

SUPPORTING INFORMATION

Gold(I)-Catalyzed 1,3-O-Transposition of Ynones: Mechanism and Catalytic Acceleration with Electron-Rich Aldehydes

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I. General procedures and methods

Aldehydes and ketones that were used as co-catalysts in the reactions were used as received from the manufacturers. Unless otherwise noted, reactions were carried out in ambient atmosphere. Other than deuterated solvents were obtained as HPLC-quality grade and used as received. Analytical thin-layer chromatography (TLC) was performed on silica gel 60 F 254 pre-coated plates (0.25 mm thickness) visualizing the reaction progress with UV light at 254 nm. Flash column chromatography was carried out using silica gel (Merck Silica Gel 60 Å, 230 X 400 mesh). ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded with VARIAN 300 MHz spectrometer at 27°C, except for the kinetic experiments. 2D ROESY, HSQC and HMBC experiments were acquired with a Varian INOVA 500 MHz spectrometer. The kinetic experiments were monitored on a Bruker Advance III HD 500 MHz spectrometer equipped with a Prodigy CryoProbe at 298 K. ^1H chemical shifts (δ) are reported in parts per million (ppm) downfield in relation to tetramethylsilane using residual non-deuterated solvent signal as an internal standard (CHCl_3 ; $\delta_{\text{H}} = 7.26$ (CHCl_2); $\delta_{\text{H}} = 6.00$ and CH_2Cl_2 ; $\delta_{\text{H}} = 5.32$) and ^{13}C signal of the solvent for carbon spectra (CHCl_3 ; $\delta_{\text{C}} = 77.16$ and (CHCl_2); $\delta_{\text{C}} = 73.78$). Multiplicities are described according to the abbreviations: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and dq (doublet of quartets). 1,1,2,2-tetrachloroethane (500 MHz, CD_2Cl_2 ; $\delta_{\text{H}} = 6.05$) and 1,2-dichloroethane (500 MHz, CD_2Cl_2 ; $\delta_{\text{H}} = 3.77$) were used as internal standards in kinetic reactions. $^{18}\text{O}[\text{H}_2\text{O}]$ (Min. 98 %; Exp. date: Mar. 10, 2016; Lot. no.: 15-0372) was received from Rotem industries Ltd. (Israel).

II. Preparation of substrates and products

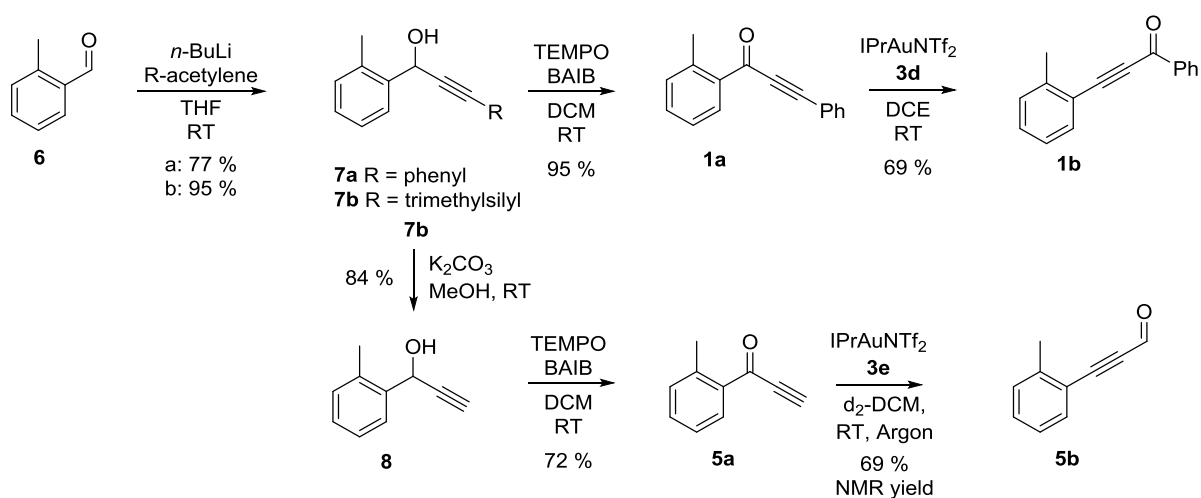


Figure S1. Synthesis of the substrates **1a** and **5a** and the products **1b** and **5b**. THF = tetrahydrofuran, DCM = dichloromethane, DCE = 1,2-dichloroethane, TEMPO = 2,2,6,6-Tetramethyl-1-piperidinyloxy, BAIB = (Diacetoxyiodo)benzene

General procedure A

3-phenyl-1-(*o*-tolyl)prop-2-yn-1-ol (7a). Phenylacetylene (1.647 ml, 15 mmol) was dissolved in dry THF (60 ml) and cooled down to -78°C under argon in a flame dried Schlenk-flask. A 1.6 M $n\text{-BuLi}$ solution in hexanes (8.75 ml, 14 mmol) was added dropwise to the mixture. After the addition, reaction mixture was let to warm at room temperature over 3 h under stirring. *O*-tolulaldehyde (1.159 ml, 10

mmol) dissolved in dry THF (5 ml) was cannulated to the reaction mixture. After the reaction had finished according to TLC monitoring, the reaction was quenched with ice. Additional 60 ml of water was added and the mixture was extracted with DCM (4 x 80 ml). Combined organic phase was dried with MgSO₄, filtered and evaporated. Crude product was purified with flash chromatography using mixtures of Hex(hexane)/EtOAc(ethyl acetate) from 1:0 to 10:1, yielding **7a** (1.72 g, 77 %) as a cream colored solid. ¹H NMR (300 MHz, CDCl₃) δ_H: 7.73 (dq, *J* = 5.8, 3.6 Hz, 1H), 7.50–7.44 (m, 2H), 7.36–7.26 (m, 4H), 7.25–7.18 (m, 2H), 5.85 (d, *J* = 5.6 Hz, 1H), 2.51 (s, 3H), 2.22 (d, *J* = 5.7 Hz, 1H) ¹³C NMR (300 MHz, CDCl₃) δ_{C(H)}: 138.6, 136.3, 132.0, 131.1, 128.8, 128.7, 128.5, 126.8, 126.5, 122.8, 88.8, 86.8, 63.2, 19.2.

General procedure B

3-phenyl-1-(*o*-tolyl)prop-2-yn-1-one (1a). Starting material **7a** (693.3 mg, 3.12 mmol) was dissolved in DCM (31 ml). TEMPO (73.1 mg, 0.47 mmol) and BAIB (1.156 g, 3.59 mmol) were added to the mixture and the mixture was left to stir overnight. Crude product was purified with flash chromatography using mixtures of Hex:EtOAc from 1:0 to 10:1 as eluents to afford the product **1a** as a yellow oil (650 mg, 95 %). ¹H NMR (300 MHz, CDCl₃) δ_H: 8.34–8.27 (m, 1H), 7.70–7.62 (m, 2H), 7.51–7.33 (m, 5H), 7.30–7.26 (m, 1H), 2.68 (s, 3H) ¹³C NMR (300 MHz, CDCl₃) δ_{C(H)}: 180.0, 140.7, 136.0, 133.4, 133.1, 132.4, 130.8, 128.9, 126.1, 120.6, 92.0, 88.6, 22.2.

Preparation of terminal ynone

1-(*o*-tolyl)-3-(trimethylsilyl)prop-2-yn-1-ol (7b). Substrate **7b** was prepared according to general procedure A with **6** (962 μl, 8.32 mmol), trimethylsilylacetylene (1.8 ml, 13 mmol), 1.6 M solution of *n*-BuLi (8 ml, 13 mmol) in hexanes and THF (55 ml in total). Product **7b** was isolated as yellow oil (1.691 g, 93 %). ¹H NMR (300 MHz, CDCl₃) δ_H: 7.69–7.62 (m, 1H), 7.26–7.16 (m, 3H), 5.60 (d, *J* = 5.8 Hz, 1H), 2.44 (s, 3H), 2.07 (d, *J* = 5.9 Hz, 1H), 0.20 (s, 9H).

1-(*o*-tolyl)prop-2-yn-1-ol (8). Starting material **7b** (1.69 g, 7.7 mmol) and K₂CO₃ were stirred in methanol (15 ml) under argon overnight. EtOAc (50 ml) was added to the mixture and the organic phase was washed with water (2 x 20 ml) and brine (20 ml), dried with Na₂SO₄, filtered and evaporated. Obtained product was used in next step without further purification (949 mg, 84 %). ¹H NMR (300 MHz, CDCl₃) δ_H: 7.71–7.64 (m, 1H), 7.27–7.17 (m, 3H), 5.63 (dd, *J* = 5.8, 2.3 Hz, 1H), 2.65 (dd, *J* = 2.3, 0.5 Hz, 1H), 2.45 (s, 3H), 2.13 (d, 1H).

1-(*o*-tolyl)prop-2-yn-1-one (5a). Substrate was prepared according to general procedure B with **8** (949.3 mg, 6.5 mmol), TEMPO (154.6 mg, 989 μmol), BAIB (2.41 g, 7.5 mmol) and DCM (65 ml). Crude product was purified with flash chromatography using mixtures of Hex:EtOAc from 1:0 to 10:1 as eluents to afford the product **5a** as a yellow solid (679 mg, 72 %). ¹H NMR (300 MHz, CDCl₃) δ_H: 8.27 (ddt, *J* = 7.8, 1.6, 0.5 Hz, 1H), 7.47 (td, *J* = 7.5, 1.4 Hz, 1H), 7.38–7.31 (m, 1H), 7.28–7.24 (m, 1H), 3.38 (s, 1H), 2.63 (s, 3H). ¹³C NMR (300 MHz, CDCl₃) δ_{C(H)}: 179.1, 141.1, 135.0, 134.0, 133.5, 126.2, 81.8, 79.7, 22.2. Note: Substrate **5a** evaporates easily from solutions.

Transposition of 1a

1-phenyl-3-(*o*-tolyl)prop-2-yn-1-one (1b). **1a** (150 mg, 0.68 mmol), **3d** (5.8 mg, 38.9 μmol) were dissolved in DCE (7 ml). After the addition of IPrAuNTf₂ (5.9 mg, 6.8 μmol) the reaction was monitored with TLC and after completion the reaction mixture was evaporated. Crude product was purified with flash chromatography using mixtures of Hex:EtOAc from 1:0 to 10:1. Product **1b** was isolated as a yellow solid (103 mg, 69 %). ¹H NMR (300 MHz, CDCl₃) δ_H: 8.27–8.21 (m, 2H), 7.68–7.60 (m, 2H), 7.56–7.48 (m, 2H), 7.42–7.33 (m, 1H), 7.32–7.20 (m, 2H), 2.59 (s, 3H) ¹³C NMR (300 MHz, CDCl₃) δ_{C(H)}: 178.3, 142.4, 137.3, 134.2, 133.9, 131.0, 130.1, 129.8, 128.9, 126.2, 120.3, 92.4, 91.0, 21.1.

Transposition of 5a

3-(*o*-tolyl)propionaldehyde (5b). Reaction was performed in a same manner than the synthesis of **1b** but in this case the reaction was conducted under an argon atmosphere in degassed solvent in a sealed NMR-tube. Reactants were used as follows: **5a** (7 mg, 49 μ mol), IPrAuNTf₂ (6.1 mg, 7 μ mol), **3e** (1.3 mg, 7 μ mol), TCE (7.5 μ l, 70 μ mol) and *d*₂-DCM (700 μ l). Product **5b** was identified from NMR-signals arising at 9.47 (s, 1H) and 2.52 (s, 3H) ppm (300 MHz, CD₂Cl₂).¹

III. NMR kinetic measurements

Standard reaction:

The reaction was prepared in an NMR tube by adding: 150 μ L of a stock solution of the internal standard (102.7 mg of (CH₂Cl)₂ in 5 mL of CD₂Cl₂), 150 μ L of a stock solution of **1a** (177.1 mg of **1a** in 1 mL of CD₂Cl₂), and 300 μ L of a stock solution of IPrAuNTf₂ (17.3 mg of IPrAuNTf₂ in 1 mL of CD₂Cl₂). The NMR tube was vigorously shaken and introduced in to the NMR spectrometer. ¹H NMR spectra were acquired using DS=2, NS=8, D1=18 s, and AQ=3.2 s. The spectra obtained were adequately processed using MestreNova.

Reaction with different [1a]₀:

The reaction was prepared in an NMR tube by adding: 100 μ L of a stock solution of the internal standard (27.7 mg of (CH₂Cl)₂ in 1 mL of CD₂Cl₂), 300 μ L of a stock solution of **1a** (175.6 mg of **1a** in 1 mL of CD₂Cl₂), and 200 μ L of a stock solution of IPrAuNTf₂ (26.2 mg of IPrAuNTf₂ in 1 mL of CD₂Cl₂). The NMR tube was vigorously shaken and introduced in to the NMR spectrometer. ¹H NMR spectra were acquired using DS=2, NS=8, D1=18 s, and AQ=3.2 s. The spectra obtained were adequately processed using MestreNova.

Reaction with different [1b]₀:

The reaction was prepared in an NMR tube by adding: 150 μ L of a stock solution of the internal standard (102.7 mg of (CH₂Cl)₂ in 5 mL of CD₂Cl₂), 150 μ L of a stock solution of **1a** (177.1 mg of **1a** in 1 mL of CD₂Cl₂), 75 μ L of a stock solution of **1b** (176.6 mg of **1b** in 1 mL of CD₂Cl₂), and 225 μ L of a stock solution of IPrAuNTf₂ (23.1 mg of IPrAuNTf₂ in 1 mL of CD₂Cl₂). The NMR tube was vigorously shaken and introduced in to the NMR spectrometer. ¹H NMR spectra were acquired using DS=2, NS=8, D1=18 s, and AQ=3.2 s. The spectra obtained were adequately processed using MestreNova.

Reaction with different [IPrAuNTf₂]₀:

The reaction was prepared in an NMR tube by adding: 100 μ L of a stock solution of the internal standard (44.0 mg of (CH₂Cl)₂ in 1 mL of CD₂Cl₂), 150 μ L of a stock solution of **1a** (175.6 mg of **1a** in 1 mL of CD₂Cl₂), and 350 μ L of a stock solution of IPrAuNTf₂ (22.6 mg of IPrAuNTf₂ in 1 mL of CD₂Cl₂). The NMR tube was vigorously shaken and introduced in to the NMR spectrometer. ¹H NMR spectra were acquired using DS=2, NS=8, D1=18 s, and AQ=3.2 s. The spectra obtained were adequately processed using MestreNova.

IV. ^{18}O -labeling experiment

IV.1. Preparation of $[\text{}^{18}\text{O}]$ -2,4,5-trimethoxybenzaldehyde (**3e'**)

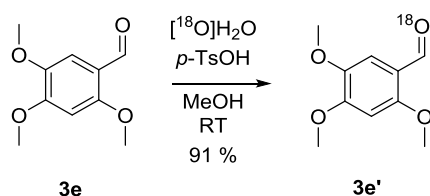


Figure S2. Preparation of $[\text{}^{18}\text{O}]$ -2,4,5-trimethoxybenzaldehyde (**3e'**).² *p*-TsOH = *para*-toluenesulfonic acid, MeOH = methanol

$[\text{}^{18}\text{O}]$ -2,4,5-trimethoxybenzaldehyde (3e'**).** Starting material **3e** (100.6 mg, 0.5 mmol) was dissolved in methanol (5 ml) and stirred for 10 min in room temperature. $[\text{}^{18}\text{O}]\text{H}_2\text{O}$ (153 μl , 7.65 mmol) and *p*-TsOH $\cdot\text{H}_2\text{O}$ (9.8 mg, 0.05 mmol) were added to the mixture and the reaction was stirred. After 24 h ethyl acetate (20 ml) was added to the reaction mixture and the organic phase was washed with water (2 x 10 ml) and brine (10 ml). Organic phase was dried with Na_2SO_2 , filtered and evaporated. Product **3e'** (92 mg, 91 %) was collected as a white solid. The degree of labelling was determined by GC-MS to be 70 %. ^1H NMR (300 MHz, CDCl_3) δ_{H} : 10.32 (s, 1H), 7.33 (s, 1H), 6.49 (s, 1H), 3.97 (s, 3H), 3.92 (s, 3H), 3.88 (s, 3H).

IV.2. ^{18}O -labeling experiment

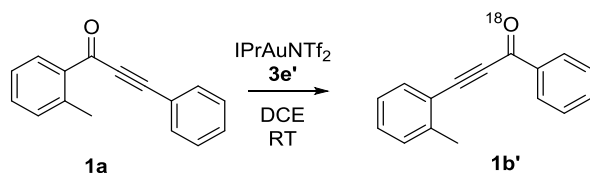


Figure S3. Labelling experiment of substrate **1a**

Substrate **1a** (10 mg 45.5 μmol), **3e'** (9.1 mg, 45.5 μmol) and IPrAuNTf₂ (3.9 mg, 4.54 μmol) were dissolved in DCE (227 μl) and stirred for 10 min. Sample was analyzed with GC-MS and accordingly **1b'** was 37 % and **3e'** 34 % labelled with ^{18}O . See spectra *vide infra*.

IV.3. MS spectra

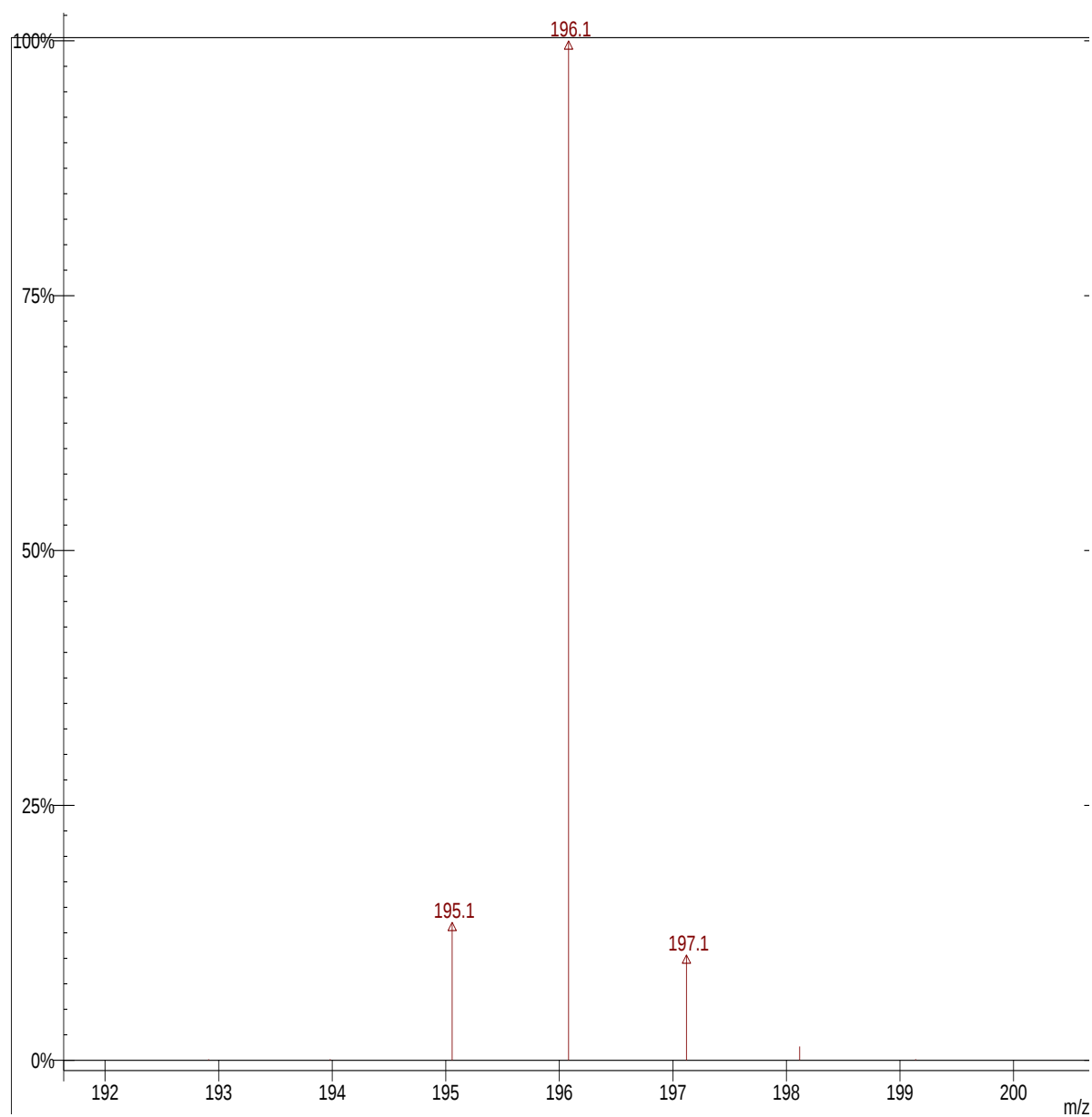


Figure S4. Reference spectrum of unlabeled **3e**

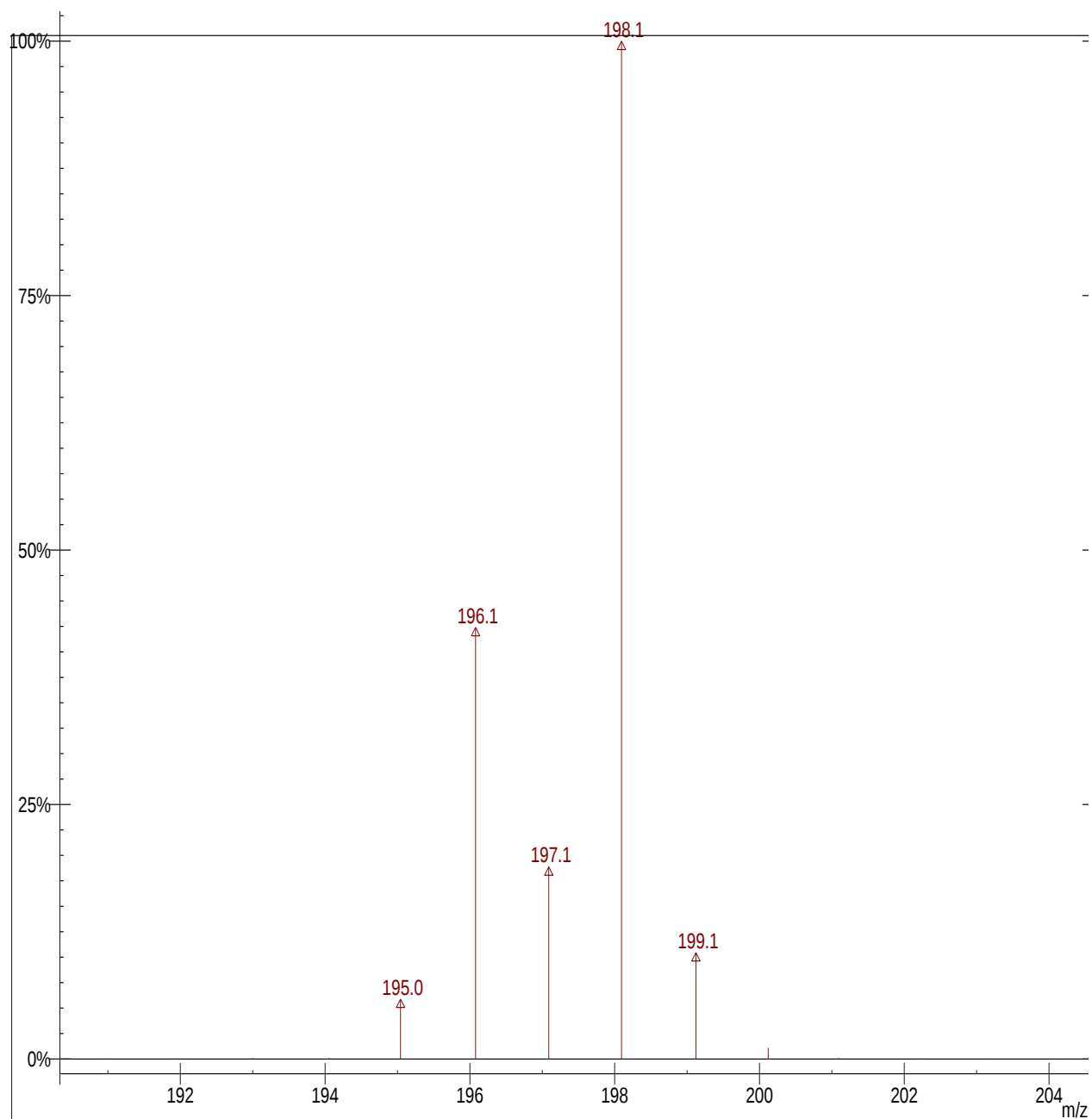


Figure S5. Labelled 3e' ($100/(100+42.5)) \times 100\% = 70.2\%$

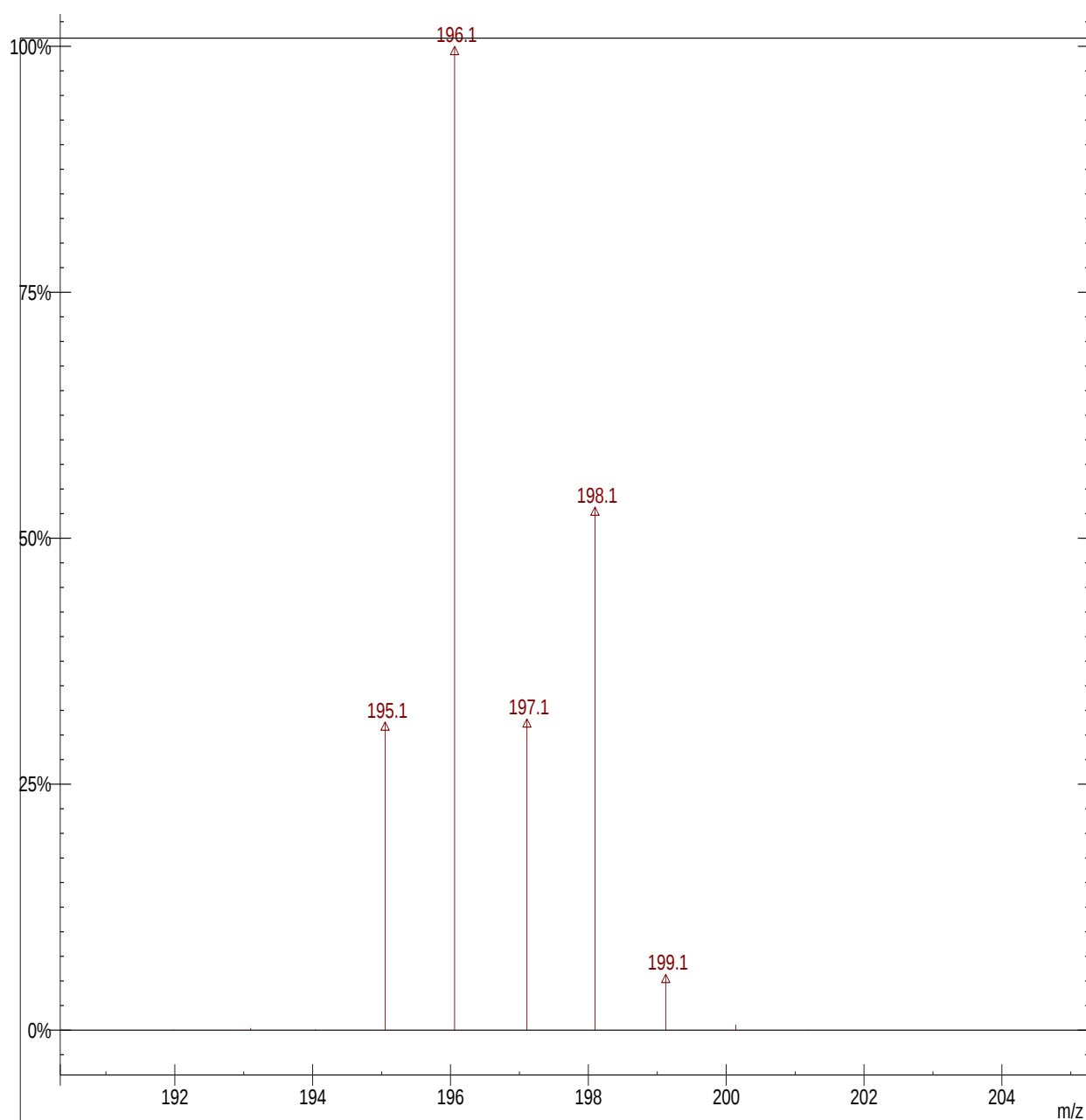


Figure S6. Spectrum of **3e'** after labelling reaction of **1b'** $(52.5/(100+52.5)) \times 100\% = 34.4\%$

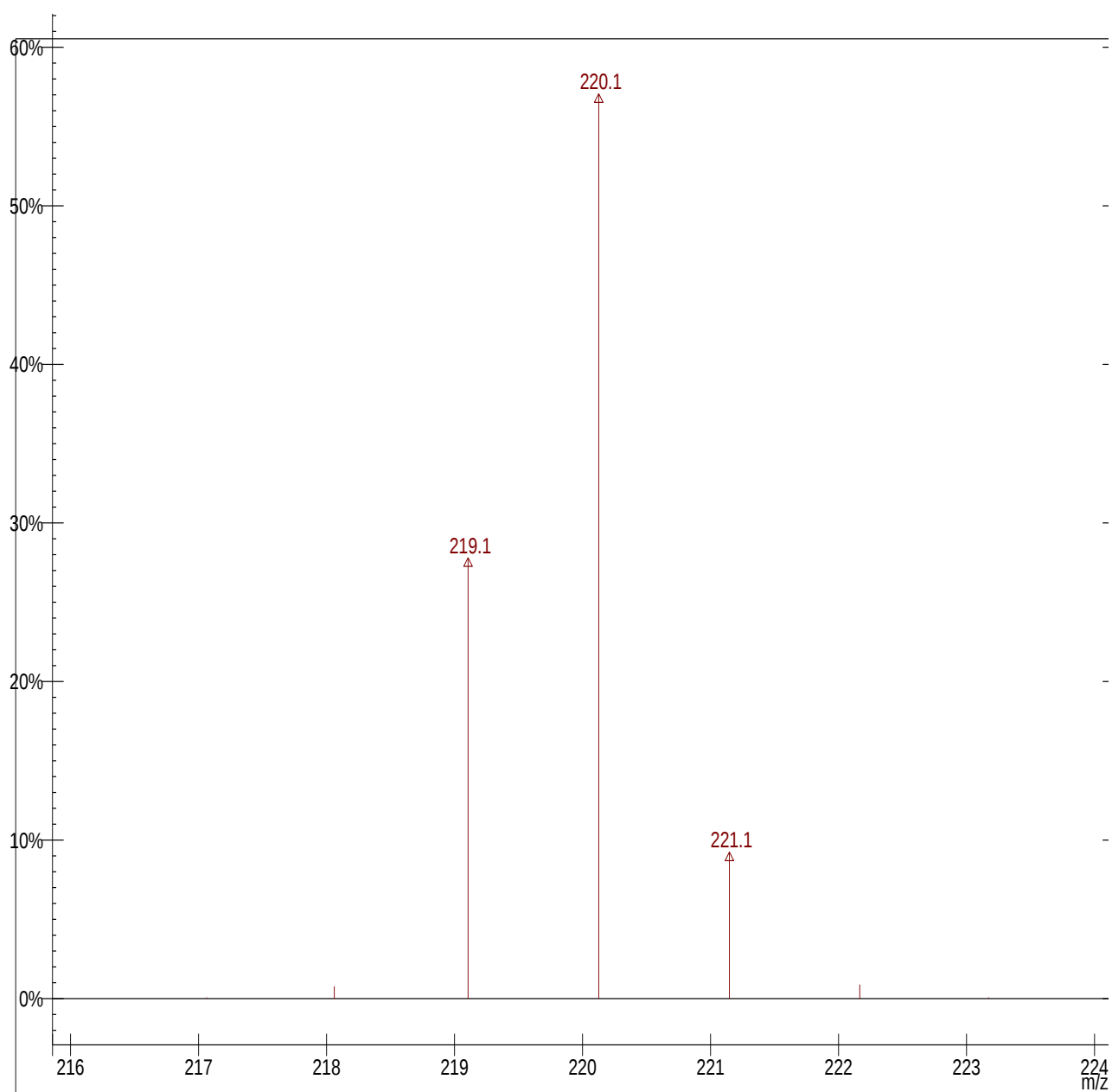


Figure S7. Reference spectrum of unlabeled **1b**

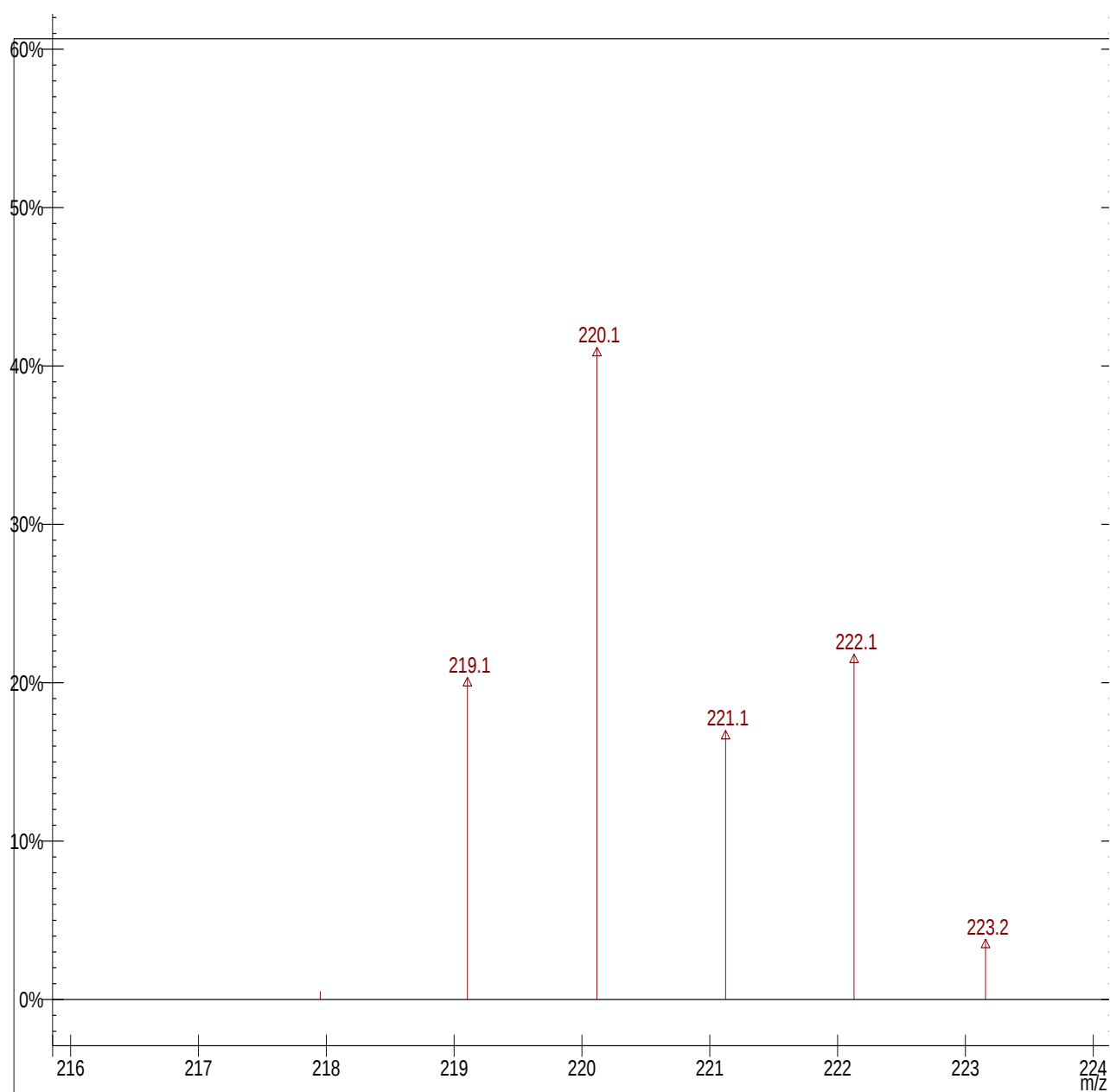


Figure S8. Spectrum of **1b'** after 10 min reaction time $(25/(25+42.5)) \times 100\% = 37.0\%$

V. Effect of **3f**, and synthesis and characterization of acetal intermediate (**4**)

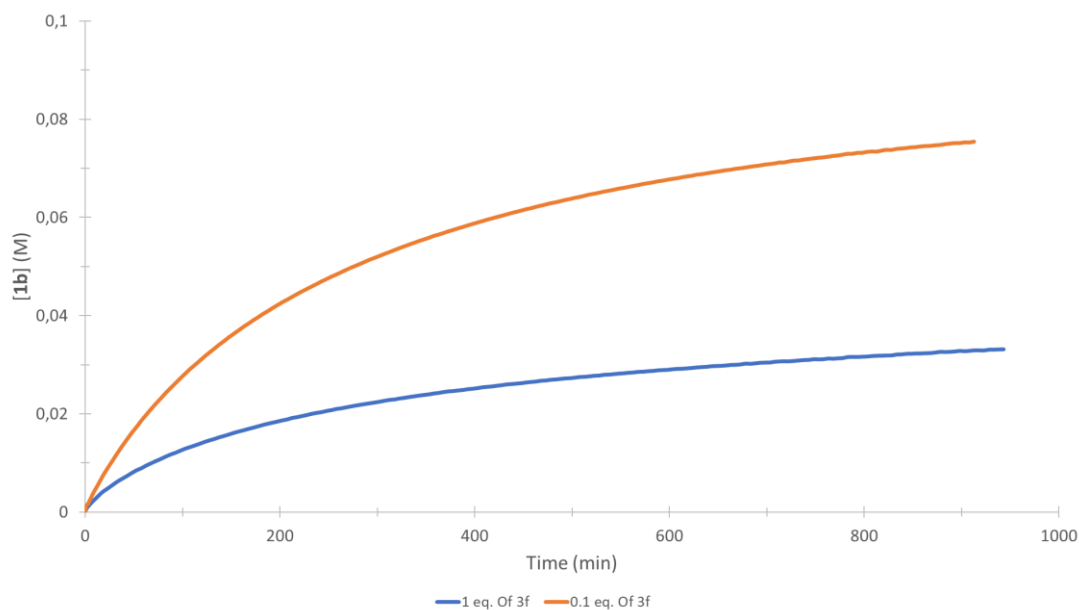


Figure S9. Effect of **3f** on conversion of **1a** to **1b**. 0.1 M solution of **1a** in d_2 -DCM, at 27 °C with 10 mol % of gold.

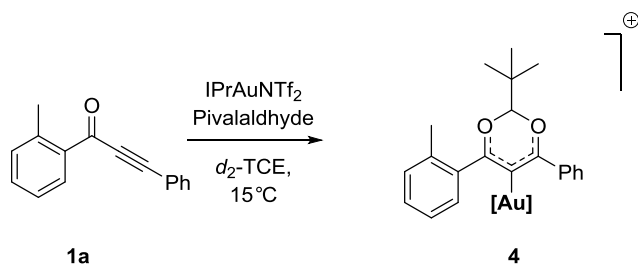
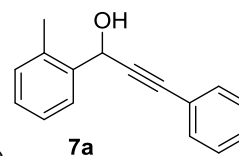


Figure S10. Synthesis of acetal intermediate **4**

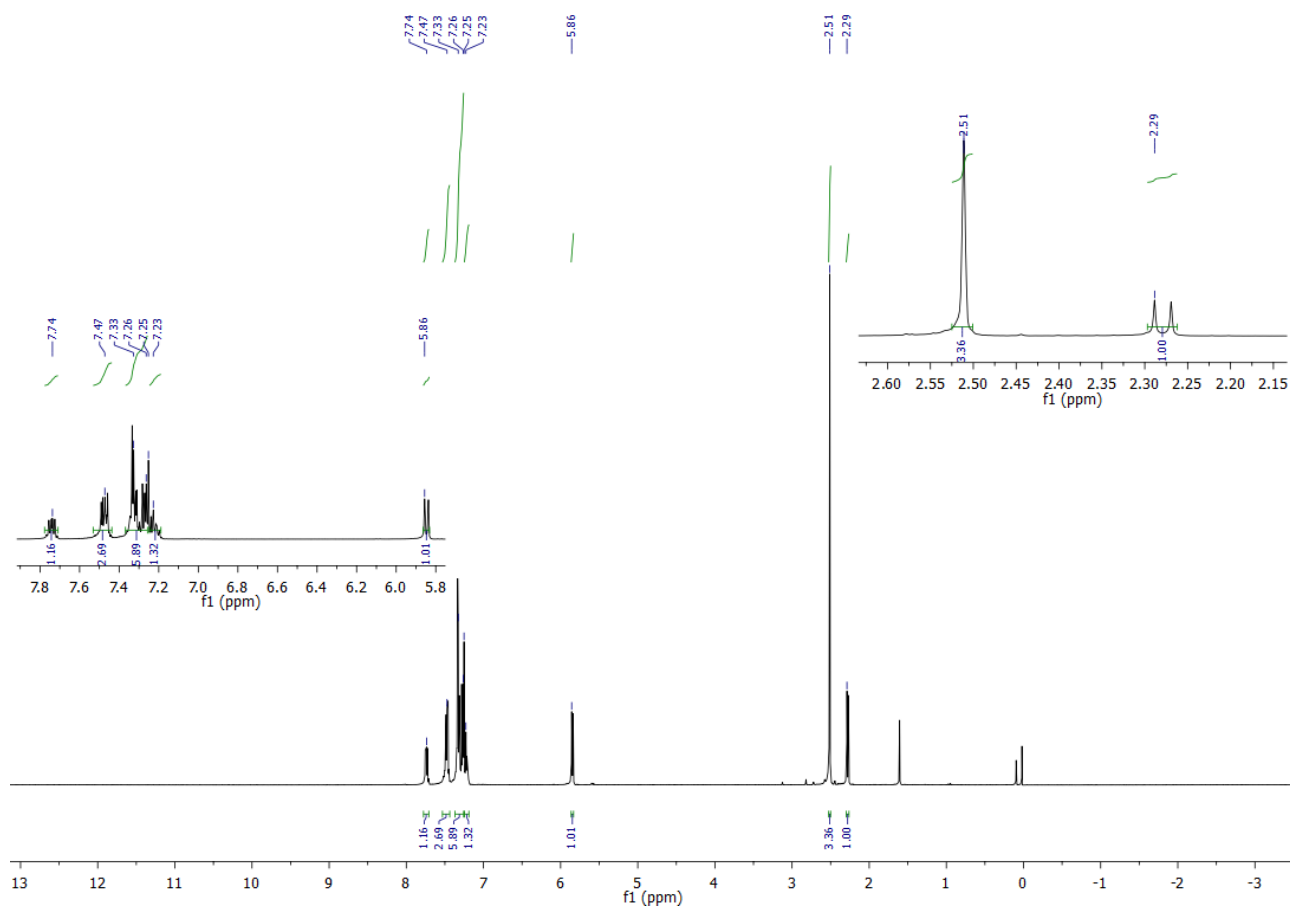
Substrate **1a** (5 mg, 22.7 μmol), **3f** (2.93 μl , 22.7 μmol) and IPrAuNTf₂ (19.1 mg, 22.7 μmol) were dissolved in d_2 -TCE (700 μl) and stirred for 18 h in cooling bath (15 °C). After inspection of ¹H spectra at 15 °C, the NMR was cooled down to 0 °C and set of 2D experiments were conducted. Assignment of signals is listed in Table S1.

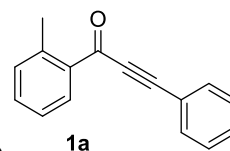
VI. NMR spectra

VII.1. Spectra of substrates and products

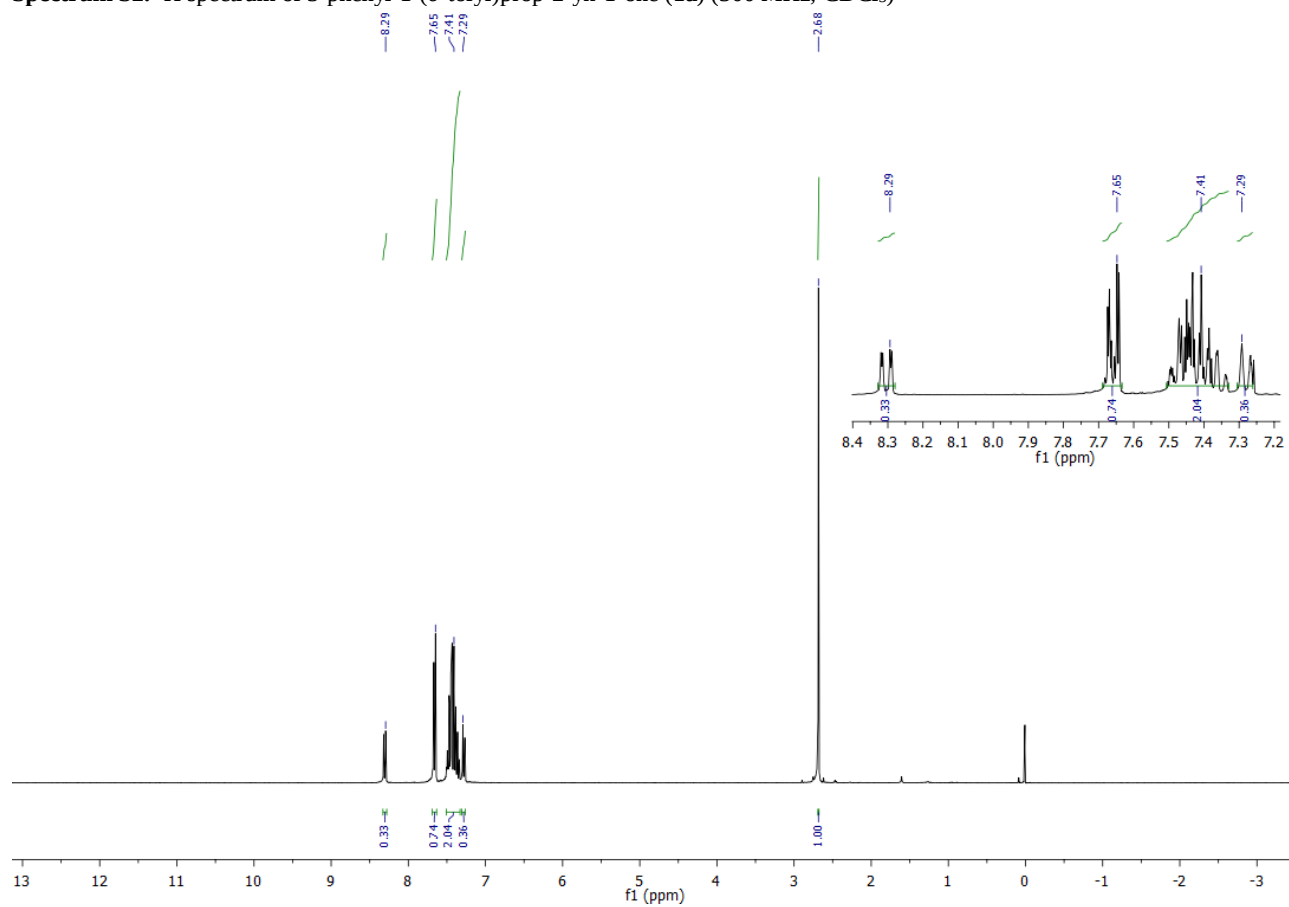


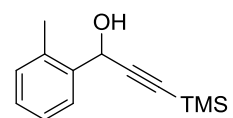
Spectrum S1. ^1H spectrum of 3-phenyl-1-(o-tolyl)prop-2-yn-1-ol (**7a**) (300 MHz, CDCl_3)





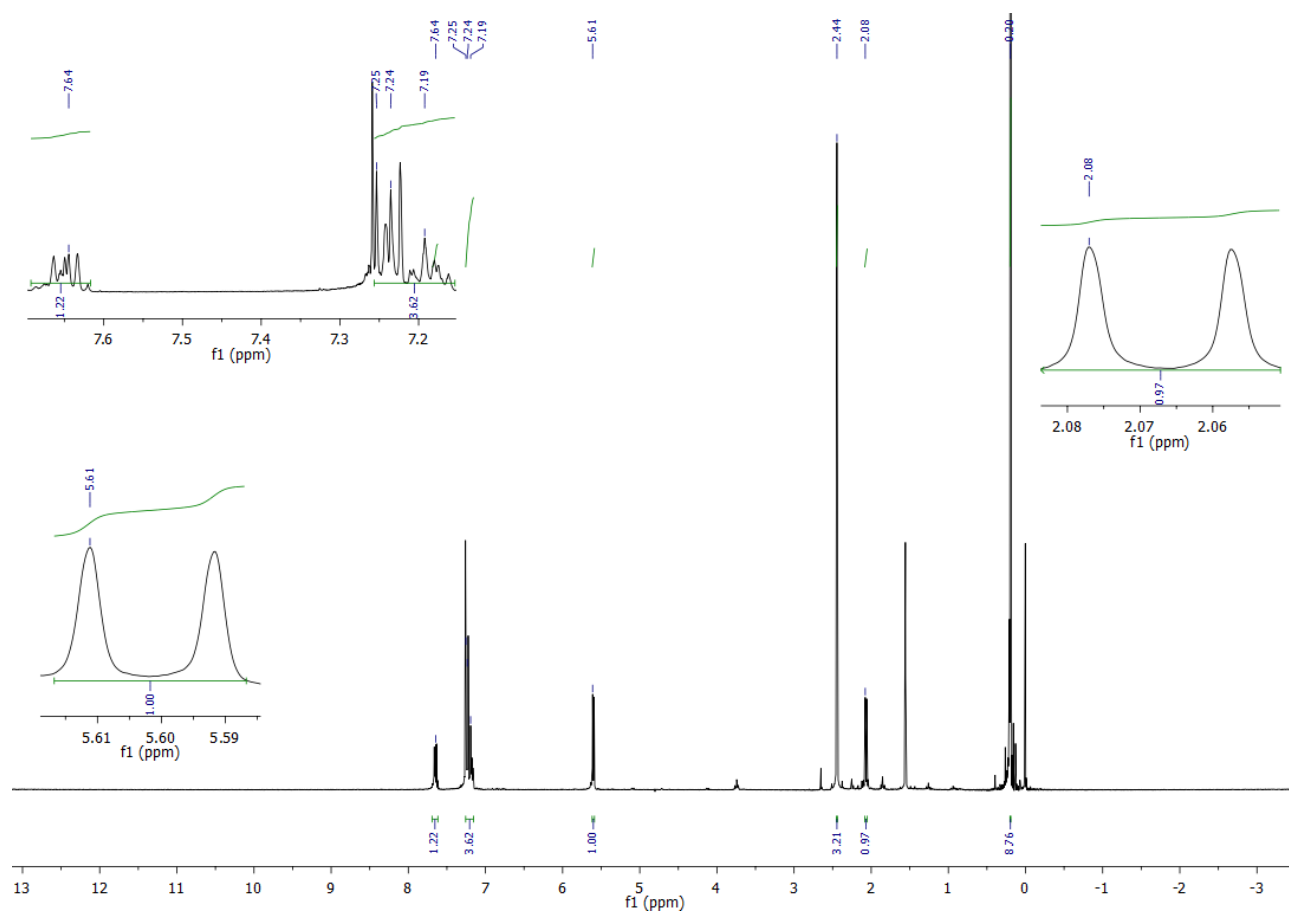
Spectrum S2. ^1H spectrum of 3-phenyl-1-(o-tolyl)prop-2-yn-1-one (**1a**) (300 MHz, CDCl_3)

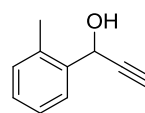




7b

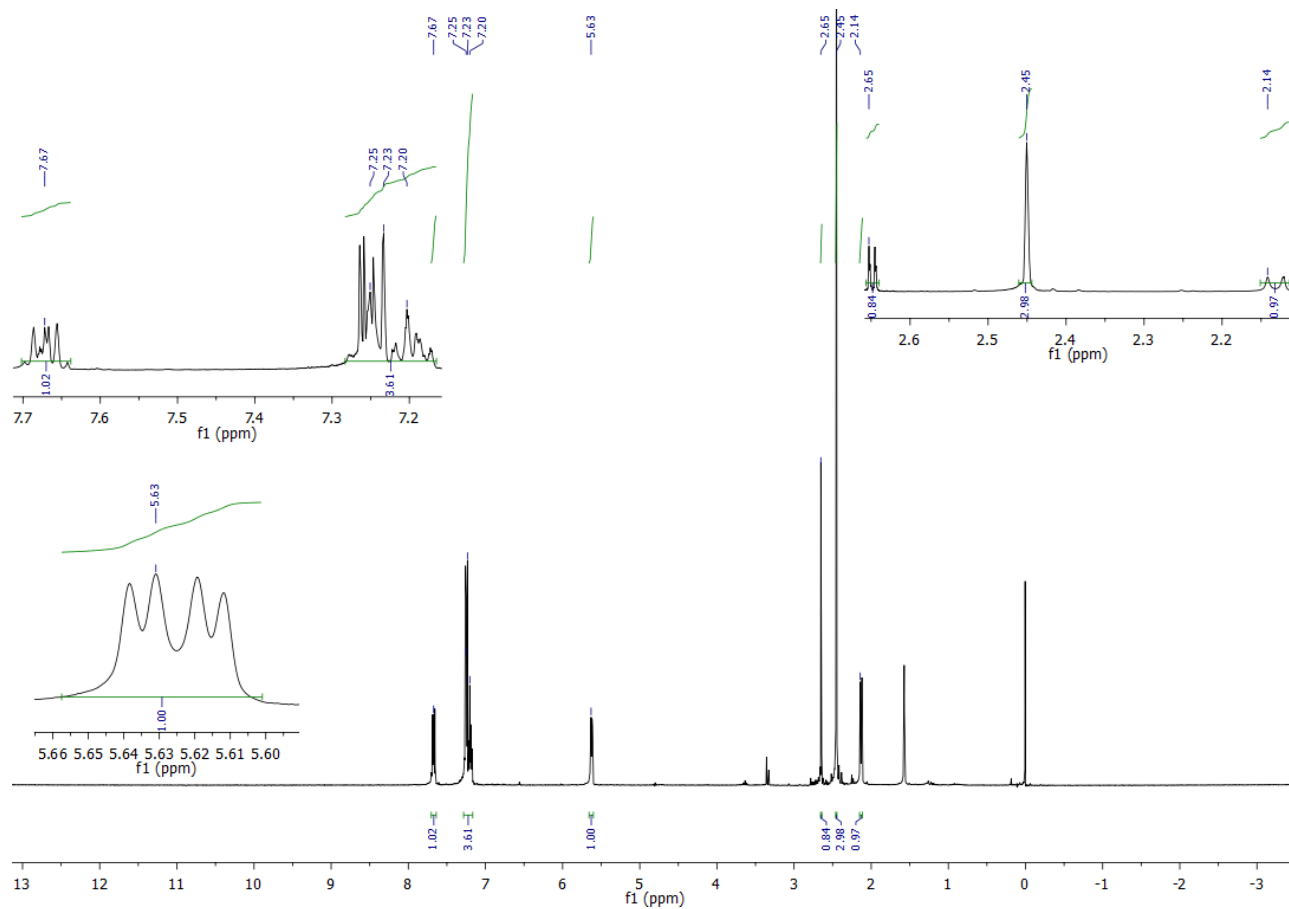
Spectrum S3. ^1H spectrum of 1-(o-tolyl)-3-(trimethylsilyl)prop-2-yn-1-ol (**7b**) (300 MHz, CDCl_3)

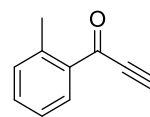




Spectrum S4. ^1H spectrum of 1-(o-tolyl)prop-2-yn-1-ol (**8**) (300 MHz, CDCl_3)

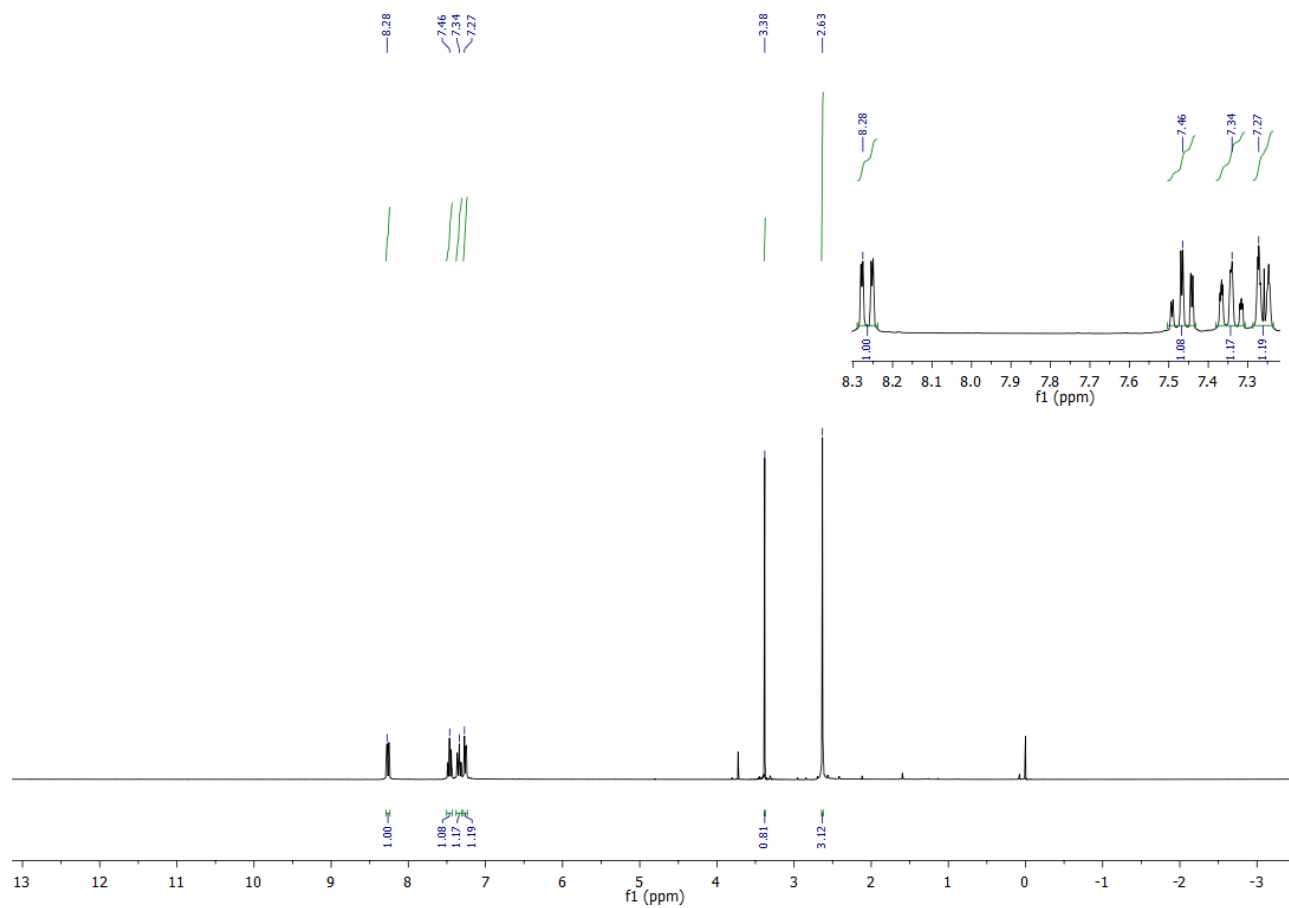
8

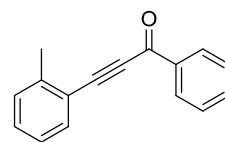




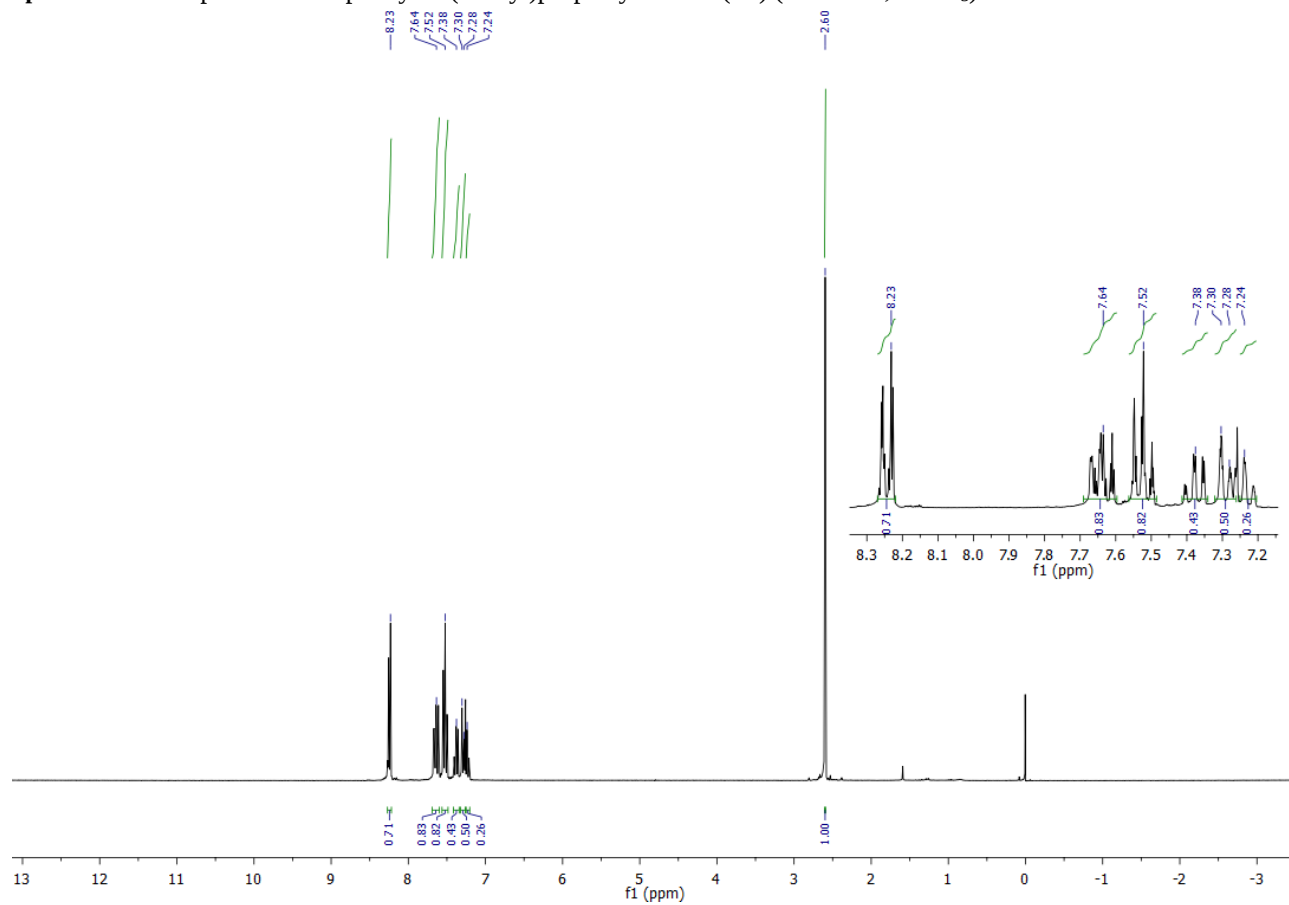
5a

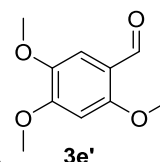
Spectrum S5. ^1H spectrum of 1-(*o*-tolyl)prop-2-yn-1-one (**5a**) (300 MHz, CDCl_3)



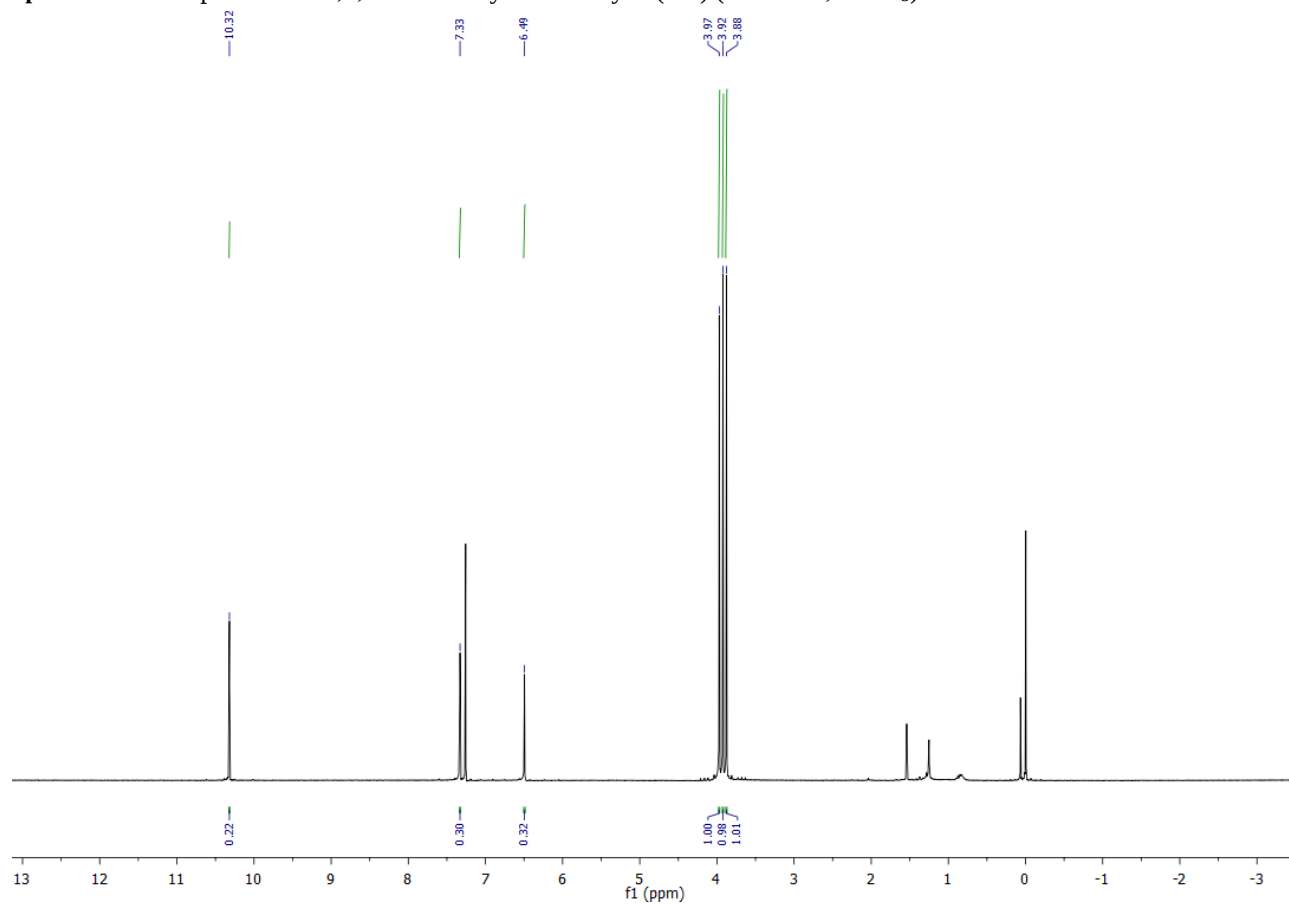


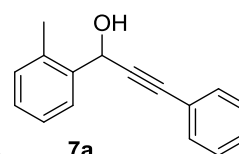
Spectrum S6. ^1H spectrum of 1-phenyl-3-(*o*-tolyl)prop-2-yn-1-one (**1b**) (300 MHz, CDCl_3)



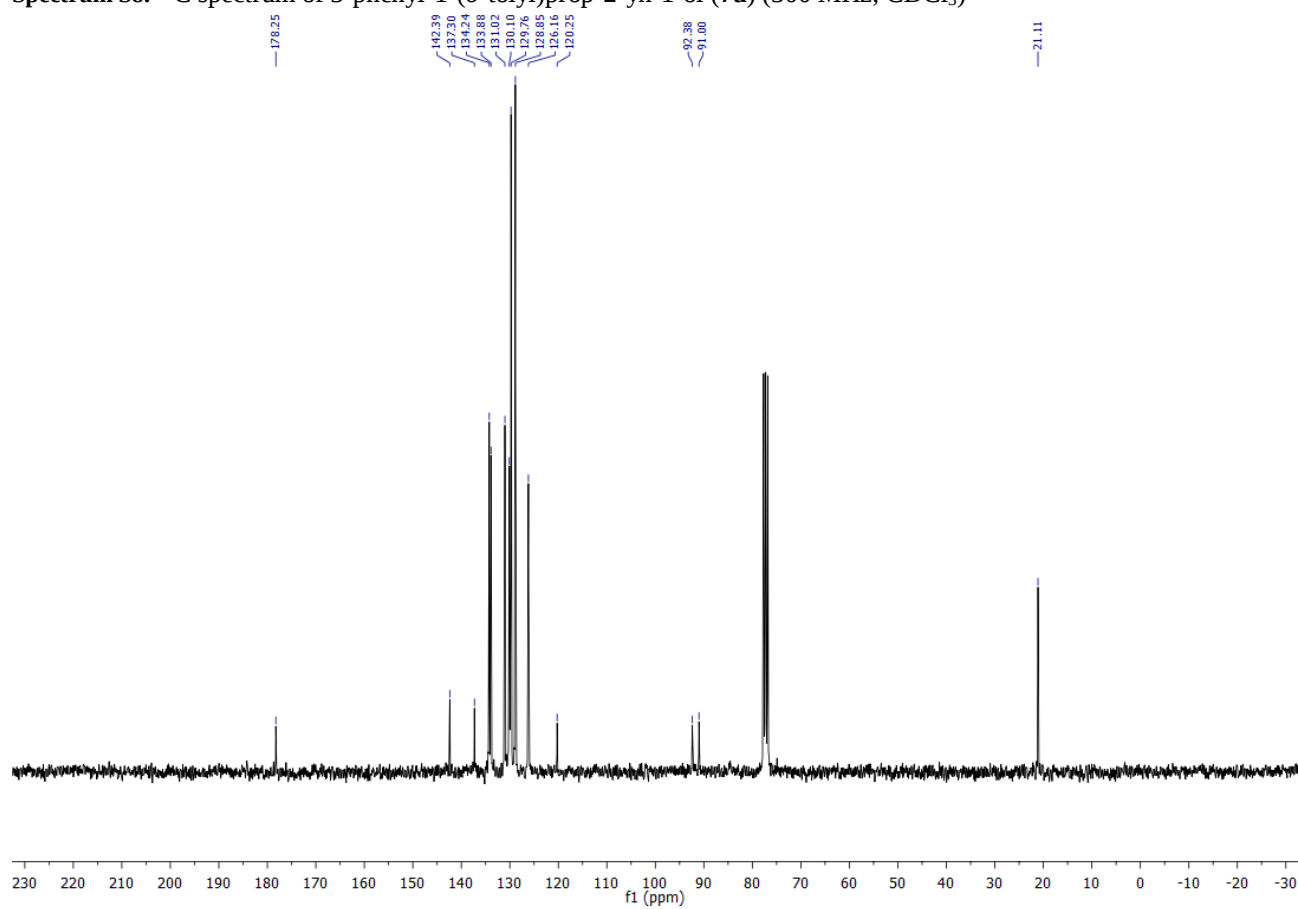


Spectrum S7. ¹H spectrum of 2,4,5-trimethoxybenzaldehyde (**3e'**) (300 MHz, CDCl₃)

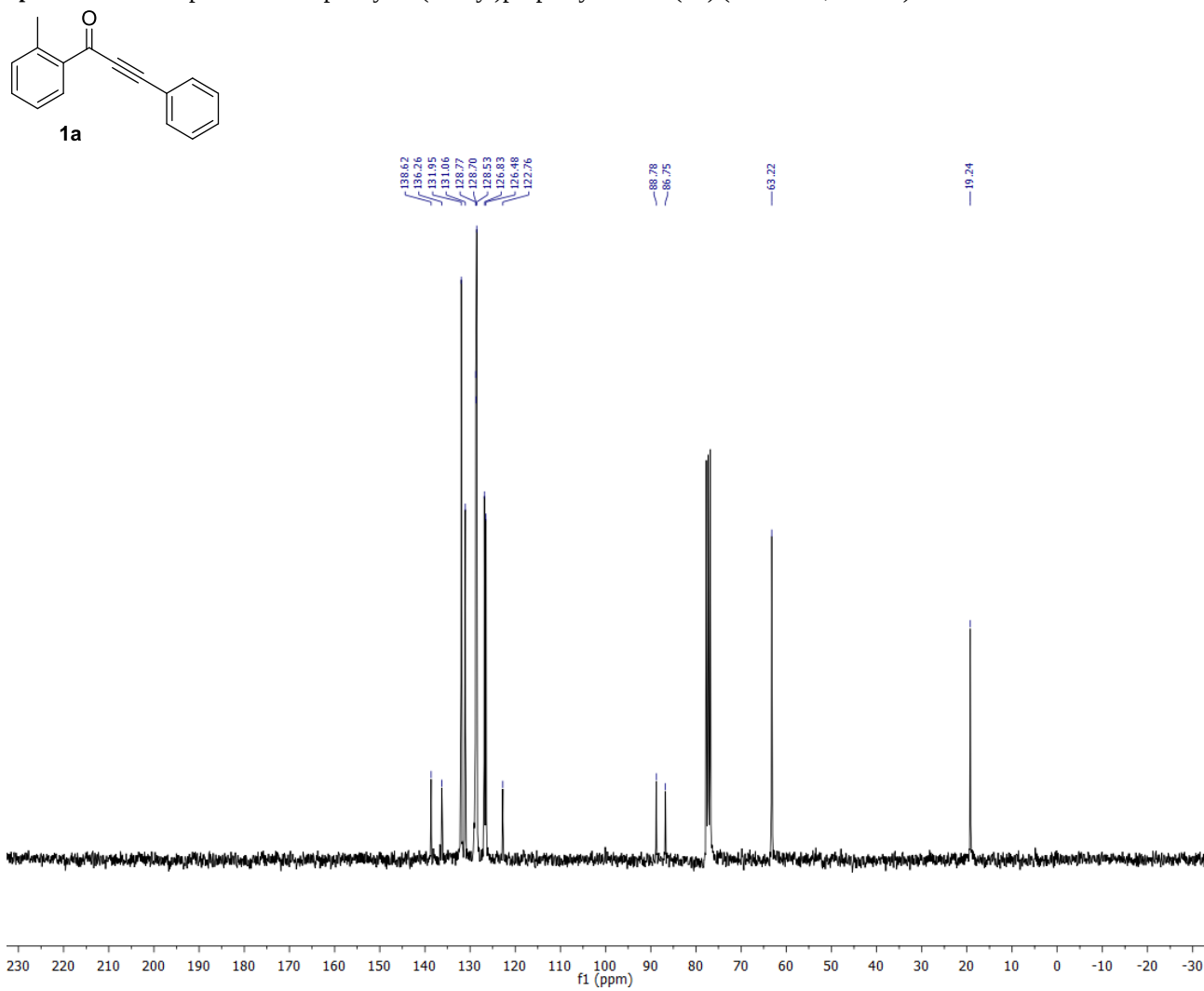


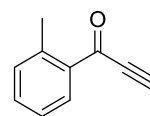


Spectrum S8. ^{13}C spectrum of 3-phenyl-1-(*o*-tolyl)prop-2-yn-1-ol (**7a**) (300 MHz, CDCl_3)



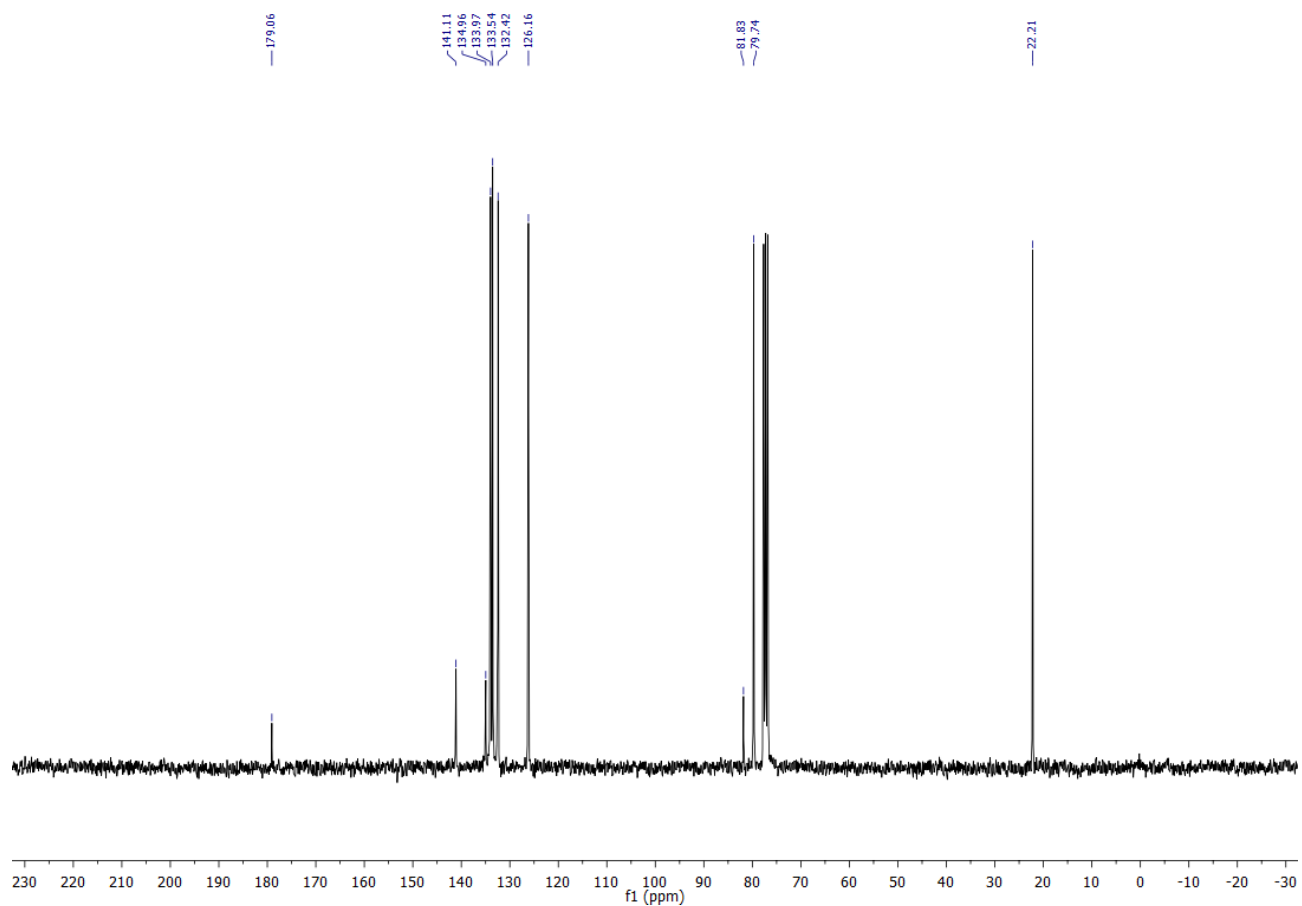
Spectrum S9. ^{13}C spectrum of 3-phenyl-1-(*o*-tolyl)prop-2-yn-1-one (**1a**) (300 MHz, CDCl_3)



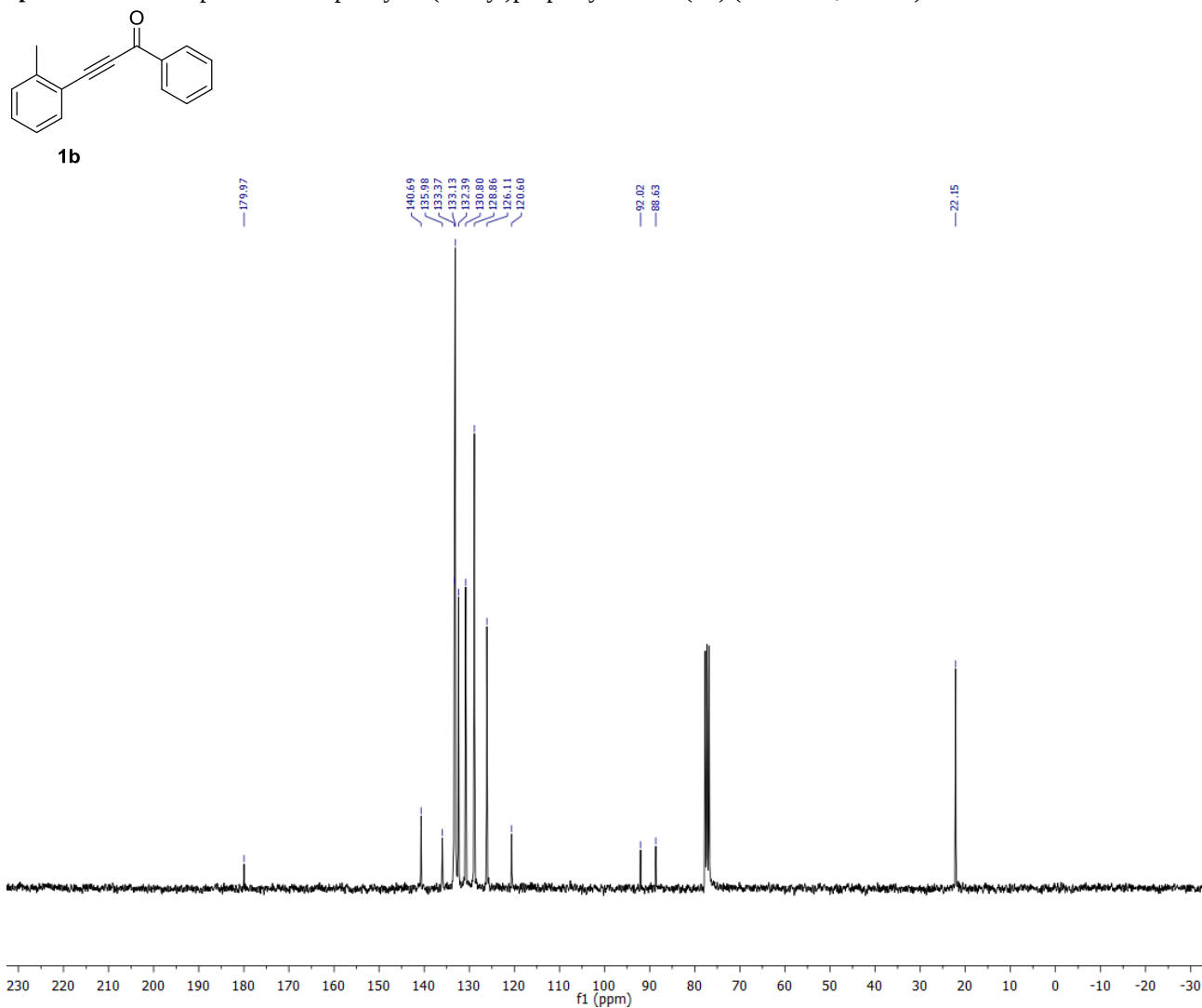


5a

Spectrum S10. ^{13}C spectrum of 1-(o-tolyl)prop-2-yn-1-one (**5a**) (300 MHz, CDCl_3)



Spectrum S11. ^{13}C spectrum of 1-phenyl-3-(*o*-tolyl)prop-2-yn-1-one (**1b**) (300 MHz, CDCl_3)



VII.2. 2D experiments for 4

2D experiments were acquired with a 500 MHz spectrometer at 0°C in d₂-TCE.

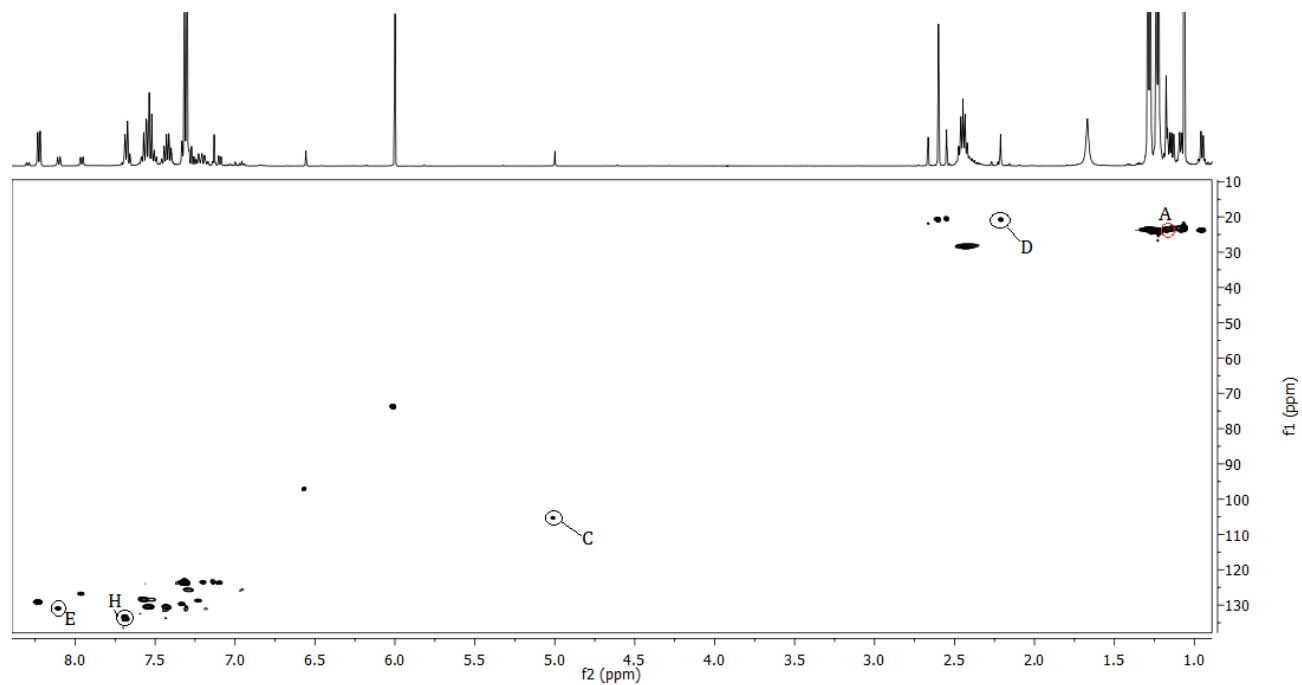


Figure S11. HSQC and selected assignments (See).

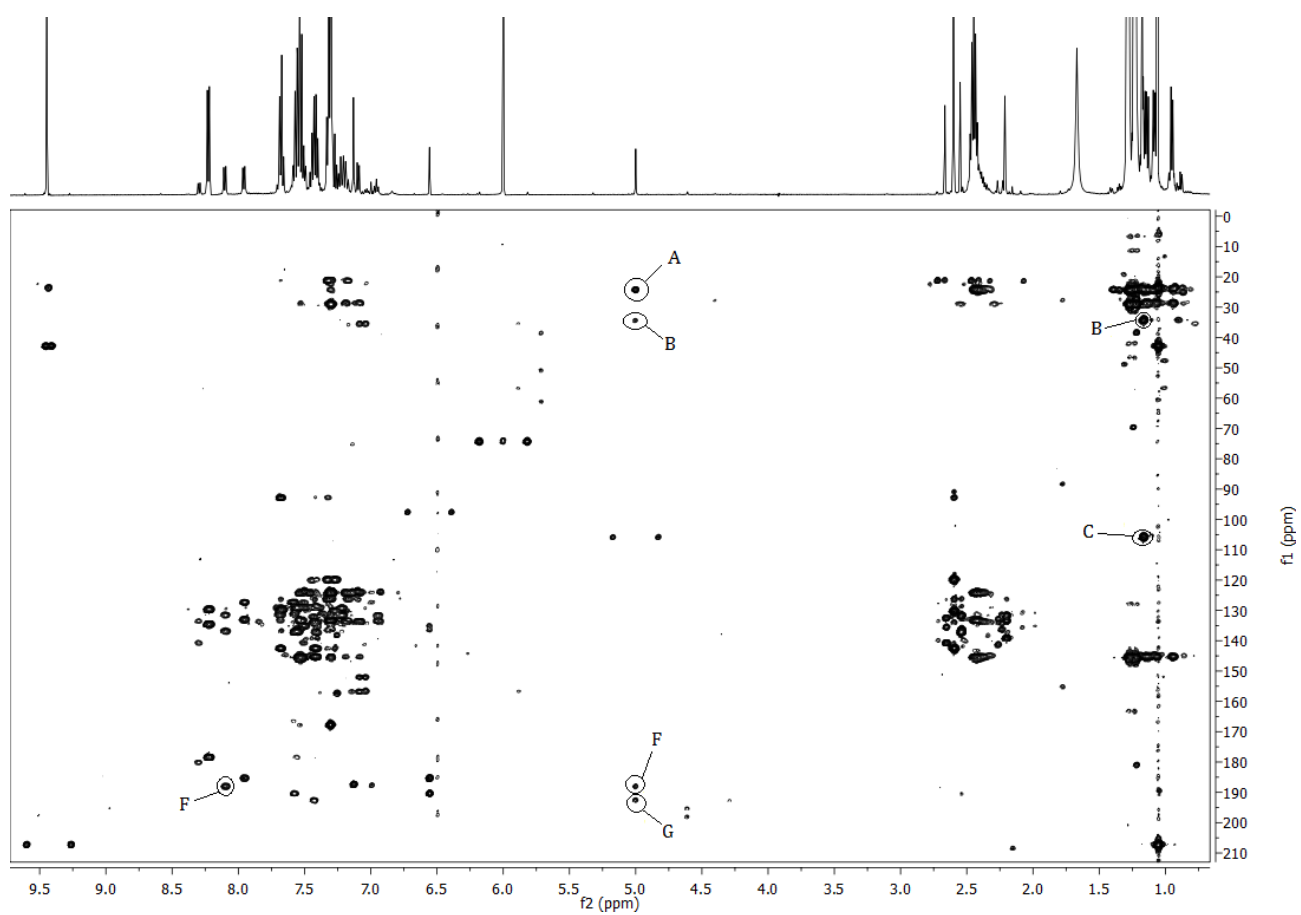


Figure S12. HMBC and selected assignments (See Table S1).

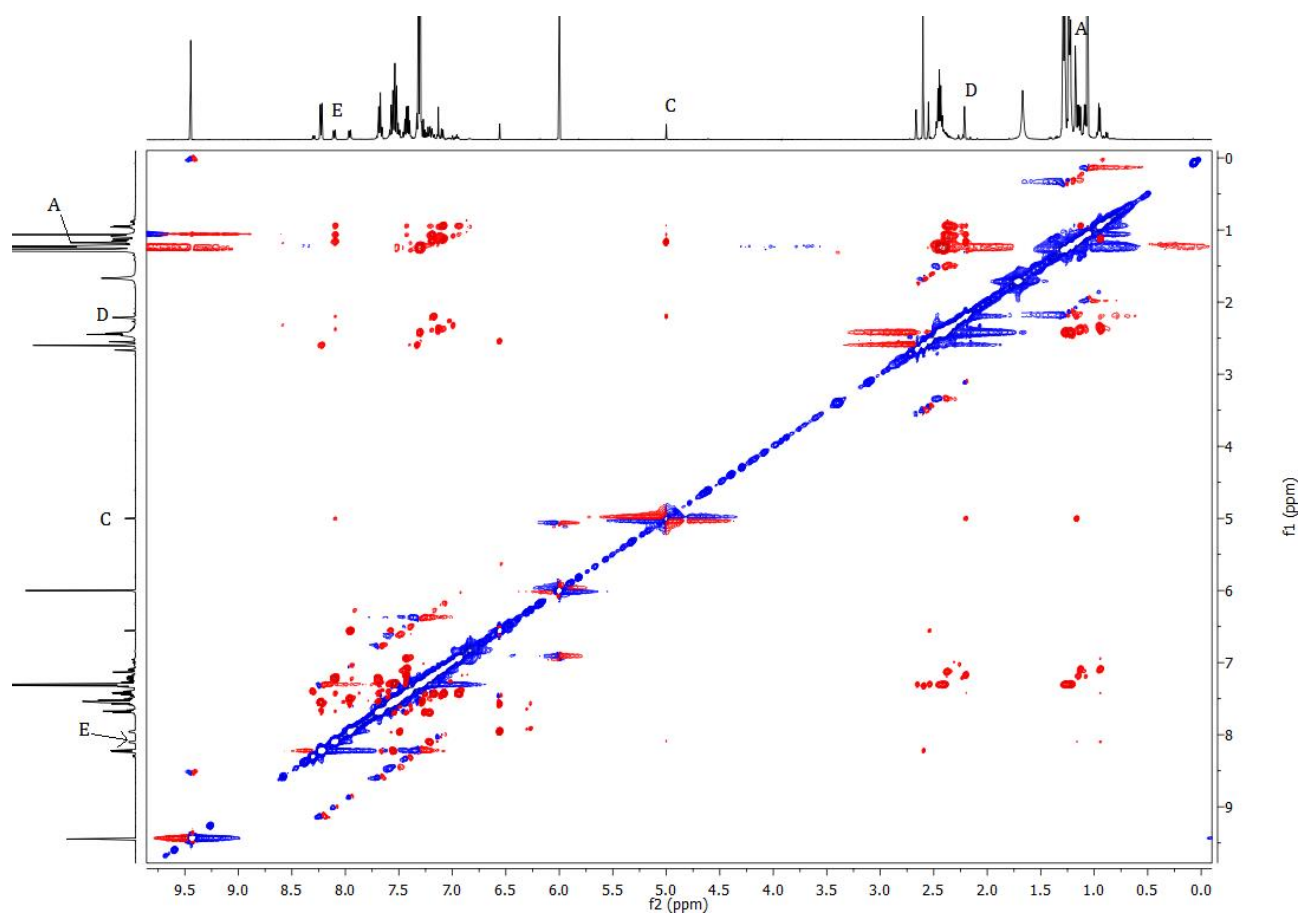
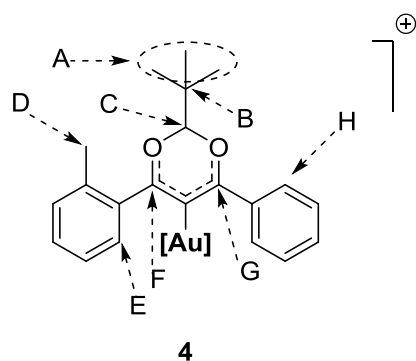


Figure S13. 2D ROESY (200ms mixing time) and selected assignments (See Table S1).

Table S1. Tabulated ^1H and ^{13}C shifts and correlations assigned for **4**



Position	Shift (ppm)		Correlation	
	^1H	^{13}C	NOE	HMBC
A	1.17	23.6	C, D, E	B, C
B	-	34.3	-	-
C	5.01	105.3	A, D, E	A, B, F, G
D	2.21	20.8	A, C, E	[1]
E	8.11	130.9	A, C, D	F, [1]
F	-	187.9	-	-
G	-	192.6	-	-
H	7.71	133.3	-	G, [1]

[1] Signals from aromatic region

VII.3. Formation of 5b

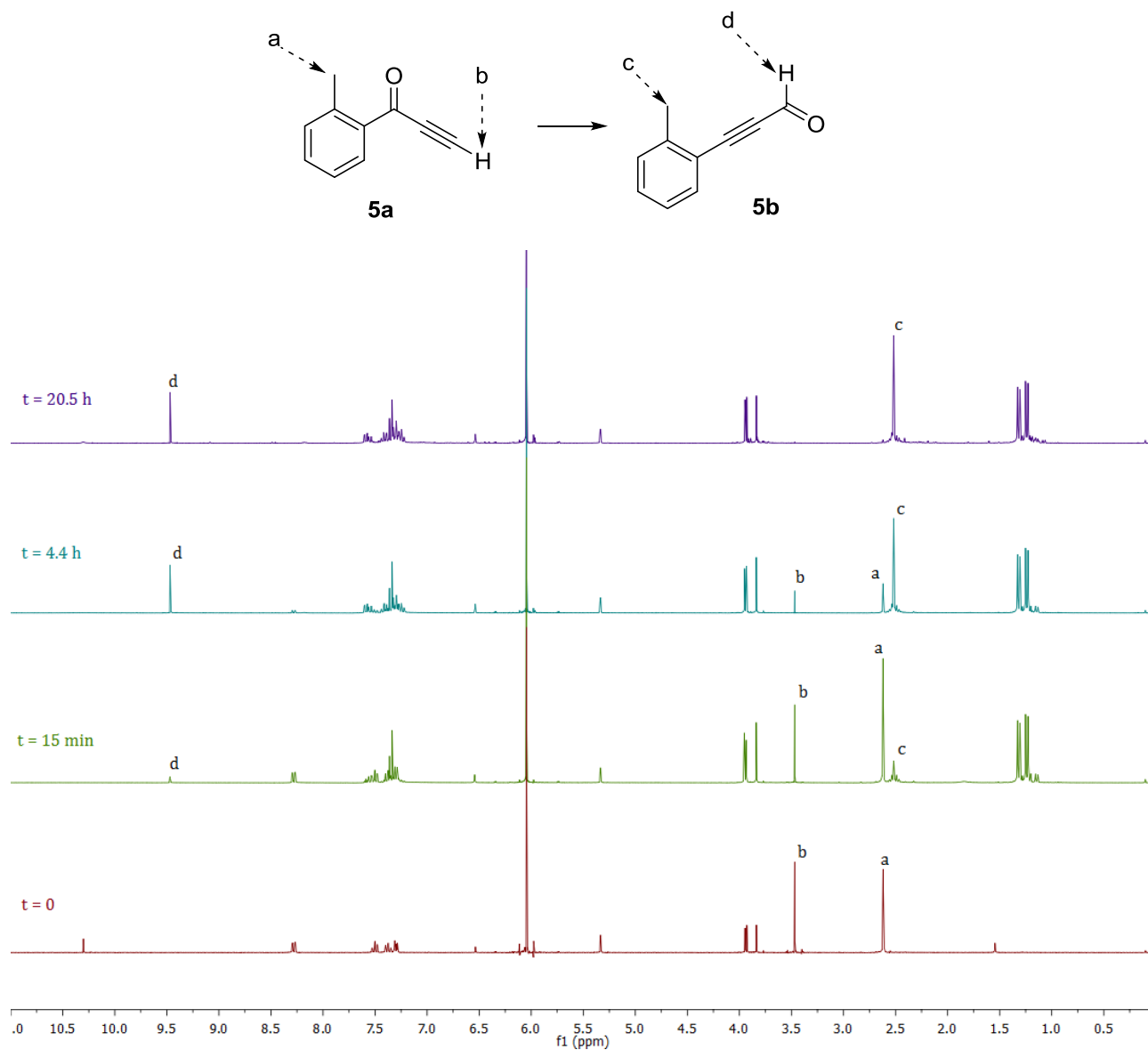


Figure S14. Reaction monitoring of **5a** → **5b** in d₂-DCM catalysed by IPrAuNTf₂ and **3e** acquired with 300 MHz spectrometer. 1,1',2,2'-tetrachloroethane was used as an internal standard.

VII. Kinetic data for COPASI

VII.1. Kinetic modelling

The experimental kinetic data of the four experiments with different initial concentrations presented in Figure 1 of the main body text (also shown below) has been used for the modelling. The exact values are provided in the corresponding tables at the end of this section.

During the experimental reactions, a small decrease in the analytical concentration of substrate and product was observed, as well as a small deactivation percentage of the catalyst. Although this is not relevant from a synthetic point of view, it is crucial to consider it when performing the kinetic modelling. Therefore, artificial reactions (shown in yellow) have been added to linearly decrease the total amount of substrate, product and active catalyst to mimic the experimental results.

The reaction network considered for the kinetic modelling is the one shown in section VII.2.

The experimental data used for the parameter estimation is shown in section VII.3.

The best fitting of **[1a]** and **[1b]** equally weighted for each experiment was obtained with the values of the nine estimated parameters (k_1 , k_{-1} , k_2 , k_{-2} , k_3 , k_4 , k_{-4} , k_5 , k_6) shown in section 1.1. Those values give the fitting shown below.

Experiment	[1a] ₀	[1b] ₀	[Au] ₀
Standard	0.2 M	–	10 mM
Dif. [1a] ₀	0.4 M	–	10 mM
Dif. [1b] ₀	0.2 M	0.1 M	10 mM
Dif. [Au] ₀	0.2 M	–	15 mM

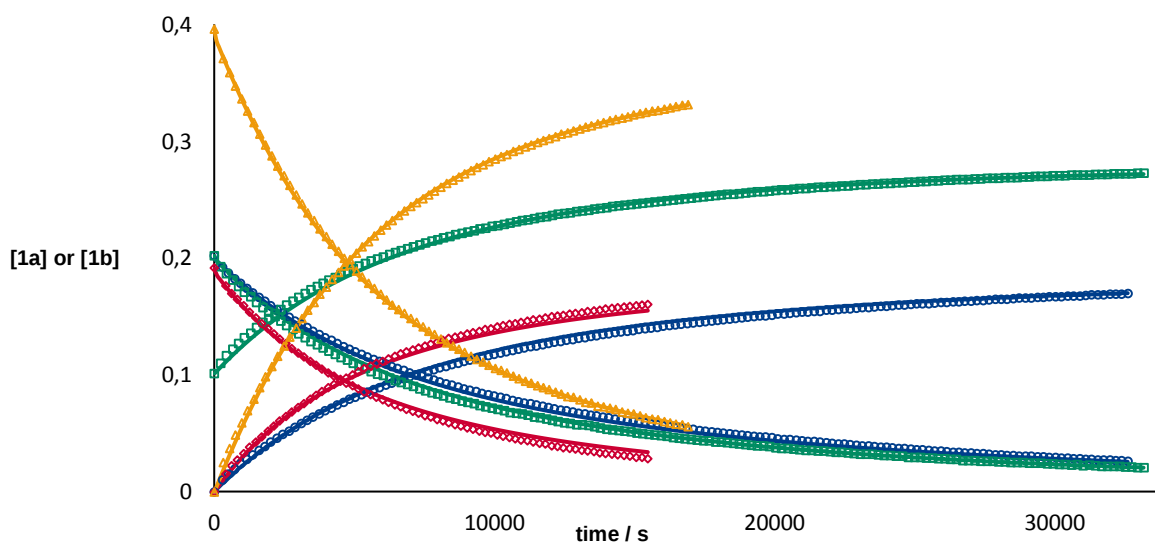


Figure S15. Results from parameter estimation on the kinetic data

Fitting results:

- objective value + 0.00518576
- root mean square 0.00168246
- standard deviation of 0.0016866

With the values obtained from the parameter estimation, the expected amount of product produced by the intramolecular pathway would be insignificant compared to the amount of product produced by the intermolecular pathway mediated by **1a** and the one mediated by **1b**.

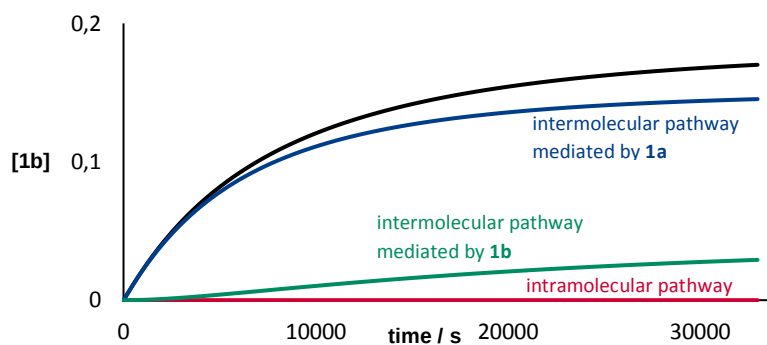


Figure S16. Formation of **1b** for the standard reaction

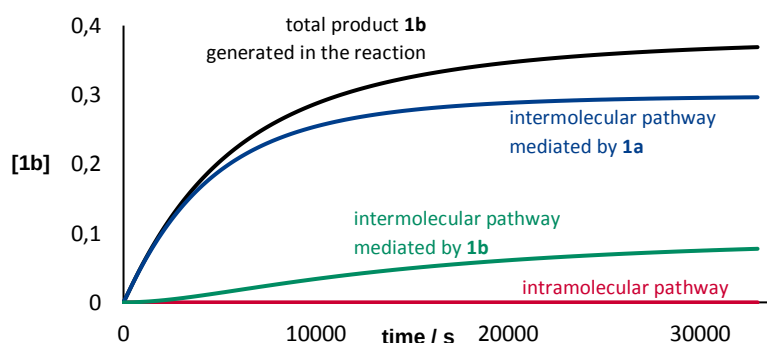


Figure S17. Formation of **1b** for the reaction with different $[1a]_0$

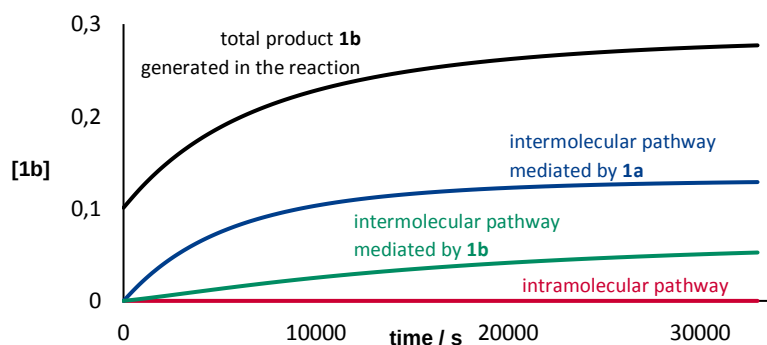


Figure S18. Formation of **1b** for the reaction with different $[1b]_0$

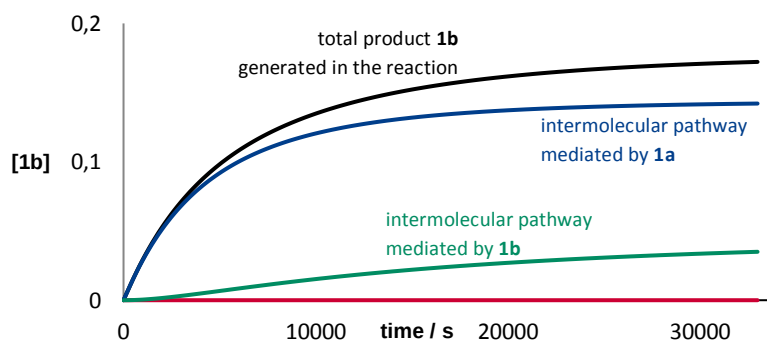


Figure S19. Formation of **1b** for the reaction with different $[Au]_0$

VII.2. Reaction network used for the modelling

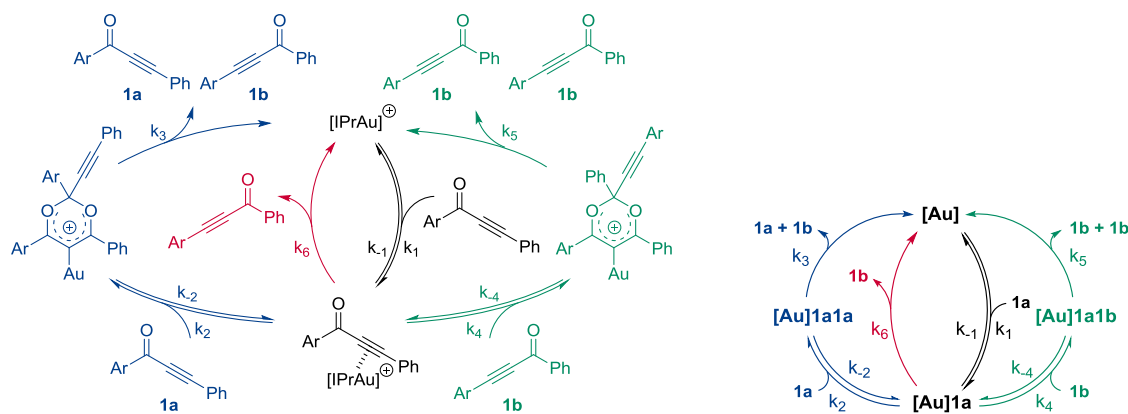
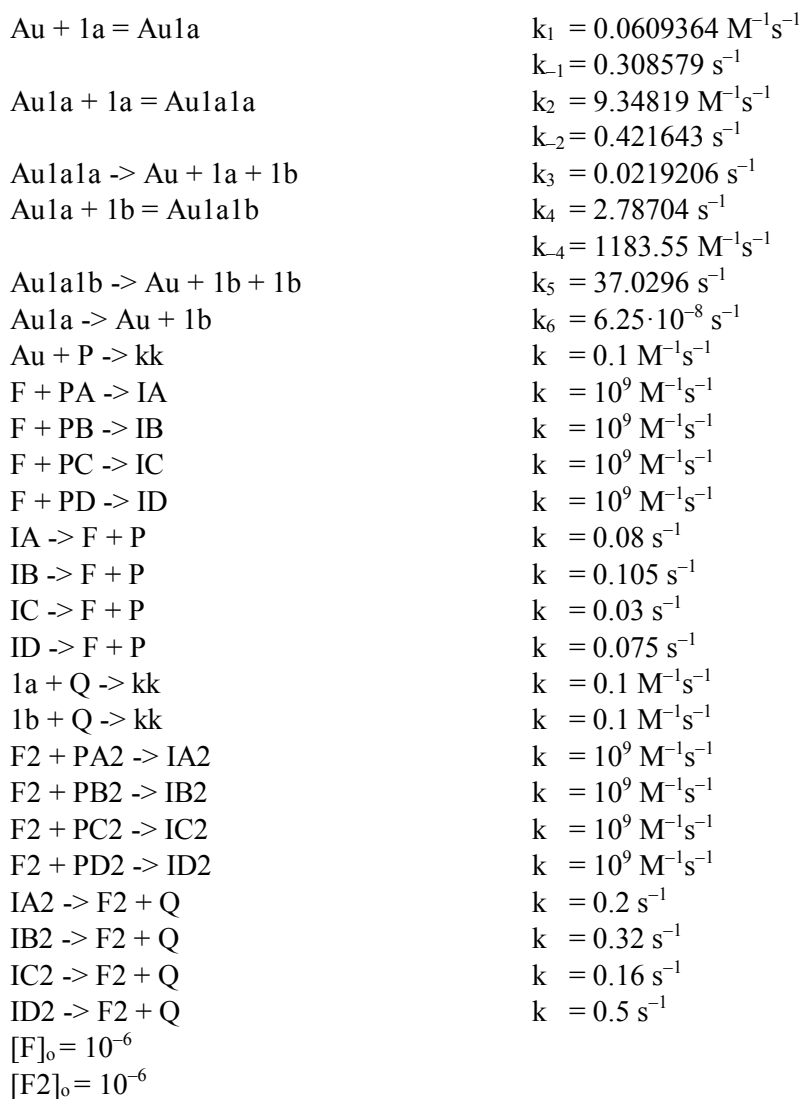


Figure S20. The catalytic cycles used for parameter estimation with COPASI

The set of reactions used in COPASI:



VII.3. Experimental data used for “Parameter Estimation”

time/s	[1a] _o	[1b] _o	[cat] _{ro}	[1a]	[1b]	[active cat]	[PA]	[PB]	[PC]	[PD]	[PA2]	[PB2]	[PC2]	[PD2]	[1a]+[1b]
0	0.201855778	0	0.00998027	0.201855778	0	0.00998027	1	0	0	0	1	0	0	0	0.201855778
289.4	0.201855778	0	0.00998027	0.191866313	0.009989464	0.00998027	1	0	0	0	1	0	0	0	0.201855778
506.4	0.201855778	0	0.00998027	0.186933411	0.014826783	0.009895565	1	0	0	0	1	0	0	0	0.201760194
721.4	0.201855778	0	0.00998027	0.182320975	0.019400769	0.009843256	1	0	0	0	1	0	0	0	0.201721744
937.4	0.201855778	0	0.00998027	0.178262101	0.023578272	0.009809224	1	0	0	0	1	0	0	0	0.201840372
1153.4	0.201855778	0	0.00998027	0.174128936	0.027851634	0.009793191	1	0	0	0	1	0	0	0	0.20198057
1369.4	0.201855778	0	0.00998027	0.17021786	0.031581869	0.009763622	1	0	0	0	1	0	0	0	0.201799729
1585.4	0.201855778	0	0.00998027	0.166385221	0.035377195	0.009755126	1	0	0	0	1	0	0	0	0.201762415
1800.4	0.201855778	0	0.00998027	0.162884175	0.038851209	0.00973413	1	0	0	0	1	0	0	0	0.201735384
2016.4	0.201855778	0	0.00998027	0.159477442	0.042283439	0.009726861	1	0	0	0	1	0	0	0	0.201760881
2231.4	0.201855778	0	0.00998027	0.155922622	0.045686313	0.009713739	1	0	0	0	1	0	0	0	0.201608934
2447.4	0.201855778	0	0.00998027	0.152607887	0.048963494	0.009710174	1	0	0	0	1	0	0	0	0.201571381
2662.4	0.201855778	0	0.00998027	0.14958459	0.051891145	0.009698453	1	0	0	0	1	0	0	0	0.201475735
2877.4	0.201855778	0	0.00998027	0.146296444	0.055250119	0.009706811	1	0	0	0	1	0	0	0	0.201546564
3093.4	0.201855778	0	0.00998027	0.143215165	0.058317457	0.009705018	1	0	0	0	1	0	0	0	0.201532622
3308.4	0.201855778	0	0.00998027	0.140414004	0.060905923	0.009679387	1	0	0	0	1	0	0	0	0.201319928
3523.4	0.201855778	0	0.00998027	0.13743676	0.063921922	0.009683477	1	0	0	0	1	0	0	0	0.201358682
3739.4	0.201855778	0	0.00998027	0.134789193	0.066456658	0.009665778	1	0	0	0	1	0	0	0	0.20124585
3955.4	0.201855778	0	0.00998027	0.132014035	0.069161952	0.009664034	1	0	0	0	1	0	0	0	0.201175988
4170.4	0.201855778	0	0.00998027	0.12936821	0.071765647	0.009657272	1	0	0	0	1	0	0	0	0.201133857
4386.4	0.201855778	0	0.00998027	0.126862309	0.074177104	0.009644044	1	0	0	0	1	0	0	0	0.201039413
4601.4	0.201855778	0	0.00998027	0.124365636	0.076670342	0.009635578	1	0	0	0	1	0	0	0	0.201035978
4817.4	0.201855778	0	0.00998027	0.121984056	0.078939025	0.009617724	1	0	0	0	1	0	0	0	0.200923081
5032.4	0.201855778	0	0.00998027	0.119859775	0.080998958	0.009599633	1	0	0	0	1	0	0	0	0.200858733
5248.4	0.201855778	0	0.00998027	0.117578878	0.083228678	0.009583413	1	0	0	0	1	0	0	0	0.200807555
5463.4	0.201855778	0	0.00998027	0.115394453	0.085337842	0.009571301	1	0	0	0	1	0	0	0	0.200732296
5679.4	0.201855778	0	0.00998027	0.113317631	0.087362748	0.009556962	1	0	0	0	1	0	0	0	0.200680379
5894.4	0.201855778	0	0.00998027	0.111407674	0.08924119	0.009537503	1	0	0	0	1	0	0	0	0.200648863
6110.4	0.201855778	0	0.00998027	0.109318444	0.091239757	0.009527088	1	0	0	0	1	0	0	0	0.200558202

6325.4	0.201855778	0	0.00998027	0.107346107	0.093136869	0.009508432	1	0	0	0	1	0	0	0	0.200482976
6541.4	0.201855778	0	0.00998027	0.105449218	0.094973309	0.009496989	1	0	0	0	1	0	0	0	0.200422527
6756.4	0.201855778	0	0.00998027	0.103709595	0.096628093	0.009471254	1	0	0	0	1	0	0	0	0.200337688
6971.4	0.201855778	0	0.00998027	0.101933306	0.098333489	0.009450441	1	0	0	0	1	0	0	0	0.200266796
7187.4	0.201855778	0	0.00998027	0.100287993	0.099865581	0.00942835	1	0	0	0	1	0	0	0	0.200153574
7402.4	0.201855778	0	0.00998027	0.098782033	0.101323684	0.009400002	1	0	0	0	1	0	0	0	0.200105717
7618.4	0.201855778	0	0.00998027	0.097103818	0.102940105	0.009390726	1	0	0	0	1	0	0	0	0.200043923
7833.4	0.201855778	0	0.00998027	0.095465604	0.104535242	0.009368967	1	0	0	0	1	0	0	0	0.200000845
8049.4	0.201855778	0	0.00998027	0.093919959	0.105952799	0.009353742	1	0	0	0	1	0	0	0	0.199872759
8264.4	0.201855778	0	0.00998027	0.092452767	0.107370224	0.009328899	1	0	0	0	1	0	0	0	0.199822991
8480.4	0.201855778	0	0.00998027	0.091067654	0.108696671	0.00930971	1	0	0	0	1	0	0	0	0.199764325
8695.4	0.201855778	0	0.00998027	0.089614147	0.110082995	0.009285605	1	0	0	0	1	0	0	0	0.199697143
8911.4	0.201855778	0	0.00998027	0.088143697	0.111465502	0.009269543	1	0	0	0	1	0	0	0	0.199609199
9126.4	0.201855778	0	0.00998027	0.086907456	0.112714569	0.009252988	1	0	0	0	1	0	0	0	0.199622024
9342.4	0.201855778	0	0.00998027	0.085653637	0.113865686	0.009224724	1	0	0	0	1	0	0	0	0.199519324
9558.4	0.201855778	0	0.00998027	0.084247845	0.1152155	0.009216881	1	0	0	0	1	0	0	0	0.199463345
9774.4	0.201855778	0	0.00998027	0.082985295	0.116381023	0.009197706	1	0	0	0	1	0	0	0	0.199366317
9989.4	0.201855778	0	0.00998027	0.081727048	0.117660237	0.009176695	1	0	0	0	1	0	0	0	0.199387285
10205.4	0.201855778	0	0.00998027	0.080592716	0.118687067	0.009155791	1	0	0	0	1	0	0	0	0.199279782
10420.4	0.201855778	0	0.00998027	0.079488712	0.119758696	0.0091349	1	0	0	0	1	0	0	0	0.199247408
10636.4	0.201855778	0	0.00998027	0.078356549	0.120861212	0.009117645	1	0	0	0	1	0	0	0	0.19921776
10851.4	0.201855778	0	0.00998027	0.077273765	0.121847656	0.009098876	1	0	0	0	1	0	0	0	0.199121421
11067.4	0.201855778	0	0.00998027	0.07616057	0.122939228	0.009076515	1	0	0	0	1	0	0	0	0.199099798
11282.4	0.201855778	0	0.00998027	0.075121981	0.123909305	0.009056744	1	0	0	0	1	0	0	0	0.199031286
11498.4	0.201855778	0	0.00998027	0.074016111	0.124888662	0.009040515	1	0	0	0	1	0	0	0	0.198904773
11714.4	0.201855778	0	0.00998027	0.073084786	0.125858373	0.009027496	1	0	0	0	1	0	0	0	0.198943159
11929.4	0.201855778	0	0.00998027	0.071979988	0.126857045	0.009008175	1	0	0	0	1	0	0	0	0.198837032
12144.4	0.201855778	0	0.00998027	0.071008236	0.12781703	0.008991621	1	0	0	0	1	0	0	0	0.198825265
12360.4	0.201855778	0	0.00998027	0.07007666	0.128633844	0.008975478	1	0	0	0	1	0	0	0	0.198710504
12576.4	0.201855778	0	0.00998027	0.069154631	0.129503956	0.008953947	1	0	0	0	1	0	0	0	0.198658587
12791.4	0.201855778	0	0.00998027	0.068273366	0.130403934	0.008939435	1	0	0	0	1	0	0	0	0.1986773

13007.4	0.201855778	0	0.00998027	0.067317673	0.131265644	0.008929125	1	0	0	0	1	0	0	0	0.198583317
13222.4	0.201855778	0	0.00998027	0.066578917	0.131986529	0.008900708	1	0	0	0	1	0	0	0	0.198565446
13438.4	0.201855778	0	0.00998027	0.065652652	0.132846707	0.008876484	1	0	0	0	1	0	0	0	0.198499359
13653.4	0.201855778	0	0.00998027	0.064739645	0.133659209	0.008865258	1	0	0	0	1	0	0	0	0.198398854
13869.4	0.201855778	0	0.00998027	0.063845341	0.134566919	0.008855909	1	0	0	0	1	0	0	0	0.198412226
14084.4	0.201855778	0	0.00998027	0.063115094	0.135128616	0.008837824	1	0	0	0	1	0	0	0	0.19824371
14300.4	0.201855778	0	0.00998027	0.062362529	0.136057495	0.008833171	1	0	0	0	1	0	0	0	0.198420024
14515.4	0.201855778	0	0.00998027	0.061575728	0.136696469	0.008803672	1	0	0	0	1	0	0	0	0.198272197
14731.4	0.201855778	0	0.00998027	0.060792974	0.137467786	0.008793317	1	0	0	0	1	0	0	0	0.19826076
14946.4	0.201855778	0	0.00998027	0.060094899	0.138007898	0.008767149	1	0	0	0	1	0	0	0	0.198102797
15162.4	0.201855778	0	0.00998027	0.059277838	0.138782441	0.008759512	1	0	0	0	1	0	0	0	0.198060278
15377.4	0.201855778	0	0.00998027	0.058687042	0.139478814	0.00873429	1	0	0	0	1	0	0	0	0.198165855
15593.4	0.201855778	0	0.00998027	0.057742147	0.140235131	0.008728817	1	0	0	0	1	0	0	0	0.197977277
15809.4	0.201855778	0	0.00998027	0.057474842	0.140695229	0.008694974	1	0	0	0	1	0	0	0	0.198170071
16024.4	0.201855778	0	0.00998027	0.056413426	0.14155648	0.008703156	1	0	0	0	1	0	0	0	0.197969905
16240.4	0.201855778	0	0.00998027	0.055768971	0.142099568	0.008676626	1	0	0	0	1	0	0	0	0.197868539
16456.4	0.201855778	0	0.00998027	0.055056498	0.142885887	0.008672521	1	0	0	0	1	0	0	0	0.197942384
16671.4	0.201855778	0	0.00998027	0.054533657	0.143286601	0.008647242	1	0	0	0	1	0	0	0	0.197820258
16887.4	0.201855778	0	0.00998027	0.053842557	0.143887426	0.008637678	1	0	0	0	1	0	0	0	0.197729983
17102.4	0.201855778	0	0.00998027	0.053237915	0.144441767	0.008624125	1	0	0	0	1	0	0	0	0.197679682
17318.4	0.201855778	0	0.00998027	0.052598594	0.145080066	0.008608061	1	0	0	0	1	0	0	0	0.19767866
17533.4	0.201855778	0	0.00998027	0.052042717	0.145562144	0.008590678	1	0	0	0	1	0	0	0	0.197604861
17749.4	0.201855778	0	0.00998027	0.051397153	0.146246906	0.008578634	1	0	0	0	1	0	0	0	0.197644059
17964.4	0.201855778	0	0.00998027	0.050916011	0.146648437	0.008555221	1	0	0	0	1	0	0	0	0.197564448
18180.4	0.201855778	0	0.00998027	0.050241615	0.147286381	0.00855062	1	0	0	0	1	0	0	0	0.197527997
18395.4	0.201855778	0	0.00998027	0.04968169	0.147831141	0.008539242	1	0	0	0	1	0	0	0	0.197512832
18611.4	0.201855778	0	0.00998027	0.049160903	0.148332706	0.008513697	1	0	0	0	1	0	0	0	0.197493609
18826.4	0.201855778	0	0.00998027	0.048541228	0.148870691	0.008505777	1	0	0	0	1	0	0	0	0.197411919
19042.4	0.201855778	0	0.00998027	0.048176228	0.149262698	0.008484568	1	0	0	0	1	0	0	0	0.197438926
19257.4	0.201855778	0	0.00998027	0.047580504	0.149747833	0.008475559	1	0	0	0	1	0	0	0	0.197328337
19473.4	0.201855778	0	0.00998027	0.047029689	0.15034231	0.008460941	1	0	0	0	1	0	0	0	0.197371998

19688.4	0.201855778	0	0.00998027	0.046601012	0.150687904	0.008444795	1	0	0	0	1	0	0	0	0.197288916
19904.4	0.201855778	0	0.00998027	0.046187497	0.151139455	0.00841883	1	0	0	0	1	0	0	0	0.197326952
20119.4	0.201855778	0	0.00998027	0.045419365	0.151820858	0.008428661	1	0	0	0	1	0	0	0	0.197240224
20335.4	0.201855778	0	0.00998027	0.044921132	0.152240886	0.008409651	1	0	0	0	1	0	0	0	0.197162018
20550.4	0.201855778	0	0.00998027	0.044606672	0.152568997	0.008393725	1	0	0	0	1	0	0	0	0.19717567
20766.4	0.201855778	0	0.00998027	0.044144349	0.153031543	0.008375446	1	0	0	0	1	0	0	0	0.197175892
20981.4	0.201855778	0	0.00998027	0.043668152	0.153477123	0.008368655	1	0	0	0	1	0	0	0	0.197145275
21197.4	0.201855778	0	0.00998027	0.043121278	0.153866638	0.008356715	1	0	0	0	1	0	0	0	0.196987916
21412.4	0.201855778	0	0.00998027	0.042773577	0.154332404	0.008341313	1	0	0	0	1	0	0	0	0.197105981
21628.4	0.201855778	0	0.00998027	0.042502028	0.154501996	0.008323036	1	0	0	0	1	0	0	0	0.197004024
21844.4	0.201855778	0	0.00998027	0.041918854	0.155141817	0.008313556	1	0	0	0	1	0	0	0	0.19706067
22059.4	0.201855778	0	0.00998027	0.041288674	0.155644795	0.008311186	1	0	0	0	1	0	0	0	0.19693347
22275.4	0.201855778	0	0.00998027	0.04092721	0.155979194	0.008296959	1	0	0	0	1	0	0	0	0.196906404
22490.4	0.201855778	0	0.00998027	0.040578144	0.156315455	0.008279796	1	0	0	0	1	0	0	0	0.196893599
22706.4	0.201855778	0	0.00998027	0.040195907	0.156632279	0.008266288	1	0	0	0	1	0	0	0	0.196828187
22921.4	0.201855778	0	0.00998027	0.03972212	0.157151365	0.008263593	1	0	0	0	1	0	0	0	0.196873485
23137.4	0.201855778	0	0.00998027	0.039343564	0.157485248	0.008243254	1	0	0	0	1	0	0	0	0.196828811
23352.4	0.201855778	0	0.00998027	0.038988559	0.157802874	0.008230109	1	0	0	0	1	0	0	0	0.196791433
23568.4	0.201855778	0	0.00998027	0.038550671	0.158205736	0.008224	1	0	0	0	1	0	0	0	0.196756407
23783.4	0.201855778	0	0.00998027	0.038254777	0.158444555	0.008204628	1	0	0	0	1	0	0	0	0.196699332
23998.4	0.201855778	0	0.00998027	0.03790728	0.158831337	0.008190844	1	0	0	0	1	0	0	0	0.196738617
24214.4	0.201855778	0	0.00998027	0.037456685	0.159238955	0.008182174	1	0	0	0	1	0	0	0	0.196695639
24429.4	0.201855778	0	0.00998027	0.037025327	0.159610885	0.008171599	1	0	0	0	1	0	0	0	0.196636213
24645.4	0.201855778	0	0.00998027	0.036735032	0.159896117	0.008155526	1	0	0	0	1	0	0	0	0.196631149
24860.4	0.201855778	0	0.00998027	0.03637305	0.16023062	0.008149197	1	0	0	0	1	0	0	0	0.19660367
25076.4	0.201855778	0	0.00998027	0.035955891	0.1606238	0.008135389	1	0	0	0	1	0	0	0	0.196579691
25291.4	0.201855778	0	0.00998027	0.035830817	0.160806026	0.008116151	1	0	0	0	1	0	0	0	0.196636842
25507.4	0.201855778	0	0.00998027	0.035426322	0.161101844	0.008106034	1	0	0	0	1	0	0	0	0.196528165
25722.4	0.201855778	0	0.00998027	0.034954189	0.161479885	0.008095511	1	0	0	0	1	0	0	0	0.196434074
25938.4	0.201855778	0	0.00998027	0.034544399	0.161882902	0.00809337	1	0	0	0	1	0	0	0	0.196427301
26153.4	0.201855778	0	0.00998027	0.034254267	0.162208924	0.008081889	1	0	0	0	1	0	0	0	0.196463191

26369.4	0.201855778	0	0.00998027	0.03385467	0.162391718	0.008074388	1	0	0	0	1	0	0	0	0.196246388
26584.4	0.201855778	0	0.00998027	0.033820655	0.162669516	0.008054327	1	0	0	0	1	0	0	0	0.196490171
26800.4	0.201855778	0	0.00998027	0.033254537	0.163123693	0.008052797	1	0	0	0	1	0	0	0	0.19637823
27015.4	0.201855778	0	0.00998027	0.032991254	0.163274669	0.008034681	1	0	0	0	1	0	0	0	0.196265923
27231.4	0.201855778	0	0.00998027	0.032723081	0.16356708	0.008027908	1	0	0	0	1	0	0	0	0.196290161
27446.4	0.201855778	0	0.00998027	0.032611997	0.16371107	0.008003731	1	0	0	0	1	0	0	0	0.196323067
27662.4	0.201855778	0	0.00998027	0.032116064	0.16414393	0.008004539	1	0	0	0	1	0	0	0	0.196259994
27877.4	0.201855778	0	0.00998027	0.03171664	0.164429349	0.008003558	1	0	0	0	1	0	0	0	0.196145989
28092.4	0.201855778	0	0.00998027	0.031637946	0.164596039	0.007980509	1	0	0	0	1	0	0	0	0.196233985
28308.4	0.201855778	0	0.00998027	0.031123386	0.164953179	0.007976221	1	0	0	0	1	0	0	0	0.196076564
28523.4	0.201855778	0	0.00998027	0.03088839	0.165287657	0.00796348	1	0	0	0	1	0	0	0	0.196176048
28739.4	0.201855778	0	0.00998027	0.030355667	0.165608723	0.007956541	1	0	0	0	1	0	0	0	0.195964391
28954.4	0.201855778	0	0.00998027	0.030395959	0.165657106	0.00793784	1	0	0	0	1	0	0	0	0.196053065
29170.4	0.201855778	0	0.00998027	0.030227454	0.165912192	0.00792575	1	0	0	0	1	0	0	0	0.196139646
29385.4	0.201855778	0	0.00998027	0.029928566	0.166116361	0.007918003	1	0	0	0	1	0	0	0	0.196044926
29601.4	0.201855778	0	0.00998027	0.029722969	0.166321343	0.007902953	1	0	0	0	1	0	0	0	0.196044312
29816.4	0.201855778	0	0.00998027	0.029305901	0.166645167	0.007901231	1	0	0	0	1	0	0	0	0.195951068
30032.4	0.201855778	0	0.00998027	0.029229481	0.166807137	0.007878575	1	0	0	0	1	0	0	0	0.196036618
30247.4	0.201855778	0	0.00998027	0.028936209	0.166955191	0.007880907	1	0	0	0	1	0	0	0	0.1958914
30463.4	0.201855778	0	0.00998027	0.02869209	0.167214996	0.007860755	1	0	0	0	1	0	0	0	0.195907085
30678.4	0.201855778	0	0.00998027	0.028347837	0.167570513	0.007862563	1	0	0	0	1	0	0	0	0.19591835
30894.4	0.201855778	0	0.00998027	0.028219201	0.16768757	0.007846035	1	0	0	0	1	0	0	0	0.195906771
31109.4	0.201855778	0	0.00998027	0.027944024	0.16807962	0.007839879	1	0	0	0	1	0	0	0	0.196023644
31324.4	0.201855778	0	0.00998027	0.027552819	0.168341554	0.007832739	1	0	0	0	1	0	0	0	0.195894373
31540.4	0.201855778	0	0.00998027	0.027370518	0.16855852	0.00782381	1	0	0	0	1	0	0	0	0.195929038
31755.4	0.201855778	0	0.00998027	0.027122895	0.168678353	0.007811901	1	0	0	0	1	0	0	0	0.195801248
31971.4	0.201855778	0	0.00998027	0.026914062	0.168894749	0.007803649	1	0	0	0	1	0	0	0	0.195808811
32186.4	0.201855778	0	0.00998027	0.026624104	0.169119453	0.007797264	1	0	0	0	1	0	0	0	0.195743558
32402.4	0.201855778	0	0.00998027	0.026676734	0.169132993	0.007785737	1	0	0	0	1	0	0	0	0.195809727
32617.4	0.201855778	0	0.00998027	0.026278811	0.169425279	0.007774082	1	0	0	0	1	0	0	0	0.19570409
32833.4	0.201855778	0	0.00998027	0.026110648	0.169613141	0.007755508	1	0	0	0	1	0	0	0	0.19572379

33048.4	0.201855778	0	0.00998027	0.025768279	0.169864021	0.007754349	1	0	0	0	1	0	0	0	0.1956323
33264.4	0.201855778	0	0.00998027	0.025596354	0.170176897	0.007741302	1	0	0	0	1	0	0	0	0.195773251

time/s	[1a] _o	[1b] _o	[cat] _{τ_o}	[1a]	[1b]	[active cat]	[PA]	[PB]	[PC]	[PD]	[PA2]	[PB2]	[PC2]	[PD2]	[1a]+[1b]
0	0.201818654	0.101	0.009994693	0.201818654	0.101	0.009994693	0	1	0	0	0	1	0	0	0.302818654
215.4	0.201818654	0.101	0.009994693	0.192834924	0.109983729	0.009994693	0	1	0	0	0	1	0	0	0.302818654
432.4	0.201818654	0.101	0.009994693	0.186461052	0.11649006	0.009865279	0	1	0	0	0	1	0	0	0.302951113
647.4	0.201818654	0.101	0.009994693	0.181196509	0.121736755	0.009762817	0	1	0	0	0	1	0	0	0.302933263
863.4	0.201818654	0.101	0.009994693	0.175557799	0.127098978	0.009712302	0	1	0	0	0	1	0	0	0.302656777
1078.4	0.201818654	0.101	0.009994693	0.170864662	0.1317871	0.009671876	0	1	0	0	0	1	0	0	0.302651762
1294.4	0.201818654	0.101	0.009994693	0.166629095	0.135912246	0.009632464	0	1	0	0	0	1	0	0	0.302541341
1509.4	0.201818654	0.101	0.009994693	0.162042918	0.140475815	0.0096303	0	1	0	0	0	1	0	0	0.302518734
1724.4	0.201818654	0.101	0.009994693	0.157748062	0.144711716	0.009622855	0	1	0	0	0	1	0	0	0.302459777
1940.4	0.201818654	0.101	0.009994693	0.153800147	0.148419679	0.00961032	0	1	0	0	0	1	0	0	0.302219826
2155.4	0.201818654	0.101	0.009994693	0.149776121	0.152422398	0.00960416	0	1	0	0	0	1	0	0	0.302198519
2371.4	0.201818654	0.101	0.009994693	0.146041195	0.15609855	0.009584716	0	1	0	0	0	1	0	0	0.302139745
2586.4	0.201818654	0.101	0.009994693	0.142438572	0.159542411	0.009571354	0	1	0	0	0	1	0	0	0.301980983
2802.4	0.201818654	0.101	0.009994693	0.138833377	0.163081968	0.009565091	0	1	0	0	0	1	0	0	0.301915345
3017.4	0.201818654	0.101	0.009994693	0.135323807	0.166427005	0.009550055	0	1	0	0	0	1	0	0	0.301750812
3232.4	0.201818654	0.101	0.009994693	0.132047785	0.169506772	0.009516542	0	1	0	0	0	1	0	0	0.301554557
3448.4	0.201818654	0.101	0.009994693	0.128572125	0.172785801	0.009526896	0	1	0	0	0	1	0	0	0.301357927
3663.4	0.201818654	0.101	0.009994693	0.126034868	0.175382882	0.009482243	0	1	0	0	0	1	0	0	0.30141775
3879.4	0.201818654	0.101	0.009994693	0.122938786	0.178255717	0.009470333	0	1	0	0	0	1	0	0	0.301194502
4094.4	0.201818654	0.101	0.009994693	0.120057659	0.18099574	0.009443302	0	1	0	0	0	1	0	0	0.301053399
4309.4	0.201818654	0.101	0.009994693	0.117407052	0.183595659	0.009423572	0	1	0	0	0	1	0	0	0.301002711
4525.4	0.201818654	0.101	0.009994693	0.11460995	0.186240278	0.009416284	0	1	0	0	0	1	0	0	0.300850229
4740.4	0.201818654	0.101	0.009994693	0.112614787	0.188429408	0.009368419	0	1	0	0	0	1	0	0	0.301044195

4956.4	0.201818654	0.101	0.009994693	0.109960607	0.19073948	0.009346969	0	1	0	0	0	1	0	0	0.300700087
5171.4	0.201818654	0.101	0.009994693	0.107558488	0.192961023	0.009321798	0	1	0	0	0	1	0	0	0.300519511
5387.4	0.201818654	0.101	0.009994693	0.105420804	0.195120774	0.009294853	0	1	0	0	0	1	0	0	0.300541577
5602.4	0.201818654	0.101	0.009994693	0.10272024	0.197364282	0.009293624	0	1	0	0	0	1	0	0	0.300084522
5818.4	0.201818654	0.101	0.009994693	0.100817666	0.199309016	0.009254881	0	1	0	0	0	1	0	0	0.300126682
6033.4	0.201818654	0.101	0.009994693	0.099277516	0.200994528	0.009207576	0	1	0	0	0	1	0	0	0.300272043
6248.4	0.201818654	0.101	0.009994693	0.097317504	0.202984614	0.00919153	0	1	0	0	0	1	0	0	0.300302118
6464.4	0.201818654	0.101	0.009994693	0.095065447	0.204837846	0.009170131	0	1	0	0	0	1	0	0	0.299903293
6679.4	0.201818654	0.101	0.009994693	0.093470193	0.206451237	0.009132461	0	1	0	0	0	1	0	0	0.29992143
6895.4	0.201818654	0.101	0.009994693	0.092071305	0.208086388	0.009109234	0	1	0	0	0	1	0	0	0.300157694
7110.4	0.201818654	0.101	0.009994693	0.089933058	0.209831343	0.009087975	0	1	0	0	0	1	0	0	0.299764401
7326.4	0.201818654	0.101	0.009994693	0.087985175	0.211496436	0.00906796	0	1	0	0	0	1	0	0	0.299481611
7542.4	0.201818654	0.101	0.009994693	0.086424828	0.212939512	0.009039655	0	1	0	0	0	1	0	0	0.29936434
7757.4	0.201818654	0.101	0.009994693	0.08488259	0.214417672	0.00901015	0	1	0	0	0	1	0	0	0.299300263
7973.4	0.201818654	0.101	0.009994693	0.083554751	0.215778321	0.00897929	0	1	0	0	0	1	0	0	0.299333073
8188.4	0.201818654	0.101	0.009994693	0.081835171	0.21724751	0.008954448	0	1	0	0	0	1	0	0	0.299082681
8404.4	0.201818654	0.101	0.009994693	0.08054453	0.218475967	0.008928125	0	1	0	0	0	1	0	0	0.299020498
8619.4	0.201818654	0.101	0.009994693	0.079099874	0.219864328	0.008916619	0	1	0	0	0	1	0	0	0.298964202
8835.4	0.201818654	0.101	0.009994693	0.077558254	0.221082767	0.008879902	0	1	0	0	0	1	0	0	0.298641021
9050.4	0.201818654	0.101	0.009994693	0.076572908	0.222256284	0.008849133	0	1	0	0	0	1	0	0	0.298829193
9266.4	0.201818654	0.101	0.009994693	0.075462533	0.223489448	0.0088336	0	1	0	0	0	1	0	0	0.298951981
9481.4	0.201818654	0.101	0.009994693	0.073648711	0.224747194	0.008816491	0	1	0	0	0	1	0	0	0.298395905
9696.4	0.201818654	0.101	0.009994693	0.07252617	0.225797357	0.008773441	0	1	0	0	0	1	0	0	0.298323527
9912.4	0.201818654	0.101	0.009994693	0.071377594	0.226981553	0.008760607	0	1	0	0	0	1	0	0	0.298359147
10127.4	0.201818654	0.101	0.009994693	0.070317355	0.227988437	0.008736922	0	1	0	0	0	1	0	0	0.298305792
10343.4	0.201818654	0.101	0.009994693	0.069445954	0.228999902	0.008706966	0	1	0	0	0	1	0	0	0.298445856
10558.4	0.201818654	0.101	0.009994693	0.067921255	0.230083984	0.008696454	0	1	0	0	0	1	0	0	0.298005239
10774.4	0.201818654	0.101	0.009994693	0.066993332	0.231051489	0.008661756	0	1	0	0	0	1	0	0	0.29804482
10989.4	0.201818654	0.101	0.009994693	0.066332605	0.231895169	0.008638083	0	1	0	0	0	1	0	0	0.298227774
11205.4	0.201818654	0.101	0.009994693	0.065460366	0.232813009	0.008610201	0	1	0	0	0	1	0	0	0.298273375
11420.4	0.201818654	0.101	0.009994693	0.063852473	0.233739287	0.008600798	0	1	0	0	0	1	0	0	0.297591761

11636.4	0.201818654	0.101	0.009994693	0.063106933	0.234738522	0.008578582	0	1	0	0	0	1	0	0	0.297845455
11851.4	0.201818654	0.101	0.009994693	0.062408618	0.235584869	0.008556851	0	1	0	0	0	1	0	0	0.297993487
12067.4	0.201818654	0.101	0.009994693	0.061205601	0.236460988	0.008537162	0	1	0	0	0	1	0	0	0.297666589
12282.4	0.201818654	0.101	0.009994693	0.060044667	0.237343153	0.008516748	0	1	0	0	0	1	0	0	0.29738782
12498.4	0.201818654	0.101	0.009994693	0.059145577	0.238073679	0.008495681	0	1	0	0	0	1	0	0	0.297219256
12713.4	0.201818654	0.101	0.009994693	0.058347243	0.238856538	0.008458796	0	1	0	0	0	1	0	0	0.297203781
12928.4	0.201818654	0.101	0.009994693	0.057278648	0.239690015	0.008455911	0	1	0	0	0	1	0	0	0.296968663
13144.4	0.201818654	0.101	0.009994693	0.057224515	0.240431194	0.008425641	0	1	0	0	0	1	0	0	0.297655709
13359.4	0.201818654	0.101	0.009994693	0.056495371	0.241101245	0.008405053	0	1	0	0	0	1	0	0	0.297596616
13575.4	0.201818654	0.101	0.009994693	0.055520412	0.241811631	0.00838304	0	1	0	0	0	1	0	0	0.297332043
13790.4	0.201818654	0.101	0.009994693	0.054649601	0.242528395	0.008365036	0	1	0	0	0	1	0	0	0.297177995
14006.4	0.201818654	0.101	0.009994693	0.053622572	0.2433283	0.008358319	0	1	0	0	0	1	0	0	0.296950872
14222.4	0.201818654	0.101	0.009994693	0.053123	0.24393959	0.008327223	0	1	0	0	0	1	0	0	0.29706259
14437.4	0.201818654	0.101	0.009994693	0.052173838	0.244600464	0.00831367	0	1	0	0	0	1	0	0	0.296774302
14653.4	0.201818654	0.101	0.009994693	0.051784597	0.245133839	0.008277776	0	1	0	0	0	1	0	0	0.296918436
14868.4	0.201818654	0.101	0.009994693	0.051048556	0.245793615	0.008269496	0	1	0	0	0	1	0	0	0.296842172
15084.4	0.201818654	0.101	0.009994693	0.050087359	0.246540595	0.008259786	0	1	0	0	0	1	0	0	0.296627955
15299.4	0.201818654	0.101	0.009994693	0.049366249	0.247127103	0.008241826	0	1	0	0	0	1	0	0	0.296493353
15515.4	0.201818654	0.101	0.009994693	0.049195742	0.247658755	0.008209862	0	1	0	0	0	1	0	0	0.296854497
15730.4	0.201818654	0.101	0.009994693	0.048585237	0.248171443	0.008186171	0	1	0	0	0	1	0	0	0.29675668
15946.4	0.201818654	0.101	0.009994693	0.047895129	0.248814398	0.008170425	0	1	0	0	0	1	0	0	0.296709527
16161.4	0.201818654	0.101	0.009994693	0.047203191	0.249348762	0.008151589	0	1	0	0	0	1	0	0	0.296551953
16377.4	0.201818654	0.101	0.009994693	0.046344118	0.24989024	0.008143699	0	1	0	0	0	1	0	0	0.296234358
16592.4	0.201818654	0.101	0.009994693	0.045538683	0.250430117	0.008129642	0	1	0	0	0	1	0	0	0.2959688
16807.4	0.201818654	0.101	0.009994693	0.045495619	0.250956058	0.008097488	0	1	0	0	0	1	0	0	0.296451677
17023.4	0.201818654	0.101	0.009994693	0.04494321	0.251381558	0.008083673	0	1	0	0	0	1	0	0	0.296324768
17239.4	0.201818654	0.101	0.009994693	0.044115184	0.252008352	0.008073804	0	1	0	0	0	1	0	0	0.296123536
17454.4	0.201818654	0.101	0.009994693	0.043730783	0.252512254	0.008049142	0	1	0	0	0	1	0	0	0.296243038
17669.4	0.201818654	0.101	0.009994693	0.043410188	0.252899749	0.008032995	0	1	0	0	0	1	0	0	0.296309937
17885.4	0.201818654	0.101	0.009994693	0.042527541	0.25350122	0.008016626	0	1	0	0	0	1	0	0	0.296028761
18100.4	0.201818654	0.101	0.009994693	0.042214356	0.253955363	0.008001622	0	1	0	0	0	1	0	0	0.296169719

18316.4	0.201818654	0.101	0.009994693	0.041744211	0.254373737	0.007979497	0	1	0	0	0	1	0	0	0.296117948
18531.4	0.201818654	0.101	0.009994693	0.041154806	0.25476043	0.00796239	0	1	0	0	0	1	0	0	0.295915236
18747.4	0.201818654	0.101	0.009994693	0.040606941	0.255314837	0.007947393	0	1	0	0	0	1	0	0	0.295921778
18962.4	0.201818654	0.101	0.009994693	0.040184927	0.255724519	0.007938803	0	1	0	0	0	1	0	0	0.295909447
19178.4	0.201818654	0.101	0.009994693	0.039835938	0.256078177	0.00790585	0	1	0	0	0	1	0	0	0.295914115
19393.4	0.201818654	0.101	0.009994693	0.039299454	0.256510669	0.007899708	0	1	0	0	0	1	0	0	0.295810123
19609.4	0.201818654	0.101	0.009994693	0.039029124	0.256904638	0.007871617	0	1	0	0	0	1	0	0	0.295933763
19824.4	0.201818654	0.101	0.009994693	0.038643845	0.257269912	0.007860739	0	1	0	0	0	1	0	0	0.295913757
20040.4	0.201818654	0.101	0.009994693	0.037512327	0.257738695	0.007863623	0	1	0	0	0	1	0	0	0.295251022
20255.4	0.201818654	0.101	0.009994693	0.037197482	0.258154853	0.007849531	0	1	0	0	0	1	0	0	0.295352336
20470.4	0.201818654	0.101	0.009994693	0.036815858	0.258450991	0.007830028	0	1	0	0	0	1	0	0	0.295266848
20686.4	0.201818654	0.101	0.009994693	0.036727923	0.258860505	0.007805402	0	1	0	0	0	1	0	0	0.295588428
20901.4	0.201818654	0.101	0.009994693	0.036121131	0.259335607	0.007798815	0	1	0	0	0	1	0	0	0.295456737
21117.4	0.201818654	0.101	0.009994693	0.035521096	0.259575298	0.007778762	0	1	0	0	0	1	0	0	0.295096394
21332.4	0.201818654	0.101	0.009994693	0.035404784	0.259942134	0.007767666	0	1	0	0	0	1	0	0	0.295346918
21548.4	0.201818654	0.101	0.009994693	0.035038299	0.260410641	0.007750116	0	1	0	0	0	1	0	0	0.29544894
21763.4	0.201818654	0.101	0.009994693	0.034865218	0.260626649	0.007728266	0	1	0	0	0	1	0	0	0.295491867
21978.4	0.201818654	0.101	0.009994693	0.034211398	0.260878875	0.007717633	0	1	0	0	0	1	0	0	0.295090273
22194.4	0.201818654	0.101	0.009994693	0.033957608	0.261402146	0.007708311	0	1	0	0	0	1	0	0	0.295359754
22409.4	0.201818654	0.101	0.009994693	0.03347173	0.261641019	0.007687527	0	1	0	0	0	1	0	0	0.295112749
22625.4	0.201818654	0.101	0.009994693	0.033415836	0.261952485	0.007670835	0	1	0	0	0	1	0	0	0.295368321
22840.4	0.201818654	0.101	0.009994693	0.032638377	0.262271975	0.00766819	0	1	0	0	0	1	0	0	0.294910351
23056.4	0.201818654	0.101	0.009994693	0.032206499	0.262639031	0.007659493	0	1	0	0	0	1	0	0	0.294845531
23271.4	0.201818654	0.101	0.009994693	0.031916782	0.262875348	0.007638737	0	1	0	0	0	1	0	0	0.29479213
23487.4	0.201818654	0.101	0.009994693	0.031803072	0.263168294	0.007618523	0	1	0	0	0	1	0	0	0.294971366
23702.4	0.201818654	0.101	0.009994693	0.031307565	0.263474126	0.00760928	0	1	0	0	0	1	0	0	0.294781691
23918.4	0.201818654	0.101	0.009994693	0.031060205	0.263798242	0.007594714	0	1	0	0	0	1	0	0	0.294858448
24133.4	0.201818654	0.101	0.009994693	0.030791471	0.26400023	0.007578101	0	1	0	0	0	1	0	0	0.294791701
24349.4	0.201818654	0.101	0.009994693	0.030602788	0.264302107	0.007552398	0	1	0	0	0	1	0	0	0.294904895
24564.4	0.201818654	0.101	0.009994693	0.030341489	0.264556746	0.007542594	0	1	0	0	0	1	0	0	0.294898235
24779.4	0.201818654	0.101	0.009994693	0.029569183	0.264819708	0.007536312	0	1	0	0	0	1	0	0	0.294388891

24995.4	0.201818654	0.101	0.009994693	0.029529067	0.265163639	0.007526943	0	1	0	0	0	1	0	0	0.294692706
25210.4	0.201818654	0.101	0.009994693	0.029223445	0.265393239	0.007510216	0	1	0	0	0	1	0	0	0.294616684
25426.4	0.201818654	0.101	0.009994693	0.02874159	0.265579442	0.007501404	0	1	0	0	0	1	0	0	0.294321032
25641.4	0.201818654	0.101	0.009994693	0.028647212	0.265949315	0.007490091	0	1	0	0	0	1	0	0	0.294596527
25856.4	0.201818654	0.101	0.009994693	0.02839348	0.266131545	0.007469475	0	1	0	0	0	1	0	0	0.294525025
26072.4	0.201818654	0.101	0.009994693	0.028218865	0.266421628	0.0074571	0	1	0	0	0	1	0	0	0.294640493
26287.4	0.201818654	0.101	0.009994693	0.027653584	0.266656821	0.007451624	0	1	0	0	0	1	0	0	0.294310405
26503.4	0.201818654	0.101	0.009994693	0.02748505	0.266935036	0.007429488	0	1	0	0	0	1	0	0	0.294420086
26718.4	0.201818654	0.101	0.009994693	0.026846765	0.267177013	0.007435882	0	1	0	0	0	1	0	0	0.294023778
26934.4	0.201818654	0.101	0.009994693	0.026701149	0.267401462	0.007421603	0	1	0	0	0	1	0	0	0.294102611
27149.4	0.201818654	0.101	0.009994693	0.026370516	0.267603766	0.00740494	0	1	0	0	0	1	0	0	0.293974282
27365.4	0.201818654	0.101	0.009994693	0.026315416	0.267748007	0.007379736	0	1	0	0	0	1	0	0	0.294063422
27580.4	0.201818654	0.101	0.009994693	0.026191366	0.268013947	0.007368866	0	1	0	0	0	1	0	0	0.294205313
27796.4	0.201818654	0.101	0.009994693	0.026218735	0.268206974	0.007350943	0	1	0	0	0	1	0	0	0.294425709
28011.4	0.201818654	0.101	0.009994693	0.025662058	0.268334219	0.007343939	0	1	0	0	0	1	0	0	0.293996277
28227.4	0.201818654	0.101	0.009994693	0.025259289	0.268597961	0.007326239	0	1	0	0	0	1	0	0	0.29385725
28442.4	0.201818654	0.101	0.009994693	0.024789741	0.268861349	0.007329108	0	1	0	0	0	1	0	0	0.29365109
28658.4	0.201818654	0.101	0.009994693	0.024711722	0.269008659	0.007308664	0	1	0	0	0	1	0	0	0.293720381
28873.4	0.201818654	0.101	0.009994693	0.024728153	0.269211466	0.007294054	0	1	0	0	0	1	0	0	0.293939619
29089.4	0.201818654	0.101	0.009994693	0.024267754	0.269376938	0.007285622	0	1	0	0	0	1	0	0	0.293644692
29304.4	0.201818654	0.101	0.009994693	0.024509376	0.26964806	0.007264444	0	1	0	0	0	1	0	0	0.294157436
29520.4	0.201818654	0.101	0.009994693	0.024131703	0.269866572	0.007250624	0	1	0	0	0	1	0	0	0.293998275
29735.4	0.201818654	0.101	0.009994693	0.023704284	0.270040777	0.007249573	0	1	0	0	0	1	0	0	0.293745061
29951.4	0.201818654	0.101	0.009994693	0.023768881	0.270269686	0.007230895	0	1	0	0	0	1	0	0	0.294038567
30166.4	0.201818654	0.101	0.009994693	0.023291032	0.270484202	0.007230927	0	1	0	0	0	1	0	0	0.293775234
30382.4	0.201818654	0.101	0.009994693	0.023187413	0.27054036	0.007203268	0	1	0	0	0	1	0	0	0.293727773
30597.4	0.201818654	0.101	0.009994693	0.022767151	0.270828513	0.007206286	0	1	0	0	0	1	0	0	0.293595664
30813.4	0.201818654	0.101	0.009994693	0.023137394	0.270950539	0.007182919	0	1	0	0	0	1	0	0	0.294087933
31028.4	0.201818654	0.101	0.009994693	0.022318992	0.271032542	0.007180793	0	1	0	0	0	1	0	0	0.293351535
31244.4	0.201818654	0.101	0.009994693	0.022493501	0.271161309	0.007148334	0	1	0	0	0	1	0	0	0.29365481
31459.4	0.201818654	0.101	0.009994693	0.022355873	0.271361889	0.007148204	0	1	0	0	0	1	0	0	0.293717762

31675.4	0.201818654	0.101	0.009994693	0.021800236	0.27162221	0.007142748	0	1	0	0	0	1	0	0	0.293422446
31890.4	0.201818654	0.101	0.009994693	0.021914878	0.271711275	0.007122869	0	1	0	0	0	1	0	0	0.293626153
32106.4	0.201818654	0.101	0.009994693	0.021548225	0.271890054	0.007119476	0	1	0	0	0	1	0	0	0.293438279
32321.4	0.201818654	0.101	0.009994693	0.021484513	0.272097221	0.007111098	0	1	0	0	0	1	0	0	0.293581733
32537.4	0.201818654	0.101	0.009994693	0.021352158	0.272299078	0.007096241	0	1	0	0	0	1	0	0	0.293651236
32752.4	0.201818654	0.101	0.009994693	0.021171585	0.272379144	0.00708841	0	1	0	0	0	1	0	0	0.293550729
32968.4	0.201818654	0.101	0.009994693	0.020747474	0.272583784	0.007077383	0	1	0	0	0	1	0	0	0.293331258
33183.4	0.201818654	0.101	0.009994693	0.020557483	0.272738555	0.007064194	0	1	0	0	0	1	0	0	0.293296038
33399.4	0.201818654	0.101	0.009994693	0.020594181	0.272799769	0.007047381	0	1	0	0	0	1	0	0	0.29339395
33614.4	0.201818654	0.101	0.009994693	0.020437441	0.272966722	0.007041069	0	1	0	0	0	1	0	0	0.293404164
33830.4	0.201818654	0.101	0.009994693	0.019900485	0.27310739	0.007030883	0	1	0	0	0	1	0	0	0.293007875
34045.4	0.201818654	0.101	0.009994693	0.020476112	0.273094228	0.006997673	0	1	0	0	0	1	0	0	0.29357034
34261.4	0.201818654	0.101	0.009994693	0.019646765	0.273426687	0.007011621	0	1	0	0	0	1	0	0	0.293073452
34476.4	0.201818654	0.101	0.009994693	0.019704511	0.273503065	0.006991115	0	1	0	0	0	1	0	0	0.293207576
34692.4	0.201818654	0.101	0.009994693	0.019391468	0.273670359	0.006987683	0	1	0	0	0	1	0	0	0.293061826
34907.4	0.201818654	0.101	0.009994693	0.019062485	0.273735862	0.006981861	0	1	0	0	0	1	0	0	0.292798347
35123.4	0.201818654	0.101	0.009994693	0.01932204	0.273960736	0.006955306	0	1	0	0	0	1	0	0	0.293282776
35338.4	0.201818654	0.101	0.009994693	0.019458337	0.274004278	0.006946255	0	1	0	0	0	1	0	0	0.293462616
35554.4	0.201818654	0.101	0.009994693	0.018877472	0.274271719	0.006942867	0	1	0	0	0	1	0	0	0.293149191
35769.4	0.201818654	0.101	0.009994693	0.018934336	0.274327395	0.006928503	0	1	0	0	0	1	0	0	0.293261731
35985.4	0.201818654	0.101	0.009994693	0.018515277	0.274407845	0.006911378	0	1	0	0	0	1	0	0	0.292923122
36200.4	0.201818654	0.101	0.009994693	0.018608929	0.274559291	0.006901367	0	1	0	0	0	1	0	0	0.29316822
36416.4	0.201818654	0.101	0.009994693	0.018480348	0.274618417	0.006888153	0	1	0	0	0	1	0	0	0.293098764
36631.4	0.201818654	0.101	0.009994693	0.018568646	0.274819299	0.006882989	0	1	0	0	0	1	0	0	0.293387945
36846.4	0.201818654	0.101	0.009994693	0.018261719	0.274876327	0.006871119	0	1	0	0	0	1	0	0	0.293138046
37062.4	0.201818654	0.101	0.009994693	0.018446857	0.274848784	0.006848491	0	1	0	0	0	1	0	0	0.293295641
37277.4	0.201818654	0.101	0.009994693	0.018105832	0.275163431	0.00684298	0	1	0	0	0	1	0	0	0.293269263
37493.4	0.201818654	0.101	0.009994693	0.017304657	0.275213052	0.006854897	0	1	0	0	0	1	0	0	0.292517709
37708.4	0.201818654	0.101	0.009994693	0.018062736	0.275424784	0.006826449	0	1	0	0	0	1	0	0	0.29348752
37924.4	0.201818654	0.101	0.009994693	0.017603472	0.275455762	0.006817377	0	1	0	0	0	1	0	0	0.293059234
38139.4	0.201818654	0.101	0.009994693	0.017509095	0.275618379	0.006800658	0	1	0	0	0	1	0	0	0.293127474

38355.4	0.201818654	0.101	0.009994693	0.017185391	0.275775923	0.006800875	0	1	0	0	0	1	0	0	0.292961314
38570.4	0.201818654	0.101	0.009994693	0.016891897	0.275724199	0.006791258	0	1	0	0	0	1	0	0	0.292616097
38785.4	0.201818654	0.101	0.009994693	0.017185823	0.275807092	0.006770256	0	1	0	0	0	1	0	0	0.292992915
39001.4	0.201818654	0.101	0.009994693	0.016937042	0.275955024	0.00676082	0	1	0	0	0	1	0	0	0.292892066
39216.4	0.201818654	0.101	0.009994693	0.016648636	0.27605002	0.006763412	0	1	0	0	0	1	0	0	0.292698655
39432.4	0.201818654	0.101	0.009994693	0.016243417	0.276182896	0.006754063	0	1	0	0	0	1	0	0	0.292426313
39647.4	0.201818654	0.101	0.009994693	0.01608045	0.276312145	0.006755171	0	1	0	0	0	1	0	0	0.292392595
39863.4	0.201818654	0.101	0.009994693	0.016577094	0.276355056	0.006717762	0	1	0	0	0	1	0	0	0.29293215
40078.4	0.201818654	0.101	0.009994693	0.016519733	0.276558599	0.006719008	0	1	0	0	0	1	0	0	0.293078332
40294.4	0.201818654	0.101	0.009994693	0.016181251	0.276613567	0.006713593	0	1	0	0	0	1	0	0	0.292794818
40509.4	0.201818654	0.101	0.009994693	0.016056979	0.27668835	0.006700868	0	1	0	0	0	1	0	0	0.292745329
40725.4	0.201818654	0.101	0.009994693	0.015847225	0.276736571	0.006680544	0	1	0	0	0	1	0	0	0.292583796
40940.4	0.201818654	0.101	0.009994693	0.015710271	0.276866522	0.006675523	0	1	0	0	0	1	0	0	0.292576793
41156.4	0.201818654	0.101	0.009994693	0.016111289	0.276946343	0.006654742	0	1	0	0	0	1	0	0	0.293057632
41371.4	0.201818654	0.101	0.009994693	0.015954453	0.277083077	0.00665591	0	1	0	0	0	1	0	0	0.29303753
41586.4	0.201818654	0.101	0.009994693	0.015019789	0.277133036	0.006661109	0	1	0	0	0	1	0	0	0.292152826
41802.4	0.201818654	0.101	0.009994693	0.014950725	0.277121119	0.006643856	0	1	0	0	0	1	0	0	0.292071844
42017.4	0.201818654	0.101	0.009994693	0.015188874	0.277286258	0.00662476	0	1	0	0	0	1	0	0	0.292475132
42233.4	0.201818654	0.101	0.009994693	0.015089795	0.277378689	0.006614207	0	1	0	0	0	1	0	0	0.292468484
42448.4	0.201818654	0.101	0.009994693	0.014841031	0.277471712	0.006612334	0	1	0	0	0	1	0	0	0.292312743
42664.4	0.201818654	0.101	0.009994693	0.015051733	0.277621301	0.006591341	0	1	0	0	0	1	0	0	0.292673034
42879.4	0.201818654	0.101	0.009994693	0.014491167	0.277686807	0.00659528	0	1	0	0	0	1	0	0	0.292177974
43094.4	0.201818654	0.101	0.009994693	0.014543442	0.27766721	0.006584478	0	1	0	0	0	1	0	0	0.292210653
43310.4	0.201818654	0.101	0.009994693	0.01455556	0.277729349	0.00657148	0	1	0	0	0	1	0	0	0.292284909
43525.4	0.201818654	0.101	0.009994693	0.015190822	0.277790007	0.006545699	0	1	0	0	0	1	0	0	0.292980829
43741.4	0.201818654	0.101	0.009994693	0.014251415	0.27794895	0.006552995	0	1	0	0	0	1	0	0	0.292200365
43956.4	0.201818654	0.101	0.009994693	0.014180649	0.277987642	0.006541208	0	1	0	0	0	1	0	0	0.292168291
44172.4	0.201818654	0.101	0.009994693	0.014795386	0.278129023	0.006520003	0	1	0	0	0	1	0	0	0.292924408
44387.4	0.201818654	0.101	0.009994693	0.014242165	0.277995882	0.006510209	0	1	0	0	0	1	0	0	0.292238047
44603.4	0.201818654	0.101	0.009994693	0.014091468	0.278201547	0.006510084	0	1	0	0	0	1	0	0	0.292293015
44818.4	0.201818654	0.101	0.009994693	0.01413628	0.278190424	0.006494492	0	1	0	0	0	1	0	0	0.292326704

45034.4	0.201818654	0.101	0.009994693	0.014263414	0.27837015	0.006477374	0	1	0	0	0	1	0	0	0.292633564
45249.4	0.201818654	0.101	0.009994693	0.01371766	0.278388844	0.006479859	0	1	0	0	0	1	0	0	0.292106504
45465.4	0.201818654	0.101	0.009994693	0.013853111	0.278472368	0.006459786	0	1	0	0	0	1	0	0	0.292325479
45680.4	0.201818654	0.101	0.009994693	0.013450646	0.278490477	0.006458167	0	1	0	0	0	1	0	0	0.291941122
45896.4	0.201818654	0.101	0.009994693	0.013434007	0.278631027	0.006452251	0	1	0	0	0	1	0	0	0.292065034
46111.4	0.201818654	0.101	0.009994693	0.013336554	0.278635244	0.006442191	0	1	0	0	0	1	0	0	0.291971797
46327.4	0.201818654	0.101	0.009994693	0.013339282	0.278697866	0.006430166	0	1	0	0	0	1	0	0	0.292037148
46542.4	0.201818654	0.101	0.009994693	0.013437045	0.278806488	0.006423094	0	1	0	0	0	1	0	0	0.292243533
46758.4	0.201818654	0.101	0.009994693	0.013366723	0.278832779	0.006411779	0	1	0	0	0	1	0	0	0.292199503
46973.4	0.201818654	0.101	0.009994693	0.01324536	0.278992523	0.006405435	0	1	0	0	0	1	0	0	0.292237883
47188.4	0.201818654	0.101	0.009994693	0.012832839	0.279014844	0.006397455	0	1	0	0	0	1	0	0	0.291847683
47404.4	0.201818654	0.101	0.009994693	0.0129716	0.279131522	0.006386809	0	1	0	0	0	1	0	0	0.292103122
47619.4	0.201818654	0.101	0.009994693	0.012715229	0.279138461	0.006373642	0	1	0	0	0	1	0	0	0.29185369
47835.4	0.201818654	0.101	0.009994693	0.012666969	0.279218977	0.006370683	0	1	0	0	0	1	0	0	0.291885946
48050.4	0.201818654	0.101	0.009994693	0.012520108	0.279395821	0.006369196	0	1	0	0	0	1	0	0	0.291915929
48266.4	0.201818654	0.101	0.009994693	0.012152772	0.279375774	0.006361078	0	1	0	0	0	1	0	0	0.291528546
48481.4	0.201818654	0.101	0.009994693	0.012234085	0.279324521	0.006341797	0	1	0	0	0	1	0	0	0.291558606
48697.4	0.201818654	0.101	0.009994693	0.012971494	0.279592839	0.00633234	0	1	0	0	0	1	0	0	0.292564334
48912.4	0.201818654	0.101	0.009994693	0.013160088	0.279481942	0.006306146	0	1	0	0	0	1	0	0	0.292642029
49128.4	0.201818654	0.101	0.009994693	0.012178847	0.279573494	0.006315804	0	1	0	0	0	1	0	0	0.291752341
49343.4	0.201818654	0.101	0.009994693	0.012659386	0.279616569	0.006294355	0	1	0	0	0	1	0	0	0.292275956
49559.4	0.201818654	0.101	0.009994693	0.012431705	0.279696521	0.006294222	0	1	0	0	0	1	0	0	0.292128226
49774.4	0.201818654	0.101	0.009994693	0.012299359	0.279637576	0.006278914	0	1	0	0	0	1	0	0	0.291936935
49990.4	0.201818654	0.101	0.009994693	0.011937915	0.279766029	0.006280797	0	1	0	0	0	1	0	0	0.291703945
50205.4	0.201818654	0.101	0.009994693	0.012141173	0.279835013	0.00626586	0	1	0	0	0	1	0	0	0.291976186
50421.4	0.201818654	0.101	0.009994693	0.012179973	0.279896922	0.006248527	0	1	0	0	0	1	0	0	0.292076895
50636.4	0.201818654	0.101	0.009994693	0.011881929	0.279887661	0.006242695	0	1	0	0	0	1	0	0	0.291769591
50852.4	0.201818654	0.101	0.009994693	0.012104707	0.279944245	0.00622716	0	1	0	0	0	1	0	0	0.292048953
51067.4	0.201818654	0.101	0.009994693	0.011377515	0.280031866	0.006235685	0	1	0	0	0	1	0	0	0.29140938
51283.4	0.201818654	0.101	0.009994693	0.011883432	0.280164392	0.006215687	0	1	0	0	0	1	0	0	0.292047825
51498.4	0.201818654	0.101	0.009994693	0.011744773	0.280053374	0.006205437	0	1	0	0	0	1	0	0	0.291798147

51714.4	0.201818654	0.101	0.009994693	0.011667782	0.280074926	0.006195879	0	1	0	0	0	1	0	0	0.291742709
51929.4	0.201818654	0.101	0.009994693	0.011563281	0.280285433	0.00620117	0	1	0	0	0	1	0	0	0.291848714
52145.4	0.201818654	0.101	0.009994693	0.011797198	0.28024789	0.006176852	0	1	0	0	0	1	0	0	0.292045088
52360.4	0.201818654	0.101	0.009994693	0.011462337	0.280332522	0.006174652	0	1	0	0	0	1	0	0	0.291794859
52576.4	0.201818654	0.101	0.009994693	0.010944242	0.280316037	0.006171252	0	1	0	0	0	1	0	0	0.291260279
52791.4	0.201818654	0.101	0.009994693	0.011023499	0.280482698	0.006166548	0	1	0	0	0	1	0	0	0.291506197
53007.4	0.201818654	0.101	0.009994693	0.010951487	0.280456274	0.006154718	0	1	0	0	0	1	0	0	0.29140776
53222.4	0.201818654	0.101	0.009994693	0.011248307	0.280491543	0.006139864	0	1	0	0	0	1	0	0	0.291739849
53438.4	0.201818654	0.101	0.009994693	0.011129565	0.28058642	0.00613151	0	1	0	0	0	1	0	0	0.291715985
53653.4	0.201818654	0.101	0.009994693	0.011119305	0.280570471	0.00612022	0	1	0	0	0	1	0	0	0.291689776
53869.4	0.201818654	0.101	0.009994693	0.010769916	0.280719692	0.006121837	0	1	0	0	0	1	0	0	0.291489607
54084.4	0.201818654	0.101	0.009994693	0.010986406	0.280598484	0.006096233	0	1	0	0	0	1	0	0	0.291584891
54300.4	0.201818654	0.101	0.009994693	0.010955676	0.280694102	0.006092038	0	1	0	0	0	1	0	0	0.291649778
54515.4	0.201818654	0.101	0.009994693	0.011172618	0.280794822	0.006083625	0	1	0	0	0	1	0	0	0.29196744
54731.4	0.201818654	0.101	0.009994693	0.01104087	0.280885227	0.006072371	0	1	0	0	0	1	0	0	0.291926097
54946.4	0.201818654	0.101	0.009994693	0.010336558	0.28082041	0.006078304	0	1	0	0	0	1	0	0	0.291156969

time/s	[1a] _o	[1b] _o	[cat] _{τ_o}	[1a]	[1b]	[active cat]	[PA]	[PB]	[PC]	[PD]	[PA2]	[PB2]	[PC2]	[PD2]	[1a]+[1b]
0	0.191292306	0	0.015210778	0.191292306	0	0.015210778	0	0	1	0	0	0	0.1	0	0.191292306
394.4	0.191292306	0	0.015210778	0.175987906	0.015304401	0.015210778	0	0	1	0	0	0	0.1	0	0.191292306
611.4	0.191292306	0	0.015210778	0.169848605	0.021967552	0.015189674	0	0	1	0	0	0	0.1	0	0.191816157
827.4	0.191292306	0	0.015210778	0.164430232	0.0271775	0.015177507	0	0	1	0	0	0	0.1	0	0.191607732
1042.4	0.191292306	0	0.015210778	0.158981287	0.032686291	0.015176291	0	0	1	0	0	0	0.1	0	0.191667578
1258.4	0.191292306	0	0.015210778	0.153618891	0.038267669	0.015196802	0	0	1	0	0	0	0.1	0	0.19188656
1473.4	0.191292306	0	0.015210778	0.148891611	0.042414399	0.015185577	0	0	1	0	0	0	0.1	0	0.191306009
1689.4	0.191292306	0	0.015210778	0.144139039	0.047136942	0.015182143	0	0	1	0	0	0	0.1	0	0.191275981
1904.4	0.191292306	0	0.015210778	0.13949157	0.051726261	0.015190204	0	0	1	0	0	0	0.1	0	0.191217831
2120.4	0.191292306	0	0.015210778	0.135115633	0.05609124	0.015199336	0	0	1	0	0	0	0.1	0	0.191206872
2335.4	0.191292306	0	0.015210778	0.130799593	0.060372545	0.015201793	0	0	1	0	0	0	0.1	0	0.191172138

2551.4	0.191292306	0	0.015210778	0.126697206	0.064461741	0.015201632	0	0	1	0	0	0	0.1	0	0.191158947
2766.4	0.191292306	0	0.015210778	0.122745154	0.068349714	0.015199974	0	0	1	0	0	0	0.1	0	0.191094869
2982.4	0.191292306	0	0.015210778	0.118911617	0.072151628	0.015204558	0	0	1	0	0	0	0.1	0	0.191063245
3197.4	0.191292306	0	0.015210778	0.115388676	0.075625999	0.015196587	0	0	1	0	0	0	0.1	0	0.191014675
3413.4	0.191292306	0	0.015210778	0.111606427	0.079423826	0.015213253	0	0	1	0	0	0	0.1	0	0.191030253
3628.4	0.191292306	0	0.015210778	0.108288535	0.082644754	0.015203046	0	0	1	0	0	0	0.1	0	0.190933289
3844.4	0.191292306	0	0.015210778	0.105116414	0.085788521	0.015195562	0	0	1	0	0	0	0.1	0	0.190904935
4059.4	0.191292306	0	0.015210778	0.101944043	0.08892292	0.015199748	0	0	1	0	0	0	0.1	0	0.190866963
4275.4	0.191292306	0	0.015210778	0.098961193	0.091826735	0.015190894	0	0	1	0	0	0	0.1	0	0.190787928
4490.4	0.191292306	0	0.015210778	0.096178992	0.094598822	0.015173223	0	0	1	0	0	0	0.1	0	0.190777814
4706.4	0.191292306	0	0.015210778	0.093172001	0.097493141	0.015171721	0	0	1	0	0	0	0.1	0	0.190665141
4921.4	0.191292306	0	0.015210778	0.090589684	0.100079432	0.015158342	0	0	1	0	0	0	0.1	0	0.190669116
5137.4	0.191292306	0	0.015210778	0.088044644	0.102559096	0.015156219	0	0	1	0	0	0	0.1	0	0.19060374
5353.4	0.191292306	0	0.015210778	0.085216205	0.105303347	0.015168421	0	0	1	0	0	0	0.1	0	0.190519552
5568.4	0.191292306	0	0.015210778	0.083054109	0.107449511	0.015156728	0	0	1	0	0	0	0.1	0	0.19050362
5783.4	0.191292306	0	0.015210778	0.080864372	0.109620167	0.015137131	0	0	1	0	0	0	0.1	0	0.190484539
5999.4	0.191292306	0	0.015210778	0.07858005	0.111809007	0.015121038	0	0	1	0	0	0	0.1	0	0.190389057
6215.4	0.191292306	0	0.015210778	0.076583776	0.113805806	0.015114357	0	0	1	0	0	0	0.1	0	0.190389583
6430.4	0.191292306	0	0.015210778	0.074406981	0.115920001	0.01510867	0	0	1	0	0	0	0.1	0	0.190326983
6645.4	0.191292306	0	0.015210778	0.072404631	0.117850962	0.015098995	0	0	1	0	0	0	0.1	0	0.190255593
6861.4	0.191292306	0	0.015210778	0.070541801	0.119685594	0.015086294	0	0	1	0	0	0	0.1	0	0.190227395
7076.4	0.191292306	0	0.015210778	0.068659143	0.121485823	0.015078516	0	0	1	0	0	0	0.1	0	0.190144965
7292.4	0.191292306	0	0.015210778	0.067035213	0.123146256	0.015066828	0	0	1	0	0	0	0.1	0	0.190181469
7507.4	0.191292306	0	0.015210778	0.065131127	0.124924775	0.015059591	0	0	1	0	0	0	0.1	0	0.190055901
7723.4	0.191292306	0	0.015210778	0.063663807	0.126394409	0.015046431	0	0	1	0	0	0	0.1	0	0.190058216
7938.4	0.191292306	0	0.015210778	0.061887717	0.128058481	0.01503327	0	0	1	0	0	0	0.1	0	0.189946198
8154.4	0.191292306	0	0.015210778	0.06040605	0.129532422	0.015016922	0	0	1	0	0	0	0.1	0	0.189938472
8369.4	0.191292306	0	0.015210778	0.058891146	0.130999173	0.015011567	0	0	1	0	0	0	0.1	0	0.189890319
8585.4	0.191292306	0	0.015210778	0.057452331	0.132384577	0.015005437	0	0	1	0	0	0	0.1	0	0.189836909
8801.4	0.191292306	0	0.015210778	0.056081688	0.13369	0.014992576	0	0	1	0	0	0	0.1	0	0.189771689
9016.4	0.191292306	0	0.015210778	0.054755442	0.134945389	0.014981721	0	0	1	0	0	0	0.1	0	0.189700832

9231.4	0.191292306	0	0.015210778	0.053263088	0.136328948	0.014971611	0	0	1	0	0	0	0.1	0	0.189592036
9447.4	0.191292306	0	0.015210778	0.05207356	0.137534304	0.014970079	0	0	1	0	0	0	0.1	0	0.189607863
9662.4	0.191292306	0	0.015210778	0.050757653	0.138763802	0.014957379	0	0	1	0	0	0	0.1	0	0.189521455
9878.4	0.191292306	0	0.015210778	0.049982348	0.139696955	0.014933948	0	0	1	0	0	0	0.1	0	0.189679303
10093.4	0.191292306	0	0.015210778	0.048336604	0.141042247	0.0149423	0	0	1	0	0	0	0.1	0	0.189378851
10309.4	0.191292306	0	0.015210778	0.047341318	0.142095962	0.014928574	0	0	1	0	0	0	0.1	0	0.18943728
10525.4	0.191292306	0	0.015210778	0.046296646	0.143164492	0.014922813	0	0	1	0	0	0	0.1	0	0.189461138
10740.4	0.191292306	0	0.015210778	0.045262437	0.144134921	0.014909795	0	0	1	0	0	0	0.1	0	0.189397358
10956.4	0.191292306	0	0.015210778	0.044399755	0.145207515	0.014905679	0	0	1	0	0	0	0.1	0	0.189607269
11171.4	0.191292306	0	0.015210778	0.043307424	0.146056319	0.014887673	0	0	1	0	0	0	0.1	0	0.189363744
11386.4	0.191292306	0	0.015210778	0.042392913	0.146909612	0.014883132	0	0	1	0	0	0	0.1	0	0.189302524
11602.4	0.191292306	0	0.015210778	0.04128218	0.147911332	0.014876065	0	0	1	0	0	0	0.1	0	0.189193512
11817.4	0.191292306	0	0.015210778	0.040596728	0.148702137	0.014855584	0	0	1	0	0	0	0.1	0	0.189298865
12033.4	0.191292306	0	0.015210778	0.039467909	0.149661844	0.014859197	0	0	1	0	0	0	0.1	0	0.189129753
12248.4	0.191292306	0	0.015210778	0.03870056	0.150403315	0.014845674	0	0	1	0	0	0	0.1	0	0.189103874
12464.4	0.191292306	0	0.015210778	0.03769804	0.151247921	0.014838709	0	0	1	0	0	0	0.1	0	0.188945961
12680.4	0.191292306	0	0.015210778	0.037220312	0.151906304	0.014821596	0	0	1	0	0	0	0.1	0	0.189126616
12895.4	0.191292306	0	0.015210778	0.036278514	0.152739169	0.014811003	0	0	1	0	0	0	0.1	0	0.189017683
13111.4	0.191292306	0	0.015210778	0.035499626	0.153423207	0.014804264	0	0	1	0	0	0	0.1	0	0.188922833
13326.4	0.191292306	0	0.015210778	0.03475665	0.154143334	0.014793624	0	0	1	0	0	0	0.1	0	0.188899984
13542.4	0.191292306	0	0.015210778	0.034084233	0.154768381	0.014787204	0	0	1	0	0	0	0.1	0	0.188852614
13757.4	0.191292306	0	0.015210778	0.033234658	0.155549353	0.01478537	0	0	1	0	0	0	0.1	0	0.188784011
13973.4	0.191292306	0	0.015210778	0.032433925	0.15620281	0.014776473	0	0	1	0	0	0	0.1	0	0.188636735
14188.4	0.191292306	0	0.015210778	0.031928683	0.156805462	0.014762602	0	0	1	0	0	0	0.1	0	0.188734145
14404.4	0.191292306	0	0.015210778	0.031422444	0.157314853	0.014740535	0	0	1	0	0	0	0.1	0	0.188737296
14619.4	0.191292306	0	0.015210778	0.030774726	0.157925408	0.0147407	0	0	1	0	0	0	0.1	0	0.188700134
14835.4	0.191292306	0	0.015210778	0.030191209	0.158559212	0.014732232	0	0	1	0	0	0	0.1	0	0.188750422
15050.4	0.191292306	0	0.015210778	0.029564329	0.159070679	0.014723121	0	0	1	0	0	0	0.1	0	0.188635008
15266.4	0.191292306	0	0.015210778	0.029099875	0.159635541	0.014708039	0	0	1	0	0	0	0.1	0	0.188735416
15481.4	0.191292306	0	0.015210778	0.028368837	0.160195073	0.014706971	0	0	1	0	0	0	0.1	0	0.188563911

time/s	[1a] _o	[1b] _o	[cat] _{to}	[1a]	[1b]	[active cat]	[PA]	[PB]	[PC]	[PD]	[PA2]	[PB2]	[PC2]	[PD2]	[1a]+[1b]
0	0.395728382	0	0.010076419	0.395728382	0	0.010076419	0	0	0	1	0	0	0	1	0.395728382
322.4	0.395728382	0	0.010076419	0.370717015	0.025011367	0.010076419	0	0	0	1	0	0	0	1	0.395728382
537.4	0.395728382	0	0.010076419	0.358733275	0.036922386	0.009992178	0	0	0	1	0	0	0	1	0.395655662
753.4	0.395728382	0	0.010076419	0.347059535	0.048340673	0.009952315	0	0	0	1	0	0	0	1	0.395400208
969.4	0.395728382	0	0.010076419	0.336378394	0.059157253	0.009939472	0	0	0	1	0	0	0	1	0.395535647
1185.4	0.395728382	0	0.010076419	0.325861609	0.069318604	0.009929073	0	0	0	1	0	0	0	1	0.395180213
1401.4	0.395728382	0	0.010076419	0.315901365	0.0793505	0.009945049	0	0	0	1	0	0	0	1	0.395251866
1617.4	0.395728382	0	0.010076419	0.30591944	0.089085074	0.00995315	0	0	0	1	0	0	0	1	0.395004515
1832.4	0.395728382	0	0.010076419	0.296554022	0.098342851	0.009951079	0	0	0	1	0	0	0	1	0.394896873
2047.4	0.395728382	0	0.010076419	0.287510944	0.107267818	0.009960231	0	0	0	1	0	0	0	1	0.394778762
2263.4	0.395728382	0	0.010076419	0.27869219	0.11594267	0.009971456	0	0	0	1	0	0	0	1	0.39463486
2479.4	0.395728382	0	0.010076419	0.270217746	0.124499293	0.009984171	0	0	0	1	0	0	0	1	0.39471704
2694.4	0.395728382	0	0.010076419	0.262077304	0.132383162	0.009977393	0	0	0	1	0	0	0	1	0.394460466
2910.4	0.395728382	0	0.010076419	0.2540594	0.140150893	0.009967746	0	0	0	1	0	0	0	1	0.394210292
3125.4	0.395728382	0	0.010076419	0.246293031	0.14818129	0.009995221	0	0	0	1	0	0	0	1	0.394474321
3341.4	0.395728382	0	0.010076419	0.238847603	0.155268244	0.00997939	0	0	0	1	0	0	0	1	0.394115847
3556.4	0.395728382	0	0.010076419	0.232099392	0.162070761	0.0099727	0	0	0	1	0	0	0	1	0.394170153
3772.4	0.395728382	0	0.010076419	0.224738699	0.169093491	0.009981404	0	0	0	1	0	0	0	1	0.39383219
3987.4	0.395728382	0	0.010076419	0.218547693	0.175263188	0.00995624	0	0	0	1	0	0	0	1	0.393810882
4203.4	0.395728382	0	0.010076419	0.212079039	0.181626911	0.009956498	0	0	0	1	0	0	0	1	0.39370595
4418.4	0.395728382	0	0.010076419	0.205911361	0.18752075	0.009943513	0	0	0	1	0	0	0	1	0.393432111
4634.4	0.395728382	0	0.010076419	0.199946703	0.193418432	0.009932448	0	0	0	1	0	0	0	1	0.393365135
4850.4	0.395728382	0	0.010076419	0.19440173	0.198913046	0.009911326	0	0	0	1	0	0	0	1	0.393314777
5065.4	0.395728382	0	0.010076419	0.188829305	0.204385588	0.009898452	0	0	0	1	0	0	0	1	0.393214893
5281.4	0.395728382	0	0.010076419	0.183704386	0.209591659	0.009897181	0	0	0	1	0	0	0	1	0.393296045
5496.4	0.395728382	0	0.010076419	0.178644845	0.214248828	0.009864637	0	0	0	1	0	0	0	1	0.392893673
5711.4	0.395728382	0	0.010076419	0.174151189	0.21899281	0.009844656	0	0	0	1	0	0	0	1	0.393143998
5927.4	0.395728382	0	0.010076419	0.168990631	0.223662529	0.009836271	0	0	0	1	0	0	0	1	0.39265316
6142.4	0.395728382	0	0.010076419	0.164355371	0.228056994	0.009815886	0	0	0	1	0	0	0	1	0.392412365

6358.4	0.395728382	0	0.010076419	0.159786425	0.232269186	0.009799801	0	0	0	1	0	0	0	1	0.392055611
6573.4	0.395728382	0	0.010076419	0.156176524	0.236351721	0.009778732	0	0	0	1	0	0	0	1	0.392528245
6789.4	0.395728382	0	0.010076419	0.152416598	0.240097854	0.009744965	0	0	0	1	0	0	0	1	0.392514453
7004.4	0.395728382	0	0.010076419	0.148205677	0.243904605	0.009728734	0	0	0	1	0	0	0	1	0.392110282
7220.4	0.395728382	0	0.010076419	0.144745966	0.247564029	0.00970325	0	0	0	1	0	0	0	1	0.392309995
7435.4	0.395728382	0	0.010076419	0.14089942	0.250928516	0.009689117	0	0	0	1	0	0	0	1	0.391827936
7651.4	0.395728382	0	0.010076419	0.137422105	0.254178184	0.009654191	0	0	0	1	0	0	0	1	0.39160029
7866.4	0.395728382	0	0.010076419	0.134334077	0.257342962	0.009629878	0	0	0	1	0	0	0	1	0.391677038
8081.4	0.395728382	0	0.010076419	0.130516376	0.260852779	0.009631851	0	0	0	1	0	0	0	1	0.391369156
8297.4	0.395728382	0	0.010076419	0.127505697	0.263750674	0.009601763	0	0	0	1	0	0	0	1	0.39125637
8512.4	0.395728382	0	0.010076419	0.124431699	0.266751178	0.009579486	0	0	0	1	0	0	0	1	0.391182878
8728.4	0.395728382	0	0.010076419	0.121825213	0.269378418	0.009543976	0	0	0	1	0	0	0	1	0.391203631
8943.4	0.395728382	0	0.010076419	0.119067543	0.272234412	0.009523756	0	0	0	1	0	0	0	1	0.391301955
9159.4	0.395728382	0	0.010076419	0.115847258	0.274960954	0.009526955	0	0	0	1	0	0	0	1	0.390808212
9375.4	0.395728382	0	0.010076419	0.113382285	0.277404772	0.009487695	0	0	0	1	0	0	0	1	0.390787058
9590.4	0.395728382	0	0.010076419	0.110965102	0.279915323	0.009471717	0	0	0	1	0	0	0	1	0.390880424
9805.4	0.395728382	0	0.010076419	0.108404022	0.282253919	0.009450039	0	0	0	1	0	0	0	1	0.39065794
10021.4	0.395728382	0	0.010076419	0.105669647	0.284613012	0.009427241	0	0	0	1	0	0	0	1	0.390282659
10237.4	0.395728382	0	0.010076419	0.10370428	0.286841355	0.009409007	0	0	0	1	0	0	0	1	0.390545636
10452.4	0.395728382	0	0.010076419	0.101535109	0.288729319	0.009362056	0	0	0	1	0	0	0	1	0.390264428
10668.4	0.395728382	0	0.010076419	0.098817115	0.291139977	0.009367592	0	0	0	1	0	0	0	1	0.389957092
10883.4	0.395728382	0	0.010076419	0.096570246	0.293117369	0.009343611	0	0	0	1	0	0	0	1	0.389687615
11098.4	0.395728382	0	0.010076419	0.094387531	0.29515373	0.009335978	0	0	0	1	0	0	0	1	0.389541261
11314.4	0.395728382	0	0.010076419	0.093003334	0.29672992	0.00928477	0	0	0	1	0	0	0	1	0.389733253
11529.4	0.395728382	0	0.010076419	0.090930037	0.298895495	0.009283367	0	0	0	1	0	0	0	1	0.389825532
11745.4	0.395728382	0	0.010076419	0.08902502	0.300579974	0.009259369	0	0	0	1	0	0	0	1	0.389604994
11960.4	0.395728382	0	0.010076419	0.087228733	0.302345324	0.00923151	0	0	0	1	0	0	0	1	0.389574057
12176.4	0.395728382	0	0.010076419	0.085418779	0.303993616	0.009210195	0	0	0	1	0	0	0	1	0.389412395
12391.4	0.395728382	0	0.010076419	0.083435961	0.305847752	0.009207555	0	0	0	1	0	0	0	1	0.389283714
12607.4	0.395728382	0	0.010076419	0.081538227	0.307209006	0.009177528	0	0	0	1	0	0	0	1	0.388747232
12823.4	0.395728382	0	0.010076419	0.080627851	0.308633348	0.009140884	0	0	0	1	0	0	0	1	0.389261199

13038.4	0.395728382	0	0.010076419	0.078870262	0.310430313	0.009136881	0	0	0	1	0	0	0	1	0.389300575
13253.4	0.395728382	0	0.010076419	0.076533601	0.311939691	0.009132718	0	0	0	1	0	0	0	1	0.388473291
13469.4	0.395728382	0	0.010076419	0.075979474	0.313211481	0.009093395	0	0	0	1	0	0	0	1	0.389190955
13684.4	0.395728382	0	0.010076419	0.073426889	0.314740051	0.0090982	0	0	0	1	0	0	0	1	0.38816694
13900.4	0.395728382	0	0.010076419	0.072886402	0.315907496	0.009059202	0	0	0	1	0	0	0	1	0.388793899
14115.4	0.395728382	0	0.010076419	0.071596931	0.317483217	0.009044619	0	0	0	1	0	0	0	1	0.389080148
14331.4	0.395728382	0	0.010076419	0.070322136	0.318684105	0.009026336	0	0	0	1	0	0	0	1	0.389006241
14546.4	0.395728382	0	0.010076419	0.068491467	0.319883975	0.009009729	0	0	0	1	0	0	0	1	0.388375442
14762.4	0.395728382	0	0.010076419	0.067128265	0.321122415	0.008996824	0	0	0	1	0	0	0	1	0.38825068
14978.4	0.395728382	0	0.010076419	0.066387081	0.322266943	0.008971466	0	0	0	1	0	0	0	1	0.388654024
15193.4	0.395728382	0	0.010076419	0.064956276	0.323446971	0.008954065	0	0	0	1	0	0	0	1	0.388403247
15409.4	0.395728382	0	0.010076419	0.063342357	0.324569695	0.008946359	0	0	0	1	0	0	0	1	0.387912052
15624.4	0.395728382	0	0.010076419	0.062069502	0.32571485	0.008924861	0	0	0	1	0	0	0	1	0.387784352
15839.4	0.395728382	0	0.010076419	0.061506864	0.326558962	0.008889664	0	0	0	1	0	0	0	1	0.388065825
16055.4	0.395728382	0	0.010076419	0.060121059	0.327727451	0.008887364	0	0	0	1	0	0	0	1	0.38784851
16270.4	0.395728382	0	0.010076419	0.058954286	0.328737209	0.00887096	0	0	0	1	0	0	0	1	0.387691495
16486.4	0.395728382	0	0.010076419	0.057849916	0.329812372	0.008861929	0	0	0	1	0	0	0	1	0.387662287
16702.4	0.395728382	0	0.010076419	0.057436833	0.330642968	0.008824398	0	0	0	1	0	0	0	1	0.388079801
16917.4	0.395728382	0	0.010076419	0.055866788	0.331512732	0.00882173	0	0	0	1	0	0	0	1	0.38737952

VIII. Computational data and procedures

All final computations were performed using TURBOMOLE 6.6. program package.³ Structures were optimized using TPSS-D3^{4,5} functional with def2-SVP⁶ basis sets and solvation effects were taken into account with COSMO⁷ solvation model ($\epsilon = 8.9$). Final energies were evaluated using higher-quality def2-TZVP basis sets. All computations were further sped-up using multipole-accelerated resolution-of-identity approximation (MARI-J) for the Coulomb term with corresponding auxiliary basis sets.^{8,9} Also, ORCA 3.0.3 program package was used for preliminary transition state optimizations.¹⁰ Exact energies are given in Hartrees and the relative energies are reported in kcal mol⁻¹. Imaginary frequencies are reported for all optimized transition states. All minima and transition states have been verified to have zero and one imaginary frequency, respectively.

VIII.1. Computed energy profile for intramolecular 1,3-*O*-transposition

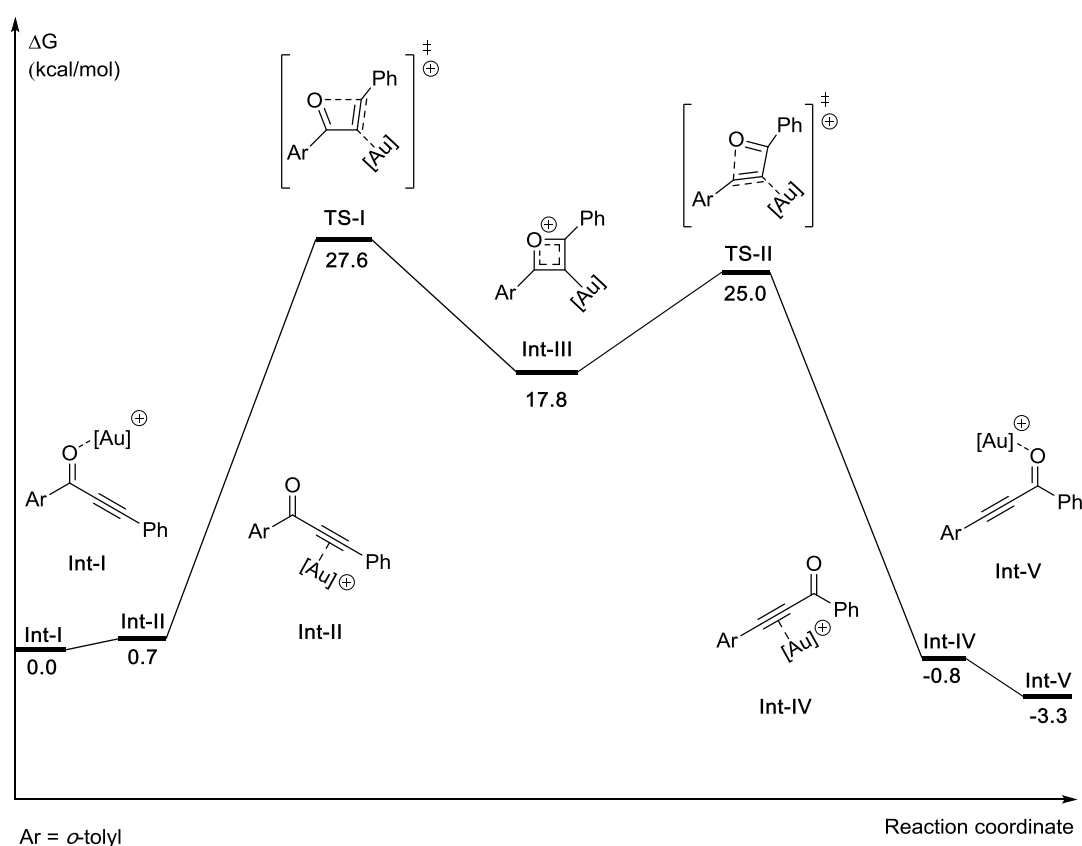


Figure S21. Energy profile for the intramolecular transposition

VIII.2. Nucleophilicity factors

Nucleophilicity (N(Theo.)) of a given reactant was calculated using formula below.¹¹ Instead of only considering energy of the HOMO regardless of the size of coefficient on C=O oxygen, orbital with a significant coefficient on carbonyl oxygen was located and used for calculating N(MO). These HOMO-X orbitals are illustrated in Figure S23. Comparison of the HOMO-LUMO gap to the ΔG gives good, close to linear correlation, but the corresponding correlation δE values is poor. This is illustrated in Figure S21 below.

$$N(\text{Theo.}) = \left| \frac{(3E_{\text{HOMO}} - E_{\text{LUMO}})^2}{8(E_{\text{HOMO}} - E_{\text{LUMO}})} \right|$$

$$N(\text{MO}) = \left| \frac{(3E_{\text{HOMO-X}} - E_{\text{LUMO}})^2}{8(E_{\text{HOMO-X}} - E_{\text{LUMO}})} \right|$$

Table S2. Tabulated values for orbital energies, N(Theo.), N(MO) and energy barriers.

Entry	Compound	E(HOMO) (eV)	E(HOMO-X) (eV)	E(LUMO) (eV)	N(Theo.) (eV)	N(MO) (eV)	ΔG (kcal/mol)	$\Delta G(\text{TS-1 - Int-1})$ (kcal/mol)	X
1	1a	-	-6.14	-3.11	-	9.67	13.51	13.51	-1
2	1b	-	-6.07	-3.18	-	9.78	14.43	14.43	0
3	3a	-6.16	-6.62	-2.75	9.67	9.45	18.72	14.89	-1
4	3b	-5.84	-5.84	-2.46	9.78	8.39	13.43	12.81	0
5	3c	-5.7	-6.15	-2.69	9.45	8.98	17.12	14.13	-1
6	3d	-5	-5	-2.18	8.39	7.29	11.34	11.34	0
7	3e	-5.03	-5.02	-2.36	8.98	7.59	11.32	10.52	0
8	3f	-5.95	-8.11	-1.76	7.29	10.03	21.99	15.27	-1
9	5a	-	-6.66	-3.09	-	9.99	-	-	-2
10	5b	-	-6.2	-3.15	-	9.78	-	-	0

Table S3. Tabulated NBO charges located on C=O oxygen

Entry	Aldehyde	NBO _{C=O}	NBO _{C=O} (rel.) ^a
1	3a	-0.5461	0.00
2	3b	-0.5655	-1.94
3	3c	-0.5450	0.11
4	3d	-0.5882	-4.21
5	3e	-0.5851	-3.90
6	3f	-0.5439	0.22

^a (3x-3a)*100

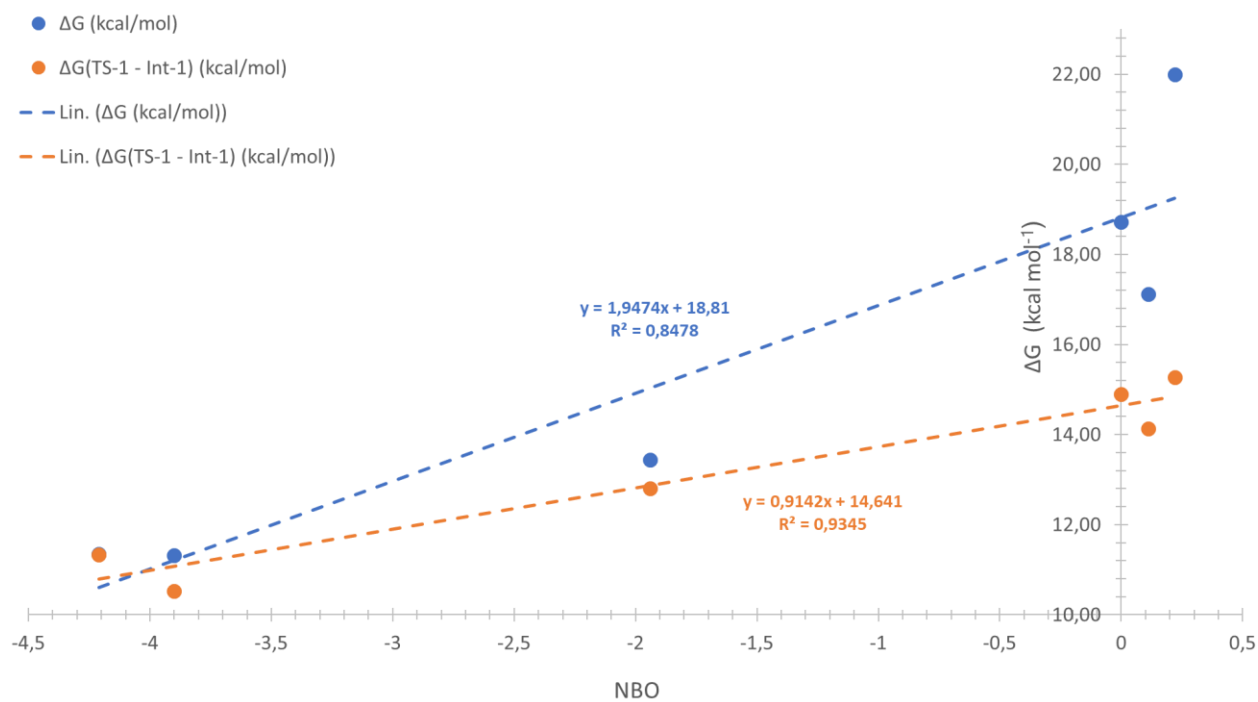


Figure S22. Correlation of ΔG (blue) and $\Delta G(\text{TS-1-Int-1})$ (orange) with NBO charge on oxygen.

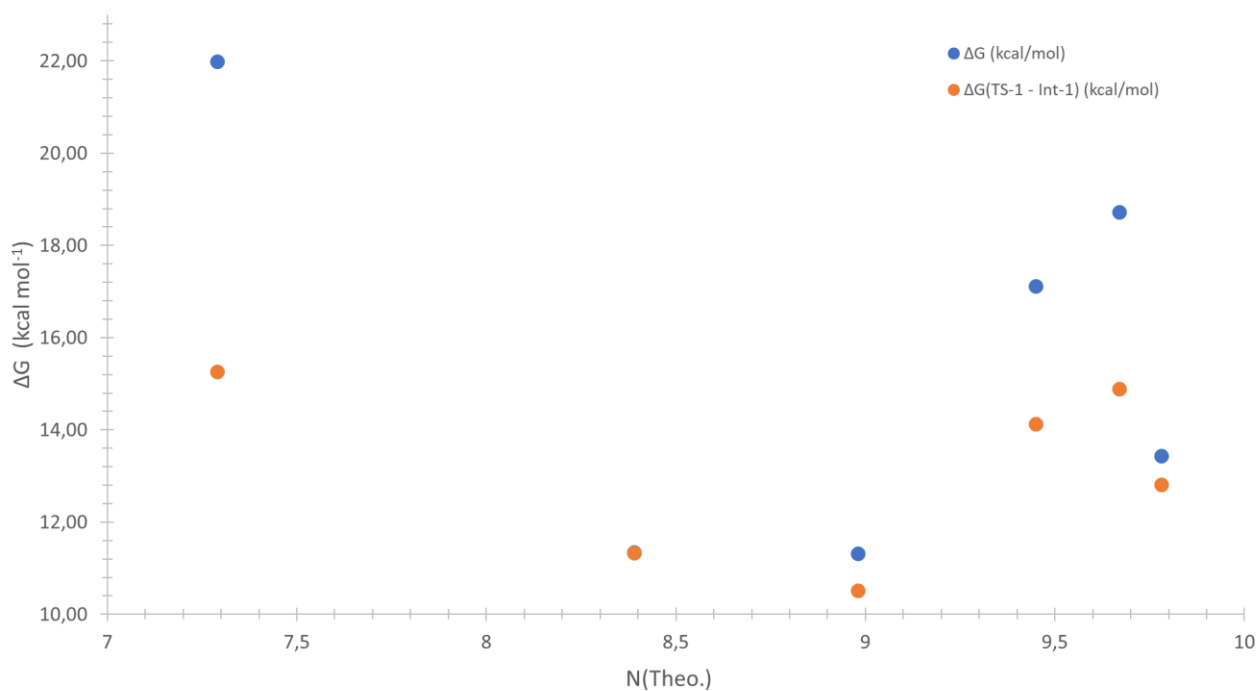


Figure S23. Correlation of ΔG (blue) and $\Delta G(\text{TS-1-Int-1})$ (orange) with N(Theo.).

VIII.3. Tabulated energies for optimized structures

Table S4. Energies for structures in Figure 2 and Table 1 (kcal mol⁻¹)

		TPSS-D3, grid m4, epsilon=8.9			
		def2-SVP		def2-TZVP	
	code	dE ^a	dG ^a	dE ^a	"dG" ^a
Ynones and aldehydes	1a	0.0	0.0	0.0	0.0
	1b	-2.4	-2.9	-2.7	-3.1
	3a	-	-	-	-
	3b	-	-	-	-
	3c	-	-	-	-
	3d	-	-	-	-
	3e	-	-	-	-
	3f	-	-	-	-
Intramolecular 1,3-O-transposition	Int-I	0.0	0.0	0.0	0.0
	Int-II	4.3	4.0	1.0	0.7
	TS-I	30.8	29.9	28.5	27.6
	Int-III	18.9	19.4	17.3	17.8
	TS-II	28.2	27.4	25.9	25.0
	Int-IV	2.3	1.8	-0.2	-0.8
	Int-V	-3.3	-3.3	-3.3	-3.3
1a as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	-1.4	11.2	0.9	13.5
	Int-3	-14.2	1.2	-9.9	5.5
	TS-2	-13.6	2.7	-8.9	7.3
	Int-4	-20.4	-4.0	-14.9	1.4
	TS-3	-12.8	3.8	-8.1	8.5
	Int-5	-15.3	0.4	-10.5	5.2
	TS-4	-5.8	6.9	-2.3	10.3
	Int-6	2.3	1.8	-0.2	-0.8
	Int-7	-3.3	-3.3	-3.3	-3.3
1b as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	-1.1	12.0	1.3	14.4
	Int-3	-15.0	0.9	-10.4	5.6
	TS-2	-15.0	1.4	-10.1	6.2
	Int-4	-21.0	-3.2	-15.8	2.0
	TS-3	-13.2	2.8	-8.7	7.4
	Int-5	-16.4	-0.2	-11.3	4.9
	TS-4	-5.9	7.1	-2.4	10.6
	Int-6	2.3	1.8	-0.2	-0.8
	Int-7	-3.3	-3.3	-3.3	-3.3

3a as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	3.1	13.8	4.2	14.9
	Int-4	-26.1	-8.9	-21.8	-4.7
	TS-4	0.1	12.4	1.8	14.1
	Int-7	-3.3	-3.3	-3.3	-3.3
3b as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	1.7	11.9	2.7	12.8
	Int-4	-25.2	-6.8	-20.6	-2.3
	TS-4	-1.8	9.6	-0.3	11.2
	Int-7	-3.3	-3.3	-3.3	-3.3
3c as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	2.5	13.1	3.6	14.1
	Int-4	-26.4	-8.7	-22.1	-4.4
	TS-4	0.1	11.2	1.6	12.7
	Int-7	-3.3	-3.3	-3.3	-3.3
3d as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	-2.0	9.3	0.1	11.3
	Int-3	-16.9	-2.4	-13.0	1.5
	TS-2	-16.5	-0.8	-12.5	3.2
	Int-4	-24.7	-6.2	-19.8	-1.3
	TS-3	-14.5	1.3	-12.5	3.4
	Int-5	-17.5	-2.8	-14.2	0.4
	TS-4	-4.0	6.1	-2.4	7.7
	Int-6	2.3	1.8	-0.2	-0.8
	Int-7	-3.3	-3.3	-3.3	-3.3
3e as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	-4.3	7.4	-1.2	10.5
	Int-3	-18.3	-3.1	-13.3	1.9
	TS-2	-15.1	-0.1	-10.9	4.2
	Int-4	-26.3	-7.7	-21.1	-2.4
	TS-3	-14.8	0.3	-10.9	4.2
	Int-5	-18.2	-3.1	-14.2	0.9
	TS-4	-5.5	6.3	-2.9	8.9
	Int-6	2.3	1.8	-0.2	-0.8
	Int-7	-3.3	-3.3	-3.3	-3.3
3f as mediator	Int-1	0.0	0.0	0.0	0.0
	Int-2	4.3	4.0	1.0	0.7
	TS-1	2.4	13.4	4.3	15.3
	Int-4	-33.5	-15.2	-28.2	-9.9
	TS-4	-0.5	10.4	1.2	12.1

Int-6	2.3	1.8	-0.2	-0.8
Int-7	-3.3	-3.3	-3.3	-3.3

^a Energies in kcal/mol

Table S5. Exact computed values

TPSS-D3, grid m4, epsilon=8.9					
def2-SVP				def2-TZVP	
code	E(0) ^a	chem.pot (298) ^a	Imaginary freq. ^b	E(0) ^a	
Ynones and aldehydes	1a	-691.76769527	0.1839	-	-692.49812376
	1b	-691.77155441	0.1832	-	-692.50239187
	3a	-345.40280347	0.0782	-	-345.77518709
	3b	-459.86800253	0.1069	-	-460.37095322
	3c	-459.86423216	0.1068	-	-460.36683946
	3d	-479.31578491	0.1449	-	-479.83007112
	3e	-688.78579386	0.1651	-	-689.54784589
	3f	-271.63522349	0.1083	-	-271.93362969
Intramolecular 1,3-O-transposition	Int-I	-1132.08195347	0.2988	-	-1133.13652716
	Int-II	-1132.07516220	0.2984	-	-1133.13497926
	TS-I	-1132.03282552	0.2973	-275.56	-1133.09110431
	Int-III	-1132.05190834	0.2996	-	-1133.10900698
	TS-II	-1132.03693647	0.2974	-267.99	-1133.09525701
	Int-IV	-1132.07823544	0.2979	-	-1133.13684575
	Int-V	-1132.08713341	0.2988	-	-1133.14171714
1a as mediator	Int-1	-1823.84964875	0.4827	-	-1825.63465092
	Int-2	-1823.84285747	0.4822	-	-1825.63310302
	TS-1	-1823.85192627	0.5028	-141.17	-1825.63322253
	Int-3	-1823.87229014	0.5072	-	-1825.65037112
	TS-2	-1823.87129458	0.5086	-74.74	-1825.64884646
	Int-4	-1823.88218889	0.5088	-	-1825.65844727
	TS-3	-1823.86999822	0.5091	76.1	-1825.64756745
	Int-5	-1823.87400353	0.5077	-	-1825.65142781
	TS-4	-1823.85881776	0.5029	-157.2	-1825.63834704
	Int-6	-1823.84593071	0.4818	-	-1825.63496951
	Int-7	-1823.85482869	0.4827	-	-1825.63984090
1b as mediator	Int-1	-1823.85350788	0.4820	-	-1825.63891904
	Int-2	-1823.84671660	0.4816	-	-1825.63737113
	TS-1	-1823.85533362	0.5029	-136.48	-1825.63684667
	Int-3	-1823.87743974	0.5074	-	-1825.65543816
	TS-2	-1823.87736875	0.5081	-82.56	-1825.65503931
	Int-4	-1823.88705198	0.5104	-	-1825.66405208

	TS-3	-1823.87459215	0.5075	-56.68	-1825.65274471
	Int-5	-1823.87969301	0.5078	-	-1825.65700054
	TS-4	-1823.86295255	0.5027	-166.32	-1825.64274877
	Int-6	-1823.84978984	0.4811	-	-1825.63923762
	Int-7	-1823.85868782	0.4820	-	-1825.64410901
3a as mediator	Int-1	-1477.48475695	0.3770		-1478.91171426
	Int-2	-1477.47796567	0.3765	-	-1478.91016635
	TS-1	-1477.47981450	0.3941	141.15	-1478.90507583
	Int-4	-1477.52628307	0.4043	-	-1478.94643848
	TS-4	-1477.48462385	0.3965	-220.72	-1478.90885837
	Int-7	-1477.48993688	0.3769		-1478.91690423
3b as mediator	Int-1	-1591.94995600	0.4057		-1593.50748038
	Int-2	-1591.94316472	0.4052		-1593.50593248
	TS-1	-1591.94721713	0.4218	-121.39	-1593.50323027
	Int-4	-1591.99006777	0.4349	-	-1593.54034532
	TS-4	-1591.95283088	0.4239	-148.39	-1593.50788216
	Int-7	-1591.95513594	0.4056	-	-1593.51267036
3c as mediator	Int-1	-1591.94618564	0.4056		-1593.50336662
	Int-2	-1591.93939436	0.4052		-1593.50181872
	TS-1	-1591.94213682	0.4225	-136.68	-1593.49770866
	Int-4	-1591.98831483	0.4339	-	-1593.53863884
	TS-4	-1591.94605482	0.4233	-154.08	-1593.50078385
	Int-7	-1591.95136557	0.4056	-	-1593.50855660
3d as mediator	Int-1	-1611.39773839	0.4437	-	-1612.96659828
	Int-2	-1611.39094711	0.4432	-	-1612.96505038
	TS-1	-1611.40095355	0.4617	-120.85	-1612.96651462
	Int-3	-1611.42462197	0.4668	-	-1612.98736125
	TS-2	-1611.42401806	0.4686	-48.9	-1612.98644646
	Int-4	-1611.43705834	0.4731	-	-1612.99812537
	TS-3	-1611.42091735	0.4690	-78.1	-1612.98644646
	Int-5	-1611.42556827	0.4670	-	-1612.98924075
	TS-4	-1611.40416749	0.4598	-134.54	-1612.97041311
	Int-6	-1611.39402035	0.4428	-	-1612.96691687
	Int-7	-1611.40291833	0.4436	-	-1612.97178826
3e as mediator	Int-1	-1820.86774733	0.4639	-	-1822.68437306
	Int-2	-1820.86095606	0.4635	-	-1822.68282515
	TS-1	-1820.87466882	0.4826	-131.57	-1822.68631771
	Int-3	-1820.89693533	0.4882	-	-1822.70556649
	TS-2	-1820.89185905	0.4879	-45.42	-1822.70166660
	Int-4	-1820.90972198	0.4936	-	-1822.71800446
	TS-3	-1820.89126881	0.4879	-79.14	-1822.70170270
	Int-5	-1820.89681620	0.4880	-	-1822.70697458
	TS-4	-1820.87653786	0.4827	-167.22	-1822.68900740
	Int-6	-1820.86402930	0.4630	-	-1822.68469164
	Int-7	-1820.87292727	0.4639	-	-1822.68956303

3f as mediator	Int-1	-1403.71717697	0.4071	-	-1405.07015686
	Int-2	-1403.71038569	0.4066	-	-1405.06860895
	TS-1	-1403.71333523	0.4246	-134.71	-1405.06334552
	Int-4	-1403.77053572	0.4363	-	-1405.11508720
	TS-4	-1403.71801507	0.4245	-141.12	-1405.06826738
	Int-6	-1403.71345893	0.4062	-	-1405.07047544
	Int-7	-1403.72235690	0.4071	-	-1405.07534683

^a Energies in Hartree; ^b Frequencies in cm⁻¹

VIII.4. Visualization of complexes with 3d as co-catalyst

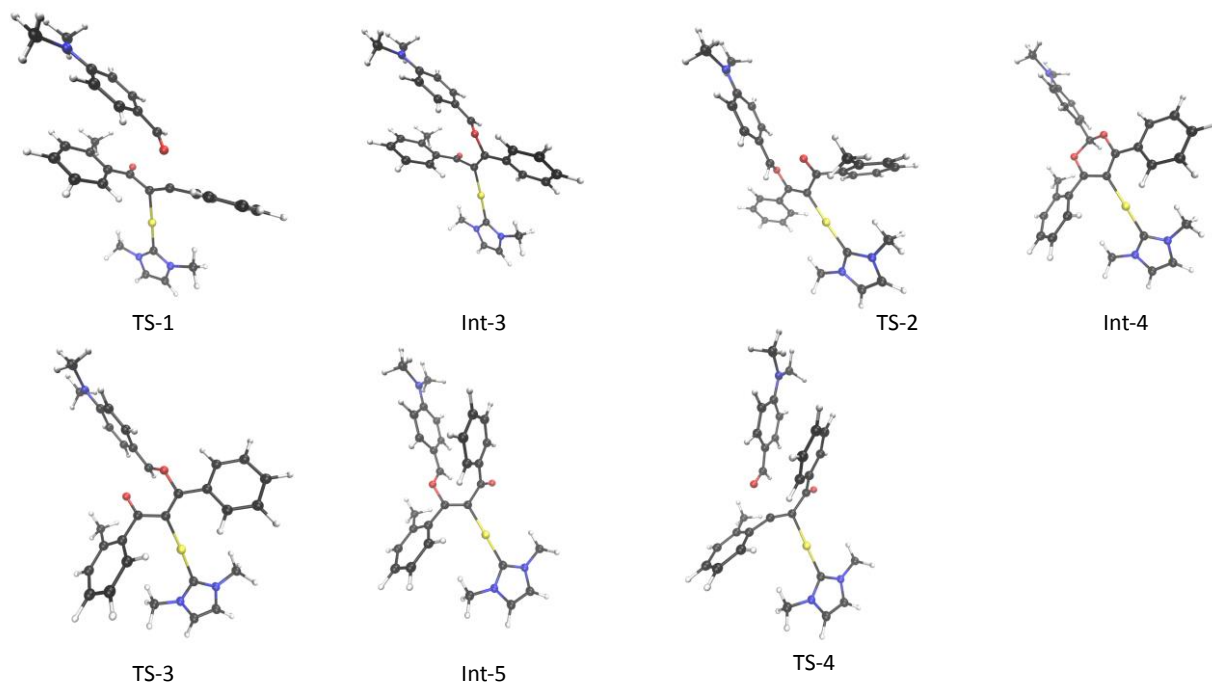


Figure S24. Optimized structures with **3d**.

VIII.5. Visualization of molecular orbitals

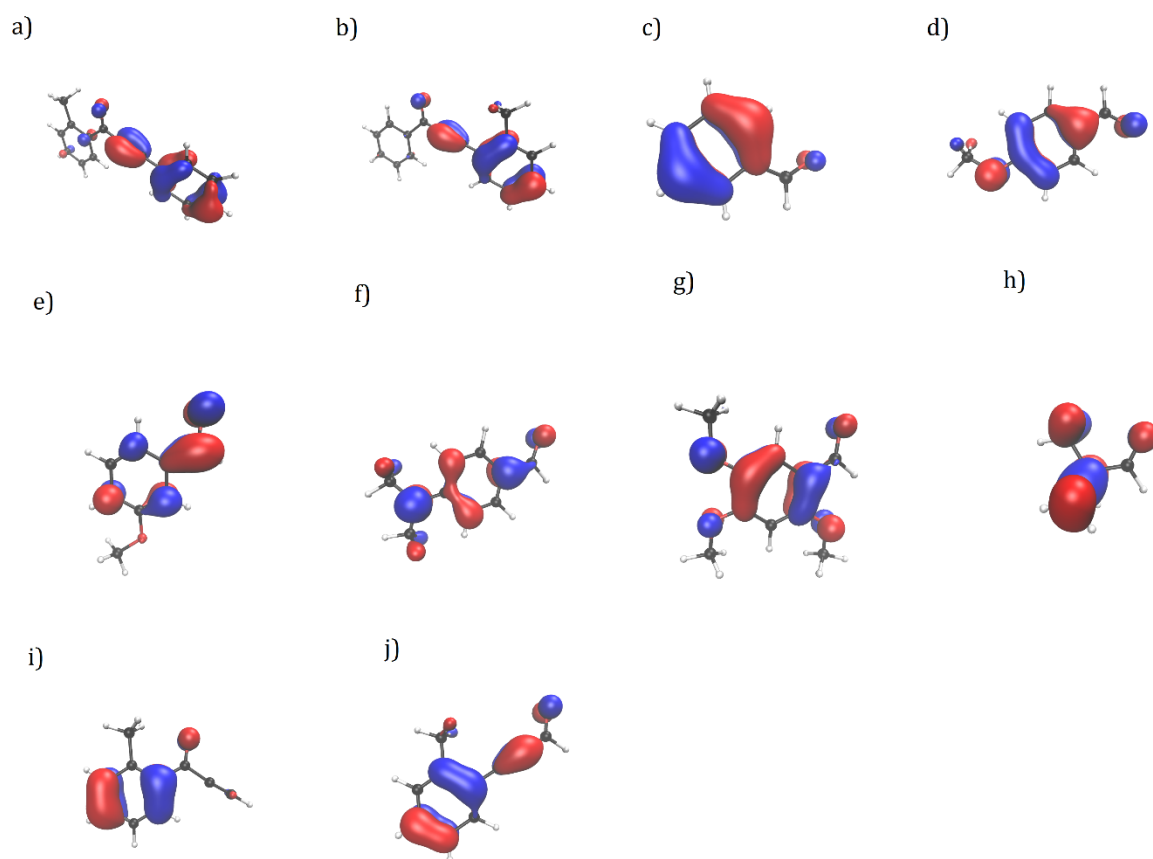


Figure S25. Visualization of HOMO-X orbitals (Table S2). a) **1a** HOMO-1, b) **1b** HOMO, c) **3a** HOMO-1, d) **3b** HOMO, e) **3c** HOMO-1, f) **3d** HOMO, g) **3e** HOMO, h) **3f** HOMO-1, i) **5a** HOMO-2, j) **5b** HOMO

VIII.6. Cartesian coordinates for the optimized structures

Substrate (1a)												
TS-1 of 1a							Int-3 of 1a					
O	0.0391372	-0.1948466	-0.0329859	O	-2.6951687	-0.3132261	1.3066226	C	-1.2467338	-0.4153005	1.3711284	
C	2.1858003	-0.1083751	-0.0208035	C	-0.5260502	0.5136216	0.6918816	C	1.5119085	0.4690350	0.3326351	
C	2.4643958	1.1460230	-0.0321096	C	3.4998801	0.5008327	-0.1700233	N	4.4434724	-0.4725726	0.0000780	
Au	4.4981966	1.4015791	-0.5361370	C	5.6770406	-0.0532409	-0.4773617	C	5.5013766	1.2160372	-0.9588619	
C	6.4123030	1.9023638	-1.0074226	N	4.1664639	1.5375628	-0.7615309	C	-1.2130339	1.5799817	-0.0948443	
N	7.3832150	1.1366811	-1.5830978	O	-2.2493165	1.3676187	-0.7549868	C	-0.8068815	-1.5517861	2.1869113	
C	8.5504494	1.8694715	-1.7418060	C	-1.6476501	-2.6766005	2.3705170	C	-1.1932243	-3.7987583	3.0736916	
C	8.2993402	3.1230850	-1.2529483	C	0.1010744	-3.8188362	3.6176460	C	0.9332831	-2.6958532	3.4716537	
N	6.9869137	3.1240094	-0.8047956	C	0.4815364	-1.5696130	2.7758636	C	4.1971970	-1.7814832	0.6098900	
C	1.6857545	2.4292927	0.0671316	C	3.5586741	2.8149130	-1.1512805	C	-3.2672837	-0.5988714	0.1391698	
O	0.7190281	2.6167386	-0.6685376	C	-2.5713773	-1.4675535	-0.7231716	C	-1.7612936	-2.1892908	-1.3059804	
C	2.5241170	-1.4923929	0.1067723	C	-0.7334490	-2.9760003	-1.8731900	C	0.4734350	-3.1278129	-1.1324347	
C	1.8519794	-2.5154796	-0.6077974	C	1.5197487	-3.8837910	-1.6646234	C	1.3808408	-4.4930887	-2.9246490	
C	2.2764671	-3.8414633	-0.4918824	C	0.1901378	-4.3475084	-3.6596487	C	-0.8674758	-3.5943534	-3.1440279	
C	3.3675537	-4.1686683	0.3322853	C	-0.5750860	2.9354932	-0.1272194	C	-0.6268551	3.7561116	-1.2890878	
C	4.0343208	-3.1633689	1.0533366	C	0.0276279	5.0035143	-1.2367511	C	0.6776054	5.4524746	-0.0781752	
C	3.6141887	-1.8344479	0.9541076	C	0.6985853	4.6486535	1.0726751	C	0.0868377	3.3921900	1.0364833	
C	7.2340660	-0.2698260	-1.9663522	C	0.1090854	2.7477024	1.9219456	H	0.1090854	2.7477024	1.9219456	
C	6.3115087	4.2931814	-0.2283675	C	-4.6442990	-0.1940909	-0.0724145	C	-5.3056483	0.7931251	0.7297897	
C	-0.4649848	0.2089969	-1.1166834	C	-5.3056483	0.7931251	0.7297897	C	-6.6402230	1.0915594	0.4042114	
C	0.3036357	0.0663433	-2.3233035	C	-7.3112407	0.4608060	-0.6543438	C	-6.6520700	-0.4976605	-1.4428301	
C	1.1448452	-0.0570797	-3.2115874	C	-5.3276324	-0.8137803	-1.1534317	H	-4.7979879	-1.5586392	-1.7560409	
C	2.1861424	-0.2114797	-4.1660199	H	1.1957419	4.9929709	1.9851736	H	1.1695894	6.4311442	-0.0758476	
C	3.4103980	-0.8078855	-3.7598472	H	0.0232995	5.6377368	-2.1306021	H	-2.6541686	-2.6826947	1.9436709	
C	4.4530950	-0.9566494	-4.6787548	H	-1.8532499	-4.6642656	3.1928346	H	-1.8532499	-4.6642656	3.1928346	
C	4.2956610	-0.5142738	-6.0038247	H	0.4540848	-4.6982732	4.1664047	H	1.9328322	-2.6898348	3.9190388	
C	3.0879745	0.0775534	-6.4129519	H	1.1182133	-0.6820585	2.6967480	H	1.1182133	-0.6820585	2.6967480	
C	2.0347986	0.2298069	-5.5055213	H	2.5202441	2.8327882	-0.7891233	H	3.5707662	2.9145761	-2.2481620	
C	2.1960700	3.4449422	1.0312285	H	4.1215429	3.6444113	-0.6963680	H	4.4251204	-2.5790436	-0.1146880	
C	1.8532248	4.8239722	0.9031692	H	3.1375568	-1.8320631	0.8996426	H	3.1375568	-1.8320631	0.8996426	
C	2.4202948	5.7227402	1.8284664	H	4.8300834	-1.9027712	1.5028824	H	6.2045674	1.9089280	-1.4179090	
C	3.2667096	5.2935944	2.8607726	H	6.5630336	-0.6842949	-0.4326344	H	-7.1670818	1.8466471	0.9970905	
C	3.5750313	3.9309535	2.9985085	H	-8.3523731	0.7248283	-0.8674896	H	-7.1670818	1.8466471	0.9970905	
C	3.0455647	3.0205946	2.0808182	H	-7.1680083	-0.9894999	-2.2726283	H	0.5620577	-2.6459594	-0.1536693	
C	3.2787335	1.9547915	2.1792135	H	0.5620577	-2.6459594	-0.1536693	H	2.4478426	-4.0057034	-1.0975881	
H	-1.8163885	0.7982954	-1.1846539	H	2.2042439	-5.0862727	-3.3356206	H	2.2042439	-5.0862727	-3.3356206	
C	-2.5187178	1.2226899	-0.0148291	H	0.0898398	-4.8252158	-4.6392188	H	-1.7965046	-3.4737792	-3.7084568	
C	-3.7968030	1.7834558	-0.1960052	C	-1.3203073	3.3335023	-2.5647290	C	-1.3203073	3.3335023	-2.5647290	
C	-4.3783526	1.9190100	-1.4654257	H	-2.4164002	3.3451400	-2.4373453	H	-2.4164002	3.3451400	-2.4373453	
C	-3.6804998	1.5014812	-2.6100526									
C	-2.4058392	0.9530274	-2.4629147									
H	-1.8456273	0.6268778	-3.3456624									
H	4.2230644	3.5833151	3.8091080									
H	3.6833465	6.0259871	3.5605450									
H	2.1880002	6.7893977	1.7335783									
H	1.0048153	-2.2585447	-1.2464086									
H	1.7543045	-4.6261549	-1.0482247									
H	3.6948605	-5.2101016	0.4169637									
H	4.8791413	-3.4172740	1.7013649									
H	4.1242065	-1.0451177	1.5149529									
H	5.3876553	3.9582441	0.2662162									
H	6.0656958	5.0141730	-1.0241132									
H	6.9748240	4.7653794	0.5113478									
H	7.4449544	-0.3838606	-3.0406890									
H	6.1995735	-0.5764627	-1.7558904									
H	7.9302773	-0.8911093	-1.3819475									
H	8.9360924	4.0034356	-1.1845244									
H	9.4499855	1.4397342	-2.1790485									
H	-4.3498340	2.1247206	0.6861358									
H	-5.3779206	2.3567834	-1.5594974									
H	-4.1250467	1.6062877	-3.6046271									
H	3.5205510	-1.1504654	-2.7262530									
H	5.3914590	-1.4251317	-4.3656459									
H	5.1153274	-0.6333475	-6.7200742									
H	2.9681466	0.4203814	-7.4456658									
H	1.0923612	0.6894692	-5.8175039									
C	0.9402491	5.3563685	-0.1763145									
H	-0.0883118	4.9789305	-0.0444574									

H	0.9232087	6.4581113	-0.1514619	H	-1.0526087	4.0131373	-3.3902531
H	1.2606524	5.0246849	-1.1792151	H	-1.0523282	2.3018856	-2.8514192
C	-1.9508020	1.1249089	1.3805945	C	-4.6469455	1.5388031	1.8641853
H	-0.9621499	1.6118349	1.4389181	H	-3.7006793	2.0018859	1.5360090
H	-2.6309943	1.6056849	2.1022093	H	-5.3182964	2.3278558	2.2375011
H	-1.7959615	0.0739632	1.6780154	H	-4.3965244	0.8623027	2.6990161
TS-2 of 1a				Int-4 of 1a			
O	0.0378988	-0.0201306	0.1133639	O	0.0423509	0.0079931	0.0711454
C	2.0237913	-0.0064807	0.0153363	C	1.5047843	0.0115228	-0.0191475
Au	-0.3928315	4.1097560	0.0534411	Au	-0.3124774	4.2566814	0.0091905
C	1.7207770	2.1089988	1.0128672	C	1.4427452	2.0245049	1.2356523
C	2.7463398	3.1108930	1.3075931	C	2.2527244	2.9019163	2.0775485
C	4.1052961	2.8327744	1.0200158	C	3.6324174	2.6235714	2.2561984
C	5.0839138	3.8150589	1.2098912	C	4.4243488	3.4708650	3.0360191
C	4.7284541	5.0807390	1.7049148	C	3.8536150	4.5946193	3.6586423
C	3.3875098	5.3566618	2.0248652	C	2.4823513	4.8674150	3.5055263
C	2.4042034	4.3803563	1.8358710	C	1.6839558	4.0286231	2.7242262
C	0.4091089	2.3007507	0.6632183	C	0.2212055	2.3491945	0.6105449
C	-0.4286892	1.1148221	0.4449918	C	-0.5242501	1.2289231	0.1818589
O	2.2365530	0.7838042	1.0955590	O	1.9790441	0.7830260	1.1212012
C	-1.2007848	5.8306007	-0.7115487	C	-0.7337015	6.0809379	-0.8226442
N	-0.5732049	1.7175819	-0.9679446	N	0.1497543	7.0911431	-1.0841026
C	-1.4602201	7.9390512	-1.5065852	C	-0.4836633	8.1480522	-1.7224538
C	-2.6744659	7.3129845	-1.5907379	C	-1.7979658	7.7923975	-1.8616983
N	-2.4962382	6.0273585	-1.1004696	N	-1.9304740	6.5271769	-1.3074869
C	0.8409788	7.2924190	-0.7012013	C	1.5831264	7.0484033	-0.7785792
C	-3.5596304	5.0206294	-1.0172384	C	-3.1903224	5.7790475	-1.2548172
C	-1.9069570	1.2192011	0.5764204	C	-1.9544617	1.2393426	-0.1367521
C	-2.7844725	0.5259012	-0.3068510	C	-2.5079298	0.4368640	-1.1836767
C	-4.1688094	0.7197907	-0.1301162	C	-3.8882549	0.5595409	-1.4312283
C	-4.6807098	1.5268139	0.8959753	C	-4.7093406	1.4102333	-0.6772160
C	-3.8079543	2.1817112	1.7799209	C	-4.1617050	2.1822271	0.3603608
C	-2.4291725	2.0378764	1.6068845	C	-2.7934077	2.0993752	0.6194092
C	2.1676824	0.6392955	-1.2455457	C	1.8969911	0.7046835	-1.2495564
C	2.2223835	1.4260695	-2.1878884	C	2.1504655	1.4306247	-2.2018666
C	2.2470813	2.4291940	-3.1902745	C	2.4024477	2.3363745	-3.2757862
C	2.2461047	3.7893732	-2.7748115	C	1.8486598	3.6413796	-3.2146270
C	2.2360902	4.8069897	-3.7319775	C	2.0814877	4.5496998	-4.2518983
C	2.2324431	4.4882112	-5.1013937	C	2.8653712	4.1747642	-5.3567581
C	2.2388873	3.1450350	-5.5174398	C	3.4163005	2.8838162	-5.4229660
C	2.2457497	2.1141522	-4.5728841	C	3.1900253	1.9639561	-4.3922505
C	2.2946308	-1.4387712	0.1902887	C	1.9867269	-1.4164467	0.1285459
C	2.1193352	-2.1074960	1.4402398	C	1.7100303	-2.1640441	1.3070586
C	2.4029262	-3.4847283	1.4761167	C	2.1831114	-3.4896922	1.3557271
C	2.8376143	-4.1875510	0.3421090	C	2.8993008	-4.0655146	0.2957517
C	2.9936574	-3.5227740	-0.8838097	C	3.1628292	-3.3161621	-0.8578854
C	2.7166314	-2.1568096	-0.9541554	C	2.7041039	-1.9953152	-0.9339052
C	-2.2970467	-0.3632496	-1.4295859	C	-1.6868359	-0.4826576	-2.0620918
C	1.6277920	-1.4250911	2.6954131	C	0.9523062	-1.6086715	2.4944143
H	-1.7359014	2.5491545	2.2825356	H	-2.3531559	2.6785786	1.4366189
H	2.8349314	-1.6222255	-1.9022599	H	2.9026048	-1.4000604	-1.8305504
H	-4.1979780	2.8602427	2.5897405	H	-4.7968073	2.8380384	0.9639328
H	-5.7642593	1.6449093	1.0037366	H	-5.7797346	1.4689041	-0.9013265
H	-4.8611875	0.2213808	-0.8177592	H	-4.3281817	-0.0256366	-2.2461982
H	4.3846350	1.8533576	0.6214863	H	4.0742826	1.7568312	1.7575660
H	6.1280661	3.5937824	0.9661226	H	5.4918499	3.2600877	3.1552911
H	5.4966674	5.8468561	1.8539039	H	4.4770536	5.2561707	4.2693381
H	3.1106517	6.3319316	2.4384954	H	2.0344636	5.7310457	4.0071139
H	1.3660195	4.5820141	2.1178880	H	0.6113937	4.2215586	2.6271834
H	-3.1407702	4.1097794	-0.5647619	H	-2.9977825	4.8103547	-0.7713399
H	-3.9381397	4.7943668	-2.0263810	H	-3.5658255	5.6131291	-2.2765989
H	-4.3803415	5.3996930	-0.3884722	H	-3.9347746	6.3438797	-0.6720561
H	1.3511904	7.5711446	-1.6367078	H	2.1600759	6.8303642	-1.6922883
H	1.2969160	6.3822904	-0.2849320	H	1.7579653	6.2554212	-0.0367984
H	0.9315420	8.1151276	0.0253520	H	1.8978091	8.0183392	-0.3658603
H	-3.6375203	7.6689029	-1.9528066	H	-2.6401513	8.3273230	-2.2973359
H	-1.1562254	8.9481621	-1.7794986	H	0.0469267	9.0524626	-2.0153162
H	2.2715523	-4.0217309	2.4217184	H	1.9800769	-4.0845938	2.2532477
H	3.0479023	-5.2596383	0.4173663	H	3.2485151	-5.1005278	0.3746200
H	3.3271270	-4.0630364	-1.7749187	H	3.7192049	-3.7514224	-1.6938859
H	2.2469471	4.0197763	-1.7047230	H	1.2390276	3.9232142	-2.3483713
H	2.2345676	5.8543158	-3.4135354	H	1.6480303	5.5544262	-4.2017589
H	2.2263765	5.2895727	-5.8474660	H	3.0460622	4.8886147	-6.1672173
H	2.2373278	2.9025517	-6.5848389	H	4.0264425	2.5920057	-6.2839251
H	2.2466426	1.0668622	-4.8887320	H	3.6176596	0.9580448	-4.4412794

H	-1.9114028	-1.3188236	-1.0344849	H	-1.4132730	-1.4064933	-1.5237657
H	-3.1200197	-0.5803241	-2.1295450	H	-2.2636416	-0.7626236	-2.9579372
H	-1.4684403	0.1017078	-1.9905638	H	-0.7446229	-0.0091754	-2.3856342
H	0.7240708	-0.8256947	2.4957414	H	-0.0148235	-1.1752104	2.1918216
H	1.3925744	-2.1750896	3.4670281	H	0.7627849	-2.4048092	3.2318351
H	2.3879836	-0.7340899	3.0984421	H	1.5260776	-0.8064324	2.9895921
TS-3 of 1a				Int-5 of 1a			
O	-0.0132080	-0.0684952	0.2123716	O	-2.1860263	-1.1132740	-0.5418118
C	1.9964672	0.0598618	0.0309133	C	-0.7635701	-1.1606989	-0.3107649
Au	-0.4105191	4.1293368	0.0322862	Au	1.9258509	-0.2655490	0.6029593
C	1.5710553	2.1561692	1.0399333	C	-0.1393722	-0.3582468	0.5936093
C	2.5205057	3.2384229	1.3561826	C	-0.8340928	0.6535644	1.4406029
C	3.7352741	3.2676790	0.6288342	C	-2.1256633	0.3022368	2.1232815
C	4.6363654	4.3248596	0.7786788	C	-3.0321631	1.3484126	2.4007716
C	4.3457026	5.3507733	1.6925747	C	-4.2867446	1.0680543	2.9530413
C	3.1719820	5.2973595	2.4566667	C	-4.6348410	-0.2577708	3.2633681
C	2.2371264	4.2520137	2.3154619	C	-3.7216377	-1.2999533	3.0288622
C	0.2557711	2.2801490	0.6853114	C	-2.4748094	-1.0243924	2.4532375
C	-0.5330533	1.0549897	0.4991131	C	-2.8789027	-0.0046106	-0.7510740
O	2.1955516	0.8772007	1.0917599	C	-4.3222785	-0.0898782	-0.6482124
C	-0.8931836	5.9370584	-0.8007000	C	-5.0332594	-1.3210586	-0.4352970
N	-0.0528439	7.0041752	-0.9620354	C	-6.4284310	-1.2341514	-0.2873578
C	-0.6943889	8.0412788	-1.6247936	C	-7.1145816	-0.0125983	-0.3437730
C	-1.9691266	7.6143246	-1.8824509	C	-6.4143963	1.1864251	-0.5652626
N	-2.0710170	6.3286271	-1.3699743	C	-5.0339451	1.1416626	-0.7190356
C	1.3421650	7.0464830	-0.5121906	C	-0.1705092	-2.2747793	-1.0855135
C	-3.2774098	5.4996538	-1.4495625	C	-0.3367921	-2.3906193	-2.4927456
C	-2.0112793	1.0788934	0.6360505	C	0.2855756	-3.4717577	-3.1468935
C	-2.7744057	0.0723703	-0.0007824	C	1.0459189	-4.4189625	-2.4464033
C	-4.1687484	0.0750625	0.1050164	C	1.2013144	-4.3023829	-1.0562025
C	-4.8144250	1.0653259	0.8662877	C	0.5942390	-3.2358627	-0.3848396
C	-4.0619287	2.0521848	1.5259566	C	3.9648807	-0.0465918	0.5164130
C	-2.6672773	2.0649507	1.4097693	N	4.8887496	-0.9480841	0.0673593
C	2.0381391	0.6882050	-1.2438251	C	6.1699653	-0.4215057	0.1443625
C	2.0163264	1.4337537	-2.2209764	C	6.0461149	0.8443955	0.6503749
C	1.9560935	2.3828125	-3.2727728	N	4.6926155	1.0553697	0.8696845
C	1.8954124	3.7620833	-2.9318819	C	4.5784187	-2.2921634	-0.4290904
C	1.7932360	4.7230730	-3.9405220	C	4.1252809	2.3015680	1.3934242
C	1.7616521	4.3290796	-5.2898307	C	-1.1180035	-1.3723263	-3.2932110
C	1.8310764	2.9671128	-5.6334081	O	-0.3551645	1.7887090	1.5701001
C	1.9263122	1.9920958	-4.6360288	C	-2.2041507	1.1789513	-1.0656401
C	2.3500731	-1.3509979	0.2142245	C	-1.5058094	2.1687288	-1.3025856
C	2.2564337	-2.0083125	1.4798771	C	-0.6270114	3.2484446	-1.5190235
C	2.6151409	-3.3674440	1.5248793	C	0.7705520	3.0307963	-1.3521392
C	3.0466120	-4.0640378	0.3858033	C	1.6580259	4.0914431	-1.5325074
C	3.1223547	-3.4121041	-0.8547975	C	1.1738691	5.3662915	-1.8805768
C	2.7690930	-2.0648241	-0.9349699	C	-0.2058478	5.5868788	-2.0484939
H	-2.2595520	-0.6917067	-0.5906928	C	-1.1101987	4.5384288	-1.8700459
C	1.7716141	-1.3338413	2.7416608	H	1.1264317	2.0346770	-1.0703290
H	-2.0791597	2.8253791	1.9327962	H	-1.7676971	-1.8372179	2.2567132
H	2.8246701	-1.5406561	-1.8944798	H	-4.4714713	2.0670052	-0.8747711
H	-4.5638361	2.8118446	2.1338851	H	-3.9875631	-2.3301721	3.2875285
H	-5.9065747	1.0652976	0.9487697	H	-5.6182218	-0.4797435	3.6911545
H	-4.7564969	-0.6933016	-0.4076993	H	-4.9987636	1.8796924	3.1354671
H	3.9470139	2.4652731	-0.0852714	H	0.1801440	-3.5618999	-4.2341723
H	5.5583854	4.3479524	0.1889431	H	1.5178645	-5.2463818	-2.9871333
H	5.0437989	6.1843023	1.8251030	H	1.7868353	-5.0398679	-0.4974040
H	2.9759314	6.0818939	3.1964271	H	0.6971794	-3.1356456	0.7007176
H	-3.1155362	4.5969801	-0.8423604	H	3.0362504	2.1750729	1.4834248
H	-3.4671791	5.2123075	-2.4959977	H	4.3472061	3.1307333	0.7026523
H	-4.1379991	6.0624933	-1.0566235	H	4.5568304	2.5209341	2.3823650
H	2.0220430	7.0091949	-1.3787742	H	4.9536662	-2.4020436	-1.4585496
H	1.5264775	6.1785522	0.1381267	H	3.4864039	-2.4214482	-0.4194434
H	1.5192008	7.9744196	0.0522677	H	5.0481768	-3.0478244	0.2201687
H	-2.8030181	8.1119308	-2.3746827	H	6.7959685	1.6027228	0.8693647
H	-0.1981180	8.9843998	-1.8472068	H	7.0493655	-0.9849301	-0.1630188
H	2.5466108	-3.8955262	2.4820173	H	-6.9940047	-2.1575661	-0.1253416
H	3.3173101	-5.1218939	0.4686747	H	-8.2020760	0.0022375	-0.2170590
H	3.4526851	-3.9484234	-1.7494057	H	-6.9434657	2.1426647	-0.6103845
H	1.9202936	4.0515575	-1.8766782	H	2.7331629	3.9302325	-1.4046957
H	1.7367775	5.7846613	-3.6790192	H	1.8766671	6.1937442	-2.0230436
H	1.6834558	5.0861540	-6.0769720	H	-0.5725039	6.5819597	-2.3185525
H	1.8076414	2.6661520	-6.6855516	H	-2.1851783	4.6974277	-1.9943620
H	1.9734869	0.9304662	-4.8951979	H	-2.7420352	2.3718820	2.1425719
H	0.8279782	-0.7911311	2.5649166	H	-0.8777587	-1.4494144	-4.3656611

H	1.6077726	-2.0827096	3.5325596	H	-2.2083099	-1.5224222	-3.1853046
H	2.5045033	-0.5935826	3.1059306	H	-0.8927215	-0.3430900	-2.9631503
C	1.0193710	4.2279100	3.2146490	C	-4.3874269	-2.6834249	-0.3861649
H	0.5830299	3.2200124	3.2925155	H	-5.1609802	-3.4617298	-0.2957443
H	1.2887214	4.5819168	4.2242422	H	-3.7862604	-2.8807704	-1.2900292
H	0.2278317	4.8966899	2.8288422	H	-3.6995423	-2.7658968	0.4721686
TS-4 of 1a							
O	-0.1006293	-0.1110502	0.0575383				
C	1.9055911	-0.0503711	0.0430503				
Au	4.4405198	1.0219028	-0.1803884				
C	2.3840737	1.1369842	0.2506624				
C	1.8017088	2.5006516	0.4468357				
C	0.6689709	2.6651626	1.4069026				
C	-0.1636431	3.7954783	1.2521389				
C	-1.2782133	3.9657013	2.0790107				
C	-1.5543981	3.0247583	3.0859601				
C	-0.7098593	1.9170538	3.2680218				
C	0.3927502	1.7297114	2.4259431				
C	-0.8259735	0.7620432	-0.5079146				
C	-2.2034540	1.0115644	-0.0508759				
C	-2.8345313	0.2052615	0.9488902				
C	-4.1224346	0.5882773	1.3666226				
C	-4.7759743	1.7102762	0.8370467				
C	-4.1550579	2.4890149	-0.1530544				
C	-2.8813074	2.1330981	-0.5923935				
C	2.1325960	-1.4685673	-0.0572911				
C	1.8967310	-2.1744738	-1.2703903				
C	2.1751819	-3.5519826	-1.2883047				
C	2.6636589	-4.2156606	-0.1522482				
C	2.8916364	-3.5102789	1.0411296				
C	2.6224201	-2.1403058	1.0903846				
C	6.4251118	1.0682563	-0.6414115				
N	7.3707905	0.1177846	-0.3859947				
C	8.6107445	0.5246362	-0.8565894				
C	8.4343796	1.7599078	-1.4188924				
N	7.0911942	2.0759470	-1.2775861				
C	7.1247025	-1.1630690	0.2842493				
C	6.4819293	3.3187323	-1.7626226				
C	1.3633901	-1.4679226	-2.4900246				
O	2.2512107	3.4514239	-0.1951389				
C	-0.2800662	1.5389874	-1.5738144				
C	0.3337314	2.1728036	-2.4313097				
C	1.1188735	2.8802297	-3.3757272				
C	2.5199971	2.6465304	-3.4194360				
C	3.3123775	3.3450954	-4.3331194				
C	2.7267647	4.2759490	-5.2094917				
C	1.3410672	4.5122676	-5.1717520				
C	0.5350395	3.8229773	-4.2612143				
H	2.9651878	1.9278439	-2.7244260				
H	1.0386378	0.8558382	2.5536489				
H	-2.3771250	2.7372427	-1.3532044				
H	-0.9203035	1.1916516	4.0604424				
H	-2.4312375	3.1535485	3.7290571				
H	-1.9401357	4.8257279	1.9350204				
H	2.0116808	-4.1144838	-2.2141576				
H	2.8712630	-5.2899971	-0.2007087				
H	3.2764487	-4.0257540	1.9268161				
H	2.7948780	-1.5687530	2.0075612				
H	5.4276471	3.3366289	-1.4495381				
H	6.5458174	3.3585017	-2.8614826				
H	7.0100112	4.1819353	-1.3296427				
H	7.3865237	-1.9910325	-0.3927610				
H	6.0572205	-1.2193213	0.5422100				
H	7.7312756	-1.2242965	1.2010972				
H	9.1412077	2.4332445	-1.9006950				
H	9.5017815	-0.0918836	-0.7513492				
H	-4.6260629	-0.0140784	2.1305640				
H	-5.7759776	1.9742719	1.1973480				
H	-4.6585236	3.3653853	-0.5724280				
H	4.3914099	3.1643288	-4.3680825				
H	3.3526256	4.8189769	-5.9253626				
H	0.8900421	5.2381644	-5.8557663				
H	-0.5435945	4.0017414	-4.2236838				
H	0.0660237	4.5097480	0.4555450				
H	1.5899625	-2.0324824	-3.4085515				

H	0.2658435	-1.3545611	-2.4210587		
H	1.7844545	-0.4522295	-2.5800612		
C	-2.2042129	-1.0212487	1.5618390		
H	-2.9284904	-1.5315888	2.2170510		
H	-1.8532029	-1.7262423	0.7896223		
H	-1.3137335	-0.7504243	2.1542974		
Product (1b)					
TS-1 of 1b				Int-3 of 1b	
O	0.0192110	-0.1195463	0.0440157	O	-2.6225913
C	2.1718938	-0.0483803	0.2284631	C	-1.2028269
C	2.4694946	1.1984733	0.1530900	C	-0.3754438
Au	4.5353360	1.3969568	-0.2541866	Au	1.6073208
C	6.4670992	1.8551050	-0.6896775	C	3.5180647
N	7.4421372	1.0509250	-1.2024387	N	4.2669692
C	8.6189070	1.7646297	-1.3758529	C	5.4921827
C	8.3705893	3.0441911	-0.9577566	C	5.5136347
N	7.0487189	3.0808594	-0.5397074	N	4.3003554
C	1.7343434	2.5103104	0.1185779	C	-0.9299840
O	0.7791604	2.6656651	-0.6376377	O	-1.9996243
C	2.4614573	-1.4260516	0.4756398	C	-0.9178824
C	1.7534376	-2.4833522	-0.1485299	C	-1.9317259
C	2.1310222	-3.8082530	0.0822780	C	-1.6414069
C	3.2122450	-4.1012554	0.9317731	C	-0.3402818
C	3.9152789	-3.0611222	1.5633948	C	0.6671981
C	3.5408649	-1.7319928	1.3504390	C	0.3802100
C	7.2725892	-0.3617917	-1.5545553	C	3.8192492
C	6.3805819	4.2815804	-0.0227793	C	3.9145427
C	-0.3883201	0.2579865	-1.0870692	C	-3.2326362
C	0.4302841	0.0968589	-2.2519908	C	-2.7285836
C	1.1830765	-0.0052085	-3.2199855	C	-2.2283163
C	2.0504661	-0.0793856	-4.3430862	C	-1.6228271
C	3.3087947	-0.7528036	-4.2499509	C	-0.4863916
C	4.1323342	-0.7647826	-5.3870935	C	0.0910267
C	3.7423201	-0.1413127	-6.5834956	C	-0.4180073
C	2.5025852	0.5132514	-6.6710968	C	-1.5348392
C	1.6597066	0.5433450	-5.5578408	C	-2.1392355
C	2.2897120	3.5973663	0.9765865	C	-0.1254139
C	2.0934708	4.9701800	0.6466084	C	-0.1556154
C	2.6995656	5.9312921	1.4803472	C	0.6547568
C	3.4411867	5.5705676	2.6145098	C	1.4405270
C	3.6037536	4.2168174	2.9491923	C	1.4417350
C	3.0378122	3.2418413	2.1239235	C	0.6714577
H	3.1603901	2.1820014	2.3728063	H	0.6720450
C	-1.7375231	0.8512797	-1.2346926	C	-4.5347323
C	-2.5001433	1.1043481	-0.0725626	C	-4.9805360
C	-3.7720258	1.6725830	-0.1820460	C	-6.2263856
C	-4.2940531	1.9900979	-1.4496309	C	-7.0333261
C	-3.5403368	1.7399285	-2.6089339	C	-6.5932493
C	-2.2649336	1.1735157	-2.5043468	C	-5.3485551
H	-1.6725130	0.9779381	-3.4040873	H	-4.9987264
H	4.1700058	3.9251084	3.8392260	H	2.0432951
H	3.8917017	6.3498383	3.2385390	H	2.0520983
H	2.5834045	6.9916949	1.2298037	H	0.6642562
H	0.9146837	-2.2525108	-0.8074163	H	-2.9468243
H	1.5801914	-4.6190953	-0.4045912	H	-2.4354994
H	3.5032256	-5.1422672	1.1064554	H	-0.1159079
H	4.7523823	-3.2870746	2.2314713	H	1.6777457
H	4.0791554	-0.9161749	1.8429083	H	1.1590291
H	5.3812709	3.9996819	0.3400489	H	2.9465592
H	6.2865539	5.0288100	-0.8261905	H	3.8222501
H	6.9692740	4.6983771	0.8083250	H	4.6765604
H	7.2374849	-0.4736635	-2.6501935	H	3.4864402
H	6.3296094	-0.7180265	-1.1167599	H	2.9817824
H	8.1127901	-0.9437453	-1.1477228	H	4.6490560
H	9.0159273	3.9199731	-0.9172338	H	6.2816243
H	9.5225363	1.3051066	-1.7725586	H	6.2365799
H	-2.0746543	0.8539848	0.9035470	H	-4.3410850
H	-4.3614969	1.8720524	0.7188156	H	-6.5729446
H	-5.2912903	2.4352338	-1.5330197	H	-8.0091228
H	-3.9484532	1.9879173	-3.5940185	H	-7.2237487
H	5.0997725	-1.2767351	-5.3355927	H	0.9585676
H	4.4095807	-0.1697062	-7.4514208	H	0.0609858
H	2.1959763	0.9978234	-7.6033697	H	-1.9293031
H	0.6916796	1.0513278	-5.6066442	H	-3.0081770

C	1.2982656	5.4272690	-0.5540891	C	-0.9902417	3.5044620	-2.6015322
H	0.2257298	5.2022033	-0.4240757	H	-2.0638857	3.6541014	-2.3943858
H	1.4195610	6.5127182	-0.7014710	H	-0.7048429	4.1304646	-3.4628439
H	1.6119839	4.9032154	-1.4734993	H	-0.8746251	2.4421062	-2.8773808
C	3.7291028	-1.4319268	-2.9714501	C	0.0622912	-3.3406942	-0.0324755
H	3.0000985	-2.2050917	-2.6733432	H	-0.7117867	-3.4627621	0.7449536
H	4.7155499	-1.9092333	-3.0798104	H	0.9059604	-4.0052075	0.2091781
H	3.7795250	-0.7065605	-2.1383648	H	0.4105400	-2.2927170	0.0338910
TS-2 of 1b				Int-4 of 1b			
O	0.0719601	0.0135728	0.1597932	O	0.0293862	0.0083593	0.0903410
C	2.0362053	0.0059937	0.0373851	C	1.4959049	-0.0109765	-0.0020228
C	0.4257415	2.3974621	0.0616585	C	0.1879734	2.4114616	0.0073830
Au	-0.5001509	3.9621234	-0.9306481	Au	-0.4627701	4.1412072	-0.9293142
C	-1.4548181	5.4046302	-2.0294416	C	-1.0329543	5.7946591	-1.9959258
N	-0.9032708	6.4647160	-2.6925645	N	-0.2656158	6.8822055	-2.3076203
C	-1.8820992	7.2055006	-3.3392265	C	-0.9847516	7.7915649	-3.0699079
C	-3.0779226	6.5947623	-3.0730908	C	-2.2352512	7.2614465	-3.2386346
N	-2.7967558	5.4973011	-2.2725418	N	-2.2449315	6.0421791	-2.5764434
C	-0.3957293	1.1932337	0.2324568	C	-0.5515635	1.2108405	-0.0885651
O	2.2714341	1.0679481	0.8421556	O	1.9731702	1.0411712	0.8744633
C	1.7550290	2.3169122	0.3858634	C	1.4413118	2.2708824	0.6321931
C	2.7905371	3.3493223	0.3438500	C	2.3089707	3.3486824	1.1023529
C	4.1491947	2.9766939	0.1904235	C	3.7084095	3.1290126	1.1785759
C	5.1410570	3.9542792	0.0537228	C	4.5627122	4.1677284	1.5594625
C	4.7999382	5.3166866	0.0826920	C	4.0360594	5.4285550	1.8891735
C	3.4597008	5.6981244	0.2684594	C	2.6473315	5.6474328	1.8472394
C	2.4644775	4.7261076	0.4080340	C	1.7867426	4.6172161	1.4599547
C	0.5290883	6.7712026	-2.7399948	C	1.1362609	7.0589404	-1.9176652
C	-3.8093710	4.5671115	-1.7622794	C	-3.4028411	5.1447797	-2.5185404
C	-1.8600392	1.3210738	0.4710864	C	-1.9926405	1.1240200	-0.3473146
C	-2.7950115	0.4290230	-0.1274215	C	-2.5544968	0.0966932	-1.1678424
C	-4.1618762	0.6488050	0.1355236	C	-3.9449608	0.1309706	-1.3854378
C	-4.5984607	1.6757287	0.9843863	C	-4.7662826	1.1096827	-0.8077207
C	-3.6660302	2.5321212	1.5921711	C	-4.2089081	2.1043296	0.0125196
C	-2.3061688	2.3618095	1.3205544	C	-2.8307996	2.1126614	0.2302733
C	2.1818433	0.2064101	-1.3614763	C	1.9105754	0.2824092	-1.3721633
C	2.3294082	0.4609970	-2.5547819	C	2.2662940	0.6243612	-2.4926696
C	2.4986475	0.7756258	-3.9272785	C	2.6778641	1.0724691	-3.7820942
C	2.5990133	2.1436079	-4.3358784	C	2.9784811	2.4551551	-3.9783084
C	2.7614021	2.4020371	-5.7063017	C	3.3713419	2.8628781	-5.2642341
C	2.8260648	1.3623632	-6.6482930	C	3.4700704	1.9499006	-6.3262410
C	2.7287261	0.0221870	-6.2378559	C	3.1746712	0.5923894	-6.1226501
C	2.5662594	-0.2721609	-4.8827214	C	2.7815635	0.1534095	-4.8547788
C	2.2911258	-1.3039687	0.6582434	C	1.9512025	-1.3370198	0.5664108
C	2.3267663	-1.4178181	2.0659015	C	1.6835207	-1.6102083	1.9218135
C	2.5518219	-2.6658931	2.6536176	C	2.0758026	-2.8356774	2.4730461
C	2.7353091	-3.8032153	1.8467141	C	2.7309561	-3.7898781	1.6750683
C	2.6957893	-3.6923103	0.4466729	C	2.9949334	-3.5155435	0.3249715
C	2.4744487	-2.4465470	-0.1500166	C	2.6069801	-2.2875838	-0.2320813
C	2.5402300	3.2623818	-3.3260038	C	2.8774958	3.4373879	-2.8369741
C	-2.3862431	-0.7018189	-1.0452424	C	-1.7321541	-0.9761608	-1.8492877
H	-1.5679598	3.0279646	1.7786593	H	-2.3823345	2.8708677	0.8793283
H	2.4447980	-2.3528497	-1.2401823	H	2.8144417	-2.0675483	-1.2838869
H	-3.9962065	3.3314917	2.2629662	H	-4.8436832	2.8632941	0.4801593
H	-5.6697979	1.8081522	1.1695504	H	-5.8442569	1.0952899	-1.0004652
H	-4.9003687	-0.0069951	-0.3390405	H	-4.3928933	-0.6302654	-2.0335207
H	4.4185677	1.9178332	0.1501231	H	4.1133356	2.1509397	0.9054335
H	6.1844993	3.6517434	-0.0815640	H	5.6434498	3.9976468	1.5944715
H	5.5779586	6.0798082	-0.0248033	H	4.7080264	6.2403584	2.1868062
H	3.1925628	6.7586632	0.3212709	H	2.2358949	6.6216297	2.1296606
H	1.4261084	5.0237341	0.5870633	H	0.7040929	4.7761750	1.4552109
H	-3.3066192	3.8141274	-1.1379547	H	-3.1440668	4.2858281	-1.8824264
H	-4.3176069	4.0717926	-2.6043835	H	-3.6528838	4.7923770	-3.5316741
H	-4.5453825	5.1166344	-1.1549351	H	-4.2642598	5.6783638	-2.0875227
H	0.9109071	6.6225457	-3.7627230	H	1.7856116	6.9822292	-2.8045449
H	1.0512490	6.0929451	-2.0497820	H	1.3987271	6.2685342	-1.1993998
H	0.6945184	7.8148055	-2.4311950	H	1.2668403	8.0455809	-1.4474845
H	-4.0919781	6.8465581	-3.3789065	H	-3.1084988	7.6445961	-3.7638111
H	-1.6479989	8.0929613	-3.9247615	H	-0.5519388	8.7269354	-3.4205248
H	2.1744747	-0.5295906	2.6848176	H	1.1732627	-0.8636532	2.5380850
H	2.5805645	-2.7561371	3.7441068	H	1.8701543	-3.0481691	3.5272059
H	2.9084270	-4.7793031	2.3118000	H	3.0361805	-4.7479930	2.1087656
H	2.8392570	-4.5779471	-0.1801123	H	3.5053875	-4.2563505	-0.2987702
H	2.8417184	3.4413881	-6.0432849	H	3.6060622	3.9194114	-5.4357748
H	2.9545097	1.6012872	-7.7092724	H	3.7805581	2.3010607	-7.3160191

H	2.7812848	-0.7878140	-6.9719944	H	3.2507749	-0.1216769	-6.9488721
H	2.4898655	-1.3093394	-4.5426564	H	2.5486150	-0.9013376	-4.6791592
H	-1.9364671	-1.5299119	-0.4705916	H	-1.4219633	-1.7542363	-1.1304730
H	-3.2627738	-1.0894177	-1.5890454	H	-2.3236191	-1.4571781	-2.6444845
H	-1.6282592	-0.3798077	-1.7795752	H	-0.8112327	-0.5661871	-2.2969406
H	3.3675632	3.1856372	-2.5979736	H	3.5295172	3.1417563	-1.9951859
H	2.6045268	4.2442493	-3.8204932	H	3.1645811	4.4510221	-3.1585939
H	1.6029526	3.2269330	-2.7395697	H	1.8464718	3.4789944	-2.4358299
TS-3 of 1b				Int-5 of 1b			
O	-0.0253313	-0.0678899	0.1245896	O	-2.0301902	-1.3603204	-0.7460025
C	2.0287075	0.0774920	0.0433967	C	-0.6087136	-1.2432874	-0.5482193
Au	-0.5327818	4.1150579	0.3118715	Au	1.9825488	-0.2785203	0.5565022
C	1.5356413	2.1201589	1.1343447	C	-0.0664449	-0.5417751	0.4819660
C	2.4791873	3.1803637	1.5328716	C	-0.8725736	0.1868760	1.5012442
C	3.7253661	3.2214079	0.8610939	C	-2.0271864	-0.5088416	2.1606712
C	4.6346917	4.2561321	1.0916827	C	-3.0796564	0.2852474	2.6660738
C	4.3184714	5.2506289	2.0316975	C	-4.2184920	-0.3170491	3.2123432
C	3.1155138	5.1804795	2.7463701	C	-4.3033099	-1.7177533	3.2836902
C	2.1753690	4.1525497	2.5281777	C	-3.2446766	-2.5145705	2.8133564
C	0.2238081	2.2417643	0.7733131	C	-2.1133075	-1.9147276	2.2474868
C	-0.5511991	1.0167837	0.5115442	C	-2.8841367	-0.3488253	-0.7086138
O	2.1633797	0.8359805	1.1478254	C	-4.2821403	-0.7128016	-0.5419031
C	-1.1485817	5.9817100	-0.2645573	C	-4.6425829	-2.0726619	-0.3554042
N	-0.3683576	7.1012254	-0.3529826	C	-5.9809246	-2.4130359	-0.1553937
C	-1.1119753	8.1866884	-0.7933740	C	-6.9678020	-1.4111961	-0.1317907
C	-2.3904610	7.7363997	-0.9845660	C	-6.6174536	-0.0602126	-0.3144582
N	-2.3926249	6.3884349	-0.6549994	C	-5.2841778	0.2915954	-0.5203744
C	1.0598911	7.1550970	-0.0248460	C	0.1001932	-2.1090975	-1.5201355
C	-3.5721161	5.5210848	-0.7283875	C	-0.0314573	-1.9195774	-2.9217932
C	-2.0287859	1.0104253	0.6883661	C	0.6962637	-2.7696550	-3.7771063
C	-2.7972047	0.0605520	-0.0230973	C	1.5229473	-3.7851932	-3.2750237
C	-4.1886067	0.0328187	0.1185306	C	1.6428515	-3.9709868	-1.8887724
C	-4.8248086	0.9335907	0.9903718	C	0.9348282	-3.1332231	-1.0197958
C	-4.0654764	1.8607500	1.7246102	C	4.0014153	0.0950464	0.5588387
C	-2.6747279	1.9053887	1.5725082	N	5.0042639	-0.6994237	0.0776909
C	2.1146348	0.7079346	-1.2207537	C	6.2379465	-0.0830433	0.2286994
C	2.1964281	1.2756387	-2.3092687	C	6.0024948	1.1315492	0.8142714
C	2.2843828	1.9236908	-3.5661371	N	4.6318741	1.2217467	1.0079455
C	2.2685730	3.3528199	-3.6453269	C	4.8148050	-2.0302627	-0.5069404
C	2.3436797	3.9332211	-4.9214578	C	3.9555821	2.3888013	1.5820251
C	2.4340396	3.1485868	-6.0826874	C	-0.8923146	-0.8150565	-3.4917974
C	2.4523420	1.7461110	-5.9959726	O	-0.6003824	1.3595513	1.7976428
C	2.3782396	1.1343601	-4.7438383	C	-2.4615247	0.9699512	-0.8502762
C	2.3485970	-1.3431523	0.2200244	C	-2.1485944	2.1608047	-0.9639124
C	2.4211354	-1.8895880	1.5221496	C	-1.7891692	3.5122805	-1.1043093
C	2.7116795	-3.2460647	1.6883695	C	-0.4046793	3.8929753	-1.1230172
C	2.9235189	-4.0653572	0.5646517	C	-0.1141390	5.2567348	-1.2744612
C	2.8462889	-3.5261998	-0.7309020	C	-1.1335574	6.2154641	-1.3973060
C	2.5604615	-2.1689875	-0.9068820	C	-2.4886937	5.8353124	-1.3721818
H	-2.2898219	-0.6355204	-0.6977721	C	-2.8185792	4.4903345	-1.2267495
H	2.2469215	-1.2464654	2.3887210	C	0.6763753	2.8623309	-0.9484570
H	-2.0824661	2.6198971	2.1526971	H	-1.2941908	-2.5343995	1.8685031
H	2.5010953	-1.7426344	-1.9130672	H	-5.0047050	1.3404982	-0.6559446
H	-4.5588341	2.5493708	2.4182079	H	-3.3078139	-3.6055889	2.8808849
H	-5.9142294	0.9100658	1.1010098	H	-5.1964803	-2.1909268	3.7051470
H	-4.7808318	-0.6902813	-0.4517552	H	-5.0450621	0.3025440	3.5754857
H	3.9572980	2.4452298	0.1247511	H	0.6190854	-2.6222568	-4.8605208
H	5.5817199	4.2873650	0.5433837	H	2.0748782	-4.4299870	-3.9673991
H	5.0202384	6.0689583	2.2254486	H	2.2807539	-4.7650695	-1.4866867
H	2.9005232	5.9346356	3.5121036	H	1.0135428	-3.2658575	0.0645012
H	-3.3036335	4.5388336	-0.3126441	H	2.8895714	2.1463966	1.7008957
H	-3.8878989	5.4053302	-1.7773055	H	4.0657887	3.2531521	0.9075972
H	-4.3917184	5.9617944	-0.1400212	H	4.3945889	2.6260271	2.5632949
H	1.6441673	7.3907313	-0.9284226	H	5.2880797	-2.0666249	-1.5002625
H	1.3632045	6.1730571	0.3672074	H	3.7353179	-2.2143450	-0.6068757
H	1.2351065	7.9272752	0.7401773	H	5.2636962	-2.7950046	0.1468589
H	-3.2873640	8.2545748	-1.3196889	H	6.6845598	1.9290863	1.1041597
H	-0.6752565	9.1748247	-0.9277649	H	7.1662436	-0.5552372	-0.0882655
H	2.7704656	-3.6703072	2.6955869	H	-3.8667629	-2.8415964	-0.3619438
H	3.1483338	-5.1284661	0.6999620	H	-6.2593217	-3.4609349	-0.0081688
H	3.0111678	-4.1654387	-1.6037283	H	-8.0154629	-1.6832685	0.0333108
H	2.3306932	5.0252352	-5.0076404	H	-7.3887277	0.7155466	-0.2923806
H	2.4899213	3.6365316	-7.0614600	H	0.9327745	5.5775690	-1.2919977
H	2.5225830	1.1350479	-6.9011478	H	-0.8679324	7.2716208	-1.5118724
H	2.3882706	0.0438828	-4.6545115	H	-3.2770436	6.5879869	-1.4672465

C	0.9379855	4.0990877	3.3995607	H	-3.8640013	4.1681943	-1.2087040
H	0.4750492	3.1002946	3.3989165	H	-2.9949956	1.3740680	2.5910506
H	1.1978737	4.3733354	4.4363542	H	0.5903838	2.0580044	-1.7015818
H	0.1722977	4.8160911	3.0501611	H	1.6772012	3.3136389	-1.0300304
C	2.1885252	4.2018590	-2.4020987	H	0.5742607	2.3740683	0.0384360
H	3.1081717	4.1051149	-1.7976325	H	-0.6431066	-0.6247513	-4.5479884
H	2.0567317	5.2644863	-2.6590383	H	-1.9658283	-1.0750757	-3.4425690
H	1.3498099	3.8928723	-1.7510794	H	-0.7571018	0.1258634	-2.9292433
TS-4 of 1b							
O	-0.0269980	-0.0498021	-0.0348672				
C	2.0116961	-0.0566234	0.0501763				
Au	4.5642576	0.9343092	0.0049613				
C	2.4850392	1.1256989	0.2826374				
C	1.8928041	2.4835594	0.4835529				
C	0.7530958	2.6218352	1.4377283				
C	-0.0856141	3.7498646	1.2991561				
C	-1.2035704	3.9000437	2.1258876				
C	-1.4781141	2.9393415	3.1137114				
C	-0.6324309	1.8284165	3.2742741				
C	0.4742779	1.6626976	2.4342327				
C	-0.6887615	0.8389675	-0.6460437				
C	-2.0837793	1.1087815	-0.2336314				
C	-2.6267440	0.3761058	0.8470876				
C	-3.9254818	0.6422358	1.2877640				
C	-4.6902347	1.6409622	0.6592823				
C	-4.1566339	2.3722479	-0.4165345				
C	-2.8594337	2.1079562	-0.8651405				
C	2.1986134	-1.4804726	-0.0243112				
C	1.9207335	-2.2176626	-1.2100211				
C	2.1926398	-3.5969601	-1.1990002				
C	2.7129724	-4.2336764	-0.0622823				
C	2.9774151	-3.4993112	1.1062688				
C	2.7157848	-2.1279256	1.1276463				
C	6.5749040	0.8511711	-0.3103834				
N	7.4106703	-0.2043928	-0.0846796				
C	8.7107143	0.1178903	-0.4460006				
C	8.6847897	1.4056407	-0.9089457				
N	7.3698258	1.8374846	-0.8180575				
C	7.0052705	-1.5057508	0.4564821				
C	6.9059615	3.1638224	-1.2384554				
C	1.3448530	-1.5496410	-2.4313970				
O	2.3349910	3.4476020	-0.1440017				
C	-0.1222016	1.6044333	-1.7039976				
C	0.3486855	2.2984898	-2.6064563				
C	0.8503296	3.1128538	-3.6522365				
C	2.2432644	3.1146235	-3.9818282				
C	2.6621506	3.9428740	-5.0351534				
C	1.7550303	4.7457848	-5.7454391				
C	0.3892404	4.7429008	-5.4142375				
C	-0.0617130	3.9323680	-4.3717413				
C	3.2252977	2.2835197	-3.1980283				
H	1.1211998	0.7877448	2.5466421				
H	-2.4368429	2.6786206	-1.6978142				
H	-0.8456196	1.0839102	4.0479727				
H	-2.3573735	3.0524361	3.7565055				
H	-1.8680727	4.7604098	1.9964468				
H	1.9972036	-4.1826792	-2.1039581				
H	2.9150701	-5.3097124	-0.0895371				
H	3.3844354	-3.9935949	1.9939790				
H	2.9190795	-1.5338905	2.0240986				
H	5.8402491	3.2561553	-0.9836386				
H	7.0383987	3.2760518	-2.3262002				
H	7.4809337	3.9401810	-0.7110518				
H	7.2298098	-2.2969885	-0.2756287				
H	5.9231610	-1.4787273	0.6509430				
H	7.5457816	-1.7014624	1.3955408				
H	9.4799118	2.0442400	-1.2897927				
H	9.5331469	-0.5878876	-0.3428975				
H	-2.0112619	-0.3871059	1.3305080				
H	-4.3442149	0.0771865	2.1266582				
H	-5.7063165	1.8511590	1.0097607				
H	-4.7541852	3.1498458	-0.9027432				
H	3.7239373	3.9612098	-5.3042693				
H	2.1181424	5.3791251	-6.5617647				
H	-0.3172904	5.3695927	-5.9671941				

H	-1.1214185	3.9138615	-4.0993929			
H	0.1433688	4.4808559	0.5177105			
H	2.9227216	1.2220356	-3.1700459			
H	4.2366800	2.3458488	-3.6293998			
H	3.2595863	2.6314723	-2.1496389			
H	1.5940236	-2.1106613	-3.3463683			
H	0.2434652	-1.4952345	-2.3555865			
H	1.7096173	-0.5142785	-2.5323551			
Benzaldehyde (3a)						
TS-1 of 3a				Int-4 of 3a		
O	0.0186192	0.0179868	0.0125787	C	-4.7350693	4.8895264
C	2.1254098	0.0320117	0.0037628	C	-4.0840435	3.6274471
C	2.4494600	1.2736311	0.1041142	C	-3.5696101	3.2550457
Au	4.5475836	1.4773163	0.1954120	C	-3.6499007	4.1156335
C	6.5393095	1.8962027	0.2439957	C	-4.2478070	5.3773284
N	7.1139269	3.0868201	-0.0979197	C	-4.7847662	5.7459178
C	8.4903498	3.0239844	0.0588692	H	-3.0950425	2.2746105
C	8.7809315	1.7631201	0.5053753	H	-3.2464387	3.8127394
N	7.5742145	1.0878426	0.6127316	H	-4.2998176	6.0746784
C	1.6761461	2.5585799	0.2225289	H	-5.2514467	6.7306180
O	0.8546301	2.6850665	1.1306994	C	-5.3292952	5.3575416
C	2.3850634	-1.3536491	-0.2383011	H	-4.6056724	5.2826872
C	1.8749386	-2.3637395	0.6153832	H	-6.1842451	4.7252927
C	2.1830039	-3.7034466	0.3683909	H	-5.6656237	6.4033184
C	2.9988496	-4.0521364	-0.7232743	C	-3.8654339	2.7089236
C	3.5067222	-3.0572979	-1.5756229	O	-4.5510502	2.7648215
C	3.1983285	-1.7132076	-1.3449441	C	-2.7630973	1.6969819
C	6.3884358	4.2834983	-0.5405306	C	-1.4579121	2.0238278
C	7.4460530	-0.3053475	1.0515240	C	-0.2539832	1.1746627
C	-0.4738440	0.3809984	1.0979613	C	-0.1570042	0.0262522
C	-1.8374778	0.8945661	1.2213540	C	0.9629372	-0.8107959
C	-2.3215671	1.2532603	2.4993687	C	2.0137503	-0.5080547
C	-3.6202571	1.7559104	2.6365485	C	1.9408668	0.6468798
C	-4.4349837	1.9012610	1.5006790	C	0.8221555	1.4866956
C	-3.9560435	1.5464739	0.2242879	H	0.7739034	2.3791521
C	-2.6610401	1.0447246	0.0810004	H	2.8906472	-1.1615248
C	2.0095475	3.6382859	-0.7470003	H	2.7589619	0.8949465
C	1.6965159	5.0030642	-0.4735326	H	-0.9587004	-0.1942884
C	2.0817940	5.9623342	-1.4309610	H	1.0213490	-1.6946737
C	2.7231321	5.6058340	-2.6257868	Au	-3.4652655	-0.2380544
C	3.0013561	4.2575741	-2.9011326	C	-4.2028575	-2.1515839
C	2.6506801	3.2875969	-1.9592644	N	-3.4988458	-3.3181982
H	2.8601267	2.2325106	-2.1665525	N	-5.4940596	-2.5408232
H	3.0027728	6.3835921	-3.3445117	C	-5.5949798	-3.9234858
H	1.8701380	7.0184636	-1.2299825	C	-4.3342109	-4.4145699
H	3.4885116	3.9668288	-3.8370707	H	-6.5435638	-4.4340668
H	3.5846331	-0.9293522	-2.0036857	H	-3.9664378	-5.4377584
H	1.2434382	-2.0879118	1.4639202	C	-2.0493383	-3.4085057
H	1.7893763	-4.4817748	1.0296440	H	-1.5495386	-3.6456666
H	3.2373409	-5.1043029	-0.9104701	H	-1.6860852	-2.4409873
H	4.1392426	-3.3307199	-2.4260895	H	-1.8334869	-4.1956530
H	9.1380558	3.8712564	-0.1596402	C	-6.6309614	-1.6311271
H	9.7320251	1.2929912	0.7491699	H	-6.2562170	-0.5982457
H	5.3501568	4.0011797	-0.7691404	H	-7.1084933	-1.8156215
H	6.8684249	4.6852360	-1.4453998	H	-7.3612013	-1.7915102
H	6.3988566	5.0434022	0.2567548	O	-1.0923363	3.3905303
H	6.3799162	-0.5735060	1.0457817	C	-1.6026688	4.4216208
H	7.8483825	-0.4104960	2.0709238	C	-1.4965558	5.7174463
H	7.9981904	-0.9628797	0.3621925	C	-1.9641814	6.8297114
H	0.1155167	0.3012658	2.0336769	C	-1.9177587	8.1067886
H	-2.2661057	0.7651859	-0.9007820	C	-1.4119153	8.2840977
H	-1.6743670	1.1390606	3.3761089	C	-0.9487869	7.1872911
H	-3.9997878	2.0362015	3.6242392	C	-0.9888687	5.9048109
H	-5.4512839	2.2952077	1.6082114	H	-2.3581860	6.6743059
H	-4.5993977	1.6656349	-0.6534570	H	-2.2750428	8.9676952
C	0.9985192	5.4579301	0.7864510	H	-1.3825896	9.2883530
H	0.9768094	6.5587921	0.8337014	H	-0.5673637	7.3428965
H	-0.0363299	5.0765209	0.8225895	H	-0.6520674	5.0395303
H	1.4990830	5.0697160	1.6903833	H	-2.0915058	4.2726827
TS-4 of 3a						
O	0.8623765	1.6428802	-0.2528084			
C	2.0230851	1.1039538	1.0893130			
C	2.6007254	2.1174552	1.6724467			

C	2.2276671	3.5595679	1.5859847
C	3.1310968	4.4743867	0.8342819
C	4.2618666	3.9914467	0.1414115
C	5.0788279	4.8756814	-0.5740101
C	4.7721639	6.2466483	-0.5996311
C	3.6452920	6.7340317	0.0874056
C	2.8260050	5.8527284	0.8000198
C	-0.3707185	1.4050887	-0.2746497
C	-1.2376051	1.0728667	0.8386160
C	-2.4527917	0.4065248	0.5327789
C	-3.3101330	0.0131603	1.5627767
C	-2.9848979	0.3226475	2.8952756
C	-1.8067622	1.0308000	3.2011511
C	-0.9261852	1.4018637	2.1838784
Au	4.1598306	1.4127131	2.8715856
C	5.6762652	0.5840687	3.9597533
N	6.5676169	1.1849345	4.7997503
C	7.4449310	0.2514903	5.3319025
C	7.0928311	-0.9639356	4.8101206
N	6.0092320	-0.7417126	3.9735053
C	2.0756743	-0.3347602	0.9133316
C	2.8957715	-0.8840572	-0.1152750
C	2.9769814	-2.2835443	-0.2106296
C	2.2749352	-3.1184263	0.6738755
C	1.4715611	-2.5679755	1.6852882
C	1.3681650	-1.1783490	1.8017914
O	1.2063050	3.9547045	2.1540296
C	6.6021428	2.6178281	5.1080308
C	5.3348060	-1.7932895	3.2037497
C	3.6927798	0.0171228	-1.0258480
H	-2.7008674	0.1825410	-0.5103212
H	-3.6638846	0.0264959	3.7017827
H	-1.5833863	1.2983593	4.2385130
H	0.7563623	-0.7307055	2.5898042
H	2.3604960	-4.2057161	0.5740896
H	3.6073771	-2.7277792	-0.9887579
H	0.9305139	-3.2176766	2.3803732
H	1.9428847	6.2096305	1.3393087
H	4.4965482	2.9222109	0.1654642
H	5.9545832	4.4979339	-1.1115916
H	5.4127879	6.9384427	-1.1570618
H	3.4098482	7.8031869	0.0641112
H	8.2337923	0.5281315	6.0292730
H	7.5153456	-1.9557087	4.9617429
H	7.5771356	3.0364292	4.8138180
H	6.4415874	2.7691169	6.1868353
H	5.8004956	3.1128483	4.5415854
H	6.0320349	-2.2189736	2.4651806
H	4.4733310	-1.3490895	2.6834650
H	4.9861774	-2.5836399	3.8860347
H	-0.8366667	1.4410836	-1.2795200
H	-0.0354699	1.9951619	2.4092975
H	-4.2357082	-0.5229381	1.3322779
H	4.1533623	-0.5516726	-1.8486315
H	3.0639269	0.8176734	-1.4502048
H	4.5014262	0.5092432	-0.4521778

Anisaldehyde (3b)						
TS-1 of 3b				Int-4 of 3b		
O	0.1157215	0.2379220	-0.0446353	O	-2.2906411	-1.3271435
C	2.2435350	0.1629736	-0.0024583	C	-0.9449938	-1.3499202
C	2.6089587	1.3868436	0.1429584	C	-0.1953085	-0.1502087
Au	4.7077785	1.5243994	0.2268601	Au	1.8439536	-0.0129409
C	6.7207122	1.8413414	0.2722263	C	3.8366919	0.1749559
N	7.3698530	2.9578688	-0.1713961	N	4.5895610	1.3156027
C	8.7371492	2.8359044	0.0254101	C	5.8993926	1.0551311
C	8.9462967	1.6121572	0.6018018	C	5.9707732	-0.2834508
N	7.7009521	1.0189027	0.7455891	N	4.7026062	-0.8033164
C	1.8493346	2.6763279	0.3209971	C	-0.9781352	1.0089352
O	1.1491382	2.8140488	1.3223640	O	-2.3190877	0.9832084
C	2.4183066	-1.2310416	-0.2624344	C	-0.4345619	-2.7013316
C	2.0949798	-2.2011960	0.7198510	C	-1.1964196	-3.8179500
C	2.2947624	-3.5568750	0.4491493	C	-0.7180421	-5.1157756
C	2.8162432	-3.9589067	-0.7941345	C	0.5150076	-5.3216701
C	3.1385260	-3.0032873	-1.7727728	C	1.2676499	-4.2229433

C	2.9372621	-1.6434745	-1.5163780	C	0.7980039	-2.9221721	-1.3193479
C	6.7220564	4.1445994	-0.7420071	C	4.0903854	2.6418521	-0.0114636
C	7.4861798	-0.3161268	1.3125051	C	4.3480945	-2.2124639	0.9951011
C	-0.4038679	0.4548944	1.0704191	C	-2.7868676	-0.1275129	0.3483723
C	-1.7713424	0.9052535	1.2415298	C	-4.2755833	-0.1392535	0.3958880
C	-2.2797084	1.1072421	2.5455019	C	-4.9407959	-0.0247316	1.6267816
C	-3.5875592	1.5480359	2.7473300	C	-6.3410139	-0.0289443	1.6920958
C	-4.4139733	1.7958218	1.6249862	C	-7.0897446	-0.1499635	0.5025483
C	-3.9115090	1.5978587	0.3101834	C	-6.4215541	-0.2646963	-0.7411685
C	-2.6106002	1.1600291	0.1233654	C	-5.0310450	-0.2587953	-0.7918694
C	2.0450284	3.7275982	-0.7139659	C	-0.4683502	2.3082931	-1.0559990
C	1.6011398	5.0684514	-0.5040869	C	-0.9819970	3.5396907	-0.5436994
C	1.8508255	6.0039825	-1.5274247	C	-0.3983404	4.7312651	-1.0140024
C	2.4930613	5.6483693	-2.7220085	C	0.6286337	4.7312732	-1.9690527
C	2.9069564	4.3234582	-2.9312732	C	1.1128542	3.5181096	-2.4837897
C	2.6828377	3.3778193	-1.9282231	C	0.5710114	2.3177004	-2.0210605
H	2.9963274	2.3401351	-2.0854549	H	0.9235369	1.3648616	-2.4270000
H	2.6665561	6.4079700	-3.4918664	H	1.0499380	5.6822906	-2.3118613
H	1.5302566	7.0412374	-1.3789749	H	-0.7572635	5.6851912	-0.6123911
H	3.3978534	4.0316296	-3.8649738	H	1.9029988	3.5080440	-3.2409315
H	3.1820636	-0.8890430	-2.2700810	H	1.3682472	-2.0677915	-1.6973394
H	1.6942291	-1.8797402	1.6854006	H	-2.1483305	-3.6531088	0.2868775
H	2.0476866	-4.3056703	1.2083594	H	-1.3042033	-5.9713459	-0.0756035
H	2.9720652	-5.0230842	-0.9999953	H	0.8869627	-6.3398299	-1.2240967
H	3.5447190	-3.3203795	-2.7385104	H	2.2171414	-4.3834786	-2.0398476
H	9.4362745	3.6203010	-0.2594074	H	6.6601400	1.8336058	0.7751734
H	9.8639679	1.1168550	0.9141225	H	6.8054166	-0.9021137	1.3414291
H	5.6835537	3.8885491	-0.9988475	H	3.0497019	2.5379632	-0.3513077
H	7.2620034	4.4513011	-1.6502364	H	4.7059007	3.0504017	-0.8279803
H	6.7292948	4.9655786	-0.0075181	H	4.1303301	3.3172243	0.8578662
H	6.4047141	-0.5119638	1.3378803	H	3.3152835	-2.3601348	0.6480452
H	7.8927212	-0.3525015	2.3348892	H	4.4194851	-2.4744699	2.0626757
H	7.9854589	-1.0706532	0.6848108	H	5.0305524	-2.8482313	0.4101481
H	0.1868553	0.3002884	1.9970832	H	-2.3151870	-0.0442096	1.3465875
H	-2.2128928	1.0069582	-0.8847384	H	-4.5211334	-0.3478192	-1.7564523
H	-1.6360190	0.9168944	3.4116769	H	-4.3638740	0.0689656	2.5537379
H	-3.9579546	1.6978637	3.7638319	H	-6.8323236	0.0610689	2.6634727
H	-4.5756149	1.8006839	-0.5352071	H	-7.0229120	-0.3569975	-1.6505934
C	0.8962066	5.5255671	0.7510573	C	-2.0699644	3.6179111	0.5058761
H	0.7179298	6.6126003	0.7122994	H	-2.1008122	4.6278038	0.9453951
H	-0.0696402	5.0061178	0.8740391	H	-3.0602400	3.3997283	0.0697307
H	1.4854578	5.2893858	1.6539445	H	-1.9073292	2.8902652	1.3194829
O	-5.6896482	2.2227812	1.7007096	O	-8.4444418	-0.1670189	0.4465473
C	-6.2838492	2.4521136	2.9904830	C	-9.1910276	-0.0544175	1.6662827
H	-5.7357345	3.2377172	3.5401695	H	-8.9803810	0.9049173	2.1734769
H	-7.3100839	2.7868216	2.7863600	H	-10.2491570	-0.0920348	1.3720052
H	-6.3046436	1.5207902	3.5837483	H	-8.9649992	-0.8937753	2.3489416
TS-4 of 3b							
O	0.2292067	0.4436019	0.1299387				
C	2.2857447	0.2671763	0.0701513				
Au	4.8835263	1.2216096	0.0571683				
O	2.4010673	3.5587003	-0.8700688				
C	2.1944609	2.8263910	0.0966705				
C	1.3310143	3.2354040	1.2425098				
C	1.1905625	2.4466290	2.4037061				
C	0.3183347	2.8495898	3.4218614				
C	-0.4236783	4.0345883	3.2837164				
C	-0.2843932	4.8275023	2.1307774				
C	0.5937022	4.4343181	1.1172674				
C	2.7975144	1.4535577	0.1197637				
C	6.9092426	0.9875212	0.0258102				
N	7.5930023	-0.1855423	0.1763488				
C	8.9603453	0.0349763	0.1018594				
C	9.1337843	1.3775760	-0.0991676				
N	7.8681459	1.9430875	-0.1430352				
C	2.3937252	-1.1616075	0.1040234				
C	2.0843353	-1.9488713	-1.0425434				
C	2.2920957	-3.3360021	-0.9560538				
C	2.7802708	-3.9311614	0.2174985				
C	3.0732052	-3.1477332	1.3470322				
C	2.8734336	-1.7667303	1.2941276				
C	1.5363637	-1.3140674	-2.2946324				
C	-0.2902226	1.3012316	-0.6207731				
C	-1.5158970	1.9956056	-0.3101238				
C	-1.9991261	2.9847825	-1.2008792				

C	-3.1226633	3.7449896	-0.8854611				
C	-3.7848799	3.5199907	0.3467858				
C	-3.3133314	2.5218260	1.2427329				
C	-2.1961966	1.7729676	0.9191771				
H	-1.4734277	3.1649420	-2.1451192				
O	-4.8658586	4.2049365	0.7611120				
C	-5.4124284	5.2437339	-0.0724836				
H	-3.8460641	2.3791387	2.1872137				
C	6.9833879	-1.5042467	0.3789794				
C	7.6126871	3.3730383	-0.3435109				
H	3.1013050	-1.1343212	2.1577716				
H	2.9334371	-5.0150733	0.2501987				
H	2.0713396	-3.9618964	-1.8275927				
H	3.4548178	-3.6122420	2.2616231				
H	0.7102448	5.0289779	0.2061636				
H	1.7575458	1.5164624	2.5036006				
H	0.2102124	2.2358668	4.3219447				
H	-1.1167061	4.3393159	4.0751252				
H	-0.8680759	5.7475052	2.0234871				
H	9.6841097	-0.7725717	0.1974730				
H	10.0385761	1.9722660	-0.2122043				
H	5.8934336	-1.3770524	0.4525630				
H	7.3670807	-1.9487021	1.3102045				
H	7.2222633	-2.1591837	-0.4734801				
H	8.0865107	3.9504585	0.4654152				
H	6.5257297	3.5366387	-0.3274703				
H	8.0204687	3.6888123	-1.3162630				
H	0.2286319	1.5936307	-1.5585980				
H	-1.8098537	1.0182258	1.6100744				
H	-3.4742050	4.5083609	-1.5827651				
H	-5.7513828	4.8312564	-1.0389082				
H	-6.2699599	5.6456127	0.4838971				
H	-4.6675787	6.0414219	-0.2414169				
H	1.7044760	-1.9561735	-3.1738396				
H	0.4468906	-1.1545317	-2.1951251				
H	1.9958484	-0.3267279	-2.4780602				
<i>m</i>-Anisaldehyde (3c)							
TS-1 of 3c				Int-4 of 3c			
O	0.1387918	0.1345403	-0.1130750	O	-2.2906802	-1.3239454	-0.2731742
C	2.2146657	0.1021775	-0.0314611	C	-0.9428976	-1.3449409	-0.4063559
C	2.5561218	1.3336757	0.1308426	C	-0.1943943	-0.1451237	-0.3858815
Au	4.6497078	1.5150383	0.2378719	Au	1.8442373	-0.0134721	-0.0338223
C	6.6601825	1.8470029	0.2984418	C	3.8374162	0.1674324	0.4123249
N	7.3112178	2.9543200	-0.1649635	N	4.5804644	1.3149006	0.4315056
C	8.6775904	2.8380406	0.0427854	C	5.8960543	1.0455843	0.7798191
C	8.8841448	1.6274589	0.6467816	C	5.9810629	-0.3051614	0.9828383
N	7.6384277	1.0361179	0.7956337	N	4.7149930	-0.8236834	0.7527695
C	1.7552750	2.5987608	0.3040804	C	-0.9748619	1.0126657	-0.6101727
O	1.0011179	2.6940589	1.2724563	O	-2.3181875	0.9873581	-0.4737836
C	2.4550009	-1.2838237	-0.2945825	C	-0.4295489	-2.6973183	-0.6286229
C	2.1585763	-2.2708030	0.6787054	C	-1.1809202	-3.8105984	-0.1721518
C	2.4223120	-3.6153107	0.4070725	C	-0.6974400	-5.1087785	-0.3576304
C	2.9794331	-3.9890330	-0.8290970	C	0.5285026	-5.3180976	-1.0127796
C	3.2744322	-3.0164018	-1.7991738	C	1.2697295	-4.2228107	-1.4905735
C	3.0109091	-1.6677119	-1.5412269	C	0.7962320	-2.9214926	-1.3042367
C	6.6667900	4.1266556	-0.7686428	C	4.0666575	2.6553338	0.1331436
C	7.4215360	-0.2864087	1.3904742	C	4.3737507	-2.2440162	0.8745071
C	-0.3927742	0.3633181	0.9901843	C	-2.7968526	-0.1167330	0.3173194
C	-1.7599223	0.8612982	1.1255761	C	-4.2941427	-0.1312667	0.3131667
C	-2.2793009	1.0360588	2.4215333	C	-4.9786606	0.0009683	1.5259206
C	-3.5880606	1.5260565	2.5952528	C	-6.3909640	-0.0057711	1.5427630
C	-4.3633180	1.8382543	1.4573866	C	-7.0988407	-0.1467499	0.3320887
C	-3.8302119	1.6599438	0.1659553	C	-6.3925934	-0.2765079	-0.8769720
C	-2.5364134	1.1744834	-0.0163031	C	-4.9947629	-0.2700569	-0.9027718
C	1.9676954	3.6794269	-0.6958768	C	-0.4623188	2.3089743	-1.0699114
C	1.4990571	5.0084949	-0.4667621	C	-0.9898612	3.5439308	-0.5799426
C	1.7607677	5.9703999	-1.4621080	C	-0.4003134	4.7325826	-1.0500649
C	2.4365654	5.6508179	-2.6481683	C	0.6444787	4.7266731	-1.9854637
C	2.8739719	4.3369322	-2.8772066	C	1.1422681	3.5101948	-2.4790976
C	2.6404371	3.3663068	-1.9010571	C	0.5950724	2.3127594	-2.0155513
H	2.9712179	2.3365717	-2.0743442	H	0.9562575	1.3573493	-2.4076223
H	2.6178916	6.4299059	-3.3963971	H	1.0685538	5.6756973	-2.3302479
H	1.4227173	6.9998608	-1.2987076	H	-0.7689196	5.6891570	-0.6638497
H	3.3905082	4.0729170	-3.8052328	H	1.9466536	3.4953156	-3.2209809

H	3.2344298	-0.9002780	-2.2882547	H	1.3562325	-2.0700049	-1.7033757
H	1.7299277	-1.9716051	1.6395342	H	-2.1279447	-3.6426246	0.3475501
H	2.1969161	-4.3769765	1.1600800	H	-1.2737356	-5.9616508	0.0146962
H	3.1847541	-5.0445371	-1.0362465	H	0.9033815	-6.3366637	-1.1582338
H	3.7084527	-3.3117659	-2.7596138	H	2.2131672	-4.3866658	-2.0208464
H	9.3776779	3.6165845	-0.2550468	H	6.6505699	1.8273129	0.8494849
H	9.8004580	1.1399395	0.9750325	H	6.8239622	-0.9337376	1.2649807
H	5.6289911	3.8651459	-1.0221202	H	3.0248191	2.5603828	-0.2058488
H	7.2099395	4.4087491	-1.6829777	H	4.6732821	3.1140323	-0.6630225
H	6.6729550	4.9668331	-0.0561195	H	4.1062870	3.2820427	1.0381782
H	6.3402381	-0.4827933	1.4128008	H	3.3371987	-2.3815317	0.5339662
H	7.8208013	-0.2996833	2.4161646	H	4.4617286	-2.5622089	1.9254271
H	7.9265099	-1.0538915	0.7833118	H	5.0529642	-2.8419814	0.2472997
H	0.1666460	0.1758854	1.9287587	H	-2.3572083	-0.0222393	1.3288611
H	-2.1101394	1.0348665	-1.0135165	H	-4.4492640	-0.3713169	-1.8453778
H	-1.6788486	0.8002869	3.3059027	H	-4.4426794	0.1099767	2.4741118
H	-4.4501481	1.9109288	-0.7007954	H	-6.9546289	-0.3836461	-1.8106568
C	0.7573542	5.4265366	0.7806675	C	-2.1010106	3.6305211	0.4441687
H	0.5694282	6.5123844	0.7655996	H	-2.1402202	4.6432576	0.8758668
H	-0.2062301	4.8953047	0.8643898	H	-3.0812352	3.4117661	-0.0134094
H	1.3259550	5.1735964	1.6924226	H	-1.9589020	2.9079397	1.2659101
H	-5.3811331	2.2222676	1.5631386	H	-8.1914625	-0.1574765	0.3184732
O	-4.0070877	1.6660311	3.8799932	O	-6.9672394	0.1272751	2.7672138
C	-5.3351216	2.1503966	4.1224966	C	-8.3977289	0.1423720	2.8558981
H	-5.4517603	2.1644852	5.2152262	H	-8.8290968	-0.8111202	2.4988554
H	-5.4646797	3.1727645	3.7221010	H	-8.6290331	0.2751912	3.9222639
H	-6.0912700	1.4784384	3.6766930	H	-8.8242073	0.9819303	2.2764564
TS-4 of 3c							
O	0.3151685	0.4957214	0.2058573				
C	2.2828934	0.3409800	0.1330960				
Au	4.9161301	1.2391243	0.0748568				
O	2.5510116	3.6552327	-0.7715749				
C	2.2677901	2.9001024	0.1583610				
C	1.3328327	3.2974651	1.2529275				
C	1.1601111	2.5228317	2.4200425				
C	0.2178996	2.9061346	3.3809044				
C	-0.5640041	4.0567174	3.1792099				
C	-0.3894285	4.8385367	2.0241041				
C	0.5610288	4.4667320	1.0688614				
C	2.8391140	1.5143131	0.1790677				
C	6.9334393	0.9473201	-0.0065809				
N	7.5856628	-0.2454893	0.1299598				
C	8.9566917	-0.0664268	0.0205666				
C	9.1652040	1.2698997	-0.1889272				
N	7.9163136	1.8729684	-0.2028244				
C	2.4280481	-1.0910860	0.1584520				
C	2.1198726	-1.8786595	-0.9868056				
C	2.3616507	-3.2614720	-0.9118859				
C	2.8817856	-3.8514593	0.2502423				
C	3.1739154	-3.0668156	1.3788241				
C	2.9412665	-1.6900767	1.3361543				
C	1.5469130	-1.2495209	-2.2316206				
C	-0.2292461	1.3562738	-0.5182946				
C	-1.5357826	1.9215505	-0.2317278				
C	-2.0493219	2.8871598	-1.1214247				
C	-3.2739494	3.5195224	-0.8387528				
C	-3.9707022	3.1733823	0.3410531				
C	-3.4473019	2.2054248	1.2198017				
C	-2.2368760	1.5708985	0.9495479				
H	-1.5027713	3.1660531	-2.0277646				
H	-4.9201608	3.6553051	0.5870651				
H	-4.0043168	1.9611130	2.1297987				
C	6.9418926	-1.5448420	0.3508946				
C	7.6984701	3.3094971	-0.4002894				
H	3.1683702	-1.0569510	2.1995077				
H	3.0614383	-4.9315329	0.2743029				
H	2.1437654	-3.8870642	-1.7844111				
H	3.5807700	-3.5263653	2.2850451				
H	0.7060724	5.0531373	0.1563379				
H	1.7572756	1.6180516	2.5681980				
H	0.0849088	2.3037097	4.2852116				
H	-1.3139045	4.3431716	3.9241703				
H	-1.0023346	5.7320504	1.8677262				
H	9.6582241	-0.8950405	0.1005568				
H	10.0842953	1.8368449	-0.3265585				

H	5.8577123	-1.3859782	0.4450049
H	7.3306127	-1.9965749	1.2765801
H	7.1449933	-2.2101414	-0.5028453
H	8.1995173	3.8737838	0.4015410
H	6.6168289	3.5033352	-0.3693971
H	8.1015091	3.6134222	-1.3787603
H	0.3109901	1.7454836	-1.4061744
H	-1.8101774	0.8315824	1.6318418
H	1.7196773	-1.8850752	-3.1146932
H	0.4549438	-1.1111333	-2.1255264
H	1.9879810	-0.2539974	-2.4167831
O	-3.6948693	4.4391131	-1.7430860
C	-4.9259496	5.1349230	-1.5008074
H	-4.8761492	5.7145176	-0.5605744
H	-5.0515947	5.8204184	-2.3505208
H	-5.7785935	4.4324512	-1.4611121

***p*-(Dimethylamino)benzaldehyde (3d)**

TS-1 of 3d				Int-3 of 3d			
O	-0.0005295	-0.0456992	-0.1161889	O	-1.5612829	0.0375380	1.7003769
C	2.2237086	-0.0570036	-0.0831176	C	-0.1300155	0.1619395	1.4925929
Au	4.6243401	0.3948483	-1.3168200	Au	2.2869325	0.2658201	-0.3941343
C	2.5483050	0.6655757	-1.0901196	C	0.3234835	0.3585366	0.2288358
C	1.8395932	1.6996462	-1.9291945	C	-0.6240539	0.6219286	-0.9040944
C	0.9615945	1.2122797	-3.0227537	C	-1.5524704	-0.4687536	-1.3456581
C	0.1404284	2.1133885	-3.7691231	C	-2.6864362	-0.1973671	-2.1698227
C	-0.6864001	1.5637503	-4.7666130	C	-3.5452569	-1.2708483	-2.4768767
C	-0.7115099	0.1888115	-5.0377393	C	-3.3034022	-2.5727148	-2.0167897
C	0.0987928	-0.6892115	-4.3019972	C	-2.1792610	-2.8366301	-1.2195687
C	0.9235193	-0.1738952	-3.2999625	C	-1.3200405	-1.7857927	-0.8857228
H	-1.8416175	3.4567859	-0.1893795	H	-4.1389394	2.8792186	0.6310033
C	-2.2799783	2.7031622	-0.8540583	C	-4.5470104	1.8633935	0.6471557
C	-1.7394013	1.3907713	-0.8708546	C	-3.7026610	0.7747631	1.0421181
C	-0.5614550	1.0733211	-0.1036777	C	-2.3520207	1.0112730	1.3110554
C	-2.3301816	0.4310233	-1.7370468	C	-4.2586393	-0.5474857	1.0581999
C	-3.3838055	0.7671564	-2.5654476	C	-5.5618258	-0.7697856	0.6867296
C	-3.9107745	2.1026669	-2.5800743	C	-6.4098125	0.3214553	0.2721273
C	-3.3351259	3.0581360	-1.6800082	C	-5.8552198	1.6510079	0.2772467
C	2.3752983	-0.9003827	1.0562334	C	0.5998579	-0.0829613	2.7490628
C	3.2526000	-0.4985370	2.0980375	C	1.8855335	0.4669281	2.9598167
C	3.4742882	-1.3485206	3.1862180	C	2.5974717	0.1910042	4.1335387
C	2.8121490	-2.5857182	3.2592649	C	2.0344102	-0.6253960	5.1285558
C	1.9270921	-2.9797790	2.2383997	C	0.7457600	-1.1518706	4.9436312
C	1.7077845	-2.1492527	1.1376802	C	0.0298023	-0.8795614	3.7703724
N	-4.9200454	2.4509103	-3.4314198	N	-7.6841502	0.0986563	-0.1226615
H	-3.7946424	0.0076845	-3.2331359	H	-5.9442096	-1.7914656	0.6874474
C	6.6313157	0.1602665	-1.5822090	C	4.2268662	0.1106375	-1.0612333
N	7.4140306	0.6897514	-2.5660141	N	4.6870198	0.2579545	-2.3398898
C	8.7329063	0.2914680	-2.4064567	C	6.0615597	0.0813681	-2.3947222
C	8.7735758	-0.5061563	-1.2951423	C	6.4757466	-0.1822646	-1.1171551
N	7.4787674	-0.5736254	-0.8026044	N	5.3420272	-0.1627811	-0.3183488
C	6.9442654	1.5634534	-3.6460459	C	3.8489182	0.5420408	-3.5084891
C	7.0878396	-1.3530773	0.3767251	C	5.3564267	-0.3712623	1.1325678
C	0.1063126	3.6031845	-3.5303712	C	-3.0223305	1.1770653	-2.7000940
O	2.0248346	2.8822730	-1.6505448	O	-0.6040981	1.7357163	-1.4477363
H	1.5527401	-0.8489423	-2.7124503	H	-0.4426203	-1.9780120	-0.2599361
H	-1.3729634	-0.1978094	-5.8205919	H	-3.9951308	-3.3802223	-2.2804871
H	-1.3337001	2.2366204	-5.3399010	H	-4.4303679	-1.0745827	-3.0928216
H	0.0836688	-1.7647722	-4.5043850	H	-1.9762760	-3.8503823	-0.8594292
H	1.0168796	-2.4375014	0.3416023	H	-0.9716835	-1.2980775	3.6347654
H	3.7587287	0.4694025	2.0302174	H	2.3140144	1.1307389	2.2011750
H	4.1590476	-1.0423583	3.9835370	H	3.5906072	0.6298379	4.2787004
H	2.9826565	-3.2452111	4.1166306	H	2.5906327	-0.8380973	6.0476718
H	1.4100245	-3.9424081	2.3036549	H	0.2938004	-1.7818831	5.7173271
H	9.5205793	0.6090291	-3.0874712	H	6.6202126	0.1531111	-3.3263738
H	9.6031818	-1.0239795	-0.8169468	H	7.4673285	-0.3812621	-0.7141278
H	5.8631606	1.7192492	-3.5214717	H	2.8166420	0.6974711	-3.1635063
H	7.1401029	1.0866765	-4.6189513	H	3.8821917	-0.3086890	-4.2073836
H	7.4661598	2.5313420	-3.5919242	H	4.2121425	1.4513063	-4.0120111
H	6.0499940	-1.0978835	0.6355022	H	4.3222013	-0.5197768	1.4738482
H	7.7508440	-1.1005496	1.2179505	H	5.7895713	0.5085666	1.6354086
H	7.1587849	-2.4295266	0.1545254	H	5.9544845	-1.2645212	1.3679214
H	-0.1170036	1.9054718	0.4887264	H	-1.8999224	2.0038466	1.1760867
H	-1.9117839	-0.5797505	-1.7601186	H	-3.6183815	-1.3888215	1.3365257
H	-3.7111917	4.0823932	-1.6484513	H	-6.4655142	2.5032210	-0.0248517

H	-0.6355783	4.0765371	-4.1939859	H	-4.0003562	1.1590859	-3.2088866
H	-0.1546378	3.8316605	-2.4835880	H	-3.0542884	1.9249552	-1.8898236
H	1.0948883	4.0604086	-3.7083356	H	-2.2531834	1.5299169	-3.4077535
C	-5.4410977	3.8194764	-3.4446571	C	-8.5410776	1.2110417	-0.5586118
C	-5.4805374	1.4689013	-4.3624430	C	-8.2395763	-1.2627608	-0.1442398
H	-4.6490855	4.5473728	-3.7010736	H	-8.1090946	1.7162231	-1.4400125
H	-6.2349172	3.8879542	-4.2005630	H	-9.5256329	0.8092164	-0.8292105
H	-5.8674221	4.0955043	-2.4628360	H	-8.6689863	1.9478136	0.2530625
H	-6.2619634	1.9561647	-4.9610057	H	-9.2793789	-1.2105128	-0.4909159
H	-4.7054701	1.0802200	-5.0486851	H	-7.6683507	-1.9083552	-0.8341246
H	-5.9329529	0.6164144	-3.8236055	H	-8.2239218	-1.7092248	0.8647768
TS-2 of 3d				Int-4 of 3d			
O	-0.0247745	-0.0317360	-0.3736171	O	-1.0535669	-1.9952627	-0.4165395
C	1.9931707	-0.0290983	-0.0721889	C	0.0239056	-2.5430813	0.3896381
Au	-0.6111881	4.0386257	0.1740966	Au	0.0996323	2.1085968	0.1481365
C	1.7534428	2.2263451	-0.6750718	C	1.3299212	-0.7205423	-0.2890865
C	2.7849898	3.2684543	-0.7515759	C	2.7053232	-0.2532120	-0.4777203
C	2.4566090	4.6107078	-1.0626010	C	2.9875214	0.9848770	-1.1067466
C	3.4460406	5.5987077	-1.0876818	C	4.3090363	1.4135271	-1.2580795
C	4.7855706	5.2653275	-0.8231204	C	5.3676710	0.6142913	-0.7915940
C	5.1296558	3.9326971	-0.5431135	C	5.1006703	-0.6249608	-0.1844113
C	4.1427093	2.9405196	-0.5127729	C	3.7816799	-1.0628121	-0.0335932
C	0.4057975	2.3454521	-0.4522876	C	0.1612026	0.0760625	-0.2523425
C	-0.4328384	1.1401989	-0.6000335	C	-1.0261862	-0.6505935	-0.5040284
O	2.3081310	0.9407561	-0.9353356	O	1.2520109	-2.0677276	-0.1985422
C	-1.7225208	5.6281042	0.8439832	C	-0.0270320	4.0987391	0.6283138
N	-3.0863867	5.6826000	0.9316586	N	-1.1609668	4.8603659	0.6907520
C	-3.5013452	6.9179473	1.4067943	C	-0.8588704	6.1685858	1.0399253
C	-2.3699069	7.6574278	1.6227286	C	0.4990011	6.2301064	1.1990609
N	-1.2947812	6.8527751	1.2737916	N	0.9887431	4.9573598	0.9434087
C	-1.8546368	1.3001549	-1.0363845	C	-2.3037512	-0.0662102	-0.9359160
C	-2.9014547	0.5487582	-0.4337774	C	-3.5535779	-0.5438767	-0.4346014
C	-4.2144437	0.7740440	-0.8940982	C	-4.7212691	0.1085579	-0.8737010
C	-4.4902983	1.6707585	-1.9363599	C	-4.6815286	1.1701931	-1.7891866
C	-3.4461739	2.3861268	-2.5438116	C	-3.4510238	1.6195658	-2.2939153
C	-2.1386602	2.2111073	-2.0803056	C	-2.2728515	1.0080947	-1.8608072
C	-2.6596134	-0.4413787	0.6843598	C	-3.6720448	-1.6663977	0.5740092
C	2.3964384	-1.3606664	-0.3721567	C	-0.0266853	-4.0247426	0.3959656
C	2.3132720	-2.3596704	0.6368511	C	-0.3095251	-4.7227149	1.5862111
C	2.6662753	-3.6723073	0.3780264	C	-0.3878170	-6.1144986	1.6069844
C	3.1244731	-4.0659003	-0.9238325	C	-0.1817904	-6.8771396	0.4171107
C	3.2023394	-3.0519581	-1.9389292	C	0.1075293	-6.1560774	-0.7847263
C	2.8430786	-1.7447451	-1.6676042	C	0.1785005	-4.7663946	-0.7870910
H	1.9633834	-2.0861726	1.6382636	H	-0.4723212	-4.1673355	2.5171115
H	3.5453570	-3.3054571	-2.9436519	H	0.2765564	-6.6911392	-1.7214842
N	3.4722548	-5.3558855	-1.1893601	N	-0.2567516	-8.2485943	0.4241345
C	-3.9959736	4.5893860	0.5732895	C	-2.5180838	4.3710685	0.4288023
C	0.1069768	7.2738371	1.3486015	C	2.4078991	4.5956416	1.0015851
H	-1.3160545	2.7717512	-2.5362685	H	-1.3075210	1.3337188	-2.2599680
H	-5.5233331	1.8127252	-2.2715983	H	-5.6148438	1.6458217	-2.1087172
H	-5.0387025	0.2279293	-0.4214816	H	-5.6877055	-0.2234962	-0.4787133
H	-3.6498697	3.0833411	-3.3627803	H	-3.4100430	2.4372578	-3.0202193
H	4.4183621	1.9069296	-0.2856032	H	3.5685749	-2.0199149	0.4498957
H	1.4195973	4.8656545	-1.3053917	H	2.1644387	1.5920428	-1.4965001
H	3.1744843	6.6308088	-1.3329750	H	4.5170894	2.3679979	-1.7520111
H	5.5598836	6.0394182	-0.8477090	H	6.4020424	0.9545617	-0.9079025
H	6.1724048	3.6649132	-0.3433426	H	5.9248104	-1.2480488	0.1772785
H	-4.5525169	7.1625462	1.5499430	H	-1.6256323	6.9345341	1.1431073
H	-2.2401984	8.6738787	1.9904957	H	1.1500179	7.0602899	1.4677536
H	-3.3949943	3.7361019	0.2269469	H	-2.4521546	3.3218312	0.1060988
H	-4.6682634	4.9149680	-0.2357108	H	-2.9806292	4.9732089	-0.3687294
H	-4.5885754	4.2948632	1.4535177	H	-3.1245410	4.4404750	1.3456875
H	0.7382308	6.4282465	1.0395999	H	2.5049512	3.5329452	0.7359298
H	0.3543948	7.5611038	2.3824520	H	2.7930882	4.7581482	2.0204635
H	0.2757882	8.1289883	0.6750732	H	2.9775341	5.2101688	0.2867955
H	1.8059684	0.2773097	0.9643485	H	-0.0640008	-2.0951359	1.3981699
H	2.9048913	-0.9905651	-2.4579537	H	0.4010057	-4.2436185	-1.7233840
H	2.5911252	-4.4069386	1.1815510	H	-0.6085738	-6.6128917	2.5530336
H	-3.6107774	-0.7130051	1.1701280	H	-4.6793618	-1.6710018	1.0201064
H	-2.1881218	-1.3611917	0.2972984	H	-3.4985530	-2.6477623	0.0998495
H	-1.9760475	-0.0348172	1.4495722	H	-2.9327092	-1.5658864	1.3871039
C	3.3871570	-6.3797970	-0.1436659	C	-0.5524704	-8.9625940	1.6640497
C	3.9384215	-5.7437792	-2.5242512	C	-0.0375690	-9.0071440	-0.8056121
H	2.3515222	-6.4854712	0.2272000	H	-1.5378965	-8.6708546	2.0749409
H	3.7063215	-7.3417525	-0.5660301	H	-0.5708848	-10.0414743	1.4564974

H	4.0457668	-6.1345658	0.7092631	H	0.2159435	-8.7702579	2.4371889
H	3.1660731	-5.5462103	-3.2894564	H	-0.7743781	-8.7375584	-1.5861154
H	4.1587229	-6.8194790	-2.5207679	H	-0.1457344	-10.0781040	-0.5847911
H	4.8587046	-5.1975684	-2.7999234	H	0.9773662	-8.8372669	-1.2130432
TS-3 of 3d				Int-5 of 3d			
O	-0.0247745	-0.0317360	-0.3736171	O	-1.5910916	-1.2947110	-0.0848742
C	1.9931707	-0.0290983	-0.0721889	C	-0.1776608	-1.0229959	0.0088690
Au	-0.6111881	4.0386257	0.1740966	Au	2.3302190	0.6139498	-0.0530040
C	1.7534428	2.2263451	-0.6750718	O	-0.4351813	2.2296052	-1.1313100
C	2.7849898	3.2684543	-0.7515759	C	-0.5925063	1.4353557	-0.1939323
C	2.4566090	4.6107078	-1.0626010	C	-1.6827493	1.6605568	0.8185515
C	3.4460406	5.5987077	-1.0876818	C	-1.7368284	0.9650354	2.0450337
C	4.7855706	5.2653275	-0.8231204	C	-2.8116820	1.1658578	2.9210341
C	5.1296558	3.9326971	-0.5431135	C	-3.8428235	2.0558262	2.5773232
C	4.1427093	2.9405196	-0.5127729	C	-3.7897758	2.7612987	1.3623288
C	0.4057975	2.3454521	-0.4522876	C	-2.7105801	2.5720186	0.4930903
C	-0.4328384	1.1401989	-0.6000335	C	0.2981911	0.2473293	-0.0489070
O	2.3081310	0.9407561	-0.9353356	C	4.3602905	0.9340085	-0.0897515
C	-1.7225208	5.6281042	0.8439832	N	5.3414812	-0.0085428	0.0510548
N	-3.0863867	5.6826000	0.9316586	C	6.5989604	0.5708160	-0.0330387
C	-3.5013452	6.9179473	1.4067943	C	6.4025898	1.9107132	-0.2316760
C	-2.3699069	7.6574278	1.6227286	N	5.0305438	2.1123145	-0.2641705
N	-1.2947812	6.8527751	1.2737916	C	0.5742183	-2.2732670	0.6242104
C	-1.8546368	1.3001549	-1.0363845	C	0.4977852	-3.3789051	-0.6252575
C	-2.9014547	0.5487582	-0.4337774	C	1.2640388	-4.5230103	-0.3301514
C	-4.2144437	0.7740440	-0.8940982	C	2.0820034	-4.5870786	0.8076157
C	-4.4902983	1.6707585	-1.9363599	C	2.1508374	-3.4927702	1.6834614
C	-3.4461739	2.3861268	-2.5438116	C	1.3988070	-2.3443906	1.4088475
C	-2.1386602	2.2111073	-2.0803056	C	-0.3460495	-3.3283038	-1.8802425
C	-2.6596134	-0.4413787	0.6843598	C	-2.3226552	-0.6838624	-0.9927968
C	2.3964384	-1.3606664	-0.3721567	C	-3.7073262	-0.5807818	-0.8541250
C	2.3132720	-2.3596704	0.6368511	C	-4.4706097	0.0590055	-1.8852384
C	2.6662753	-3.6723073	0.3780264	C	-5.8271785	0.2448363	-1.7548771
C	3.1244731	-4.0659003	-0.9238325	C	-6.5190701	-0.2001151	-0.5717452
C	3.2023394	-3.0251981	-1.9389292	C	-5.7485380	-0.8468521	0.4625729
C	2.8430786	-1.7447451	-1.6676042	C	-4.3939872	-1.0280529	0.3237026
H	1.9633834	-2.0861726	1.6382636	H	-3.9605439	0.4121513	-2.7873025
H	3.5453570	-3.3054571	-2.9436519	N	-7.8504038	-0.0099073	-0.4292413
N	3.4722548	-5.3558855	-1.1893601	H	-6.2360978	-1.1872965	1.3772942
C	-3.9959736	4.5893860	0.5732895	C	5.1086173	-1.4416044	0.2542070
C	0.1069768	7.2738371	1.3486015	C	4.3958316	3.4197516	-0.4535622
H	-1.3160545	2.7717512	-2.5362685	H	1.4370607	-1.4838578	2.0852110
H	-5.5233331	1.8127252	-2.2715983	H	2.6675406	-5.4910798	1.0071123
H	-5.0387025	0.2279293	-0.4214816	H	1.2273743	-5.3760509	-1.0175526
H	-3.6498697	3.0833411	-3.3627803	H	2.7839036	-3.5330541	2.5760128
H	4.4183621	1.9069296	-0.2856032	H	-2.6507018	3.1034257	-0.4620253
H	1.4195973	4.8656545	-1.3053917	H	-0.9364500	0.2674019	2.3110693
H	3.1744843	6.6308088	-1.3329750	H	-2.8476474	0.6253875	3.8727736
H	5.5598836	6.0394182	-0.8477090	H	-4.6890039	2.2005613	3.2577629
H	6.1724048	3.6649132	-0.3433426	H	-4.5944605	3.4542916	1.0944370
H	-4.5525169	7.1625462	1.5499430	H	7.5144053	-0.0119772	0.0540658
H	-2.2401984	8.6738787	1.9904957	H	7.1130509	2.7270796	-0.3503162
H	-3.3949943	3.7361019	0.2269469	H	4.0255165	-1.6089215	0.3443235
H	-4.6682634	4.9149680	-0.2357108	H	5.6106753	-1.7707345	1.1774651
H	-4.5885754	4.2948632	1.4535177	H	5.5009193	-2.0096998	-0.6041875
H	0.7382308	6.4282465	1.0395999	H	4.6703873	4.0911484	0.3753162
H	0.3543948	7.56111038	2.3824520	H	3.3060117	3.2748299	-0.4675769
H	0.2757882	8.1289883	0.6750732	H	4.7239904	3.8564200	-1.4097841
H	1.8059684	0.2773097	0.9643485	H	-1.7950406	-0.2527836	-1.8550398
H	2.9048913	-0.9905651	-2.4579537	H	-3.8197229	-1.5009743	1.1247953
H	2.5911252	-4.4069386	1.1815510	H	-6.3737154	0.7412494	-2.5579689
H	-3.6107774	-0.7130051	1.1701280	H	-0.0531736	-4.1246548	-2.5832775
H	-2.1881218	-1.3611917	0.2972984	H	-1.4189641	-3.4616785	-1.6496985
H	-1.9760475	-0.0348172	1.4495722	H	-0.2367298	-2.3569620	-2.3958118
C	3.3871570	-6.3797970	-0.1436659	C	-8.5509920	-0.4589854	0.7832637
C	3.9384215	-5.7437792	-2.5242512	C	-8.6305037	0.6617697	-1.4791502
H	2.3515222	-6.4854712	0.2272000	H	-8.1580982	0.0565916	1.6768967
H	3.7063215	-7.3417525	-0.5660301	H	-8.4422913	-1.5488292	0.9173682
H	4.0457668	-6.1345658	0.7092631	H	-9.6170578	-0.2209519	0.6793166
H	3.1660731	-5.5462103	-3.2894564	H	-8.5727148	0.1015716	-2.4283733
H	4.1587229	-6.8194790	-2.5207679	H	-9.6793528	0.7084159	-1.1599994
H	4.8587046	-5.1975684	-2.7999234	H	-8.2628078	1.6895767	-1.6431214
TS-4 of 3d							

O	0.1295534	0.1709298	0.1526250
C	2.2936077	0.1093338	0.1007391
Au	4.7927728	1.2174529	0.0072211
O	2.1260483	3.3838806	-0.8863807
C	2.0074768	2.6638985	0.1034991
C	1.1828883	3.0489380	1.2843608
C	1.1283416	2.2666535	2.4565015
C	0.3018106	2.6545904	3.5183587
C	-0.4795237	3.8166072	3.4123259
C	-0.4306147	4.5993795	2.2450135
C	0.4011717	4.2221408	1.1879138
C	2.6954601	1.3317418	0.1274355
C	6.8269510	1.1202292	-0.0841483
N	7.5972610	0.0067286	0.0948246
C	8.9421387	0.3191094	-0.0376180
C	9.0122862	1.6595005	-0.3049403
N	7.7084813	2.1319382	-0.3299998
C	2.4397485	-1.3098028	0.1464410
C	2.1843920	-2.1107662	-1.0054983
C	2.4251530	-3.4910038	-0.9049480
C	2.8919349	-4.0676603	0.2868172
C	3.1298079	-3.2721462	1.4211491
C	2.8981779	-1.8971558	1.3546307
C	1.6479763	-1.4958057	-2.2713442
C	-0.4047755	1.0200260	-0.6025025
C	-1.5783075	1.7754008	-0.2621466
C	-2.0651243	2.7759888	-1.1452361
C	-3.1142473	3.6052227	-0.7844675
C	-3.7401495	3.4744594	0.4992707
C	-3.2603567	2.4438016	1.3770953
C	-2.2113907	1.6266795	1.0026251
H	-1.5869730	2.9086084	-2.1226246
N	-4.7511287	4.3074422	0.8806019
H	-3.7082312	2.3108966	2.3636076
C	7.0911198	-1.3401898	0.3791628
C	7.3446674	3.5302327	-0.5808372
H	3.0837395	-1.2550552	2.2211032
H	3.0706956	-5.1473145	0.3303039
H	2.2451513	-4.1271529	-1.7783945
H	3.4941816	-3.7232573	2.3493366
H	0.4473929	4.8090553	0.2658711
H	1.7272569	1.3544766	2.5320768
H	0.2611628	2.0464835	4.4278321
H	-1.1355158	4.1097898	4.2390194
H	-1.0493551	5.4985981	2.1604922
H	9.7246408	-0.4303990	0.0677370
H	9.8679266	2.3101337	-0.4771168
H	5.9954839	-1.2904544	0.4609967
H	7.5163279	-1.7019247	1.3280127
H	7.3699965	-2.0218716	-0.4393592
H	7.7700181	4.1711168	0.2070992
H	6.2482138	3.6106105	-0.5713300
H	7.7301702	3.8410323	-1.5640970
H	0.0714057	1.2582206	-1.5796424
H	-1.8330678	0.8660005	1.6921177
H	-3.4493446	4.3718100	-1.4855827
H	1.8348935	-2.1446254	-3.1416867
H	0.5562116	-1.3472687	-2.1829796
H	2.0959635	-0.5038798	-2.4576139
C	-5.3629766	4.1788278	2.2057734
C	-5.2263985	5.3606687	-0.0200812
H	-4.6149120	4.3221936	3.0071483
H	-5.8335638	3.1873112	2.3358164
H	-6.1386619	4.9489627	2.3120019
H	-5.6144891	4.9347177	-0.9631116
H	-6.0392256	5.9085598	0.4751904
H	-4.4180827	6.0750852	-0.2624752

2,4,5-trimethoxybenzaldehyde (3e)					
TS-1 of 3e			Int-3 of 3e		
O	-0.0084804	0.0409026	0.0747758	O	-1.3219136
C	2.1787457	0.0070782	0.0008514	C	0.1041820
C	-2.2635524	5.0202932	-0.0262956	C	-4.5724506
C	-5.4711604	3.4204588	-3.5289321	C	-8.0967865
C	-3.5311861	-1.6542156	-3.0687425	C	-4.9845424
					0.0753352
					1.7208596
					0.1939950
					1.4864429
					3.9726007
					-0.2984257
					0.4554367
					-1.1012909
					-3.3103399
					1.2947372

Au	4.5439939	0.3993770	-1.3365757	Au	2.5186813	0.2494114	-0.3897619
C	2.4950368	0.7475608	-0.9981616	C	0.5497914	0.3644663	0.2153142
C	1.7925814	1.8250370	-1.7841972	C	-0.3869403	0.6132886	-0.9290339
C	0.8479824	1.3936232	-2.8466730	C	-1.3398844	-0.4681344	-1.3435516
C	-0.0375697	2.3254073	-3.4715433	C	-2.4826691	-0.1852183	-2.1520860
C	-0.9311491	1.8256410	-4.4373469	C	-3.3705604	-1.2438066	-2.4263804
C	-0.9486671	0.4730117	-4.8056073	C	-3.1419146	-2.5464220	-1.9609284
C	-0.0672954	-0.4327165	-4.1959739	C	-2.0056999	-2.8227363	-1.1857173
C	0.8123544	0.0291939	-3.2140152	C	-1.1240295	-1.7832586	-0.8726434
O	-1.7882663	3.6673911	0.0488634	O	-3.8301532	2.9267900	0.3626685
C	-2.3452260	2.7212958	-0.7439299	C	-4.3270540	1.6845521	0.4145326
C	-1.7850713	1.4127588	-0.6791806	C	-3.4699404	0.6748714	0.9841679
C	-0.5717171	1.1604455	0.0564453	C	-2.1347878	0.9899486	1.2473042
C	-2.3458064	0.3732345	-1.4737006	C	-3.9483950	-0.6712080	1.1104202
C	-3.3915730	0.6159258	-2.3473969	C	-5.1912322	-1.0279900	0.6344478
C	-3.9178843	1.9503942	-2.4383430	C	-6.0212560	-0.0117971	0.0172091
C	-3.4058509	2.9802778	-1.6314607	C	-5.5894608	1.3233006	-0.0753128
C	2.3800001	-0.8668225	1.1115518	C	0.8485808	-0.0301018	2.7391858
C	3.3223898	-0.5026646	2.1091897	C	2.1217268	0.5518031	2.9390702
C	3.5941668	-1.3813515	3.1627355	C	2.8486521	0.2959743	4.1085124
C	2.9187896	-2.6107070	3.2459805	C	2.3125334	-0.5313804	5.1089835
C	1.9694779	-2.9672596	2.2702610	C	1.0353720	-1.0889295	4.9351120
C	1.6987553	-2.1070247	1.2041042	C	0.3045719	-0.8370034	3.7665620
O	-4.9022150	2.1143372	-3.3390794	O	-7.1882911	-0.4533347	-0.4420235
O	-3.9642839	-0.2939855	-3.1797199	O	-5.7306967	-2.2654445	0.6512107
C	6.5226502	0.0782693	-1.7040443	C	4.4684010	0.0740103	-1.0204290
N	7.2696285	0.5452782	-2.7455916	N	4.9748182	0.3208029	-2.2658021
C	8.5792723	0.1003072	-2.6439142	C	6.3427863	0.0939798	-2.2973332
C	8.6507769	-0.6631675	-1.5104108	C	6.7045650	-0.3064981	-1.0396355
N	7.3832707	-0.6643914	-0.9473547	N	5.5476255	-0.3123022	-0.2746534
C	6.7740135	1.4004796	-3.8288488	C	4.1892252	0.7640014	-3.4211564
C	7.0310578	-1.3854856	0.2802657	C	5.5019236	-0.6951031	1.1395522
C	-0.0692181	3.7968185	-3.1352921	C	-2.7951481	1.1869045	-2.7034681
O	2.0330749	2.9948459	-1.4931031	O	-0.3382593	1.7074982	-1.5094972
H	1.4924431	-0.6708527	-2.7189901	H	-0.2407836	-1.9846919	-0.2578455
H	-1.6632363	0.1257910	-5.5589848	H	-3.8557065	-3.3420293	-2.1997614
H	-1.6352332	2.5193241	-4.9099374	H	-4.2661180	-1.0374185	-3.0236399
H	-0.0704968	-1.4904641	-4.4775510	H	-1.8108484	-3.8373518	-0.8232610
H	0.9593455	-2.3678091	0.4430111	H	-0.6876637	-1.2797071	3.6397781
H	3.8380573	0.4597447	2.0346420	H	2.5278559	1.2252775	2.1767383
H	4.3287311	-1.1036618	3.9254017	H	3.8315806	0.7594233	4.2456226
H	3.1292818	-3.2931168	4.0760756	H	2.8806520	-0.7290787	6.0241303
H	1.4426461	-3.9240506	2.3429236	H	0.6043542	-1.7273461	5.7137656
H	9.3394794	0.3638083	-3.3772144	H	6.9349456	0.2357635	-3.1998358
H	9.4851265	-1.1988245	-1.0609716	H	7.6739197	-0.5844492	-0.6294156
H	5.7085924	1.6044686	-3.6505318	H	3.1414671	0.8710236	-3.1056600
H	6.8960223	0.8836240	-4.7933235	H	4.2595158	0.0166826	-4.2271061
H	7.3354211	2.3474872	-3.8383408	H	4.5691867	1.7337543	-3.7787890
H	5.9961557	-1.1298865	0.5499830	H	4.4713750	-0.5677052	1.5006452
H	7.7101154	-1.0823538	1.0917287	H	6.1805859	-0.0509358	1.7202742
H	7.1109490	-2.4708183	0.1114257	H	5.8033757	-1.7485787	1.2509598
H	-0.1037981	2.0239370	0.5708641	H	-1.7179053	1.9792486	1.0210793
H	-1.8755517	-0.6095705	-1.4052678	H	-3.2696481	-1.4132677	1.5322486
H	-3.8290458	3.9815137	-1.7046576	H	-6.2400117	2.0714409	-0.5262287
H	-4.6987848	4.1394310	-3.8564582	H	-7.6208596	0.8880485	-1.9979347
H	-6.2273102	3.3009219	-4.3166842	H	-8.9602890	-0.1575030	-1.3896918
H	-5.9505057	3.7784045	-2.6004510	H	-8.4107132	1.2533261	-0.4071985
H	-1.6497833	5.5882201	0.6860822	H	-3.9367247	4.8648677	-0.2323628
H	-2.1279929	5.4290719	-1.0439345	H	-4.7472539	3.7085979	-1.3557286
H	-3.3270738	5.0793529	0.2659965	H	-5.5300770	4.1493449	0.2198776
H	-4.1305714	-2.2206297	-3.7954977	H	-5.6054730	-4.2127953	1.2130001
H	-2.4583406	-1.7522326	-3.3152003	H	-4.0179720	-3.4718683	0.7854002
H	-3.7110403	-2.0437081	-2.0491445	H	-4.8110824	-3.0659876	2.3587108
H	-0.9085988	4.2863793	-3.6554661	H	-3.8026538	1.1961180	-3.1517587
H	-0.1702214	3.9594722	-2.0500784	H	-2.7359712	1.9630771	-1.9232579
H	0.8730472	4.2908359	-3.4302919	H	-2.0591104	1.4802781	-3.4715784
TS-2 of 3e				Int-4 of 3e			
O	0.0077793	-0.0088787	-0.1978652	O	0.0780232	-0.0320020	-0.0004094
C	2.0501430	-0.0074346	-0.0501899	C	1.5339255	0.0328537	-0.0278296
Au	-0.7178110	4.0561872	-0.0182532	C	2.0029814	4.1664629	0.0487205
C	1.7686704	2.2491174	-0.6029846	C	3.5595889	3.8860967	4.8271565
C	2.8353796	3.2600660	-0.6034682	C	2.9741015	-1.5396155	4.7228293
C	2.6226475	4.5610027	-0.0879003	Au	-0.1950954	-1.9952517	-3.8221068
C	3.6484683	5.5091047	-0.0868532	C	-0.7021060	-2.3813612	-5.7716022
C	4.9126954	5.1849875	-0.6104558	N	-1.8151371	-1.9513805	-6.4391541

C	5.1412168	3.8976920	-1.1210467	C	-1.8163519	-2.4138846	-7.7471423
C	4.1195159	2.9401245	-1.1117138	C	-0.6764354	-3.1547902	-7.9038143
C	0.4148019	2.3625977	-0.4262167	N	-0.0102188	-3.1240900	-6.6872211
C	-0.4035850	1.1342719	-0.5315709	O	2.0073359	-1.3090535	-0.1503756
O	2.2918496	0.9571378	-0.9326649	C	1.5169231	-1.9562837	-1.2359940
C	-1.9826217	5.6266246	0.3668015	C	0.3445591	-1.5029376	-1.8822060
N	-3.3436627	5.5470529	0.4778762	C	-0.4396339	-0.6269904	-1.0902735
C	-3.8920453	6.7947369	0.7338557	O	1.8511726	2.7433977	0.0957164
C	-2.8496692	7.6805029	0.7828040	C	2.1831124	2.0764432	1.2398597
N	-1.6934812	6.9492745	0.5525097	C	2.0449903	0.6733872	1.2113290
C	-1.8107278	1.2323642	-1.0304540	C	2.3373945	-0.0857868	2.3644650
C	-2.8684654	0.5222557	-0.3983854	C	2.7869072	0.5278618	3.5354133
C	-4.1636267	0.6676400	-0.9351215	O	3.1067739	-0.1166321	4.6933589
C	-4.4090590	1.4467939	-2.0749915	C	2.6338756	2.7103183	2.4157243
C	-3.3530409	2.1226692	-2.7064078	C	2.9357843	1.9491123	3.5564396
C	-2.0640507	2.0266595	-2.1725640	O	3.3762820	2.4685869	4.7272100
C	-2.6549060	-0.3428693	0.8244043	C	2.3052361	-3.1435964	-1.5737300
C	2.4083312	-1.3404834	-0.4020221	C	1.7337500	-4.2356515	-2.2731206
C	2.3696370	-2.3553951	0.5990837	C	2.5135615	-5.3482080	-2.6005285
C	2.7110565	-3.6772242	0.2603443	C	3.8697338	-5.3922782	-2.2316215
C	3.0756943	-3.9963748	-1.0580747	C	4.4417725	-4.3240700	-1.5193822
C	3.1031384	-2.9825621	-2.0799329	C	3.6671817	-3.2095990	-1.1840019
C	2.7642360	-1.6821998	-1.7392651	C	-1.8588454	-0.3220911	-1.3069133
O	1.9942967	-1.9699500	1.8366865	C	-2.3917234	0.9832997	-1.0652431
C	1.9291134	-2.9404080	2.8936613	C	-3.7550454	1.1889157	-1.3518645
O	3.4662244	-3.4157190	-3.3144133	C	-4.5816536	0.1607494	-1.8266629
C	3.5082781	-2.4512122	-4.3720145	C	-4.0571556	-1.1247867	-2.0361373
O	3.4165947	-5.2266984	-1.4713079	C	-2.7043269	-1.3567141	-1.7838086
C	3.4199548	-6.3128848	-0.5280856	C	-2.8670559	-1.1074849	-5.8639336
C	-4.1297417	4.3171325	0.3351472	C	1.2682438	-3.7944934	-6.4327178
C	-0.3453069	7.5239267	0.5483374	C	-1.5670842	2.1499219	-0.5659214
H	-1.2325879	2.5568140	-2.6488948	H	-2.2861381	-2.3584769	-1.9205962
H	-5.4283857	1.5295584	-2.4670694	H	-5.6384244	0.3645578	-2.0296144
H	-4.9976907	0.1533408	-0.4444074	H	-4.1766205	2.1889260	-1.2016418
H	-3.5332427	2.7285969	-3.6000428	H	-4.6976833	-1.9392099	-2.3885341
H	4.3126483	1.9390255	-1.5052861	H	4.1117797	-2.3699775	-0.6428481
H	1.6384373	4.8139048	0.3237940	H	0.6707951	-4.2132602	-2.5327182
H	3.4641168	6.5061283	0.3272175	H	2.0613666	-6.1899834	-3.1345515
H	5.7147522	5.9305625	-0.6147406	H	4.4794569	-6.2634120	-2.4934986
H	6.1233101	3.6341817	-1.5272491	H	5.4972558	-4.3589163	-1.2312671
H	-4.9637904	6.9456787	0.8513263	H	-2.6192617	-2.1821258	-8.4449196
H	-2.8329062	8.7554817	0.9543384	H	-0.2892280	-3.6966493	-8.7650137
H	-3.4438331	3.4905260	0.1000432	H	-2.6687036	-0.9897635	-4.7886481
H	-4.8545136	4.4332771	-0.4853559	H	-3.8462555	-1.5898327	-6.0078173
H	-4.6621161	4.1041775	1.2752982	H	-2.8641872	-0.1197170	-6.3515229
H	0.3337988	6.8138103	0.0565634	H	1.1827482	-4.8621578	-6.6879401
H	-0.0079066	7.7076540	1.5811528	H	1.5092351	-3.6869376	-5.3651438
H	-0.3549631	8.4698334	-0.0134122	H	2.0622392	-3.3301053	-7.0387516
H	1.9507009	0.2809446	1.0009887	H	1.8030783	0.5889648	-0.9448537
H	2.7666748	-0.8866799	-2.4865260	H	2.2179267	-1.1698924	2.3144884
H	2.6911540	-4.4598722	1.0179255	H	2.7456255	3.7940071	2.4451814
H	2.4095786	-6.4698586	-0.1106516	H	2.6057632	4.4224210	4.6686292
H	3.7292137	-7.1975541	-1.1008080	H	3.9196332	4.0683789	5.8494391
H	4.1416016	-6.1206470	0.2855778	H	4.3122559	4.2418523	4.0994430
H	1.6021382	-2.3846717	3.7829719	H	1.6991112	4.4645381	-0.9646086
H	1.1944021	-3.7299650	2.6550753	H	1.3487461	4.6597300	0.7908594
H	2.9215758	-3.3892696	3.0771420	H	3.0539913	4.4613357	0.2229917
H	3.8206506	3.0026716	-5.2693148	H	3.2755177	-1.8493216	5.7337937
H	2.5116222	-2.0015106	-4.5394435	H	1.9277960	-1.8490046	4.5377140
H	4.2416868	-1.6526287	-4.1522956	H	3.6356969	-2.0198357	3.9767122
H	-3.6191158	-0.5756711	1.3045815	H	-2.1054912	3.0949762	-0.7422136
H	-2.1612840	-1.2913914	0.5505083	H	-1.3718194	2.0603316	0.5168517
H	-2.0013845	0.1497748	1.5647908	H	-0.5814323	2.2084970	-1.0555012
TS-3 of 3e				Int-5 of 3e			
O	0.0144085	-0.0691095	-0.3915797	O	-0.1033485	0.3728420	0.1139551
C	1.9953771	-0.0208579	-0.0831574	C	3.2533107	0.3438000	-0.3121913
Au	-0.6549100	4.1144218	-0.2046649	Au	-0.2230906	3.7686191	-0.1034469
C	1.6998178	2.2357571	-0.6257490	C	2.5288141	2.5897014	-0.0112752
C	2.6931772	3.3256824	-0.5473010	C	3.1670425	3.8732200	-0.3797004
C	2.6272357	4.2125382	0.5520144	C	3.9759369	3.9930928	-1.5420420
C	3.5369053	5.2675695	0.6800586	C	4.5265350	5.2543249	-1.8405972
C	4.5220633	5.4508915	-0.3020898	C	4.2954488	6.3701744	-1.0225531
C	4.5926881	4.5734191	-1.3936116	C	3.4974167	6.2445827	0.1249631
C	3.6978924	3.4958405	-1.5409622	C	2.9386702	5.0004649	0.4404521
C	0.3380322	2.3191967	-0.5235362	C	0.7464874	1.0124202	0.7482373

C	-0.4372881	1.0743710	-0.6909333	C	1.2216481	2.3408048	0.2607118
O	2.3120060	0.9800088	-0.9056928	O	3.5183778	1.5499408	0.1452507
C	-1.6723151	5.8700953	0.1041239	C	3.8587012	-0.7778097	0.2519625
N	-3.0283456	6.0479865	0.1035412	C	3.4895921	-2.0836704	-0.2399819
C	-3.3528268	7.3747101	0.3459322	C	3.8965986	-3.2266695	0.4612917
C	-2.1708729	8.0477428	0.4979366	C	4.6786056	-3.0943410	1.6223508
N	-1.1571310	7.1129322	0.3464099	C	5.0910335	-1.7902240	2.1063502
C	-1.8293035	1.1105170	-1.2205638	C	4.6889396	-0.6672399	1.4167161
C	-2.7524092	0.1373389	-0.7772204	C	-1.6299585	5.2066236	-0.5246361
C	-4.0666919	0.1435372	-1.2582815	N	-1.3919433	6.4823322	-0.9569732
C	-4.4618845	1.0969700	-2.2123733	C	-2.5818160	7.1684651	-1.1500841
C	-3.5385087	2.0436926	-2.6872036	C	-3.5921810	6.3023090	-0.8302279
C	-2.2301064	2.0601587	-2.1879311	N	-2.9912856	5.1107874	-0.4517626
H	-2.4314597	-0.6041694	-0.0392274	C	-0.0645994	7.0521255	-1.2076476
C	2.4369686	-1.3292550	-0.4468951	C	-3.7279894	3.9178679	-0.0248506
C	2.3858843	-2.3777084	0.5161816	C	1.3106962	0.4617440	2.0308547
C	2.8144410	-3.6692610	0.1585575	C	2.0398667	1.2534035	2.9419804
C	3.2759409	-3.9256117	-1.1431563	C	2.5871689	0.6746057	4.0960526
C	3.3177073	-2.8770070	-2.1276214	C	2.4298978	-0.6997039	4.3379045
C	2.8924344	-1.6073300	-1.7676594	C	1.7035630	-1.4948496	3.4331911
O	1.9147578	-2.0535359	1.7400055	C	1.1349577	-0.9142895	2.2949166
C	1.8591865	-3.0568988	2.7667248	O	2.7396121	-2.1100583	-1.3465008
O	3.7796125	-3.2463903	-3.3502400	C	2.2084441	-3.3614786	-1.8299873
C	3.8476076	-2.2403932	-4.3663616	O	5.8279710	-1.8149786	3.2370548
O	3.7016146	-5.1242108	-1.5727544	C	6.2975550	-0.5602456	3.7547846
C	3.6969783	-6.2409773	-0.6664609	O	5.0941334	-4.1165366	2.3633707
C	-4.0160360	4.9833279	-0.0973117	C	4.7316160	-5.4673057	2.0015612
C	0.2715660	7.4312515	0.4206409	C	4.2135468	2.8181980	-2.4654670
H	-1.5088545	2.7907736	-2.5673857	H	2.3190498	4.8839068	1.3359649
H	-5.4895597	1.0979984	-2.5911317	H	4.7371407	7.3378267	-1.2840699
H	-4.7854114	-0.5963411	-0.8909990	H	5.1381936	5.3642778	-2.7435362
H	-3.8385856	2.7723472	-3.4472456	H	3.3131466	7.1083107	0.7722052
H	1.8641919	4.0485101	1.3201509	H	0.5683843	-1.5131247	1.5744110
H	3.4797821	5.9375048	1.5442364	H	2.1728656	2.3225951	2.7488022
H	5.2371197	6.2764306	-0.2197221	H	3.1417332	1.2972561	4.8060994
H	5.3579402	4.7302890	-2.1623826	H	2.8770559	-1.1538304	5.2285171
H	-4.3836303	7.7225804	0.3874173	H	1.5849628	-2.5676467	3.6190798
H	-1.9675401	9.0991545	0.6939204	H	-2.6080985	8.2011137	-1.4938689
H	-3.4910388	4.0837846	-0.4500286	H	-4.6731982	6.4313369	-0.8378915
H	-4.7498970	5.3024206	-0.8531397	H	0.6940252	6.3324089	-0.8674891
H	-4.5316563	4.7637129	0.8512776	H	0.0436793	7.9944792	-0.6487072
H	0.8413832	6.5018787	0.2787698	H	0.0639014	7.2426658	-2.2850688
H	0.5054272	7.8635497	1.4062120	H	-4.3085375	4.1434655	0.8835627
H	0.5350133	8.1494331	-0.3717454	H	-3.0003355	3.1218150	0.1886360
H	1.8195140	0.2302110	0.9680478	H	-4.4069681	3.5937376	-0.8289804
H	2.9007468	-0.7869499	-2.4872379	H	2.5074151	0.2547682	-1.1113756
H	2.7859859	-4.4776597	0.8883001	H	4.9365749	0.3345437	1.7696137
H	2.6708610	-6.4586573	-0.3207047	H	3.6128013	-4.2182398	0.1109471
H	4.0840859	-7.0902891	-1.2454259	H	5.1396041	-5.7197771	1.0082891
H	4.3553543	-6.0447288	0.1983471	H	5.1859255	-6.1043887	2.7711613
H	1.4567906	-2.5481987	3.6532733	H	3.6343262	-5.5832362	2.0099623
H	1.1864918	-3.8819602	2.4720109	H	1.5940152	-3.0980637	-2.7005460
H	2.8676839	-3.4502413	2.9864511	H	3.0283601	-4.0340800	-2.1342115
H	4.2498903	-2.4989081	-5.2582960	H	1.5847883	-3.8384619	-1.0545149
H	2.8440201	-1.8321158	-4.5898104	H	6.8809752	-0.8082312	4.6518693
H	4.5236115	-1.4173405	-4.0659771	H	6.9406466	-0.0492941	3.0150912
C	3.8050928	2.5883753	-2.7476621	H	5.4490371	0.0925419	4.0263720
C	2.8112671	2.3430331	-3.1611590	H	4.5974483	3.1565073	-3.4412949
H	4.4051361	3.0656147	-3.5390604	H	4.9516401	2.1140580	-2.0397019
H	4.2901168	1.6321146	-2.4809248	H	3.2797804	2.2535322	-2.6400685
TS-4 of 3e							
O	-0.0046652	0.0067509	-0.0606214				
C	2.1249204	0.0141873	-0.0307066				
Au	4.5947165	1.2319548	0.0076722				
O	1.8110740	3.2353301	-1.0887042				
C	1.7724793	2.5646751	-0.0582005				
C	1.0304364	3.0035391	1.1588162				
C	0.9961340	2.2349856	2.3404994				
C	0.2465315	2.6742752	3.4398704				
C	-0.4805889	3.8730528	3.3627982				
C	-0.4523683	4.6411033	2.1849177				
C	0.3042606	4.2136183	1.0908396				
C	2.4921424	1.2494307	-0.0048419				
C	6.6330271	1.2109871	0.0400098				
N	7.4305396	0.1223990	0.2511831				

C	8.7689857	0.4826435	0.2005502
C	8.8071928	1.8281002	-0.0471225
N	7.4911928	2.2556858	-0.1422111
C	2.3436317	-1.3957231	0.0544432
C	2.1261930	-2.2433603	-1.0710719
C	2.4430144	-3.6050096	-0.9320567
C	2.9480875	-4.1201029	0.2720800
C	3.1481812	-3.2794549	1.3807774
C	2.8397446	-1.9219313	1.2758949
C	1.5506363	-1.6970170	-2.3511212
C	-0.4673776	0.8765702	-0.8437722
C	-1.5560462	1.7456183	-0.5002488
C	-1.8865905	2.8387613	-1.3561791
C	-2.7389905	3.8552165	-0.8868914
C	-3.2807612	3.7758391	0.4062088
C	-3.0001569	2.6482377	1.2569903
C	-2.1489282	1.6616144	0.7925881
O	-1.3174582	2.8483779	-2.5799441
C	-1.3908839	4.0350251	-3.3853364
O	-4.0696263	4.7141376	0.9536751
C	-4.3771343	5.9021254	0.2036553
O	-3.5830979	2.6893022	2.4829972
C	-3.3863628	1.5630541	3.3457160
C	6.9563465	-1.2450049	0.4898980
C	7.0937181	3.6426194	-0.4043161
H	2.9941995	-1.2455182	2.1223047
H	3.1864219	-5.1865234	0.3455509
H	2.2935050	-4.2753077	-1.7855359
H	3.5423062	-3.6818941	2.3191741
H	0.3330815	4.7904902	0.1617262
H	1.5509169	1.2938151	2.3953226
H	0.2259202	2.0772414	4.3574252
H	-1.0795959	4.2055674	4.2167516
H	-1.0320024	5.5677853	2.1220200
H	9.5699825	-0.2405357	0.3439115
H	9.6479702	2.5101128	-0.1614296
H	5.8574333	-1.2306218	0.5322179
H	7.3580847	-1.6126795	1.4465914
H	7.2858915	-1.9013058	-0.3306056
H	7.4860640	4.2962050	0.3900870
H	5.9955153	3.6923800	-0.4157362
H	7.4890847	3.9624758	-1.3808734
H	0.0277759	1.0571079	-1.8173878
H	-1.8515934	0.8210909	1.4227009
H	-2.9783578	4.7085195	-1.5207287
H	-4.9295697	5.6505151	-0.7187991
H	-5.0094805	6.5110068	0.8637651
H	-3.4536319	6.4541683	-0.0466999
H	-0.7862379	3.8233480	-4.2777181
H	-2.4330266	4.2459912	-3.6842330
H	-0.9689846	4.8995619	-2.8424845
H	-3.9570229	1.7816513	4.2592778
H	-3.7674148	0.6367246	2.8768554
H	-2.3173375	1.4368639	3.5957565
H	1.7737451	-2.3574781	-3.2040484
H	0.4523819	-1.6103714	-2.2617610
H	1.9384447	-0.6856964	-2.5662992

Pivalaldehyde (3f)

TS-1 of 3f				Int-4 of 3f			
O	-0.0107080	0.0554790	0.0092364	O	-3.2040575	-0.7550403	-0.0106876
C	2.0992894	0.0657059	-0.0468721	C	-1.8983697	-1.0333877	-0.2208980
C	2.4201949	1.3118478	0.0104884	C	-0.9283853	-0.0060839	-0.1862761
Au	4.5188704	1.5037510	0.1358188	Au	1.1173785	-0.2779510	0.0091016
C	6.5120139	1.9082271	0.2264451	C	3.1362929	-0.4884861	0.2983198
N	7.1014543	3.0997460	-0.0855372	N	4.0770712	0.5036172	0.3014070
C	8.4744091	3.0235705	0.0941115	C	5.3424973	-0.0165090	0.5309900
C	8.7476416	1.7533213	0.5246443	C	5.1923838	-1.3694264	0.6729781
N	7.5341778	1.0858092	0.5997881	N	3.8391449	-1.6381766	0.5268645
C	1.6390359	2.5938513	0.0642661	C	-1.4749941	1.2943602	-0.2834948
O	0.7305108	2.7209201	0.8875467	O	-2.7807963	1.5305407	-0.0473740
C	2.3592360	-1.3255923	-0.2468922	C	-1.6728476	-2.4448318	-0.5362236
C	1.8342092	-2.3127916	0.6250073	C	-2.6006973	-3.4160972	-0.0804712
C	2.1415977	-3.6589742	0.4163937	C	-2.3902714	-4.7713051	-0.3498987
C	2.9706051	-4.0374575	-0.6552323	C	-1.2652560	-5.1768708	-1.0886379

C	3.4933729	-3.0659647	-1.5254947	C	-0.3518606	-4.2203135	-1.5659426
C	3.1872003	-1.7156740	-1.3328347	C	-0.5521752	-2.8639648	-1.2959363
C	6.3930020	4.3094330	-0.5202253	C	3.7960873	1.9295422	0.1071109
C	7.3881264	-0.3134801	1.0128938	C	3.2535052	-2.9791021	0.6121323
C	-0.4627331	0.4479050	1.0923750	C	-3.4438238	0.4779778	0.6764325
C	-1.9053898	0.8622230	1.2749362	C	-4.9486561	0.7447802	0.7556760
C	2.0627346	3.6816115	-0.8594738	C	-0.7244462	2.4835486	-0.7126975
C	1.7988886	5.0513968	-0.5631760	C	-0.8815319	3.7489316	-0.0720027
C	2.2704525	6.0153580	-1.4764954	C	-0.0788304	4.8125143	-0.5272987
C	2.9439526	5.6587129	-2.6533880	C	0.8246827	4.6606636	-1.5883346
C	3.1715052	4.3060980	-2.9533153	C	0.9591919	3.4173274	-2.2269149
C	2.7405612	3.3033585	-2.0515540	C	0.1965682	2.3363967	-1.7811548
H	2.9117827	2.2720358	-2.2769134	H	0.2787621	1.3651910	-2.2782195
H	3.2895918	6.4401069	-3.3386214	H	1.4255778	5.5157108	-1.9156512
H	2.1015377	7.0750456	-1.2549543	H	-0.1623181	5.7840405	-0.0278300
H	3.6834512	4.0163355	-3.8761933	H	1.6522399	3.2915902	-3.0645223
H	3.5848985	-0.9499367	-2.0058699	H	0.1409807	-2.1156363	-1.6926453
H	1.1929221	-2.0145979	1.4583186	H	-3.4656820	-3.0989544	0.5080142
H	1.7367541	-4.4190311	1.0918722	H	-3.1012073	-5.5161476	0.0214126
H	3.2077801	-5.0947189	-0.8128297	H	-1.1033425	-6.2393851	-1.2983930
H	4.1359859	-3.3628013	-2.3603544	H	0.5117706	-4.5337906	-2.1609318
H	9.1321774	3.8692884	-0.0988909	H	6.2307191	0.6118125	0.5705231
H	9.6907473	1.2718501	0.7772041	H	5.9240270	-2.1536970	0.8596159
H	5.3558731	4.0401063	-0.7684460	H	2.7458587	2.0384221	-0.2001681
H	6.8895082	4.7204099	-1.4119430	H	4.4537988	2.3298116	-0.6797135
H	6.3987203	5.0570803	0.2885815	H	3.9657953	2.4776757	1.0475421
H	6.3200812	-0.5726348	0.9861199	H	2.1796541	-2.9021704	0.3884619
H	7.7735829	-0.4389605	2.0364895	H	3.3911128	-3.3835444	1.6273043
H	7.9457569	-0.9639400	0.3212587	H	3.7389278	-3.6424670	-0.1206034
H	0.1656240	0.4049560	2.0083506	H	-2.9611716	0.4088654	1.6723613
C	1.0672663	5.5063992	0.6778989	C	-1.8212397	3.9825094	1.0897032
H	1.1418328	6.6007767	0.7841197	H	-1.5168176	4.8799644	1.6513121
H	0.0002460	5.2278585	0.6279360	H	-2.8531859	4.1417680	0.7315126
H	1.4687754	5.0289073	1.5879653	H	-1.8457240	3.1273685	1.7851233
C	-1.9931813	1.9880396	2.3286405	C	-5.1623507	2.0744724	1.5107944
H	-3.0537791	2.2071676	2.5412567	H	-6.2429214	2.2454274	1.6514856
H	-1.5090075	1.6874920	3.2750702	H	-4.6853914	2.0529270	2.5069425
H	-1.5045332	2.9051867	1.9636753	H	-4.7512021	2.9258380	0.9442841
C	-2.6045952	-0.4201773	1.8212862	C	-5.5887327	-0.4179788	1.5472111
H	-3.6632762	-0.1845490	2.0270884	H	-6.6690063	-0.2288244	1.6656077
H	-2.5619998	-1.2387600	1.0825998	H	-5.4629230	-1.3784479	1.0199142
H	-2.1405969	-0.7654231	2.7620833	H	-5.1437440	-0.5090621	2.5541451
C	-2.5245743	1.2906768	-0.0664749	C	-5.5426097	0.8271329	-0.6657127
H	-2.0083368	2.1833279	-0.4603443	H	-5.0750632	1.6446341	-1.2407452
H	-2.4442043	0.4855922	-0.8157076	H	-5.3860836	-0.1177182	-1.2133338
H	-3.5909863	1.5357938	0.0744537	H	-6.6270571	1.0197957	-0.6045970
TS-4 of 3f							
O	0.0373544	0.0457533	-0.0272108				
C	1.9880300	0.0200320	0.0374262				
C	2.3871934	1.2529196	0.1357020				
Au	4.4736085	1.4202244	0.2671679				
C	6.4948182	1.6883614	0.3750694				
N	7.1910472	2.7949884	-0.0192827				
C	8.5483971	2.6235354	0.2070987				
C	8.7039623	1.3776623	0.7523078				
N	7.4371328	0.8212631	0.8471264				
C	1.5804499	2.5118914	0.2262441				
O	0.7493502	2.6518545	1.1282644				
C	2.2874787	-1.3677876	-0.1775807				
C	2.0637982	-2.3039417	0.8625217				
C	2.3618364	-3.6540155	0.6715824				
C	2.8809566	-4.0770545	-0.5642322				
C	3.0991349	-3.1549525	-1.5988761				
C	2.8066137	-1.7890363	-1.4392942				
C	6.5967164	4.0155430	-0.5754946				
C	7.1649709	-0.5196332	1.3742384				
C	-0.5101556	0.2890771	1.0611064				
C	-1.9807572	0.5781376	1.1782668				
C	1.8457733	3.5835936	-0.7746233				
C	1.2763593	4.8584051	-0.5627777				
C	1.4982362	5.8879418	-1.4830036				
C	2.2772014	5.6505718	-2.6297517				
C	2.8309851	4.3794460	-2.8578749				
C	2.6190391	3.3494315	-1.9332675				
H	3.0441008	2.3566933	-2.1159303				

H	2.4497774	6.4579883	-3.3493965
H	1.0657223	6.8787990	-1.3098991
H	3.4264002	4.1914663	-3.7570992
H	1.6637517	-1.9547399	1.8194671
H	2.1928976	-4.3738656	1.4784436
H	3.1158435	-5.1346302	-0.7246851
H	3.5004830	-3.5029364	-2.5568967
H	9.2790899	3.3924861	-0.0377731
H	9.5972433	0.8444710	1.0729803
H	5.5493078	3.8064053	-0.8379874
H	7.1517591	4.3120971	-1.4781308
H	6.6360064	4.8254051	0.1701190
H	7.6917744	-1.2708865	0.7655467
H	6.0810289	-0.6969821	1.3257442
H	7.5032463	-0.5822954	2.4201057
H	0.0751870	0.2264263	2.0006528
H	0.6707807	5.0221891	0.3339183
C	-2.1721230	1.7798123	2.1365323
H	-3.2519715	1.9355106	2.3017368
H	-1.6952683	1.5923997	3.1144781
H	-1.7368013	2.6961112	1.7073388
C	-2.5828311	-0.7062100	1.8266188
H	-3.6620545	-0.5406750	1.9875535
H	-2.4555006	-1.5815587	1.1671531
H	-2.1180010	-0.9238983	2.8040371
C	-2.6076164	0.8462780	-0.1996115
H	-2.1531484	1.7364187	-0.6676925
H	-2.4631715	-0.0120165	-0.8768383
H	-3.6899147	1.0256227	-0.0860138
C	3.0544376	-0.8028157	-2.5536535
H	3.3089571	-1.3213978	-3.4909103
H	2.1723020	-0.1628418	-2.7283716
H	3.8937676	-0.1293905	-2.2930503

Intramolecular 1,3-*O*-transposition

Int-I				Int-II			
C	-7.6168132	1.5945451	-4.6998375	O	-3.8770566	0.7848127	0.5848776
C	-7.7373384	2.4938371	-5.7640118	C	-1.7236387	-1.3757634	-0.4083902
C	-6.8051037	3.5074095	-5.9905298	Au	0.2418393	-0.4133235	-0.1212735
C	-5.7035480	3.6547072	-5.1425985	C	2.2440803	-0.0806033	0.0724092
C	-5.5542117	2.7800443	-4.0785325	N	3.0477598	0.5999994	-0.7963513
C	-6.4911214	1.7491914	-3.8389486	C	4.3436494	0.6495559	-0.3168033
H	-4.7033226	2.8796256	-3.4109293	C	4.3511429	-0.0250026	0.8770597
H	-6.9400547	4.1826694	-6.8308105	N	3.0574527	-0.4595161	1.1000515
H	-4.9745501	4.4405954	-5.3125899	C	-2.7498901	1.0376745	0.1601256
H	-8.5879531	2.3943930	-6.4328898	C	-1.9185706	-0.1459658	-0.1773744
C	-6.2461887	0.8802202	-2.6933846	C	-1.9776407	-2.7687466	-0.6278477
O	-7.0372011	-0.0858696	-2.4199443	C	-3.3019962	-3.2270043	-0.3997191
C	-5.1194379	1.0850186	-1.8589627	C	-3.6077328	-4.5752530	-0.6025133
C	-4.1947524	1.1278295	-1.0626548	C	-2.6092343	-5.4709396	-1.0248350
C	-3.1628555	1.1012659	-0.0998985	C	-1.2971081	-5.0190897	-1.2491304
C	-2.2542660	2.1729365	0.0332441	C	-0.9755167	-3.6727104	-1.0536218
C	-3.0512503	-0.0232735	0.7492769	C	2.5938249	1.2602125	-2.0262401
C	-2.0532503	-0.0658768	1.7146616	C	2.6471143	-1.2600799	2.2602348
C	-1.1610042	1.0041989	1.8469661	C	-2.1828108	2.3952591	-0.0111713
C	-1.2626100	2.1181046	1.0066149	C	-1.1526597	2.5918562	-0.9614763
H	-3.7463473	-0.8487586	0.6274903	C	-0.5905209	3.8537309	-1.1679677
H	-1.9663859	-0.9314001	2.3647060	C	-1.0495491	4.9369812	-0.4023066
H	-0.3836898	0.9682726	2.6045635	C	-2.0732830	4.7522497	0.5385166
H	-0.5654377	2.9436621	1.1119074	C	-2.6758847	3.4973912	0.7494966
H	-2.3412074	3.0332359	-0.6226832	C	-3.7862318	3.3669937	1.7650868
Au	-6.8322973	-1.2984252	-0.7453272	H	-0.6146608	5.9324322	-0.5415596
C	-6.6904261	-2.4595583	0.8546919	H	-2.4202042	5.6075921	1.1283405
N	-6.8106709	-3.8129713	0.9184226	H	0.1900758	3.9947884	-1.9221177
N	-6.4253274	-2.0631975	2.1305962	H	-4.6281357	-4.9311123	-0.4283694
C	-6.3821279	-3.1563221	2.9780418	H	-4.0662055	-2.5182652	-0.0665693
C	-6.6233348	-4.2560386	2.2156654	H	-2.8550918	-6.5266576	-1.1791708
H	-6.1887437	-3.0535070	4.0340884	H	-0.5237948	-5.7199392	-1.5788344
H	-6.6782977	-5.3011950	2.4760922	H	0.0425150	-3.3110979	-1.2291225
C	-7.0992932	-4.6979076	-0.2155607	H	1.5490110	-1.2888973	2.2960956
H	-6.2724666	-5.3985204	-0.3488699	H	3.0350225	-0.7916411	3.1765559
H	-8.0249452	-5.2432097	-0.0209052	H	3.0440888	-2.2827895	2.1644523
H	-7.2126137	-4.0843905	-1.1093788	H	1.7159621	0.7247021	-2.4150105
C	-6.2407714	-0.6768257	2.5734184	H	3.4032280	1.2248996	-2.7687211
H	-5.2684116	-0.5761758	3.0596831	H	2.3302824	2.3083277	-1.8121445

H	-6.2864097	-0.0274178	1.6989068	H	5.1433868	1.1543891	-0.8559039
H	-7.0355105	-0.4094943	3.2726196	H	5.1615877	-0.2329872	1.5734085
C	-8.6704196	0.5318338	-4.5303231	H	-0.8207618	1.7466252	-1.5753689
H	-9.1560056	0.6064129	-3.5518529	H	-3.6121197	2.5225675	2.4543569
H	-9.4273504	0.6332744	-5.3121252	H	-3.8776553	4.2947993	2.3521178
H	-8.2349298	-0.4712224	-4.5841731	H	-4.7503295	3.1665797	1.2666031
TS-I				Int-III			
O	-0.0142502	0.1000357	0.2681749	O	-1.2199392	-2.8982136	0.2520566
C	1.9767364	0.0454046	0.3969786	C	0.0288237	-2.2798970	0.1345544
Au	3.3783574	2.7123952	0.0873777	Au	0.3297596	0.9634479	-0.1030378
C	4.8784738	4.1156292	0.0029356	C	1.0754952	2.8752739	-0.2672300
N	4.9620419	5.1832795	-0.8456574	N	0.4412215	3.9741321	-0.7768754
C	6.1073241	5.9231791	-0.5934176	C	1.2537333	5.0953908	-0.6999741
C	6.7587733	5.3016300	0.4373674	C	2.4307632	4.6900039	-0.1316537
N	5.9927673	4.2002578	0.7878343	N	2.3029788	3.3328571	0.1240721
C	0.3724067	1.2935177	-0.0192745	C	-1.6861507	-1.5093071	0.1852943
C	1.8473127	1.3456944	0.1595249	C	-0.4258726	-0.9184281	0.0665576
C	2.5577269	-1.2283860	0.5393919	C	1.2667671	-2.9762397	0.1112521
C	2.0965135	-2.1378050	1.5317986	C	1.3774583	-4.4076829	0.2176521
C	2.7153785	-3.3801370	1.6606458	C	2.6708698	-4.9504671	0.1805759
C	3.7971406	-3.7211199	0.8258631	C	3.8118839	-4.1427951	0.0450094
C	4.2580237	-2.8257124	-0.1559801	C	3.6986818	-2.7425823	-0.0606857
C	3.6356289	-1.5874561	-0.3214066	C	2.4357898	-2.1669397	-0.0272879
C	3.9646866	5.5357370	-1.8612351	C	-0.9297569	3.9877849	-1.2957957
C	6.3508253	3.2598383	1.8542478	C	3.3490822	2.5161510	0.7456460
C	-0.5201368	2.3478098	-0.4664276	C	-3.0703950	-1.2004567	0.2536815
C	0.0400120	3.6281900	-0.7252186	C	-3.4943521	0.1579669	0.1980448
C	-0.7503378	4.6907234	-1.1556129	C	-4.8522186	0.4573284	0.2668997
C	-2.1283345	4.4835901	-1.3363560	C	-5.7973380	-0.5826464	0.3905981
C	-2.6970384	3.2257731	-1.0843271	C	-5.3858624	-1.9272945	0.4465455
C	-1.9282409	2.1330659	-0.6475935	C	-4.0285778	-2.2440808	0.3792661
C	-2.6046987	0.8096694	-0.3939855	H	-3.6893127	-3.2828374	0.4216045
H	-2.7667496	5.3065963	-1.6745313	H	-6.8636618	-0.3400691	0.4444780
H	-3.7735045	3.0857837	-1.2299873	H	-6.1297088	-2.7239728	0.5431517
H	-0.3038787	5.6709900	-1.3477859	H	-5.1875863	1.4981228	0.2263990
H	2.3607693	-4.0892153	2.4147744	H	2.7904232	-6.0358868	0.2595265
H	1.2531903	-1.8560594	2.1678891	H	4.8010430	-4.6119571	0.0206560
H	4.2803736	-4.6971006	0.9377837	H	4.5916090	-2.1201797	-0.1685256
H	5.0951328	-3.1029868	-0.8039199	H	2.3111105	-1.0820194	-0.1102230
H	3.9696243	-0.8845900	-1.0900295	H	3.0193470	1.4675568	0.7386672
H	5.5628281	2.4964118	1.9236048	H	3.5111928	2.8431616	1.7849109
H	6.4286251	3.7986214	2.8112757	H	4.2846727	2.6149652	0.1739429
H	7.3129215	2.7792234	1.6177210	H	-1.2308428	2.9531388	-1.5142833
H	3.3033955	4.6713815	-2.0171022	H	-0.9631863	4.5834966	-2.2201734
H	4.4758916	5.7809162	-2.8041043	H	-1.6123943	4.4235783	-0.5483275
H	3.3726919	6.4013505	-1.5228894	H	0.9317883	6.0723066	-1.0566844
H	6.3594170	6.8157139	-1.1636007	H	3.3385506	5.2430358	0.1032700
H	7.6928482	5.5434179	0.9415044	H	-2.7437677	0.9499809	0.1056409
H	1.1160179	3.7707293	-0.5723967	C	0.1860647	-5.3191304	0.3647341
H	-2.4598446	0.4838019	0.6507889	H	-0.5039492	-5.2102475	-0.4893609
H	-3.6839724	0.8866963	-0.6007382	H	0.5133479	-6.3682666	0.4275693
H	-2.1717451	0.0139789	-1.0247644	H	-0.3934563	-5.0704317	1.2700751
TS-II				Int-IV			
O	0.0247662	0.1401379	0.3459097	O	-2.2938592	-3.3318901	0.5307381
C	1.9127482	0.0514482	0.5187286	C	0.4650337	-1.9876599	-0.1343918
Au	3.4104755	2.7199137	0.1495259	Au	0.3123189	0.2193901	-0.0170001
C	4.9279351	4.1044879	0.0416123	C	0.8276194	2.1933689	-0.0507336
N	4.9970059	5.1988754	-0.7739617	N	0.3026150	3.1600962	-0.8584189
C	6.1670918	5.9080644	-0.5488086	C	0.8776508	4.3868499	-0.5783901
C	6.8503695	5.2396364	0.4306417	C	1.7906828	4.1778932	0.4223794
N	6.0777569	4.1420121	0.7784086	N	1.7407346	2.8311241	0.7360604
C	0.4163397	1.3421521	0.0617560	C	-2.1399720	-2.1232457	0.3483952
C	1.8804895	1.3642257	0.2526123	C	-0.7323007	-1.6852934	0.1549193
C	2.4945138	-1.2215130	0.6912160	C	1.7013515	-2.6676874	-0.3631912
C	2.0802450	-2.0906165	1.7521755	C	1.9295567	-3.9023356	0.3237217
C	2.7327816	-3.3269081	1.8615924	C	3.1380458	-4.5686107	0.0623203
C	3.7620525	-3.6205237	0.9779678	C	4.0900903	-4.0467391	-0.8277071
C	4.1682200	-2.8286250	-0.0551927	C	3.8577077	-2.8286326	-1.4891778
C	3.5300150	-1.5996798	-0.2121088	C	2.6676021	-2.1386225	-1.2565279
C	3.9690671	5.6008439	-1.7387813	C	-0.7782441	2.9543560	-1.8299944
C	6.4653339	3.1565106	1.7925576	C	2.6004267	2.1852746	1.7353557
C	-0.4959677	2.3725381	-0.3857919	C	-3.2734179	-1.1665394	0.3059922
C	-0.0285413	3.6833973	-0.6558756	C	-3.1092975	0.2272394	0.1669516
C	-0.9223179	4.6659517	-1.0867327	C	-4.2222319	1.0741512	0.1274319

C	-2.2823508	4.3484859	-1.2526876	C	-5.5149508	0.5336199	0.2254790
C	-2.7555792	3.0486801	-0.9860209	C	-5.6908145	-0.8551047	0.3661674
C	-1.8709648	2.0614331	-0.5525073	C	-4.5794535	-1.7008383	0.4076931
H	-2.2186925	1.0462041	-0.3397410	H	-4.6981359	-2.7831190	0.5156323
H	-2.9814842	5.1202884	-1.5913538	H	-6.3870816	1.1951362	0.1936114
H	-3.8164039	2.8148293	-1.1181052	H	-6.6990261	-1.2745179	0.4427962
H	-0.5666924	5.6799192	-1.2935830	H	-4.0836287	2.1552727	0.0238829
H	2.4375453	-4.0146794	2.6610041	H	3.3368375	-5.5180955	0.5710211
H	4.2526402	-4.6640730	1.0972538	H	5.0207162	-4.5957932	-1.0052317
H	4.9692159	-3.1215138	-0.7406227	H	4.5996180	-2.4233437	-2.1838179
H	3.8126192	-0.9143545	-1.0164945	H	2.4625072	-1.1922601	-1.7671144
H	5.6514692	2.4245093	1.8947997	H	2.1945159	1.1879299	1.9562570
H	6.6297050	3.6633275	2.7560043	H	2.6056771	2.7930586	2.6518929
H	7.3880420	2.6434510	1.4791507	H	3.6245871	2.0922244	1.3411111
H	3.2418945	4.7818899	-1.8343030	H	-0.7590469	1.9083376	-2.1680369
H	4.4376092	5.7903924	-2.7163329	H	-0.6171973	3.6204810	-2.6893339
H	3.4599099	6.5123568	-1.3870925	H	-1.7505327	3.1795416	-1.3628781
H	6.4116011	6.8151188	-1.0989534	H	0.5926711	5.2952909	-1.1061614
H	7.8096995	5.4472618	0.9015595	H	2.4667320	4.8662457	0.9266197
H	1.0331917	3.9146068	-0.5163307	H	-2.1010909	0.6550099	0.0966147
C	0.9900661	-1.6765467	2.7038152	C	0.9226446	-4.4480963	1.3046784
H	0.0309645	-1.5609707	2.1680882	H	-0.0896117	-4.4922905	0.8674747
H	0.8621091	-2.4171760	3.5081773	H	1.2122827	-5.4541783	1.6454030
H	1.2192256	-0.6946996	3.1564159	H	0.8544734	-3.7894738	2.1910169
Int-V							
C	-7.6137414	1.7035089	-4.4344278				
C	-7.8144086	2.5522476	-5.5249344				
C	-6.8439665	3.5167841	-5.8552139				
C	-5.6683423	3.6327102	-5.0931628				
C	-5.4593127	2.7864444	-4.0006414				
C	-6.4317462	1.8147199	-3.6624053				
H	-4.5458580	2.8727440	-3.4037071				
H	-7.0057437	4.1809570	-6.7107014				
H	-4.9162945	4.3840616	-5.3530516				
H	-8.7274759	2.4669242	-6.1224945				
C	-6.2332890	0.9162813	-2.5153109				
O	-7.1392335	0.0581604	-2.2356729				
C	-5.0535945	1.0028462	-1.7343454				
C	-4.0339873	1.0499496	-1.0421444				
C	-2.8653271	1.0981083	-0.2454480				
C	-1.8454132	2.0354098	-0.5642395				
C	-2.7172684	0.2098689	0.8680268				
C	-1.5373748	0.3007472	1.6215275				
C	-0.5326730	1.2287500	1.3009105				
C	-0.6847208	2.0986075	0.2073381				
H	-1.4012844	-0.3679824	2.4783113				
H	0.3755891	1.2727395	1.9110723				
H	0.0993641	2.8210033	-0.0393228				
H	-1.9843096	2.7029335	-1.4199657				
Au	-7.0767984	-1.2980625	-0.6441518				
C	-7.0492951	-2.6009542	0.8585251				
N	-6.8751933	-3.9522701	0.7813724				
N	-7.1516189	-2.3224360	2.1915523				
C	-7.0417321	-3.4861622	2.9381087				
C	-6.8676918	-4.5121023	2.0501644				
H	-7.0997383	-3.4830293	4.0250930				
H	-6.7427743	-5.5817508	2.2090449				
C	-6.7143494	-4.7259480	-0.4548794				
H	-5.7349699	-5.2288348	-0.4497377				
H	-7.5188520	-5.4739232	-0.5269906				
H	-6.7723626	-4.0359331	-1.3084510				
C	-7.3528807	-0.9922796	2.7761842				
H	-6.4945295	-0.7357018	3.4160757				
H	-7.4401189	-0.2615978	1.9596718				
H	-8.2772823	-0.9894677	3.3737892				
H	-8.3586215	0.9496619	-4.1649031				
C	-3.7989712	-0.7827621	1.2112276				
H	-3.9602942	-1.4964030	0.3830256				
H	-3.5447580	-1.3528799	2.1182012				
H	-4.7619363	-0.2684488	1.3762864				
Ynones and Aldehydes							
1a				1b			

C	-1.0952065	-0.8525023	-0.0583272	C	-1.1318989	-0.8000017	-0.0878501
C	0.1819556	-1.3989712	0.1403331	C	0.1259406	-1.4040698	0.0751259
C	1.2789445	-0.5399792	0.2406683	C	1.2771548	-0.6105690	0.1641627
C	1.1297344	0.8644029	0.1498313	C	1.1757363	0.7950087	0.0899835
C	-0.1679966	1.4265747	-0.0531431	C	-0.0915384	1.3951514	-0.0750951
C	-1.2559534	0.5374085	-0.1535553	C	-1.2391982	0.6008734	-0.1629938
H	-1.9693810	-1.5075692	-0.1403260	H	-2.0314286	-1.4214040	-0.1561761
H	0.3204620	-2.4822857	0.2160717	H	0.2083774	-2.4944832	0.1329448
H	2.2809031	-0.9539995	0.3948356	H	2.2597175	-1.0774938	0.2912144
H	-2.2582359	0.9517547	-0.3115311	H	-2.2209754	1.0691129	-0.2905841
C	-0.4284062	2.9105895	-0.1670400	H	-0.1496611	2.4867551	-0.1315410
H	0.1605012	3.3597584	-0.9849035	O	2.2852397	2.9186692	0.1119847
H	-1.5001482	3.0940394	-0.3503530	C	2.3752749	1.6849041	0.1790453
H	-0.1232518	3.4419000	0.7507478	C	4.7882361	0.5705120	0.4989163
O	2.3190112	2.9621401	0.2554604	C	3.6677449	1.0555695	0.3493880
C	2.3451061	1.7231116	0.2735737	C	6.0913768	0.0246267	0.6720499
C	4.7574635	0.5845672	0.5473353	C	7.2245703	0.8926905	0.7499858
C	3.6276276	1.0534322	0.4225631	C	8.4899530	0.3070665	0.9208627
C	6.0601935	0.0236458	0.6897842	C	8.6480017	-1.0850899	1.0143973
C	7.1939926	0.8666866	0.8233169	C	7.5304627	-1.9327276	0.9371243
C	8.4694977	0.3090611	0.9600916	C	6.2580323	-1.3811462	0.7665029
C	8.6349239	-1.0866907	0.9664924	H	9.3705740	0.9562920	0.9816805
C	7.5176630	-1.9296387	0.8366430	H	9.6490631	-1.5088307	1.1484391
C	6.2369952	-1.3845326	0.6986772	H	7.6518259	-3.0183427	1.0093591
H	7.0591264	1.9525325	0.8182827	H	5.3759103	-2.0260465	0.7035477
H	9.3401699	0.9654037	1.0609182	C	7.0551062	2.3890429	0.6527720
H	9.6358509	-1.5181619	1.0732249	H	8.0285273	2.9025190	0.6988925
H	7.6465855	-3.0170043	0.8431755	H	6.5521388	2.6696570	-0.2901523
H	5.3637881	-2.0361135	0.5959438	H	6.4195490	2.7669170	1.4743638
3a				3b			
C	-6.6302378	1.5054476	0.0146154	C	-6.4216989	1.5813197	0.0058284
C	-5.4577380	0.7210420	0.0085959	C	-5.2277461	0.8312986	0.0190210
C	-5.5527689	-0.6883619	-0.0050855	C	-5.3054299	-0.5841601	0.0083354
C	-6.8083232	-1.3024258	-0.0124928	C	-6.5377890	-1.2230626	-0.0147338
C	-7.9756872	-0.5144941	-0.0065145	C	-7.7333929	-0.4586419	-0.0273482
C	-7.8879894	0.8877036	0.0069601	C	-7.6711683	0.9534056	-0.0169896
H	-6.5493762	2.5990594	0.0250853	H	-6.3706678	2.6768334	0.0135671
H	-4.6293562	-1.2772464	-0.0097470	H	-4.3746567	-1.1612143	0.0184743
H	-6.8862826	-2.3948374	-0.0228562	H	-6.6179657	-2.3145228	-0.0236072
H	-8.9585076	-0.9983399	-0.0122404	H	-8.5813410	1.5577476	-0.0265842
H	-8.7992037	1.4949781	0.0113548	C	-3.9244886	1.5139533	0.0439324
C	-4.1318644	1.3815748	0.0164960	O	-2.8336152	0.9478154	0.0580480
O	-3.0589364	0.7891431	0.0121528	H	-3.9854692	2.6344132	0.0499170
H	-4.1672284	2.5023069	0.0271263	O	-8.8837914	-1.1721934	-0.0490793
				C	-10.1382801	-0.4749545	-0.0624760
				H	-10.9114794	-1.2557776	-0.0788182
				H	-10.2553451	0.1463653	0.8439285
				H	-10.2293349	0.1584853	-0.9634556
3c				3d			
C	-6.4205685	1.5055699	0.0663258	C	-6.4285054	1.5593077	-0.0001178
C	-5.2057285	0.8025184	0.0134621	C	-5.2030497	0.8520914	0.0183122
C	-5.1944385	-0.6114568	-0.0071665	C	-5.2517071	-0.5642964	0.0144023
C	-6.4086528	-1.2988178	0.0245719	C	-6.4600840	-1.2459413	-0.0069896
C	-7.6336503	-0.6052889	0.0773048	C	-7.7047105	-0.5339552	-0.0258145
C	-7.6438193	0.8055015	0.0992974	C	-7.6505990	0.8960046	-0.0216959
H	-6.4360375	2.6010554	0.0827834	H	-6.4151936	2.6564345	0.0024326
H	-4.2348714	-1.1356574	-0.0479757	H	-4.3060894	-1.1175374	0.0287889
H	-6.4218364	-2.3939891	0.0086819	H	-6.4520369	-2.3382018	-0.0091509
C	-3.9346828	1.5647378	-0.0207305	H	-8.5715246	1.4828432	-0.0357484
O	-2.8210080	1.0561185	-0.0673059	C	-3.9265611	1.5662355	0.0404033
H	-4.0555043	2.6793027	-0.0008649	O	-2.8125849	1.0370557	0.0568826
H	-8.5677881	-1.1722990	0.1010173	H	-4.0212760	2.6854897	0.0416081
O	-8.7690487	1.5707908	0.1513723	N	-8.9026794	-1.2006212	-0.0470438
C	-10.0429916	0.9177335	0.1909291	C	-8.9379406	-2.6626356	-0.0552881
H	-10.7905006	1.7227404	0.2345508	H	-9.9864368	-2.9906836	-0.0746350
H	-10.2084246	0.3082689	-0.7170608	H	-8.4274654	-3.0749998	-0.9459615
H	-10.1363955	0.2772281	1.0877334	H	-8.4577837	-3.0844152	0.8477367
				C	-10.1613236	-0.4567470	-0.0660819
				H	-10.9953737	-1.1719773	-0.0769775
				H	-10.2647801	0.1856452	0.8287452
				H	-10.2394629	0.1838319	-0.9649015
3e				3f			

C	-6.5097089	1.6225090	-0.0218007	C	0.3419009	0.7651910	-0.0193388
C	-5.2694802	0.9311742	-0.0252380	O	-0.2027290	1.7727600	-0.4364803
C	-5.2700582	-0.4886232	-0.0478436	H	1.3797396	0.8159218	0.4122293
C	-6.4512062	-1.2200820	-0.0663671	C	-0.2672063	-0.6316178	-0.0145860
C	-7.6968308	-0.5105194	-0.0619614	C	-1.6685280	-0.6104895	-0.6431667
C	-7.7170210	0.8932764	-0.0401923	H	-2.1077352	-1.6233252	-0.6308983
H	-4.2915244	-0.9764423	-0.0497717	H	-2.3382382	0.0683212	-0.0875739
H	-8.6736240	1.4153792	-0.0371731	H	-1.6248395	-0.2610973	-1.6892538
C	-3.9885056	1.6423116	-0.0059606	C	-0.3230702	-1.0954405	1.4637755
O	-2.8863359	1.0854532	-0.0076612	H	-0.6958563	-2.1340253	1.5112549
H	-4.0593891	2.7559075	0.0110846	H	0.6778489	-1.0702845	1.9313390
O	-8.8030148	-1.2868147	-0.0797047	H	-1.0009300	-0.4555686	2.0557373
C	-10.0920734	-0.6586222	-0.0756515	C	0.6916104	-1.5540485	-0.8090290
H	-10.8225088	-1.4795755	-0.0909687	H	0.7499607	-1.2492406	-1.8687872
H	-10.2334852	-0.0513431	0.8370788	H	1.7115058	-1.5350913	-0.3839019
H	-10.2259789	-0.0242345	-0.9709024	H	0.3239159	-2.5946701	-0.7669783
O	-6.5509172	-2.5803044	-0.0885148				
C	-5.3333993	-3.3298285	-0.0918781				
H	-5.6310511	-4.3882823	-0.1095574				
H	-4.7242508	-3.1005564	-0.9867848				
H	-4.7358837	-3.1273570	0.8172138				
O	-6.4634171	2.9809647	-0.0000693				
C	-7.6862373	3.7255011	-0.0015794				
H	-8.2927609	3.4983587	0.8945082				
H	-7.3897696	4.7838783	0.0137815				
H	-8.2770128	3.5201135	-0.9132807				

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