Supporting Information

Unraveling Innate Substrate Control in Site-Selective Palladium-Catalyzed C-H Heterocycle Functionalization

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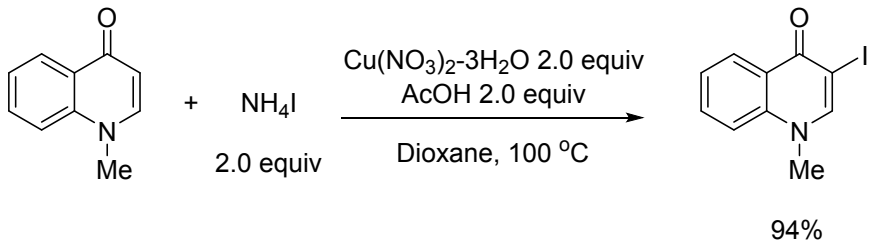
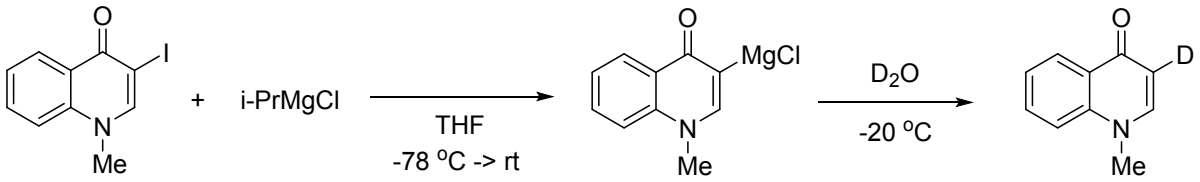
1. EXPERIMENT

1.1 SYNTHESIS OF 1-METHYLQUINOLIN-4(1H)-ONE-3-D



94%

A mixture of 1-methyl-4-quinolone (1 equiv), NH_4I (2 equiv), $Cu(NO_3)_2$-$3H_2O$ (2 equiv), AcOH (2 equiv) in 1,4-dioxane was heated to 100 °C for 1 h. After cooled to room temperature, 1,4-dioxane was removed under vacuo. The residue was diluted with CH_2Cl_2 and then added aqueous sodium thiosulfate and aqueous NH_4Cl. When the residue was changed from dark red to pale yellow, it was extracted three times with CH_2Cl_2. After removal of solvent, the residue was purified by flash chromatography on silica gel (CH_2Cl_2 / MeOH = 25 : 1) to give 3-iodo-1-methylquinolin-4(1H)-one. (94% yield)

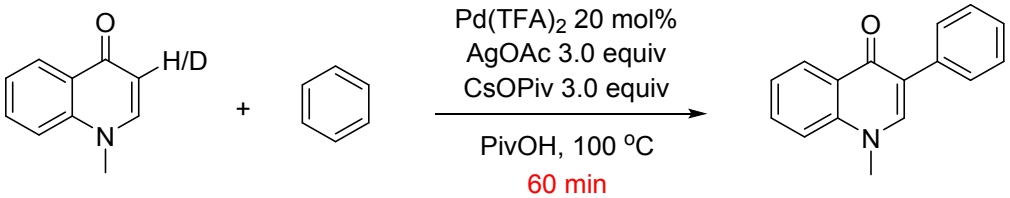


66%

To an over-dried round bottom flask were added 3-iodo-1-methylquinolin-4(1H)-one (1 mmol, 1.0 equiv), THF (10 mL) under N_2. The solution was cooled to -78 °C and *i*PrMgCl (0.5 mL, 2 M in THF) was added slowly. After stirring for 1 h, the reaction mixture was allowed to warm to room temperature and re-cool to -20 °C. D_2O (0.6 mL) was added slowly and the mixture was diluted with ethyl acetate, washed with water, dried over Na_2SO_4, filtered and concentrated. The product was purified with silica gel chromatography (CH_2Cl_2 / MeOH = 15 : 1) to give 1-methylquinolin-4(1H)-one-3-*d* as a colorless solid. (66% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 8.56 – 8.34 (m, 1H), 7.69 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.51 (s, 1H), 7.46 – 7.34 (m, 2H), 3.80 (s, 3H).

[Ref] *Org. Lett.* **2012**, 14, 1176.

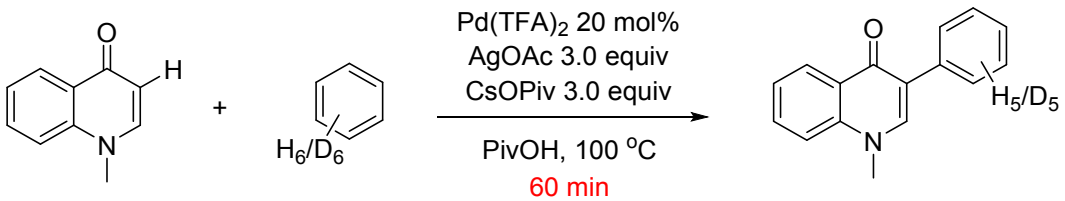
1.2 General Procedure for the Kinetic isotope experiments:



K_H/K_D = 1.13

H : 12.0%
D : 10.6%

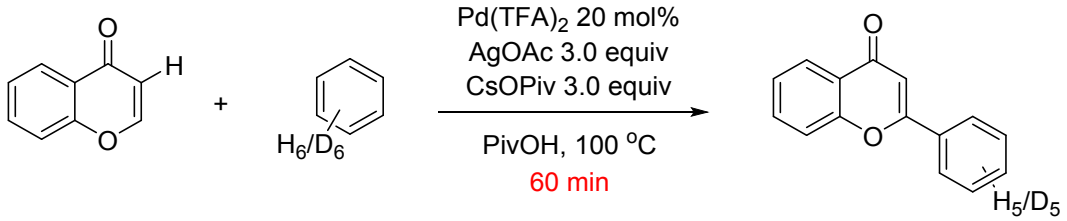
To two capped sealed tubes, were added $Pd(TFA)_2$ (20 mol%), AgOAc (3.0 equiv), CsOPiv (3.0 equiv). In one tube, 1-methylquinolin-4(1H)-one (0.1 mmol), Benzene (0.5 mL) and Pivalic acid (0.5 mL) were added subsequently. In the other tube, 1-methylquinolin-4(1H)-one-3-d (0.1 mmol), Benzene (0.5 mL) and Pivalic acid (0.5 mL) were added. The reactions were stirred at 100 °C for 60 min. the The reaction mixture was cooled to room temperature, and then diluted with CH_2Cl_2 and $NaHCO_3$. After stirring for 10 min, the mixture was washed sequentially with aqueous $NaHCO_3$ and NH_4Cl. The combined organic layers were dried over $MgSO_4$. The filtrate was concentrated in vacuo and the yield was analyzed by ^1H NMR.



K_H/K_D = 4.28

H : 12.0%
D : 2.8%

To two capped sealed tubes, were added 1-methylquinolin-4(1H)-one (0.1 mmol), $Pd(TFA)_2$ (20 mol%), AgOAc (3.0 equiv), CsOPiv (3.0 equiv). In one tube, Benzene (0.5 mL) and Pivalic acid (0.5 mL) were added subsequently. In the other tube, Benzene-*d*6 (0.5 mL) and Pivalic acid (0.5 mL) were added. The reactions were stirred at 100 °C for 60 min. the The reaction mixture was cooled to room temperature, and then diluted with CH_2Cl_2 and $NaHCO_3$. After stirring for 10 min, the mixture was washed sequentially with aqueous $NaHCO_3$ and NH_4Cl. The combined organic layers were dried over $MgSO_4$. The filtrate was concentrated in vacuo and the yield was analyzed by ^1H NMR.

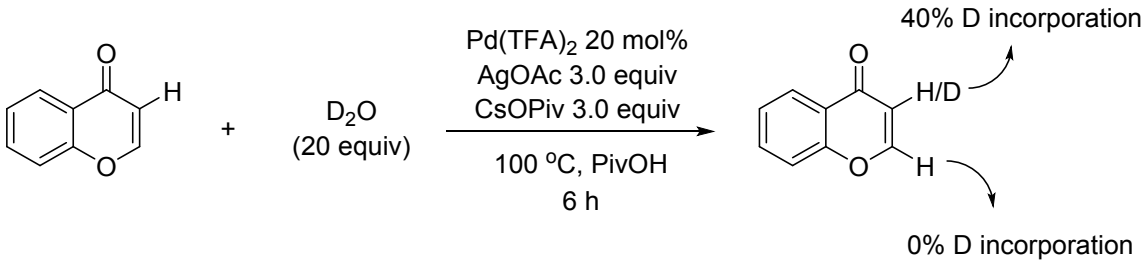


K_H/K_D = 2.90

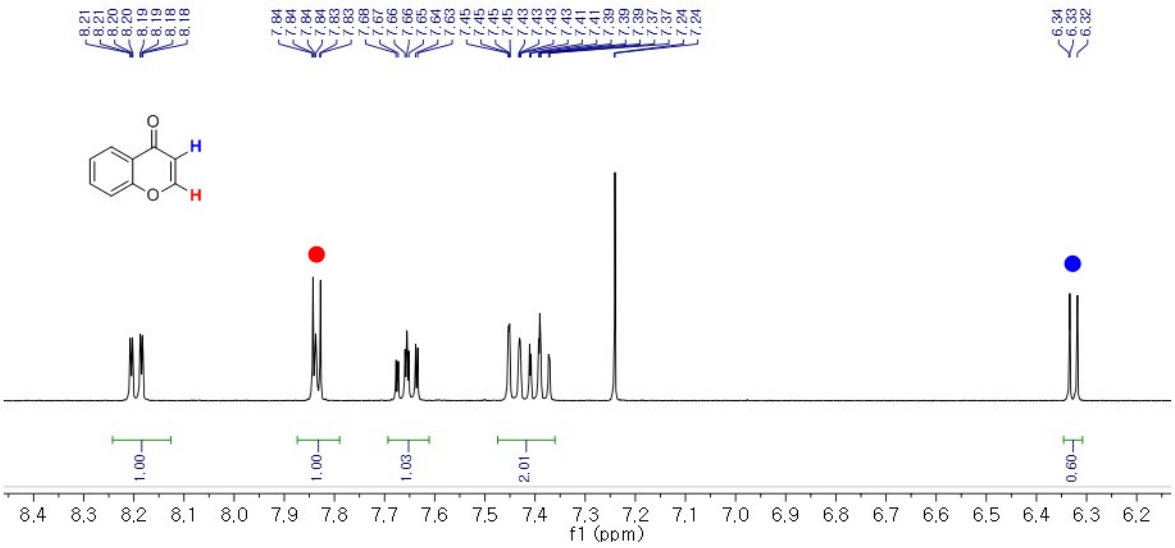
H : 20.3%
D : 7.0%

To two capped sealed tubes, were added chromone (0.1 mmol), $Pd(TFA)_2$ (20 mol%), AgOAc (3.0 equiv), CsOPiv (3.0 equiv). In one tube, Benzene (0.5 mL) and Pivalic acid (0.5 mL) were added subsequently. In the other tube, Benzene-*d*6 (0.5 mL) and Pivalic acid (0.5 mL) were added. The reactions were stirred at 100 °C for 60 min. the The reaction mixture was cooled to room temperature, and then diluted with CH_2Cl_2 and $NaHCO_3$. After stirring for 10 min, the mixture was washed sequentially with aqueous $NaHCO_3$ and NH_4Cl. The combined organic layers were dried over $MgSO_4$. The filtrate was concentrated in vacuo and the yield was analyzed by ^1H NMR.

1.3 General Procedure for the H/D Exchange Experiments:



Chromone (0.1 mmol), $Pd(TFA)_2$ (20 mol%), AgOAc (3.0 equiv), CsOPiv (3.0 equiv) and D_2O (20 equiv) were combined in PivOH (1.0 mL). The reactions were stirred at 100 °C for 6 h. The reaction mixture was diluted with CH_2Cl_2 and the excess $NaHCO_3$ was added to neutralize PivOH. After stirring the mixture for 10 min, the residue was washed with sequentially aqueous $NaHCO_3$ and NH_4Cl. The organic layer was dried over $MgSO_4$. The residue was concentrated, and evaporated to dryness under high vacuum. The extent of H/D exchange was determined by integration of ^1H-NMR.



2. DFT CALCULATIONS

2.1 Stationary points:

All stationary points were fully optimized at the wB97XD/6-31G(d) level of theory, with the LANL2DZ basis set for Pd, using *Gaussian 09* with default convergence criteria for the optimizations and grid spacing for numerical integrations. Minima and transition structures were verified by the presence of zero and a single imaginary frequency, respectively, following calculation of harmonic vibrations. The effects of solvation due to toluene were described through incorporation of a conductor-like polarizable continuum model (CPCM) on single point energies. Single point energies were evalauted using a larger 6-311+G(d,p) basis set including the LANL2TZ ECP for Pd. The B3LYP functional with a D3-dispersion correction with zero-damping at short range was used to corroborate these results. Free energies were computed employing a standard state in solution of 1 mol/l in the Sackur-Tetrode expression. The experimental use of benzene in 40-fold excess causes a corresponding increase in its chemical potential by RTln(40) relative to the aforementioned standard state, which was applied to our computed free energy profile. Entropic contributions of low frequency mode vibrations (below 100 cm^{-1}) were treated according to a quasi-rigid-rotor harmonic oscillator (RRHO) approximation to avoid supriously large values, switching from the harmonic approximation using a Head-Gordon damping function as previously described by Grimme. Translational entropies were corrected for the inadequacy of the ideal gas approximation in solution by using the number density according to the effective free space of the solvent (rather than the total volume, since the solute and solvent molecules are not free to move), as proposed by Shakhnovich. This was computed for acetic acid as solvent, to model pivalic acid, using a molarity for AcOH of 17.4 mol/l and a solvent volume (computed with B3LYP/6-31G*) of 86.1 $Å^3$ per molecule.

2.2 Computational details

Quantum chemical calculations have provided important insights into the mechanisms of Pd(II)-catalyzed C-H activation of arenes,[1] however, the mechanism of direct cross-coupling reactions between two arenes has received relatively little computational attention.[2] All calculations were performed with *Gaussian 09* revision D.01.[3] Stationary points were located

with the range-separated, density independent atom-pairwise London dispersion-corrected wB97XD density functional of Chai and Head-Gordon,[4] using the 6-31G(d) basis set along with a LANL2DZ effective core potential (ECP) and associated valence basis set for Pd.[5] Tests of Pd–ligand bond dissociation energies against correlated *ab initio* results show the wB97XD functional to give lowest errors (<1 kcal/mol) compared with a variety of other hybrid and non-hybrid functionals employing the generalized gradient approximation (GGA),[6] and this method has been employed in previous studies of oxidative C-H functionalization.[7] Single point energies were further evaluated using a larger 6-311+G(d,p) basis set including the LANL2TZ ECP for Pd,[8] taking into account effects due to solvation (acetic acid) with an implicit conductor-like polarizable continuum model.[9] The B3LYP functional[10] with a D3-dispersion correction[11] with zero-damping at short range[12] was also used to corroborate these results as described in the Supporting Information (SI). Stationary points were fully optimized, and minima and transition structures (TSs) were characterized by the presence of zero or a single vibrational imaginary frequency, respectively. Free energies are quoted in kcal/mol, and were computed employing a standard state in solution of 1 mol/l in the Sackur-Tetrode expression for translational entropies. The experimental use of benzene in 40-fold excess causes a corresponding increase in its chemical potential by RTln(40) relative to the aforementioned standard state, which was applied to our computed free energy profile. Entropic contributions of low frequency mode vibrations (below 100 cm^{-1}) were treated according to a quasi-rigid-rotor harmonic oscillator (RRHO) approximation to avoid spuriously large values as previously described by Grimme to improve estimates of supramolecular thermochemistry.[13] Translational entropies were corrected for the inadequacy of the ideal gas approximation in solution by using the number density according to the effective free space of the solvent (rather than the total volume, since the solute and solvent molecules are not free to move), as proposed by Shakhnovich.[14] This was computed for acetic acid as solvent, to model pivalic acid, using a molarity for AcOH of 17.4 mol/l and a solvent volume (computed with B3LYP/6-31G*) of 86.1 $Å^3$ per molecule. All molecular graphics were produced with *Pymol.*[15]

2.2.1 **Genration of grid based Potential Energy Surface (PES) of C-H arylation selectivity**

Potential energy surfaces of palladium catalyzed selective C-H arylation were probed through the frozen method of energy calculations with the version of Gaussian 09 code. These quantum chemical calculations were carried out based on density functional calculations using the PBE1PBE/LanL2DZ level with geometric optimization. LanL2DZ basis was used for facilitating to describe palladium electronic structures.[16] In detail, the energy functions were obtained to vary two geometric parameters and distances between 1.35 and 3.55 Å by the step of 0.1 Å, respectively. The scanning grid based points were generated through 386 transition chemical structures (Figure S1). Two-dimensional potential energy surfaces (PES) were constructed with relaxed scans; the bond lengths and bond angles of the molecules except the each scan point of geometric parameters (Υ1andΥ2) were allowed to relax for each sample conformation.

For obtaining an accurate description of the palladium catalyzed direct C–H arylation of chromone selectivity, characterization of the Potential Energy Surface (PES) using grid based method help us understand overall landscapes of potential energies in the vicinity of energy minima of those catalytic processes. A detailed method is described in the section of computational details (Figure S1 in the Supporting Information). Our calculation results support C2 arylation of chromone through carbopalladation (Figure 5). We can easily notice the potential energy surfaces have three different energy minima. Specifically, C2 region and C3 region have lower energies than those of C6 region. This result suggests palladium catalyzed arylation of chromone would have carbopalladation process. To further investigate the selectivity of C2

region and C3 region of potential energy surfaces, C2 region has lower energy than C3 region by -2.96 kcal/mol. However, this energy gap between C2 selectivity and C3 selectivity is not so large, it can also produce slightly C3-arylation at the temperature of 373K. Detail description of palladium catalyzed C–H arylation shows that benzene is spilt from palladium to attach perpendicularly to the chromone. It should be noted to find the distance of C2-C3 of chromone is extended 1.53 Å during arylation process, which means breaking up double bond of C2-C3 into single bond in the transition state (Figure 5). This extension of C–C bond supports a loss of aromaticity during carbopalladation process.

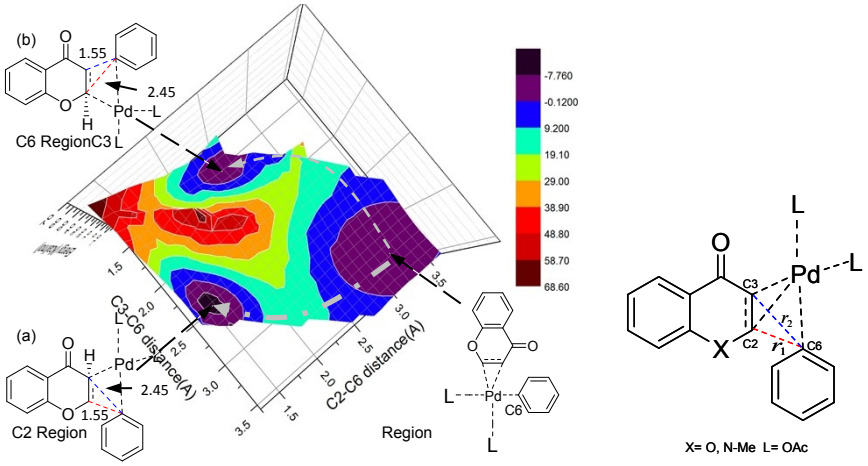


Figure S1. Potential Energy Surface of C–H Regioselectivity of Chromone through Carbopalladation; (a) Arylation of C3 Position, (b) Arylation of C2 Position. The pathway of C2 position is preferred. (G_{rel} in kcal/mol). Schematic Representation of the Palladium Catalysis Geometry. O, Oxygen; N-Me; nitrogen-methyl; L=OTFA, trifluoroacetate. Palladium catalysis geometric parameters considered here are: $\Upsilon 1$, distance between C6 and C2; Υ_2, distance between C6 and C3.

2.2.2 Calculated pathway for the reaction

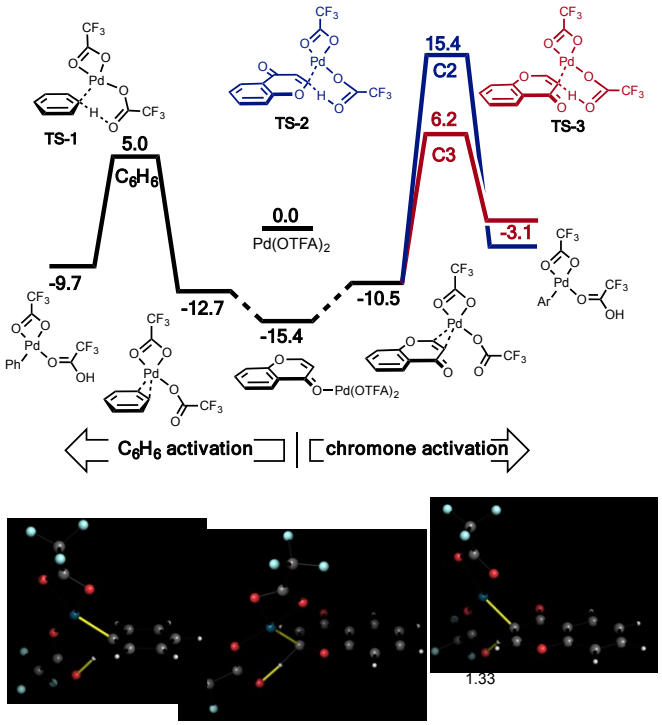


Figure S2. Palladation of benzene (40-fold excess) with $Pd(OTFA)_2$ is marginally faster than for the C3-position of chromone; the process is reversible (G_{rel}(373K) is shown in kcal/mol and has been used throughout). Structures are colored as follows: Pd(dark blue), F(light blue), O(red), C(grey), H(white).

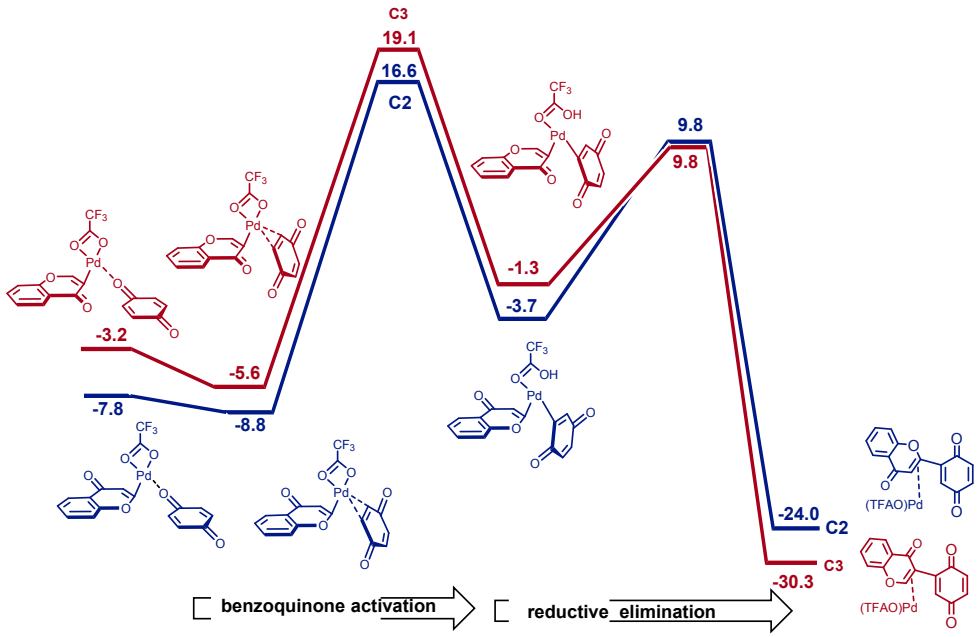


Figure S3. Energy profile of unfavorable pathway for reaction of benzoquinone

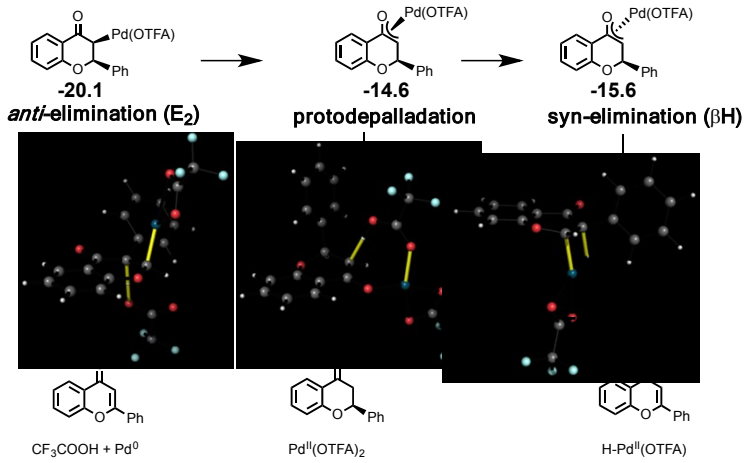


Figure S4. Possible fates for the intermediate of carbopalladation.

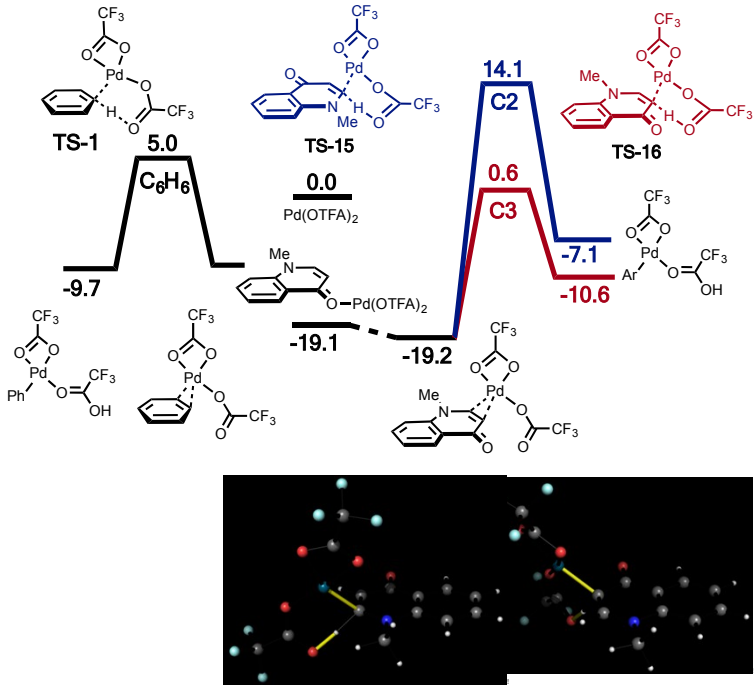


Figure S5. C–H activation of C2 and C3 Positions of enaminone; the process is reversible (G_{rel} shown in kcal/mol) and the C3 position outcompetes benzene activation.

2.2.3 **Calculated frontier orbital and transition state structure**

Table S1. Frontier orbitals of calculated substrates and electrostatic potential map (ESP)

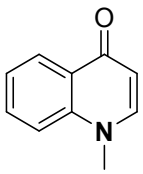
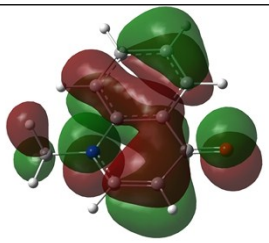
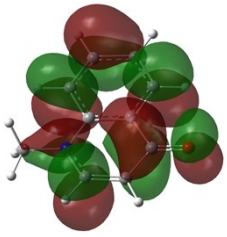
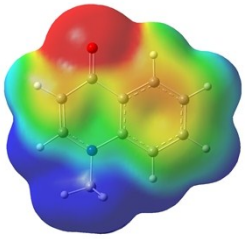
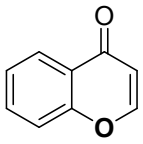
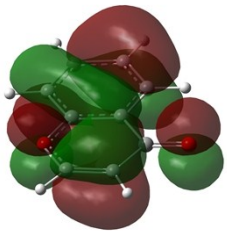
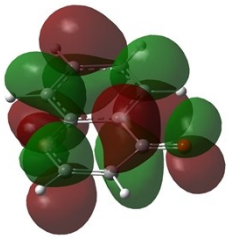
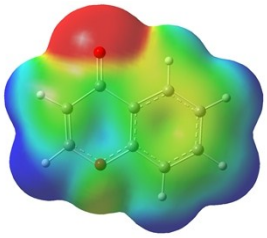
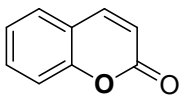
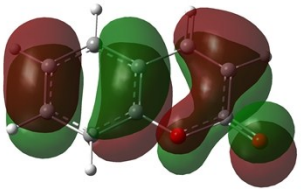
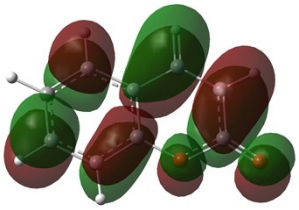
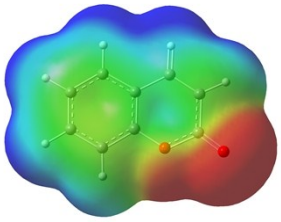
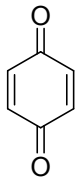
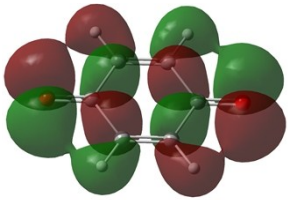
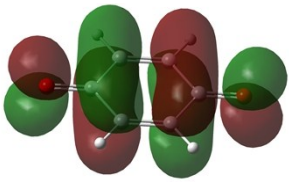
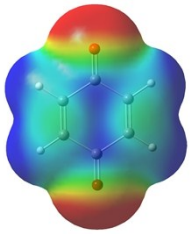
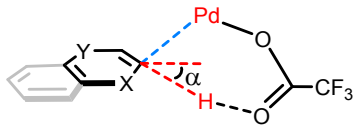
	HOMO	LUMO	ESP
	 -7.95 ev	 0.25 ev	
	 -8.89 ev	 -0.11 ev	
	 -8.79 ev	 -0.39 ev	
	 -9.96 ev	 -2.02 ev	

Table S2. Calculated structure parameters correlated with relative energy in transition states



X&Y=CH,C=O,O,N-Me

	Bond distance(Å)							Angle(degree)		Energy
	Pd-C*i*	Pd-H	C*i*-H	O-H	X-C2	C2-C3	C3-C4	Pd-C*i*-H	Angle α[1]	(kcal/mol)
TS16	2.046	2.399	1.323	1.294	1.334	1.393	1.474	88.1	53.3	0.6
TS3	2.083	2.376	1.293	1.328	1.317	1.374	1.484	86.1	47.7	6.2
TS1	2.081	2.291	1.317	1.329	1.412, 1.395, 1.388			81.4	47.0	7.7[2]
TS15	2.106	2.300	1.338	1.295	1.378	1.37	1.463	80.4	39.8	14.1
TS2	2.104	2.274	1.322	1.318	1.358	1.359	1.474	79.4	37.9	15.4
TS21	2.120	2.240	1.298	1.349	1.496	1.351	1.500	77.8	37.7	14.9
R^2	**0.923**	**0.781**	0.011	0.120	0.362	**0.830**	0.011	**0.877**	**0.992**	-

1. Angle α is the distortion of the C-H bond out of the ring-plane (chromone, benzene, enaminone). [2] this energy is shown before the entropy correlation

2.3 Cartesian coordinates:

Chromone stationary points:

C_6H_6:
E(wB97XD/6-31G(d)&LANL2DZ) = -232.161046983
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.101811
H(wB97XD/6-31G(d)&LANL2DZ) = -232.05136
G(wB97XD/6-31G(d)&LANL2DZ) = -232.077235

C 0.109812 1.388597 -0.000258
C 1.257757 0.599192 0.000107
H 2.238318 1.066461 0.000271
C -0.109919 -1.388634 -0.000084
C -1.257660 -0.599274 -0.000044
C -1.147784 0.789663 0.000106
C 1.147793 -0.789531 -0.000022
H 2.042886 -1.404995 0.000195
H -0.195564 -2.471554 0.000069
H -2.238336 -1.066368 0.000225
H -2.043068 1.404805 0.000319
H 0.195770 2.471574 0.000100

TS1, C6H6_PdOTFA2_CMD_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1410.96565115
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.156726
H(wB97XD/6-31G(d)&LANL2DZ) = -1410.77885
G(wB97XD/6-31G(d)&LANL2DZ) = -1410.870204

Pd -0.219083 -0.169286 -0.127763
O 1.591227 -1.056006 -0.476830
C 2.598016 -0.663555 0.162206
O 2.687918 0.357255 0.881116
C 3.864780 -1.540359 0.067866
H 1.569766 1.035562 0.644306
C 0.565071 1.736455 0.160707
C -0.071334 2.510730 1.155281
H -0.413819 2.031060 2.067244
C 0.171274 4.480150 -0.204119
C 0.795510 3.737703 -1.206143
C 0.991013 2.375771 -1.024104
F 4.072223 -2.130208 1.248022
F 4.921301 -0.779632 -0.222082
F 3.745269 -2.477838 -0.864515
C -2.572271 -0.848655 -0.052370

O -2.197334 0.340129 0.196203
O -1.755202 -1.745044 -0.350626
C -4.076392 -1.146788 0.034600
F -4.332790 -2.412018 -0.276850
F -4.509911 -0.912166 1.277626
F -4.747165 -0.351009 -0.803039
C -0.255398 3.873236 0.978650
H -0.735967 4.464748 1.751259
H 0.017739 5.546224 -0.344360
H 1.127461 4.222698 -2.118451
H 1.497800 1.793885 -1.789719

3, C6H6_PdOTFA2_CMD_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1410.99073596
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.162342
H(wB97XD/6-31G(d)&LANL2DZ) = -1410.797522
G(wB97XD/6-31G(d)&LANL2DZ) = -1410.890577

Pd -0.372696 -0.112385 -0.298050
O 1.531349 -1.055207 -0.504076
C 2.498421 -0.877831 0.220919
O 2.667215 0.064620 1.101477
C 3.709155 -1.829610 0.154205
H 1.928729 0.716602 1.038141
C 0.447908 1.662335 -0.164176
C 0.044989 2.518540 0.863935
H -0.727785 2.209133 1.561145
C 1.582899 4.200070 0.055423
C 1.972092 3.350204 -0.977352
C 1.410091 2.079279 -1.090116
F 3.914442 -2.370011 1.353977
F 4.791890 -1.138348 -0.202337
F 3.492047 -2.789129 -0.729706
C -2.812245 -0.637525 -0.067433
O -2.307441 0.530836 0.018622
O -2.140435 -1.657054 -0.285160
C -4.333843 -0.724920 0.139874
F -4.782504 -1.956668 -0.081805
F -4.636798 -0.382664 1.399574
F -4.966808 0.114687 -0.685183
C 0.622754 3.784187 0.973650
H 0.310516 4.448011 1.774356
H 2.027463 5.186603 0.142961
H 2.714754 3.673896 -1.700585
H 1.721079 1.420749 -1.896862

2, C6H6_PdOTFA2_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1410.99790892
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.162333
H(wB97XD/6-31G(d)&LANL2DZ) = -1410.804878
G(wB97XD/6-31G(d)&LANL2DZ) = -1410.896645

Pd -0.051925 0.159249 -0.223520
O 1.833887 -0.304682 -0.625335
C 2.567047 -0.574205 0.409818
O 2.265627 -0.486556 1.582501
C 3.990904 -0.999747 -0.019788
H 1.542642 1.858813 1.148771
C 0.627219 2.197385 0.674708
C -0.442126 2.658501 1.475465
H -0.374501 2.562931 2.553491
C -1.626420 3.354043 -0.520017
C -0.592194 2.920514 -1.321498
C 0.550617 2.325070 -0.735549
F 3.952845 -1.991100 -0.914584
F 4.705374 -1.401240 1.026409
F 4.618940 0.046496 -0.582170
C -2.184354 -1.025963 -0.070532
O -2.106860 0.236180 0.043574
O -1.159854 -1.712892 -0.286055
C -3.564039 -1.682149 0.073550
F -3.490621 -2.993639 -0.112161
F -4.047682 -1.441648 1.295238
F -4.405015 -1.161782 -0.824811
C -1.550805 3.222689 0.881470
H -2.375814 3.570065 1.494729
H -2.507701 3.801636 -0.967547
H -0.639939 3.034579 -2.399111
H 1.421791 2.099516 -1.342931

1, PdOTFA2:
E(wB97XD/6-31G(d)&LANL2DZ) = -1178.81149962
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.058804
H(wB97XD/6-31G(d)&LANL2DZ) = -1178.733331
G(wB97XD/6-31G(d)&LANL2DZ) = -1178.795663

Pd 0.000003 0.000000 -0.000016
O 1.759972 1.088673 0.038033
C 2.400226 -0.000002 0.041532
O 1.759980 -1.088684 0.038025
C 3.933591 0.000003 0.001876
F 4.409340 1.084385 0.603670
F 4.332278 0.000033 -1.272651
F 4.409344 -1.084406 0.603614
C -2.400223 -0.000020 -0.041544
O -1.759995 1.088669 -0.038056
O -1.759958 -1.088691 -0.038051
C -3.933587 -0.000011 -0.001851
F -4.409385 -1.084607 -0.603201
F -4.332249 0.000469 1.272687
F -4.409344 1.084176 -0.604001

Chromone:
E(wB97XD/6-31G(d)&LANL2DZ) = -496.834375623

ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.129783
H(wB97XD/6-31G(d)&LANL2DZ) = -496.691712
G(wB97XD/6-31G(d)&LANL2DZ) = -496.734359

C -2.342894 -0.151041 -0.000349
C -1.925360 -1.427543 -0.000183
H -2.587759 -2.285252 -0.000793
C 0.335963 -0.858676 0.000213
C 0.028465 0.503644 0.000364
C 1.080413 1.428614 0.000189
H 0.823327 2.483013 0.000328
C 1.657067 -1.308515 -0.000136
H 1.853939 -2.375083 -0.000272
C 2.678728 -0.374186 -0.000321
H 3.710089 -0.713631 -0.000708
C 2.394507 0.998351 -0.000100
H 3.205142 1.719704 -0.000266
C -1.384180 0.953472 -0.000103
O -1.704557 2.132490 0.000086
H -3.402716 0.072651 -0.001253
O -0.637728 -1.818255 0.000605

TS3, Chromone_PdOTFA2_CMD_C3_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.64541044
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.185075
H(wB97XD/6-31G(d)&LANL2DZ) = -1675.425218
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.52842

Pd -0.532478 0.810867 0.051777
O -2.425607 0.136118 -0.246114
C -2.834211 -0.964846 0.195637
O -2.186265 -1.821797 0.835850
C -4.332263 -1.257799 -0.037862
H -0.924823 -1.408884 0.804347
C 0.284298 -1.045544 0.525023
C 1.061664 -1.035954 1.657971
H 0.783827 -0.505366 2.563397
C 2.739154 -2.381884 0.758604
C 2.070006 -2.483559 -0.459698
C 2.666142 -3.226054 -1.484376
H 2.139905 -3.297495 -2.430510
C 3.967561 -2.990936 0.984672
H 4.451632 -2.880965 1.948568
C 4.538021 -3.722819 -0.046440
H 5.497786 -4.204467 0.110329
C 3.889508 -3.842915 -1.280698
H 4.347199 -4.418701 -2.078202
C 0.769818 -1.798276 -0.657846
O 0.154131 -1.852640 -1.707453
O 2.209151 -1.663740 1.815231
F -5.021147 -0.825251 1.025785
F -4.540338 -2.564424 -0.175546
F -4.783944 -0.634183 -1.120091
C 0.648222 2.949802 -0.100771
O 1.221948 1.869858 0.255163
O -0.564905 2.981386 -0.390395
C 1.513512 4.217358 -0.160227
F 0.780020 5.283967 -0.453663
F 2.109551 4.413473 1.020078
F 2.460549 4.073427 -1.092326

15, Chromone_PdOTFA2_CMD_C3_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.6682454
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.190584
H(wB97XD/6-31G(d)&LANL2DZ) = -1675.441906
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.543429

Pd -1.031638 0.339397 0.246148
O 0.237850 1.938221 0.686547
C 0.877573 2.493149 -0.201285
O 0.536749 2.606810 -1.457073
C 2.082149 3.373534 0.172721
H -0.234674 2.036062 -1.635576
C 0.514480 -0.881112 0.126743
C 0.237047 -2.176629 0.397612
H -0.759427 -2.543372 0.613998
C 2.431362 -2.906441 0.150741
C 2.846797 -1.614490 -0.172785
C 4.206440 -1.395398 -0.447231
H 4.515089 -0.386113 -0.697228
C 3.331050 -3.973189 0.206819
H 2.964725 -4.961813 0.460471
C 4.664705 -3.730937 -0.065371
H 5.375066 -4.550752 -0.024404
C 5.107517 -2.439831 -0.393033
H 6.157731 -2.265374 -0.602167
C 1.881590 -0.498708 -0.224463
O 2.262268 0.626195 -0.559109
O 1.128730 -3.183202 0.421240
F 1.620625 4.606256 0.426189
F 2.959440 3.443698 -0.817534
F 2.670931 2.905304 1.261322
C -3.443039 -0.246869 -0.024339
O -2.480107 -1.080608 -0.110998
O -3.268195 0.963707 0.184755
C -4.854809 -0.831715 -0.192598
F -5.782280 0.115874 -0.111139
F -4.960629 -1.433928 -1.382110
F -5.085723 -1.741434 0.760830

TS2, Chromone_PdOTFA2_CMD_C2_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.62971657
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.184516

H(wB97XD/6-31G(d)&LANL2DZ) = -1675.410013
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.512476

Pd -0.612447 0.682586 0.078750
O -2.569298 0.168494 0.272885
C -2.990664 -0.874348 -0.291395
O -2.306508 -1.753490 -0.858660
C -4.521730 -1.065982 -0.230531
H -1.056022 -1.450675 -0.573070
C 0.157023 -1.269462 -0.078643
C 0.322308 -1.876794 1.126135
H -0.482690 -1.856102 1.853478
C 2.591456 -2.515199 0.427564
C 2.317750 -1.868677 -0.782641
C 3.274936 -1.793540 -1.796347
H 3.027553 -1.281365 -2.719442
C 3.855715 -3.094159 0.613920
H 4.048306 -3.591393 1.558963
C 4.810631 -3.023669 -0.380813
H 5.787642 -3.471601 -0.233416
C 4.514797 -2.369485 -1.586726
H 5.267095 -2.311240 -2.367039
O 1.111329 -1.290398 -1.044415
C 1.566105 -2.582723 1.482334
O 1.718979 -3.139565 2.556864
F -4.886559 -1.237181 1.041782
F -5.130235 0.016051 -0.712451
F -4.902171 -2.124716 -0.933301
C 0.659437 2.755440 0.068549
O 1.211776 1.621542 -0.081206
O -0.582162 2.847755 0.213607
C 1.539489 4.012712 0.112362
F 0.906627 5.040218 -0.446531
F 1.805796 4.313216 1.387354
F 2.687016 3.806195 -0.527650

14, Chromone_PdOTFA2_CMD_C2_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.66442521
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.189747
H(wB97XD/6-31G(d)&LANL2DZ) = -1675.438727
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.543316

Pd 0.920237 0.370983 0.153415
O 0.027101 2.286638 -0.054937
C -1.089128 2.776649 -0.135575
O -2.233758 2.192034 0.036059
C -1.241232 4.281058 -0.444774
H -2.109861 1.247511 0.322178
C -0.749625 -0.595252 0.344864
C -1.635661 -0.412866 1.361020
H -1.402237 0.268626 2.173737
C -2.993008 -2.227157 0.387778
C -2.028671 -2.313961 -0.615128
C -2.126184 -3.238291 -1.652173
H -1.350650 -3.273916 -2.409133
C -4.086841 -3.099914 0.342593
H -4.828139 -3.022837 1.131323
C -4.201197 -4.024962 -0.679458
H -5.048709 -4.701727 -0.710832
C -3.217652 -4.091800 -1.675087
H -3.305347 -4.821215 -2.474170
O -0.930108 -1.483238 -0.634426
C -2.844950 -1.239074 1.480060
O -3.651235 -1.119233 2.387415
F -0.093357 4.780112 -0.873364
F -2.176941 4.462823 -1.372683
F -1.607454 4.910811 0.672387
C 3.202571 -0.598673 0.121123
O 2.136722 -1.290047 0.232717
O 3.190355 0.641884 0.037140
C 4.531951 -1.365901 0.034815
F 4.458611 -2.534460 0.669680
F 4.816872 -1.600034 -1.253161
F 5.522177 -0.650930 0.563551

12, Chromone_PdOTFA2_COIp:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.68443619
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.190815
H(wB97XD/6-31G(d)&LANL2DZ) = -1675.458041
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.561218

Pd 1.101557 0.177869 -0.427139
C 3.328212 -0.737527 -0.170125
O 2.350496 -1.518684 -0.338534
O 3.155030 0.510086 -0.134619
C 4.731908 -1.320424 0.040223
C -2.044878 -1.983720 2.206086
C -1.149779 -1.393488 1.387099
H -1.842407 -2.240583 3.238182
H -0.168776 -1.128930 1.759516
C -3.717249 -2.042928 0.593916
C -2.878135 -1.435869 -0.346447
C -1.520312 -1.080785 0.038082
O -0.768093 -0.544172 -0.811738
C -3.383339 -1.170874 -1.632098
C -5.032786 -2.391031 0.283865
C -5.504753 -2.120578 -0.986457
H -6.527462 -2.380840 -1.239843
C -4.682026 -1.509792 -1.947857
H -5.073067 -1.303064 -2.938146
H -2.728762 -0.693198 -2.352566
H -5.651489 -2.857720 1.041940
F 4.863054 -2.471175 -0.615407
F 4.917166 -1.550052 1.345970

F 5.664001 -0.470812 -0.379825
O -3.289232 -2.317074 1.856434
C -0.510687 2.292958 0.438155
O 0.335547 2.007257 -0.493124
O -0.877376 1.604515 1.372194
C -1.088734 3.714223 0.237143
F -1.941817 4.027406 1.211108
F -0.113853 4.630258 0.222309
F -1.745806 3.786148 -0.930278

13, Chromone_PdOTFA2_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1675.6750434
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.190086
H(wB97XD/6-31G(d)&LANL2DZ) = -1675.449347
G(wB97XD/6-31G(d)&LANL2DZ) = -1675.551881

Pd 0.969638 -0.205338 -0.293198
C 3.376369 0.174581 -0.009243
O 2.836214 -0.975547 0.110533
O 2.696618 1.181781 -0.289008
C 4.892513 0.271229 0.215415
C -0.082969 -1.948451 0.972221
C -0.085977 -2.087915 -0.416470
H 0.769108 -2.209973 1.592263
H 0.709152 -2.664674 -0.883336
C -2.336717 -1.342889 1.061186
C -2.507479 -1.534120 -0.310638
C -1.380235 -1.991745 -1.149965
O -1.480045 -2.282152 -2.323701
O -1.131501 -1.609794 1.689632
C -3.757302 -1.256356 -0.871327
C -3.357119 -0.871823 1.874910
C -4.585636 -0.593613 1.293410
H -5.389837 -0.208970 1.911778
C -4.789960 -0.788663 -0.076196
H -5.752820 -0.557258 -0.518416
H -3.878460 -1.398383 -1.939670
H -3.168224 -0.709157 2.929338
F 5.524400 -0.583134 -0.592401
F 5.174282 -0.053224 1.481045
F 5.331302 1.499524 -0.023829
C -1.202116 1.439277 0.189402
O -0.643934 0.829568 -0.808145
O -0.886482 1.380762 1.361203
C -2.386881 2.327719 -0.255787
F -3.013521 1.833971 -1.327618
F -3.277373 2.441470 0.731372
F -1.938887 3.551795 -0.560843

10-2, Chromone_PdPhOAc_13_C3_flip:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20333738
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.253509
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.916886
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.012197

Pd -1.218479 0.422510 -0.823820
C -3.453989 -0.196983 0.058862
O -3.459622 0.791242 -0.697657
O -2.389757 -0.824913 0.359580
C -4.765428 -0.736993 0.650848
C 2.568042 -1.737685 0.106485
C 3.539635 -1.234389 -0.763107
C 2.777654 -2.974704 0.716392
C 4.701714 -1.956371 -1.013380
H 3.395627 -0.273708 -1.249594
C 3.937886 -3.700630 0.463377
H 2.028074 -3.370901 1.396768
C 4.901997 -3.191837 -0.402104
H 5.449313 -1.556297 -1.691513
H 4.087174 -4.663849 0.941574
H 5.807585 -3.756585 -0.601912
C 1.309893 -0.951961 0.432123
C 0.690239 -0.326997 -0.795633
H 0.583926 -1.621465 0.900245
C 2.080553 1.225323 1.099859
C 1.760889 1.836951 -0.124885
C 0.924459 1.077820 -1.043166
O 0.187987 1.595311 -1.942247
O 1.584109 0.020396 1.457875
C 2.197135 3.137332 -0.400642
C 2.851413 1.916852 2.033815
C 3.292805 3.198649 1.737746
H 3.896850 3.730665 2.466624
C 2.973760 3.815771 0.522690
H 3.326068 4.819461 0.311125
H 1.916106 3.590866 -1.345844
H 3.082529 1.437378 2.978331
H 0.648270 -0.974016 -1.672638
F -4.627795 -0.965443 1.959974
F -5.082337 -1.893642 0.054015
F -5.766002 0.119728 0.471175

10-1, Chromone_PdPhOAc_13_C2_ii:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20689018
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.254059
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.920206
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.013000

Pd -0.732544 -1.168631 0.082203
C -3.165550 -0.606021 0.076102
O -2.827176 -1.307961 1.042970
O -2.363795 -0.270526 -0.852809

C -4.591553 -0.044056 -0.034474
C 0.943455 1.706459 -0.554669
C 1.828323 2.327497 0.325705
C -0.396250 2.106581 -0.566163
C 1.371389 3.309884 1.202411
H 2.879757 2.062847 0.336189
C -0.852352 3.079224 0.315407
H -1.096920 1.638208 -1.250225
C 0.031448 3.681872 1.207688
H 2.071234 3.783385 1.884501
H -1.900894 3.360730 0.302083
H -0.321572 4.441159 1.898838
C 1.353206 0.584004 -1.495807
C 0.894797 -0.800864 -1.049779
H 0.951794 0.793167 -2.488694
H 0.816897 -1.521146 -1.871383
C 3.574343 -0.034161 -0.793616
C 3.096566 -0.933485 0.180494
C 1.718144 -1.324270 0.055996
O 1.067624 -2.053717 0.844422
O 2.783705 0.561977 -1.706696
C 3.969349 -1.470870 1.140979
C 4.936973 0.279465 -0.825524
C 5.784124 -0.273759 0.120545
H 6.839507 -0.018979 0.093667
C 5.309605 -1.143409 1.115060
H 5.992927 -1.555664 1.849234
H 3.566081 -2.155489 1.880623
H 5.297254 0.969169 -1.580651
F -5.399810 -0.573930 0.877961
F -4.557588 1.285228 0.148968
F -5.100157 -0.282754 -1.247015

TS-12, Chromone_PdPhOAc_C3_bH_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.18735702
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.248617
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.905878
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.001325

Pd -0.588853 -0.392867 -0.060139
C -3.064756 -0.518053 -0.153890
O -2.533613 -0.167596 0.927813
O -2.397917 -0.812967 -1.181027
C -4.597892 -0.573991 -0.259557
C 1.797908 -0.281486 0.045361
C 1.005099 0.031280 1.203030
H 0.970628 -0.705685 2.002127
C 1.996630 2.007314 -0.514949
C 1.248103 2.427467 0.585181
C 0.831303 1.447743 1.613572
O 0.378706 1.763963 2.696388
O 2.388648 0.701906 -0.678768
C 0.934838 3.784958 0.708880
C 2.424507 2.903899 -1.489421
C 2.093810 4.243927 -1.352462
H 2.418307 4.951482 -2.108837
C 1.349166 4.688898 -0.254231
H 1.098084 5.739976 -0.159367
H 0.359450 4.094667 1.575193
H 3.003025 2.539067 -2.330936
C 2.560885 -1.568106 -0.033481
C 1.939318 -2.783783 0.258856
C 3.919873 -1.538794 -0.346103
C 2.676811 -3.960213 0.254413
H 0.872047 -2.810743 0.466426
C 4.653590 -2.721620 -0.351476
H 4.401956 -0.595523 -0.575655
C 4.036615 -3.931355 -0.050268
H 2.185866 -4.902294 0.475858
H 5.711886 -2.693220 -0.591024
H 4.610313 -4.852900 -0.059301
H 0.663766 -0.659591 -1.002038
F -5.030681 0.418423 -1.048491
F -5.175936 -0.446488 0.932247
F -4.985554 -1.734635 -0.797315

Chromone_PdPhOAc_C3_bH_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20237122
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.250303
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.918513
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.013887

Pd -0.275163 0.784725 0.030065
C -2.767741 1.033563 -0.169132
O -2.416542 0.229589 0.716970
O -1.956363 1.679549 -0.898210
C -4.263832 1.287848 -0.424785
C 1.198059 -1.017042 0.342919
C 1.187514 -0.047268 1.359416
H 0.592011 -0.213910 2.252091
C 3.199310 -0.139993 -0.564834
C 3.331035 0.815870 0.441237
C 2.343857 0.863691 1.542219
O 2.466546 1.573109 2.521694
O 2.178775 -1.057165 -0.573125
C 4.416651 1.695756 0.397432
C 4.110774 -0.227470 -1.612536
C 5.175452 0.660593 -1.641780
H 5.893392 0.604010 -2.453770
C 5.332581 1.623631 -0.638192
H 6.168858 2.313743 -0.674583
H 4.505873 2.429709 1.191633
H 3.973479 -0.982558 -2.378639

C 0.304671 -2.193448 0.263266
C -0.732355 -2.374167 1.187818
C 0.486295 -3.135915 -0.757541
C -1.567706 -3.478195 1.092803
H -0.918568 -1.645408 1.967769
C -0.351958 -4.239282 -0.844834
H 1.281365 -3.001002 -1.480742
C -1.379691 -4.413705 0.079041
H -2.372834 -3.599843 1.809494
H -0.203558 -4.964019 -1.639001
H -2.037172 -5.274426 0.005350
H 0.850922 1.502216 -0.690638
F -4.562003 2.568703 -0.177584
F -5.026717 0.520869 0.352249
F -4.566067 1.026727 -1.701966

TS6，Chromone_PdPhOAc_CMD_C3_RE_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.167832
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.251088
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.883547
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.978233

Pd	1.5671576	1.2108638	-0.9092792
C	-0.0419454	2.1429868	-0.1521482
C	-0.6169744	3.1555638	-0.9389672
C	-1.1892944	4.2725458	-0.3414942
C	-1.2223864	4.3895238	1.0476028
C	-0.6718374	3.3829518	1.8350168
C	-0.0874264	2.2640298	1.2453778
O	3.5639976	0.2089888	-1.0829232
C	3.9233066	-0.5475552	-0.1957492
O	3.2388896	-1.0251012	0.7960008
C	5.3742356	-1.0713832	-0.1726832
H	-0.6103754	3.0762918	-2.0229862
H	-1.6125714	5.0557968	-0.9643222
H	-1.6790104	5.2589448	1.5108658
H	-0.6956644	3.4653348	2.9181128
H	0.3230446	1.4730118	1.8646158
H	2.2639786	-0.7596942	0.8154008
C	-0.2397604	0.2781478	-0.7537732
C	-1.1255524	0.1706218	-1.7780452
H	-1.2145774	0.8976118	-2.5752052
C	-2.1542764	-1.7629882	-0.9876302
C	-1.2991974	-1.7908632	0.1164148
C	-1.4565384	-2.8169182	1.0646028
C	-3.1549814	-2.7232512	-1.1623252
H	-3.7963374	-2.6682332	-2.0350202
C	-3.2955844	-3.7145902	-0.2099792
H	-4.0710274	-4.4645662	-0.3319592
C	-2.4469264	-3.7644472	0.9088878
H	-2.5698604	-4.5511752	1.6459448
C	-0.2313854	-0.7957332	0.2360978
O	0.6321576	-0.9032392	1.1248868
F	5.3791196	-2.3946512	-0.3594152
F	5.9410106	-0.8056742	1.0063148
F	6.0932886	-0.5018182	-1.1315152
O	-2.0397934	-0.8067642	-1.9404832
H	-0.7769024	-2.8345702	1.9097618

8(C3), Chromone_PdPhOAc_CMD_C3_RETS_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.21858523
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.253186
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.931632
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.029617

Pd -0.101705 -0.834182 0.442228
C -2.997571 -0.559524 -0.040751
C -4.010909 -0.644234 0.919586
C -5.070473 -1.532139 0.758180
C -5.140380 -2.337026 -0.374400
C -4.147658 -2.243081 -1.347730
C -3.085131 -1.363132 -1.185527
O 1.889310 -1.851453 0.310181
C 2.799567 -1.116451 -0.025473
O 2.711219 0.163069 -0.278746
C 4.236527 -1.642400 -0.195005
H -3.984154 0.002510 1.792509
H -5.847087 -1.584579 1.515426
H -5.967563 -3.028854 -0.502481
H -4.199870 -2.860432 -2.239605
H -2.319092 -1.284789 -1.948126
H 1.761619 0.431106 -0.152240
C -1.844015 0.366821 0.146910
C -1.332382 0.623417 1.432815
H -1.749822 0.158227 2.319815
C -0.180088 2.565081 0.808035
C -0.497889 2.360496 -0.538737
C 0.037330 3.234012 -1.495162
H -0.229671 3.066475 -2.533503
C 0.660284 3.607889 1.202482
H 0.886090 3.732437 2.256028
C 1.183172 4.452245 0.237315
H 1.841124 5.261833 0.537990
C 0.875038 4.267549 -1.116906
H 1.290325 4.935634 -1.864295
C -1.430745 1.279088 -0.953224
O -1.816006 1.171655 -2.106711
O -0.659469 1.759897 1.790592
F 5.047426 -1.009995 0.654924
F 4.655314 -1.414776 -1.440463
F 4.282597 -2.943476 0.047652

TS5, Chromone_PdPhOAc_CMD_C3_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.14804281

ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.246117
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.868241
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.967384

Pd 0.746410 1.299588 0.083435
C -1.090286 1.967769 0.044268
C -1.542605 2.638230 -1.095503
C -2.746393 3.341743 -1.052864
C -3.510149 3.349947 0.111474
C -3.073375 2.651590 1.235044
C -1.872065 1.944656 1.201920
O 2.866006 0.773207 0.166706
C 3.170439 -0.416523 -0.026307
O 2.398610 -1.379418 -0.291267
C 4.671660 -0.779276 0.005556
H -0.961136 2.626307 -2.014651
H -3.090500 3.874246 -1.935121
H -4.452133 3.889612 0.139550
H -3.673117 2.646848 2.140963
H -1.550177 1.376859 2.070864
H 1.178484 -0.954561 -0.300480
C -0.105715 -0.587067 -0.307191
C -0.627459 -0.709956 -1.569770
H -0.124874 -0.337205 -2.456472
C -2.542512 -1.858404 -0.907689
C -2.153854 -1.812768 0.429893
C -3.001278 -2.380664 1.387592
H -2.692167 -2.332155 2.426581
C -3.732443 -2.454131 -1.313220
H -3.992285 -2.466801 -2.365945
C -4.552301 -3.015190 -0.346215
H -5.484096 -3.484796 -0.645072
C -4.189382 -2.980018 1.005599
H -4.841449 -3.421989 1.751799
C -0.890513 -1.140213 0.818156
O -0.548405 -1.038560 1.985889
O -1.759649 -1.314765 -1.901944
F 5.124515 -0.876305 -1.253947
F 4.870616 -1.949887 0.612555
F 5.385479 0.150691 0.635885

7, Chromone_PdPhOAc_CMD_C3_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.183928
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.251512
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.898645
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.999385

Pd	1.4697917	1.2182544	-0.3961705
C	0.1369927	2.5922494	0.0307725
C	-0.0902433	3.5921884	-0.9231715
C	-0.8707083	4.7048894	-0.6076355
C	-1.4451213	4.8210384	0.6547335
C	-1.2399843	3.8191344	1.6011325
C	-0.4630773	2.7048234	1.2896975
O	3.3273977	0.0785854	-0.8429145
C	3.9103447	-0.7481976	-0.1531175
O	3.4296597	-1.4715946	0.7948225
C	5.4048037	-1.0323596	-0.4071895
H	0.3421737	3.5118034	-1.9183765
H	-1.0320593	5.4784294	-1.3537115
H	-2.0572503	5.6844224	0.8989085
H	-1.6926313	3.9013414	2.5856335
H	-0.3251163	1.9222174	2.0300935
H	2.4018187	-1.3798356	0.8852545
C	-0.0662243	-0.0447556	-0.4806325
C	-1.1683713	0.1861834	-1.2347045
H	-1.3338933	1.0902674	-1.8056455
C	-2.2309013	-1.8125056	-0.6894305
C	-1.1715013	-2.1661436	0.1487185
C	-1.2404043	-3.3883166	0.8403275
C	-3.3447333	-2.6421876	-0.8519615
H	-4.1447033	-2.3296456	-1.5139735
C	-3.3877113	-3.8370186	-0.1599875
H	-4.2460363	-4.4912946	-0.2778525
C	-2.3347053	-4.2144806	0.6904095
H	-2.3840833	-5.1575016	1.2247905
C	-0.0085043	-1.2807296	0.2736935
O	0.9375417	-1.6289196	1.0091245
F	5.5415777	-2.2478476	-0.9462955
F	6.0868497	-0.9953156	0.7386415
F	5.9192247	-0.1352456	-1.2406695
O	-2.2195343	-0.6478946	-1.3793635
H	-0.4106783	-3.6540386	1.4860495

TS7, Chromone_PdPhOAc_CMD_C2_RETS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.16077053
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.250258
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.876838
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.974222

Pd 0.345701 -1.574316 -0.261236
C -1.631017 -1.885524 0.023246
C -2.029155 -2.497456 1.219289
C -3.199151 -3.248911 1.264431
C -3.994253 -3.374379 0.126507
C -3.619436 -2.742896 -1.056731
C -2.448846 -1.990387 -1.108105
O 2.523981 -1.119267 -0.451738
C 3.015852 -0.106723 0.011161
O 2.418903 0.836744 0.684675
C 4.518676 0.190979 -0.165574
H -1.433181 -2.375218 2.119287
H -3.497168 -3.726514 2.193226

H -4.914223 -3.949958 0.167657
H -4.244414 -2.827508 -1.941106
H -2.176847 -1.471544 -2.022012
H 1.454394 0.646544 0.806194
C -0.799757 -0.026285 0.229696
C -0.680774 0.548902 1.465721
H -0.375104 -0.060306 2.309673
C -1.587474 2.637087 0.536467
C -1.654958 1.975329 -0.688326
C -2.139035 2.606841 -1.833417
H -2.174921 2.057987 -2.768300
C -2.021630 3.965805 0.607688
H -1.961304 4.463224 1.570319
C -2.506082 4.607074 -0.518499
H -2.841426 5.637460 -0.458764
C -2.563266 3.922401 -1.739405
H -2.944437 4.422998 -2.624224
O -1.242975 0.677024 -0.836144
C -1.070676 1.929286 1.731306
O -0.979598 2.463357 2.828287
F 5.098313 -0.772129 -0.867482
F 4.676060 1.351437 -0.803303
F 5.104492 0.273095 1.029842

9(C2), Chromone_PdPhOAc_CMD_C3_RETS_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.23109159
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.252591
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.945085
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.041142

Pd -0.185790 0.456996 -0.757302
C 2.439865 1.651573 0.242743
C 1.746980 2.800124 0.649818
C 2.389886 4.029462 0.709908
C 3.732394 4.137341 0.353651
C 4.424367 3.003901 -0.061741
C 3.786382 1.768903 -0.116745
O -2.439991 0.377454 -0.882424
C -3.213543 0.120249 0.024396
O -2.996712 -0.452869 1.164919
C -4.700698 0.514909 -0.111863
H 0.692467 2.735035 0.902380
H 1.836985 4.908144 1.027773
H 4.233241 5.099612 0.396436
H 5.471072 3.077889 -0.341309
H 4.333629 0.888986 -0.433459
H -2.068126 -0.841122 1.328967
C 1.754512 0.333782 0.198352
C 0.691838 -0.026911 1.066168
H 0.328771 0.659633 1.826282
C 1.151161 -2.391622 0.520133
C 2.278273 -1.950034 -0.182271
C 3.158214 -2.863341 -0.768147
H 4.019290 -2.489890 -1.311671
C 0.911122 -3.769060 0.628091
H 0.027210 -4.087856 1.170518
C 1.782223 -4.678440 0.059852
H 1.597339 -5.743606 0.150727
C 2.907433 -4.218129 -0.639191
H 3.592569 -4.930376 -1.088900
O 2.566086 -0.638461 -0.351984
C 0.247697 -1.409646 1.130165
O -0.816626 -1.750835 1.683093
F -4.926648 1.096391 -1.284221
F -5.478351 -0.565903 -0.012268
F -5.033755 1.369629 0.860866

TS4, Chromone_PdPhOAc_CMD_C2_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.13567001
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.245644
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.856183
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.954258

Pd -0.779746 1.223697 0.018353
C 1.094641 1.753658 -0.110717
C 1.696017 2.375415 0.982970
C 2.945510 2.975231 0.820940
C 3.594411 2.919926 -0.409396
C 3.000158 2.263833 -1.485440
C 1.753136 1.660177 -1.335853
O -2.934238 0.817837 0.066984
C -3.295158 -0.367141 -0.005698
O -2.561181 -1.399992 0.004018
C -4.803798 -0.647525 -0.176709
H 1.210648 2.389872 1.955169
H 3.417847 3.465382 1.667074
H 4.573356 3.374700 -0.526159
H 3.512018 2.208011 -2.441646
H 1.306070 1.118426 -2.164828
H -1.384295 -1.060653 0.078202
C -0.028955 -0.761954 0.238691
C 0.468845 -0.835055 1.508085
H -0.158819 -0.536838 2.341715
C 2.593699 -1.678019 0.607803
C 1.991276 -1.608318 -0.651990
C 2.690903 -1.972017 -1.805630
H 2.192468 -1.906293 -2.766688
C 3.922010 -2.117434 0.701525
H 4.370000 -2.164001 1.688777
C 4.623071 -2.476200 -0.433105
H 5.650736 -2.816063 -0.356918
C 4.000529 -2.401016 -1.688189
H 4.550310 -2.682064 -2.581410
O 0.711188 -1.182338 -0.829792

C 1.833571 -1.291277 1.808622
O 2.289329 -1.313339 2.942198
F -5.534641 0.378820 0.250670
F -5.061785 -0.840394 -1.477203
F -5.169352 -1.739712 0.493175

6, Chromone_PdPhOAc_CMD_C2_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.16803283
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.251108
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.882484
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.983405

Pd -0.248740 1.565877 -0.176354
C 1.619410 2.181667 -0.011025
C 1.989579 2.881497 1.142043
C 3.229171 3.516397 1.207981
C 4.114057 3.435869 0.136109
C 3.760261 2.713528 -1.001171
C 2.522603 2.076496 -1.072264
O -2.429557 1.060173 -0.352350
C -3.032467 0.057458 -0.017647
O -2.555007 -1.009949 0.555429
C -4.552009 -0.064959 -0.255242
H 1.318055 2.932392 1.995242
H 3.506712 4.063245 2.104894
H 5.082954 3.923239 0.192601
H 4.454701 2.636942 -1.833424
H 2.265882 1.492354 -1.951413
H -1.580951 -0.930629 0.728947
C 0.539486 -0.183211 0.249334
C 0.388791 -0.799342 1.455990
H -0.022151 -0.245941 2.294146
C 1.524845 -2.778506 0.533878
C 1.618204 -2.070922 -0.663502
C 2.216940 -2.625745 -1.793980
H 2.268726 -2.043790 -2.707818
C 2.053587 -4.073540 0.594116
H 1.973741 -4.605266 1.536819
C 2.652227 -4.638125 -0.517585
H 3.061841 -5.641760 -0.467460
C 2.731340 -3.909284 -1.711907
H 3.200389 -4.351433 -2.585531
O 1.120072 -0.799653 -0.797425
C 0.883225 -2.153491 1.712487
O 0.777055 -2.720618 2.789858
F -5.015830 1.028888 -0.842687
F -4.801820 -1.118437 -1.033542
F -5.176113 -0.232010 0.911282

4, Chromone_PdPhOAc_COIp:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20359756
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.252321
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.917195
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.016834

Pd 0.830584 0.341757 0.094845
C 2.767112 -1.301435 0.038927
O 1.671443 -1.885715 0.130915
O 2.900855 -0.044127 -0.023190
C 4.067223 -2.125455 0.036449
C 0.891106 2.291569 -0.004279
C 2.029923 2.869246 -0.562096
C -0.146797 3.085403 0.477731
C 2.119577 4.258177 -0.648070
H 2.845353 2.245616 -0.914826
C -0.040383 4.473865 0.395613
H -1.029153 2.632241 0.916320
C 1.087268 5.061612 -0.170864
H 3.005082 4.710158 -1.086284
H -0.845336 5.096522 0.777357
H 1.164289 6.142993 -0.236860
C -2.443541 -2.966074 -0.241416
C -1.549649 -1.963533 -0.117512
H -2.169872 -4.008485 -0.348831
H -0.486870 -2.184871 -0.115705
C -4.290897 -1.558526 -0.123636
C -3.467995 -0.436088 0.012433
C -2.017144 -0.608256 0.026759
O -1.278605 0.390759 0.159154
C -4.067126 0.829929 0.126369
C -5.681990 -1.447521 -0.141866
C -6.246777 -0.191250 -0.023832
H -7.327329 -0.089882 -0.037291
C -5.441385 0.951795 0.108589
H -5.902759 1.929490 0.196488
H -3.419984 1.695288 0.220147
H -6.283994 -2.342972 -0.248110
F 3.825923 -3.412085 -0.217601
F 4.658231 -2.039106 1.236453
F 4.922409 -1.668655 -0.883190
O -3.772008 -2.812049 -0.247136

11, Chromone_PdPhOAc_CP_C3:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20939986
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.253553
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.922879
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.016769

Pd -0.311706 0.791712 -0.563409
C -2.602158 -0.136094 0.053969
O -1.801536 -0.734578 -0.725873
O -2.374490 0.962806 0.588483
C -3.915511 -0.874459 0.369810
C 1.645075 1.828030 -0.102031

C 1.701767 1.956087 1.307191
C 0.907150 2.792537 -0.835613
C 1.043140 2.992206 1.940465
H 2.281575 1.249490 1.888751
C 0.248016 3.844683 -0.169719
H 0.965060 2.812553 -1.920902
C 0.308608 3.936045 1.206173
H 1.097073 3.074898 3.021056
H -0.301381 4.577251 -0.751175
H -0.206507 4.739790 1.721710
C 2.361544 0.714511 -0.897205
C 1.191198 0.074230 -1.658839
H 3.108703 1.154985 -1.568634
H 1.050787 0.455681 -2.671986
C 2.518148 -1.584191 0.201330
C 1.534325 -2.043087 -0.681464
C 0.976047 -3.310055 -0.536414
C 2.954634 -2.427085 1.232435
C 2.404435 -3.686890 1.387237
H 2.735997 -4.334235 2.192123
C 1.412993 -4.121939 0.499481
H 0.971669 -5.106096 0.623377
H 0.203077 -3.624342 -1.228147
H 3.726695 -2.058679 1.900330
C 3.101978 -0.245289 0.030068
O 4.102578 0.126670 0.613449
O 1.123160 -1.302355 -1.746574
F -4.419020 -1.456261 -0.723476
F -3.682784 -1.833641 1.280263
F -4.836008 -0.047414 0.864676

10, Chromone_PdPhOAc_CP_C2:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.20772888
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.253331
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.92145
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.015047

Pd -0.421751 0.647893 -0.577270
C -2.547926 -0.502326 0.083598
O -1.718936 -1.038102 -0.707917
O -2.385259 0.629244 0.587231
C -3.792033 -1.318969 0.472452
C 1.305364 2.021749 -0.172033
C 1.416287 2.060736 1.238513
C 0.360651 2.863655 -0.807585
C 0.610997 2.907663 1.973065
H 2.144315 1.424452 1.728200
C -0.446815 3.725578 -0.039702
H 0.345537 2.943589 -1.891852
C -0.325528 3.739014 1.335474
H 0.701562 2.929431 3.054171
H -1.160364 4.371538 -0.539481
H -0.955561 4.392629 1.929559
C 2.205454 1.132347 -1.049631
C 1.196365 0.191773 -1.714135
H 2.737383 1.746777 -1.781902
H 0.948864 0.455223 -2.744689
C 3.032873 -0.725420 0.236113
C 2.175911 -1.660897 -0.352478
C 1.395948 -1.278508 -1.549490
O 0.919847 -2.087370 -2.323065
O 3.220453 0.525705 -0.274915
C 2.086010 -2.946591 0.187062
C 3.797559 -1.071284 1.349136
C 3.687585 -2.351037 1.877349
H 4.278878 -2.617475 2.748458
C 2.829377 -3.293485 1.304154
H 2.747648 -4.287862 1.730023
H 1.415322 -3.651434 -0.294025
H 4.471815 -0.335449 1.775097
F -4.106172 -2.211782 -0.464859
F -3.549770 -1.976574 1.616438
F -4.843190 -0.519901 0.666088

10 + AcOH**,** Chromone_PdPhOAc_CP_C3_AcOH:
E(wB97XD/6-31G(d)&LANL2DZ) = -1610.24395404
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.318727
H(wB97XD/6-31G(d)&LANL2DZ) = -1609.897157
G(wB97XD/6-31G(d)&LANL2DZ) = -1609.987166

C -2.679614 0.586026 -0.631144
O -2.114720 -0.486536 -0.276220
O -2.100533 1.693132 -0.655226
C -4.149992 0.481873 -1.070163
C 1.008947 -0.758994 0.939798
C 1.948527 0.247088 1.586050
H 0.364041 -1.332974 1.614425
H 1.819952 0.245209 2.670123
C 2.943126 -1.324732 -0.569433
C 3.761870 -0.505373 0.223053
C 5.090188 -0.279254 -0.141622
C 3.471699 -1.908605 -1.727885
C 4.784185 -1.676038 -2.099916
H 5.187189 -2.124865 -3.001448
C 5.590207 -0.862206 -1.296328
H 6.623338 -0.679321 -1.576423
H 5.704957 0.352038 0.490512
H 2.820359 -2.547246 -2.315874
C 1.561256 -1.611991 -0.142643
O 0.912221 -2.525238 -0.646090
F -4.232066 -0.170835 -2.235175
F -4.863432 -0.197360 -0.160733
F -4.702417 1.683436 -1.219774

C -2.022826 -2.945015 1.310979
O -1.307241 -2.388610 2.124951
O -1.603684 -3.396001 0.136641
H -0.686574 -3.078741 -0.038067
C -3.495691 -3.173429 1.514495
H -4.027342 -2.377251 0.983729
H -3.808732 -4.130788 1.092186
H -3.737270 -3.119379 2.576559
Pd -0.288625 0.573116 0.118313
C 1.467966 1.594215 1.035353
C 0.932001 2.588064 1.894724
C 1.594171 1.887176 -0.347137
C 0.543625 3.811526 1.393007
H 0.834511 2.370710 2.954343
C 1.204556 3.150502 -0.837102
H 2.112928 1.201699 -1.010551
C 0.679174 4.093509 0.021322
H 0.132211 4.562073 2.059860
H 1.318340 3.365386 -1.893923
H 0.365855 5.059338 -0.361277
O 3.343201 0.061697 1.381206

TS-11, Chromone_PdPhOAc_CP_C3_PDM_TFA_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1907.82956968
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.290823
H(wB97XD/6-31G(d)&LANL2DZ) = -1907.495863
G(wB97XD/6-31G(d)&LANL2DZ) = -1907.615759

Pd 1.805607 0.054781 -0.501351
C 4.020541 -0.348290 0.374232
O 3.232009 -1.307318 0.127472
O 3.660166 0.839102 0.164101
C 5.400170 -0.646179 0.975760
C -3.065582 -0.134715 1.897925
C -2.906510 0.838386 2.885002
C -4.118698 -0.015127 0.990130
C -3.775483 1.922935 2.958862
H -2.094632 0.748699 3.604025
C -4.990425 1.066790 1.066083
H -4.265408 -0.765529 0.219617
C -4.819925 2.040644 2.046489
H -3.639704 2.672609 3.732821
H -5.805463 1.149218 0.353127
H -5.501395 2.884164 2.101734
C -2.030882 -1.243788 1.788624
C -0.839742 -0.821897 0.935570
H -1.670864 -1.473605 2.795802
H 0.042374 -0.484644 1.481636
C -2.636707 -2.777962 0.042444
C -1.696258 -2.256265 -0.857747
C -0.655694 -1.374755 -0.321154
O 0.338574 -1.119006 -1.111600
O -2.641494 -2.464931 1.355727
C -1.734977 -2.641336 -2.201794
C -3.594026 -3.691210 -0.402572
C -3.617461 -4.061182 -1.739867
H -4.369181 -4.767014 -2.080579
C -2.694008 -3.535960 -2.648382
H -2.725472 -3.828661 -3.692435
H -0.994300 -2.229994 -2.879258
H -4.307297 -4.086944 0.312195
F 5.906403 -1.757291 0.446875
F 6.235323 0.363089 0.755710
F 5.270393 -0.819498 2.295463
C -0.394122 2.135519 -0.806427
O -1.316525 1.597337 -0.121197
O 0.753517 1.741292 -1.054958
H -1.121849 0.589693 0.293182
C -0.815898 3.492840 -1.412886
F 0.203877 4.084626 -2.020460
F -1.271944 4.294668 -0.451024
F -1.790782 3.288805 -2.301879

TS-8, Chromone_PdPhOAc_Heck_C3_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.16782572
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.250914
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.883967
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.977891

Pd -0.662479 0.102312 -0.520189
C -3.053939 -0.352098 0.147342
O -2.420730 -1.173023 -0.572913
O -2.566269 0.709423 0.590566
C -4.529182 -0.658581 0.461102
C 0.708290 1.582713 -0.124648
C 1.247160 1.463509 1.160864
C 0.514101 2.838407 -0.701790
C 1.538968 2.614041 1.885546
H 1.429913 0.486472 1.597811
C 0.815544 3.981183 0.032607
H 0.117428 2.928482 -1.708411
C 1.328763 3.870632 1.322158
H 1.939892 2.525208 2.890532
H 0.653294 4.959241 -0.409435
H 1.572232 4.765474 1.886328
C 1.396369 0.298512 -1.571674
C 0.711586 -0.953334 -1.620613
H 1.234867 0.961588 -2.415709
H 0.143591 -1.253672 -2.497549
C 3.127266 -0.845525 -0.192861
C 2.271258 -1.951916 -0.155274
C 2.544371 -3.040190 0.672054

C 4.279423 -0.848361 0.603337
C 4.556715 -1.921022 1.431372
H 5.443589 -1.915259 2.056115
C 3.682838 -3.015196 1.462396
H 3.896329 -3.858464 2.111863
H 1.861203 -3.882280 0.676056
H 4.930798 0.018443 0.554916
O 1.168421 -2.056268 -0.951569
C 2.808792 0.308293 -1.051148
O 3.593480 1.183850 -1.347427
F -5.316917 0.071240 -0.343601
F -4.819986 -1.945867 0.270213
F -4.822905 -0.345355 1.725864

TS-9, Chromone_PdPhOAc_Heck_C2_TS:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.17221909
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.25111
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.888164
G(wB97XD/6-31G(d)&LANL2DZ) = -1380.982298

Pd -0.328401 0.372108 -0.589757
C -2.597691 -0.324912 0.184085
O -1.989669 -1.013579 -0.679782
O -2.123449 0.714923 0.696664
C -4.009418 -0.783370 0.587673
C 0.891999 1.985322 -0.182552
C 1.305038 2.113236 1.145374
C 0.573984 3.121476 -0.935219
C 1.345063 3.372773 1.734191
H 1.581764 1.233130 1.718596
C 0.616029 4.378059 -0.339693
H 0.291069 3.024125 -1.980642
C 0.999292 4.502321 0.994353
H 1.645155 3.473618 2.772705
H 0.354587 5.259519 -0.917259
H 1.037710 5.483606 1.457110
C 2.058806 0.634774 -1.220423
C 1.156693 -0.273883 -1.865909
H 2.468945 1.468439 -1.774864
H 0.836089 -0.018847 -2.875103
C 2.779636 -1.018891 0.288140
C 1.983662 -2.007790 -0.293226
C 1.270041 -1.725435 -1.562250
O 0.801875 -2.589798 -2.275146
O 2.952126 0.212050 -0.300332
C 1.893064 -3.255168 0.329560
C 3.476307 -1.248355 1.470055
C 3.361434 -2.490161 2.080018
H 3.893309 -2.677564 3.007501
C 2.569970 -3.495145 1.514480
H 2.486166 -4.459604 2.003917
H 1.273076 -4.012339 -0.139220
H 4.093213 -0.459111 1.886054
F -4.048100 -2.107502 0.760226
F -4.878800 -0.462222 -0.381244
F -4.409231 -0.200254 1.717333

5, Chromone_PdPhOAc_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1381.19806632
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.251738
H(wB97XD/6-31G(d)&LANL2DZ) = -1380.912452
G(wB97XD/6-31G(d)&LANL2DZ) = -1381.008865

Pd -0.790259 -0.238961 0.237397
C -3.281121 -0.060271 -0.056813
O -2.861372 -1.214880 0.177281
O -2.533910 0.956322 -0.147574
C -4.785631 0.164519 -0.290754
C 0.596300 1.146723 0.124416
C 1.033762 1.769457 1.287677
C 1.089824 1.514036 -1.122133
C 2.001029 2.770137 1.196644
H 0.656643 1.467107 2.260413
C 2.062256 2.510503 -1.199636
H 0.738880 1.025515 -2.027170
C 2.520784 3.134418 -0.042333
H 2.353886 3.255157 2.102062
H 2.461523 2.795213 -2.168775
H 3.282076 3.905857 -0.106428
C 0.496724 -2.044808 -0.374492
C 0.632582 -1.748535 0.974590
H -0.313385 -2.646010 -0.775720
H -0.040185 -2.209416 1.693597
C 2.639528 -1.263533 -0.907199
C 2.917667 -0.952255 0.424317
C 1.925100 -1.229127 1.484179
O 2.139025 -1.058724 2.669521
O 1.446886 -1.833456 -1.291231
C 4.140505 -0.345821 0.728089
C 3.550435 -1.004628 -1.925614
C 4.756915 -0.405165 -1.599725
H 5.474089 -0.190552 -2.385718
C 5.053711 -0.069283 -0.273977
H 5.996844 0.410701 -0.035393
H 4.334770 -0.094709 1.765399
H 3.295396 -1.261948 -2.947679
F -5.504128 -0.877579 0.123303
F -5.010668 0.336904 -1.601428
F -5.209190 1.254341 0.353435

Benzoquinone
E(wB97XD/6-31G(d)&LANL2DZ) = -381.3147464
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.08655

H(wB97XD/6-31G(d)&LANL2DZ) = -381.217769
G(wB97XD/6-31G(d)&LANL2DZ) = -381.254925

C	0.6687742	-1.2699605	0.0000981
C	-0.6687758	-1.2699655	0.0000431
C	-0.6687668	1.2699655	0.0000531
C	0.6687702	1.2699685	0.0000921
H	1.2547232	-2.1843145	0.0001841
H	-1.2547248	-2.1843195	0.0001311
H	-1.2547318	2.1843095	0.0001311
H	1.2547342	2.1843135	0.0001671
C	1.4441552	-0.0000005	-0.0000519
O	2.6611512	0.0000025	-0.0003899
C	-1.4441568	-0.0000095	-0.0001179
O	-2.6611518	0.0000105	-0.0003399

Benzoquinone_COlp
E(wB97XD/6-31G(d)&LANL2DZ) = -1560.152535
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.146953
H(wB97XD/6-31G(d)&LANL2DZ) = -1559.982366
G(wB97XD/6-31G(d)&LANL2DZ) = -1560.063018

Pd	1.3139553	0.3594195	-0.8689046
C	3.5528203	-0.5167875	-0.6501336
O	2.5820563	-1.3114545	-0.8007486
O	3.3528713	0.7279455	-0.6108306
C	4.9704433	-1.0759245	-0.4720836
C	-1.8153947	-1.7422555	1.8361014
C	-0.9480547	-1.1682535	0.9949624
H	-1.5586607	-1.9739475	2.8644354
H	0.0570873	-0.8897615	1.2922184
C	-3.5820647	-1.7706485	0.0071374
C	-2.7092487	-1.2102105	-0.8370016
C	-1.3457607	-0.8815045	-0.3909246
O	-0.5774277	-0.3873455	-1.2302986
F	5.1441793	-2.1440555	-1.2468086
F	5.1354703	-1.4407465	0.8039374
F	5.8803413	-0.1591985	-0.7786586
C	-0.3493347	2.4639345	-0.0499186
O	0.5516333	2.1865035	-0.9320226
O	-0.7960767	1.7490035	0.8285694
C	-0.9002477	3.8965275	-0.2462956
F	-1.6464957	4.2638965	0.7925594
F	0.0847253	4.7853405	-0.3954726
F	-1.6677377	3.9315245	-1.3470226
H	-2.9502147	-0.9637825	-1.8655726
H	-4.5975327	-2.0211375	-0.2819046
C	-3.1985137	-2.0901365	1.4110234
O	-3.9828167	-2.6169455	2.1736584

Benzoquinone_pi
E(wB97XD/6-31G(d)&LANL2DZ) = -1560.149886
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.147
H(wB97XD/6-31G(d)&LANL2DZ) = -1559.980021
G(wB97XD/6-31G(d)&LANL2DZ) = -1560.058432

Pd	0.9032603	-0.0124461	-0.2938447
C	3.2952343	0.4216579	-0.0813357
O	2.7907323	-0.7356331	0.0946983
O	2.5686773	1.3917379	-0.3921157
C	4.8085103	0.5878819	0.1200663
C	-0.0470717	-1.7470161	0.7056123
C	-0.1844947	-1.8908691	-0.6638817
H	0.8177443	-2.1380281	1.2374143
H	0.5488953	-2.4259221	-1.2644037
C	-2.5071227	-1.1124631	0.8817573
C	-2.6398347	-1.2324251	-0.4456597
C	-1.5215457	-1.6612181	-1.3210737
O	-1.6610117	-1.8771021	-2.5046477
F	5.4593723	-0.3364121	-0.5868207
F	5.0991853	0.4233559	1.4121903
F	5.2039563	1.7927679	-0.2658917
C	-1.2562707	1.6686649	0.1119533
O	-0.6931557	1.0156089	-0.8600567
O	-0.9830927	1.6042889	1.2917503
C	-2.4162977	2.5505939	-0.4038777
F	-3.4086997	1.7666339	-0.8588837
F	-2.9000807	3.3106129	0.5710063
F	-2.0144987	3.3361779	-1.4041077
C	-1.2307557	-1.4068361	1.5739173
O	-1.1276437	-1.4620921	2.7788223
H	-3.5755227	-1.0258151	-0.9536157
H	-3.3284697	-0.8057051	1.5210283

TS-15, Benzoquinone_CMD
E(wB97XD/6-31G(d)&LANL2DZ) = -1560.11343
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.141405
H(wB97XD/6-31G(d)&LANL2DZ) = -1559.939287
G(wB97XD/6-31G(d)&LANL2DZ) = -1560.036992

Pd	-0.5903063	0.8769410	-0.0915484
O	-2.5444613	0.3870600	0.1166326
C	-2.9137123	-0.8099040	-0.0202644
O	-2.1852583	-1.8105670	-0.1686204
C	-4.4450463	-1.0107550	-0.0216414
H	-0.9256103	-1.3379480	-0.0703764
C	0.3119307	-1.0242040	0.1655946
C	0.6908317	-1.2947350	1.4346006
H	0.0392927	-1.1123940	2.2860996
C	2.9288887	-2.1754140	0.6235356
C	2.5603547	-1.9315740	-0.6396924
C	1.2422257	-1.3296520	-0.9710764
O	0.9295057	-1.0891740	-2.1202124
F	-4.9902133	-0.3730110	1.0129486

F	-4.7593923	-2.2979640	0.0526226
F	-4.9443343	-0.5072260	-1.1517654
C	0.6412687	2.9356460	-0.4919854
O	1.2230727	1.8132390	-0.3573334
O	-0.6056023	3.0234430	-0.4151034
C	1.5132487	4.1720840	-0.7531274
F	0.7715777	5.2705720	-0.8097254
F	2.4111877	4.3016490	0.2261316
F	2.1622987	4.0232670	-1.9097414
C	2.0304817	-1.8738960	1.7627206
O	2.3473907	-2.0777110	2.9179856
H	3.2057007	-2.1477150	-1.4856454
H	3.8946797	-2.6000560	0.8789876

16(C2)

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.350821
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.236756
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.089133
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.173199

Pd	2.0958384	-1.1658357	-0.2662514
C	3.6951464	-3.0260717	0.1445706
O	2.4289044	-3.1583807	0.1811856
O	4.2499334	-1.9437797	-0.1165524
C	4.5425454	-4.2595837	0.4957196
C	1.5338884	3.1195253	-0.9456524
C	0.7408164	1.6914223	0.9986446
C	0.7894504	4.1395823	-0.5034404
H	2.1520234	3.1769103	-1.8355604
C	-0.0011206	2.7109913	1.4452816
H	0.7903674	0.7369233	1.5145796
H	0.7594464	5.1015953	-1.0049844
H	-0.5962586	2.6436023	2.3499826
C	0.1521314	-1.2340897	-0.1946374
C	-0.5283136	-2.2156857	0.4295556
C	-1.8010846	-0.0185887	-0.6950944
C	-2.6013706	-0.9660557	-0.0616224
C	-1.9884636	-2.1792897	0.5356506
O	-2.6513326	-3.0443737	1.0862426
C	-3.9810386	-0.7367337	0.0043326
C	-2.3353776	1.1432553	-1.2519094
C	-3.7029696	1.3499983	-1.1712584
H	-4.1326256	2.2497383	-1.6009534
C	-4.5302276	0.4094973	-0.5431944
H	-5.5999496	0.5829723	-0.4879244
H	-4.5914186	-1.4858867	0.4984636
H	-1.6753696	1.8534743	-1.7399434
F	3.8970534	-5.3890247	0.2101766
F	4.8120214	-4.2459397	1.8084606
F	5.6954934	-4.2442517	-0.1707654
O	-0.4446386	-0.1752127	-0.7906024
C	1.5063044	1.8183183	-0.2536994
O	2.1175104	0.8742073	-0.7664324
C	-0.0538636	4.0083303	0.7179226
O	-0.7477556	4.9262153	1.1060476
H	0.0043044	-3.0477747	0.8736606

17(C3)

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.353537
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.237203
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.079869
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.183322

Pd	1.8257604	-0.9555393	-0.3419341
C	3.4797624	-2.6582483	0.4352369
O	2.2156934	-2.8145873	0.4855299
O	4.0180274	-1.6307113	-0.0081811
C	4.3288434	-3.8191703	0.9788839
C	1.2120654	3.1428937	-1.5522231
C	1.7630014	2.1476807	0.7168209
C	1.1299254	4.3572237	-0.9997951
H	1.0428524	2.9578407	-2.6075491
C	1.7034134	3.3642717	1.2666799
H	1.9862234	1.2538787	1.2928179
H	0.8839384	5.2445517	-1.5742581
H	1.8738794	3.5322537	2.3248619
C	-0.6255946	-2.3519183	-0.3577531
C	-0.1415586	-1.0923613	-0.2871521
H	0.0024094	-3.2334033	-0.4085781
C	-2.8611106	-1.7160343	-0.2694121
C	-2.4965856	-0.3735023	-0.1627721
C	-1.0727166	0.0276977	-0.1501851
O	-0.7661586	1.2147607	-0.0224431
C	-3.5123866	0.5910497	-0.0696641
C	-4.2007916	-2.1123983	-0.2870991
C	-5.1819406	-1.1425933	-0.1971511
H	-6.2265156	-1.4381183	-0.2111401
C	-4.8408726	0.2144197	-0.0880411
H	-5.6212716	0.9651017	-0.0183361
H	-3.2156356	1.6308547	0.0163019
H	-4.4387966	-3.1670763	-0.3703411
F	3.9634094	-4.9700723	0.4041539
F	4.1449594	-3.9338693	2.3003539
F	5.6228714	-3.6211003	0.7479329
O	-1.9279606	-2.6985803	-0.3563641
C	1.5442844	1.9665117	-0.7297681
O	1.7092224	0.8826147	-1.3062431
C	1.3736234	4.5642017	0.4547129
O	1.3057304	5.6714767	0.9520989

18(C2)

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.352836
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.236419
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.080065

G(wB97XD/6-31G(d)&LANL2DZ) = -1530.181891

Pd	1.9955567	-0.1597038	-0.3652567
C	3.8790687	-1.7864828	-0.3842947
O	2.6767767	-2.1766568	-0.4785827
O	4.1970157	-0.5780278	-0.2989637
C	4.9883887	-2.8501738	-0.3217147
C	-0.6134223	2.5925232	-0.8699907
C	1.8601817	1.9734932	-0.9146487
C	-0.6164913	2.5356922	0.4679043
H	-1.5052013	2.8252942	-1.4434107
C	1.8501487	1.8916822	0.4660583
H	2.7872667	2.0557722	-1.4793597
H	-1.5122283	2.7183552	1.0531243
H	2.7698667	1.8972492	1.0483033
C	0.0710337	-0.4526088	-0.4633127
C	-0.6042253	-0.6846418	-1.6030557
C	-1.8409073	-0.5350088	0.8851603
C	-2.6518003	-0.7698468	-0.2221417
C	-2.0590553	-0.8796868	-1.5773067
O	-2.7276793	-1.0835308	-2.5766207
C	-4.0329943	-0.8852578	-0.0217847
C	-2.3583273	-0.4034688	2.1715213
C	-3.7283753	-0.5206438	2.3428593
H	-4.1495503	-0.4220758	3.3384473
C	-4.5688373	-0.7637278	1.2480783
H	-5.6393183	-0.8569428	1.3990053
H	-4.6548753	-1.0697698	-0.8918257
H	-1.6853233	-0.2088078	2.9995223
F	4.5723797	-4.0162778	-0.8070607
F	5.3516477	-3.0239998	0.9554493
F	6.0553067	-2.4517468	-1.0140767
O	-0.4777683	-0.4039038	0.7567373
C	0.6138907	2.3456812	-1.6692517
O	0.6405377	2.4753332	-2.8742477
C	0.5994367	2.1926672	1.2460023
O	0.6145677	2.1889082	2.4588863
H	-0.0966913	-0.7096608	-2.5601527

19(C3)

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.352062
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.236904
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.078889
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.180525

Pd	1.9727559	-0.0896289	-0.3653923
C	3.7656169	-1.8160229	-0.3859373
O	2.5411389	-2.1387549	-0.4412003
O	4.1543549	-0.6273909	-0.3330243
C	4.8072839	-2.9470639	-0.3376043
C	-0.5525951	2.7605041	-0.5269873
C	1.7958819	1.9703561	-1.1218423
C	-0.2141381	2.8371401	0.7660507
H	-1.5543321	2.9867041	-0.8788273
C	2.1367009	2.0279291	0.2185517
H	2.5487639	1.9339361	-1.9070253
H	-0.9203081	3.1295051	1.5360857
H	3.1755479	2.0158411	0.5436137
C	-0.6115651	-0.7146029	-1.5293483
C	0.0195339	-0.3444289	-0.4005933
C	-2.6762121	-0.9499219	-0.4721113
C	-2.1278331	-0.5831539	0.7596027
C	-0.6934111	-0.2546019	0.8679957
O	-0.1666611	0.0915321	1.9212317
C	-2.9694731	-0.5192559	1.8803277
C	-4.0324301	-1.2546049	-0.6033233
C	-4.8415811	-1.1844979	0.5163307
H	-5.8980151	-1.4169599	0.4251837
C	-4.3136401	-0.8148299	1.7628147
H	-4.9626061	-0.7630389	2.6308297
H	-2.5266521	-0.2314249	2.8282717
H	-4.4197041	-1.5383349	-1.5756523
F	4.3538799	-4.0449819	-0.9404213
F	5.0749309	-3.2431399	0.9401277
F	5.9392029	-2.5702619	-0.9306893
O	-1.9216521	-1.0209619	-1.6039123
C	0.4169209	2.3595301	-1.5757783
O	0.1356249	2.3661081	-2.7571853
C	1.1657759	2.5547391	1.2372597
O	1.5409009	2.8304061	2.3551377
H	-0.1420071	-0.7963659	-2.5025583

TS-13

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.326472
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.235665
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.055368
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.156458

Pd	-1.2425842	-1.0602661	-1.0412356
C	-3.5062612	-1.4981461	-0.1334886
O	-2.9380842	-2.3426961	-0.8827206
O	-2.9694922	-0.4131421	0.1896934
C	-4.9281182	-1.8055401	0.3644894
C	0.0802548	0.4872119	-0.7893036
C	-0.1348482	1.6785019	-1.3853536
C	0.9786118	1.4619459	1.1470234
H	-0.5373412	1.7288069	-2.3901436
C	0.7730778	2.7458969	0.6435214
C	0.8863788	-0.8481611	-2.0255776
C	0.1268808	-2.0484831	-2.2152476
H	0.9424128	-0.1613511	-2.8641786
H	-0.3716812	-2.2147791	-3.1695656
C	2.3867058	-2.1184311	-0.3852146
C	1.6029748	-3.1990271	-0.4831306

C	2.2033128	-0.9391391	-1.2607516
O	3.0538028	-0.0933381	-1.4129656
F	-5.8173692	-1.2556191	-0.4730046
F	-5.1490422	-3.1176671	0.4123934
F	-5.1222892	-1.2948561	1.5800914
C	1.5492208	1.2445979	2.3989834
C	1.9249858	2.3433839	3.1535244
C	1.7341608	3.6446359	2.6690454
C	1.1625548	3.8405899	1.4253004
H	1.6823418	0.2291239	2.7556154
H	2.3710608	2.1911209	4.1313064
H	2.0331888	4.4951619	3.2725754
H	0.9981988	4.8335239	1.0197154
H	1.7628268	-4.0849071	0.1240044
H	3.2257908	-2.0689941	0.3017374
C	0.5142488	-3.3028301	-1.4947906
O	-0.0101332	-4.3673831	-1.7464786
C	0.1641268	2.9367449	-0.6906186
O	-0.0522712	4.0315239	-1.1816816
O	0.6223978	0.3419869	0.4364304

TS-14

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.332655
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.236854
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.060628
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.159105

Pd	-1.1488591	-1.3631943	-0.3901736
C	-3.4606431	-1.5087543	0.4945314
O	-3.0116001	-2.4406313	-0.2244356
O	-2.7768461	-0.5027023	0.8092274
C	-4.9136761	-1.5790083	0.9917114
C	0.2941029	0.0675177	-0.1784066
C	0.8767979	0.0907837	1.0447294
C	0.6442779	2.5047797	-0.2540786
H	1.0252469	-0.7855723	1.6663124
C	1.2107179	2.3974137	1.0171454
C	0.9062889	-1.3923613	-1.5595306
C	0.0649459	-2.5332573	-1.6095936
H	0.8400989	-0.6651743	-2.3652236
H	-0.5788141	-2.6944043	-2.4735276
C	2.4788079	-2.6463883	0.0062964
C	1.6191599	-3.6720733	0.0575314
C	2.2822079	-1.5229703	-0.9429196
O	3.1795349	-0.7740143	-1.2599466
F	-5.6579091	-0.6880783	0.3248184
F	-5.4356621	-2.7885983	0.8065914
F	-4.9721551	-1.2840433	2.2934634
C	0.5470549	3.7746187	-0.8404256
C	1.0044849	4.8914237	-0.1668316
C	1.5705769	4.7567557	1.1087024
C	1.6785429	3.5136657	1.7081954
H	0.1052819	3.8441767	-1.8288186
H	0.9259399	5.8726637	-0.6228316
H	1.9301659	5.6345217	1.6362084
H	2.1121939	3.3854177	2.6936204
H	1.7799339	-4.5286743	0.7056064
H	3.3889689	-2.6183663	0.5981674
C	0.4376379	-3.7653213	-0.8499856
O	-0.1691241	-4.8084613	-0.9775476
C	0.1659819	1.3038517	-0.9650656
O	-0.2846611	1.3345037	-2.1017176
O	1.3409989	1.1899567	1.6481994

20(C2)

E(wB97XD/6-31G(d)&LANL2DZ) = -1530.377762
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.238141
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.104181
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.204689

Pd	1.1667082	0.1316773	-0.8974132
C	2.8491482	-1.3072837	0.2356988
O	3.0807402	-0.0811897	0.0231918
O	1.7759062	-1.8621847	-0.0903492
C	3.9622162	-2.1502657	0.8797208
C	-0.9700848	0.9183063	-0.9455712
C	-0.7278758	-0.0083127	-1.9601512
C	-2.0799118	-0.6637267	0.3882508
H	-0.4437238	0.3369543	-2.9504002
C	-1.9162318	-1.6752287	-0.5585082
C	-0.4813388	2.3535683	-1.0740192
C	0.9989122	2.1079773	-1.4068392
H	-1.0268008	2.8597323	-1.8777112
H	1.2310432	2.1665863	-2.4722632
C	0.3588522	3.4363483	1.1220618
C	1.6390052	3.2861633	0.7575588
C	-0.7671318	3.1464803	0.2089238
O	-1.8960438	3.5159933	0.4482428
F	4.7376952	-2.6675067	-0.0815352
F	4.7241112	-1.4075677	1.6823968
F	3.4467242	-3.1531417	1.5903578
C	-2.6928308	-0.8946697	1.6136428
C	-3.1422968	-2.1761467	1.8954838
C	-2.9859318	-3.2109007	0.9661238
C	-2.3813408	-2.9585117	-0.2531522
H	-2.8051378	-0.0760687	2.3157078
H	-3.6199088	-2.3740267	2.8497468
H	-3.3364828	-4.2094277	1.2040118
H	-2.2461228	-3.7371447	-0.9964672
H	2.4585382	3.5622173	1.4144888
H	0.0797312	3.8411333	2.0905498
C	2.0301192	2.8304173	-0.6050902
O	3.1479352	3.0415533	-1.0314632

C	-1.2872978	-1.3797007	-1.8632422
O	-1.2274398	-2.1717447	-2.7826042
O	-1.6534528	0.6296423	0.1606208

21 (C3)
E(wB97XD/6-31G(d)&LANL2DZ) = -1530.381149
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.238559
H(wB97XD/6-31G(d)&LANL2DZ) = -1530.107166
G(wB97XD/6-31G(d)&LANL2DZ) = -1530.207569

Pd	1.2079734	0.1913156	-0.0800163
C	2.7389894	-1.7418954	0.3090327
O	3.1656514	-0.6584474	-0.1829143
O	1.5484134	-1.9146244	0.6551267
C	3.7428444	-2.8997324	0.4398037
C	-0.7566966	1.0422366	-0.4174003
C	-0.7470866	0.7598416	0.9433007
C	-2.0422246	-1.0657514	-0.6953593
H	-0.4163696	1.4654676	1.6995997
C	-1.9379626	-1.2368794	0.6874537
C	-0.1756786	2.3540006	-0.9511113
C	1.3137194	2.0430176	-0.9183213
H	-0.5524186	2.4699146	-1.9713493
H	1.7675084	1.8393296	-1.8910543
C	0.2690644	4.1650866	0.8290197
C	1.5670074	3.8347826	0.8858387
C	-0.6743886	3.5349856	-0.1235373
O	-1.8287306	3.9002926	-0.2023763
F	3.9386064	-3.4553224	-0.7635343
F	4.9165754	-2.4599864	0.8960617
F	3.2905814	-3.8401554	1.2677417
C	-2.6805016	-2.0595024	-1.4486743
C	-3.1885086	-3.1866024	-0.8294253
C	-3.0669946	-3.3357854	0.5580397
C	-2.4439346	-2.3646644	1.3249697
H	-2.7550816	-1.9151074	-2.5213233
H	-3.6777636	-3.9568744	-1.4159233
H	-3.4628476	-4.2223844	1.0428687
H	-2.3343696	-2.4613714	2.3990517
H	2.2471714	4.3170836	1.5827017
H	-0.1590966	4.9248716	1.4773667
C	2.2079274	2.8789106	-0.0641333
O	3.4203814	2.8273526	-0.1414263
C	-1.4909026	0.1364776	-1.3459923
O	-1.6035976	0.3861716	-2.5314223
O	-1.3472586	-0.2960504	1.4973187

Enaminone stationary points:

Enaminone:

E(wB97XD/6-31G(d)&LANL2DZ) = -516.286390271
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.171569
H(wB97XD/6-31G(d)&LANL2DZ) = -516.099532
G(wB97XD/6-31G(d)&LANL2DZ) = -516.147319

C	-2.052089	1.120728	0.000210
C	-2.218677	-0.221587	-0.000156
H	-3.209072	-0.665041	-0.000255
C	0.124769	-0.666258	-0.000440
C	0.377076	0.719702	-0.000162
C	1.700017	1.177327	0.000193
H	1.847898	2.252623	0.000395
C	1.207922	-1.564463	-0.000407
H	1.040292	-2.635311	-0.000719
C	2.504870	-1.082203	-0.000022
H	3.329513	-1.788959	-0.000001
C	2.761697	0.293275	0.000303
H	3.783563	0.658825	0.000692
C	-0.726199	1.712883	-0.000022
O	-0.517881	2.922150	0.000039
N	-1.190299	-1.123422	-0.000817
C	-1.470251	-2.548695	0.000750
H	-1.053625	-3.030014	-0.890274
H	-1.053982	-3.028027	0.893033
H	-2.550480	-2.698600	0.000637
H	-2.913771	1.777000	0.000411

TS-17, Enaminone_PdChromOC3OAc_CMD_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.61122541
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.288352
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.287003
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.386926

Pd	0.566293	-0.366126	-0.052471
C	-1.327209	0.123326	-0.026383
C	-2.189841	1.162347	-0.002273
C	-4.089289	-0.307667	0.021820
C	-3.236587	-1.438535	-0.001867
O	2.519312	-1.303654	-0.061624
C	3.520234	-0.568102	-0.054233
O	3.543856	0.693353	-0.070903
C	4.895719	-1.260967	0.042828
H	-1.867431	2.198881	0.001190
H	2.316112	1.092362	-0.062137
C	1.112631	1.691700	-0.030314
C	0.881552	2.352998	1.193740
H	1.112780	1.839699	2.123022
C	0.092187	4.315057	0.042916
C	0.326111	3.695170	-1.185237
C	0.831975	2.400540	-1.216837
F	5.853245	-0.532664	-0.532098
F	4.873926	-2.460329	-0.536382

F 5.210403 -1.422970 1.336597
C 0.375029 3.647001 1.234865
H 1.022459 1.923738 -2.174276
H 0.119086 4.224864 -2.110615
H -0.297834 5.329133 0.071210
H 0.206192 4.139415 2.188093
C -3.779566 -2.734602 0.001505
C -5.484487 -0.518141 0.048128
C -5.143230 -2.923233 0.027813
H -5.564164 -3.923082 0.030890
C -5.989762 -1.802521 0.050880
H -7.066354 -1.943292 0.072445
H -3.086743 -3.569984 -0.016587
H -6.171840 0.319115 0.066616
C -1.809803 -1.210692 -0.027884
O -0.902047 -2.098544 -0.050404
N -3.552704 0.970159 0.020213
C -4.431978 2.130125 0.044176
H -5.084433 2.143523 -0.834672
H -5.046978 2.135023 0.949822
H -3.820657 3.032858 0.035723

26, Enaminone_PdChromOC3OAc_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.64435781
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.29417
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.313863
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.41551

Pd 1.055573 0.597089 -0.109359
C -0.754969 -0.090782 0.147800
C -1.254184 -0.308375 1.384929
C -3.316296 -1.174395 0.559194
C -2.849014 -0.991821 -0.758412
O 2.149051 -1.209924 0.196459
C 3.243688 -0.618619 -0.038012
O 3.333636 0.600540 -0.295302
C 4.520318 -1.474757 0.040867
H -0.681709 -0.071900 2.275975
H 1.098475 2.638217 -1.748759
C 0.336064 2.655712 -0.973934
C 0.692713 2.894687 0.371151
H 1.736231 3.044844 0.636778
C -1.640943 3.119876 0.949811
C -1.998570 2.882549 -0.389511
C -1.028036 2.656134 -1.342868
F 4.823567 -1.704724 1.328002
F 5.555075 -0.858805 -0.527577
F 4.344330 -2.652653 -0.561935
C -0.314600 3.125715 1.331543
H -1.296254 2.458084 -2.373527
H -3.046490 2.874730 -0.672399
H -2.417000 3.303772 1.686907
H -0.035013 3.327180 2.360688
C -3.675276 -1.340189 -1.836382
C -4.604904 -1.705641 0.764909
C -4.937234 -1.858853 -1.629690
H -5.568096 -2.127840 -2.470714
C -5.395808 -2.039600 -0.318229
H -6.385401 -2.450978 -0.142350
H -3.273808 -1.186346 -2.832768
H -4.986502 -1.859694 1.767583
C -1.508276 -0.432925 -1.042150
O -1.100954 -0.260828 -2.192507
N -2.501117 -0.829260 1.626264
C -2.946588 -1.038013 2.993041
H -3.853241 -0.460518 3.202912
H -3.146796 -2.098013 3.180904
H -2.162035 -0.709684 3.675479

TS-18, Enaminone_PdChromOC2OAc_CMD_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.59330551
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.287876
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.269537
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.371076

Pd 0.707878 -0.570304 -0.554845
C -1.226925 -0.645399 -0.234983
C -1.551775 -1.723102 0.534503
C -3.920361 -1.132322 0.265679
C -3.519000 -0.009357 -0.481252
O 2.842157 -0.806660 -0.820377
C 3.547102 -0.403600 0.126603
O 3.171661 0.256126 1.132273
C 5.061912 -0.686769 0.034530
H -0.779665 -2.314929 1.019989
H 1.929567 0.623778 0.917884
C 0.793647 1.235109 0.542026
C -0.150267 1.440711 1.574038
H -0.434317 0.607057 2.208072
C -0.346712 3.764102 0.972702
C 0.592241 3.596658 -0.046108
C 1.151075 2.344355 -0.260033
F 5.650733 0.333967 -0.605947
F 5.301258 -1.805011 -0.647309
F 5.610248 -0.799322 1.242158
C -0.713460 2.691536 1.786777
H 1.902486 2.215554 -1.035316
H 0.885877 4.441410 -0.661665
H -0.788858 4.742037 1.141189
H -1.438581 2.834840 2.581672
C -2.932385 -2.105505 0.787883
O -3.259454 -3.103981 1.419988
C -4.496936 0.898051 -0.929514

C -5.277934 -1.332239 0.541991
C -5.832390 0.677754 -0.639998
H -6.571712 1.392232 -0.990056
C -6.235130 -0.441863 0.095448
H -7.285805 -0.605292 0.312171
H -4.218390 1.781695 -1.490739
H -5.538151 -2.213896 1.119195
N -2.166305 0.187415 -0.775288
C -1.792265 1.252376 -1.692849
H -1.928995 2.236032 -1.230809
H -0.741815 1.137911 -1.952886
H -2.387584 1.190093 -2.608683

25, Enaminone_PdChromOC2OAc_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.64457476
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.29323
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.314838
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.416624

Pd 1.016332 0.545666 -0.098415
C -0.745815 -0.185536 0.324111
C -1.283423 0.147543 1.522215
C -3.372361 -0.924754 0.788904
C -2.731755 -1.284387 -0.411017
O 3.282687 0.713154 -0.302140
C 3.296964 -0.473134 0.087135
O 2.249068 -1.133718 0.358841
C 4.639411 -1.199910 0.281301
H -0.726713 0.744104 2.235448
H 0.793788 2.057427 -2.294316
C 0.065372 2.241369 -1.508242
C 0.465498 2.872099 -0.309764
H 1.506232 3.153400 -0.167248
C -1.847009 3.079685 0.353712
C -2.248863 2.459718 -0.841454
C -1.309144 2.049158 -1.765331
F 5.649229 -0.492360 -0.218724
F 4.614966 -2.391584 -0.324044
F 4.861801 -1.395046 1.586238
C -0.508053 3.294091 0.616037
H -1.619628 1.583621 -2.695242
H -3.304504 2.295484 -1.031626
H -2.596072 3.382898 1.077663
H -0.197301 3.783801 1.532801
C -2.654431 -0.190827 1.857992
O -3.197515 0.136607 2.909037
C -3.463817 -1.967624 -1.400374
C -4.718712 -1.255708 0.980728
C -4.794718 -2.280436 -1.184625
H -5.344126 -2.804991 -1.961001
C -5.433673 -1.929377 0.009159
H -6.477224 -2.181729 0.166903
H -3.003231 -2.245917 -2.340510
H -5.168520 -0.960322 1.923278
N -1.392080 -0.945731 -0.613024
C -0.707549 -1.425086 -1.804335
H -1.078476 -0.923568 -2.706064
H 0.361798 -1.239037 -1.707931
H -0.848139 -2.504443 -1.907948

TS-16, Enaminone_PdOTFA2_CMD_C3_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1695.10788623
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.227252
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.823973
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.930983

Pd 0.994076 0.526195 -0.092512
O 0.276844 2.432506 -0.292422
C -0.718919 2.829869 0.349724
O -1.452832 2.167418 1.125384
C -1.071031 4.326141 0.214123
H -1.131554 0.927033 0.945817
C -0.842449 -0.236828 0.387828
C -0.790612 -1.265789 1.324844
H -0.034815 -1.247005 2.103944
C -2.617682 -2.472097 0.385708
C -2.729623 -1.517673 -0.637608
C -3.715972 -1.673034 -1.614585
H -3.769645 -0.917223 -2.391112
C -3.493609 -3.563614 0.422099
H -3.425609 -4.313546 1.200806
C -4.468687 -3.692575 -0.555981
H -5.145383 -4.540492 -0.518785
C -4.586255 -2.748824 -1.578146
H -5.354653 -2.857977 -2.336263
C -1.811917 -0.349359 -0.717385
O -1.894866 0.465773 -1.623007
F -0.717778 4.957395 1.341290
F -2.383456 4.477830 0.038747
F -0.434907 4.890219 -0.805279
C 3.138140 -0.706373 -0.230144
O 2.033104 -1.249639 0.101610
O 3.233324 0.500170 -0.512248
C 4.368933 -1.625943 -0.265770
F 4.205620 -2.571424 -1.198341
F 5.475232 -0.944293 -0.538734
F 4.519970 -2.230892 0.919586
N -1.613481 -2.315126 1.366572
C -1.467997 -3.317874 2.418085
H -2.377488 -3.369628 3.022604
H -1.262832 -4.296618 1.977133
H -0.631794 -3.039144 3.058701

24, Enaminone_PdOTFA2_CMD_C2_prod:

E(wB97XD/6-31G(d)&LANL2DZ) = -1695.13274442
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.23354
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.850468
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.960231

Pd 1.106173 0.546604 -0.137412
O -0.172998 2.066688 -0.375847
C -1.300095 2.053961 0.286311
O -1.195559 1.991733 1.674021
C -2.170010 3.272158 -0.115181
H -0.312750 2.327177 1.880979
C -0.415109 -0.672336 -0.007050
C -0.138545 -2.025257 0.027143
H 0.893475 -2.361606 0.044517
C -2.415577 -2.673056 -0.009190
C -2.780903 -1.309906 -0.035478
C -4.150801 -0.962372 -0.062197
H -4.410348 0.089762 -0.069386
C -3.417467 -3.665918 -0.017954
H -3.156985 -4.716964 0.000944
C -4.742708 -3.295052 -0.051421
H -5.507826 -4.064643 -0.058773
C -5.116704 -1.938259 -0.072058
H -6.166721 -1.667115 -0.092597
C -1.761478 -0.297697 -0.022370
O -2.211422 0.932950 -0.038794
F -1.548870 4.396936 0.251217
F -3.365138 3.240465 0.488672
F -2.375599 3.309976 -1.433471
C 3.562853 -0.028628 -0.059566
O 2.621471 -0.884814 0.020435
O 3.368873 1.187186 -0.194307
C 4.988451 -0.596329 0.035659
F 5.907117 0.355225 -0.091924
F 5.161789 -1.197993 1.220896
F 5.186597 -1.510579 -0.923967
N -1.072720 -2.997423 0.032589
C -0.653540 -4.398113 0.076185
H -1.055884 -4.883379 0.968743
H -0.998455 -4.923220 -0.817966
H 0.434367 -4.437218 0.112500

TS-15, Enaminone_PdOTFA2_CMD_C2_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1695.08776723
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.226232
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.823973
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.930983

Pd -0.683105 0.707871 0.158956
O -2.589092 0.020202 0.395899
C -2.952627 -1.000739 -0.239009
O -2.222348 -1.784545 -0.889522
C -4.467115 -1.295228 -0.184213
H -1.011677 -1.445384 -0.579343
C 0.202098 -1.188856 -0.077459
C 0.322092 -1.791353 1.147266
H -0.506316 -1.765303 1.848024
C 2.626374 -2.418310 0.567572
C 2.447400 -1.780879 -0.679279
C 3.527217 -1.739665 -1.583998
H 3.427339 -1.241732 -2.540466
C 3.863642 -3.000212 0.879659
H 3.954626 -3.480654 1.848393
C 4.913684 -2.958923 -0.013146
H 5.867925 -3.411778 0.234270
C 4.734878 -2.320211 -1.247660
H 5.555979 -2.272918 -1.956635
C 1.538618 -2.491865 1.558821
O 1.640722 -3.054587 2.641790
F -4.838398 -1.460346 1.085278
F -5.135676 -0.263399 -0.699852
F -4.770819 -2.390502 -0.868462
C 0.462627 2.864255 0.134154
O 1.065940 1.764258 -0.076530
O -0.769820 2.892768 0.343364
C 1.285820 4.160098 0.169209
F 0.595455 5.161218 -0.371093
F 1.565618 4.466995 1.439052
F 2.428303 4.011334 -0.497268
N 1.222929 -1.212853 -1.002376
C 1.015967 -0.618827 -2.316046
H 1.606550 0.295952 -2.426817
H 1.280198 -1.331352 -3.102492
H -0.039908 -0.367073 -2.424419

23, Enaminone_PdOTFA2_CMD_C3_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1695.11995025
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.231186
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.850468
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.960231

Pd 1.037119 0.370855 0.094327
O 0.054666 2.235081 -0.143497
C -1.064784 2.703097 0.019915
O -2.117295 2.121540 0.492364
C -1.335797 4.172299 -0.368446
H -1.918988 1.174203 0.770771
C -0.635157 -0.633133 0.267403
C -1.308923 -0.486711 1.455509
H -0.848774 0.051779 2.280167
C -3.029423 -2.023591 0.598353
C -2.310571 -2.099578 -0.607364
C -2.824392 -2.874364 -1.661238
H -2.300424 -2.953230 -2.605368

C -4.234294 -2.721102 0.734663
H -4.748665 -2.634655 1.686248
C -4.736681 -3.481898 -0.303419
H -5.674273 -4.016411 -0.192251
C -4.022058 -3.551789 -1.502491
H -4.403344 -4.144487 -2.328500
C -2.535992 -1.221433 1.742194
O -3.122301 -1.166841 2.814972
F -0.241092 4.730172 -0.860962
F -2.301215 4.212781 -1.287250
F -1.731714 4.850659 0.706790
C 3.354900 -0.539689 0.121541
O 2.299885 -1.258228 0.159575
O 3.322815 0.700252 0.069871
C 4.690819 -1.300610 0.106163
F 4.714828 -2.223589 1.069472
F 4.833582 -1.918559 -1.074246
F 5.715944 -0.473393 0.278462
N -1.097174 -1.400653 -0.751393
C -0.354013 -1.547230 -2.000015
H -0.929272 -1.144227 -2.839080
H 0.588618 -1.008606 -1.925165
H -0.129087 -2.601803 -2.179405

22-1, Enaminone_PdOTFA2_COlp:
E(wB97XD/6-31G(d)&LANL2DZ) = -1695.14383934
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.232649
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.873276
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.981614

Pd 1.325929 0.376822 -0.455849
C 3.585454 -0.458058 -0.154422
O 2.695873 -1.227335 -0.614750
O 3.319735 0.736049 0.141773
C 5.003817 -0.992363 0.087359
C -1.590679 -2.837317 1.088725
C -0.710612 -2.023412 0.440009
H -1.241283 -3.572931 1.803978
H 0.350929 -2.107300 0.638690
C -3.480067 -1.884790 0.013304
C -2.626255 -1.015190 -0.695350
C -1.189769 -1.069062 -0.492670
O -0.457033 -0.280787 -1.164621
C -3.176231 -0.056415 -1.565503
C -4.871579 -1.798410 -0.182803
C -5.381907 -0.857574 -1.054124
H -6.456668 -0.795864 -1.193785
C -4.538120 0.023699 -1.747693
H -4.958334 0.768551 -2.414645
H -2.494524 0.619601 -2.068548
H -5.549243 -2.455733 0.348096
F 5.209027 -2.119872 -0.588519
F 5.163402 -1.242646 1.392598
F 5.911230 -0.092047 -0.285642
C -0.574386 2.053266 0.697911
O 0.382021 2.105866 -0.165174
O -0.889197 1.140036 1.439036
C -1.434468 3.338044 0.672217
F -2.106322 3.489807 1.813772
F -0.711625 4.440247 0.462901
F -2.334868 3.236852 -0.325480
N -2.930536 -2.800130 0.902148
C -3.796500 -3.692489 1.664998
H -4.469766 -3.114285 2.303844
H -4.382664 -4.324686 0.992565
H -3.178417 -4.331549 2.295288

22, Enaminone_PdOTFA2_pi:
E(wB97XD/6-31G(d)&LANL2DZ) = -1695.14458929
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.232472
H(wB97XD/6-31G(d)&LANL2DZ) = -1694.874269
G(wB97XD/6-31G(d)&LANL2DZ) = -1694.981252

Pd 1.042408 -0.146665 -0.360651
C 3.466238 0.193959 -0.090932
O 2.905820 -0.947060 0.014584
O 2.813979 1.224327 -0.343394
C 4.985987 0.248481 0.125581
C -0.176801 -1.829852 1.056386
C 0.009490 -2.008255 -0.334983
H 0.642506 -2.027406 1.740512
H 0.828321 -2.652721 -0.648626
C -2.471586 -1.237837 0.808982
C -2.427944 -1.527363 -0.565670
C -1.185269 -2.010809 -1.213461
O -1.141760 -2.384764 -2.369876
C -3.567216 -1.335406 -1.346490
C -3.644352 -0.729922 1.373050
C -4.761708 -0.533041 0.573280
H -5.661212 -0.121891 1.019464
C -4.732948 -0.841251 -0.785859
H -5.609737 -0.674258 -1.402069
H -3.494011 -1.564208 -2.404189
H -3.692674 -0.462835 2.420660
F 5.595430 -0.624944 -0.679672
F 5.266066 -0.079142 1.392924
F 5.461645 1.463338 -0.117383
C -1.156619 1.493706 0.195162
O -0.596825 0.916703 -0.808945
O -0.848750 1.424407 1.374014
C -2.354722 2.377042 -0.226095
F -2.996451 1.885241 -1.289121
F -3.233402 2.480966 0.776362
F -1.923628 3.607735 -0.530512

N -1.322873 -1.457302 1.610257
C -1.355504 -1.093736 3.025648
H -1.505085 -0.014581 3.109029
H -2.149833 -1.643558 3.534958
H -0.397856 -1.352781 3.476392

TS-19, Enaminone_PdPhOAc_CMD_C3_RETS_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.62313
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.292732
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.295009
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.394673

Pd	1.5865866	-1.7312091	0.3571715
C	-0.3521074	-2.2423481	0.2741495
C	-0.8869214	-2.9114041	1.3890495
C	-1.8824764	-3.8691081	1.2307195
C	-2.3803104	-4.1641331	-0.0375775
C	-1.8679014	-3.4976391	-1.1471405
C	-0.8647204	-2.5429681	-0.9985095
O	3.7122726	-1.2841091	-0.1769535
C	3.9581976	-0.7470131	-1.2457345
O	3.1465076	-0.2282501	-2.1081875
C	5.4235996	-0.6121001	-1.7092815
H	-0.5166304	-2.6913631	2.3876085
H	-2.2703104	-4.3894391	2.1025075
H	-3.1636064	-4.9066580	-0.1575575
H	-2.2505644	-3.7205401	-2.1394665
H	-0.4848374	-2.0092191	-1.8638015
H	2.1572786	-0.2291191	-1.8537105
C	0.1066236	-0.3312931	0.4647685
C	-0.3903744	0.1735069	1.6369765
H	-0.3854794	-0.4261821	2.5397605
C	-1.1039394	2.2358759	0.6946135
C	-0.6048694	1.8108659	-0.5531135
C	-0.7359964	2.6574349	-1.6687135
H	-0.3293964	2.3046989	-2.6101125
C	-1.7319934	3.4934679	0.8008585
H	-2.1261784	3.8371729	1.7497235
C	-1.8536424	4.2958019	-0.3149805
H	-2.3425394	5.2607199	-0.2210315
C	-1.3552794	3.8829009	-1.5605895
H	-1.4556514	4.5270789	-2.4277555
C	0.0818806	0.5274939	-0.6982985
O	0.6244346	0.2284209	-1.7892135
F	5.7553186	0.6801329	-1.7958145
F	5.5811976	-1.1717841	-2.9116945
F	6.2455036	-1.2056711	-0.8519225
N	-0.9578714	1.4039700	1.7889275
C	-1.4329754	1.8226549	3.0998445
H	-0.9385754	2.7481739	3.4097005
H	-2.5165174	1.9768019	3.0889725
H	-1.1977354	1.0443759	3.8258095

29(C3), Enaminone_PdPhOAc_CMD_C3_RETS_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.66988233
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.294551
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.338997
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.443443

Pd -0.154692 -0.995594 0.229458
C -3.076545 -0.495584 -0.055941
C -4.050307 -0.451528 0.946964
C -5.202759 -1.227048 0.858205
C -5.406904 -2.048152 -0.245666
C -4.453287 -2.083419 -1.261399
C -3.299407 -1.314843 -1.171008
O 1.856294 -2.006729 0.159596
C 2.755907 -1.234681 -0.115384
O 2.633725 0.040933 -0.375667
C 4.223176 -1.695349 -0.177874
H -3.920747 0.214893 1.795767
H -5.947558 -1.177390 1.647144
H -6.308163 -2.649423 -0.320510
H -4.609077 -2.713804 -2.131943
H -2.564513 -1.335289 -1.967264
H 1.662664 0.266191 -0.320037
C -1.835722 0.325221 0.053974
C -1.254581 0.564984 1.315160
H -1.675727 0.082142 2.192265
C 0.032888 2.450284 0.588963
C -0.410927 2.231517 -0.733098
C 0.087358 3.032252 -1.767879
H -0.296500 2.843389 -2.765083
C 0.996833 3.446914 0.829918
H 1.372260 3.622794 1.830928
C 1.481389 4.213241 -0.216200
H 2.226518 4.975576 -0.009052
C 1.027994 4.015068 -1.524080
H 1.413289 4.623183 -2.335823
C -1.434531 1.204297 -1.069180
O -1.900713 1.115460 -2.197401
F 4.937661 -1.034863 0.737034
F 4.729232 -1.439052 -1.384550
F 4.311229 -2.995289 0.062038
N -0.468214 1.666461 1.616778
C 0.112440 1.750898 2.944447
H 1.176806 1.483172 2.933964
H 0.000408 2.759895 3.351446
H -0.411969 1.057881 3.603234

TS-20, Enaminone_PdPhOAc_CMD_C2_RETS_opt:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.6075561
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.292327
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.279521

G(wB97XD/6-31G(d)&LANL2DZ) = -1400.38021

Pd 0.311160 -1.634434 -0.312354
C -1.684611 -1.832674 0.062665
C -1.941018 -2.401580 1.322797
C -3.042068 -3.224284 1.525338
C -3.932068 -3.473051 0.482474
C -3.703949 -2.902019 -0.764829
C -2.591216 -2.090767 -0.976152
O 2.502006 -1.201207 -0.462694
C 2.981942 -0.215421 0.068516
O 2.374738 0.697468 0.770477
C 4.489963 0.084519 -0.056283
H -1.282172 -2.193857 2.159983
H -3.211585 -3.662077 2.504568
H -4.802244 -4.101702 0.645070
H -4.393404 -3.087831 -1.583364
H -2.440970 -1.666757 -1.961056
H 1.399907 0.519363 0.866142
C -0.849312 -0.031738 0.122328
C -0.679281 0.453915 1.403967
H -0.477218 -0.234452 2.216475
C -1.410157 2.680077 0.670996
C -1.539352 2.160718 -0.628488
C -1.998313 3.009327 -1.652996
H -2.120235 2.644940 -2.665409
C -1.737088 4.015320 0.927130
H -1.614934 4.364644 1.947420
C -2.187092 4.844521 -0.082640
H -2.433968 5.881398 0.120924
C -2.316830 4.328084 -1.375049
H -2.673194 4.963663 -2.180441
C -0.928132 1.830409 1.781981
O -0.766896 2.262080 2.920274
F 5.095970 -0.876141 -0.740474
F 4.664004 1.245890 -0.690655
F 5.039861 0.169547 1.155212
N -1.200401 0.826809 -0.898390
C -1.073994 0.438103 -2.296434
H -2.045553 0.436428 -2.801639
H -0.403209 1.129480 -2.816470
H -0.633599 -0.558101 -2.348326

30(C2), Enaminone_PdPhOAc_CMD_C2_RETS_prod:
E(wB97XD/6-31G(d)&LANL2DZ) = -1400.67772195
ZPE(wB97XD/6-31G(d)&LANL2DZ) = 0.293787
H(wB97XD/6-31G(d)&LANL2DZ) = -1400.34813
G(wB97XD/6-31G(d)&LANL2DZ) = -1400.449356

Pd -0.352332 0.502642 -0.788209
C 2.388591 1.671178 0.271334
C 3.717432 1.669121 0.713266
C 4.392939 2.864211 0.929323
C 3.750477 4.080990 0.709510
C 2.428578 4.092870 0.275169
C 1.753030 2.895533 0.055623
O -2.604706 0.379446 -0.870713
C -3.344856 0.152594 0.072413
O -3.084583 -0.358917 1.230877
C -4.843381 0.509805 -0.040487
H 4.215232 0.721055 0.897544
H 5.421584 2.845760 1.277159
H 4.277685 5.015234 0.877306
H 1.920330 5.036295 0.100591
H 0.721588 2.902601 -0.289866
H -2.140919 -0.729905 1.392863
C 1.666296 0.367637 0.107309
C 0.613892 0.053887 1.002146
H 0.302187 0.782823 1.746052
C 1.030613 -2.347318 0.613932
C 2.132232 -1.995118 -0.198660
C 2.922020 -3.031014 -0.739898
H 3.777095 -2.799364 -1.363510
C 0.750251 -3.697553 0.872994
H -0.112293 -3.917078 1.493588
C 1.541136 -4.699756 0.351870
H 1.323176 -5.742031 0.559248
C 2.630243 -4.352004 -0.458562
H 3.263614 -5.129730 -0.875421
C 0.155316 -1.313480 1.162551
O -0.904313 -1.598098 1.764286
F -5.111925 1.049942 -1.224553
F -5.593349 -0.585492 0.109157
F -5.177459 1.385908 0.912829
N 2.415654 -0.671323 -0.477934
C 3.253463 -0.359753 -1.631140
H 2.927356 -0.939622 -2.500903
H 3.155381 0.699142 -1.863709
H 4.309448 -0.571130 -1.432433

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