**Which DFT factors influence the accuracy of 1H, 13C and 195Pt NMR chemical shift predictions in organopolymetallic square-planed complexes? New scaling parameters for homo- and hetero- multimetallic compounds and their direct applications**

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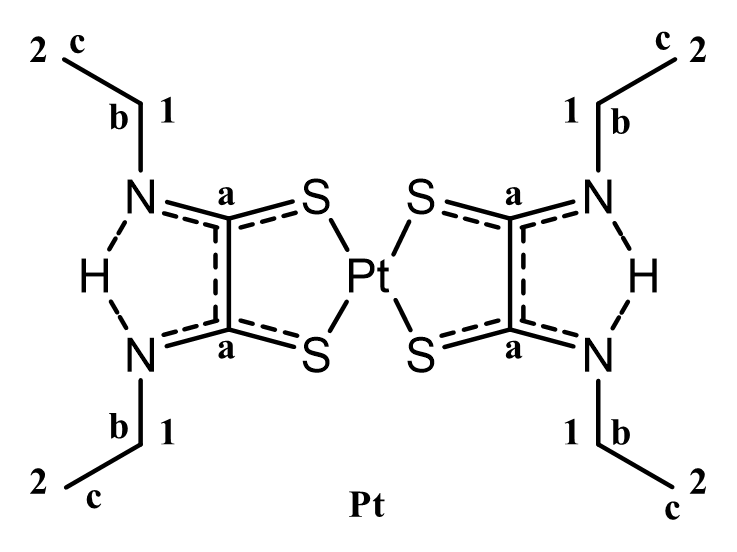
**Cartesian coordinates**…………………………………………………………………………………………………………………………….…45

**Table S1.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pt** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1 | 27.6943 | 3.7731 | 3.6700 | 0.1031 | 0.1448 |
| 2 | 30.3848 | 1.1935 | 1.3800 | 0.1865 |

**Table S2.** Experimental and predicted 13C NMR chemical shifts (in ppm). Letters are related to carbon resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pt** (13C) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| a | -7.7641 | 178.9844 | 179.6000 | 0.6156 | 1.0992 |
| b | 140.5227 | 43.0911 | 44.1500 | 1.0589 |
| c | 174.1472 | 12.2769 | 13.9000 | 1.6231 |

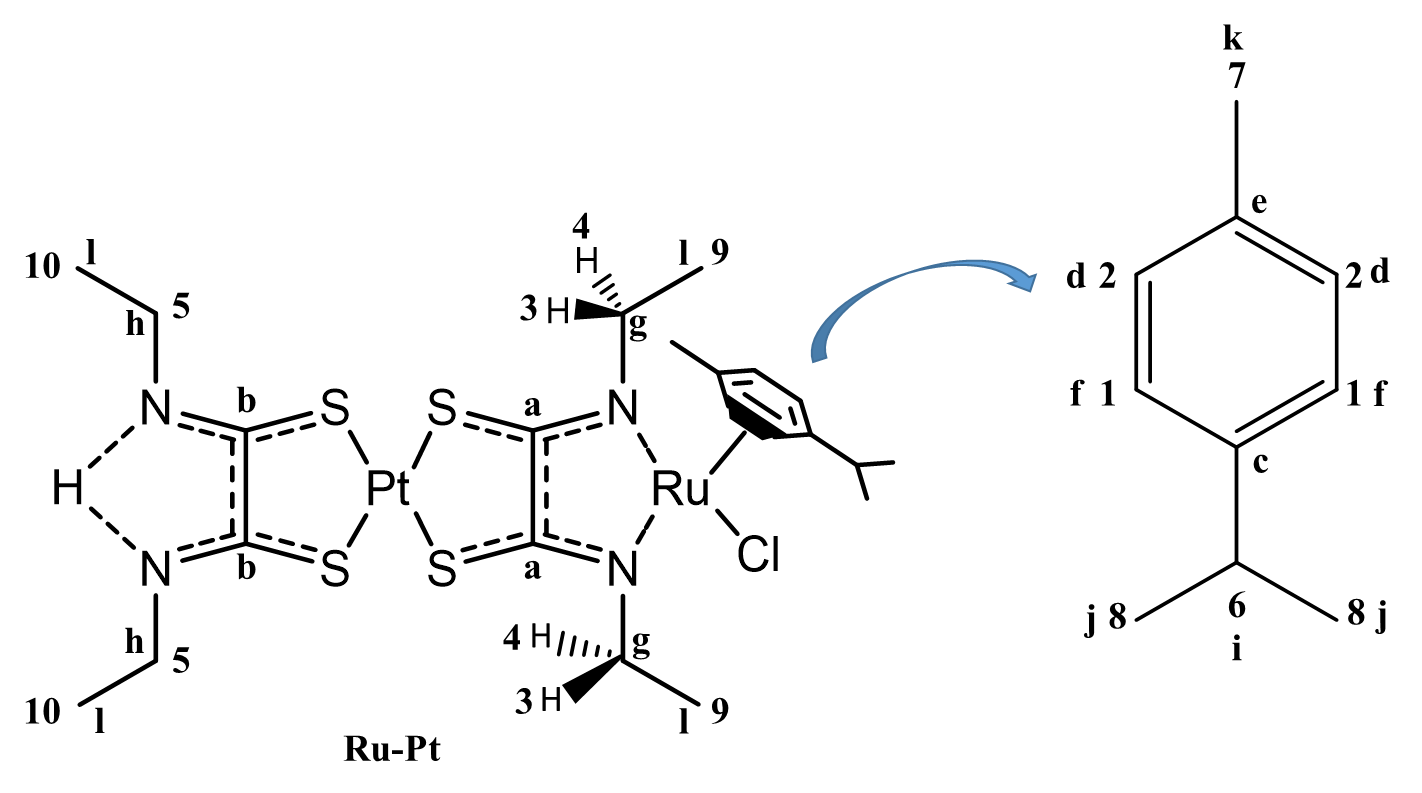


**Table S3.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Ru-Pt** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1 | 26.4188 | 4.9959 | 5.4400 | 0.4441 | 0.2451 |
| 2 | 26.7403 | 4.6877 | 5.1600 | 0.4723 |
| 3 | 27.2177 | 4.2300 | 4.4900 | 0.2600 |
| 4 | 27.2713 | 4.1785 | 4.0000 | 0.1785 |
| 5 | 27.7460 | 3.7234 | 3.6200 | 0.1034 |
| 6 | 28.3999 | 3.0965 | 2.7600 | 0.3365 |
| 7 | 29.5593 | 1.9849 | 2.2500 | 0.2651 |
| 8 | 30.2948 | 1.2797 | 1.1800 | 0.0997 |
| 9 | 30.2415 | 1.3308 | 1.4400 | 0.1092 |
| 10 | 30.4222 | 1.1575 | 1.3400 | 0.1825 |

**Table S4.** Experimental and predicted 13C NMR chemical shifts (in ppm). Letters are related to carbon resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Ru-Pt** (13C) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| a | -8.2056 | 179.3890 | 180.5000 | 1.1110 | 3.1163 |
| b | -18.4786 | 188.8034 | 188.9200 | 0.1166 |
| c | 62.7236 | 114.3879 | 103.4400 | 10.9479 |
| d | 87.7892 | 91.4172 | 84.8400 | 6.5772 |
| e | 89.2160 | 90.1097 | 101.7200 | 11.6103 |
| f | 97.6523 | 82.3785 | 83.1500 | 0.7715 |
| g | 128.3657 | 54.2320 | 56.9800 | 2.7480 |
| h | 140.5806 | 43.0381 | 44.1400 | 1.1019 |
| i | 152.3857 | 32.2196 | 31.2500 | 0.9696 |
| j | 163.4820 | 22.0507 | 22.5500 | 0.4993 |
| k | 167.6058 | 18.2715 | 19.0500 | 0.7785 |
| l | 174.3655 | 12.0768 | 12.2400 | 0.1632 |

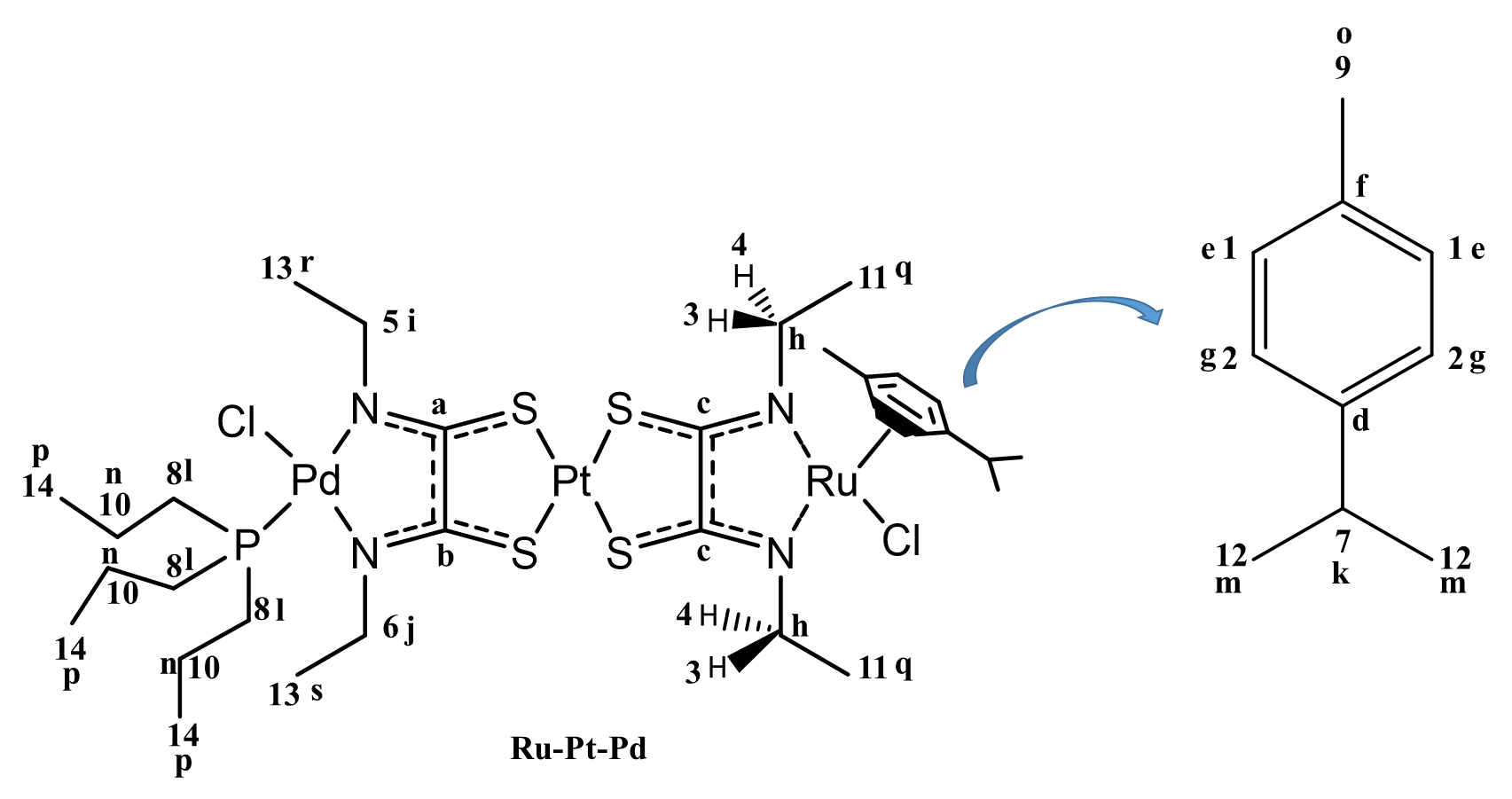
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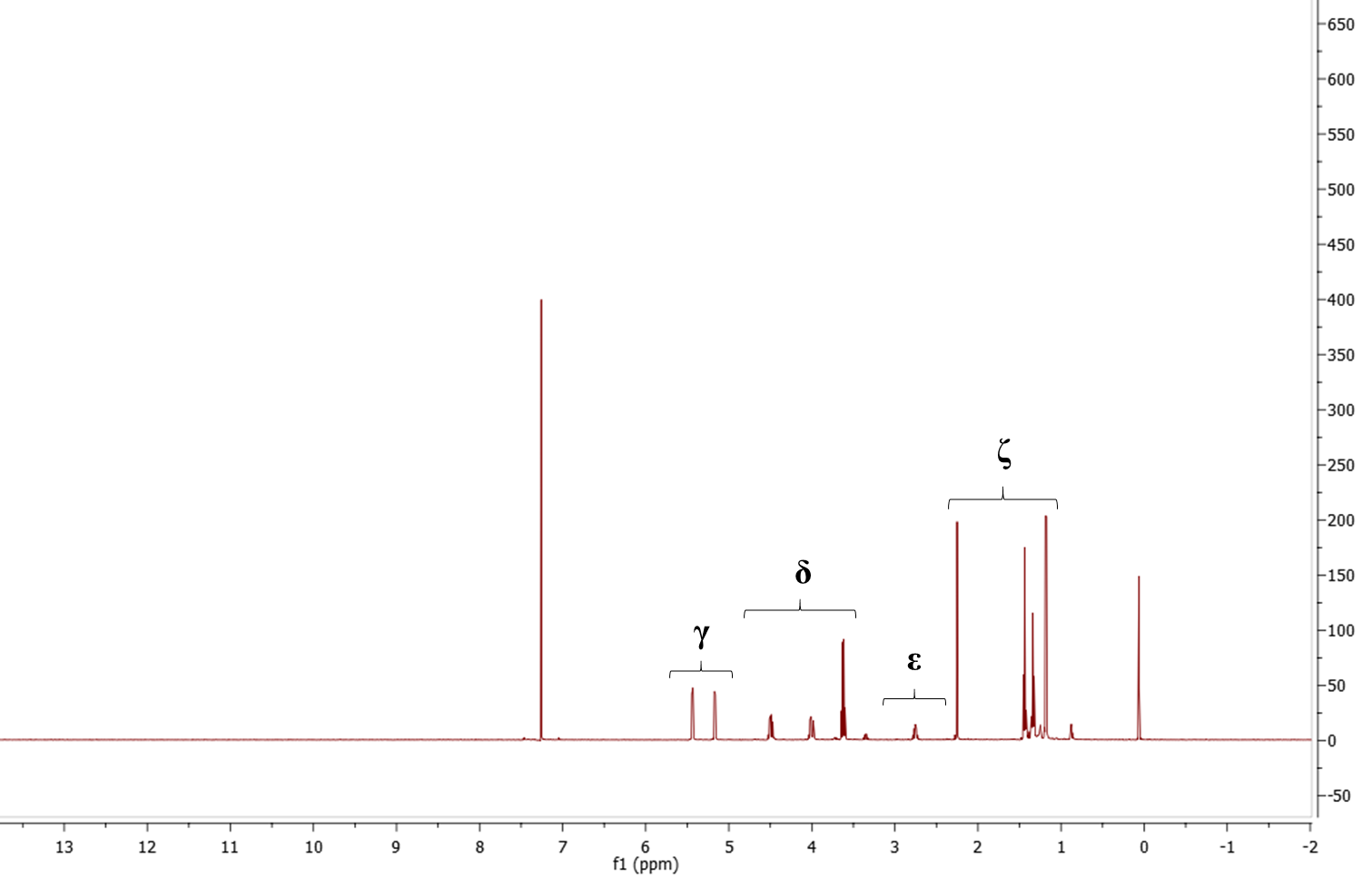
**Table S5.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Ru-Pt-Pd** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1 | 26.4526 | 4.9635 | 5.4300 | 0.4665 | 0.1940 |
| 2 | 26.7294 | 4.6981 | 5.1600 | 0.4619 |
| 3 | 27.2277 | 4.2204 | 4.4600 | 0.2396 |
| 4 | 27.3029 | 4.1483 | 3.9800 | 0.1683 |
| 5 | 27.4835 | 3.9751 | 3.7200 | 0.2551 |
| 6 | 27.9120 | 3.5643 | 3.5600 | 4.2857e-3 |
| 7 | 28.3592 | 3.1355 | 2.7500 | 0.3855 |
| 8 | 29.5398 | 2.0035 | 1.7900 | 0.2135 |
| 9 | 29.5580 | 1.9861 | 2.2400 | 0.2539 |
| 10 | 29.9539 | 1.6065 | 1.6500 | 0.0435 |
| 11 | 30.2637 | 1.3095 | 1.4100 | 0.1005 |
| 12 | 30.3122 | 1.2630 | 1.2400 | 0.0230 |
| 13 | 30.4049 | 1.1742 | 1.1800 | 5.8389e-3 |
| 14 | 30.6023 | 0.9848 | 1.0800 | 0.0952 |

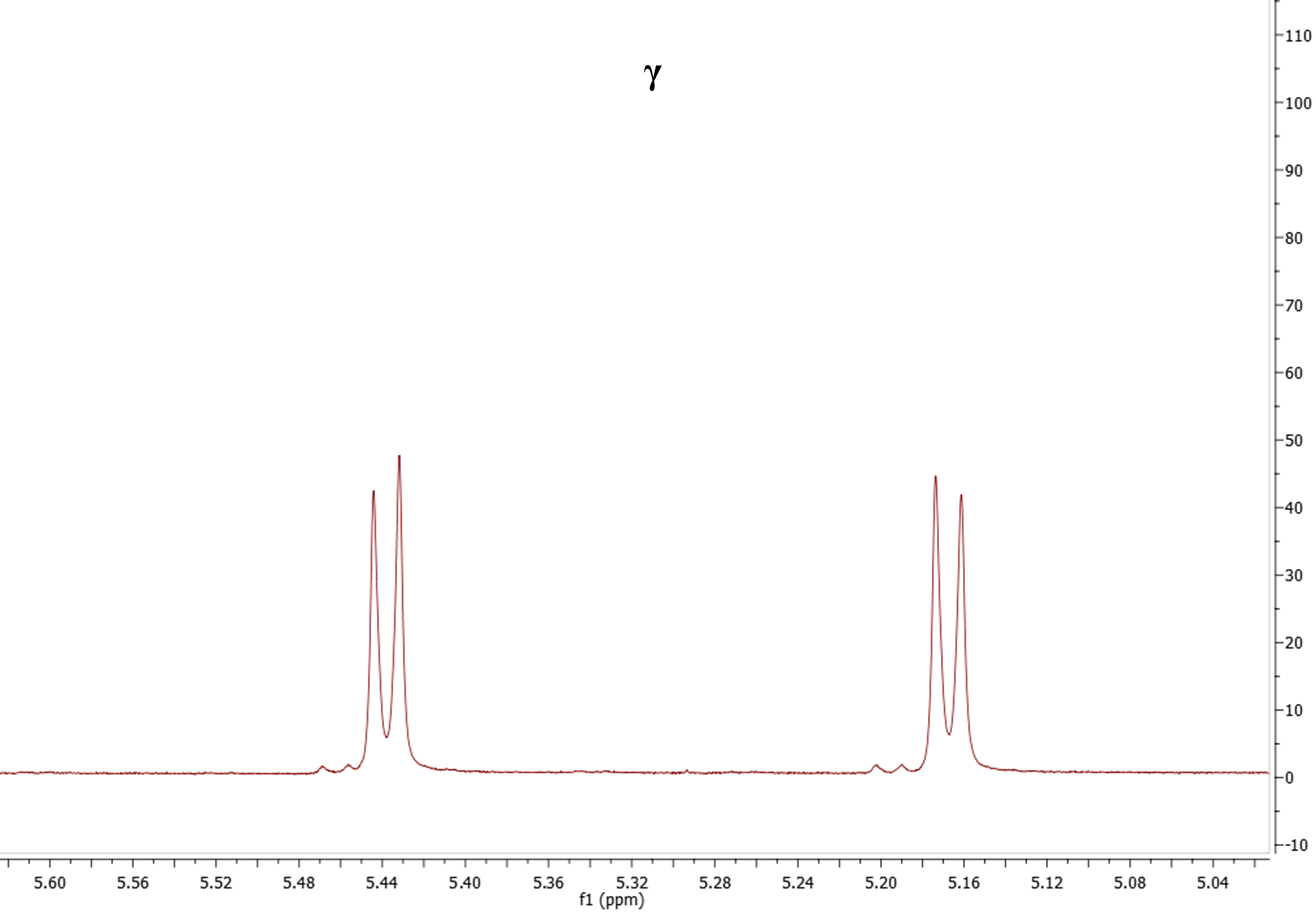
**Table S6.** Experimental and predicted 13C NMR chemical shifts (in ppm). Letters are related to carbon resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Ru-Pt-Pd** (13C) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| a | -27.8528 | 197.3942 | 197.9800 | 0.5858 | 2.2875 |
| b | -21.8365 | 191.8807 | 192.2800 | 0.3993 |
| c | -18.5817 | 188.8979 | 189.0500 | 0.1521 |
| d | 63.5497 | 113.6309 | 103.1700 | 10.4609 |
| e | 88.7370 | 90.5487 | 84.7900 | 5.7587 |
| f | 88.5961 | 90.6778 | 101.4800 | 10.8022 |
| g | 96.7324 | 83.2215 | 83.1100 | 0.1115 |
| h | 128.4780 | 54.1292 | 56.8900 | 2.7608 |
| i | 134.6435 | 48.4789 | 51.8100 | 3.3311 |
| j | 136.3651 | 46.9012 | 47.6000 | 0.6988 |
| k | 152.8785 | 31.7680 | 31.2300 | 0.5380 |
| l | 156.7023 | 28.2637 | 25.6500 | 2.6137 |
| m | 163.5654 | 21.9743 | 22.5500 | 0.5757 |
| n | 165.2104 | 20.4667 | 18.2200 | 2.2467 |
| o | 167.7370 | 18.1513 | 19.0400 | 0.8887 |
| p | 169.4792 | 16.5547 | 15.8500 | 0.7047 |
| q | 174.3313 | 12.1081 | 12.2300 | 0.1219 |
| r | 173.6191 | 12.7608 | 12.1300 | 0.6308 |
| s | 173.9031 | 12.5005 | 12.4200 | 0.0805 |

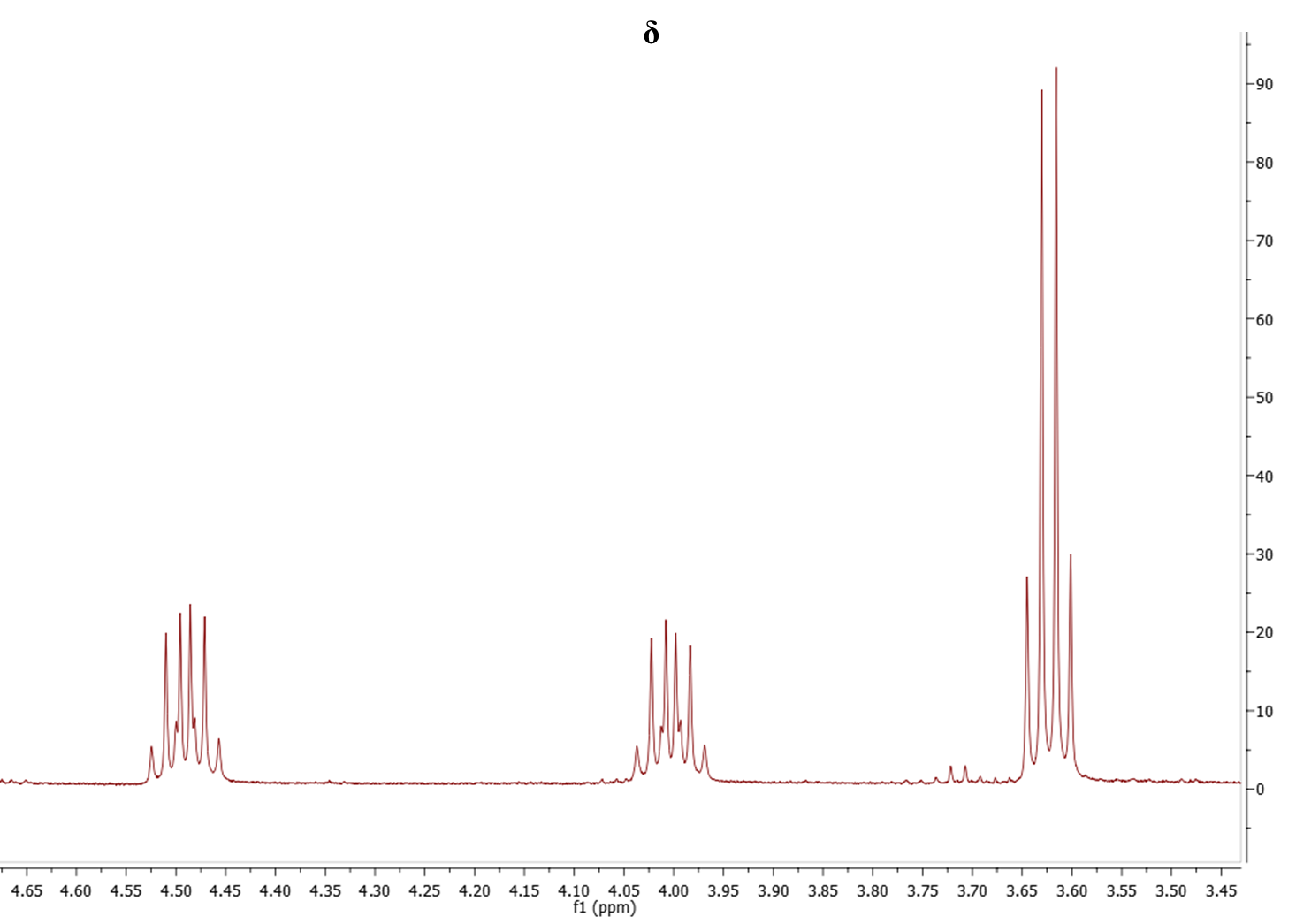
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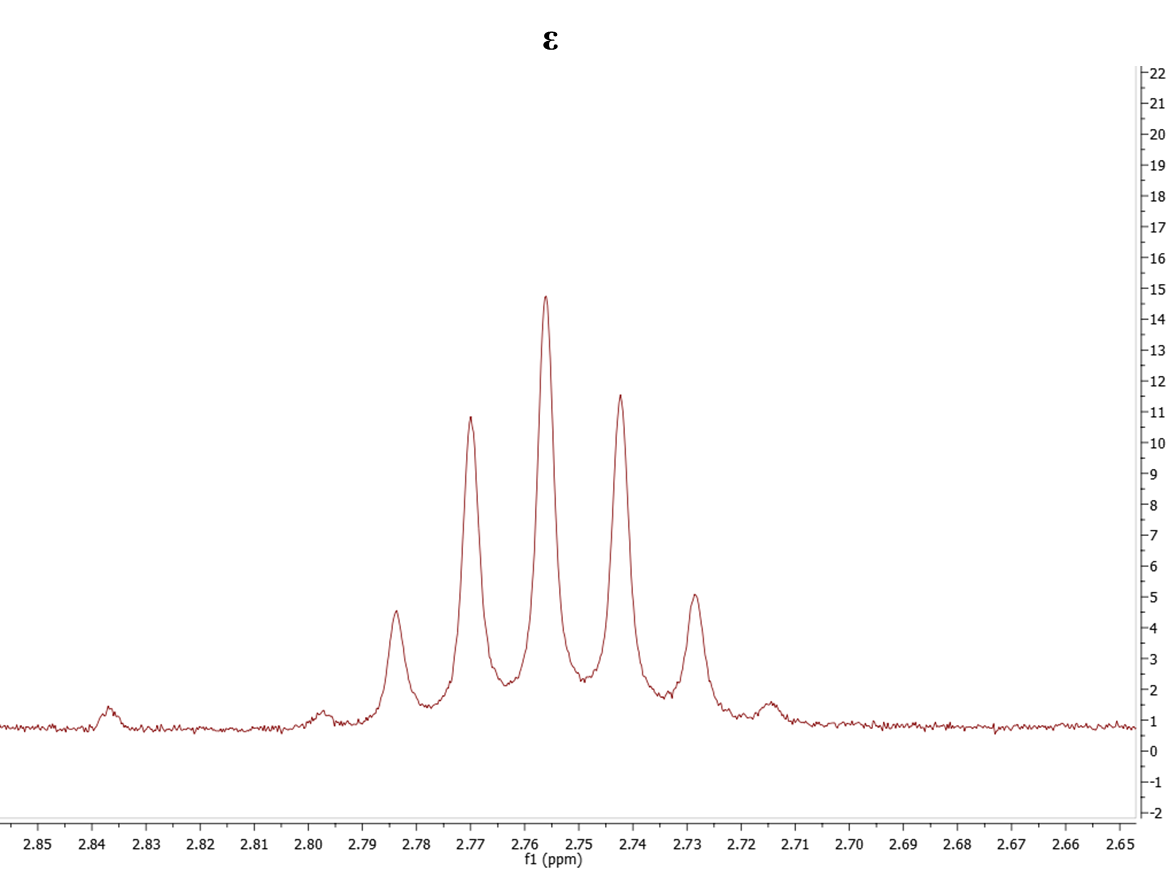
**Figure S1.** 1H NMR spectrum of **Ru-Pt** recorded in chloroform.



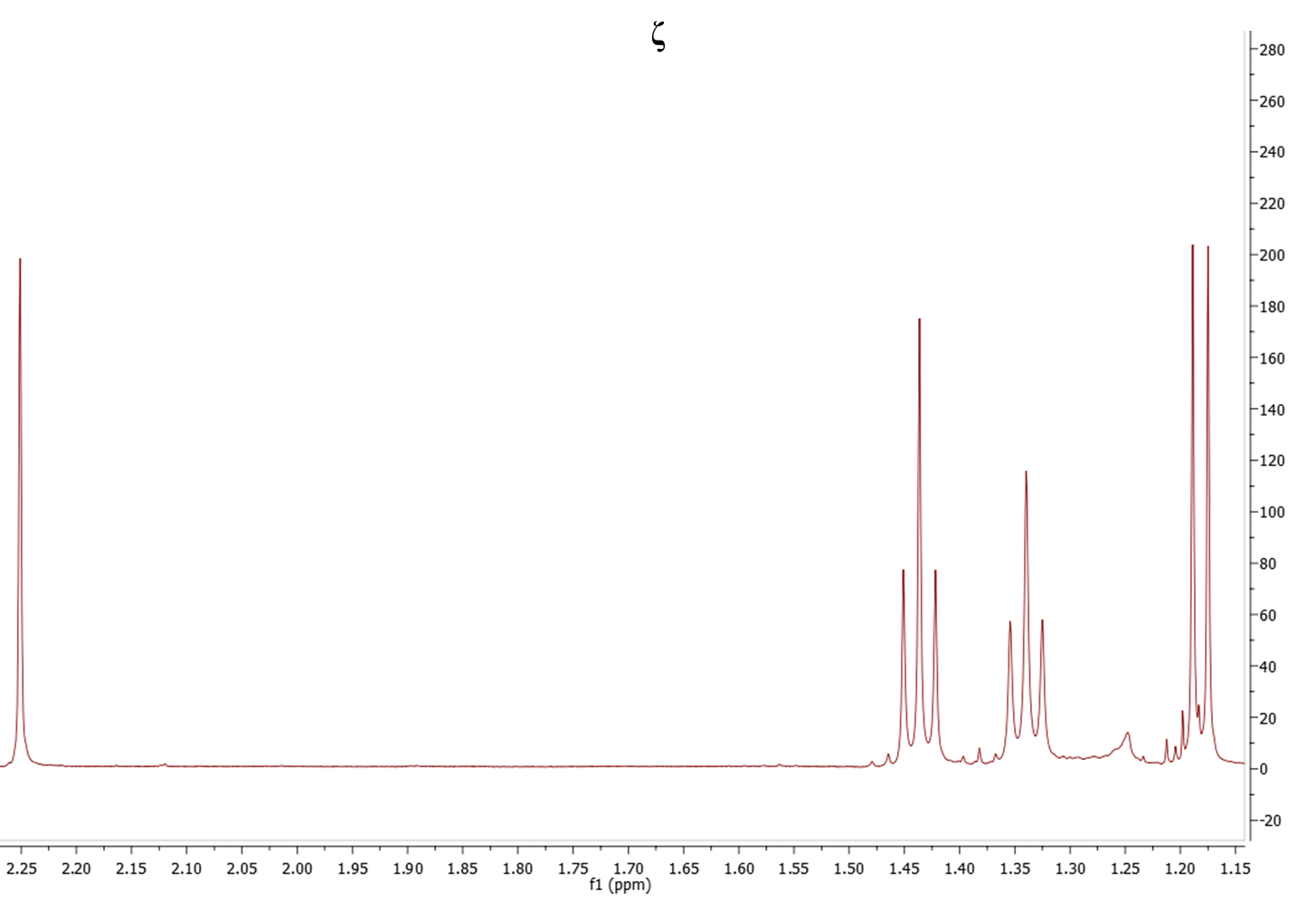
**Figure S2.** 5.60-5.04 ppm expansion of **γ** 1H spectrum section**.**

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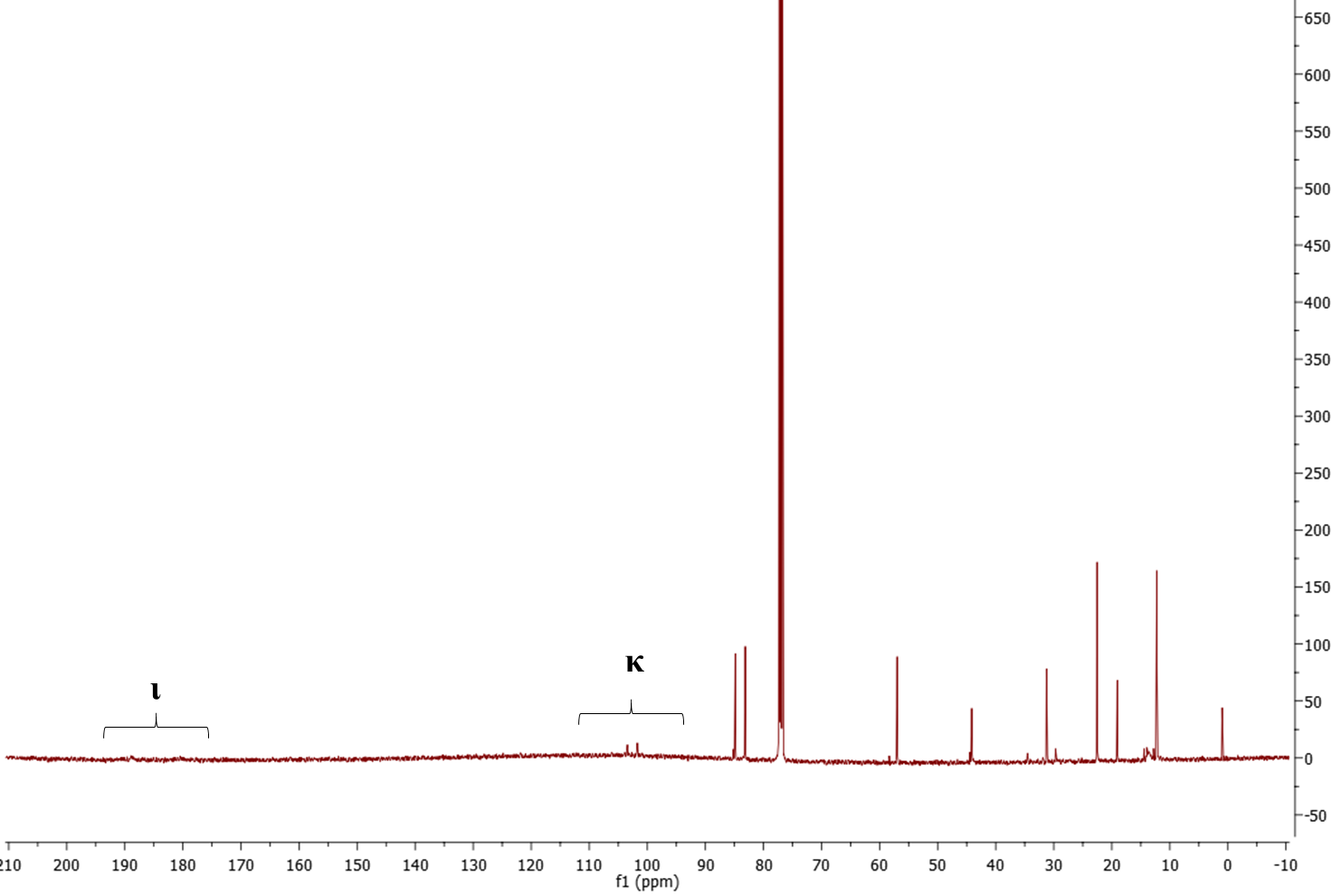
**Figure S3.** 4.65-3.45 ppm expansion of **δ** 1H spectrum section**.**

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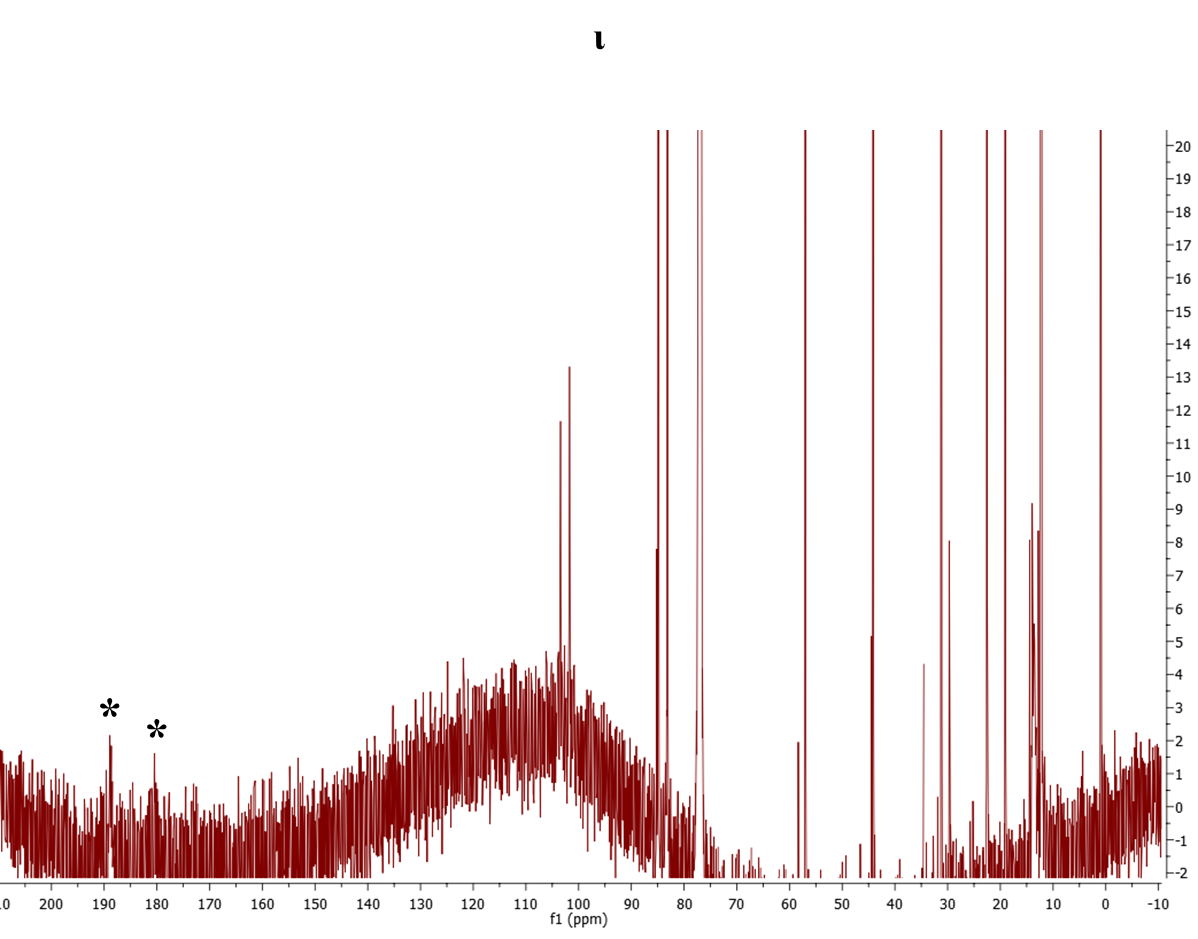
**Figure S4.** 2.85-2.65 ppm expansion of **ε** 1H spectrum section**.**

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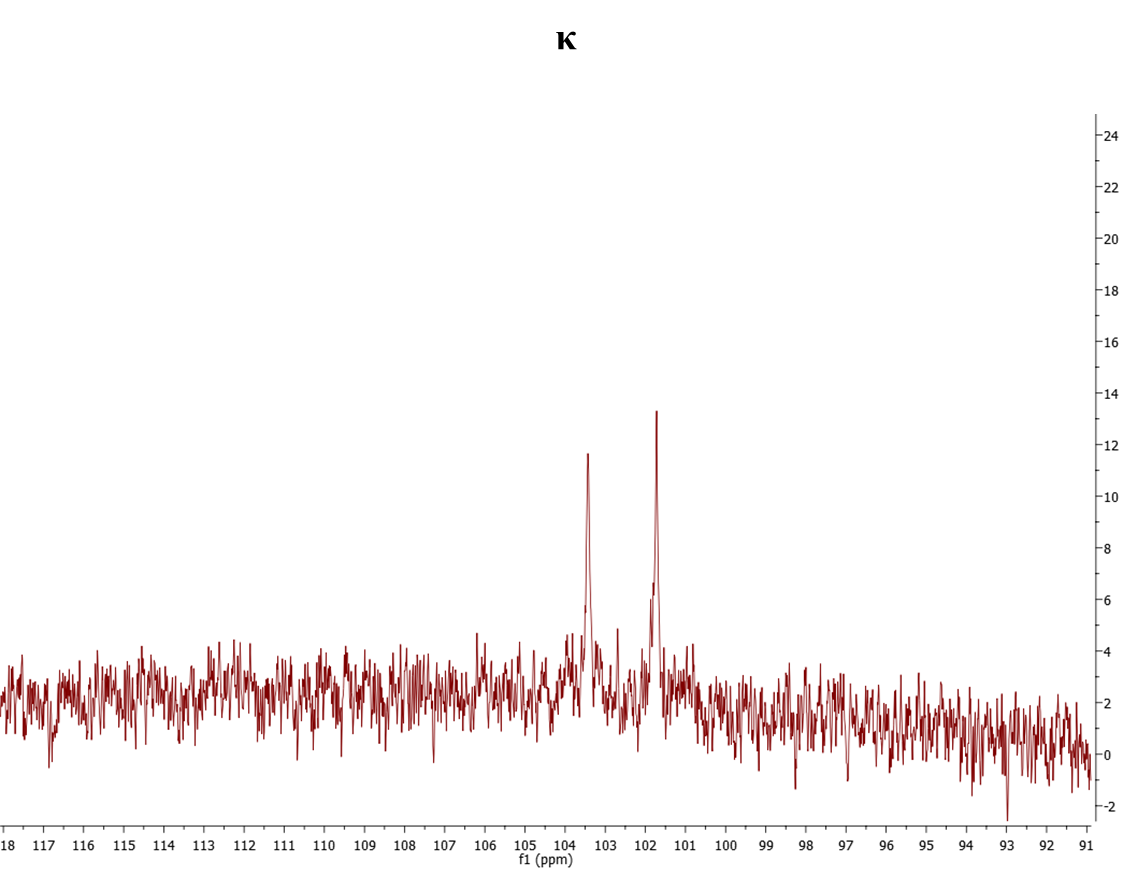
**Figure S5.** 2.25-1.15 ppm expansion of **ζ** 1H spectrum section**.**

****

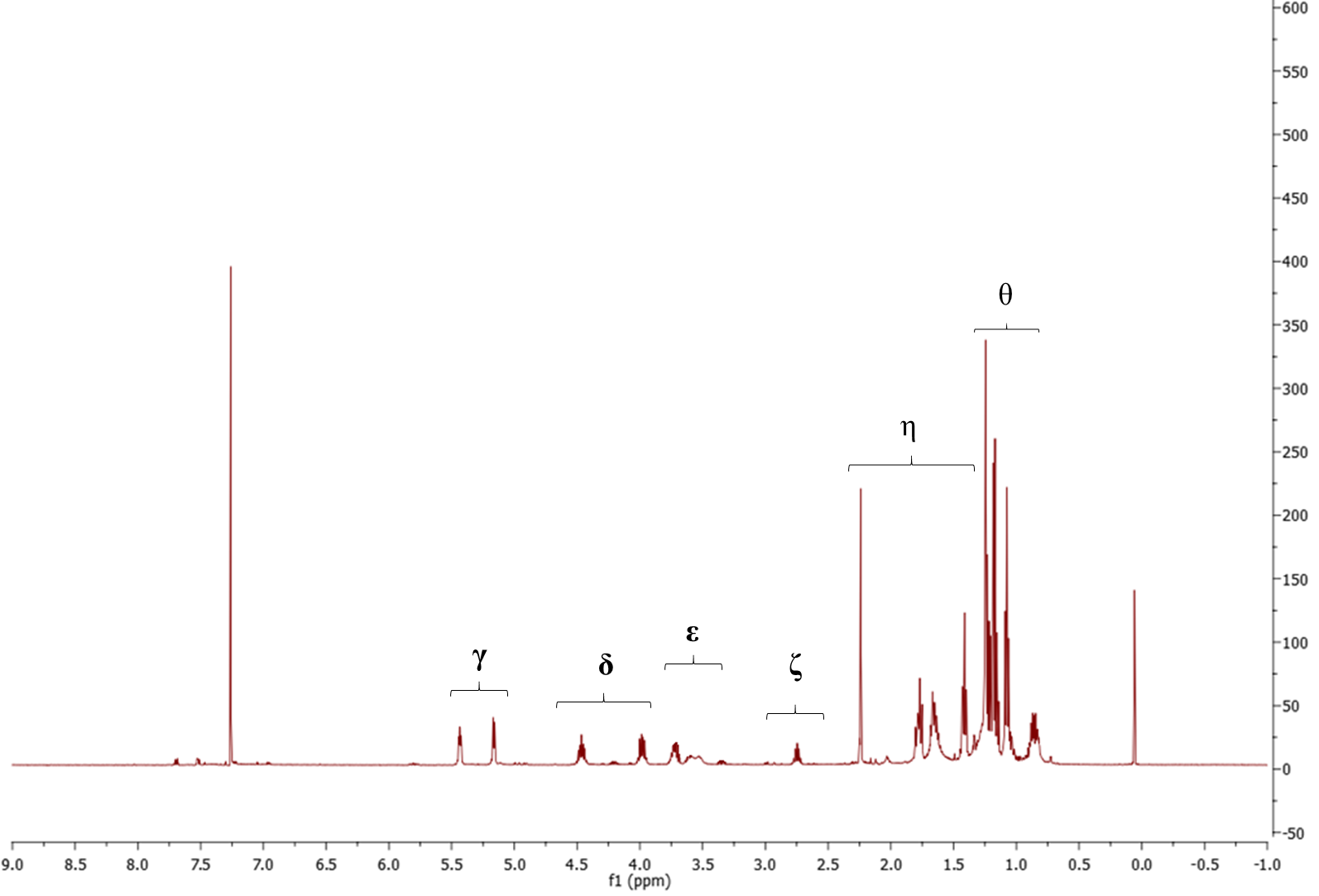
**Figure S6.** 13C NMR spectrum of **Ru-Pt** recorded in chloroform.

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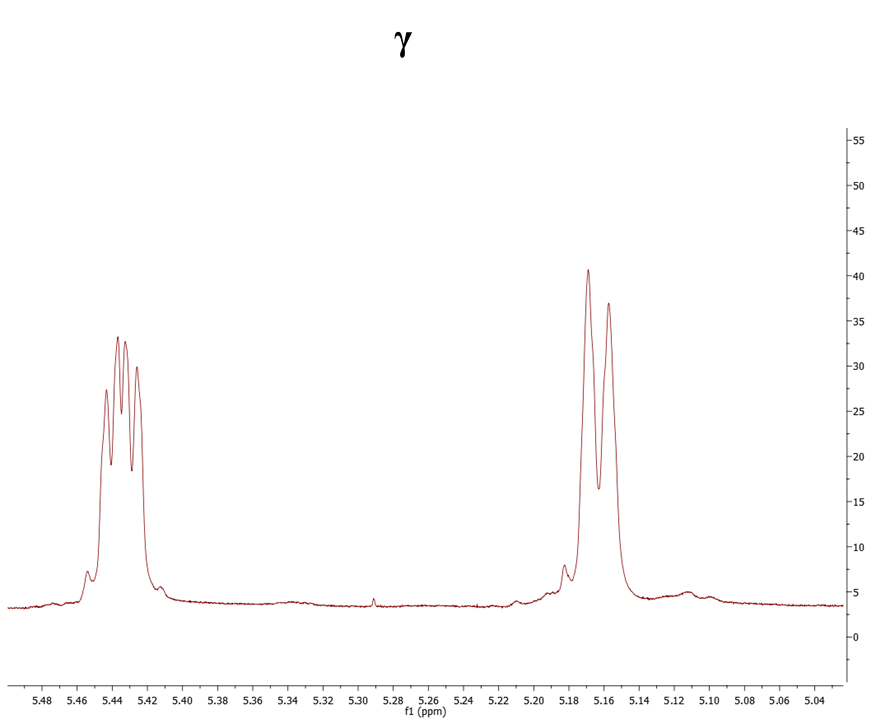
**Figure S7.** Zoomed vision of **ι** 13C spectrum section**.** The asterisks indicate the apparently hidden quaternary dithiooxamide carbon signals between 180 and 190 ppm.

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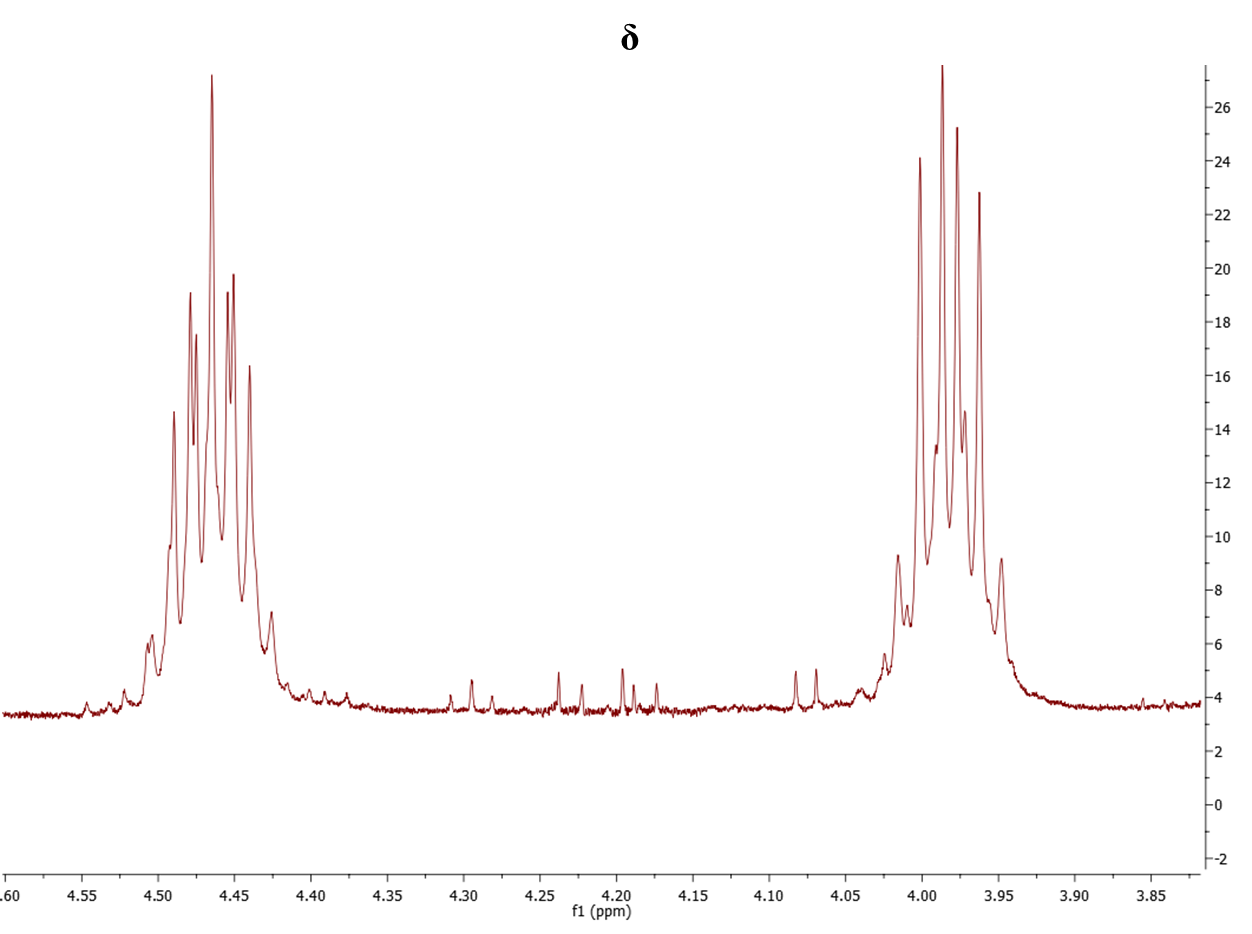
**Figure S8.** 118-91 ppm expansion of **κ** 13C spectrum section**.**



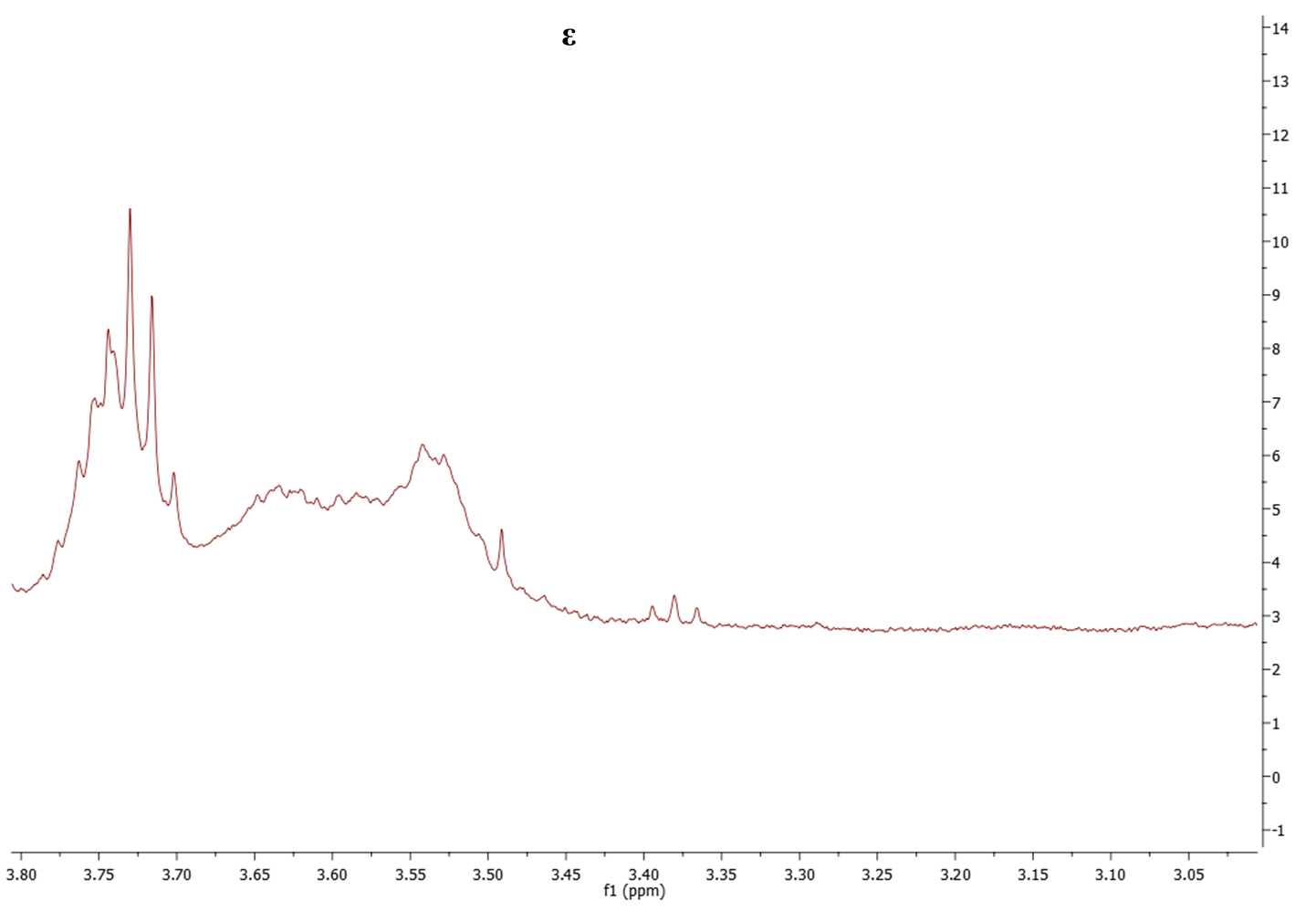
**Figure S9.** 1H NMR spectrum of **Ru-Pt-Pd** recorded in chloroform.



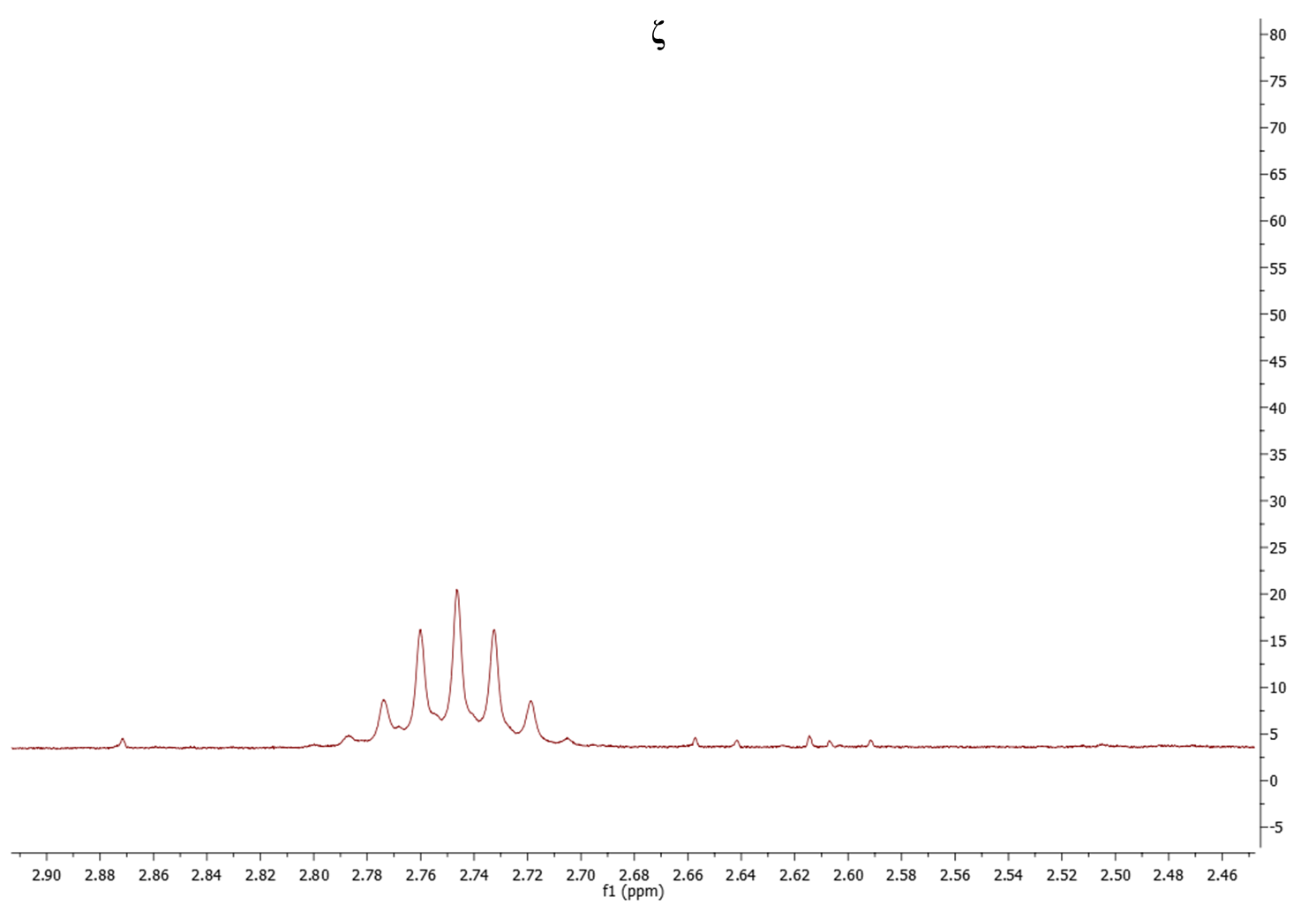
**Figure S10.** 5.48-5.04 ppm expansion of **γ** 1H spectrum section**.**



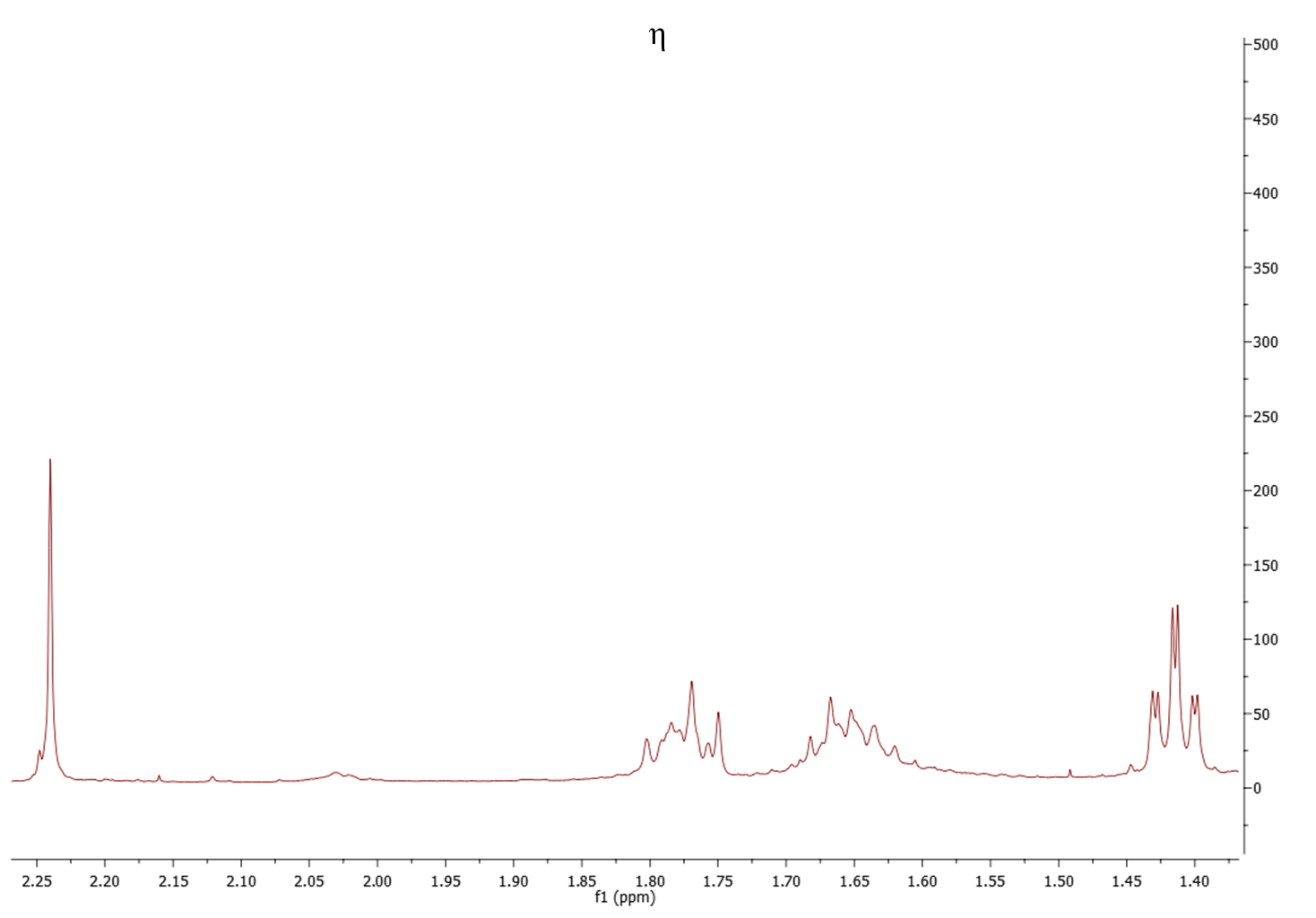
**Figure S11.** 4.55-3.85 ppm expansion of **δ** 1H spectrum section**.**



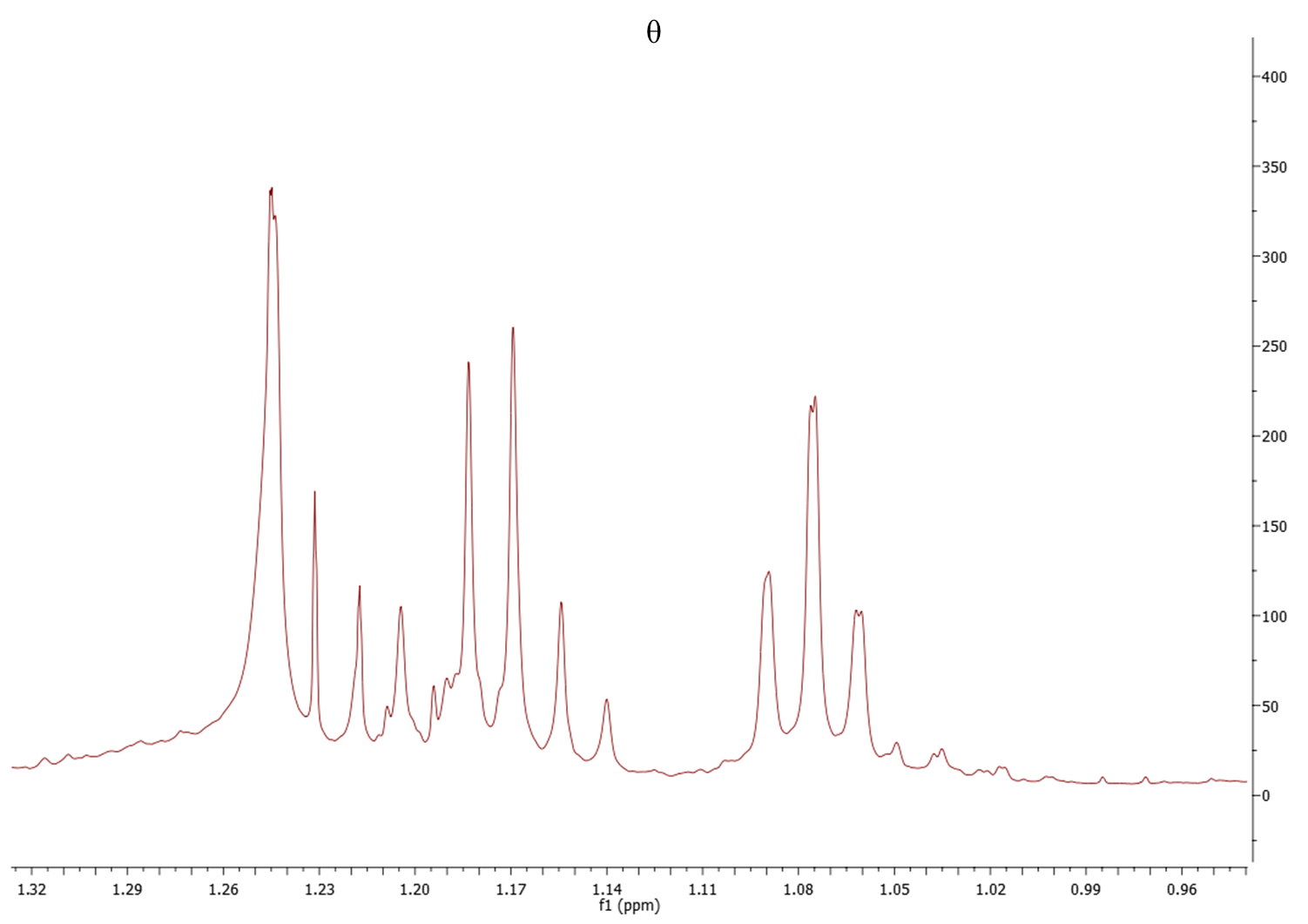
**Figure S12.** 3.80-3.05 ppm expansion of **ε** 1H spectrum section**.**



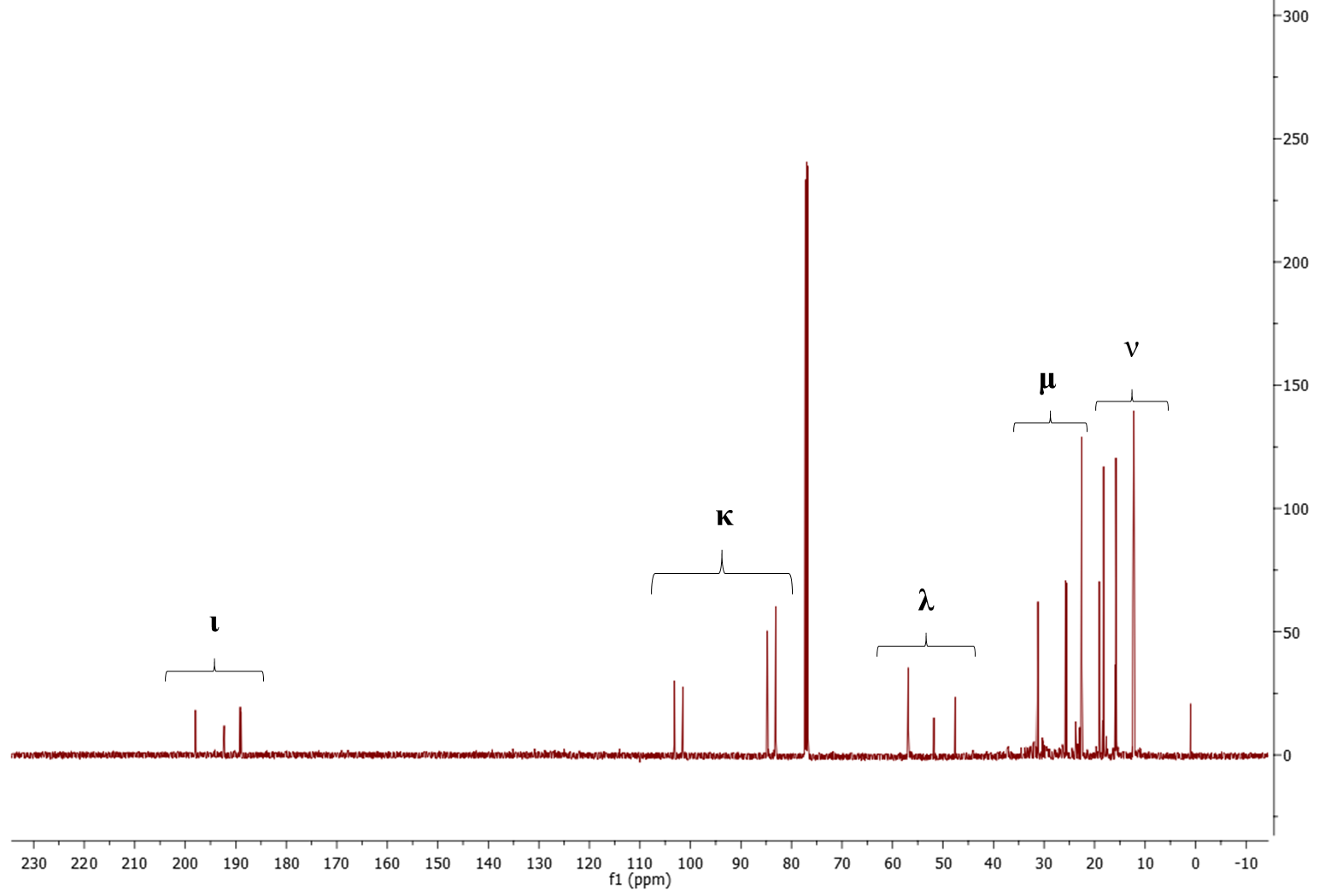
**Figure S13.** 2.90-2.45 ppm expansion of **ζ** 1H spectrum section**.**



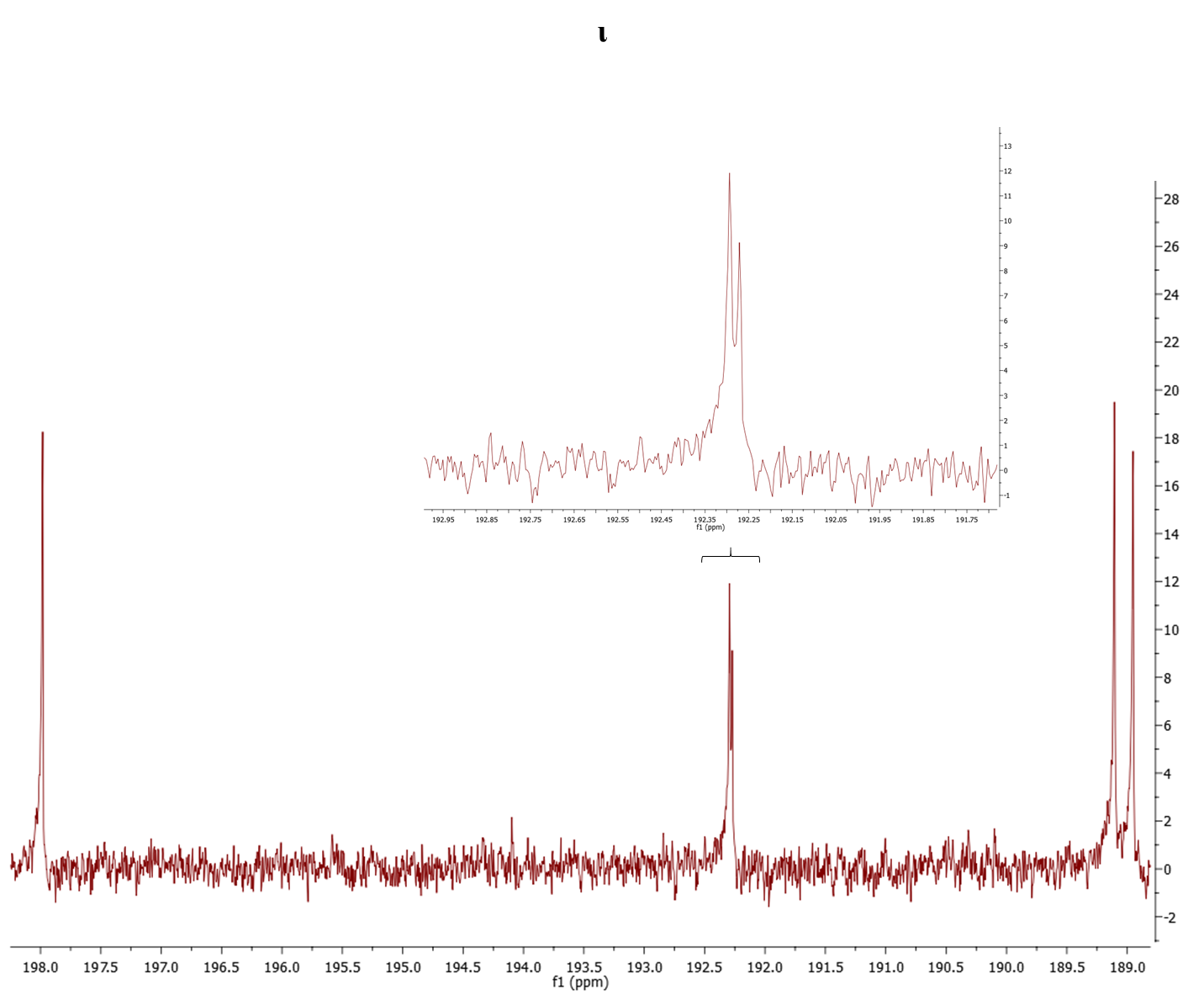
**Figure S14.** 2.25-1.40 ppm expansion of **η** 1H spectrum section**.**



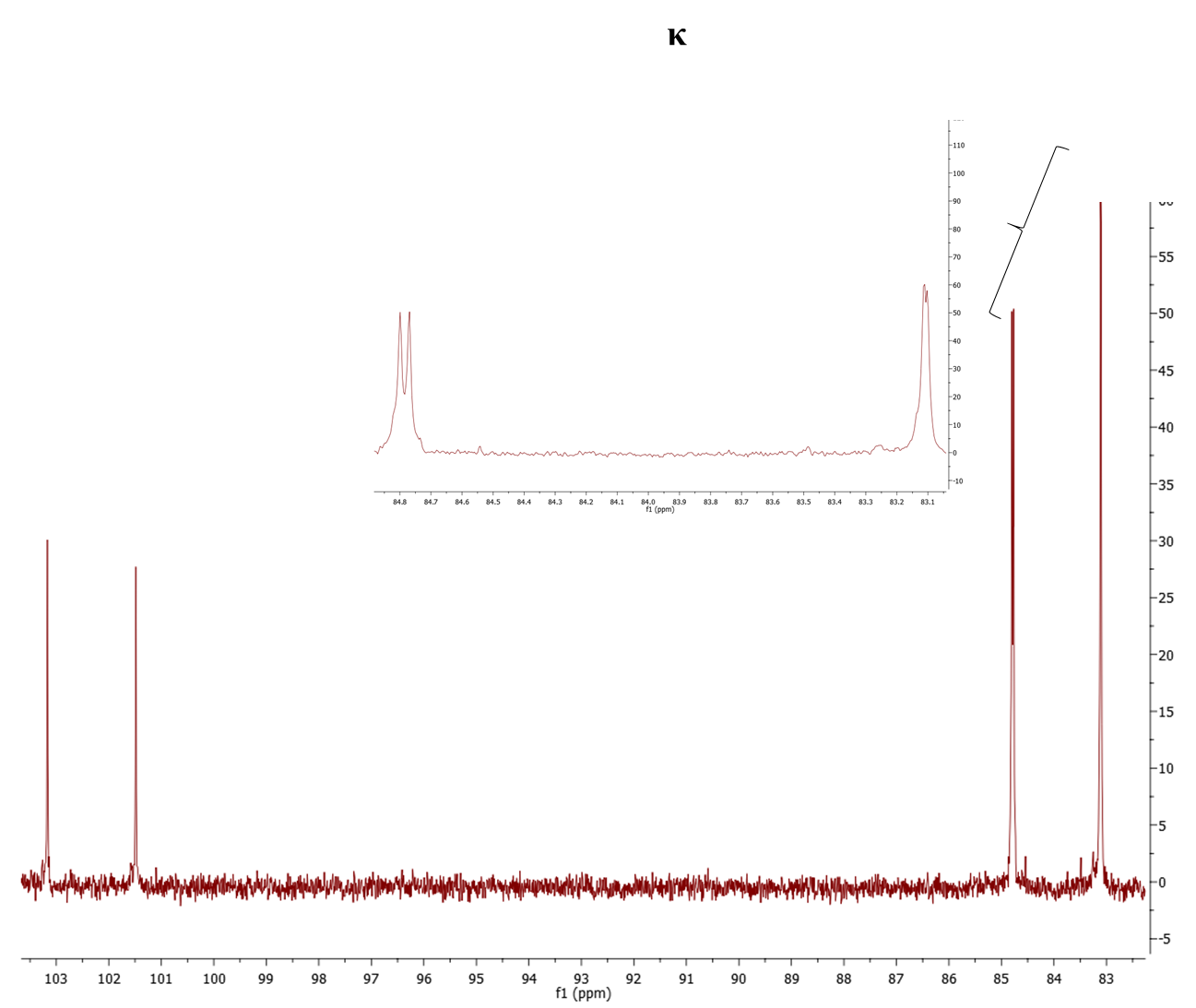
**Figure S15.** 1.32-0.96 ppm expansion of **θ** 1H spectrum section**.**



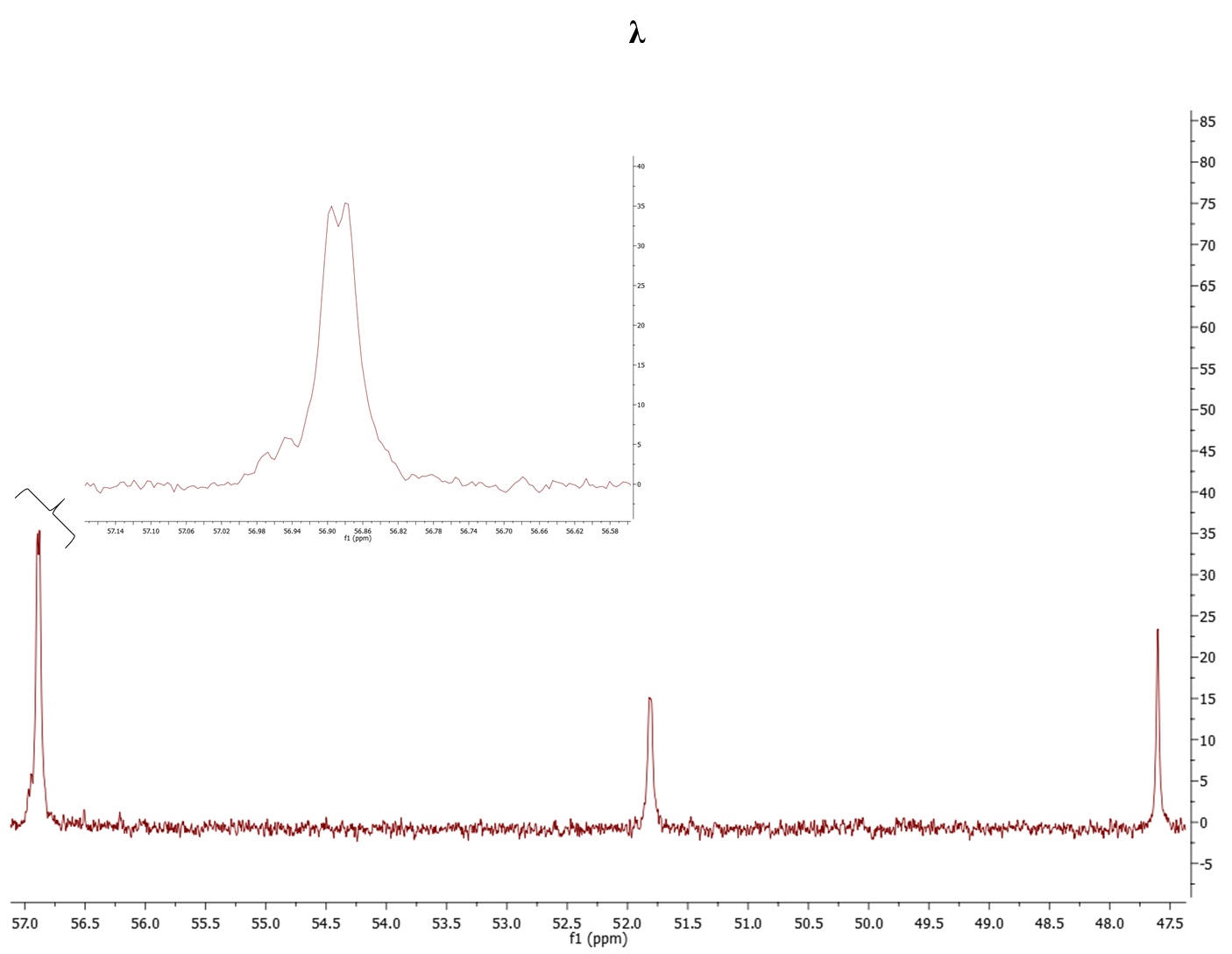
**Figure S16.** 13C NMR spectrum of **Ru-Pt-Pd** recorded in chloroform.



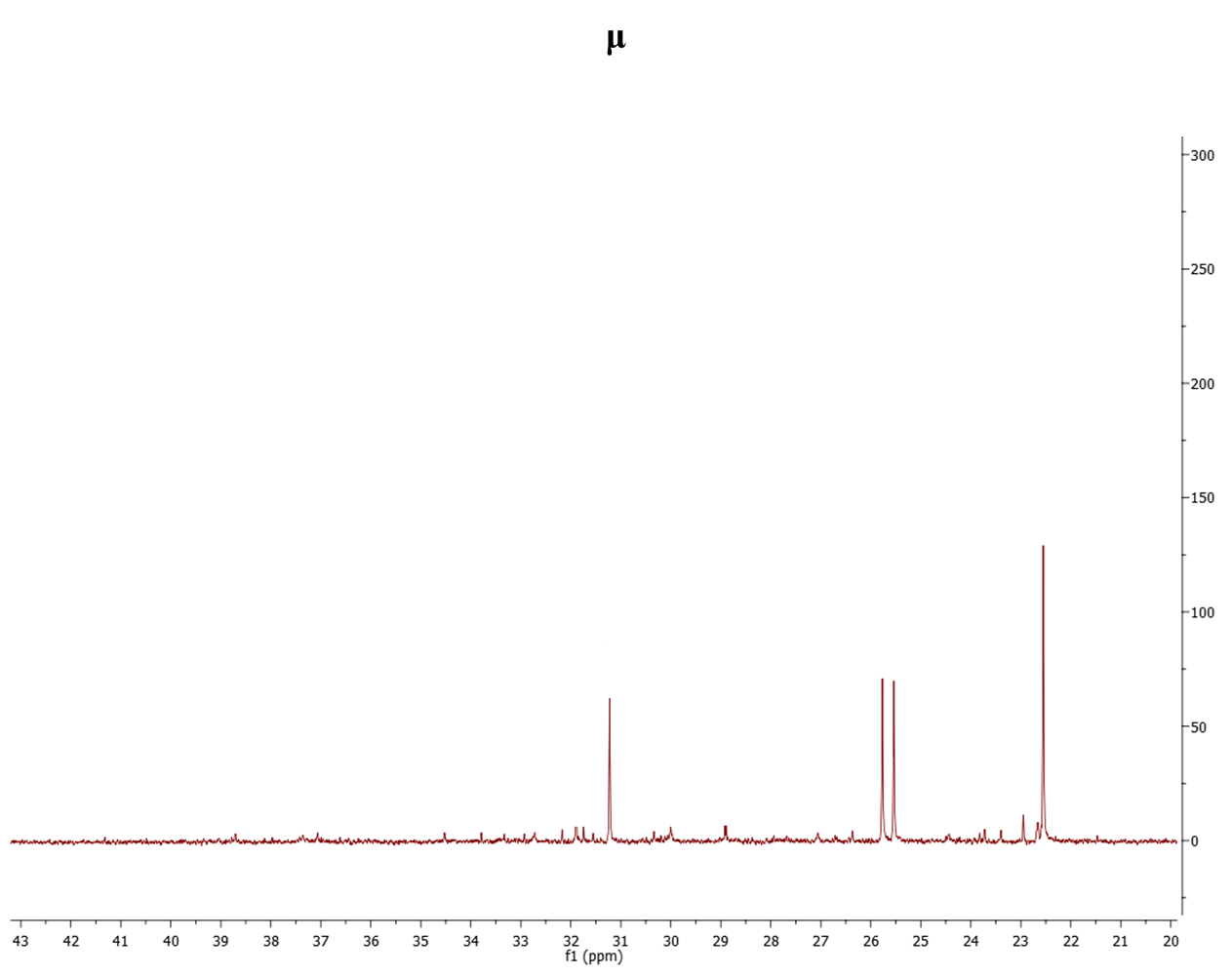
**Figure S17.** 198-189 ppm expansion of **ι** 13C spectrum section**.**



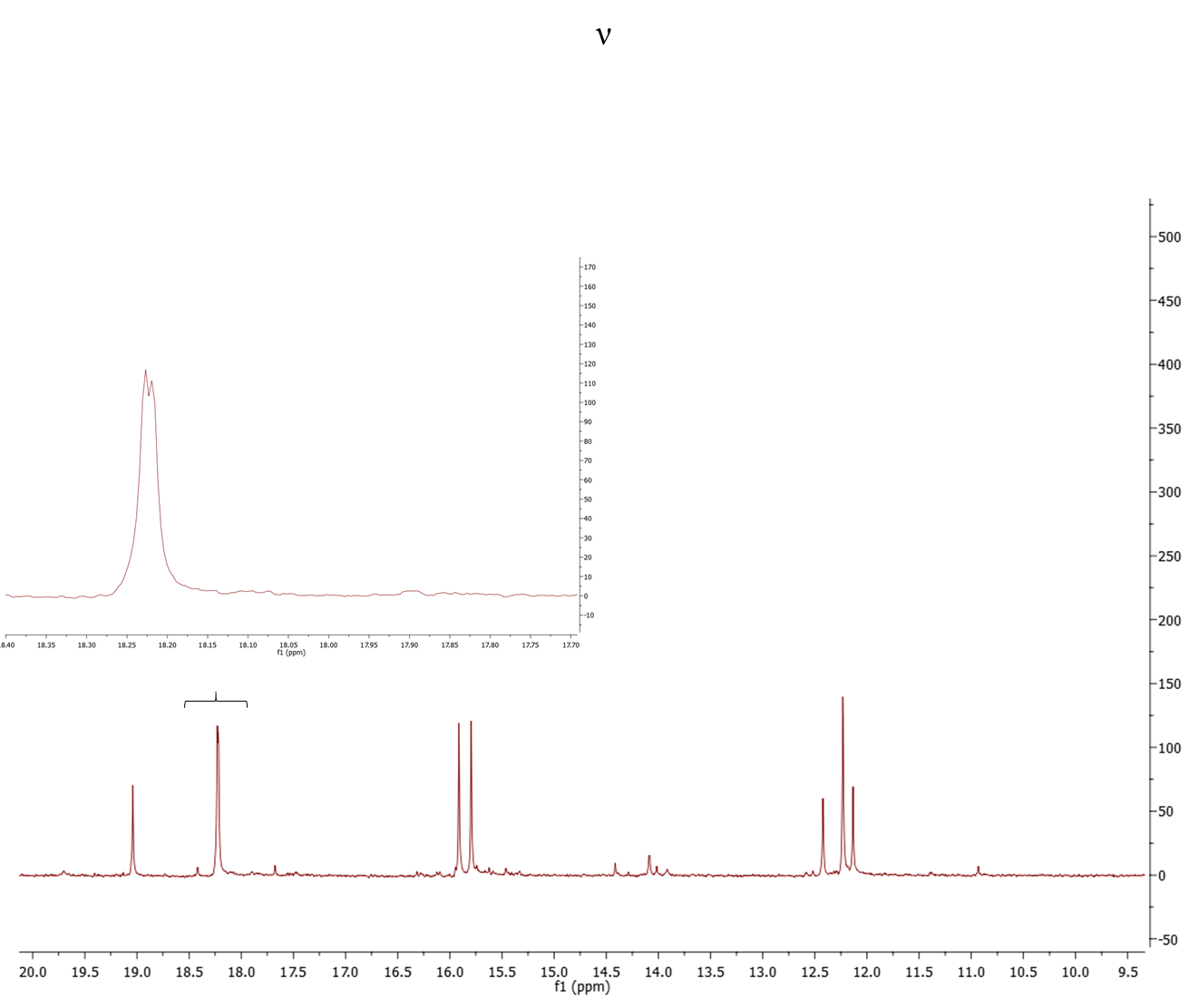
**Figure S18.** 103-83 ppm expansion of **κ** 13C spectrum section**.**



**Figure S18.** 57-47.5 ppm expansion of **λ** 13C spectrum section**.**



**Figure S19.** 43-20 ppm expansion of **μ** 13C spectrum section**.**



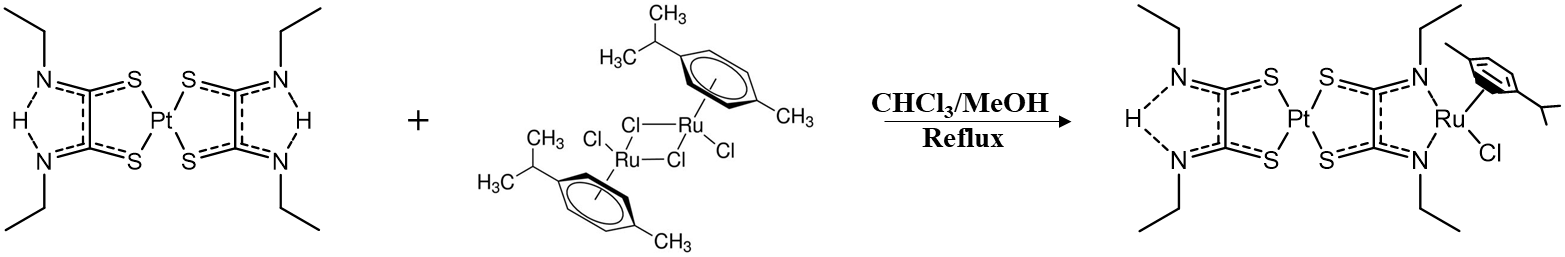
**Figure S20.** 20-9.5 ppm expansion of **ν** 13C spectrum section**.**

**Synthetic procedures**

**General notes**

Chemicals and solvents were purchased from commercial suppliers and were used without further purification. Column chromatography was performed on silica gel 60 from Merck. For thin layer chromatography (TLC) aluminium backed silica gel was used. Room temperature 1H and 13C NMR spectra were recorded on a Varian 500 instrument and were referenced internally to residual protio-solvent, and solvent resonances, respectively, are reported relative to tetramethylsilane (δ = 0 ppm).

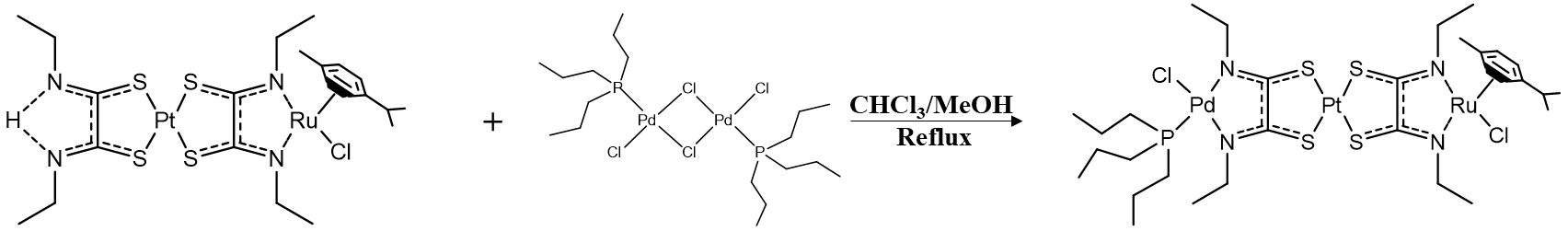
**Synthesis of Ru-Pt**

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**Pt** compound(synthetized according to literature preparation[1]) (0.1 g, 1.8\*10-4 mol, 1eq) and dichloro(p-cymene)ruthenium(II) dimer (0.055g, 9\*10-5 mol, 0.5 eq) were dissolved in a chloroform/methanol 95:5 solvent mixture (20ml) and refluxed in argon atmosphere for 3h. To the hot mixture was added sodium bicarbonate to neutralize the hydrochloric acid, then the suspension was filtered and concentrated to a small volume. The solution was purified by column chromatography (SiO2, CHCl3/petroleum ether 70:30). A red powdery solid (41%, 0.06g, 7.23\*10-5 mol) was isolated as pure final product.

1H NMR (500 MHz, CDCl3,298K) δ 5.44, 5.16 (2d, *J* = 6.2 Hz, 4H, cymene ring protons), 5.49, 4.00 (m, 4H, N-methylene groups near ruthenium), 3.62 (q, *J* = 7.3, 3H, methylene groups far from ruthenium), 2.76 (sep, 3*J* = 6.9 Hz, 1H, cymene isopropyl proton), 2.25 (s, 3H, cymene methyl group), 1.44 (t, *J* = 7.24, 6H methyl groups near ruthenium), 1,34 (t, *J* = 7.24, 6H, methyl groups far from ruthenium), 1.18 (d, 6H, *J* = 6.9 cymene isopropyl methyl groups). 13C NMR (500 MHz, CDCl3,room temp) δ 188.92, 180.5 (quaternary dithiooxamide carbons), 103.44, 101.72 (quaternary cymene carbons), 84.84, 83.15 (non-substituted *C*H cymene ring carbons), 56.98 (N-*C*H2 methylene carbons near ruthenium), 44.14 (N-*C*H2 methylene carbons far from ruthenium), 31.25 (*C*H(CH3)2 isopropyl carbon), 22.55 (CH(*C*H3)2 isopropyl methyl carbons), 19.05 (cymene methyl carbon), 12.24 (N-CH2-*C*H3 methyl carbons near and far from ruthenium).

**Synthesis of Ru-Pt-Pd**



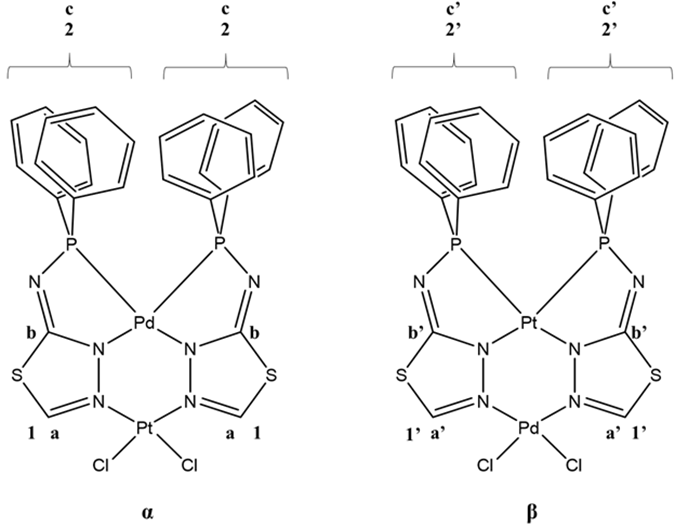
The hetero tri-metallic compound **Ru-Pt-Pd** was obtained by reaction of the **Ru-Pt** compound (0.04g, 5\*10-5 mol,1 eq) and tri-normalpropyl-phosphine palladium(II) chloride dimer (0.017 g, 2.5\*10-5 mol, 0.5 eq) in a chloroform/methanol 95:5 solvent mixture (20ml) and refluxed for 6h under inert atmosphere (Ar). Once cooled to room temperature the stirring mixture was added sodium bicarbonate to neutralize the hydrochloric acid, then the suspension was filtered and the solvent was removed by rotatory evaporation. The crude material was purified by column chromatography using (SiO2, CHCl3/hexane 75:25) as eluent mixture. A dark red solid was obtained (42%, 0.022 g, 1.86\*10-5 mol) as final product. 1H NMR (500 MHz, CDCl3,room temp) δ 5.43, 5.16 (dd, d *J* = 5.9 Hz, 4H, cymene ring protons), 4.46, 3.98 (m, 4H, N-methylene groups near ruthenium), 3.72 (m, 2H, N-methylene group trans P), 3.56 (m, 2H, N-methylene group cis P), 2.75 (sep, *J* = 6.9 Hz, 1H, cymene isopropyl proton), 2.24 (s, 3H, cymene methyl group), 1.79 (m, 6H, P-CH2-C*H*2-CH3), 1.65(m, 6H, P-CH2-C*H*2-CH3), 1.41 (td, *J* = 7.3Hz, 6H, methyl groups near ruthenium), 1.24 (d broad, 6H, cymene isopropyl methyl groups), 1.18 (m, 6H, methyl groups near palladium), 1.08 (t, *J* = 6.1 Hz, P-CH2-CH2-C*H*3). 13C NMR (500 MHz, CDCl3,room temp) δ 197.98 , 192.28 , 189.05 (quaternary dithiooxamide carbons), 103.17 , 101.48 (quaternary cymene carbons), 84.79 , 83.11 (non-substituted *C*H cymene ring carbons), 56.89 (N-*C*H2 methylene carbons near ruthenium), 51.81 (N-*C*H2 methylene carbon trans P), 47.60 (N-*C*H2 methylene carbon cis P), 31.23 (*C*H(CH3)2 isopropyl carbon), 25.65 (d, *J*c-p = 28.7 P-*C*H2-CH2-CH3), 22.55 (CH(*C*H3)2 isopropyl methyl carbons), 19.04 (cymene methyl carbon), 18.22 (P-CH2-*C*H2-CH3), 15.85 ( P-CH2-CH2-*C*H3), 12.42, 12,13 (N-CH2-*C*H3 methyl carbons near palladium), 12,23 (N-CH2-*C*H3 methyl carbons near ruthenium)

**Table S7.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **α** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1 | 23.1590 | 8.1213 | 8.8300 | 0.0359 | 0.3723 |
| 2 | 24.1104 | 7.2091 | 7.2450 | 0.7087 |

**Table S8.** Experimental and predicted 13C NMR chemical shifts (in ppm). Letters are related to carbon resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **α** (13C) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| a | 15.2725 | 157.8732 | 149.4000 | 8.4732 | 3.2373 |
| b | -7.9192 | 179.1266 | 178.8000 | 0.3266 |
| c | 46.4102 | 129.3379 | 130.2500 | 0.9121 |

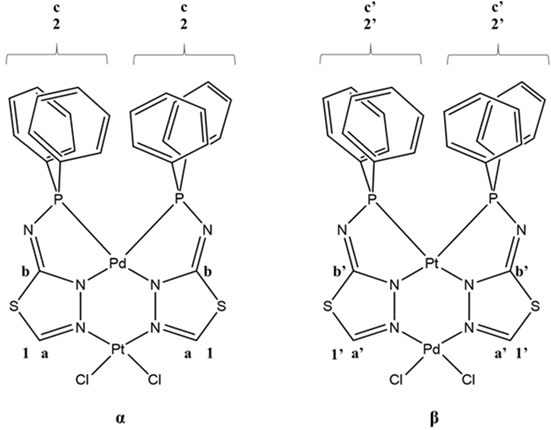


**Table S9.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **β** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1’ | 23.0719 | 8.2048 | 8.9200 | 0.0359 | 0.3755 |
| 2’ | 24.0322 | 7.2841 | 7.3200 | 0.7152 |

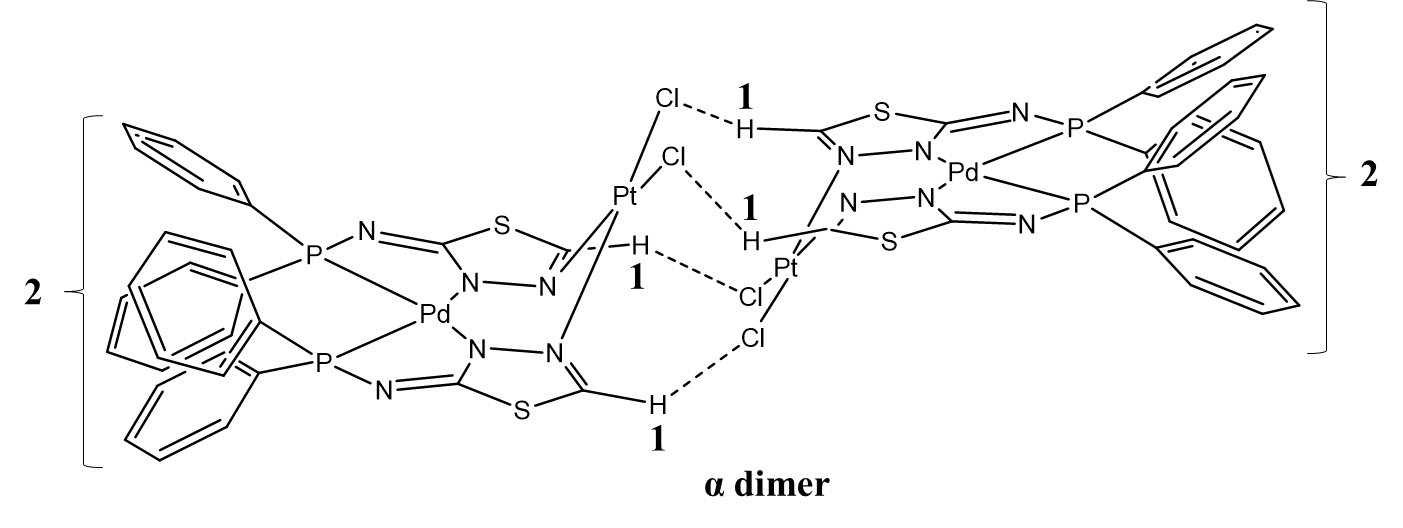
**Table S10.** Experimental and predicted 13C NMR chemical shifts (in ppm). Letters are related to carbon resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **β** (13C) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| a’ | 14.4318 | 158.6436 | 151.5000 | 7.1436 | 4.1292 |
| b’ | -7.5721 | 178.8084 | 183.2000 | 4.3916 |
| c’ | 46.3451 | 129.3975 | 130.2500 | 0.8525 |



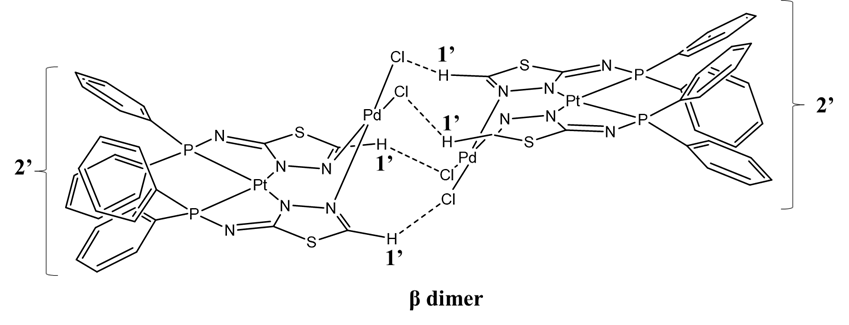
**Table S11.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **α dimer** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1 | 21.8725 | 7.2314 | 8.8300 | 0.0136 | 0.2692 |
| 2 | 24.0872 | 9.3548 | 7.2450 | 0.5248 |



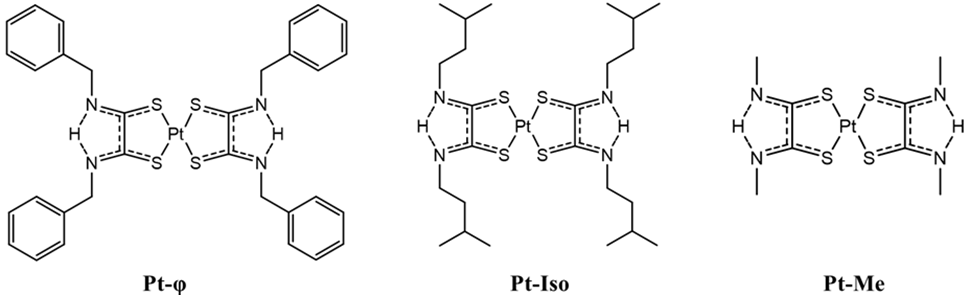
**Table S12.** Experimental and predicted 1H NMR chemical shifts (in ppm). Numbers are related to proton resonances.

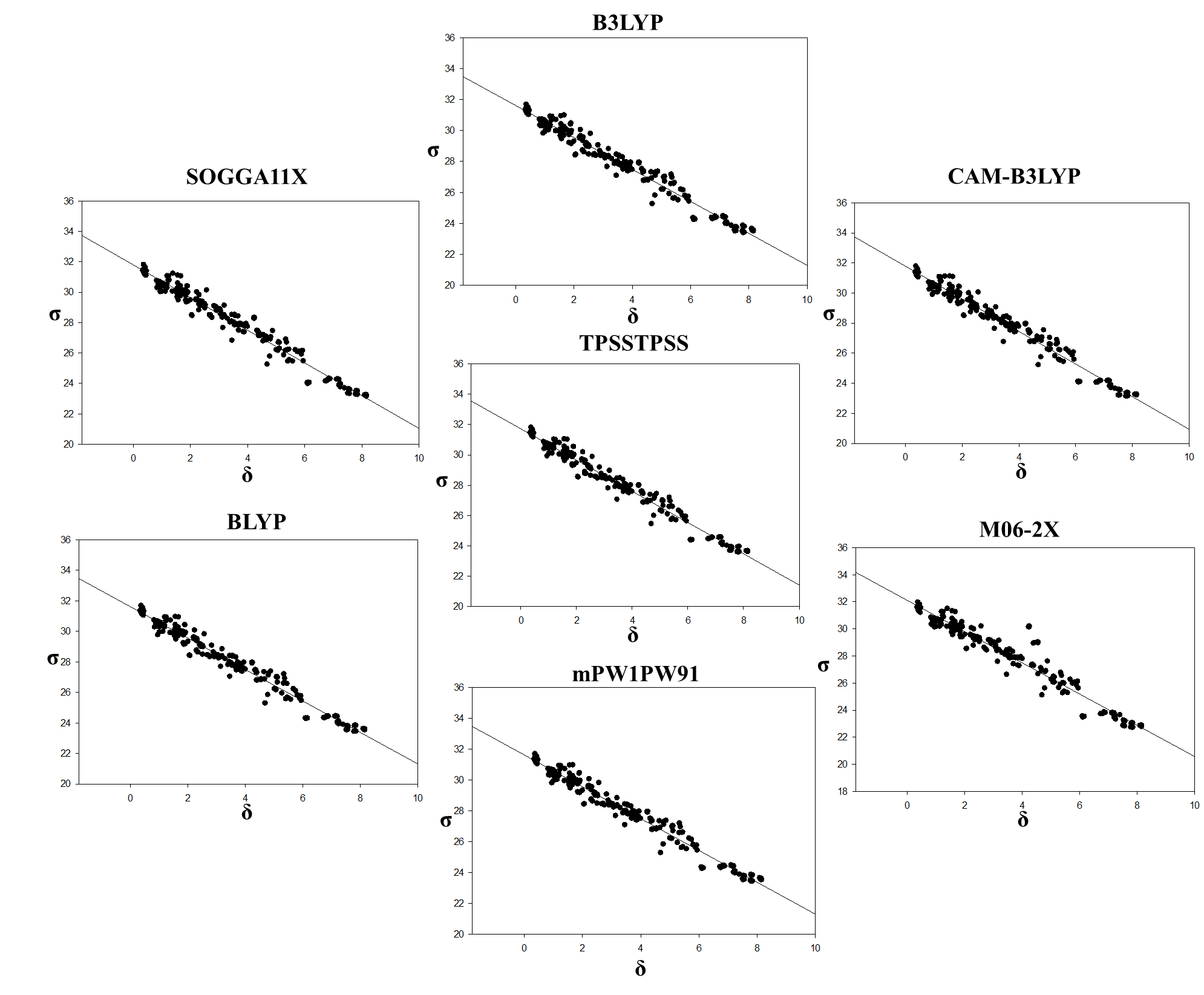
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **β dimer** (1H) | | | | | |
| Atom labels | Isotropic shielding values | δcalc (ppm) | δexp (ppm) | Δ(calc-exp) | MAE |
| 1’ | 21.8492 | 9.3771 | 8.9200 | 0.4571 | 0.2333 |
| 2’ | 24.0047 | 7.3104 | 7.3200 | 9.5805e-3 |



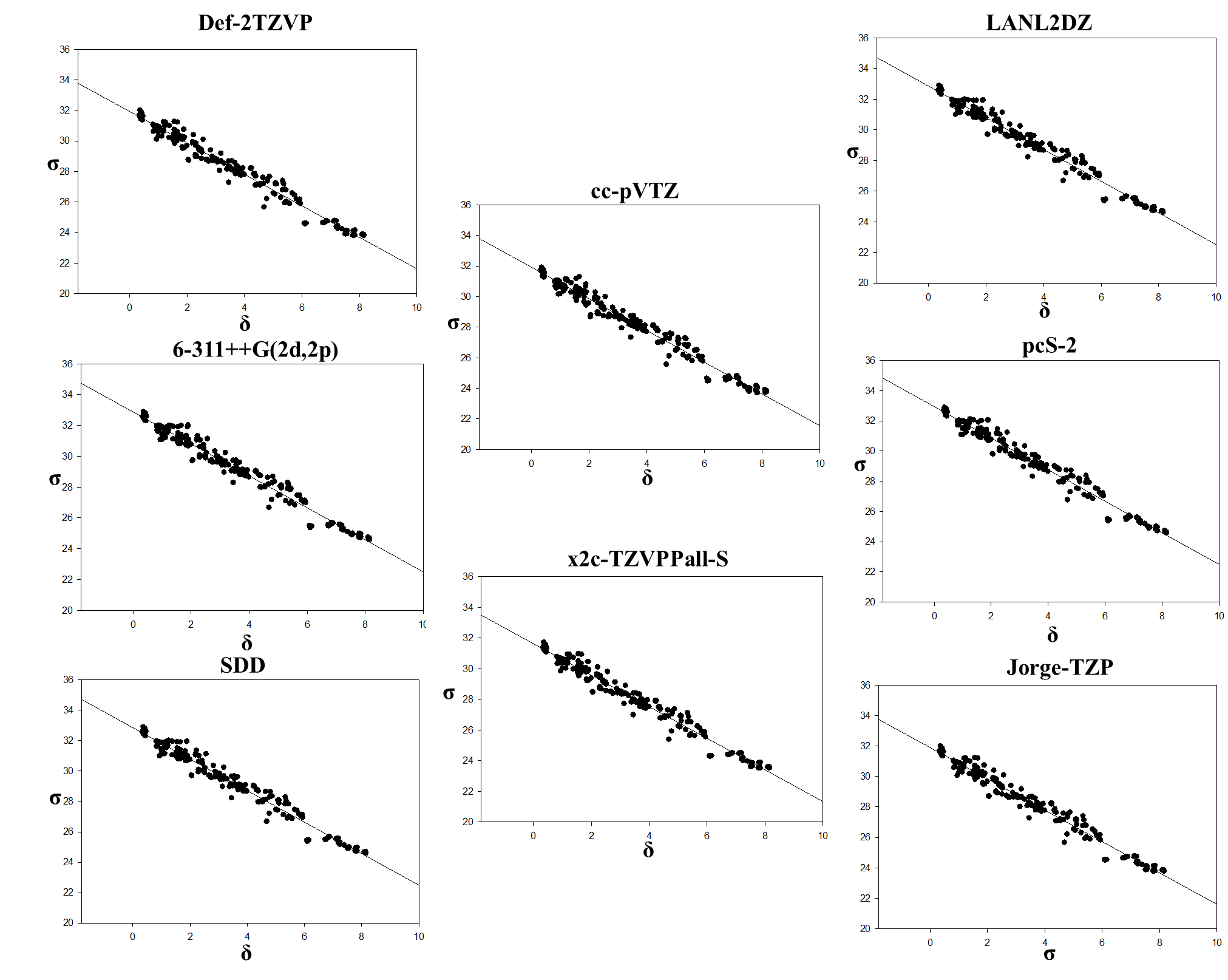
**Table S13.** Experimental and predicted 195Pt NMR chemical shifts (in ppm).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Label compounds | 195Pt | | | |
| Isotropic shielding values | δcal | δexp | Δδcal-exp |
| Pt-φ | 74.0708 | 122.2795 | 120.0000 | 2.2795 |
| Pt-Iso | 75.6882 | 96.1502 | 110.0000 | 13.8498 |
| Pt-Me | 73.7104 | 128.1018 | 110.0000 | 18.1018 |
| MAE | 11.41 | | | |

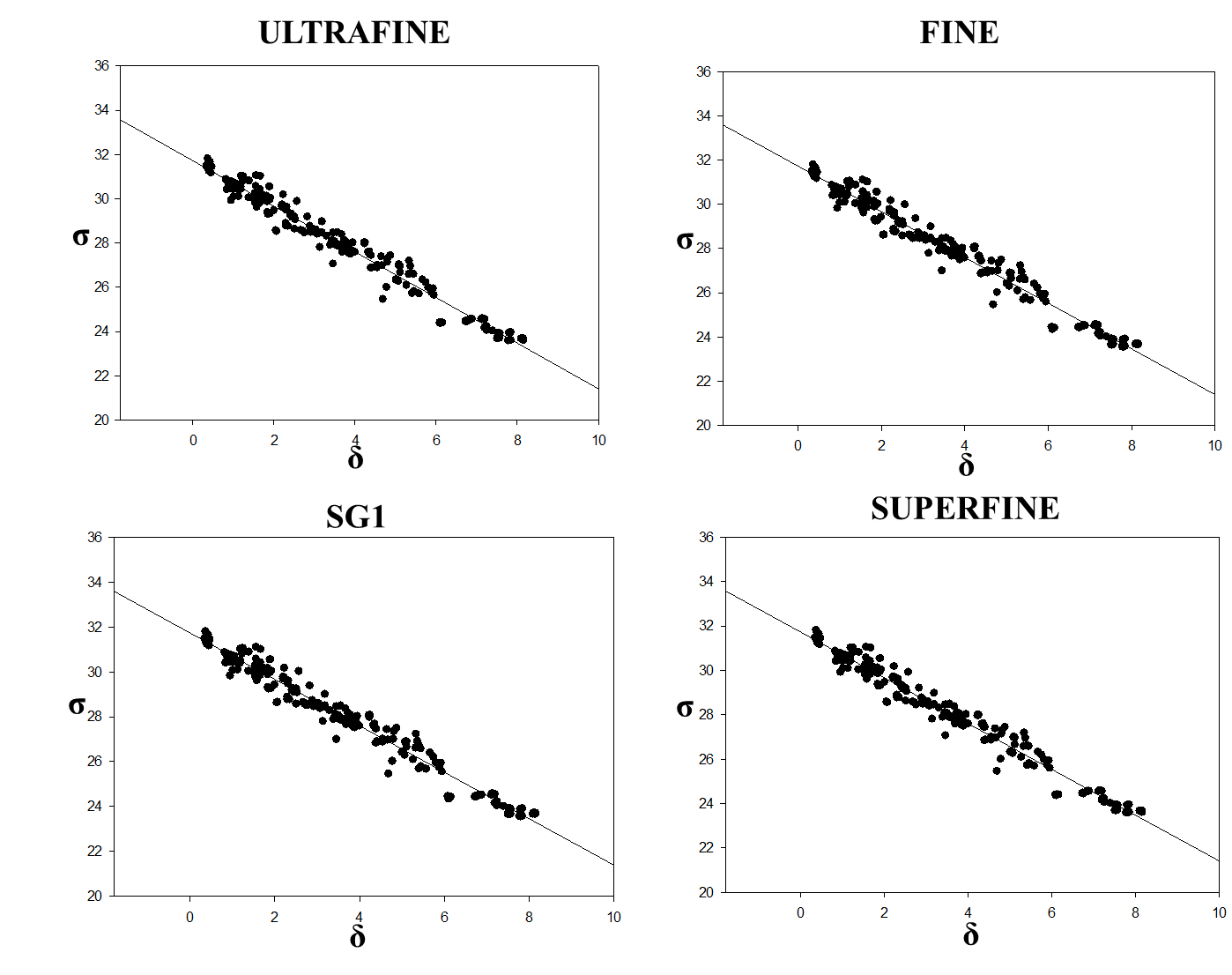




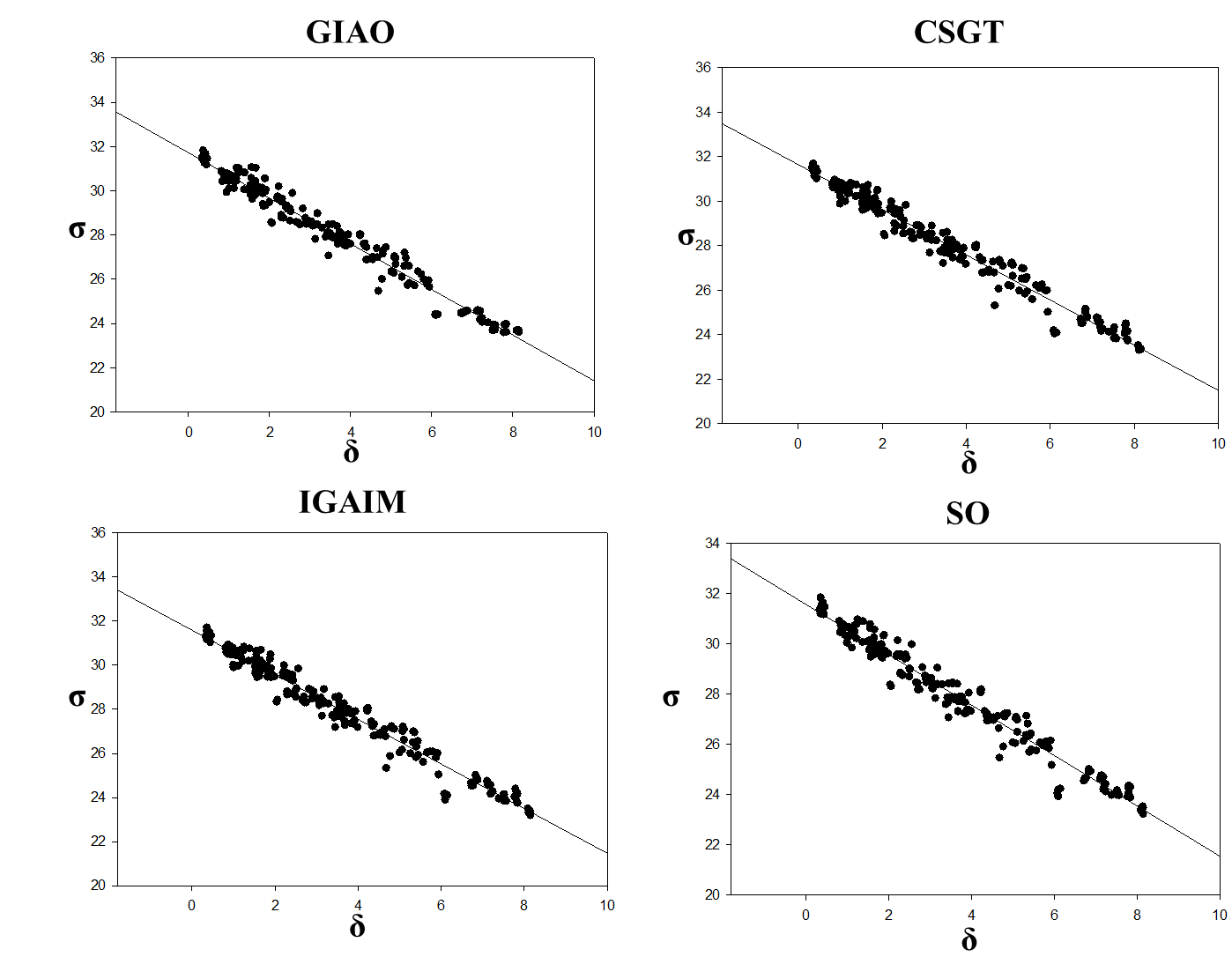
**Figure S21.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the functional evaluation for our calibration set.



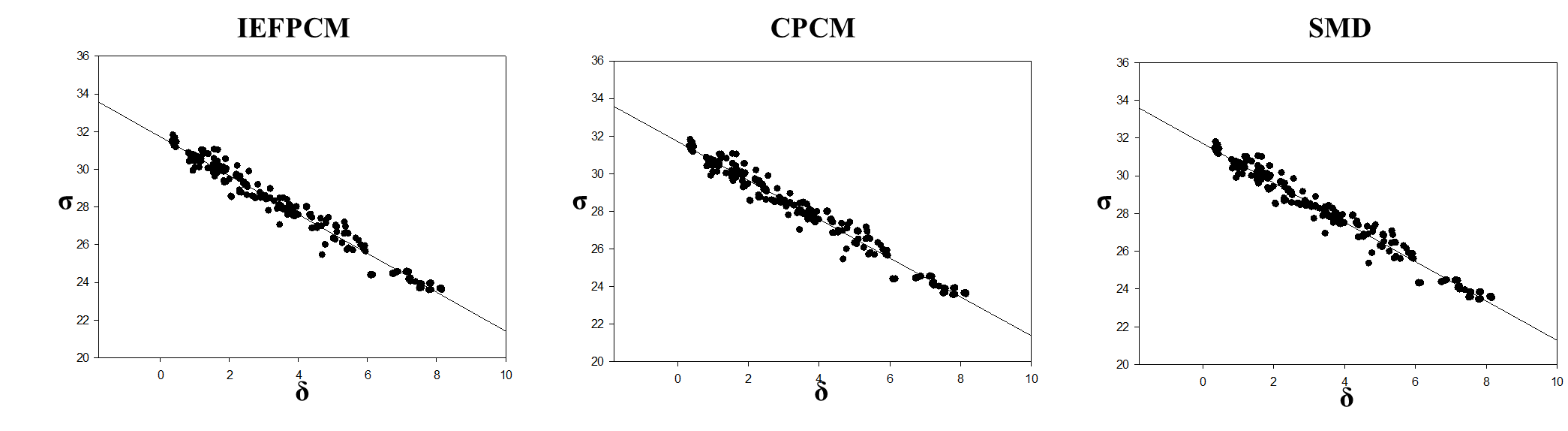
**Figure S22.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the basis set evaluation for our calibration set.



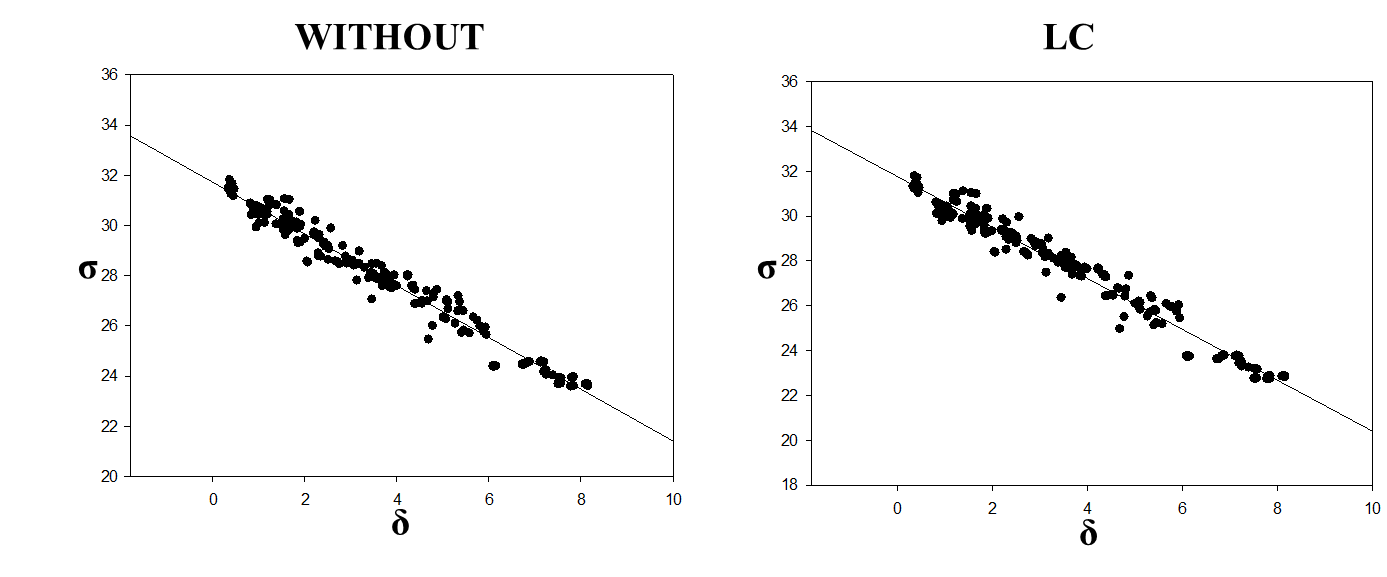
**Figure S23.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the integration grid evaluation for our calibration set.



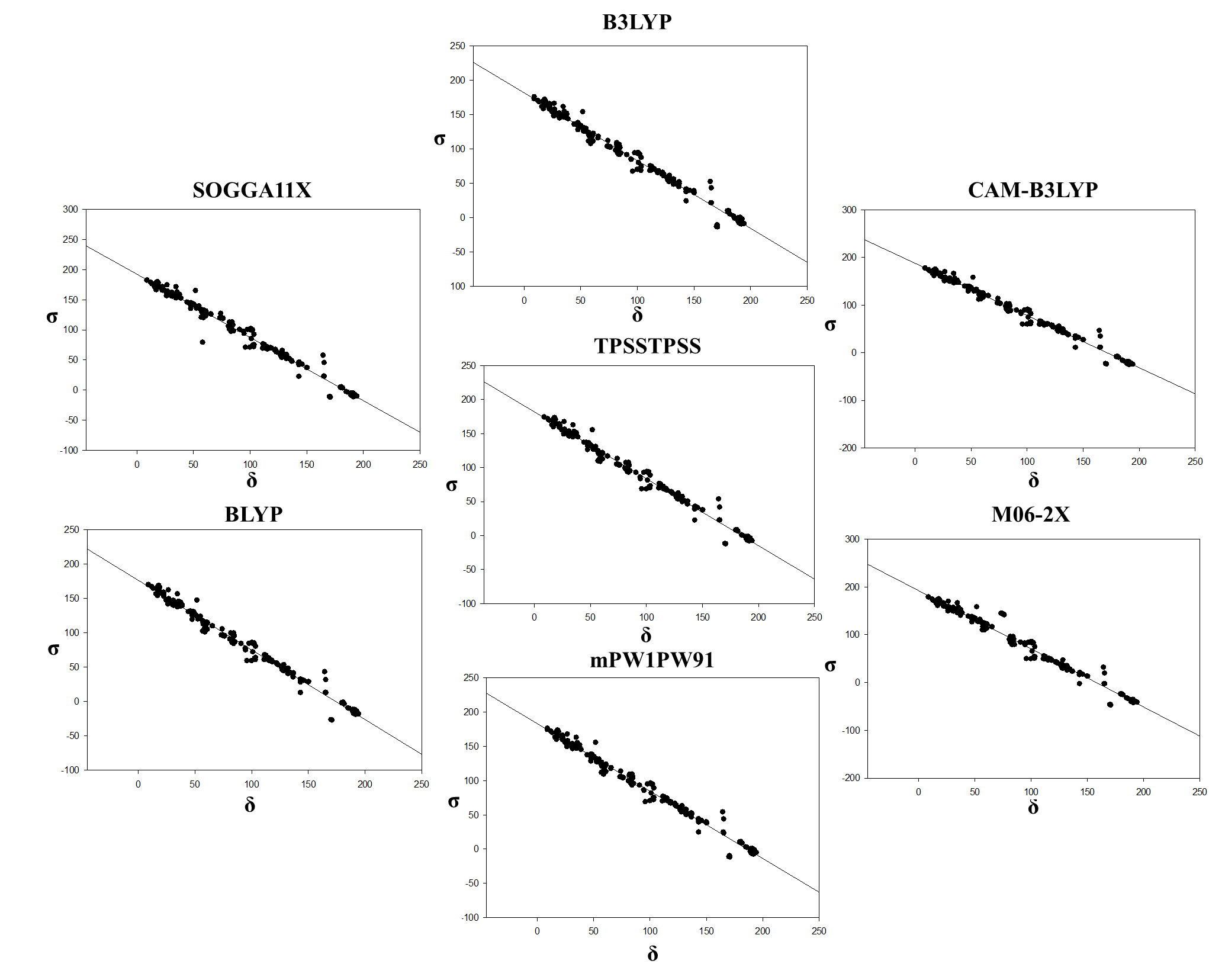
**Figure S24.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the NMR method evaluation for our calibration set.



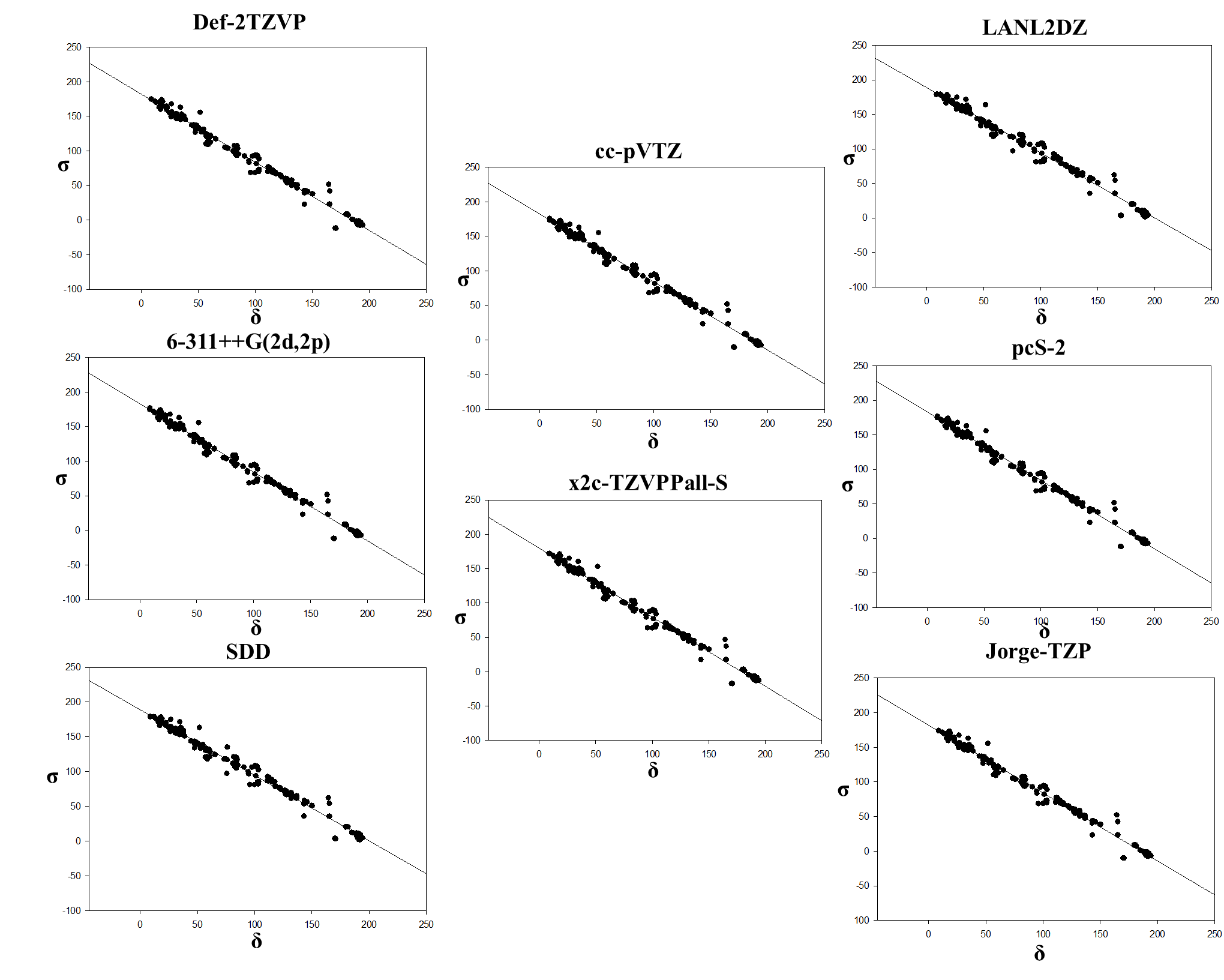
**Figure S25.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the solvent model evaluation for our calibration set.



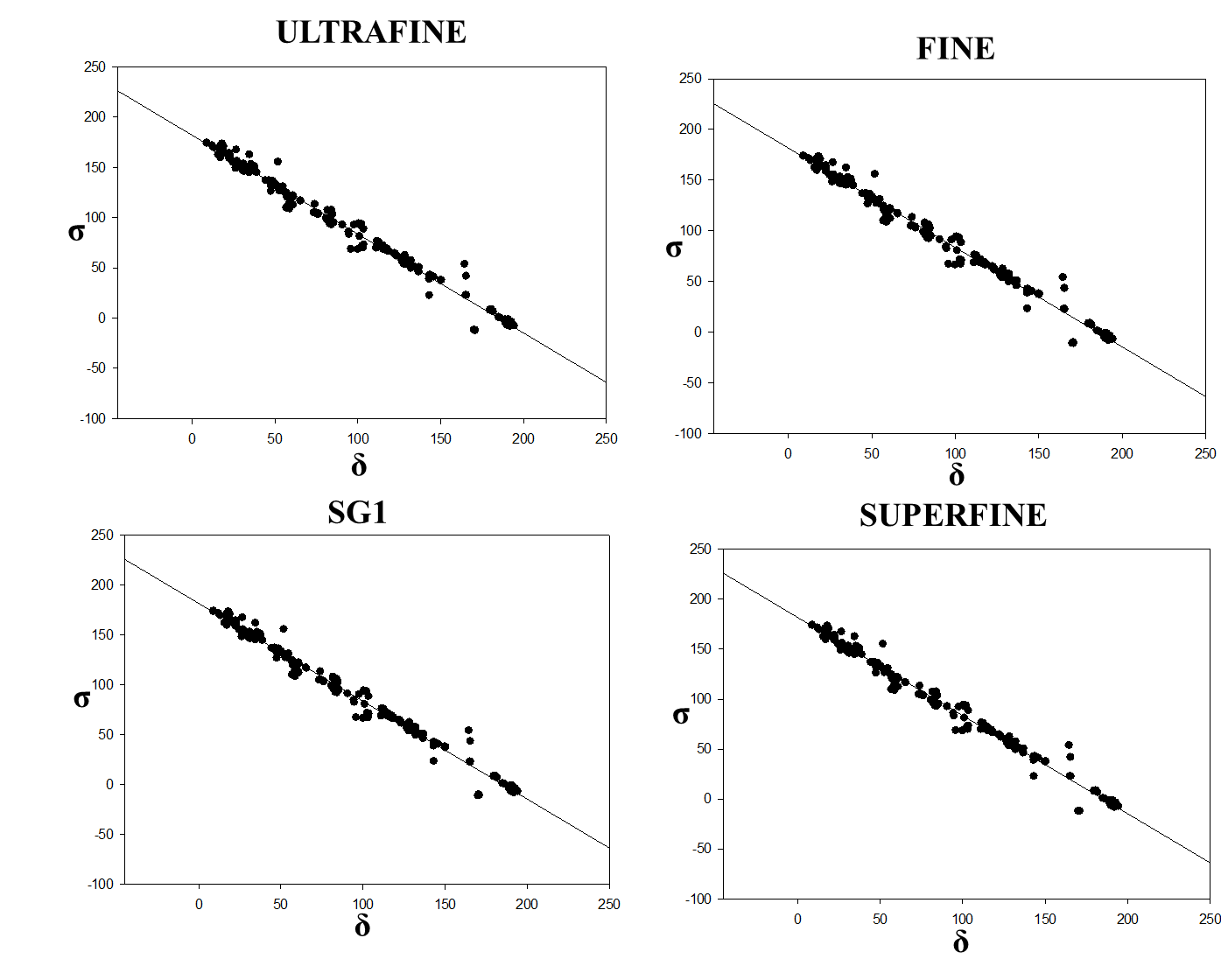
**Figure S26.** Correlation between experimental chemical shifts (δ 1H) and the isotropic shielding values (σ) in the process of the LC correction evaluation for our calibration set.



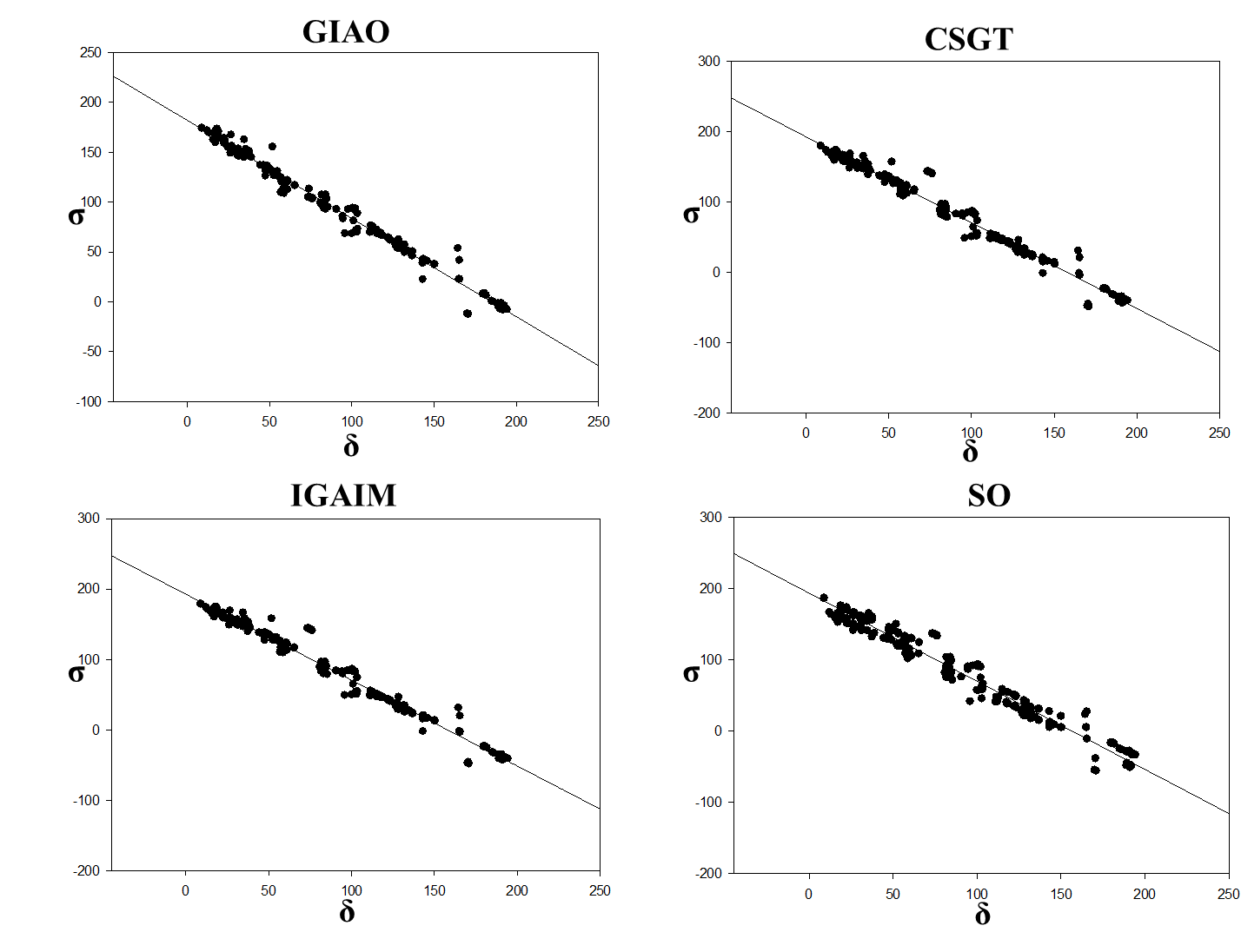
**Figure S27.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the functional evaluation for our calibration set.



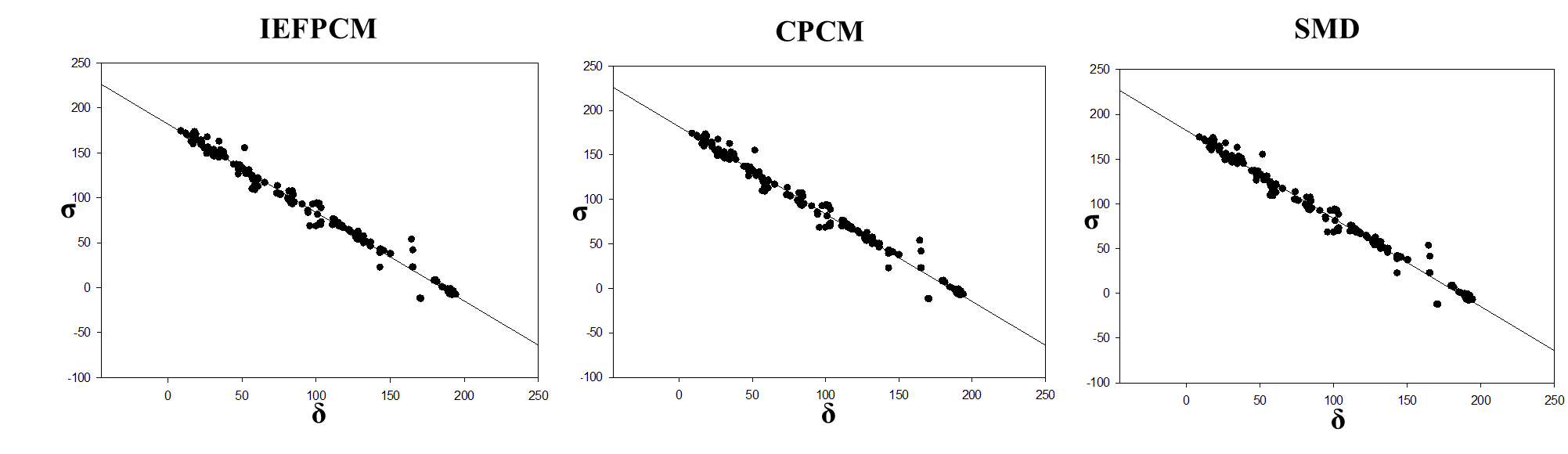
**Figure S28.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the basis set evaluation for our calibration set.



**Figure S29.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the integration grid evaluation for our calibration set.

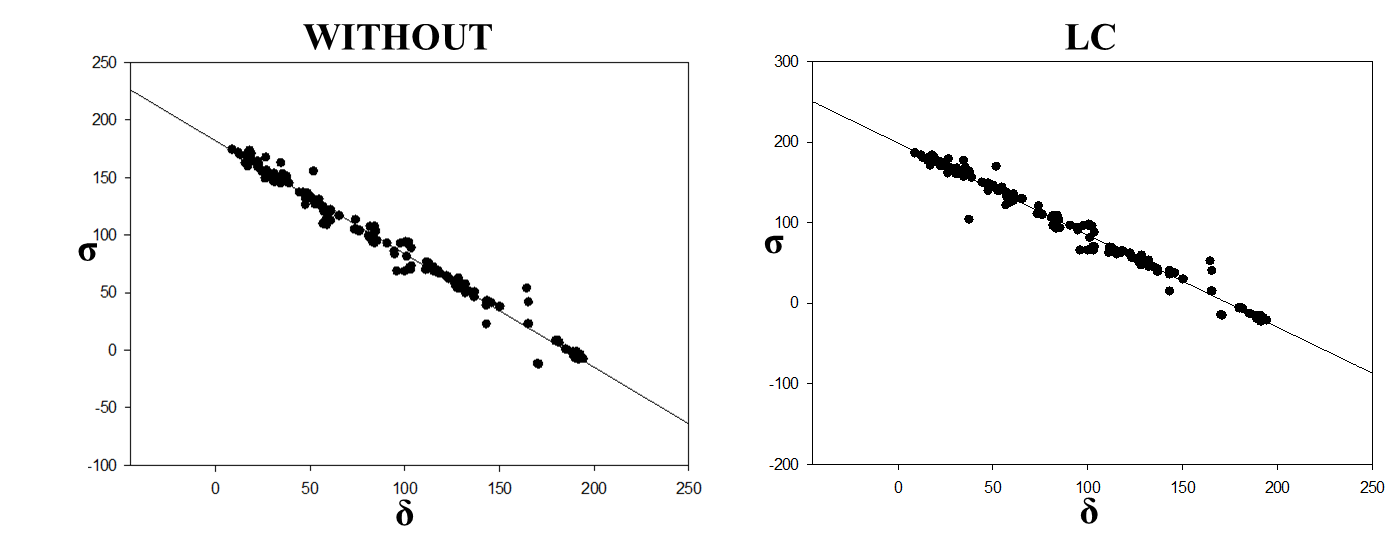


**Figure S30.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the NMR method evaluation for our calibration set.

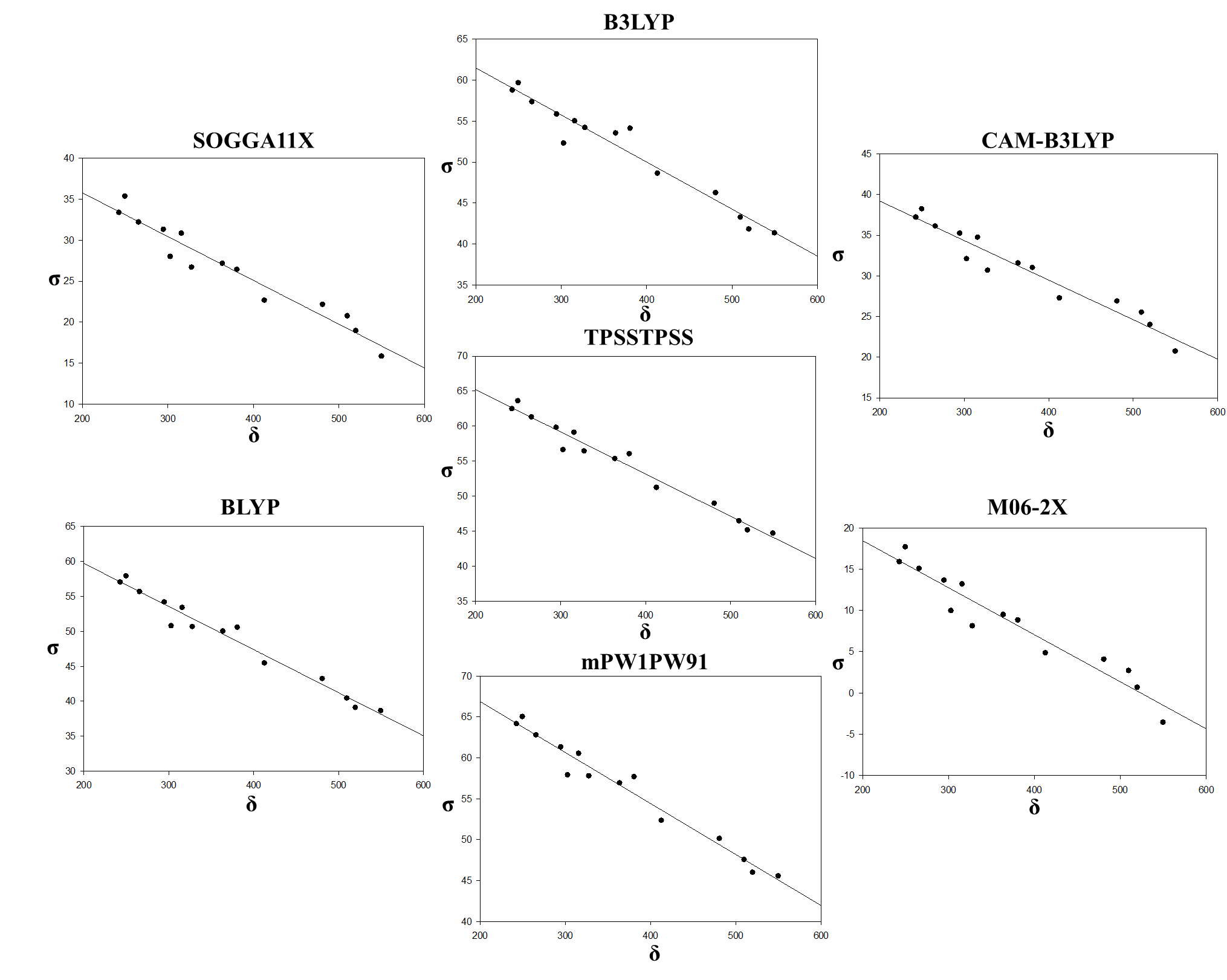


**Figure S31.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the solvent model evaluation for our calibration set.

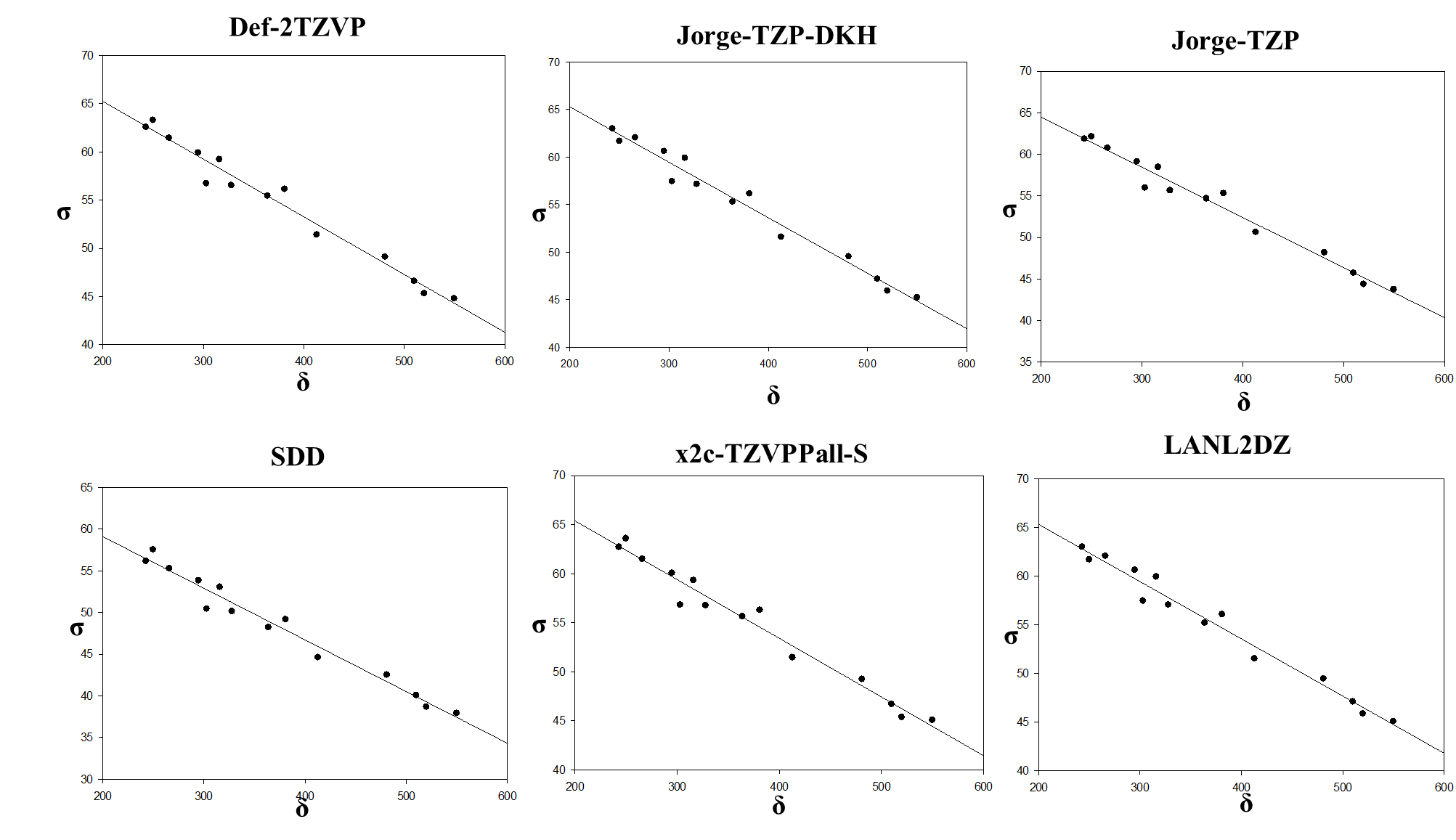
.



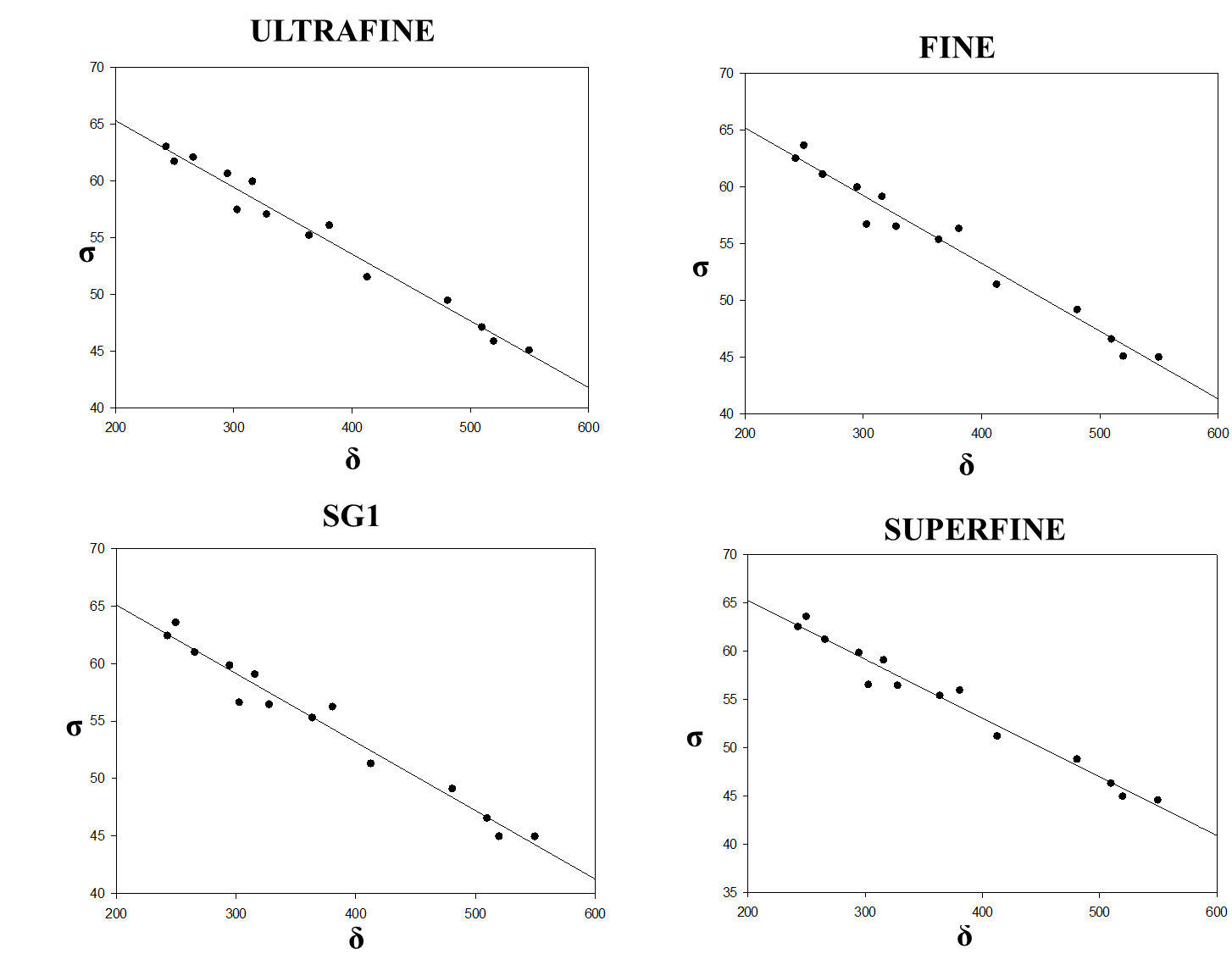
**Figure S32.** Correlation between experimental chemical shifts (δ 13C) and the isotropic shielding values (σ) in the process of the LC correction evaluation for our calibration set.



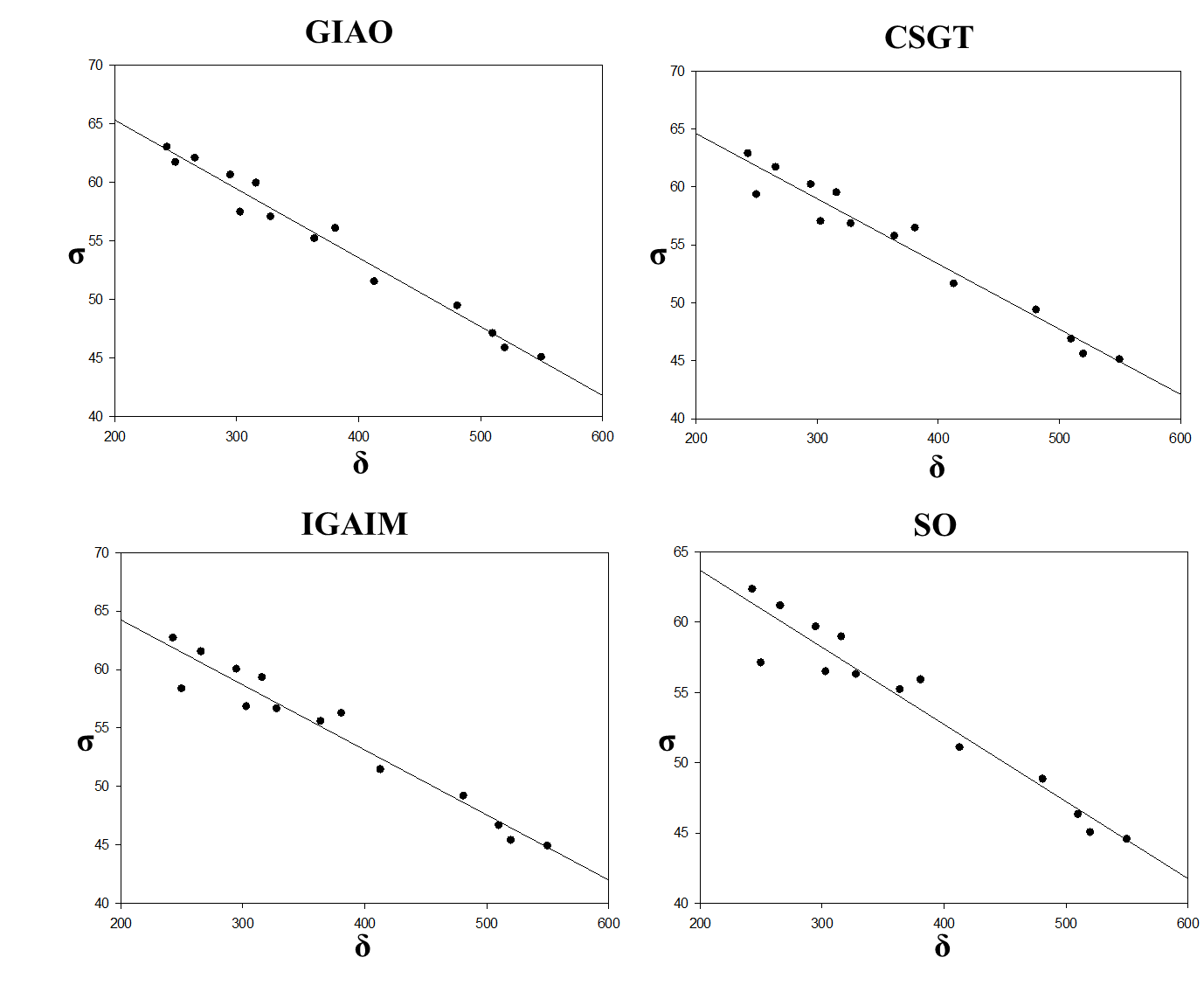
**Figure S33.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the functional evaluation for our calibration set.



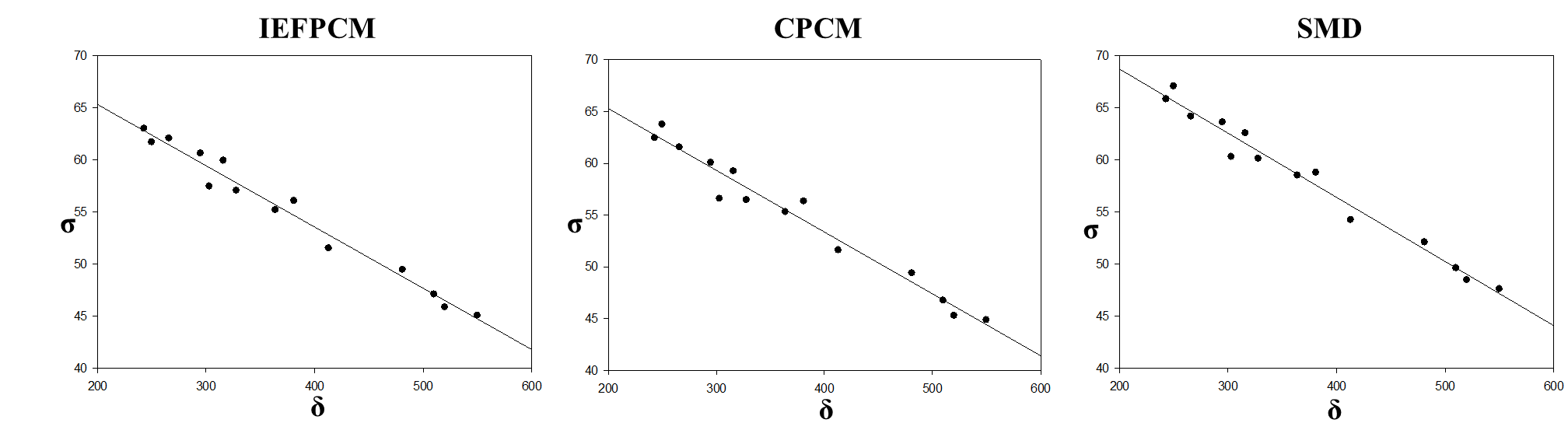
**Figure S34.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the basis set evaluation for our calibration set.



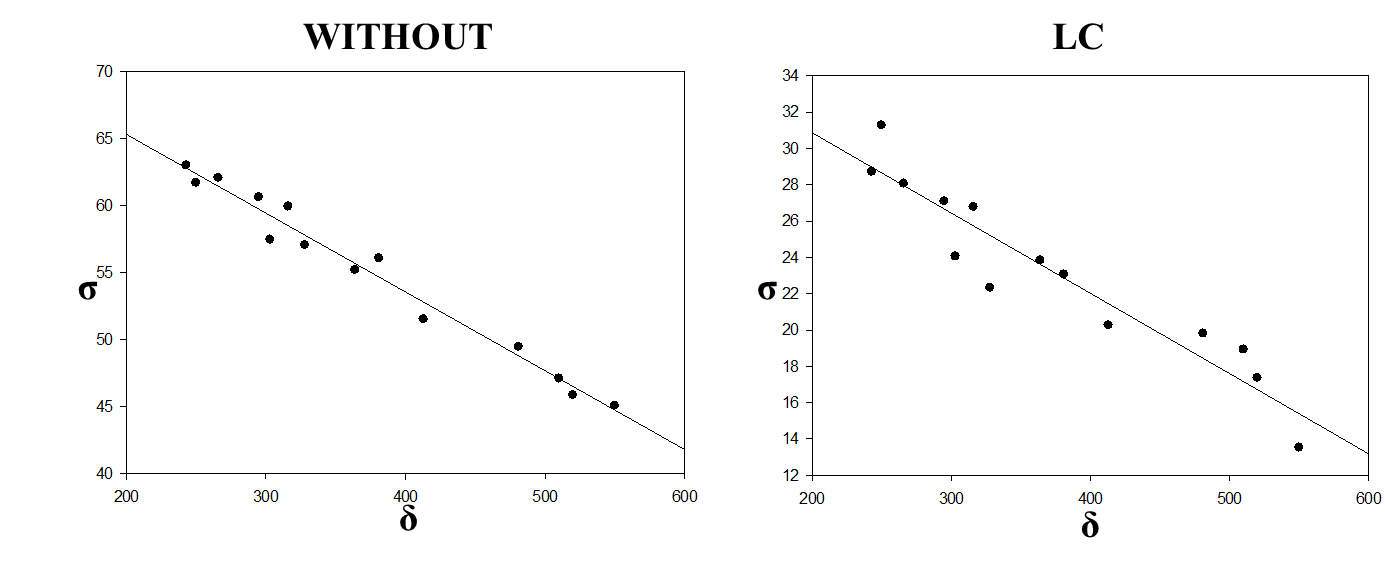
**Figure S35.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the integration grid evaluation for our calibration set.



**Figure S36.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the NMR method evaluation for our calibration set.



**Figure S37.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the solvent model evaluation for our calibration set.



**Figure S38.** Correlation between experimental chemical shifts (δ 195Pt) and the isotropic shielding values (σ) in the process of the LC correction evaluation for our calibration set.

**Table S14.** Evaluation of the functional for calculating 1H isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Class | Functional | Bi-metallic set (1H) | | | | Tri-metallic set(1H) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| GGA | BLYP | 0.9728 | 0.4219 | -1.0325 | 31.5949 | 0.9741 | 0.3546 | -1.0212 | 31.6227 |
| R-S-Hybrid | CAM-B3LYP | 0.9740 | 0.4331 | -1.0855 | 31.7511 | 0.9725 | 0.3847 | -1.0752 | 31.8111 |
| H-M-GGA | M06-2X | 0.9439 | 0.6907 | -1.1603 | 32.0780 | 0.9210 | 0.7048 | -1.1304 | 32.1019 |
| Hybrid | SOGGA11X | 0.9717 | 0.4290 | -1.0762 | 31.7996 | 0.9697 | 0.4023 | -1.0689 | 31.8215 |
| B3LYP | 0.9726 | 0.4288 | -1.0421 | 31,6070 | 0.9737 | 0.3666 | -1.0349 | 31,6341 |
| mPW1PW191 | 0.9723 | 0,4200 | -1.0399 | 31,5989 | 0.9735 | 0.3722 | -1.0299 | 31,6134 |
| Meta-GGA | TPSSTPSS | 0.9742 | 0.4103 | -1.0331 | 31.7055 | 0.9769 | 0.3349 | -1.0230 | 31.7310 |

**Table S15.** Evaluation of the functional for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Class | Functional | Bi-metallic set (13C) | | | | Tri-metallic set(13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| GGA | BLYP | 0.9844 | 7.0944 | -1.0112 | 176.2728 | 0.9908 | 5.3399 | -1.0132 | 176.0869 |
| R-S-Hybrid | CAM-B3LYP | 0.9881 | 6.7032 | -1.0955 | 187.7796 | 0.9931 | 5.0134 | -1.1000 | 187.6947 |
| H-M-GGA | M06-2X | 0.9769 | 10.4659 | -1.2184 | 192.3861 | 0.9760 | 10.4760 | -1.2197 | 192.7633 |
| Hybrid | SOGGA11X | 0.9875 | 6.6008 | -1.0491 | 192.5539 | 0.9844 | 7.2282 | -1.0470 | 191.6968 |
| B3LYP | 0.9879 | 6.6673 | -1.0798 | 181.2290 | 0.9890 | 6.1552 | -1.0322 | 180.9921 |
| mPW1PW191 | 0.9877 | 6.6553 | -1.0678 | 183.0083 | 0.9860 | 6.9034 | -1.0399 | 183.1902 |
| Meta-GGA | TPSSTPSS | 0.9860 | 6.5435 | -0.9828 | 181.9709 | 0.9927 | 4.6650 | -0.9848 | 181.6487 |

**Table S16.** Evaluation of the basis set for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported. (\*) In those cases metals were treated with LANL2DZ basis set.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Family | Basis set | Bi-metallic set (13C) | | | | Tri-metallic set (13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| Ahlrichs | Def2-TZVP | 0.9863 | 6.4818 | -0.9848 | 182.2463 | 0.9922 | 4.8102 | -0.9867 | 182.1053 |
| Jorge | Jorge-TZP | 0.9867 | 6.3384 | -0.9787 | 181.8637 | 0.9924 | 4.7047 | -0.9804 | 181.6361 |
| Lanl | LANL2DZ | 0.9849 | 6.5211 | -0.9446 | 188.8084 | 0.9912 | 4.8624 | -0.9440 | 188.7469 |
| Stuttgard | SDD | 0.9845 | 6.6035 | -0.9433 | 188.9527 | 0.9913 | 4.8389 | -0.9420 | 188.7626 |
| Pople | 6-311++G(2d,2p)\* | 0.9859 | 6.5067 | -0.9689 | 187.0076 | 0.9918 | 4.8433 | -0.9521 | 183.9945 |
| Jensen | pcS-2\* | 0.9861 | 6.4966 | -0.9733 | 183.2267 | 0.9920 | 4.8222 | -0.9801 | 182.2855 |
| Dunning | cc-pVTZ\* | 0.9866 | 6.3778 | -0.9801 | 182.9921 | 0.9923 | 4.7758 | -0.9854 | 182.3401 |
| Ahlrichs\_x2c | x2c-TZVPPall-S | 0.9866 | 6.4571 | -1.0040 | 179.7221 | 0.9922 | 4.8891 | -1.0054 | 179.5659 |

**Table S17.** Evaluation of the solvent model for calculating 1H isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Solvent Model | Bi-metallic set (1H) | | | | Tri-metallic set(1H) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| CPCM | 0.9746 | 0.4087 | -1.0359 | 31.7055 | 0.9774 | 0.3321 | -1.0266 | 31.7307 |
| IEFPCM | 0.9738 | 0.3574 | -1.0235 | 31.7372 | 0.9769 | 0.3349 | -1.0230 | 31.7310 |
| SMD | 0.9746 | 0.4124 | -1.0461 | 31.6968 | 0.9785 | 0.3276 | -1.0373 | 31.7277 |

**Table S18.** Evaluation of the solvent model for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Solvent Model | Bi-metallic set (13C) | | | | Tri-metallic set(13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| CPCM | 0.9860 | 6.5384 | -0.9821 | 181.9024 | 0.9921 | 4.7976 | -0.9831 | 181.6038 |
| IEFPCM | 0.9860 | 6.5436 | -0.9827 | 181.9747 | 0.9922 | 4.7877 | -0.9845 | 181.7259 |
| SMD | 0.9859 | 6.5780 | -0.9844 | 182.1188 | 0.9920 | 4.8621 | -0.9853 | 181.8219 |

**Table S19.** Evaluation of the integration grid for calculating 1H isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Grid | Bi-metallic set (1H) | | | | Tri-metallic set(1H) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| SG1 | 0.9739 | 0.4143 | -1.0353 | 31.7111 | 0.9758 | 0.3446 | -1.0267 | 31.7538 |
| Fine | 0.9737 | 0.4159 | -1.0351 | 31.7107 | 0.9757 | 0.3449 | -1.0263 | 31.7522 |
| Ultrafine | 0.9738 | 0.3574 | -1.0235 | 31.7372 | 0.9769 | 0.3349 | -1.0230 | 31.7310 |
| Superfine | 0.9744 | 0.4091 | -1.0332 | 31.7056 | 0.9771 | 0.3339 | -1.0234 | 31.7328 |

**Table S20.** Evaluation of the integration grid for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Grid | Bi-metallic set (13C) | | | | Tri-metallic set(13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| SG1 | 0.9859 | 6.5302 | -0.9799 | 181.6647 | 0.9917 | 4.9425 | -0.9826 | 181.3460 |
| Fine | 0.9859 | 6.5333 | -0.9799 | 181.6655 | 0.9917 | 4.9398 | -0.9825 | 181.3301 |
| Ultrafine | 0.9860 | 6.5435 | -0.9828 | 181.9709 | 0.9927 | 4.6650 | -0.9848 | 181.6487 |
| Superfine | 0.9859 | 6.5271 | -0.9832 | 181.9229 | 0.9921 | 4.8544 | -0.9803 | 181.2142 |

**Table S21.** Evaluation of the NMR method for calculating 1H isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NMR method | Bi-metallic set (1H) | | | | Tri-metallic set(1H) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| GIAO | 0.9742 | 0.4103 | -1.0331 | 31.7055 | 0.9769 | 0.3349 | -1.0230 | 31.7310 |
| CSGT | 0.9724 | 0.4194 | -1.0192 | 31.6416 | 0.9678 | 0.3892 | -1.0017 | 31.6365 |
| IGAIM | 0.9722 | 0.4195 | -1.0164 | 31.6173 | 0.9659 | 0.4007 | -1.0017 | 31.5466 |
| SO | 0.9707 | 0.4272 | -1.0062 | 31.5842 | 0.9645 | 0.4064 | -0.9948 | 31.5456 |

**Table S22.** Evaluation of the NMR method for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NMR method | Bi-metallic set (13C) | | | | Tri-metallic set(13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| GIAO | 0.9860 | 6.5435 | -0.9828 | 181.9709 | 0.9927 | 4.6650 | -0.9848 | 181.6487 |
| CSGT | 0.9772 | 10.4169 | -1.2211 | 192.7550 | 0.9767 | 10.3474 | -1.2221 | 193.2791 |
| IGAIM | 0.9771 | 10.4286 | -1.2195 | 192.4336 | 0.9764 | 10.4066 | -1.2207 | 192.8696 |
| SO | 0.9682 | 12.5008 | -1.2358 | 192.6469 | 0.9689 | 12.1230 | -1.2352 | 193.9647 |

**Table S23.** Evaluation of the LC correction for calculating 13C isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| LC | Bi-metallic set (1H) | | | | Tri-metallic set(1H) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| YES | 0.9735 | 0.4592 | -1.1387 | 31.7454 | 0.9734 | 0.3974 | -1.1287 | 31.7881 |
| NOT | 0.9742 | 0.4103 | -1.0331 | 31.7055 | 0.9769 | 0.3349 | -1.0230 | 31.7310 |

**Table S24.** Evaluation of the LC correction for calculating 1H isotropic shielding values referred to bi-metallic and tri-metallic subset. Coefficient of determination (R2), standard error (stdErr) and fitted empirical scaling parameters (slope and intercept) are reported.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| LC | Bi-metallic set (13C) | | | | Tri-metallic set(13C) | | | |
| R2 | stdErr | Slope | Intercept | R2 | stdErr | Slope | Intercept |
| YES | 0.9863 | 7.5125 | -1.1418 | 198.6355 | 0.9937 | 5.0153 | -1.1475 | 198.8490 |
| NOT | 0.9860 | 6.5435 | -0.9828 | 181.9709 | 0.9927 | 4.6650 | -0.9848 | 181.6487 |

**Cartesian coordinates**

Compound **Pt**

Tag Symbol X Y Z

1 N -4.2927890 1.3071870 -0.4538280

2 N -4.2677210 -1.2799080 -0.4451150

3 C -3.1305340 0.7976800 -0.3093090

4 C -3.0986010 -0.7059680 -0.3042160

5 S -1.6219060 1.6582140 -0.1216530

6 S -1.6652650 -1.5875230 -0.1384980

7 Pt 0.0000640 -0.0000060 0.0003220

8 S 1.6653930 1.5875080 0.1390210

9 S 1.6220330 -1.6582380 0.1220980

10 C 3.0988370 0.7059450 0.3037520

11 C 3.1307580 -0.7977010 0.3089080

12 N 4.2680440 1.2798930 0.4438950

13 N 4.2930400 -1.3072080 0.4532530

14 C -4.4690760 2.7424030 -0.4581180

15 H -3.6132650 3.2426890 -0.9316280

16 H -5.3596740 2.9638500 -1.0533170

17 C -4.6583940 3.2738500 0.9597760

18 H -3.7738020 3.0723910 1.5691500

19 H -5.5226960 2.8031400 1.4358220

20 C -4.5386950 -2.7058190 -0.4481770

21 H -3.7254380 -3.2045190 -0.9833300

22 H -5.4547500 -2.8538900 -1.0232590

23 C -4.6839220 -3.2684020 0.9586400

24 H -3.7683660 -3.1175130 1.5349250

25 H -5.5121840 -2.7897060 1.4867190

26 C 4.4692690 -2.7424310 0.4578600

27 H 5.3600880 -2.9637520 1.0527700

28 H 3.6136280 -3.2425600 0.9318500

29 C 4.6580180 -3.2742970 -0.9599610

30 H 5.5221210 -2.8037200 -1.4364930

31 H 3.7731830 -3.0730520 -1.5690500

32 C 4.5389820 2.7058190 0.4470840

33 H 3.7265570 3.2042860 0.9837380

34 H 5.4559430 2.8536670 1.0207730

35 C 4.6820500 3.2690570 -0.9596890

36 H 5.5092920 2.7903460 -1.4893550

37 H 3.7655240 3.1187990 -1.5345780

38 H -5.0263630 -0.5974450 -0.5201980

39 H 5.0266950 0.5974300 0.5188560

40 H -4.8222530 4.3546460 0.9377480

41 H -4.8826170 -4.3416690 0.9064920

42 H 4.8218950 -4.3550860 -0.9376710

43 H 4.8812390 4.3422200 -0.9072760

Compound **Ru-Pt**

Tag Symbol X Y Z

1 N 6.6903000 -1.0863360 -0.4478340

2 N 6.5734010 1.4747770 -0.1060310

3 C 5.5032260 -0.6312680 -0.3166320

4 C 5.4171830 0.8563170 -0.1124540

5 S 4.0179020 -1.5487950 -0.3503700

6 S 3.9465350 1.6639860 0.0848520

7 Pt 2.3292450 0.0285660 -0.1568860

8 S 0.7312950 -1.6166880 -0.3983640

9 S 0.6273640 1.5922300 0.0410710

10 C -0.7608580 -0.8217260 -0.0457940

11 C -0.8125980 0.6448480 0.1181200

12 N -1.9073290 -1.4218740 0.0911120

13 N -2.0045990 1.1196410 0.3317900

14 Cl -3.4318410 0.0174740 -2.1271020

15 C 6.9140560 -2.5025730 -0.6357610

16 H 6.1123130 -2.9500850 -1.2392350

17 H 7.8528000 -2.6186480 -1.1852370

18 C 7.0155440 -3.2258570 0.7041180

19 H 6.0816270 -3.1345880 1.2643760

20 H 7.8253010 -2.8073680 1.3078500

21 C 6.7951550 2.8956020 0.0843400

22 H 5.9958650 3.4351240 -0.4322760

23 H 7.7364170 3.1399270 -0.4122000

24 C 6.8423550 3.2824020 1.5556150

25 H 5.9017040 3.0355630 2.0530070

26 H 7.6556970 2.7641050 2.0693690

27 C -2.1840630 2.5575090 0.4823200

28 H -3.0799720 2.7225520 1.0811940

29 H -1.3332520 2.9621180 1.0435300

30 C -2.3144110 3.2600420 -0.8617880

31 H -3.1247750 2.8196320 -1.4443190

32 H -1.3931250 3.1637520 -1.4399720

33 C -1.9725410 -2.8696250 -0.0549520

34 H -1.0133940 -3.2982060 0.2552700

35 H -2.7302670 -3.2425000 0.6351170

36 C -2.3055480 -3.2937880 -1.4770730

37 H -3.2605480 -2.8699130 -1.7932390

38 H -1.5365130 -2.9483840 -2.1716770

39 C -5.1732210 1.0456900 1.1211480

40 C -4.3543700 0.4698290 2.1386480

41 C -4.1670980 -0.9274620 2.2388300

42 C -4.8033540 -1.7357170 1.2480200

43 C -5.5521750 -1.1727850 0.2083060

44 C -5.7586510 0.2429310 0.1333340

45 H -5.2613580 2.1230830 1.0593600

46 H -3.8264490 1.1216500 2.8272320

47 H -4.6343320 -2.8068020 1.2497090

48 H -5.9337830 -1.8087740 -0.5820670

49 C -6.5808980 0.7938800 -1.0035130

50 H -6.2940550 0.2160030 -1.8890740

51 C -8.0620020 0.5352060 -0.7074640

52 H -8.6742780 0.8614860 -1.5526030

53 H -8.2626060 -0.5258560 -0.5340410

54 H -8.3831320 1.0911220 0.1795110

55 C -6.3215930 2.2624720 -1.3011180

56 H -6.6552860 2.9094970 -0.4829450

57 H -5.2600120 2.4402430 -1.4845560

58 H -6.8739720 2.5594960 -2.1961250

59 Ru -3.5756360 -0.2158110 0.2652070

60 C -3.3122610 -1.5330160 3.3063600

61 H -2.5836460 -0.8110990 3.6791370

62 H -3.9352440 -1.8571160 4.1463940

63 H -2.7720400 -2.4050080 2.9322690

64 H 7.3570740 0.8279290 -0.2241610

65 H 7.2178260 -4.2884220 0.5439820

66 H 7.0066930 4.3588240 1.6481640

67 H -2.3592020 -4.3846400 -1.5307660

68 H -2.5170980 4.3231260 -0.7061770

Compound **Ru-Pt-Pd**

Tag Symbol X Y Z

1 N 3.8042200 -1.7747910 -0.5295370

2 N 3.9533170 0.7538130 0.0806690

3 C 2.6615320 -1.1857090 -0.3473080

4 C 2.7482320 0.2527390 0.0160230

5 S 1.1295500 -1.9650890 -0.4861960

6 S 1.3131470 1.1479550 0.3427770

7 Pt -0.4307790 -0.2971670 -0.1200900

8 S -2.1723670 -1.7504910 -0.5792410

9 S -1.9882280 1.3748150 0.2549640

10 C -3.5937500 -0.8654270 -0.1586090

11 C -3.5102790 0.5640700 0.2033190

12 N -4.7976460 -1.3595790 -0.1265930

13 N -4.6552750 1.1168280 0.4790240

14 Cl -6.1195580 0.5289400 -2.1306060

15 C 3.8435330 -3.1895160 -0.8671680

16 H 2.9697200 -3.4322880 -1.4824180

17 H 4.7411630 -3.3620890 -1.4607910

18 C 3.8761380 -4.0549280 0.3847270

19 H 2.9890650 -3.8860410 1.0005090

20 H 4.7682580 -3.8274250 0.9724230

21 C 4.0961760 2.1362140 0.5078560

22 H 3.2318380 2.7123800 0.1603480

23 H 4.9696040 2.5479650 0.0132670

24 C 4.2236540 2.2414090 2.0202190

25 H 3.3156980 1.8817140 2.5096820

26 H 5.0640170 1.6431320 2.3820800

27 C -4.6975150 2.5281930 0.8372650

28 H -5.5814100 2.6904830 1.4546750

29 H -3.8195660 2.7612040 1.4517320

30 C -4.7390680 3.4299190 -0.3883480

31 H -5.5819460 3.1649630 -1.0281480

32 H -3.8249730 3.3268390 -0.9766240

33 C -5.0034430 -2.7578020 -0.4773790

34 H -4.0912760 -3.3184890 -0.2478800

35 H -5.7931210 -3.1519960 0.1637750

36 C -5.3797490 -2.9343810 -1.9401880

37 H -6.2894670 -2.3783780 -2.1752460

38 H -4.5826840 -2.5642320 -2.5888580

39 C -7.8248740 1.2376400 1.2384350

40 C -7.1008240 0.4156510 2.1536810

41 C -7.0678280 -0.9908180 2.0197340

42 C -7.7569950 -1.5498410 0.8998250

43 C -8.4085550 -0.7425020 -0.0388660

44 C -8.4644510 0.6803530 0.1241890

45 H -7.7964910 2.3132380 1.3582510

46 H -6.5279330 0.8822980 2.9483050

47 H -7.7032380 -2.6181610 0.7221350

48 H -8.8294890 -1.1924300 -0.9306620

49 C -9.1919850 1.4981300 -0.9123410

50 H -8.9101330 1.0721860 -1.8819460

51 C -10.7004180 1.3136290 -0.7150590

52 H -11.2470390 1.8397310 -1.5024610

53 H -10.9895430 0.2594660 -0.7495340

54 H -11.0182800 1.7217310 0.2499950

55 C -8.8121720 2.9706800 -0.9200400

56 H -9.1296440 3.4776200 -0.0025010

57 H -7.7341090 3.0976540 -1.0387910

58 H -9.3046660 3.4730940 -1.7562950

59 Ru -6.3456040 -0.0327640 0.1998180

60 C -6.3206940 -1.8549700 2.9851720

61 H -5.5311750 -1.2912120 3.4849880

62 H -7.0050600 -2.2378890 3.7493240

63 H -5.8669610 -2.7113780 2.4825140

64 H 3.9049960 -5.1117010 0.1052150

65 H 4.3833690 3.2825250 2.3145110

66 H -5.5393370 -3.9949980 -2.1529670

67 H -4.8357990 4.4736160 -0.0770640

68 Pd 5.4651220 -0.5869190 -0.2126670

69 P 7.4159410 0.6422920 0.0481820

70 C 7.4140940 2.4678020 0.2787610

71 H 6.7172080 2.7119790 1.0845780

72 H 8.4098090 2.7296620 0.6556200

73 C 8.5232590 0.4196890 -1.3999720

74 H 8.5686480 -0.6558950 -1.5837850

75 H 7.9946380 0.8587070 -2.2539220

76 C 8.3496030 0.0390370 1.5064730

77 H 8.6249900 -0.9950150 1.2804440

78 H 9.2715360 0.6254900 1.5886250

79 C 7.5541200 0.1023900 2.8070750

80 H 7.2874140 1.1419010 3.0316980

81 H 6.6116570 -0.4432720 2.6799320

82 C 8.3348700 -0.4833620 3.9755370

83 H 7.7555160 -0.4330160 4.9015620

84 H 8.5829160 -1.5331100 3.7904050

85 H 9.2725250 0.0586330 4.1358770

86 C 9.9263990 1.0072390 -1.2706210

87 H 10.4553020 0.5183890 -0.4456720

88 H 9.8785710 2.0732910 -1.0218550

89 C 10.7195590 0.8262070 -2.5588600

90 H 11.7296160 1.2337520 -2.4608530

91 H 10.8072190 -0.2329700 -2.8196580

92 H 10.2307860 1.3356930 -3.3954690

93 C 7.1070740 3.2732470 -0.9839810

94 H 7.9443170 3.1830900 -1.6835130

95 H 6.2391530 2.8549830 -1.5079740

96 C 6.8603100 4.7421130 -0.6690870

97 H 6.6762020 5.3159820 -1.5810520

98 H 5.9907770 4.8637150 -0.0146980

99 H 7.7229640 5.1842800 -0.1606160

100 Cl 6.9404290 -2.3669610 -0.4435630

Compound **α**

Tag Symbol X Y Z

1 Pd 0.1303320 -0.0068100 -0.2537110

2 Pt -3.6174310 -0.0174510 -0.0709260

3 P 1.5841550 1.7818720 -0.1168330

4 P 1.6019950 -1.7693230 0.0495770

5 N 0.6179860 3.1035790 -0.8501140

6 N -1.1619300 1.5094470 -0.7217960

7 N -2.5260910 1.4283180 -0.9556940

8 N 0.6634030 -3.1358210 -0.6376760

9 N -1.1440170 -1.5699940 -0.5934260

10 N -2.5105230 -1.5266530 -0.8156460

11 Cl -4.9403900 1.6834370 0.8633400

12 Cl -4.8807920 -1.6327240 1.0731290

13 S -1.8732250 3.7959910 -1.8021910

14 S -1.8308380 -3.9415920 -1.4880120

15 C -0.6125310 2.7242810 -1.0368630

16 C -3.0403850 2.4783780 -1.5291840

17 H -4.0877460 2.5777460 -1.7393580

18 C 2.0746060 2.4166650 1.5454520

19 C 1.8310900 3.7497460 1.8762580

20 H 1.3495610 4.3974920 1.1561860

21 C 2.2061790 4.2217760 3.1331780

22 H 2.0175100 5.2542520 3.3945890

23 C 2.8178300 3.3672760 4.0497110

24 H 3.1027880 3.7367170 5.0257520

25 C 3.0550880 2.0339340 3.7138250

26 H 3.5190270 1.3651060 4.4262000

27 C 2.6831890 1.5544630 2.4606570

28 H 2.8519900 0.5135440 2.2167040

29 C 3.1132110 1.7274130 -1.1440890

30 C 4.2904500 2.3410680 -0.7186670

31 H 4.3333690 2.8304000 0.2455090

32 C 5.4126540 2.3175790 -1.5455590

33 H 6.3280690 2.7927240 -1.2192140

34 C 5.3531890 1.6878430 -2.7870690

35 H 6.2271300 1.6676170 -3.4245400

36 C 4.1722940 1.0742020 -3.2071270

37 H 4.1296720 0.5724850 -4.1639690

38 C 3.0502170 1.0917900 -2.3862900

39 H 2.1373280 0.5989140 -2.6981590

40 C -0.5773480 -2.7945940 -0.8280780

41 C -3.0161670 -2.6251040 -1.2989500

42 H -4.0641210 -2.7542320 -1.4892110

43 C 1.9603730 -2.1818470 1.8152740

44 C 2.9933780 -3.0603790 2.1502030

45 H 3.6206120 -3.4849670 1.3776470

46 C 3.2156640 -3.3802680 3.4874830

47 H 4.0165290 -4.0582100 3.7500320

48 C 2.4059610 -2.8322770 4.4828680

49 H 2.5828430 -3.0824480 5.5204240

50 C 1.3681570 -1.9644680 4.1440350

51 H 0.7376490 -1.5400980 4.9132260

52 C 1.1405760 -1.6391480 2.8090460

53 H 0.3403220 -0.9592670 2.5440560

54 C 3.2032170 -1.8856110 -0.8522710

55 C 4.3474830 -1.2771440 -0.3304600

56 H 4.3147240 -0.7613020 0.6203910

57 C 5.5440910 -1.3435070 -1.0366580

58 H 6.4285820 -0.8678280 -0.6361410

59 C 5.5973180 -2.0116050 -2.2600670

60 H 6.5289120 -2.0588690 -2.8081530

61 C 4.4529350 -2.6159450 -2.7771860

62 H 4.4940390 -3.1394710 -3.7229260

63 C 3.2502640 -2.5536780 -2.0757950

64 H 2.3587900 -3.0337400 -2.4555820

Compound **β**

Tag Symbol X Y Z

1 P 1.3181290 1.7809460 -0.0591500

2 P 1.3119100 -1.7793210 0.0498460

3 N 0.3565080 3.1450560 -0.7221400

4 N -1.4149130 1.5332680 -0.6894350

5 N -2.7745340 1.4599070 -0.9372790

6 N 0.3767720 -3.1451040 -0.6509140

7 N -1.4104020 -1.5527710 -0.6279090

8 N -2.7722200 -1.4959220 -0.8583120

9 Cl -5.2035810 1.6839880 0.9044720

10 Cl -5.1547620 -1.6313980 1.0470200

11 S -2.1290100 3.8691840 -1.6605540

12 S -2.1178230 -3.9177610 -1.5276010

13 C -0.8685340 2.7733260 -0.9368210

14 C -3.2902510 2.5319270 -1.4570830

15 H -4.3384770 2.6408680 -1.6597590

16 C 1.8470640 2.3578820 1.6124560

17 C 1.6733670 3.6943650 1.9719440

18 H 1.2164180 4.3796060 1.2709140

19 C 2.0821830 4.1214550 3.2345460

20 H 1.9466940 5.1562690 3.5187610

21 C 2.6585650 3.2191810 4.1279810

22 H 2.9699560 3.5539980 5.1084660

23 C 2.8259640 1.8829400 3.7633190

24 H 3.2617090 1.1769820 4.4574820

25 C 2.4202610 1.4488980 2.5040290

26 H 2.5330540 0.4064210 2.2372400

27 C 2.8261600 1.7470450 -1.1166540

28 C 4.0091790 2.3591030 -0.7062380

29 H 4.0691240 2.8359090 0.2634050

30 C 5.1150370 2.3498750 -1.5550580

31 H 6.0356290 2.8231510 -1.2407300

32 C 5.0328790 1.7351280 -2.8029160

33 H 5.8941100 1.7259330 -3.4577700

34 C 3.8460750 1.1222880 -3.2070670

35 H 3.7865680 0.6319260 -4.1689060

36 C 2.7402390 1.1254230 -2.3641100

37 H 1.8217010 0.6340720 -2.6608450

38 C -0.8559580 -2.7925800 -0.8543070

39 C -3.2878330 -2.5849120 -1.3414830

40 H -4.3377070 -2.7053690 -1.5289400

41 C 1.6725430 -2.2323740 1.8040990

42 C 2.7185110 -3.1038160 2.1152850

43 H 3.3520760 -3.4967850 1.3311750

44 C 2.9445870 -3.4593990 3.4429370

45 H 3.7554970 -4.1323760 3.6867470

46 C 2.1253340 -2.9530030 4.4522110

47 H 2.3043090 -3.2306960 5.4823900

48 C 1.0744430 -2.0920620 4.1364460

49 H 0.4361590 -1.7006250 4.9166430

50 C 0.8428600 -1.7308250 2.8114090

51 H 0.0312970 -1.0571000 2.5659230

52 C 2.9083330 -1.8717350 -0.8650580

53 C 4.0534440 -1.2677940 -0.3413770

54 H 4.0274680 -0.7720310 0.6203970

55 C 5.2434170 -1.3120200 -1.0608970

56 H 6.1288920 -0.8387000 -0.6597370

57 C 5.2886300 -1.9549330 -2.2978980

58 H 6.2148400 -1.9846210 -2.8562650

59 C 4.1431100 -2.5563070 -2.8157090

60 H 4.1778420 -3.0600400 -3.7724080

61 C 2.9472650 -2.5158860 -2.1010570

62 H 2.0549970 -2.9935080 -2.4821770

63 Pt -0.1159750 -0.0007070 -0.2485640

64 Pd -3.8838100 0.0013600 -0.0679340

Compound **α dimer**

Tag Symbol X Y Z

1 P -7.0707720 1.7106770 0.2836020

2 P -6.9627550 -1.8360040 -0.1048110

3 N -6.0645790 3.0413840 0.9442810

4 N -4.2685210 1.5371570 0.4690540

5 N -2.8826160 1.4975220 0.5046870

6 N -5.8957040 -3.1772370 0.4294760

7 N -4.1782820 -1.5295760 0.2173810

8 N -2.7983210 -1.4184900 0.2986390

9 Cl -1.0116930 1.9313590 -1.8413600

10 Cl -0.8453530 -1.4068060 -2.0286500

11 S -3.4792940 3.7921540 1.5546730

12 S -3.2842770 -3.8679320 1.0010260

13 C -4.8049030 2.7093590 0.9277100

14 C -2.3198740 2.5363790 1.0479900

15 H -1.2526180 2.6390520 1.1438610

16 C -7.8390310 2.4051440 -1.2438270

17 C -7.8285250 3.7831650 -1.4615570

18 H -7.3488810 4.4328630 -0.7419800

19 C -8.4247160 4.2977980 -2.6117580

20 H -8.4168450 5.3652870 -2.7863150

21 C -9.0238340 3.4411840 -3.5350590

22 H -9.4813130 3.8447870 -4.4285280

23 C -9.0248420 2.0635470 -3.3144690

24 H -9.4759240 1.3947270 -4.0351310

25 C -8.4310160 1.5417590 -2.1679810

26 H -8.4129340 0.4703960 -2.0146100

27 C -8.4252640 1.5226960 1.5200450

28 C -9.6702290 2.1178790 1.3215960

29 H -9.8719170 2.6718430 0.4141560

30 C -10.6546910 1.9907780 2.3003640

31 H -11.6219060 2.4515210 2.1500690

32 C -10.3924680 1.2746770 3.4665800

33 H -11.1601610 1.1733810 4.2222380

34 C -9.1453940 0.6786620 3.6587290

35 H -8.9456990 0.1101930 4.5565630

36 C -8.1593120 0.8009730 2.6860070

37 H -7.1964070 0.3230150 2.8208580

38 C -4.6565490 -2.7805230 0.4919550

39 C -2.1893640 -2.4905970 0.7117630

40 H -1.1231640 -2.5442150 0.8372130

41 C -7.4991250 -2.2063750 -1.8363450

42 C -8.5595550 -3.0802270 -2.0865470

43 H -9.1020570 -3.5280110 -1.2645800

44 C -8.9199000 -3.3651780 -3.4016440

45 H -9.7428530 -4.0393720 -3.5973200

46 C -8.2198050 -2.7869160 -4.4607210

47 H -8.5037280 -3.0094620 -5.4806960

48 C -7.1537840 -1.9237930 -4.2079430

49 H -6.6072650 -1.4760770 -5.0266450

50 C -6.7888500 -1.6331750 -2.8956030

51 H -5.9657280 -0.9575010 -2.6993250

52 C -8.4516500 -2.0574320 0.9558600

53 C -9.6516650 -1.4282890 0.6147070

54 H -9.7282180 -0.8336210 -0.2866550

55 C -10.7623450 -1.5733990 1.4392950

56 H -11.6892900 -1.0810120 1.1796720

57 C -10.6743510 -2.3404880 2.6013420

58 H -11.5389790 -2.4480380 3.2427900

59 C -9.4748830 -2.9647980 2.9379380

60 H -9.4063070 -3.5634890 3.8363420

61 C -8.3573720 -2.8242200 2.1167790

62 H -7.4235420 -3.3145170 2.3552160

63 P 7.0709020 1.7106400 -0.2841110

64 P 6.9626090 -1.8359890 0.1057100

65 N 6.0648630 3.0410900 -0.9455500

66 N 4.2686910 1.5372300 -0.4696310

67 N 2.8828010 1.4976310 -0.5053580

68 N 5.8954190 -3.1773820 -0.4279120

69 N 4.1781630 -1.5294100 -0.2169100

70 N 2.7982170 -1.4182530 -0.2983160

71 Cl 1.0119640 1.9323840 1.8407290

72 Cl 0.8449570 -1.4056810 2.0286150

73 S 3.4796360 3.7916990 -1.5564710

74 S 3.2839960 -3.8680740 -0.9994840

75 C 4.8051630 2.7091520 -0.9288880

76 C 2.3201250 2.5362260 -1.0492360

77 H 1.2528750 2.6387570 -1.1453860

78 C 7.8390860 2.4059000 1.2429940

79 C 7.8277050 3.7839450 1.4604860

80 H 7.3475050 4.4331890 0.7408700

81 C 8.4238010 4.2991840 2.6104680

82 H 8.4152680 5.3667000 2.7848260

83 C 9.0236860 3.4431370 3.5337930

84 H 9.4810950 3.8472060 4.4270870

85 C 9.0255620 2.0654590 3.3134470

86 H 9.4772420 1.3970690 4.0341310

87 C 8.4318410 1.5430760 2.1671790

88 H 8.4144460 0.4716710 2.0140080

89 C 8.4254930 1.5218260 -1.5203190

90 C 9.6705350 2.1169000 -1.3220150

91 H 9.8722060 2.6712670 -0.4148170

92 C 10.6550810 1.9891860 -2.3006190

93 H 11.6223560 2.4498420 -2.1504330

94 C 10.3928610 1.2726010 -3.4665370

95 H 11.1606150 1.1708300 -4.2220700

96 C 9.1457070 0.6767110 -3.6585480

97 H 8.9460100 0.1078660 -4.5561420

98 C 8.1595450 0.7996180 -2.6859820

99 H 7.1965720 0.3217670 -2.8207230

100 C 4.6563260 -2.7805510 -0.4907620

101 C 2.1891920 -2.4904930 -0.7109940

102 H 1.1229810 -2.5440750 -0.8363450

103 C 7.4991130 -2.2055910 1.8373560

104 C 8.5592700 -3.0796900 2.0878600

105 H 9.1014650 -3.5281310 1.2660480

106 C 8.9197440 -3.3640410 3.4030510

107 H 9.7424860 -4.0384240 3.5989600

108 C 8.2200410 -2.7849380 4.4619290

109 H 8.5040640 -3.0070160 5.4819780

110 C 7.1542810 -1.9215800 4.2088570

111 H 6.6080620 -1.4732200 5.0274060

112 C 6.7892190 -1.6315630 2.8964190

113 H 5.9662820 -0.9557360 2.6999090

114 C 8.4513780 -2.0581440 -0.9550160

115 C 9.6516960 -1.4294740 -0.6140610

116 H 9.7286050 -0.8347660 0.2872410

117 C 10.7622490 -1.5751950 -1.4387180

118 H 11.6894340 -1.0831830 -1.1792370

119 C 10.6738360 -2.3424360 -2.6006290

120 H 11.5383690 -2.4504710 -3.2421250

121 C 9.4740710 -2.9662880 -2.9370250

122 H 9.4051730 -3.5651180 -3.8353120

123 C 8.3566880 -2.8250830 -2.1158060

124 H 7.4226440 -3.3150570 -2.3540720

125 Pt -1.9146860 0.1379890 -0.6112940

126 Pt 1.9146900 0.1385920 0.6110550

127 Pd 5.5477920 -0.0132460 -0.1041600

128 Pd -5.5477880 -0.0133410 0.1042250

Compound **β dimer**

Tag Symbol X Y Z

1 P 7.0305630 1.7564580 -0.1898890

2 P 6.9926420 -1.8096870 0.0888120

3 N 6.0107430 3.1070560 -0.7963860

4 N 4.2506830 1.5219240 -0.4653950

5 N 2.8709750 1.4444600 -0.5466880

6 N 5.9726630 -3.1759880 -0.4826920

7 N 4.2249280 -1.5542560 -0.2992220

8 N 2.8478460 -1.4692950 -0.3989010

9 Cl 0.9688900 1.7967850 1.8070890

10 Cl 0.9188120 -1.5473380 1.9689670

11 S 3.4236190 3.8074970 -1.4567970

12 S 3.3825820 -3.9084990 -1.0955420

13 C 4.7643100 2.7413760 -0.8398260

14 C 2.2912710 2.4888470 -1.0507120

15 H 1.2227380 2.5691970 -1.1642390

16 C 7.7765590 2.3994240 1.3698120

17 C 7.7998410 3.7728700 1.6146580

18 H 7.3566660 4.4506240 0.8976850

19 C 8.3791330 4.2476850 2.7902760

20 H 8.3965450 5.3113230 2.9864080

21 C 8.9281430 3.3560810 3.7118330

22 H 9.3725800 3.7289180 4.6250550

23 C 8.8952630 1.9836940 3.4638460

24 H 9.3069610 1.2879200 4.1826010

25 C 8.3180210 1.5017420 2.2915150

26 H 8.2721100 0.4349370 2.1157090

27 C 8.3909720 1.6462480 -1.4290510

28 C 9.6193580 2.2677990 -1.2114430

29 H 9.8062740 2.7990870 -0.2873400

30 C 10.6069290 2.1963500 -2.1927440

31 H 11.5619430 2.6772100 -2.0279810

32 C 10.3636380 1.5085650 -3.3800360

33 H 11.1336660 1.4506160 -4.1379280

34 C 9.1328590 0.8856500 -3.5907700

35 H 8.9483410 0.3394310 -4.5055460

36 C 8.1438570 0.9522640 -2.6154730

37 H 7.1927440 0.4552240 -2.7630400

38 C 4.7295240 -2.8048340 -0.5646760

39 C 2.2614380 -2.5479780 -0.8150610

40 H 1.1952720 -2.6233110 -0.9358900

41 C 7.5126670 -2.2194390 1.8156910

42 C 8.6076480 -3.0515270 2.0567390

43 H 9.1850490 -3.4447450 1.2305690

44 C 8.9564910 -3.3666250 3.3682350

45 H 9.8065120 -4.0084360 3.5569660

46 C 8.2104050 -2.8593770 4.4320930

47 H 8.4851090 -3.1046960 5.4493770

48 C 7.1093770 -2.0385940 4.1874750

49 H 6.5267960 -1.6467130 5.0099650

50 C 6.7558070 -1.7178130 2.8791330

51 H 5.9055690 -1.0748380 2.6886930

52 C 8.4977940 -1.9534890 -0.9628780

53 C 9.6719480 -1.2936970 -0.5930330

54 H 9.7206480 -0.7223950 0.3251740

55 C 10.7933180 -1.3765590 -1.4121040

56 H 11.7003160 -0.8593910 -1.1310980

57 C 10.7411050 -2.1132490 -2.5956130

58 H 11.6136800 -2.1720680 -3.2326210

59 C 9.5670390 -2.7695250 -2.9596360

60 H 9.5262040 -3.3444400 -3.8751060

61 C 8.4391810 -2.6912220 -2.1441350

62 H 7.5250950 -3.2068450 -2.4047290

63 Pt 5.5719150 -0.0115600 -0.1163960

64 Pd 1.9195240 0.0471170 0.5518650

65 P -7.0740230 1.7341600 0.2495970

66 P -6.9476120 -1.8175380 -0.1371100

67 N -6.0799880 3.0991290 0.8653160

68 N -4.2838220 1.5673500 0.4778720

69 N -2.9020590 1.5270290 0.5323310

70 N -5.8946240 -3.1738110 0.3949170

71 N -4.1861750 -1.5054570 0.2614590

72 N -2.8110320 -1.3892680 0.3738440

73 Cl -1.0500740 1.9322010 -1.8495050

74 Cl -0.8318310 -1.4053390 -1.9574630

75 S -3.5006630 3.8641720 1.4799310

76 S -3.2927460 -3.8553810 1.0130840

77 C -4.8236090 2.7672370 0.8791180

78 C -2.3413370 2.5824990 1.0350610

79 H -1.2740130 2.6890710 1.1272810

80 C -7.8678000 2.3931220 -1.2796650

81 C -7.9383310 3.7711440 -1.4870450

82 H -7.5013370 4.4431120 -0.7609560

83 C -8.5558250 4.2585240 -2.6377660

84 H -8.6101590 5.3259220 -2.8045090

85 C -9.0955540 3.3747860 -3.5722920

86 H -9.5700350 3.7574650 -4.4661080

87 C -9.0144380 1.9980670 -3.3625490

88 H -9.4182140 1.3088560 -4.0920220

89 C -8.3989360 1.5036210 -2.2150780

90 H -8.3151330 0.4344780 -2.0707600

91 C -8.4091000 1.5528380 1.5082120

92 C -9.6541330 2.1546800 1.3335310

93 H -9.8677030 2.7164390 0.4335630

94 C -10.6243990 2.0228230 2.3257210

95 H -11.5922620 2.4878590 2.1938910

96 C -10.3478690 1.2944450 3.4811730

97 H -11.1049020 1.1887050 4.2469610

98 C -9.1003610 0.6924130 3.6494660

99 H -8.8895570 0.1151660 4.5391840

100 C -8.1282360 0.8197640 2.6632460

101 H -7.1642620 0.3391260 2.7772340

102 C -4.6615460 -2.7736420 0.4942030

103 C -2.2028090 -2.4625980 0.7721000

104 H -1.1359770 -2.5163200 0.9030690

105 C -7.4594170 -2.1828340 -1.8763500

106 C -8.5385720 -3.0273890 -2.1437740

107 H -9.1076450 -3.4577130 -1.3304050

108 C -8.8827530 -3.3063760 -3.4647000

109 H -9.7206140 -3.9577620 -3.6738720

110 C -8.1476290 -2.7506290 -4.5118170

111 H -8.4187190 -2.9678620 -5.5364330

112 C -7.0624230 -1.9170100 -4.2411320

113 H -6.4887950 -1.4869910 -5.0507560

114 C -6.7136090 -1.6320980 -2.9233070

115 H -5.8767210 -0.9778740 -2.7127770

116 C -8.4479110 -2.0329120 0.9097640

117 C -9.6345360 -1.3783960 0.5716360

118 H -9.6964770 -0.7677420 -0.3200790

119 C -10.7519570 -1.5166260 1.3885620

120 H -11.6685670 -1.0035750 1.1322860

121 C -10.6837220 -2.3035990 2.5384600

122 H -11.5534190 -2.4058450 3.1739120

123 C -9.4973960 -2.9545500 2.8708330

124 H -9.4440430 -3.5685710 3.7598930

125 C -8.3732680 -2.8206700 2.0573640

126 H -7.4493310 -3.3308430 2.2928470

127 Pt -5.5706020 0.0078780 0.1160520

128 Pd -1.9173850 0.1557690 -0.5686360

Compound **Pt-φ**

Tag Symbol X Y Z

1 N -3.9664120 1.2101840 0.2460980

2 N -3.9005580 -1.3727090 0.3117050

3 C -2.8021010 0.7127420 0.0751770

4 C -2.7492100 -0.7855370 0.0993110

5 S -1.3251210 1.5959530 -0.1806520

6 S -1.3219450 -1.6560310 -0.1372250

7 Pt 0.2962440 -0.0439640 -0.4728340

8 S 1.9143030 1.5637470 -0.7974870

9 S 1.9149360 -1.6832840 -0.7554650

10 C 3.3294290 0.6999140 -1.1247170

11 C 3.3810170 -0.8054540 -1.1157870

12 N 4.4770530 1.2773560 -1.3853730

13 N 4.5360520 -1.2923210 -1.3612470

14 C -4.1439390 2.6357680 0.2316500

15 H -3.7121120 3.0543210 -0.6930570

16 C -4.1401600 -2.8039550 0.3561230

17 H -3.6394120 -3.2607150 -0.5058890

18 C 4.7647530 -2.7186560 -1.3501930

19 H 5.3772760 -2.9635310 -2.2229900

20 C 4.7600450 2.6954990 -1.4183780

21 H 5.3638440 2.8953290 -2.3071560

22 H -4.6702960 -0.7129890 0.4491140

23 H -3.5688880 3.0951070 1.0496060

24 C -5.5923820 3.0386740 0.3327490

25 C -6.6101340 2.2129600 -0.1428330

26 C -5.9309490 4.2800520 0.8711690

27 C -7.9388340 2.6201890 -0.0819360

28 H -6.3554780 1.2424550 -0.5558710

29 C -7.2581070 4.6915410 0.9301180

30 H -5.1477680 4.9303300 1.2522040

31 C -8.2680370 3.8616400 0.4530570

32 H -8.7200040 1.9642280 -0.4537140

33 H -7.5041400 5.6594320 1.3555110

34 H -9.3047700 4.1788420 0.5019750

35 H -3.6763350 -3.2209090 1.2567300

36 C -5.6173260 -3.0783440 0.3290630

37 C -6.3632580 -2.7504980 -0.8047600

38 C -6.2610300 -3.6338890 1.4316860

39 C -7.7339670 -2.9736140 -0.8325160

40 H -5.8653030 -2.3207620 -1.6697610

41 C -7.6333190 -3.8639780 1.4027050

42 H -5.6868550 -3.8868770 2.3181150

43 C -8.3713850 -3.5319320 0.2724810

44 H -8.3051640 -2.7169200 -1.7186540

45 H -8.1254840 -4.2987170 2.2664650

46 H -9.4417120 -3.7088480 0.2504540

47 H 3.8268070 -3.2850030 -1.4320680

48 C 5.5032170 -3.1453940 -0.1014990

49 C 6.5830720 -4.0223230 -0.1860770

50 C 5.1017460 -2.6886340 1.1548640

51 C 7.2463050 -4.4446510 0.9623890

52 H 6.9104800 -4.3770430 -1.1594610

53 C 5.7650790 -3.1057460 2.3024820

54 H 4.2620770 -2.0050760 1.2346460

55 C 6.8394170 -3.9866600 2.2105180

56 H 8.0863880 -5.1270040 0.8794390

57 H 5.4413530 -2.7426630 3.2728780

58 H 7.3576910 -4.3111420 3.1070950

59 C 5.4840440 3.1756070 -0.1819380

60 C 5.1866740 2.6570870 1.0776720

61 C 6.4432610 4.1800720 -0.2954030

62 C 5.8369760 3.1409510 2.2068210

63 H 4.4448830 1.8714380 1.1817410

64 C 7.0906300 4.6679540 0.8346780

65 H 6.6883310 4.5823070 -1.2744250

66 C 6.7890240 4.1488840 2.0891430

67 H 5.5982160 2.7285810 3.1817360

68 H 7.8372110 5.4488710 0.7326680

69 H 7.2970600 4.5244800 2.9712690

70 H 3.8132460 3.2295930 -1.5395210

71 H 5.2308410 0.5967080 -1.5199590

Compound **Pt-Me**

Tag Symbol X Y Z

1 N 4.3107330 -1.3113920 -0.0090660

2 N 4.2825590 1.2892500 -0.0026230

3 C 3.1423580 -0.7935310 0.0033190

4 C 3.1099890 0.7048370 0.0031960

5 S 1.6300290 -1.6592710 0.0224060

6 S 1.6716590 1.5906720 0.0094180

7 Pt 0.0000260 -0.0000610 0.0007650

8 S -1.6716970 -1.5906500 -0.0103930

9 S -1.6298620 1.6592340 -0.0195120

10 C -3.1099510 -0.7047900 -0.0049540

11 C -3.1422340 0.7935590 -0.0030950

12 N -4.2826650 -1.2889480 -0.0017940

13 N -4.3106300 1.3113070 0.0091220

14 C 4.4434920 -2.7448560 -0.0111740

15 H 3.9450960 -3.1884810 -0.8842010

16 C 4.5063240 2.7150030 -0.0067250

17 H 4.0492780 3.1700720 -0.8904650

18 C -4.4435100 2.7447350 0.0129460

19 H -5.4997820 3.0152770 0.0317520

20 C -4.5068310 -2.7146080 -0.0001370

21 H -5.5791730 -2.8992760 0.0080190

22 H 5.0585720 0.6251800 -0.0072490

23 H 3.9777520 -3.1880490 0.8798210

24 H 4.0663790 3.1728740 0.8841880

25 H -3.9773080 3.1890840 -0.8772320

26 H -4.0652410 -3.1713760 -0.8907920

27 H 5.4997140 -3.0155710 -0.0302070

28 H 5.5785910 2.8999700 -0.0172500

29 H -3.9456450 3.1872960 0.8868030

30 H -4.0516930 -3.1710320 0.8838850

31 H -5.0584630 -0.6246100 0.0027850

Compound **Pt-iso**

Tag Symbol X Y Z

1 N 4.1743470 -1.3698410 -1.0423750

2 N 4.1862740 1.2194830 -1.0205650

3 C 3.0531310 -0.8440310 -0.7278890

4 C 3.0424930 0.6587420 -0.7143670

5 S 1.5769610 -1.6862770 -0.3231230

6 S 1.6599370 1.5594890 -0.3416260

7 Pt 0.0020200 -0.0077610 -0.0100700

8 S -1.6571690 -1.5737680 0.3241850

9 S -1.5713760 1.6715630 0.3026390

10 C -3.0359820 -0.6718080 0.7075930

11 C -3.0434760 0.8309920 0.7253340

12 N -4.1787200 -1.2310500 1.0203320

13 N -4.1593100 1.3580300 1.0564980

14 C 4.3192250 -2.8067090 -1.0767050

15 H 3.3950980 -3.2897190 -1.4271800

16 H 5.1141690 -3.0397550 -1.7899410

17 C 4.6797590 -3.3517580 0.3068820

18 H 3.9413770 -2.9788190 1.0257430

19 H 5.6535840 -2.9450280 0.6096850

20 C 4.7174810 -4.8785560 0.3810260

21 H 3.7299420 -5.2501330 0.0721260

22 C 4.9602000 -5.3241220 1.8198380

23 H 5.9379270 -4.9750140 2.1723730

24 H 4.1980750 -4.9231670 2.4952830

25 H 4.9464550 -6.4153530 1.9035900

26 C 5.7658520 -5.4805500 -0.5507400

27 H 5.5636410 -5.2571740 -1.6020000

28 H 6.7627710 -5.0922300 -0.3097350

29 H 5.7989840 -6.5695890 -0.4470800

30 C 4.4655140 2.6413050 -1.0544920

31 H 3.5815660 3.1471140 -1.4519660

32 H 5.2849220 2.7949210 -1.7610160

33 C 4.8385670 3.1805910 0.3234510

34 H 4.0199660 2.9727350 1.0234920

35 H 5.7139410 2.6287700 0.6847890

36 C 5.1426870 4.6796220 0.3312160

37 H 5.9174940 4.8718980 -0.4251840

38 C 5.6999780 5.0867670 1.6918690

39 H 4.9611920 4.9041880 2.4806690

40 H 6.6028000 4.5203920 1.9405960

41 H 5.9519780 6.1513120 1.7113920

42 C 3.9142890 5.5175090 -0.0156640

43 H 3.5374790 5.3138710 -1.0218200

44 H 3.1018650 5.3183910 0.6925610

45 H 4.1478770 6.5851820 0.0350540

46 C -4.3005300 2.7952850 1.0936910

47 H -5.0886320 3.0370040 1.8145120

48 H -3.3701080 3.2672160 1.4356600

49 C -4.6956610 3.3382190 -0.2806460

50 H -5.6091160 2.8231950 -0.6008390

51 H -3.9136420 3.0786830 -1.0054800

52 C -4.9288550 4.8495000 -0.3096560

53 H -5.6665020 5.0925130 0.4691290

54 C -5.5133720 5.2600620 -1.6580800

55 H -4.8121320 5.0274190 -2.4679970

56 H -6.4501770 4.7331960 -1.8652180

57 H -5.7152300 6.3352940 -1.6912550

58 C -3.6519880 5.6353220 -0.0215650

59 H -3.2494550 5.4253940 0.9730570

60 H -2.8761040 5.3859250 -0.7546770

61 H -3.8361460 6.7125460 -0.0819780

62 C -4.4600810 -2.6523220 1.0622950

63 H -3.5799880 -3.1645050 1.4656280

64 H -5.2805260 -2.7923260 1.7679320

65 C -4.8099210 -3.2062180 -0.3164690

66 H -5.7410690 -2.7420210 -0.6658810

67 H -4.0226960 -2.9089520 -1.0178630

68 C -4.9546610 -4.7281800 -0.3420350

69 H -4.0114860 -5.1581100 0.0242160

70 C -5.1654120 -5.2046280 -1.7756990

71 H -6.0974140 -4.7976960 -2.1848550

72 H -4.3457570 -4.8860360 -2.4269140

73 H -5.2299080 -6.2959020 -1.8219190

74 C -6.0856980 -5.2176570 0.5589230

75 H -5.9159280 -4.9754680 1.6120100

76 H -7.0391740 -4.7673060 0.2583810

77 H -6.1942500 -6.3040240 0.4882760

78 H 4.9200750 0.5305200 -1.2027120

79 H -4.9082940 -0.5407050 1.2137230

Compound **1** (calibration set)

Tag Symbol X Y Z

1 N 6.2110030 -1.1322900 -0.9053550

2 N 6.0899190 1.4524860 -0.8255740

3 C 5.0380310 -0.6697280 -0.6946750

4 C 4.9517830 0.8292850 -0.6356200

5 S 3.5710990 -1.5931490 -0.4772970

6 S 3.5003920 1.6474730 -0.3541560

7 Pt 1.8942320 -0.0104040 -0.2323830

8 S 0.3005910 -1.6766990 -0.1332070

9 S 0.2117550 1.5656610 0.0184940

10 C -1.1752700 -0.8452450 0.2023730

11 C -1.2183310 0.6300700 0.2493150

12 N -2.3156750 -1.4235320 0.4447180

13 N -2.3956210 1.1231690 0.5015990

14 Cl -3.8319150 -0.1546540 -1.8664030

15 C 6.4286880 -2.5593030 -0.9633280

16 H 5.5712490 -3.0737950 -1.4217350

17 H 7.3039510 -2.7331840 -1.5948570

18 C 6.6699590 -3.1293020 0.4360550

19 H 5.8417680 -2.8147780 1.0811280

20 H 7.5841860 -2.6846750 0.8510110

21 C 6.7792340 -4.6537950 0.4763790

22 H 5.8515730 -5.0643350 0.0527270

23 C 6.8888610 -5.1298160 1.9217630

24 H 7.8028700 -4.7425660 2.3874280

25 H 6.0380020 -4.7881610 2.5193890

26 H 6.9243580 -6.2224080 1.9769990

27 C 7.9521760 -5.1745370 -0.3498590

28 H 7.8531860 -4.9289910 -1.4108940

29 H 8.8954060 -4.7447560 0.0085140

30 H 8.0311900 -6.2633000 -0.2706940

31 C 6.3005980 2.8856040 -0.7928580

32 H 5.4318450 3.3622470 -1.2548900

33 H 7.1716590 3.1008390 -1.4169750

34 C 6.5208230 3.3974180 0.6278690

35 H 5.6556530 3.1249370 1.2448150

36 H 7.3890490 2.8789100 1.0508640

37 C 6.7417820 4.9088940 0.7065640

38 H 7.5711480 5.1656960 0.0315860

39 C 7.1489800 5.2991860 2.1241720

40 H 6.3513150 5.0541290 2.8348770

41 H 8.0538010 4.7711790 2.4408280

42 H 7.3412780 6.3738970 2.1968230

43 C 5.5070620 5.6942070 0.2703440

44 H 5.2363510 5.5058090 -0.7721840

45 H 4.6446980 5.4293730 0.8928490

46 H 5.6767770 6.7701220 0.3740290

47 C -2.5677930 2.5646940 0.5861280

48 H -3.4158350 2.7637200 1.2450620

49 H -1.6780820 2.9995400 1.0555280

50 C -2.8215680 3.1880000 -0.7838650

51 H -3.5368090 2.5546850 -1.3163090

52 H -1.8950700 3.1600550 -1.3693570

53 C -3.3440310 4.6211880 -0.7116940

54 H -4.2684840 4.6102250 -0.1138660

55 C -3.6952310 5.1180620 -2.1103520

56 H -2.8024630 5.1409780 -2.7455800

57 H -4.4295800 4.4650880 -2.5924440

58 H -4.1093710 6.1307780 -2.0788750

59 C -2.3515040 5.5636180 -0.0360080

60 H -2.1465810 5.2759440 0.9994360

61 H -1.3978320 5.5653920 -0.5764460

62 H -2.7317940 6.5898540 -0.0240560

63 C -2.3998390 -2.8747390 0.4514240

64 H -1.4178440 -3.2931150 0.6997210

65 H -3.0824730 -3.1605660 1.2526450

66 C -2.8785500 -3.4280070 -0.8849860

67 H -3.8413560 -2.9704680 -1.1406020

68 H -2.1737830 -3.1065580 -1.6590420

69 C -3.0070180 -4.9508960 -0.9017240

70 H -2.0449930 -5.3788860 -0.5853690

71 C -3.2929300 -5.4296710 -2.3217350

72 H -4.2429780 -5.0185390 -2.6825560

73 H -2.5079100 -5.1109560 -3.0139700

74 H -3.3623240 -6.5211010 -2.3655950

75 C -4.0889800 -5.4471530 0.0550680

76 H -3.8706510 -5.2003000 1.0984020

77 H -5.0592990 -5.0048350 -0.2024280

78 H -4.1945030 -6.5347100 -0.0042830

79 C -5.5479570 1.1322180 1.3303460

80 C -4.7457550 0.5848710 2.3763640

81 C -4.5908760 -0.8105770 2.5386090

82 C -5.2386240 -1.6500800 1.5804220

83 C -5.9678370 -1.1149450 0.5129070

84 C -6.1477590 0.3009890 0.3763540

85 H -5.6113900 2.2076980 1.2202160

86 H -4.2084360 1.2543760 3.0400590

87 H -5.0909190 -2.7235960 1.6264360

88 H -6.3537590 -1.7756220 -0.2550050

89 C -6.9552170 0.8194030 -0.7863610

90 H -6.6494950 0.2235180 -1.6537320

91 C -8.4395400 0.5575530 -0.5097150

92 H -9.0393230 0.8599550 -1.3725010

93 H -8.6369330 -0.5004090 -0.3151690

94 H -8.7794000 1.1317270 0.3584910

95 C -6.7040750 2.2835950 -1.1128920

96 H -7.0547410 2.9451580 -0.3135520

97 H -5.6425060 2.4720100 -1.2851780

98 H -7.2462290 2.5562100 -2.0217600

99 Ru -3.9745220 -0.2013130 0.5383410

100 C -3.7644860 -1.3822400 3.6462780

101 H -3.0204600 -0.6617950 3.9902600

102 H -4.4073000 -1.6428570 4.4935070

103 H -3.2452710 -2.2886850 3.3294750

104 H 6.8686560 0.8039500 -0.9629230

Compound **2** (calibration set)

Tag Symbol X Y Z

1 N -5.7688090 1.1211320 0.0368860

2 N -5.6556990 -1.4465470 0.2947850

3 C -4.5811740 0.6481720 0.0387290

4 C -4.4974050 -0.8408920 0.1914860

5 S -3.1061190 1.5547580 -0.1285530

6 S -3.0312260 -1.6743520 0.2198190

7 Pt -1.4201670 -0.0397460 -0.0751240

8 S 0.1718750 1.6030240 -0.3582050

9 S 0.2719990 -1.6240690 -0.0179780

10 C 1.6799400 0.7657360 -0.3091210

11 C 1.7222330 -0.7079970 -0.2018740

12 N 2.8472210 1.3290320 -0.4288160

13 N 2.9171740 -1.2127240 -0.3021160

14 Cl 3.9168830 0.0155400 -2.8645860

15 C -5.9727560 2.5354720 -0.1148260

16 H -5.4665900 2.8867930 -1.0298080

17 C -5.8724680 -2.8759630 0.4068240

18 H -5.1964730 -3.3775790 -0.2962060

19 C 3.0998230 -2.6525140 -0.3921020

20 H 3.8361030 -2.8319960 -1.1792920

21 C 2.9406470 2.7412050 -0.7752860

22 H 3.7517210 2.8334010 -1.5009620

23 C 6.2156130 -1.2207560 -0.1027200

24 C 5.6284670 -0.7599230 1.1087490

25 C 5.4625030 0.6135580 1.3822360

26 C 5.8674290 1.5288750 0.3657770

27 C 6.4189780 1.0854020 -0.8460420

28 C 6.6051900 -0.3114960 -1.0981290

29 H 6.2786590 -2.2861780 -0.2806230

30 H 5.2564630 -1.4869150 1.8215300

31 H 5.6696340 2.5862420 0.5051430

32 H 6.6423520 1.8015470 -1.6287870

33 C 7.1873280 -0.7480130 -2.4184860

34 H 6.7772390 -0.0672840 -3.1722380

35 C 8.7075950 -0.5638400 -2.3667810

36 H 9.1467350 -0.8071650 -3.3382080

37 H 8.9827410 0.4651260 -2.1182540

38 H 9.1535740 -1.2254230 -1.6169290

39 C 6.8090400 -2.1672980 -2.8173740

40 H 7.2592700 -2.9112760 -2.1516730

41 H 5.7234070 -2.2926580 -2.8152730

42 H 7.1717640 -2.3743930 -3.8274100

43 Ru 4.4951210 0.0920820 -0.5299670

44 C 4.8784170 1.0793920 2.6769580

45 H 4.1650860 0.3505330 3.0676780

46 H 5.6775910 1.2010000 3.4160250

47 H 4.3737910 2.0389130 2.5614780

48 H -6.4488280 -0.8004610 0.2827080

49 H -5.4852680 3.0786690 0.7086190

50 C -7.4324100 2.9032610 -0.1794850

51 C -8.3767690 2.0269390 -0.7130870

52 C -7.8537690 4.1578370 0.2603870

53 C -9.7141940 2.3974570 -0.8051690

54 H -8.0580620 1.0461360 -1.0506950

55 C -9.1899270 4.5328350 0.1663350

56 H -7.1289530 4.8475600 0.6850460

57 C -10.1259680 3.6524220 -0.3671070

58 H -10.4376210 1.7025050 -1.2204480

59 H -9.5011150 5.5119140 0.5169140

60 H -11.1698290 3.9410400 -0.4372650

61 H -5.5959500 -3.2113580 1.4124380

62 C -7.3063700 -3.2079080 0.1012680

63 C -7.8451800 -2.8807080 -1.1447970

64 C -8.1129300 -3.8310510 1.0497130

65 C -9.1722540 -3.1706430 -1.4345980

66 H -7.2201100 -2.3971890 -1.8906960

67 C -9.4407550 -4.1291100 0.7576950

68 H -7.7018220 -4.0829010 2.0229100

69 C -9.9727460 -3.7971980 -0.4828840

70 H -9.5814640 -2.9125400 -2.4058840

71 H -10.0605630 -4.6155340 1.5037530

72 H -11.0089840 -4.0258320 -0.7095070

73 H 2.1592310 -3.1190610 -0.7087640

74 C 3.5690370 -3.2718720 0.8999280

75 C 4.5753380 -4.2357390 0.8850340

76 C 3.0132860 -2.8918010 2.1228480

77 C 5.0304310 -4.8044440 2.0709590

78 H 5.0135830 -4.5387240 -0.0624900

79 C 3.4687610 -3.4559840 3.3081620

80 H 2.2279360 -2.1431140 2.1467480

81 C 4.4817290 -4.4115750 3.2867530

82 H 5.8193900 -5.5492480 2.0441890

83 H 3.0319690 -3.1479090 4.2527690

84 H 4.8395600 -4.8482600 4.2134150

85 C 3.1934610 3.6579920 0.3954380

86 C 2.5003720 3.5158260 1.5980720

87 C 4.1163840 4.6963590 0.2688280

88 C 2.7319580 4.3916960 2.6526670

89 H 1.7764800 2.7157900 1.7111740

90 C 4.3494120 5.5738240 1.3229870

91 H 4.6624950 4.8156010 -0.6634690

92 C 3.6580090 5.4221690 2.5201400

93 H 2.1861120 4.2672700 3.5824780

94 H 5.0741660 6.3735980 1.2089070

95 H 3.8387320 6.1034240 3.3451900

96 H 2.0170700 3.0461160 -1.2832310

Compound **3** (calibration set)

Tag Symbol X Y Z

1 N 6.8967770 -1.0588040 -0.2389070

2 N 6.7534210 1.4831030 0.2892560

3 C 5.7059580 -0.6002950 -0.1555290

4 C 5.6062480 0.8632840 0.1494900

5 S 4.2341230 -1.5098430 -0.3627960

6 S 4.1294790 1.6657810 0.3018440

7 Pt 2.5296480 0.0327630 -0.0535070

8 S 0.9477580 -1.6142630 -0.4138810

9 S 0.8167660 1.5704200 0.2732650

10 C -0.5594040 -0.8050330 -0.2114430

11 C -0.6195940 0.6358460 0.1040270

12 N -1.7204320 -1.3717570 -0.3507780

13 N -1.8250040 1.1122660 0.1993270

14 Cl -3.3724940 0.2635030 -2.2928930

15 C 7.0907490 -2.4549350 -0.5314100

16 H 6.6397740 -2.7251060 -1.4963770

17 C 6.9151600 2.8863350 0.5828820

18 H 6.4535580 3.4960100 -0.1996730

19 C -2.0150500 2.5318680 0.4058430

20 H -3.0407490 2.7971790 0.1577260

21 C -1.7957370 -2.7438230 -0.8054190

22 H -2.7936560 -2.9376510 -1.1948190

23 C -4.9002420 0.8791890 1.2036640

24 C -4.0136940 0.1739560 2.0718780

25 C -3.8093230 -1.2182500 1.9511070

26 C -4.5098780 -1.8892050 0.9003550

27 C -5.3452740 -1.1948540 0.0162950

28 C -5.5529670 0.2178510 0.1536280

29 H -4.9858980 1.9539720 1.3016760

30 H -3.4372370 0.7293180 2.8041880

31 H -4.3123890 -2.9415170 0.7245730

32 H -5.7789030 -1.7148870 -0.8303300

33 C -6.4359930 0.9258590 -0.8426890

34 H -6.2626120 0.4305540 -1.8044320

35 C -7.8994560 0.7165710 -0.4415750

36 H -8.5608040 1.1576950 -1.1924000

37 H -8.1466880 -0.3453320 -0.3540110

38 H -8.1101890 1.1949300 0.5205260

39 C -6.1059000 2.4012820 -1.0178320

40 H -6.3240970 2.9798650 -0.1140090

41 H -5.0542010 2.5329330 -1.2846750

42 H -6.7136240 2.8201330 -1.8240010

43 Ru -3.3806720 -0.2290610 0.0608890

44 C -2.8656470 -1.9544490 2.8481160

45 H -2.0970960 -1.2870780 3.2420310

46 H -3.4123500 -2.3836390 3.6941140

47 H -2.3742410 -2.7717380 2.3167620

48 H 7.5567200 0.8647420 0.1664940

49 H 6.6163500 -3.0904940 0.2292290

50 H 6.4410100 3.1340270 1.5373980

51 H -1.3326340 3.1084710 -0.2270170

52 H -1.0610900 -2.9278640 -1.5960100

53 H 8.1577420 -2.6783850 -0.5644290

54 H 7.9785970 3.1117460 0.6373910

55 H -1.8141380 2.7991130 1.4506020

56 H -1.5848070 -3.4377780 0.0175260

Compound **4** (calibration set)

Tag Symbol X Y Z

1 C 6.9773160 -0.1735200 0.4802950

2 H 7.2053620 -0.0949430 1.5380890

3 C 2.1478890 0.6701740 -0.0247970

4 C 2.0995900 -0.8135540 0.0265850

5 C 3.3697280 -2.8717300 0.1247540

6 H 2.4724030 -3.3026000 0.5738410

7 C 3.5862130 -3.4163340 -1.2874100

8 H 4.4368110 -2.8880030 -1.7309860

9 H 2.7089800 -3.1807010 -1.9001780

10 C 3.5505250 2.6418080 -0.1381810

11 H 2.6857250 3.1409710 -0.5846540

12 C 3.7877620 3.1741880 1.2755790

13 H 4.6517420 2.6576450 1.7108540

14 H 2.9197890 2.9160030 1.8901660

15 C 6.6146060 -1.4238300 -0.0679250

16 H 6.6508860 -2.3087480 0.5551200

17 H 6.7157980 -1.6006850 -1.1355970

18 C 6.6733650 0.9908300 -0.2600880

19 H 6.7787840 0.9929390 -1.3419880

20 H 6.7537740 1.9601040 0.2165920

21 N 3.3385500 1.1936030 -0.1100710

22 N 3.2562430 -1.4123990 0.0983710

23 S 0.6530840 1.6345800 0.0685260

24 S 0.5412210 -1.6714280 -0.0412560

25 Pd 4.8978670 -0.1581410 -0.0060300

26 C -4.2748470 -0.5723280 -0.0127880

27 C -4.2621090 0.9170830 0.0477790

28 C -5.5885960 2.9164520 0.1618630

29 H -4.7632540 3.3864740 0.7066470

30 C -5.6714730 3.4814500 -1.2610270

31 H -6.4613560 2.9456510 -1.7969690

32 H -4.7308670 3.2727580 -1.7824840

33 C -5.7852320 -2.5361930 -0.0697060

34 H -5.0570140 -3.0380670 -0.7113440

35 C -5.7678770 -3.1535420 1.3307180

36 H -6.5743930 -2.7163540 1.9298140

37 H -4.8258790 -2.8857960 1.8178840

38 N -5.4722040 -1.1136720 -0.0403950

39 N -5.4201520 1.4694040 0.1244210

40 S -2.8236510 -1.5313980 -0.0430880

41 S -2.6789350 1.7794560 -0.0010850

42 H -6.2193650 -0.4176080 0.0033600

43 H -6.5188090 3.1287870 0.6912350

44 H -6.7652940 -2.6358210 -0.5333800

45 C -5.9083410 -4.6817370 1.3215140

46 H -5.0902720 -5.0871890 0.7110460

47 C -5.7541980 -5.2261490 2.7433190

48 H -4.7969810 -4.9306070 3.1791590

49 H -6.5517190 -4.8447000 3.3883930

50 H -5.8085210 -6.3171630 2.7518640

51 C -7.2361860 -5.1369940 0.7101080

52 H -7.3299830 -6.2241880 0.7586710

53 H -8.0776740 -4.7032750 1.2596990

54 H -7.3310900 -4.8474910 -0.3387530

55 C -5.9542010 4.9889650 -1.3145480

56 H -6.8787970 5.1790510 -0.7521240

57 C -4.8275400 5.8093100 -0.6804800

58 H -4.7075130 5.5938950 0.3829650

59 H -3.8758810 5.5932360 -1.1757050

60 H -5.0247770 6.8794230 -0.7804520

61 C -6.1823660 5.4229610 -2.7647690

62 H -6.4199360 6.4879420 -2.8229130

63 H -5.2823970 5.2462340 -3.3618020

64 H -7.0043670 4.8661230 -3.2214810

65 H 4.4166310 2.8236390 -0.7716490

66 C 4.0175730 4.6903680 1.3343770

67 H 3.1592480 5.1794680 0.8549530

68 C 5.2881530 5.1099820 0.5899680

69 H 6.1614260 4.6014960 1.0120990

70 H 5.2416640 4.8748940 -0.4753630

71 H 5.4523870 6.1861500 0.6814130

72 C 4.0731160 5.1514920 2.7926480

73 H 3.1575670 4.8864420 3.3265430

74 H 4.9147110 4.6810820 3.3108830

75 H 4.2022510 6.2345050 2.8567880

76 H 4.2235230 -3.1218070 0.7549010

77 C 3.8477910 -4.9276550 -1.3325210

78 H 4.7077890 -5.1394720 -0.6819270

79 C 2.6496150 -5.7335590 -0.8233780

80 H 2.4252340 -5.5232270 0.2241790

81 H 1.7571050 -5.4990030 -1.4115100

82 H 2.8391470 -6.8059760 -0.9115100

83 C 4.2143620 -5.3504540 -2.7570510

84 H 4.4387270 -6.4187340 -2.8038010

85 H 3.3829320 -5.1513070 -3.4400560

86 H 5.0877320 -4.8036720 -3.1212920

87 Pt -1.0749520 0.0515890 -0.0041890

Compound **5** (calibration set)

Tag Symbol X Y Z

1 N 6.9098280 1.1417720 -0.5995980

2 N 6.9151190 -1.2239170 0.4558790

3 C 5.7267140 0.6236300 -0.3689140

4 C 5.7487080 -0.7668760 0.1991560

5 S 4.2900680 1.4543730 -0.6861020

6 S 4.2256400 -1.5890240 0.4375430

7 Pt 2.6052410 -0.0294410 -0.1340860

8 S 0.9785170 1.5255900 -0.6917620

9 S 0.9392330 -1.5228050 0.4208850

10 C -0.5241920 0.7359630 -0.3460930

11 C -0.5408870 -0.6567650 0.1838990

12 N -1.6909990 1.2702900 -0.5124890

13 N -1.7144860 -1.1477000 0.4496010

14 C -1.8378670 -2.4853040 1.0080970

15 H -0.9819530 -2.6912100 1.6632090

16 H -2.7447470 -2.4927000 1.6136790

17 C -1.9165930 -3.5417060 -0.0888900

18 H -1.0233640 -3.4584610 -0.7179980

19 C -1.8293360 2.6313120 -0.9914960

20 H -1.0249110 2.8741690 -1.6979300

21 H -2.7787220 2.6882380 -1.5296130

22 C -1.8184060 3.6194190 0.1720930

23 H -2.5874760 3.3236840 0.8943570

24 H -0.8555630 3.5295120 0.6870510

25 C -2.0423740 5.0726280 -0.2439590

26 H -1.2826570 5.3344420 -0.9944750

27 C -1.8513480 5.9865520 0.9628050

28 H -2.5858850 5.7506710 1.7419360

29 H -0.8544260 5.8680620 1.3982970

30 H -1.9796690 7.0385450 0.6889460

31 C -3.4223380 5.2884470 -0.8610730

32 H -3.5647930 4.7120410 -1.7795830

33 H -4.2076580 4.9898070 -0.1567820

34 H -3.5778170 6.3431010 -1.1092020

35 Rh -3.3182590 0.0282890 0.0252320

36 C 7.1793440 2.4779010 -1.0907020

37 H 8.1470440 2.4506050 -1.5980700

38 C 7.0671070 -2.5605370 0.9830220

39 H 7.9924420 -2.5834490 1.5652670

40 C 7.1468500 -3.5784040 -0.1591210

41 H 6.2684510 -3.4440580 -0.8006730

42 H 8.0262970 -3.3402980 -0.7693560

43 C -3.3952500 0.7934920 1.8537140

44 C -2.5786640 0.4962090 2.9477260

45 C -2.7693890 1.1210550 4.1766990

46 C -3.7834710 2.0636960 4.3458160

47 C -4.6034730 2.3832930 3.2747220

48 C -4.4121350 1.7572270 2.0383750

49 H -1.7777630 -0.2291050 2.8457600

50 H -2.1195970 0.8738360 5.0115830

51 H -3.9280310 2.5475680 5.3060560

52 H -5.3864480 3.1239450 3.4071280

53 C -5.1996260 2.0640250 0.8505260

54 C -6.2412420 2.9910280 0.7780340

55 C -6.8856000 3.2139060 -0.4251780

56 H -6.5376180 3.5346040 1.6663500

57 C -5.4506420 1.5944120 -1.4209670

58 C -6.4810540 2.5065120 -1.5527080

59 H -7.6939880 3.9345260 -0.4862490

60 H -5.1033240 1.0111630 -2.2649530

61 H -6.9535900 2.6492650 -2.5166500

62 N -4.8256930 1.3767270 -0.2582090

63 C -2.7065590 -0.5873030 -2.9801000

64 C -2.8691760 -1.2123450 -4.2042310

65 C -3.8746200 -2.1662420 -4.3235570

66 C -4.6634670 -2.4633280 -3.2252940

67 C -4.4444530 -1.8011690 -2.0143930

68 H -1.9371910 0.1612200 -2.8247750

69 H -2.2217430 -0.9579930 -5.0344450

70 H -4.0374610 -2.6802440 -5.2649920

71 H -5.4405920 -3.2131770 -3.3021050

72 C -5.1685830 -2.0591750 -0.7651690

73 C -6.1874980 -3.0156030 -0.6767000

74 C -4.7576080 -1.3258370 0.3739610

75 C -6.8117600 -3.2639200 0.5356190

76 H -6.4963390 -3.5781100 -1.5524350

77 C -5.4068180 -1.5985820 1.5820720

78 C -6.4149780 -2.5543430 1.6670700

79 H -7.5983640 -4.0084950 0.6002740

80 H -5.1177820 -1.0561780 2.4770620

81 H -6.8955600 -2.7472350 2.6222390

82 N -3.4728970 -0.8647900 -1.9223090

83 H -2.7797230 -3.3246860 -0.7262030

84 C -2.0370540 -4.9709710 0.4381670

85 H -1.1669410 -5.1719260 1.0794330

86 C -3.3040950 -5.1718840 1.2663980

87 H -4.1926180 -4.9008150 0.6839600

88 H -3.4058910 -6.2176910 1.5731800

89 H -3.3080640 -4.5618740 2.1738670

90 C -2.0013410 -5.9512450 -0.7304870

91 H -1.0876680 -5.8343310 -1.3217520

92 H -2.0489930 -6.9874390 -0.3811420

93 H -2.8558670 -5.7834520 -1.3970650

94 H 6.4175420 2.7201440 -1.8363950

95 C 7.1945930 3.5063790 0.0367100

96 H 7.9602490 3.2108140 0.7633150

97 H 6.2310150 3.4773120 0.5601650

98 C 7.4685690 4.9337340 -0.4398040

99 H 8.4061260 4.9250450 -1.0146130

100 C 6.3565040 5.4618460 -1.3431630

101 H 6.2486210 4.8777720 -2.2613390

102 H 5.3943910 5.4413000 -0.8185570

103 H 6.5555600 6.4969950 -1.6364820

104 C 7.6607110 5.8526770 0.7628680

105 H 7.8879950 6.8748140 0.4452840

106 H 6.7491530 5.8869020 1.3705320

107 H 8.4778360 5.5076380 1.4039690

108 H 6.2354660 -2.8113550 1.6552550

109 C 7.2181240 -5.0436560 0.2857300

110 H 7.3285590 -5.6308230 -0.6362200

111 C 8.4368480 -5.3294360 1.1595730

112 H 9.3606660 -4.9864850 0.6819440

113 H 8.3567140 -4.8318280 2.1320260

114 H 8.5350940 -6.4025580 1.3508740

115 C 5.9318030 -5.5046210 0.9674040

116 H 5.7850400 -5.0043060 1.9302440

117 H 5.0555750 -5.2935780 0.3466610

118 H 5.9597950 -6.5816780 1.1605690

119 H 7.6687280 0.5177890 -0.3158230

Compound **6** (calibration set)

Tag Symbol X Y Z

1 N 5.8945460 1.2183470 -0.5178210

2 N 5.9347120 -1.2478790 0.2786610

3 C 4.7212540 0.6749390 -0.3012990

4 C 4.7619650 -0.7708410 0.1046800

5 S 3.2745860 1.5344870 -0.4628320

6 S 3.2474710 -1.6243750 0.2855500

7 Pt 1.6093190 -0.0194520 -0.0567310

8 S -0.0451470 1.5630080 -0.4113590

9 S -0.0420580 -1.5704110 0.3629560

10 C -1.5344460 0.7118920 -0.2351170

11 C -1.5315990 -0.7105420 0.2188050

12 N -2.7076850 1.2310890 -0.4592930

13 N -2.6998480 -1.2265460 0.4717400

14 C -2.7836630 -2.6243890 0.8620890

15 H -1.9449590 -2.8775860 1.5231620

16 H -3.7007940 -2.7558250 1.4380770

17 C -2.7778450 -3.5472780 -0.3552470

18 H -1.8548690 -3.3721040 -0.9176670

19 C -2.7970710 2.6295630 -0.8447630

20 H -1.9713220 2.8824250 -1.5221210

21 H -3.7257670 2.7643470 -1.4012030

22 C -2.7638550 3.5494310 0.3743410

23 H -3.5793760 3.2736740 1.0556100

24 H -1.8305810 3.3689890 0.9178930

25 C -2.8666340 5.0351290 0.0283610

26 H -2.0732490 5.2669650 -0.6964980

27 C -2.6255980 5.8771160 1.2774610

28 H -3.3910250 5.6705790 2.0347740

29 H -1.6489440 5.6609850 1.7212540

30 H -2.6645590 6.9464600 1.0476640

31 C -4.2107550 5.3900730 -0.6032280

32 H -4.3843130 4.8595860 -1.5437040

33 H -5.0326710 5.1421500 0.0793710

34 H -4.2693500 6.4616890 -0.8170210

35 C 6.1495200 2.6000120 -0.8724530

36 H 7.0950170 2.6261570 -1.4200550

37 C 6.1044750 -2.6334030 0.6518380

38 H 7.0437860 -2.7136580 1.2057480

39 C 6.1598340 -3.5197380 -0.5963650

40 H 5.2613410 -3.3282500 -1.1941350

41 H 7.0183270 -3.2058690 -1.2020820

42 H -3.6057110 -3.2702400 -1.0209310

43 C -2.8791210 -5.0316710 -0.0031630

44 H -2.0727700 -5.2642730 0.7068830

45 C -4.2121870 -5.3802450 0.6548610

46 H -5.0461290 -5.1319090 -0.0128710

47 H -4.2700280 -6.4509870 0.8731770

48 H -4.3663350 -4.8463860 1.5968230

49 C -2.6647800 -5.8777070 -1.2543590

50 H -1.6957000 -5.6665120 -1.7166600

51 H -2.7034230 -6.9462620 -1.0209190

52 H -3.4435120 -5.6702110 -1.9977620

53 H 5.3583680 2.9213080 -1.5550300

54 C 6.2178570 3.5004630 0.3577390

55 H 7.0100670 3.1260230 1.0163800

56 H 5.2760770 3.4184800 0.9142680

57 C 6.4833580 4.9698910 0.0261570

58 H 7.3960390 5.0196420 -0.5853280

59 C 5.3391170 5.5962110 -0.7674690

60 H 5.1874670 5.1138260 -1.7370580

61 H 4.3997410 5.5244660 -0.2073520

62 H 5.5351200 6.6557340 -0.9574940

63 C 6.7330430 5.7531530 1.3114080

64 H 6.9537540 6.8029580 1.0960100

65 H 5.8484300 5.7239290 1.9579120

66 H 7.5743700 5.3391340 1.8757490

67 H 5.2901800 -2.9613070 1.3118780

68 C 6.2588580 -5.0234600 -0.3150280

69 H 6.3385300 -5.5062050 -1.2986090

70 C 7.5121770 -5.3877490 0.4768490

71 H 8.4145330 -4.9855110 0.0045580

72 H 7.4661290 -4.9984580 1.4995850

73 H 7.6250320 -6.4740420 0.5477080

74 C 5.0031820 -5.5704850 0.3601910

75 H 4.8934200 -5.1842190 1.3789110

76 H 4.1012740 -5.2986910 -0.1970030

77 H 5.0441740 -6.6621390 0.4285270

78 H 6.6631590 0.5693940 -0.3335140

79 C -5.8340640 -1.5009130 0.1385230

80 C -6.9852470 -1.2529090 -0.8152230

81 C -6.9696440 1.2615190 0.9066460

82 C -6.6253500 -0.1853890 -1.8562630

83 C -5.8350150 1.5090620 -0.0668690

84 C -5.7021690 0.8722300 -1.3056980

85 H -7.8795040 -0.9675910 -0.2551710

86 H -6.1119340 -0.6636050 -2.6962920

87 H -7.2099090 2.1958350 1.4217310

88 H -5.3288210 -2.4545300 0.0084440

89 H -7.2345600 -2.1871070 -1.3261940

90 H -7.8734530 0.9763480 0.3620900

91 H -7.5314070 0.2780500 -2.2721850

92 H -5.3270140 2.4624140 0.0545290

93 H -5.1026990 1.3754490 -2.0649160

94 C -5.6792060 -0.8640430 1.3747180

95 H -5.0667750 -1.3675860 2.1233140

96 C -6.5921410 0.1939770 1.9413350

97 H -7.4910080 -0.2690580 2.3729860

98 H -6.0640240 0.6719700 2.7723370

99 Rh -4.3151100 0.0037030 0.0223250

Compound **7** (calibration set)

Tag Symbol X Y Z

1 N 2.4541700 -1.3081900 -0.0758560

2 N 2.4521050 1.2260760 -0.5197620

3 C 1.2814160 -0.7527090 -0.0627640

4 C 1.2792980 0.7067130 -0.3195980

5 S -0.1947420 -1.5987490 0.2361180

6 S -0.2011930 1.5945040 -0.3306320

7 C 2.5801550 2.6568880 -0.7265030

8 C 2.5827200 -2.7258900 0.2091430

9 H 3.4714030 -3.0869470 -0.3060380

10 H 1.7186940 -3.2570060 -0.2113660

11 H 1.7074300 3.0204580 -1.2843560

12 H 3.4593840 2.8247910 -1.3469680

13 C 2.6859570 -3.0031420 1.7064160

14 H 3.6111970 -2.5589410 2.0900880

15 H 1.8640780 -2.4843270 2.2104980

16 C 2.7059790 3.4111520 0.5943620

17 H 1.9015320 3.0764520 1.2571900

18 H 3.6434510 3.1235740 1.0834560

19 Pt -1.8465400 -0.0197590 -0.0740100

20 S -3.4798550 -1.6472910 0.1693940

21 S -3.5170280 1.5545680 -0.3537040

22 C -4.9969430 -0.7900770 0.0486360

23 C -4.9613050 0.6864550 -0.2276380

24 N -6.1690590 -1.2856160 0.1711420

25 N -6.1389440 1.2472700 -0.3643760

26 Rh 4.0789840 -0.0341500 -0.2577140

27 Cl 3.8671350 0.3712940 2.0978500

28 C 5.1178530 0.3505350 -2.0986360

29 C 5.8094330 1.0193850 -1.0216510

30 C 5.1330800 -1.0538870 -1.8308580

31 C 6.2538360 0.0148040 -0.1091690

32 C 5.8258480 -1.2652970 -0.5824880

33 C 6.1541890 2.4670540 -0.9344640

34 C 4.5631820 0.9863060 -3.3253150

35 C 7.0550200 0.2558680 1.1181960

36 C 6.1858060 -2.5701330 0.0416340

37 C 4.5986620 -2.1045230 -2.7405720

38 H 5.5535480 3.0725310 -1.6135730

39 H 6.0133830 2.8507990 0.0777940

40 H 7.2048110 2.6161700 -1.2062670

41 H 6.8637510 1.2459630 1.5317810

42 H 6.8333440 -0.4814700 1.8896780

43 H 8.1197830 0.1853710 0.8662060

44 H 7.2349840 -2.8075100 -0.1653690

45 H 6.0565870 -2.5399690 1.1252670

46 H 5.5827910 -3.3907060 -0.3475690

47 H 5.3362570 -2.3178330 -3.5222000

48 H 4.3974570 -3.0387070 -2.2158900

49 H 3.6772930 -1.7812860 -3.2276030

50 H 5.3187170 0.9726940 -4.1188060

51 H 3.6840070 0.4519980 -3.6884850

52 H 4.2826560 2.0263420 -3.1558050

53 C -6.4012850 2.6554470 -0.5828160

54 H -7.3684060 2.7246410 -1.0836820

55 H -5.6404460 3.0440640 -1.2680730

56 C -6.3358120 -2.6994240 0.4170740

57 H -5.5321420 -3.0874560 1.0603310

58 H -7.2842460 -2.8324150 0.9442350

59 C -6.3518480 -3.4823360 -0.8976090

60 H -7.2175820 -3.1641510 -1.4933810

61 H -5.4559500 -3.2121790 -1.4680680

62 C -6.3919250 3.4463130 0.7230340

63 H -7.2184200 3.1024600 1.3581110

64 H -5.4633720 3.2181310 1.2575040

65 H -6.9030870 0.5810970 -0.2294180

66 C 2.6322750 4.9292890 0.4373790

67 H 1.6777060 5.1686350 -0.0532460

68 C 2.6365030 5.5925480 1.8110810

69 H 2.5432920 6.6798930 1.7264830

70 H 1.8116930 5.2280420 2.4308340

71 H 3.5720490 5.3765750 2.3400540

72 C 3.7624650 5.4827880 -0.4267760

73 H 4.7370550 5.2350330 0.0099520

74 H 3.7392960 5.0859500 -1.4462530

75 H 3.6986050 6.5728860 -0.4998290

76 C 2.6278430 -4.4909830 2.0505660

77 H 1.6830380 -4.8892600 1.6533550

78 C 3.7757960 -5.2806100 1.4265150

79 H 3.7620610 -5.2409690 0.3329800

80 H 4.7416130 -4.8891940 1.7669800

81 H 3.7243440 -6.3351990 1.7143880

82 C 2.6168040 -4.6719800 3.5651800

83 H 3.5428860 -4.2849480 4.0060340

84 H 1.7801320 -4.1358580 4.0231960

85 H 2.5327950 -5.7288870 3.8372260

86 C -6.3854530 -5.0002300 -0.7170500

87 H -5.5077290 -5.2824860 -0.1182680

88 C -6.2719100 -5.6885250 -2.0739270

89 H -7.1294600 -5.4349540 -2.7083740

90 H -5.3631190 -5.3822150 -2.6013200

91 H -6.2491300 -6.7773950 -1.9647020

92 C -7.6365100 -5.4707670 0.0198130

93 H -8.5397400 -5.1610700 -0.5197010

94 H -7.6540640 -6.5622320 0.0992460

95 H -7.6964080 -5.0669120 1.0342980

96 C -6.4949040 4.9584080 0.5216570

97 H -5.6607550 5.2651170 -0.1254950

98 C -7.8010060 5.3647610 -0.1561350

99 H -8.6615960 5.0280600 0.4340560

100 H -7.8670390 6.4529030 -0.2491740

101 H -7.8975940 4.9453370 -1.1617590

102 C -6.3398210 5.6714580 1.8612210

103 H -7.1518390 5.3933330 2.5430710

104 H -5.3928640 5.4119590 2.3442510

105 H -6.3687470 6.7579100 1.7344290

Compound **8** (calibration set)

Tag Symbol X Y Z

1 S 2.5399830 1.4446380 -0.8234800

2 S 2.5022130 -1.3665530 0.7896400

3 C 1.0339090 0.7059440 -0.3872000

4 C 1.0164860 -0.5903540 0.3599270

5 N -0.1361400 1.1895020 -0.6580340

6 N -0.1631090 -1.0516140 0.6550040

7 C -0.2996910 -2.2853530 1.4138010

8 H 0.5327390 -2.3757630 2.1218270

9 H -1.2295640 -2.2077680 1.9783460

10 C -0.3297620 -3.5011840 0.4945730

11 H 0.5888330 -3.5056410 -0.1027670

12 C -0.2835200 2.4566370 -1.3463070

13 H 0.5387220 2.6052430 -2.0572840

14 H -1.2177970 2.4095510 -1.9113940

15 C -0.3230660 3.6107050 -0.3483780

16 H -1.1068990 3.4132490 0.3915780

17 H 0.6272170 3.6183820 0.1970990

18 C -0.5582480 4.9787510 -0.9871820

19 H 0.2149740 5.1354160 -1.7531300

20 C -0.4087000 6.0710210 0.0676340

21 H -1.1568650 5.9440670 0.8590990

22 H 0.5798930 6.0397000 0.5359630

23 H -0.5470960 7.0658630 -0.3675610

24 C -1.9261960 5.0727500 -1.6590620

25 H -2.0400860 4.3560990 -2.4773370

26 H -2.7236380 4.8763430 -0.9328420

27 H -2.0892730 6.0724510 -2.0739300

28 Rh -1.7639350 0.0141360 -0.0003890

29 C -1.9272050 1.0384990 1.6899370

30 C -1.1544060 0.9201030 2.8481520

31 C -1.4061010 1.7130580 3.9638980

32 C -2.4393000 2.6501250 3.9524820

33 C -3.2168630 2.7939960 2.8138460

34 C -2.9644710 1.9984580 1.6910400

35 H -0.3401590 0.2035210 2.8852520

36 H -0.7895480 1.6026550 4.8517030

37 H -2.6316170 3.2655600 4.8250560

38 H -4.0152960 3.5299120 2.8050350

39 C -3.7074750 2.1114650 0.4417370

40 C -4.7594540 2.9957600 0.1943290

41 C -5.3585530 3.0258060 -1.0517460

42 H -5.0993990 3.6577820 0.9808540

43 C -3.8605960 1.3076690 -1.7427350

44 C -4.8986350 2.1687130 -2.0463580

45 H -6.1746610 3.7125740 -1.2488140

46 H -3.4709750 0.6141480 -2.4778920

47 H -5.3342260 2.1582920 -3.0378410

48 N -3.2791150 1.2764410 -0.5382660

49 C -1.0271210 -1.0219560 -2.8578700

50 C -1.1350050 -1.8195310 -3.9838660

51 C -2.1214210 -2.8002820 -3.9991990

52 C -2.9465880 -2.9513910 -2.8978590

53 C -2.7828880 -2.1173470 -1.7884750

54 H -0.2751830 -0.2437070 -2.7854320

55 H -0.4613140 -1.6737910 -4.8193930

56 H -2.2421000 -3.4470650 -4.8618450

57 H -3.7106970 -3.7183840 -2.8935840

58 C -3.5530270 -2.2037710 -0.5431200

59 C -4.5613750 -3.1568700 -0.3540980

60 C -3.2000610 -1.3015110 0.4893060

61 C -5.2338290 -3.2346580 0.8553290

62 H -4.8241670 -3.8497480 -1.1475270

63 C -3.8982600 -1.4041510 1.6967680

64 C -4.8964560 -2.3559740 1.8826110

65 H -6.0120160 -3.9770790 0.9988280

66 H -3.6557860 -0.7290710 2.5117890

67 H -5.4156740 -2.4135100 2.8353570

68 N -1.8282620 -1.1593020 -1.7983790

69 H -1.1667890 -3.3962820 -0.2031320

70 C -0.4646260 -4.8319800 1.2333230

71 H 0.3832080 -4.9233680 1.9274440

72 C -1.7588930 -4.9125810 2.0396730

73 H -2.6274080 -4.7385600 1.3935540

74 H -1.8699300 -5.9000230 2.4989930

75 H -1.7941840 -4.1710620 2.8424980

76 C -0.3854640 -5.9823440 0.2340840

77 H 0.5467270 -5.9501730 -0.3388140

78 H -0.4400430 -6.9520050 0.7389970

79 H -1.2180490 -5.9288380 -0.4777020

80 C 5.7047750 -0.8918850 1.2256880

81 C 6.8552480 0.0443370 1.5417010

82 C 6.8764510 -0.0523730 -1.5100220

83 C 6.5196490 1.4988080 1.1895340

84 C 5.7418280 0.9084690 -1.2104530

85 C 5.6110250 1.6175680 -0.0084880

86 H 7.7537870 -0.2861570 1.0126940

87 H 6.0017630 1.9592730 2.0369780

88 H 7.1292820 0.0105970 -2.5725190

89 H 5.1825720 -1.2971670 2.0905450

90 H 7.0915630 -0.0243430 2.6075860

91 H 7.7742950 0.2594690 -0.9686760

92 H 7.4377880 2.0851100 1.0355510

93 H 5.2417890 1.3257550 -2.0827080

94 H 5.0382940 2.5437500 -0.0416070

95 C 5.5765020 -1.5986600 0.0220420

96 H 4.9853530 -2.5135460 0.0472910

97 C 6.5058840 -1.4994560 -1.1619710

98 H 7.4095990 -2.1038870 -0.9934360

99 H 5.9922570 -1.9504220 -2.0171870

100 Rh 4.2055790 0.0242610 -0.0038010

Compound **9** (calibration set)

Tag Symbol X Y Z

1 S -3.0976840 1.4845370 0.7991910

2 S -3.0556590 -1.4078860 -0.7822700

3 C -1.6047510 0.7133240 0.3718810

4 C -1.5855570 -0.6006330 -0.3541180

5 N -0.4317130 1.1947110 0.6370820

6 N -0.4018890 -1.0612350 -0.6370270

7 C -0.2551480 -2.3058740 -1.3757460

8 H -1.0849830 -2.4134580 -2.0845870

9 H 0.6757090 -2.2306210 -1.9389200

10 C -0.2176160 -3.5071780 -0.4379990

11 H -1.1383860 -3.5120270 0.1559000

12 C -0.2770270 2.4701840 1.3080820

13 H -1.0977470 2.6325350 2.0179910

14 H 0.6575340 2.4256330 1.8729570

15 C -0.2314870 3.6113770 0.2957160

16 H 0.5525840 3.4010320 -0.4403710

17 H -1.1808870 3.6164300 -0.2511730

18 C 0.0088890 4.9865900 0.9169250

19 H -0.7664240 5.1579490 1.6775890

20 C -0.1303570 6.0652410 -0.1532180

21 H 0.6204180 5.9235600 -0.9397150

22 H -1.1171220 6.0328770 -0.6253180

23 H 0.0115890 7.0651800 0.2689740

24 C 1.3747240 5.0821670 1.5928920

25 H 1.4809510 4.3769250 2.4220230

26 H 2.1738530 4.8703360 0.8728820

27 H 1.5422800 6.0868530 1.9937210

28 Rh 1.1982400 0.0147300 -0.0000660

29 C 1.3600870 1.0086900 -1.7083340

30 C 0.5851660 0.8713190 -2.8631310

31 C 0.8363950 1.6437370 -3.9932790

32 C 1.8712610 2.5790070 -4.0003060

33 C 2.6509200 2.7416970 -2.8656510

34 C 2.3990920 1.9666920 -1.7284420

35 H -0.2303250 0.1555790 -2.8861840

36 H 0.2182350 1.5185310 -4.8780120

37 H 2.0631390 3.1785430 -4.8839770

38 H 3.4504150 3.4765090 -2.8711370

39 C 3.1443640 2.1010150 -0.4825940

40 C 4.1999450 2.9860680 -0.2539540

41 C 4.8010840 3.0381630 0.9904090

42 H 4.5412370 3.6311980 -1.0538140

43 C 3.2979830 1.3392120 1.7167200

44 C 4.3393660 2.2024220 2.0021960

45 H 5.6200630 3.7255580 1.1728610

46 H 2.9070820 0.6615270 2.4658750

47 H 4.7762390 2.2098570 2.9931410

48 N 2.7147240 1.2863470 0.5138590

49 C 0.4642930 -0.9710860 2.8757660

50 C 0.5764800 -1.7452540 4.0175820

51 C 1.5678830 -2.7204790 4.0523700

52 C 2.3935770 -2.8894730 2.9540440

53 C 2.2256590 -2.0784910 1.8282670

54 H -0.2915720 -0.1982660 2.7876910

55 H -0.0975790 -1.5860160 4.8503510

56 H 1.6920220 -3.3491620 4.9278100

57 H 3.1615190 -3.6525640 2.9649300

58 C 2.9966090 -2.1855200 0.5850040

59 C 4.0105810 -3.1363430 0.4155100

60 C 2.6388580 -1.3060160 -0.4653040

61 C 4.6839220 -3.2346030 -0.7919420

62 H 4.2773670 -3.8113460 1.2228930

63 C 3.3375330 -1.4297180 -1.6705260

64 C 4.3414010 -2.3791020 -1.8369360

65 H 5.4666400 -3.9750590 -0.9201850

66 H 3.0913820 -0.7726760 -2.4991380

67 H 4.8609980 -2.4530470 -2.7883480

68 N 1.2658560 -1.1255690 1.8190000

69 H 0.6156500 -3.3831810 0.2609840

70 C -0.0657700 -4.8477190 -1.1555050

71 H -0.9127070 -4.9615650 -1.8474040

72 C 1.2291420 -4.9239570 -1.9613350

73 H 2.0951850 -4.7221820 -1.3200470

74 H 1.3558240 -5.9187790 -2.4002910

75 H 1.2516980 -4.1987780 -2.7793760

76 C -0.1291070 -5.9826890 -0.1377000

77 H -1.0605620 -5.9526480 0.4365360

78 H -0.0635880 -6.9596860 -0.6269330

79 H 0.7040630 -5.9074900 0.5714550

80 Pd -4.7284140 0.0204170 -0.0025000

81 C -6.7978230 -0.2237130 0.3656370

82 C -6.5006590 1.1528390 0.4024280

83 C -6.4635220 -0.9624600 -0.7860490

84 H -7.0259850 -0.7477460 1.2910710

85 H -6.5929330 1.6923050 1.3395600

86 H -6.5260170 -2.0456020 -0.7604200

87 H -6.5822160 1.7545000 -0.5004360

88 H -6.5420910 -0.5063620 -1.7707030

Compound **10** (calibration set)

Tag Symbol X Y Z

1 S -2.1480170 0.7109940 0.4131740

2 S -1.4052610 -2.1661460 -0.8828440

3 C -0.4916940 0.2477690 0.1765810

4 C -0.1504080 -1.0579230 -0.4574480

5 N 0.5163390 0.9817110 0.5153420

6 N 1.1186130 -1.2669900 -0.6531920

7 C 1.5626950 -2.4868050 -1.3099410

8 H 0.8140650 -2.7981750 -2.0489830

9 H 2.4876210 -2.2444480 -1.8346620

10 C 1.7937010 -3.6106690 -0.3057240

11 H 0.8631790 -3.7784190 0.2478440

12 C 0.3255870 2.2826270 1.1265490

13 H -0.5570110 2.2717900 1.7800400

14 H 1.2028010 2.4770620 1.7480730

15 C 0.1738130 3.3705470 0.0667410

16 H 1.0448650 3.3434800 -0.5973690

17 H -0.6973340 3.1273760 -0.5514520

18 C 0.0148860 4.7766500 0.6432750

19 H -0.8438270 4.7686240 1.3306280

20 C -0.2875120 5.7619140 -0.4816770

21 H 0.5432920 5.7940420 -1.1963300

22 H -1.1886300 5.4739050 -1.0319670

23 H -0.4351270 6.7748100 -0.0939790

24 C 1.2502460 5.2208890 1.4232680

25 H 1.4444150 4.5882070 2.2940100

26 H 2.1397310 5.1865510 0.7831800

27 H 1.1355910 6.2479490 1.7837040

28 Rh 2.4032940 0.1609200 0.0197790

29 C 2.4357020 1.1228090 -1.7147600

30 C 1.7843540 0.7798230 -2.9023780

31 C 1.9139350 1.5644910 -4.0445790

32 C 2.6987180 2.7175840 -4.0303920

33 C 3.3501650 3.0852740 -2.8632110

34 C 3.2203630 2.2979560 -1.7140510

35 H 1.1631290 -0.1092030 -2.9426420

36 H 1.3966510 1.2766590 -4.9556150

37 H 2.7969960 3.3252900 -4.9237860

38 H 3.9545550 3.9874070 -2.8533370

39 C 3.8383170 2.6310710 -0.4362790

40 C 4.6349750 3.7491620 -0.1816740

41 C 5.1348710 3.9667410 1.0892710

42 H 4.8554920 4.4434470 -0.9827570

43 C 4.0462250 1.9675670 1.7906370

44 C 4.8328720 3.0611260 2.1012390

45 H 5.7528150 4.8348820 1.2917250

46 H 3.7890750 1.2280780 2.5391100

47 H 5.2007060 3.1901570 3.1116610

48 N 3.5595340 1.7557500 0.5624880

49 C 1.7315250 -0.8948000 2.8848280

50 C 1.9383060 -1.6055320 4.0542400

51 C 3.1143630 -2.3387920 4.1751840

52 C 4.0238070 -2.3419430 3.1314070

53 C 3.7531250 -1.6079980 1.9733660

54 H 0.8321840 -0.3086160 2.7298330

55 H 1.1947150 -1.5851980 4.8415360

56 H 3.3170850 -2.9105760 5.0746070

57 H 4.9362770 -2.9196160 3.2083160

58 C 4.6004740 -1.5705680 0.7768370

59 C 5.8061780 -2.2776190 0.6932360

60 C 4.1197780 -0.8185200 -0.3221500

61 C 6.5519230 -2.2549070 -0.4747850

62 H 6.1680280 -2.8560540 1.5376740

63 C 4.8946950 -0.8147630 -1.4860860

64 C 6.0898940 -1.5232870 -1.5668000

65 H 7.4839380 -2.8070220 -0.5364050

66 H 4.5576590 -0.2495470 -2.3495620

67 H 6.6660200 -1.5049200 -2.4878100

68 N 2.6118800 -0.8881320 1.8809090

69 H 2.5463810 -3.2874870 0.4203970

70 C 2.2510030 -4.9226590 -0.9420090

71 H 1.4887200 -5.2305350 -1.6718410

72 C 3.5846840 -4.7732510 -1.6705180

73 H 4.3552580 -4.3913980 -0.9902730

74 H 3.9247380 -5.7380180 -2.0601620

75 H 3.5211990 -4.0821200 -2.5155000

76 C 2.3460010 -6.0048980 0.1293050

77 H 1.3903790 -6.1403590 0.6454650

78 H 2.6370560 -6.9673450 -0.3031880

79 H 3.0978930 -5.7348450 0.8806810

80 Pd -3.3936840 -1.0421860 -0.3443490

81 P -5.3750110 0.0220270 0.1032300

82 C -5.2694310 1.6480610 0.9481110

83 H -4.5289450 2.2400430 0.3992680

84 H -6.2334790 2.1571000 0.8317190

85 C -6.5125090 -0.9798190 1.1314020

86 H -6.5922560 -1.9452050 0.6223560

87 H -5.9828960 -1.1704520 2.0717050

88 C -6.2688360 0.3677430 -1.4567900

89 H -6.5244330 -0.6119730 -1.8744170

90 H -7.2029390 0.8893060 -1.2181390

91 C -5.4405200 1.1702240 -2.4569100

92 H -5.1614770 2.1368550 -2.0213350

93 H -4.5030120 0.6375920 -2.6520420

94 C -6.1911960 1.3959750 -3.7619880

95 H -5.5858140 1.9674220 -4.4712230

96 H -6.4491950 0.4422810 -4.2331090

97 H -7.1217770 1.9481500 -3.5936700

98 C -7.8887920 -0.3765660 1.3977590

99 H -8.4183790 -0.2289370 0.4505570

100 H -7.7860510 0.6146950 1.8542420

101 C -8.7209530 -1.2697080 2.3093810

102 H -9.7094960 -0.8383610 2.4909030

103 H -8.8617300 -2.2599870 1.8652500

104 H -8.2304080 -1.4067490 3.2784380

105 C -4.8791660 1.5534890 2.4215400

106 H -5.7009920 1.1049240 2.9908500

107 H -4.0207920 0.8818310 2.5316270

108 C -4.5334970 2.9175360 3.0026810

109 H -4.2791760 2.8429170 4.0637570

110 H -3.6754530 3.3540810 2.4807660

111 H -5.3731900 3.6137260 2.9068760

112 Cl -4.6670830 -2.8380160 -1.2069340

Compound **11** (calibration set)

Tag Symbol X Y Z

1 S 0.1948840 -1.9045850 -0.2658910

2 S -1.0705570 0.6158170 1.1585710

3 Cl -1.7031270 0.0947470 -2.0715790

4 C -3.8384430 -0.9795370 1.1823770

5 C -3.0196140 -2.0169250 1.7187000

6 C -2.5717450 -3.0808430 0.9022670

7 C -2.9951190 -3.1088160 -0.4648410

8 C -3.7819960 -2.0691270 -0.9821690

9 C -4.2240710 -0.9728690 -0.1731210

10 H -4.0784310 -0.1298520 1.8115370

11 H -2.6698550 -1.9477600 2.7425800

12 H -2.6197720 -3.8805490 -1.1276380

13 H -3.9771770 -2.0375240 -2.0485610

14 C -5.0156220 0.1473940 -0.8010430

15 H -4.7056270 0.1777460 -1.8518250

16 C -6.5091580 -0.1819670 -0.7418280

17 H -7.0886130 0.5856350 -1.2631500

18 H -6.7274590 -1.1474790 -1.2079670

19 H -6.8558640 -0.2214020 0.2964150

20 C -4.7105560 1.5126540 -0.1969360

21 H -5.0631210 1.5906130 0.8371650

22 H -3.6374990 1.7199760 -0.2192510

23 H -5.2197130 2.2924590 -0.7699560

24 C -1.6767770 -4.1485210 1.4466180

25 H -1.0892740 -3.7774340 2.2878160

26 H -2.2834680 -4.9924820 1.7915930

27 H -0.9883700 -4.5150520 0.6826330

28 C 4.8049150 2.7168340 -0.8468020

29 H 4.6490510 3.1654940 -1.8252160

30 C 1.1282710 -0.4688780 -0.1351340

31 C 0.5152130 0.7418000 0.5168530

32 C 0.8453810 3.0474630 1.2190490

33 C 3.1125510 -1.4217740 -1.1624680

34 C 4.2434930 3.3189910 0.2946060

35 H 3.7447280 4.2781400 0.1922800

36 H 4.6432590 3.0982460 1.2829770

37 C 5.2220390 1.3753370 -0.7515330

38 H 5.6981950 1.0127850 0.1581330

39 H 5.4727520 0.8369190 -1.6607060

40 N 2.3689580 -0.3332890 -0.5070830

41 N 1.2795320 1.7942850 0.5812820

42 Pd 3.1954990 1.5331030 -0.1606960

43 H 4.1447770 -1.0646410 -1.1938260

44 H 1.6248650 3.7659480 0.9539980

45 C 3.1526000 -2.6912450 -0.3274290

46 C 3.4145690 -2.5882990 1.0413020

47 C 2.9999560 -3.9598400 -0.8822570

48 C 3.5018180 -3.7217930 1.8380450

49 H 3.5309740 -1.6039920 1.4857590

50 C 3.0918120 -5.0986710 -0.0872510

51 H 2.7841030 -4.0689090 -1.9391940

52 C 3.3394380 -4.9852670 1.2757710

53 H 3.6959210 -3.6199330 2.9013130

54 H 2.9622910 -6.0783820 -0.5368050

55 H 3.4056490 -5.8732800 1.8962680

56 C -0.4377450 3.6107710 0.6275460

57 C -0.6056650 3.6004340 -0.7585860

58 C -1.4189810 4.2123680 1.4128730

59 C -1.7340510 4.1579260 -1.3433000

60 H 0.1433750 3.1213500 -1.3809190

61 C -2.5475940 4.7806260 0.8286800

62 H -1.3215360 4.2257970 2.4927550

63 C -2.7115380 4.7531010 -0.5509410

64 H -1.8555140 4.1180280 -2.4210110

65 H -3.3054470 5.2368080 1.4583140

66 H -3.5970700 5.1851380 -1.0061470

67 C 2.6590570 -1.5824090 -2.6090330

68 H 1.6380450 -1.9623130 -2.6729090

69 H 2.6969360 -0.6085200 -3.1026630

70 H 3.3275390 -2.2603190 -3.1456310

71 C 0.8750330 2.9148330 2.7375510

72 H 0.0837460 2.2568680 3.1028150

73 H 1.8398140 2.5008890 3.0410730

74 H 0.7648470 3.8937600 3.2104910

75 Ru -2.0450080 -1.1794410 -0.0184390

Compound **12** (calibration set)

Tag Symbol X Y Z

1 S 0.8493190 0.5064010 -0.7954800

2 S -0.5944550 -2.0917020 0.3626000

3 Pd 1.6395450 -1.4535020 0.0408880

4 P 3.8267950 -0.7793800 -0.1312050

5 C 4.1316140 0.8154650 -0.9845550

6 H 3.4616830 1.5528800 -0.5291230

7 H 5.1574860 1.1302400 -0.7587610

8 C 4.9102720 -1.9931650 -0.9717060

9 H 4.7586880 -2.9379700 -0.4409340

10 H 4.4898440 -2.1340910 -1.9738660

11 C 4.5202730 -0.5411410 1.5464860

12 H 4.5450300 -1.5348850 2.0064420

13 H 5.5530740 -0.1861050 1.4505430

14 C 3.6926970 0.4220490 2.3937440

15 H 3.6115690 1.3912780 1.8899240

16 H 2.6698450 0.0372400 2.4750780

17 C 4.2856410 0.6180590 3.7815680

18 H 3.6776860 1.3084730 4.3737240

19 H 4.3392720 -0.3312720 4.3239150

20 H 5.2994650 1.0283980 3.7252160

21 C 6.3906170 -1.6310600 -1.0515330

22 H 6.8005870 -1.5219460 -0.0417020

23 H 6.5168190 -0.6606670 -1.5453540

24 C 7.1823640 -2.6901050 -1.8083900

25 H 8.2437250 -2.4306370 -1.8575590

26 H 7.0961380 -3.6663990 -1.3214530

27 H 6.8140010 -2.7964640 -2.8337790

28 C 3.9030060 0.7564430 -2.4925810

29 H 4.6445760 0.0941030 -2.9533880

30 H 2.9231480 0.3117440 -2.7006560

31 C 3.9815400 2.1367420 -3.1299900

32 H 3.8313640 2.0826880 -4.2118370

33 H 3.2149030 2.7978370 -2.7146630

34 H 4.9565980 2.6007020 -2.9483970

35 Cl 2.4157800 -3.4749530 0.9878700

36 C -5.3227610 2.1322310 -0.7114630

37 H -5.5340090 1.8333440 -1.7356250

38 C -0.7677410 0.6228270 -0.2151200

39 C -1.4664710 -0.6092670 0.3175820

40 C -3.6000210 -1.3992740 1.2800100

41 C -0.9234880 3.0249250 -0.6134190

42 C -5.5845490 1.2388400 0.3444220

43 H -6.0668270 0.2897060 0.1305970

44 H -5.6971890 1.6137240 1.3605440

45 C -4.4557720 3.2142530 -0.4620460

46 H -4.4880570 3.7299020 0.4964580

47 H -4.0834280 3.7981750 -1.2985100

48 N -1.4662210 1.7176740 -0.2102070

49 N -2.7007950 -0.4128400 0.6761820

50 Pd -3.4954210 1.3993390 0.0471490

51 H -1.6775170 3.7401040 -0.2704150

52 H -4.3281830 -0.7787970 1.8114480

53 C 0.3527380 3.3881970 0.1296960

54 C 0.4115020 3.1875640 1.5112920

55 C 1.4456340 3.9732040 -0.5048310

56 C 1.5436770 3.5368040 2.2338200

57 H -0.4329380 2.7309210 2.0190730

58 C 2.5810750 4.3296730 0.2177140

59 H 1.4294210 4.1371600 -1.5764090

60 C 2.6372500 4.1086680 1.5884530

61 H 1.5761420 3.3576740 3.3039780

62 H 3.4270070 4.7737770 -0.2979390

63 H 3.5250020 4.3787130 2.1514780

64 C -4.3901930 -2.1569190 0.2273430

65 C -3.9748300 -2.2618990 -1.0978770

66 C -5.5900220 -2.7648210 0.6043210

67 C -4.7360800 -2.9703110 -2.0237270

68 H -3.0516190 -1.7907290 -1.4149150

69 C -6.3512390 -3.4720310 -0.3174940

70 H -5.9357470 -2.6777080 1.6310180

71 C -5.9248800 -3.5783710 -1.6386120

72 H -4.3948950 -3.0448030 -3.0514800

73 H -7.2814440 -3.9364830 -0.0055630

74 H -6.5177850 -4.1289400 -2.3618010

75 C -0.8644200 3.1369290 -2.1321160

76 H -0.0909750 2.4929340 -2.5562290

77 H -1.8295510 2.8401380 -2.5499670

78 H -0.6682680 4.1690290 -2.4324480

79 C -2.9993920 -2.3273400 2.3399700

80 H -2.4483250 -3.1623880 1.9124570

81 H -2.3323610 -1.7699460 3.0024880

82 H -3.8208120 -2.7263360 2.9414420

Compound **13** (calibration set)

Tag Symbol X Y Z

1 C 3.8068580 -2.5990510 -0.3780460

2 C 4.1749680 -1.8762090 -1.5449900

3 C 3.4970510 -0.6312770 -1.5291310

4 C 2.6876320 -0.5837630 -0.3469180

5 C 2.8916880 -1.8118010 0.3662060

6 H 4.1297880 -3.5974690 -0.1197290

7 H 4.8294170 -2.2261730 -2.3303790

8 H 3.5489260 0.1359300 -2.2873340

9 H 2.4155450 -2.0948980 1.2929950

10 Fe 2.1333300 -2.1487640 -1.4849640

11 C 1.3044210 -2.5066180 -3.3393040

12 C 1.5116870 -3.7318400 -2.6490280

13 C 0.4669740 -1.6865370 -2.5427910

14 H 1.7455780 -2.2274280 -4.2853270

15 C 0.8031980 -3.6817410 -1.4208950

16 H 2.1416120 -4.5464900 -2.9769350

17 C 0.1554020 -2.4061450 -1.3410340

18 H 0.1415660 -0.6795450 -2.7635600

19 H 0.8091230 -4.4467400 -0.6599470

20 P 1.5934910 0.7845400 0.1139160

21 P -0.8067260 -1.6769260 -0.0070690

22 C -2.4831740 -2.3540810 -0.2565030

23 C -3.3362740 -2.5330070 0.8348440

24 C -2.9432490 -2.6186390 -1.5475200

25 C -4.6350610 -2.9831990 0.6341740

26 H -2.9868540 -2.3263970 1.8414640

27 C -4.2440600 -3.0676720 -1.7419970

28 H -2.2868760 -2.4817260 -2.4009580

29 C -5.0903690 -3.2502440 -0.6531250

30 H -5.2914130 -3.1271250 1.4859600

31 H -4.5949420 -3.2790440 -2.7465770

32 H -6.1042990 -3.6043480 -0.8075110

33 C -0.2848780 -2.4268050 1.5658420

34 C 0.1401630 -1.6112440 2.6139330

35 C -0.3326170 -3.8131970 1.7452210

36 C 0.5616800 -2.1747610 3.8136470

37 H 0.1418120 -0.5343380 2.4963350

38 C 0.0923760 -4.3724570 2.9422780

39 H -0.7205580 -4.4554490 0.9616820

40 C 0.5489660 -3.5549680 3.9741430

41 H 0.8978370 -1.5300790 4.6189230

42 H 0.0588960 -5.4486790 3.0744000

43 H 0.8804790 -3.9968280 4.9079590

44 C 2.2164300 2.1154800 -0.9702460

45 C 1.7076910 2.2075510 -2.2677790

46 C 3.2178310 2.9908210 -0.5533550

47 C 2.2125750 3.1549540 -3.1478340

48 H 0.9040620 1.5493820 -2.5814020

49 C 3.7111180 3.9469540 -1.4347060

50 H 3.6092520 2.9357960 0.4567040

51 C 3.2148660 4.0261500 -2.7312750

52 H 1.8144600 3.2212900 -4.1547690

53 H 4.4841260 4.6326760 -1.1042510

54 H 3.6032050 4.7727860 -3.4161040

55 C 2.1259230 1.2094660 1.8059890

56 C 3.4069050 0.8754520 2.2536690

57 C 1.2507910 1.8876140 2.6584420

58 C 3.8043400 1.2166850 3.5409670

59 H 4.0937580 0.3457280 1.6025920

60 C 1.6537500 2.2247390 3.9443280

61 H 0.2555120 2.1485570 2.3145900

62 C 2.9289430 1.8884780 4.3876970

63 H 4.7999920 0.9539710 3.8822570

64 H 0.9677530 2.7483970 4.6017120

65 H 3.2404370 2.1486370 5.3939670

66 Pt -0.7038710 0.6256010 -0.0586200

67 S -3.0599660 0.6838280 -0.1838140

68 S -0.7337080 2.9826290 -0.1528420

69 C -3.4508850 2.3281010 -0.0782740

70 C -2.4215830 3.4132610 -0.0131880

71 N -2.8803090 4.5957980 0.1063360

72 N -4.6934840 2.7301630 -0.0506440

73 C -1.9733170 5.7133470 0.1674870

74 H -1.2315890 5.5826600 0.9665970

75 H -1.4157340 5.8151540 -0.7728970

76 H -2.5355360 6.6303190 0.3438830

77 C -5.8568220 1.8731220 -0.0903350

78 H -5.8728460 1.2962010 -1.0191790

79 H -5.8419300 1.1750860 0.7514630

80 H -6.7478240 2.4948640 -0.0336550

81 H -4.7850930 3.7455690 0.0188550

Compound **14** (calibration set)

Tag Symbol X Y Z

1 C -4.8459560 -0.4420480 -0.2333950

2 C -4.7054900 -1.2178880 -1.4157390

3 C -3.3845560 -1.7309480 -1.4568000

4 C -2.6905570 -1.2582600 -0.2953180

5 C -3.6105210 -0.4600750 0.4629340

6 H -5.7263260 0.1085870 0.0660270

7 H -5.4611100 -1.3649440 -2.1740640

8 H -2.9590590 -2.3422070 -2.2387810

9 H -3.3930360 0.0531750 1.3876840

10 Fe -3.3216810 0.3090010 -1.3903270

11 C -3.0021100 1.1494350 -3.2465480

12 C -3.9192170 1.9386960 -2.5006310

13 C -1.7985370 1.0506420 -2.5045960

14 H -3.2008730 0.6685800 -4.1935430

15 C -3.2911530 2.3364280 -1.2922040

16 H -4.9399960 2.1588850 -2.7789950

17 C -1.9709440 1.7798060 -1.2808950

18 H -0.9110180 0.4978690 -2.7776780

19 H -3.7550470 2.9025580 -0.4993170

20 P -0.9578490 -1.6065970 0.1018480

21 P -0.7082100 1.8282250 0.0006780

22 C 0.1276650 3.4265780 -0.2758540

23 C 0.7091900 4.1087210 0.7951520

24 C 0.2578350 3.9290500 -1.5715720

25 C 1.4053200 5.2896700 0.5699570

26 H 0.6156910 3.7212920 1.8047400

27 C 0.9572440 5.1097770 -1.7908680

28 H -0.1914400 3.4046020 -2.4087340

29 C 1.5307720 5.7907490 -0.7218980

30 H 1.8490750 5.8197630 1.4060500

31 H 1.0496590 5.5001160 -2.7989110

32 H 2.0731100 6.7143980 -0.8952260

33 C -1.5224870 2.0522730 1.6108730

34 C -1.2888220 1.1317620 2.6315890

35 C -2.3579730 3.1489270 1.8462180

36 C -1.9215750 1.2742790 3.8618320

37 H -0.6104110 0.3033830 2.4645420

38 C -2.9911610 3.2859280 3.0737470

39 H -2.4980220 3.9067180 1.0825320

40 C -2.7814440 2.3441440 4.0790960

41 H -1.7379360 0.5474370 4.6461020

42 H -3.6434350 4.1345670 3.2503900

43 H -3.2791140 2.4555800 5.0367540

44 C -0.6101240 -3.0169560 -1.0040670

45 C -0.2384440 -2.7487880 -2.3235600

46 C -0.7497180 -4.3358840 -0.5758610

47 C -0.0287250 -3.7934170 -3.2132320

48 H -0.0977040 -1.7229760 -2.6484240

49 C -0.5262480 -5.3792910 -1.4680380

50 H -1.0233480 -4.5530240 0.4509550

51 C -0.1719420 -5.1102210 -2.7853500

52 H 0.2589810 -3.5800030 -4.2371790

53 H -0.6271870 -6.4049720 -1.1292930

54 H 0.0015380 -5.9271480 -3.4780430

55 C -1.0371050 -2.2945350 1.7909960

56 C -2.2250230 -2.8494940 2.2749820

57 C 0.1002260 -2.2842880 2.6029770

58 C -2.2733590 -3.3810400 3.5582780

59 H -3.1146400 -2.8649150 1.6551080

60 C 0.0448330 -2.8162520 3.8850690

61 H 1.0283140 -1.8629630 2.2326720

62 C -1.1411730 -3.3620260 4.3656980

63 H -3.1998980 -3.8085470 3.9265730

64 H 0.9313450 -2.8012210 4.5102810

65 H -1.1830210 -3.7726020 5.3691910

66 Pt 0.6919240 -0.0016490 -0.1116090

67 S 2.5301700 1.4660190 -0.2425710

68 S 2.2207130 -1.7862990 -0.2718520

69 C 3.8867750 0.4555460 -0.1501960

70 C 3.7938130 -1.0386230 -0.1217870

71 N 4.9040220 -1.6545090 -0.0215260

72 N 5.0962890 0.9445620 -0.1007470

73 H 5.8191430 0.2219000 -0.0496770

74 C 4.9367270 -3.0986350 0.0086260

75 H 4.2536420 -3.4644840 0.7898120

76 H 4.5353340 -3.4856990 -0.9396730

77 C 5.4509950 2.3540150 -0.0946940

78 H 5.1157650 2.7998020 -1.0379820

79 H 4.8875140 2.8445720 0.7067670

80 C 6.3446620 -3.6100600 0.2396500

81 H 6.3564990 -4.7029930 0.2565370

82 H 7.0156970 -3.2726600 -0.5548340

83 H 6.7368100 -3.2491170 1.1943550

84 C 6.9428760 2.5280240 0.0950440

85 H 7.1899770 3.5910900 0.0947590

86 H 7.2722340 2.1039950 1.0473240

87 H 7.5031510 2.0515720 -0.7136970

Compound **15** (calibration set)

Tag Symbol X Y Z

1 C 4.8027420 -1.2327790 0.4198750

2 C 5.0944650 -0.6168850 -0.8272850

3 C 4.0467470 0.2883750 -1.1319860

4 C 3.0866080 0.2263610 -0.0701140

5 C 3.5677070 -0.7210220 0.8935880

6 H 5.3933320 -1.9959850 0.9063370

7 H 5.9476960 -0.8262130 -1.4564300

8 H 3.9635070 0.8966920 -2.0204670

9 H 3.0667200 -1.0097770 1.8055760

10 Fe 3.2829680 -1.5936720 -0.9163670

11 C 2.9635330 -2.5260080 -2.7279420

12 C 3.4401410 -3.4620810 -1.7703560

13 C 1.7727870 -1.9452380 -2.2245940

14 H 3.4478110 -2.2654760 -3.6581080

15 C 2.5480020 -3.4706850 -0.6673140

16 H 4.3537670 -4.0348280 -1.8427580

17 C 1.5085250 -2.5222530 -0.9374430

18 H 1.1770860 -1.1765420 -2.6961600

19 H 2.6730610 -4.0442410 0.2383400

20 P 1.5425480 1.1703730 0.0000920

21 P 0.1441580 -1.9802180 0.1023020

22 C -1.1682190 -3.2143930 -0.1881070

23 C -2.1135500 -3.4710540 0.8081970

24 C -1.2962390 -3.8206460 -1.4382340

25 C -3.1731500 -4.3322230 0.5550800

26 H -2.0234420 -2.9976870 1.7808940

27 C -2.3592560 -4.6820670 -1.6858200

28 H -0.5665140 -3.6255620 -2.2176390

29 C -3.2983700 -4.9369640 -0.6920140

30 H -3.9038210 -4.5289350 1.3325910

31 H -2.4511990 -5.1561300 -2.6573380

32 H -4.1273290 -5.6090630 -0.8882900

33 C 0.5972110 -2.2632510 1.8407970

34 C 0.5746250 -1.2022930 2.7448640

35 C 0.9376050 -3.5444850 2.2867480

36 C 0.9356990 -1.4055100 4.0725950

37 H 0.2730420 -0.2159340 2.4134400

38 C 1.3013510 -3.7430450 3.6114230

39 H 0.8979400 -4.3903270 1.6082560

40 C 1.3097130 -2.6726500 4.5033910

41 H 0.9213120 -0.5707710 4.7655360

42 H 1.5701550 -4.7373060 3.9520290

43 H 1.5945690 -2.8330380 5.5379490

44 C 1.8434590 2.4606730 -1.2563660

45 C 1.5424170 2.1692240 -2.5888960

46 C 2.4004380 3.6944990 -0.9236320

47 C 1.8139530 3.0996150 -3.5831390

48 H 1.0802110 1.2207950 -2.8440640

49 C 2.6595530 4.6272410 -1.9218990

50 H 2.6239060 3.9347240 0.1101440

51 C 2.3721430 4.3300460 -3.2497260

52 H 1.5782390 2.8686460 -4.6165270

53 H 3.0843950 5.5901850 -1.6587810

54 H 2.5758210 5.0609140 -4.0253450

55 C 1.6206630 2.0056330 1.6199070

56 C 2.8508030 2.2431750 2.2388510

57 C 0.4424330 2.4301310 2.2392970

58 C 2.8977400 2.9007670 3.4625490

59 H 3.7718350 1.9130960 1.7706070

60 C 0.4957550 3.0875670 3.4616310

61 H -0.5129200 2.2442990 1.7604410

62 C 1.7223150 3.3228390 4.0750010

63 H 3.8562070 3.0814310 3.9374750

64 H -0.4239660 3.4140600 3.9358810

65 H 1.7622860 3.8333150 5.0316450

66 Pt -0.5033740 0.1781320 -0.3817990

67 S -2.6872840 -0.6066800 -0.7787440

68 S -1.3136270 2.3391330 -0.8574940

69 C -3.6379000 0.7957900 -0.7409680

70 C -3.0480740 2.1702830 -0.6314530

71 N -3.8826960 3.1098040 -0.4315320

72 N -4.9421640 0.7437620 -0.8037080

73 C -3.4232560 4.4732000 -0.2752820

74 H -2.5752600 4.6895660 -0.9387070

75 H -4.2459290 5.1381750 -0.5539130

76 C -5.7456210 -0.4654500 -0.8687880

77 H -6.7061300 -0.1898990 -1.3092350

78 H -5.2537250 -1.1638980 -1.5532560

79 H -5.3835640 1.6617510 -0.7253160

80 C -3.0173860 4.7460940 1.1744890

81 H -3.8806000 4.5625320 1.8233360

82 H -2.2421970 4.0270440 1.4600810

83 C -2.5024450 6.1650170 1.3600610

84 H -3.2592990 6.9034990 1.0768660

85 H -2.2304330 6.3501040 2.4027260

86 H -1.6138360 6.3434360 0.7463120

87 C -5.9426460 -1.1161940 0.4978530

88 H -6.4786010 -0.4205320 1.1519710

89 H -4.9621490 -1.2950940 0.9504450

90 C -6.7034720 -2.4276300 0.3735650

91 H -6.1534790 -3.1409890 -0.2483110

92 H -6.8522990 -2.8848840 1.3547310

93 H -7.6895350 -2.2768380 -0.0769550

Compound **16** (calibration set)

Tag Symbol X Y Z

1 Pt -0.0128960 -0.0040310 -0.6931410

2 S 1.5756700 1.6753000 -0.5900350

3 S 1.6913470 -1.5665380 -0.5939210

4 C 3.0815930 0.8470350 -0.4611430

5 C 3.1364150 -0.6295340 -0.5117130

6 N 4.2468530 1.4239390 -0.3808520

7 N 4.3437300 -1.1157080 -0.5282090

8 Cl 5.6190790 0.3879320 -2.8044360

9 C 4.5585380 -2.5353870 -0.7566410

10 H 5.3833680 -2.6234190 -1.4683350

11 C 4.3564160 2.8657650 -0.5533140

12 H 5.2502920 3.0444430 -1.1551490

13 C 7.6033060 -1.1282050 0.0486710

14 C 6.8700130 -0.8156070 1.2272970

15 C 6.6438870 0.5154540 1.6350470

16 C 7.1424680 1.5457070 0.7837050

17 C 7.8413810 1.2505240 -0.3973010

18 C 8.0858060 -0.1060060 -0.7833470

19 H 7.7105150 -2.1652320 -0.2408710

20 H 6.4339610 -1.6234530 1.8036100

21 H 6.9056440 2.5782370 1.0172030

22 H 8.1380720 2.0543070 -1.0615570

23 C 8.8260510 -0.3819510 -2.0674750

24 H 8.4892780 0.3763770 -2.7824350

25 C 10.3256250 -0.1899630 -1.8184860

26 H 10.8788610 -0.3161040 -2.7532550

27 H 10.5466750 0.8063760 -1.4252360

28 H 10.6977770 -0.9287390 -1.1011170

29 C 8.5293510 -1.7498310 -2.6652070

30 H 8.9177150 -2.5602210 -2.0392800

31 H 7.4538880 -1.8855350 -2.8037330

32 H 9.0102530 -1.8362110 -3.6429410

33 Ru 5.9160700 0.2123380 -0.4244550

34 C 5.9038320 0.8229060 2.8969470

35 H 5.1636300 0.0494040 3.1128350

36 H 6.6081610 0.8613920 3.7348850

37 H 5.3975620 1.7864490 2.8341190

38 H 3.6681500 -2.9655950 -1.2310980

39 C 4.8848120 -3.2957790 0.5036630

40 C 5.8967590 -4.2537990 0.4971610

41 C 4.1904130 -3.0529550 1.6901690

42 C 6.2218500 -4.9505670 1.6572470

43 H 6.4414800 -4.4516690 -0.4223710

44 C 4.5158660 -3.7450290 2.8502830

45 H 3.3987820 -2.3106780 1.7068930

46 C 5.5356240 -4.6935780 2.8390510

47 H 7.0168150 -5.6892300 1.6379790

48 H 3.9715540 -3.5429900 3.7673080

49 H 5.7917830 -5.2304030 3.7466250

50 C 4.4426390 3.6471090 0.7342630

51 C 3.6275200 3.3500140 1.8269540

52 C 5.3332730 4.7165770 0.8304030

53 C 3.7071850 4.1048780 2.9918630

54 H 2.9277660 2.5232800 1.7672260

55 C 5.4145590 5.4729560 1.9951410

56 H 5.9737280 4.9566950 -0.0143580

57 C 4.6014680 5.1674660 3.0813510

58 H 3.0673900 3.8602230 3.8338190

59 H 6.1163990 6.2987610 2.0539130

60 H 4.6636040 5.7540560 3.9921620

61 H 3.4974620 3.2212800 -1.1365510

62 S -1.6055900 -1.6817780 -0.7513190

63 S -1.7192410 1.5567870 -0.7718270

64 C -3.1049920 -0.8531820 -0.5560670

65 C -3.1606610 0.6233380 -0.6142040

66 N -4.2661350 -1.4287280 -0.4268640

67 N -4.3671660 1.1104370 -0.5864890

68 Cl -5.7281000 -0.4047610 -2.8044500

69 C -4.5886530 2.5302830 -0.8090500

70 H -5.4417250 2.6192470 -1.4863720

71 C -4.3811020 -2.8727190 -0.5821630

72 H -5.2979810 -3.0571080 -1.1463660

73 C -7.5958510 1.1335270 0.1204740

74 C -6.8206130 0.8171340 1.2709980

75 C -6.5873360 -0.5151500 1.6703220

76 C -7.1229420 -1.5429060 0.8385220

77 C -7.8630640 -1.2437360 -0.3158310

78 C -8.1150150 0.1142520 -0.6925780

79 H -7.7074740 2.1712160 -0.1648900

80 H -6.3592710 1.6225450 1.8307700

81 H -6.8835790 -2.5766130 1.0639300

82 H -8.1882350 -2.0457820 -0.9687380

83 C -8.9042030 0.3941290 -1.9463480

84 H -8.6026290 -0.3672710 -2.6737240

85 C -10.3936810 0.2130470 -1.6356600

86 H -10.9841060 0.3415430 -2.5470460

87 H -10.6052930 -0.7810190 -1.2315560

88 H -10.7307360 0.9556810 -0.9050320

89 C -8.6231470 1.7594270 -2.5573680

90 H -8.9781770 2.5730820 -1.9160630

91 H -7.5537770 1.8873840 -2.7424080

92 H -9.1451830 1.8489780 -3.5134960

93 Ru -5.9352370 -0.2156620 -0.4153710

94 C -5.8041720 -0.8263930 2.9049840

95 H -5.0483480 -0.0602470 3.0908580

96 H -6.4777000 -0.8541630 3.7683060

97 H -5.3106930 -1.7954050 2.8276550

98 H -3.7189390 2.9597720 -1.3206430

99 C -4.8610310 3.2919840 0.4635060

100 C -5.8693310 4.2531830 0.4986460

101 C -4.1182160 3.0478020 1.6200510

102 C -6.1432170 4.9518330 1.6708220

103 H -6.4513280 4.4525510 -0.3974210

104 C -4.3922720 3.7419400 2.7921200

105 H -3.3283240 2.3037880 1.6035840

106 C -5.4086290 4.6937050 2.8229080

107 H -6.9359360 5.6930320 1.6843020

108 H -3.8101850 3.5391110 3.6854670

109 H -5.6244990 5.2322480 3.7399020

110 C -4.4156510 -3.6405510 0.7160370

111 C -3.5513180 -3.3372680 1.7686340

112 C -5.3073290 -4.7033490 0.8626790

113 C -3.5840400 -4.0795000 2.9438220

114 H -2.8496100 -2.5161570 1.6689140

115 C -5.3419040 -5.4469090 2.0380370

116 H -5.9853770 -4.9487760 0.0493430

117 C -4.4800740 -5.1351600 3.0840840

118 H -2.9061550 -3.8302870 3.7540320

119 H -6.0453670 -6.2675380 2.1364610

120 H -4.5055630 -5.7116930 4.0030550

121 H -3.5469530 -3.2348310 -1.1960120

Compound **17** (calibration set)

Tag Symbol X Y Z

1 N 4.2484000 -1.3858060 0.4161520

2 N 4.2315770 1.1755890 0.5689270

3 C 3.0800940 -0.8341880 0.2436880

4 C 3.0692450 0.6404900 0.3341730

5 S 1.6194380 -1.7013230 -0.0579150

6 S 1.6015680 1.5274640 0.1508860

7 Pt -0.0443220 -0.0962480 0.0464870

8 S -1.6906160 -1.7227070 -0.0602570

9 S -1.7070080 1.5133000 0.1474130

10 C -3.1592790 -0.8645680 0.2274420

11 C -3.1694280 0.6111980 0.2914080

12 N -4.3243670 -1.4169330 0.4102550

13 N -4.3467040 1.1309370 0.4850770

14 Cl -5.7366300 -0.0949670 -1.9442030

15 C 4.3517630 2.6239840 0.6391770

16 H 5.1898980 2.8606260 1.2934030

17 C -4.4879900 2.5759600 0.5657960

18 H -5.3620900 2.7958430 1.1826030

19 H -3.6113550 2.9881190 1.0782820

20 C -4.6594300 3.2054000 -0.8139030

21 H -5.3770150 2.5993740 -1.3743150

22 H -3.7111810 3.1385200 -1.3603120

23 C -5.1260480 4.6587960 -0.7660570

24 H -6.0702930 4.6887000 -0.2007340

25 C -5.4082400 5.1610350 -2.1784210

26 H -4.4940950 5.1425840 -2.7825780

27 H -6.1523330 4.5360580 -2.6822190

28 H -5.7804150 6.1903650 -2.1662830

29 C -4.1202140 5.5649900 -0.0609920

30 H -3.9617180 5.2753620 0.9820170

31 H -3.1496200 5.5259730 -0.5688010

32 H -4.4597240 6.6055400 -0.0664290

33 C -4.4436410 -2.8653320 0.3956020

34 H -3.4830670 -3.3090130 0.6812470

35 H -5.1676380 -3.1433670 1.1625700

36 C -4.8758160 -3.3944820 -0.9660150

37 H -5.8140690 -2.9096510 -1.2599520

38 H -4.1290110 -3.0850020 -1.7048190

39 C -5.0423630 -4.9133200 -1.0034220

40 H -4.1063190 -5.3690340 -0.6498360

41 C -5.2783820 -5.3722380 -2.4390760

42 H -6.2009580 -4.9332840 -2.8365370

43 H -4.4561720 -5.0679010 -3.0935650

44 H -5.3737620 -6.4610960 -2.4967780

45 C -6.1773720 -5.3898150 -0.0993970

46 H -5.9977810 -5.1592980 0.9550160

47 H -7.1234850 -4.9187390 -0.3933040

48 H -6.3091630 -6.4735100 -0.1753740

49 C 7.7516140 -1.2120650 0.7931710

50 C 6.9279900 -1.3955600 1.9263770

51 C 6.4178390 -0.3110360 2.6853820

52 C 6.7384820 0.9850490 2.2141480

53 C 7.5621880 1.1978410 1.0790090

54 C 8.0752790 0.0972060 0.3527320

55 H 8.0755210 -2.0758130 0.2288800

56 H 6.6359510 -2.4028690 2.2037000

57 H 6.2906970 1.8392190 2.7113060

58 H 7.7427890 2.2065790 0.7252940

59 C 8.9305020 0.3580260 -0.8643650

60 H 8.4182370 1.1411200 -1.4346130

61 C 10.2886940 0.8968620 -0.3999870

62 H 10.9090390 1.1373660 -1.2676990

63 H 10.1846150 1.8020830 0.2041870

64 H 10.8192560 0.1482220 0.1974940

65 C 9.1071570 -0.8500980 -1.7735580

66 H 9.6783680 -1.6445660 -1.2810520

67 H 8.1417120 -1.2469460 -2.0932540

68 H 9.6638700 -0.5552880 -2.6668560

69 Ru -5.9568700 -0.1561510 0.4549260

70 C 5.5411010 -0.5263050 3.8779080

71 H 4.9614170 -1.4457430 3.7752240

72 H 6.1495920 -0.6076160 4.7846610

73 H 4.8467590 0.3059700 4.0077170

74 Ru 5.8610120 -0.0879020 0.5731600

75 C -7.5225610 1.2090890 1.2057540

76 C -6.7681860 0.6352920 2.2729860

77 C -6.6519750 -0.7645920 2.4288270

78 C -7.2884800 -1.5812150 1.4435210

79 C -7.9694410 -1.0213270 0.3570360

80 C -8.1096380 0.3995850 0.2254310

81 H -7.5567310 2.2864320 1.1019280

82 H -6.2359850 1.2871870 2.9580340

83 H -7.1675490 -2.6581550 1.4857480

84 H -8.3452280 -1.6673430 -0.4281320

85 C -8.8635100 0.9465470 -0.9601010

86 H -8.5405350 0.3508310 -1.8213420

87 C -10.3624330 0.7175330 -0.7389920

88 H -10.9238050 1.0416010 -1.6195950

89 H -10.5912900 -0.3371110 -0.5616780

90 H -10.7196460 1.2920070 0.1220610

91 C -8.5676970 2.4073660 -1.2641970

92 H -8.9344930 3.0701140 -0.4730530

93 H -7.4965040 2.5742160 -1.3944210

94 H -9.0687420 2.6989480 -2.1906310

95 C -5.8758650 -1.3647530 3.5576320

96 H -5.1222250 -0.6675240 3.9276260

97 H -6.5508750 -1.6107600 4.3839730

98 H -5.3734580 -2.2842610 3.2513570

99 H 3.4455290 3.0345740 1.1025290

100 C 4.5645810 3.2535470 -0.7338060

101 H 5.4661410 2.8253590 -1.1852010

102 H 3.7287800 2.9652910 -1.3797790

103 C 4.6767250 4.7772050 -0.6902740

104 H 3.7882790 5.1713360 -0.1759040

105 C 4.6858910 5.3345680 -2.1104750

106 H 5.5526610 4.9576550 -2.6657950

107 H 3.7857670 5.0401560 -2.6584050

108 H 4.7397750 6.4278560 -2.1074800

109 C 5.9164520 5.2416420 0.0712820

110 H 5.9999570 6.3327370 0.0542280

111 H 5.9032490 4.9328850 1.1208070

112 H 6.8229100 4.8309590 -0.3901310

113 C 4.3335470 -2.8419560 0.3904570

114 H 3.4259660 -3.2367630 0.8616470

115 H 5.1752270 -3.1421070 1.0140580

116 C 4.4799980 -3.4347620 -1.0130480

117 H 4.0971570 -4.4639120 -0.9874630

118 H 3.8249590 -2.8798950 -1.6919760

119 C 5.9064390 -3.4489750 -1.5652770

120 H 6.3176700 -2.4430680 -1.4346920

121 C 6.7941610 -4.4492420 -0.8309860

122 H 7.8242260 -4.4024620 -1.1998060

123 H 6.8246790 -4.2730630 0.2494060

124 H 6.4330220 -5.4732600 -0.9839570

125 C 5.8887710 -3.7500610 -3.0592810

126 H 5.4331510 -4.7284280 -3.2552000

127 H 5.3146720 -2.9945390 -3.6035000

128 H 6.9027910 -3.7656830 -3.4720220

129 Cl 5.6942360 0.1044270 -1.8182670

Compound **18** (calibration set)

Tag Symbol X Y Z

1 N 4.2845940 1.2707210 0.2887500

2 N 4.2822260 -1.3029300 0.2865160

3 C 3.1154530 0.7261820 0.1370700

4 C 3.1132770 -0.7563790 0.1409090

5 S 1.6457090 1.6054150 -0.0747920

6 S 1.6386270 -1.6327280 -0.0509510

7 C 4.4109310 -2.7483150 0.2464280

8 C 4.4152880 2.7159160 0.2522410

9 H 5.2833020 2.9848330 0.8522260

10 H 3.5324620 3.1674130 0.7240790

11 H 3.5306390 -3.2005950 0.7220870

12 H 5.2822860 -3.0199250 0.8402190

13 C 4.5706670 3.2441290 -1.1712490

14 H 5.5110310 2.8694170 -1.5912250

15 H 3.7691820 2.8208790 -1.7857690

16 C 4.5576110 -3.2705330 -1.1802410

17 H 3.7520410 -2.8446980 -1.7876120

18 H 5.4951220 -2.8931240 -1.6041040

19 Pt -0.0113080 -0.0086670 0.0146120

20 S -1.6555640 1.6201080 0.0594330

21 S -1.6699340 -1.6229240 0.0898530

22 C -3.1342780 0.7475400 0.2328180

23 C -3.1419540 -0.7348420 0.2383030

24 N -4.3026990 1.2980510 0.3663150

25 N -4.3171270 -1.2738330 0.3650260

26 Rh 5.9079350 -0.0177100 0.3480460

27 Cl 5.8650410 -0.0149820 -2.0511030

28 C 6.8307950 -0.7409670 2.1489040

29 C 7.6062020 -1.1819410 1.0138430

30 C 6.8279990 0.6888940 2.1565870

31 C 8.0891880 -0.0138430 0.3465960

32 C 7.6031150 1.1447070 1.0269420

33 C 7.9858330 -2.5813080 0.6672770

34 C 6.2066180 -1.6056520 3.1880220

35 C 8.9775970 -0.0057420 -0.8439540

36 C 7.9791910 2.5491800 0.6975620

37 C 6.2026010 1.5412500 3.2050280

38 H 7.3646250 -3.3135860 1.1836460

39 H 7.9016750 -2.7617080 -0.4062360

40 H 9.0247170 -2.7697520 0.9590020

41 H 8.8151210 -0.8840660 -1.4686570

42 H 8.8142310 0.8804190 -1.4572990

43 H 10.0213080 -0.0072790 -0.5078460

44 H 9.0181340 2.7358160 0.9902200

45 H 7.8932870 2.7433780 -0.3733900

46 H 7.3574410 3.2733290 1.2246550

47 H 6.8968440 1.6576200 4.0447200

48 H 5.9649550 2.5383780 2.8333470

49 H 5.2839750 1.0936050 3.5873480

50 H 6.8904960 -1.7088910 4.0378110

51 H 5.2739650 -1.1756980 3.5565710

52 H 5.9935800 -2.6069630 2.8129880

53 C -4.4534330 -2.7191600 0.3344050

54 H -5.3409810 -2.9793990 0.9091210

55 H -3.5897660 -3.1725640 0.8383680

56 C -4.4265120 2.7437870 0.3469500

57 H -5.2766270 3.0179550 0.9737880

58 C -4.5641220 -3.2529500 -1.0911060

59 H -5.4843710 -2.8689570 -1.5453850

60 H -3.7362400 -2.8411620 -1.6774580

61 C 4.5072580 -4.7947800 -1.2771220

62 H 3.5521640 -5.1264850 -0.8447950

63 C 4.5360230 -5.2211430 -2.7415420

64 H 4.4589840 -6.3086730 -2.8393410

65 H 3.7119090 -4.7704250 -3.3026900

66 H 5.4734380 -4.9074420 -3.2154470

67 C 5.6383300 -5.4671550 -0.5029330

68 H 6.6126980 -5.1289300 -0.8747430

69 H 5.5938010 -5.2528800 0.5691890

70 H 5.5970850 -6.5545940 -0.6194540

71 C 4.5193170 4.7688830 -1.2606510

72 H 3.5602020 5.0968360 -0.8343960

73 C 5.6427900 5.4388930 -0.4734320

74 H 5.5898820 5.2185190 0.5970700

75 H 6.6208800 5.1047160 -0.8390730

76 H 5.6003640 6.5268900 -0.5841830

77 C 4.5593730 5.2032910 -2.7223980

78 H 5.5011990 4.8938460 -3.1903090

79 H 3.7406480 4.7542930 -3.2927340

80 H 4.4811970 6.2912150 -2.8147900

81 C -4.5269480 -4.7783970 -1.1737770

82 H -3.5928990 -5.1169150 -0.7024910

83 C -5.6944120 -5.4320950 -0.4387510

84 H -6.6495230 -5.0924810 -0.8564110

85 H -5.6567370 -6.5213510 -0.5382530

86 H -5.6928660 -5.2031820 0.6313910

87 C -4.5041030 -5.2167770 -2.6347870

88 H -5.4178720 -4.8947630 -3.1476820

89 H -3.6525990 -4.7816890 -3.1665880

90 H -4.4379640 -6.3060220 -2.7209070

91 Rh -5.9351450 0.0191950 0.3449740

92 C -6.9229340 0.6715320 2.1345180

93 C -7.6195980 1.2206710 0.9936230

94 C -6.9963490 -0.7541330 2.0515520

95 C -8.1095220 0.1267870 0.2224110

96 C -7.7109850 -1.0999890 0.8483950

97 C -7.9208160 2.6573820 0.7275000

98 H -8.9833360 2.8524020 0.9074200

99 H -7.3533370 3.3192810 1.3824270

100 H -7.7031160 2.9298380 -0.3074610

101 C -6.3224880 1.4388210 3.2603170

102 H -5.4872840 0.8979520 3.7076420

103 H -5.9596100 2.4163590 2.9403780

104 H -7.0758370 1.6026770 4.0390630

105 C -6.4808190 -1.6939640 3.0859410

106 H -7.1518140 -1.6826360 3.9517900

107 H -6.4345330 -2.7200090 2.7211290

108 H -5.4855890 -1.4061280 3.4298120

109 C -8.1130770 -2.4624420 0.3978170

110 H -9.1423290 -2.6746600 0.7074080

111 H -8.0647970 -2.5479200 -0.6894050

112 H -7.4757400 -3.2383460 0.8228600

113 C -8.9247310 0.2434450 -1.0139420

114 H -8.7464160 -0.5926740 -1.6897290

115 H -9.9865010 0.2494270 -0.7404920

116 H -8.7023020 1.1653870 -1.5515430

117 H -3.5294730 3.1826070 0.7974040

118 C -4.6450710 3.2758580 -1.0654410

119 H -3.7837370 3.0036390 -1.6876290

120 H -5.5074650 2.7565490 -1.4947550

121 C -4.8632190 4.7875190 -1.1200280

122 H -5.6932770 5.0349550 -0.4409060

123 C -3.6301320 5.5672290 -0.6700310

124 H -3.3583040 5.3545790 0.3677490

125 H -2.7684490 5.3136560 -1.2979860

126 H -3.7990960 6.6455870 -0.7517940

127 C -5.2714390 5.2002760 -2.5309390

128 H -6.1748320 4.6739940 -2.8549240

129 H -5.4642190 6.2762120 -2.5896150

130 H -4.4747280 4.9637030 -3.2453550

131 Cl -5.7653510 -0.0028040 -2.0499840

Compound **19** (calibration set)

Tag Symbol X Y Z

1 C -7.9605590 0.1089280 0.5140860

2 H -8.1551670 -0.0084260 1.5777470

3 C -3.1545650 -0.6763240 -0.0829020

4 C -3.1203700 0.8186510 0.0095650

5 C -4.3805540 2.8417220 0.1965850

6 H -3.4728490 3.2559060 0.6479460

7 C -4.6182950 3.4351510 -1.1884570

8 H -5.4869640 2.9307020 -1.6288650

9 H -3.7580070 3.2021630 -1.8290020

10 C -4.5125770 -2.6408050 -0.2277950

11 H -3.6412690 -3.1137880 -0.6968470

12 C -4.7197390 -3.2049140 1.1747490

13 H -5.5885010 -2.7104330 1.6304520

14 H -3.8483550 -2.9346820 1.7821730

15 C -7.6254000 1.3767020 0.0003460

16 H -7.6569540 2.2409690 0.6567120

17 H -7.7515820 1.5853930 -1.0607010

18 C -7.6646360 -1.0219950 -0.2718610

19 H -7.7925770 -0.9848910 -1.3524560

20 H -7.7244910 -2.0097380 0.1753210

21 N -4.3379340 -1.2005410 -0.1752680

22 N -4.2773770 1.3954590 0.1260850

23 S -1.6870860 -1.5828550 -0.0371090

24 S -1.6130810 1.6567320 -0.0661940

25 Pd -5.9146690 0.1305660 -0.0014250

26 C 3.1563130 0.6734950 -0.0015560

27 C 3.1244430 -0.8216940 0.0897880

28 C 4.3869650 -2.8467820 0.2219360

29 H 3.4972930 -3.2645730 0.7045310

30 C 4.5687190 -3.4249580 -1.1780800

31 H 5.4279570 -2.9253610 -1.6418230

32 H 3.6896040 -3.1716210 -1.7843700

33 C 4.5108140 2.6368040 -0.1956260

34 H 3.6236650 3.1070070 -0.6372430

35 C 4.7664760 3.2114680 1.1944120

36 H 5.6464120 2.7157140 1.6266760

37 H 3.9135880 2.9528360 1.8324070

38 N 4.3364120 1.1973110 -0.1301990

39 N 4.2843120 -1.3994740 0.1671920

40 S 1.6910590 1.5799010 0.0981830

41 S 1.6154970 -1.6593410 0.0701560

42 H 5.2546420 -3.0948570 0.8397330

43 H 5.3597200 2.8290410 -0.8546630

44 C 4.9735840 4.7260970 1.2133750

45 H 4.1043730 5.1906800 0.7265650

46 C 5.0307350 5.2253390 2.6538280

47 H 4.1211990 4.9632070 3.2029190

48 H 5.8817730 4.7800320 3.1826010

49 H 5.1475670 6.3128730 2.6912890

50 C 6.2291580 5.1457350 0.4529740

51 H 6.3722620 6.2293670 0.5053930

52 H 7.1171200 4.6719440 0.8890900

53 H 6.1876920 4.8722190 -0.6050310

54 C 4.7858470 -4.9379700 -1.2035580

55 H 5.6401220 -5.1666060 -0.5493960

56 C 3.5692300 -5.7019600 -0.6870130

57 H 3.3414790 -5.4652350 0.3558850

58 H 2.6831800 -5.4593540 -1.2849630

59 H 3.7317850 -6.7823060 -0.7517470

60 C 5.1398030 -5.3889570 -2.6174450

61 H 5.3311430 -6.4659490 -2.6531900

62 H 4.3156470 -5.1736380 -3.3073710

63 H 6.0309790 -4.8740660 -2.9902210

64 H -5.3831050 -2.8382900 -0.8563010

65 C -4.9158580 -4.7205010 1.2150130

66 H -4.0585650 -5.1842110 0.7067060

67 C -6.1909070 -5.1559710 0.4971900

68 H -7.0685920 -4.6838170 0.9553310

69 H -6.1831630 -4.8924270 -0.5641630

70 H -6.3248910 -6.2399630 0.5643250

71 C -4.9256270 -5.2052820 2.6615230

72 H -4.0016190 -4.9313890 3.1798600

73 H -5.7632020 -4.7602500 3.2115900

74 H -5.0335980 -6.2931380 2.7135480

75 H -5.2243240 3.0817180 0.8498600

76 C -4.8565480 4.9452310 -1.1837390

77 H -5.6919010 5.1513650 -0.4983710

78 C -3.6346020 5.7187430 -0.6947090

79 H -3.3686430 5.4677770 0.3357470

80 H -2.7656620 5.5001620 -1.3260960

81 H -3.8151570 6.7974150 -0.7350670

82 C -5.2632140 5.4129270 -2.5777940

83 H -5.4707570 6.4874430 -2.5898680

84 H -4.4593960 5.2204400 -3.2977870

85 H -6.1589440 4.8910260 -2.9293080

86 Pd 5.9171670 -0.1355080 -0.0136410

87 C 7.6564770 1.0154090 -0.3503270

88 H 7.7371950 2.0008020 0.0987220

89 C 7.9826510 -0.1199130 0.4170470

90 H 8.2218120 -0.0079940 1.4721650

91 C 7.6236770 -1.3846360 -0.0879350

92 H 7.7048120 -1.5885390 -1.1542980

93 H 7.6809060 -2.2520140 0.5625640

94 H 7.7391720 0.9835580 -1.4355070

95 Pt 0.0015580 -0.0002000 0.0165750

Compound **20** (calibration set)

Tag Symbol X Y Z

1 N -4.3365940 -1.2733730 -0.0046820

2 N -4.2958710 1.2828540 0.4715030

3 C -3.1635240 -0.7119940 -0.0423530

4 C -3.1380030 0.7530620 0.2379200

5 S -1.6915870 -1.5690060 -0.3363320

6 S -1.6373690 1.6163500 0.2690880

7 Pt -0.0119950 -0.0041690 -0.0385080

8 S 1.6122360 -1.6296200 -0.3197050

9 S 1.6666590 1.5655240 0.2336490

10 C 3.1184030 -0.7932850 -0.1473760

11 C 3.1430640 0.6728650 0.1213940

12 N 4.2837920 -1.3515360 -0.2332500

13 N 4.3230010 1.2006730 0.2673020

14 C 4.4570560 2.6168230 0.5697350

15 H 3.6146230 2.9416110 1.1934020

16 H 5.3762610 2.7320390 1.1452880

17 C 4.5122770 3.4553770 -0.7028530

18 H 3.6054440 3.2621280 -1.2867580

19 C 4.4148490 -2.7774270 -0.4567510

20 H 3.5985530 -3.1441470 -1.0926710

21 H 5.3549060 -2.9348790 -0.9913590

22 C 4.4238730 -3.5349830 0.8685810

23 H 5.2054990 -3.1143770 1.5111810

24 H 3.4699880 -3.3483200 1.3740160

25 C 4.6397780 -5.0407970 0.7237320

26 H 3.8706290 -5.4324740 0.0425810

27 C 4.4611150 -5.7176270 2.0794790

28 H 5.2044240 -5.3452500 2.7944090

29 H 3.4691740 -5.5182880 2.4963430

30 H 4.5852160 -6.8024420 2.0017080

31 C 6.0119160 -5.3718000 0.1412260

32 H 6.1454460 -4.9717160 -0.8678760

33 H 6.8060280 -4.9542160 0.7713150

34 H 6.1615830 -6.4547300 0.0866790

35 Rh 5.9191460 -0.0370490 0.0332630

36 C -4.4654050 -2.7121970 -0.1714730

37 H -3.5990650 -3.2101830 0.2829440

38 C -4.4193410 2.6655540 0.8845030

39 H -5.2558750 2.7107390 1.5870210

40 C -4.6802940 3.5840950 -0.3066100

41 H -3.8383980 3.4960880 -1.0039540

42 H -5.5720920 3.2225520 -0.8319480

43 C 6.0365430 -0.4480790 1.9697110

44 C 5.2452060 0.0523570 3.0069620

45 C 5.4652370 -0.3303020 4.3268010

46 C 6.4844520 -1.2270850 4.6474030

47 C 7.2790690 -1.7460850 3.6369920

48 C 7.0579370 -1.3637650 2.3094600

49 H 4.4408730 0.7473830 2.7884290

50 H 4.8344390 0.0716490 5.1147930

51 H 6.6520080 -1.5215420 5.6781100

52 H 8.0661620 -2.4507790 3.8883580

53 C 7.8184230 -1.8910090 1.1831450

54 C 8.8558050 -2.8222760 1.2628390

55 C 9.4748190 -3.2679200 0.1093200

56 H 9.1680470 -3.1944870 2.2305090

57 C 8.0235240 -1.8516130 -1.1402610

58 C 9.0493820 -2.7780730 -1.1213660

59 H 10.2796620 -3.9928170 0.1666370

60 H 7.6605640 -1.4322780 -2.0706670

61 H 9.5020320 -3.0991530 -2.0513780

62 N 7.4223240 -1.4192830 -0.0259870

63 C 5.2399630 0.0077200 -3.0195400

64 C 5.3737370 0.3929290 -4.3422350

65 C 6.3728780 1.3072280 -4.6598230

66 C 7.1843010 1.8040960 -3.6540430

67 C 6.9940300 1.3798920 -2.3361900

68 H 4.4770900 -0.6982650 -2.7096820

69 H 4.7094790 -0.0120870 -5.0958110

70 H 6.5136180 1.6359610 -5.6841300

71 H 7.9572260 2.5256180 -3.8868430

72 C 7.7446860 1.8656130 -1.1732290

73 C 8.7609330 2.8221390 -1.2874910

74 C 7.3628370 1.3559120 0.0913620

75 C 9.4121680 3.2908170 -0.1573080

76 H 9.0462020 3.2130740 -2.2593550

77 C 8.0398250 1.8472740 1.2121230

78 C 9.0454340 2.8022650 1.0949420

79 H 10.1964660 4.0348700 -0.2501640

80 H 7.7743740 1.4797410 2.1986530

81 H 9.5476340 3.1683080 1.9862380

82 N 6.0282420 0.4776520 -2.0495750

83 H 5.3611300 3.1218070 -1.3082840

84 C 4.6446390 4.9563090 -0.4487380

85 H 3.7900920 5.2742530 0.1656420

86 C 5.9310900 5.3004220 0.2985600

87 H 6.8057150 4.9267870 -0.2469110

88 H 6.0381260 6.3842110 0.4094250

89 H 5.9587610 4.8635500 1.3004980

90 C 4.5805250 5.7075720 -1.7752110

91 H 3.6527310 5.4889340 -2.3132670

92 H 4.6369450 6.7899230 -1.6219920

93 H 5.4184560 5.4171060 -2.4203810

94 H -5.3619040 -3.0126220 0.3725030

95 C -4.5740400 -3.1074370 -1.6404360

96 H -3.6916470 -2.7312310 -2.1696530

97 H -5.4461200 -2.6110360 -2.0769190

98 C -4.6995220 -4.6136720 -1.8656810

99 H -3.8265320 -5.1006510 -1.4078750

100 C -5.9624900 -5.1858040 -1.2256340

101 H -5.9606620 -5.0810690 -0.1372190

102 H -6.8533250 -4.6706560 -1.6042530

103 H -6.0651090 -6.2516380 -1.4531500

104 C -4.6779010 -4.9110460 -3.3620370

105 H -4.7321190 -5.9872970 -3.5541070

106 H -5.5345320 -4.4393190 -3.8583990

107 H -3.7665250 -4.5279330 -3.8318400

108 H -3.5139240 2.9745970 1.4181490

109 C -4.8775420 5.0595120 0.0585820

110 H -5.0759260 5.5796110 -0.8884500

111 C -6.0899170 5.2742910 0.9619390

112 H -6.9896320 4.8148830 0.5404770

113 H -5.9309550 4.8438830 1.9562860

114 H -6.2869230 6.3421680 1.0984500

115 C -3.6207820 5.6776990 0.6663660

116 H -3.3996440 5.2511680 1.6502600

117 H -2.7469670 5.5134280 0.0281110

118 H -3.7451730 6.7568980 0.7996290

119 Rh -5.9313510 -0.0330230 0.2294630

120 C -5.9989480 -0.2328990 2.1997200

121 C -5.2105430 -1.0572500 3.0066770

122 C -5.3692820 -1.0705530 4.3889940

123 C -6.3189740 -0.2537560 5.0035920

124 C -7.1090600 0.5792610 4.2270980

125 C -6.9525980 0.5922000 2.8362650

126 H -4.4587160 -1.6968360 2.5550530

127 H -4.7445330 -1.7199800 4.9959090

128 H -6.4373020 -0.2667130 6.0820090

129 H -7.8444640 1.2161340 4.7096830

130 C -7.7457690 1.4288800 1.9426960

131 C -8.7596230 2.3080830 2.3301920

132 C -9.4475760 3.0330880 1.3746000

133 H -9.0058720 2.4130340 3.3792990

134 C -8.0997780 1.9952490 -0.2924610

135 C -9.1152590 2.8745770 0.0326790

136 H -10.2370830 3.7153680 1.6707060

137 H -7.8017890 1.8341760 -1.3211620

138 H -9.6280770 3.4183170 -0.7511110

139 N -7.4281960 1.2972350 0.6301560

140 C -5.2491900 0.8459630 -2.6974780

141 C -5.3816930 0.8804690 -4.0749660

142 C -6.4010680 0.1315210 -4.6532390

143 C -7.2287820 -0.6284980 -3.8441360

144 C -7.0359580 -0.6283720 -2.4601930

145 H -4.4714130 1.4062090 -2.1913000

146 H -4.7008660 1.4756160 -4.6711350

147 H -6.5429800 0.1315680 -5.7288520

148 H -8.0135850 -1.2310550 -4.2838360

149 C -7.7900930 -1.4415830 -1.5000930

150 C -8.8238500 -2.2996210 -1.8950320

151 C -7.3854600 -1.3632810 -0.1461810

152 C -9.4691060 -3.0940960 -0.9603570

153 H -9.1278220 -2.3583010 -2.9356560

154 C -8.0566560 -2.1758670 0.7731870

155 C -9.0790350 -3.0325830 0.3761000

156 H -10.2674120 -3.7603050 -1.2706170

157 H -7.7731860 -2.1414450 1.8208200

158 H -9.5770920 -3.6561210 1.1135140

159 N -6.0568210 0.1281760 -1.9136010

Compound **21** (calibration set)

Tag Symbol X Y Z

1 N 4.3454160 1.2283440 -0.5140890

2 N 4.3544390 -1.2394210 0.3875120

3 C 3.1762180 0.7084450 -0.2701410

4 C 3.1806450 -0.7186760 0.1692320

5 S 1.6855720 1.5647080 -0.4093040

6 S 1.6925770 -1.5742380 0.3401240

7 Pt 0.0335400 -0.0061610 -0.0243720

8 S -1.6267960 1.5606700 -0.3910130

9 S -1.6182600 -1.5768350 0.3628650

10 C -3.1139910 0.7026560 -0.2285090

11 C -3.1096690 -0.7239870 0.2129510

12 N -4.2876020 1.2206420 -0.4547770

13 N -4.2794580 -1.2459030 0.4498100

14 C -4.3622950 -2.6481010 0.8234270

15 H -3.5278260 -2.9065860 1.4878150

16 H -5.2835850 -2.7893290 1.3904870

17 C -4.3437820 -3.5562160 -0.4047940

18 H -3.4178700 -3.3691850 -0.9585550

19 C -4.3786930 2.6227920 -0.8266060

20 H -3.5506120 2.8849390 -1.4974960

21 H -5.3051150 2.7610720 -1.3859960

22 C -4.3534950 3.5297570 0.4023450

23 H -5.1708900 3.2438840 1.0772060

24 H -3.4218110 3.3464080 0.9475990

25 C -4.4596830 5.0188260 0.0724170

26 H -3.6647770 5.2610300 -0.6473170

27 C -4.2249660 5.8476510 1.3314980

28 H -4.9917840 5.6300970 2.0843510

29 H -3.2487890 5.6298050 1.7754590

30 H -4.2668580 6.9193780 1.1135580

31 C -5.8029830 5.3766630 -0.5592920

32 H -5.9722660 4.8556280 -1.5058190

33 H -6.6261730 5.1191500 0.1182420

34 H -5.8640730 6.4503220 -0.7619200

35 C 4.4271970 2.6312130 -0.8849620

36 H 5.3466240 2.7812450 -1.4570610

37 C 4.4434210 -2.6438580 0.7526790

38 H 5.3682530 -2.7880810 1.3139700

39 C 4.4273190 -3.5358730 -0.4898790

40 H 3.4832820 -3.3718190 -1.0200750

41 H 5.2254360 -3.2032110 -1.1642080

42 H -5.1685060 -3.2749590 -1.0726410

43 C -4.4400480 -5.0453820 -0.0722710

44 H -3.6370920 -5.2831790 0.6399590

45 C -5.7755000 -5.4085310 0.5728960

46 H -6.6064350 -5.1550730 -0.0966630

47 H -5.8299690 -6.4822820 0.7769200

48 H -5.9376900 -4.8874770 1.5206510

49 C -4.2138130 -5.8745430 -1.3326760

50 H -3.2430300 -5.6526880 -1.7863810

51 H -4.2486120 -6.9462030 -1.1131580

52 H -4.9889330 -5.6613920 -2.0782500

53 H 3.5885970 2.8837870 -1.5435160

54 C 4.4378260 3.5344550 0.3473280

55 H 5.1942050 3.1539950 1.0440080

56 H 3.4731100 3.4550470 0.8621240

57 C 4.7271720 5.0016750 0.0316560

58 H 5.6840590 5.0476180 -0.5095810

59 C 3.6487840 5.6220370 -0.8530770

60 H 3.5765280 5.1291230 -1.8265740

61 H 2.6681360 5.5501750 -0.3686840

62 H 3.8561570 6.6811580 -1.0348210

63 C 4.8796070 5.7927300 1.3270750

64 H 5.1216670 6.8407180 1.1246910

65 H 3.9474530 5.7706000 1.9033000

66 H 5.6722150 5.3775720 1.9577160

67 H 3.6130270 -2.9010740 1.4200140

68 C 4.5898680 -5.0330090 -0.2055820

69 H 4.5318190 -5.5301680 -1.1831230

70 C 5.9527460 -5.3687800 0.3959430

71 H 6.7693340 -4.9860730 -0.2253520

72 H 6.0667340 -4.9455000 1.3996980

73 H 6.0806350 -6.4519460 0.4856650

74 C 3.4565420 -5.5840310 0.6566290

75 H 3.5018210 -5.1907260 1.6777790

76 H 2.4779030 -5.3234090 0.2416460

77 H 3.5163710 -6.6746070 0.7254640

78 C -7.4105330 -1.5244390 0.0963130

79 C -8.5579390 -1.2684440 -0.8599210

80 C -8.5557220 1.2273140 0.8890670

81 C -8.1955880 -0.1888480 -1.8875340

82 C -7.4169030 1.4876410 -0.0762270

83 C -7.2768980 0.8643880 -1.3212060

84 H -9.4553440 -0.9910920 -0.3008560

85 H -7.6774190 -0.6568030 -2.7304310

86 H -8.8002160 2.1554660 1.4132650

87 H -6.9027380 -2.4756100 -0.0417020

88 H -8.8030390 -2.1975150 -1.3822050

89 H -9.4564560 0.9465190 0.3371230

90 H -9.1007260 0.2773330 -2.3024520

91 H -6.9116030 2.4407160 0.0577660

92 H -6.6749360 1.3770510 -2.0721010

93 C -7.2630330 -0.9006540 1.3401700

94 H -6.6532540 -1.4110660 2.0862740

95 C -8.1811390 0.1491440 1.9137710

96 H -9.0811880 -0.3204070 2.3358980

97 H -7.6580460 0.6190730 2.7525220

98 Rh -5.8943850 -0.0155520 0.0040470

99 C 7.3357570 -0.8783120 1.2713540

100 C 8.2478960 0.1764260 1.8452670

101 C 8.2594330 -0.1576130 -1.9570680

102 C 8.6157510 1.2573080 0.8209760

103 C 7.3357630 0.8899020 -1.3881730

104 C 7.4743490 1.5127720 -0.1427720

105 H 9.1508250 -0.2880370 2.2668510

106 H 8.8563790 2.1860720 1.3457890

107 H 7.7422370 -0.6278770 -2.7992840

108 H 6.7296110 -1.3935650 2.0171160

109 H 7.7223230 0.6429240 2.6844060

110 H 9.1610290 0.3140780 -2.3734640

111 H 9.5171520 0.9813920 0.2676860

112 H 6.7296030 1.3998300 -2.1374390

113 H 6.9640920 2.4631680 -0.0067780

114 C 7.4857000 -1.4994940 0.0265700

115 H 6.9828300 -2.4530480 -0.1117550

116 C 8.6300120 -1.2360310 -0.9311750

117 H 9.5268020 -0.9540680 -0.3734540

118 H 8.8795300 -2.1631790 -1.4548120

119 Rh 5.9604900 0.0005090 -0.0617410

Compound **22** (calibration set)

Tag Symbol X Y Z

1 N -4.3544610 1.0934950 -0.0723580

2 N -4.2476640 -1.4489410 -0.0350860

3 C -3.1477960 0.6106350 -0.0518930

4 C -3.0859630 -0.8648100 -0.0458350

5 S -1.7126930 1.5616940 -0.0636540

6 S -1.5782370 -1.6931580 -0.1015640

7 Pt 0.0025930 0.0036330 -0.1563860

8 S 1.5844720 1.7000690 -0.1823080

9 S 1.7182810 -1.5545790 -0.2340590

10 C 3.0905880 0.8694130 -0.1156730

11 C 3.1517170 -0.6054150 -0.1473730

12 N 4.2525050 1.4519860 -0.0818410

13 N 4.3576360 -1.0908180 -0.1456870

14 Cl 5.9968990 0.3327510 -2.2965160

15 C -4.3243860 -2.8874630 -0.1717870

16 H -5.3307480 -3.1646970 -0.4805450

17 C 4.5506220 -2.5176980 -0.2894180

18 H 5.5829360 -2.7140110 -0.5718040

19 H 4.3271230 -3.0344790 0.6520340

20 C 4.3308060 2.8918680 -0.2029540

21 H 4.0566400 3.3773590 0.7419730

22 H 5.3465060 3.1743300 -0.4737540

23 C -7.4149460 1.1054810 0.9830440

24 C -6.5178570 0.6228730 1.9831180

25 C -6.3116500 -0.7588440 2.1906720

26 C -7.0230950 -1.6578420 1.3357860

27 C -7.8710600 -1.1901280 0.3240040

28 C -8.0788450 0.2154720 0.1264560

29 H -7.4985300 2.1732610 0.8246400

30 H -5.9331260 1.3338460 2.5575400

31 H -6.8250580 -2.7220930 1.4098850

32 H -8.3142840 -1.8943230 -0.3709190

33 C -8.9744020 0.6678170 -0.9992270

34 H -8.8073540 -0.0390840 -1.8195410

35 C -10.4334120 0.5551730 -0.5465430

36 H -11.1030800 0.8027620 -1.3747720

37 H -10.6742220 -0.4562320 -0.2066540

38 H -10.6392920 1.2480830 0.2758890

39 C -8.6528810 2.0616300 -1.5187760

40 H -8.8651130 2.8352640 -0.7733540

41 H -7.6043460 2.1290450 -1.8196730

42 H -9.2698140 2.2785490 -2.3945940

43 Ru 5.9056480 0.2414440 0.1059300

44 C -5.3535220 -1.2634740 3.2223200

45 H -4.5820570 -0.5216130 3.4361530

46 H -5.8861840 -1.4818890 4.1536520

47 H -4.8662900 -2.1820550 2.8898690

48 Ru -5.9069480 -0.2425570 0.1172070

49 C 7.3791410 -1.1165280 1.0151570

50 C 6.4519670 -0.6347480 1.9875870

51 C 6.2451240 0.7469120 2.1936800

52 C 6.9886290 1.6465630 1.3671150

53 C 7.8659940 1.1793170 0.3806810

54 C 8.0737990 -0.2264480 0.1836720

55 H 7.4647650 -2.1840820 0.8563110

56 H 5.8460960 -1.3455390 2.5397070

57 H 6.7939560 2.7114600 1.4408000

58 H 8.3344320 1.8845030 -0.2965170

59 C 9.0043260 -0.6795420 -0.9128420

60 H 8.8782830 0.0384840 -1.7308040

61 C 10.4464480 -0.5933370 -0.4036350

62 H 11.1440920 -0.8420060 -1.2081140

63 H 10.6884640 0.4105870 -0.0430000

64 H 10.6100380 -1.2980930 0.4183150

65 C 8.6826120 -2.0629660 -1.4596610

66 H 8.8558490 -2.8476330 -0.7157280

67 H 7.6451550 -2.1115390 -1.7999750

68 H 9.3288990 -2.2796430 -2.3141150

69 C 5.2554900 1.2514180 3.1952400

70 H 4.4703940 0.5148890 3.3754290

71 H 5.7568580 1.4572440 4.1465970

72 H 4.7884830 2.1771560 2.8538610

73 H -4.0862310 -3.3816670 0.7782970

74 C -4.5566550 2.5211130 -0.1880660

75 H -4.4519350 3.0061180 0.7900970

76 H -5.5566520 2.7093550 -0.5752320

77 Cl -5.9227630 -0.3110470 -2.2874270

78 H 3.6425270 3.2503470 -0.9754460

79 H 3.8860820 -2.9204890 -1.0607340

80 H -3.6093890 -3.2409050 -0.9219690

81 H -3.8192540 2.9629390 -0.8656130

Compound **23** (calibration set)

Tag Symbol X Y Z

1 Pd 5.9480540 -0.0220180 -0.0076350

2 S 1.6588570 1.6118840 -0.0034700

3 S 1.6519170 -1.6182660 -0.0503570

4 N 4.3228500 1.2925570 -0.1499860

5 N 4.3104460 -1.3112230 0.1645820

6 C 3.1510020 0.7421440 -0.0586130

7 C 3.1448650 -0.7544280 0.0392450

8 C 4.4396670 2.7468320 -0.2403640

9 H 3.4536350 3.1506960 -0.5070710

10 C 4.8117560 3.2937550 1.1319610

11 H 4.0912880 2.9360490 1.8710500

12 H 4.7848300 4.3855500 1.1414720

13 H 5.8110600 2.9609590 1.4254570

14 C 5.3827670 3.1238980 -1.3638820

15 C 6.2440360 4.2164550 -1.2724140

16 H 6.2750090 4.8144060 -0.3685550

17 C 7.0904520 4.5456610 -2.3280090

18 H 7.7589890 5.3956040 -2.2336520

19 C 7.0869300 3.7872800 -3.4926740

20 H 7.7509720 4.0402200 -4.3128900

21 C 6.2205890 2.7025530 -3.5988480

22 H 6.2037580 2.1056580 -4.5053550

23 C 5.3752420 2.3784860 -2.5456190

24 H 4.7097600 1.5253860 -2.6316250

25 C 4.4166520 -2.7634030 0.2944080

26 H 3.4309250 -3.1481570 0.5903880

27 C 4.7593710 -3.3596850 -1.0641460

28 H 4.0165970 -3.0378100 -1.7975530

29 H 4.7439090 -4.4513490 -1.0293100

30 H 5.7461460 -3.0280920 -1.3988900

31 C 5.3732400 -3.1048190 1.4177410

32 C 5.3158900 -2.3674490 2.6037830

33 H 4.6045520 -1.5516210 2.6878610

34 C 6.1660500 -2.6536480 3.6634980

35 C 7.0889690 -3.6911520 3.5583670

36 H 7.7572420 -3.9150060 4.3836190

37 C 7.1437950 -4.4401730 2.3891410

38 H 7.8575490 -5.2527240 2.2964000

39 C 6.2907570 -4.1495360 1.3276070

40 H 6.3600400 -4.7396810 0.4205400

41 C 7.7008190 1.1774920 0.0194790

42 H 7.7496140 2.0583530 -0.6104630

43 H 7.8241620 1.3462970 1.0882270

44 C 7.9999950 -0.0824530 -0.5260950

45 H 8.1891250 -0.1770040 -1.5929960

46 C 7.6789390 -1.2204970 0.2355010

47 H 7.7964560 -1.2149010 1.3175580

48 H 7.7170320 -2.2004220 -0.2267770

49 S -1.6588600 -1.6119000 -0.0033350

50 C -3.1510050 -0.7421420 -0.0586050

51 N -4.3228480 -1.2925540 -0.1500730

52 Pd -5.9480630 0.0220050 -0.0077830

53 N -4.3104760 1.3112140 0.1645400

54 C -3.1448800 0.7544330 0.0392710

55 S -1.6519290 1.6183010 -0.0502140

56 C -4.4167000 2.7633920 0.2943710

57 H -3.4309840 3.1481550 0.5903740

58 C -4.7593980 3.3596750 -1.0641890

59 H -4.0166060 3.0378100 -1.7975810

60 H -4.7439490 4.4513380 -1.0293490

61 H -5.7461630 3.0280720 -1.3989520

62 C -5.3733030 3.1048050 1.4176930

63 C -5.3159570 2.3674410 2.6037390

64 H -4.6046160 1.5516160 2.6878250

65 C -6.1661250 2.6536410 3.6634460

66 H -6.1092600 2.0652470 4.5738540

67 C -7.0890460 3.6911420 3.5583050

68 H -7.7573260 3.9149970 4.3835510

69 C -7.1438650 4.4401600 2.3890770

70 H -7.8576190 5.2527090 2.2963280

71 C -6.2908180 4.1495220 1.3275490

72 H -6.3600950 4.7396650 0.4204810

73 C -7.7008220 -1.1775130 0.0192080

74 H -7.7495790 -2.0583630 -0.6107510

75 H -7.8242310 -1.3463350 1.0879460

76 C -7.9999700 0.0824380 -0.5263690

77 C -7.6789670 1.2204740 0.2352610

78 H -8.1890350 0.1770010 -1.5932810

79 H -7.7965520 1.2148630 1.3173110

80 H -7.7170370 2.2004030 -0.2270080

81 C -4.4396530 -2.7468270 -0.2404830

82 H -3.4536050 -3.1506760 -0.5071560

83 C -4.8118020 -3.2937830 1.1318120

84 H -4.0913730 -2.9360880 1.8709440

85 H -4.7848680 -4.3855780 1.1412990

86 H -5.8111230 -2.9610010 1.4252680

87 C -5.3826910 -3.1238810 -1.3640570

88 C -6.2439620 -4.2164400 -1.2726530

89 H -6.2749860 -4.8144050 -0.3688050

90 C -7.0903180 -4.5456320 -2.3283010

91 H -7.7588580 -5.3955770 -2.2339950

92 C -7.0867320 -3.7872320 -3.4929550

93 H -7.7507270 -4.0401610 -4.3132110

94 C -6.2203860 -2.7025030 -3.5990640

95 H -6.2035030 -2.1055950 -4.5055610

96 C -5.3750980 -2.3784520 -2.5457820

97 H -4.7096100 -1.5253510 -2.6317380

98 H 6.1091810 -2.0652490 4.5739020

99 Pd -0.0000220 0.0000050 -0.0260730

Compound **24** (calibration set)

Tag Symbol X Y Z

1 C -6.0839760 -0.7876580 -0.2936270

2 C -5.8619090 -1.5456640 -1.4751170

3 C -4.5054770 -1.9581710 -1.4902110

4 C -3.8726330 -1.4401700 -0.3134930

5 C -4.8648630 -0.7162770 0.4278120

6 H -7.0089890 -0.3056820 -0.0108140

7 H -6.5888440 -1.7450700 -2.2493780

8 H -4.0192350 -2.5318330 -2.2653780

9 H -4.7054960 -0.1920580 1.3582640

10 Fe -4.5981280 0.0801200 -1.4183620

11 C -4.3222790 0.9475840 -3.2683990

12 C -5.2978020 1.6689630 -2.5277280

13 C -3.1203850 0.9297230 -2.5171970

14 H -4.4800920 0.4568000 -4.2180250

15 C -4.7079910 2.1052110 -1.3133500

16 H -6.3291500 1.8189970 -2.8137510

17 C -3.3524680 1.6415660 -1.2933150

18 H -2.1950450 0.4396330 -2.7848180

19 H -5.2155750 2.6361580 -0.5226040

20 P -2.1256990 -1.6574950 0.1165610

21 P -2.1079080 1.7819570 -0.0003100

22 C -1.3922880 3.4390970 -0.2660750

23 C -0.8456600 4.1440150 0.8086440

24 C -1.3195930 3.9714290 -1.5538840

25 C -0.2424650 5.3766280 0.5951540

26 H -0.8925150 3.7328120 1.8120200

27 C -0.7128810 5.2045540 -1.7618380

28 H -1.7400340 3.4285520 -2.3941530

29 C -0.1747680 5.9077610 -0.6892100

30 H 0.1756420 5.9229720 1.4340130

31 H -0.6640870 5.6170380 -2.7641070

32 H 0.2955550 6.8716630 -0.8536410

33 C -2.9631440 1.9501220 1.5966940

34 C -2.7098170 1.0379500 2.6199570

35 C -3.8586040 3.0020780 1.8151560

36 C -3.3788480 1.1437460 3.8346790

37 H -1.9886060 0.2437140 2.4696880

38 C -4.5273490 3.1030140 3.0272390

39 H -4.0181280 3.7538240 1.0492490

40 C -4.2952660 2.1690610 4.0348130

41 H -3.1781770 0.4235900 4.6209930

42 H -5.2251600 3.9175410 3.1900640

43 H -4.8201240 2.2521100 4.9807930

44 C -1.6536310 -3.0343980 -0.9883370

45 C -1.2390220 -2.7299370 -2.2872240

46 C -1.7418250 -4.3651090 -0.5825580

47 C -0.9353500 -3.7502510 -3.1784380

48 H -1.1367830 -1.6938390 -2.5940630

49 C -1.4244380 -5.3833240 -1.4752240

50 H -2.0494980 -4.6107980 0.4280990

51 C -1.0273110 -5.0783800 -2.7725240

52 H -0.6146910 -3.5081360 -4.1861060

53 H -1.4865350 -6.4174280 -1.1530400

54 H -0.7812720 -5.8756190 -3.4661900

55 C -2.1877420 -2.3648960 1.7989880

56 C -3.3360000 -3.0192230 2.2534790

57 C -1.0738880 -2.2662850 2.6372080

58 C -3.3681260 -3.5640300 3.5317560

59 H -4.2082330 -3.1003190 1.6140870

60 C -1.1122840 -2.8124610 3.9139950

61 H -0.1771340 -1.7617820 2.2945540

62 C -2.2587760 -3.4594150 4.3639810

63 H -4.2642090 -4.0687650 3.8770050

64 H -0.2444400 -2.7278380 4.5595460

65 H -2.2881940 -3.8805980 5.3635060

66 Pt -0.5846100 0.0607550 -0.0885890

67 S 1.1306140 1.6438090 -0.2916150

68 S 1.0851400 -1.6029420 -0.1835210

69 C 2.5995960 0.7438570 -0.1668710

70 C 2.5798690 -0.7431390 -0.1005390

71 N 3.7321890 -1.3333080 -0.0126770

72 N 3.7685530 1.3068220 -0.1338140

73 C 3.7520180 -2.7813560 0.0567720

74 H 3.1269150 -3.1377710 0.8833960

75 H 3.3594910 -3.2184760 -0.8688250

76 H 4.7696020 -3.1355660 0.2070320

77 C 3.8281970 2.7530730 -0.2217200

78 H 3.3693820 3.1035080 -1.1534160

79 H 3.2823850 3.2134710 0.6100400

80 H 4.8625850 3.0887270 -0.1942710

81 C 6.8323570 -1.4136090 0.6899490

82 C 7.9578360 -0.7473610 1.4555110

83 C 8.0808690 0.6221420 -1.2639270

84 C 7.6059520 0.6991580 1.8261890

85 C 6.9138040 1.3142090 -0.5883450

86 C 6.7272360 1.3643910 0.7971570

87 H 8.8778180 -0.7873500 0.8671600

88 H 7.0613030 0.7042650 2.7753040

89 H 8.3631710 1.1857750 -2.1571510

90 H 6.2753790 -2.1627550 1.2504760

91 H 8.1570410 -1.3166470 2.3673300

92 H 8.9533610 0.6419160 -0.6058840

93 H 8.5165980 1.2919520 1.9910280

94 H 6.4189170 2.0755770 -1.1892890

95 H 6.1159570 2.1738810 1.1952500

96 C 6.7550470 -1.4619370 -0.7059920

97 H 6.1599510 -2.2596310 -1.1499490

98 C 7.7264940 -0.8167500 -1.6621740

99 H 8.6337400 -1.4298600 -1.7564410

100 H 7.2572780 -0.8099560 -2.6507100

101 Rh 5.3654080 -0.0326960 -0.0109460

Compound **25** (calibration set)

Tag Symbol X Y Z

1 C -5.5589350 -0.7701480 -0.1884220

2 C -5.3743810 -1.5295520 -1.3754590

3 C -4.0211480 -1.9493240 -1.4287180

4 C -3.3524990 -1.4345420 -0.2705410

5 C -4.3194910 -0.7050970 0.4981880

6 H -6.4730330 -0.2832820 0.1203000

7 H -6.1239770 -1.7252530 -2.1287700

8 H -3.5597240 -2.5256040 -2.2170180

9 H -4.1308710 -0.1813870 1.4234560

10 Fe -4.1003940 0.0892640 -1.3545650

11 C -3.8629070 0.9539390 -3.2111020

12 C -4.8190440 1.6794350 -2.4495060

13 C -2.6445690 0.9324690 -2.4868790

14 H -4.0434800 0.4630070 -4.1565920

15 C -4.2006010 2.1145840 -1.2490270

16 H -5.8560490 1.8328910 -2.7123660

17 C -2.8468010 1.6456540 -1.2584980

18 H -1.7267800 0.4397150 -2.7751800

19 H -4.6884480 2.6481120 -0.4477540

20 P -1.5935730 -1.6553790 0.1049360

21 P -1.5710450 1.7846350 0.0043930

22 C -0.8636810 3.4417510 -0.2837100

23 C -0.3078530 4.1609740 0.7765260

24 C -0.8096620 3.9610250 -1.5779670

25 C 0.2852100 5.3949360 0.5425550

26 H -0.3399670 3.7602390 1.7846160

27 C -0.2127020 5.1951050 -1.8064770

28 H -1.2376340 3.4073290 -2.4073140

29 C 0.3340380 5.9129210 -0.7479130

30 H 0.7102170 5.9525560 1.3704590

31 H -0.1786010 5.5970940 -2.8136170

32 H 0.7964840 6.8778070 -0.9282170

33 C -2.3832220 1.9498930 1.6235010

34 C -2.0913710 1.0386980 2.6375020

35 C -3.2813400 2.9934380 1.8692930

36 C -2.7257740 1.1366040 3.8713200

37 H -1.3668630 0.2520110 2.4632240

38 C -3.9153840 3.0864430 3.1005100

39 H -3.4701940 3.7447470 1.1096850

40 C -3.6455810 2.1530920 4.0992990

41 H -2.4960420 0.4170900 4.6502470

42 H -4.6156800 3.8941570 3.2850850

43 H -4.1437950 2.2299200 5.0600970

44 C -1.1633970 -3.0376260 -1.0094550

45 C -0.7750170 -2.7391040 -2.3175080

46 C -1.2635880 -4.3669860 -0.6014700

47 C -0.5086410 -3.7640330 -3.2156840

48 H -0.6631280 -1.7042330 -2.6253160

49 C -0.9839090 -5.3897200 -1.5011990

50 H -1.5511540 -4.6075490 0.4163650

51 C -0.6126510 -5.0904720 -2.8076840

52 H -0.2077700 -3.5268240 -4.2305790

53 H -1.0549470 -6.4228620 -1.1777410

54 H -0.3957760 -5.8913450 -3.5068790

55 C -1.6029990 -2.3569670 1.7917000

56 C -2.7437630 -2.9863430 2.2971450

57 C -0.4543370 -2.2743640 2.5836680

58 C -2.7346710 -3.5205910 3.5804350

59 H -3.6422660 -3.0560820 1.6939600

60 C -0.4514930 -2.8100220 3.8653650

61 H 0.4373380 -1.7910010 2.1996070

62 C -1.5912700 -3.4305820 4.3668790

63 H -3.6255030 -4.0054980 3.9654540

64 H 0.4432660 -2.7377040 4.4746840

65 H -1.5885550 -3.8429790 5.3705000

66 Pt -0.0552850 0.0593850 -0.1284990

67 S 1.6630400 1.6451350 -0.3110870

68 S 1.6038440 -1.6067950 -0.3271690

69 C 3.1253460 0.7350530 -0.1664880

70 C 3.0968380 -0.7566570 -0.1377380

71 N 4.2389450 -1.3479130 -0.0008190

72 N 4.2932540 1.2853720 -0.0808990

73 C 4.2933960 -2.7957640 0.0388780

74 H 3.5604250 -3.1942170 0.7499100

75 H 4.0606100 -3.2151280 -0.9471980

76 H 5.2925370 -3.1121460 0.3296440

77 C 4.3989550 2.7312760 -0.0925350

78 H 4.0894080 3.1327280 -1.0649400

79 H 3.7471010 3.1738490 0.6699160

80 H 5.4294670 3.0205440 0.0993590

81 Pd 5.8845320 -0.0621190 0.0290780

82 C 7.5741760 -1.2940760 0.3091770

83 C 7.9615130 -0.1186180 -0.3616080

84 H 7.6309940 -2.2445280 -0.2125140

85 C 7.6250020 1.1132970 0.2309910

86 H 8.2269900 -0.1582900 -1.4153580

87 H 7.7217620 2.0241080 -0.3520820

88 H 7.6829640 1.2342890 1.3114440

89 H 7.6276540 -1.3462370 1.3955690

[1] A. Giannetto, F. Puntoriero, A. Barattucci, S. Lanza, S. Campagna, *Inorganic chemistry* **2009**, *48*, 10397-10404.