

Supplementary Information for

Synthesis of Novel 3-Hydroxy-2-naphthoic hydrazones as Selective Chemosensors for Cyanide Ion

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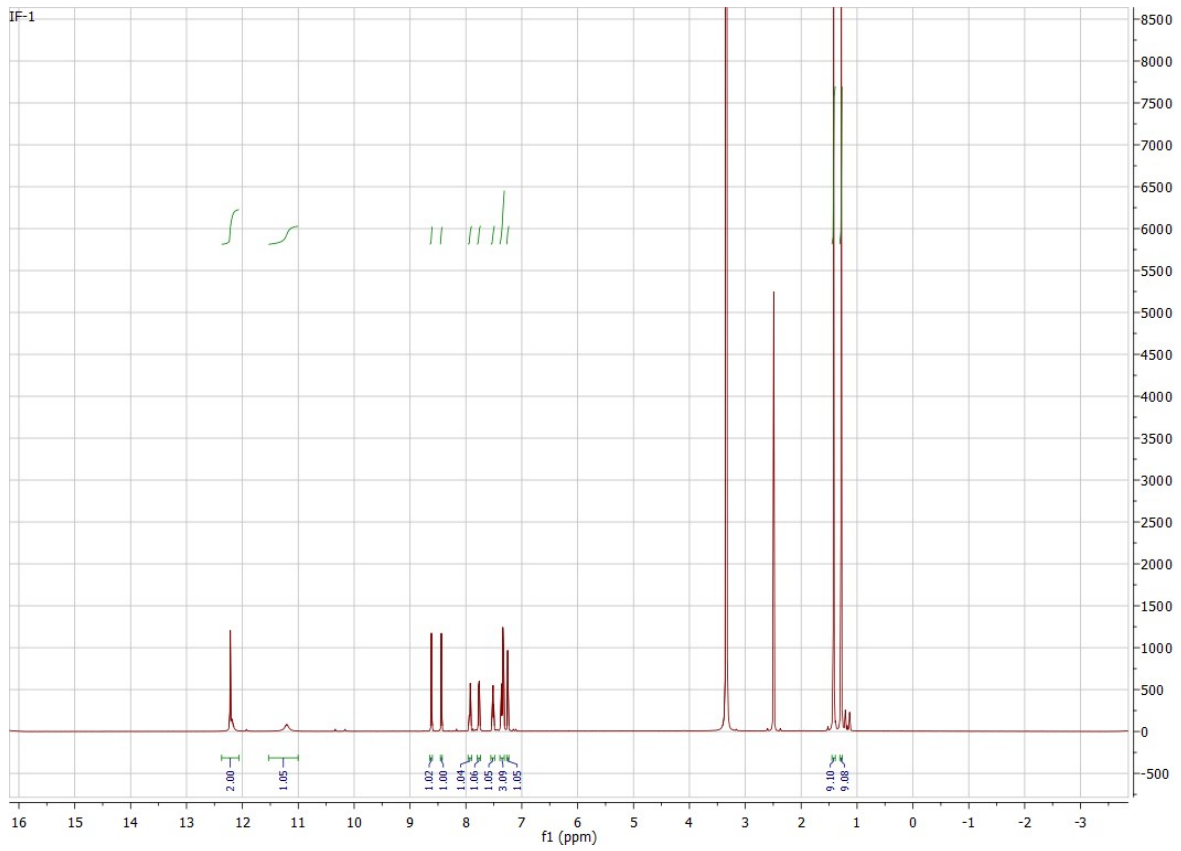
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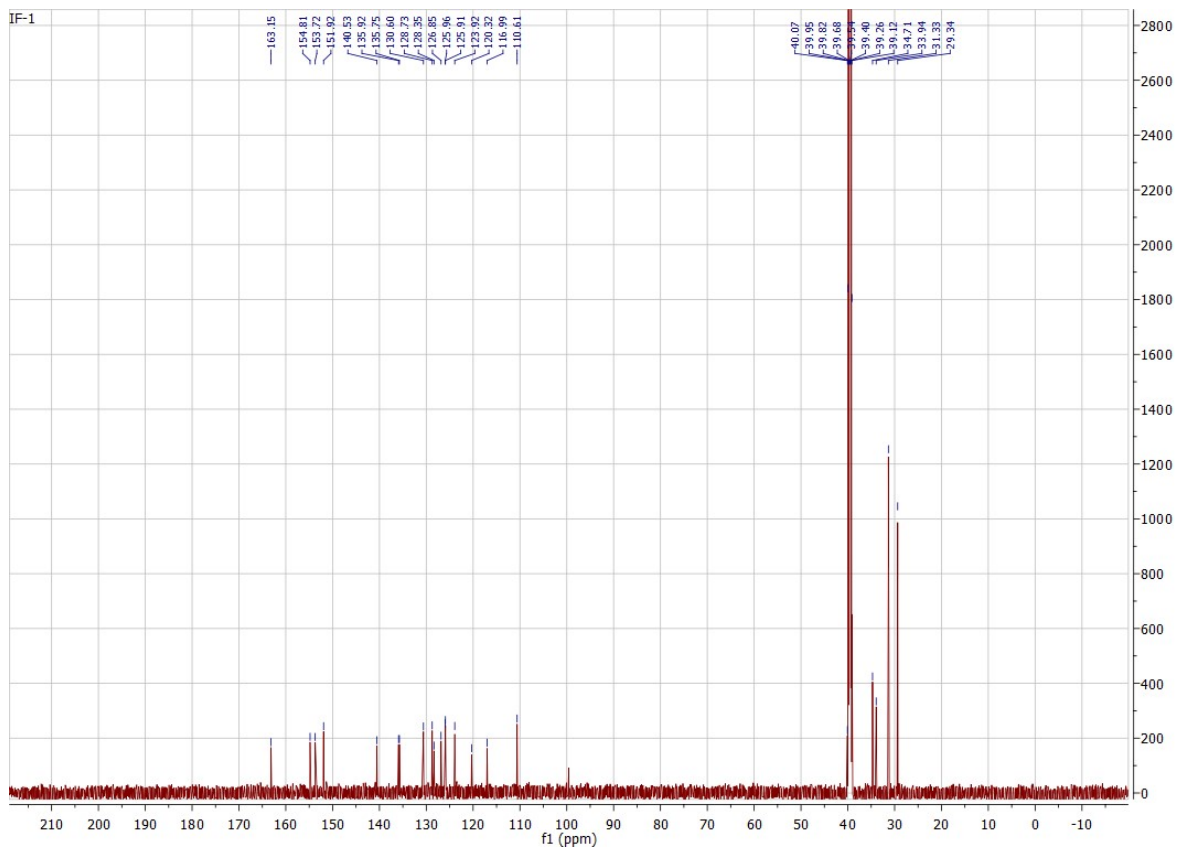
^e Department of Chemistry, Division of Science and Technology, University of Education Lahore, Pakistan

Content

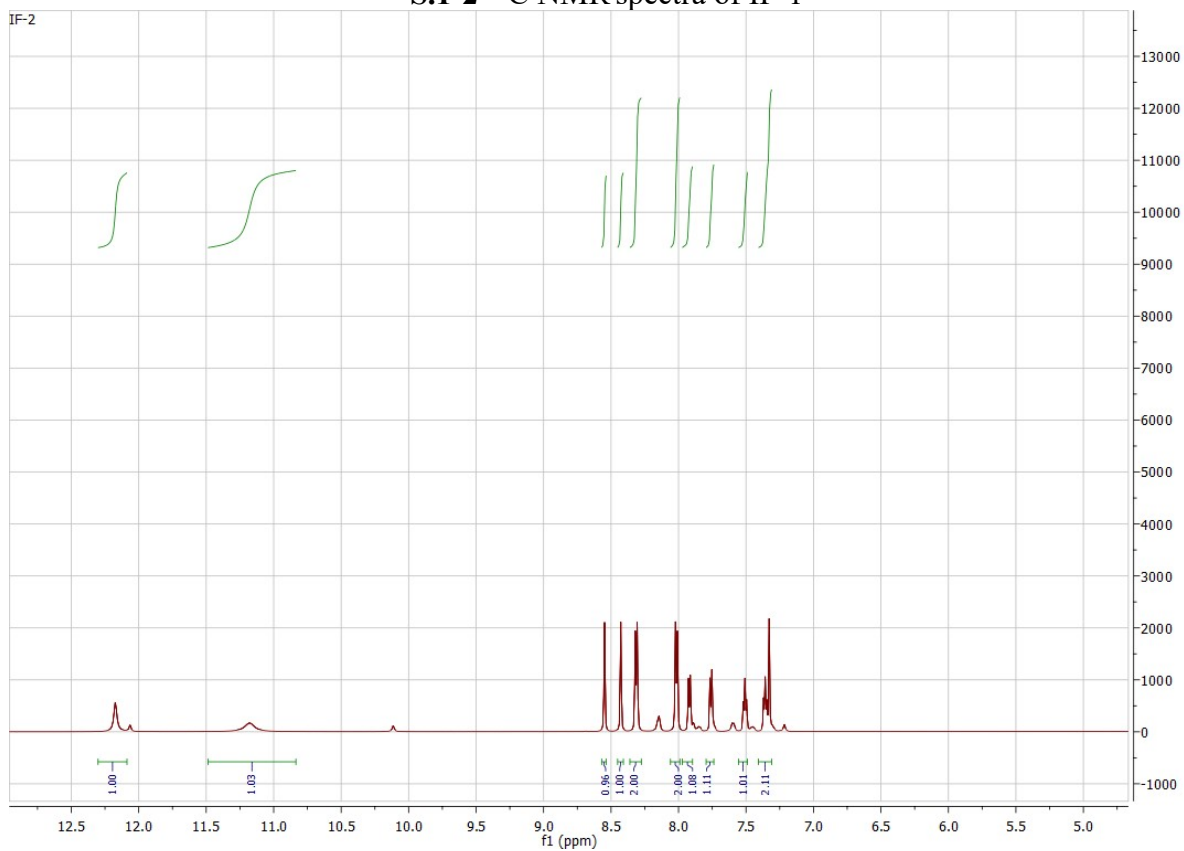
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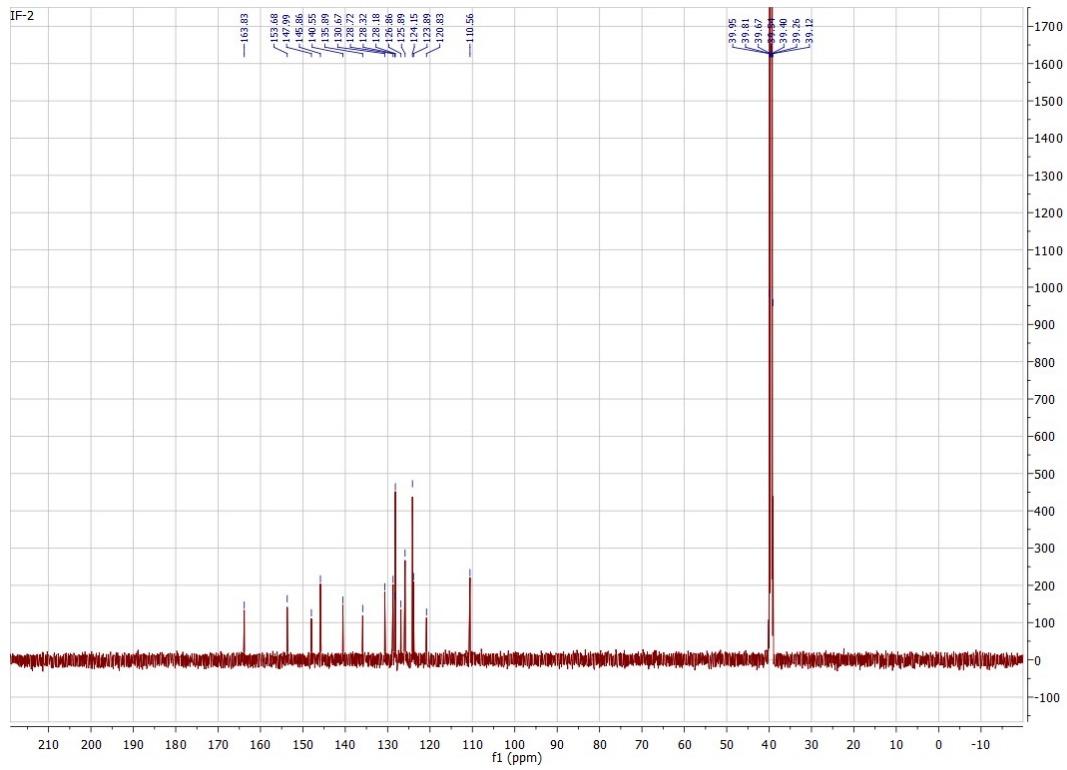
S.I-1 ¹H NMR spectra of IF-1



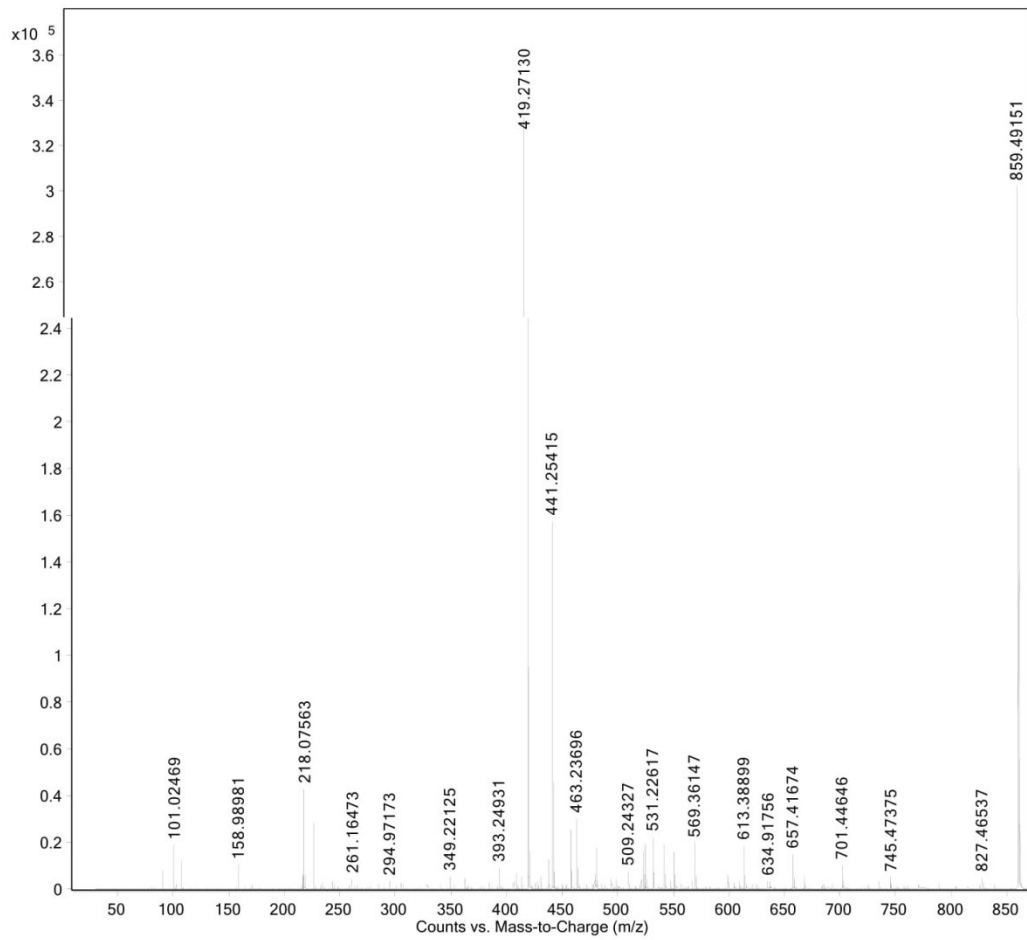
S.I-2 ^{13}C NMR spectra of IF-1



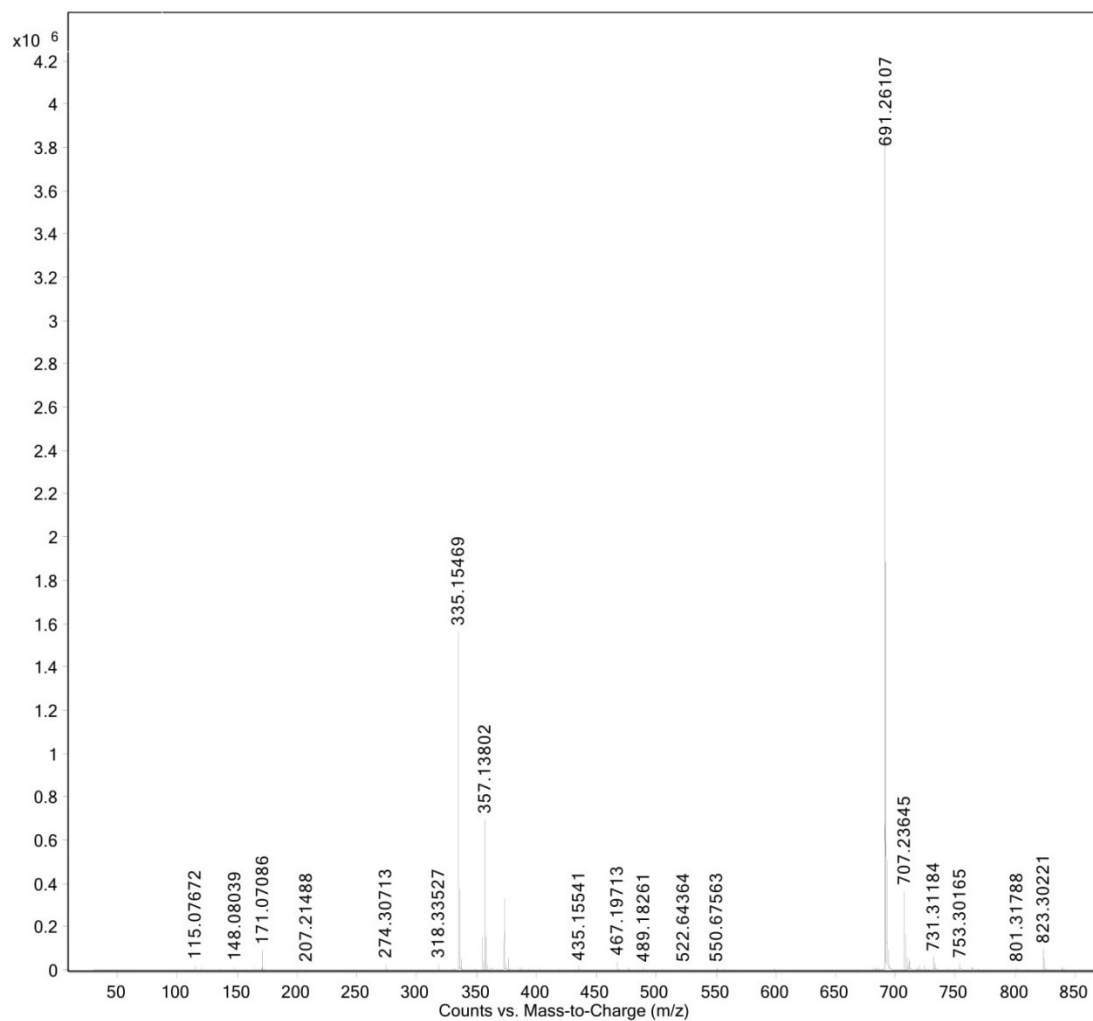
S.I-3 ^1H NMR spectra of IF-2



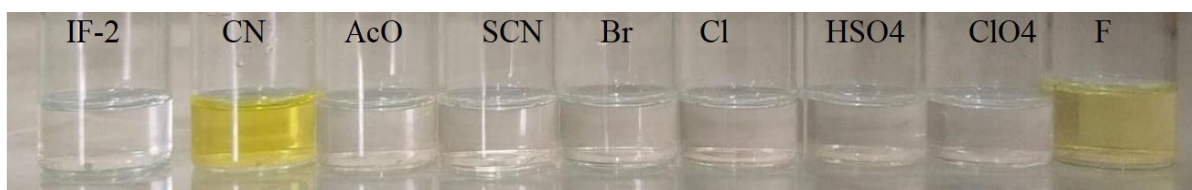
S.1-4 ¹³C NMR spectra of IF-2



S.I-5 HRMS of IF-1

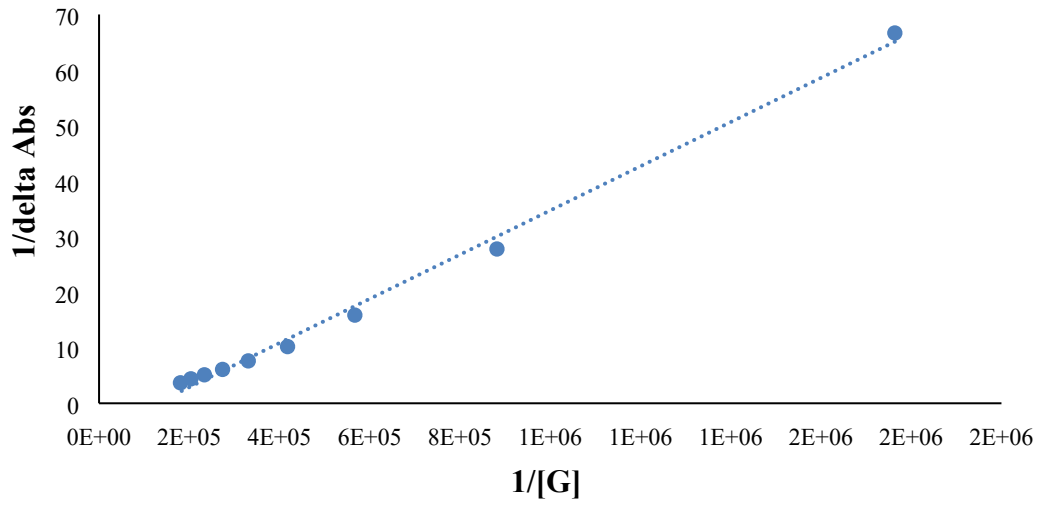


S.I-6 HRMS of IF-2

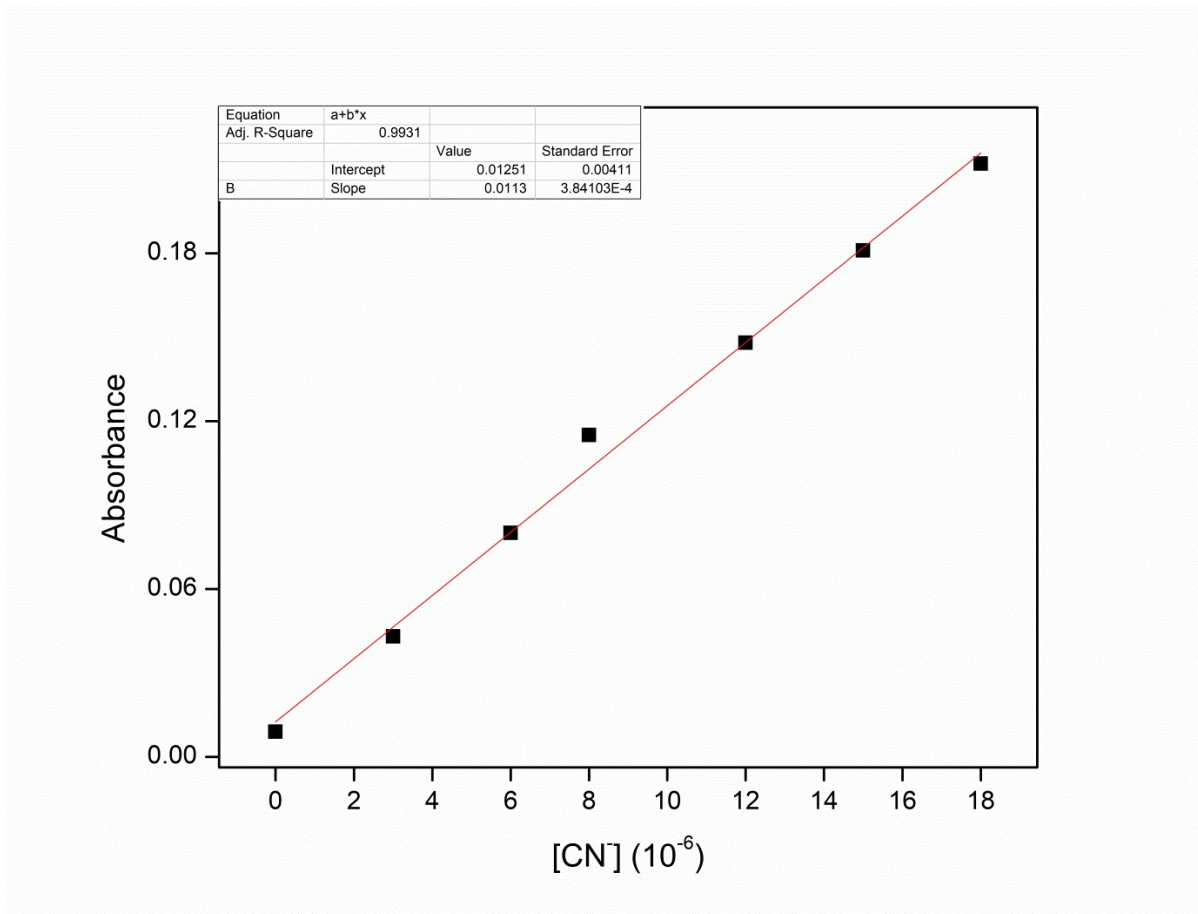


S.I.7 Color change of IF-2

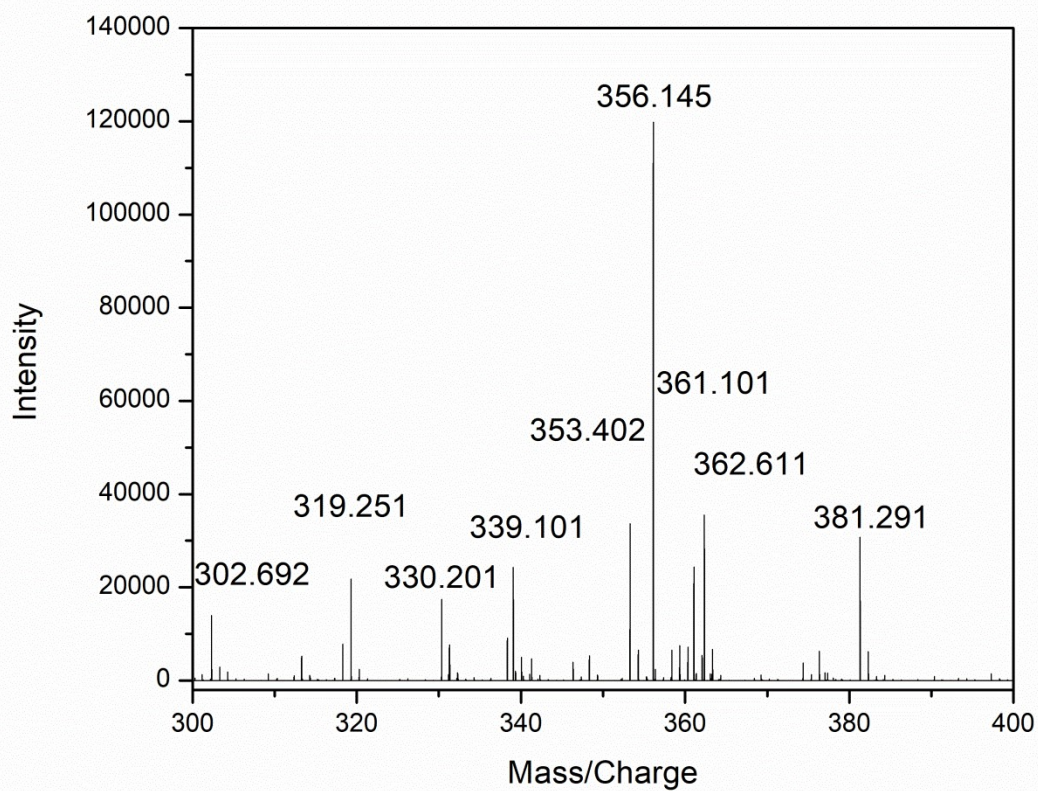
BH Plot of IF-2 (CN)



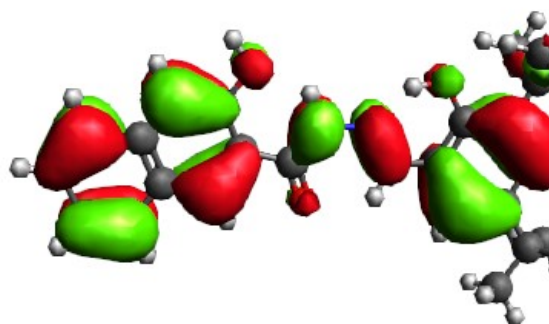
S.I-8 BH plot of chemosensor IF-2



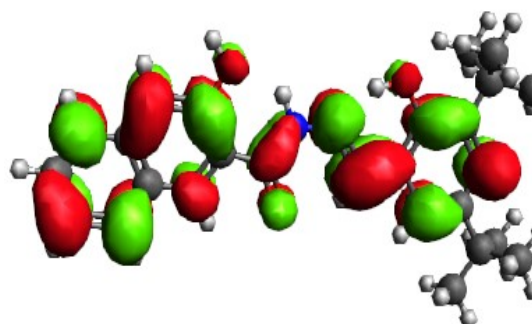
S.I-9 Linear plot of chemosensor IF-2



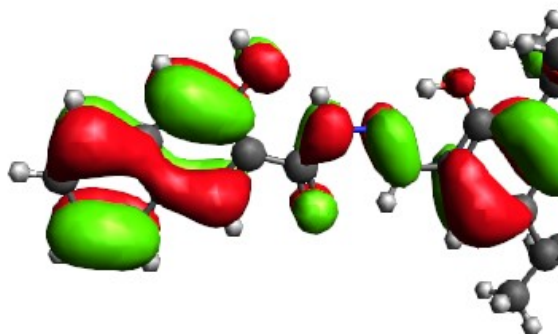
S.I-10 HRMS Spectra of IF-2 after the addition of CN⁻ ions



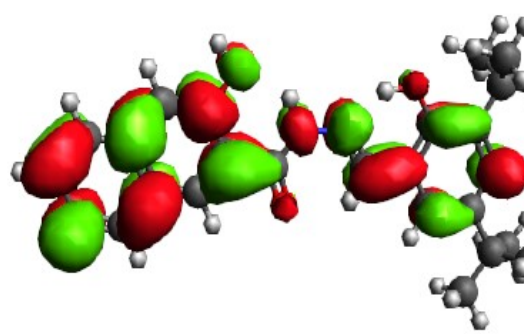
HOMO -1



LUMO +1



HOMO -2



LUMO +2

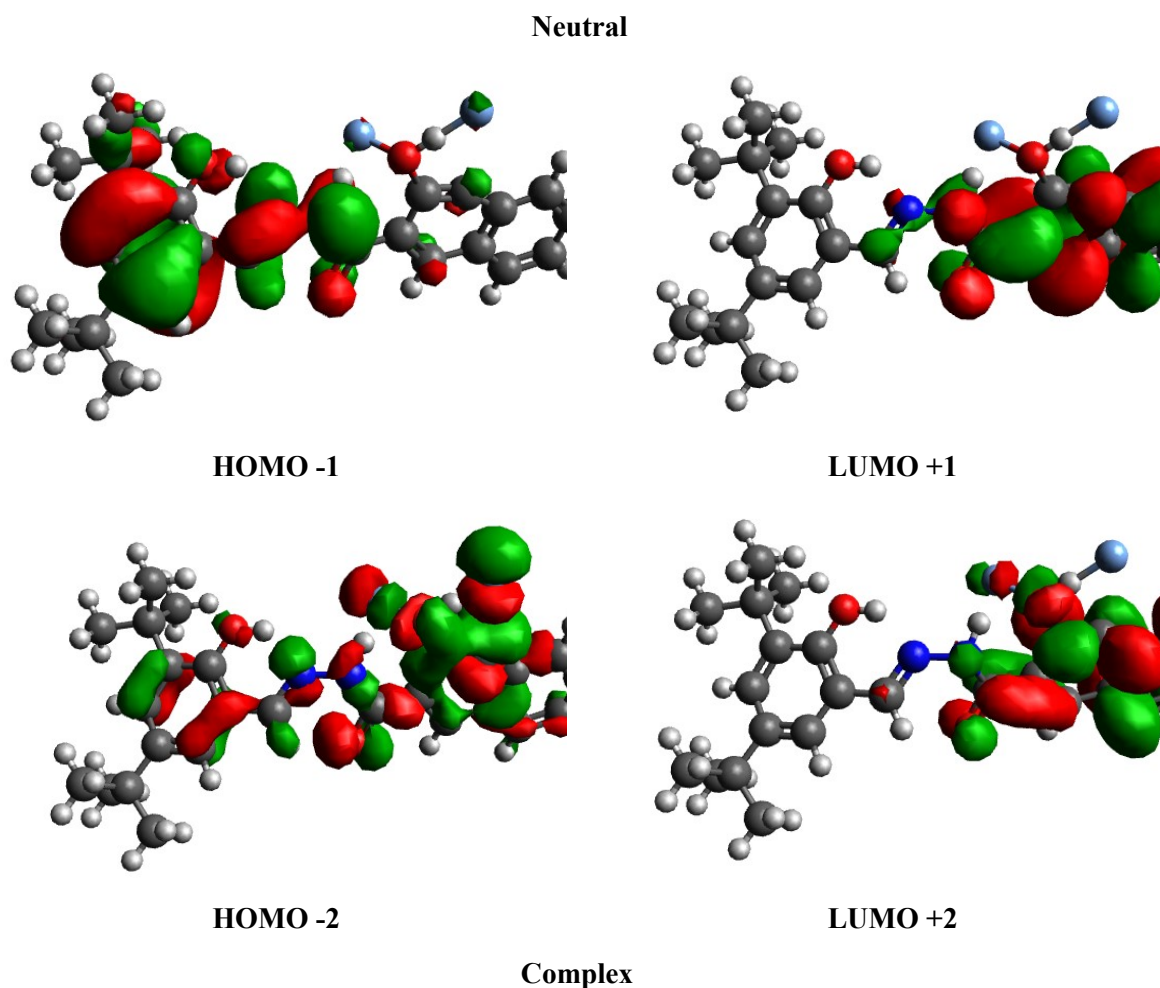


Fig-S1-11: The HOMO-LUMO structures of IF-1 and it's Complex

Table S1: Calculated E_{HOMO} , E_{LUMO} and band gap of IF-1 and its **Complex**

| MOs | IF-1 | | Complex | |
|--------|---------|----------------|---------|----------------|
| | $E(eV)$ | $\Delta E(eV)$ | $E(eV)$ | $\Delta E(eV)$ |
| HOMO | -5.717 | 4.1 | -5.827 | 0.776 |
| HOMO | -5.717 | 4.1 | -5.827 | 0.776 |
| LUMO+1 | -0.855 | 5.479 | -2.921 | 3.514 |
| HOMO-1 | -6.334 | | -6.435 | |
| LUMO+2 | -0.419 | 5.969 | -1.867 | 4.944 |
| HOMO-2 | -6.388 | | -6.811 | |

Table S2: Global reactivity descriptors of IF-1 and its complex; unit in eV

| GRPs | IF-1 | Complex |
|----------|--------|---------|
| IP | 5.717 | 5.827 |
| EA | 1.617 | 5.051 |
| X | 3.667 | 5.439 |
| η | 2.05 | 0.388 |
| μ | -3.667 | -5.439 |
| ω | 3.279 | 38.122 |
| σ | 0.243 | 1.289 |

Table S3. AIM properties of the main intra- and intermolecular interactions for **test**. Electronic density (ρ), Laplacian of density ($\nabla^2\rho$), ellipticity (ϵ) and density of potential energy (V).

| BCP | Bond | ρ (e/a ³) | $\nabla^2\rho$ (e/a ⁵) | ϵ | V (hartree.e/a ³) |
|-----|-----------|----------------------------|------------------------------------|------------|------------------------------------|
| 1 | C15 - C17 | +0.260591 | -0.633727 | +0.109318 | -0.279848 |
| 2 | C1 - C2 | +0.298101 | -0.783177 | +0.145642 | -0.370323 |
| 3 | C3 - C4 | +0.322605 | -0.884760 | +0.247868 | -0.446372 |
| 4 | C2 - C3 | +0.300853 | -0.797958 | +0.151006 | -0.378164 |
| 5 | C4 - C5 | +0.300411 | -0.793371 | +0.153115 | -0.379662 |
| 6 | C1 - C11 | +0.304448 | -0.816547 | +0.143797 | -0.386473 |
| 7 | C5 - C6 | +0.323276 | -0.888397 | +0.247176 | -0.448326 |
| 8 | C1 - C6 | +0.300200 | -0.795053 | +0.149703 | -0.375710 |
| 9 | C2 - C13 | +0.300761 | -0.793071 | +0.167232 | -0.380027 |
| 10 | C3 - H7 | +0.278226 | -0.947581 | +0.016918 | -0.325957 |
| 11 | C4 - H8 | +0.280494 | -0.967125 | +0.008441 | -0.328379 |
| 12 | C11 - C15 | +0.319176 | -0.863023 | +0.230587 | -0.436137 |
| 13 | C5 - H9 | +0.280229 | -0.963506 | +0.014491 | -0.328763 |
| 14 | C17 - O18 | +0.400304 | +0.010220 | +0.084542 | -1.365782 |
| 15 | C6 - H10 | +0.279350 | -0.960453 | +0.010612 | -0.326233 |
| 16 | C17 - N19 | +0.315764 | -0.973627 | +0.132504 | -0.718714 |
| 17 | C11 - H12 | +0.282540 | -1.006134 | +0.004621 | -0.329534 |
| 18 | C15 - C16 | +0.296031 | -0.782293 | +0.198340 | -0.369310 |
| 19 | C13 - C16 | +0.324880 | -0.907016 | +0.320180 | -0.460855 |
| 20 | C13 - H14 | +0.273586 | -0.907779 | +0.029835 | -0.321925 |
| 21 | C16 - O31 | +0.280437 | -0.229374 | +0.025085 | -0.788371 |
| 22 | N19 - N20 | +0.345595 | -0.617600 | +0.071904 | -0.507204 |
| 23 | N20 - C21 | +0.358345 | -0.572297 | +0.190753 | -1.065192 |
| 24 | O18 - H22 | +0.023161 | +0.079227 | +0.098176 | -0.018668 |
| 25 | C21 - H22 | +0.286344 | -1.053367 | +0.013619 | -0.335000 |
| 26 | C21 - C23 | +0.282920 | -0.730376 | +0.119934 | -0.331092 |
| 27 | C23 - C25 | +0.304954 | -0.804367 | +0.191732 | -0.393287 |
| 28 | C24 - O60 | +0.298358 | -0.271880 | +0.002879 | -0.856314 |
| 29 | C23 - C24 | +0.305390 | -0.816512 | +0.235346 | -0.392414 |
| 30 | C25 - H28 | +0.279414 | -0.957926 | +0.012279 | -0.328965 |
| 31 | C25 - C27 | +0.316586 | -0.850063 | +0.231697 | -0.429727 |
| 32 | C27 - C29 | +0.304925 | -0.801158 | +0.180219 | -0.394769 |
| 33 | C26 - C33 | +0.245742 | -0.562991 | +0.031725 | -0.252964 |
| 34 | C24 - C26 | +0.305669 | -0.825299 | +0.225395 | -0.394250 |
| 35 | C29 - H59 | +0.281265 | -0.971260 | +0.008712 | -0.333769 |
| 36 | C27 - C34 | +0.249085 | -0.578434 | +0.031556 | -0.257286 |
| 37 | C34 - C35 | +0.248467 | -0.573394 | +0.001469 | -0.257241 |
| 38 | C26 - C29 | +0.311200 | -0.818976 | +0.224720 | -0.415608 |
| 39 | C51 - H59 | +0.014580 | +0.067393 | +0.576660 | -0.010382 |
| 40 | N19 - H30 | +0.343432 | -1.853141 | +0.052946 | -0.563466 |
| 41 | H30 - O31 | +0.030738 | +0.109129 | +0.064231 | -0.025906 |
| 42 | O31 - H32 | +0.361821 | -2.079663 | +0.021704 | -0.670397 |
| 43 | C33 - C51 | +0.247796 | -0.569810 | +0.000729 | -0.256127 |
| 44 | C35 - H36 | +0.271446 | -0.885890 | +0.006845 | -0.317395 |
| 45 | C35 - H37 | +0.271473 | -0.886033 | +0.006798 | -0.317468 |
| 46 | C35 - H38 | +0.271638 | -0.886691 | +0.006027 | -0.318116 |
| 47 | C34 - C39 | +0.245055 | -0.557986 | +0.002874 | -0.252039 |
| 48 | C39 - H40 | +0.271818 | -0.889965 | +0.007724 | -0.317241 |
| 49 | C39 - H41 | +0.270678 | -0.879930 | +0.007516 | -0.316103 |

| | | | | | |
|----|-----------|-----------|-----------|-----------|-----------|
| 50 | C39 - H42 | +0.272135 | -0.890573 | +0.007487 | -0.319007 |
| 51 | C33 - C43 | +0.243879 | -0.552569 | +0.006145 | -0.250099 |
| 52 | C43 - H44 | +0.270070 | -0.873727 | +0.011126 | -0.316024 |
| 53 | H45 - O60 | +0.015346 | +0.053709 | +0.123776 | -0.011619 |
| 54 | C43 - H45 | +0.276594 | -0.931694 | +0.007932 | -0.324465 |
| 55 | C43 - H46 | +0.270844 | -0.879973 | +0.011860 | -0.316812 |
| 56 | C33 - C47 | +0.243895 | -0.552648 | +0.006142 | -0.250131 |
| 57 | C47 - H48 | +0.270875 | -0.880318 | +0.011833 | -0.316840 |
| 58 | C47 - H50 | +0.270110 | -0.874007 | +0.011081 | -0.316122 |
| 59 | H49 - O60 | +0.015196 | +0.053293 | +0.126335 | -0.011490 |
| 60 | C47 - H49 | +0.276623 | -0.931848 | +0.007937 | -0.324561 |
| 61 | C51 - H53 | +0.271854 | -0.888478 | +0.005117 | -0.318537 |
| 62 | C51 - H52 | +0.271190 | -0.883421 | +0.006940 | -0.317259 |
| 63 | C51 - H54 | +0.271202 | -0.883418 | +0.006917 | -0.317301 |
| 64 | C34 - C55 | +0.245081 | -0.558026 | +0.002913 | -0.252097 |
| 65 | C55 - H56 | +0.270692 | -0.880032 | +0.007472 | -0.316134 |
| 66 | C55 - H57 | +0.271845 | -0.890253 | +0.007708 | -0.317272 |
| 67 | C55 - H58 | +0.272072 | -0.890144 | +0.007459 | -0.318870 |
| 68 | N20 - H61 | +0.046131 | +0.126499 | +0.044858 | -0.035598 |
| 69 | O60 - H61 | +0.335223 | -1.951311 | +0.017202 | -0.637722 |

Table S4. AIM properties of the main intra- and intermolecular interactions for **mode**. Electronic density (ρ), Laplacian of density ($\nabla^2\rho$), ellipticity (ϵ) and density of potential energy (V).

| BCP | Bond | ρ (e/a ³) | $\nabla^2\rho$ (e/a ⁵) | ϵ | V (hartree.e/a ³) |
|-----|-----------|----------------------------|------------------------------------|------------|------------------------------------|
| 1 | C1 - C2 | +0.317371 | -0.885953 | +0.151275 | -0.431628 |
| 2 | C2 - C3 | +0.302809 | -0.818853 | +0.137741 | -0.389187 |
| 3 | C4 - C5 | +0.295493 | -0.770641 | +0.130857 | -0.365201 |
| 4 | C4 - H8 | +0.281963 | -0.986086 | +0.006340 | -0.328468 |
| 5 | C3 - C4 | +0.335519 | -0.964180 | +0.241055 | -0.481468 |
| 6 | C1 - C11 | +0.253939 | -0.561839 | +0.152795 | -0.274877 |
| 7 | C5 - C6 | +0.317012 | -0.850813 | +0.235586 | -0.430991 |
| 8 | C1 - C6 | +0.302524 | -0.809074 | +0.143395 | -0.384199 |
| 9 | C2 - C13 | +0.342954 | -1.062420 | +0.114489 | -0.555937 |
| 10 | C3 - H7 | +0.291268 | -1.066905 | +0.013027 | -0.350769 |
| 11 | C5 - H9 | +0.294536 | -1.082264 | +0.006201 | -0.361119 |
| 12 | C6 - H10 | +0.295836 | -1.092912 | +0.010342 | -0.367308 |
| 13 | C11 - C14 | +0.259835 | -0.553294 | +0.254361 | -0.297032 |
| 14 | C11 - H12 | +0.292531 | -1.096101 | +0.020349 | -0.354106 |
| 15 | C14 - C15 | +0.303607 | -0.815316 | +0.177834 | -0.404719 |
| 16 | C13 - C15 | +0.387336 | -1.291055 | +0.257111 | -0.690716 |
| 17 | C14 - C16 | +0.305752 | -0.878997 | +0.111766 | -0.379380 |
| 18 | C16 - O17 | +0.363952 | -0.373064 | +0.090185 | -1.127424 |
| 19 | C16 - N18 | +0.247157 | -0.520242 | +0.163607 | -0.318680 |
| 20 | N18 - N19 | +0.294064 | -0.433909 | +0.062124 | -0.396424 |
| 21 | O17 - C20 | +0.014112 | +0.055000 | +2.565047 | -0.010274 |
| 22 | N19 - C20 | +0.355993 | -0.686926 | +0.176688 | -1.026931 |
| 23 | C20 - H21 | +0.305435 | -1.189628 | +0.005468 | -0.384076 |
| 24 | C20 - C22 | +0.286517 | -0.749770 | +0.125467 | -0.341617 |
| 25 | C22 - C23 | +0.306794 | -0.829336 | +0.222838 | -0.392064 |
| 26 | C22 - C24 | +0.303782 | -0.798464 | +0.186351 | -0.390321 |
| 27 | C23 - C25 | +0.311212 | -0.860509 | +0.224681 | -0.408972 |
| 28 | C24 - H27 | +0.289943 | -1.036846 | +0.012822 | -0.356407 |
| 29 | C24 - C26 | +0.327463 | -0.915063 | +0.230564 | -0.460300 |
| 30 | C26 - C33 | +0.238037 | -0.526767 | +0.030712 | -0.237842 |

| | | | | | |
|----|-----------|-----------|-----------|-----------|-----------|
| 31 | C33 - C54 | +0.239177 | -0.529808 | +0.002659 | -0.242200 |
| 32 | C25 - C28 | +0.304506 | -0.780582 | +0.220094 | -0.397700 |
| 33 | C26 - C28 | +0.308086 | -0.821354 | +0.170587 | -0.401454 |
| 34 | C15 - O30 | +0.241645 | -0.421150 | +0.036918 | -0.525674 |
| 35 | N18 - H29 | +0.343246 | -1.818020 | +0.037073 | -0.586412 |
| 36 | H29 - F62 | +0.103923 | +0.370556 | +0.032733 | -0.156409 |
| 37 | O30 - F62 | +0.216821 | +0.710127 | +0.052328 | -0.375318 |
| 38 | H31 - F61 | +0.105879 | +0.146570 | +0.006114 | -0.132312 |
| 39 | O30 - H31 | +0.304463 | -1.814718 | +0.021042 | -0.680613 |
| 40 | C25 - C32 | +0.242932 | -0.548337 | +0.031384 | -0.248741 |
| 41 | C33 - C34 | +0.244009 | -0.550633 | +0.002457 | -0.249822 |
| 42 | C34 - H36 | +0.286831 | -0.994862 | +0.001971 | -0.359881 |
| 43 | C33 - C38 | +0.239588 | -0.531281 | +0.001868 | -0.242482 |
| 44 | C34 - H35 | +0.289526 | -1.020171 | +0.002579 | -0.365842 |
| 45 | H27 - H36 | +0.016899 | +0.074250 | +0.759255 | -0.011513 |
| 46 | C34 - H37 | +0.285540 | -0.988988 | +0.002817 | -0.355730 |
| 47 | C38 - H40 | +0.285245 | -0.987242 | +0.004326 | -0.355058 |
| 48 | C38 - H39 | +0.287509 | -1.005359 | +0.004097 | -0.359707 |
| 49 | H41 - H58 | +0.013787 | +0.056128 | +0.600833 | -0.008630 |
| 50 | C38 - H41 | +0.287367 | -0.999862 | +0.003423 | -0.361193 |
| 51 | C32 - C42 | +0.243938 | -0.550806 | +0.004931 | -0.250924 |
| 52 | C42 - H44 | +0.288342 | -1.014571 | +0.003977 | -0.359130 |
| 53 | C42 - H43 | +0.286044 | -0.991734 | +0.006649 | -0.358495 |
| 54 | H44 - O59 | +0.009388 | +0.036102 | +0.346187 | -0.006797 |
| 55 | C42 - H45 | +0.287815 | -1.005496 | +0.007444 | -0.362516 |
| 56 | C32 - C46 | +0.241311 | -0.538721 | +0.005619 | -0.246247 |
| 57 | C23 - O59 | +0.321050 | +0.034937 | +0.012558 | -1.013323 |
| 58 | C46 - H47 | +0.284633 | -0.979199 | +0.013387 | -0.355460 |
| 59 | H48 - O59 | +0.025059 | +0.089138 | +0.032475 | -0.020774 |
| 60 | C46 - H48 | +0.294000 | -1.065751 | +0.005795 | -0.367929 |
| 61 | C46 - H49 | +0.285058 | -0.982196 | +0.013201 | -0.357687 |
| 62 | C50 - H51 | +0.287896 | -1.007836 | +0.002496 | -0.361640 |
| 63 | H53 - H58 | +0.017807 | +0.076497 | +0.786464 | -0.012251 |
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| 69 | C54 - H56 | +0.288775 | -1.015645 | +0.005079 | -0.363111 |
| 70 | C54 - H57 | +0.285645 | -0.990724 | +0.004715 | -0.355429 |
| 71 | N19 - H60 | +0.049501 | +0.141469 | +0.036608 | -0.040771 |
| 72 | O59 - H60 | +0.356605 | -2.310350 | +0.012261 | -0.740936 |
