ARTICLE

Electronic Supporting Information for:

New Binding Modes for CSe: Coinage Metal Coordination to a Tungsten Selenocarbonyl Complex

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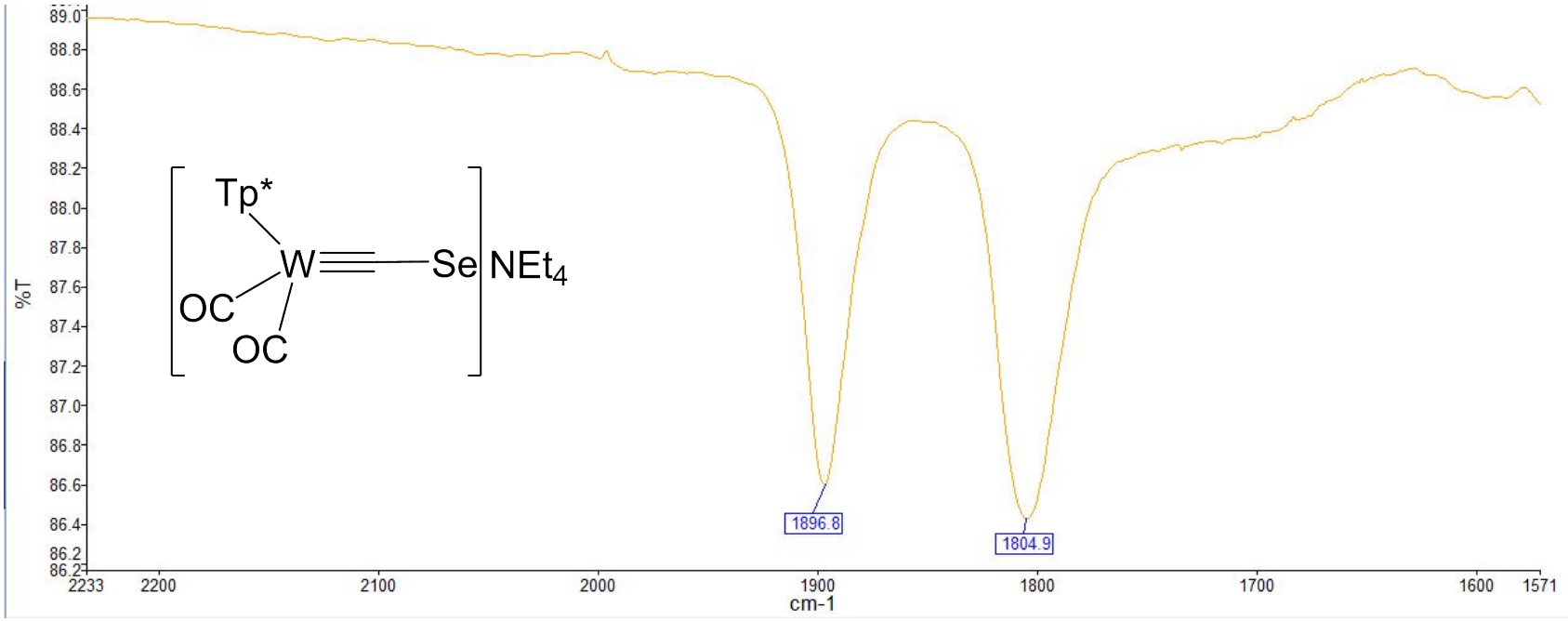
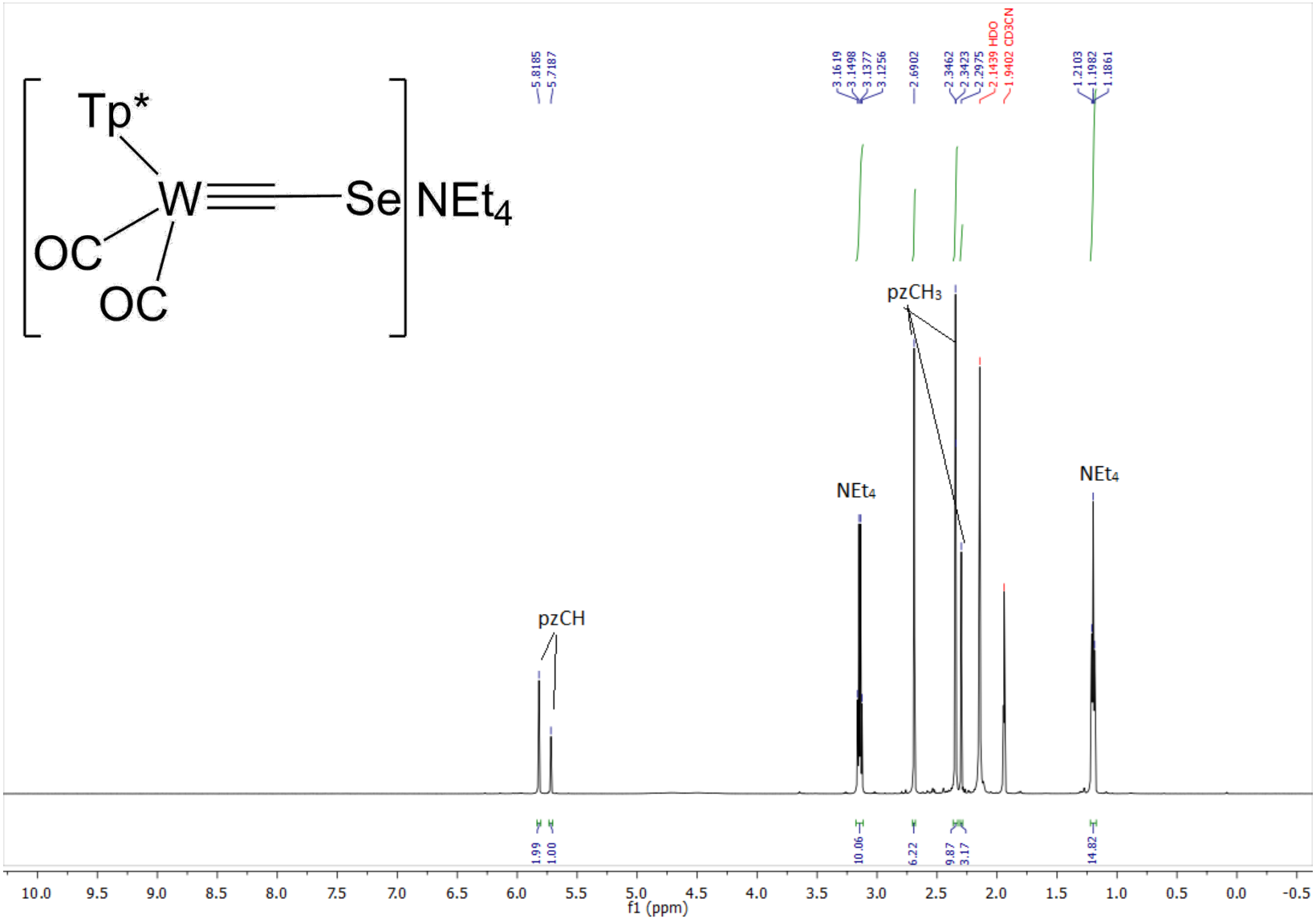
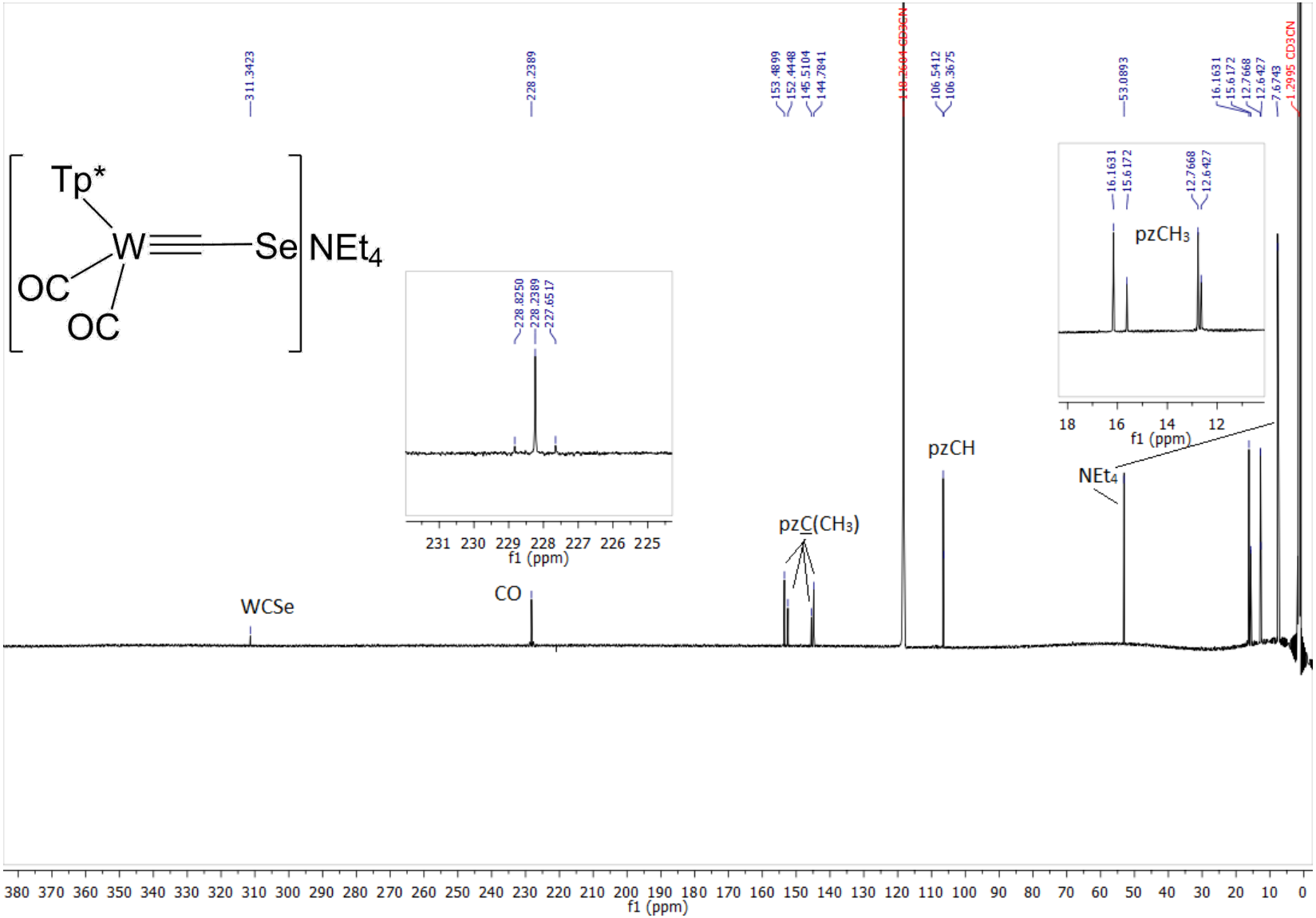
CCDC 1919338 – 1919344 contain the supplementary crystallographic data for this paper, and are available free of charge from The Cambridge Crystallographic Data Centre.



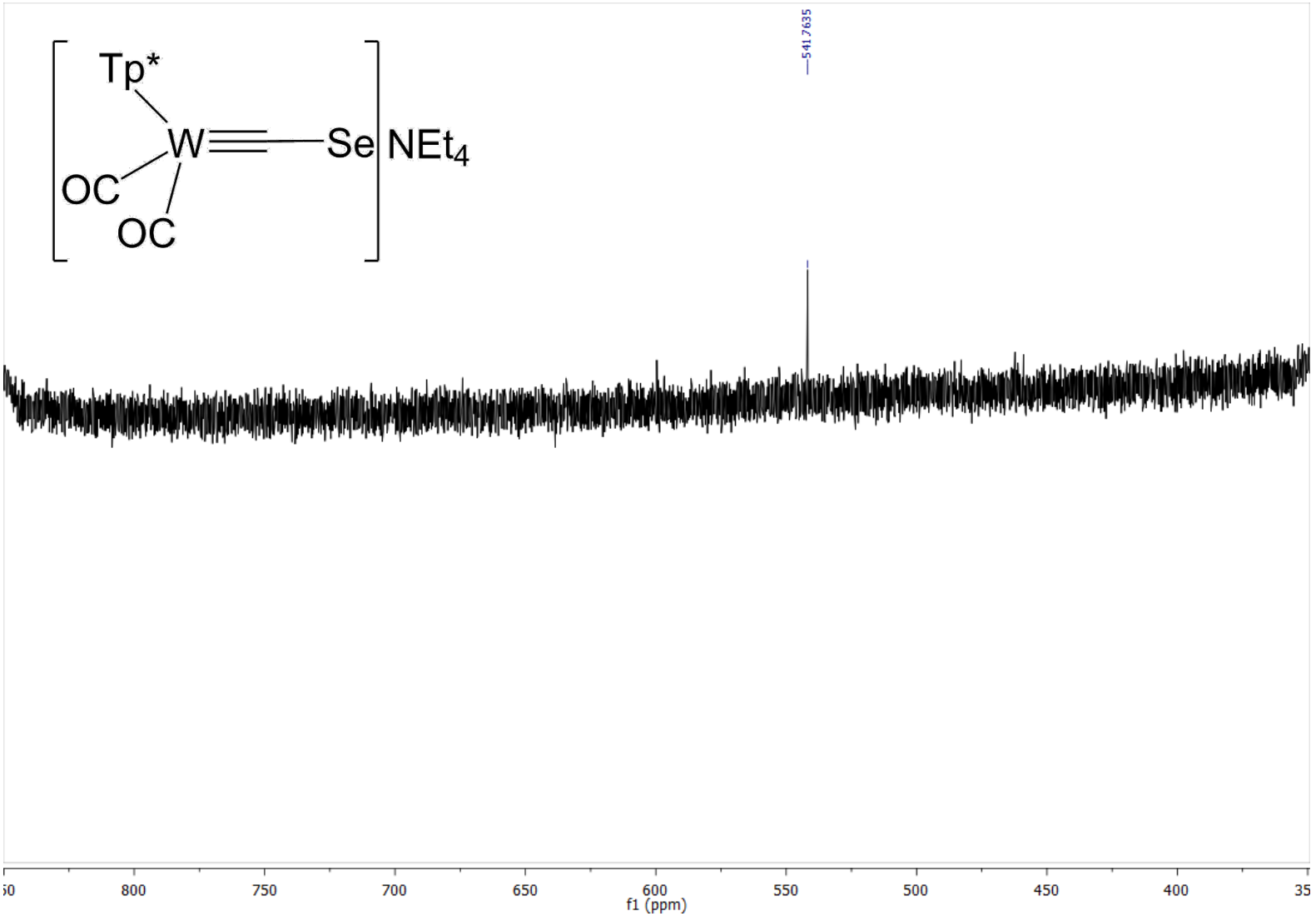
IR (CH_2Cl_2) for [W(≡CSe)$(CO)_2$(Tp*)]NEt_4 ([**2**]NEt_4).



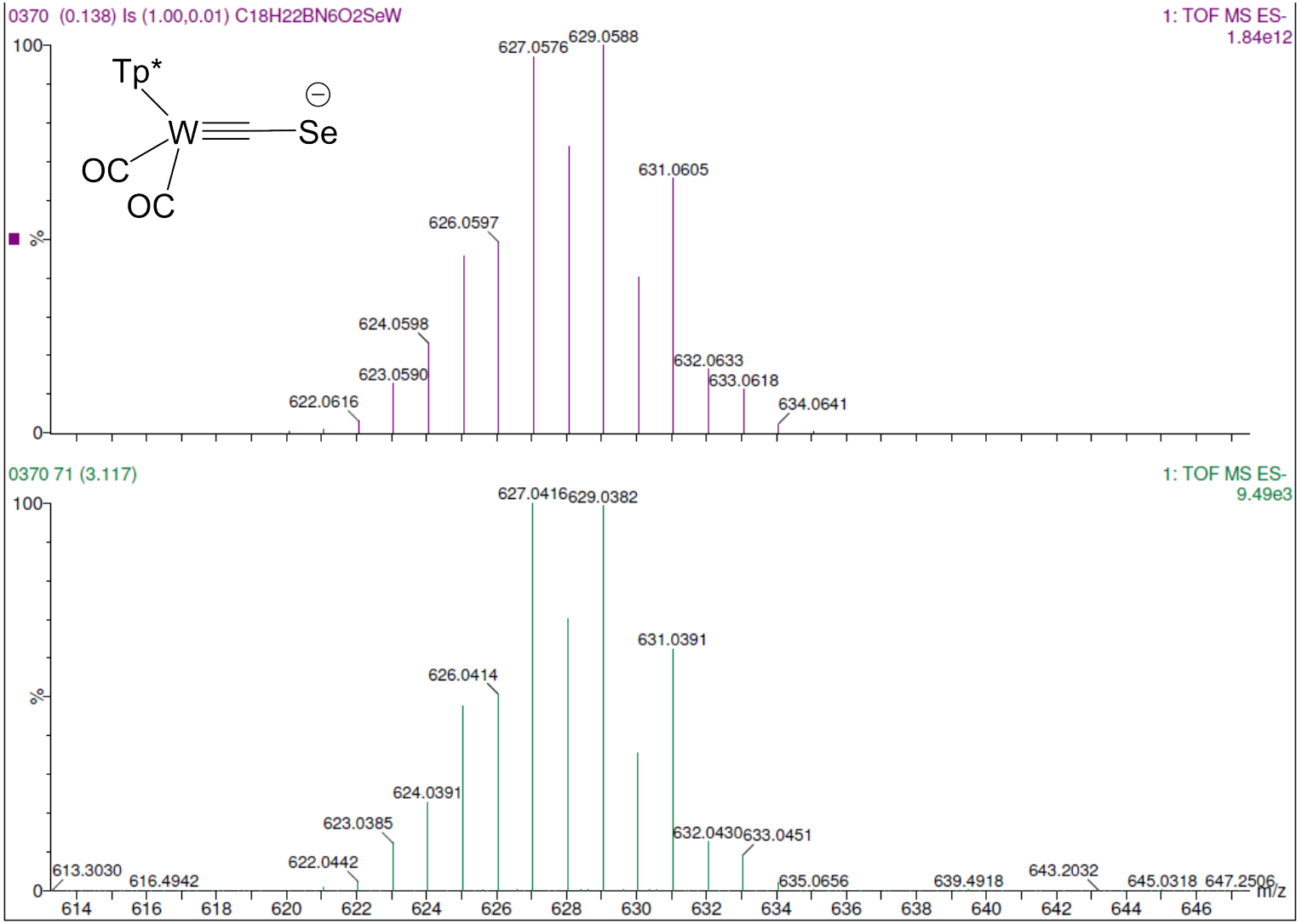
^{1}H NMR (600 MHz, CD_3CN, 298 K, δ) for [W(≡CSe)$(CO)_2$(Tp*)]NEt_4 ([**2**]NEt_4).



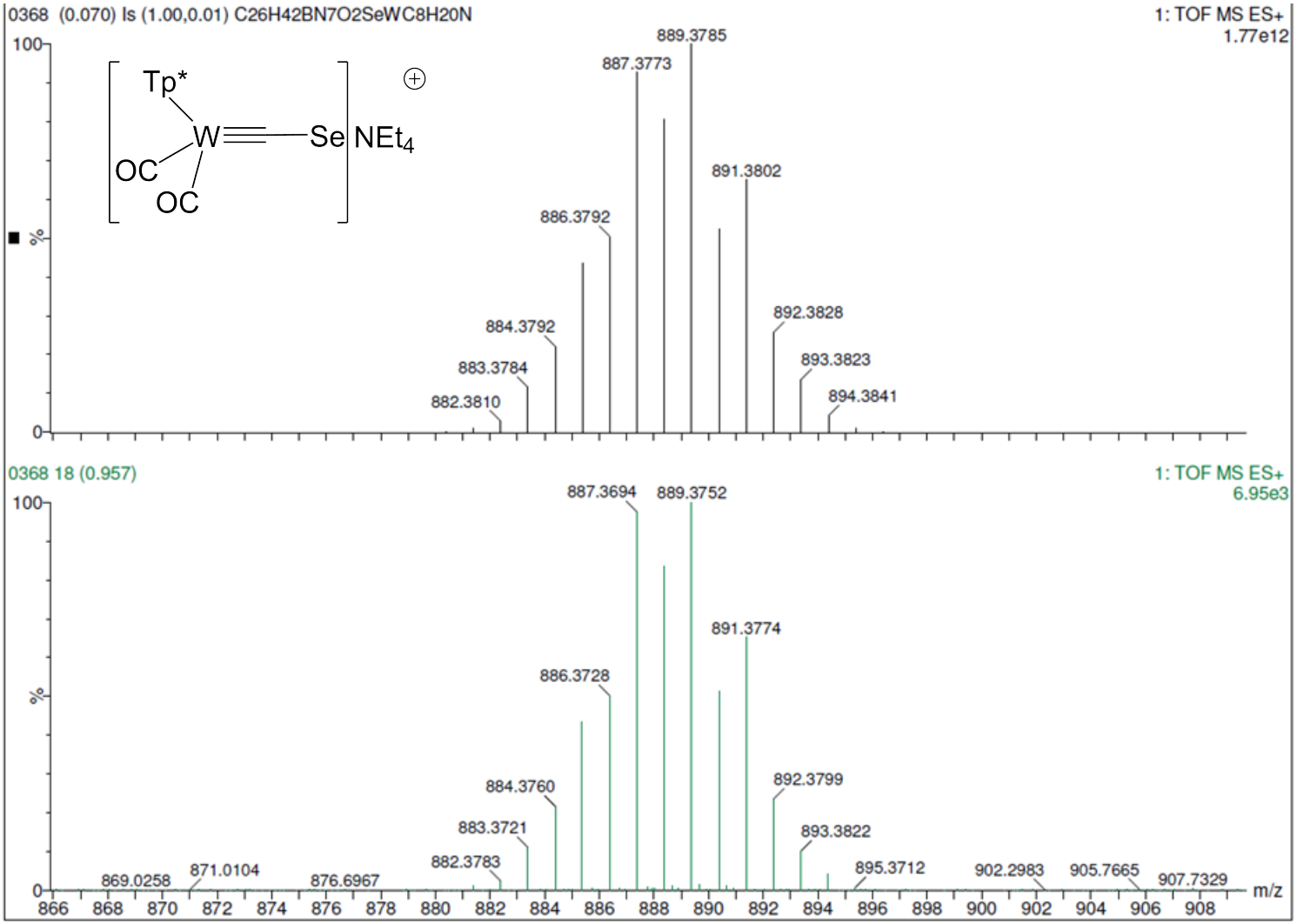
$^{13}C\{^{1}H\}$ NMR (151 MHz, CD_3CN, 298 K, δ) for $[W(\equiv CSe)(CO)_2(Tp^*)]NEt_4$ ([**2**]NEt_4).



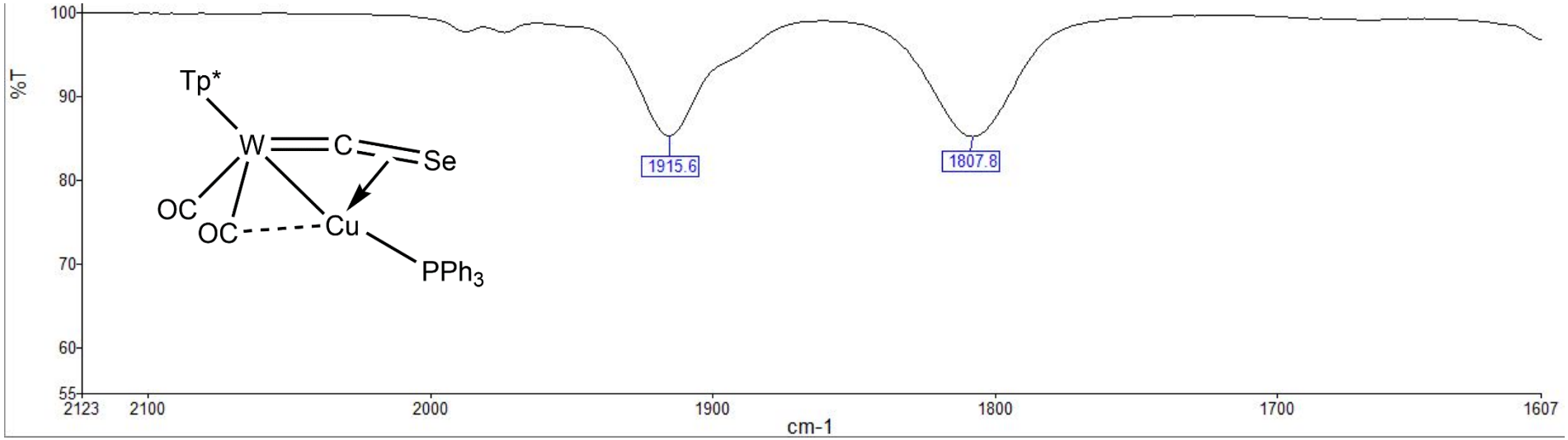
^{77}Se NMR (76 MHz, CD_3CN, 298 K, δ) for $[W(\equiv CSe)(CO)_2(Tp^*)]NEt_4$ ([**2**]NEt_4).



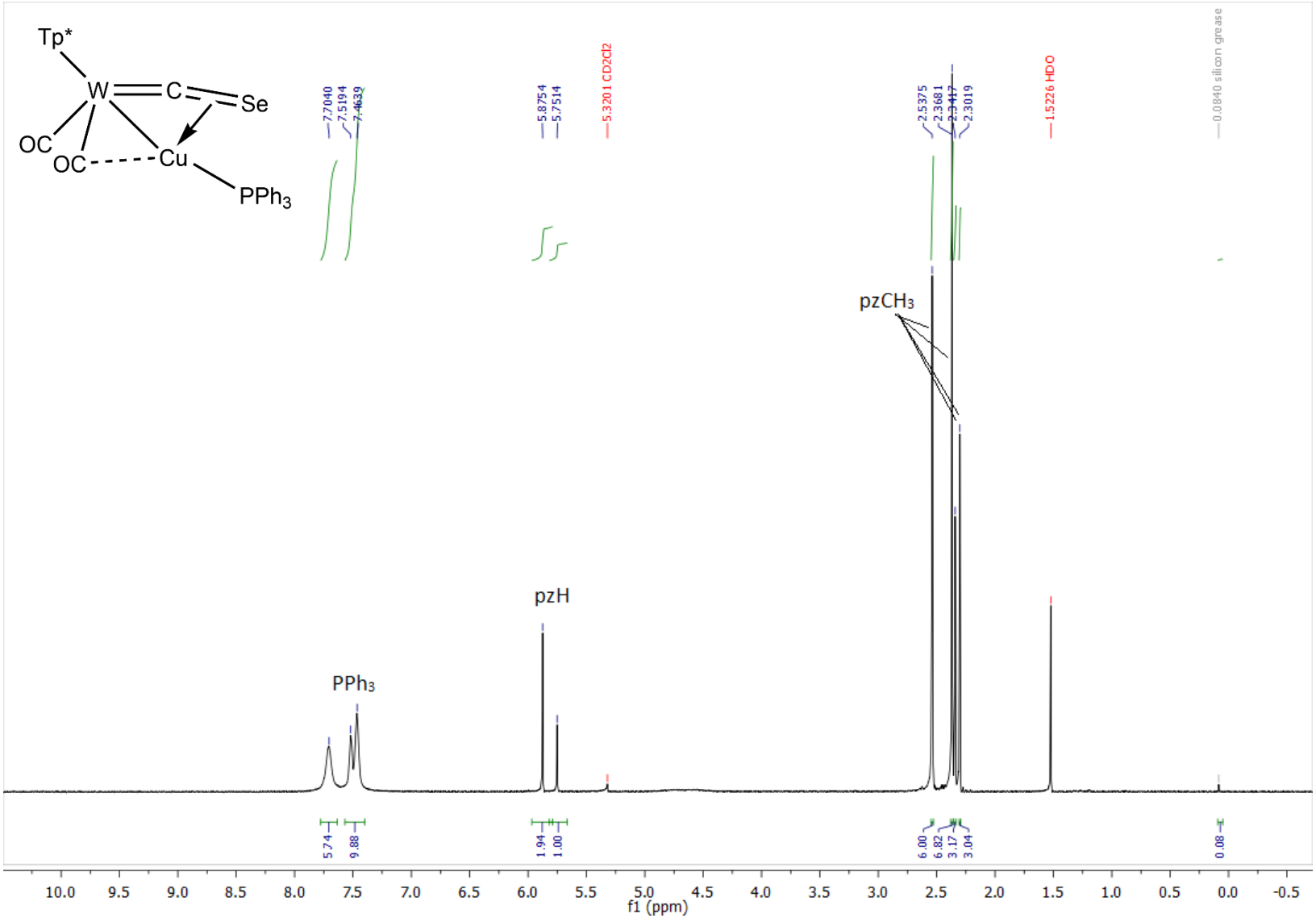
MS (ESI, -ve ion) of $[M]^-$, for $[W(\equiv CSe)(CO)_2(Tp^*)]NEt_4$ ([**2**]NEt_4).



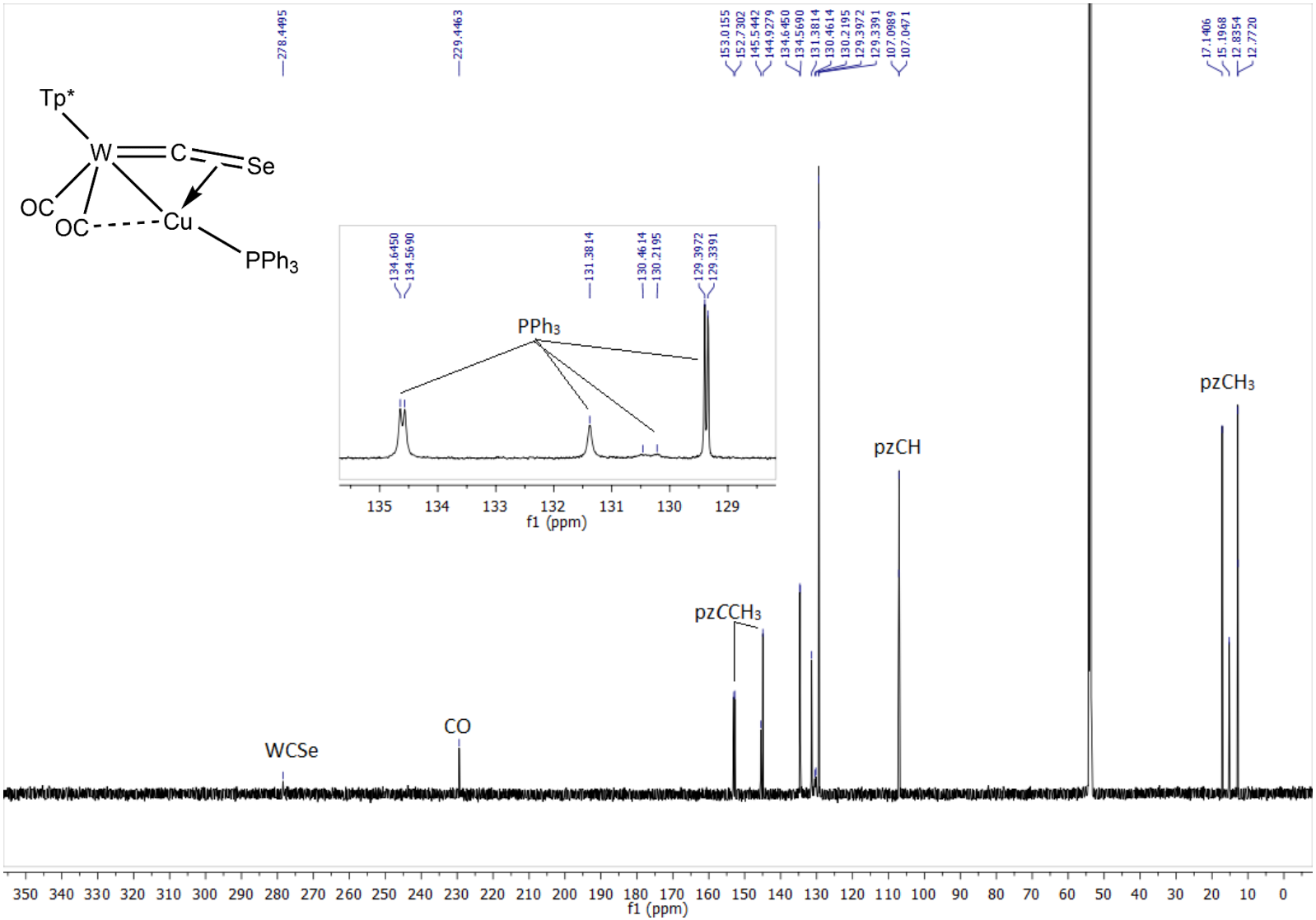
MS (ESI, +ve ion) for $[M+NEt_4]^+$, for $[W(\equiv CSe)(CO)_2(Tp^*)]NEt_4$ ([**2**]NEt_4).



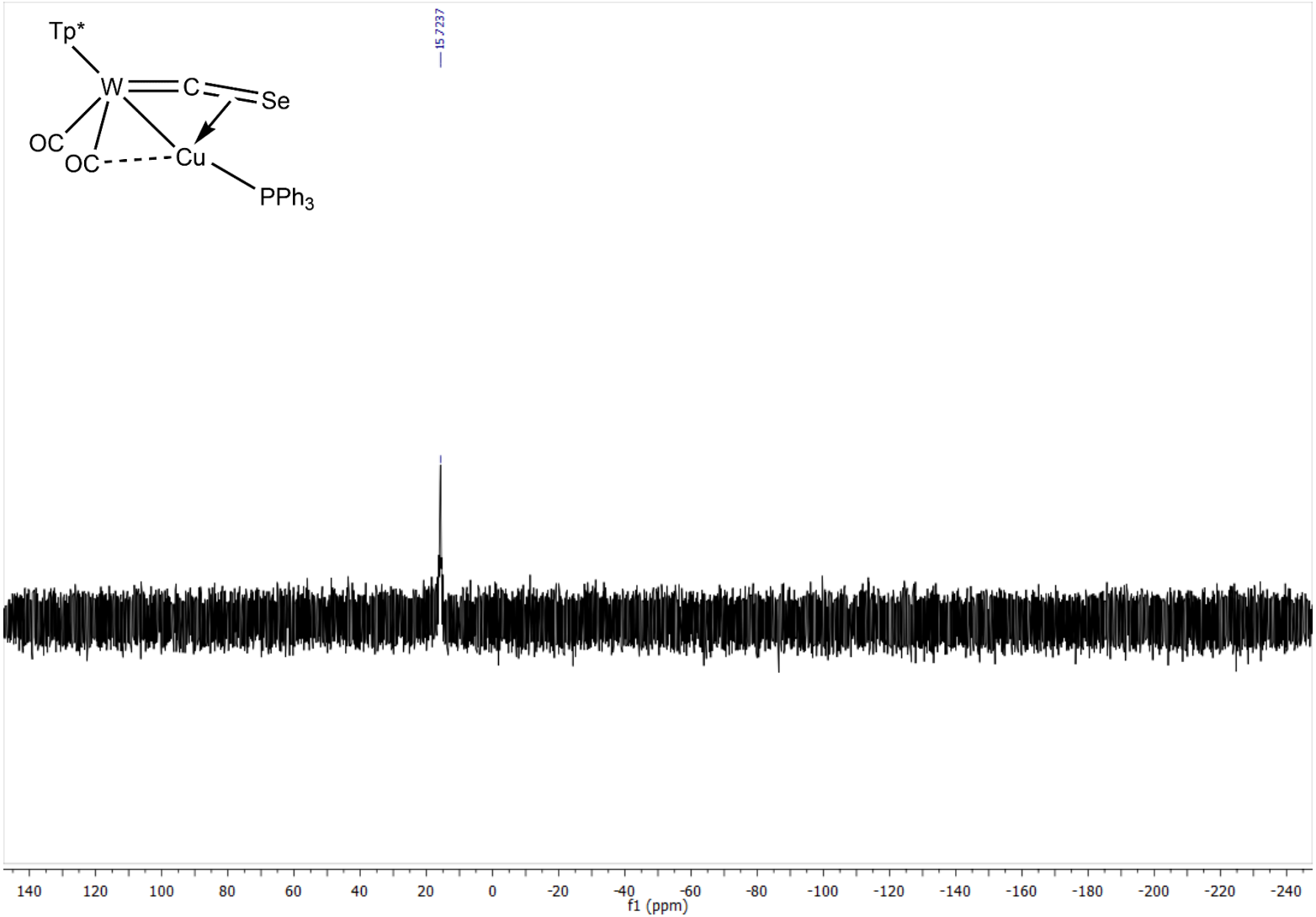
IR (CH_2Cl_2, cm^{-1}) for [WCu(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**3**).



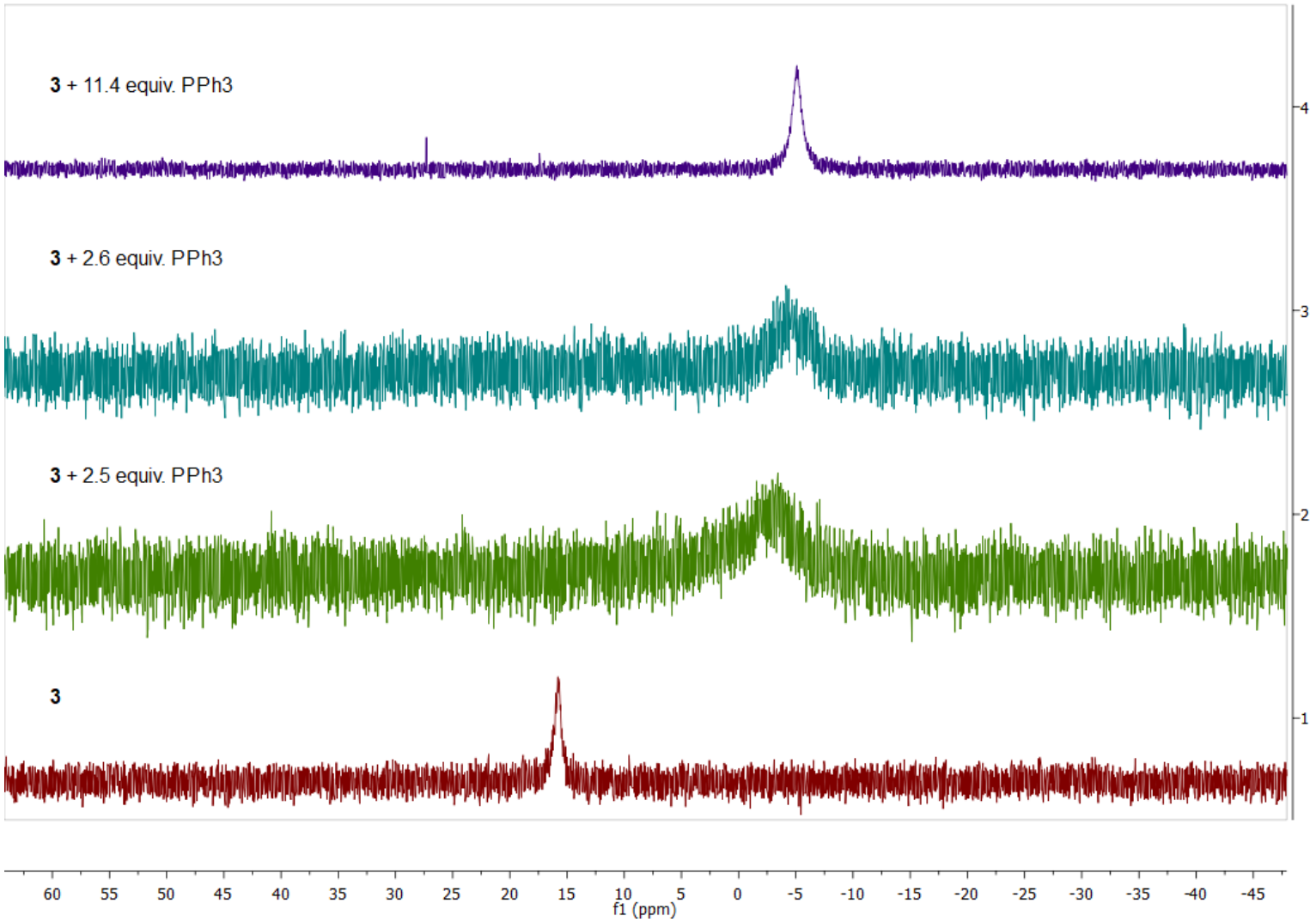
^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, δ) for [WCu(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**3**).



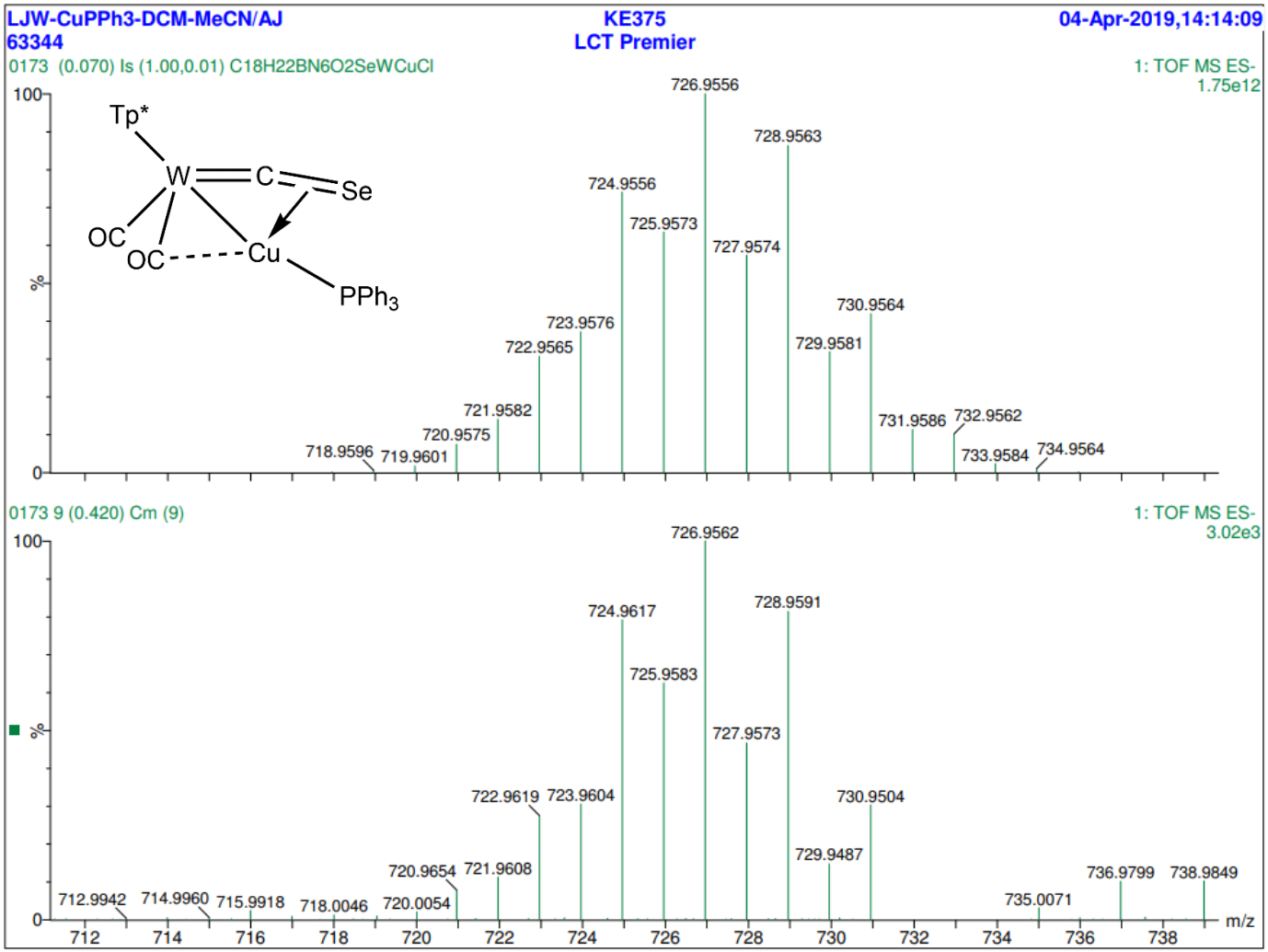
$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 298 K, δ) for $[WCu(\mu\text{-}CSe)(PPh_3)(CO)_2(Tp^*)]$ (**3**).



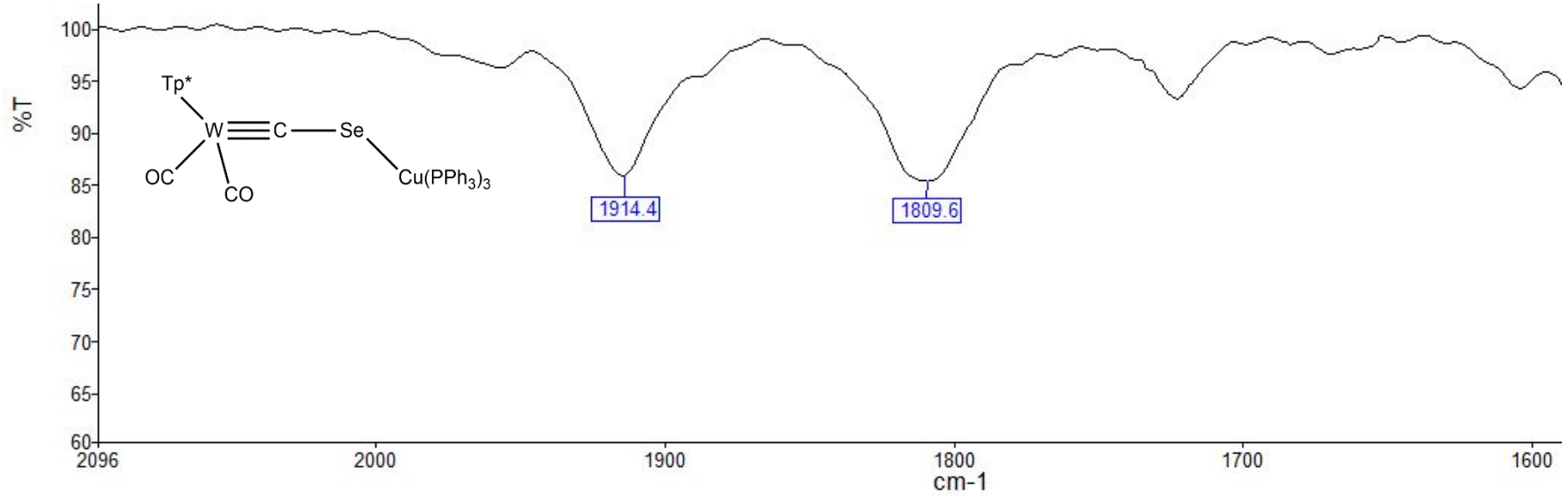
$^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$, 298 K, δ) for $[WCu(\mu\text{-}CSe)(PPh_3)(CO)_2(Tp^*)]$ (**3**).



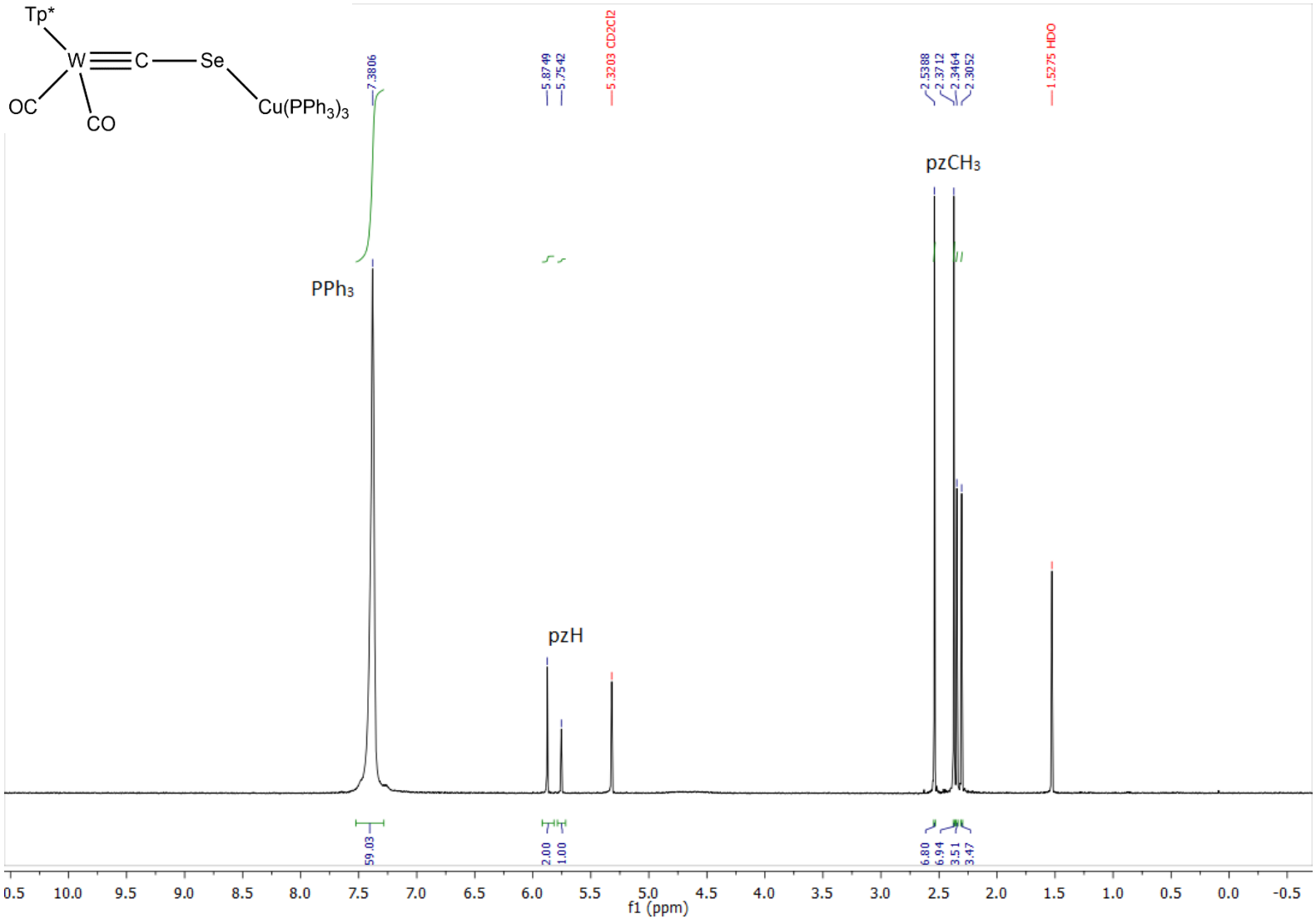
Variation in the $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2, 298 K, δ) of [WCu(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**3**) on addition of further PPh_3.



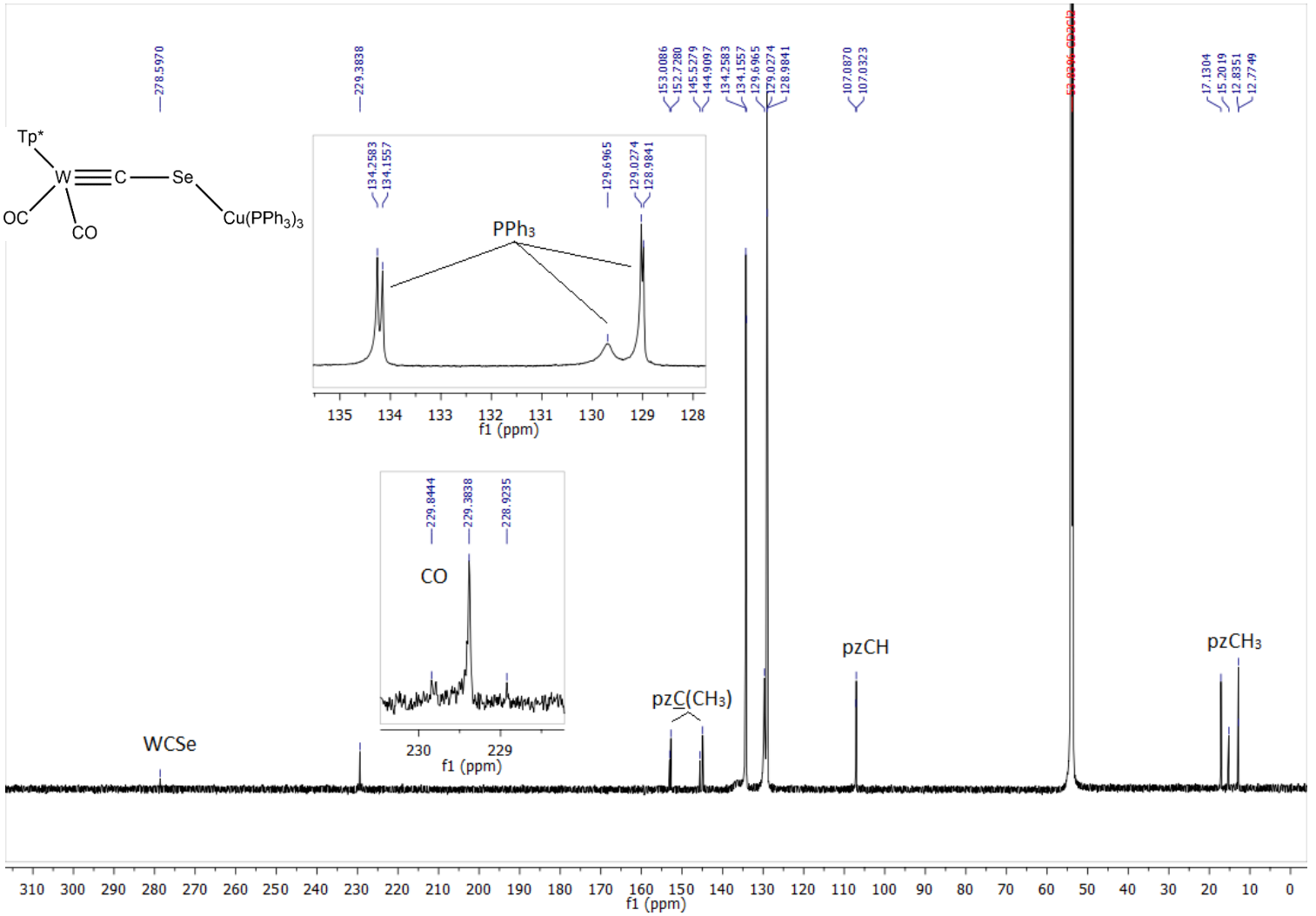
MS (ESI, +ve ion) of $[M\text{-}PPh_3+Cl]^+$ for $[WCu(\mu\text{-}CSe)(PPh_3)(CO)_2(Tp^*)]$ (**3**).



IR (CH_2Cl_2, cm^{-1}) for [W{≡CSeCu(PPh_3)$_3$}(CO)$_2$(Tp*)] (**4**).



^{1}H NMR (700 MHz, CD_2Cl_2, 298K, δ) for [W{≡CSeCu(PPh_3)$_3$}(CO)$_2$(Tp*)] (**4**).



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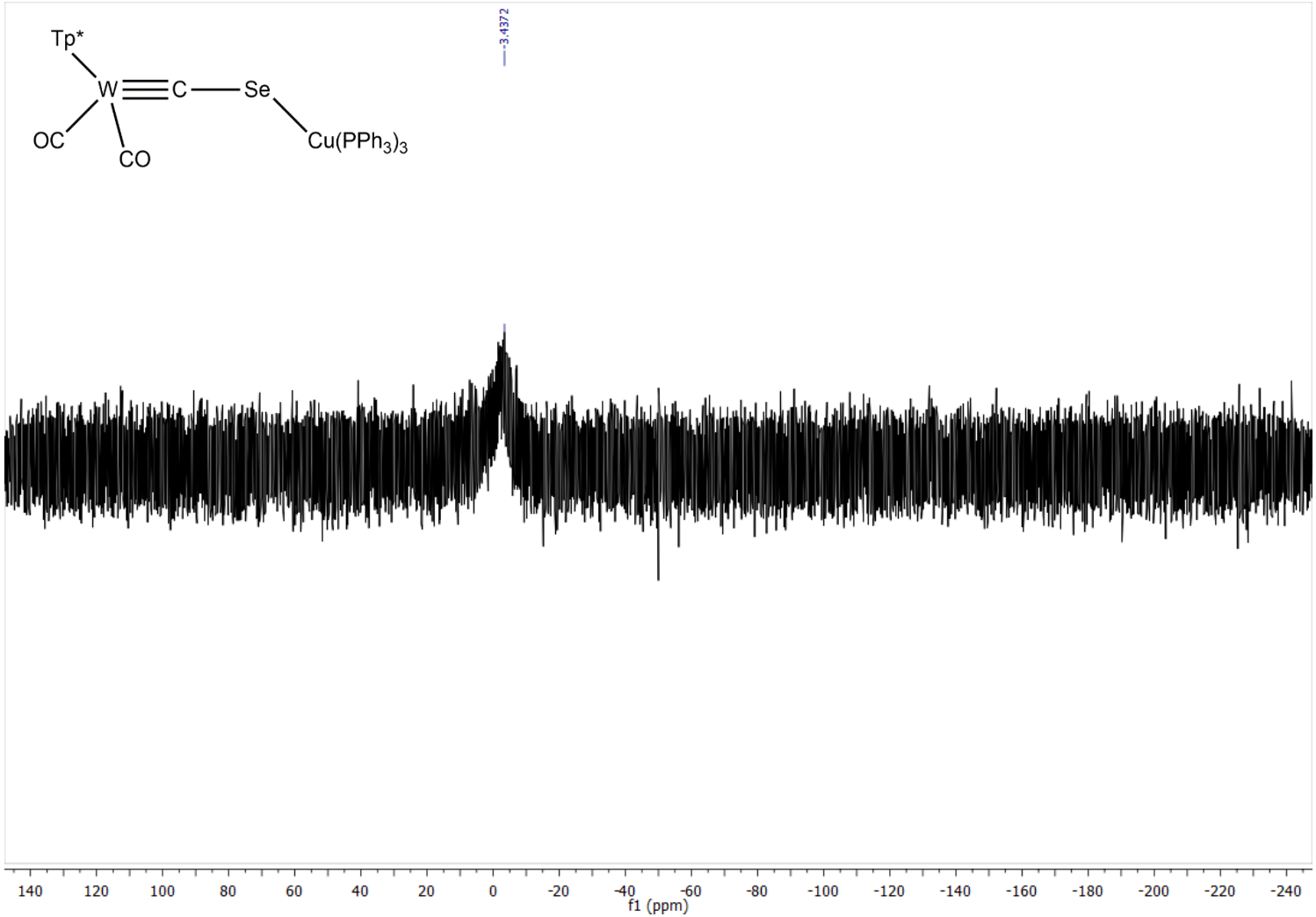

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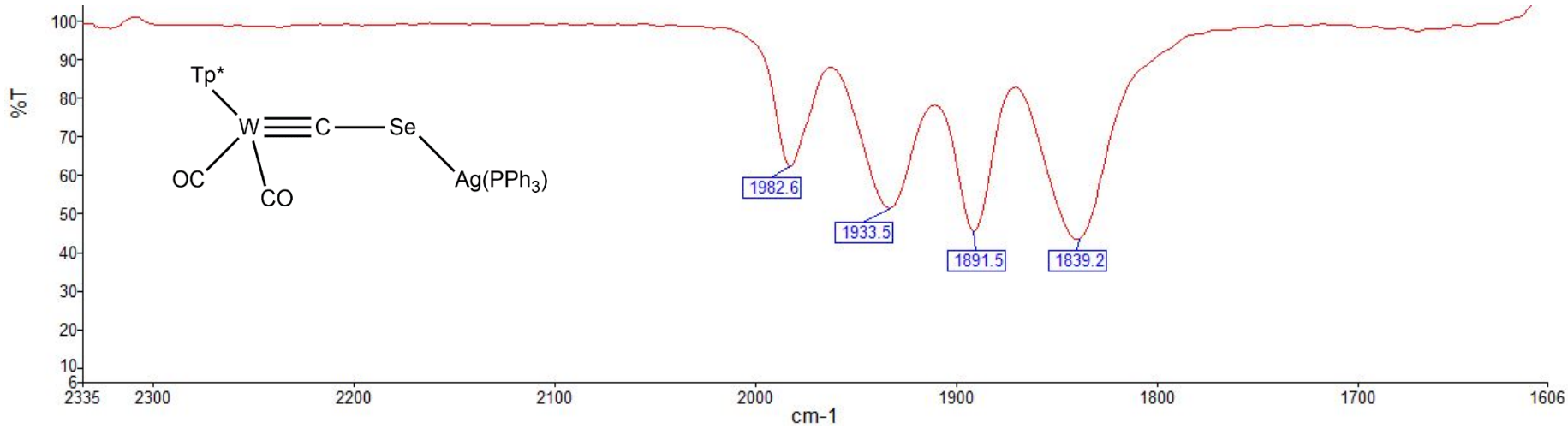
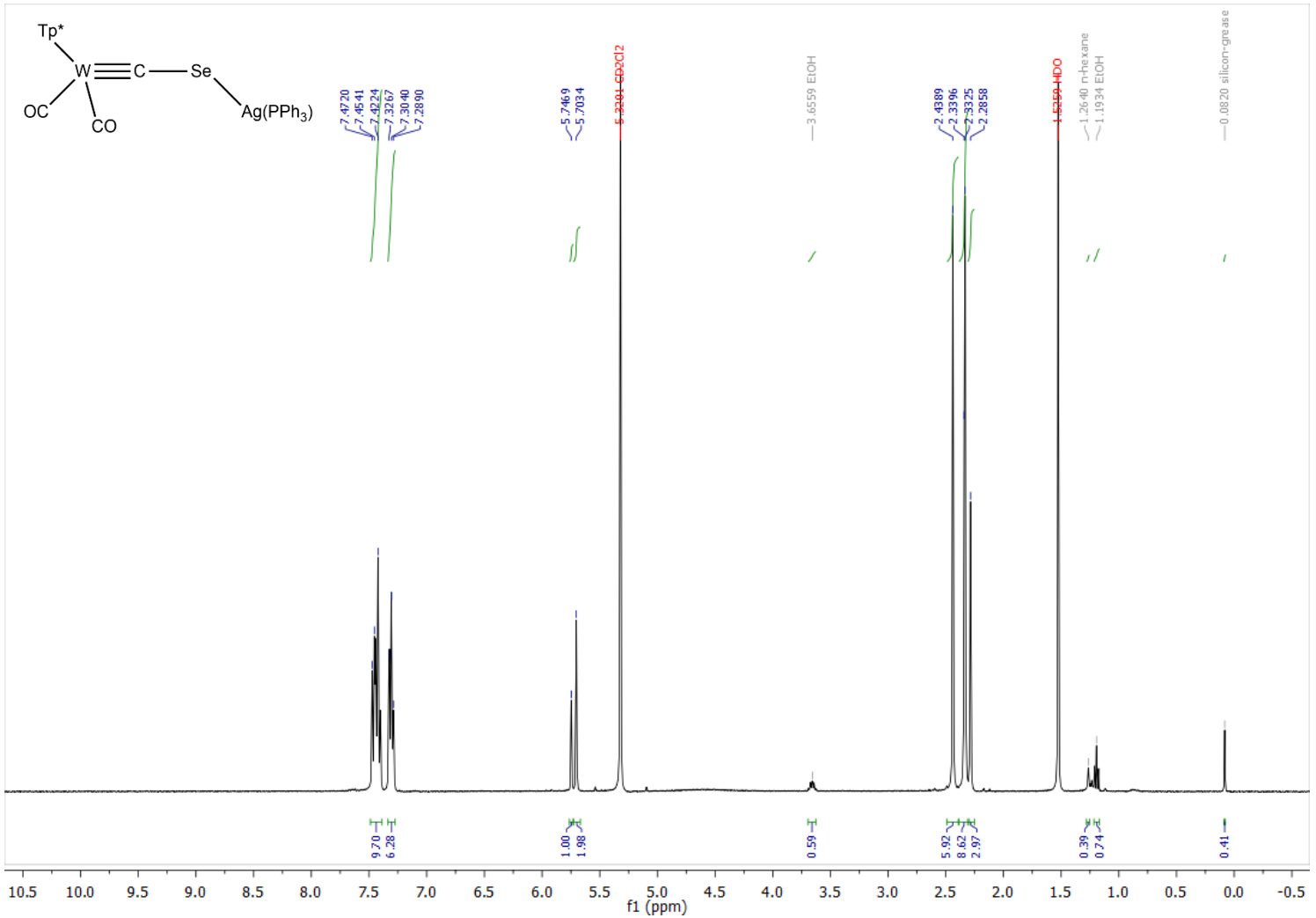
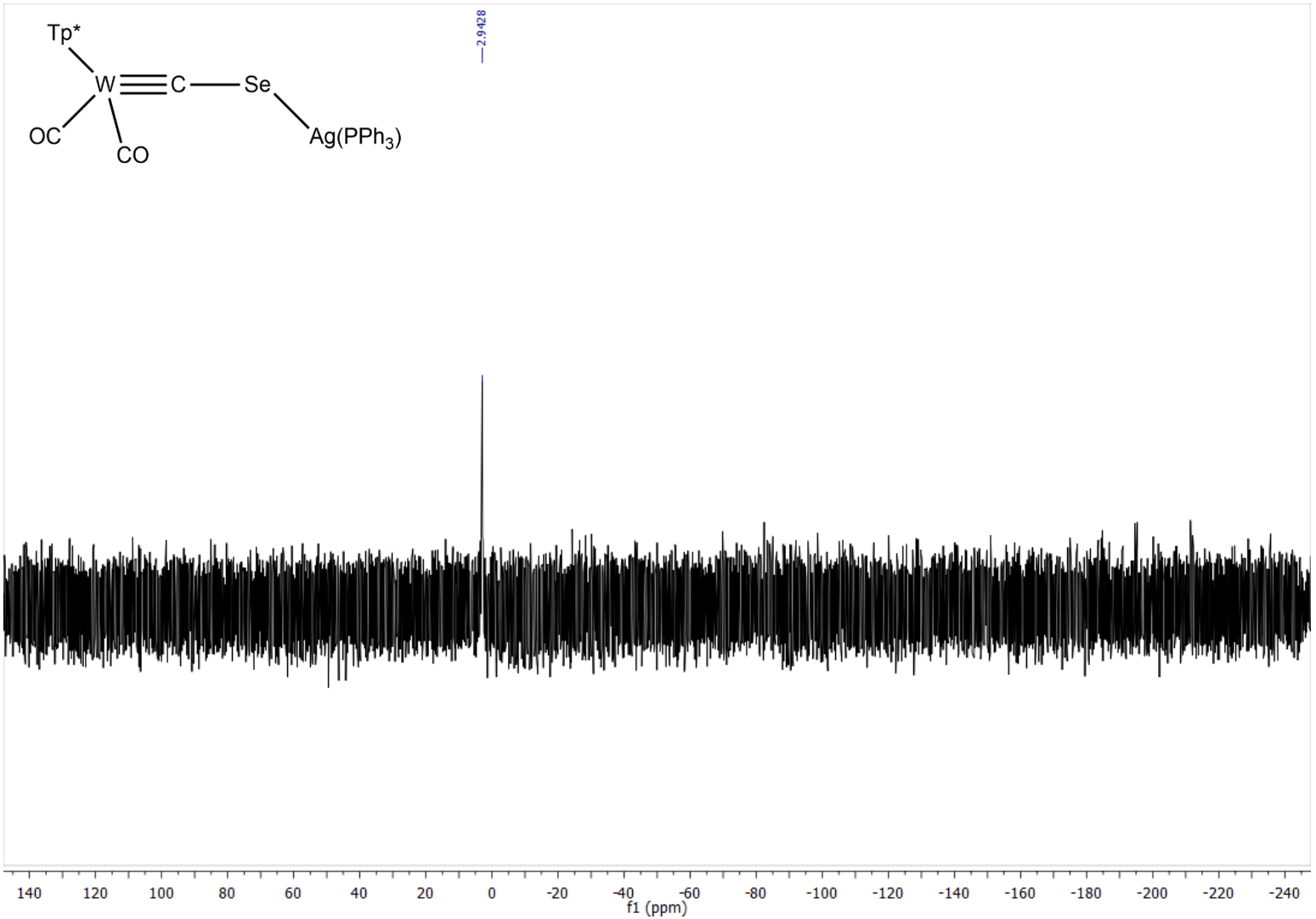


IR (CH_2Cl_2, cm^{-1}) for [WAg(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**5**).



^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, δ) for [WAg(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**5**).



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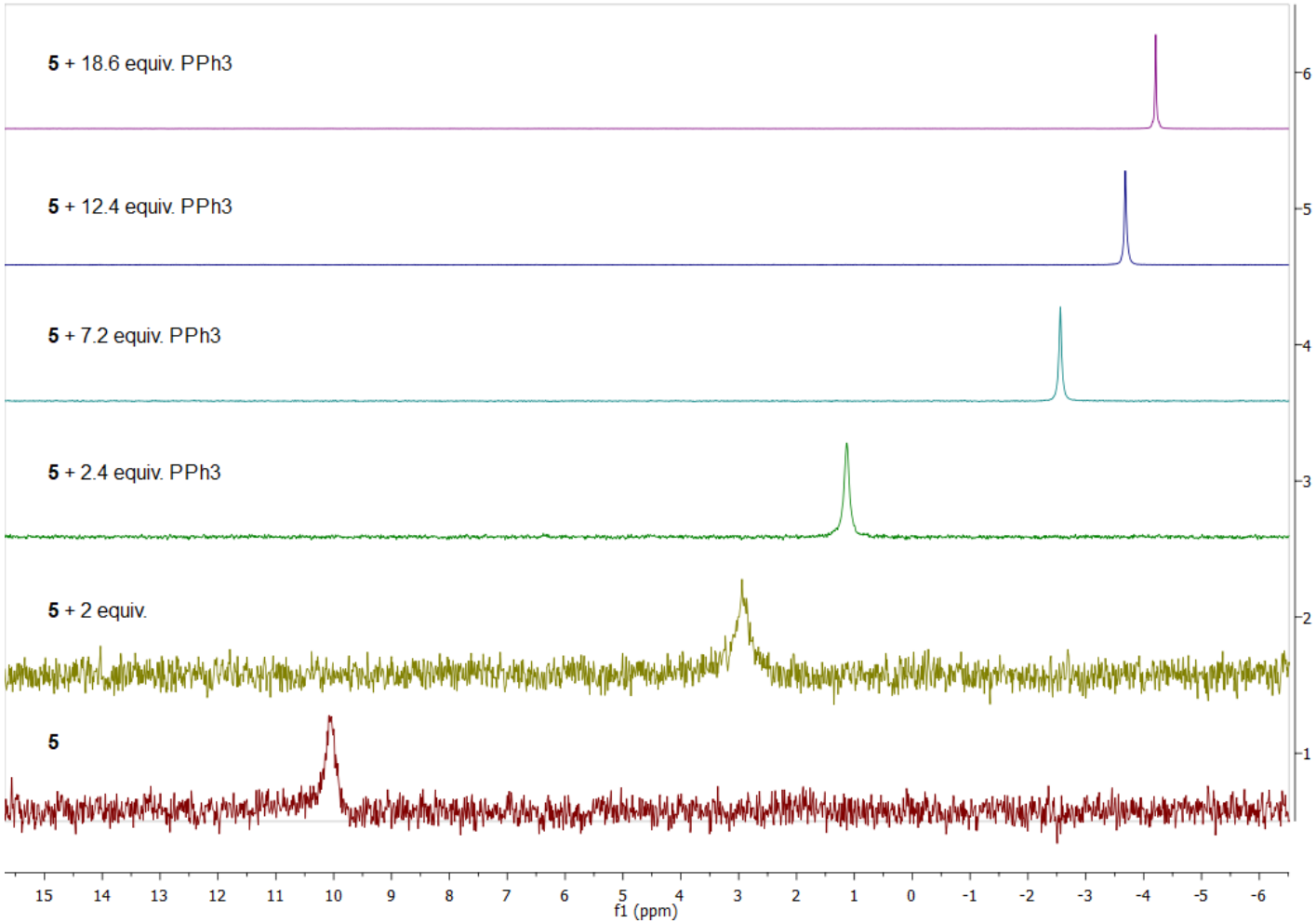
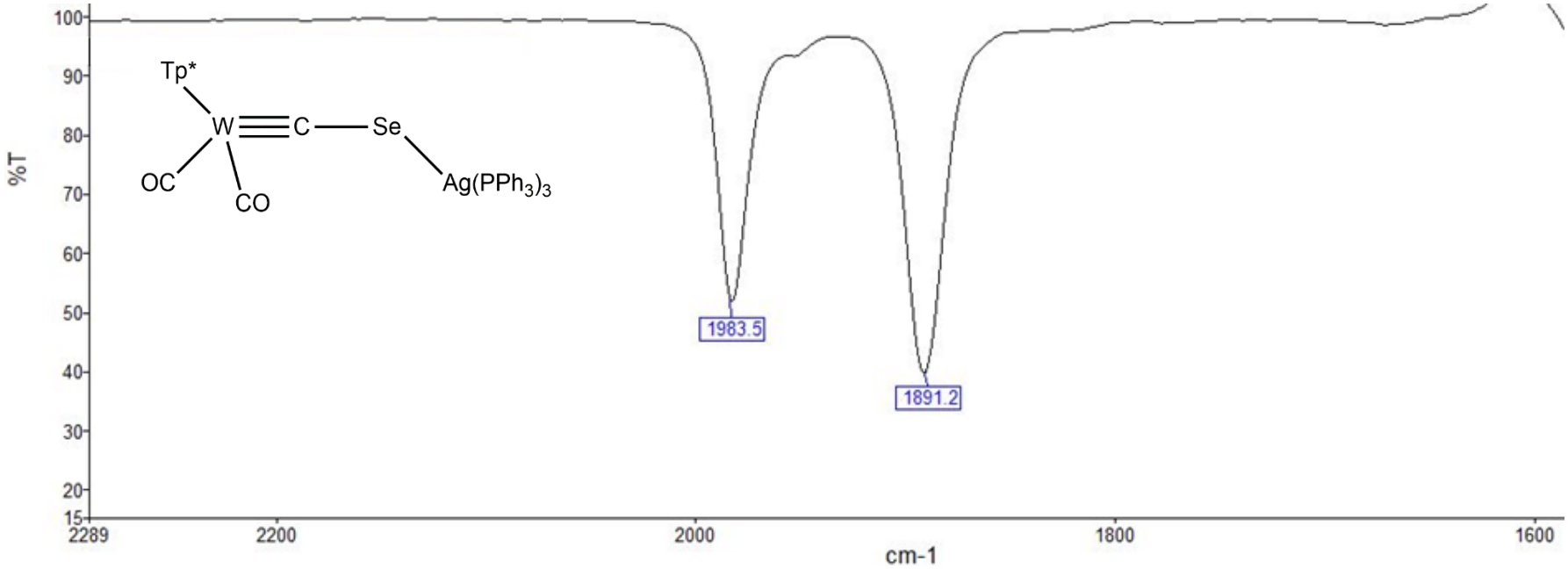
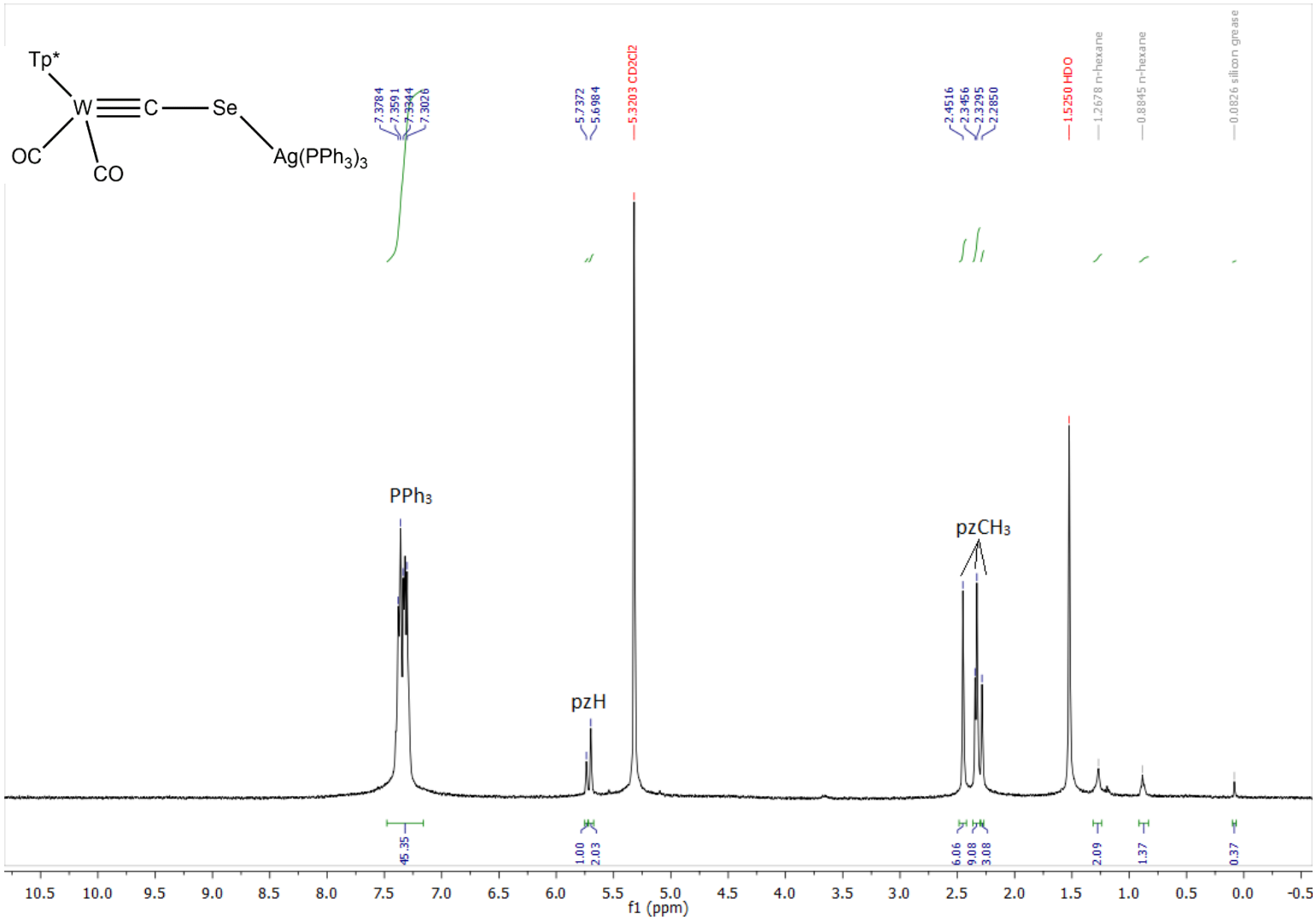


Variation in the $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2, 298 K, δ) of [WAg(μ-CSe)(PPh_3)$(CO)_2$(Tp*)] (**5**) on addition of further PPh_3.



IR (CH_2Cl_2) for [W{≡CSeAg(PPh_3)$_3$}(CO)$_2$(Tp*)] (**6**).



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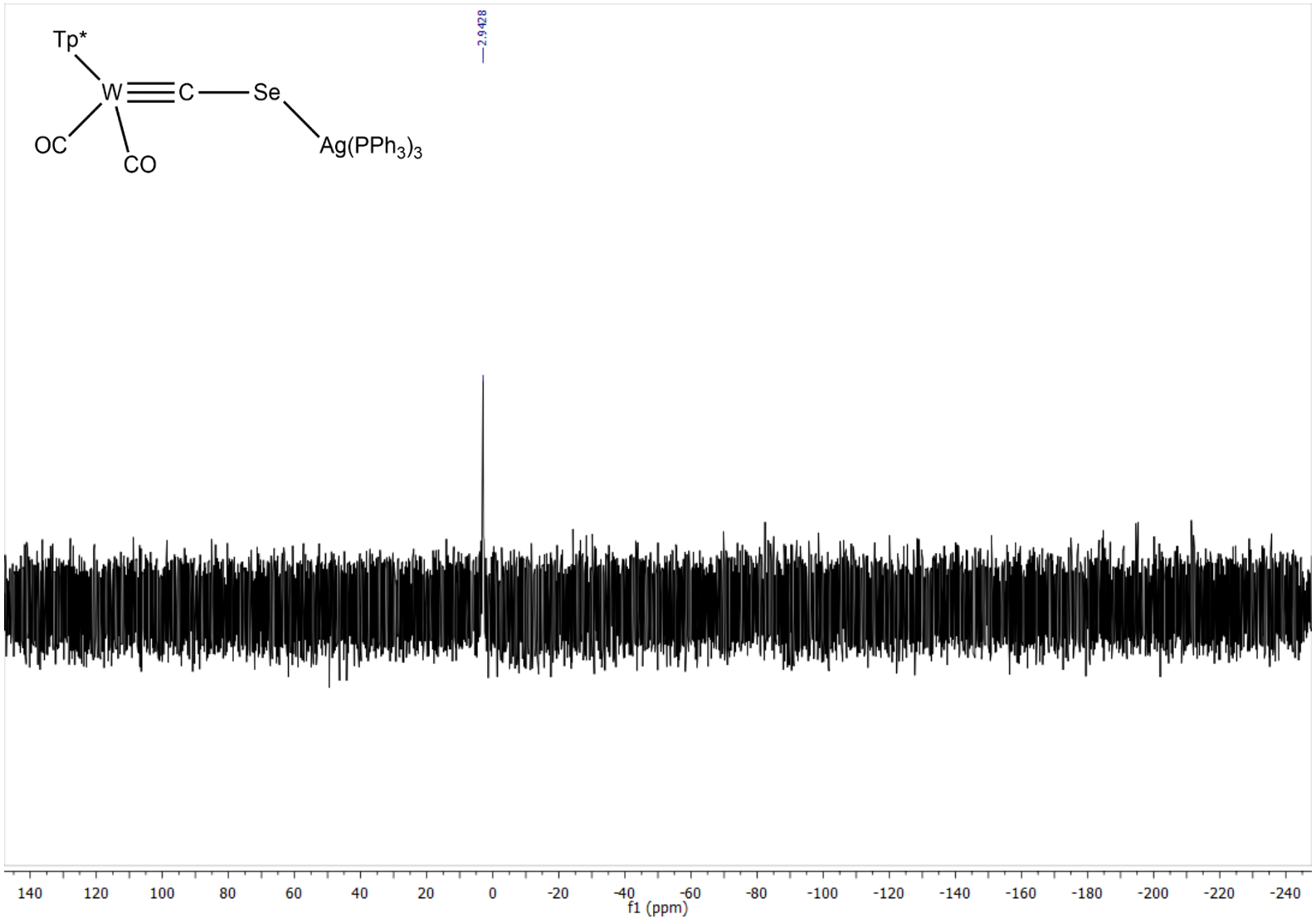

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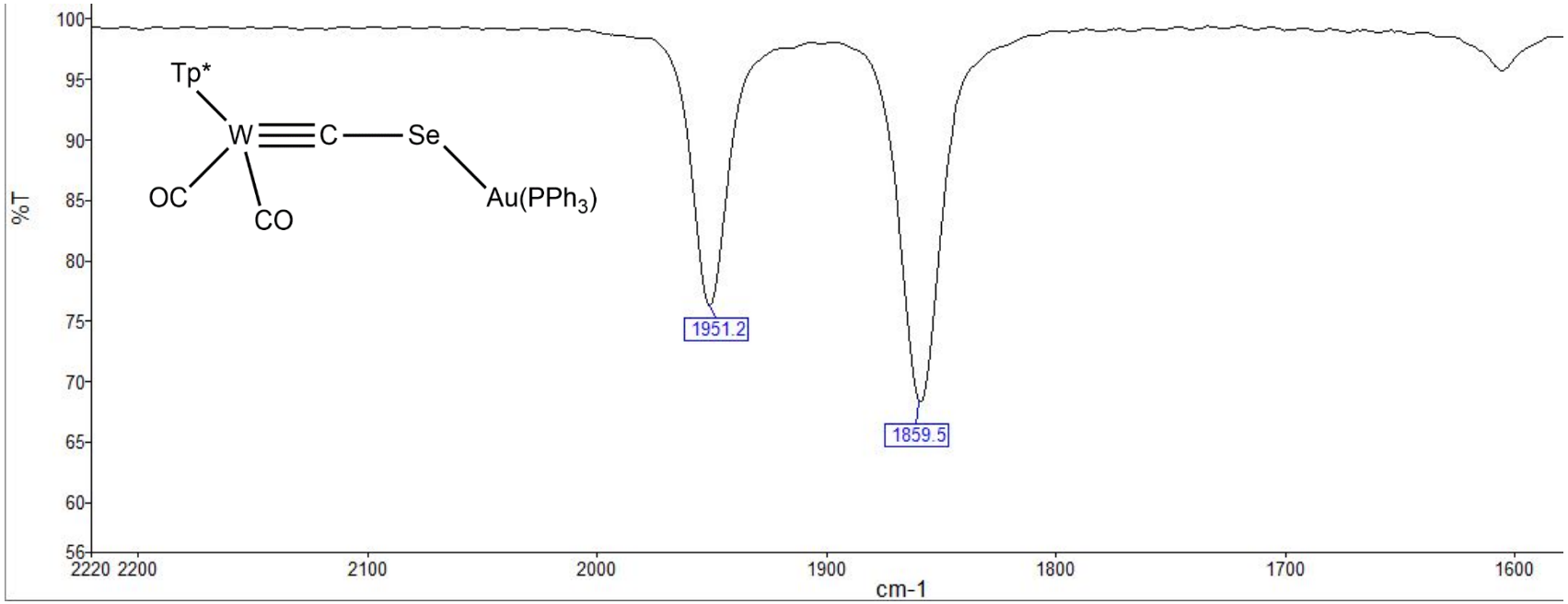
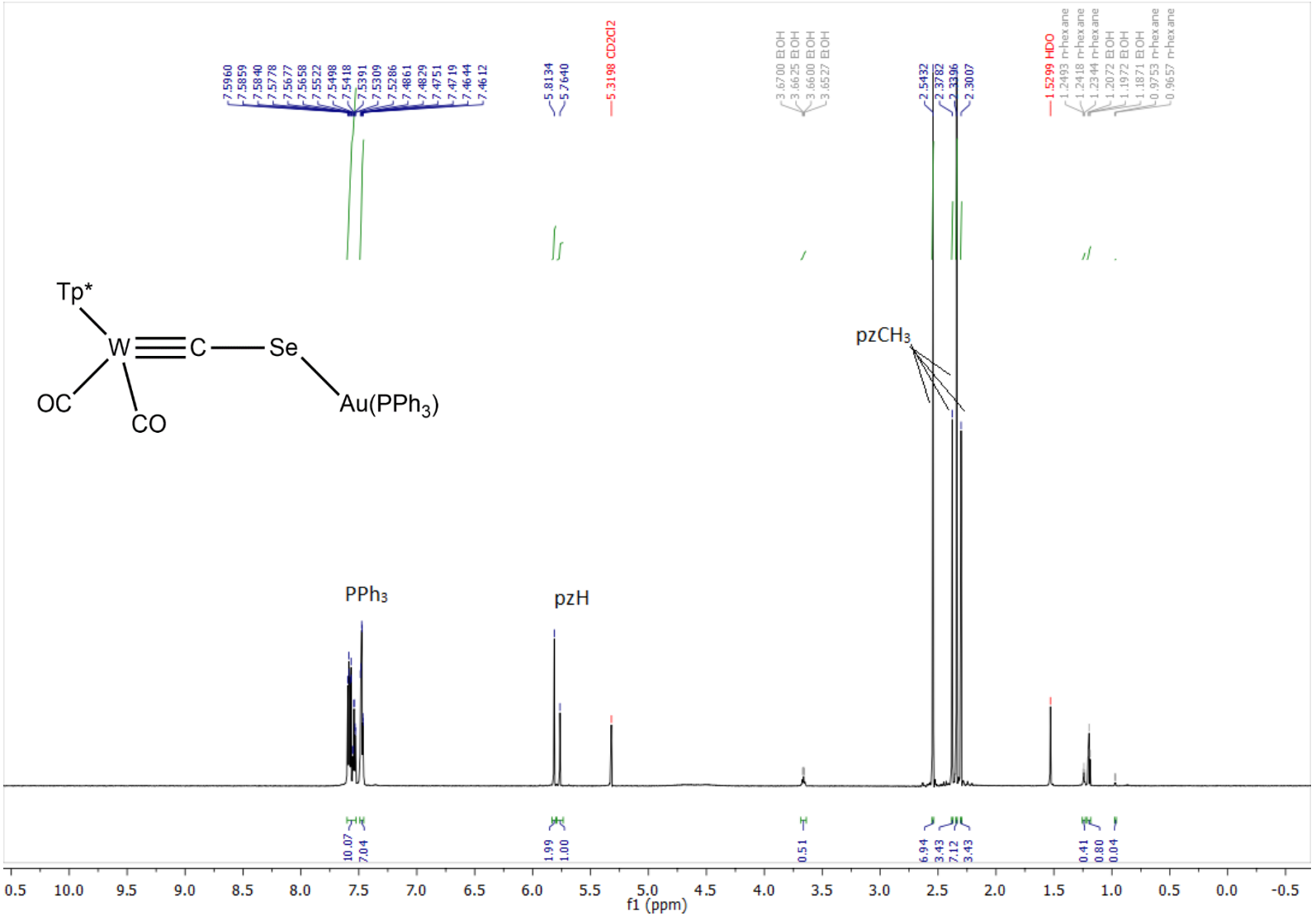
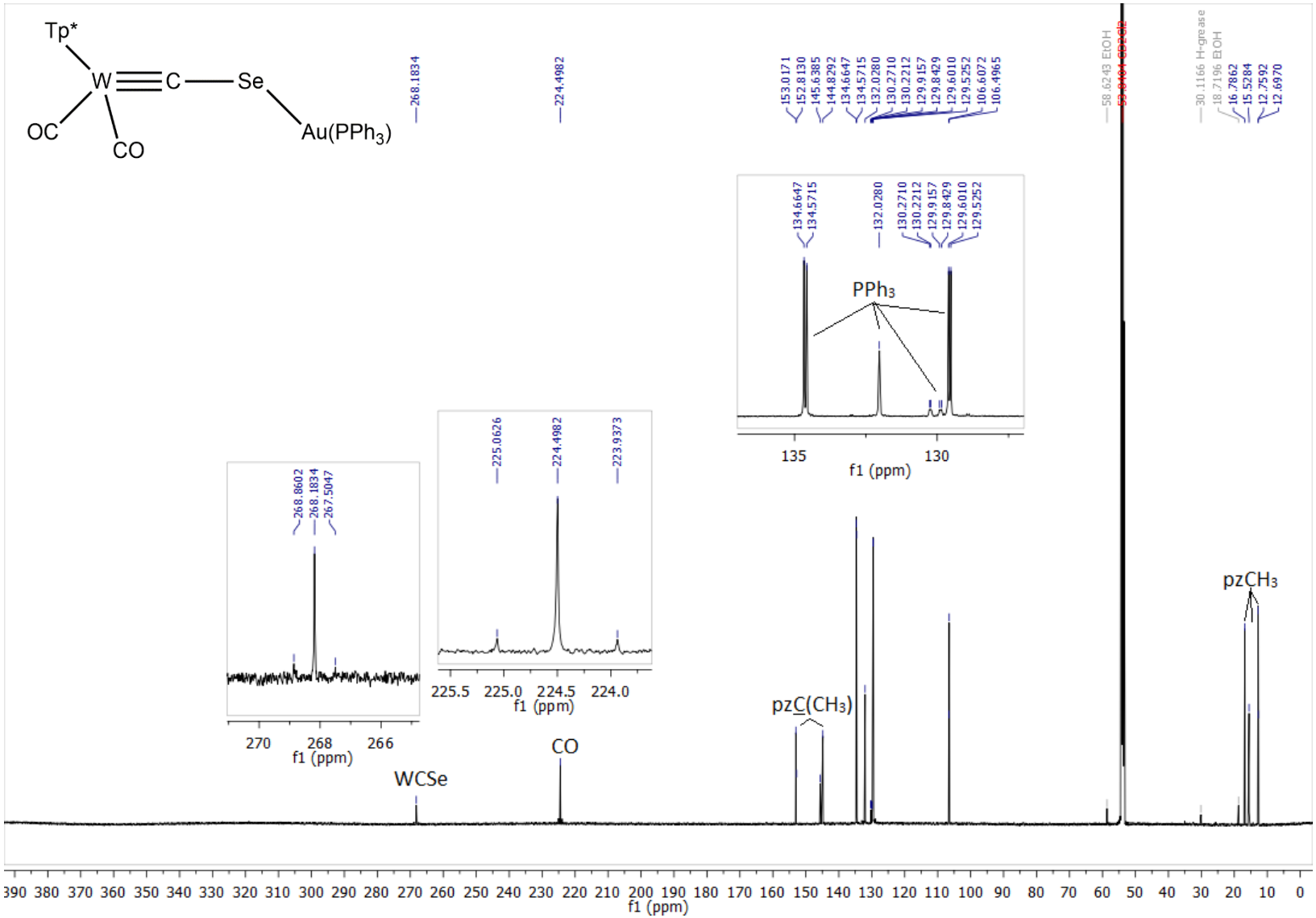


IR (CH_2Cl_2, cm^{-1}) for [W(≡CSeAuPPh$_3$)(CO)$_2$(Tp*)] (**7**).



^{1}H NMR (700 MHz, CD_2Cl_2, 298 K, δ) for [W(≡CSeAuPPh$_3$)(CO)$_2$(Tp*)] (**7**).



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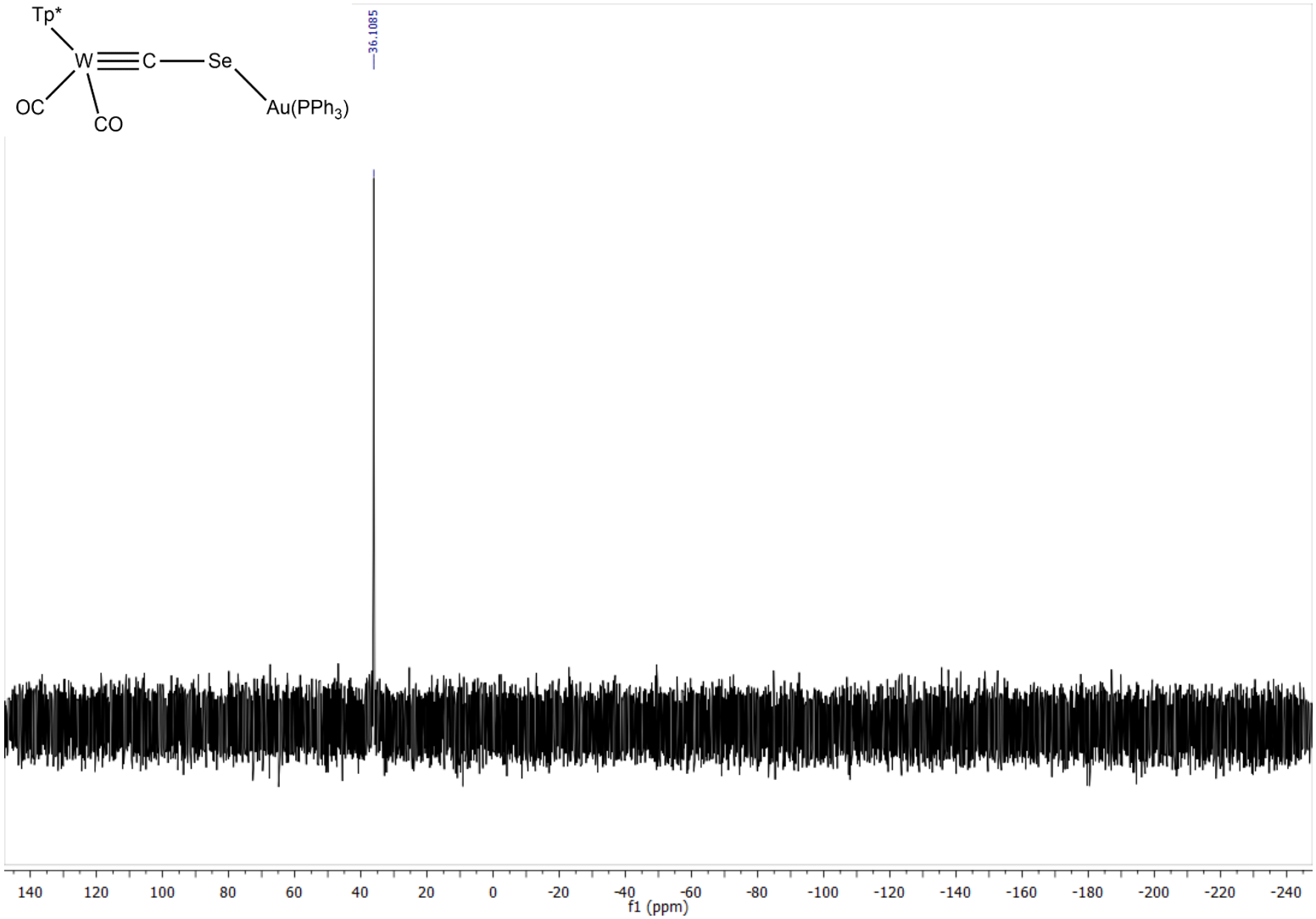

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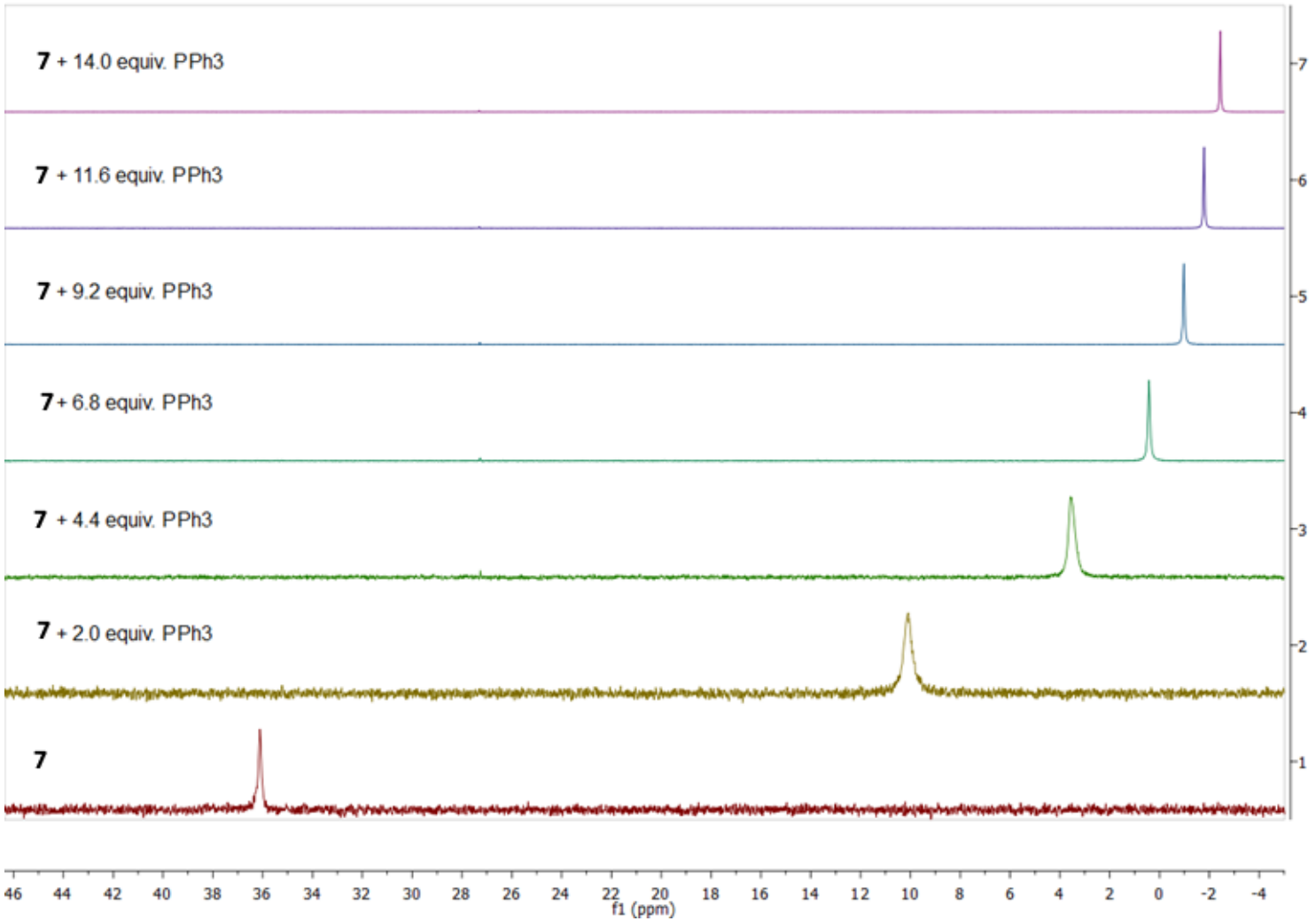
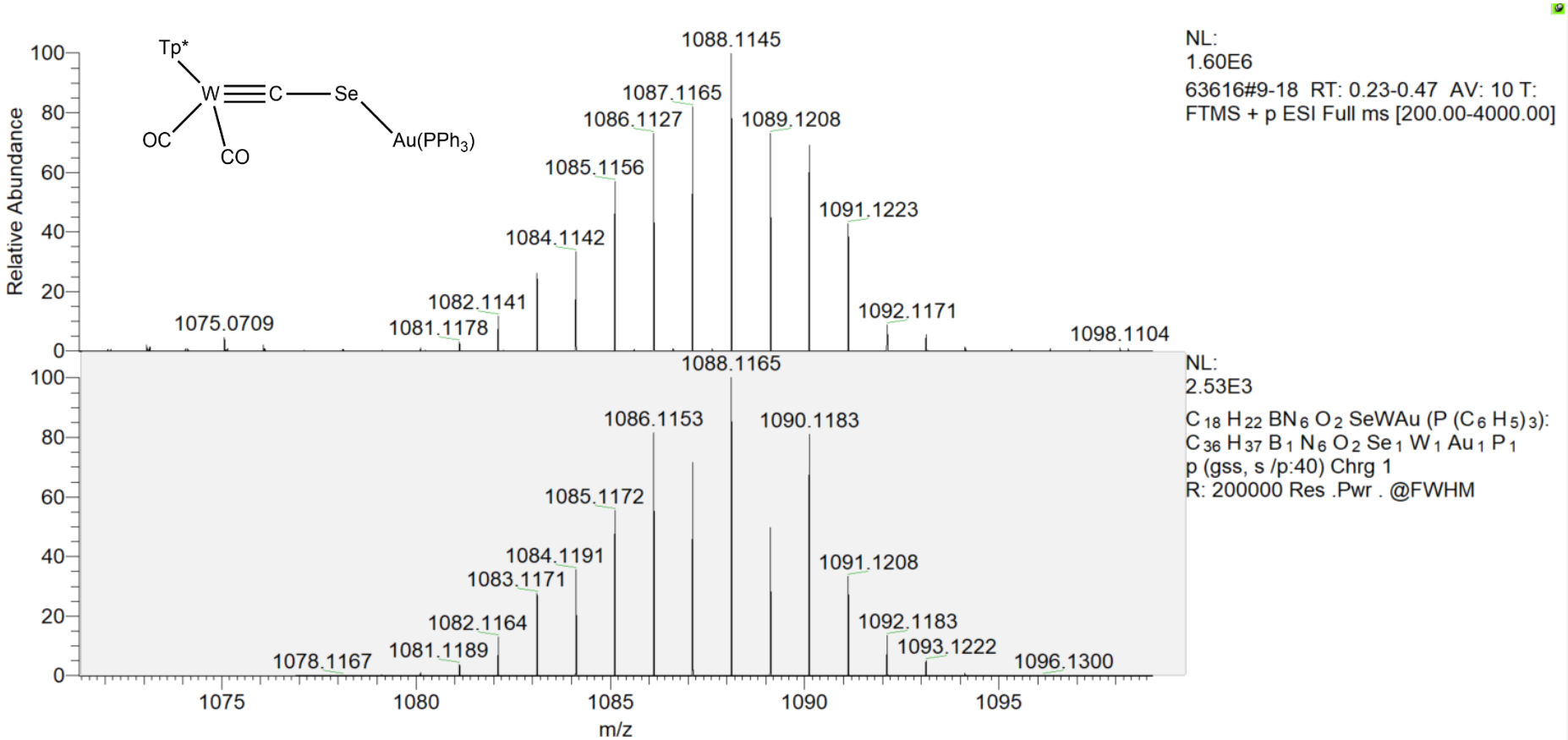
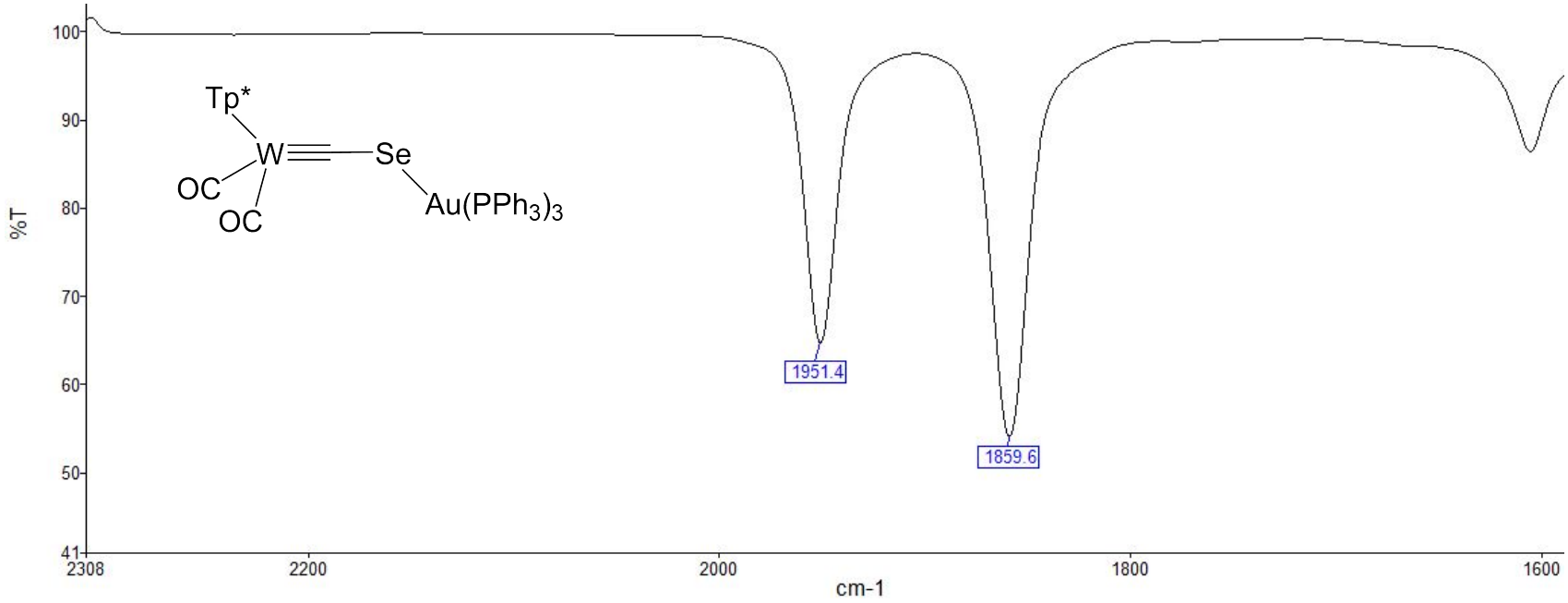


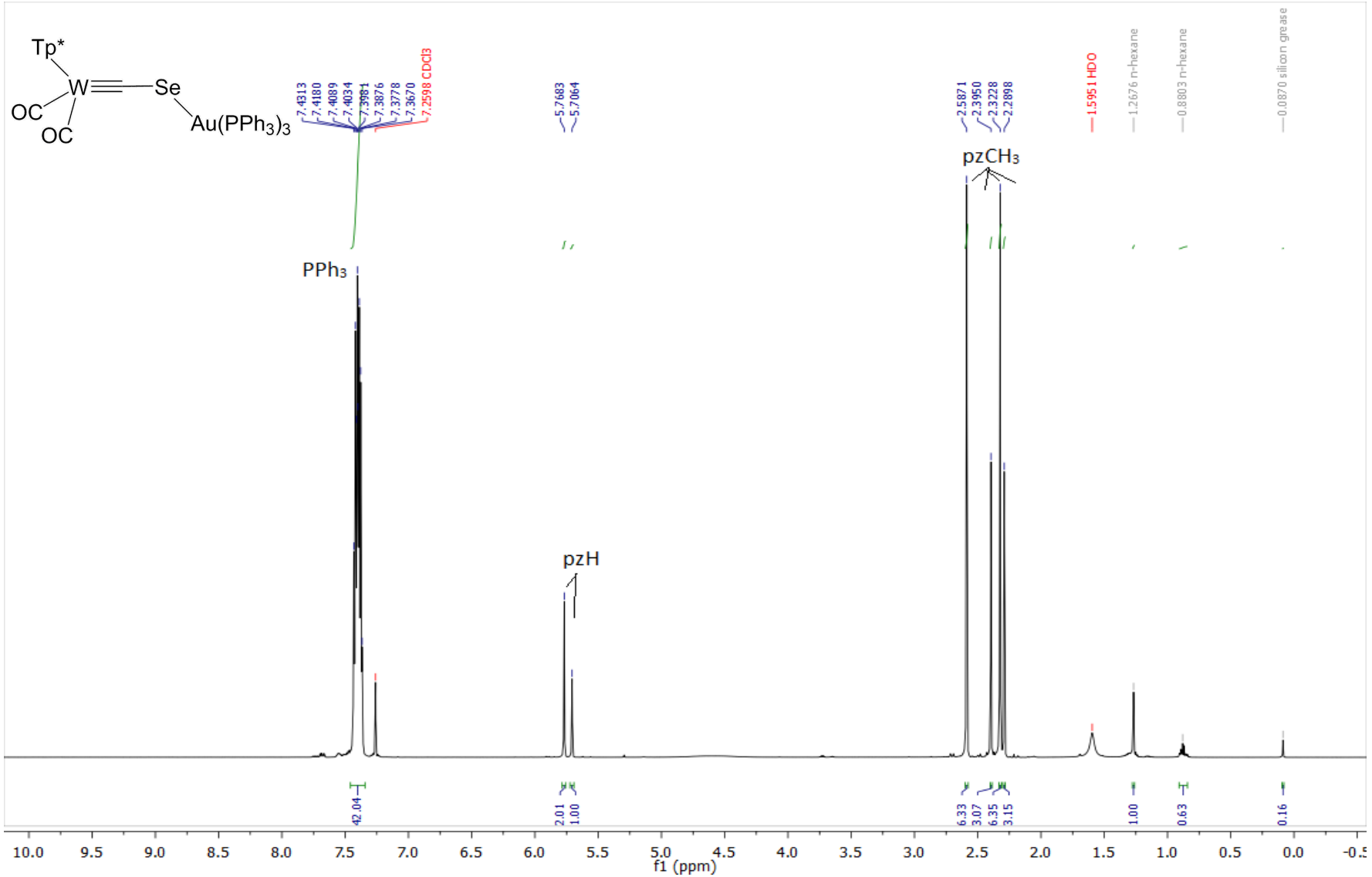
Variation in the $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2, 298 K, δ) of [W(≡CSeAuPPh$_3$)(CO)$_2$(Tp*)] (**7**) on addition of further PPh$_3$.



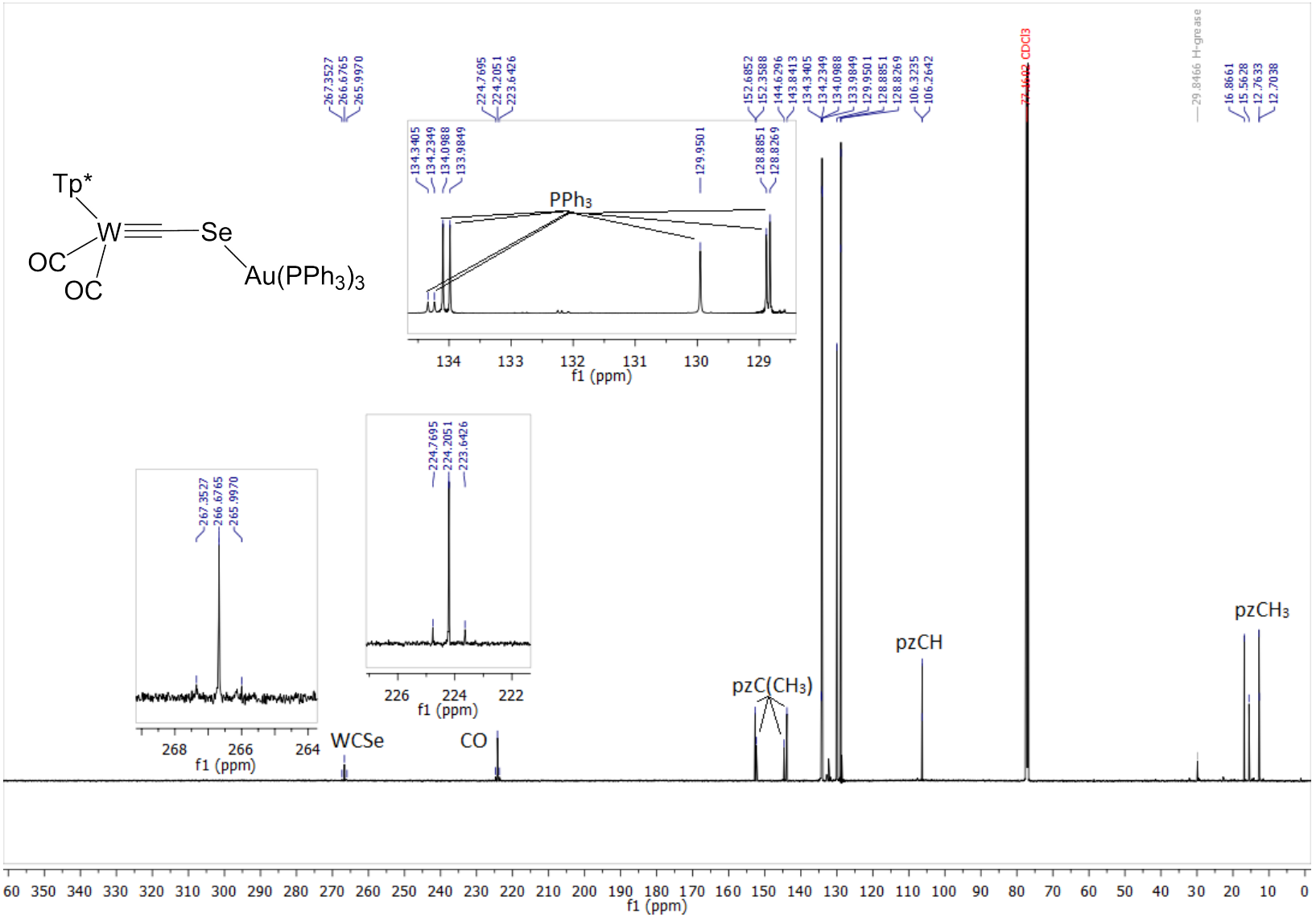
MS (ESI, +ve mode, *m/z*): of $[M–2PPh_3+H]^+$ for $[W(\equiv CSeAuPPh_3)(CO)_2(Tp^*)]$ (**7**).



IR (CH_2Cl_2) for [W{≡CSeAu(PPh_3)$_3$}$(CO)_2$(Tp*)] (**8**).



^{1}H NMR (600 MHz, $CDCl_3$, 298 K, δ) for [W{≡CSeAu(PPh_3)$_3$}(CO)$_2$(Tp*)] (**8**).



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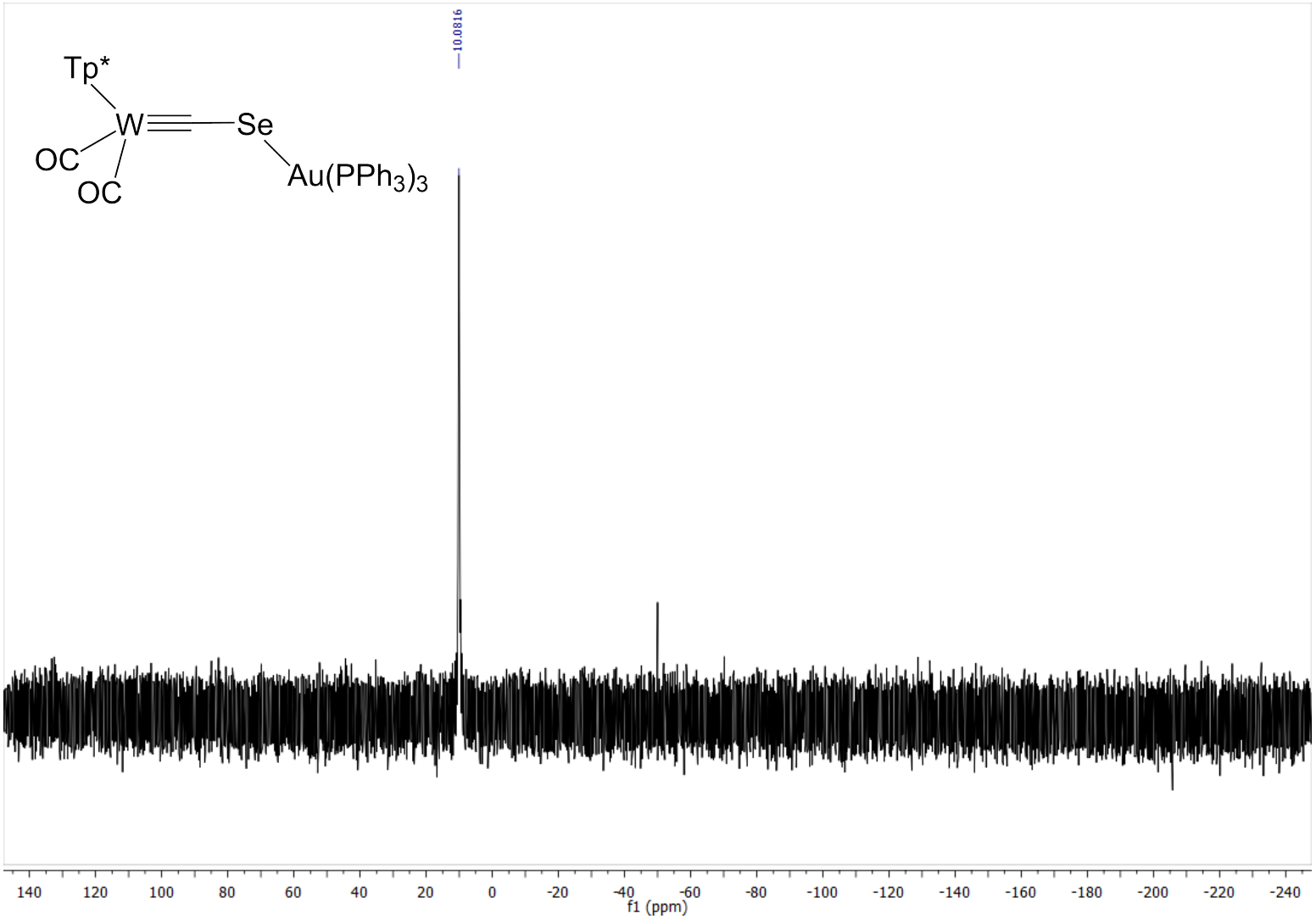

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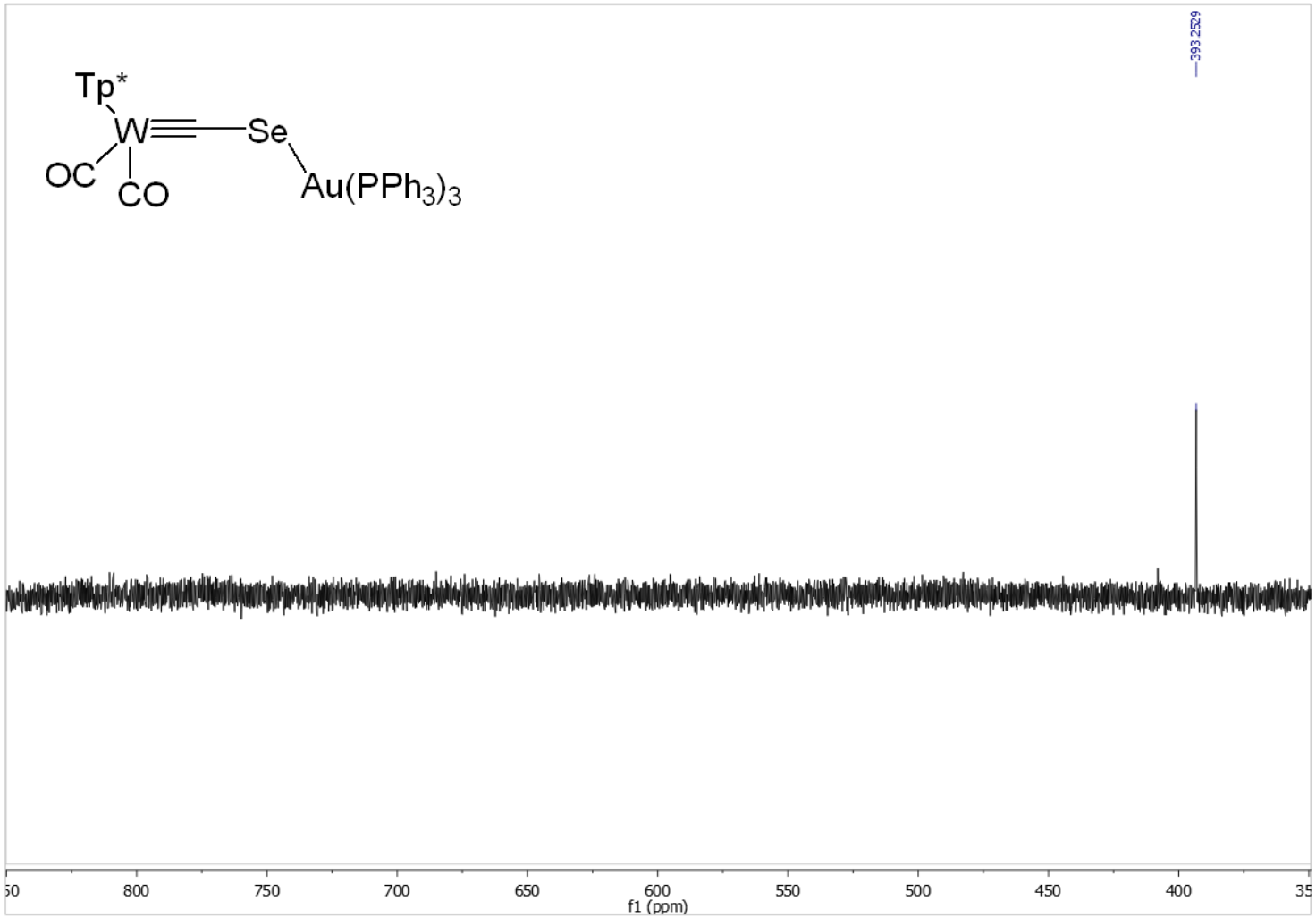

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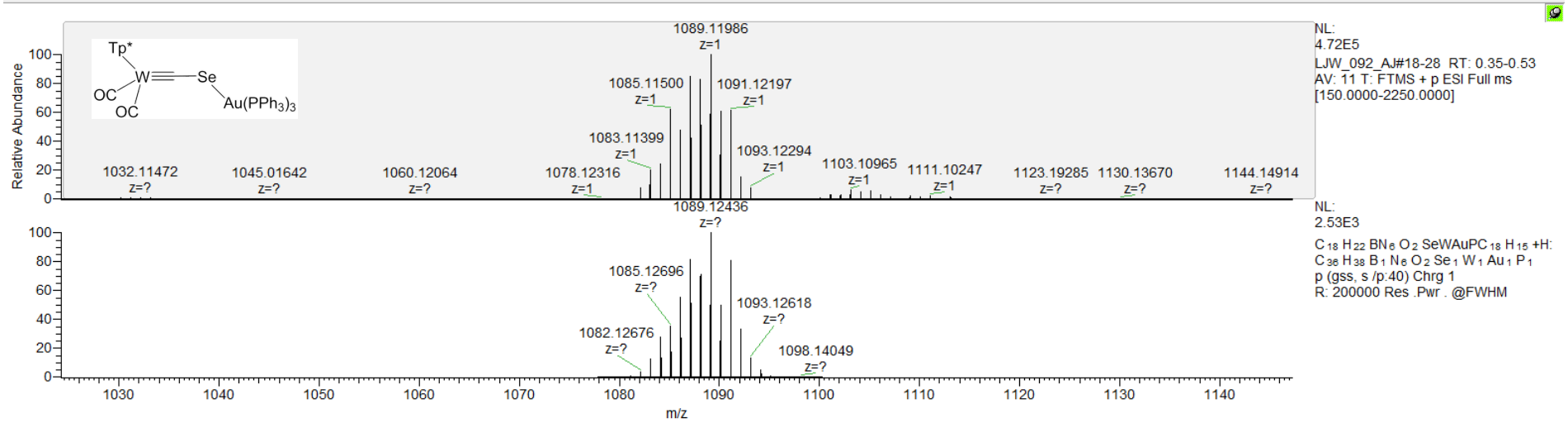
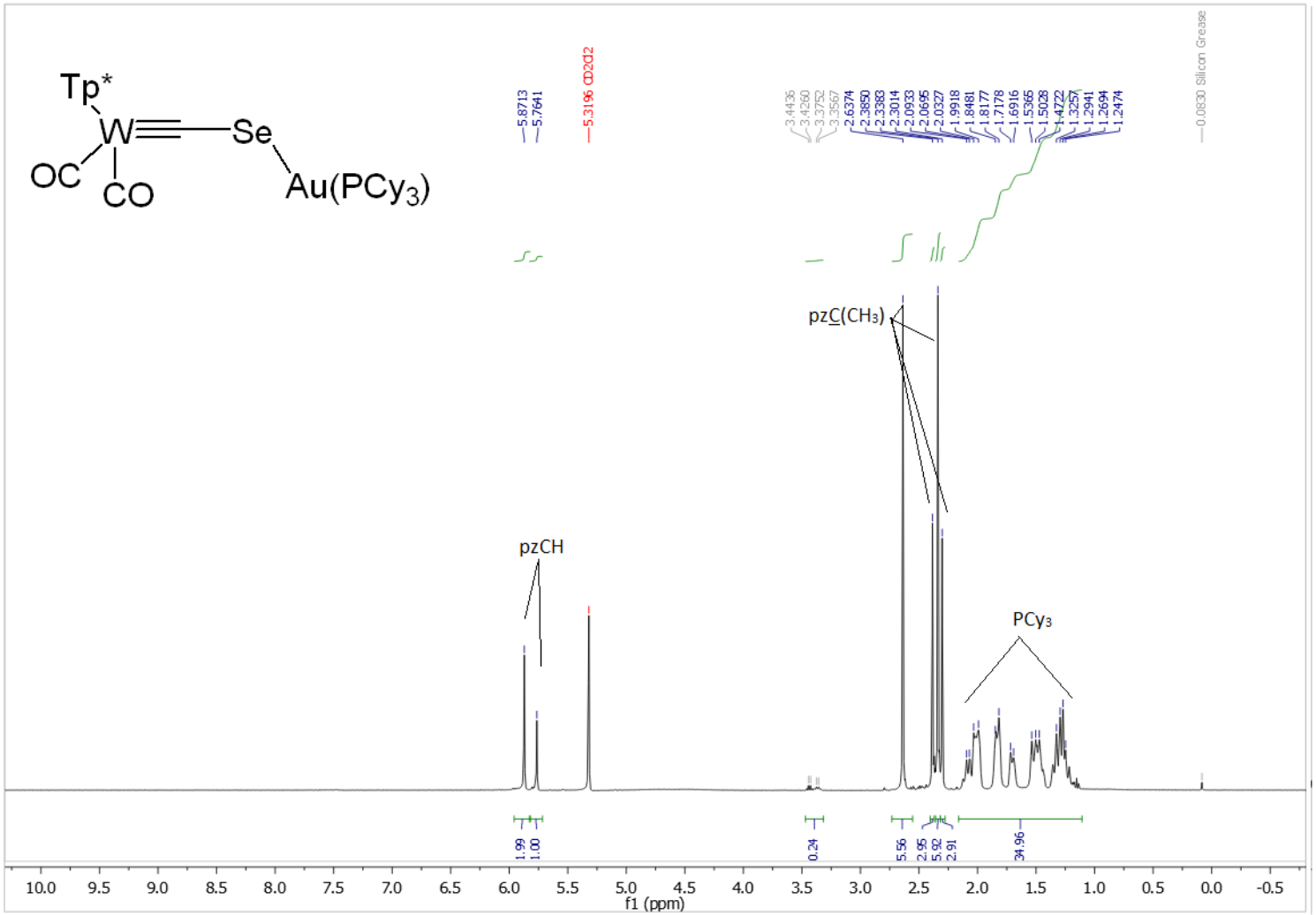
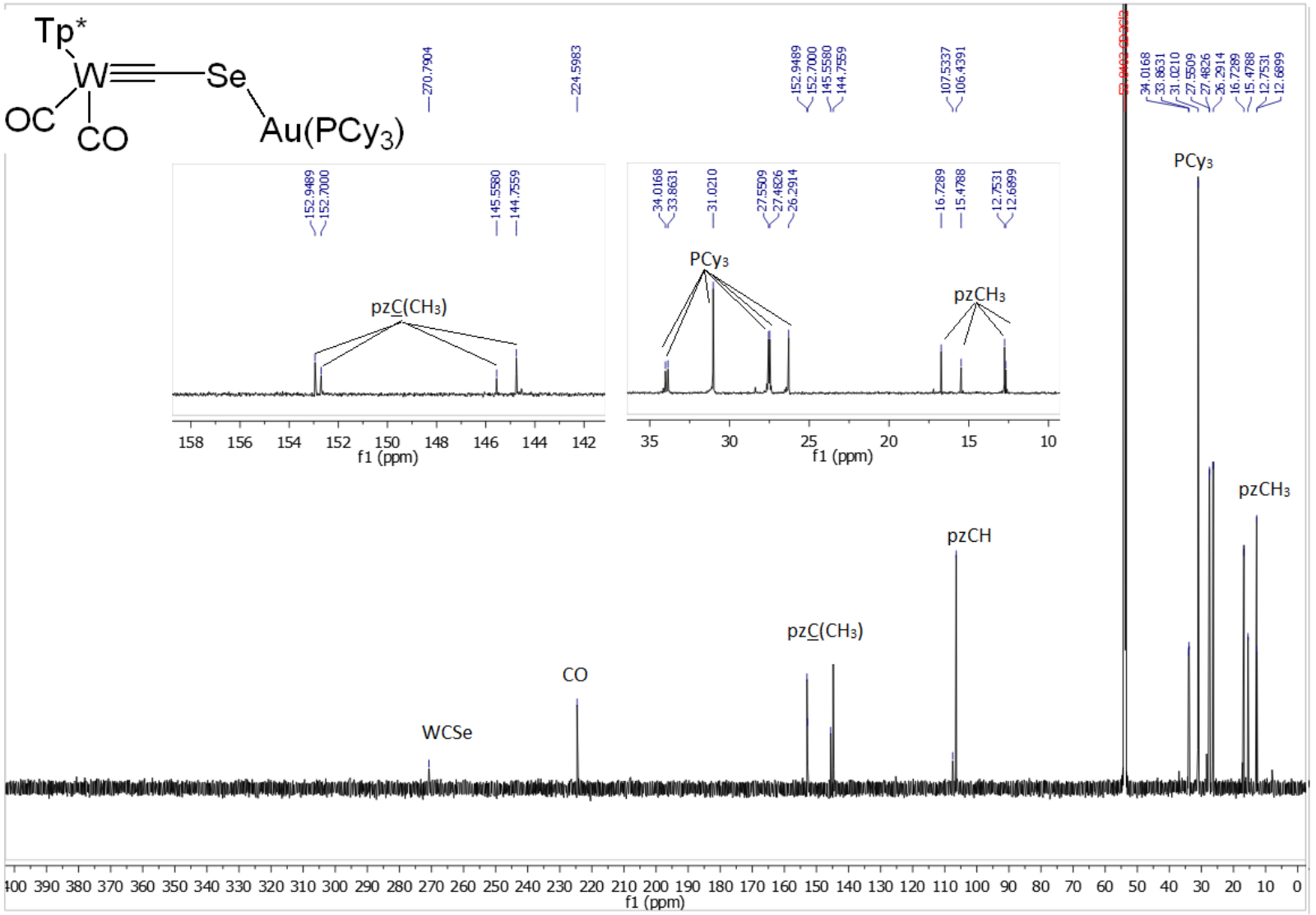


MS (ESI, +ve ion) for [W{≡CSeAu(PPh$_3$)$_3$}(CO)$_2$(Tp*)] (**8**).



^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, δ) for [W(≡CSeAuPCy$_3$)(CO)$_2$(Tp*)] (**9**).



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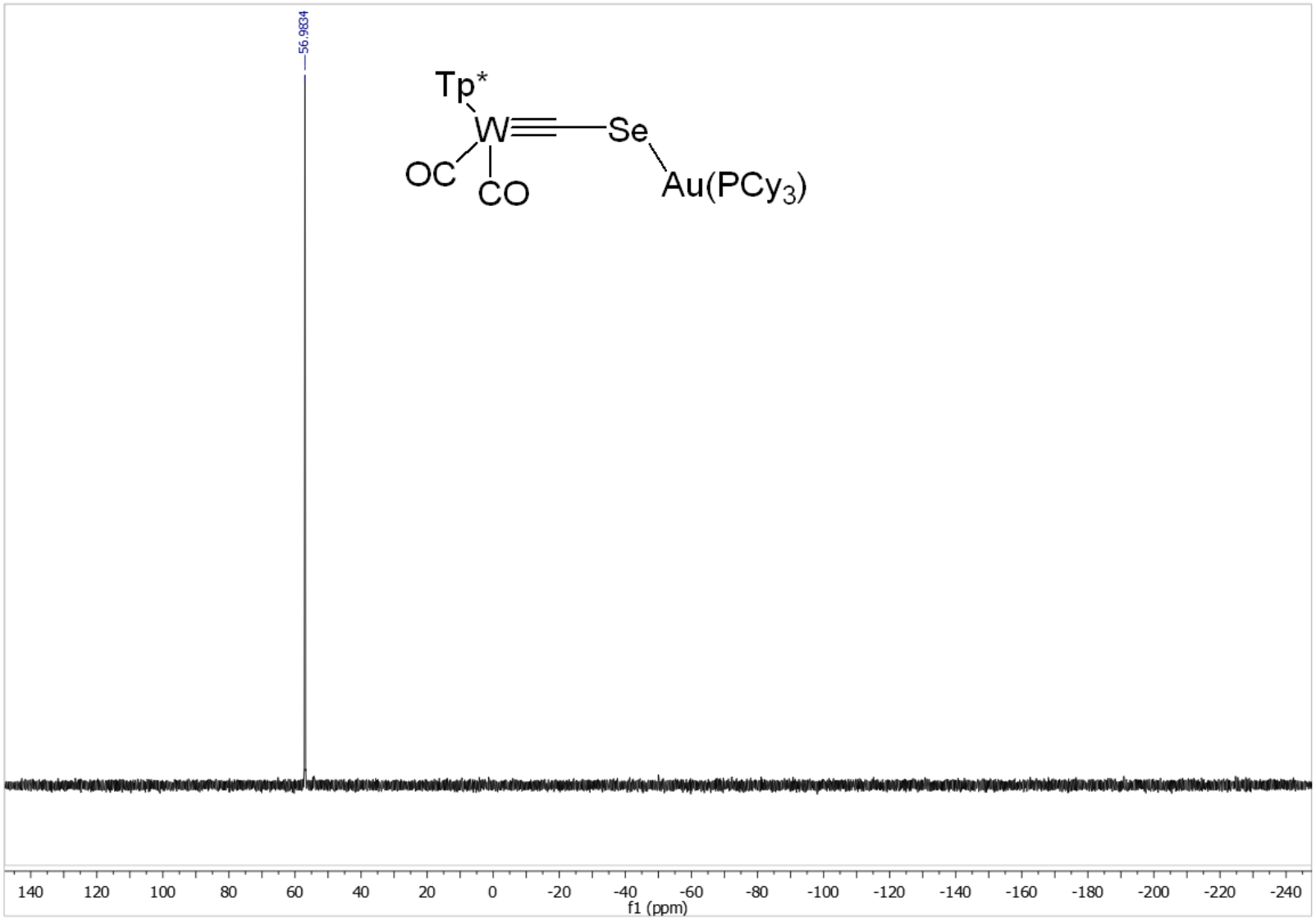

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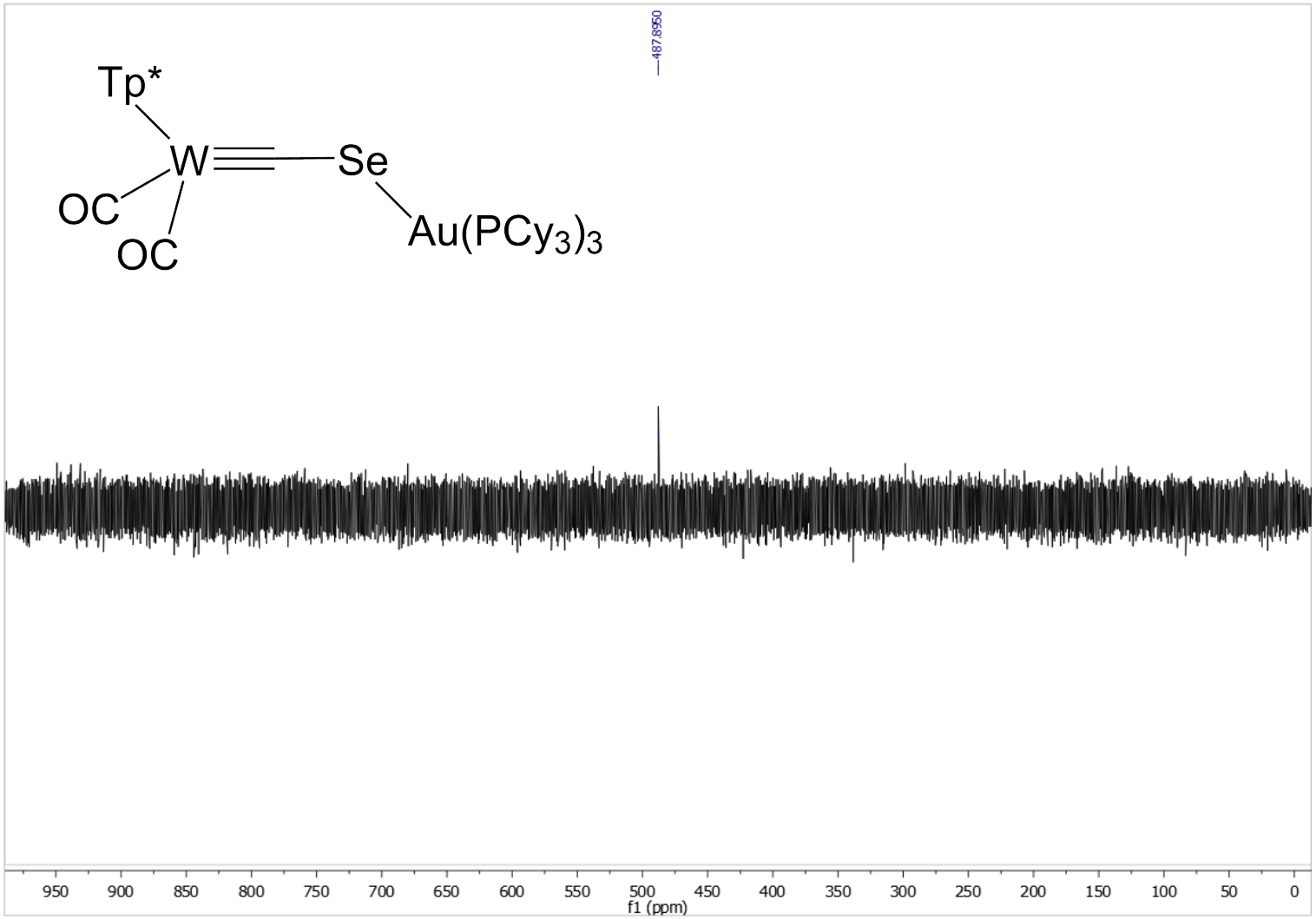

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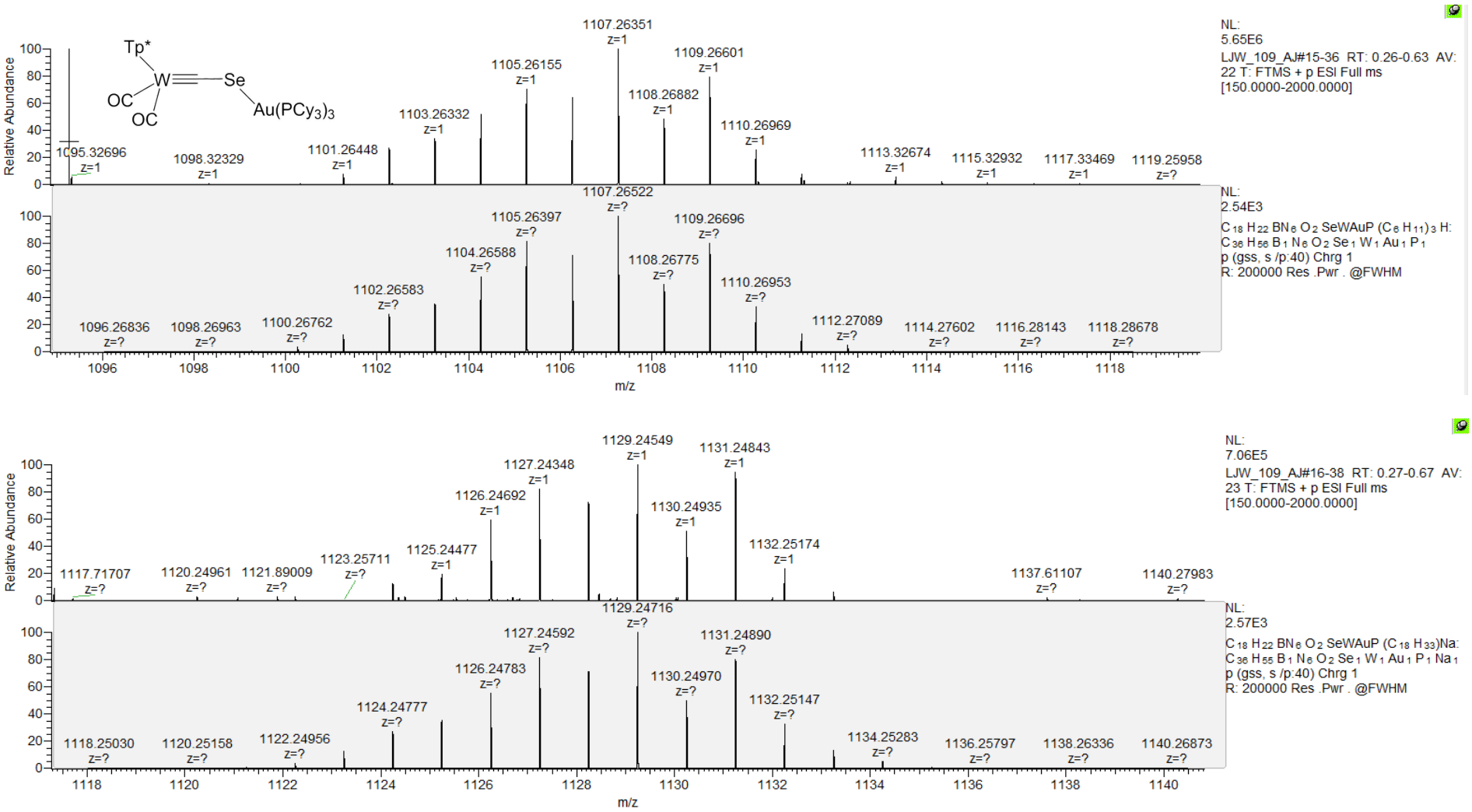

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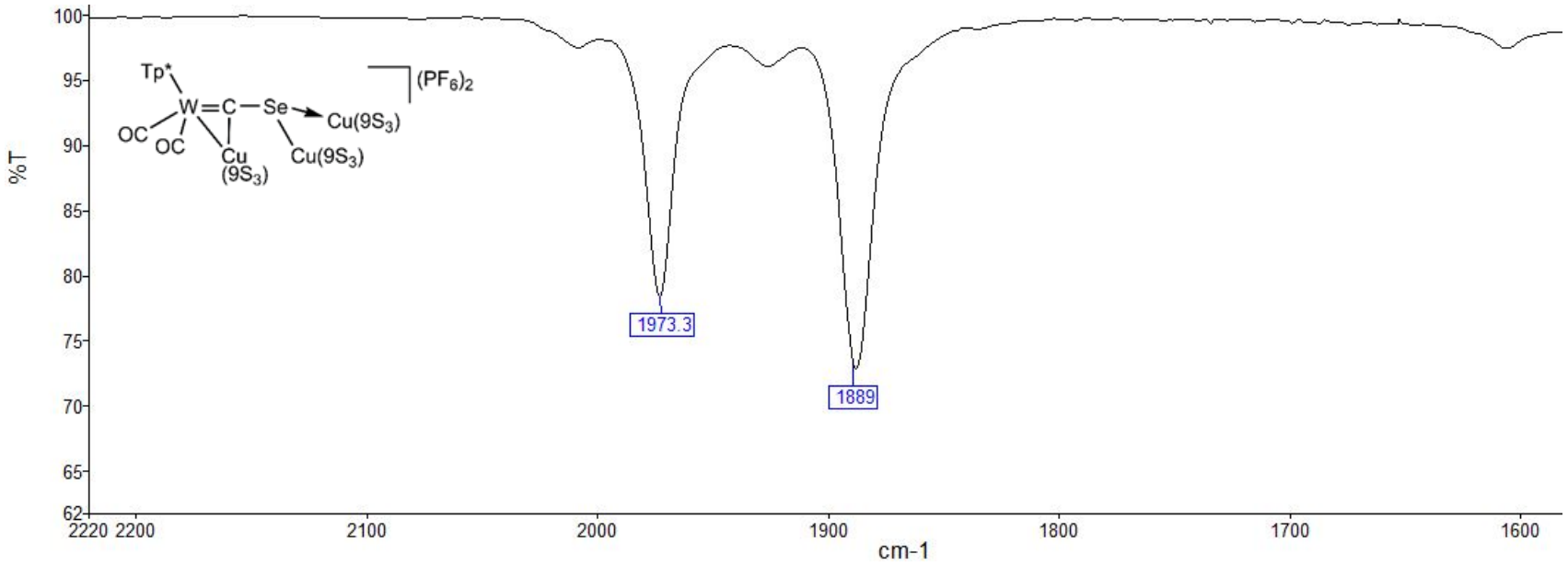
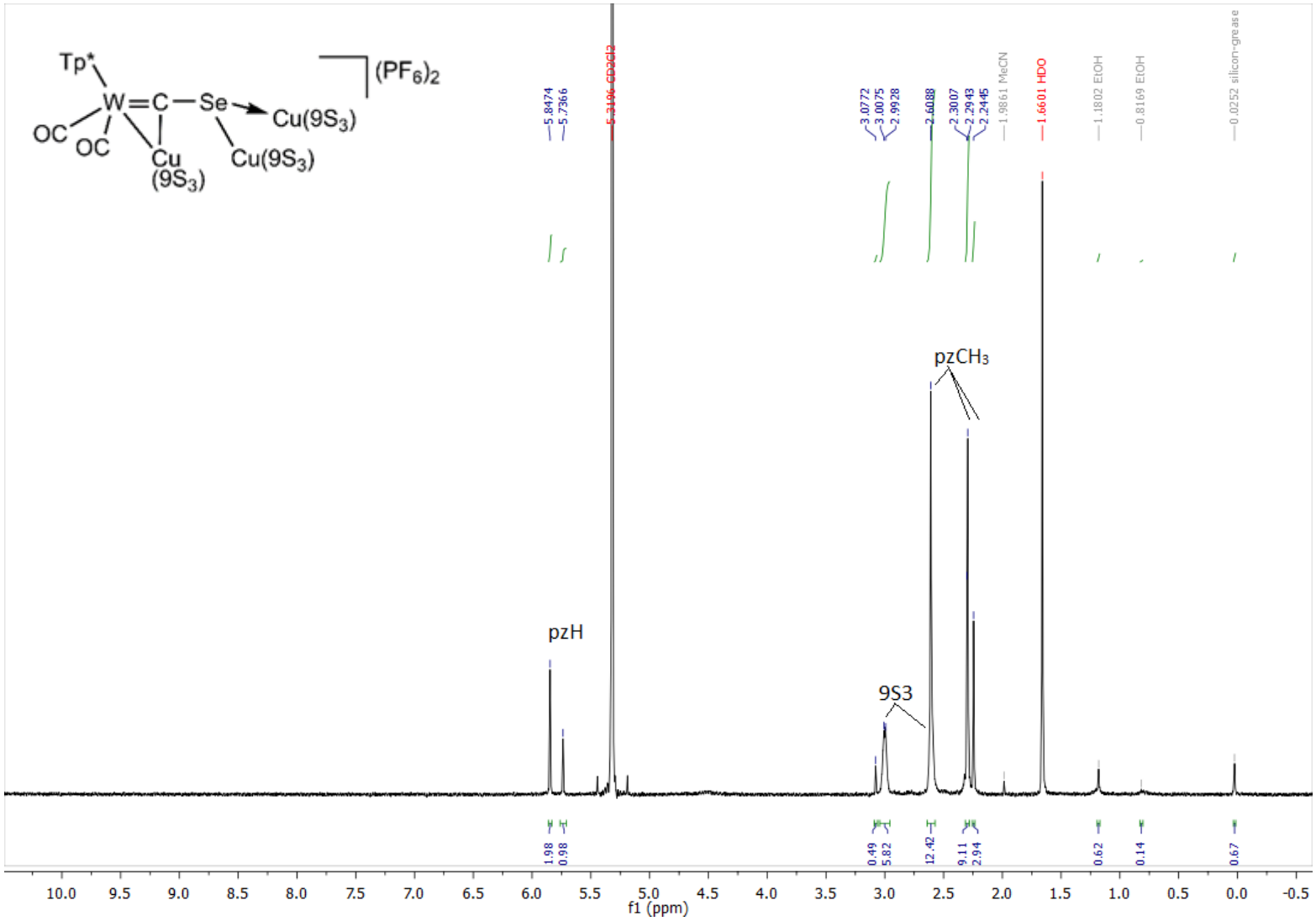
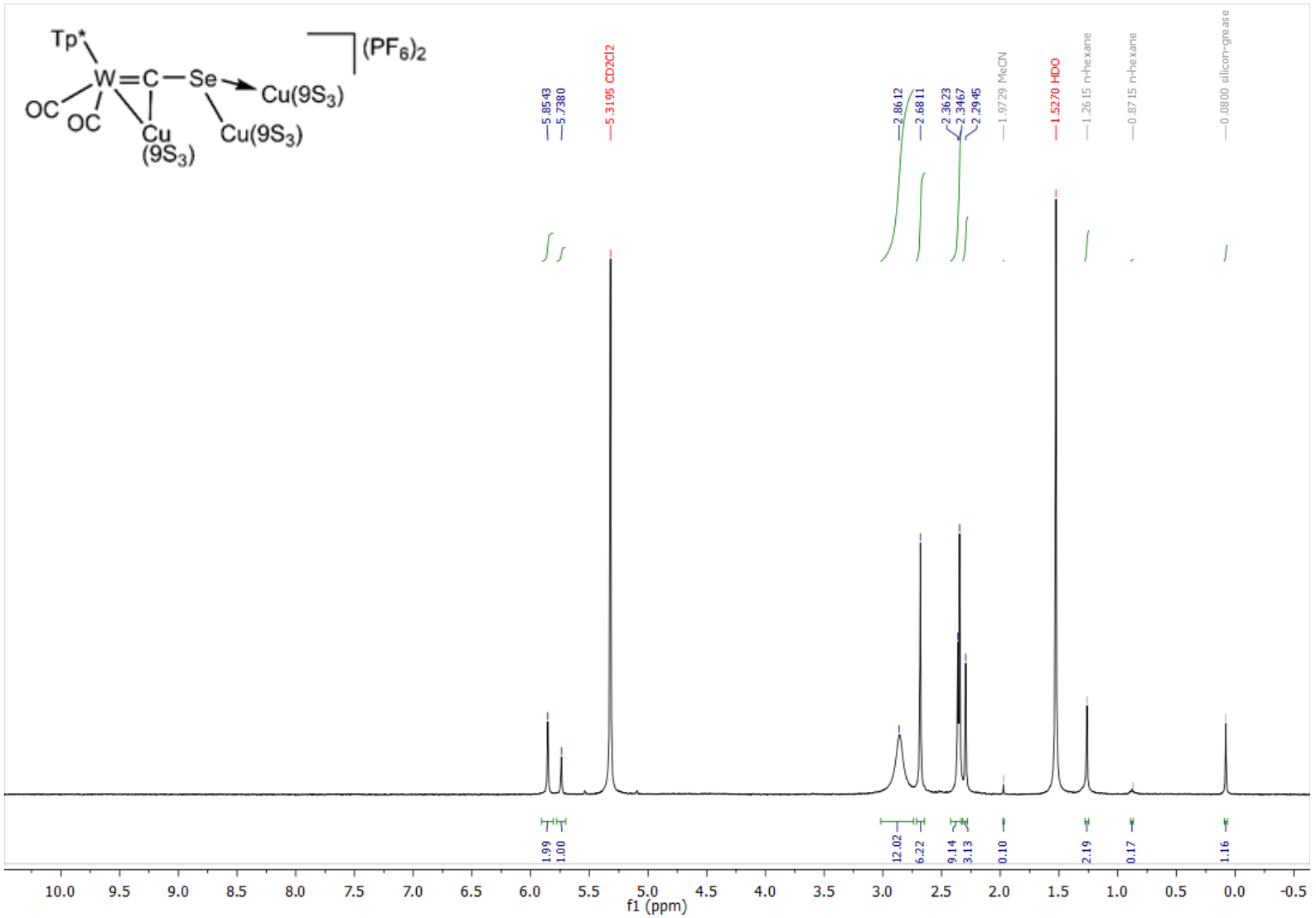


IR (CH_2Cl_2, cm^{-1}) for $[WCu[9S_3]\{\mu\text{-}CSe(Cu[9S_3])_2\}(CO)_2(Tp^*)](PF_6)_2$ (**10**).



^{1}H NMR (700 MHz, CD_2Cl_2, 210 K, δ) for $[WCu[9S_3]\{\mu\text{-}CSe(Cu[9S_3])_2\}(CO)_2(Tp^*)](PF_6)_2$ (**10**).



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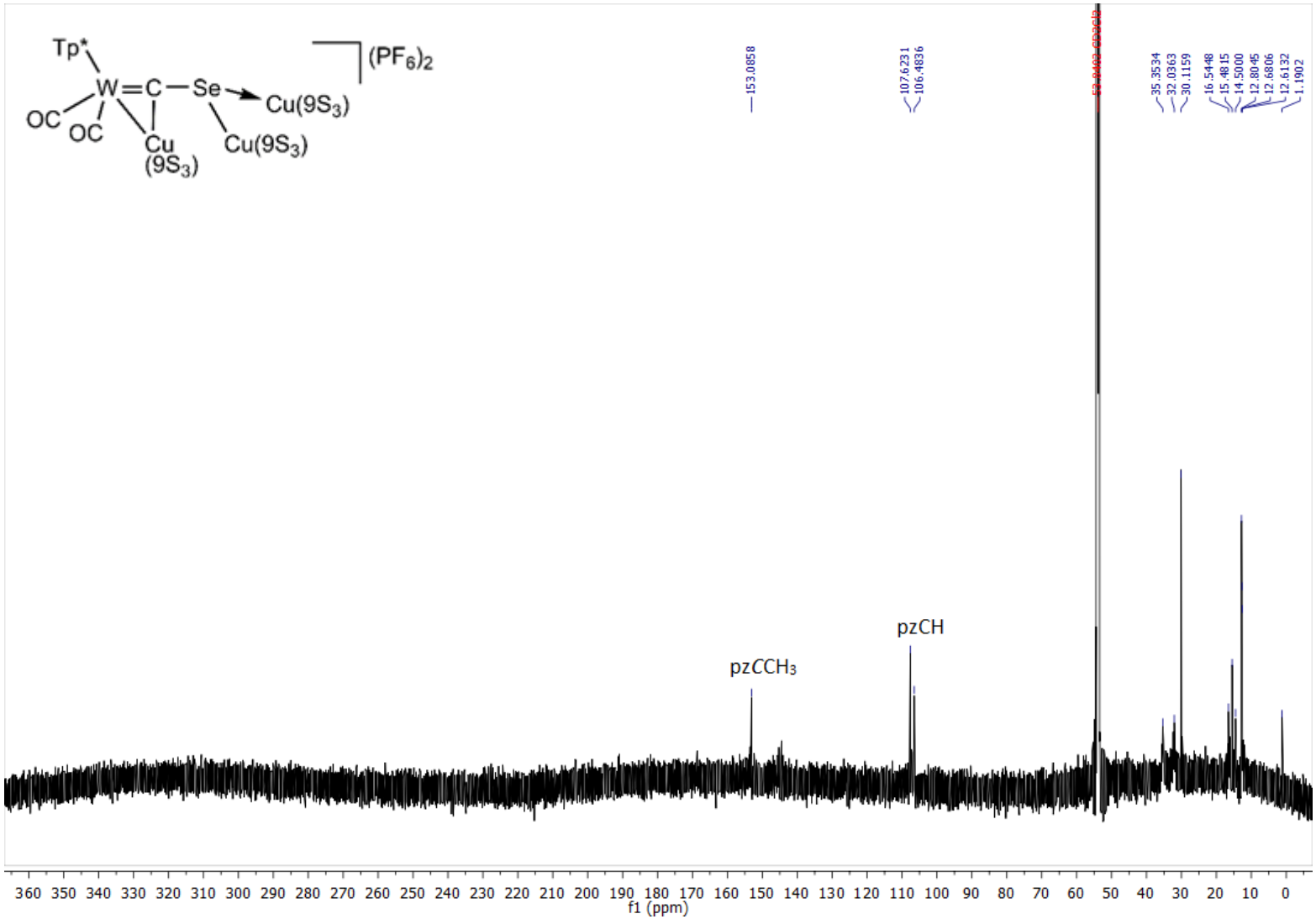
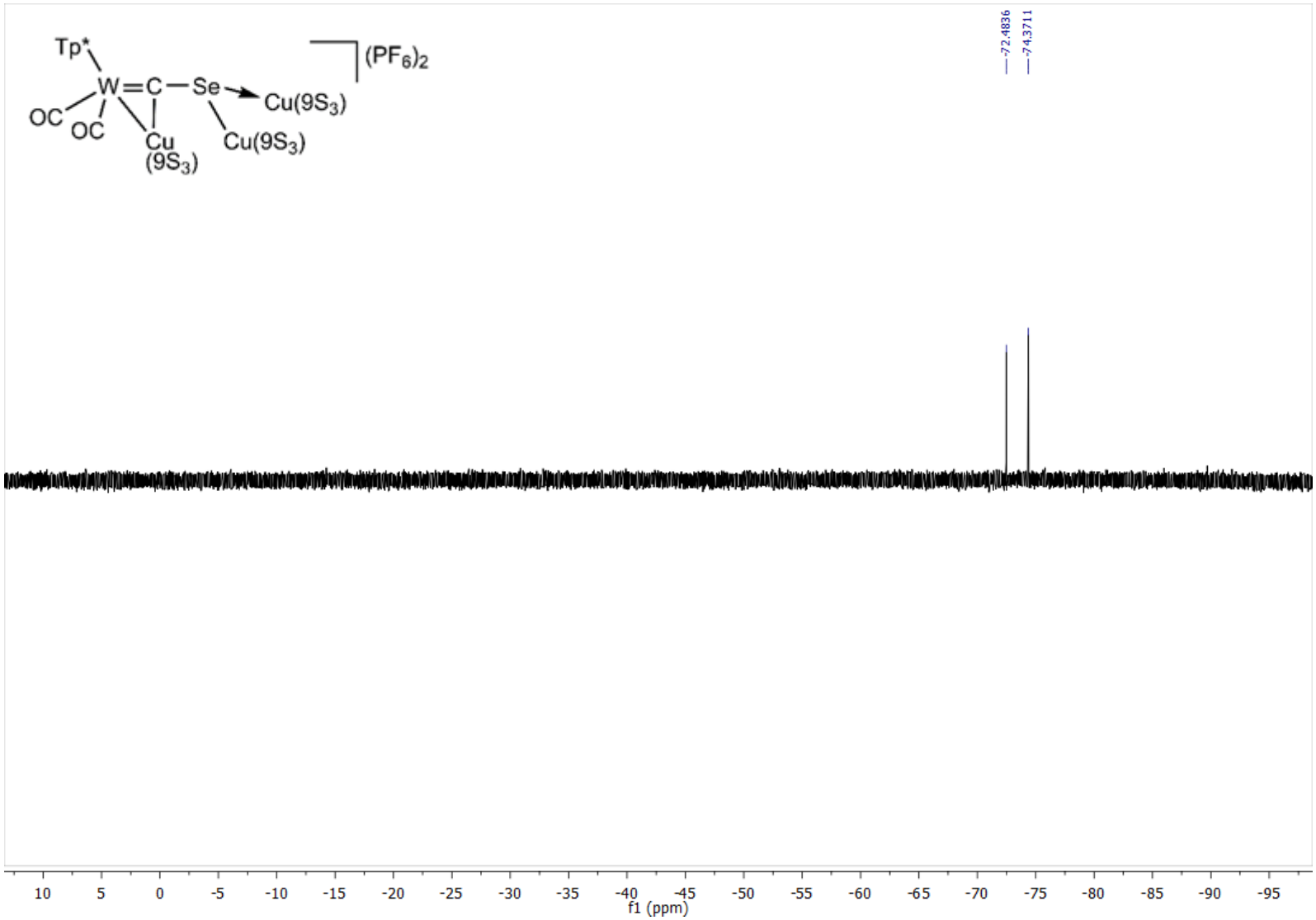
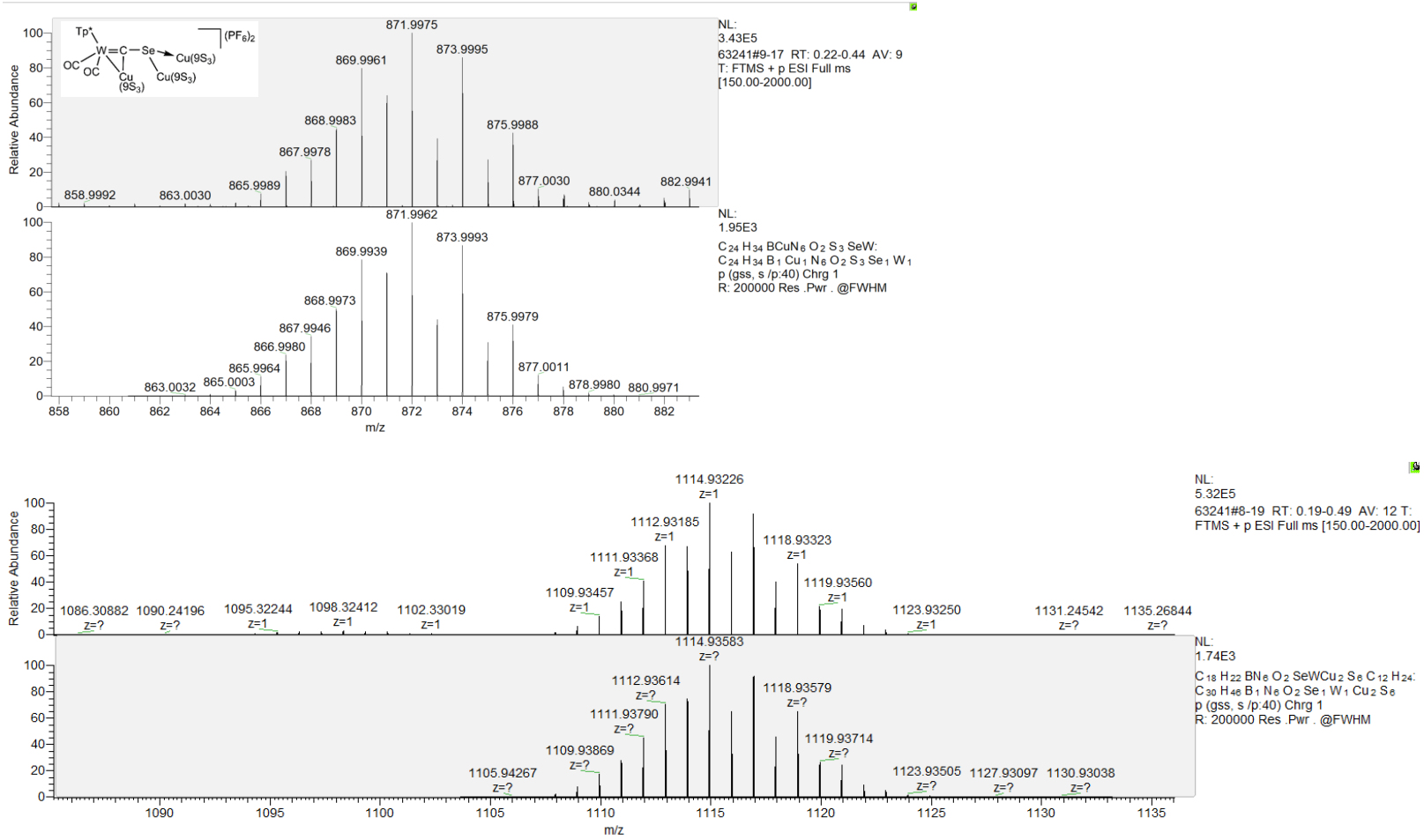


$^{13}C\{^{1}H\}$ NMR (151 MHz, CD_2Cl_2, 298 K, δ) for $[WCu[9S_3]\{\mu\text{-}CSe(Cu[9S_3])_2\}(CO)_2(Tp^*)](PF_6)_2$ (**10**).



$^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2, 300 K, δ): for $[WCu[9S_3]\{\mu\text{-}CSe(Cu[9S_3])_2\}(CO)_2(Tp^*)](PF_6)_2$ (**10**).



MS (ESI, +ve ion) for $[WCu[9S_3]\{\mu\text{-}CSe(Cu[9S_3])_2\}(CO)_2(Tp^*)](PF_6)_2$ (**10**).