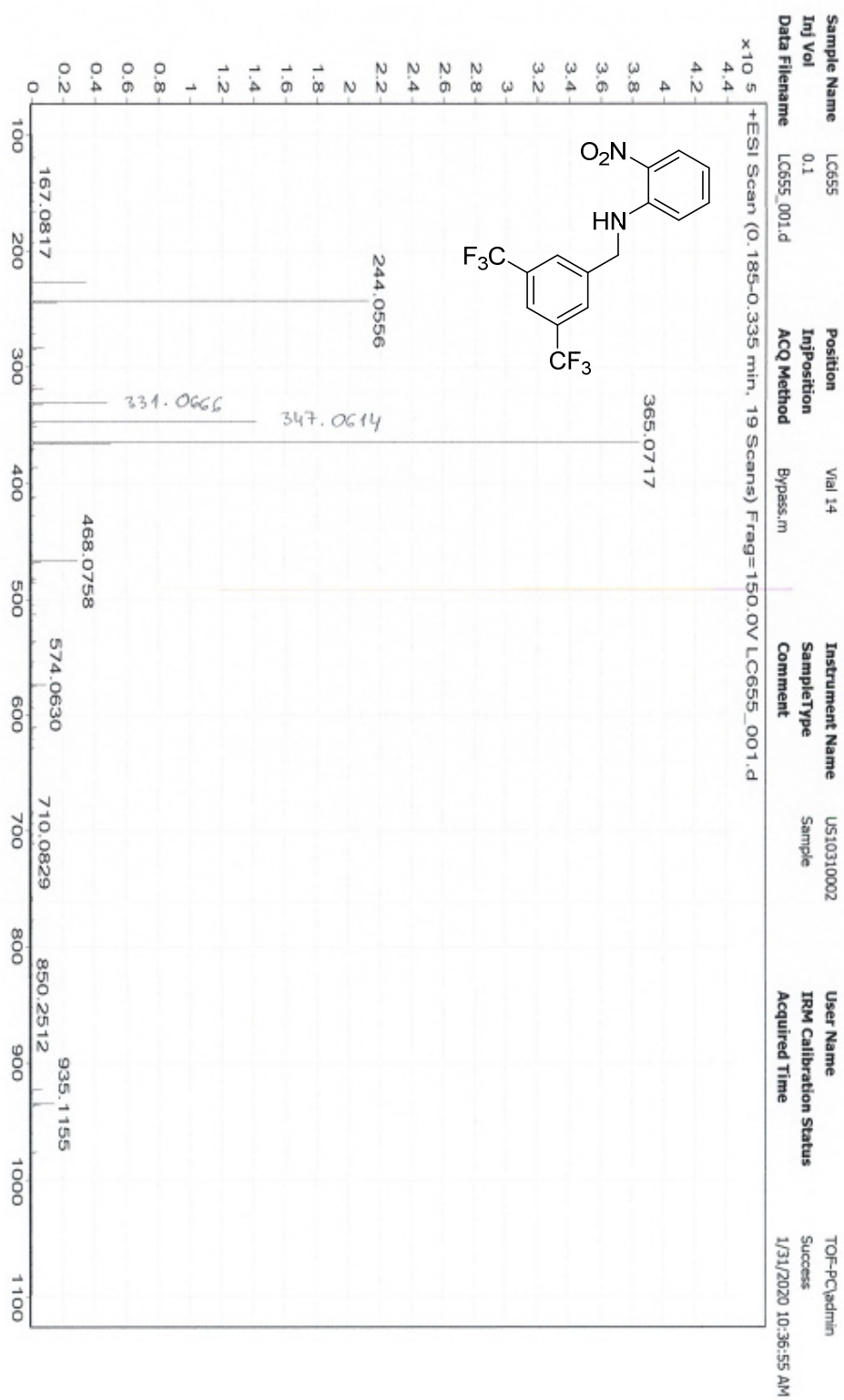


***N,N*-Bis(2-nitrophenyl)-3,5-bis(trifluoromethyl)aniline (7)**

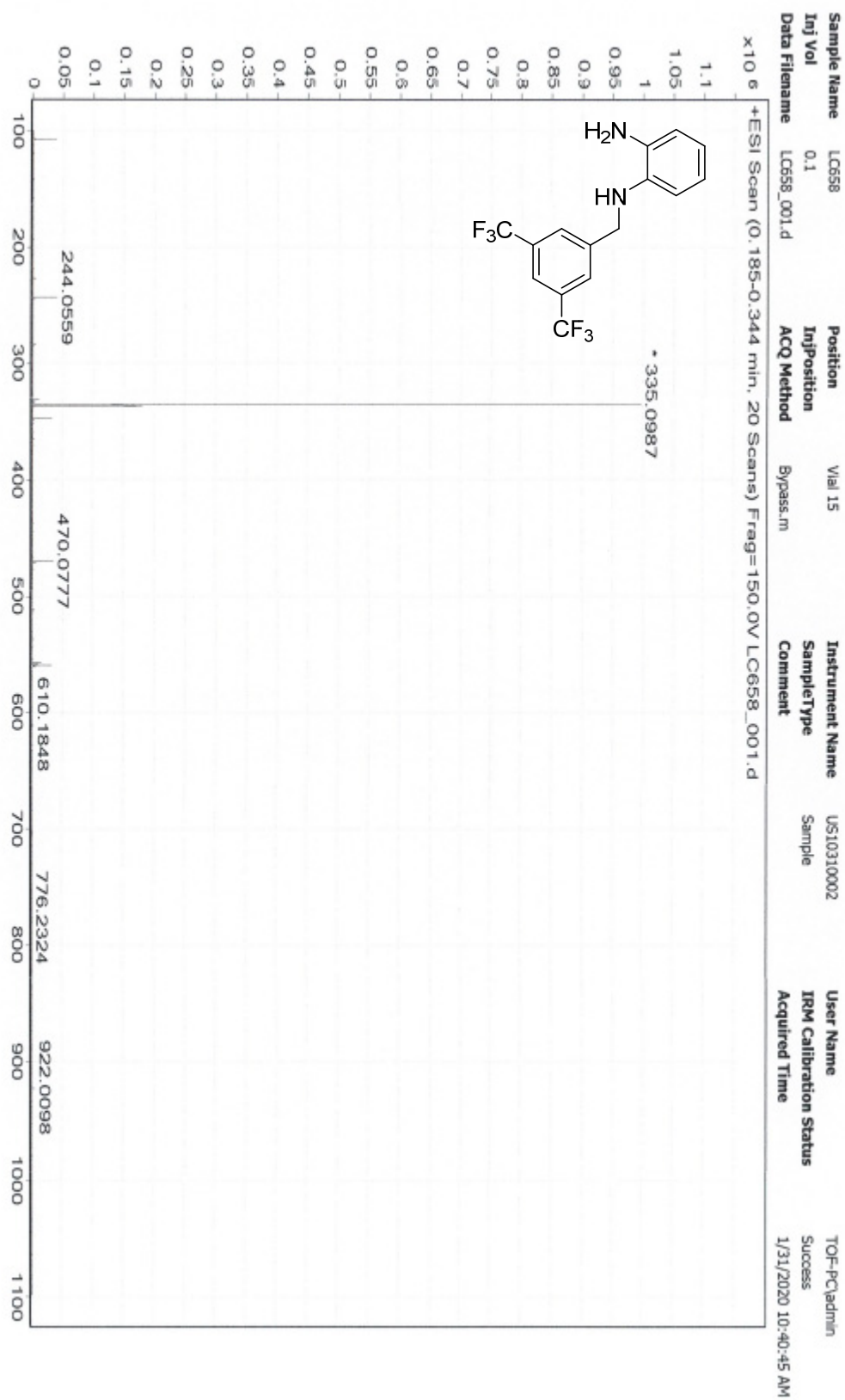


3. MS spectra

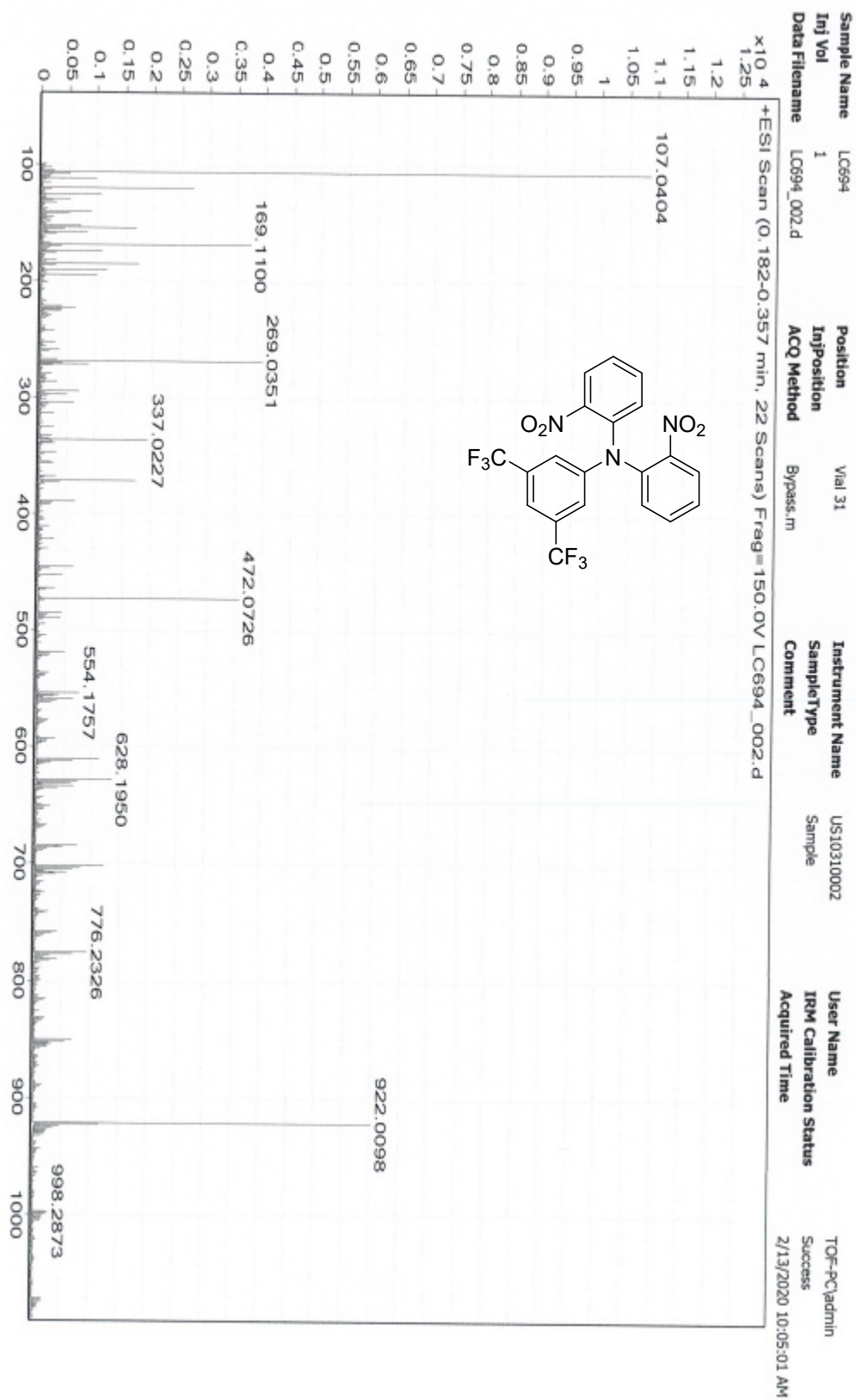
N-(3,5-Bis(trifluoromethyl)benzyl)-2-nitroaniline (3)



***N*¹-(3,5-Bis(trifluoromethyl)benzyl)benzene-1,2-diamine (4a)**



***N,N*-Bis(2-nitrophenyl)-3,5-bis(trifluoromethyl)aniline (7)**



4. Structure determination by X-ray diffraction analysis

Table S1 Crystal data and structure refinement for compound **3**.

Empirical formula	C ₁₅ H ₁₀ F ₆ N ₂ O ₂
Formula weight	364.25
Temperature/K	150(2)
Crystal system	Triclinic
Space group	P-1
<i>a</i> [Å ³]	8.3598(5)
<i>b</i> [Å ³]	8.8785(4)
<i>c</i> [Å ³]	10.0104(5)
<i>α</i> [°]	88.538(4)
<i>β</i> [°]	82.936(4)
<i>γ</i> [°]	83.704(4)
<i>V</i> [Å ³]	732.86(7)
<i>Z</i>	2
ρ_{calc} [g/cm ³]	1.651
μ [mm ⁻¹]	0.162
<i>F</i> (000)	368.0
Crystal size/mm ³	0.5 × 0.3 × 0.2
Radiation	MoK α (λ = 0.71073)
Reflections collected	9527
Independent reflections	3938
<i>R</i> _{int}	0.0260
Data/restraints/parameters	3938/0/227
GOF	1.031
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> ≥ 2σ (<i>I</i>)]	0.0466, 0.1026
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0669, 0.1179
(Δρ) _{max} [e Å ⁻³]	0.48
(Δρ) _{min} [e Å ⁻³]	−0.32

Table S2. Crystal data and structure refinement for compound **7**.

Empirical formula	C ₂₀ H ₁₁ F ₆ N ₃ O ₄
Formula weight	471.32
Temperature/K	150.00(10)
Crystal system	Monoclinic
Space group	P2 ₁ /c
<i>a</i> [Å ³]	17.9155(5)
<i>b</i> [Å ³]	12.6121(3)
<i>c</i> [Å ³]	8.4701(2)
<i>α</i> [°]	90
<i>β</i> [°]	103.197(3)
<i>γ</i> [°]	90
<i>V</i> [Å ³]	1863.29(8)
<i>Z</i>	4
<i>ρ</i> _{calc} [g/cm ³]	1.680
<i>μ</i> [mm ⁻¹]	1.401
<i>F</i> (000)	952.0
Crystal size/mm ³	0.4 × 0.2 × 0.2
Radiation	CuKα (<i>λ</i> = 1.54184)
Reflections collected	13055
Independent reflections	3659
<i>R</i> _{int}	0.0401
Data/restraints/parameters	3659/0/299
GOF	1.037
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> ≥ 2σ (<i>I</i>)]	0.0427, 0.1092
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0505, 0.1160
(Δ <i>ρ</i>) _{max} [e Å ⁻³]	0.34
(Δ <i>ρ</i>) _{min} [e Å ⁻³]	−0.47