**SUPPLEMENTARY MATERIAL for**

# *1-Fluoro-2,5-dimethoxy-4-nitrobenzene*

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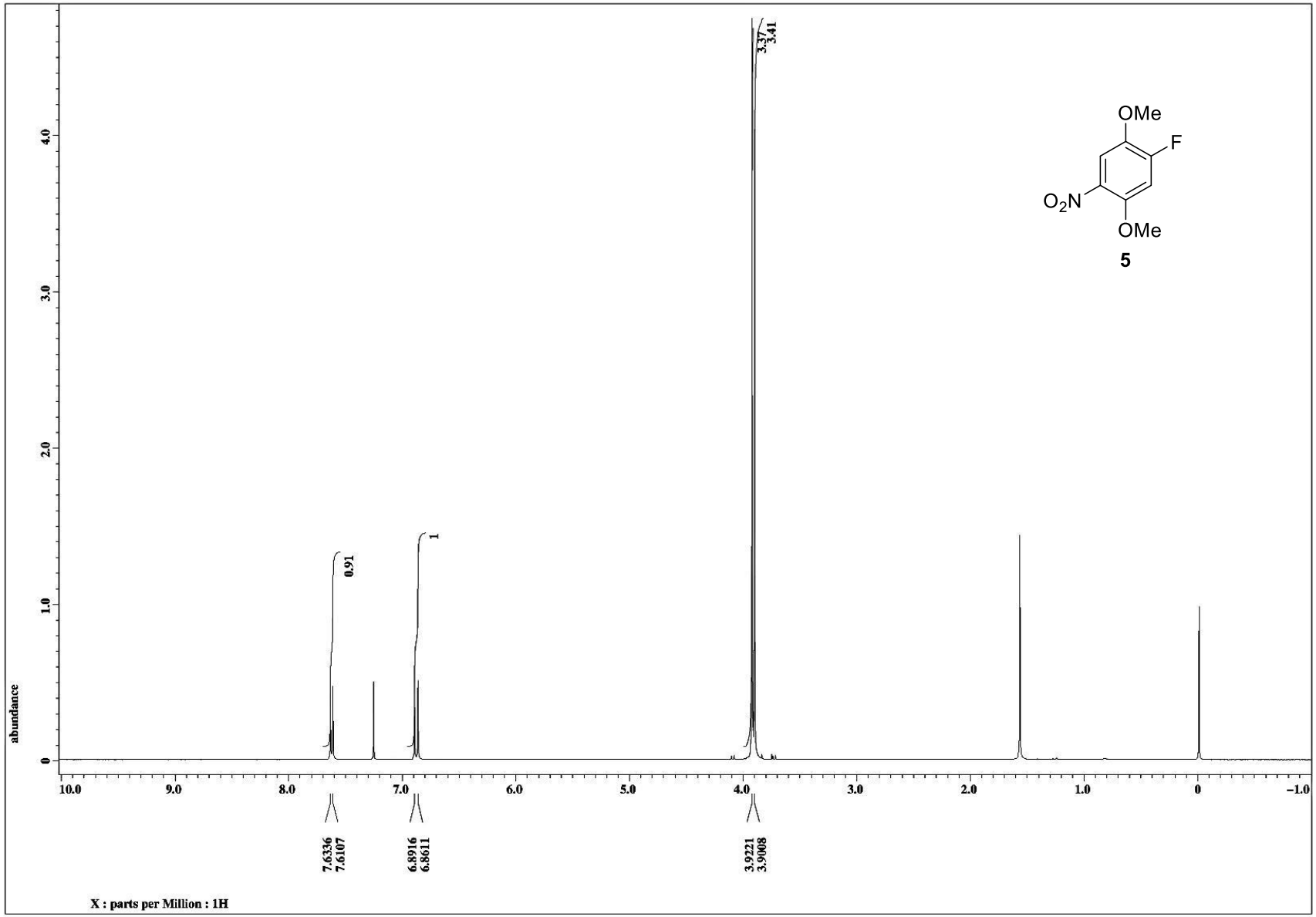
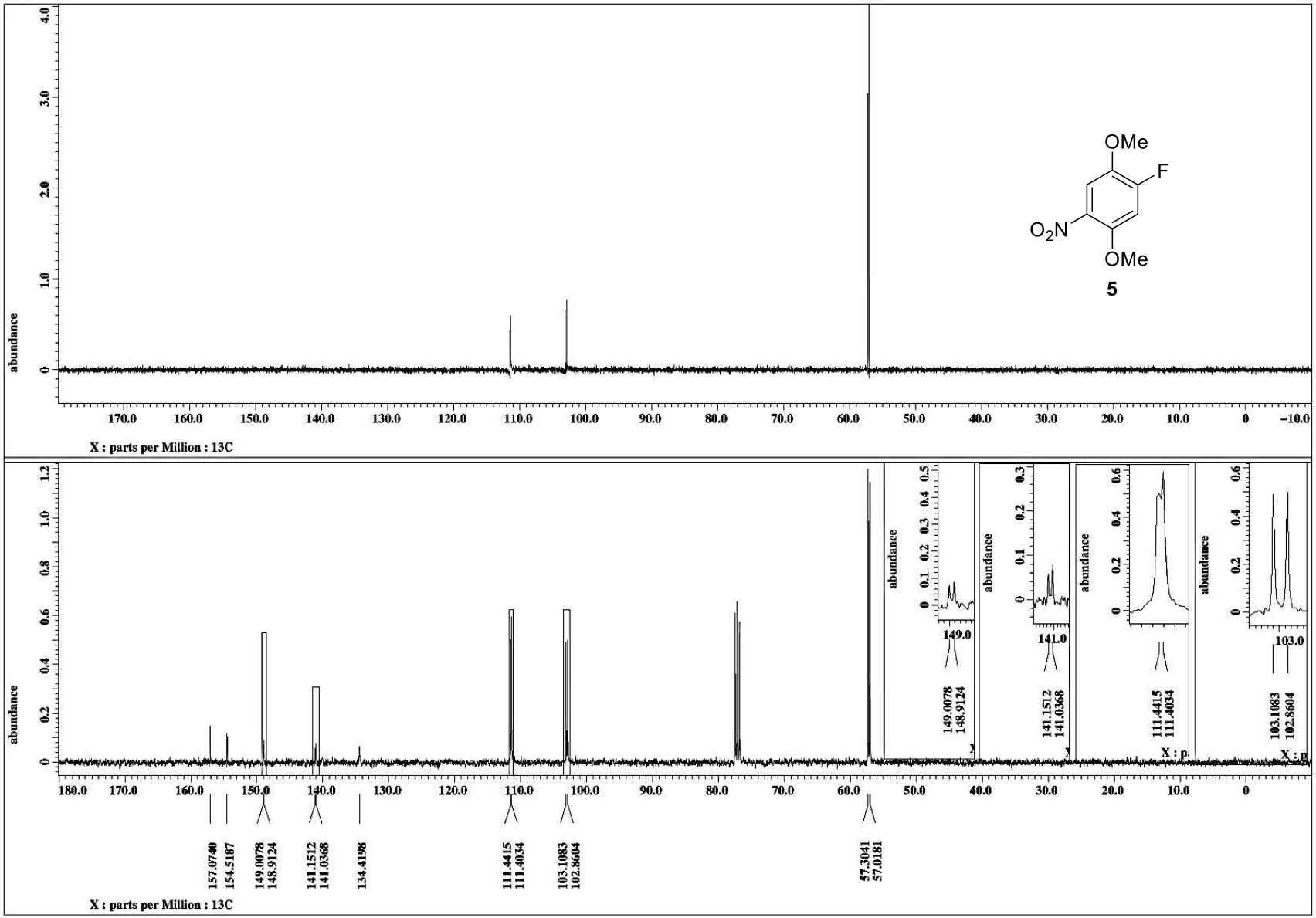
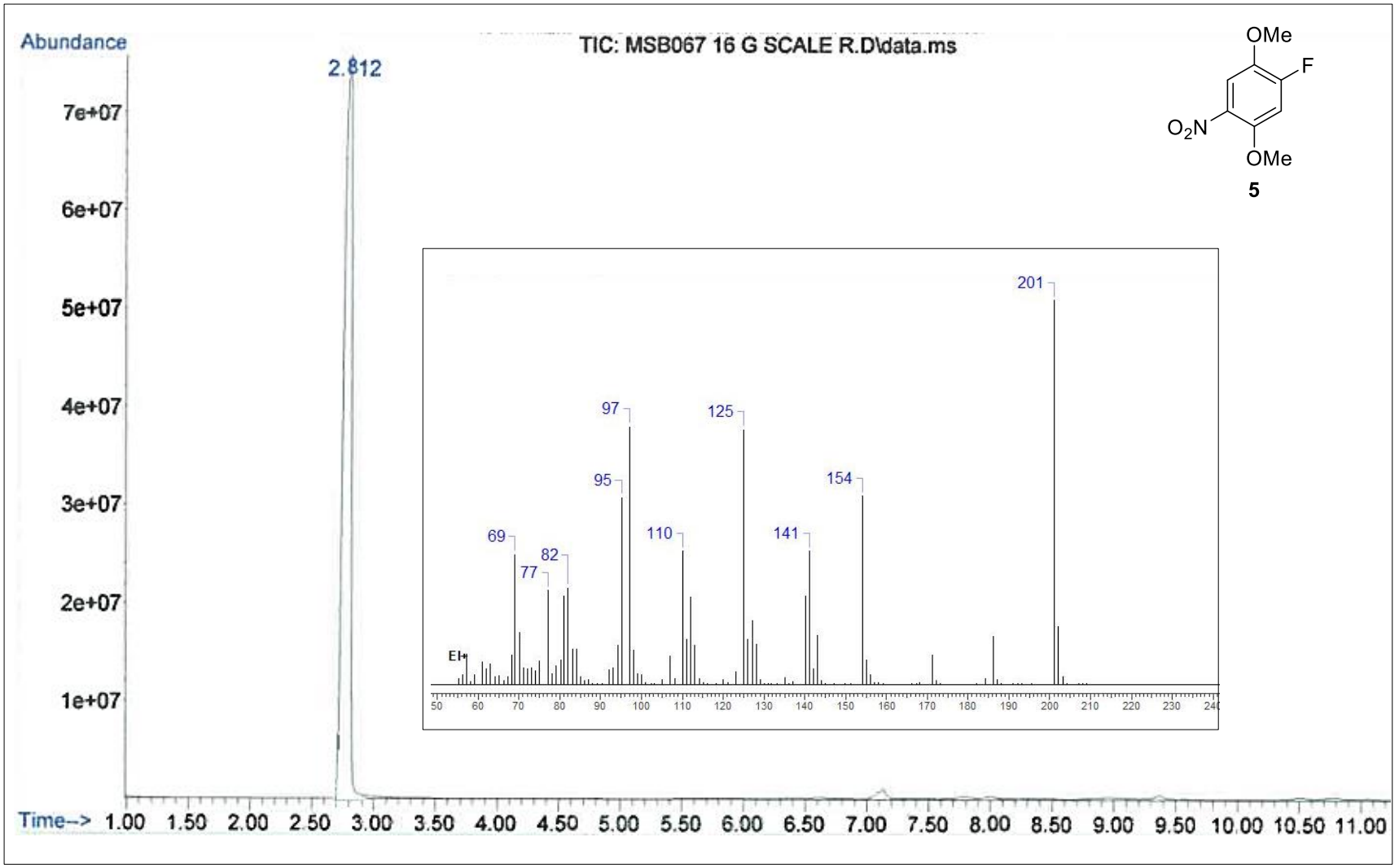
**$^{1}$H NMR (400 MHz) of 1-fluoro-2,5-dimethoxy-4-nitrobenzene in $CDCl_3$ (5)**



**$^{13}$C NMR (100 MHz) of 1-fluoro-2,5-dimethoxy-4-nitrobenzene in $CDCl_3$ (5)**



**GC-MS chromatogram with EI-MS inset spectrum of 1-fluoro-2,5-dimethoxy-4-nitrobenzene (5)**



## Crystal data and structure refinement for 1-fluoro-2,5-dimethoxy-4-nitrobenzene (5)

| | | |
|---|---|---|
| Identification code | ms_6_1 | |
| Empirical formula | $C_8H_8F\,NO_4$ | |
| Formula weight | 201.15 | |
| Temperature | 298.4(4) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | Cc | |
| Unit cell dimensions | a = 7.9538(6) Å | α = 90°. |
| | b = 13.5379(11) Å | β = 89.983(6)°. |
| | c = 16.0790(13) Å | γ = 90°. |
| Volume | 1731.4(2) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.543 $Mg/m^3$ | |
| Absorption coefficient | 0.138 $mm^{-1}$ | |
| F(000) | 832 | |
| Crystal size | 0.50 x 0.40 x 0.20 $mm^3$ | |
| Theta range for data collection | 3.905 to 29.220°. | |
| Index ranges | -10<=h<=9, -18<=k<=17, -20<=l<=20 | |
| Reflections collected | 6792 | |
| Independent reflections | 3164 [R(int) = 0.0214] | |
| Completeness to theta = 25.242° | 99.6 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 1.00000 and 0.92979 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3164 / 2 / 258 | |
| Goodness-of-fit on $F^2$ | 1.059 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0755, wR2 = 0.1838 | |
| R indices (all data) | R1 = 0.0903, wR2 = 0.2067 | |
| Absolute structure parameter | 1(2) | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.725 and -0.227 $e.Å^{-3}$ | |