10.1071/CH17624_AC

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# Supplementary Material

## Is it reasonable to obtain information on the polarizability and hyperpolarizability from the electron density?

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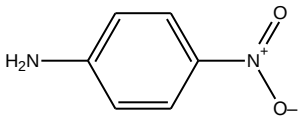
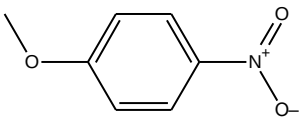
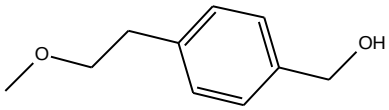
Jha, Kunal; Shiv Nadar University, Chemistry
Munshi, Parthapratim; Shiv Nadar University, Chemistry. E-mail: parthapratim.munshi@snu.edu.in



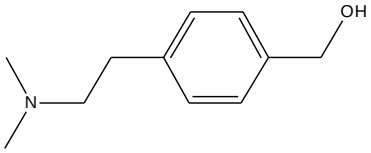
**K1** (4-nitrobenzenamine)



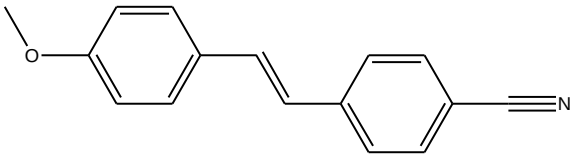
**K2** (1-methoxy-4-nitrobenzene)



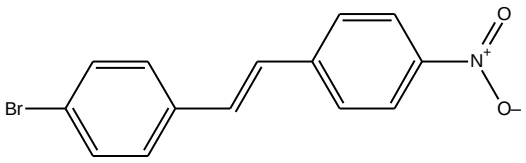
**K3** ((4-(2-methoxyethyl)phenyl)methanol)



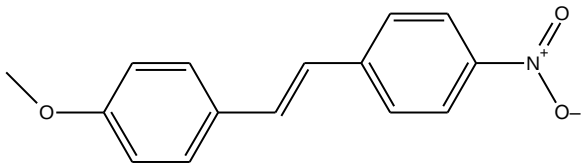
**K4** ((4-(2-(dimethylamino)ethyl)phenyl)methanol)



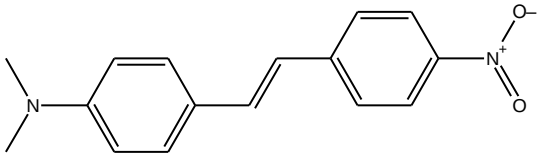
**K5** ((*E*)-4-(4-methoxystyryl)benzonitrile)



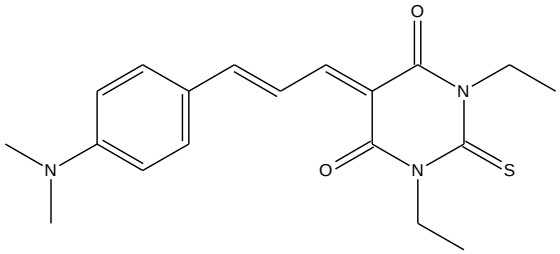
**K6** (*E*)-1-(4-bromostyryl)-4-nitrobenzene



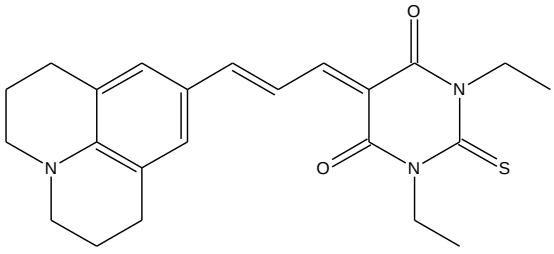
**K7** ((*E*)-1-(4-nitrostyryl)-4-methoxybenzene)



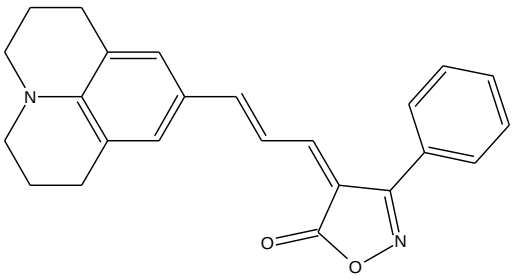
**K8** ((*E*)-4-(4-nitrostyryl)-*N*,*N*-dimethylbenzenamine)



**K9** ((*E*)-5-(3-(4-(dimethylamino)phenyl)allylidene)-1,3 -diethyl -2-thioxo-dihydropyrimidine-4,6(1*H*,5*H*)-dione)

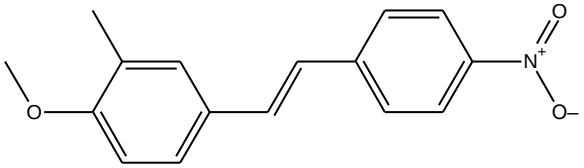


**K10** (1,3-dimethyl-2-sulfanylidene-5-[(2*E*) -3-(2,3,6,7-tetrahydro-1*H*,5*H*-pyrido [3,2,1-*ij*]quinolin-9-yl)prop-2-en-1-ylidene] dihydropyrimidine-4,6(1*H*,5*H*)-dione )

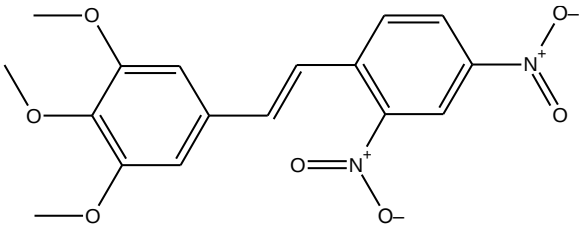


**K11** (4*Z*)-3-phenyl-4-[(2*E*)-3-(2,3,6,7-tetrahydro-1*H*,5*H*-pyrido [3,2,1-*ij*]quinolin-9-yl)prop-2-en-1-ylidene]-1,2-oxazol-5(4*H*)-one

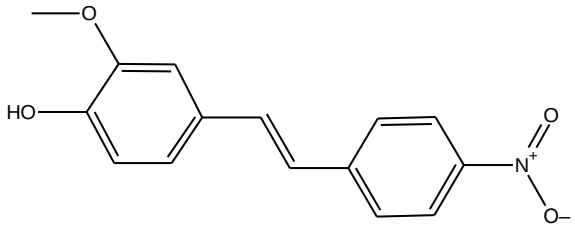
**Fig. S1** Chemical diagrams and IUPAC names of Molecules(K1-11) from Kuzyk *et al.*[23]



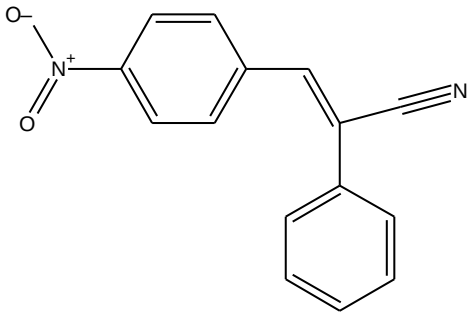
**NS1a/b(**(*E*)-4-(4-nitrostyryl)-1-methoxy-2-methylbenzene
)



**NS2** ((*E*)-5-(2,4-dinitrostyryl)-1,2,3-trimethoxybenzene)

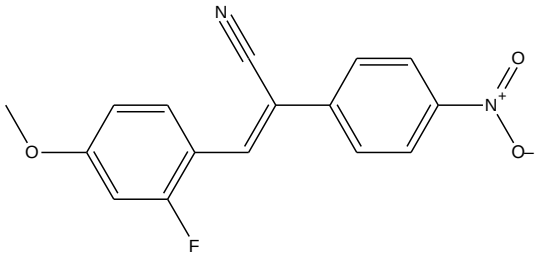


**NS3** ((*E*)-4-(4-nitrostyryl)-2-methoxyphenol)

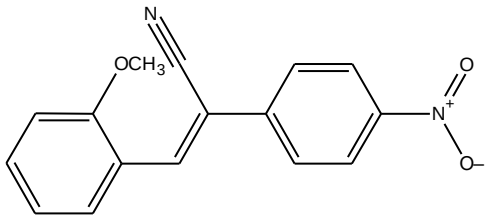


**NS4** ((*E*)-3-(4-nitrophenyl)-2-phenylacrylonitrile)

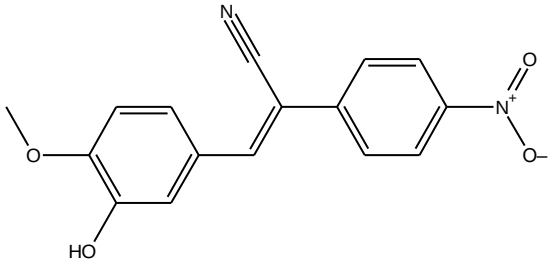
**Fig. S2** Chemical diagrams and IUPAC names of Nitrostilbene derivatives (NS1-4) .



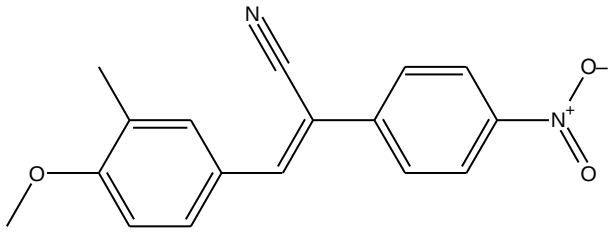
**NCS1**((*Z*)-3-(2-fluoro-4-methoxyphenyl)-2-(4-nitrophenyl)acrylonitrile)



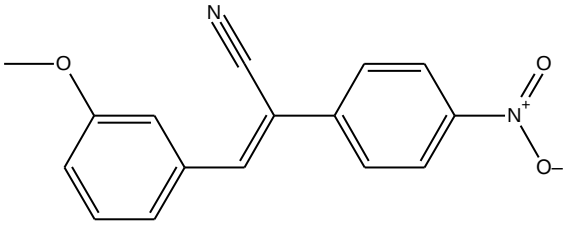
**NCS2**((*Z*)-3-(2-methoxyphenyl)-2-(4-nitrophenyl)acrylonitrile)



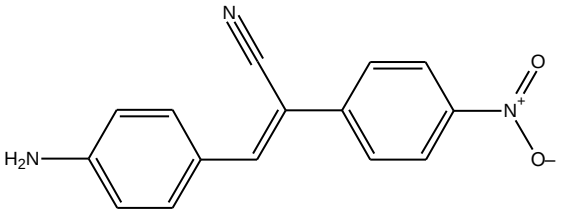
**NCS3**((*Z*)-3-(3-hydroxy-4-methoxyphenyl)-2-(4-nitrophenyl)acrylonitrile)



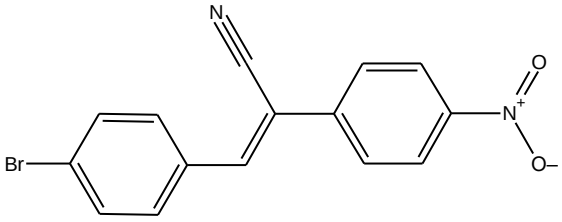
**NCS4**(*Z*)-3-(4-methoxy-3-methylphenyl)-2-(4-nitrophenyl)acrylonitrile



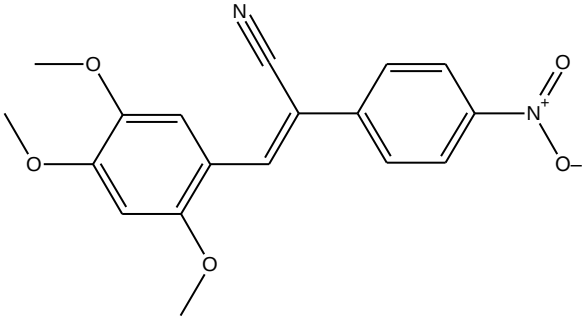
**NCS5**((*Z*)-3-(3-methoxyphenyl)-2-(4-nitrophenyl) acrylonitrile)



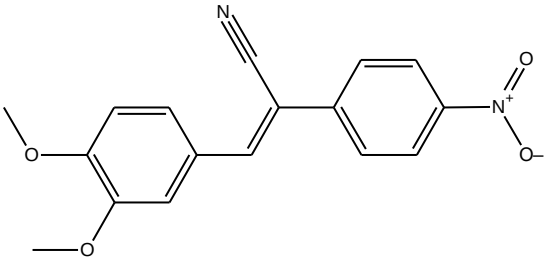
**NCS6(**(*Z*)-3-(4-aminophenyl)-2-(4-nitrophenyl) acrylonitrile)



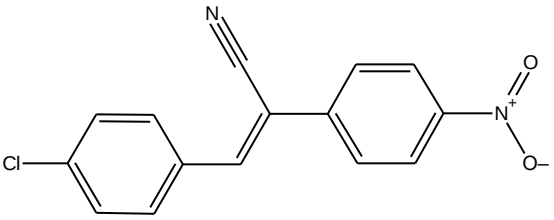
**NCS7**((*Z*)-3-(4-bromophenyl)-2-(4-nitrophenyl)acrylonitrile)



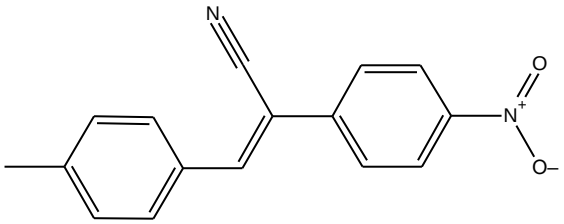
**NCS8**((*Z*)-2-(4-nitrophenyl)-3-(2,4,5-trimethoxyphenyl) acrylonitrile)



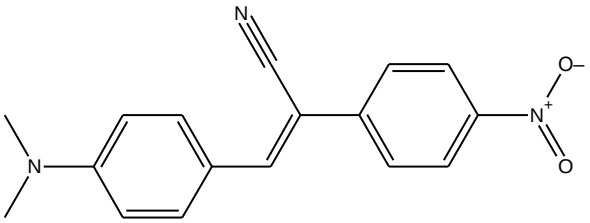
**NCS9**((*Z*)-3-(3,4-dimethoxyphenyl)-2-(4-nitrophenyl) acrylonitrile)



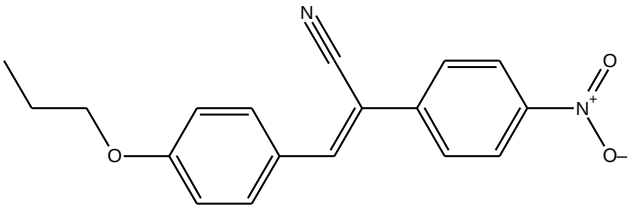
**NCS10**((*Z*)-3-(4-chlorophenyl)-2-(4-nitrophenyl)acr ylonitrile)



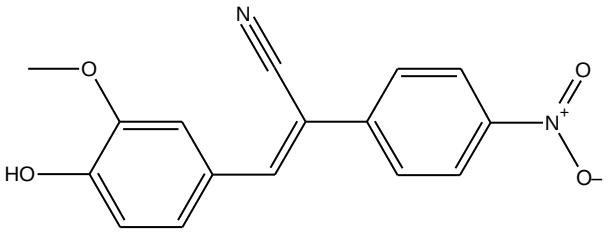
**NCS11**((*Z*)-2-(4-nitrophenyl)-3-*p*-tolyla crylonitrile)



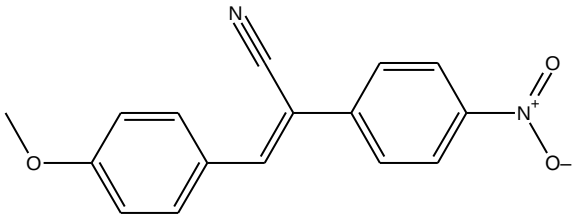
**NCS12**(*Z*)-3-(4-(dimethylamino)phenyl)-2-(4-nitrophenyl) acrylonitrile



**NCS13**(*Z*)-2-(4-nitrophenyl)-3-(4-propoxyphenyl)acry lonitrile

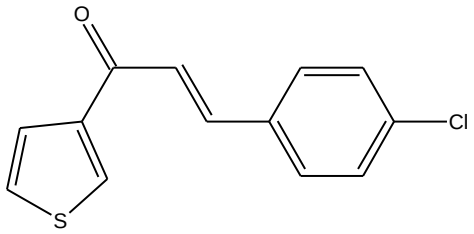


**NCS14**(*Z*)-3-(4-hydroxy-3-methoxyphenyl)-2-(4-nitrophe nyl)acrylonitrile

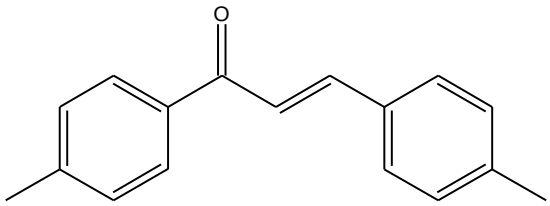


**NCS15a/b/c**(*Z*)-3-(4-methoxyphenyl)-2-(4-nitrophenyl )acrylonitrile

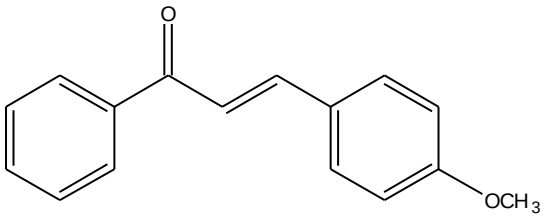
**Fig. S3** Chemical diagrams and IUPAC names of Nitrocyanostilbene derivatives (NCS1-15).



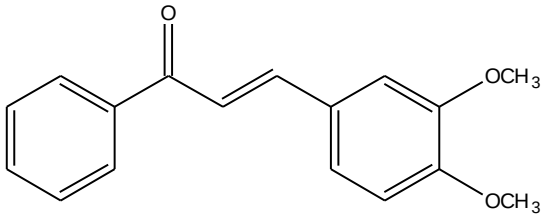

**C1 (**(*E*)-3-(4-chlorophenyl)-1-(thiophen-3-yl)prop-2-en-1-one)



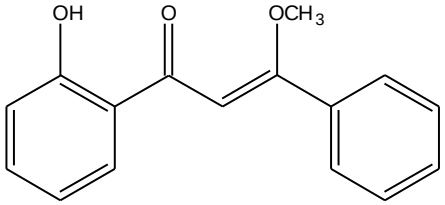

**C2** ((*E*)-1,3-di*p*-tolylprop-2-en-1-one



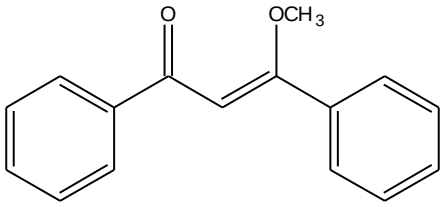

**C3** ((*E*)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one)




**C4** (*E*)-3-(3,4-dimethoxyphenyl)-1-phenylprop-2-en-1-one)




**C5** ((*Z*)-1-(2-hydroxyphenyl)-3-methoxy-3-phenylprop-2-en-1-one)




**C6a/b** ((*Z*)-3-methoxy-1,3-diphenylprop-2-en-1-one)

**Fig. S4** Chemical diagrams and IUPAC names of Chalcone derivatives(C1-6).

**Table.S1:** Polarizability(α), hyperpolarizability(β) and band gap($\varepsilon_{LUMO} - \varepsilon_{HOMO}$) calculated from the different approaches as denoted in the subscript.

| Compound name | $\alpha_{HF}$ (au) | $\beta_{HF}$(au) | $\alpha_{SC}$(au) | $\beta_{SC}$(au) | $\alpha_{JJM}$(au) | $\beta_{JJM}$(au) | $\varepsilon_{LUMO} - \varepsilon_{HOMO}$ (au) |
|---|---|---|---|---|---|---|---|
| k1 | 76.15 | 633.21 | 82.35 | 11.58 | 1134.78 | 5055.46 | 0.40107 |
| k2 | 81.08 | 229.76 | 89.64 | 18.83 | 1497.68 | 8200.16 | 0.42614 |
| k3 | 109.82 | 939.85 | 110.65 | 68.57 | 2587.03 | 23370.57 | 0.38048 |
| k4 | 123.61 | 626.79 | 126.96 | 63.42 | 3214.34 | 10424.87 | 0.38749 |
| k5 | 181.22 | 1391.31 | 167.57 | 43.42 | 6887.69 | 43418.52 | 0.35340 |
| k6 | 189.06 | 2308.63 | 147.20 | 18.01 | 8566.63 | 84575.55 | 0.33831 |
| k7 | 180.51 | 2194.46 | 169.03 | 43.80 | 7800.37 | 38898.17 | 0.34283 |
| k8 | 201.57 | 3667.49 | 186.72 | 54.96 | 9210.98 | 19440.98 | 0.32833 |
| k9 | 283.08 | 6065.47 | 240.40 | 103.85 | 13465.71 | 391813.60 | 0.30971 |
| k10 | 326.57 | 8340.31 | 280.20 | 131.54 | 17394.52 | 166681.90 | 0.30018 |
| k11 | 294.03 | 7481.90 | 263.09 | 150.76 | 14752.57 | 126422.69 | 0.30610 |
| NS1a | 194.56 | 2997.40 | 189.13 | 71.81 | 9035.76 | 26036.11 | 17000.35 |
| NS1b | 195.36 | 3145.72 | 196.74 | 53.82 | 9345.62 | 29858.85 | 20513.23 |
| NS2 | 221.33 | 2856.07 | 229.07 | 151.98 | 11778.04 | 96859.28 | 85081.24 |
| NS3 | 184.51 | 2898.65 | 185.40 | 100.83 | 8641.02 | 74739.60 | 66098.59 |
| NS4 | 163.87 | 514.11 | 166.35 | 17.88 | 4665.01 | 30132.93 | 25467.93 |
| NCS1 | 191.98 | 2149.82 | 176.42 | 33.39 | 7974.47 | 20790.48 | 0.34474 |
| NCS2 | 181.98 | 990.80 | 177.54 | 35.15 | 6412.81 | 67179.20 | 0.35947 |
| NCS3 | 195.92 | 2556.92 | 182.46 | 70.01 | 8506.97 | 43956.05 | 0.33428 |
| NCS4 | 205.36 | 2651.76 | 189.84 | 66.57 | 8663.36 | 57097.90 | 0.34011 |
| NCS5 | 186.12 | 1102.77 | 177.38 | 42.20 | 7461.02 | 23212.93 | 0.35432 |
| NCS6 | 188.97 | 3343.21 | 171.70 | 67.29 | 6769.95 | 47404.87 | 0.33152 |
| NCS7 | 194.28 | 1604.48 | 155.69 | 20.91 | 8616.91 | 73353.72 | 0.35173 |
| NCS8 | 222.61 | 2461.58 | 210.69 | 58.79 | 10026.27 | 133754.24 | 0.33680 |
| NCS9 | 206.90 | 2405.92 | 193.89 | 51.72 | 9373.29 | 82512.12 | 0.33941 |
| NCS10 | 185.83 | 1545.96 | 164.64 | 30.55 | 7404.52 | 41507.23 | 0.35413 |
| NCS11 | 187.30 | 1661.88 | 173.41 | 27.50 | 6828.13 | 50675.18 | 0.34946 |

| Compound name | $\alpha_{HF}$ (au) | $\beta_{HF}$(au) | $\alpha_{SC}$(au) | $\beta_{SC}$(au) | $\alpha_{JJM}$(au) | $\beta_{JJM}$(au) | $\varepsilon_{LUMO} - \varepsilon_{HOMO}$ (au) |
|---|---|---|---|---|---|---|---|
| k1 | 76.15 | 633.21 | 82.35 | 11.58 | 1134.78 | 5055.46 | 0.40107 |
| k2 | 81.08 | 229.76 | 89.64 | 18.83 | 1497.68 | 8200.16 | 0.42614 |
| k3 | 109.82 | 939.85 | 110.65 | 68.57 | 2587.03 | 23370.57 | 0.38048 |
| k4 | 123.61 | 626.79 | 126.96 | 63.42 | 3214.34 | 10424.87 | 0.38749 |
| k5 | 181.22 | 1391.31 | 167.57 | 43.42 | 6887.69 | 43418.52 | 0.35340 |
| k6 | 189.06 | 2308.63 | 147.20 | 18.01 | 8566.63 | 84575.55 | 0.33831 |
| k7 | 180.51 | 2194.46 | 169.03 | 43.80 | 7800.37 | 38898.17 | 0.34283 |
| k8 | 201.57 | 3667.49 | 186.72 | 54.96 | 9210.98 | 19440.98 | 0.32833 |
| k9 | 283.08 | 6065.47 | 240.40 | 103.85 | 13465.71 | 391813.60 | 0.30971 |
| k10 | 326.57 | 8340.31 | 280.20 | 131.54 | 17394.52 | 166681.90 | 0.30018 |
| k11 | 294.03 | 7481.90 | 263.09 | 150.76 | 14752.57 | 126422.69 | 0.30610 |
| NS1a | 194.56 | 2997.40 | 189.13 | 71.81 | 9035.76 | 26036.11 | 17000.35 |
| NS1b | 195.36 | 3145.72 | 196.74 | 53.82 | 9345.62 | 29858.85 | 20513.23 |
| NS2 | 221.33 | 2856.07 | 229.07 | 151.98 | 11778.04 | 96859.28 | 85081.24 |
| NS3 | 184.51 | 2898.65 | 185.40 | 100.83 | 8641.02 | 74739.60 | 66098.59 |
| NS4 | 163.87 | 514.11 | 166.35 | 17.88 | 4665.01 | 30132.93 | 25467.93 |
| NCS1 | 191.98 | 2149.82 | 176.42 | 33.39 | 7974.47 | 20790.48 | 0.34474 |
| NCS2 | 181.98 | 990.80 | 177.54 | 35.15 | 6412.81 | 67179.20 | 0.35947 |
| NCS3 | 195.92 | 2556.92 | 182.46 | 70.01 | 8506.97 | 43956.05 | 0.33428 |
| NCS4 | 205.36 | 2651.76 | 189.84 | 66.57 | 8663.36 | 57097.90 | 0.34011 |
| NCS5 | 186.12 | 1102.77 | 177.38 | 42.20 | 7461.02 | 23212.93 | 0.35432 |
| NCS6 | 188.97 | 3343.21 | 171.70 | 67.29 | 6769.95 | 47404.87 | 0.33152 |
| NCS7 | 194.28 | 1604.48 | 155.69 | 20.91 | 8616.91 | 73353.72 | 0.35173 |
| NCS8 | 222.61 | 2461.58 | 210.69 | 58.79 | 10026.27 | 133754.24 | 0.33680 |
| NCS9 | 206.90 | 2405.92 | 193.89 | 51.72 | 9373.29 | 82512.12 | 0.33941 |
| NCS10 | 185.83 | 1545.96 | 164.64 | 30.55 | 7404.52 | 41507.23 | 0.35413 |
| NCS11 | 187.30 | 1661.88 | 173.41 | 27.50 | 6828.13 | 50675.18 | 0.34946 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| NCS12 | 218.14 | 4793.14 | 195.68 | 71.79 | 9257.31 | 60287.03 | 0.32275 |
| NCS13 | 216.60 | 2812.24 | 200.94 | 43.70 | 11400.87 | 134724.42 | 0.34139 |
| NCS14 | 193.12 | 2182.51 | 182.80 | 66.51 | 8165.91 | 61428.69 | 0.34539 |
| NCS15a | 192.96 | 2501.63 | 191.22 | 70.39 | 8496.32 | 51945.87 | 43449.55 |
| NCS15b | 192.96 | 2500.72 | 184.73 | 43.89 | 8214.36 | 48410.76 | 40196.40 |
| NCS15c | 192.95 | 2501.60 | 183.25 | 61.75 | 8143.86 | 47717.79 | 39573.93 |
| C1 | 160.84 | 755.74 | 144.47 | 25.02 | 5834.36 | 48213.87 | 42379.51 |
| C2 | 180.59 | 781.79 | 181.67 | 18.02 | 6920.42 | 75560.27 | 68639.85 |
| C3 | 171.41 | 1418.75 | 161.34 | 55.79 | 6188.89 | 57669.13 | 51480.24 |
| C4 | 186.63 | 1544.35 | 190.72 | 90.86 | 8035.66 | 90503.50 | 82467.84 |
| C5 | 167.39 | 294.64 | 177.59 | 69.62 | 5253.53 | 53788.73 | 48535.20 |
| C6a | 162.17 | 323.45 | 173.09 | 45.18 | 4877.84 | 53204.17 | 48326.33 |
| C6b | 159.38 | 67.79 | 176.35 | 51.60 | 4675.80 | 41310.91 | 36635.11 |

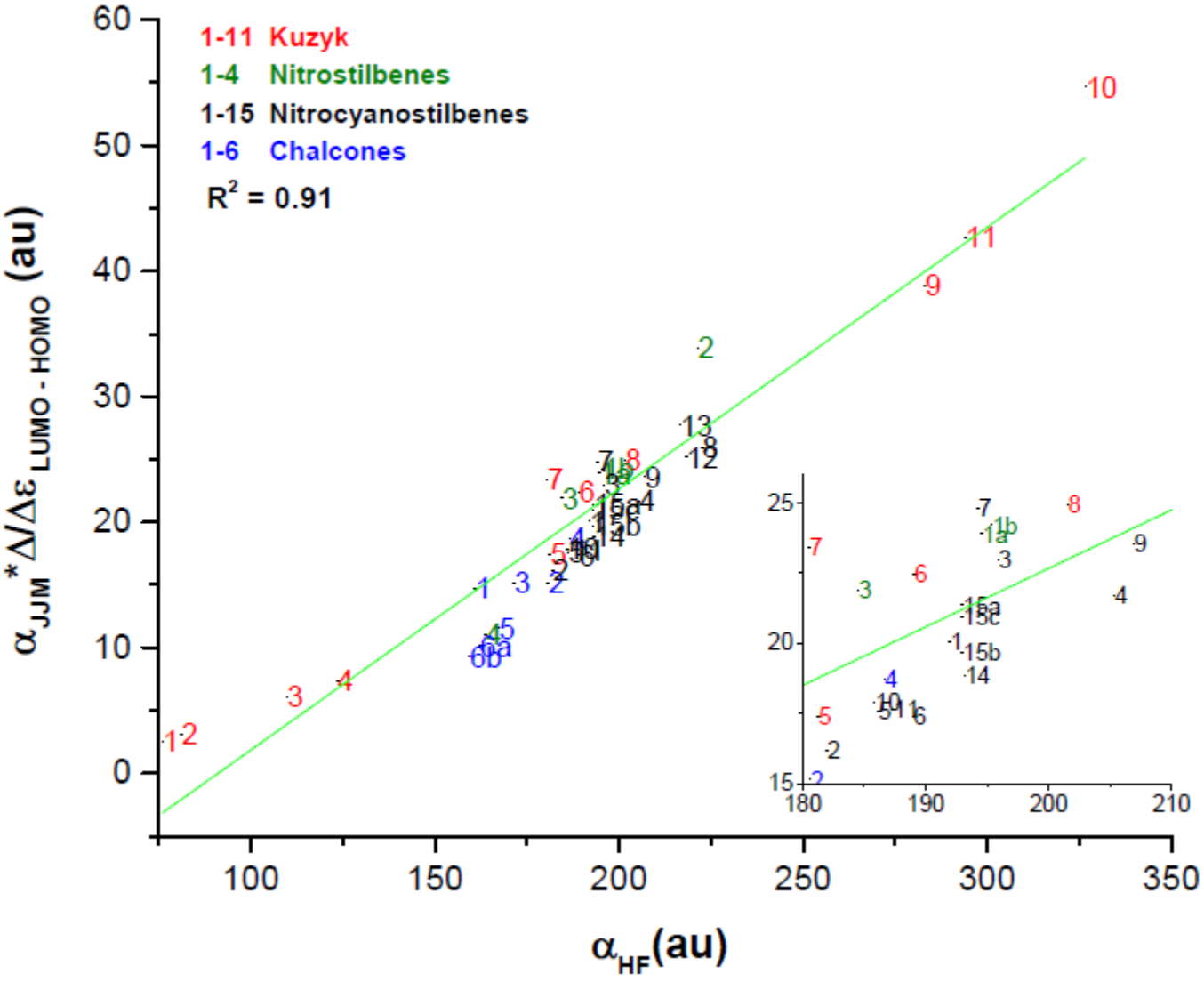



**Figure S5**. Polarizabilities from this work (JJM) with modified energy denominator vs the polarizabilities from CPHF, in atomic units.