

Electronic Supporting Information for

Dissecting the complex recognition interfaces of highly potent tetrazole- and pyrrole-based anion binders

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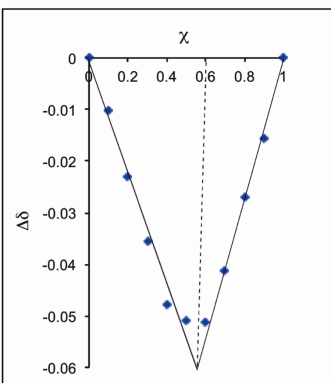
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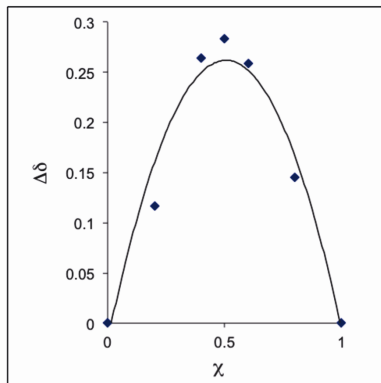
Section 1: Supplementary NMR titration data

Job plots were recorded in CD₃CN at 500 MHz with a representative amide host (**14**) and the ester-derived host **11**. Chloride, an alternate halide (Br⁻), and a representative oxyanion (HSO₄⁻) were employed as guests. Data for host **14** is shown in a) guest = chloride, b) guest = bromide and c) guest = hydrogensulfate. Data for host **11** is shown in d) guest = chloride, e) guest = bromide and f) guest = hydrogensulfate.

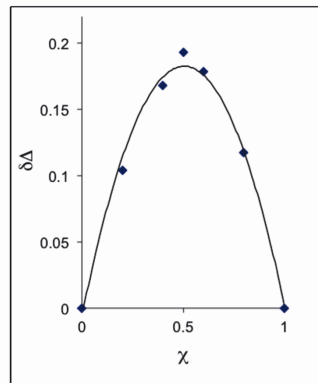
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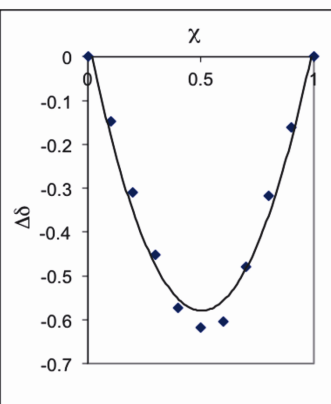
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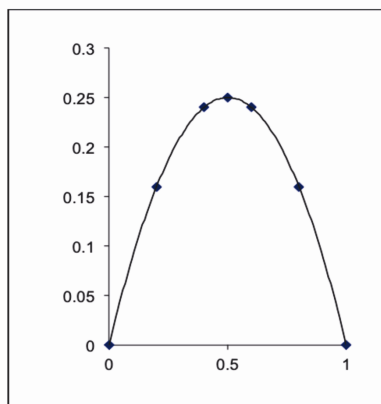
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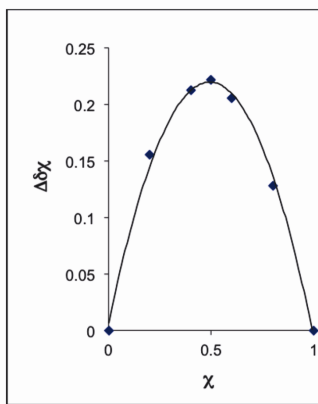
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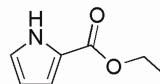
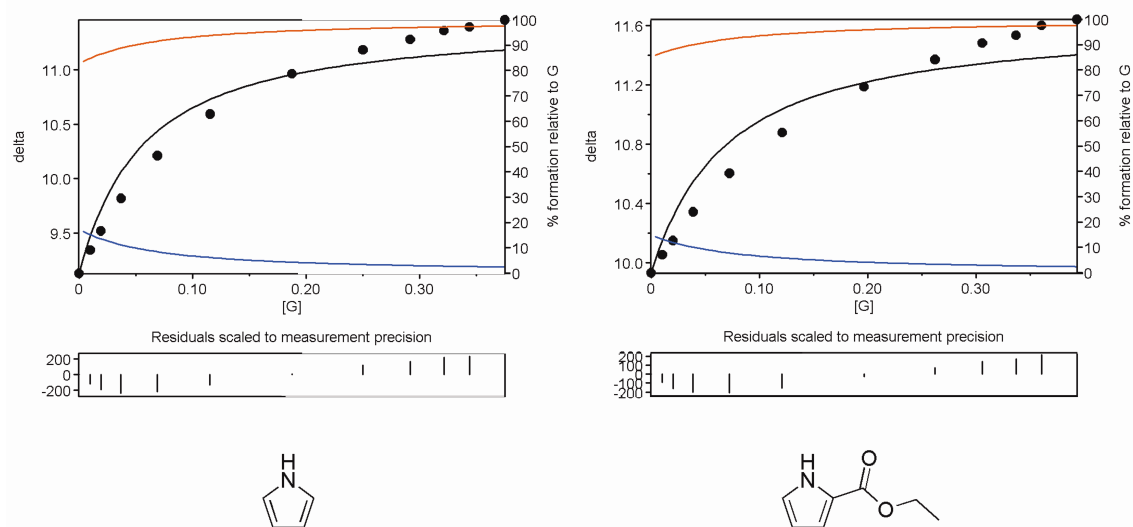


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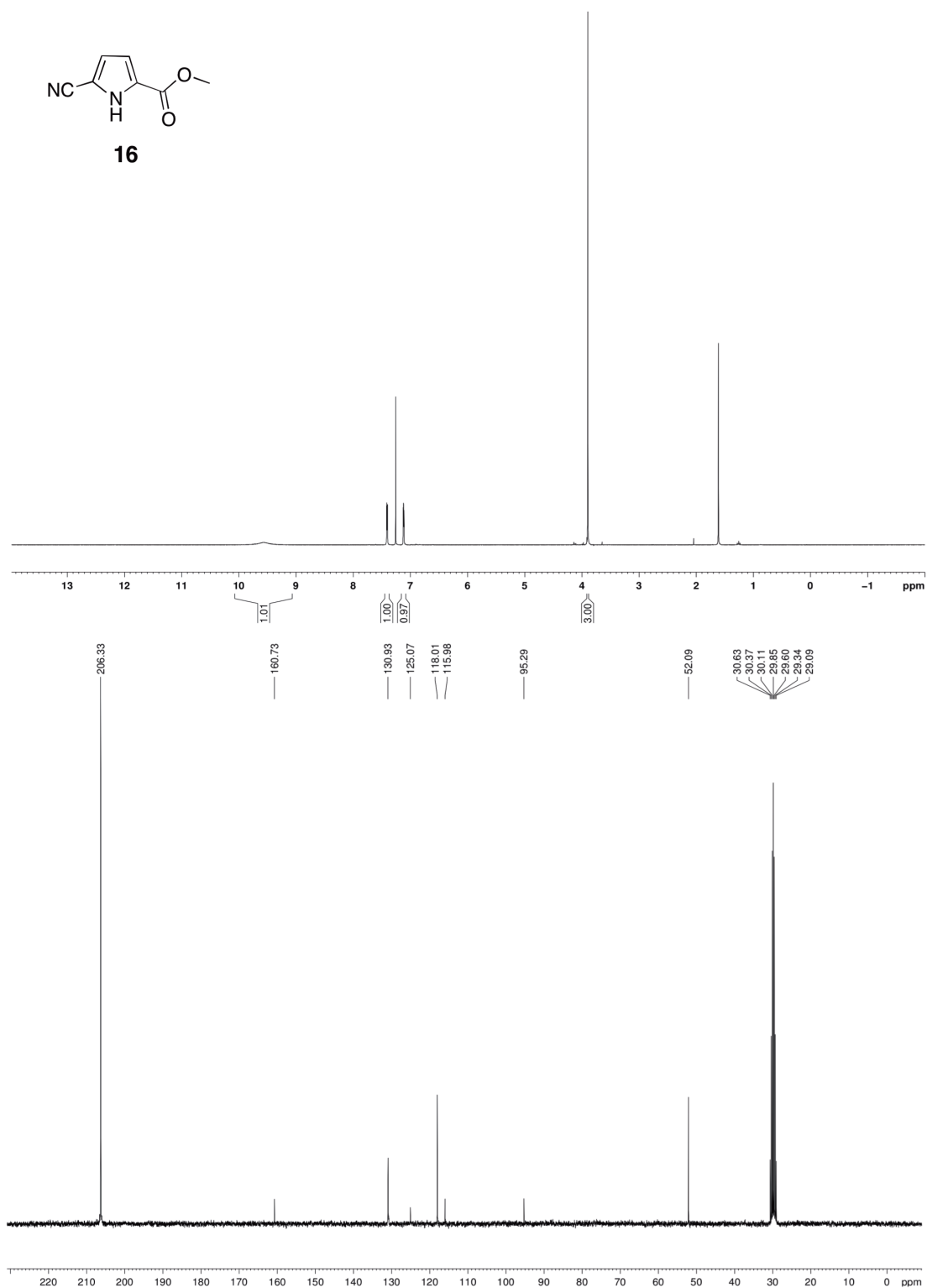
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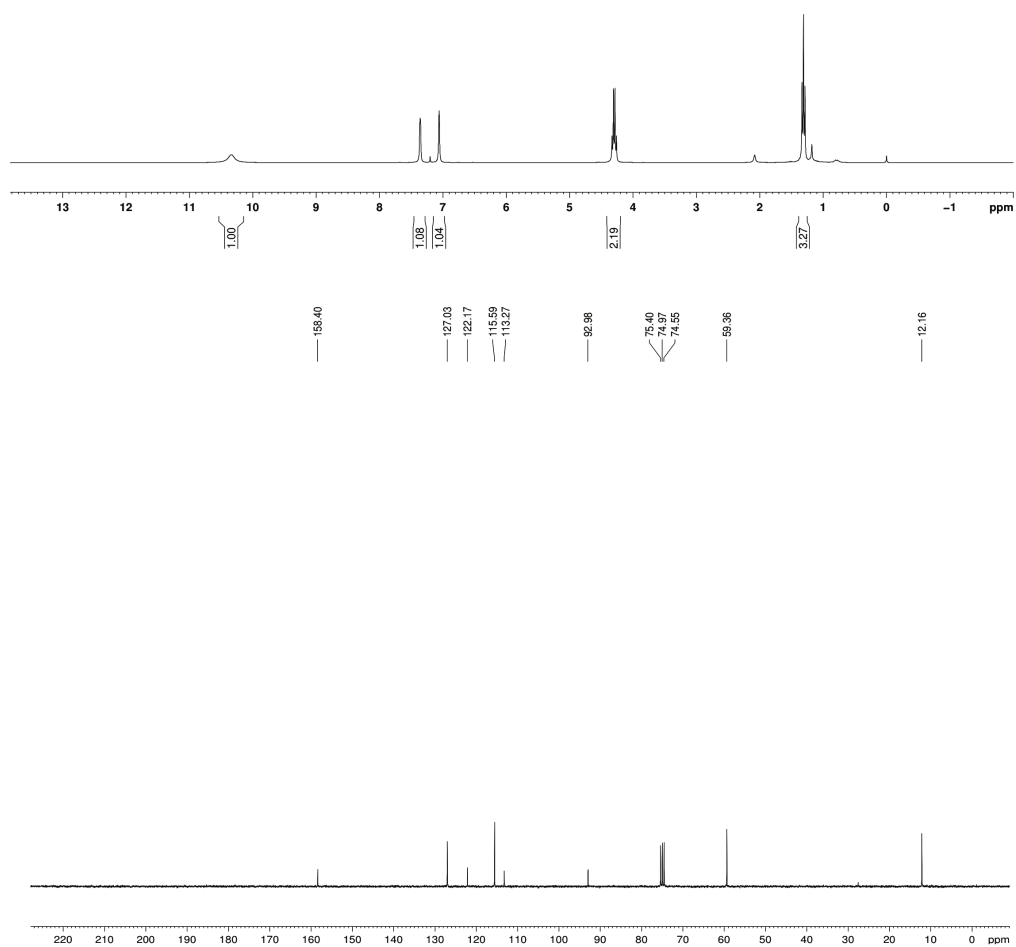
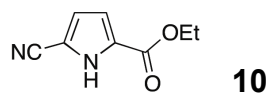


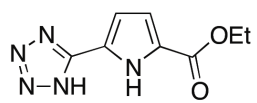


Binding curves for pyrrole and ethyl-2-pyrrole carboxylate titrated with tetrabutylammonium chloride. Data was acquired through ^1H NMR titrations in CD_3CN . Host solutions (~ 10 mM) were used to make guest solutions (~ 500 mM) to ensure host concentrations were kept constant. Black points = experimental chemical shift data for pyrrole NH. Black lines = 1:1 binding isotherm. **Truth in advertising:** The systematic deviations of fitted lines from experimental points show that the 1:1 binding isotherm is close, but not strictly correct for these systems. The use of 1:2 and/or 2:1 binding isotherms (and attempts to collect this data at different concentrations of pyrrole) did not improve the quality of the fits. We assume deviations arising from changing ionic strength and/or an unanticipated self-association are behind the non-ideal behavior. The simplicity of these systems (monotopic NH donors mated with a simple, spherical H-bond acceptor) lead us to stick with the 1:1 fits as the best possible method for getting an estimate of K_{11} for these systems. The fitted K_{11} value for pyrrole- Cl^- is 200 M^{-1} and for the ester is 150 M^{-1} . While the shapes of the curves show that these values *must* be overestimates of the true association constants, we conservatively use the relatively small deviation of fitted data from experimental data to estimate a binding constant of $\geq 10\text{ M}^{-1}$ for each system. In any case, these values are not central to the conclusions of this paper.

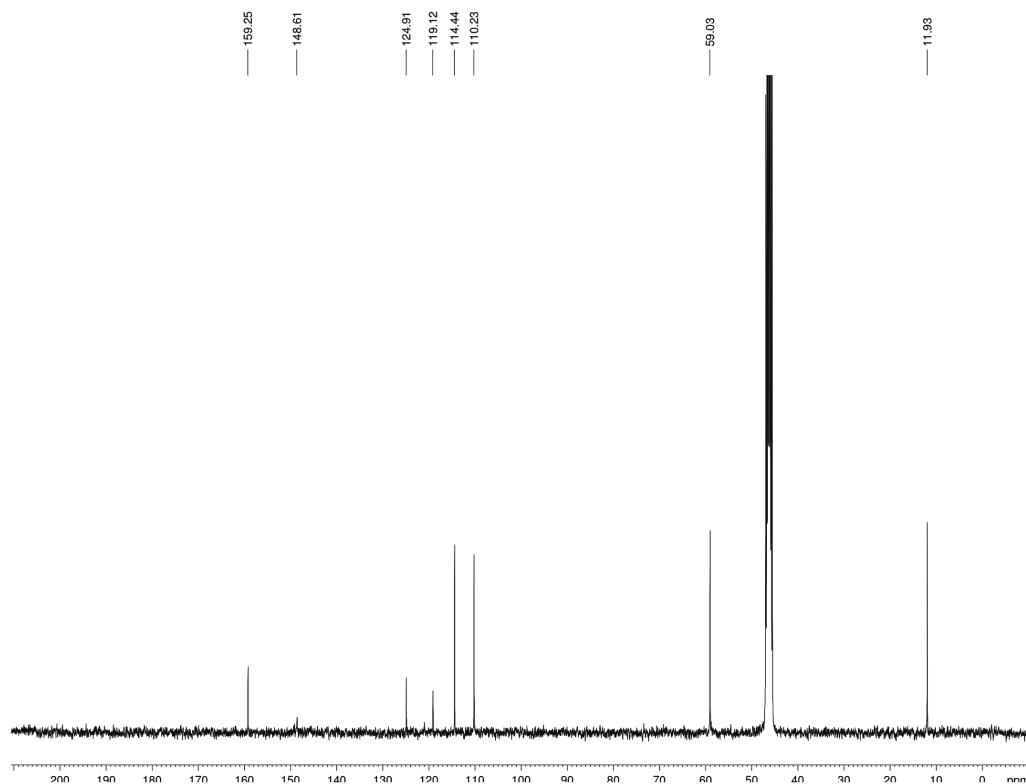
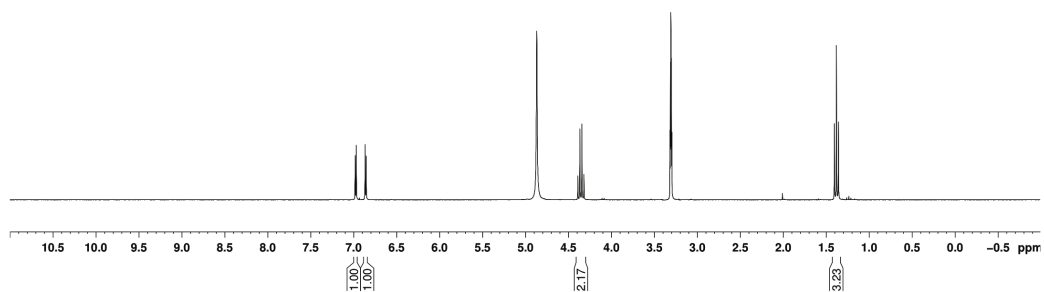
Section 2. ^1H and ^{13}C NMR spectra of all newly synthesized compounds

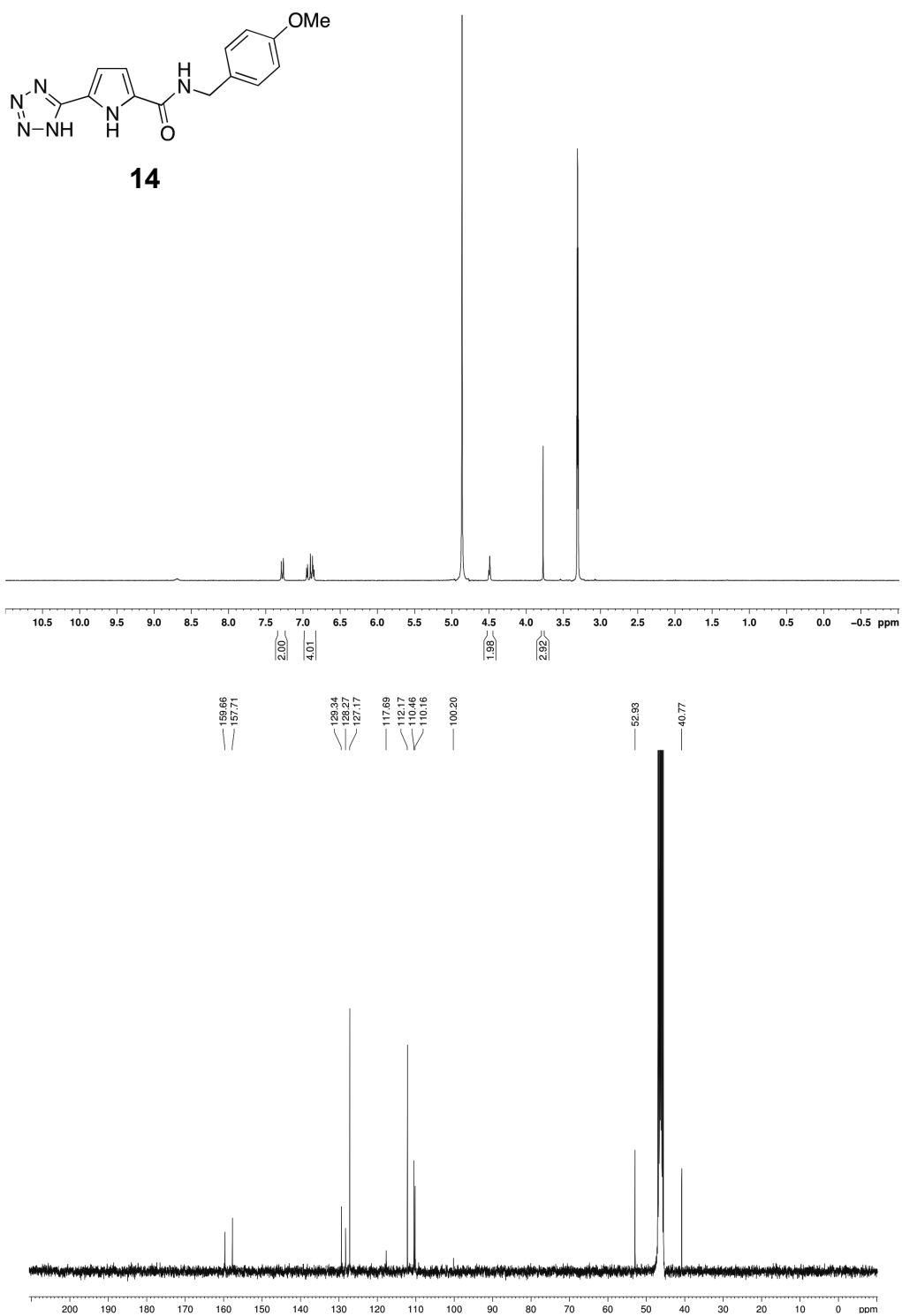


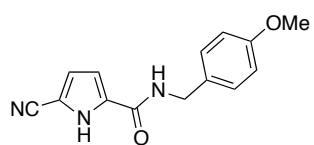




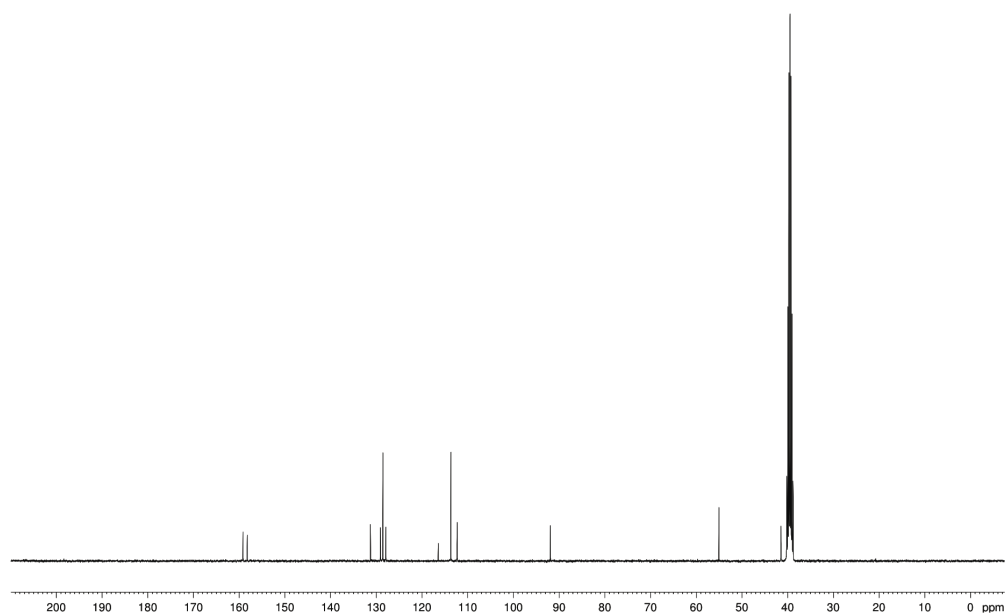
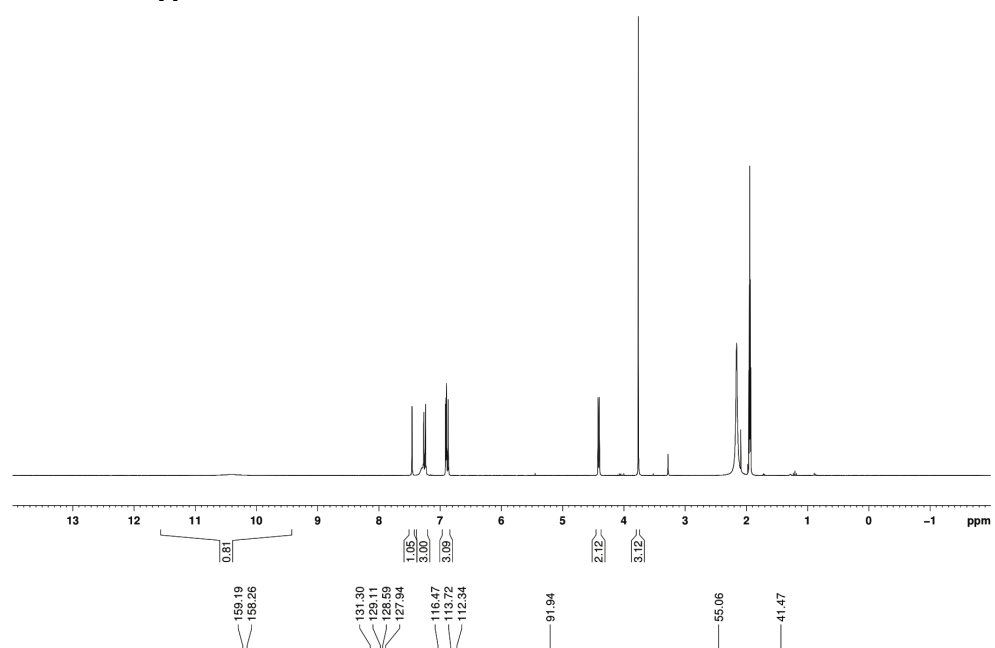
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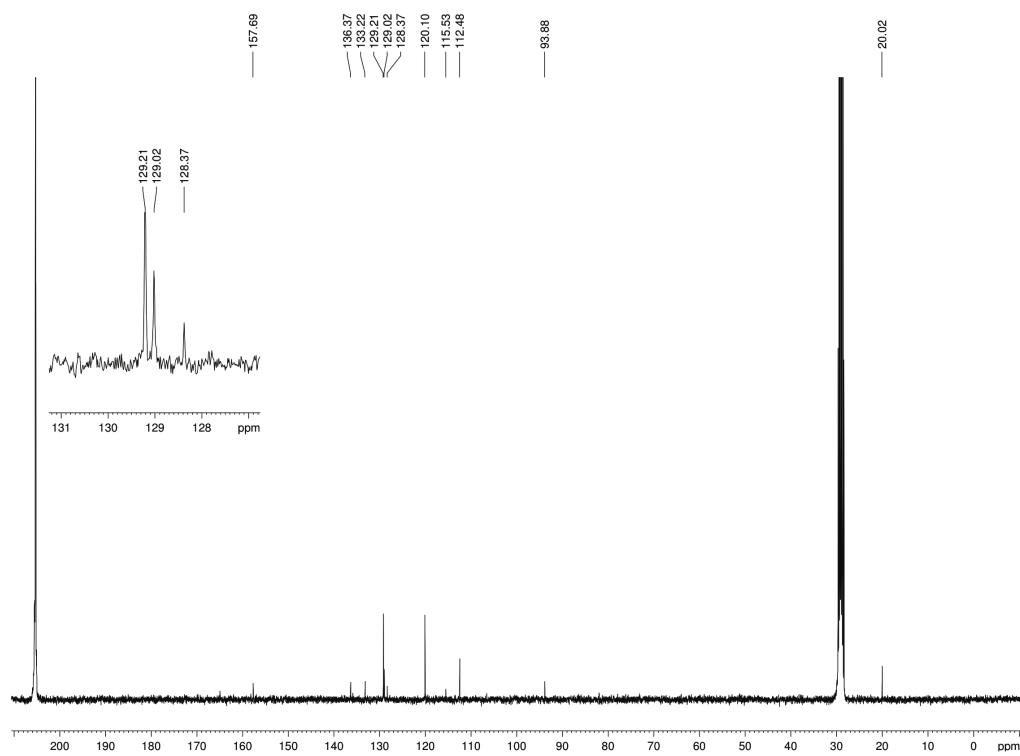
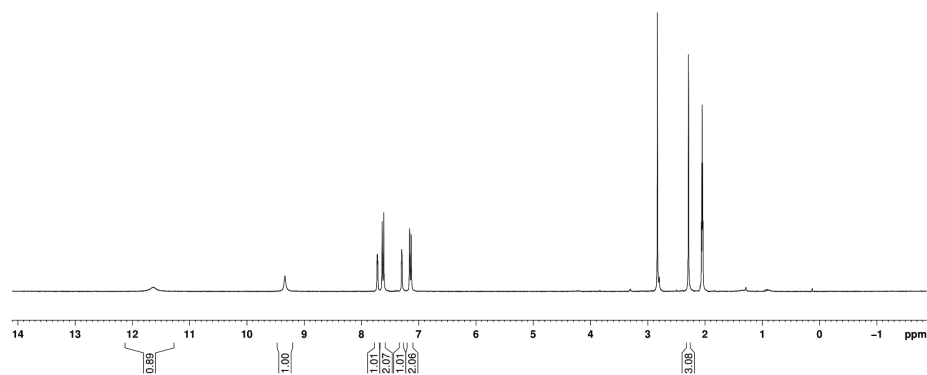
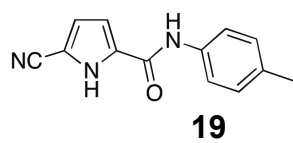


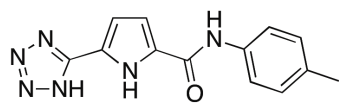




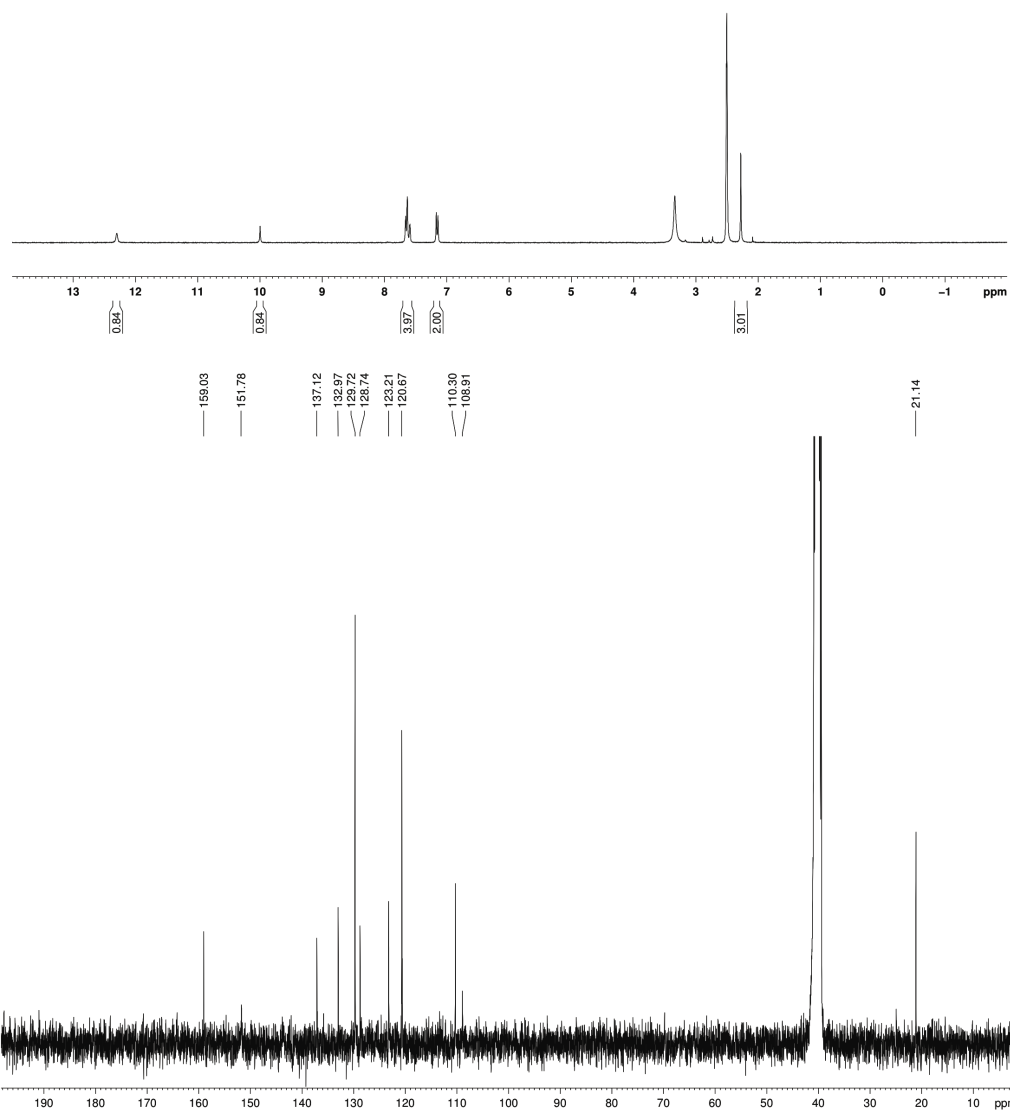
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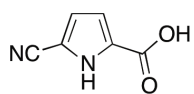






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