Electronic Supplementary Material (ESI) for Chemical Science.

Directing Group Assisted *meta*-Hydroxylation by C-H Activation

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I. General considerations:

Reagent Information: Unless otherwise stated, all reactions were carried out under atmospheric condition in screw cap reaction tubes. All solvents were bought from Merck/Aldrich/ TCI in sure-seal bottle and were used as received. For column chromatography, silica gel (60–120 mesh or 100–200 mesh) obtained from SRL Co. and neutral activated alumina from Spectrochem was used. A gradient elution using pet ether and ethyl acetate was performed, based on Merck aluminum TLC sheets (silica gel $60F_{254}$). Benzyl halides were obtained from Aldrich/ TCI/Alfa Aeser and Spectrochem. HFIP was used from TCI.

Analytical Information: All isolated compounds were characterized by ^{1}H, ^{13}C NMR spectroscopy, mass analysis and IR spectroscopy. Copies of the ^{1}H NMR, ^{13}C NMR and few NOE spectra can be found in the supporting information. Unless otherwise stated, all Nuclear Magnetic Resonance spectra were recorded on a Bruker 400 MHz instrument. Some Nuclear Magnetic Resonance was taken on a Bruker 500 MHz instrument. All ^{1}H NMR experiments are reported in units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvent, unless otherwise stated. All ^{13}C NMR spectra were reported in ppm relative to deuterochloroform (77.23 ppm), unless otherwise stated, and all were obtained with ^{1}H decoupling. The NMR yields were calculated using 1,3,5-trimethoxybenzene as the reference. High-resolution mass spectra (HRMS) were recorded on a micro-mass ESI TOF (time of flight) mass spectrometer. Neat infrared spectra were recorded on a Perkin-Elmer spectrum one FT-IR spectrometer. The data was recorded in transmittance mode (%T, cm^{-1}).

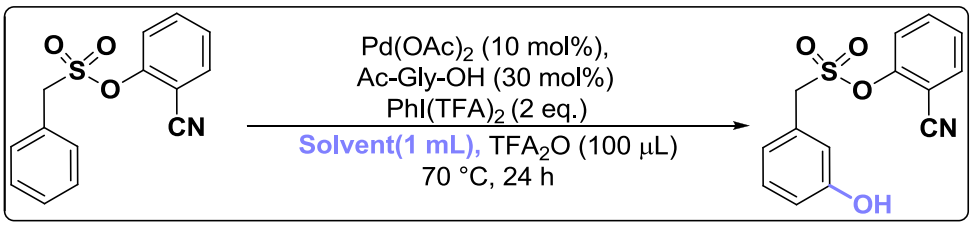
Description of Reaction Tube:

Fig A. Pictorial description of reaction tube for demethylenation: Fisher brand Disposable Borosilicate Glass Tubes (16*125mm) with Threaded End (Fisher Scientific Order No.1495935A) [left]; Kimble Black Phenolic Screw Thread Closures with Open Tops (Fisher Scientific Order No. 033407E) [middle]; Thermo Scientific National PTFE/Silicone Septa for Sample Screw Thread Caps (Fisher Scientific Order No. 03394A) [right].

II. Optimization:

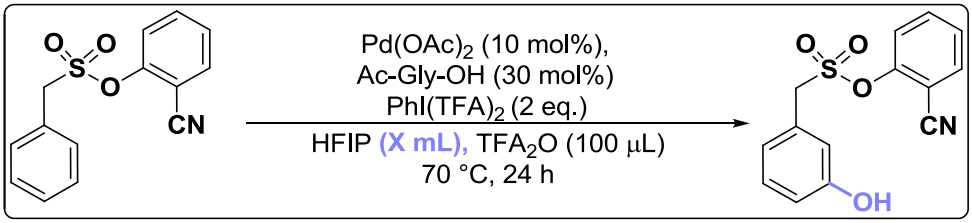
A. Optimization details for *meta* –hydroxylation:

Table S1: Solvent Optimization



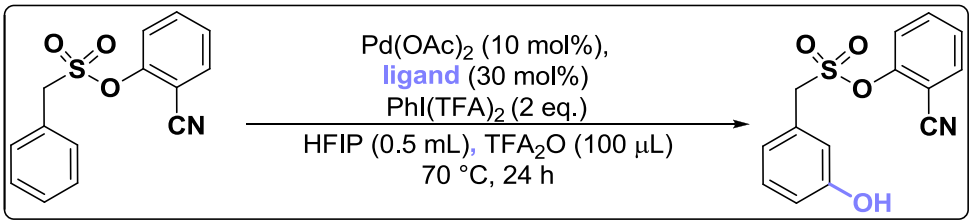
	Solvent	Yield (meta:others)
1	**HFIP**	**28% (multiple pdts)**
2	Trifluoroethanol(TFE)	10% (multiple pdts)
3	DCE	n.d
4	DCM	n.d
5	Trifluorotoluene	n.d
6	Toluene	n.d
7	MeCN	n.d
8	Dioxane	n.d
9	DMF	n.d
10	DMSO	n.d
11	NMP	n.d
12	DMA	n.d
13	Sulpholane	n.d
14	THF	n.d
15	Isopropanol	n.d
16	MeOH	n.d
17	EtOH	n.d
18	t-BuOH	n.d
19	HFIP:DCE (1:1)	18% (multiple pdts)
20	HFIP:DCE (1:9)	5% (multiple pdts)
21	HFIP:DCE (9:1)	23% (multiple pdts)
22	HFIP : TFE (1:1)	21% (multiple pdts)
23	HFIP : TFE (1:9)	8% (multiple pdts)
24	HFIP : TFE (9:1)	25% (multiple pdts)

Table S2: Solvent amount optimization



	Amount	Yield (meta:others)
1	0.3 mL	20% (multiple pdts)
2	**0.5 mL**	**32% (multiple pdts)**
3	0.7 mL	30% (multiple pdts)
4	1.0 mL	28% (multiple pdts)
5	1.25 mL	27% (multiple pdts)
6	1.5 mL	25% (multiple pdts)
7	2 mL	18% (multiple pdts)
8	3 mL	5% (multiple pdts)
9	4 mL	n.d

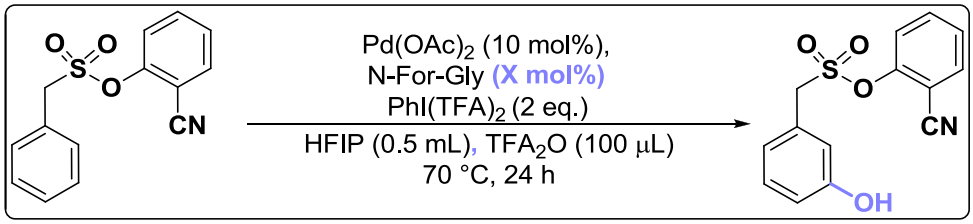
Table S3: Ligand optimization



	Ligand (30%)	Yield (meta:others)
1	Ac-Gly-OH	32% (multiple pdts)
2	**For-Gly-OH**	**44% (5:2:1)**
3	Boc-Gly-OH	23% (multiple pdts)
4	Ac-Ala-OH	25% (multiple pdts)
5	Piv-Ala-OH	23% (multiple pdts)
6	Benzoyl-Ala-OH	23% (multiple pdts)
7	Boc-Ala-OH	27% (multiple pdts)
8	Ac-Phe-OH	23% (multiple pdts)
9	Boc-Phe-OH	23% (multiple pdts)
10	Z-Gly-OH	36% (multiple pdts)
11	Boc-PheGly-OH	27% (multiple pdts)
12	Ac-Gly-ethylester	18% (multiple pdts)

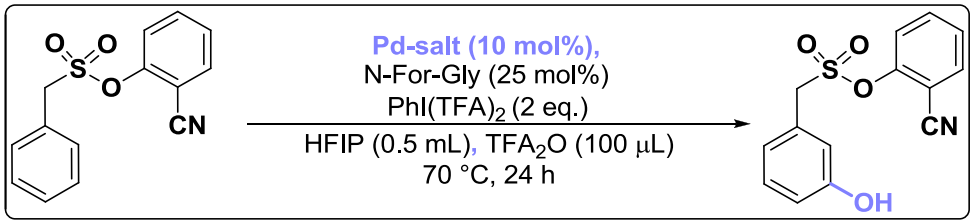
13	Ac-PheGly-OH	14% (multiple pdts)
14	Z-Ala-OH	32% (multiple pdts)
15	Z-Phe-OH	36% (multiple pdts)
16	Benzoyl-b-Ala-OH	27% (multiple pdts)
17	Boc-Aib-OH	23% (multiple pdts)
18	**1-(Boc-amino)cyclopentane carboxylic acid**	**42% (6:1)**
19	Glycylglycine	12% (multiple pdts)
20	Fmoc-L-Ala-OH	5% (multiple pdts)
21	Glycine	5% (multiple pdts)

Table S4: Ligand amount optimization



	Amount	Yield (meta:others)
1	10%	30% (multiple pdts)
2	15%	36% (multiple pdts)
3	20%	42% (6:2)
4	**25%**	**48% (7:2)**
5	30%	44% (5:2)

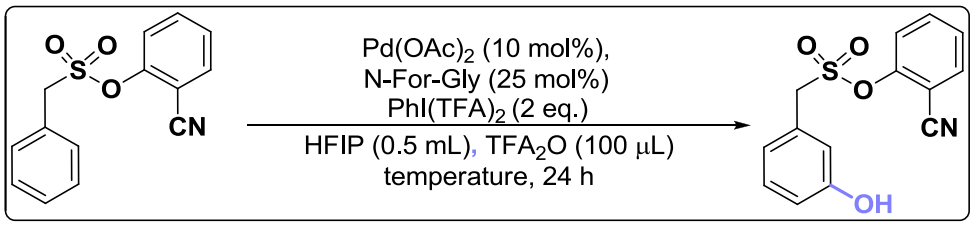
Table S5: Pd-salt optimization



	Pd-salt	Yield (meta:others)
1	**$Pd(OAc)_2$**	**48% (7:2)**
2	**$Pd(CF_3COO)_2$**	**44% (7:3)**
3	$Pd(piv)_2$	42% (5:2)
4	$Pd(acac)_2$	10% (3:1)

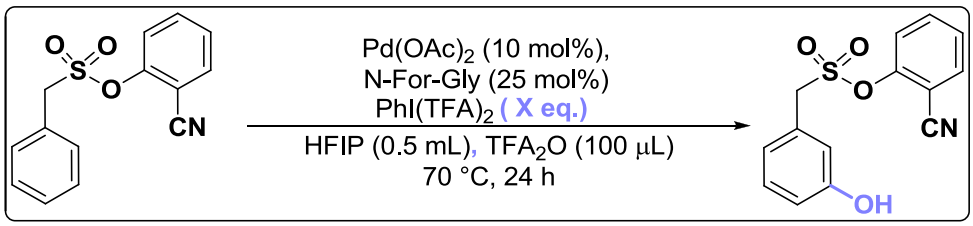
5	$PdSO_4$	n.d
6	$Pd(PPh_3)_2Cl_2$	n.d
7	$Pd(dppf)Cl_2$	n.d
8	$PdCl_2$	25% (multiple pdts)
9	$Pd(CH_3CN)_2Cl_2$	20% (multiple pdts)
10	$Pd_2(dba)_3$	n.d
11	$Pd(COD)Cl_2$	n.d

Table S6: Temperature optimization



	Temperature	Yield (meta:others)
1	RT	n.d
2	40 °C	10% (5:1)
3	60 °C	25% (5:1)
4	**70 °C**	**48% (7:3)**
5	80 °C	45% (7:3)
6	90 °C	43% (7:3)
7	100 °C	41% (7:3)
8	110 °C	27% (7:4)
9	120 °C	n.d
10	130 °C	n.d

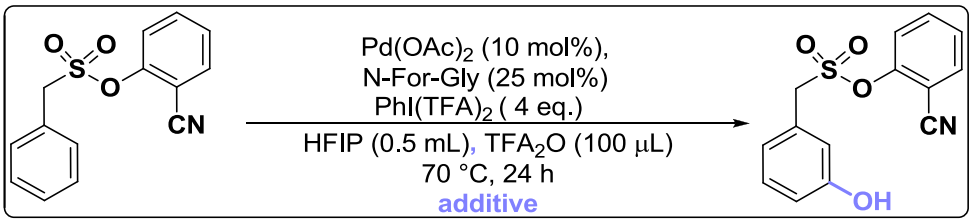
Table S7: Reagent amount optimization



	Amount	Yield (meta:others)
1	1 eq.	27% (3:2)

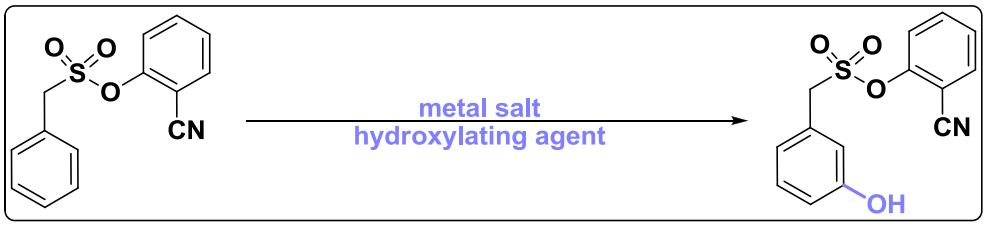
2	1.5 eq	42% (4:2)
3	2 eq	48% (7:3)
4	2.5 eq	54% (7:2)
5	3 eq	58% (8:2)
6	3.5 eq	61% (10:1)
7	**4 eq**	**65% (12:1)**
8	4.5 eq.	64% (6:1)
9	5 eq.	58% (3:1)

Table S8: Effect of additive



	Additive (2 eq)	**Yield (meta:others)**
1	K_2CO_3	n.d
2	K_3PO_4	n.d
3	NaOAc	n.d
4	Cs_2CO_3	n.d
5	TFA	n.d
6	AcOH	n.d
7	$AgNO_3$	n.d
8	Ag_2CO_3	45% (10:1)
9	AgOAc	41% (9:1)
10	$Cu(OAc)_2$	31%(multiple pdts)
11	BQ	n.d
12	$K_2S_2O_8$	18% (3:1)
13	$Na_2S_2O_8$	17% (3:1)
14	-	65% (12:1)
15	**No- $(TFA)_2O$**	**78% (>20:1)**

Table S9: Different hydroxylating reagent:

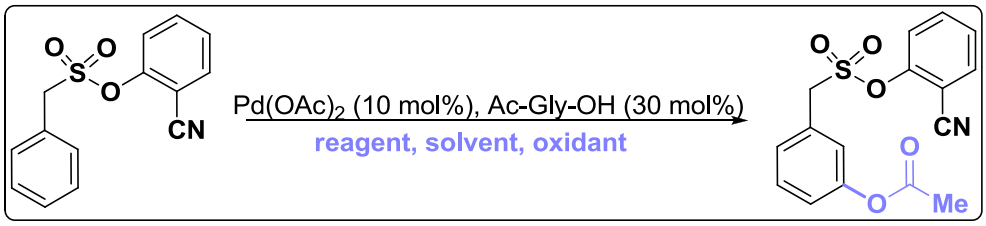


	Metal salt	-OH source	Yield (meta:others)
1	$PdCl_2$ / $Pd(OAc)_2$	TBHP	0
2	$PdCl_2$	H_2O_2	0
3	$PdCl_2$	NHPI	0
4	$Cu(OAc)_2$	$(PhCO)_2O$, HFIP	0
5	$PdCl_2$ / $Pd(OAc)_2$	TEMPO	0
6	$Cu(OAc)_2$	TBAI, Ag_2CO_3,	0
7	$PdCl_2$	$K_2S_2O_8$, CF_3COOH	0
8	$Pd(OAc)_2$	$Na_2S_2O_8$; Dioxane	0
9	$Pd(OAc)_2$	$PhI(TFA)_2$, $(CF_3CO)_2O$	11 %
10	**$Pd(OAc)_2$**	**$PhI(TFA)_2$, HFIP**	**78 % (>20:1)**
11*	**$Pd(TFA)_2$**	**$PhI(TFA)_2$, HFIP**	**74% (>20:1)**

**Ligand is 1-(Boc-amino)cyclopentane carboxylic acid instead of For-Gly-OH.*

B. Optimization details for *meta* –acetoxylation:

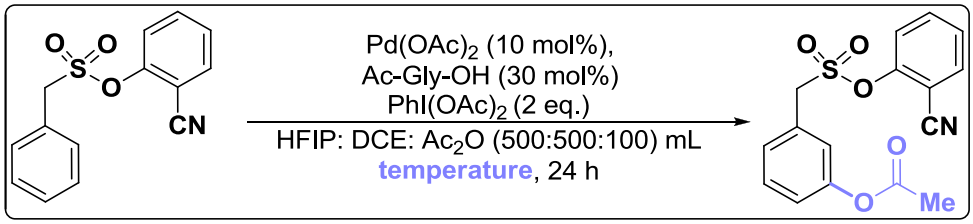
Table S10: Various acetoxylation condition.



	Reagent	Solvent	Oxidant	Product:Substrate
1	$PhI(OAc)_2$ (2 eq.)	DCE : HFIP : Ac_2O (500:500:100) µL	--	42 % (multiple pdts) : 48%
2	$PhI(OAc)_2$ (2 eq.)	DCE: HFIP: Ac_2O (500:500:100) µL	Ag_2CO_3 (2 eq)	35% (multiple pdts) : 65%
3	**$PhI(OAc)_2$ (2 eq.)**	**DCE: HFIP (500:500) µL**	**--**	**27% (*m:other =10:1*): 71%**

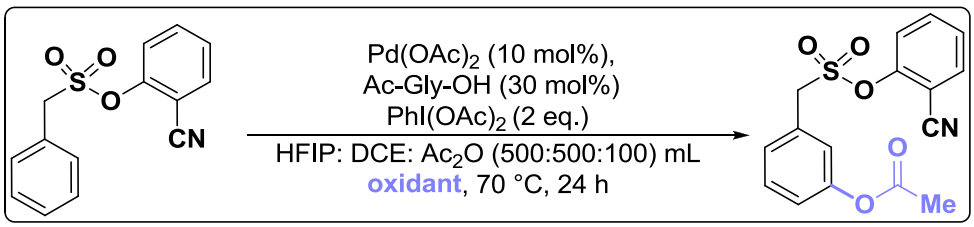
4	Ac_2O (10 eq.)	DCE: HFIP (500:500) µL	--	No product
5	$PhI(OAc)_2$ (2 eq.)	AcOH (1mL)	--	No Product
6	Ac_2O (10 eq.)	AcOH (1mL)	--	Undesired product (X)
7	Ac_2O (10 eq.)	AcOH (1mL)	Oxone (2 eq.)	Undesired product (X)
8	Ac_2O (10 eq.)	AcOH (1mL)	$K_2S_2O_8$ (2 eq.)	Undesired product (X)
9	-	AcOH (1mL)	--	Undesired product (X)
10	$PhI(OAc)_2$ (2 eq.)	AcOH: $CHCl_3$(500:500) µL	--	No Product

Table S11: Variation of temperature



	Temperature	Product:Substrate
1	rt	n.d
2	40 °C	n.d
3	60 °C	10% (multiple products): 85%
4	**70 °C**	**36 % (multiple product): 64 %**
5	80 °C	31 % (multiple product): 69 %
6	90 °C	36 % (multiple product): 40 %
7	100 °C	34 % (multiple product): 35 %
8	110 °C	31 % (multiple product): 40 %
9	120 °C	25 % (multiple product): 35 %

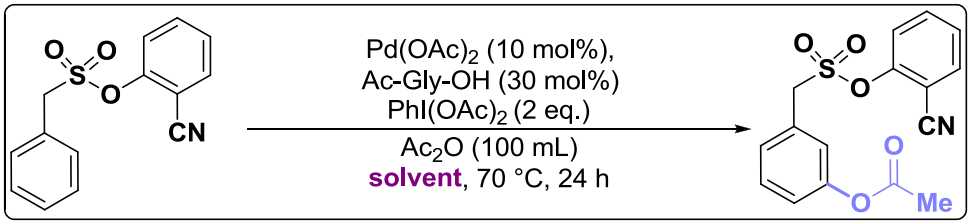
Table S12: Variation of oxidant



	Oxidant (2 eq.)	Product : Substrate
1	Ag_2CO_3	35% (multiple product):65%
2	AgOAc	18% (multiple product):62%
3	$Cu(OAc)_2$	No Product
4	$AgNO_3$	18% (multiple product):62%
5	$CuBr_2$	No Product
6	BQ	No Product
7	Oxone	36% (multiple product):36%
8	$K_2S_2O_8$	23% (multiple product):31%
9	$Fe(NO_3)_3$, $9H_20$	No Product
10	--	42% (multiple product):48%
11*	--	**59% (multiple product):31%**

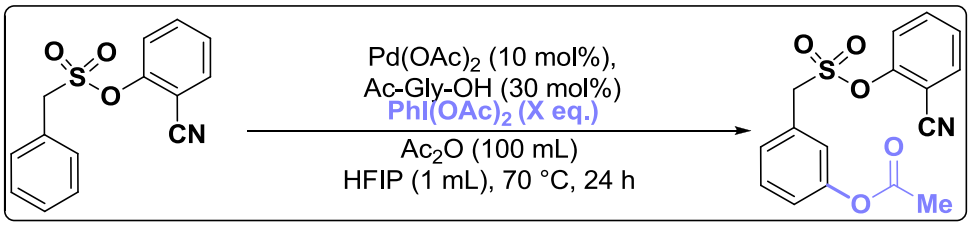
** Solvent is HFIP:Ac_2O (1 mL:100 μL)*

Table S13: Variation of oxidants



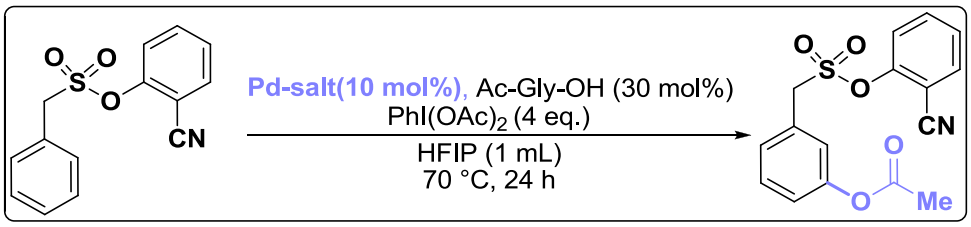
	Solvent (1 mL)	Product: Substrate
1	HFIP:DCE (1:1)	42% (multiple product):48%
2	**HFIP**	**59% (multiple product):31%**
3	DCE	No Product
4	MeCN	No Product
5	*t*-amyl –OH	No Product
6	Toluene	No Product
7	AcOH	Undesired product (X)
8	DMF	No Product
9	H_2O	Undesired product (X)

Table S14: Variation of reagent amount



Entry	Amount (X eq.)	Temperature	Product : Substrate
1	2	70 °C	59% (multiple product):31%
2	2.5	70 °C	54% (multiple product):40%
3	3	70 °C	54% (multiple product):35%
4	3.5	70 °C	59% (multiple product):31%
5	**4**	**70 °C**	**63% (multiple product):27%**
6	4	80 °C	54% (multiple product):20%
7	4	90 °C	49% (multiple product):10%
8	4	100 °C	48% (multiple product):5%
9*	**4**	**70 °C**	**61% (7:3):27%**

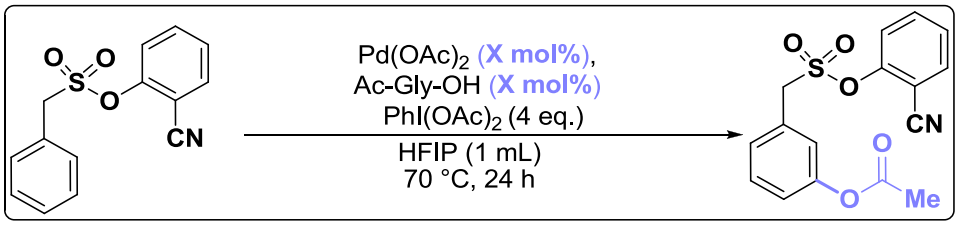
Table S15: Variation of Pd-salt



Entry	Pd-salt	Yield (*meta:others*)
1	**$Pd(OAc)_2$**	**61% (7:3)**
2	$Pd(CF_3COO)_2$	50% (5:1)
3	**$Pd(piv)_2$**	**60% (5:2)**
4	$Pd(acac)_2$	58% (4:1)
5	$PdSO_4$	No Product
6	$Pd(PPh_3)_2Cl_2$	54% (6:1)
7	$Pd(dppf)Cl_2$	No Product
8	$PdCl_2$	54% (6:1)
9	$Pd(CH_3CN)_2Cl_2$	58%

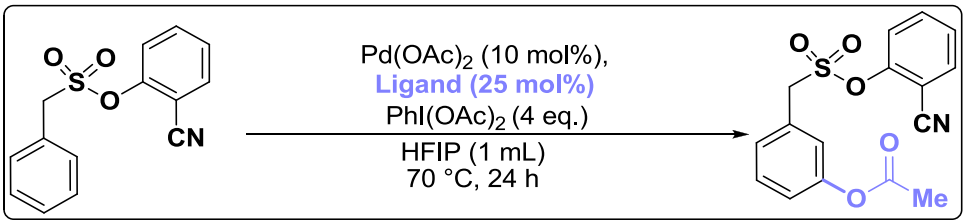
10	$Pd_2(dba)_3$	54% (7:1)
11	$Pd(COD)Cl_2$	54% (6:1)

Table S16: Variation of Pd-salt and ligand amount



	$Pd(OAc)_2$	**Ac-Gly-OH**	**Yield (meta:others)**
1	2.5 mol%	30 mol%	45% (2:1)
2	5 mol%	20 mol%	49% (4:1)
3	5 mol%	30 mol%	45% (2:1)
4	10 mol%	10 mol%	55% (3:1)
5	10 mol%	20 mol%	55% (5:1)
6	10 mol%	30 mol%	61%(7:3)
7	10 mol%	40 mol%	54% (4:1)
8	10 mol%	50 mol%	35% (2:1)
9	**10 mol%**	**25 mol%**	**69% (12:1)**

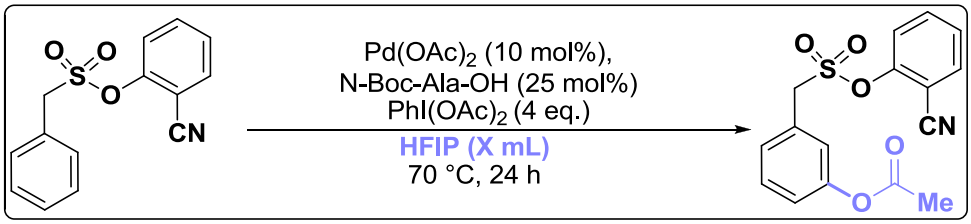
Table S17: Variation of ligand



Entry	**Ligand**	**Yield (*meta:others*)**
1	Ac-Gly-OH	69% (12:1)
2	DL-Proline	No Product
3	Boc-D-Valine	54% (7:6)
4	Ac-L-Leucine	54% (7:6)
5	Ac-DL-Valine	49% (11:3)

6	Ac-L-Phenylalanine	61% (1:1)
7	Boc-L-Proline	54% (3:1)
8	Ac-Alanine	40% (9:13)
9	Bathophen.	No Product
10	1,1'-Bi(2-Napthylamine)	No Product
11	4,7-dimethoxy-1,10-Phen.	No Product
12	**N-Boc-Ala**	**72% (12:1)**

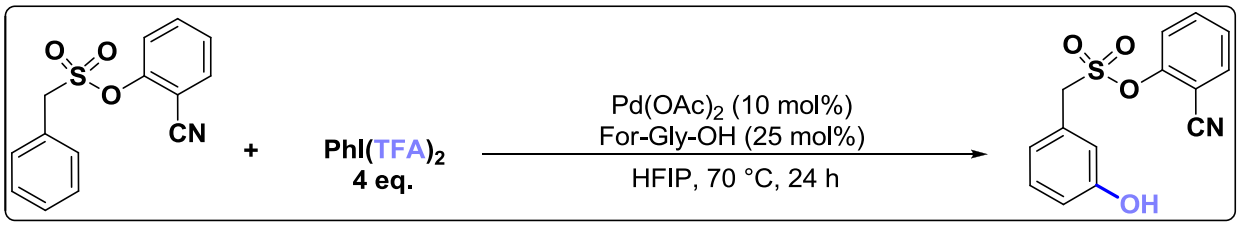
Table S18: Variation of solvent amount



Entry	HFIP	Yield (meta:others)
1	**0.3**	**75% (11:1)**
2	**0.5**	**76% (12:1)**
3	0.5+ DCE (100 µL)	67% (7:1)
4	0.75	70% (9:1)
5	1	72% (12:1)
6	1.25	63% (10:1)
7	1.5	59% (9:1)
8	2	35% (5:1)
9	3	25% (3:1)
10	100 mL+ DCE (0.5 µL)	24%

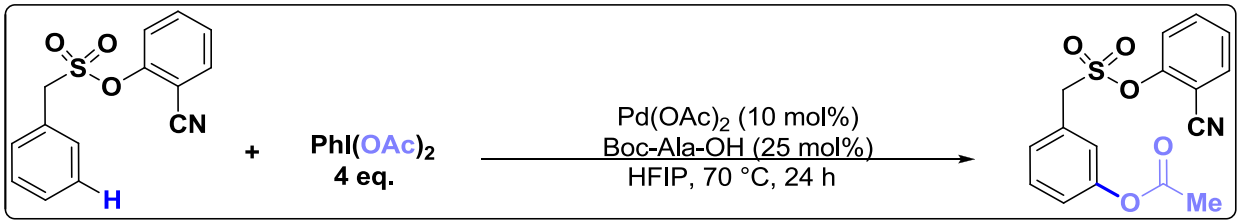
III. General Procedure:

A. General Procedure A: Procedure for *meta*-hydroxylation



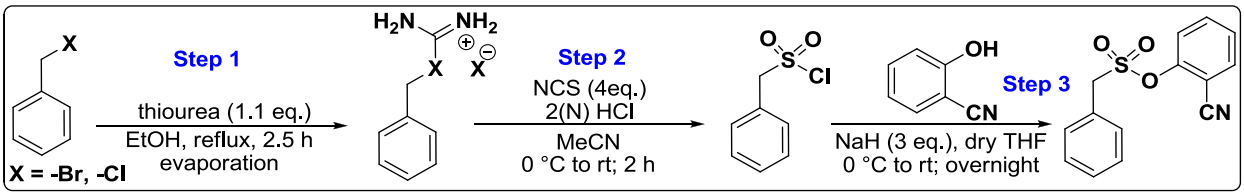
In a oven dried reaction tube, charged with magnetic stir-bar, $Pd(OAc)_2$ (10 mol%; 4.48 mg), For-Gly-OH (25 mol%; 5.15 mg) and arylmethanesuphonic ester substrate (0.2 mmol) were added. The hydroxylating agent $PhI(TFA)_2$ (0.8 mmol; 344 mg) was added to the reaction mixture followed by the HFIP (1 mL). The reaction tube was capped and stirred at room temperature for 15 mins and then placed to a preheated oil-bath at 70 °C for 24 h. Upon completion, the reaction was taken out to cool and diluted with ethyl acetate. The solution was filtered through celite bed. The filtrate was evaporated under reduced pressure and passed through the column for purification. Petroleum ether and ethyl acetate mixture was used as the eluent.

B. General Procedure B: Procedure for *meta*-acetoxylation



In a oven dried reaction tube, charged with magnetic stir-bar, $Pd(OAc)_2$ (10 mol%; 4.48 mg), N-Boc-Ala-OH (25 mol%; 9.45 mg) and arylmethanesuphonic ester substrate (0.2 mmol) were added. The hydroxylating agent $PhI(OAc)_2$ (0.8 mmol; 258 mg) was added to the reaction mixture followed by the HFIP(1 mL). The reaction tube was capped and stirred at room temperature for 15 mins and then placed to a preheated oil-bath at 70 °C for 24 h. Upon completion, the reaction was taken out to cool and diluted with ethyl acetate. The solution was filtered through celite bed. The filtrate was evaporated under reduced pressure and passed through the column for purification. Petroleum ether and ethyl acetate mixture was used as the eluent.

C. General Procedure C: Procedure for sulphonate ester synthesis



The synthesis was done following the literature procedure with few modifications.[1]

Step 1: In an oven dried 250 mL round bottomed flask the desired benzyl chloride/bromide was added along with thiourea. Absolute ethanol was added to it as solvent and refluxed for 2.5 h. Upon completion the round bottomed flask was cooled and evaporated under reduced pressure yielding white solid compound, which was directly used in the next step.

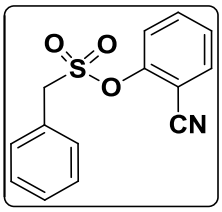
Step 2: N-chlorosuccinimide (4 eq.) was taken in clean round bottomed flask charged with stir-bar. 2(N) HCl was added to it along with MeCN. The reaction mixture was stirred on an ice cooled water bath. The solid salt obtained from the first step was added slowly to this reaction mixture and stirred vigorously. The addition led to an exothermic reaction. However the temperature was maintained below 25 °C. Upon forming a clear solution the mixture was warmed to the room temperature and stirred for 2 h. The reaction was evaporated under reduced

pressure to remove the acetonitrile. The remaining solution was diluted with water and extracted with ethyl acetate. The organic portion was dried over anhydrous Na_2SO_4. The solution was concentrated under reduced pressure and purified through column chromatography.

Step 3: In an oven dried round bottomed flask 2-hydroxybenzonitrile was dissolved in dry THF and cooled to 0 °C on an ice bath. NaH was added to the reaction mixture slowly until effervescence stopped. The mixture was stirred further for another 30 mins. Benzylsulphonyl chloride, dissolved in THF, was added to the reaction mixture slowly. Upon completion of addition the reaction was taken out of the ice bath and stirred at room temperature overnight. Once completed the reaction was quenched with distilled water and extracted with ethyl acetate. The organic portion was dried over anhydrous Na_2SO_4. The solution was concentrated under reduced pressure and purified through column chromatography.

IV. Characterization:

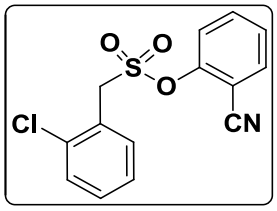
A. Characterization of substrate:



2-cyanophenyl phenylmethanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.74 – 7.65 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.66 – 7.56 (m, 1H), 7.57 – 7.49 (m, 1H), 7.49 – 7.34 (m, 4H), 4.75 – 4.70 (s, 2H).

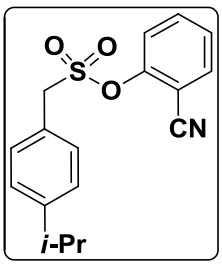
^{13}C NMR (101 MHz, $CDCl_3$): δ = 58.67, 76.91, 77.55, 107.43, 115.22, 123.57, 126.48, 127.48, 129.29, 129.76, 131.26, 133.97, 134.67, 150.27.



2-cyanophenyl (2-chlorophenyl)methanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.68 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.69 – 7.58 (m, 2H), 7.53 – 7.39 (m, 2H), 7.43 – 7.31 (m, 3H), 5.02 – 4.94 (s, 2H).

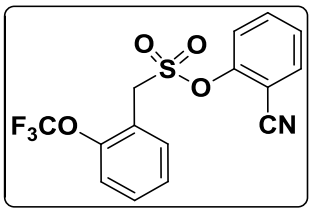
^{13}C NMR (101 MHz, $CDCl_3$) δ 55.50, 76.91, 77.55, 107.57, 115.06, 123.54, 125.02, 127.59, 127.67, 130.47, 131.27, 133.25, 134.09, 134.69, 135.81, 150.02.



2-cyanophenyl (4-isopropylphenyl)methanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.68 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.65 – 7.56 (m, 1H), 7.48 – 7.40 (m, 2H), 7.43 – 7.34 (m, 2H), 7.32 – 7.24 (m, 2H), 4.72 – 4.68 (s, 2H), 3.01 – 2.85 (hept, *J* = 7.0 Hz, 1H), 1.27 – 1.24 (d, *J* = 6.9 Hz, 6H).

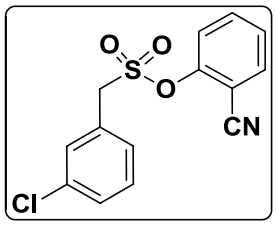
^{13}C NMR (101 MHz, $CDCl_3$) δ 24.04, 34.14, 58.52, 76.91, 77.54, 107.46, 110.19, 115.26, 123.57, 123.64, 127.44, 131.23, 133.96, 134.63, 150.46, 150.69.



2-cyanophenyl (2-(trifluoromethoxy)phenyl)methanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.68 (ddd, *J* = 7.9, 6.2, 1.6 Hz, 2H), 7.66 – 7.60 (ddd, *J* = 8.3, 7.5, 1.7 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.45 – 7.42 (m, 1H), 7.41 – 7.34 (m, 3H), 4.90 – 4.78 (s, 2H).

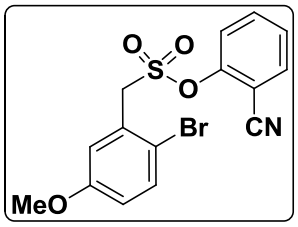
^{13}C NMR (101 MHz, $CDCl_3$) δ 52.42, 76.91, 77.55, 107.62, 114.99, 119.18, 120.17, 123.51, 127.22, 127.64, 129.67, 131.61, 132.27, 132.43, 133.38, 134.11, 134.69, 138.50, 148.54, 149.97.



2-cyanophenyl (3-chlorophenyl)methanesulfonate:

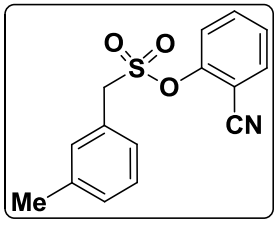
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.68 – 7.60 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.54 – 7.50 (t, *J* = 1.9 Hz, 1H), 7.47 – 7.34 (m, 5H), 4.75 – 4.66 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.07, 76.91, 77.54, 107.49, 115.18, 123.66, 127.68, 128.38, 129.46, 130.07, 130.55, 131.24, 134.02, 134.75, 135.16, 150.15.



2-cyanophenyl (2-bromo-5-methoxyphenyl)methanesulfonate:

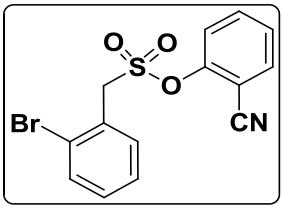
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.67 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.67 – 7.60 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.60 – 7.53 (d, *J* = 9.0 Hz, 1H), 7.52 – 7.44 (m, 1H), 7.45 – 7.38 (td, *J* = 7.6, 1.1 Hz, 1H), 6.95 – 6.86 (d, *J* = 9.0 Hz, 1H), 5.36 – 5.26 (s, 2H), 3.93 – 3.91 (s, 3H).



2-cyanophenyl m-tolylmethanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.66 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.65 – 7.58 (ddd, *J* = 8.6, 7.6, 1.7 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.35 – 7.28 (dd, *J* = 6.0, 2.6 Hz, 3H), 7.26 – 7.20 (m, 1H), 4.74 – 4.60 (s, 2H), 2.43 – 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 21.48, 58.70, 76.91, 77.54, 107.42, 115.23, 123.56, 126.26, 127.43, 128.29, 129.15, 130.54, 131.89, 133.96, 134.66, 139.14, 150.36.

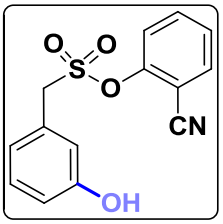


2-cyanophenyl (2-bromophenyl)methanesulfonate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.68 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.68 – 7.64 (ddd, *J* = 8.0, 2.6, 1.5 Hz, 2H), 7.64 – 7.59 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.45 – 7.41 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.41 – 7.36 (tt, *J* = 7.6, 1.3 Hz, 2H), 7.31 – 7.26 (m, 1H), 5.02 – 4.96 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 57.92, 76.91, 77.55, 107.51, 115.02, 123.49, 126.10, 126.80, 127.57, 128.25, 131.34, 133.18, 133.76, 134.03, 134.65, 149.93.

B. Characterization of *meta*-hydroxylated compounds:



2-cyanophenyl (3-hydroxyphenyl)methanesulfonate (**1a**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl phenylmethanesulfonate (0.2 mmol; 54.6 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether(10:90) mixture as the eluent. Yellow viscous liquid. Yield 74%; 43 mg.

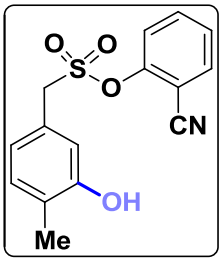
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.66 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.64 – 7.57 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.46 – 7.42 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.40 – 7.34 (td, *J* = 7.7, 1.1 Hz, 1H), 7.31 – 7.22 (t, *J* = 7.8 Hz, 1H), 7.08 – 7.00 (m, 2H), 6.94 – 6.87 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 4.68 – 4.63 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.52, 106.80, 115.37, 117.21, 118.26, 123.12, 123.34, 127.35, 127.64, 130.54, 134.06, 134.86, 150.31, 156.50.

Dept: ^{13}C NMR (101 MHz, $CDCl_3$) δ 58.35, 117.03, 118.08, 122.95, 123.16, 127.18, 130.37, 133.89, 134.68.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{12}NO_4S$: 290.0482; found: 290.0481

IR: 3375, 3000, 2952, 2725, 2596, 2245, 1696, 1601, 1486, 1360, 1286, 1155, 997, 775 cm^{-1}.



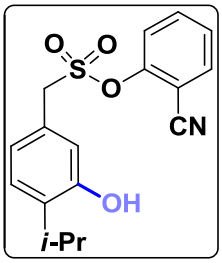
2-cyanophenyl (3-hydroxy-4-methylphenyl)methanesulfonate (**1b**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl *p*-tolylmethanesulfonate (0.2 mmol; 57.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (9:91) mixture as the eluent. Colourless solid; melting point: 126-128 °C; Yield 77%; 47 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.66 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.67 – 7.57 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.52 – 7.47 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.41 – 7.33 (td, *J* = 7.7, 1.1 Hz, 1H), 7.18 – 7.13 (m, 1H), 7.05 – 7.01 (d, *J* = 1.8 Hz, 1H), 6.98 – 6.92 (dd, *J* = 7.7, 1.8 Hz, 1H), 4.66 – 4.61 (s, 2H), 2.28 – 2.21 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 15.90, 58.57, 106.64, 115.55, 117.75, 122.95, 123.36, 124.91, 126.48, 127.15, 131.81, 134.06, 134.80, 150.56, 154.55.

HRMS: Calculated $[M+H]^+$ for $C_{15}H_{14}NO_4S^+$: 304.0638; found: 304.0640

IR: 3378, 3023, 2932, 2854, 2246, 1659, 1368, 1259, 1217, 1164, 1098, 870, 767 cm-^{1}.



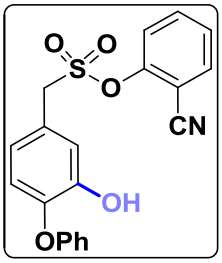
2-cyanophenyl (3-hydroxy-4-isopropylphenyl)methanesulfonate (**1c**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (4-isopropylphenyl)methanesulfonate (0.2 mmol; 63 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (10:90) mixture as the eluent. Colorless solid. Yield 63%; 42 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.66 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.65 – 7.57 (ddd, *J* = 8.5, 7.6, 1.7 Hz, 1H), 7.53 – 7.46 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.41 – 7.32 (td, *J* = 7.7, 1.1 Hz, 1H), 7.26 – 7.18 (d, *J* = 7.7 Hz, 1H), 7.08 – 6.94 (m, 2H), 4.67 – 4.60 (s, 2H), 3.35 – 3.13 (hept, *J* = 6.9 Hz, 1H), 1.25 – 1.23 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 22.59, 27.17, 58.53, 106.61, 115.59, 118.11, 122.86, 123.62, 124.46, 127.12, 127.38, 134.06, 134.78, 136.91, 150.64, 153.59.

HRMS: Calculated $[M+H]^+$ for $C_{17}H_{18}NO_4S^+$: 332.0951: found: 332.0957 .

IR: 3522, 3012, 2942, 2857, 2254, 1642, 1451, 1373, 1263, 1161, 1030, 920, 760 cm-^{1}.



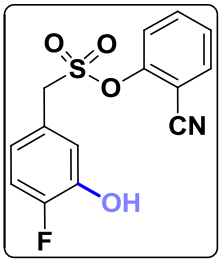
2-cyanophenyl (3-hydroxy-4-phenoxyphenyl)methanesulfonate (**1d**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (4-phenoxyphenyl)methanesulfonate (0.2 mmol; 73 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yellow viscous liquid. Yield 62%; 47 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.67 – 7.60 (ddd, *J* = 8.5, 7.6, 1.7 Hz, 1H), 7.48 – 7.37 (m, 3H), 7.33 – 7.24 (m, 3H), 7.19 – 7.14 (t, *J* = 2.1 Hz, 1H), 7.09 – 7.02 (ddd, *J* = 8.3, 2.6, 1.1 Hz, 1H), 6.99 – 6.93 (m, 2H), 4.75 – 4.65 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.29, 107.48, 115.11, 119.44, 119.86, 120.64, 121.30, 123.66, 126.24, 127.62, 128.31, 130.05, 130.72, 134.01, 134.71, 150.12, 155.36, 157.67.

HRMS: Calculated $[M+H]^+$ for $C_{20}H_{16}NO_5S^+$: 382.0749; found: 382.0749.

IR: 3400, 3101, 3012, 2989, 2942, 2857, 2261, 1649, 1498, 1219, 1188, 1158, 1136, 1095, 1032, 993, 959, 871, 771 cm-^{1}.



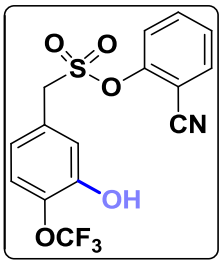
2-cyanophenyl (4-fluoro-3-hydroxyphenyl)methanesulfonate (**1e**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (4-fluorophenyl)methanesulfonate (0.2 mmol; 58.2 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Colourless solid; melting point: 147-150 °C; Yield 53%; 32.5 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.67 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.67 – 7.60 (ddd, *J* = 9.2, 7.6, 1.7 Hz, 1H), 7.50 – 7.45 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.43 – 7.37 (td, *J* = 7.7, 1.2 Hz, 1H), 7.23 – 7.18 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.16 – 7.07 (dd, *J* = 10.2, 8.4 Hz, 1H), 7.05 – 6.98 (ddd, *J* = 8.4, 4.4, 2.2 Hz, 1H), 5.90 – 5.51 (s, 1H), 4.68 – 4.61 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.10, 107.18, 115.29, 116.46, 116.65, 120.43 (*J* = 3 Hz.), 123.19, 123.22, 123.43, 123.82 (*J* = 7 Hz.), 127.50, 134.05, 134.79, 144.34 (*J* = 15 Hz.), 150.29, 153.37.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{11}FNO_4S^+$: 308.0393; found: 308.0374.

IR: 3372, 2925, 2861, 2250, 1601, 1510, 1488, 1449, 1359, 1308, 1278, 1217, 1161, 1020, 966, 868, 770 cm-^{1}.



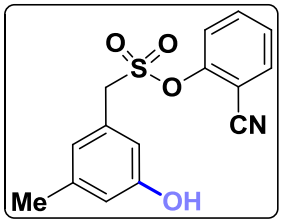
2-cyanophenyl(3-hydroxy-4-(trifluoromethoxy)phenyl)methanesulfonate (**1f**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (4-(trifluoromethoxy)phenyl)methanesulfonate (0.2 mmol; 71.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Colorless solid; melting point: 136-138 °C. Yield 51%; 38 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.68 – 7.61 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.52 – 7.44 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.44 – 7.36 (td, *J* = 7.7, 1.1 Hz, 1H), 7.29 – 7.26 (s, 2H), 7.16 – 7.05 (dd, *J* = 8.4, 2.2 Hz, 1H), 4.70 – 4.64 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.03, 107.17, 115.30, 120.39, 120.54, 121.60, 123.34, 123.40, 123.54 (*J* = 270 Hz.), 123.70, 126.55, 134.07, 134.81, 137.71, 148.40, 150.27.

HRMS: Calculated $[M+H]^+$ for $C_{15}H_{11}F_3NO_5S^+$: 374.0310; found: 374.0314.

IR: 3647, 2932, 2854, 2249, 1601, 1486, 1447, 1374, 1310, 1259, 1164, 1100, 1019, 973, 871, 773 cm-^{1}.



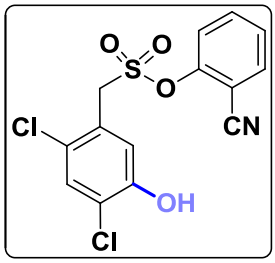
2-cyanophenyl(3-hydroxy-5-methylphenyl)methanesulfonate (**1g**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl m-tolylmethanesulfonate (0.2 mmol; 57.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether(9:91) mixture as the eluent. Colourless solid. Yield 75%; 45.5 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.66 – 7.59 (ddd, *J* = 8.4, 7.6, 1.8 Hz, 1H), 7.52 – 7.46 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.41 – 7.34 (td, *J* = 7.7, 1.1 Hz, 1H), 6.89 – 6.83 (dd, *J* = 5.2, 3.1 Hz, 2H), 6.76 – 6.71 (d, *J* = 1.9 Hz, 1H), 4.66 – 4.59 (s, 2H), 2.35 – 2.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 21.48, 29.91, 58.63, 106.79, 115.42, 115.45, 117.89, 123.06, 124.36, 127.25, 127.35, 134.06, 134.79, 140.93, 150.47, 156.29.

HRMS: Calculated $[M+H]^+$ for $C_{15}H_{14}NO_4S^+$: 304.0638; found: 304.0644

IR: 3344, 3023, 2932, 2854, 2243, 1169, 1368, 1259, 1217, 1164, 1098, 1029, 870, 767 cm-^{1}.



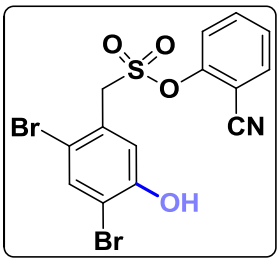
2-cyanophenyl (2,4-dichloro-5-hydroxyphenyl)methanesulfonate (**1h**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2,4-dichlorophenyl)methanesulfonate (0.2 mmol; 68 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (12:88) mixture as the eluent. Yellow viscous liquid. Yield 65%; 46 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.69 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.69 – 7.60 (ddd, *J* = 8.9, 7.6, 1.6 Hz, 1H), 7.62 – 7.58 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.50 (d, *J* = 2.1 Hz, 1H), 7.46 – 7.37 (td, *J* = 7.7, 1.1 Hz, 1H), 7.39 – 7.31 (dd, *J* = 8.4, 2.1 Hz, 1H), 4.99 – 4.87 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 55.01, 107.56, 110.20, 115.07, 123.57, 123.73, 127.71, 128.15, 130.40, 133.94, 134.12, 134.76, 136.59, 136.85, 149.94.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{10}Cl_2NO_4S^+$:357.9702; found: 357.9708.

IR: 3440, 2930, 2850, 2239, 1607, 1515, 1460, 1371 1230, 1161, 1090, 988, 867, 770 cm-^{1}.



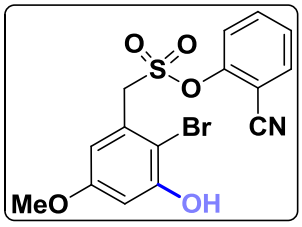
2-cyanophenyl (2,4-dibromo-5-hydroxyphenyl)methanesulfonate (**1i**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2,4-dibromophenyl)methanesulfonate (0.2 mmol; 85.8 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yellow solid. Yield 63%; 56.5 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.69 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.68 – 7.63 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.55 – 7.50 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.50 – 7.46 (s, 1H), 7.45 – 7.39 (td, *J* = 7.7, 1.1 Hz, 1H), 7.37 – 7.35 (s, 1H), 4.89 – 4.86 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 55.20, 107.14, 115.26, 120.43, 122.85, 123.29, 125.01, 126.99, 127.58, 130.44, 134.17, 134.86, 150.06, 151.02.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{10}Br_2NO_4S^+$: 445.8692; found: 445.8677.

IR: 3422, 2921, 2848, 2234, 1628, 1607, 1518, 1449, 1362, 1220, 1153, 1094, 990, 870, 770 cm-^{1}.



2-cyanophenyl (2-bromo-3-hydroxy-5-methoxyphenyl)methanesulfonate (**1j**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2-bromo-5-methoxyphenyl)methanesulfonate (0.2 mmol; 76 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. White solid. Yield 58%; 46 mg.

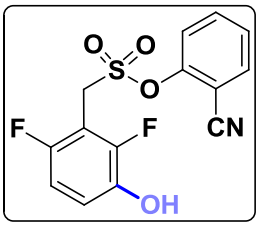
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.66 – 7.60 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.57 – 7.52 (d, *J* = 8.9 Hz, 1H), 7.51 – 7.46 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.44

– 7.37 (td, *J* = 7.7, 1.1 Hz, 1H), 6.92 – 6.87 (d, *J* = 8.9 Hz, 1H), 5.34 – 5.27 (s, 2H), 3.92 – 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 56.78, 56.86, 107.91, 114.35, 114.90, 117.21, 123.80, 126.31, 126.77, 127.68, 132.13, 134.13, 134.63, 149.74, 155.40.

HRMS: Calculated $[M+H]^+$ for $C_{15}H_{13}BrNO_5S^+$: 397.9698; found: 397.9690.

IR: 3392, 2930, 2861, 2239, 1627, 1610, 1523, 1450, 1363, 1199, 1092, 993, 870, 772 cm-^{1}.



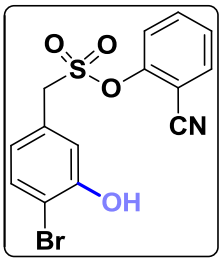
2-cyanophenyl (2,6-difluoro-3-hydroxyphenyl)methanesulfonate (**1k**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2,6-difluorophenyl)methanesulfonate (0.2 mmol; 61.8 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yellow solid. Yield 59%; 38 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.67 – 7.60 (ddd, *J* = 8.4, 7.5, 1.7 Hz, 1H), 7.56 – 7.50 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.44 – 7.36 (td, *J* = 7.6, 1.1 Hz, 1H), 7.13 – 7.04 (td, *J* = 9.3, 5.4 Hz, 1H), 6.96 – 6.87 (td, *J* = 8.9, 2.0 Hz, 1H), 4.88 – 4.84 (d, *J* = 1.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 46.95, 76.91, 77.55, 104.31, 104.62, 107.27, 111.69 (*J* = 4 Hz.), 111.92 (*J* = 4 Hz.), 114.74, 119.67 (*J* = 3 Hz.), 119.76 (*J* = 3 Hz.), 123.01, 127.52, 134.29, 134.75, 140.63 (*J* = 10 Hz.), 149.91, 153.77, 153.81.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{10}F_2NO_4S^+$: 326.0299: found: 326.0289.

IR: 3440, 2925, 2850, 2237, 1630, 1601, 1522, 1451, 1369 1225, 1158, 1095, 993, 871, 773 cm-^{1}.



2-cyanophenyl (4-bromo-3-hydroxyphenyl)methanesulfonate (**1l**): The compound was synthesized following the general **procedure A** 2-cyanophenyl (4-bromophenyl)methanesulfonate (0.2 mmol; 70.2 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Colorless Solid; melting point: 170-172 °C; Yield 55%; 40.5 mg.

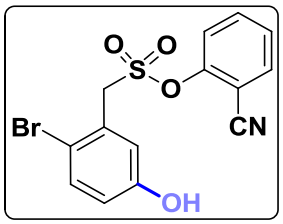
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.69 (ddd, *J* = 7.7, 1.8, 0.5 Hz, 1H), 7.68 – 7.61 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.55 – 7.51 (d, *J* = 8.2 Hz, 1H), 7.49 – 7.45 (ddd, *J* = 8.4, 1.1, 0.4 Hz, 1H), 7.44 – 7.38 (td, *J* = 7.7, 1.1 Hz, 1H), 7.22 – 7.19 (d, *J* = 2.1 Hz, 1H), 7.02 – 6.95 (dd, *J* = 8.2, 2.1 Hz, 1H), 4.69 – 4.59 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 58.14, 107.27, 112.16, 115.30, 118.94, 123.52, 124.46, 127.58,

127.73, 133.02, 134.05, 134.80, 150.23, 153.00.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{11}BrNO_4S^+$: 367.9592; found: 367.9588.

IR: 3397, 3018, 2945, 2866, 2245, 1623, 1589, 1401, 1366, 1264, 1220, 1168, 990, 873, 771, 673 cm-[1].



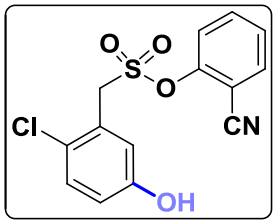
2-cyanophenyl (2-bromo-5-hydroxyphenyl)methanesulfonate (**1m**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2-bromophenyl)methanesulfonate (0.2 mmol; 70 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yellow viscous liquid. Yield 60%; 44 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.66 (ddd, *J* = 9.5, 7.7, 1.7 Hz, 2H), 7.67 – 7.59 (ddt, *J* = 8.3, 7.5, 2.0 Hz, 2H), 7.57 – 7.50 (dd, *J* = 9.3, 3.2 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.41 – 7.36 (s, 0H), 7.33 – 7.25 (dd, *J* = 8.8, 7.1 Hz, 1H), 7.27 – 7.19 (m, 1H), 7.12 – 7.05 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.84 – 6.79 (dd, *J* = 8.8, 2.8 Hz, 1H), 4.98 (s, 2H), 4.91 (s, 1H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 58.07, 58.34, 107.53, 114.33, 115.08, 115.51, 115.97, 117.69, 119.43, 120.26, 122.79, 123.60, 125.13, 127.29, 127.34, 127.39, 127.66, 129.16, 134.12, 134.17, 134.53, 134.76, 134.95, 149.98, 150.23, 153.52, 155.96.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{11}BrNO_4S^+$: 367.9592; found: 369.9572.

IR: 3391, 3022, 2944, 2848, 2245, 1634, 1588, 1400, 1369, 1255, 1218, 1167, 991, 872, 771cm-[1].



2-cyanophenyl (2-chloro-5-hydroxyphenyl)methanesulfonate (**1n**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2-chlorophenyl)methanesulfonate (0.2 mmol; 61.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yellow viscous liquid. Yield 55%; 35.5 mg.

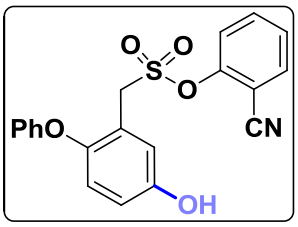
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.67 (td, *J* = 7.5, 1.7 Hz, 2H), 7.69 – 7.59 (m, 2H), 7.57 – 7.50 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.48 – 7.40 (m, 1H), 7.43 – 7.34 (m, 1H), 7.34 – 7.29 (d, *J* = 8.7 Hz, 1H), 7.30 – 7.18 (m, 4H), 7.13 – 7.08 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.93 – 6.85 (dd, *J* = 8.8, 2.9 Hz, 1H), 4.97 – 4.92 (s, 2H), 4.91 – 4.86 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 55.56, 55.78, 76.91, 77.54, 106.43, 107.47, 115.07, 115.51, 117.95, 119.10, 120.07, 121.84, 122.73, 123.54, 124.98, 125.43, 125.48, 126.63, 127.28, 127.65, 128.40, 134.12, 134.17, 134.77, 134.95, 149.96, 150.21, 152.46, 155.24.

HRMS: Calculated $[M+H]^+$ for $C_{14}H_{11}ClNO_4S^+$: 324.0097; found: 324.0103.

IR: 3367, 2920, 2868, 2248, 1600, 1516, 1482, 1450, 1361, 1305, 1278, 1219, 1160, 1022, 967,

863, 766 cm-^{1}.



2-cyanophenyl (5-hydroxy-2-phenoxyphenyl)methanesulfonate (**1o**): The compound was synthesized following the general **procedure A** with 2-cyanophenyl (2-phenoxyphenyl)methanesulfonate (0.2 mmol; 73 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. White solid. Yield 50%; 38 mg.

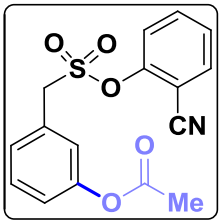
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 – 8.08 (m, 1H), 7.73 – 7.64 (m, 1H), 7.64 – 7.58 (m, 1H), 7.57 – 7.53 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.44 – 7.32 (m, 2H), 7.31 – 7.26 (t, *J* = 2.1 Hz, 1H), 7.24 – 7.20 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.09 – 7.04 (d, *J* = 2.4 Hz, 1H), 6.96 – 6.91 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H), 6.91 – 6.87 (d, *J* = 8.7 Hz, 1H), 6.87 – 6.80 (dd, *J* = 8.6, 2.4 Hz, 1H), 4.72 – 4.67 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 58.18, 107.00, 114.61, 117.55, 120.86, 121.31, 123.29, 125.95, 127.54, 128.69, 130.39, 130.71, 133.89, 134.31, 134.86, 141.19, 149.12, 149.85, 157.66.

HRMS: Calculated $[M+H]^+$ for $C_{20}H_{16}NO_5S^+$: 382.0749; found: 382.0756

IR: 3377, 3110, 3012, 2988, 2940, 2866, 2250, 1650, 1476, 1219, 1187, 1148, 1126, 1088, 993, 959, 872, 770 cm-^{1}.

C. Characterization of *meta*-acetoxylated compounds:



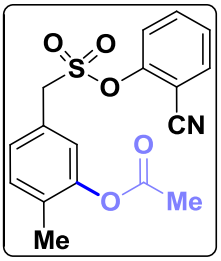
3-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (**2a**): The compound was synthesized following the general **procedure B** 2-cyanophenyl phenylmethanesulfonate (0.2 mmol; 54.6 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Pale yellow solid; melting point: 113-115 °C; Yield 71%; 47 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.65 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.65 – 7.56 (ddd, *J* = 8.5, 7.6, 1.7 Hz, 1H), 7.47 – 7.41 (t, *J* = 7.8 Hz, 1H), 7.43 – 7.34 (m, 3H), 7.31 – 7.28 (t, *J* = 2.0 Hz, 1H), 7.21 – 7.16 (m, 1H), 4.72 – 4.71 (s, 2H), 2.33 – 2.27 (d, *J* = 2.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 21.27, 58.14, 107.43, 115.18, 123.15, 123.55, 124.46, 127.55, 127.98, 128.67, 130.28, 133.98, 134.71, 150.15, 151.15, 169.36.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{14}NO_5S^+$: 332.0593; found: 332.0591

IR: 3019, 2967, 2867, 2240, 1602, 1558, 1498, 1442, 1262, 1198, 1023, 997. 860, 774 cm^{-1}.



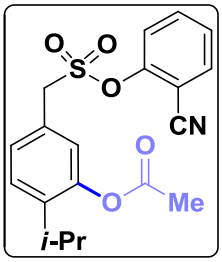
5-((2-cyanophenoxysulfonyl)methyl)-2-methylphenyl acetate (**2b**): The compound was synthesized following the general **procedure B** 2-cyanophenyl p-tolylmethanesulfonate (0.2 mmol; 57.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (14:86) mixture as the eluent. Colorless solid: 88-90 °C; Yield 71%; 49 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.71 – 7.67 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.42 – 7.35 (m, 2H), 7.33 – 7.27 (m, 2H), 7.25 – 7.20 (d, *J* = 1.5 Hz, 1H), 4.75 – 4.63 (s, 2H), 2.39 – 2.29 (s, 3H), 2.24 – 2.14 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 16.31, 20.98, 58.03, 76.98, 77.48, 107.46, 115.23, 123.60, 124.79, 125.25, 127.48, 128.86, 132.01, 132.28, 133.98, 134.71, 149.78, 150.26, 169.19.

HRMS: Calculated $[M+H]^+$ for $C_{17}H_{16}NO_5S^+$: 346.0749; found: 349.0745

IR: 2925, 2857, 2232, 1756, 1600, 1574, 1486, 1448, 1420, 1317, 1216, 1161, 1115, 1096, 958, 868, 773 cm^{-1}.



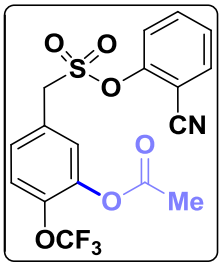
5-((2-cyanophenoxysulfonyl)methyl)-2-isopropylphenyl acetate (**2c**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (4-isopropylphenyl)methanesulfonate (0.2 mmol; 63 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (12:88) mixture as the eluent. Solid. Yield 61%; 45.5 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.70 – 7.66 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.62 – 7.57 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.39 – 7.34 (m, 4H), 7.21 – 7.18 (d, *J* = 1.3 Hz, 1H), 4.71 – 4.70 (s, 0H), 4.69 – 4.66 (s, 2H), 3.08 – 2.97 (hept, *J* = 6.9 Hz, 1H), 2.35 – 2.29 (s, 3H), 1.23 – 1.16 (d, *J* = 7.0 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 21.09, 22.99, 27.62, 57.98, 76.91, 77.55, 107.45, 115.20, 123.53, 124.87, 125.19, 127.44, 127.76, 129.12, 133.95, 134.66, 142.17, 148.51, 150.33, 169.61.

HRMS: Calculated $[M+H]^+$ for $C_{19}H_{20}NO_5S^+$: 374.1062; found: 374.1068.

IR: 3019, 2941, 2849, 2252, 1641, 1449, 1375, 1263, 1215 1161, 1041, 920, 871 765 cm-^{1}.



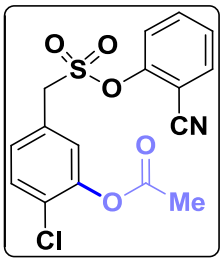
5-((2-cyanophenoxysulfonyl)methyl)-2-(trifluoromethoxy)phenyl acetate (**2d**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (4-(trifluoromethoxy)phenyl)methanesulfonate (0.2 mmol; 71.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Solid. Yield 56%; 46.5 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.66 – 7.59 (td, *J* = 7.8, 1.8 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.42 – 7.35 (m, 3H), 4.76 – 4.68 (s, 2H), 2.41 – 2.25 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 20.64, 57.56, 107.36, 115.20, 120.39, 122.87, 123.17 (*J* = 267 Hz.), 123.29, 126.37, 127.68, 129.78, 134.02, 134.79, 141.98, 143.03, 150.08, 168.33.

HRMS: Calculated $[M+Na]^+$ for $C_{17}H_{12}F_3NNaO_6S^+$: 438.0235; found: 438.0236.

IR: 3010, 2931, 2854, 2247, 1610, 1488, 1442, 1371, 1310, 1262, 1166, 1105, 1018, 970, 872, 770 cm^{-1}.



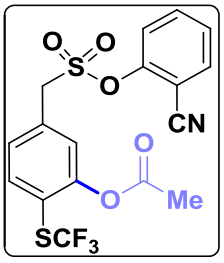
2-chloro-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (**2e**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (4-chlorophenyl)methanesulfonate (0.2 mmol; 51.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (17:83) mixture as the eluent. Solid. Yield 55%; 40 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.66 (m, 1H), 7.68 – 7.58 (m, 1H), 7.54 – 7.47 (m, 1H), 7.44 – 7.33 (m, 4H), 4.74 – 4.65 (s, 2H), 2.41 – 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 20.79, 57.69, 107.40, 110.19, 115.22, 123.57, 126.57, 127.65, 128.99, 129.77, 131.15, 134.01, 134.78, 147.58, 150.10, 168.39.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{13}ClNO_5S^+$: 366.0203; found: 366.0210

IR: 2928, 2854, 2237, 1607, 1486, 1449, 1367, 1293, 1219, 1161, 1095, 869, 771 cm^{-1}.



5-((2-cyanophenoxysulfonyl)methyl)-2-(trifluoromethylthio)phenyl acetate (**2f**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (4-(trifluoromethylthio)phenyl)methanesulfonate (0.2 mmol; 74.6 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (22:78) mixture as the eluent. Solid. Yield 52%; 45 mg.

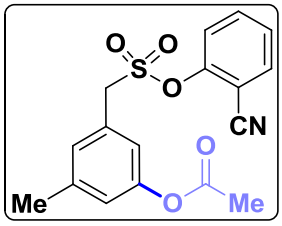
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.81 – 7.77 (d, *J* = 8.0 Hz, 1H), 7.72 – 7.67 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.50 – 7.46 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.47 – 7.43 (d, *J* = 2.0 Hz, 1H), 7.44 – 7.35 (m, 2H), 4.78 – 4.69 (s, 2H), 2.40 – 2.31 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 20.91, 57.76, 107.38, 115.21, 122.92 (*J* = 252 Hz.), 126.44, 127.74, 127.89, 129.57, 131.69, 134.03, 134.81, 138.73, 139.39, 150.06, 153.03, 168.89.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -41.46 – -41.59

HRMS: Calculated $[M+Na]^+$ for $C_{17}H_{12}F_3NNaO_5S_2^+$: 454.0007;found: 453.9997

IR: 2926, 2856, 2239, 1605, 1487, 1440, 1372, 1278, 1221, 1155, 1095, 970, 861, 767 cm^{-1}.



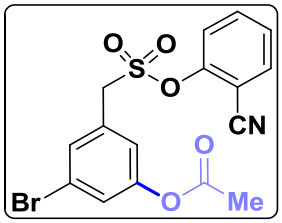
3-((2-cyanophenoxysulfonyl)methyl)-5-methylphenyl acetate (**2g**): The compound was synthesized following the general **procedure B** 2-cyanophenyl m-tolylmethanesulfonate (0.2 mmol; 57.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (13:87) mixture as the eluent. Solid. Yield 71%; 49 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.72 – 7.65 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.43 – 7.34 (m, 2H), 7.23 – 7.16 (s, 1H), 7.13 – 7.06 (d, *J* = 2.0 Hz, 1H), 7.01 – 6.91 (d, *J* = 2.0 Hz, 1H), 4.70 – 4.64 (s, 2H), 2.41 – 2.33 (s, 3H), 2.31 – 2.26 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 21.25, 21.39, 58.15, 107.38, 115.17, 121.46, 123.50, 123.77, 127.49, 129.46, 133.95, 134.68, 140.72, 150.20, 151.04, 169.47.

HRMS: Calculated $[M+H]^+$ for $C_{17}H_{16}NO_5S^+$: 346.0749; found: 349.0748.

IR: 2935, 2858, 2236, 1758, 1605, 1576, 1510, 1478, 1445, 1423, 1317, 1272, 1115, 1016, 958, 868, 773, cm^{-1}.



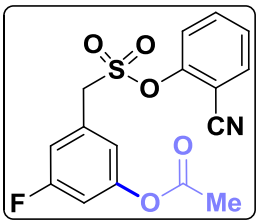
3-bromo-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (**2h**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (3-bromophenyl)methanesulfonate (0.2 mmol; 71.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Solid. Yield 55%; 45 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.66 – 7.60 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.56 – 7.51 (t, *J* = 1.7 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.38 – 7.35 (t, *J* = 1.9 Hz, 1H), 7.31 – 7.25 (t, *J* = 1.8 Hz, 1H), 4.69 (s), 4.67 (s, 2H), 2.36 (s), 2.30 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 21.19, 57.57, 107.46, 115.16, 123.05, 123.46, 123.61, 126.60, 127.73, 129.46, 131.50, 134.03, 134.78, 150.05, 151.53, 168.89.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{13}BrNO_5S^+$: 409.9698; found: 409.9695.

IR: 3017, 2931, 2819, 1740, 1602, 1450, 1267, 1221, 1167, 990, 872, 772, 672 cm^{-1}.



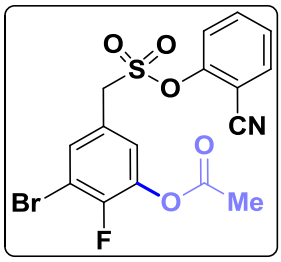
3-((2-cyanophenoxysulfonyl)methyl)-5-fluorophenyl acetate (**2i**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (3-fluorophenyl)methanesulfonate (0.2 mmol; 58.2 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (12:88) mixture as the eluent. Solid. Yield 54%; 38 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.67 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.67 – 7.60 (ddd, *J* = 8.3, 7.5, 1.7 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.18 – 7.09 (m, 2H), 7.00 – 6.94 (dt, *J* = 9.0, 2.2 Hz, 1H). 4.69 (s, 2H), 4.62 (s), 2.34 (s), 2.30 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 20.70, 21.24, 57.72, 57.80, 76.98, 77.48, 100.17, 107.46, 111.23, 111.43, 115.17, 115.72, 115.90, 119.57, 119.73, 120.46, 123.10, 123.63, 124.69, 127.43, 127.74, 129.23, 134.04, 134.80, 150.01, 151.90, 151.99, 161.95, 163.93, 168.93.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{13}FNO_5S^+$: 350.0498; found: 350.0495.

IR: 3045, 2930, 2821, 1743, 1608, 1461, 1432, 1278, 1231, 1166, 987, 872, 765, 671cm^{-1}.



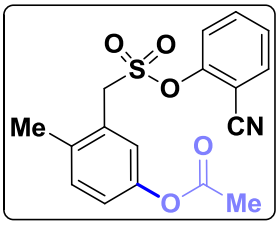
3-bromo-5-((2-cyanophenoxysulfonyl)methyl)-2-fluorophenyl acetate (**2j**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (3-bromo-4-fluorophenyl)methanesulfonate (0.2 mmol; 73.8 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (21:79) mixture as the eluent. Solid. Yield 57%; 49 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.69 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.68 – 7.62 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.62 – 7.58 (dd, *J* = 5.5, 2.2 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.35 – 7.31 (dd, *J* = 6.3, 2.2 Hz, 1H), 4.71 – 4.61 (s, 2H), 2.39 – 2.29 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 20.64, 57.14, 107.39, 110.94 (*J* = 18 Hz.), 115.21, 123.62, 123.89 (*J* = 5 Hz.), 126.01, 127.80, 133.28, 134.04, 134.85, 139.27 (*J* = 15 Hz.), 150.00, 151.51, 153.52, 167.93.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{12}BrFNO_5S^+$: 427.9604: found: 427.9610.

IR: 3001, 2928, 2861, 2241, 1604, 1480, 1438, 1372, 1305, 1268, 1168, 1121, 989, 869, 774 cm-1.



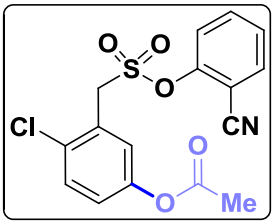
3-((2-cyanophenoxysulfonyl)methyl)-4-methylphenyl acetate (**2k**): The compound was synthesized following the general **procedure B** 2-cyanophenyl o-tolylmethanesulfonate (0.2 mmol; 57.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (12:88) mixture as the eluent. Pale yellow solid; melting point: 133-135 °C; Yield 75%; 52 mg.

^{1}H NMR (500 MHz, Chloroform-*d*): δ = 7.74 – 7.68 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.66 – 7.58 (m, 1H), 7.44 – 7.37 (m, 2H), 7.31 – 7.23 (m, 2H), 7.09 – 7.05 (dd, *J* = 8.3, 2.5 Hz, 1H), 4.77 (s, 2H), 4.82 (s), 2.49 – 2.45 (s, 3H), 2.29 – 2.27 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ = 19.37, 21.27, 55.80, 107.62, 115.19, 123.23, 123.72, 125.24, 126.10, 127.60, 132.18, 134.01, 134.74, 136.41, 149.12, 150.06, 169.62.

HRMS: Calculated $[M+H]^+$ for $C_{17}H_{16}NO_5S^+$: 346.0749; found: 349.0744.

IR: 2930, 2856, 2234, 1751, 1612, 1575, 1488, 1452, 1412, 1311, 1210, 1112, 1088, 954, 859, 770 cm^{-1}.



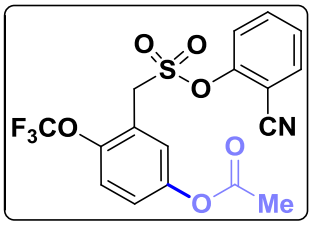
4-chloro-3-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (**2l**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (2-chlorophenyl)methanesulfonate (0.2 mmol; 61.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (18:82) mixture as the eluent. Solid. Yield: 63%; 46 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.66 – 7.59 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.51 – 7.46 (d, *J* = 8.7 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.43 – 7.36 (td, *J* = 7.6, 1.1 Hz, 1H), 7.18 – 7.13 (dd, *J* = 8.7, 2.7 Hz, 1H). 4.99(s), 4.94(s, 2H), 2.36 (s), 2.30 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 21.21, 55.27, 107.55, 115.02, 123.49, 123.55, 124.69, 125.35, 126.15, 126.23, 127.63, 127.93, 130.56, 131.16, 132.66, 134.08, 134.10, 134.71, 149.58, 149.90, 169.13.

HRMS: Calculated $[M+Na]^+$ for $C_{16}H_{12}ClNNaO_5S^+$:388.0022; found: 388.0028.

IR: 2941, 2852, 2237, 1606, 1481, 1454, 1364, 1297, 1218, 1160, 1092, 869, 771 cm^{-1}.



3-((2-cyanophenoxysulfonyl)methyl)-4-(trifluoromethoxy)phenylacetate (**2m**): The

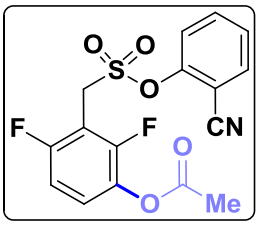
compound was synthesized following the general **procedure B** 2-cyanophenyl (2-(trifluoromethoxy)phenyl)methanesulfonate (0.2 mmol; 71.4 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Solid. Yield 57%; 47.5 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.49 – 7.46 (d, *J* = 2.8 Hz, 1H), 7.46 – 7.43 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.25 – 7.22 (dd, *J* = 9.0, 2.8 Hz, 1H), 4.86 – 4.79 (s, 2H), 2.32 – 2.29 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 21.20, 52.11, 107.61, 114.94, 120.62, 122.78, 124.50 (*J* = 271 Hz.), 126.23, 129.82, 132.66, 134.12, 134.71, 139.11, 145.74, 148.79, 149.83, 169.12.

HRMS: Calculated $[M+Na]^+$ for $C_{17}H_{12}F_3NNaO_6S^+$: 438.0235; found: 438.0240.

IR: 2943, 2850, 2242, 1605, 1478, 1448, 1375, 1301, 1266, 1155, 1100, 1014, 970, 877, 778 cm-[1].



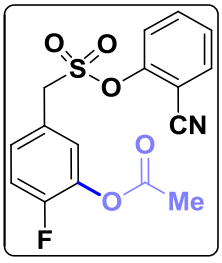
3-((2-cyanophenoxysulfonyl)methyl)-2,4-difluorophenyl acetate (**2n**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (2,6-difluorophenyl)methanesulfonateulfonate (0.2 mmol; 61.8 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. liquid. Yield 51%; 37.5 mg.

^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.72 – 7.68 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.66 – 7.60 (ddd, *J* = 8.5, 7.5, 1.7 Hz, 1H), 7.49 – 7.44 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.44 – 7.37 (td, *J* = 7.7, 1.1 Hz, 1H), 7.29 – 7.19 (td, *J* = 8.8, 5.5 Hz, 1H), 7.06 – 6.99 (td, *J* = 8.8, 2.0 Hz, 1H), 4.87(s, 2H), 4.86 (s) 2.37 – 2.29 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ = 20.60, 22.90, 29.90, 46.69, 107.90, 111.70, 111.92, 114.70, 123.03, 123.56, 125.92, 125.95, 125.97, 126.05, 126.08, 127.79, 134.20, 134.71, 149.63, 152.06, 168.34.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{12}F_2NO_5S^+$: 368.0404; found: 368.0406

IR: 2929, 2848, 2235, 1625, 1602, 1525, 1450, 1363 1220, 1153, 1091, 990, 872, 768 cm-[1].



5-((2-cyanophenoxysulfonyl)methyl)-2-fluorophenyl acetate (**2o**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (4-fluorophenyl)methanesulfonate (0.2 mmol; 58.2 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (12:88) mixture as the eluent. Solid; melting point:100-102 °C; Yield 55%; 38.5 mg.

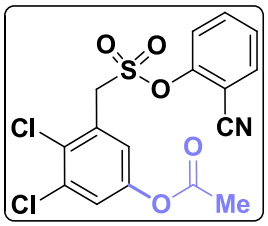
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.67 – 7.58 (m, 1H),

7.43 – 7.40 (t, *J* = 0.9 Hz, 1H), 7.41 – 7.38 (dd, *J* = 2.1, 1.1 Hz, 1H), 7.38 – 7.34 (m, 2H), 7.25 – 7.18 (dd, *J* = 9.7, 8.4 Hz, 1H), 4.71 – 4.65 (s, 2H), 2.37 – 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 20.64, 57.60, 107.37, 115.21, 117.65 (*J* = 19 Hz.), 123.14, 123.18, 123.53, 126.80, 126.82, 127.62, 130. 03 (*J* = 8 Hz.), 134.00, 134.77, 138.65 (*J* = 13 Hz.), 150.11, 153.86, 156.37, 168.21.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{13}FNO_5S^+$: 350.0498; found: 350.0497.

IR: 2945, 2856, 2238, 1611, 1491, 1459, 1368, 1291, 1211, 1145, 1088, 859, 768 cm^{-1}.



3,4-dichloro-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (**2p**): The compound was synthesized following the general **procedure B** 2-cyanophenyl (2,3-dichlorophenyl)methanesulfonate (0.2 mmol; 68.2 mg) as the substrate. The pure compound was purified through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Solid. Yield: 50%; 40 mg.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.67 – 7.61 (ddd, *J* = 8.5, 7.6, 1.7 Hz, 1H), 7.51 – 7.44 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.44 – 7.36 (m, 3H), 5.01 – 5.00 (s, 0H), 5.01 – 4.96 (s, 2H), 2.36 – 2.25 (s, 3H).

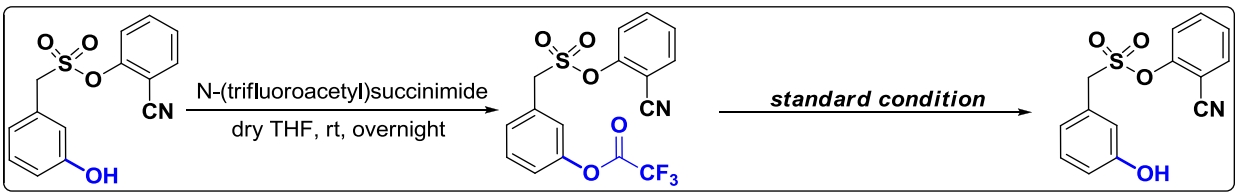
^{13}C NMR (126 MHz, $CDCl_3$) δ 21.17, 55.88, 107.47, 115.01, 123.48, 124.77, 125.57, 127.76, 131.42, 131.46, 134.12, 134.70, 134.78, 149.04, 149.70, 168.78.

HRMS: Calculated $[M+H]^+$ for $C_{16}H_{12}Cl_2NO_5S$+: 399.9813; found: 399.9818

IR: 2939, 2841, 2236, 1618, 1600, 1527, 1455, 1360 1228, 1167, 1088, 991, 872, 770 cm-^{1}.

V. Mechanistic Study:

A. Identification of intermediate (hydroxylation):



In order to confirm the intermediacy of the *meta*-trifluoroacetoxy moiety, the compound was synthesized separately and administrated under the optimized condition of *meta*-hydroxylation.

Synthesis of meta-trifluoroacetoxy moiety [3-((2-cyanophenoxysulfonyl)methyl)phenyl 2,2,2-trifluoroacetate]: The meta-hydroxylated compound (**1a**)(0.5 mmol; 145 mg) was dissolved in dry THF (3mL) and N-(trifluoroacetyl)succinimide[2] (0.8 mmol; 156 mg) was added to it. The reaction was refluxed overnight under N_2 atmosphere. After the reaction was finished, the precipitated succinimide was filtered off, and solvent was evaporated under reduced pressure forming the trifluoroacetate esters. The crude product was dissolved in diethylether (3 X 5 mL) and filtered to remove the succinimide. The organic part was evaporated to obtain the pure product (yield **92**%).

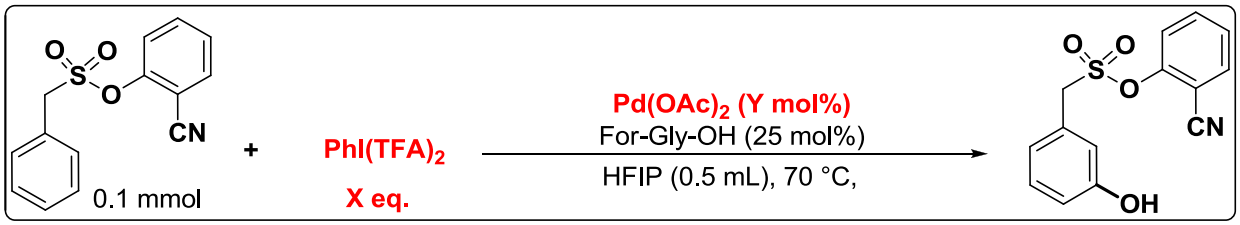
The obtained solid compound was directly used under optimized condition (general

procedure A). Both in presence and absence of $PhI(TFA)_2$ meta-hydroxylated compound was obtained in quantitative yield.

B. Determination of order and KIE:

The order of the reaction with respect to the palladium and $PhI(TFA)_2$ was determined using Initial slope method. Multiple sets of standard reaction were performed with the variation of the palladium and $PhI(TFA)_2$ loading keeping other parameters intact (Table S19).

Table S19. Different sets of reaction



	Substrate	$Pd(OAc)_2$	N-For-Gly-OH	$PhI(TFA)_2$	HFIP
Run 1	0.1 mmol	10 mol% = 0.02(M)	25 mol% = 0.05(M)	0.4 mmol	0.5 mL
Run 2	0.1 mmol	**15 mol% = 0.03(M)**	25 mol% = 0.05(M)	0.4 mmol	0.5 mL
Run 3	0.1 mmol	10 mol% = 0.02(M)	25 mol% = 0.05(M)	**0.2 mmol**	0.5 mL
Run 4	0.1 mmol	10 mol% = 0.02(M)	25 mol% = 0.05(M)	**0.3 mmol**	0.5 mL
Run 5	**0.15 mmol**	10 mol% = 0.02(M)	25 mol% = 0.05(M)	0.4 mmol	0.5 mL
Run 6	**0.1 mmol-d_5**	10 mol% = 0.02(M)	25 mol% = 0.05(M)	0.4 mmol	0.5 mL

Procedure: In a oven dried reaction tube, charged with magnetic stir-bar, $Pd(OAc)_2$ (Y mol%), N-For-Gly-OH (25 mol%), phenylmethanesuphonic ester substrate (0.1 mmol) were added. The hydroxylating agent $PhI(TFA)_2$ (X eq.) was added to the reaction mixture followed by the HFIP(0.5 mL). The reaction tube was capped and stirred at room temperature for 15 mins and then placed to a preheated oil-bath at 70 °C. The reaction was stirred vigorously for a definite amount of time and then taken out to cool it to the room temperature. The reaction mixture was diluted with ethyl acetate and equivalent amount of 1,3,5-trimethoxybenzene (TMB) (0.1 mmol; 16.8 mg) was added to the reaction mixture. 200 µL aliquot was taken out from the mixture, evaporated and dissolved in $CDCl_3$ for NMR study.

Comparing the initial rate for the ***Run 1*** and ***Run 2*** an enhancement in rate can be observed with the increase in loading of palladium catalyst amount.

Initial slope for Run 1 = 2.32×10^{-2} (M)/h

Initial slope for Run 2 = 3.56×10^{-2} (M)/h

Considering a simplified rate equation Rate (r) = $k\,[sub]^a\,[Pd]^b\,[lig]^c\,[PhI(TFA)_2]^d$

(all terms are of usual significance)

Now, $r_1 = 2.32 \times 10^{-2}$ (M)/h = $k\,[sub]^a\,[0.02]^b\,[lig]^c\,[PhI(TFA)_2]^d$ …….. (1)

and $r_2 = 3.56 \times 10^{-2}$ (M)/h = $k\,[sub]^a\,[0.03]^b\,[lig]^c\,[PhI(TFA)_2]^d$ …….. (2)

Comparing the initial rate for for the Run

$[r_2/\, r_1] = [3.56/2.32] = [0.03/0.02]^a$

or, $1.53 = [1.5]^a$

or, a = [log1.53/log1.5] = 1.04 ~ 1

Therefore the kinetics of the reaction follows a first order rate dependence with respect to the palladium catalyst.

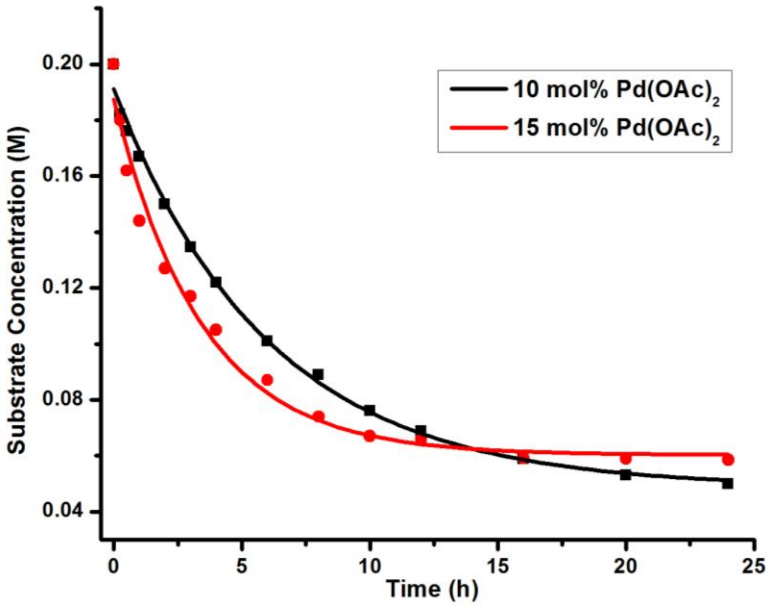


Figure B: Overlay kinetics plot for ***Run 1*** and ***Run 2***

The initial rate for the ***Run 1, Run 3*** and ***Run 4*** was found to be almost same. As the only parameter of difference was the amount of $PhI(TFA)_2$, therefore it is evident that the rate of the reaction is indifferent towards the amount of the $PhI(TFA)_2$. So it can be concluded that the order of the reaction w.r.t $PhI(TFA)_2$ is zero.

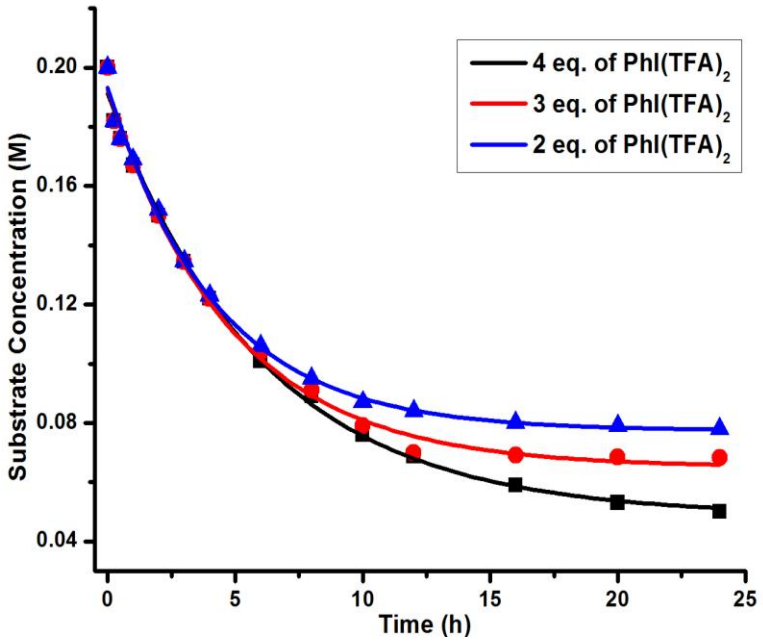


Figure C: Overlay of ***Run 1, 3*** and ***4***

Comparing the initial rate for the ***Run 1*** and ***Run 5*** an enhancement in rate can be observed with

the increase in loading of substrate.

Initial slope for Run 1 = 2.32 x 10^{-2} (M)/h

Initial slope for Run 5 = 3.06 x 10^{-2} (M)/h

Considering a simplified rate equation Rate (r) = k $[sub]^a$ $[Pd]^b$ $[lig]^c$ $[PhI(TFA)_2]^0$

(all terms are of usual significance)

Now, r_1 = 2.32 x 10^{-2} (M)/h = k $[0.2]^a$ $[Pd]^1$ $[lig]^c$

and r_5 = 3.06 x 10^{-2} (M)/h = k $[0.3]^a$ $[Pd]^1$ $[lig]^c$

Comparing the initial rate for for the Run

$[r_5/ r_1] = [3.06/2.32] = [0.3/0.2]^a$

or, $1.31 = [1.5]^a$

or, a = [log1.31/log1.5] = 0.88 ~ 1

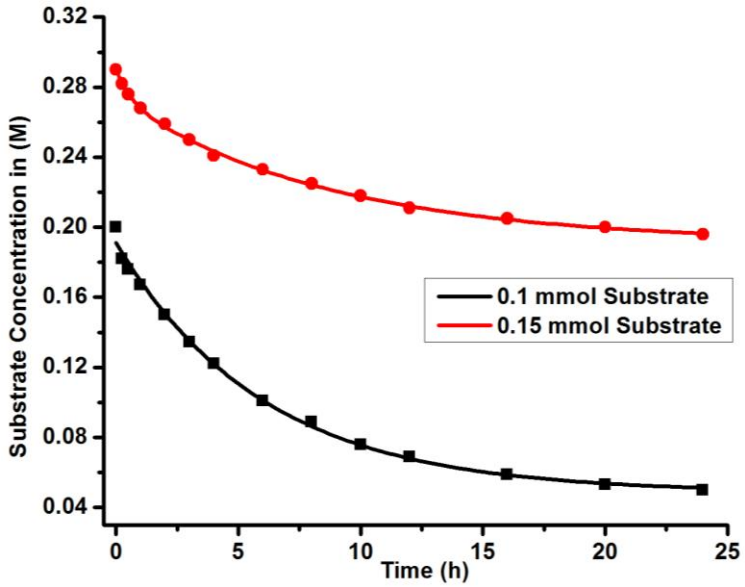


Figure D: Overlay of ***Run 1*** and ***5***

Comparing the initial rate for the ***Run 1*** and ***Run 6*** an variation in rate can be observed on shifting from model substrate to d_5-substate.

Initial slope for Run 1 = 2.32 x 10^{-2} (M)/h

Initial slope for Run 6 = 7.67 x 10^{-3} (M)/h

Considering a simplified rate equation Rate (r) = k $[sub]^1$ $[Pd]^1$ $[lig]^c$ $[PhI(TFA)_2]^0$

(all terms are of usual significance)

Now, r_1 = 2.32 x 10^{-2} (M)/h = k $[0.2]^1$ $[Pd]^1$ $[lig]^c$

and r_6 = 7.67 x 10^{-3} (M)/h = k_6 $[0.2]^1$ $[Pd]^1$ $[lig]^c$

Comparing the initial rate for for the Run

$[r_1/ r_6] = [2.32/0.767] = k/k_6$

or, $3.02 = k/k_6$

or, $k/k_6 = k_H/k_D = 3.02$ = KIE

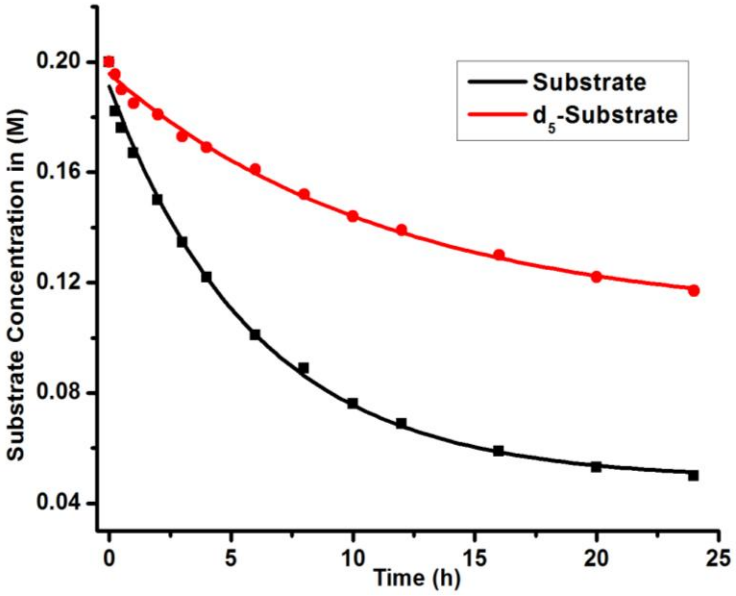


Figure E: Overlay of ***Run 1*** and ***6***

C. NMR Study:

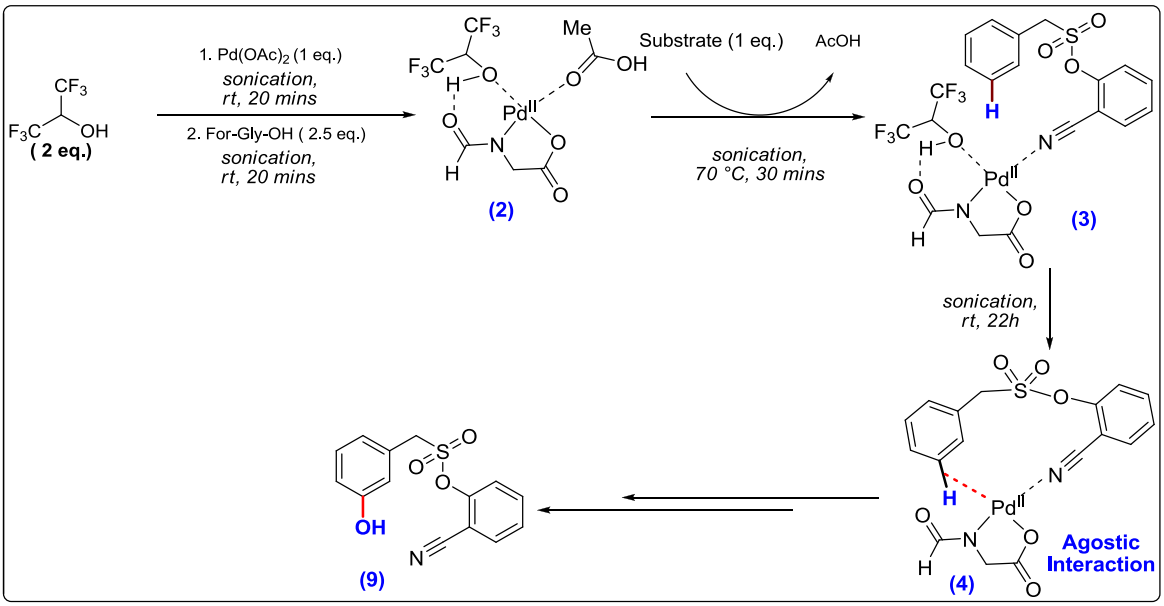
This experiment was performed to monitor the progress of the reaction from the shift of the characteristic ^{1}H-NMR signal.

In this experiment following peaks were considered

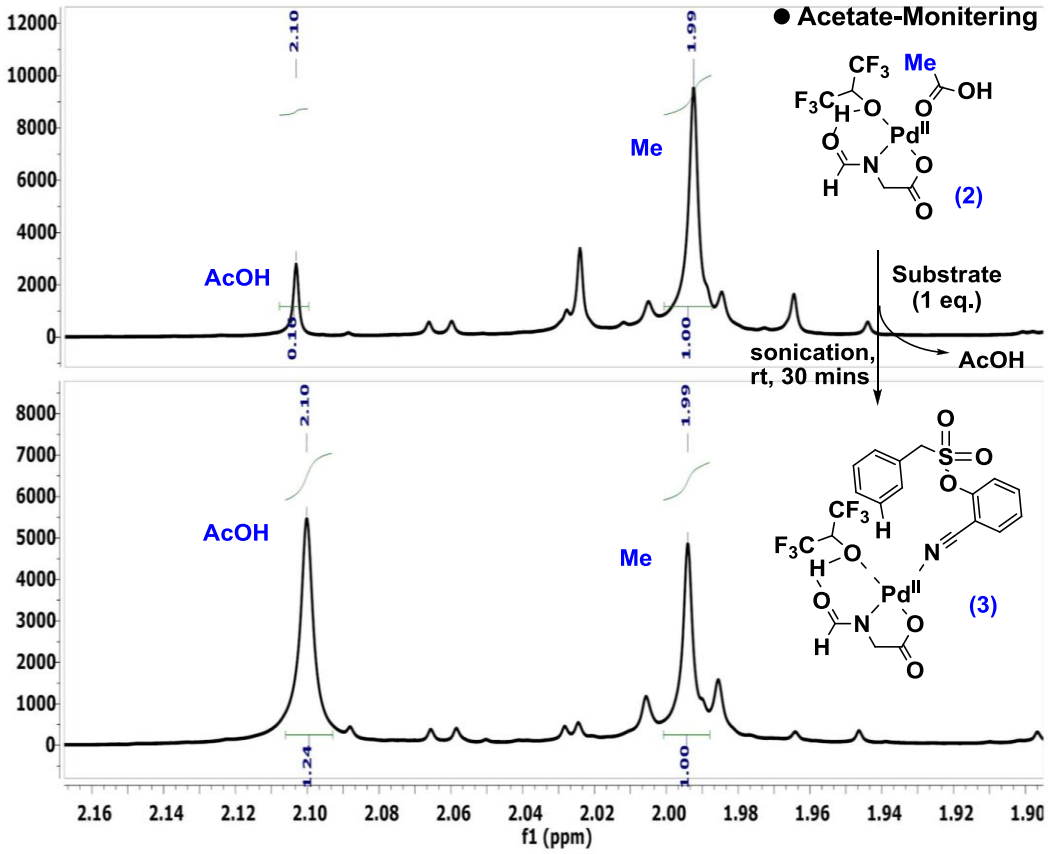
(a) –Me peak of acetate and acetic acid
(b) Aromatic *meta* C-H peak

Procedure:

In a clean NMR tube HFIP (2 eq.; 6.2 μL) was added to 510 μL of $CDCl_3$ and the ^{1}H-NMR was recorded. In the same NMR tube $Pd(OAc)_2$ (1eq.; 0.03 mmol; 6.72 mg) was added and put for sonication for 20 mins at room temperature. The ^{1}H-NMR of the reaction mixture was recorded again. Following the same procedure 2.5 eq. of For-Gly-OH (7.73 mg) was added to the NMR tube followed by sonication and the NMR monitoring of the reaction. 1 eq. of the model substrate was added to the same NMR tube was placed in sonicator for 20 mins at 70 °C. The ^{1}H-NMR of the mixture was recorded. Afterwards the tube was kept for 22 hrs under sonic ation. The reaction was cooled in a salted ice-bath to nearly -20 °C and kept for 30 mins. Any change of the mixture was monitored by ^{1}H-NMR.



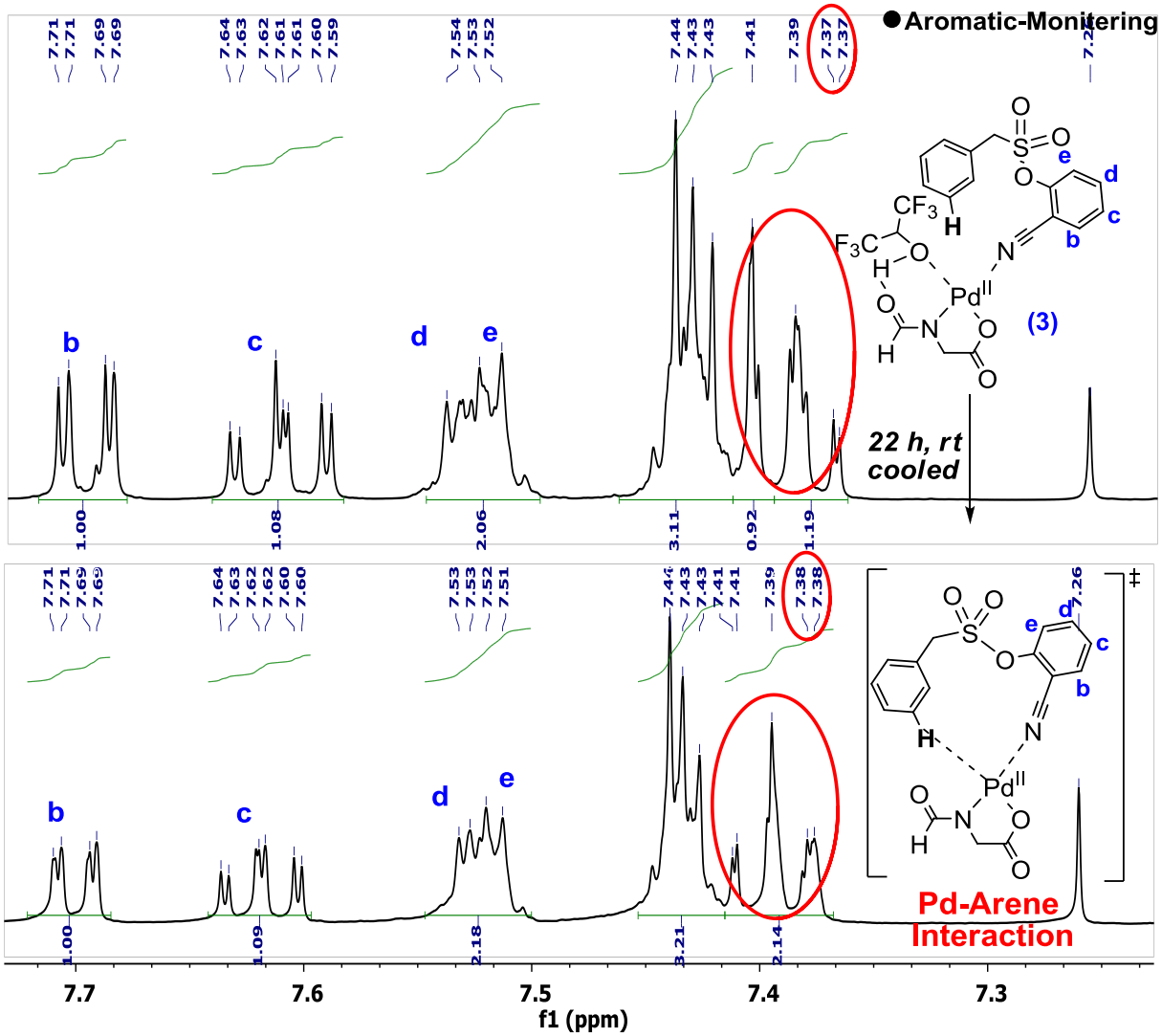
Acetate Monitoring: Upon addition of substrate (**1**) (1 eq.) to the mixture of $Pd(OAc)_2$, ligand (2.5 eq.) and HFIP (**2**), the signal for AcOH intensifies (integration changes from 0.22 to 1.24 w.r.t to –Me signal of acetate of unreacted $Pd(OAc)_2$, as 1.00). Notably same observation was not **observed in absence of ligand** signifies that simple $Pd(OAc)_2$ does not release AcOH in presence of substrate in the similar fashion.



Aromatic Monitoring: The addition of substrate (**1**) to the mixture of $Pd(OAc)_2$, ligand and HFIP does not show any change in aromatic signal of **1**. However upon sonication for 22 h followed by cooling at 0 °C, a distinct variation in peak patterns and slight change in peak values

were observed, with no change in number of aromatic protons (δ, 7.37-7.41 ppm). According to the literature,[3] the interaction of the metal with the –H will be reflected in the change of *J* values. Thus the interaction of the aromatic C–H bond (likely *meta* C–H bond) with palladium (as shown above) will hinder the interaction with neighboring C–H and the H-H coupling will be disturbed. The extend of variation will depend on the strength of the interaction. The distinct change in the splitting pattern (as circled in the above figure) is likely to indicate the weak interaction between which eventually leads to the C–H activation via agostic interaction.

In order to verify the above conclusion various control experiments were done omitting various components separately. In case of $Pd(OAc)_2$, same experiment was conducted following the same procedure **without addition of $Pd(OAc)_2$**. Even after 48h of standing **no variation** was observed in the aromatic region of the spectra. These observation suggests the presence of $Pd(OAc)_2$ along with the substrate is essential for the above mentioned changes.

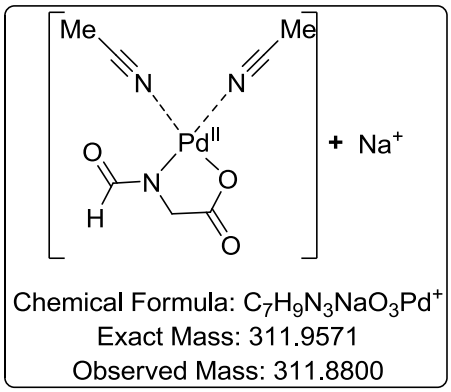


D. Mass Study:

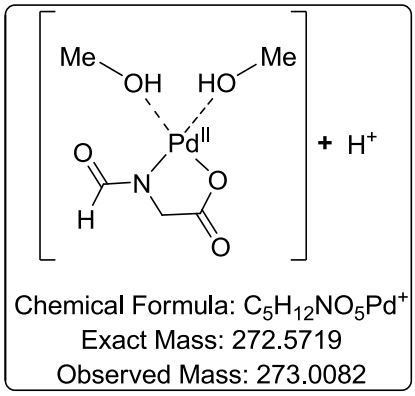
In order to study the metal-ligand interaction, the following experiment was performed.

Experiment 1: In a clean oven dried reaction tube, charged with magnetic stir-bar, $Pd(OAc)_2$ (1 eq.) was added with For-Gly-OH (2 eq.) and HFIP. The mixture was stirred at 70 °C for 2 hrs. The mixture was cooled to the room temperature and divided in three portions.

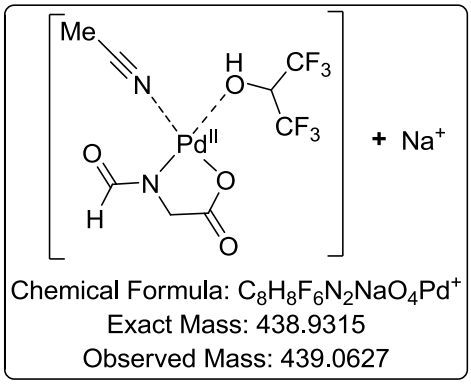
Portion 1: The reaction mixture was diluted with MeCN and subjected to mass analysis.



Portion 2: The reaction mixture was diluted with MeOH and kept overnight for stirring at room temperature.



Portion 3: The reaction mixture was diluted with HFIP, water and few drops of MeCN and subjected to mass analysis.



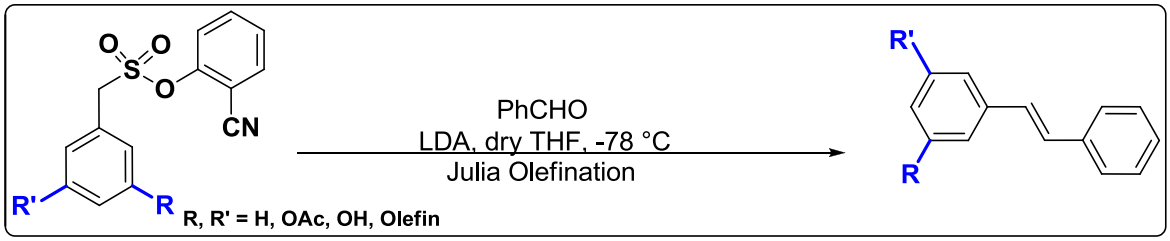
E. IR Study:

Substrate = 2237 cm^{-1}

[Substrate + $Pd(OAc)_2$] = 2247 cm^{-1}

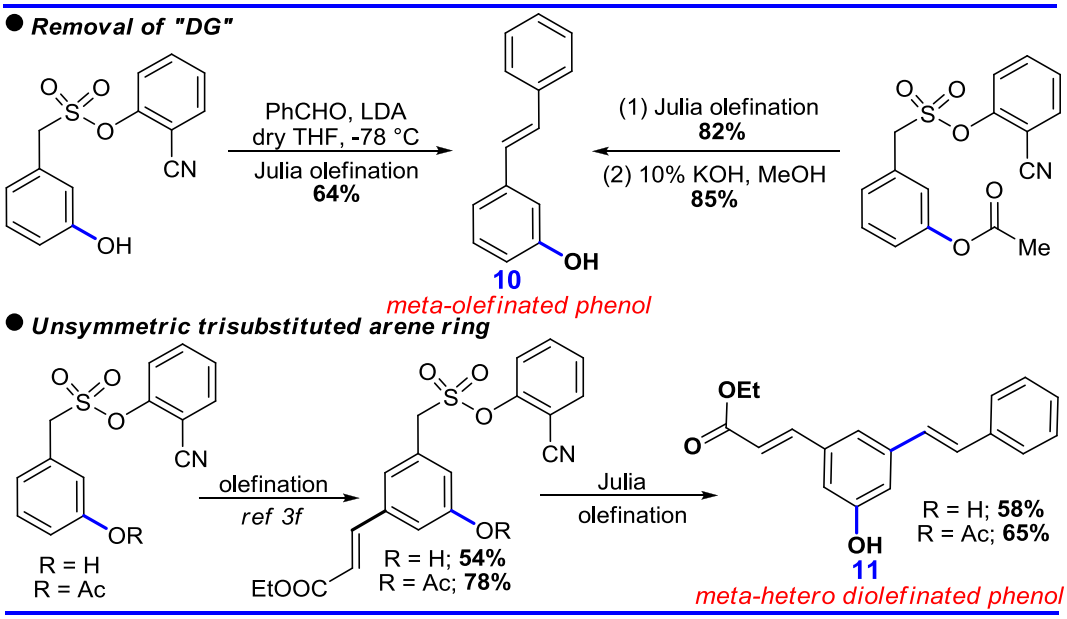
[Substrate + $Pd(OAc)_2$ + *N*-For-Gly] = 2250 cm^{-1}

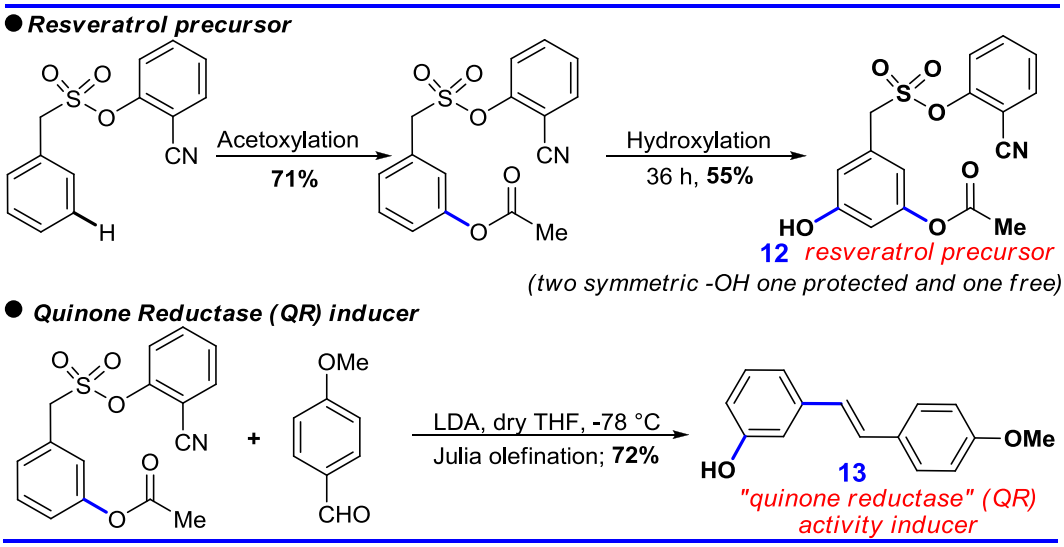
VI. Application:



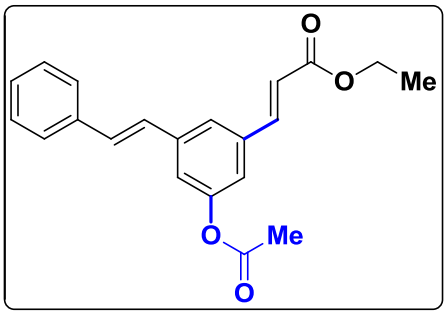
To a flame dried round bottomed flask equipped with magnetic stir-bar, freshly prepared LDA (2(M); 240 µL) and dry THF (6 mL) was added. The solution was cooled to -78 °C. Separately a solution of benzaldehyde and the *meta*-functionalized compound (0.2 mmol) in dry THF (15 mL) was prepared and slowly added to the LDA/THF solution at -78 °C. The reaction mixture was stirred overnight while warmed it to room temperature. Upon completion the reaction was quenched with saturated NH_4Cl solution and extracted with ethyl acetate. The organic portion was dried over anhydrous Na_2SO_4, concentrated under reduced pressure and purified through column chromatography.

The above mentioned procedure was followed for the following reactions.





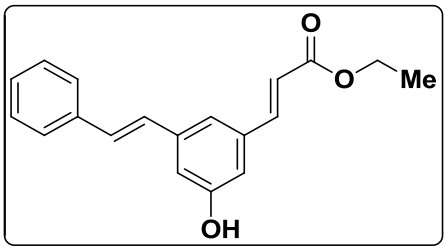
In case of synthesis of **11** from hydroxylated substrate (R=H), the double amount of LDA was used. For the synthesis of compound **12**, hydroxylation reaction was continued for 36 h.



(E)-ethyl 3-(3-acetoxy-5-((2-cyanophenoxysulfonyl)methyl)phenyl)acrylate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.68 – 7.60 (m, 2H), 7.56 – 7.49 (t, *J* = 1.6 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.35 – 7.30 (t, *J* = 1.8 Hz, 2H), 6.51 – 6.42 (d, *J* = 16.0 Hz, 1H), 4.75 – 4.71 (s, 2H), 4.30 – 4.22 (q, *J* = 7.1 Hz, 2H), 2.35 – 2.28 (s, 3H), 1.40 – 1.29 (t, *J* = 7.1 Hz, 3H).

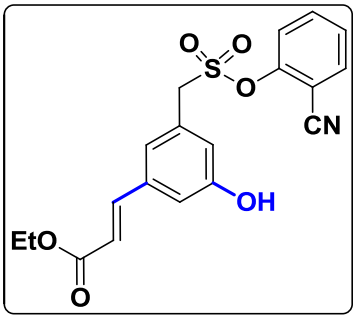
^{13}C NMR (101 MHz, $CDCl_3$) δ 14.48, 21.29, 58.00, 60.96, 107.46, 114.88, 120.88, 122.20, 123.64, 125.89, 127.69, 128.19, 128.72, 134.02, 134.78, 137.12, 142.51, 150.12, 151.56, 166.58, 169.19.



(E)-ethyl 3-(3-hydroxy-5-styrylphenyl)acrylate:

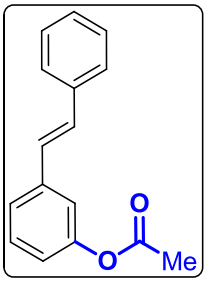
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.48 (d, *J* = 16.0 Hz, 1H), 7.25 – 7.19 (s, 3H), 6.99 – 6.95 (s, 1H), 6.86 – 6.82 (t, *J* = 2.0 Hz, 1H), 6.73 – 6.70 (s, 1H), 6.67 – 6.62 (d, *J* = 12.2 Hz, 1H), 6.55 – 6.48 (d, *J* = 12.3 Hz, 1H), 6.30 – 6.22 (d, *J* = 16.0 Hz, 1H), 4.28 – 4.20 (q, *J* = 7.1 Hz, 2H), 1.37 – 1.29 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 14.52, 60.75, , 113.40, 117.61, 118.99, 121.97, 127.65, 128.57, 129.06, 129.21, 129.24, 131.70, 136.25, 139.58, 144.27, 155.97, 167.12.



(E)-ethyl 3-(3-((2-cyanophenoxysulfonyl)methyl)-5-hydroxyphenyl)acrylate:

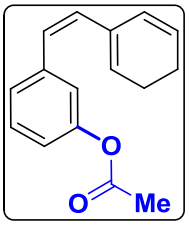
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.67 – 7.56 (m, 2H), 7.55 – 7.48 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.43 – 7.35 (td, *J* = 7.7, 1.1 Hz, 1H), 7.21 – 7.16 (t, *J* = 1.5 Hz, 1H), 7.15 – 7.11 (t, *J* = 1.9 Hz, 1H), 7.10 – 7.05 (m, 1H), 6.47 – 6.40 (d, *J* = 16.1 Hz, 1H), 4.71 – 4.62 (s, 2H), 4.31 – 4.21 (q, *J* = 7.2 Hz, 2H), 1.36 – 1.29 (t, *J* = 7.1 Hz, 3H).



(E)-3-styrylphenyl acetate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.15 (ddd, *J* = 13.2, 4.7, 2.2 Hz, 5H), 7.13 – 7.06 (m, 1H), 6.99 – 6.95 (t, *J* = 1.9 Hz, 1H), 6.95 – 6.88 (dd, *J* = 8.6, 2.2 Hz, 1H), 6.67 – 6.62 (s, 0H), 6.63 – 6.55 (d, *J* = 17.1 Hz, 1H), 6.55 – 6.50 (s, 0H), 2.27 – 2.20 (s, 3H).

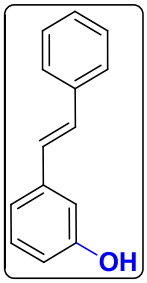
^{13}C NMR (101 MHz, $CDCl_3$) δ 21.32, 76.91, 77.54, 110.22, 120.48, 122.14, 126.58, 127.52, 128.50, 129.09, 129.33, 129.37, 131.33, 136.95, 139.02, 150.83, 169.55.



(Z)-3-(2-(cyclohexa-1,5-dienyl)vinyl)phenyl acetate:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.47 (dt, *J* = 8.1, 1.0 Hz, 2H), 7.41 – 7.32 (m, 4H), 7.32 – 7.22 (m, 2H), 7.10 – 7.07 (d, *J* = 2.5 Hz, 2H), 7.02 – 6.95 (ddd, *J* = 5.0, 3.9, 2.3 Hz, 1H), 2.41 – 2.27 (s, 3H).

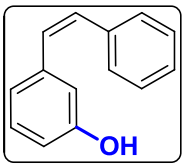
^{13}C NMR (101 MHz, $CDCl_3$) δ 21.39, 76.91, 77.55, 119.47, 120.86, 124.41, 126.83, 127.93, 128.10, 128.93, 129.81, 130.02, 137.21, 139.30, 151.31, 169.69.



(E)-3-styrylphenol:

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.59 – 7.16 (m, 5H), 7.14 – 7.08 (t, *J* = 7.8 Hz, 1H), 6.85 – 6.79 (d, *J* = 7.6 Hz, 1H), 6.73 – 6.65 (m, 2H), 6.62 – 6.51 (m, 2H).

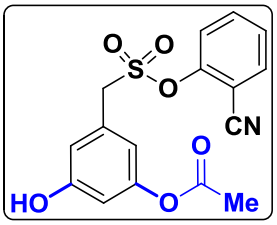
^{13}C NMR (126 MHz, $CDCl_3$) δ 29.91, 76.98, 77.48, 114.39, 115.66, 121.83, 127.39, 128.45, 129.13, 129.74, 130.03, 130.85, 139.11, 155.59.



(Z)-3-styrylphenol:

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 – 7.49 (m, 2H), 7.40 – 7.31 (td, *J* = 7.6, 1.4 Hz, 2H), 7.30 – 7.19 (m, 2H), 7.12 – 7.04 (m, 3H), 7.02 – 6.98 (q, *J* = 1.7 Hz, 1H), 6.77 – 6.72 (m, 1H).

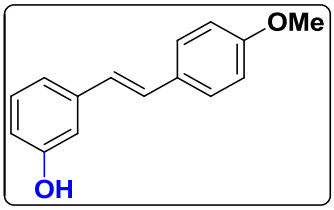
^{13}C NMR (126 MHz, $CDCl_3$) δ 29.93, 76.98, 77.48, 113.16, 114.88, 119.65, 126.77, 127.95, 128.46, 128.91, 129.40, 130.08, 137.36, 156.05.



3-((2-cyanophenoxysulfonyl)methyl)-5-hydroxyphenyl acetate:

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.68 – 7.61 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 7.48 – 7.39 (m, 2H), 7.42 – 7.37 (m, 1H), 7.24 – 7.21 (d, *J* = 1.7 Hz, 2H), 4.71 – 4.65 (s, 2H), 2.34 – 2.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 21.22, 57.80, 76.91, 77.55, 107.44, 111.44, 115.16, 115.69, 115.91, 120.45, 123.62, 127.74, 129.24, 134.04, 134.80, 149.99, 151.87, 168.93.



(E)-3-(4-methoxystyryl)phenol:

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.48 – 7.41 (m, 2H), 7.25 – 7.19 (t, *J* = 7.9 Hz, 1H), 7.09 – 7.00 (m, 2H), 6.98 – 6.96 (t, *J* = 2.0 Hz, 1H), 6.95 – 6.87 (m, 3H), 6.75 – 6.68 (ddd, *J* = 8.1, 2.6, 0.9 Hz, 1H), 3.84 – 3.82 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 55.56, 76.91, 77.55, 112.92, 114.36, 114.49, 119.35, 126.40, 127.99, 128.89, 130.02, 130.20, 139.62, 156.07, 159.57.

^{13}C NMR DEPT (101 MHz, $CDCl_3$) δ 55.35, 112.71, 114.15, 114.28, 119.14, 126.19, 127.78, 128.68, 129.81.

Reference:

1. M. Bera; A. Maji; S. K. Sahoo; D. Maiti *Angew. Chem. Int. Ed.* 2015, **54**, 8515.
2. A. R. Katritzky; B. Yang; G. Qiu; Z. Zhang *Synthesis* 1999, **1**, 55.
3. M. Brookhart; M. L. H. Green *J. Organomet. Chem.* 1983, **250,** 395.

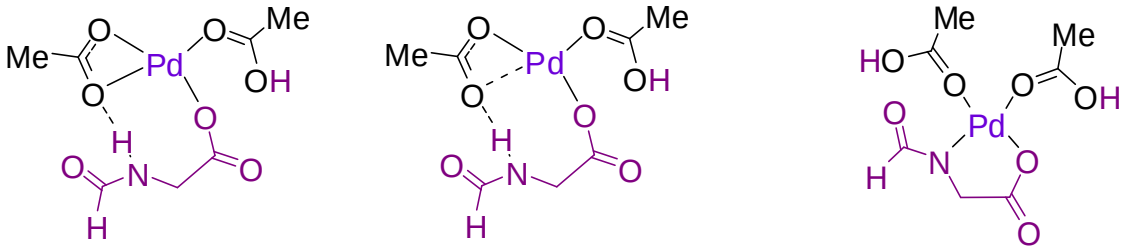
VII. Computational Methods

Computations were performed using Gaussian09 (Revision D.01) suite of quantum chemical program.[1] The geometries were optimized in the solvent phase using the M06[2] hybrid density functional theory using Pople's 6-31G** basis set for all atoms except Palladium. Los Alamos pseudopotential (LANL2DZ) basis set consisting of an effective core potential (ECP) for 28 core electrons and a double-ζ quality valence basis set for 18 valence electrons was employed for Palladium atom.[3] All the stationary points were characterized, as minima or a first-order saddle point (transition states) by evaluating the corresponding Hessian indices. The transition states were verified by examining whether it has a unique imaginary frequency representing the desired reaction coordinate. Intrinsic reaction coordinate (IRC) calculations were additionally carried out to further characterise the true nature of the transition states.[4] The effect of a solvent continuum in dielectric (dielectric constant ε=16.7 is nearly equal to the solvent HFIP used in the reaction) was evaluated using the Cramer−Truhlar continuum solvation model that employs quantum mechanical charge densities of solutes, designated as SMD.[5] Graphical representation of the optimized geometries are created by using CYLView.[6] Further analysis of the transition states (*meta, ortho and para*) were performed using the *Activation Strain* model, wherein the *distortion energy* of each of the reacting partner at the transition state is computed with respect to the native undistorted reactant(s) and the *interaction energy* between such distorted reactants are then estimated.[7] Weinhold's natural bond orbital (NBO) approaches also carried out for further analysis of *meta, ortho* and *para* C-H activation.[8]

VIII. Case Study:

A. Hydroxylation product using N-Formyl-Glycine

(1) N-H activation of the N-For-Gly ligand



a **[a-b]‡** **b**

Figure S4: Deprotonation of N-H of the ligand at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory.

(2) Palladium Acetate with Different Ligand Combinations and the Potential Active Catalyst

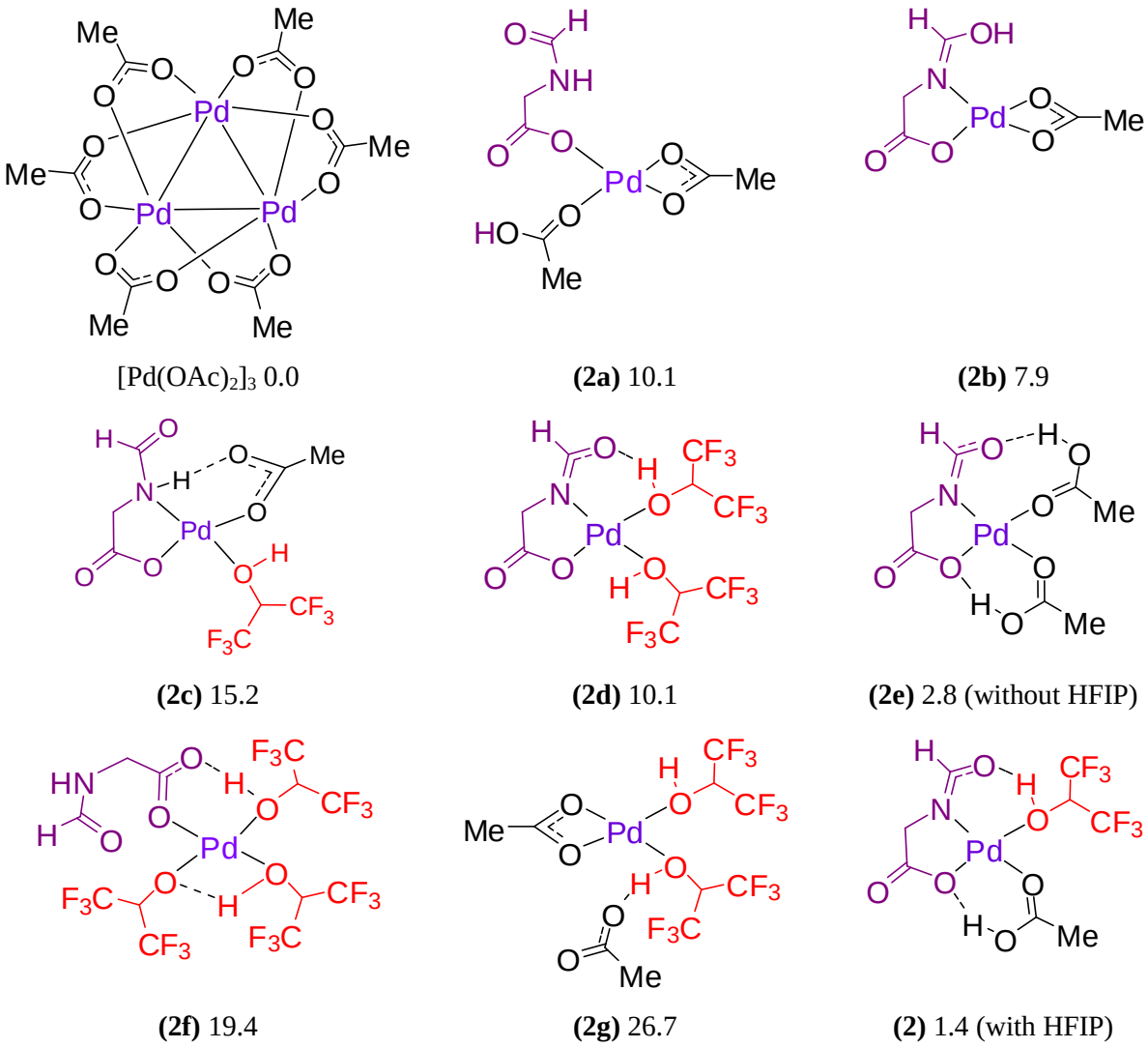
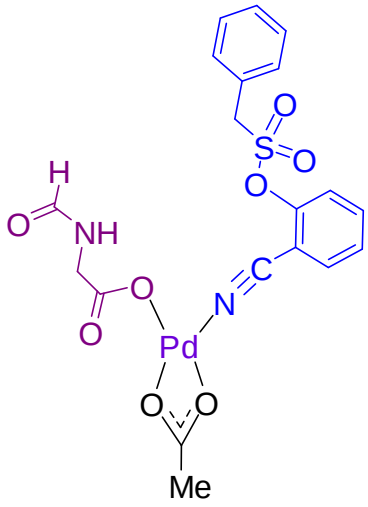
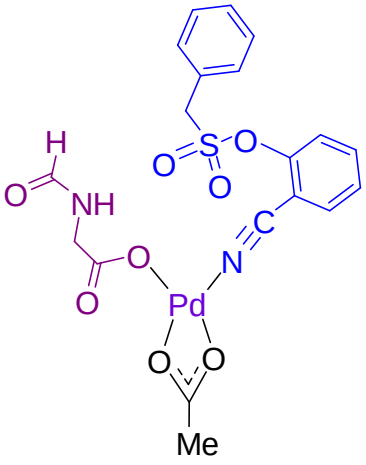


Figure S5: Different possibilities of potential active catalyst at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. The lowest energy species (**2**) is highlighted.

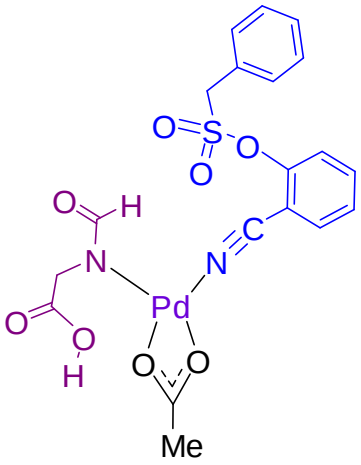
(3) Various Binding Modes between Palladium Acetate, N-For-Gly Ligand and the Substrate



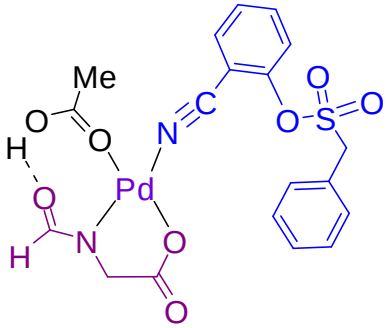
(3a) 11.5



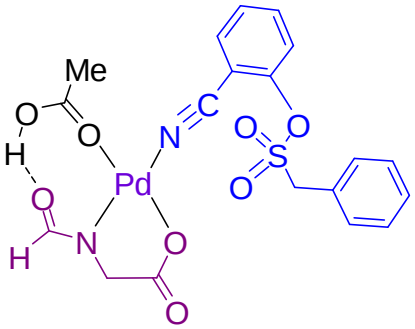
(3b) 11.4



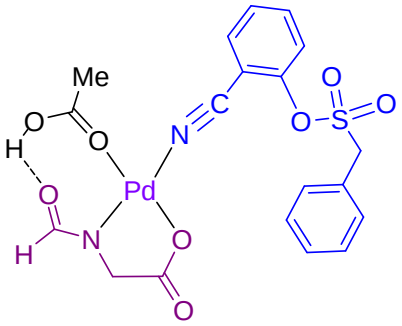
(3c) 13.6



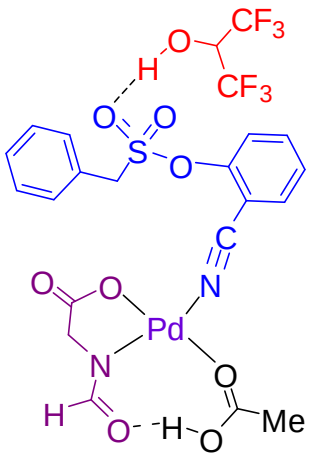
(3d) 4.1



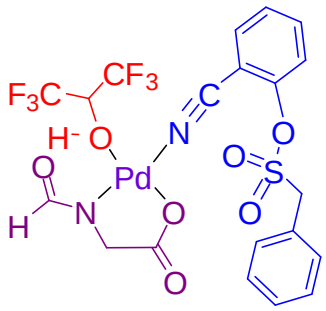
(3e) 3.9



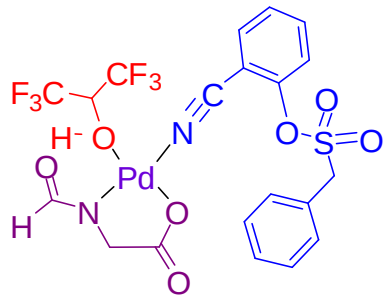
(3f) 1.4



(3g) 10.8



(3h) 3.2



(3) 0.1

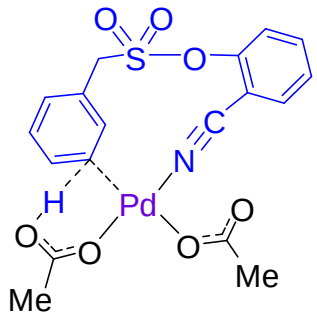
Figure S6: Relative energies of different possible combinations of palladium acetate, ligand and the substrate at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. The lowest energy species (**3**) is highlighted.

(4) C-H activation

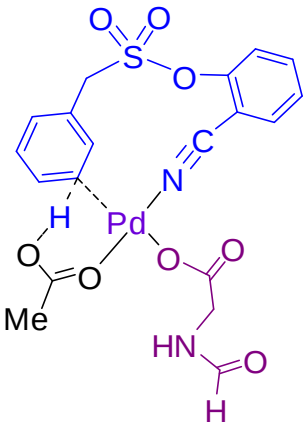
Table S20: Relative Gibbs Free Energies (in kcal/mol) of the C-H Bond Activation Transition States at the *meta*, *ortho* and *para* Positions at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** Level of Theory

Conformation/Configuration	*meta*	*ortho*	*para*
A	28.3	33.8	30.8
B	21.0	26.0	21.9
C	16.4	20.9	17.9
D	32.3	38.2	34.4
E	36.9	36.1	37.2
F	27.4	27.4	25.0
G	51.9	-	37.2*
H	26.1		30.7

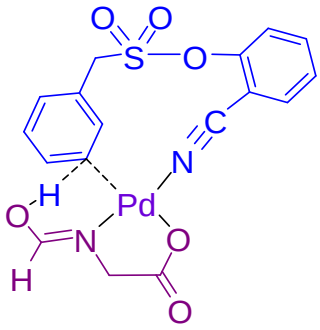
The lowest energy possibility (**C**) is highlighted



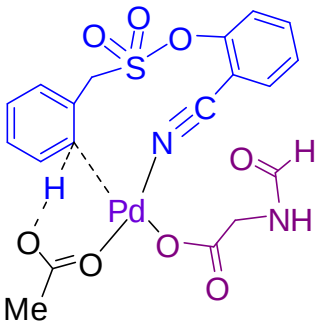
(A)



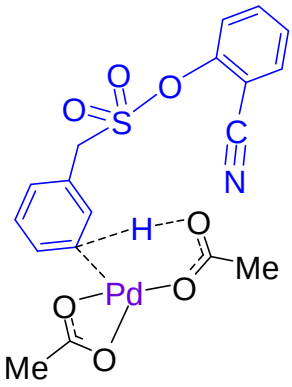
(B)



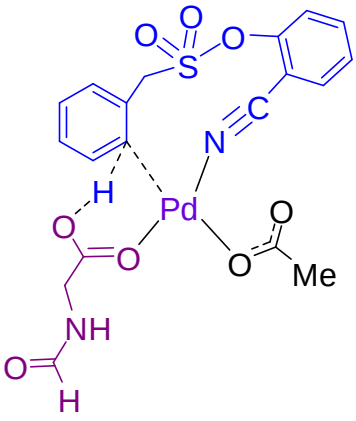
(C) [4-5]‡



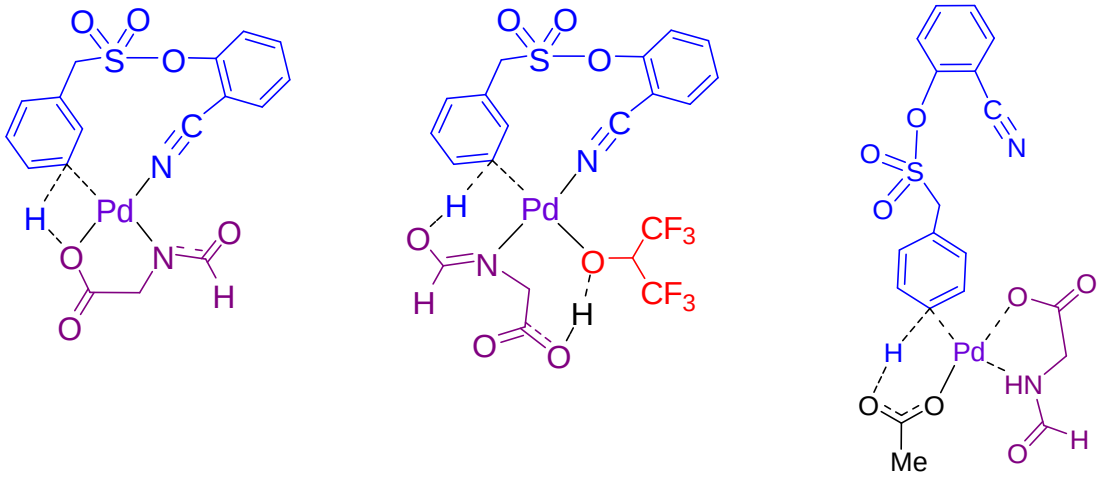
(D)



(E)



(F)

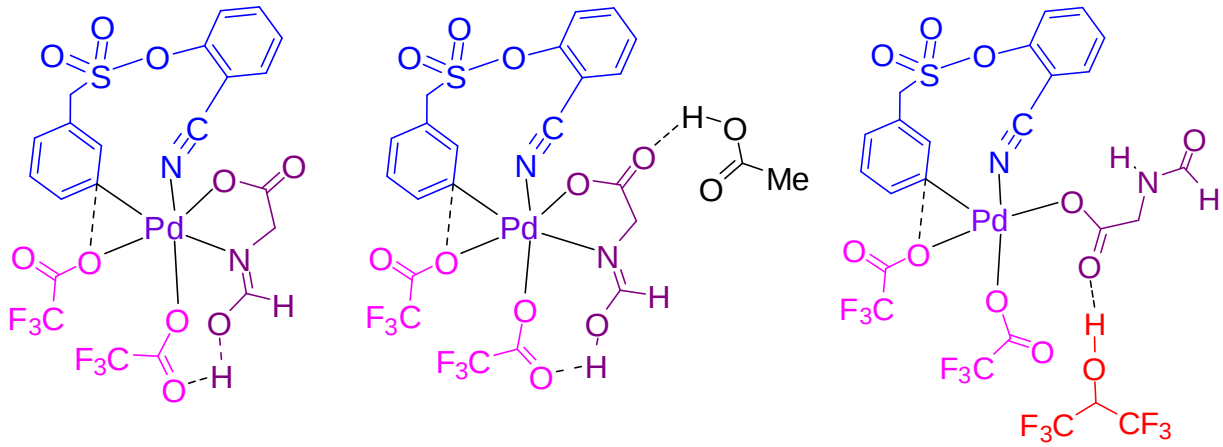


(G) **(H)** **(G*)**

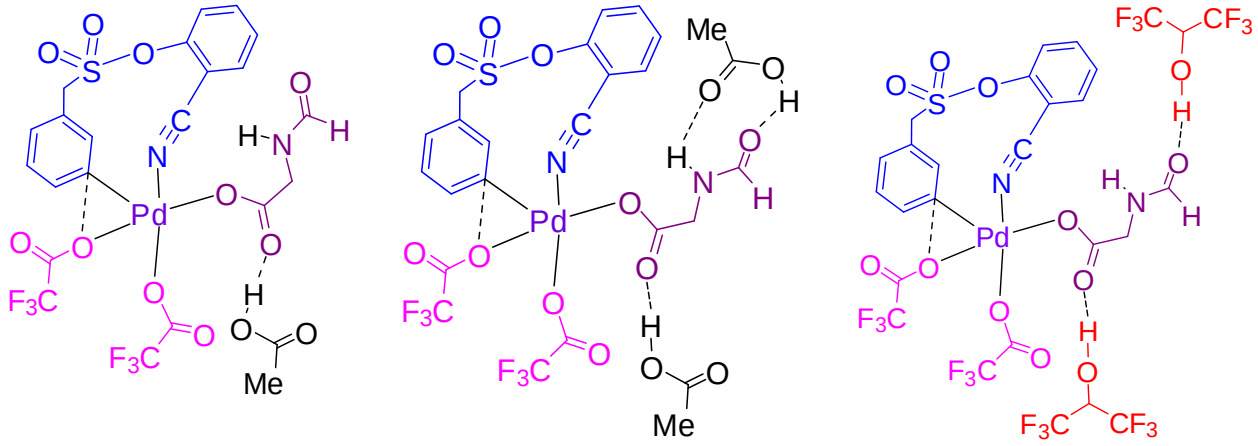
Figure S7: *meta* C-H bond activation transition states at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. (Similar possibilities for the *ortho* and *para* C-H bond activation were also examined).

(4) Reductive Elimination

hexa-coordination penta-coordination



(conf-1) 20.5 (conf-2) 22.5 penta-coordination (conf-3) 18.3



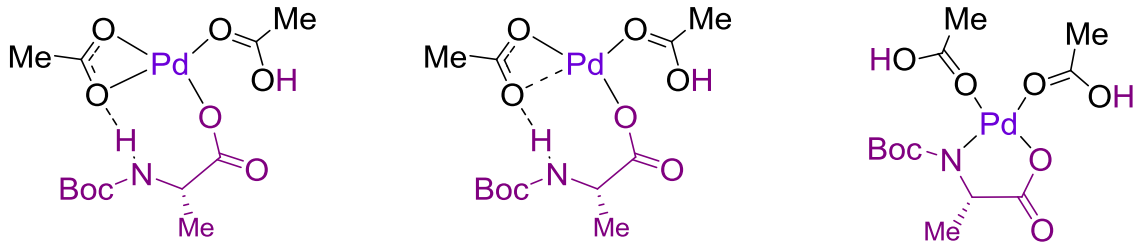
(conf-4) 15.9 (conf-5) 15.1 **[6-7]**‡ (conf-6) 23.0

Figure S8: Different possibilities of reductive elimination transition states at the SMD$_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. The lowest energy possibility is highlighted.

B. Acetoxylation product using Boc-Ala-OH

The acetoxylation pathway has been initially investigated in the gas phase. Transition states and intermediates that are found to be energetically lower were then re-optimized in the solvent phase. Free Energy values in parenthesis are obtained through the gas phase optimization.

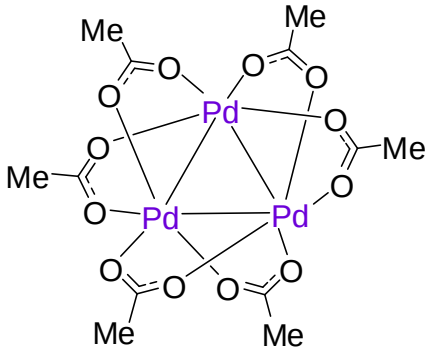
(1) N-H activation of the Boc-Ala-OH ligand



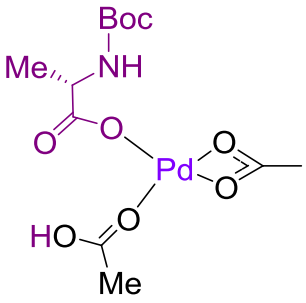
a' ***[a'-b']**‡ **b'**

Figure S9: The N-H deprotonation of the ligand at the SMD$_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. **(*=**SMD$_{(\varepsilon=16.7)}$/M06/6-31G**//M06/6-31G**)

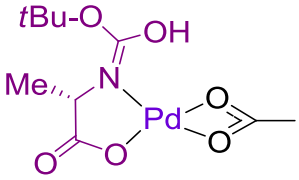
(2) Palladium Acetate with Different Ligand Combinations and the Potential Active Catalyst



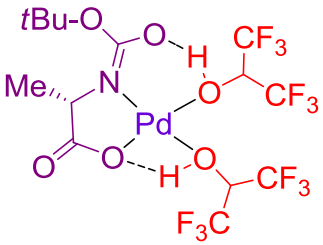
$[Pd(OAc)_2]_3$ 0.0 (0.0)



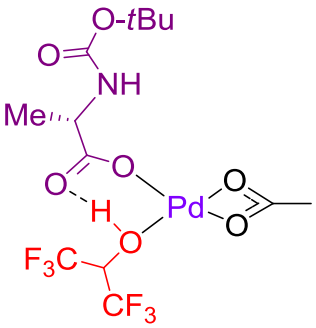
(2a') 21.5 (21.9)



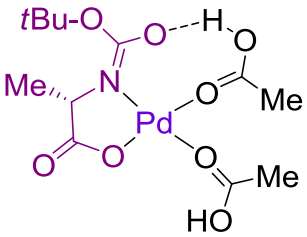
(2b') 16.8 (33.9)



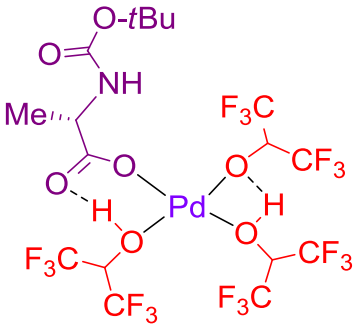
(2c') (31.7)



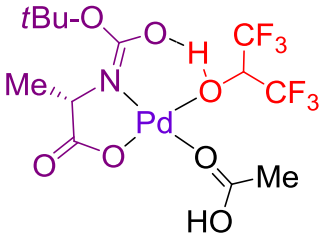
(2d') 17.4 (24.1)



(2e') 11.3 (18.0)



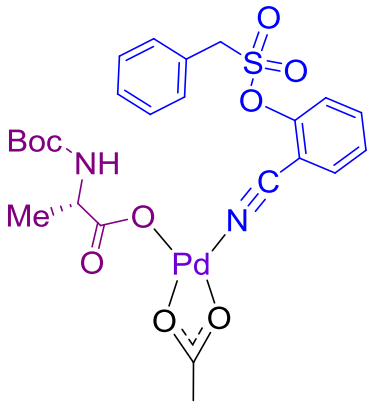
(2f') 30.1 (35.6)



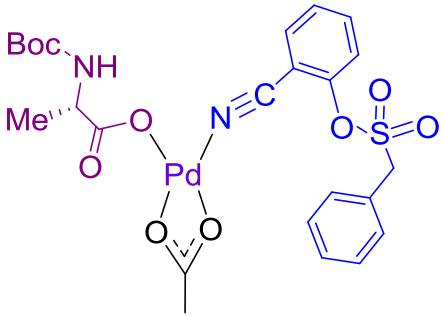
(2') 9.8 (16.0)

Figure S10: Different possibilities of potential active catalyst at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. The values in parenthesis are at the M06/6-31G** level of theory. The lowest energy species (**2'**) is highlighted.

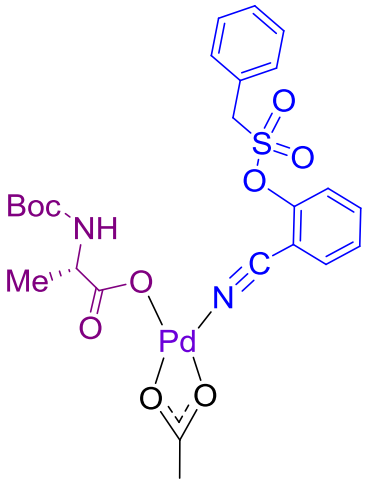
(3) Various Binding Modes between Palladium Acetate, Boc-Ala-OH Ligand and the Substrate



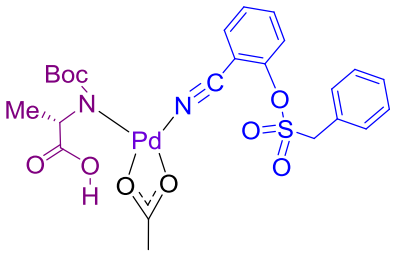
(3a') 16.5 (30.7)



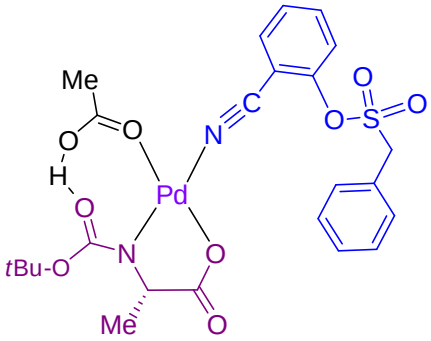
(3b') 19.3 (32.5)



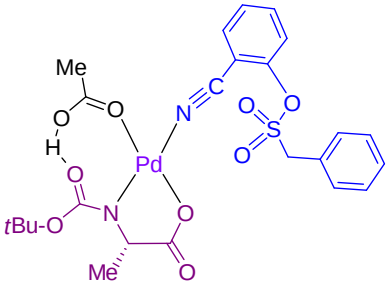
(3c') 19.9 (33.3)



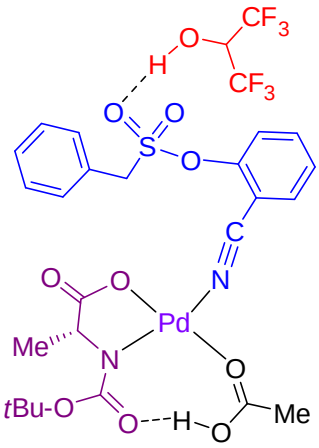
(3d') 21.8 (37.2)



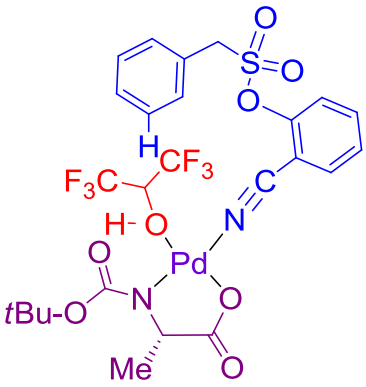
(3e') 12.4 (21.9)



(3f') 13.9 (23.5)



(3g') 19.0 (23.6)



(3') 11.4 (21.7)

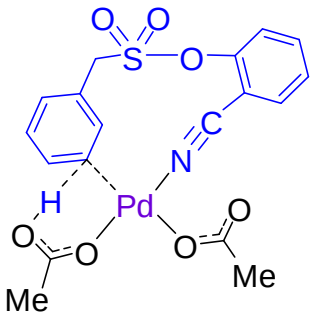
Figure S11: Different possible combinations of palladium acetate, ligand and the substrate at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory. The values in parenthesis is M06/6-31G** level of theory. The lowest energy species (**3'**) is highlighted.

(4) C-H activation

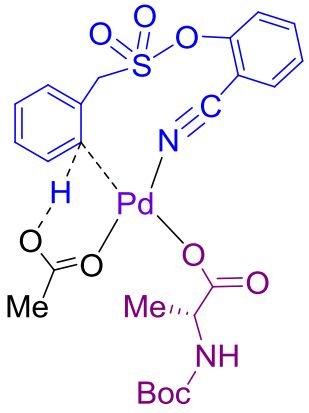
Table S21: Relative Gibbs Free Energies (in kcal/mol) of the C-H Bond Activation Transition States at the *meta*, *ortho* and *para* Positions at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** Level of Theory. The Values in Parenthesis are at the M06/6-31G** Level of Theory

Conformation/Configuration	*meta*	*Ortho*	*para*
A'	(34.5)	(39.0)	(33.2)
B'	27.8 (32.3)	33.9 (35.7)	29.8 (33.2)
C'	26.4 (36.4)	29.9 (41.4)	28.5 (37.0)
D'	35.9 (45.3)	-	36.9 (46.2)
E'	(36.2)	(37.9)	(40.0)
F'	-	(38.6)	30.3 (36.0)

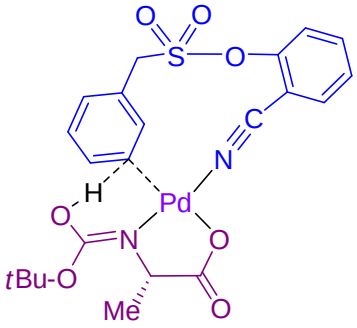
The lowest energy possibility (**C'**) is highlighted.



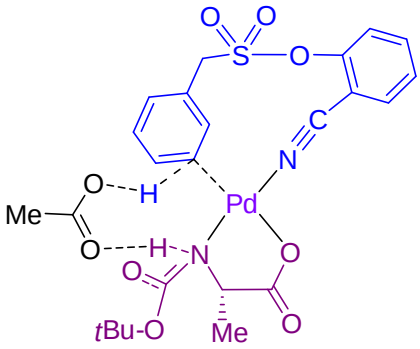
meta-**(A')**



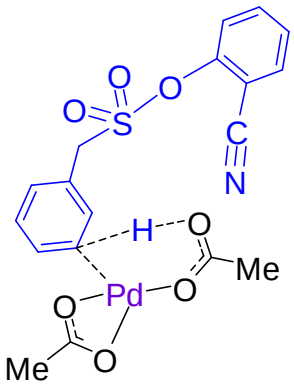
meta-**(B')**



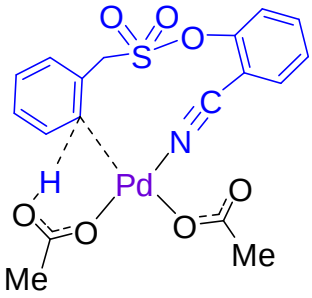
meta-**C' [4'-5']**‡



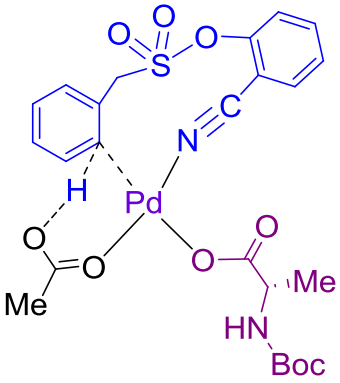
meta-**(D')**



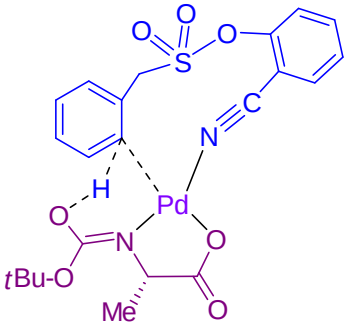
meta-**(E')**



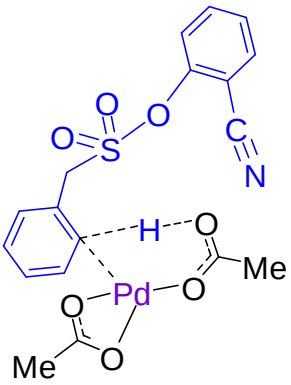
ortho-**(A')**



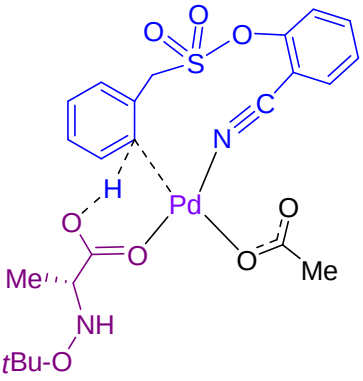
ortho-**(B')**



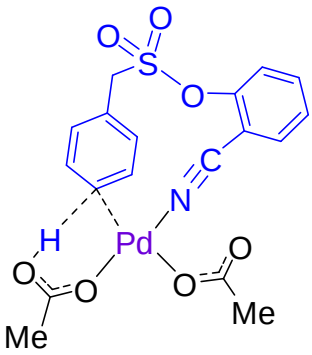
ortho-**(C')**



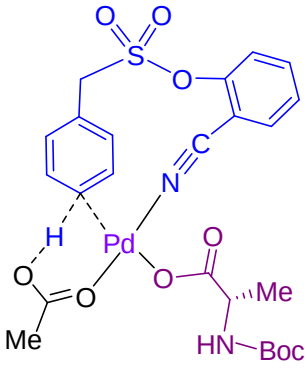
ortho-**(E')**



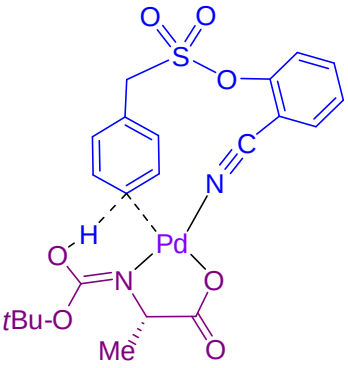
ortho-**(F')**



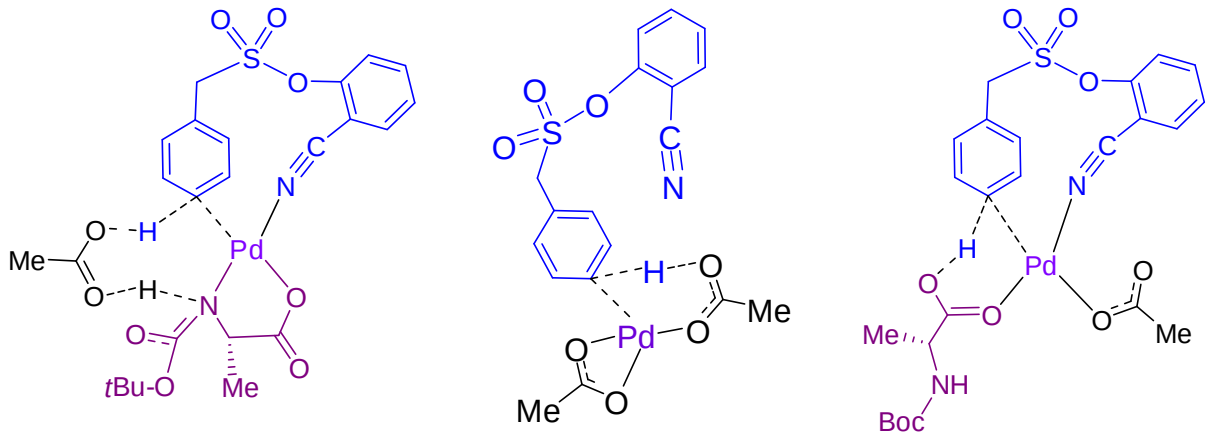
para-**(A')**



para-**(B')**



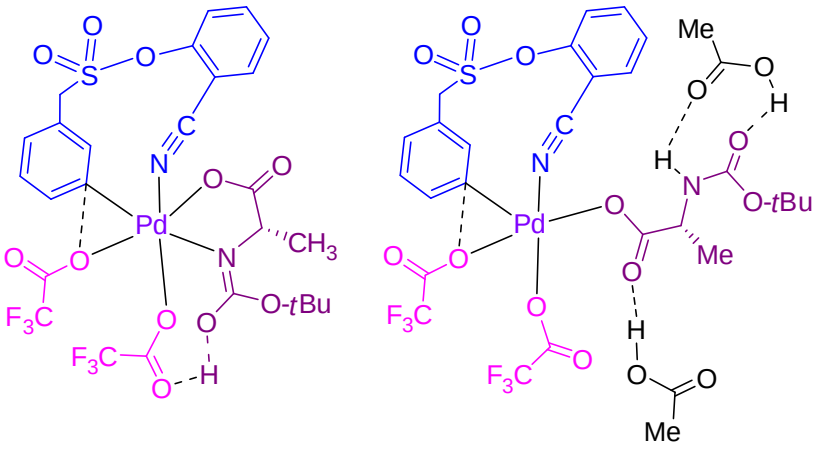
para-**(C')**



para-**(D')** *para*-**(E')** *para*-**(F')**

Figure S12: Different possibilities for the C-H bond activation transition states at the *meta*, *ortho* and *para* positions obtained at the SMD$_{(\varepsilon=16.7)}$/M06/6-31G** level of theory.

(5) Reductive Elimination



(conf-1') 29.2 (40.5) (conf-5') 21.6 **[6'-7']**‡

Figure S13: Different possibilities for the reductive elimination transition states for the *meta* product at the SMD$_{(\varepsilon=16.7)}$/M06/6-31G**Level of Theory. The values in parenthesis are at the M06/6-31G** level of theory.

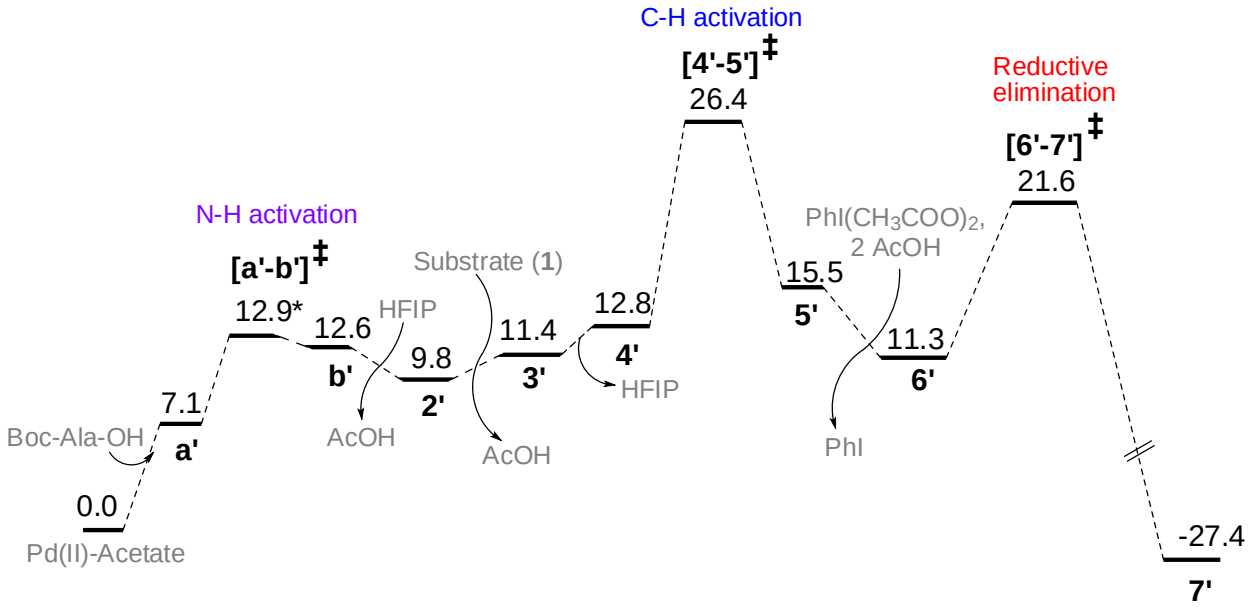
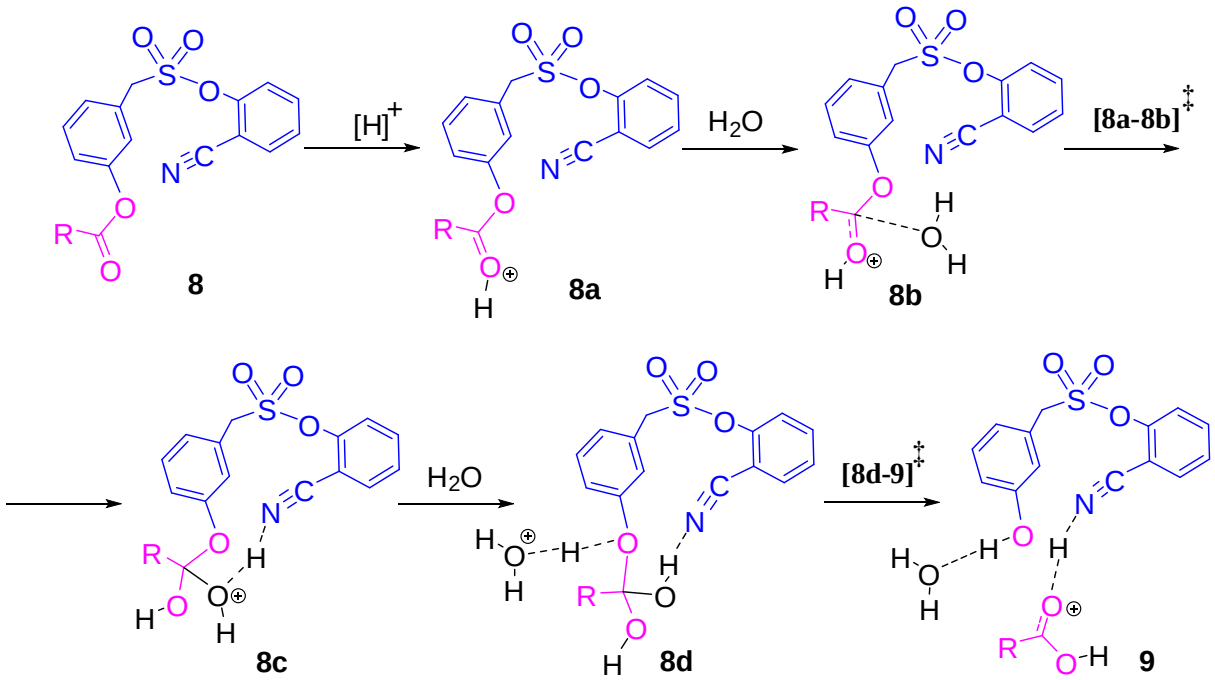


Figure S14: Gibbs free energy profile (kcal/mol) of the acetoxylation obtained at the SMD/M06/6-31G**,LANL2DZ(Pd) level of theory.

IX. Hydrolysis of Trifluoroacetoxy and Acetoxy Products

(a) Mechanism of acid-catalyzed hydrolysis of acetate/trifluoroacetate (R=CF_3/CH_3)



(b) comparison of hydrolysis of trifluoroacetoxylated and acetoxylated products

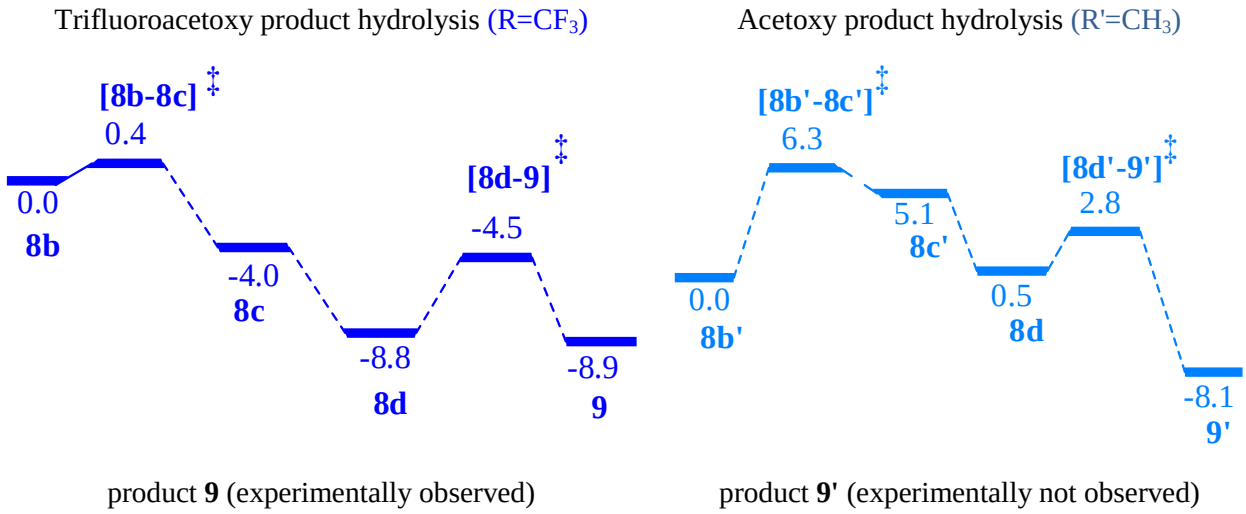


Figure S15: (a) Mechanism of acid-catalyzed hydrolysis and (b) Free energy profile for the hydrolysis of triflouroacetoxylation and acetoxylation at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory.

XIX. Comparison of *meta*, *ortho*, and *para* C-H activation transition states leading to hydroxylated product with N-For-Gly as the ligand by using activation strain analysis

$E_{act}=E_{interaction(i)}+E_{distortion(d)}$

f1=Pd-ligand and f2=Substrate

$E_d= \{(E_{f1(TS)}+ E_{f2(TS)})-(E_{f1}+E_{f2})\}$

$E_i=\{(E_{(TS)}-(E_{f1(TS)}+E_{f2(TS)})\}$

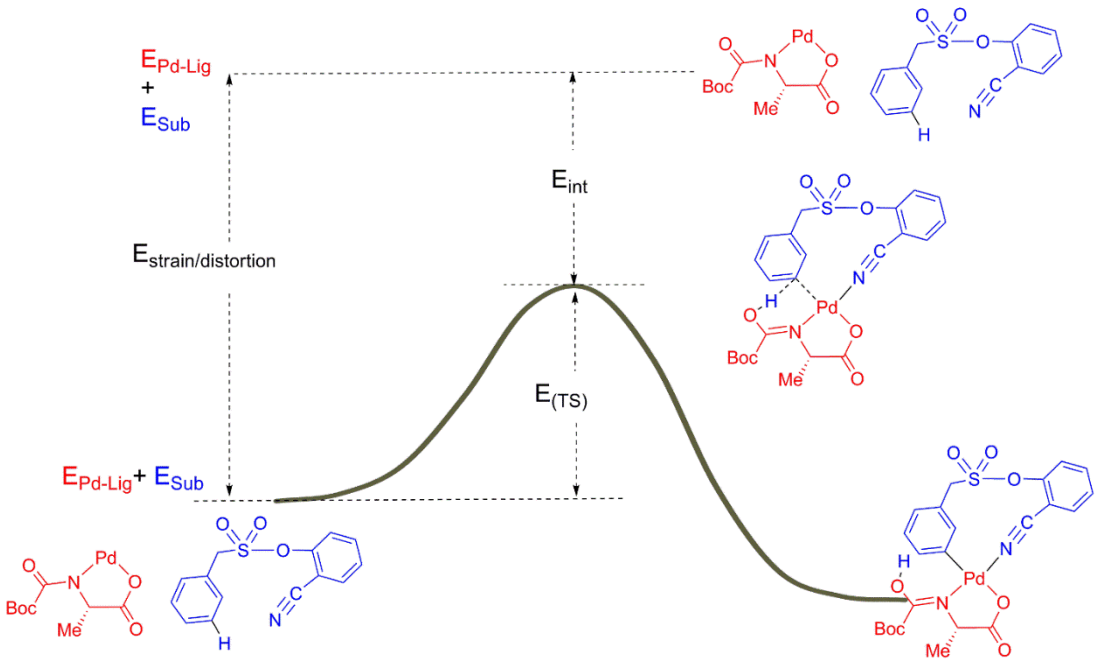


Figure S16. Illustration of distortion and interaction energies within the *Activation Strain Model* for the lowest energy C-H activation transition states

Table S22: Computed Relative Distortion Energies in each Fragment, Total Relative Distortion Energies ($\Delta E^{\ddagger}_{d}$) and Relative Interaction Energies ($\Delta E^{\ddagger}_{i}$) (in kcal/mol) in the C-H Activation Transition State Obtained at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** Level of Theory

C-H activation	Distortion Energy (ΔE_d)	Interaction Energy(ΔE_i)	Activation Energy ($\Delta E^{\ddagger}=[\Delta E^{\ddagger}_{d}+ \Delta E^{\ddagger}_{i}]$)
meta	32.1	-59.9	-27.8
ortho	35.2	-58.3	-23.1
para	32.0	-58.9	-26.9

VI. Natural Bond Orbital Analysis

[4-5]‡		
meta	*ortho*	*Para*

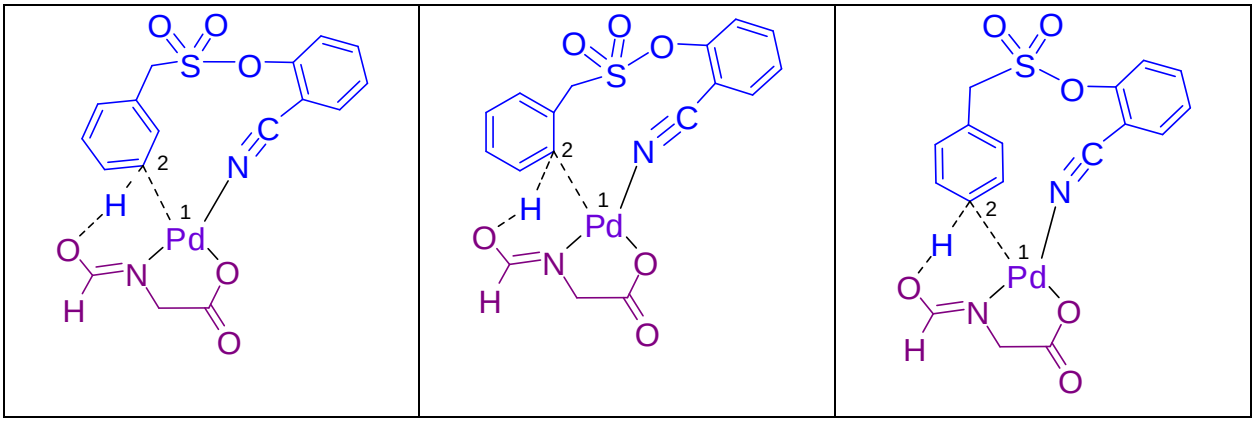


Figure S17: *meta*, *ortho* and *para* C-H bond activation transition states at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G** level of theory (atom numbering used in NBO is shown).

Summary of Natural Population Analysis

Table S23: Natural Charges

C-H activation	Pd1	C2
meta	0.51594	-0.41797
ortho	0.50341	-0.40361
para	0.51560	-0.41358

Table S24: Natural Bond Orbitals, its Occupancy and Orbital energies

C-H_activation	Natural Bond Orbitals	Occupancy	Energy
meta	BD(1) Pd 1 - C 2	1.65521	-0.34506
ortho	BD(1) Pd 1 - C 2	1.23779	0.04631
para	BD(1) Pd 1 - C 2	1.27785	0.02805

We find that the bonding orbital between Pd1 and C2 has the highest occupancy or population in case of *meta*- C-H activation.

XX. References:

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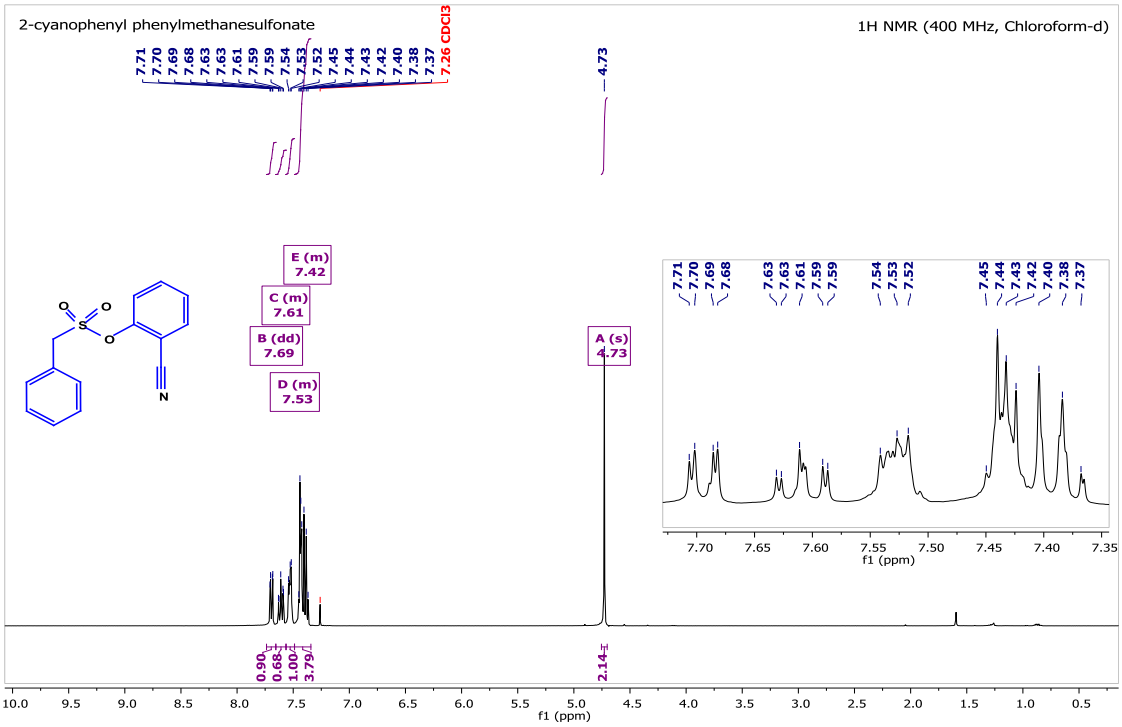
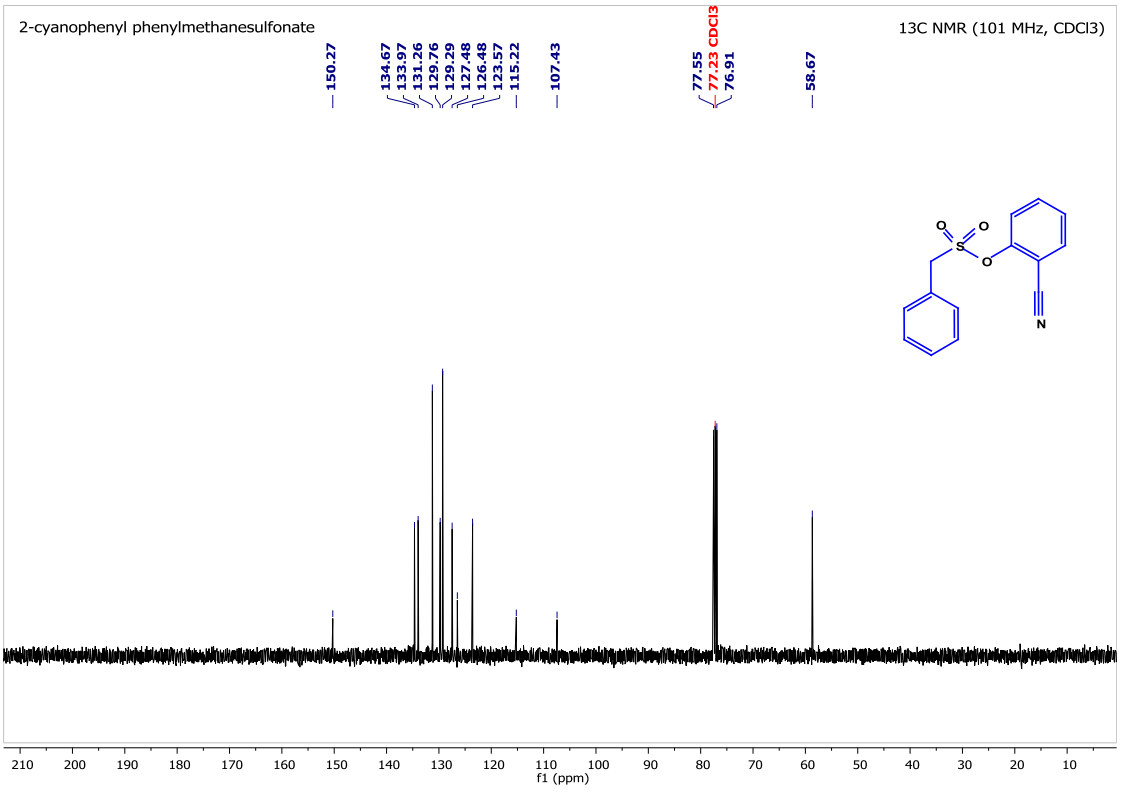
XII. NMR Characterization

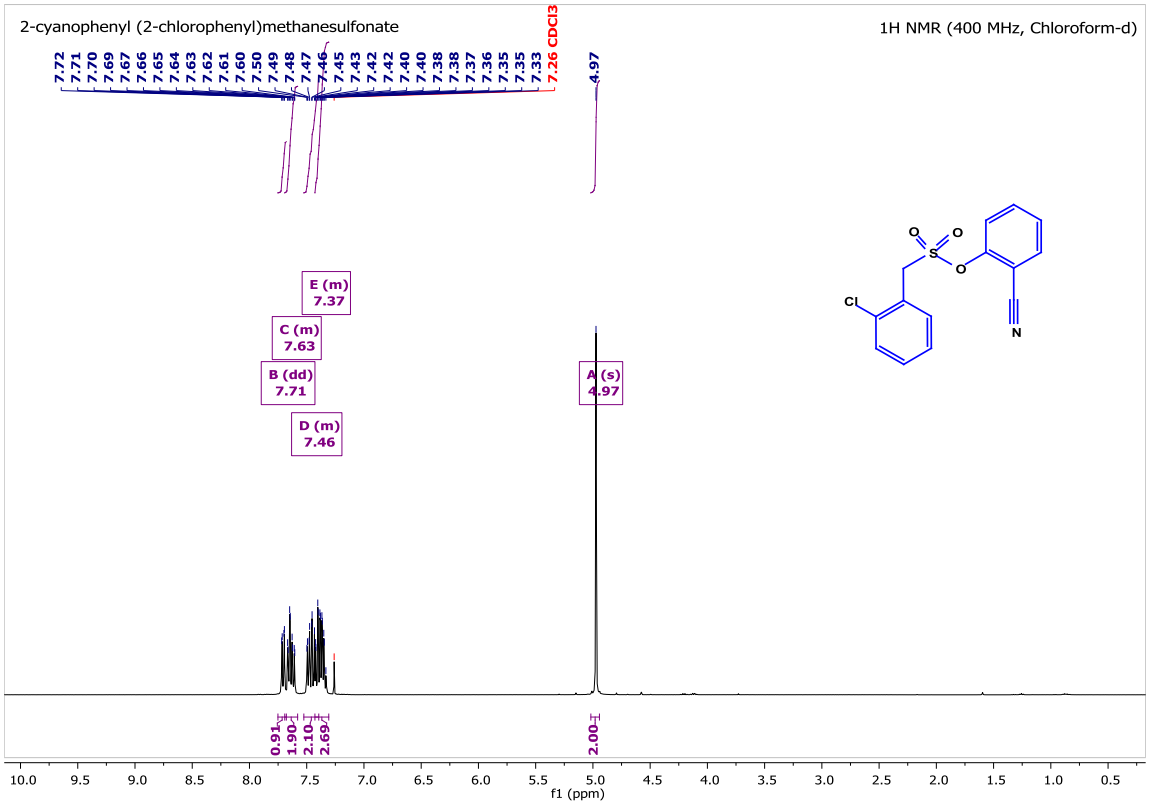
A. NMR Characterization of Substrates

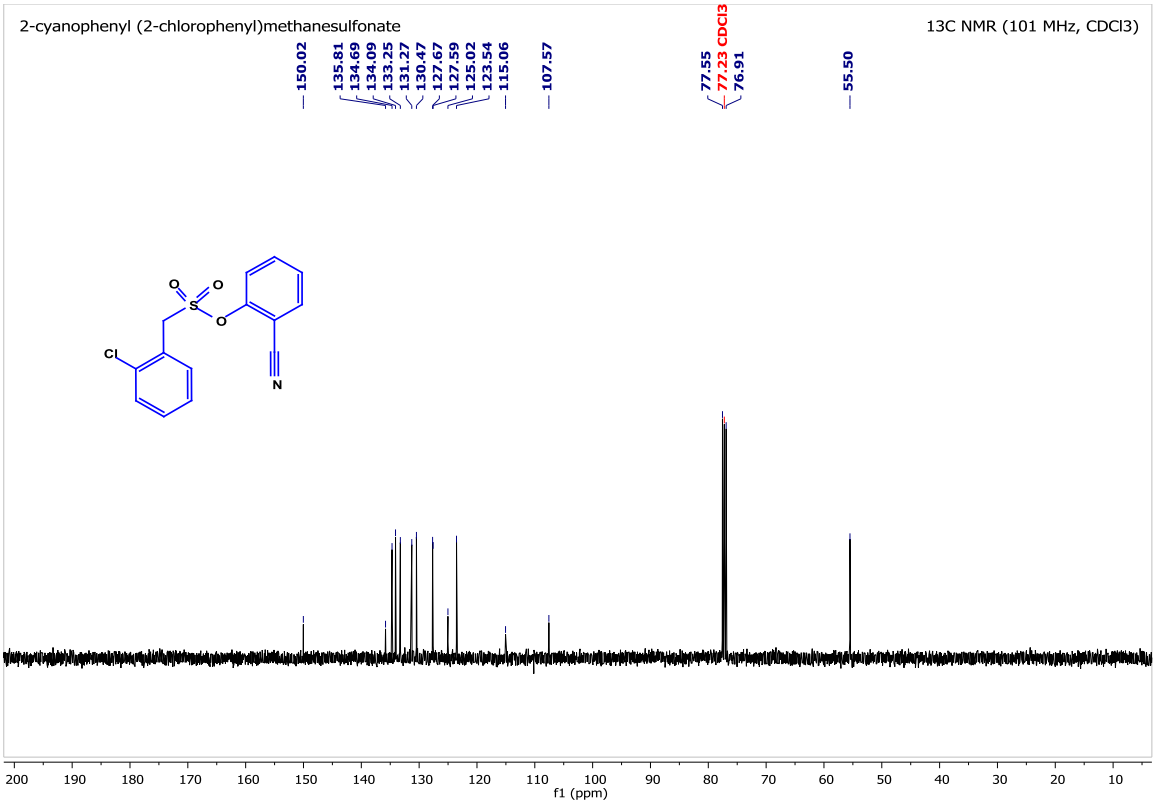
2-cyanophenyl phenylmethanesulfonate:



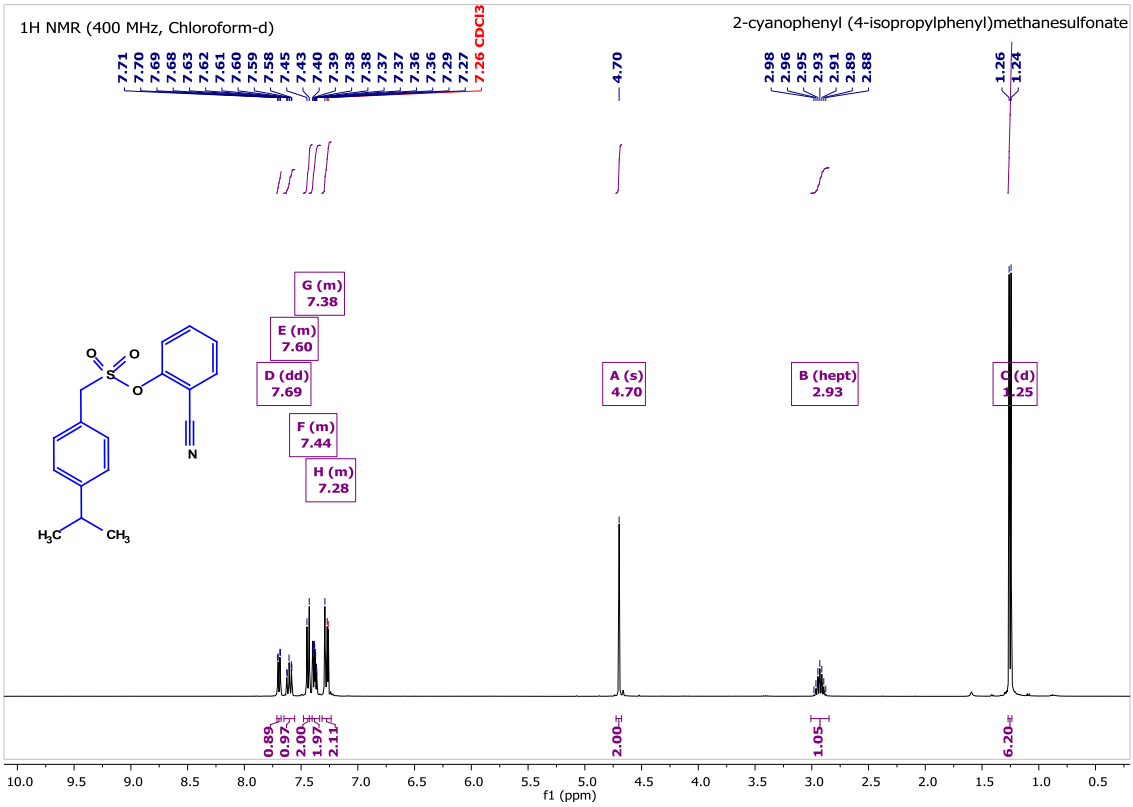


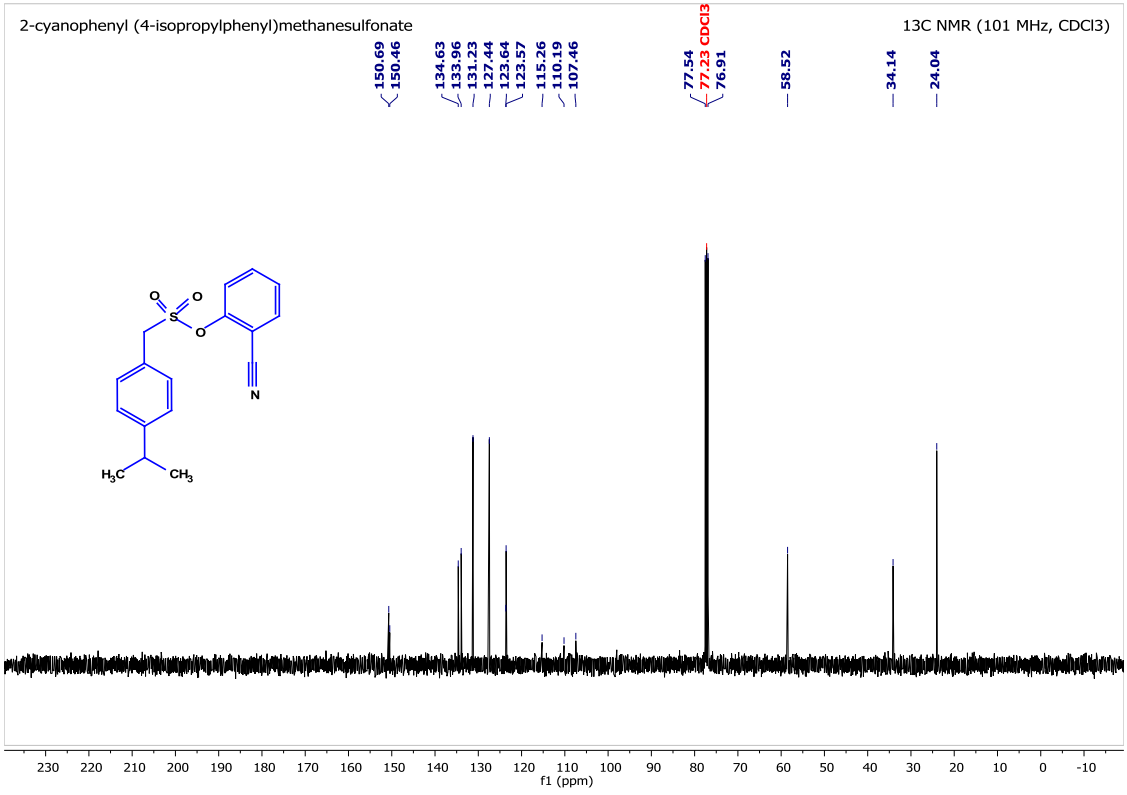
2-cyanophenyl (2-chlorophenyl)methanesulfonate:



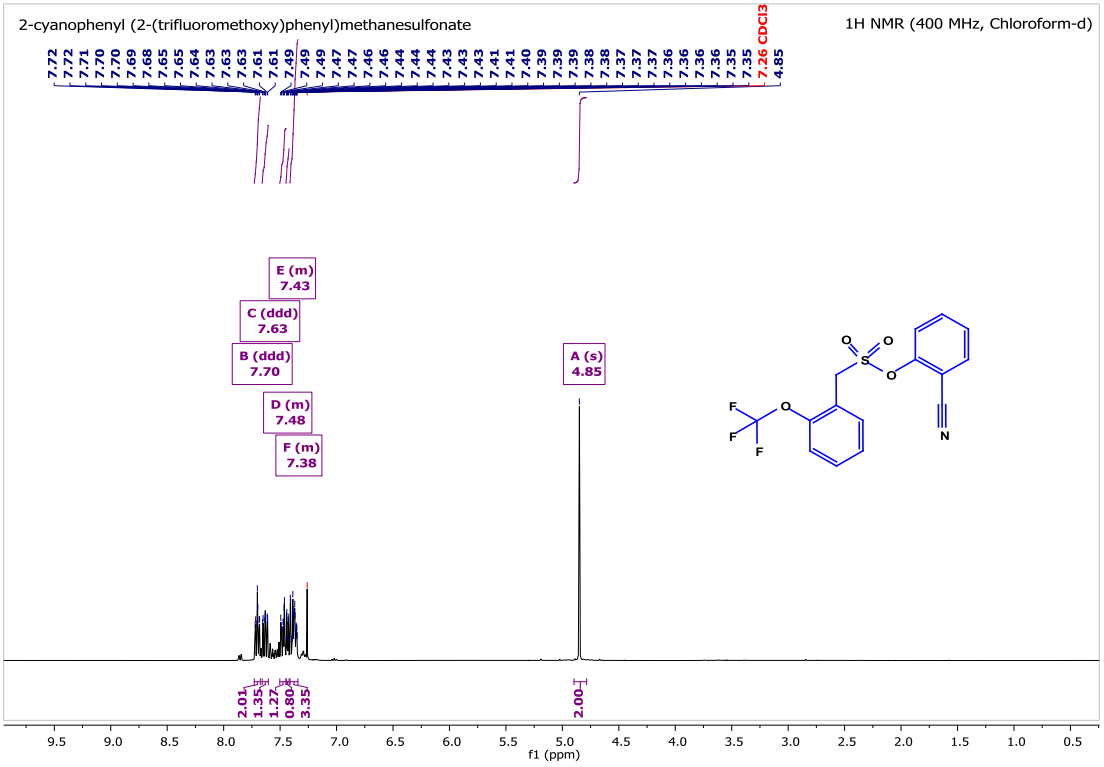


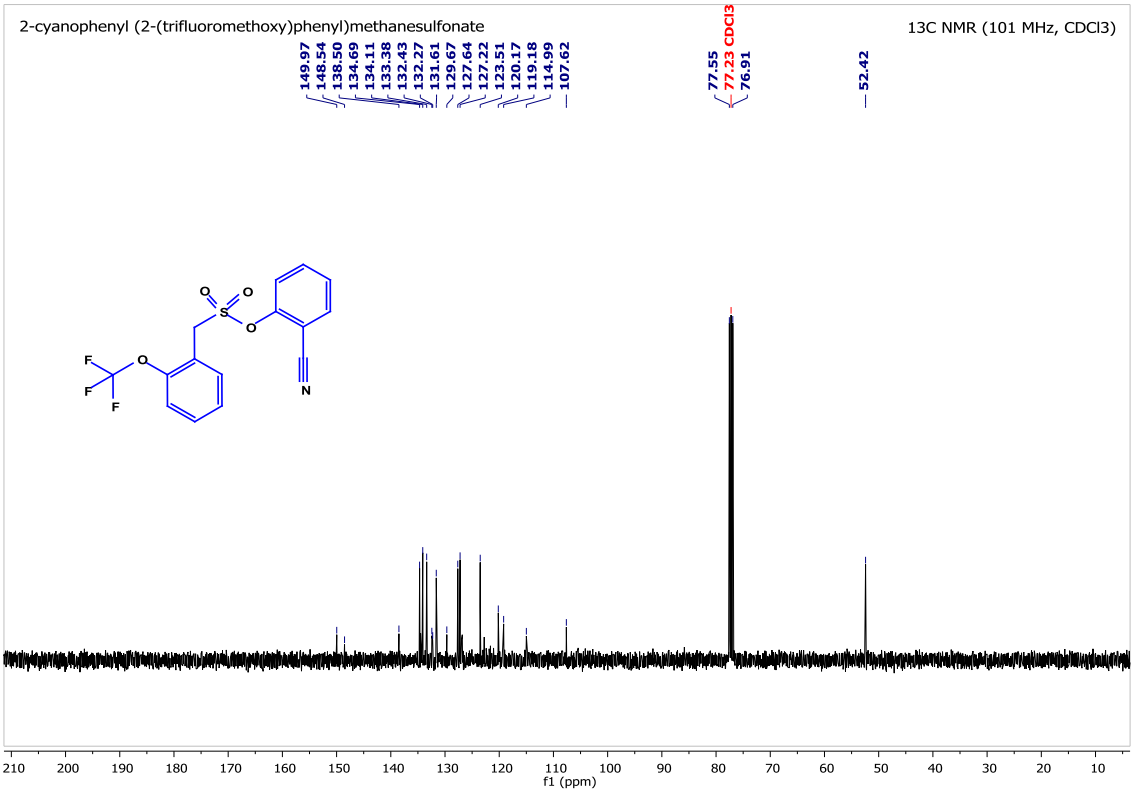
2-cyanophenyl (4-isopropylphenyl)methanesulfonate:



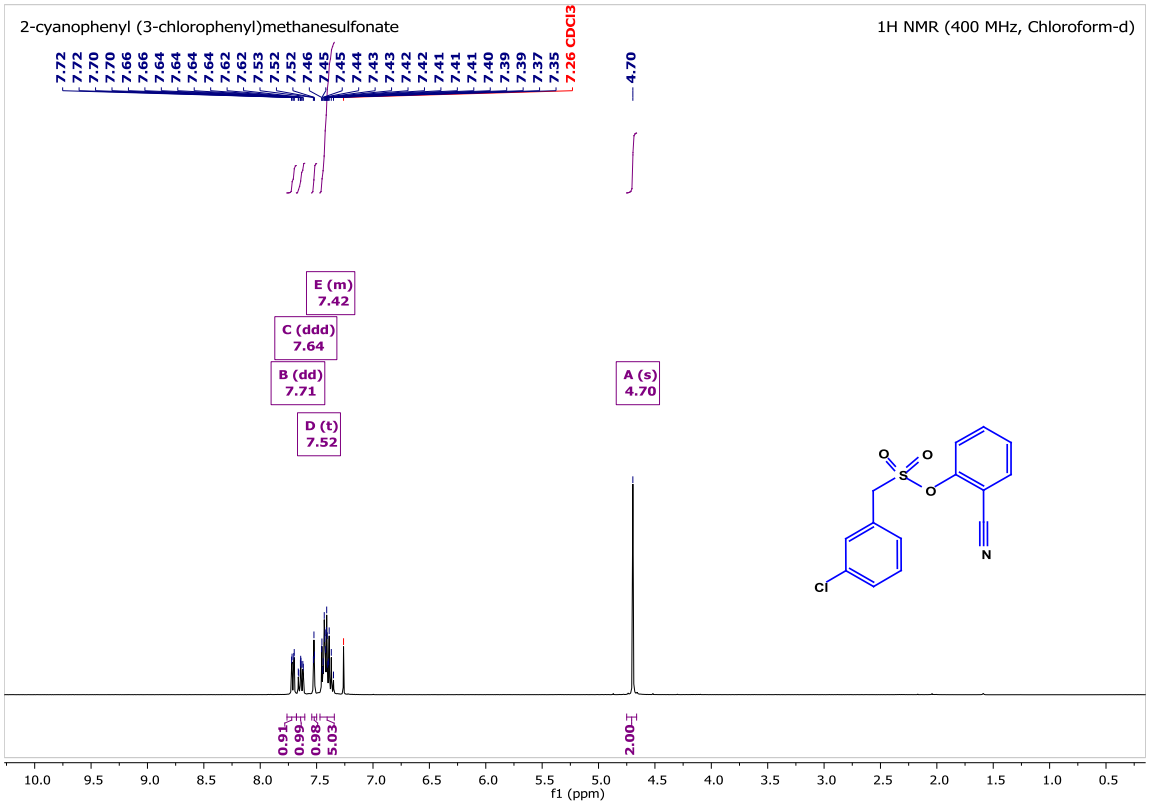


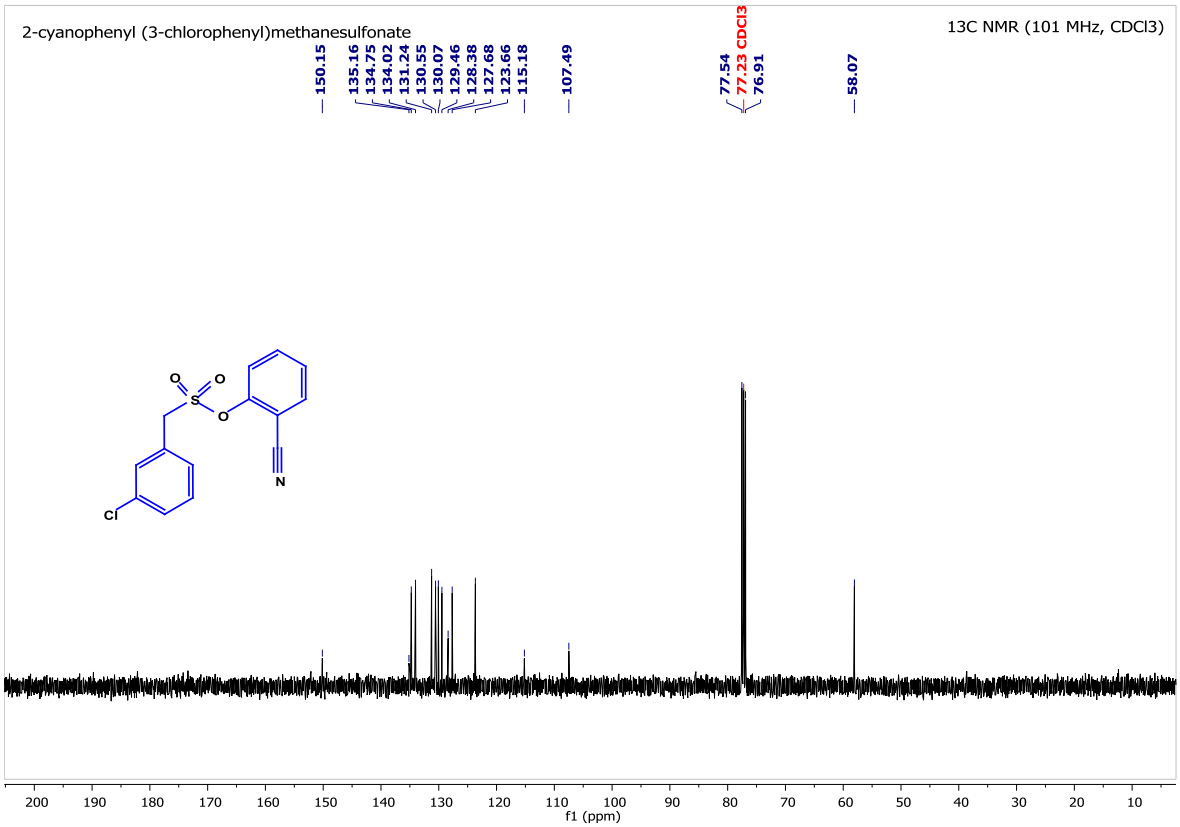
2-cyanophenyl (2-(trifluoromethoxy)phenyl)methanesulfonate:



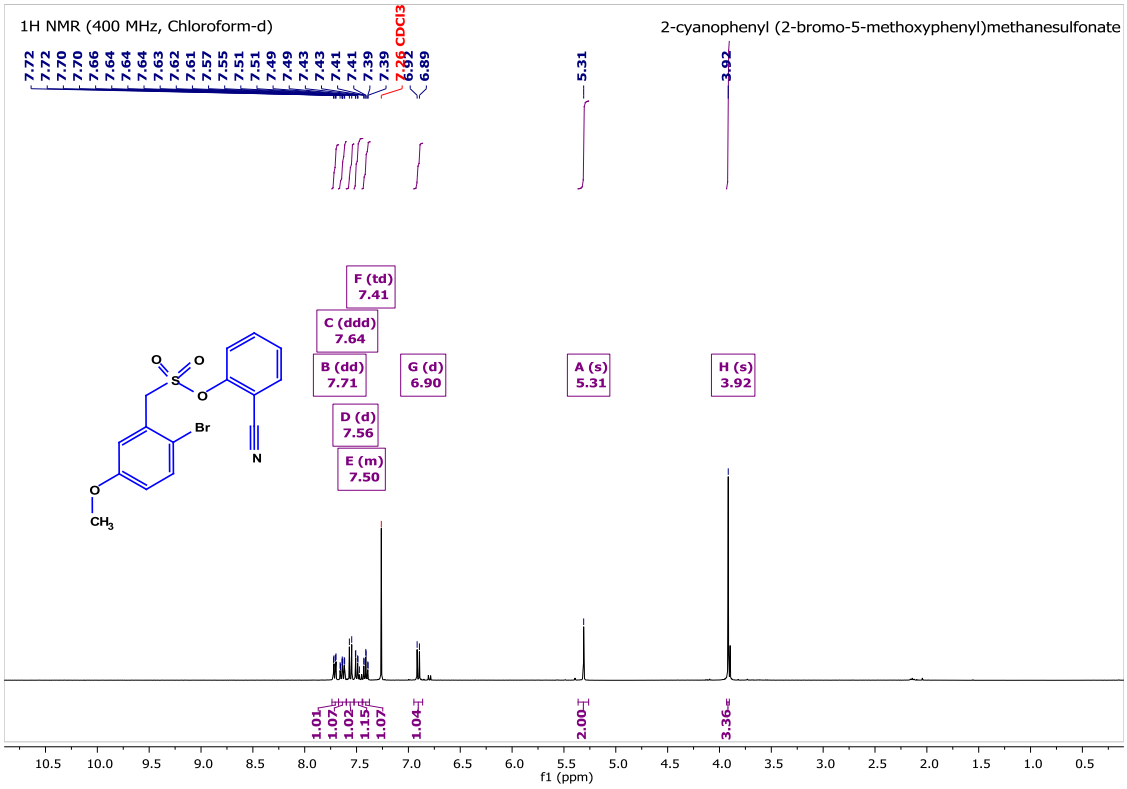


2-cyanophenyl (3-chlorophenyl)methanesulfonate:

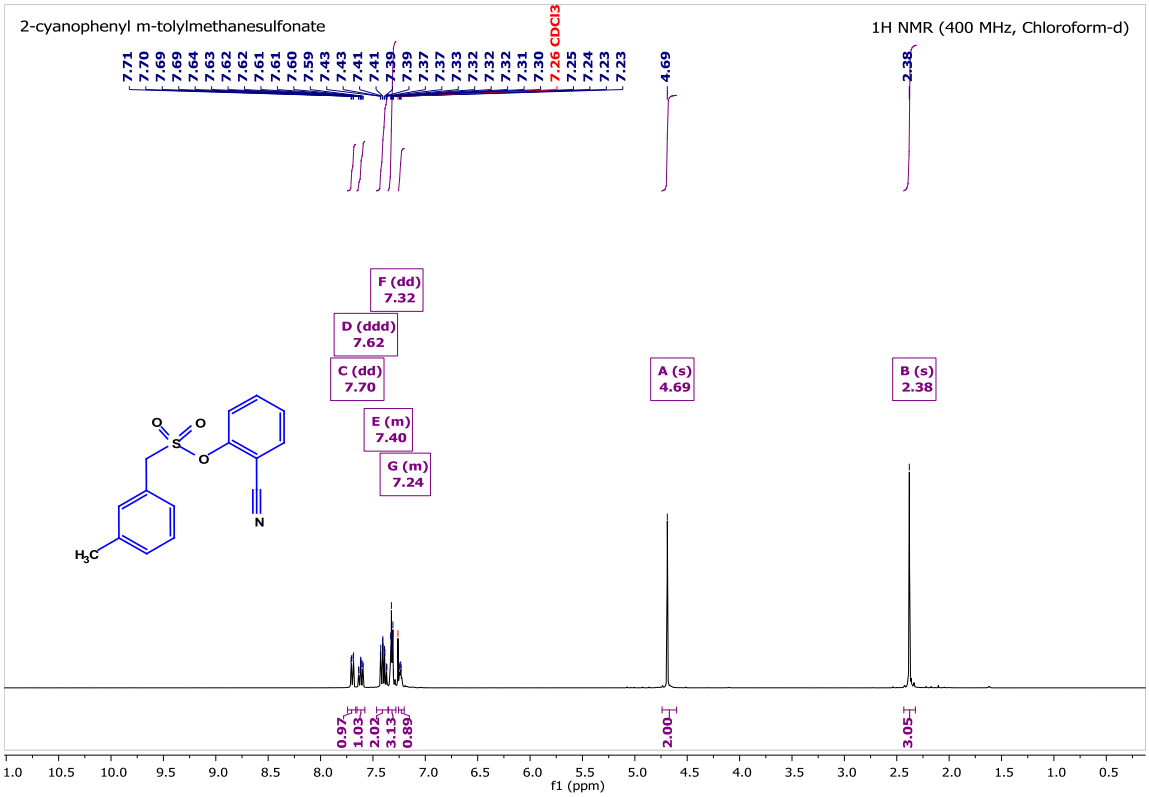

2-cyanophenyl (3-chlorophenyl)methanesulfonate
1H NMR (400 MHz, Chloroform-d)
7.72 7.72 7.70 7.70 7.66 7.64 7.64 7.64 7.62 7.62 7.53 7.52 7.52 7.46 7.45 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.41 7.41 7.40 7.39 7.39 7.37 7.35 7.26 CDCl3
4.70
E (m) 7.42
C (ddd) 7.64
B (dd) 7.71
D (t) 7.52
A (s) 4.70
0.91 0.99 0.98 5.03 2.00
f1 (ppm)

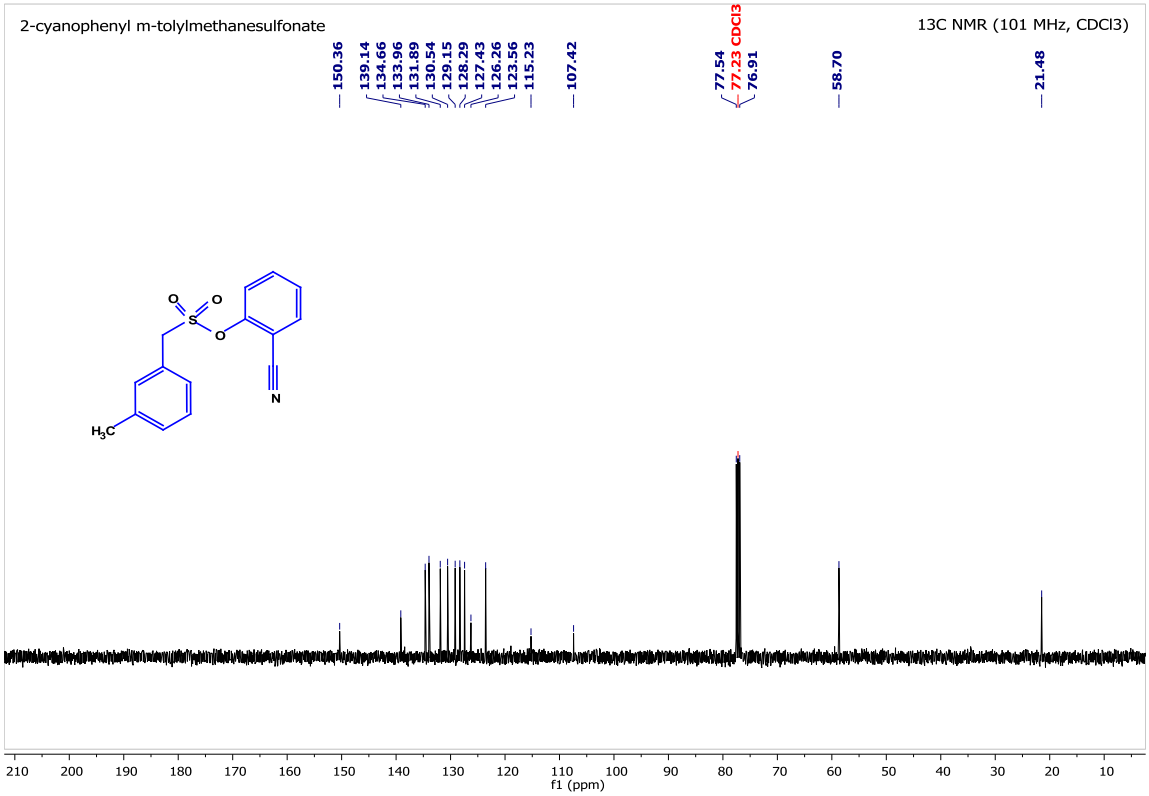

2-cyanophenyl (3-chlorophenyl)methanesulfonate
13C NMR (101 MHz, CDCl3)
150.15 135.16 134.75 134.02 131.24 130.55 130.07 129.46 128.38 127.68 123.66 115.18 107.49 77.54 77.23 CDCl3 76.91 58.07
f1 (ppm)

2-cyanophenyl (2-bromo-5-methoxyphenyl)methanesulfonate:

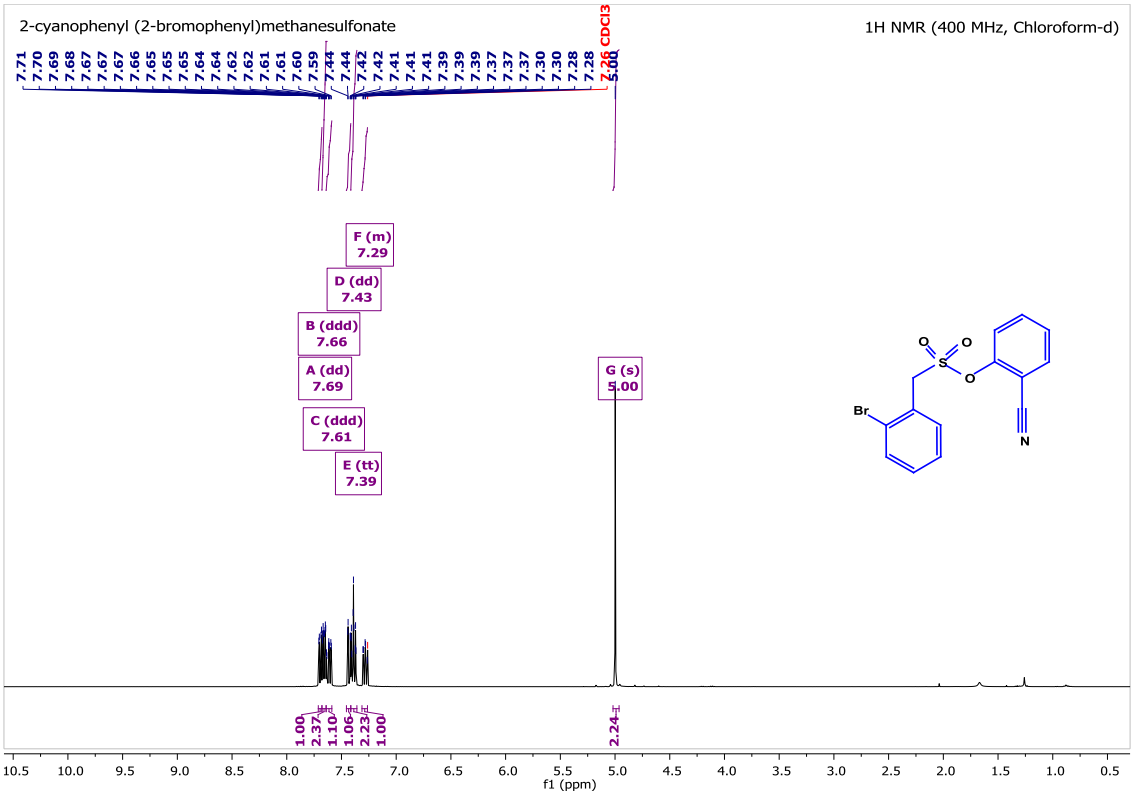


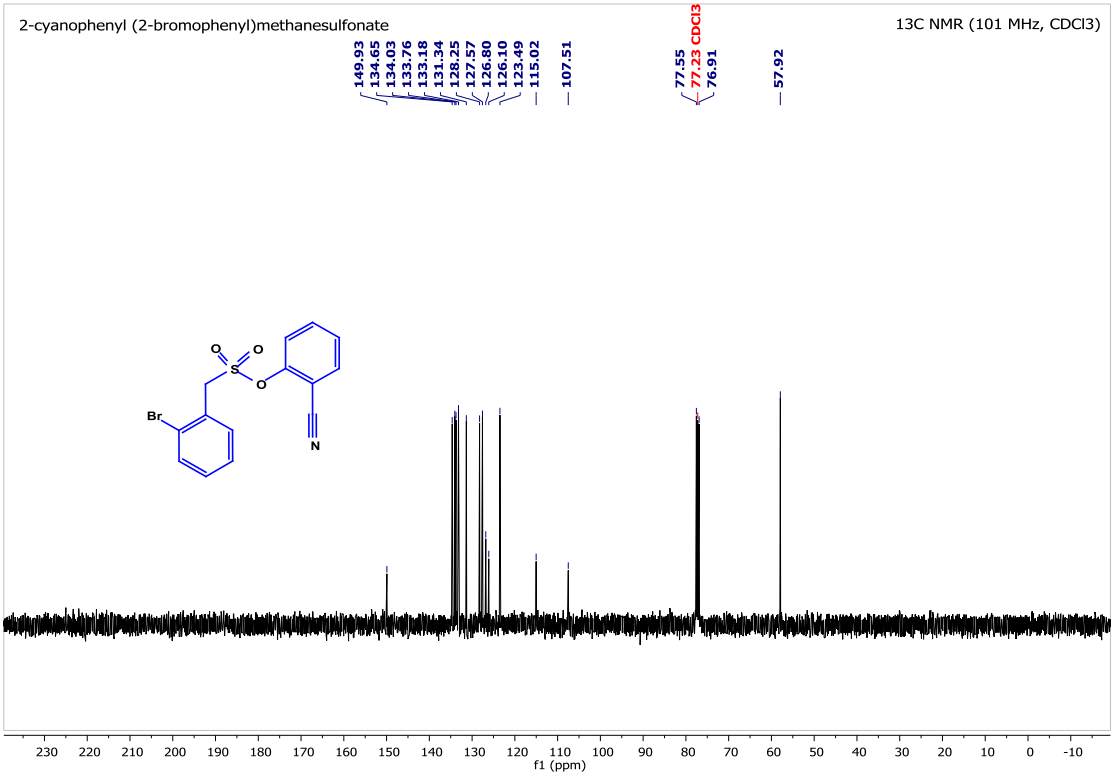
2-cyanophenyl m-tolylmethanesulfonate:



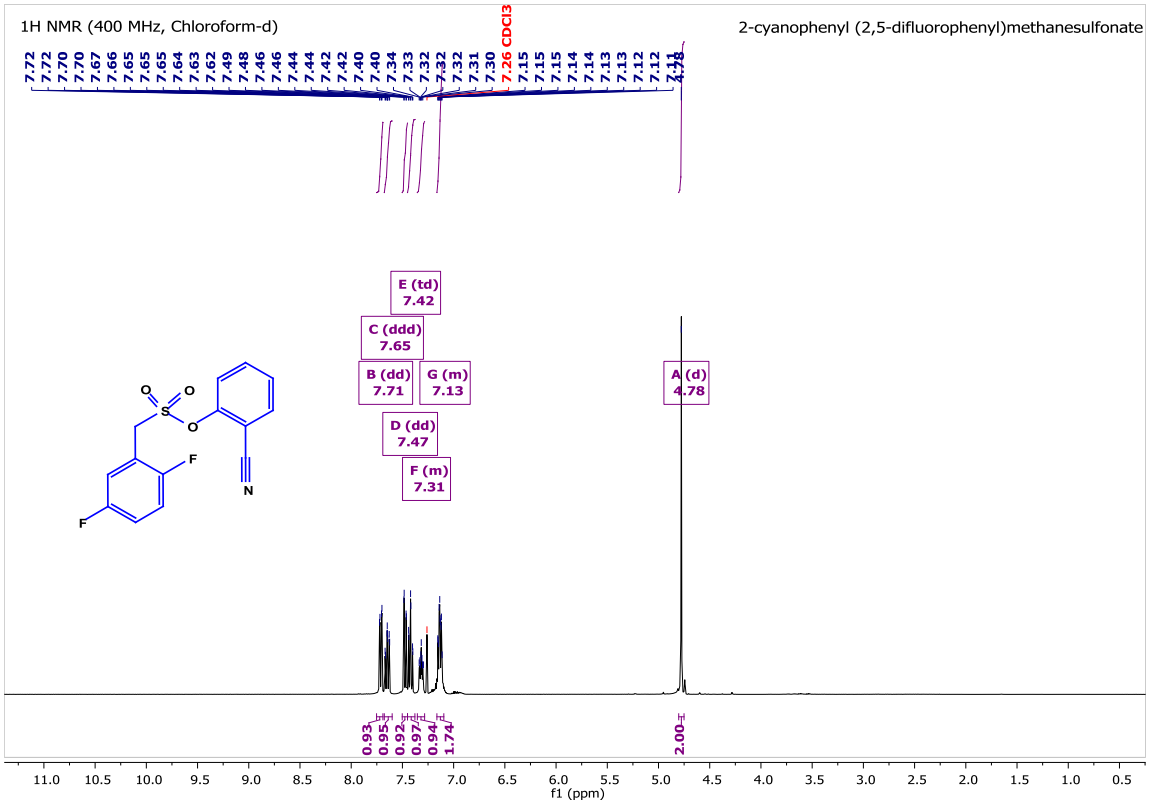


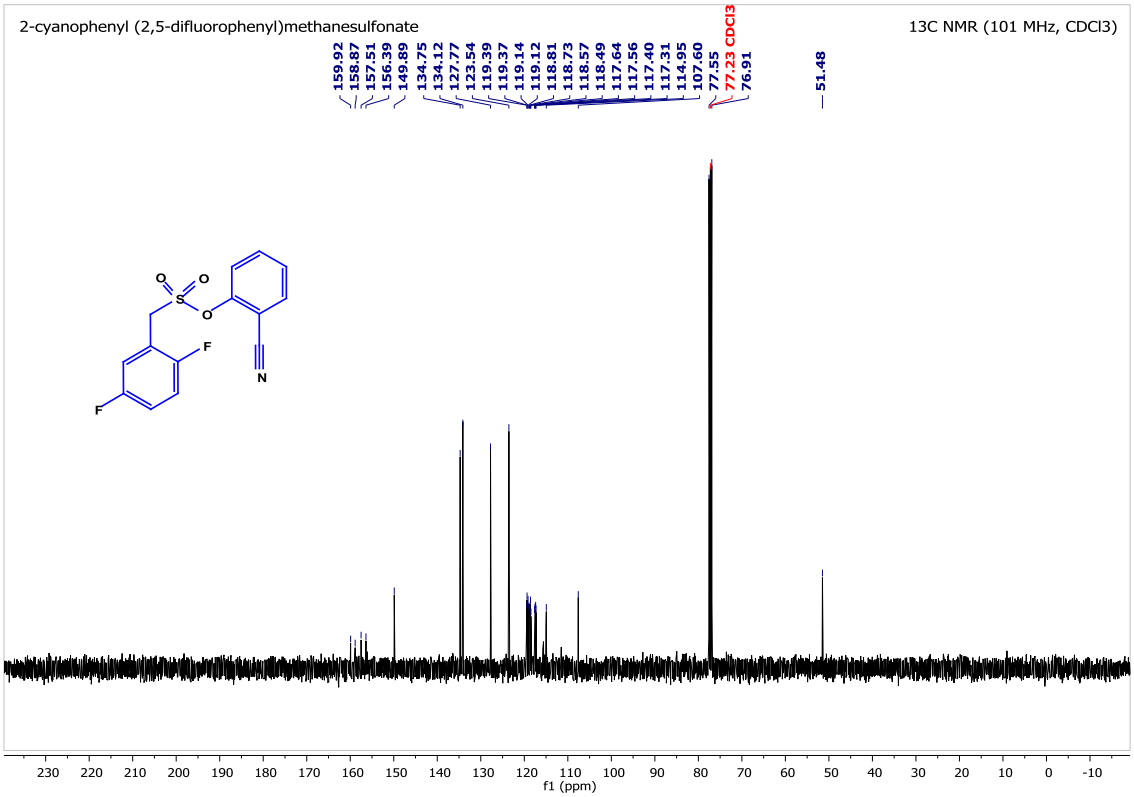
2-cyanophenyl (2-bromophenyl)methanesulfonate:





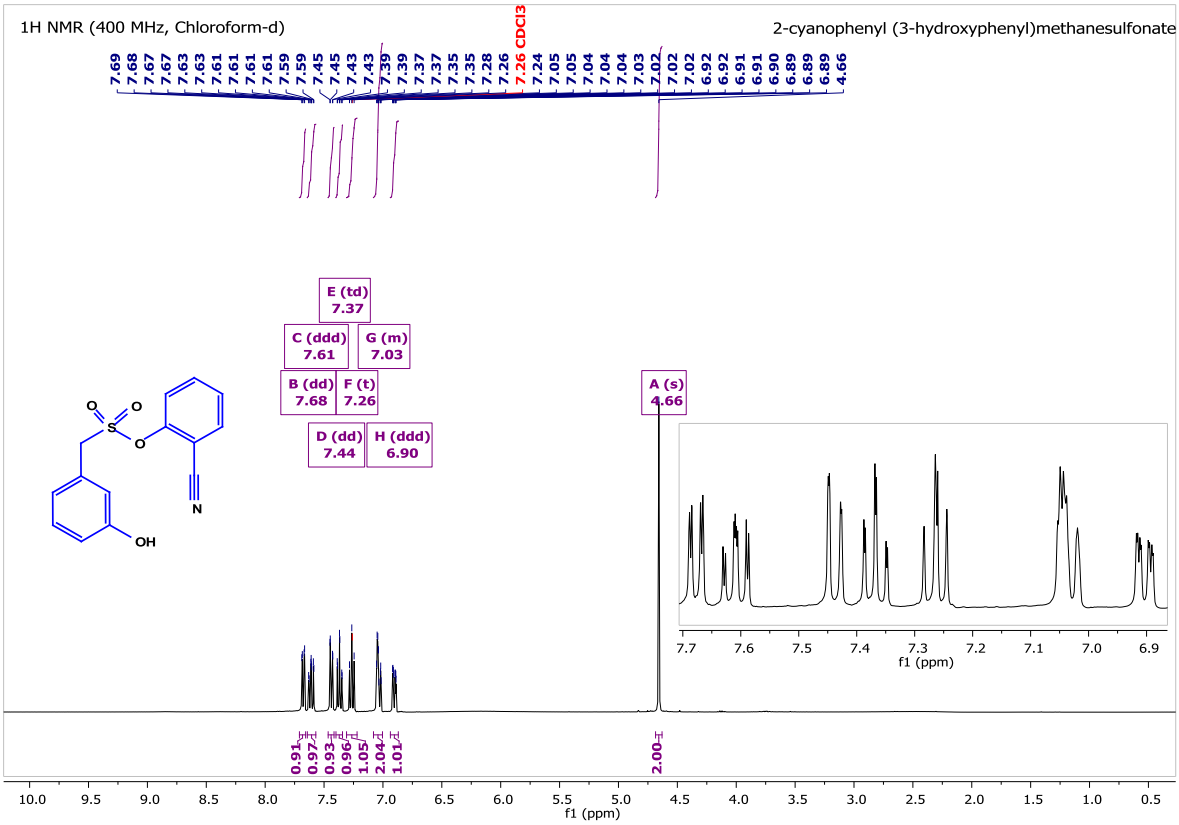
2-cyanophenyl (2,5-difluorophenyl)methanesulfonate:

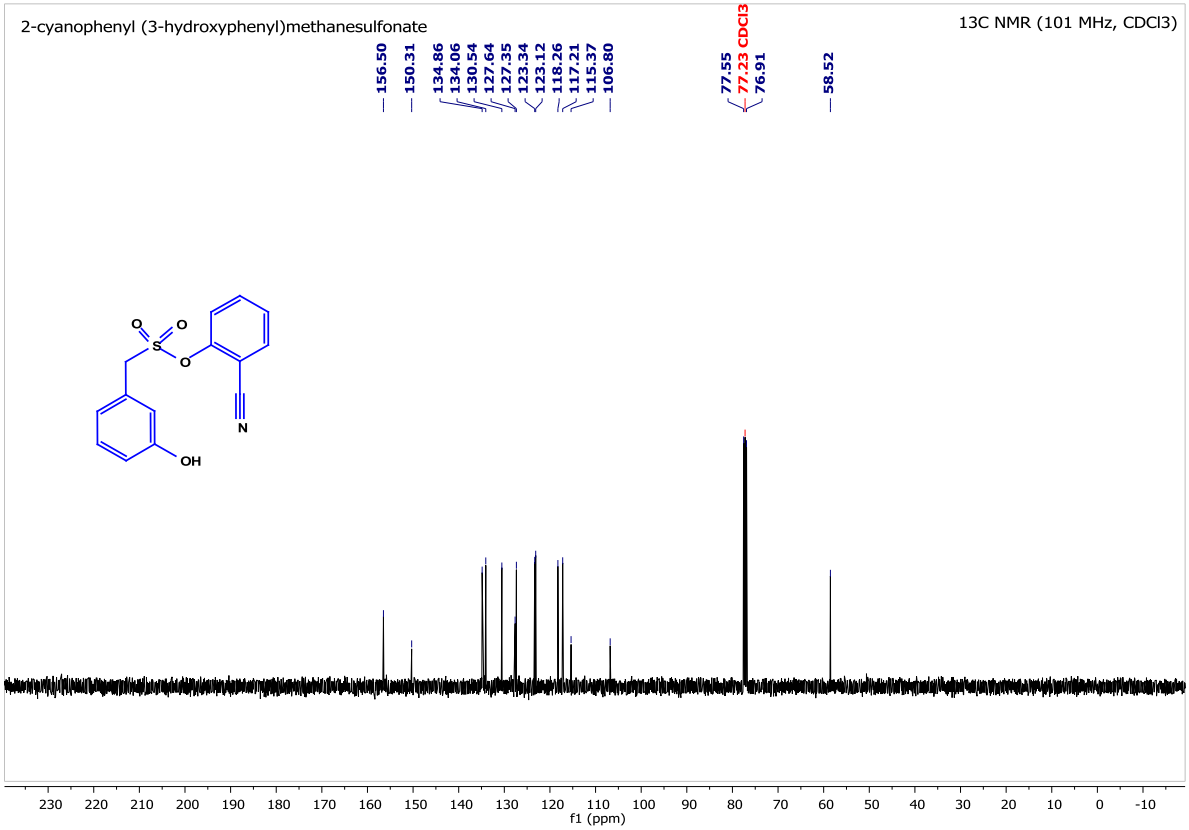


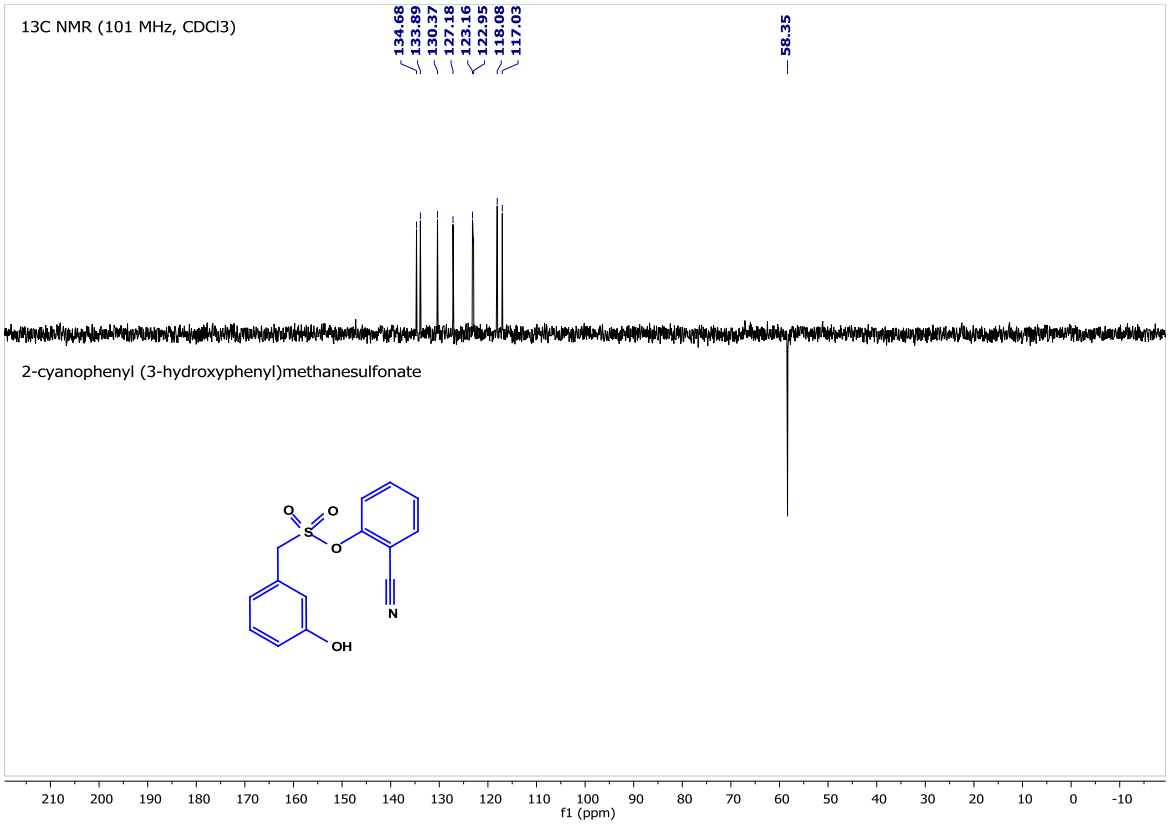


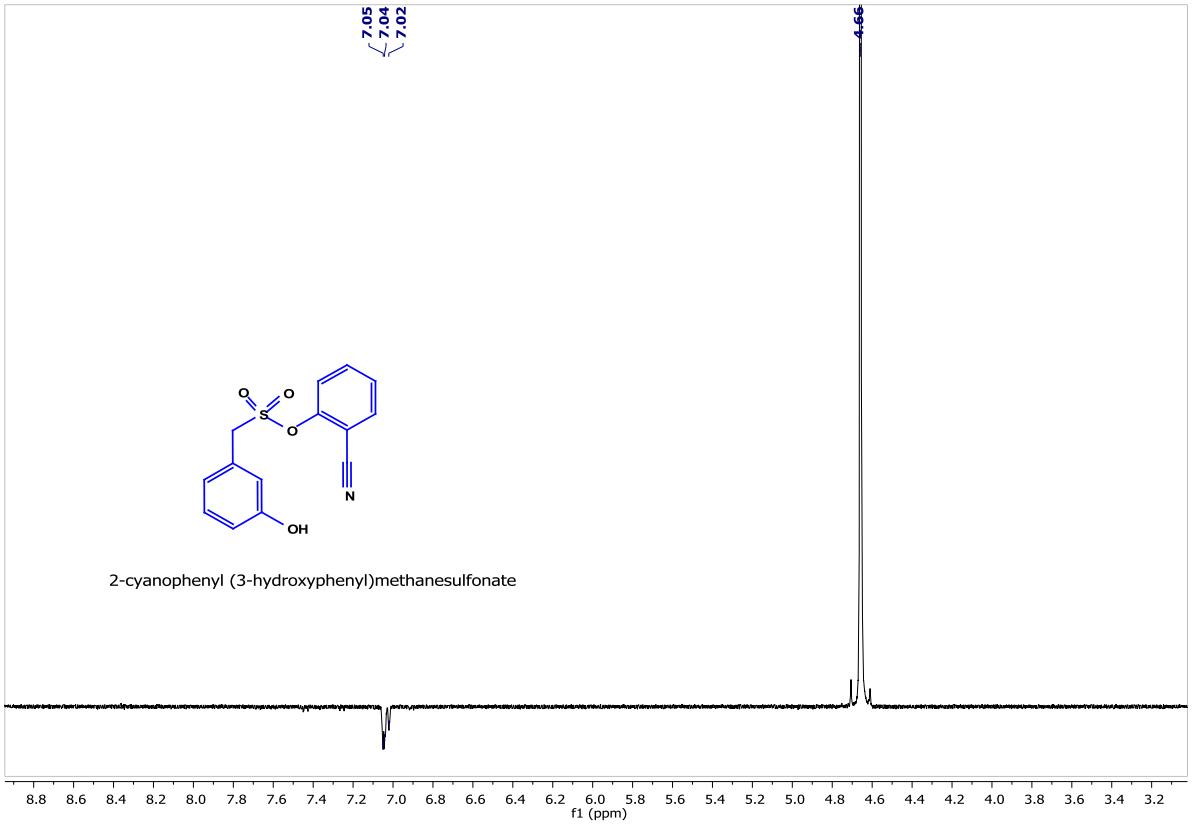
B. NMR Characterization of the *meta*-hydroxylated compounds:

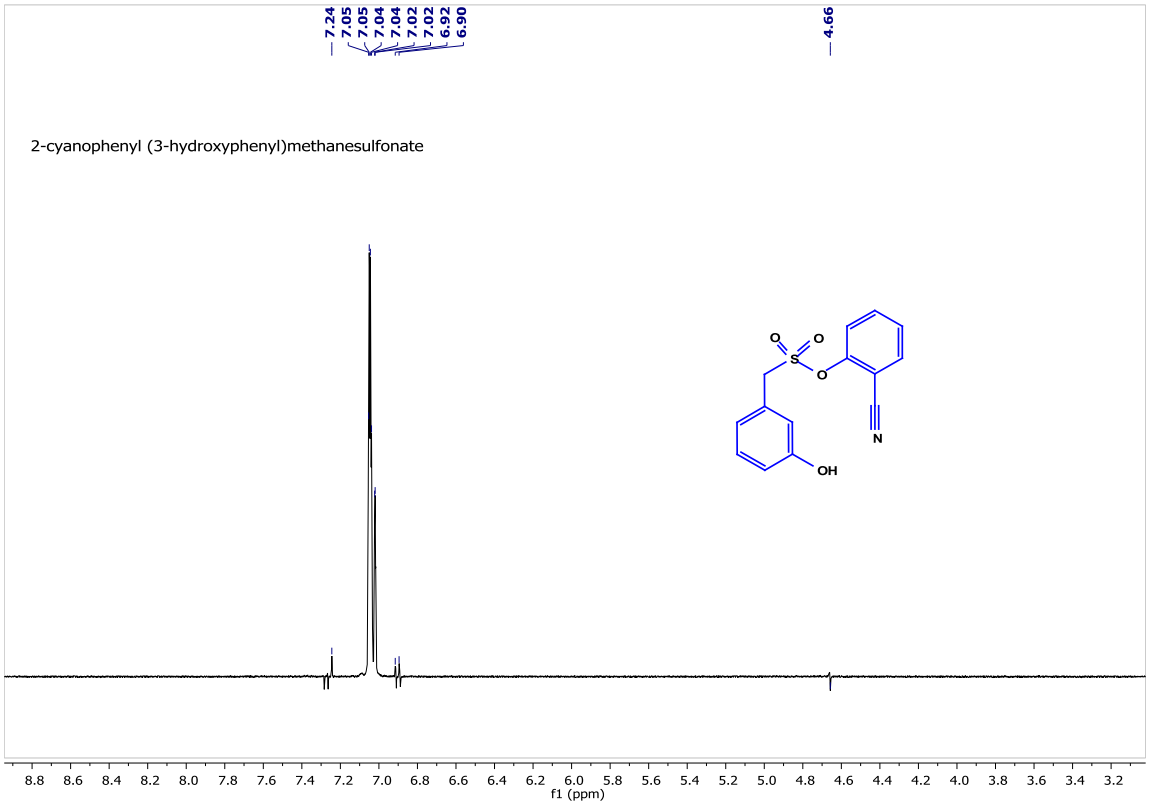
2-cyanophenyl (3-hydroxyphenyl)methanesulfonate (1a):



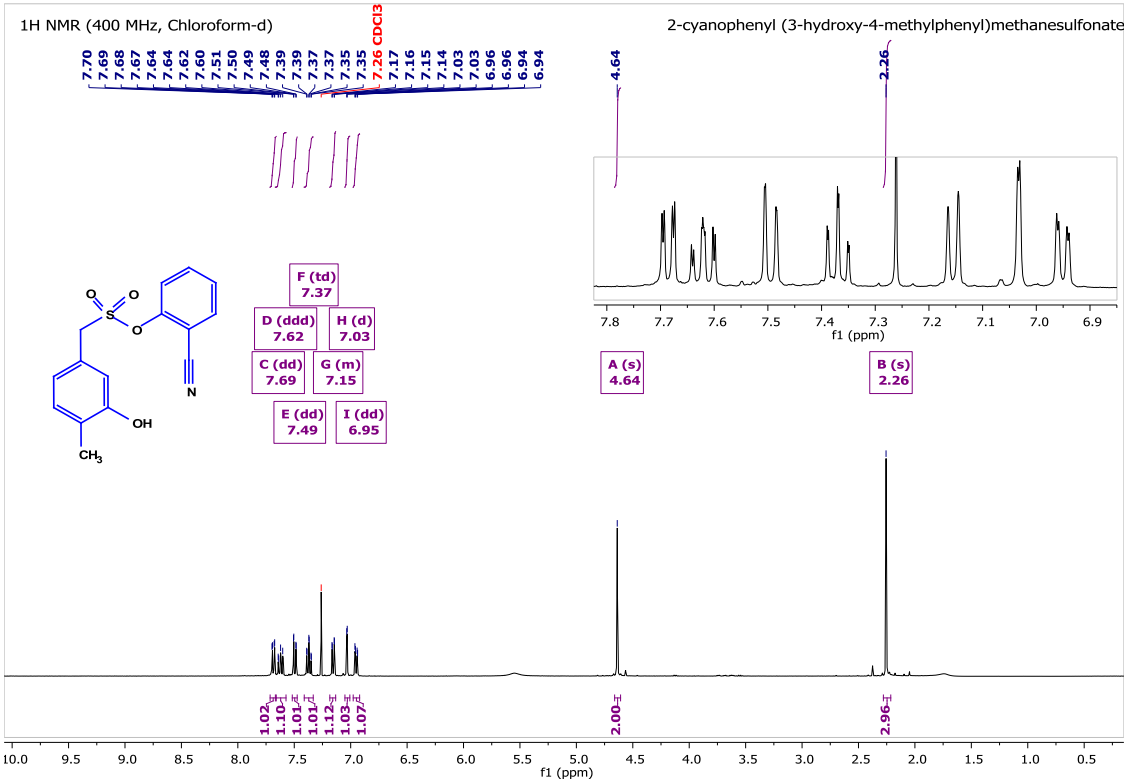

2-cyanophenyl (3-hydroxyphenyl)methanesulfonate
13C NMR (101 MHz, CDCl3)
156.50
150.31
134.86
134.06
130.54
127.64
127.35
123.34
123.12
118.26
117.21
115.37
106.80
77.55
77.23 CDCl3
76.91
58.52
O
O
S
O
N
OH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

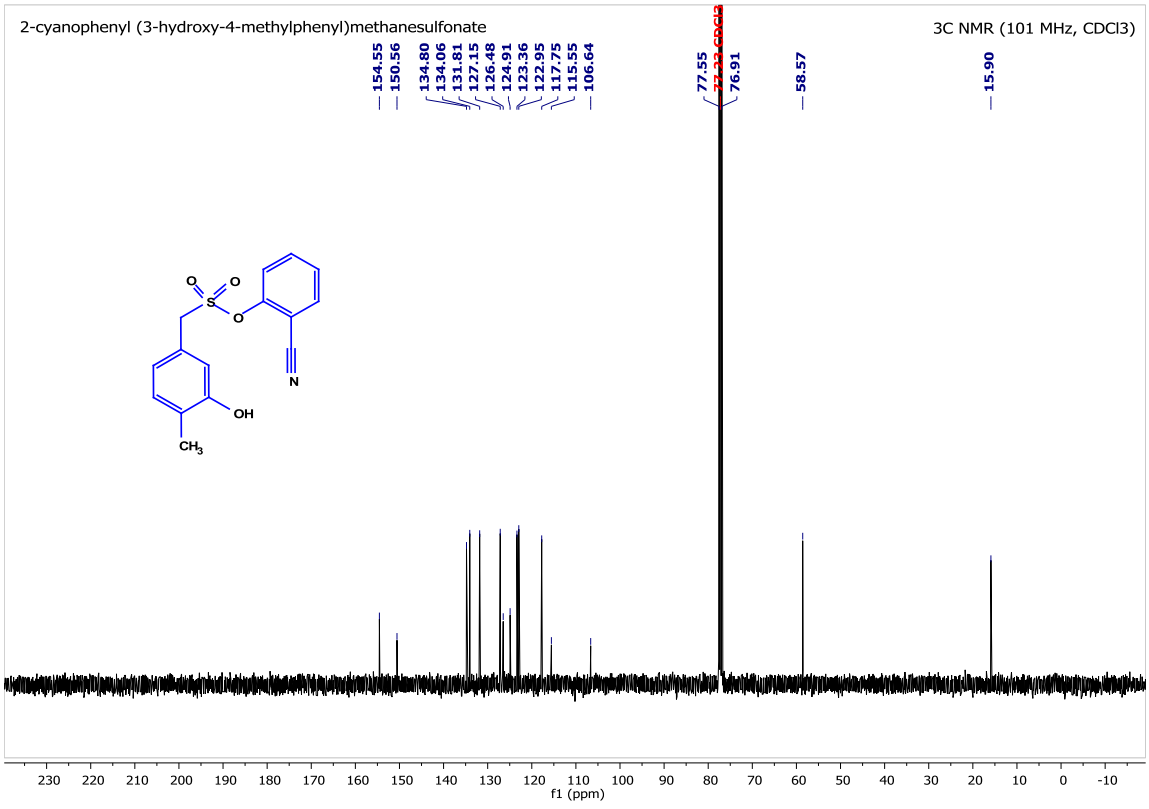

13C NMR (101 MHz, CDCl3)
134.68
133.89
130.37
127.18
123.16
122.95
118.08
117.03
58.35
2-cyanophenyl (3-hydroxyphenyl)methanesulfonate
O
O
S
O
N
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.05
7.04
7.02
4.66
O
O
S
O
N
OH
2-cyanophenyl (3-hydroxyphenyl)methanesulfonate
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2
f1 (ppm)

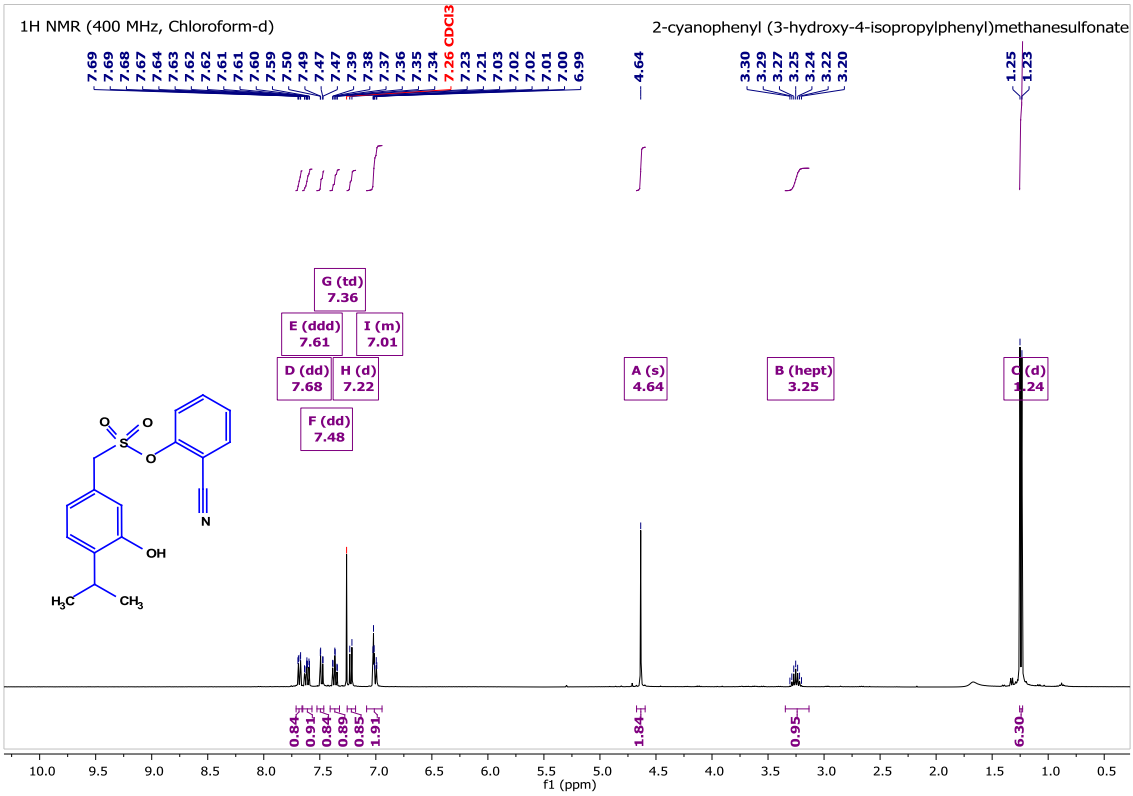

7.24
7.05
7.05
7.04
7.04
7.02
7.02
6.92
6.90
4.66
2-cyanophenyl (3-hydroxyphenyl)methanesulfonate
O
O
S
O
N
OH
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2
f1 (ppm)

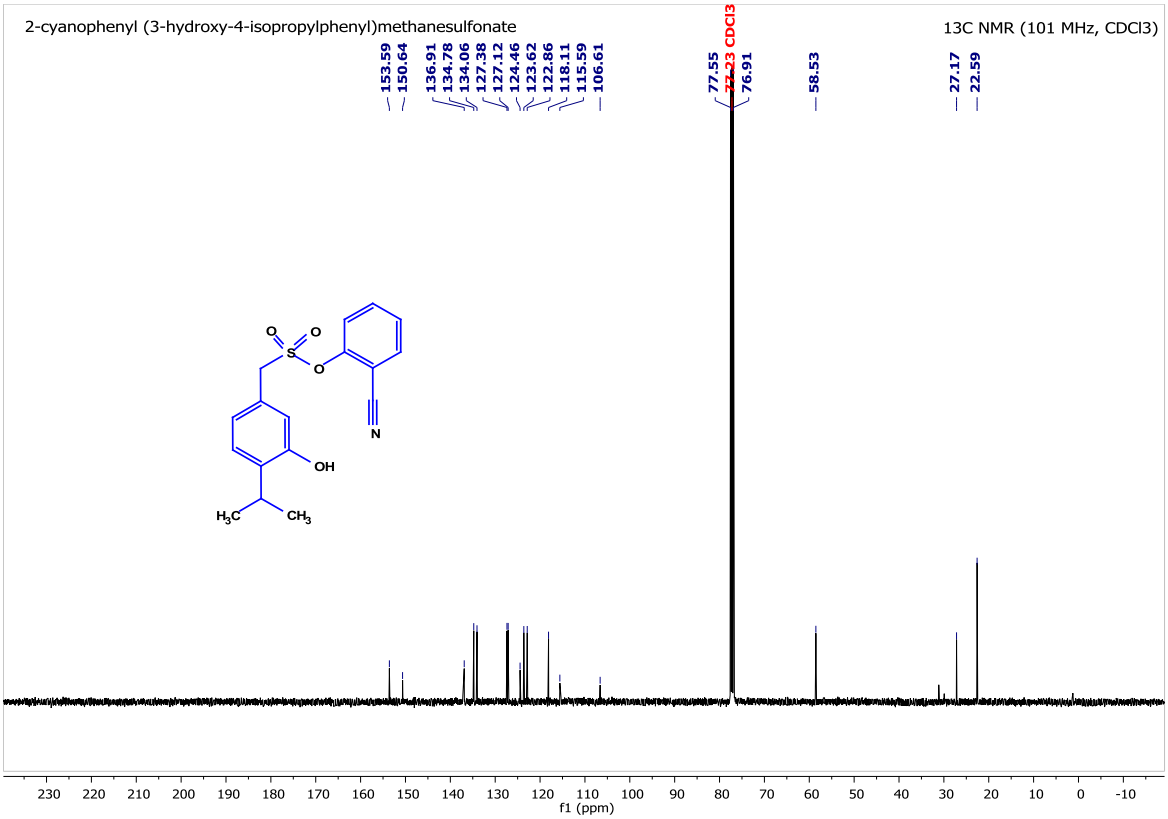
2-cyanophenyl (3-hydroxy-4-methylphenyl)methanesulfonate (1b):



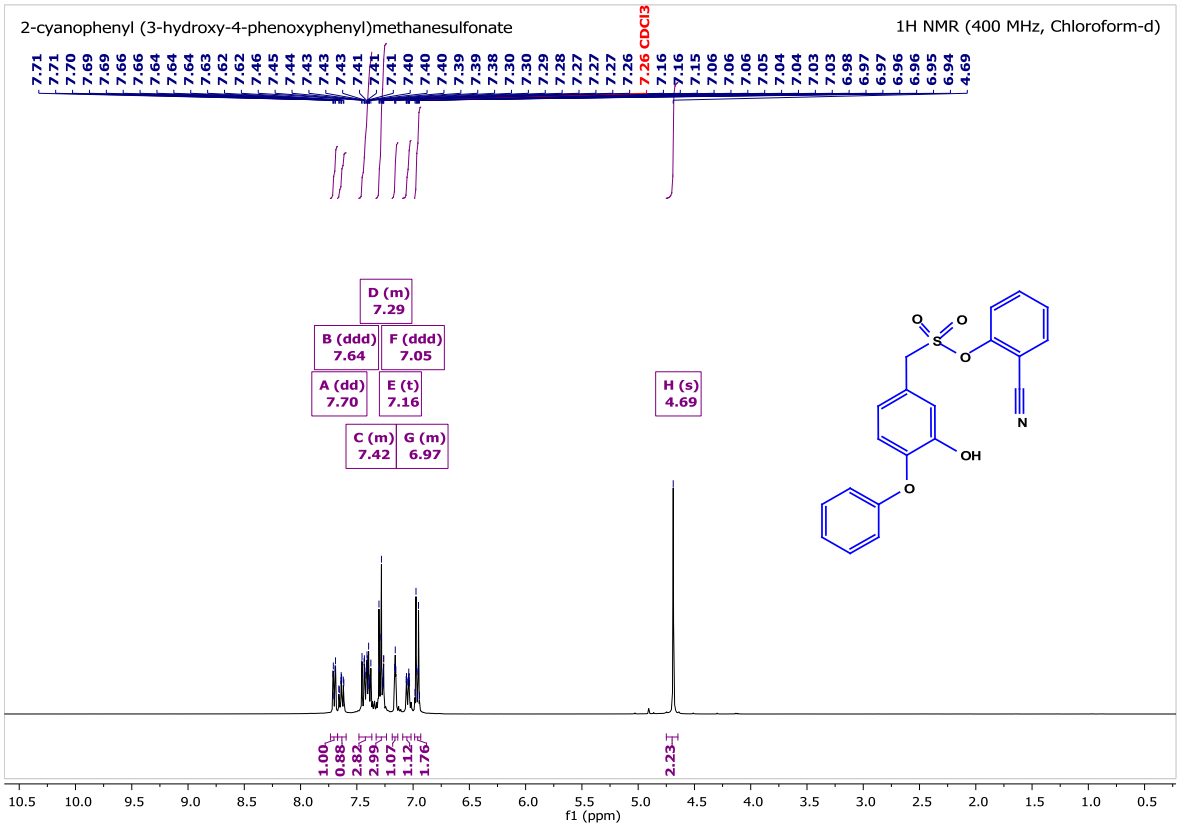


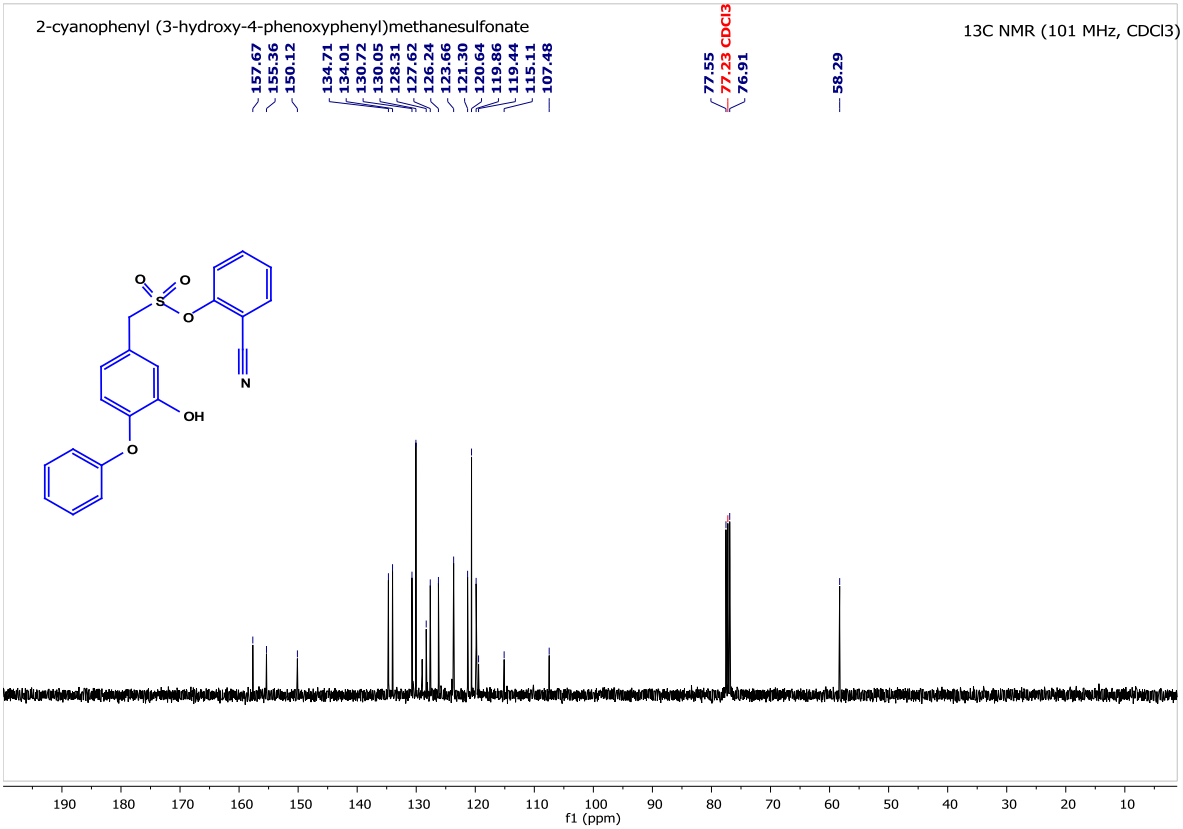
2-cyanophenyl (3-hydroxy-4-isopropylphenyl)methanesulfonate (1c):



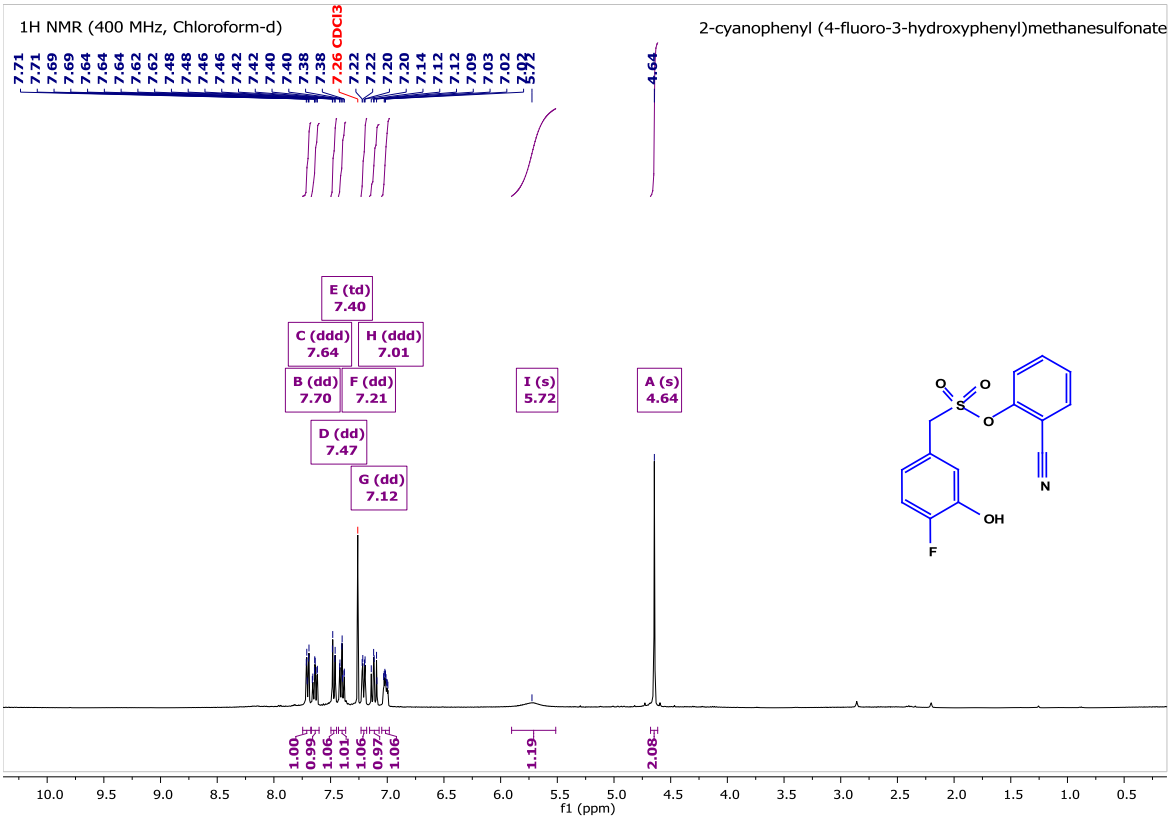


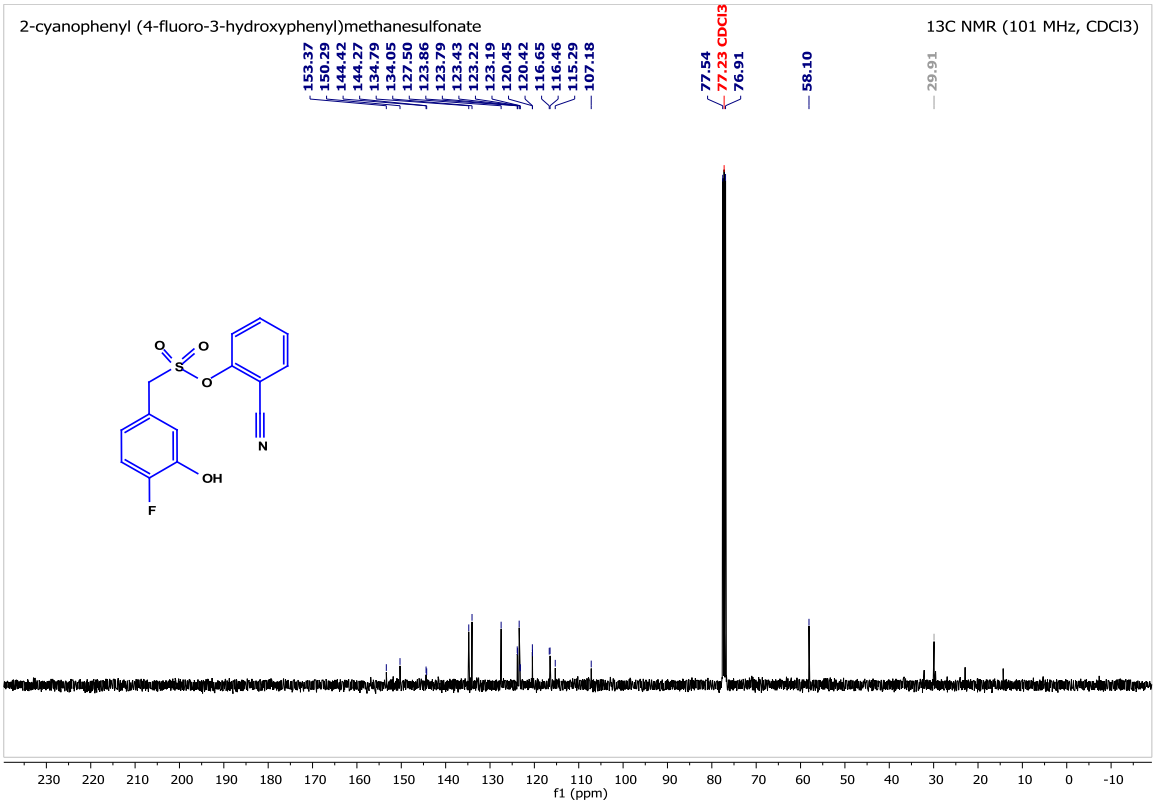
2-cyanophenyl (3-hydroxy-4-phenoxyphenyl)methanesulfonate (1d):



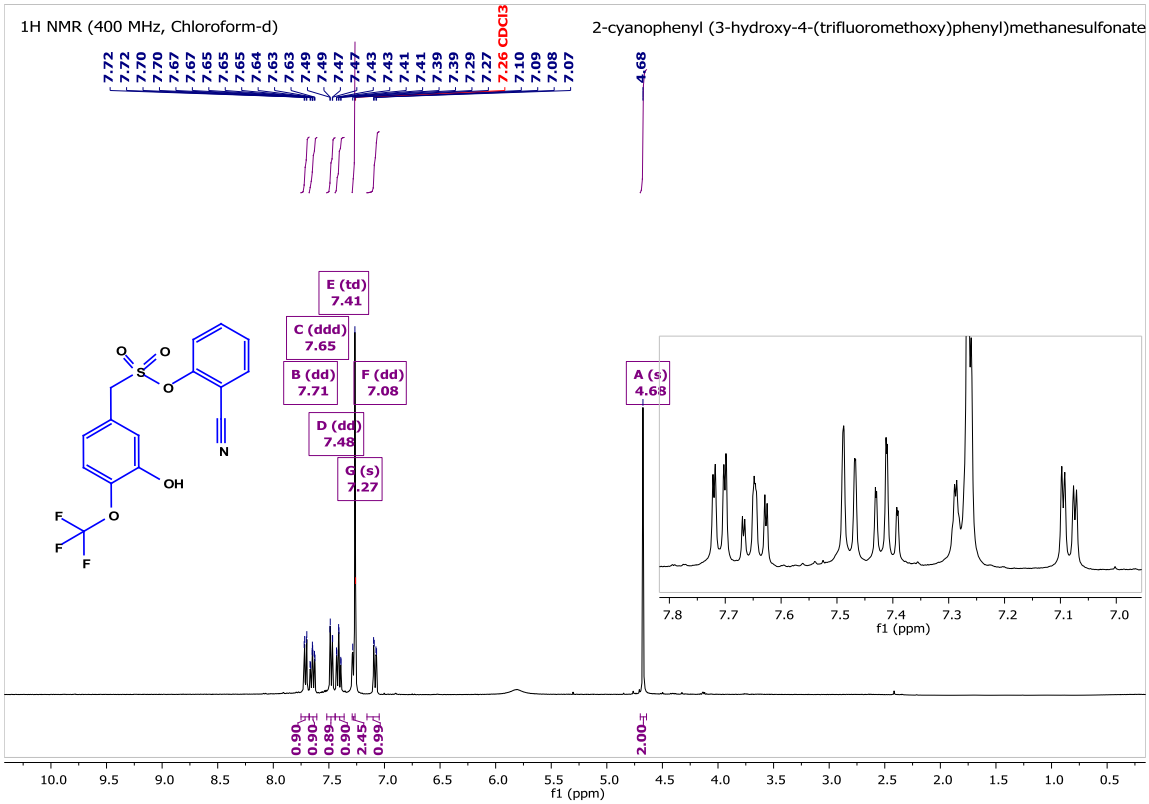


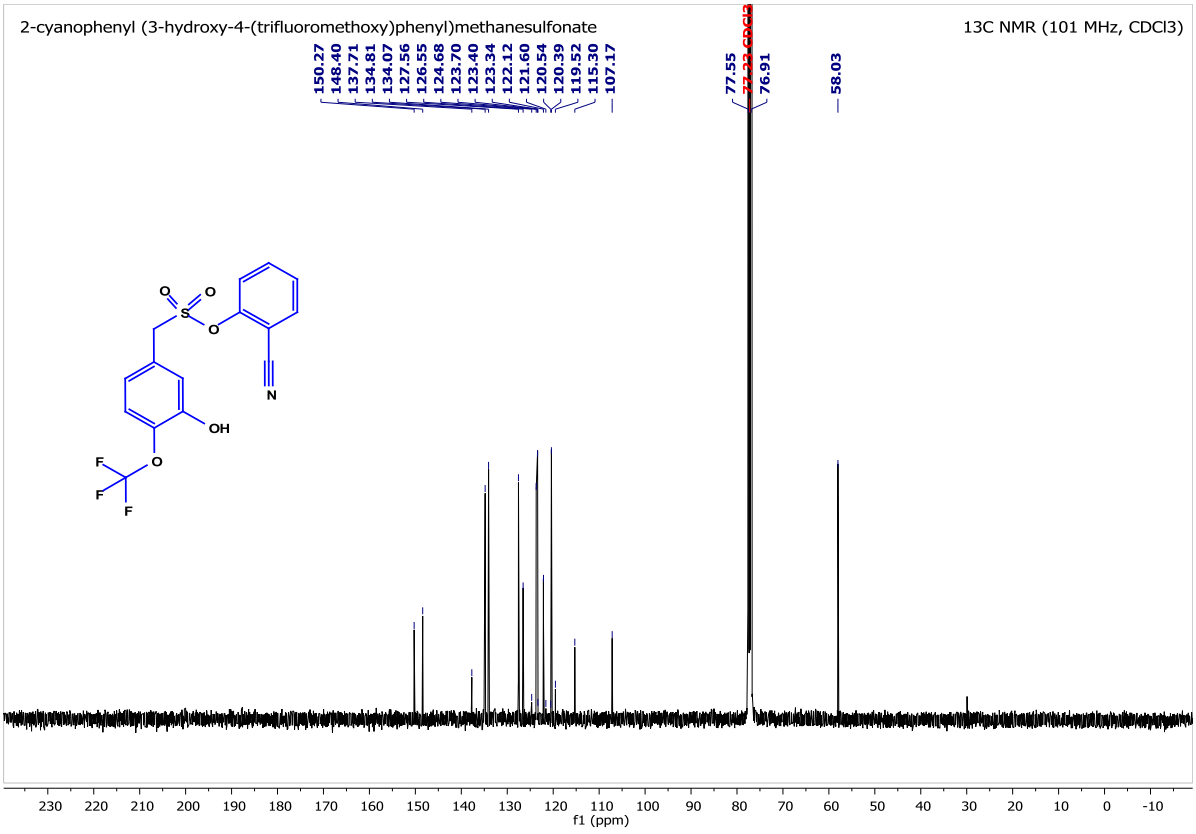
2-cyanophenyl (4-fluoro-3-hydroxyphenyl)methanesulfonate (1e):



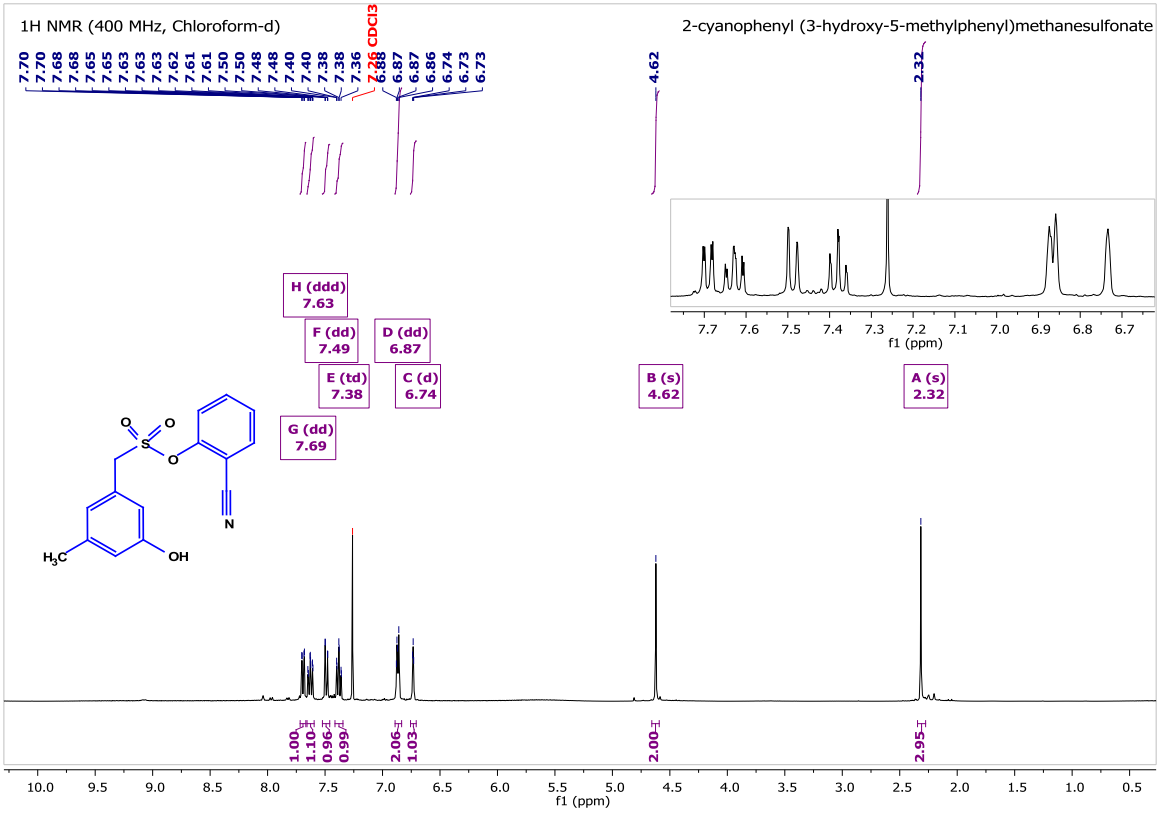


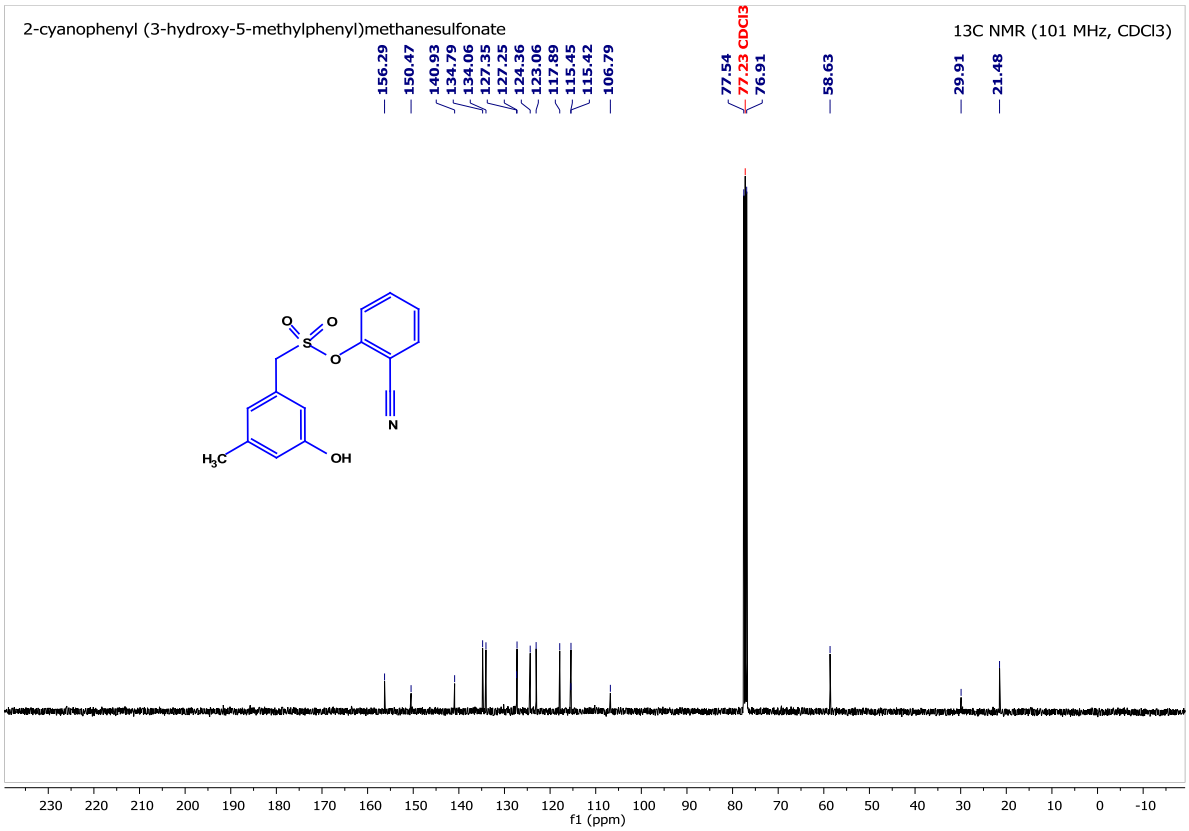
2-cyanophenyl (3-hydroxy-4-(trifluoromethoxy)phenyl)methanesulfonate (1f):



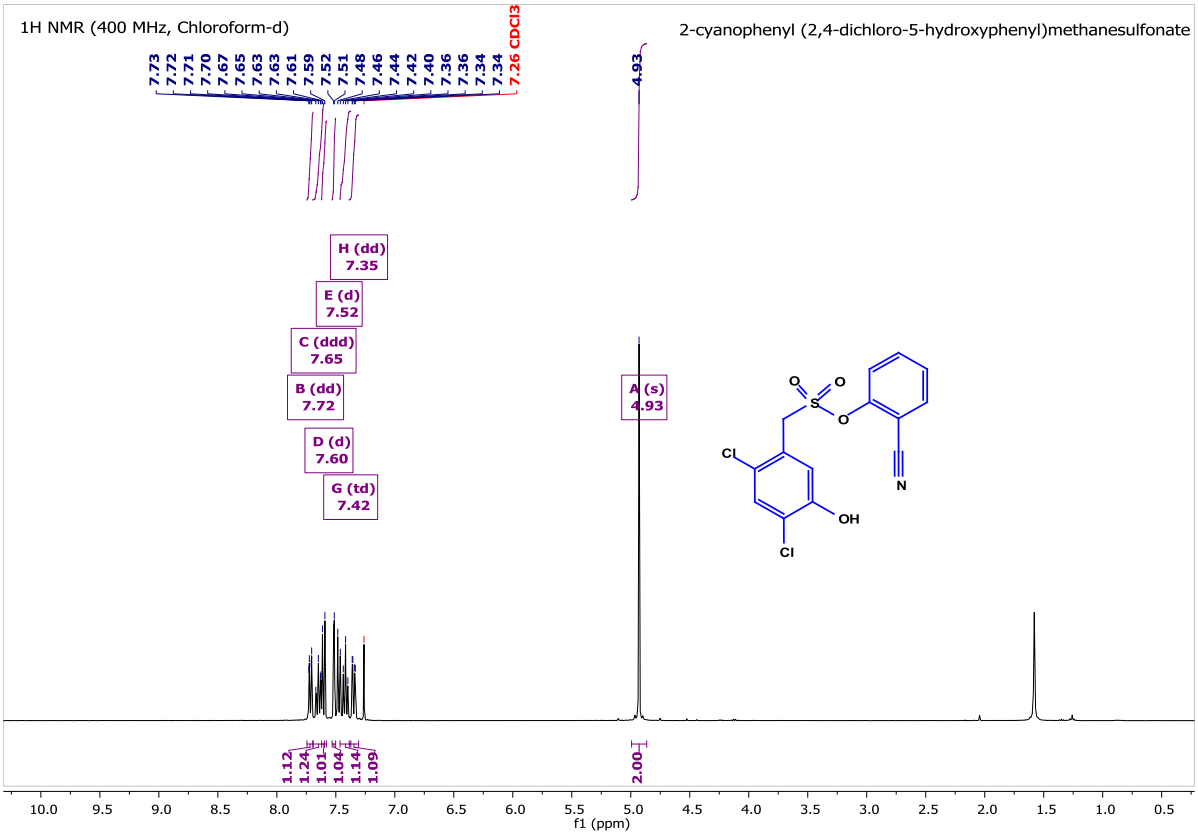


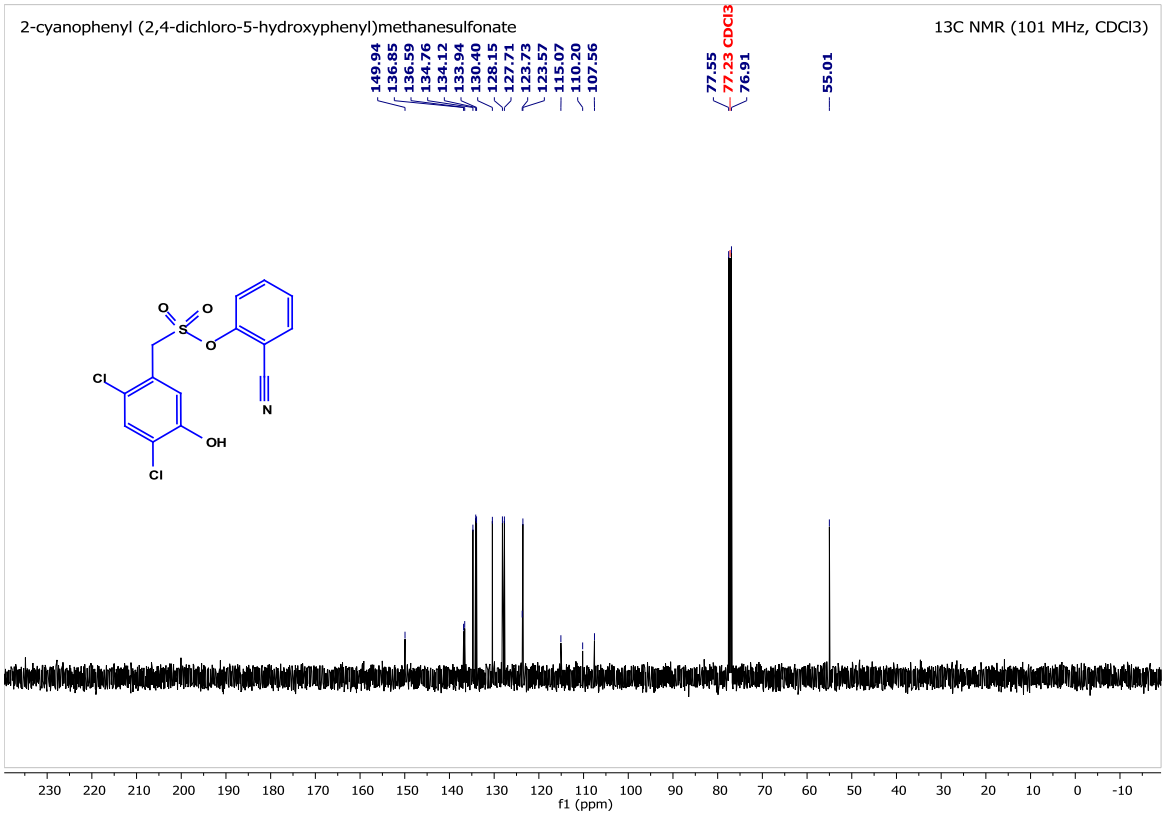
2-cyanophenyl (3-hydroxy-5-methylphenyl)methanesulfonate (1g):



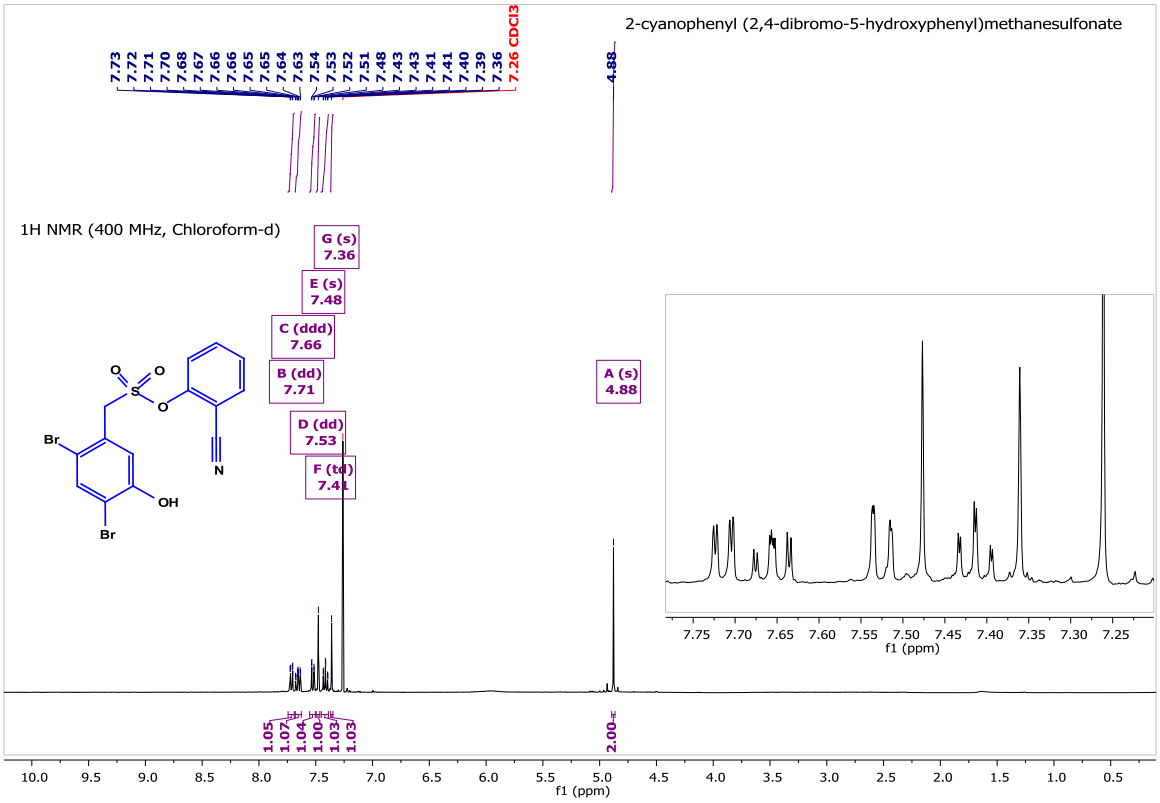


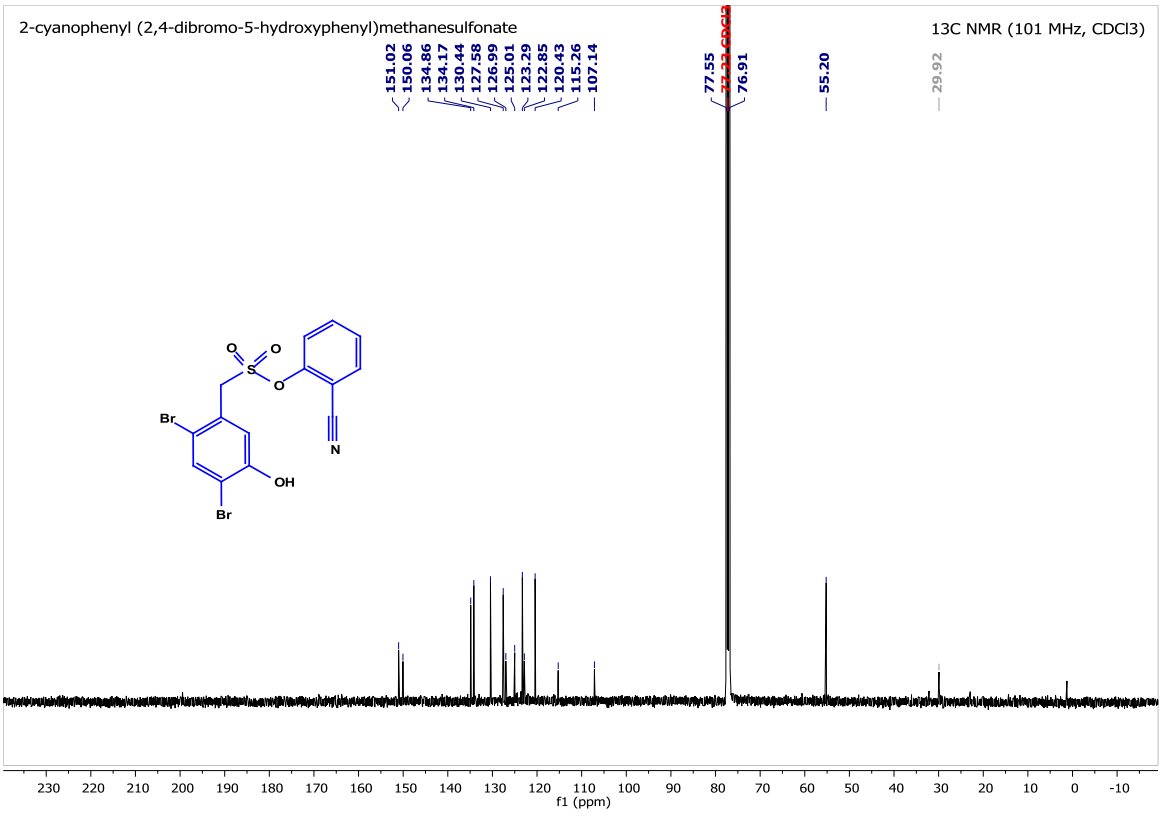
2-cyanophenyl (2,4-dichloro-5-hydroxyphenyl)methanesulfonate (1h):



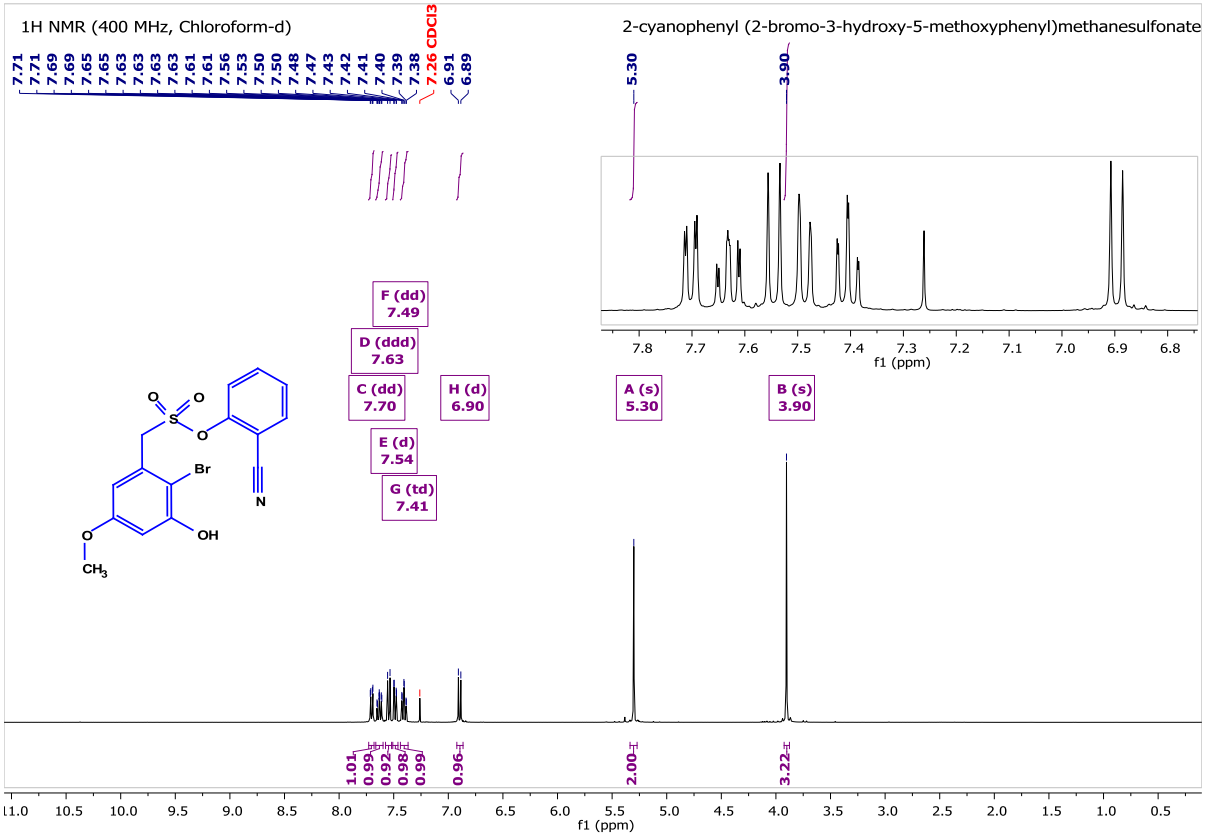


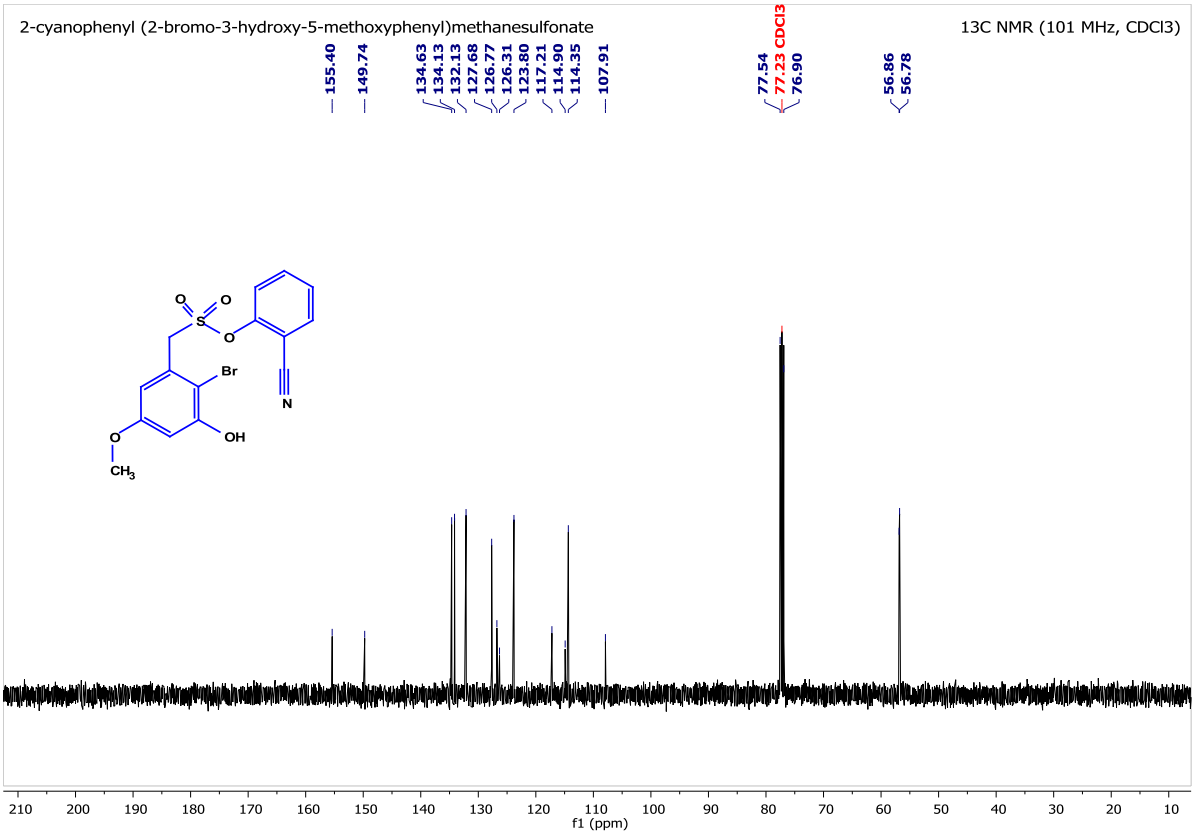
2-cyanophenyl (2,4-dibromo-5-hydroxyphenyl)methanesulfonate (1i):



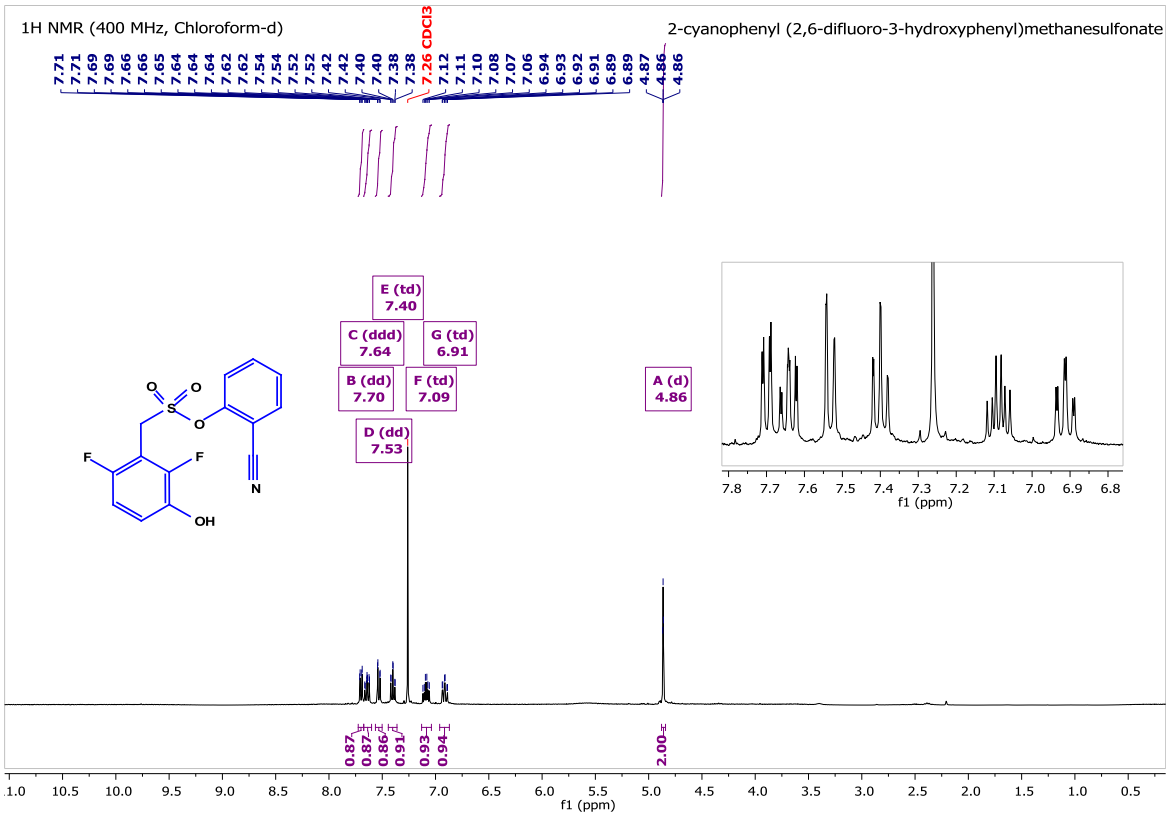


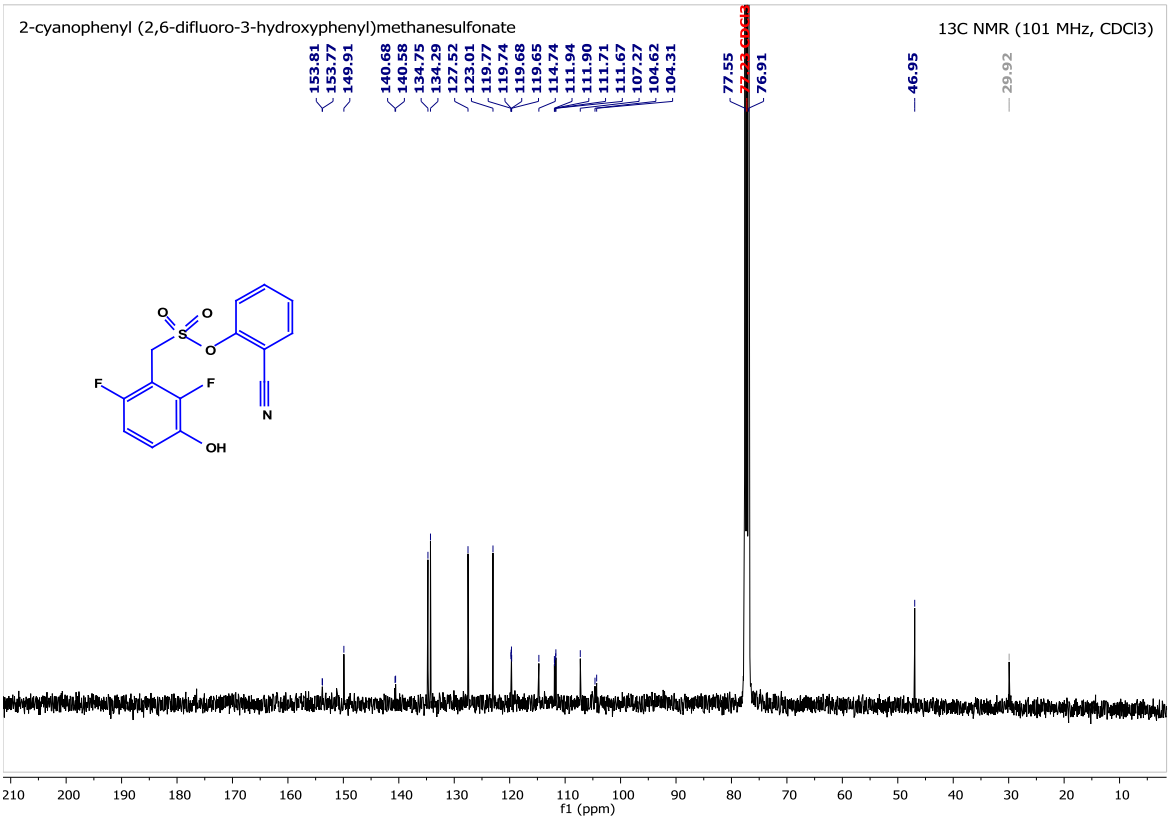
2-cyanophenyl (2-bromo-3-hydroxy-5-methoxyphenyl)methanesulfonate (1j) :



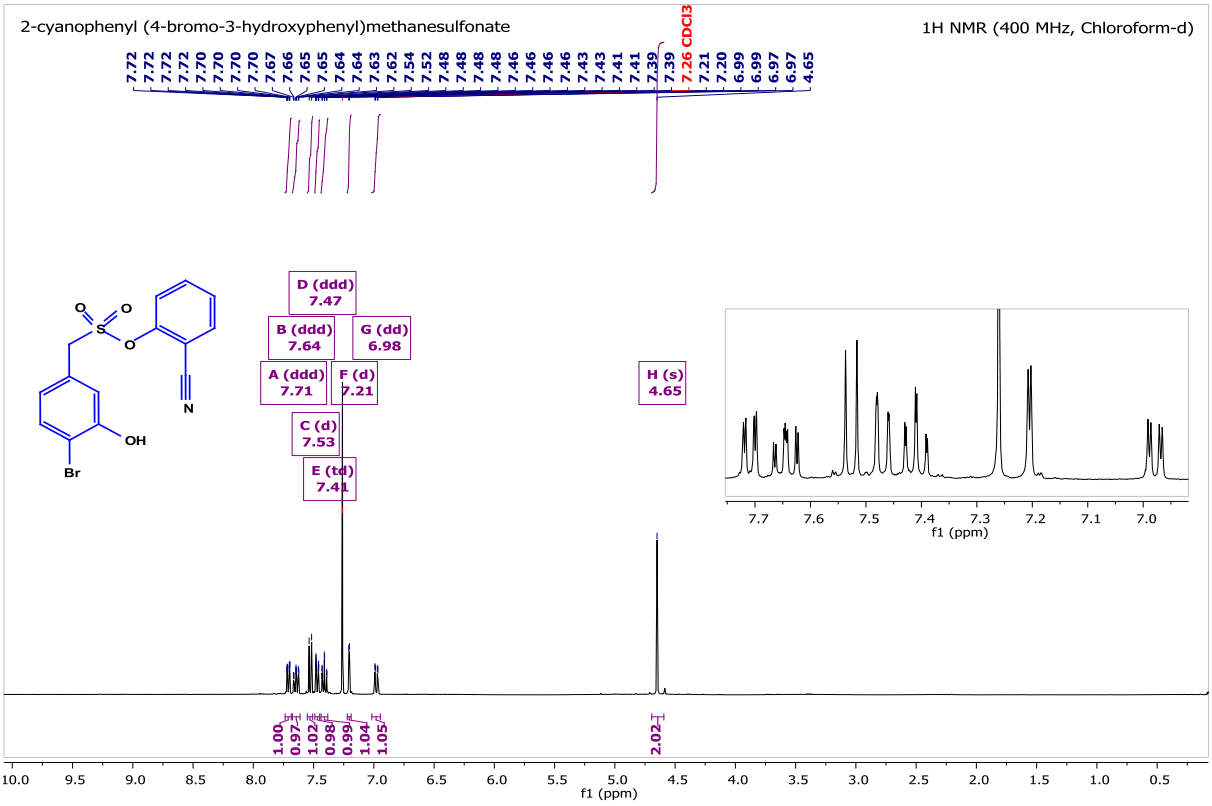


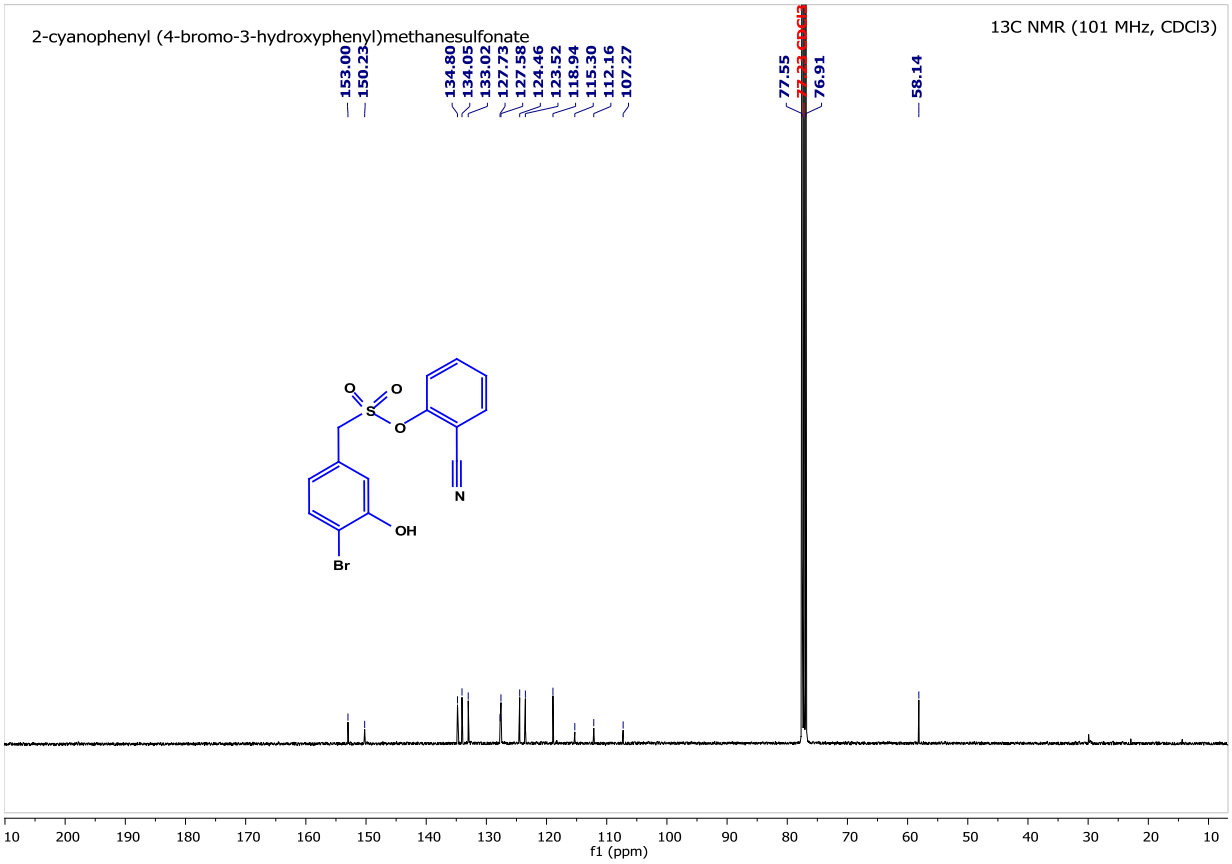
2-cyanophenyl (2,6-difluoro-3-hydroxyphenyl)methanesulfonate (1k):



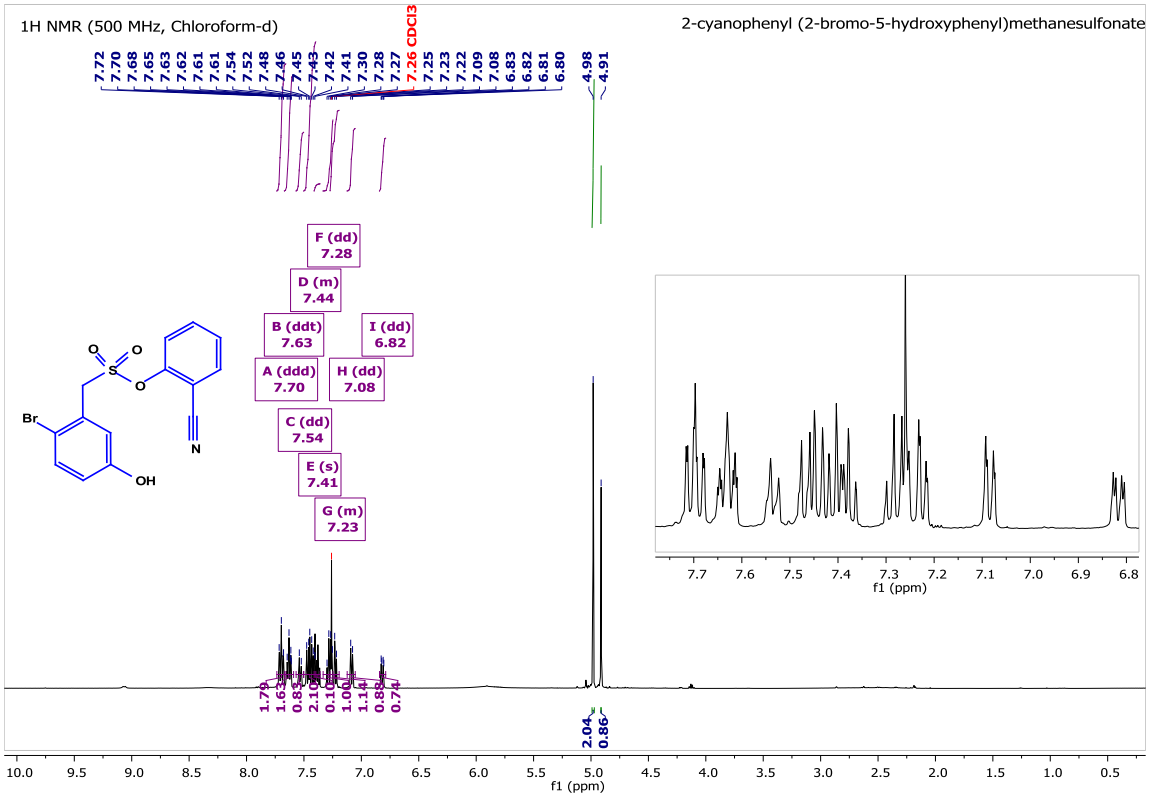


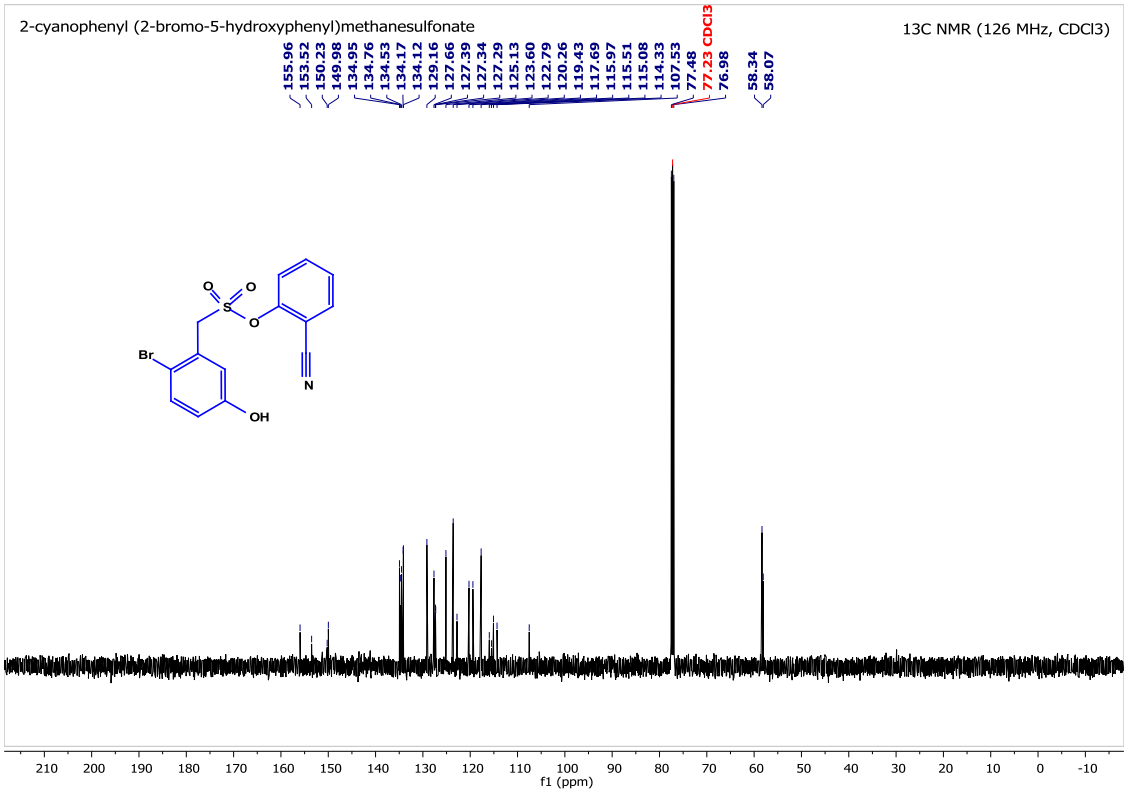
2-cyanophenyl (4-bromo-3-hydroxyphenyl)methanesulfonate (1l):



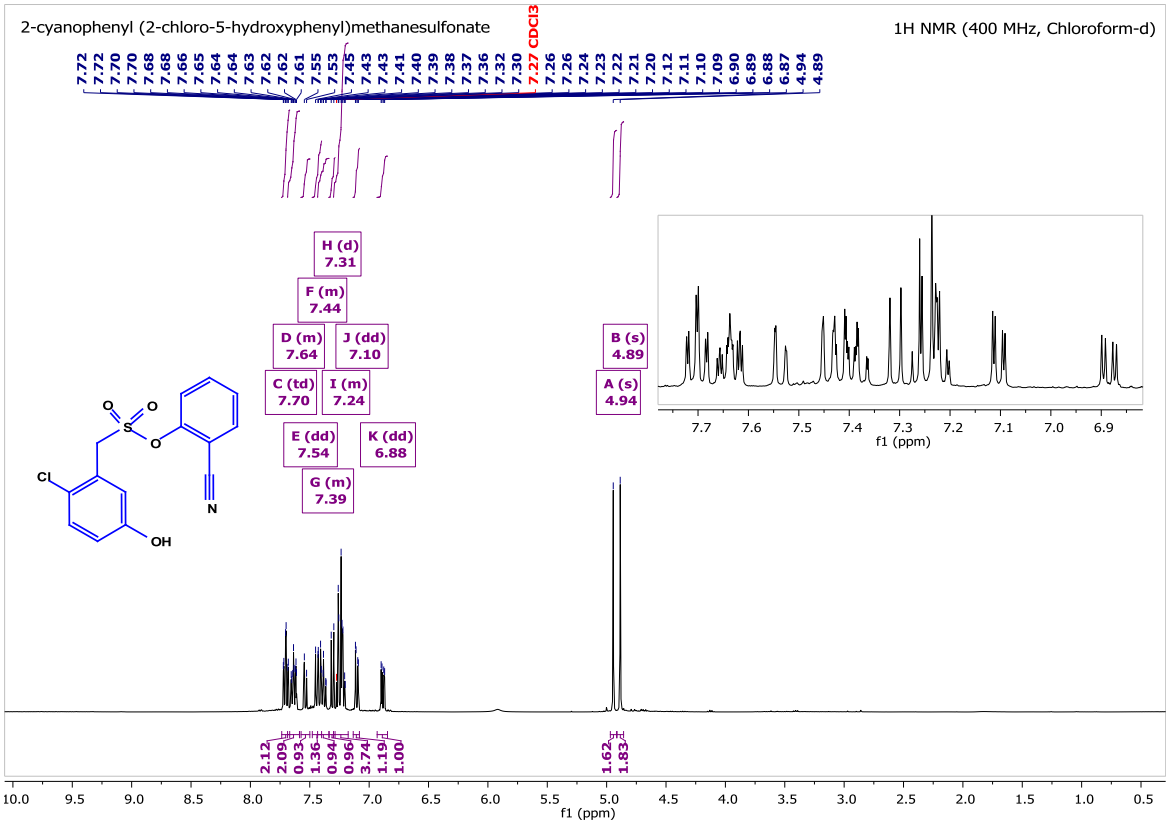


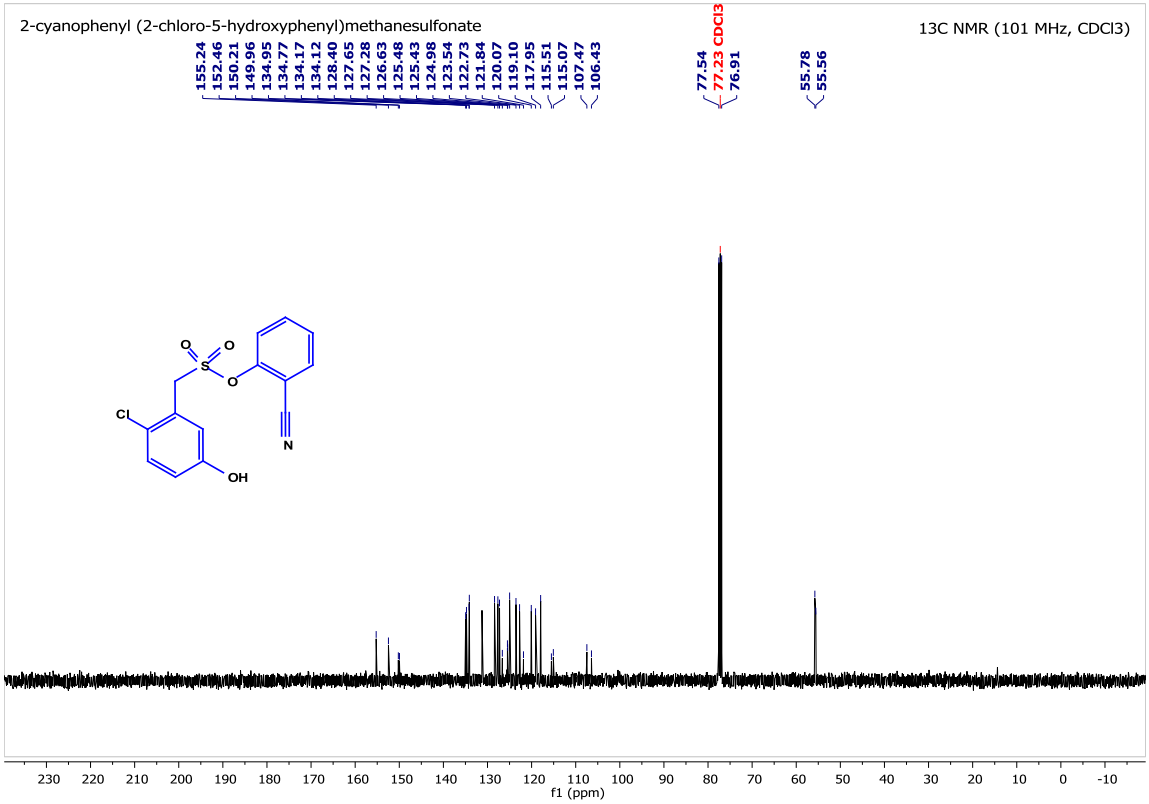
2-cyanophenyl (2-bromo-5-hydroxyphenyl)methanesulfonate (1m):



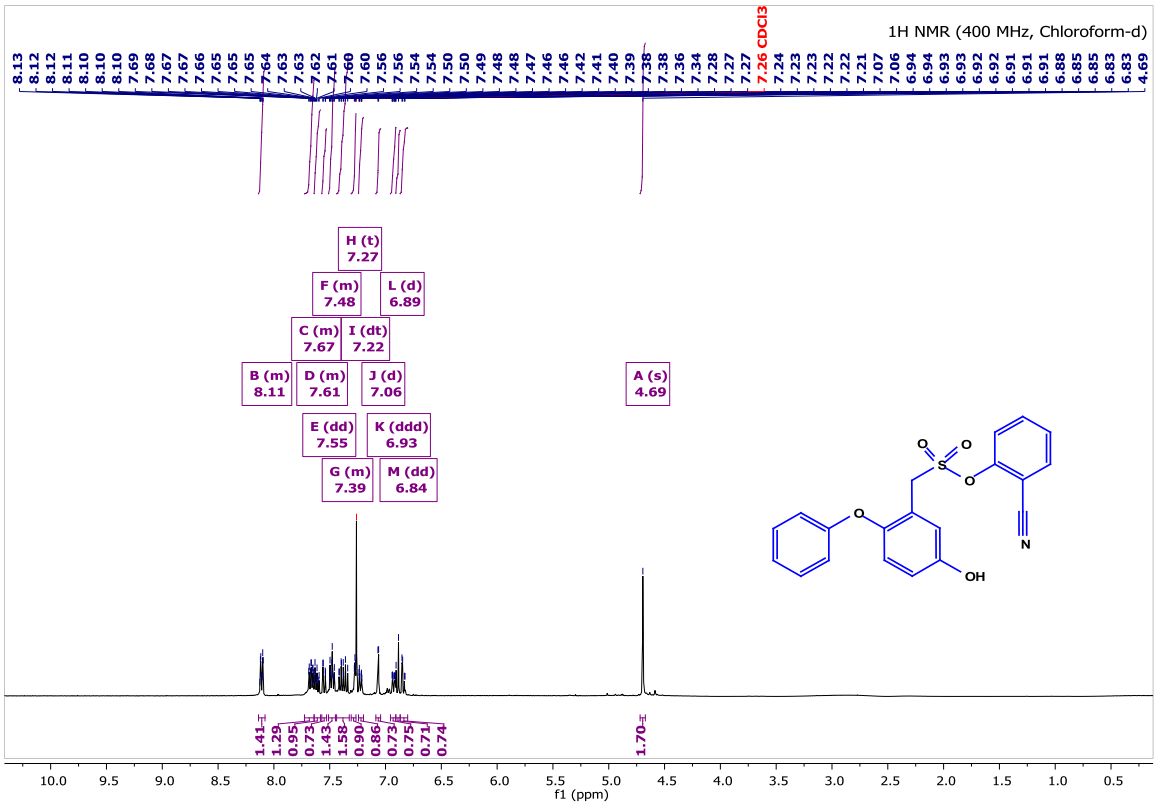


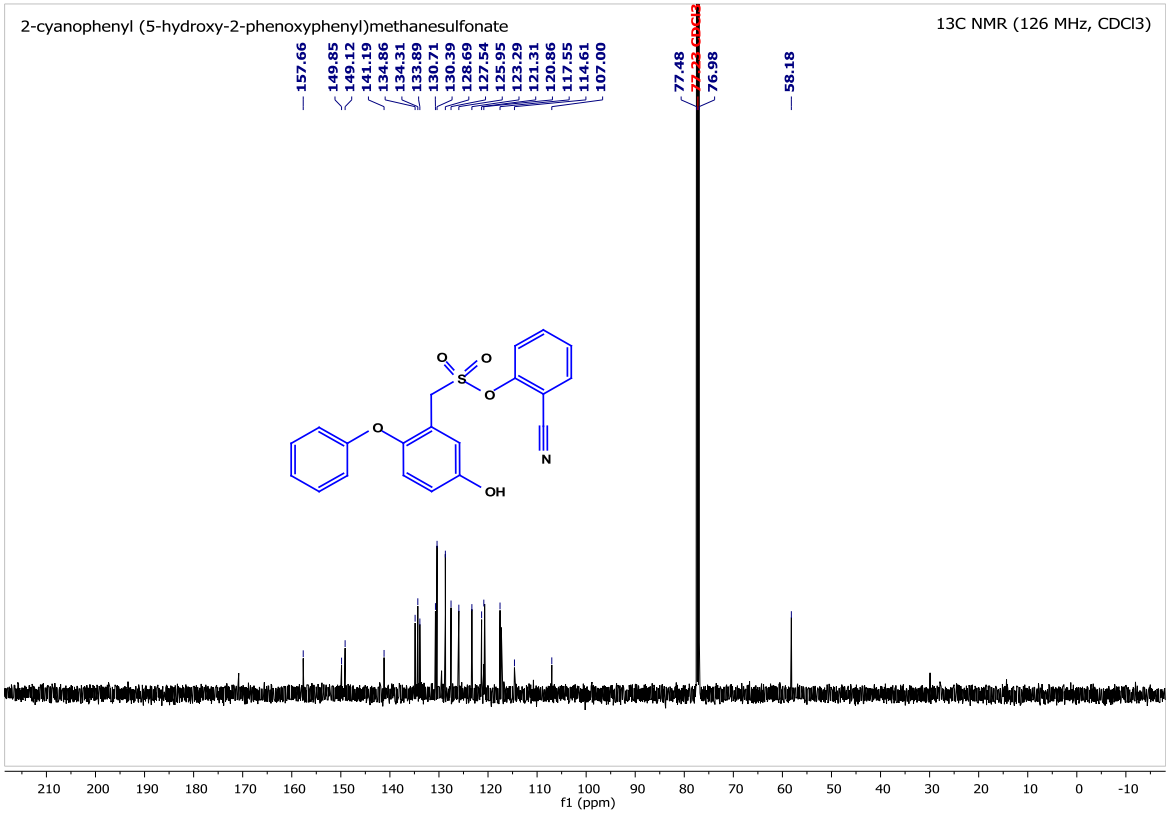
2-cyanophenyl (2-chloro-5-hydroxyphenyl)methanesulfonate (1n):





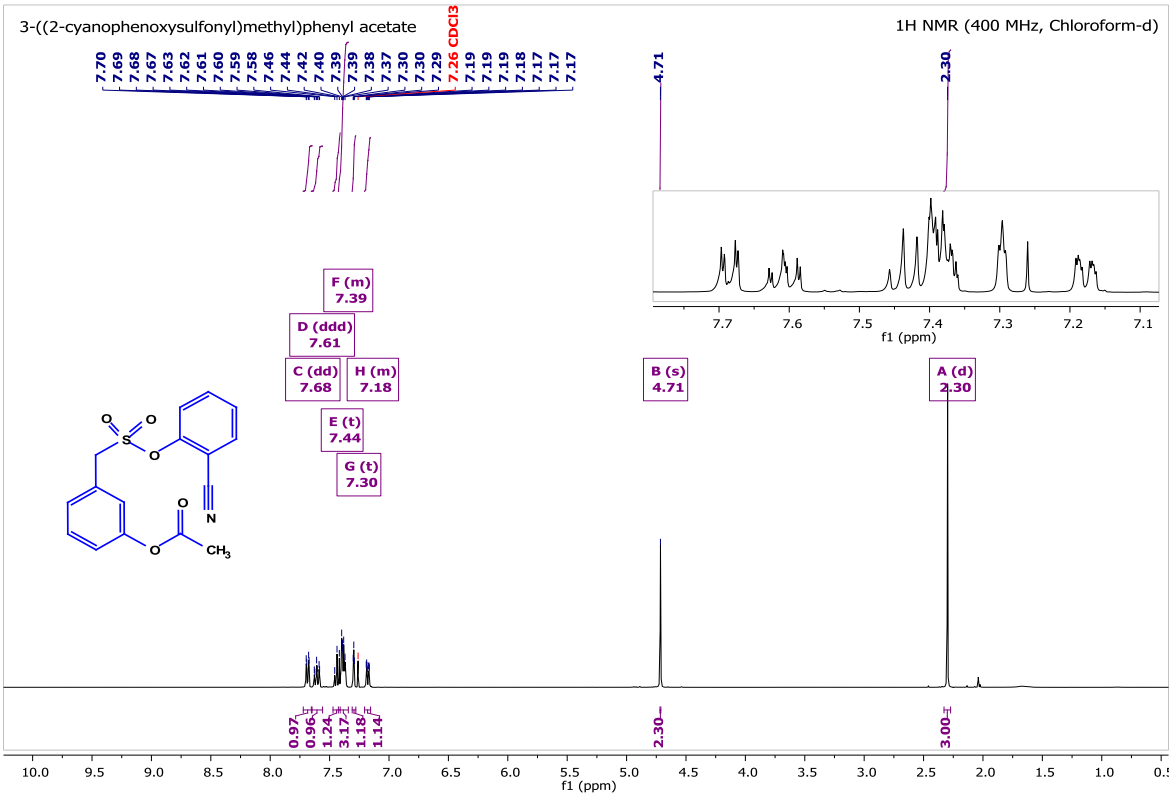
2-cyanophenyl (5-hydroxy-2-phenoxyphenyl)methanesulfonate (1o):

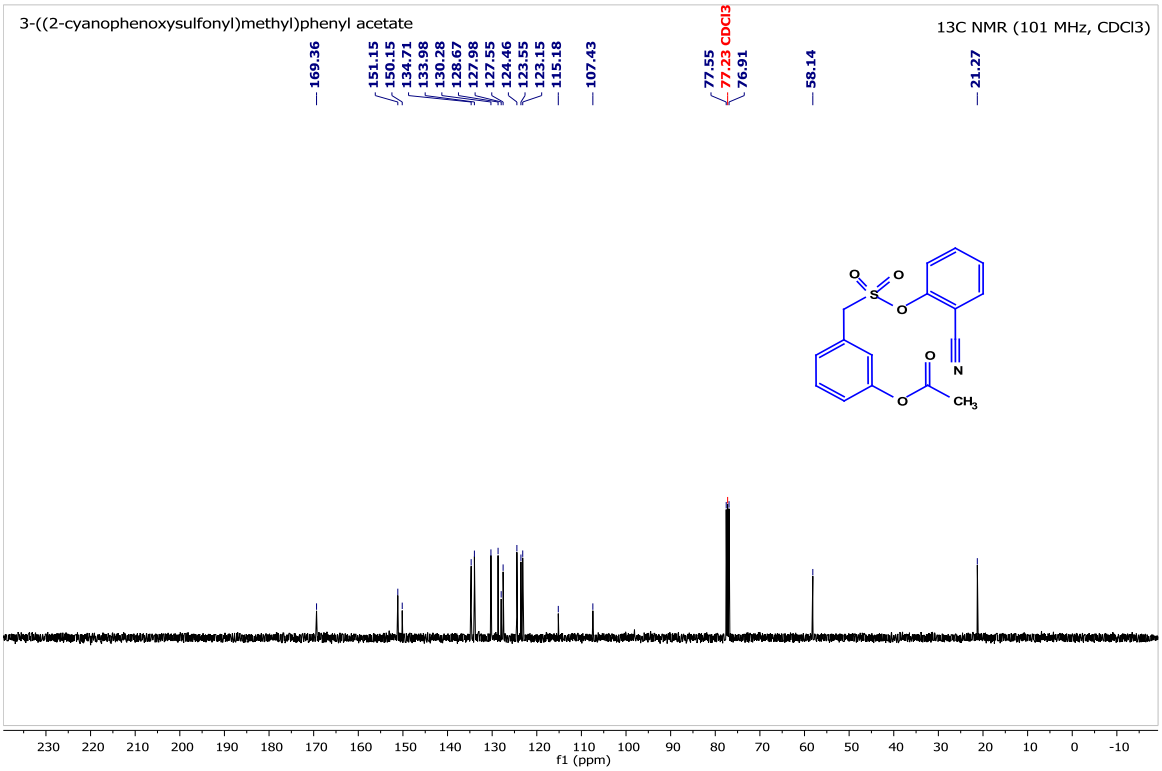




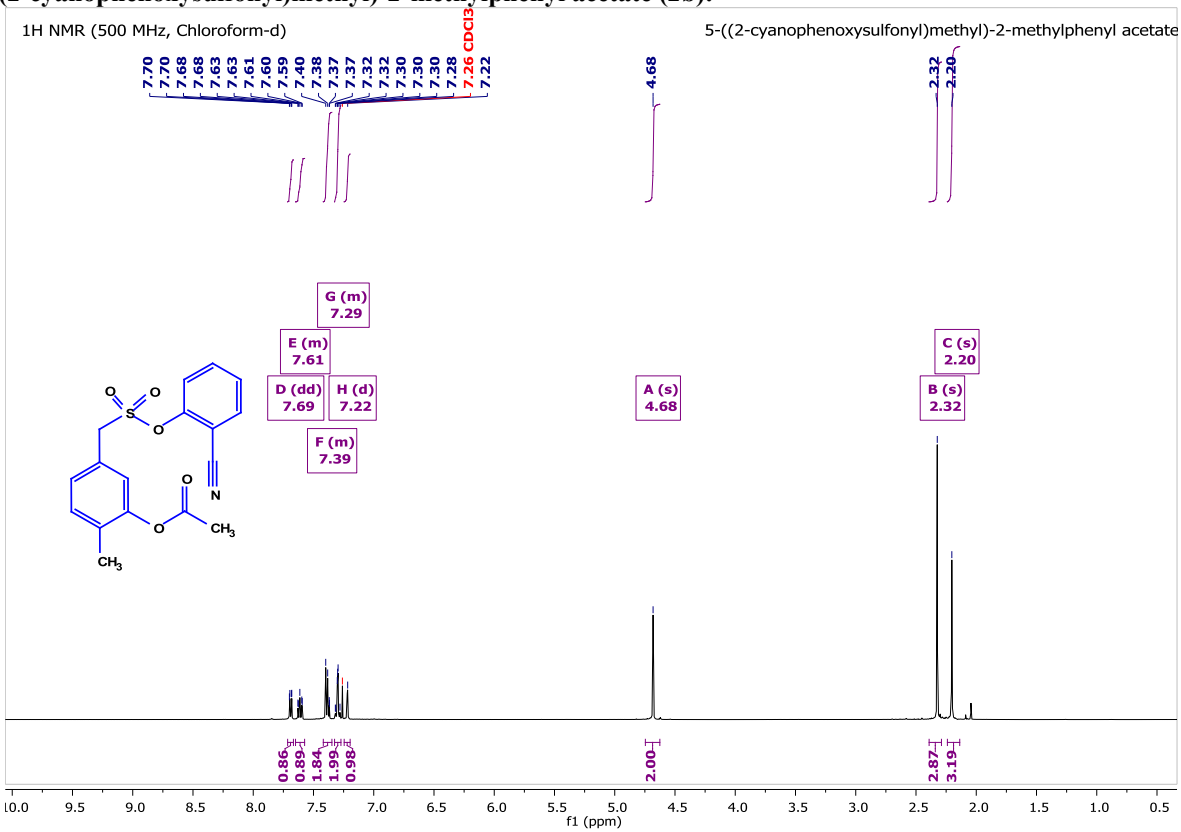
C. NMR Characterization of the *meta*-acetoxylated compounds:

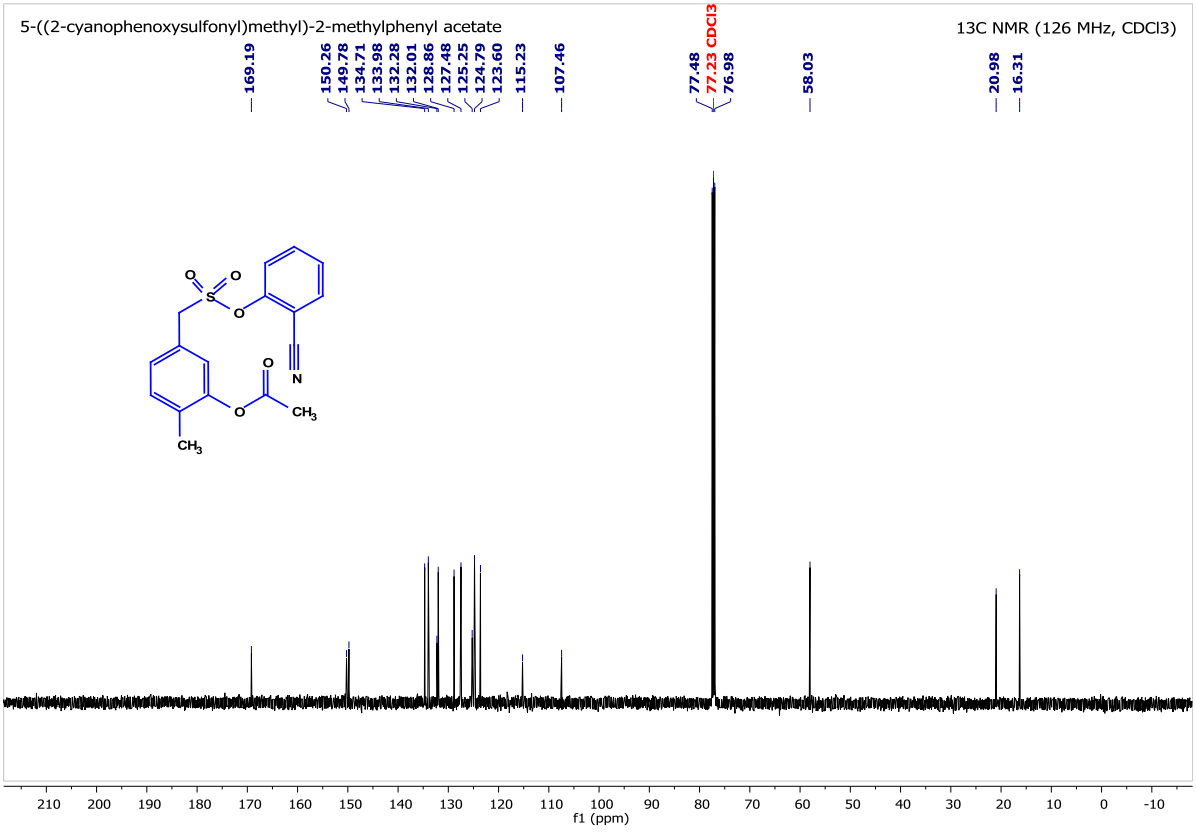
3-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (2a):



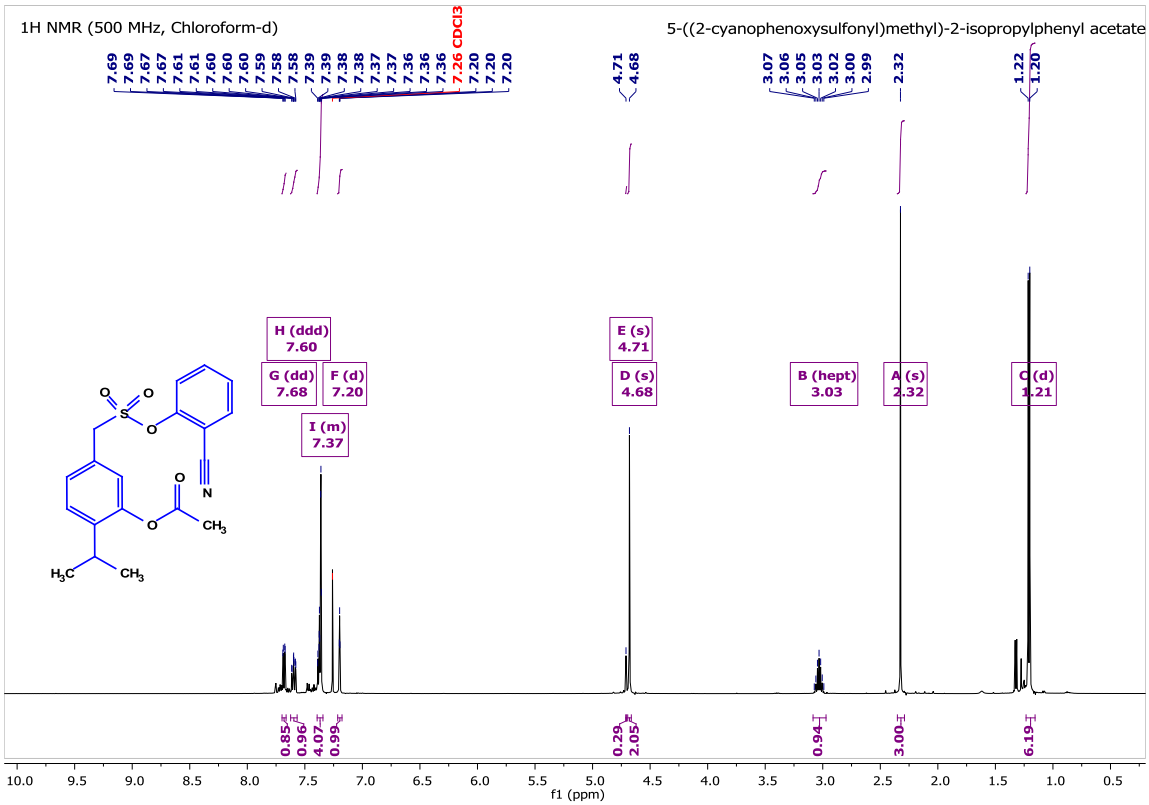


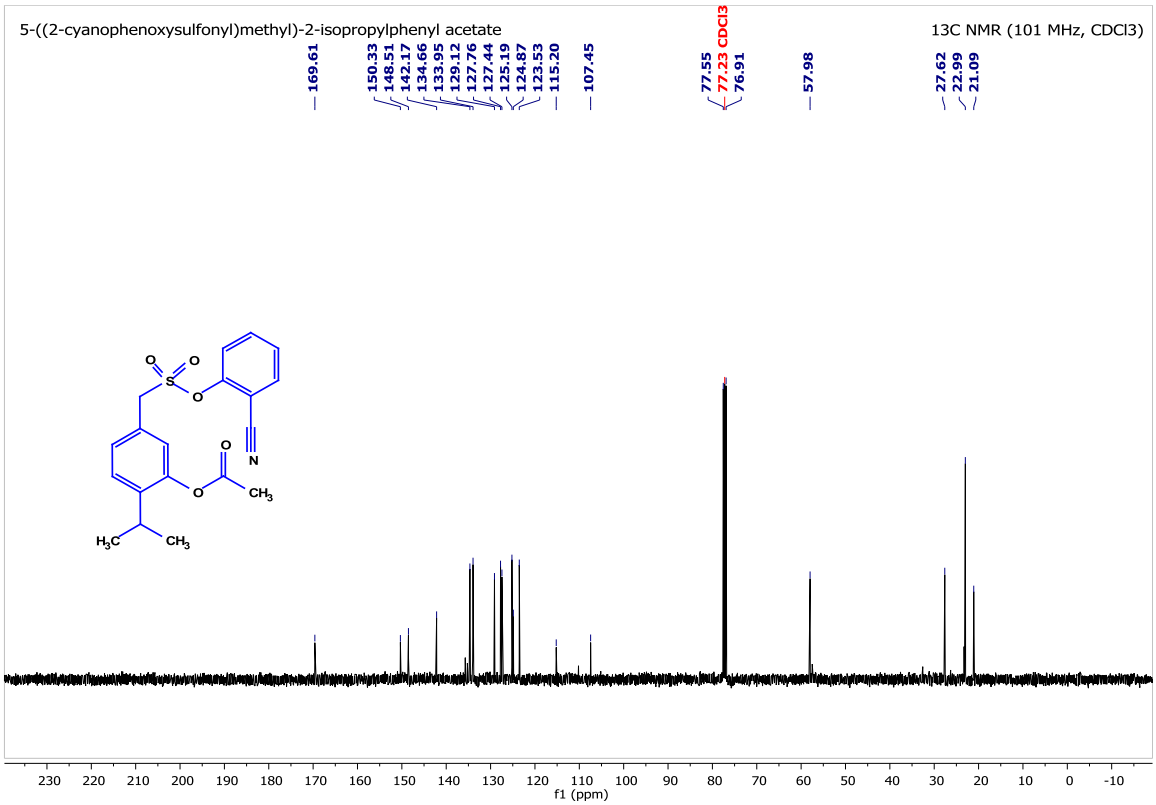
5-((2-cyanophenoxysulfonyl)methyl)-2-methylphenyl acetate (2b):



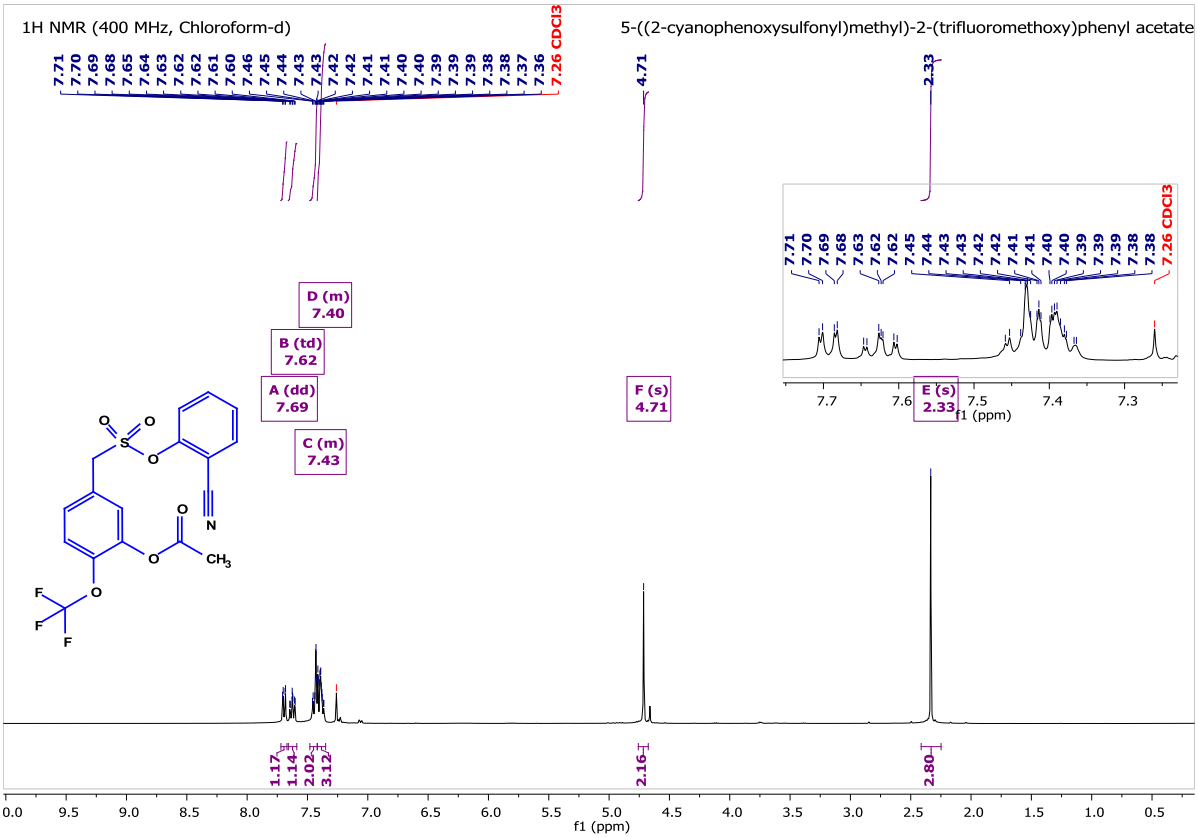


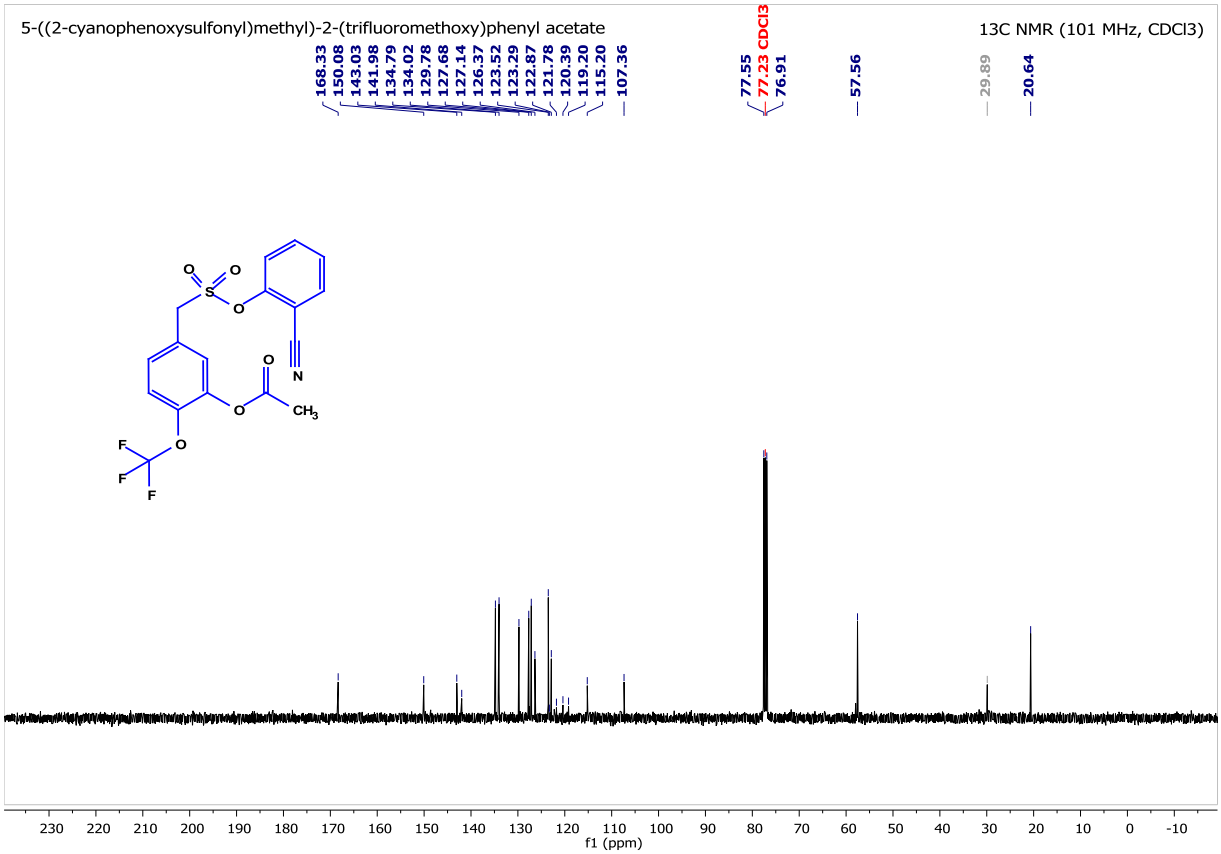
5-((2-cyanophenoxysulfonyl)methyl)-2-isopropylphenyl acetate (2c):



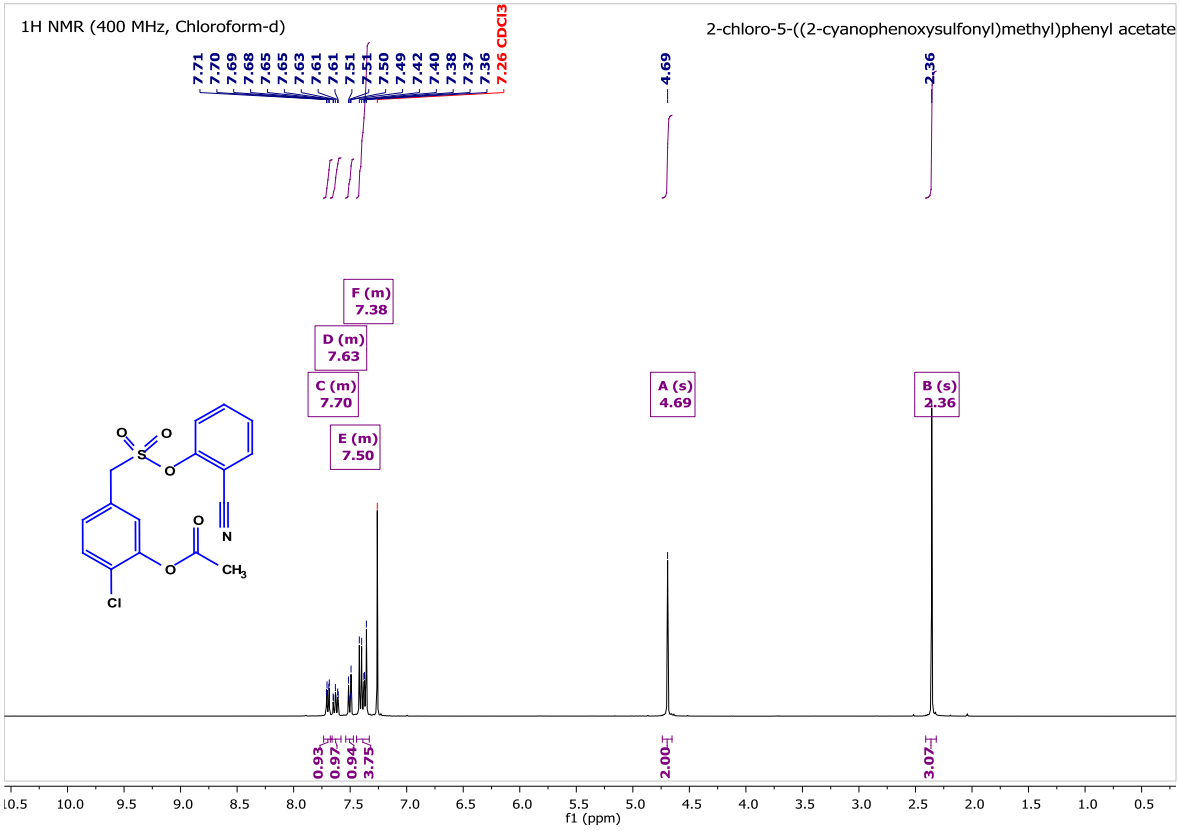


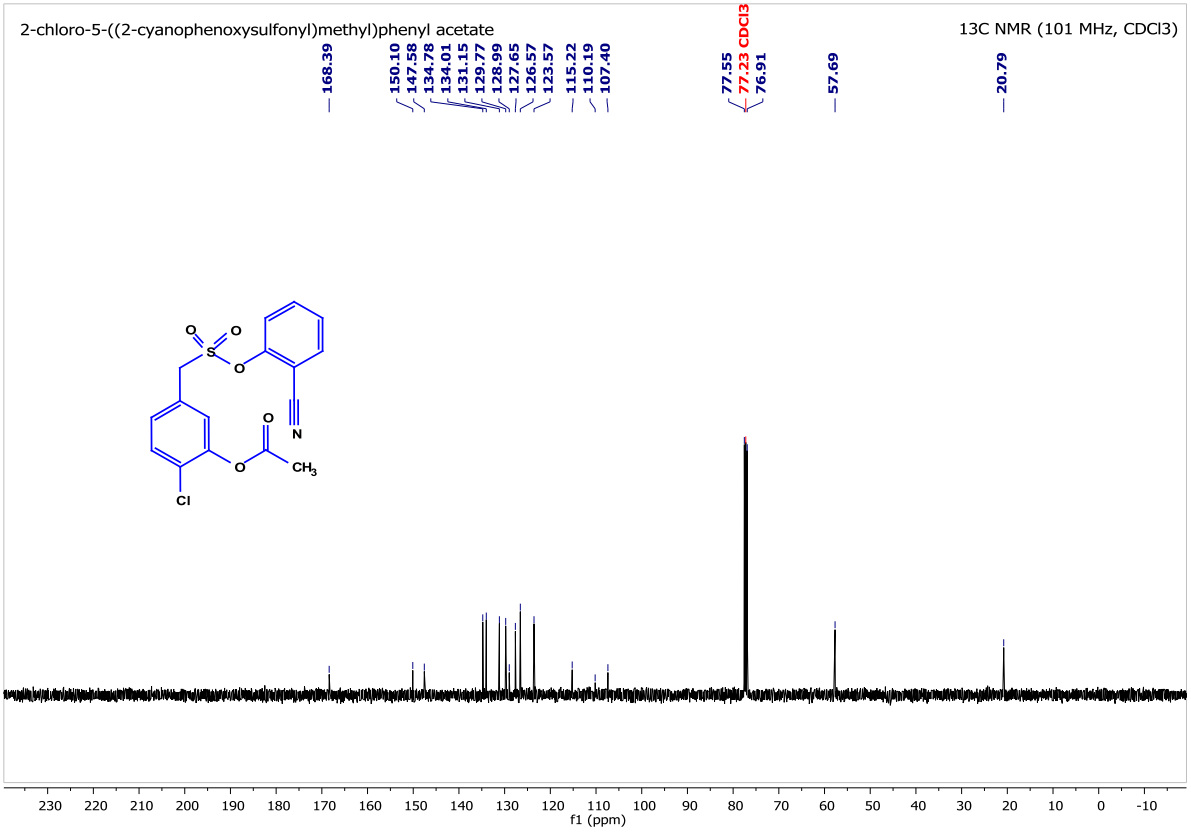
5-((2-cyanophenoxysulfonyl)methyl)-2-(trifluoromethoxy)phenyl acetate (2d):



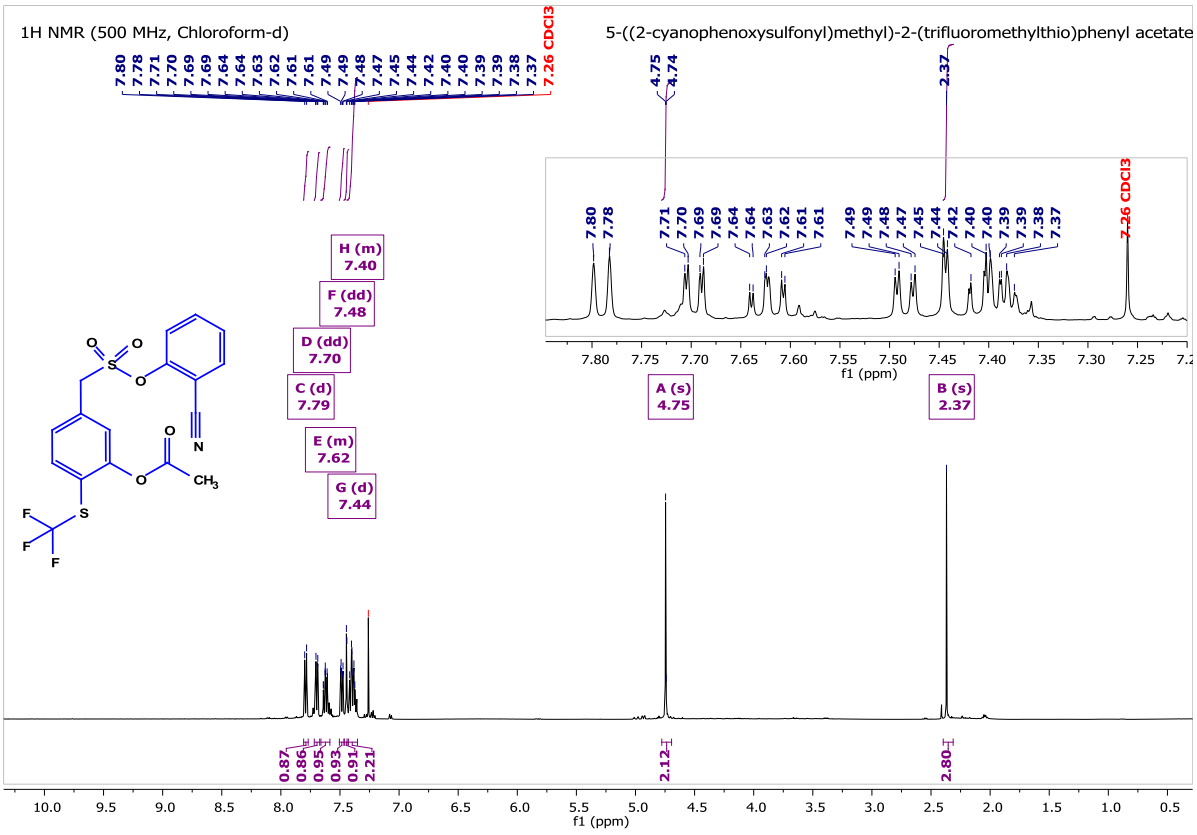


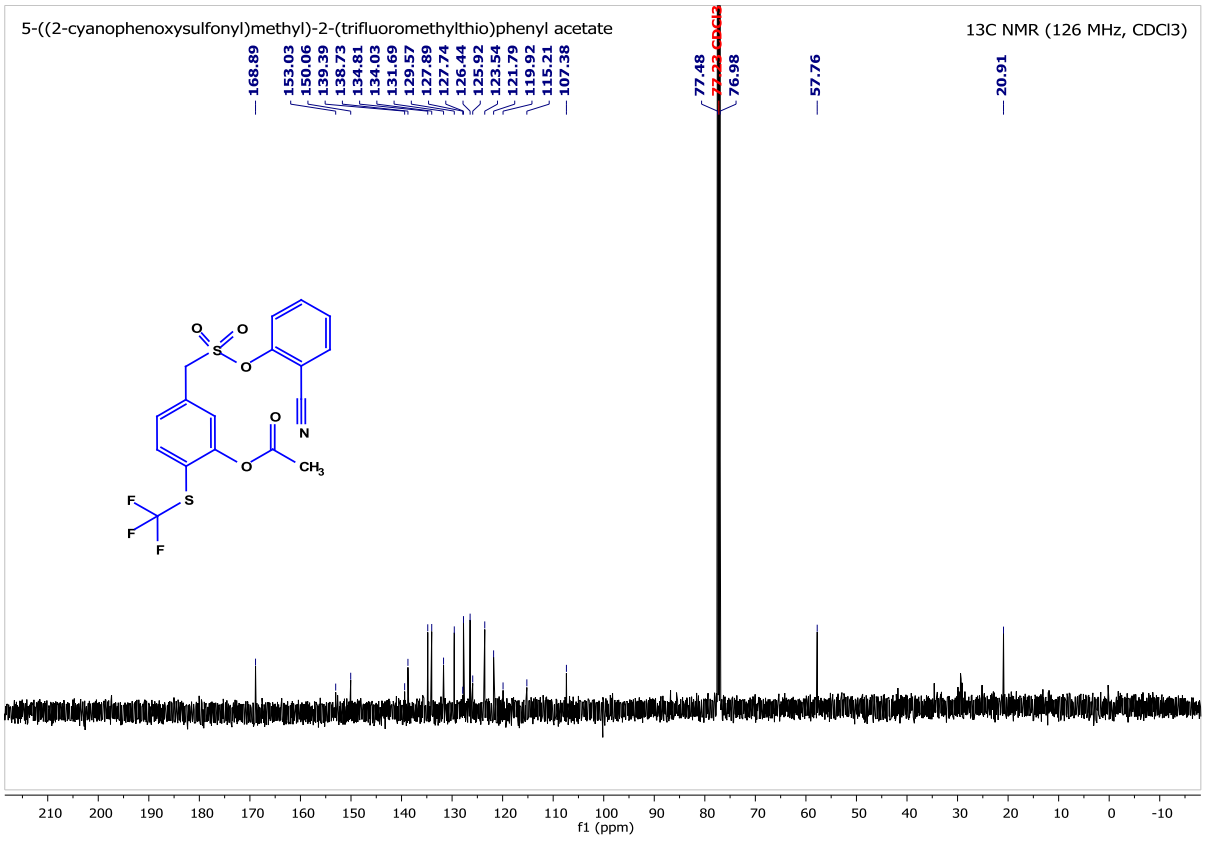
2-chloro-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (2e):

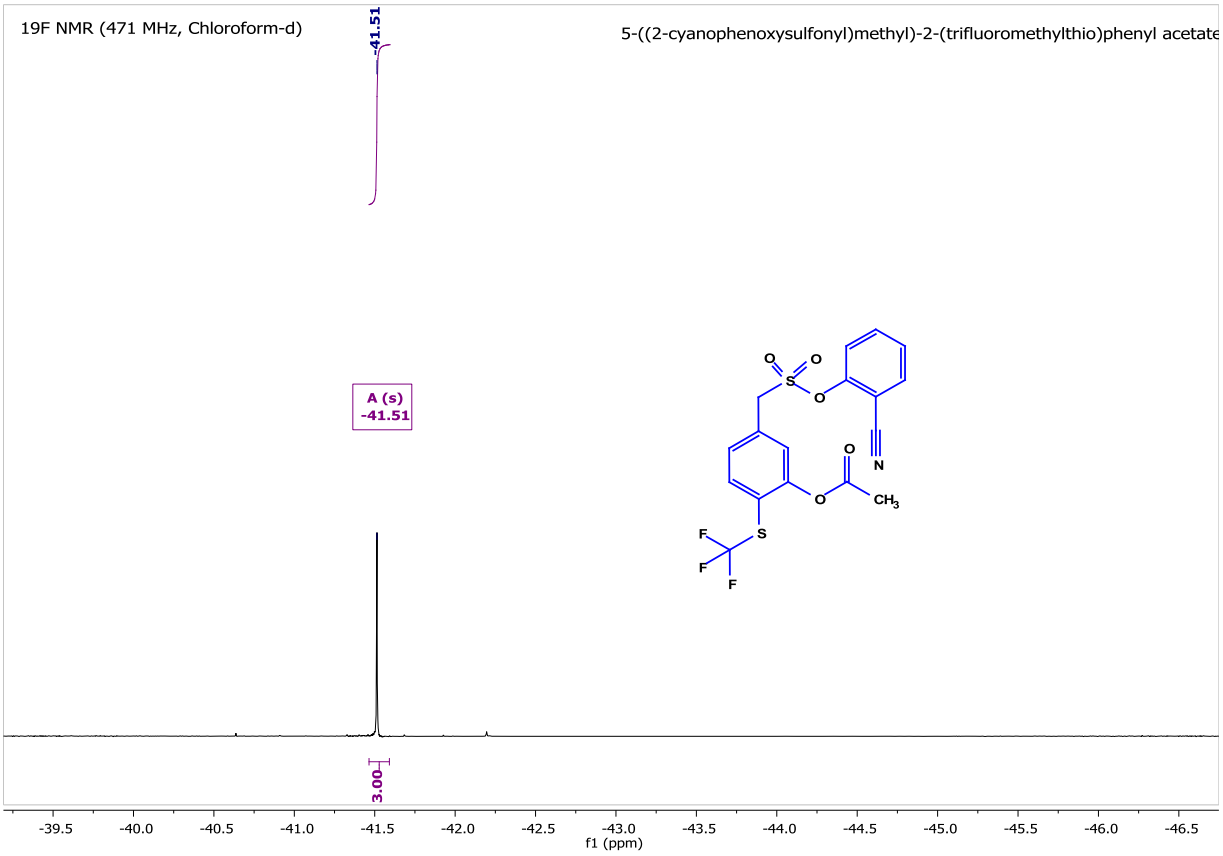




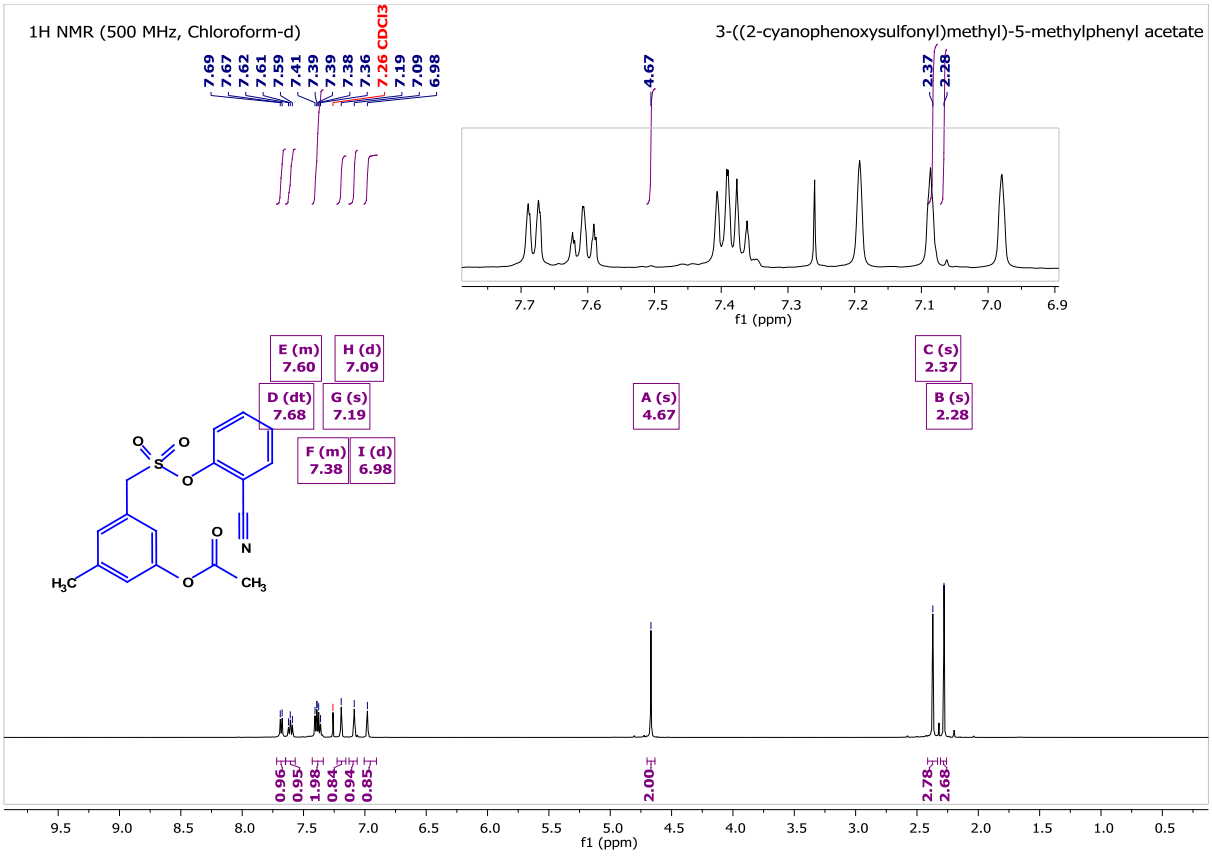
5-((2-cyanophenoxysulfonyl)methyl)-2-(trifluoromethylthio)phenyl acetate (2f):

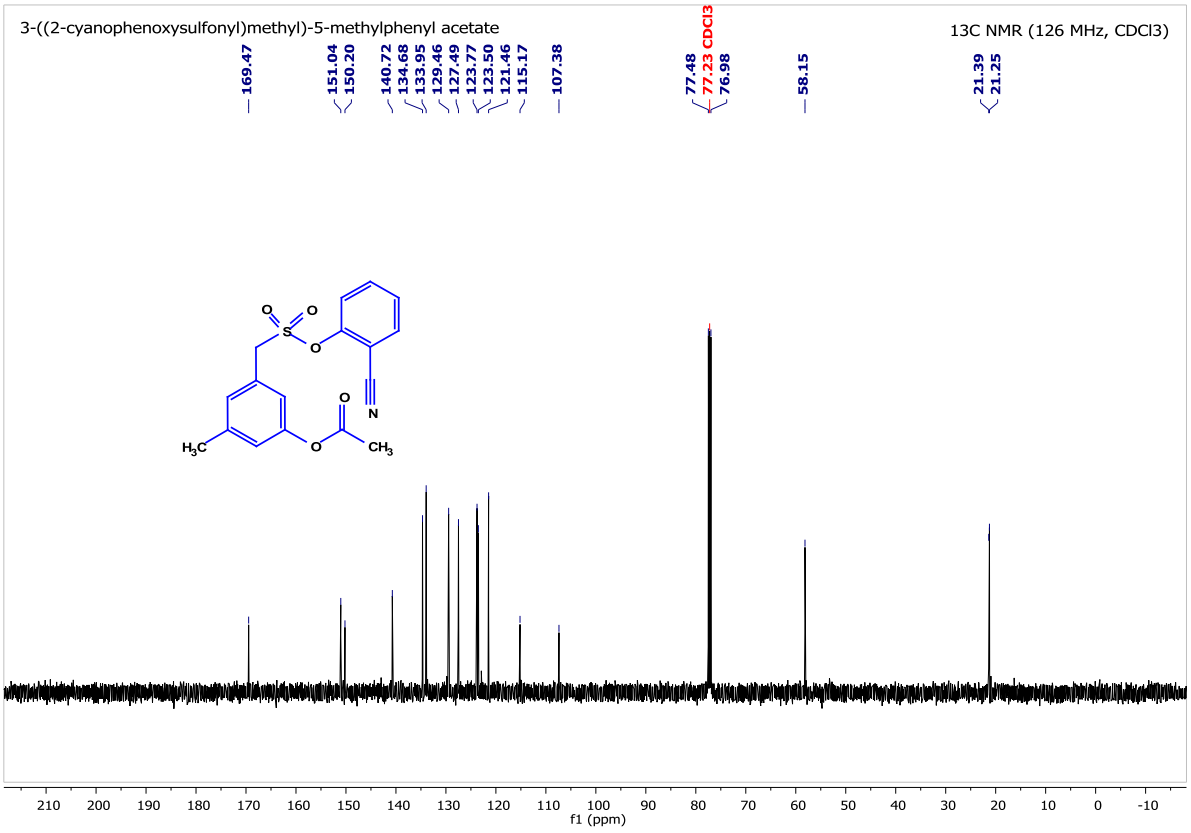




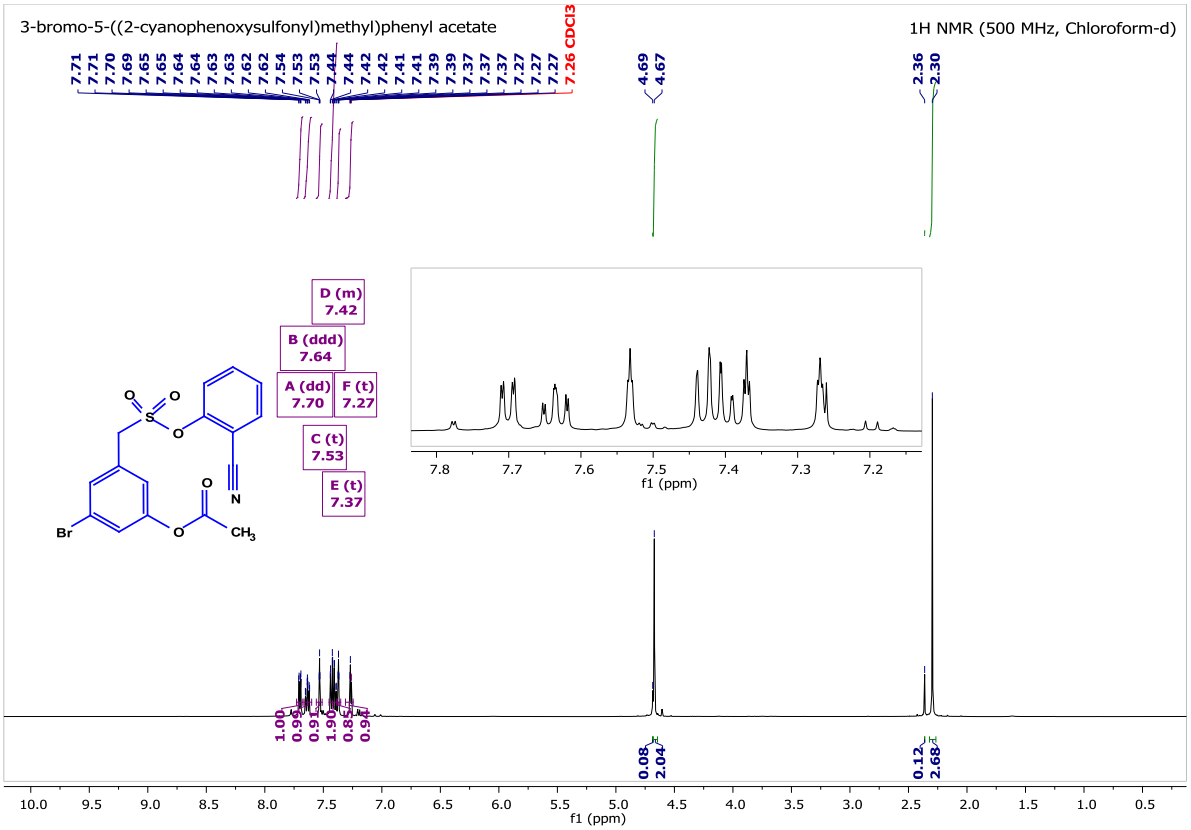


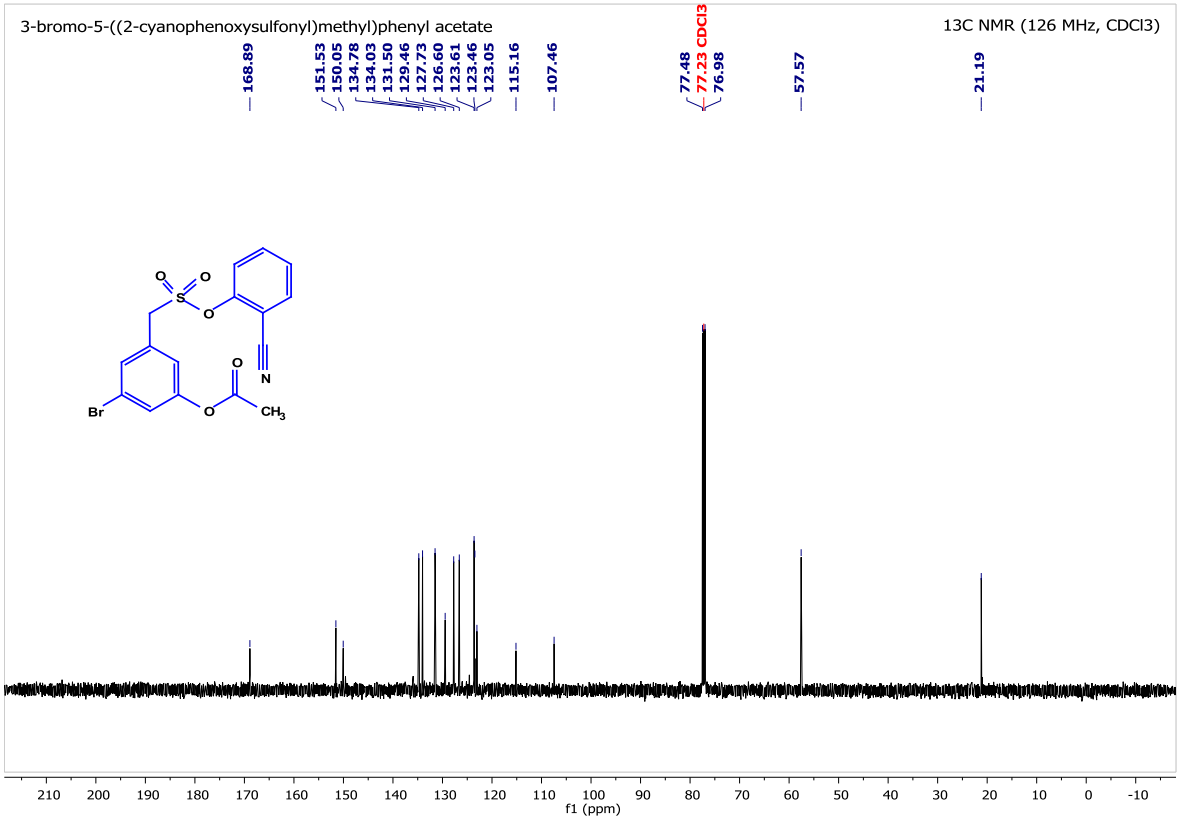
3-((2-cyanophenoxysulfonyl)methyl)-5-methylphenyl acetate (2g):



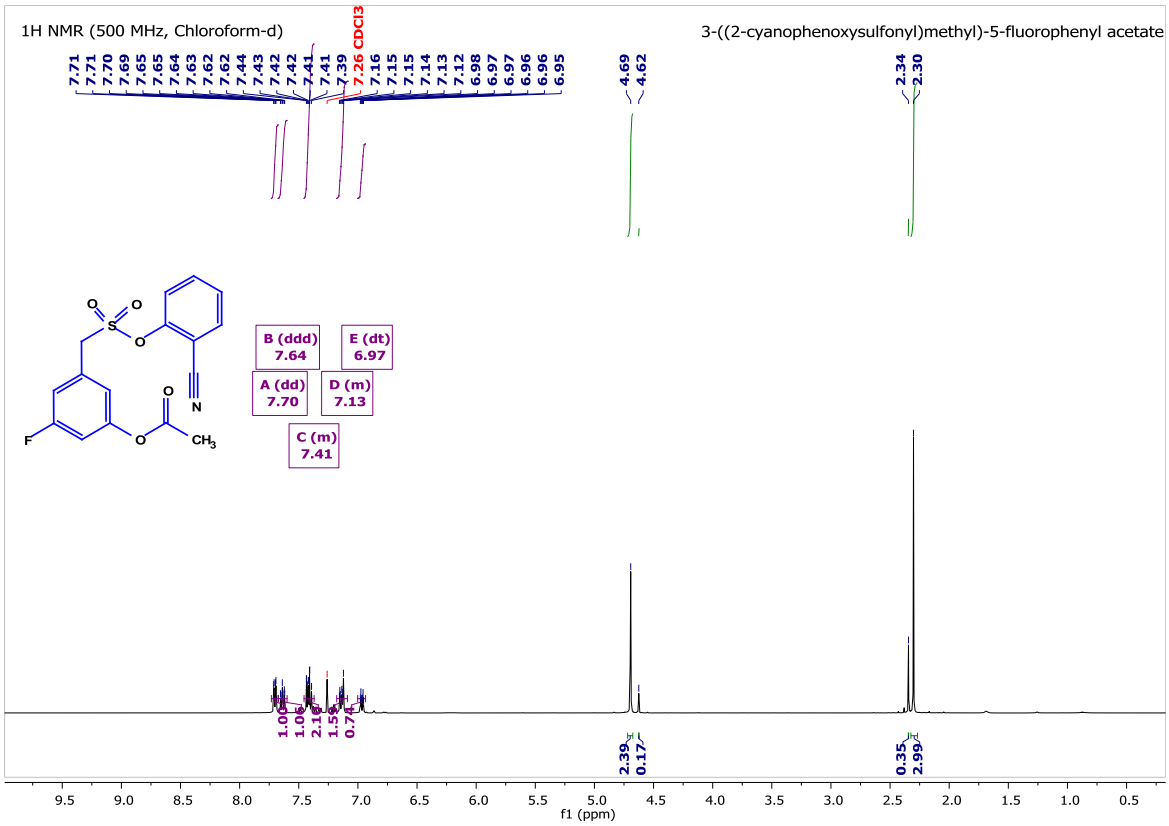


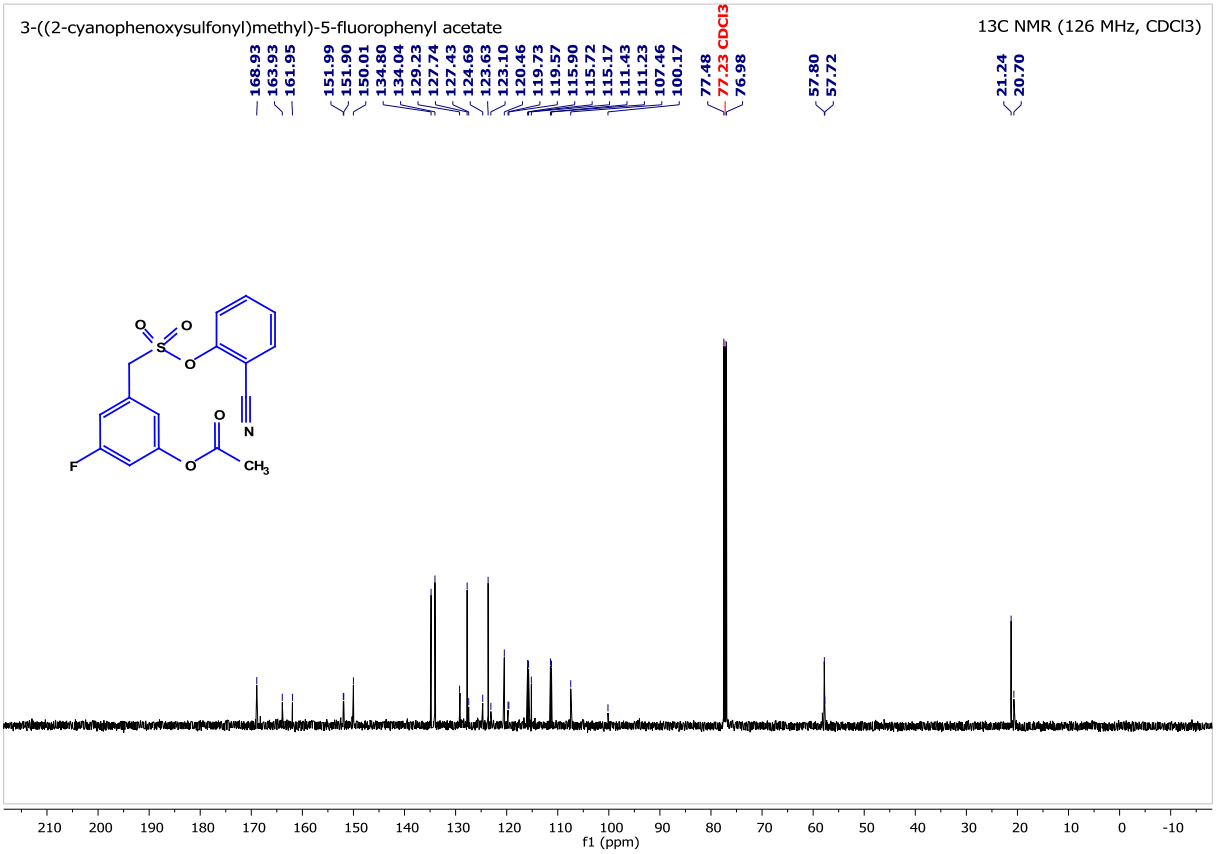
3-bromo-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (2h):



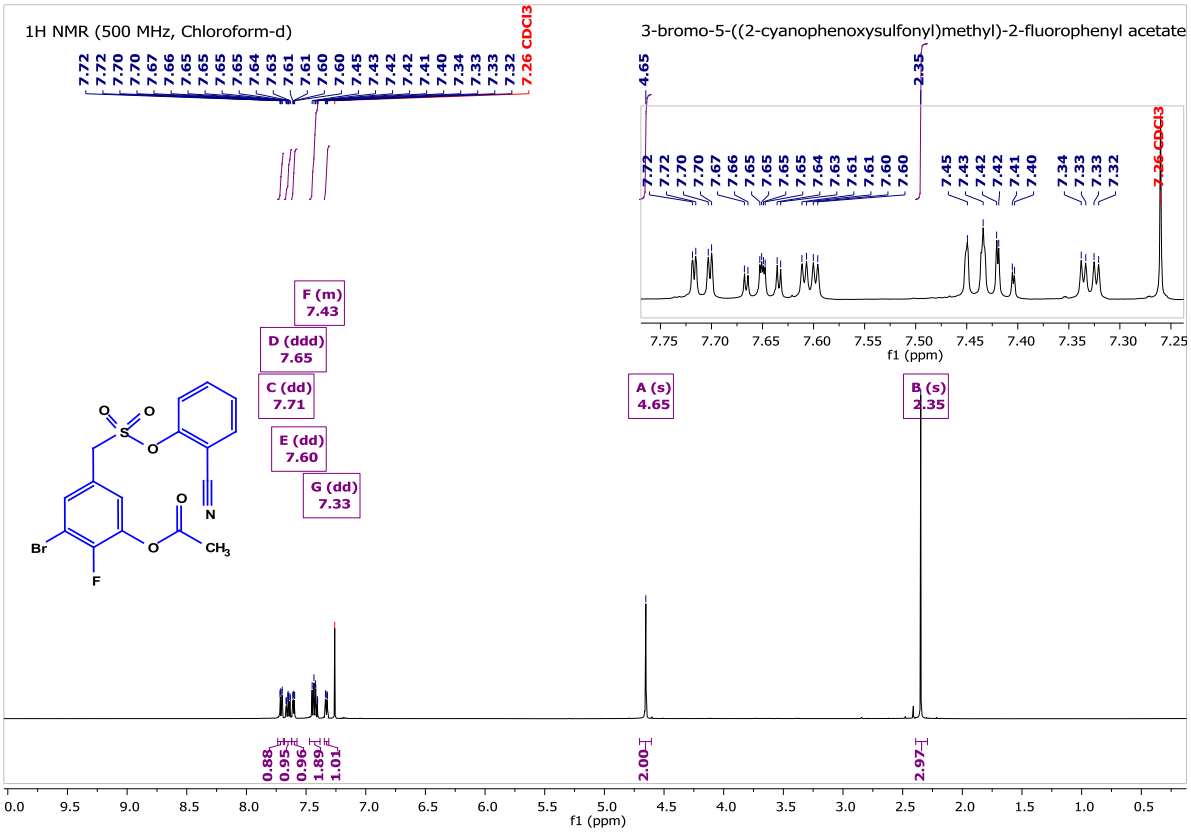


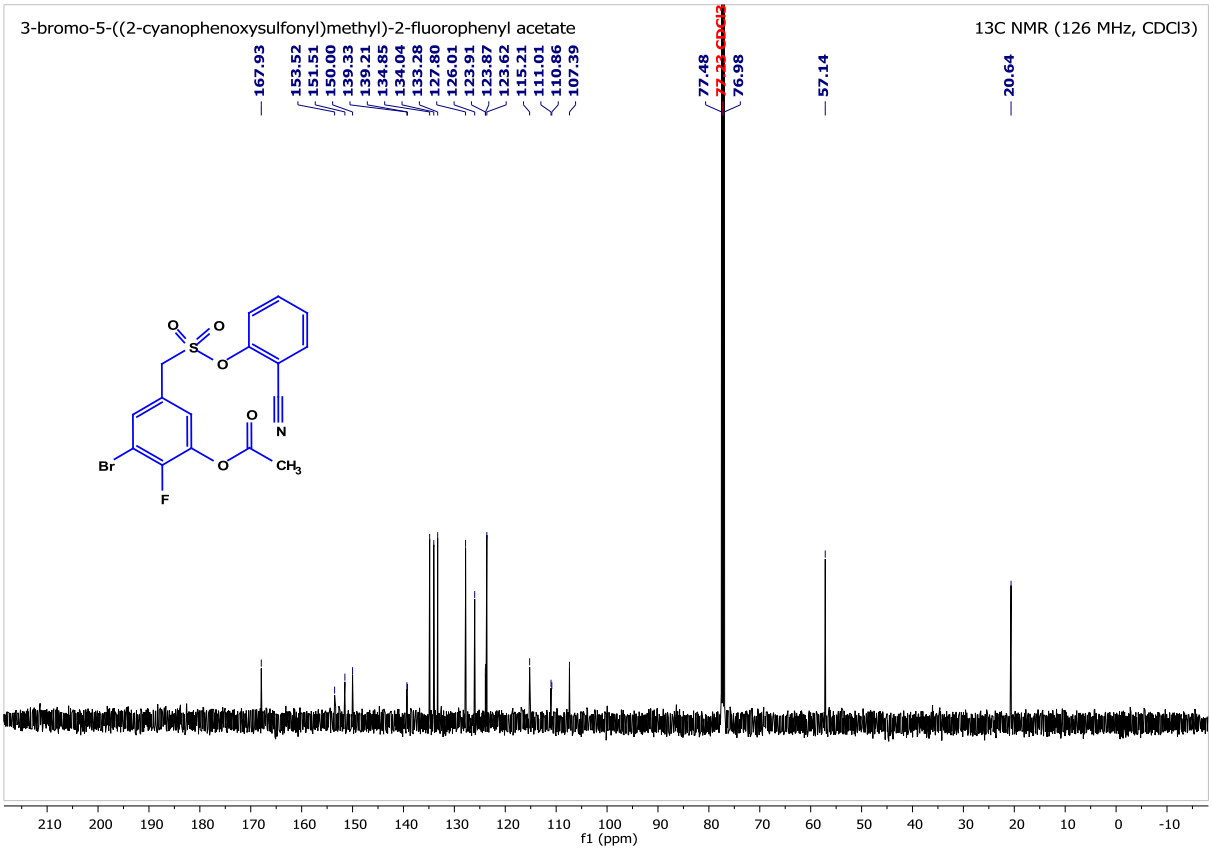
3-((2-cyanophenoxysulfonyl)methyl)-5-fluorophenyl acetate (2i):



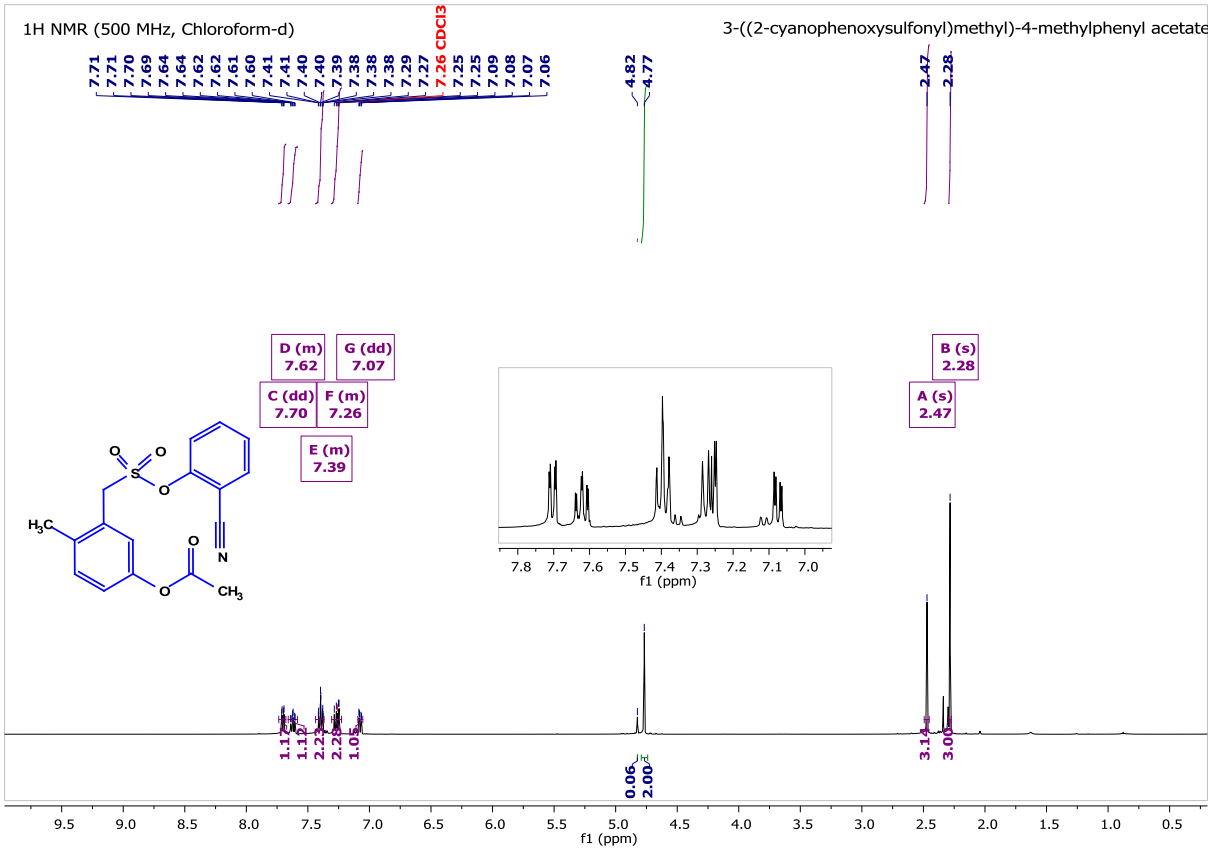


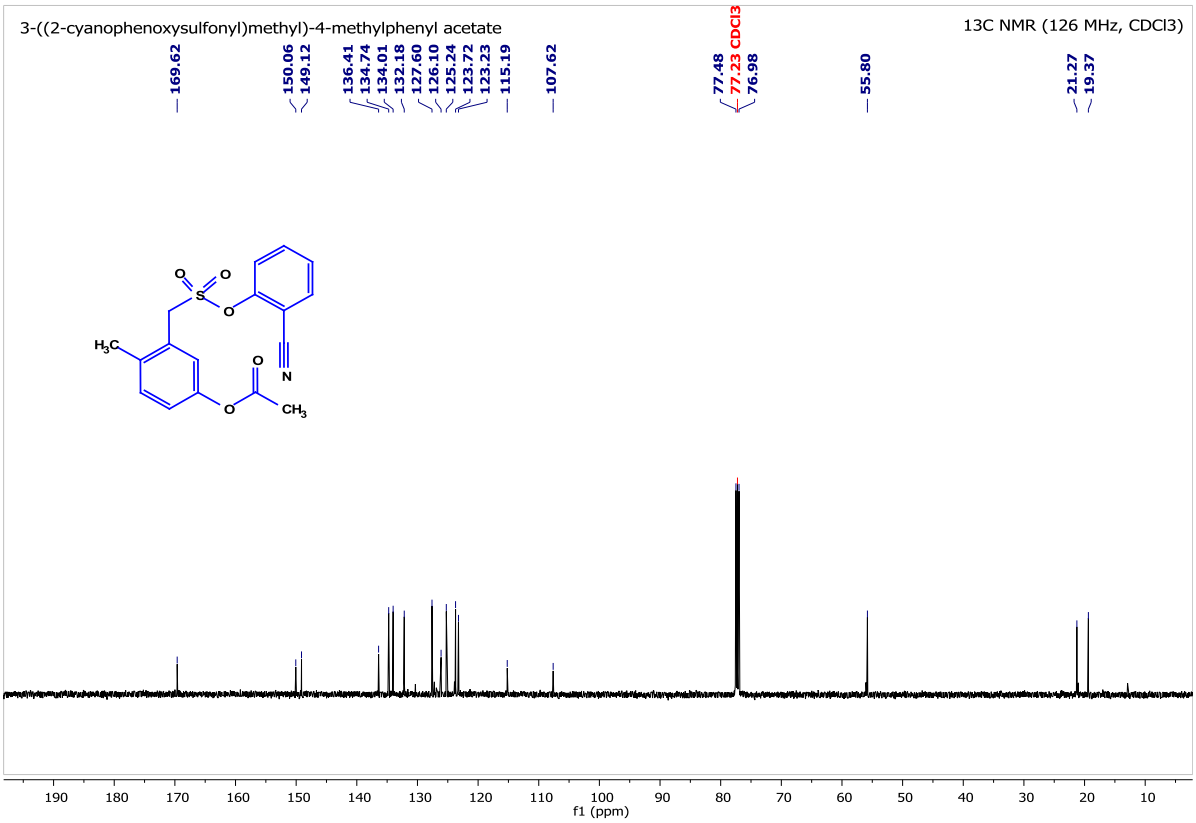
3-bromo-5-((2-cyanophenoxysulfonyl)methyl)-2-fluorophenyl acetate (2j):



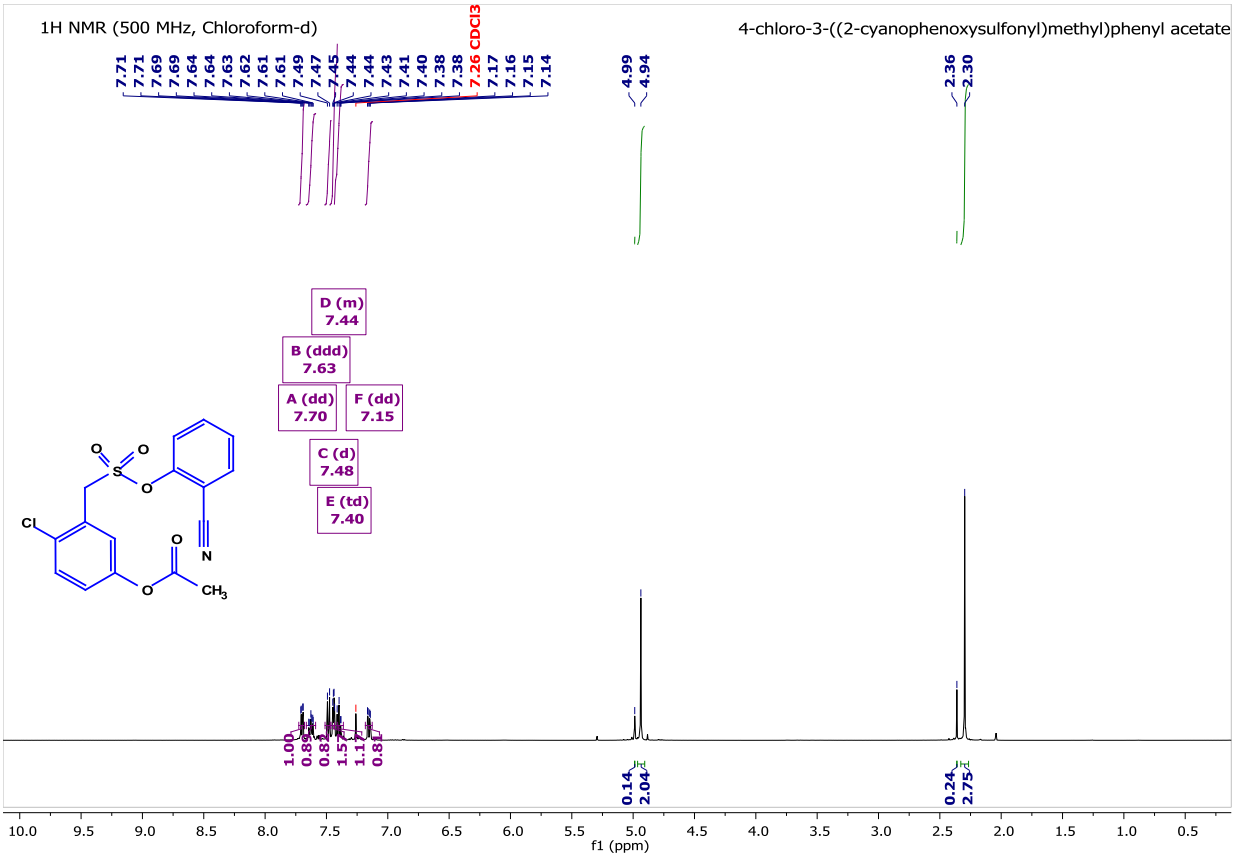


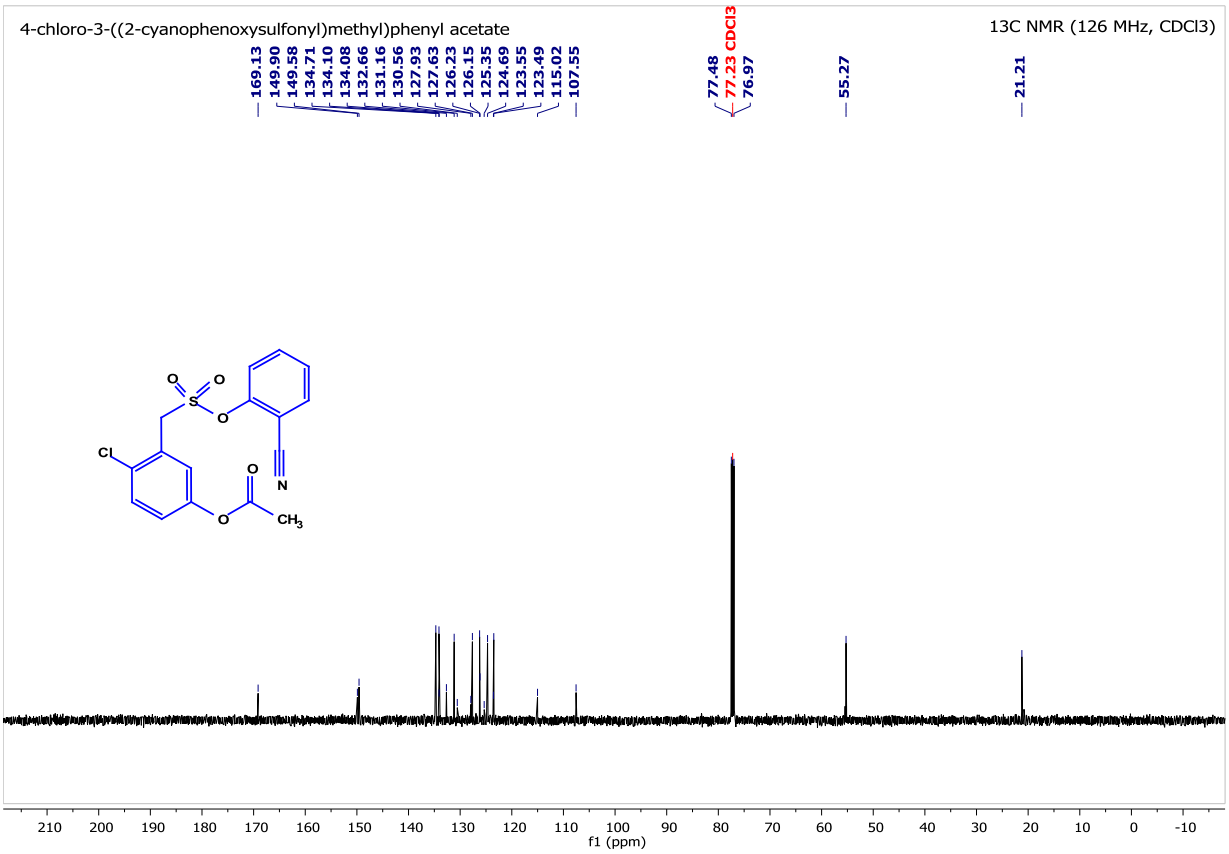
3-((2-cyanophenoxysulfonyl)methyl)-4-methylphenyl acetate (2k):



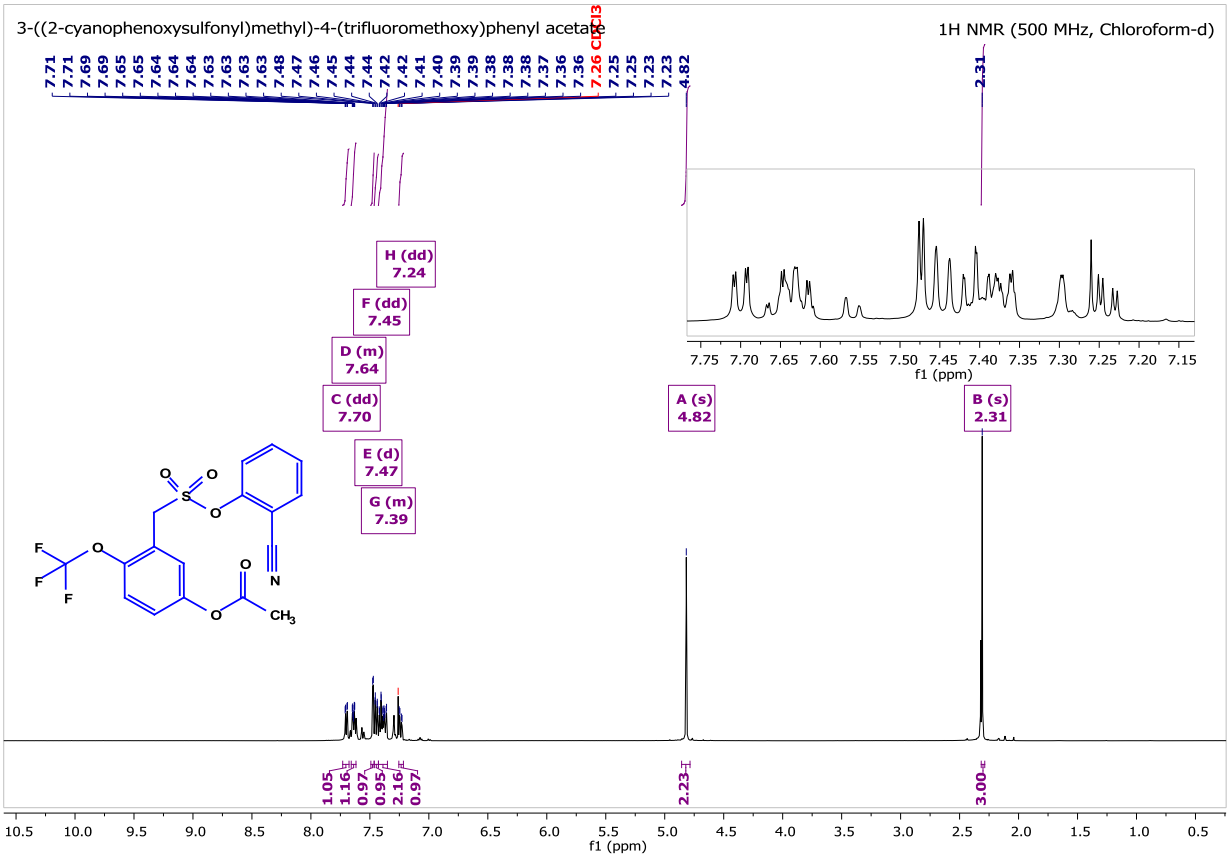


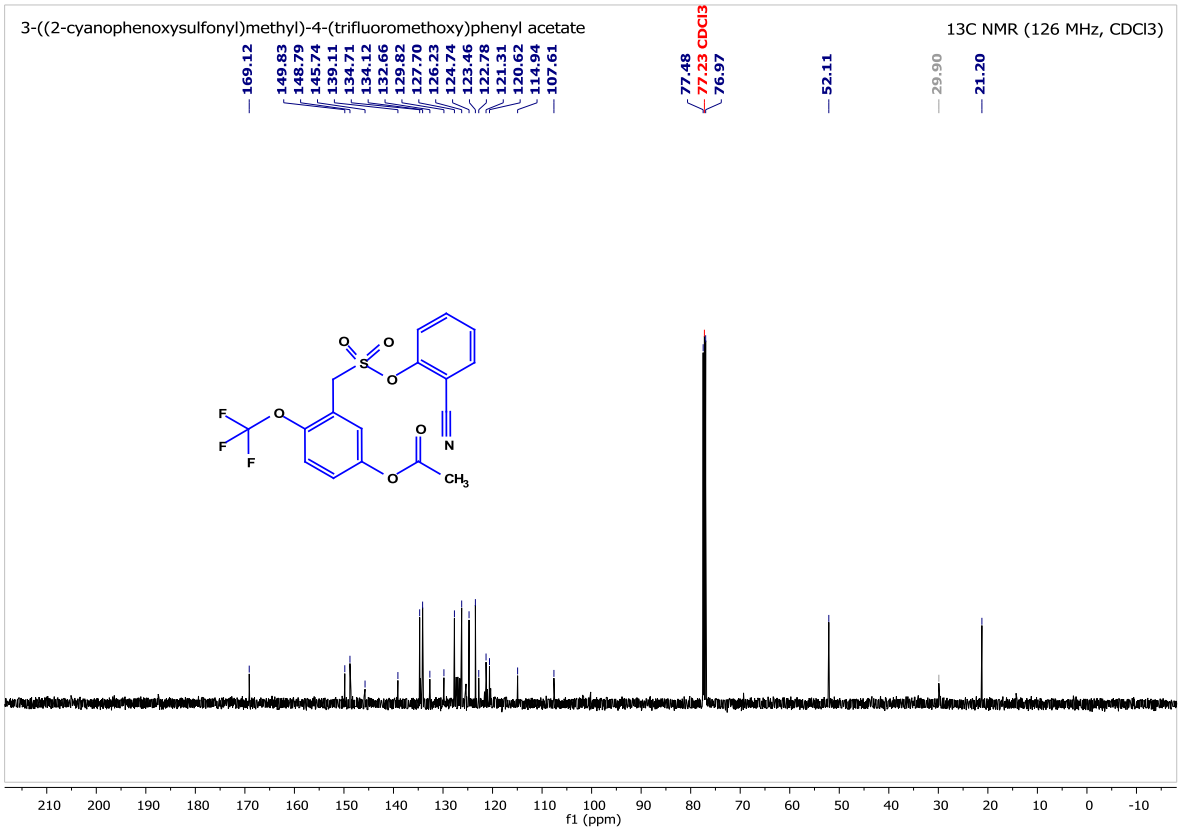
4-chloro-3-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (2l):



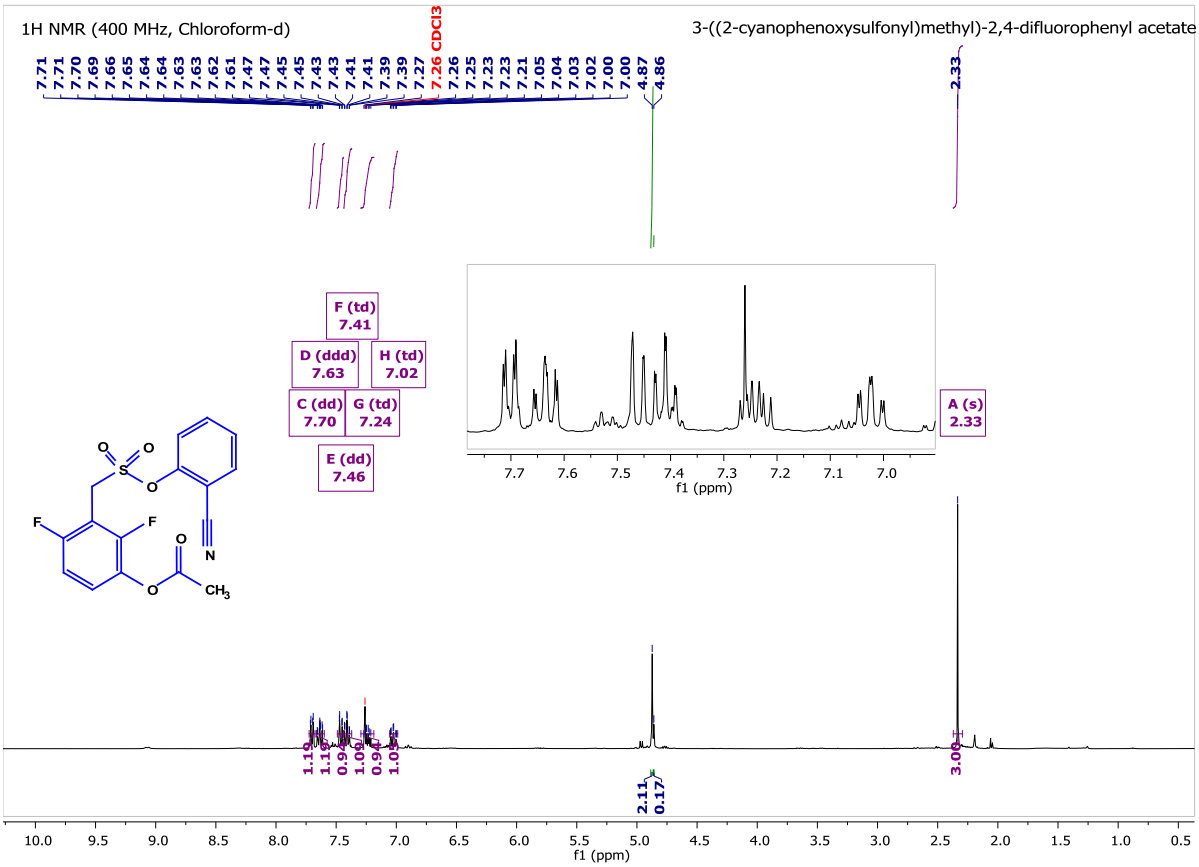


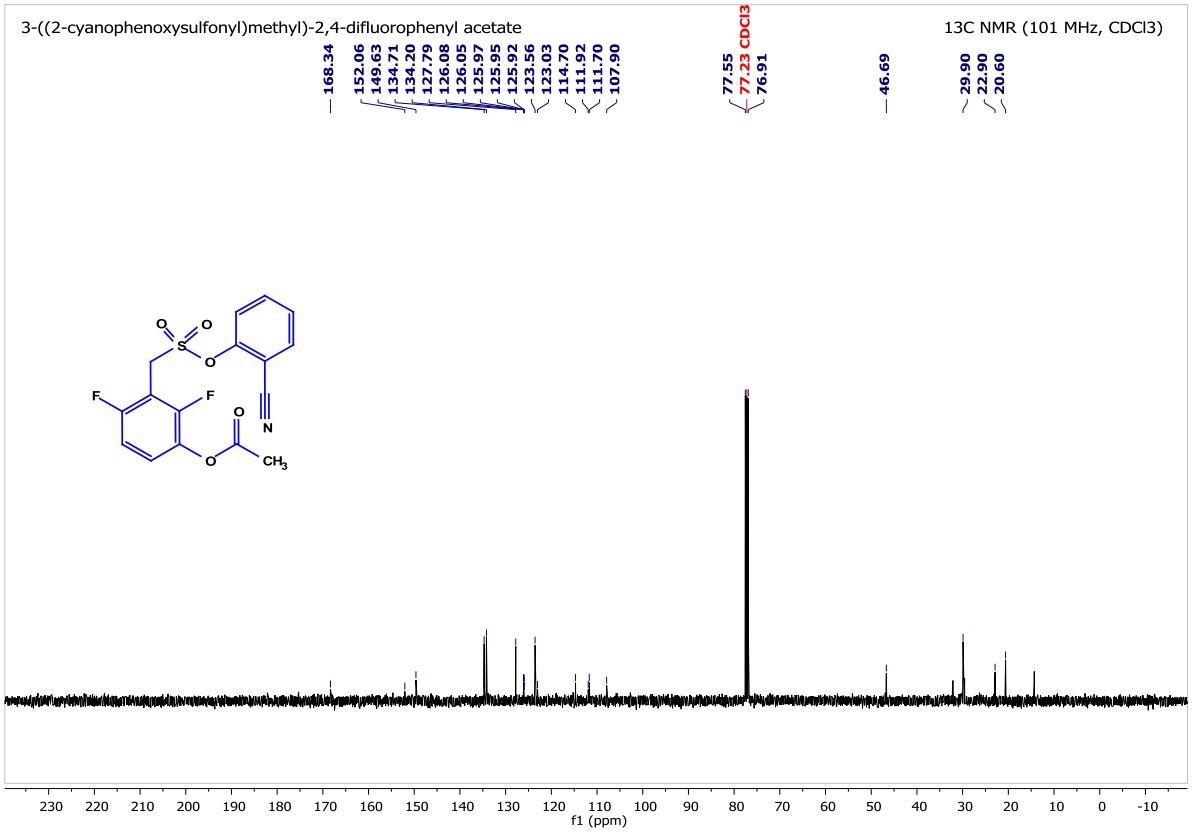
3-((2-cyanophenoxysulfonyl)methyl)-4-(trifluoromethoxy)phenyl acetate (2m):



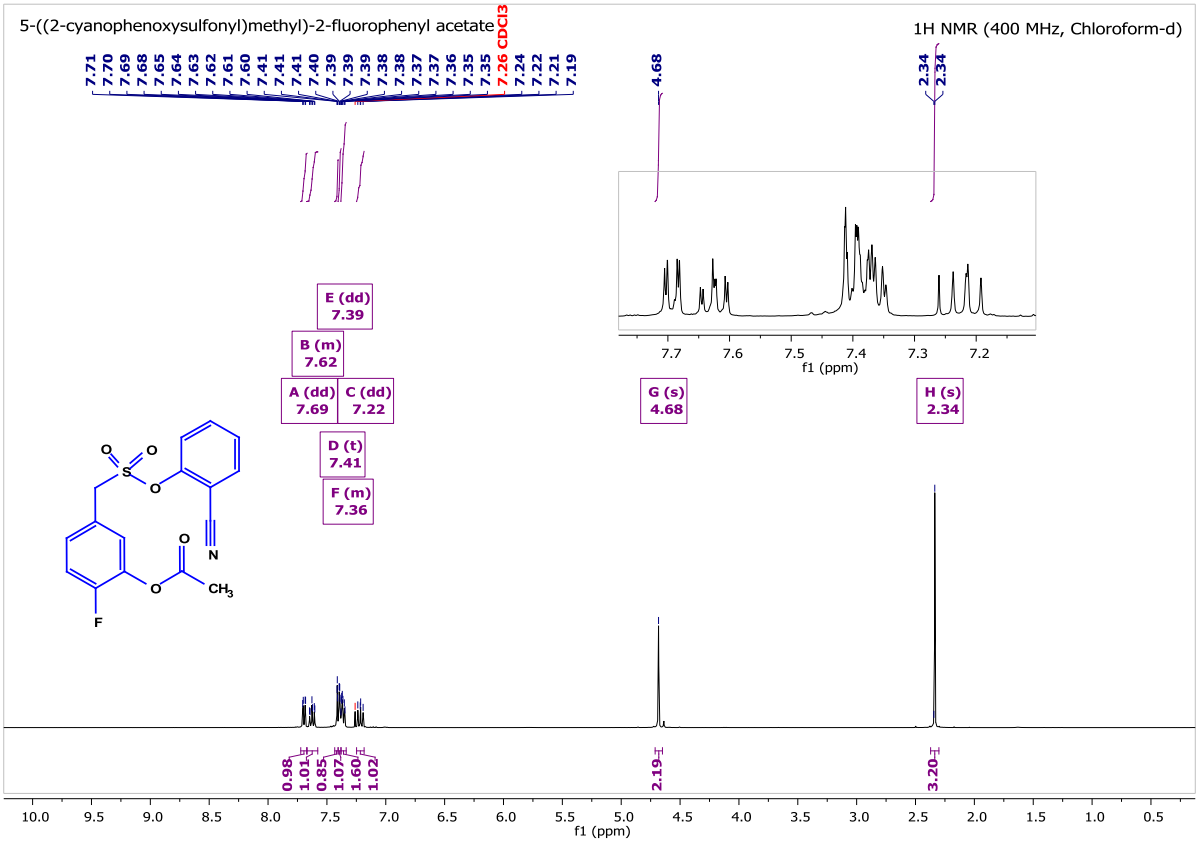


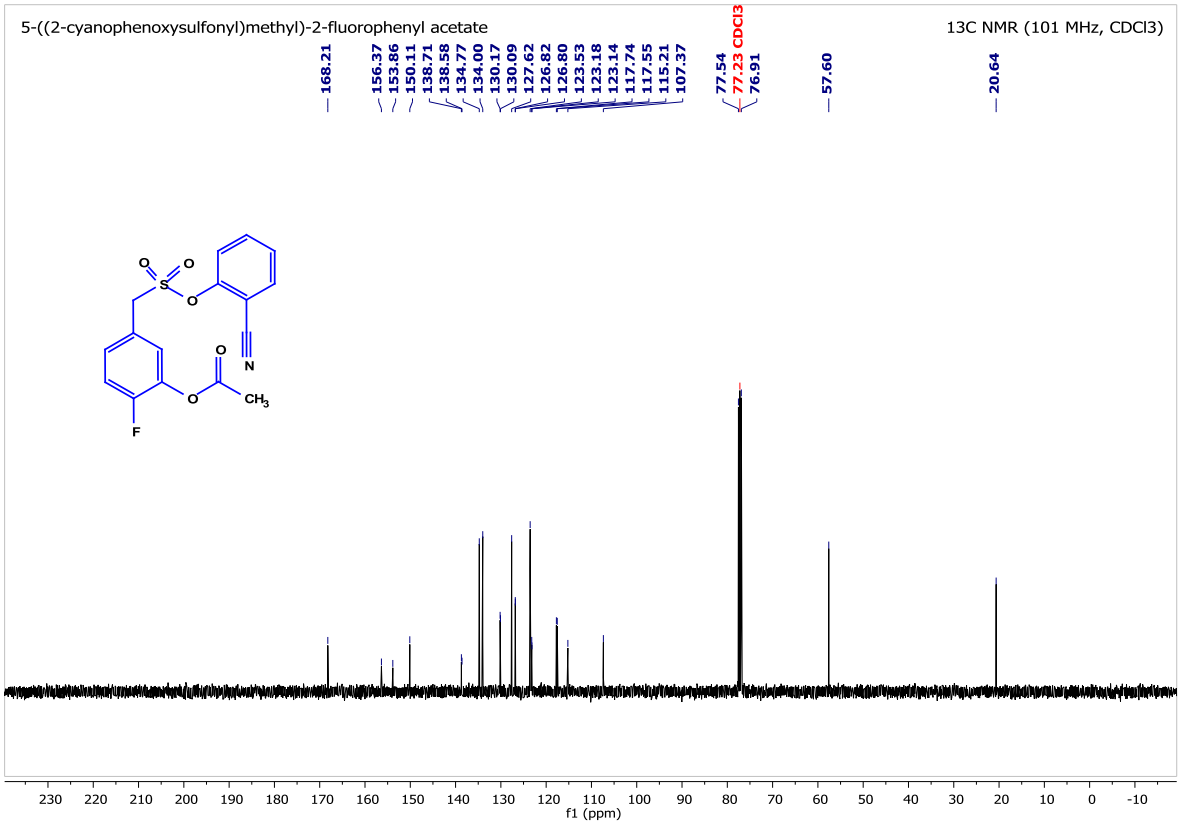
3-((2-cyanophenoxysulfonyl)methyl)-2,4-difluorophenyl acetate (2n):



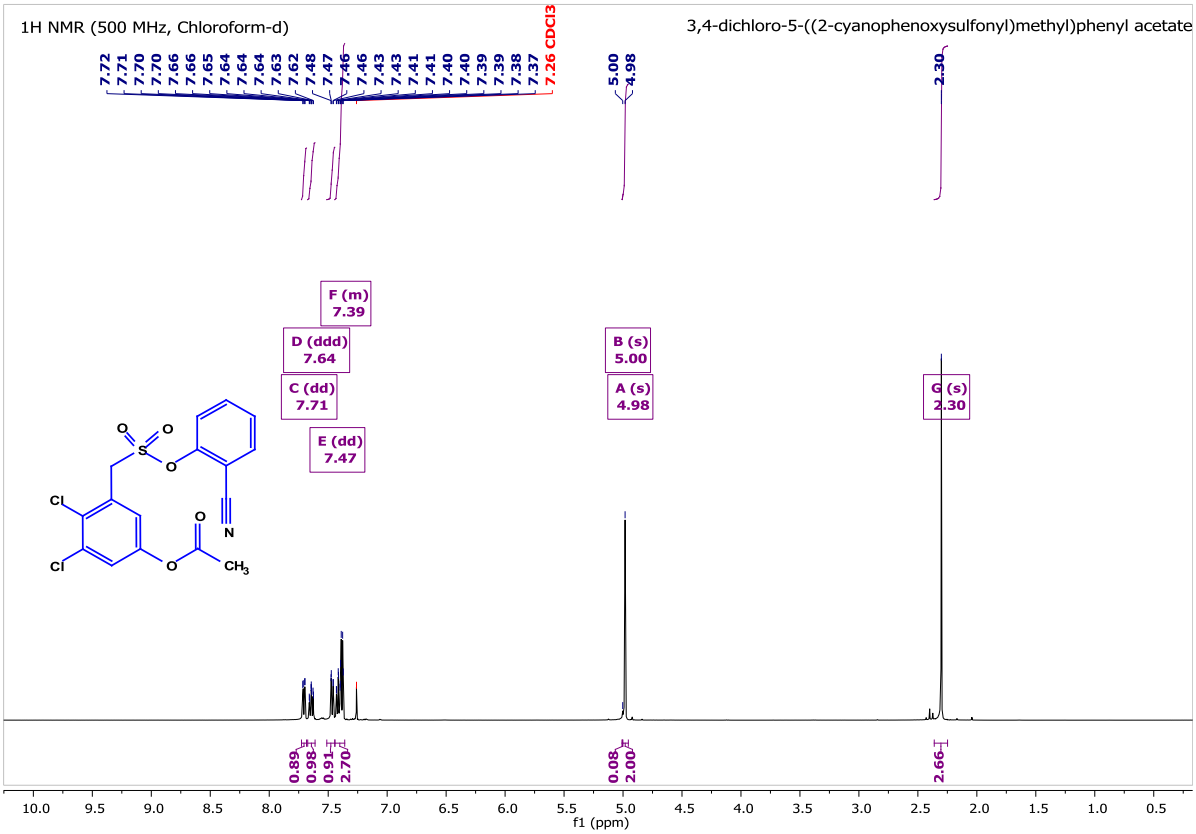


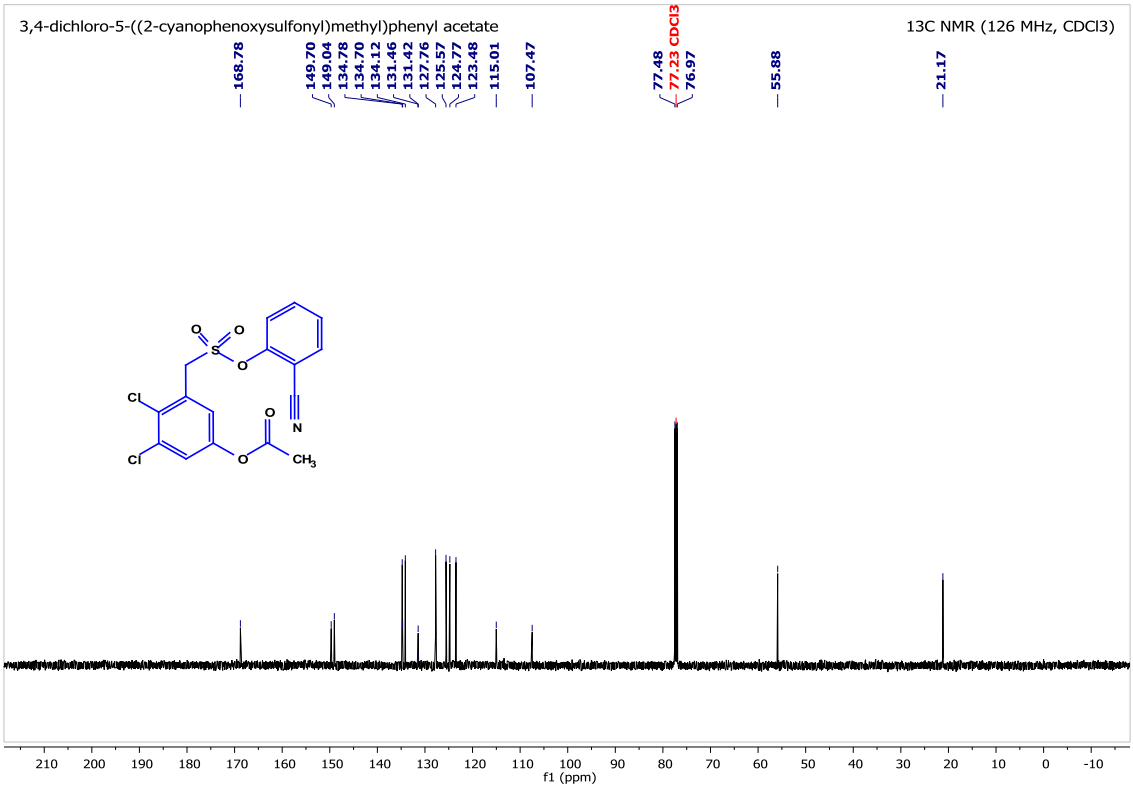
5-((2-cyanophenoxysulfonyl)methyl)-2-fluorophenyl acetate (2o):





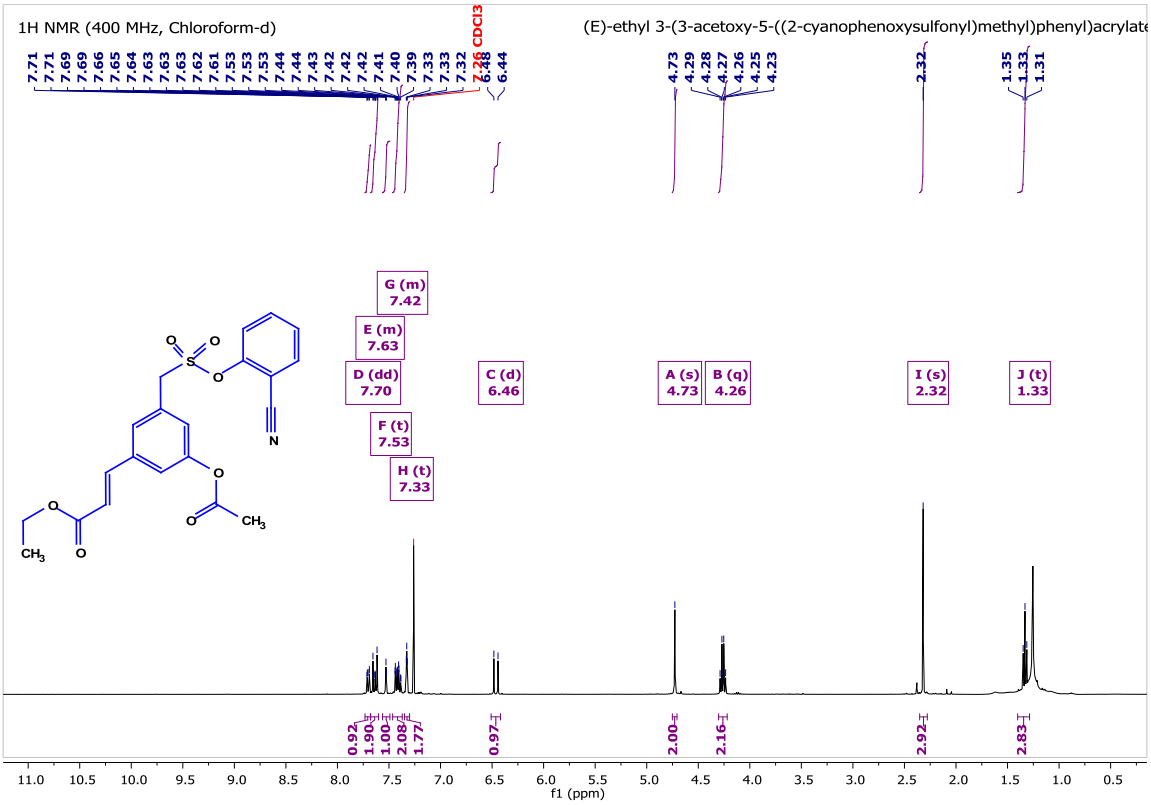
3,4-dichloro-5-((2-cyanophenoxysulfonyl)methyl)phenyl acetate (2p):

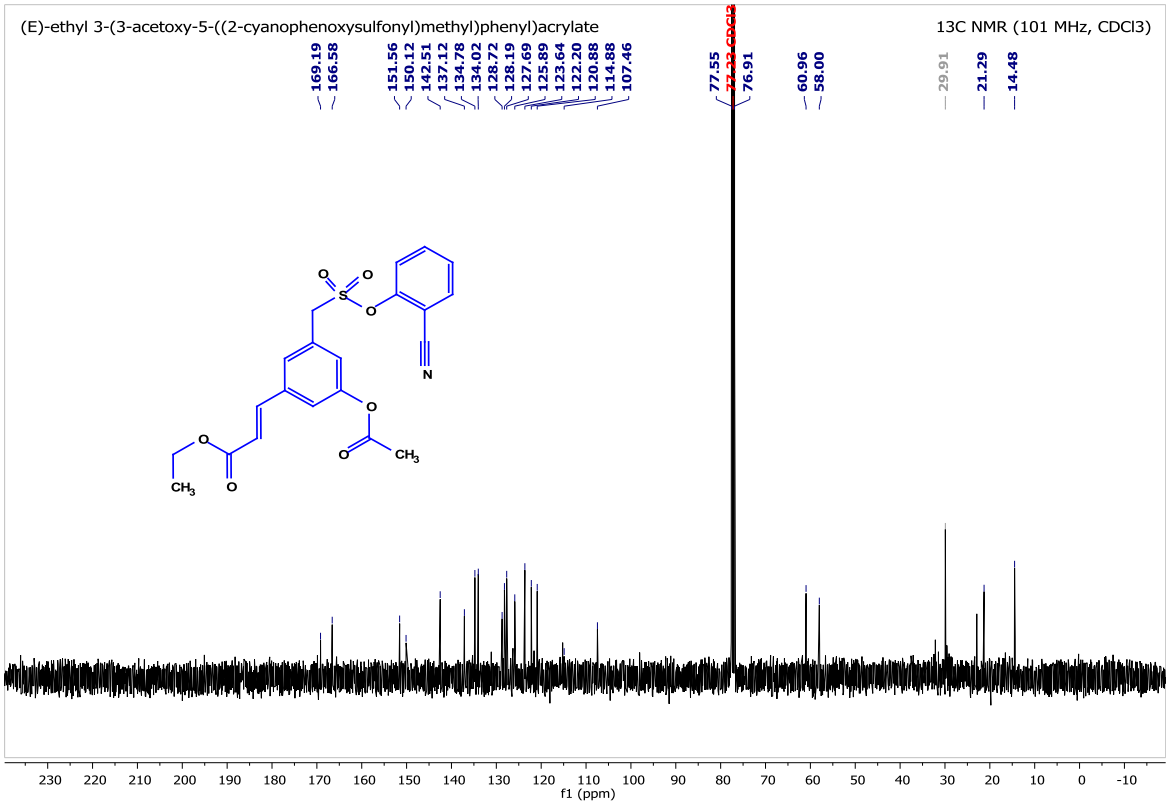




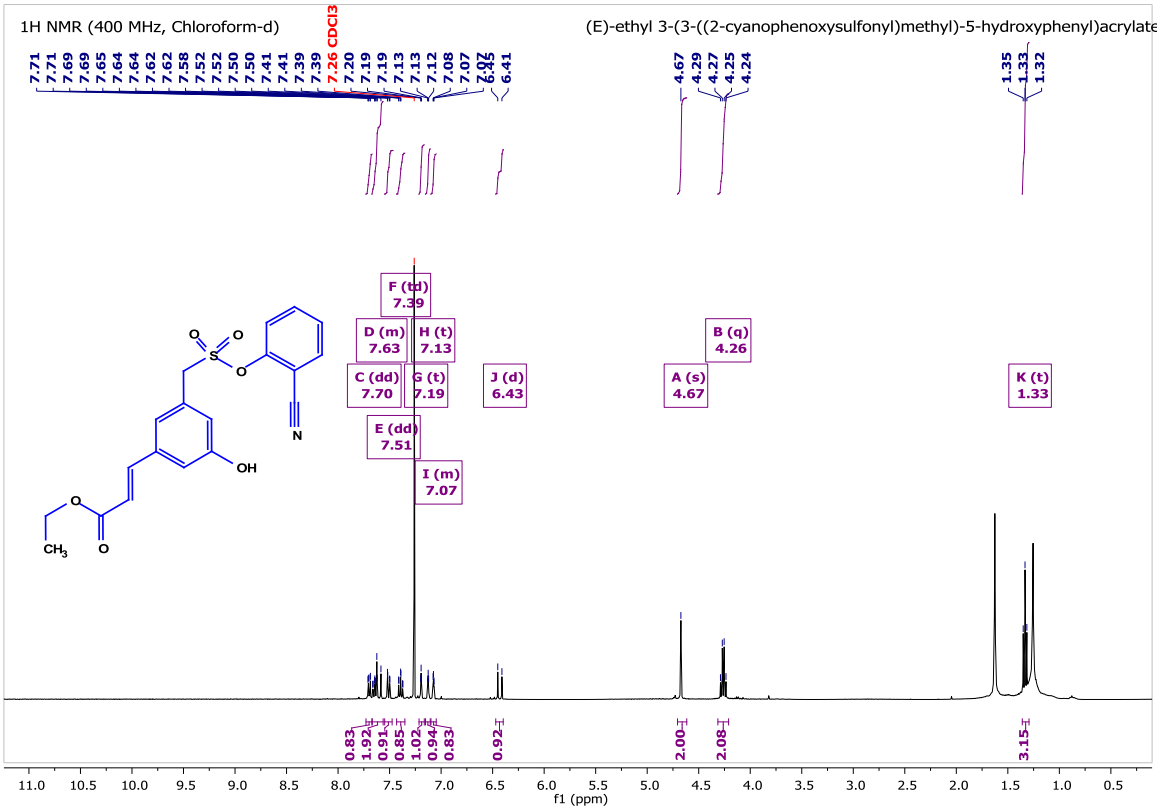
Application:

(E)-ethyl 3-(3-acetoxy-5-((2-cyanophenoxysulfonyl)methyl)phenyl)acrylate:

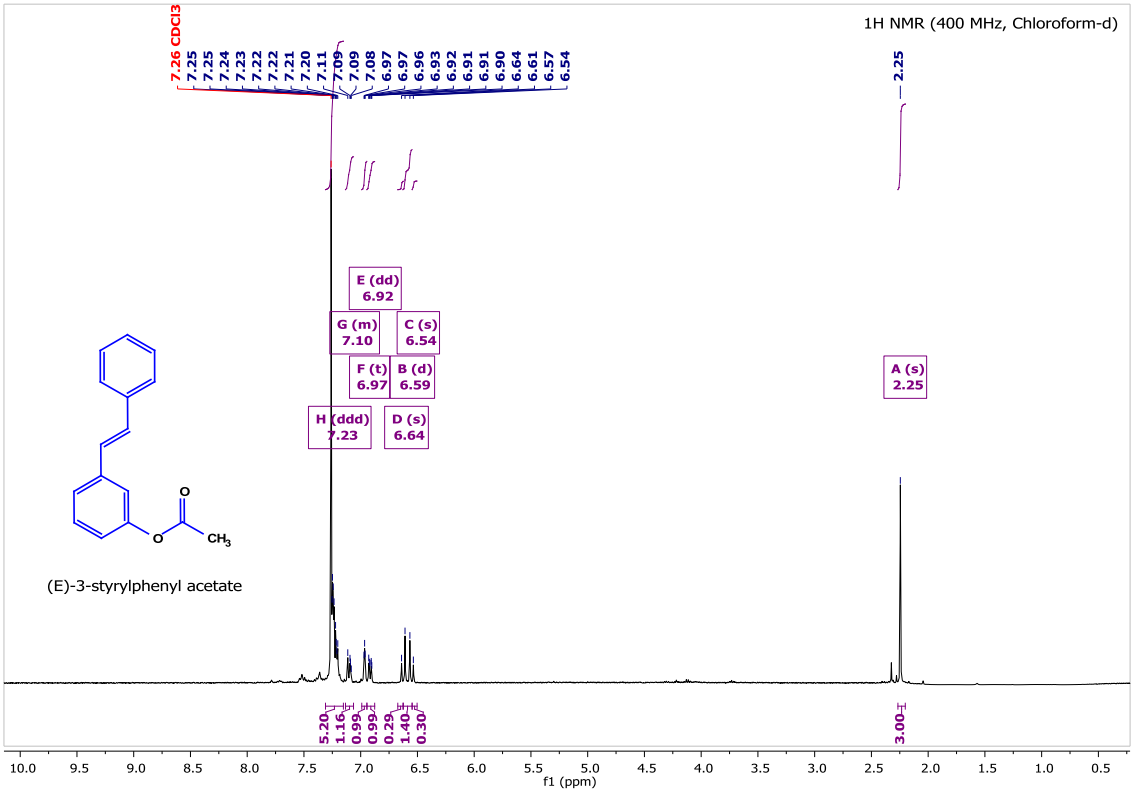


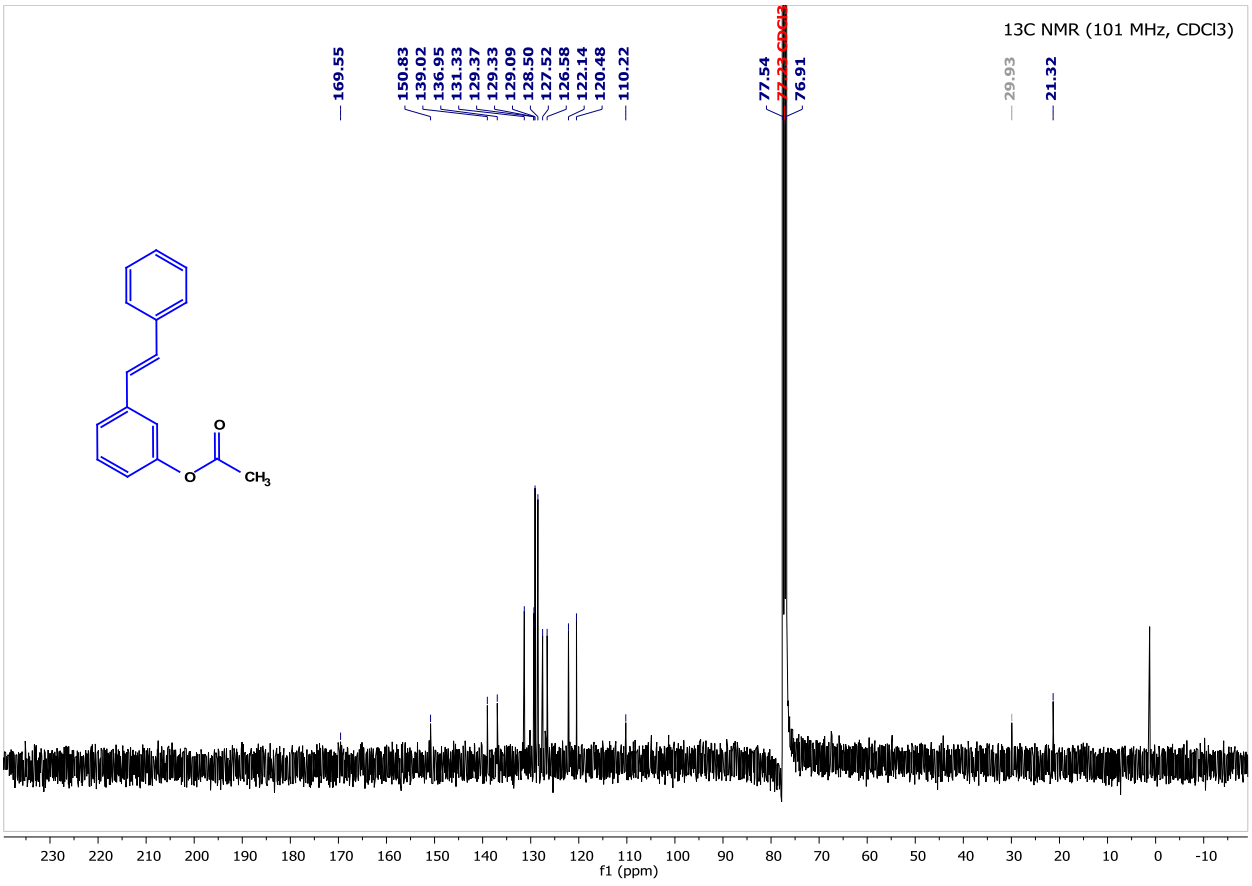


(E)-ethyl 3-(3-((2-cyanophenoxysulfonyl)methyl)-5-hydroxyphenyl)acrylate:

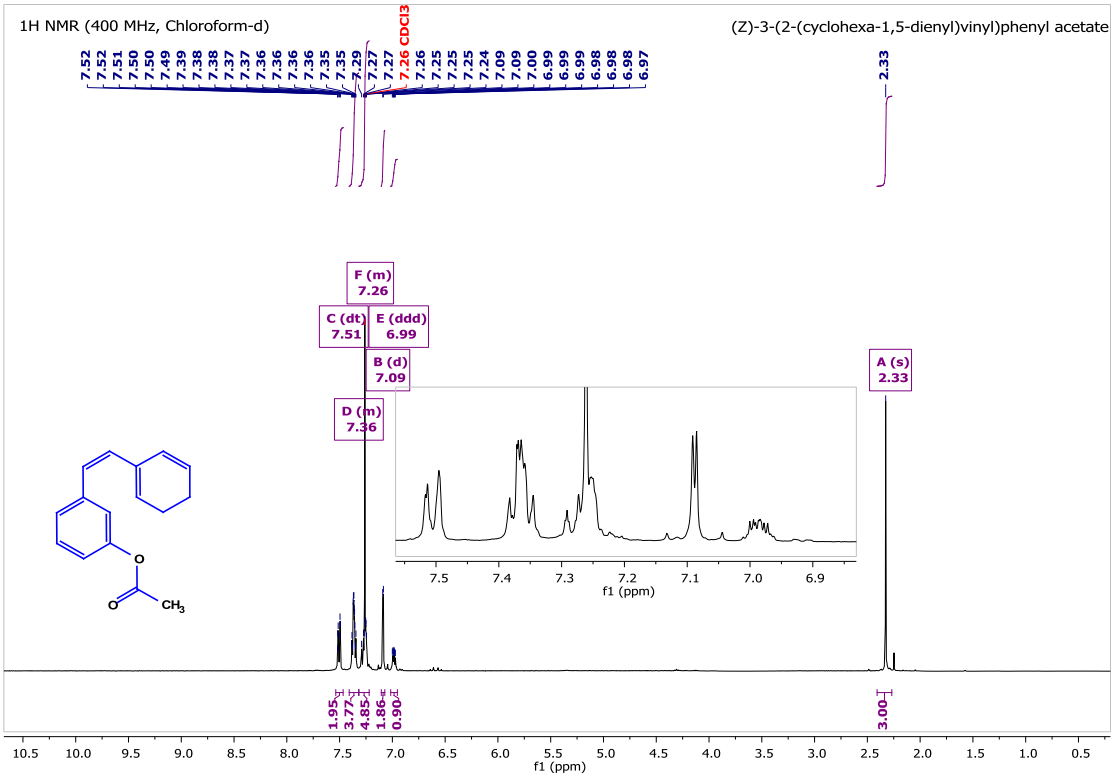


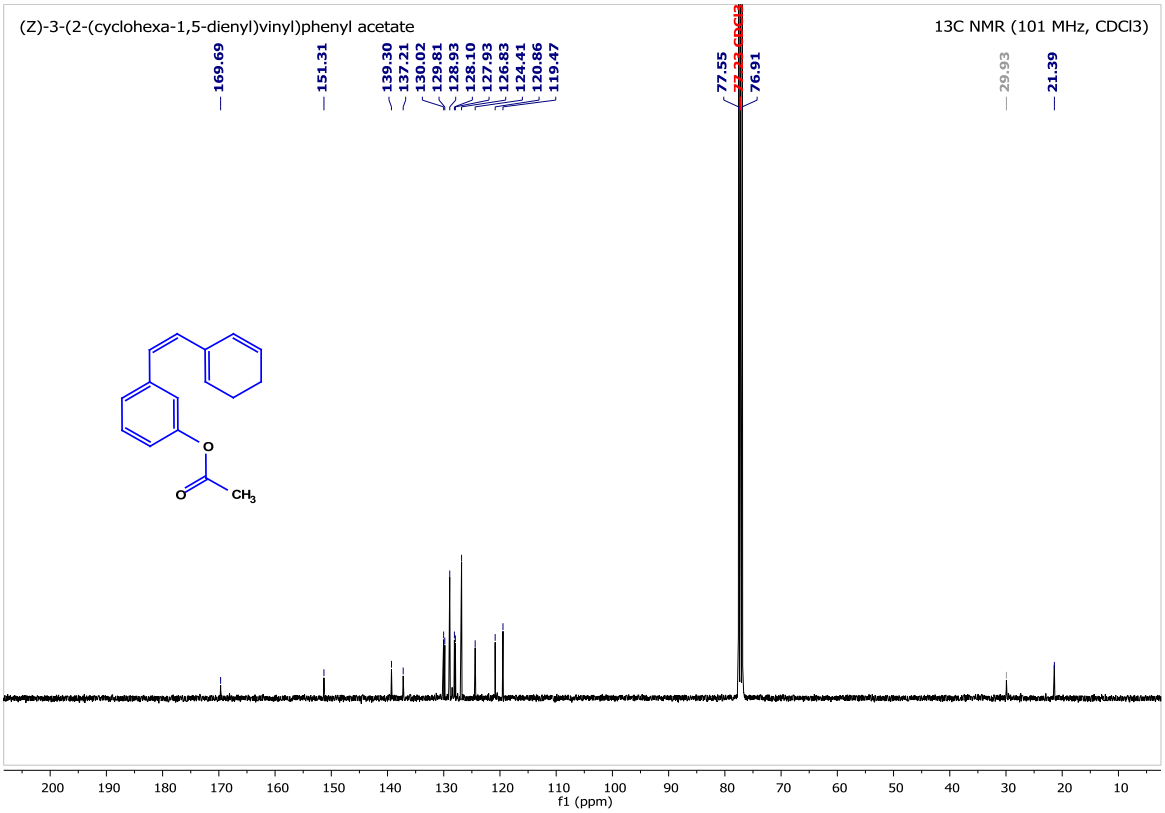
(E)-3-styrylphenyl acetate:



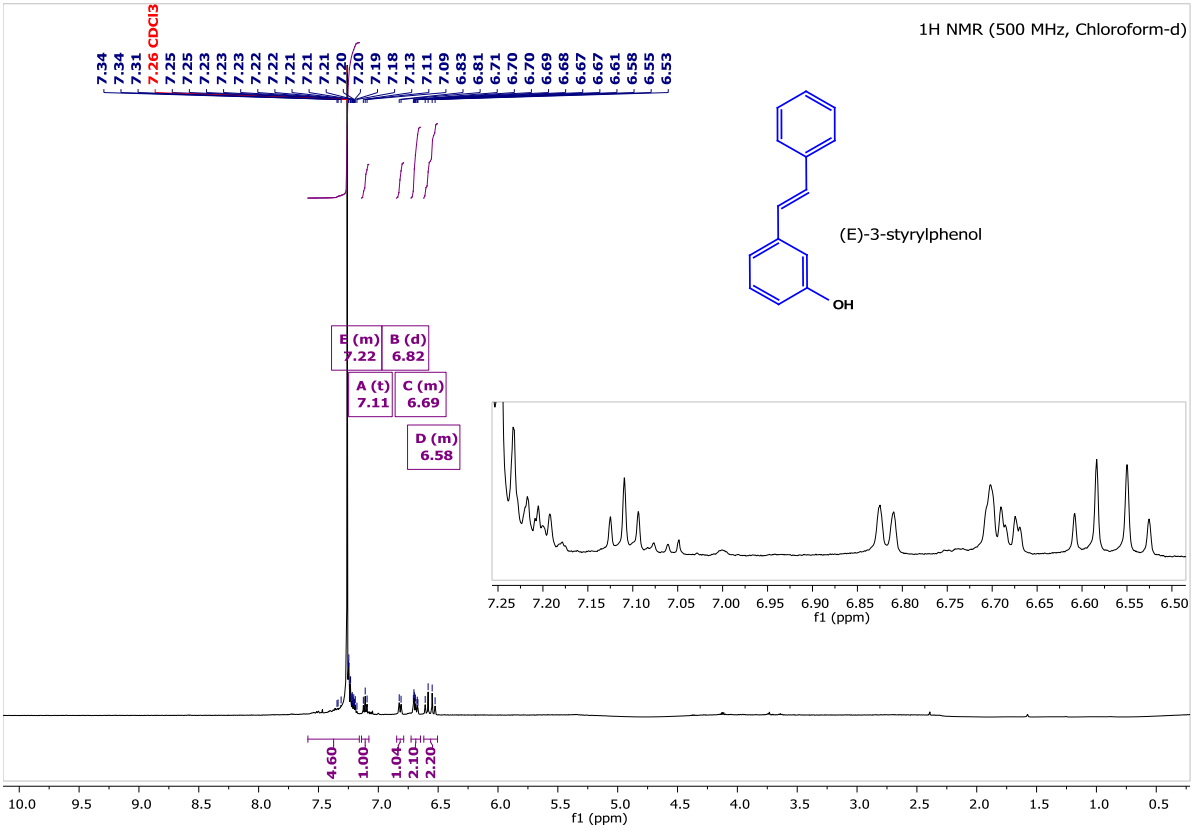


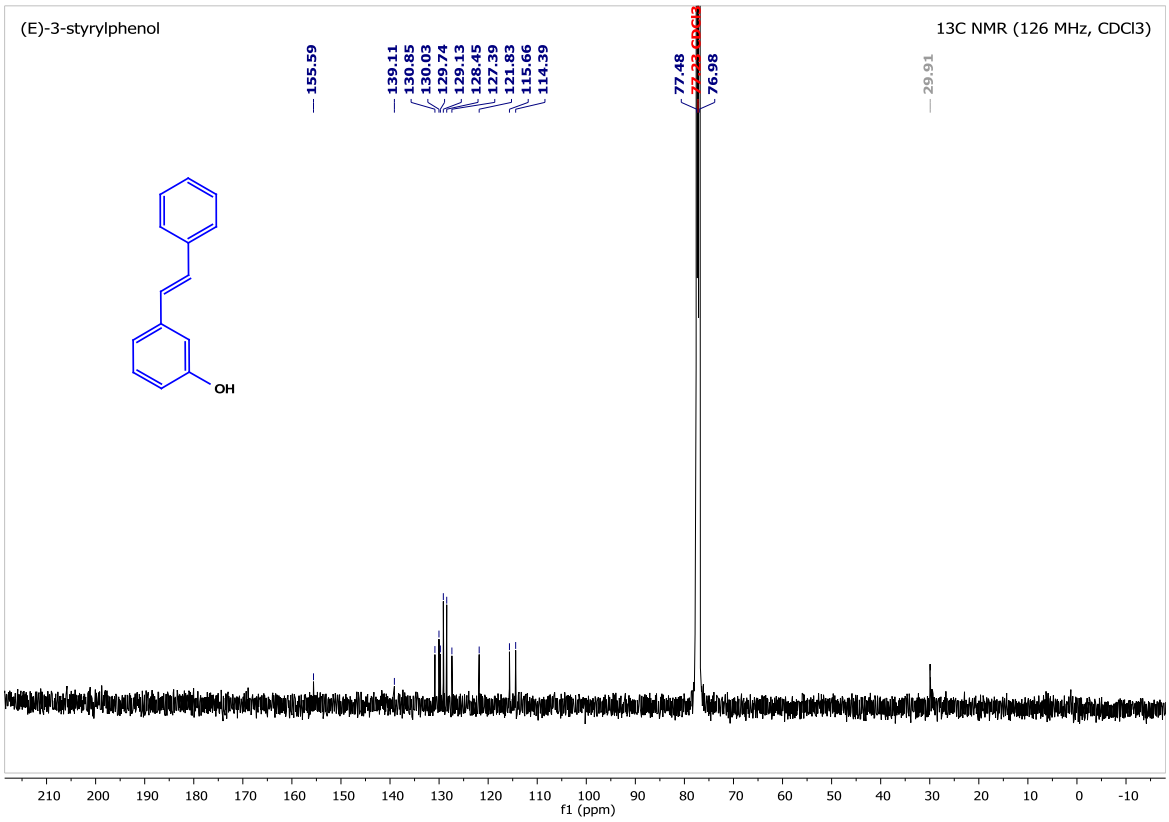
(Z)-3-(2-(cyclohexa-1,5-dienyl)vinyl)phenyl acetate:



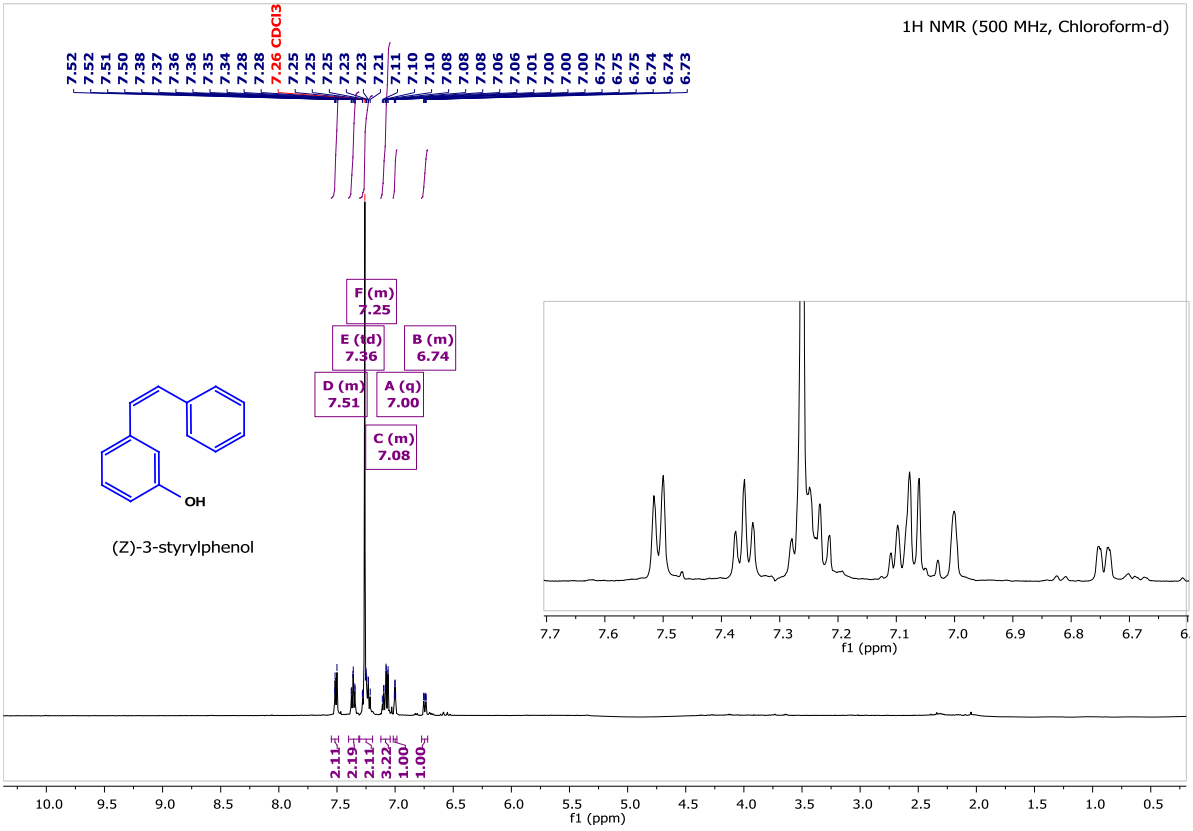


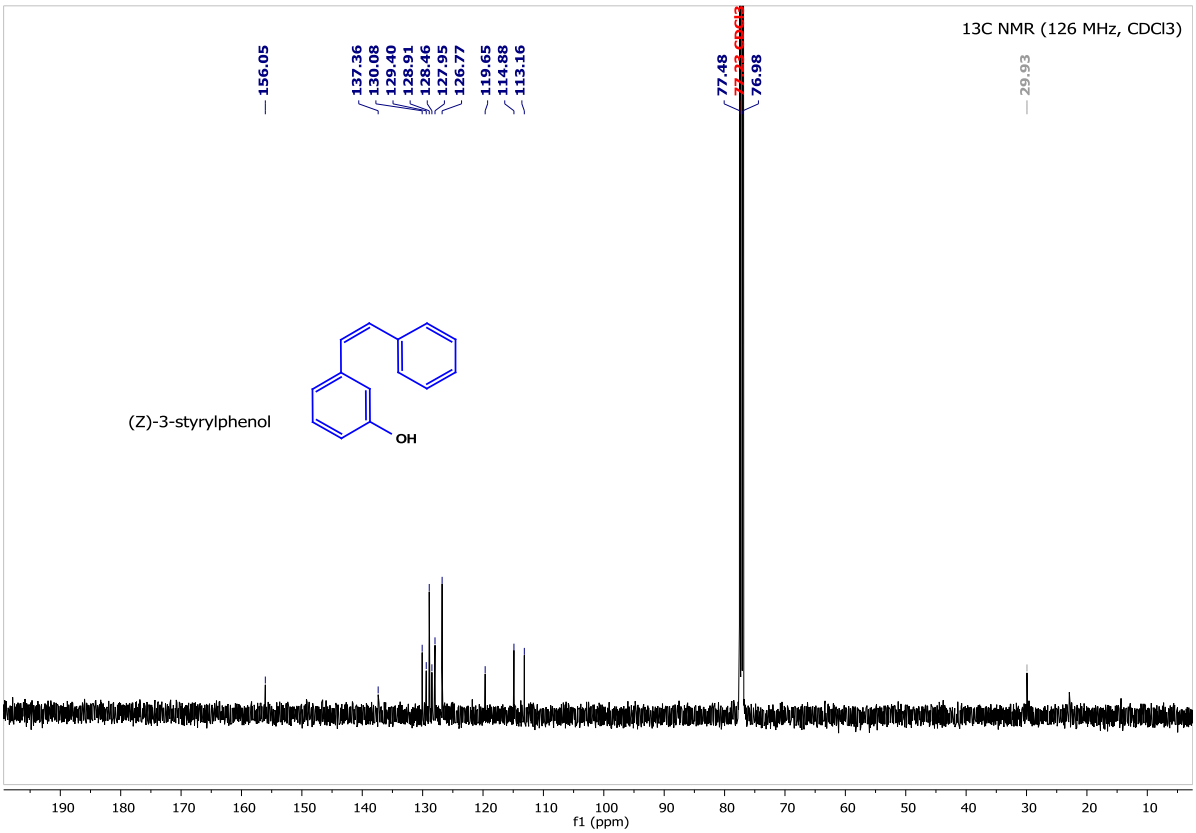
(E)-3-styrylphenol:



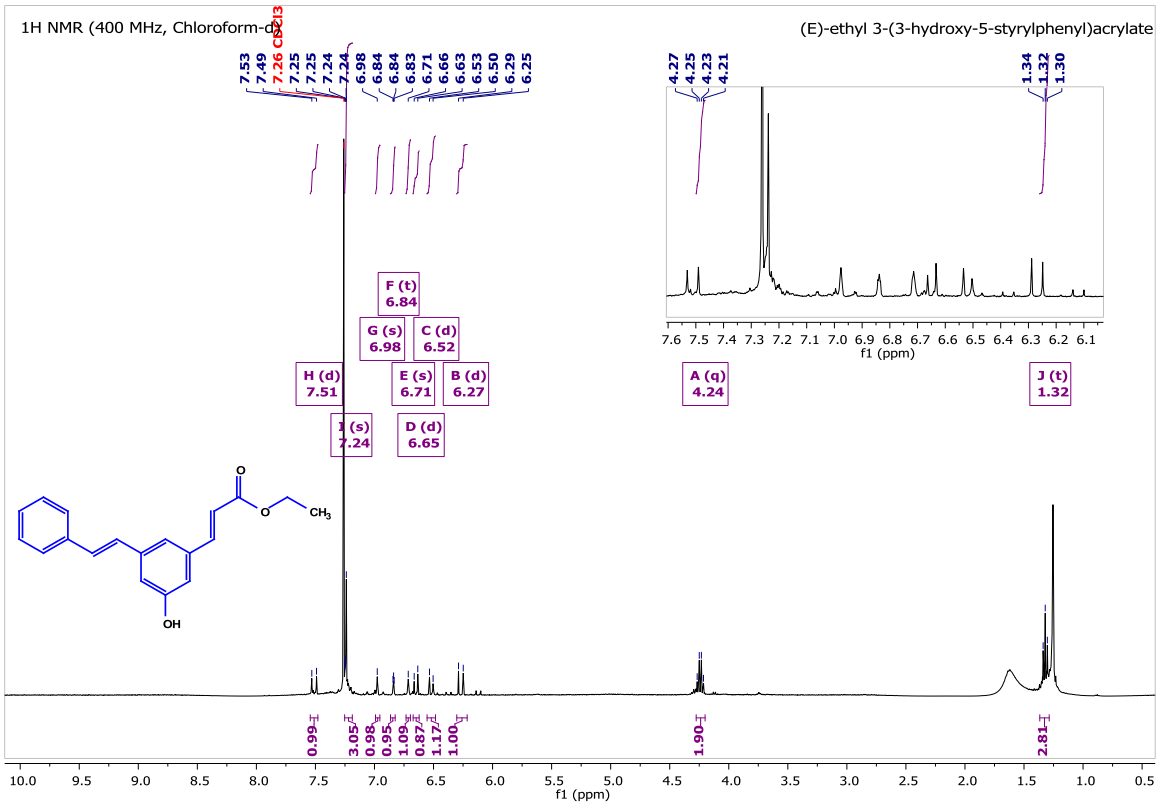


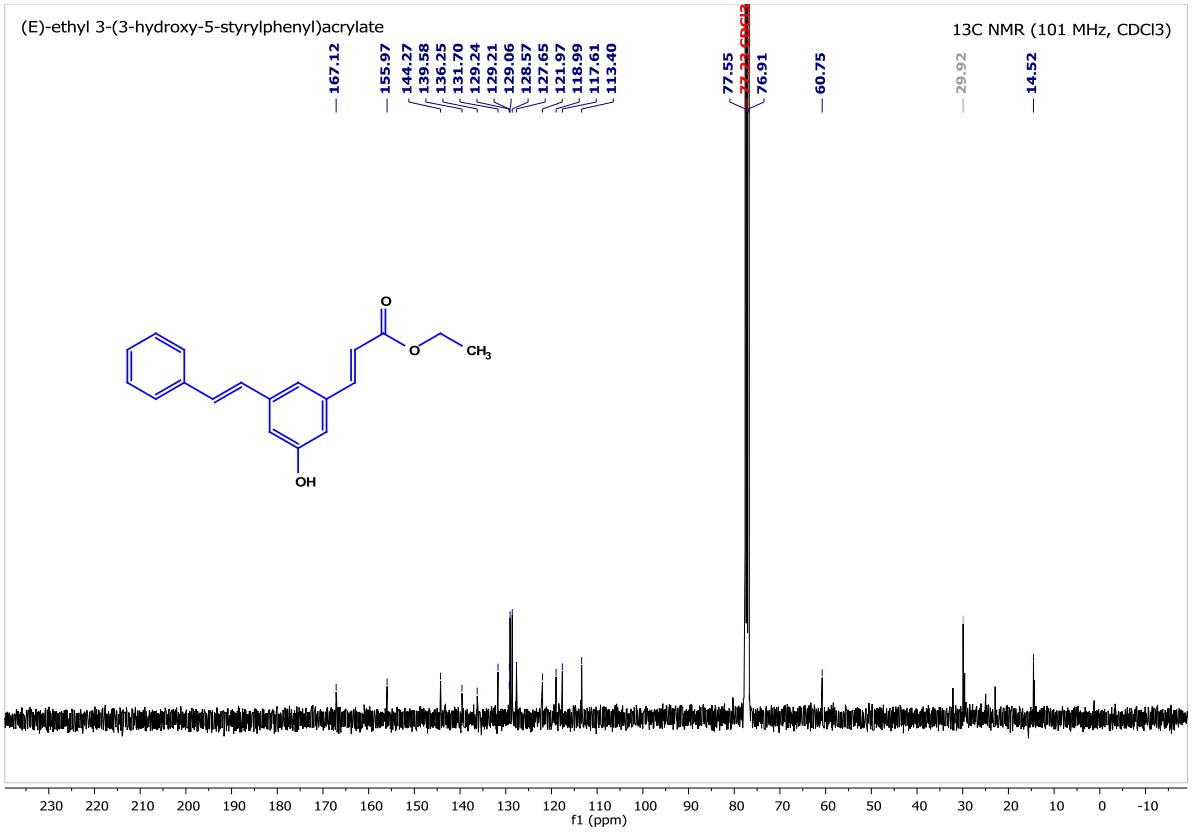
(Z)-3-styrylphenol:



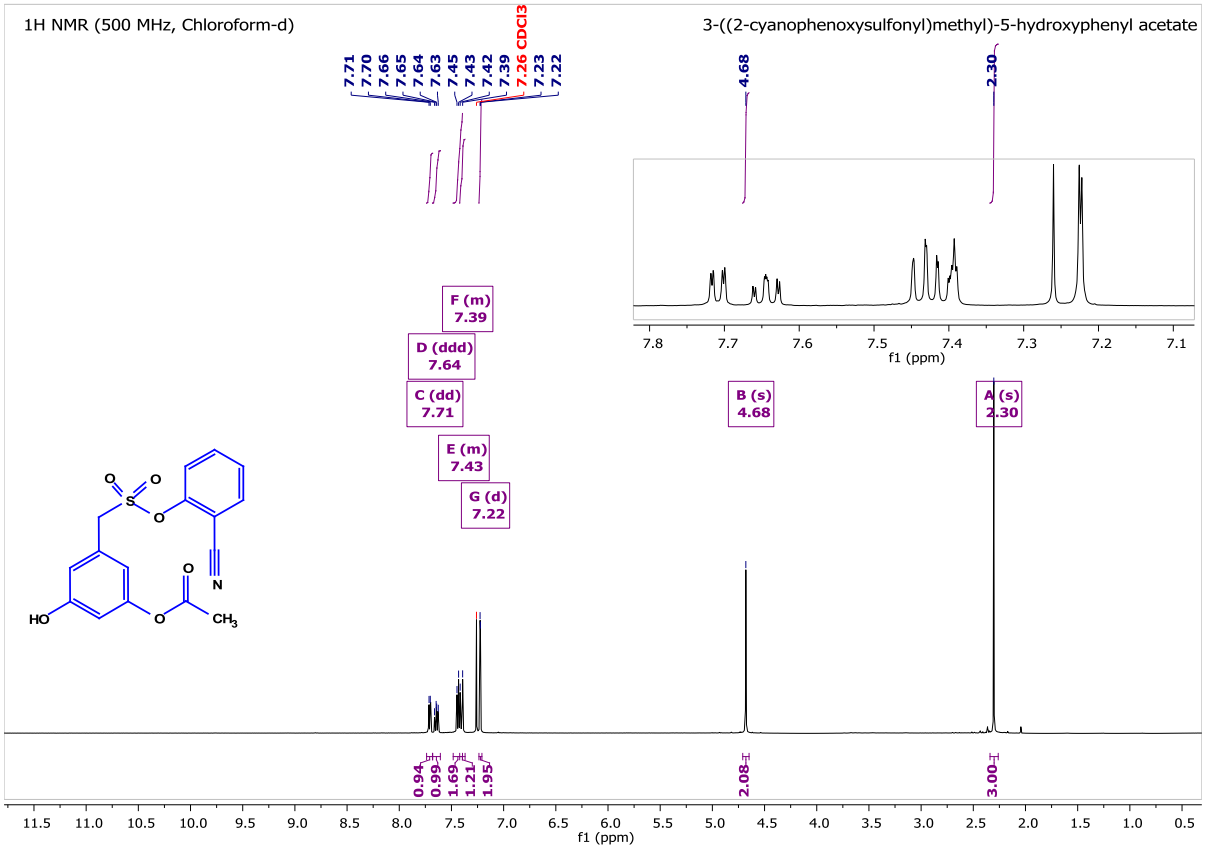


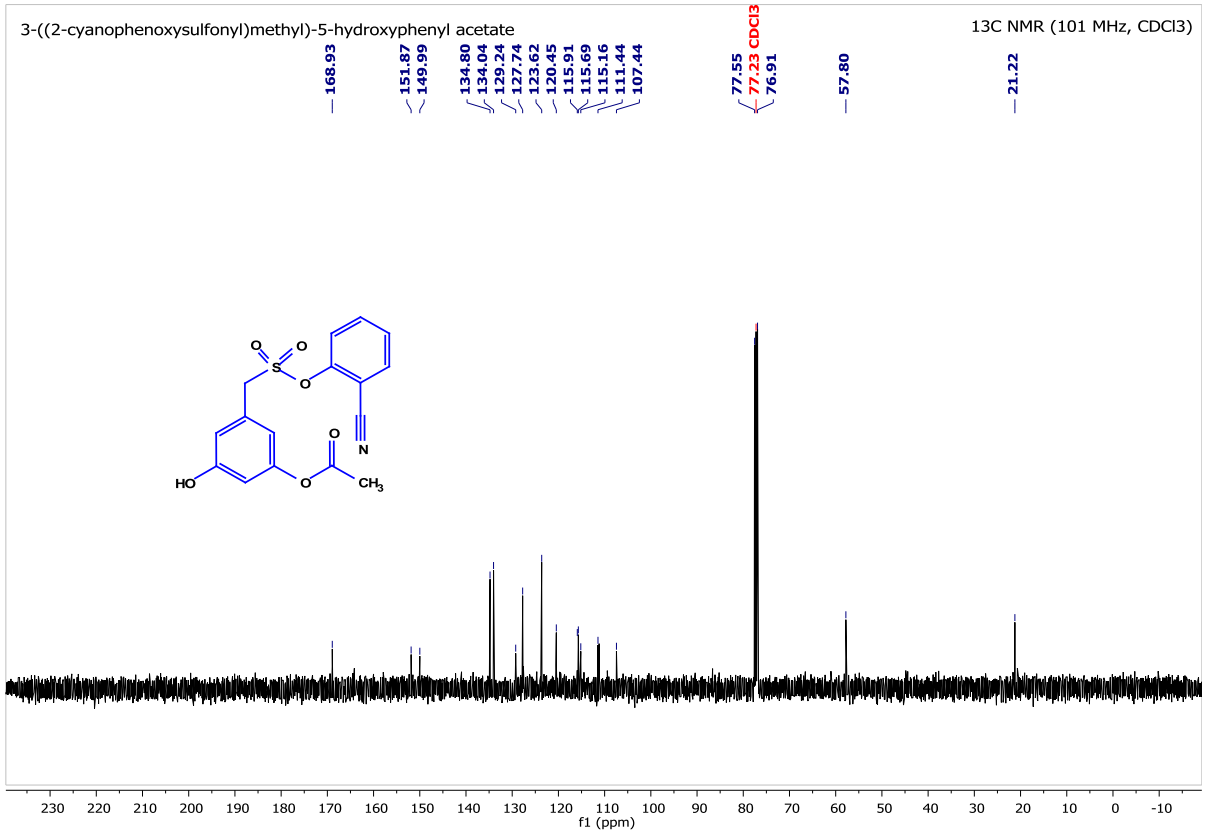
(E)-ethyl 3-(3-hydroxy-5-styrylphenyl)acrylate:



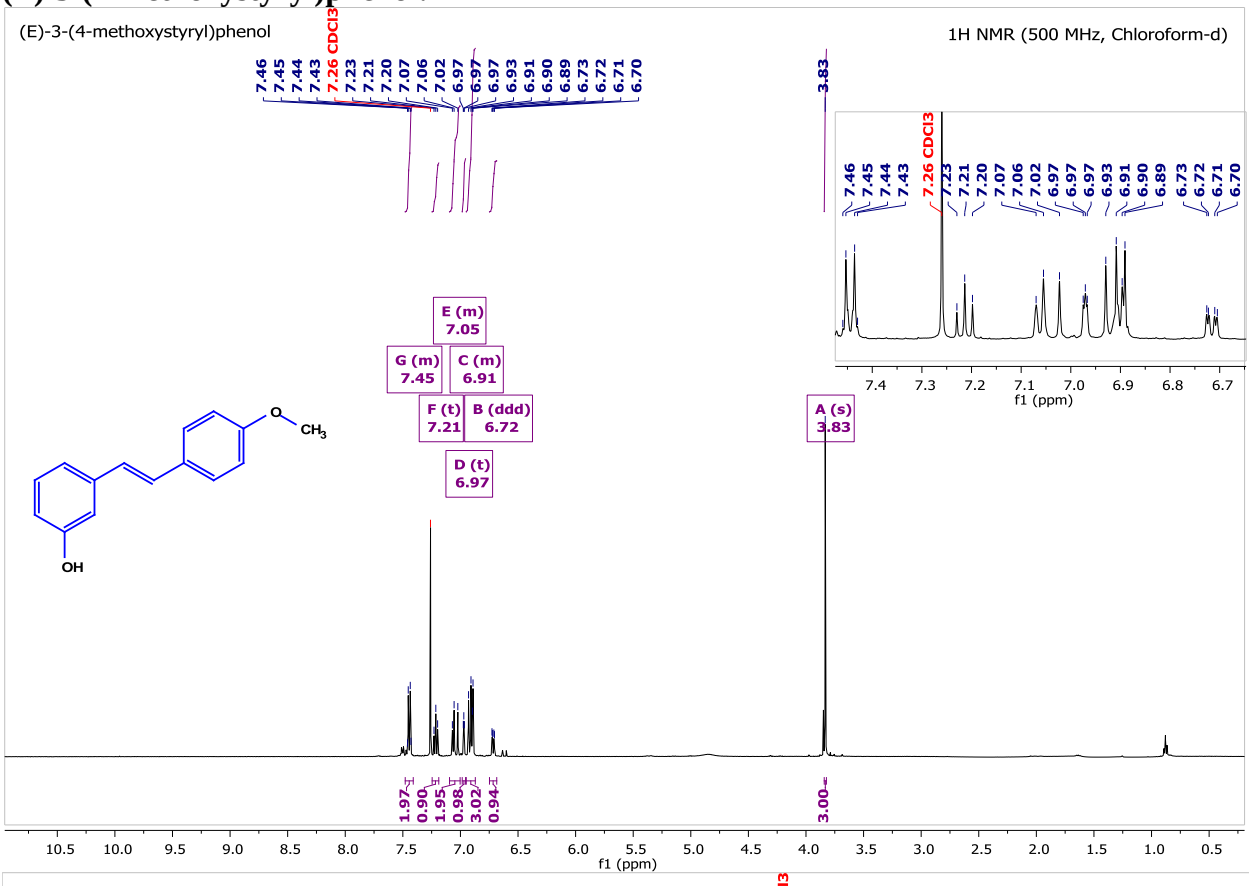


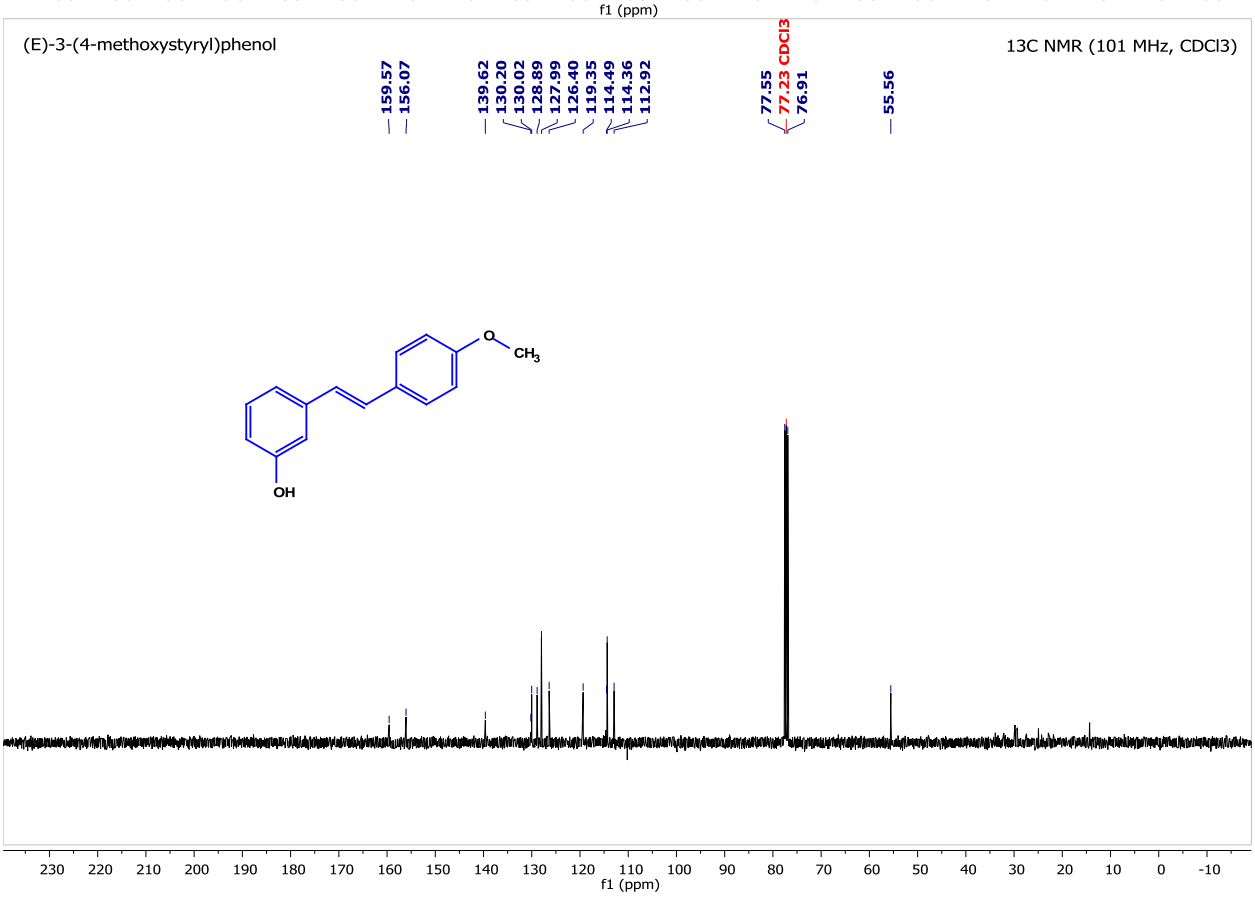
3-((2-cyanophenoxysulfonyl)methyl)-5-hydroxyphenyl acetate:

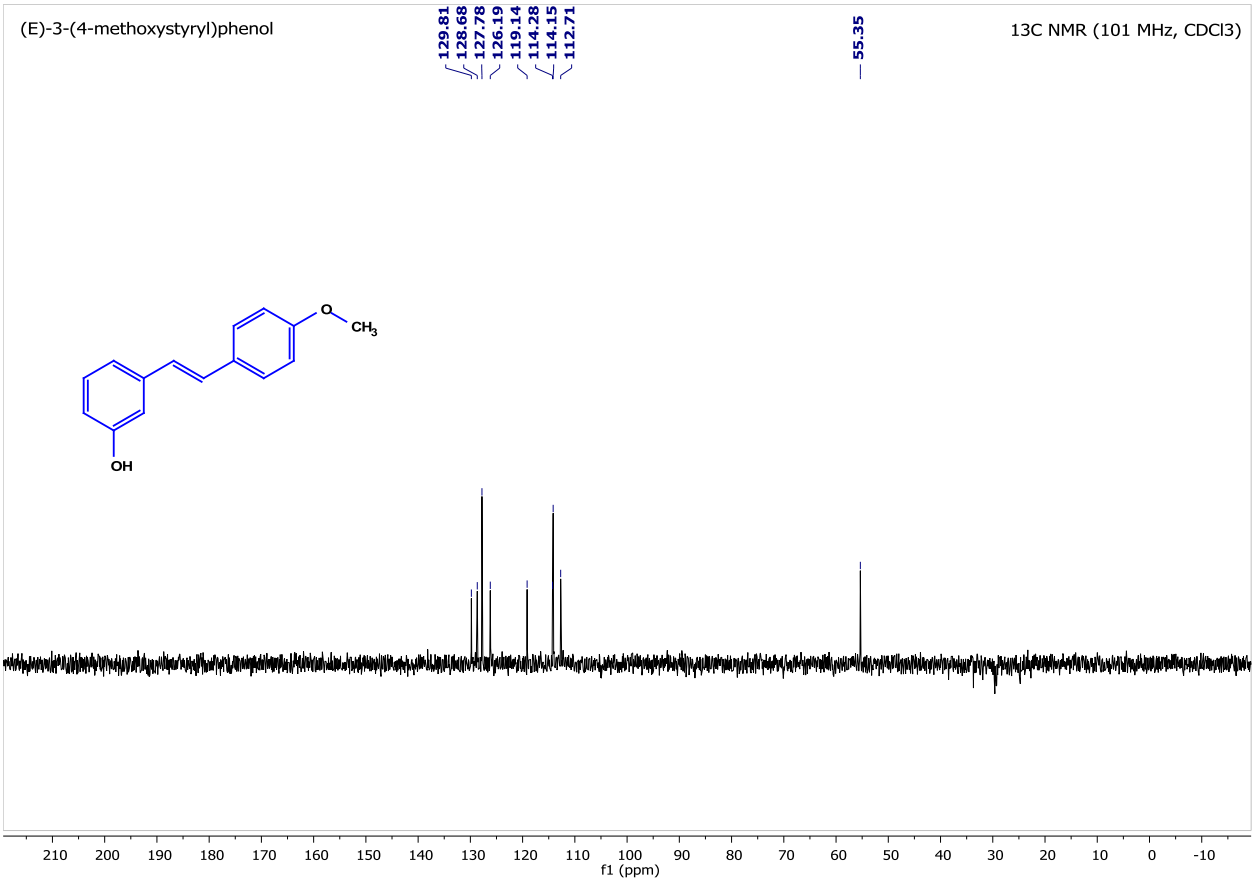


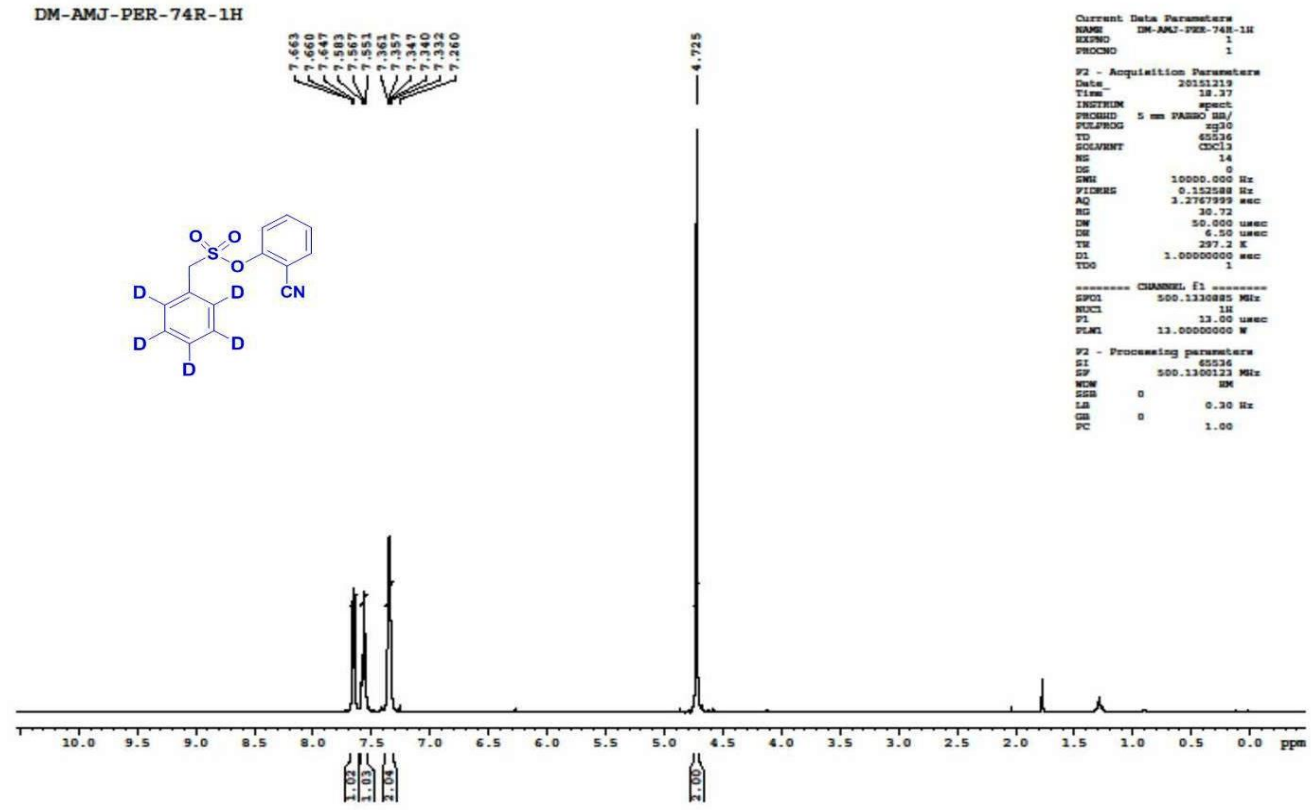


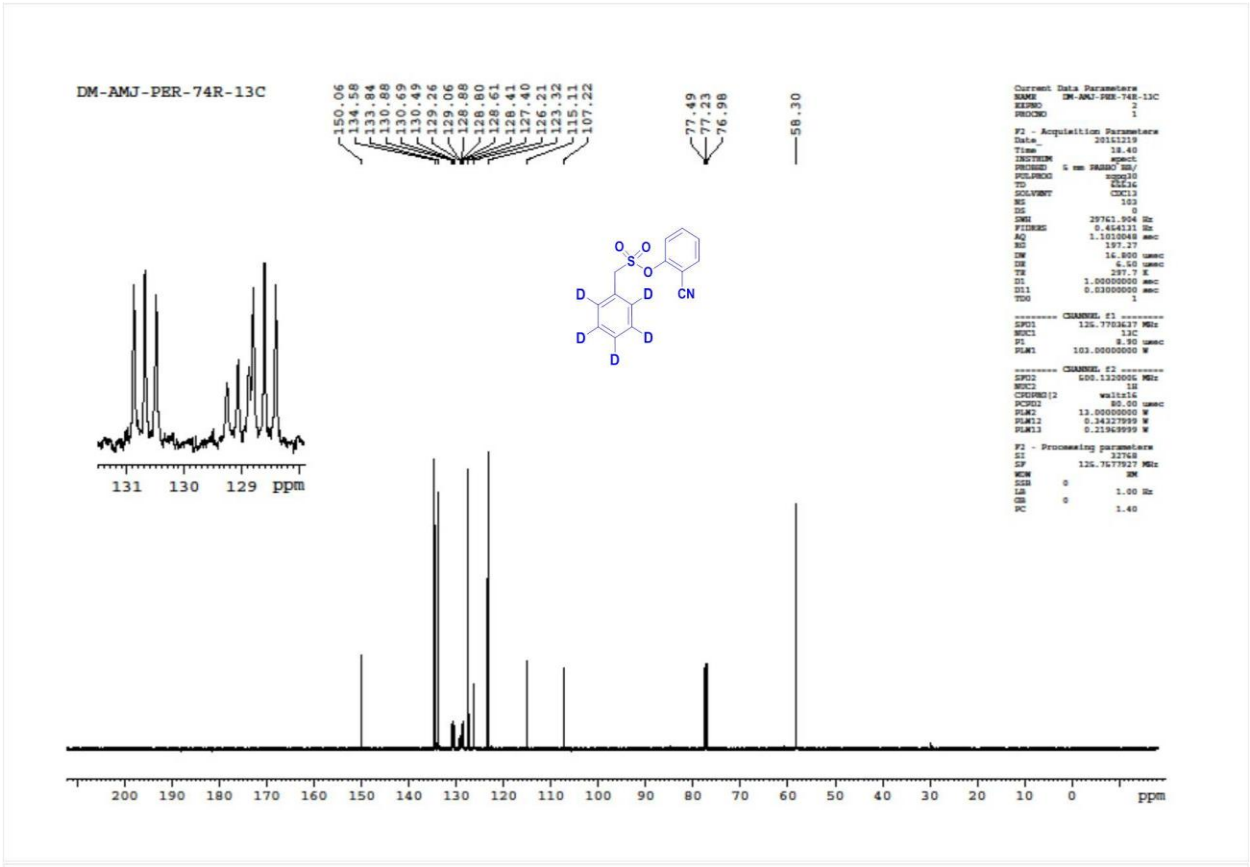
(E)-3-(4-methoxystyryl)phenol:

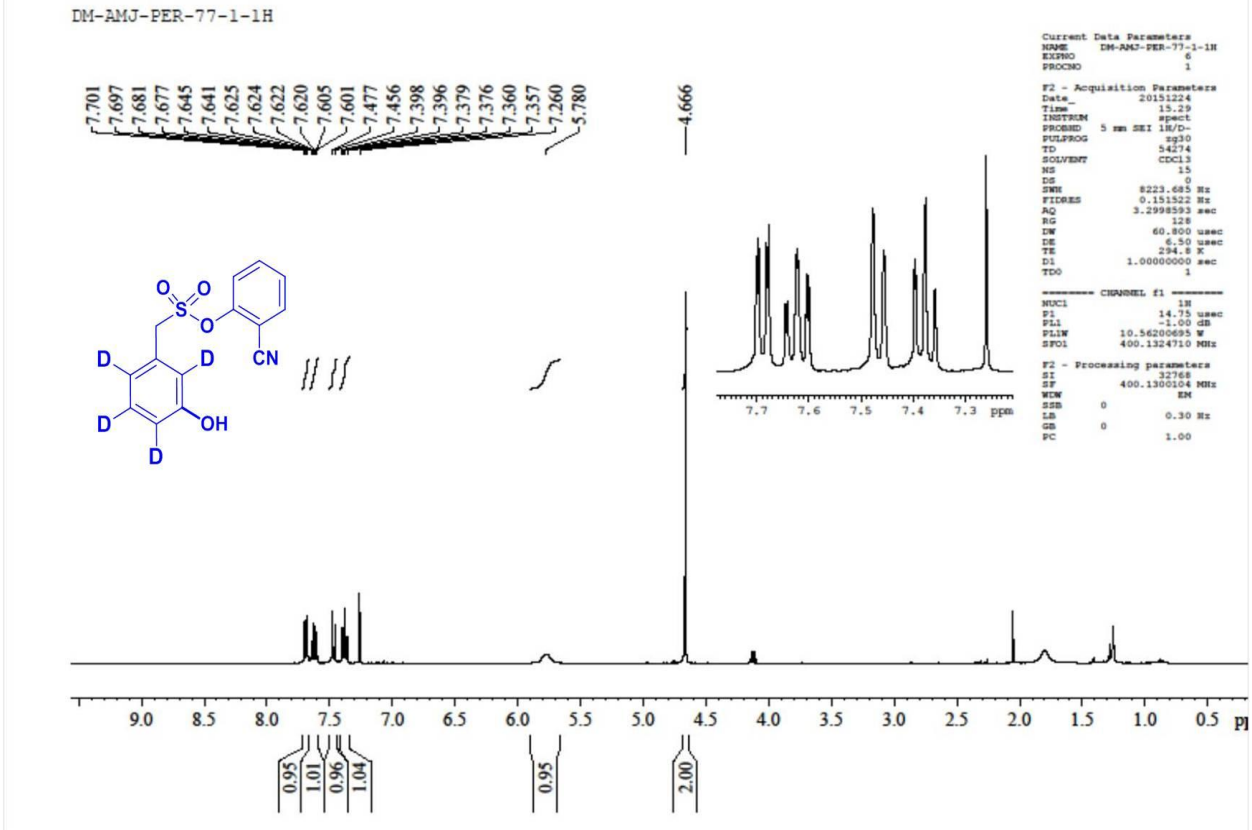


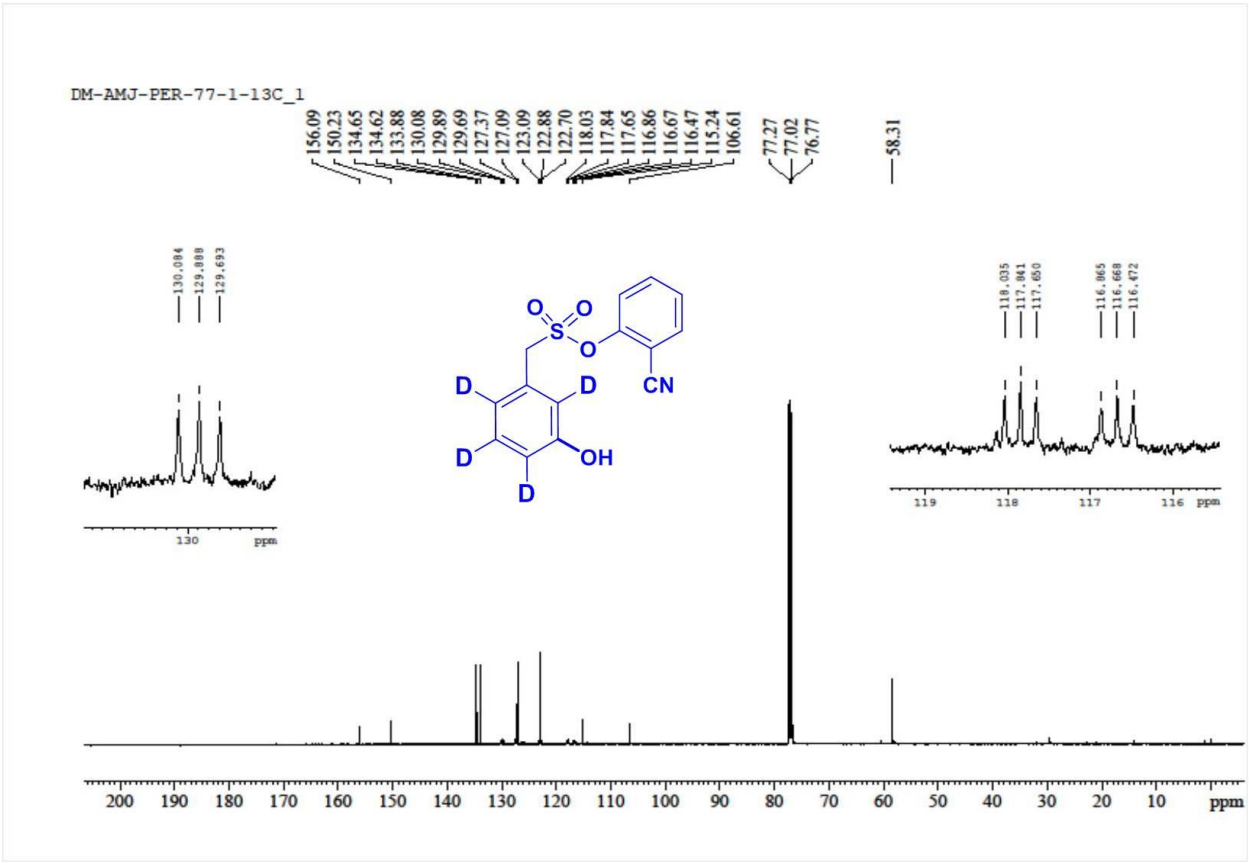



(E)-3-(4-methoxystyryl)phenol
13C NMR (101 MHz, CDCl3)
129.81
128.68
127.78
126.19
119.14
114.28
114.15
112.71
55.35
O
CH3
OH
f1 (ppm)


DM-AMJ-PER-74R-1H
7.663
7.660
7.647
7.583
7.567
7.551
7.361
7.357
7.347
7.340
7.332
7.260
4.725
O
S
O
O
CN
D
D
D
D
D
1.02
1.03
2.04
2.00
ppm


DM-AMJ-PER-74R-13C
150.06
134.58
133.84
130.88
130.69
130.49
129.26
129.06
128.88
128.80
128.61
128.41
127.40
126.21
123.32
115.11
107.22
77.49
77.23
76.98
58.30
131 130 129 ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


DM-AMJ-PER-77-1-1H
7.701
7.697
7.681
7.677
7.645
7.641
7.625
7.624
7.622
7.620
7.605
7.601
7.477
7.456
7.398
7.396
7.379
7.376
7.360
7.357
7.260
5.780
4.666
7.7 7.6 7.5 7.4 7.3 ppm
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
0.95
1.01
0.96
1.04
0.95
2.00


DM-AMJ-PER-77-1-13C_1
156.09
150.23
134.65
134.62
133.88
130.08
129.89
129.69
127.37
127.09
123.09
122.88
122.70
118.03
117.84
117.65
116.86
116.67
116.47
115.24
106.61
77.27
77.02
76.77
58.31
130.084
129.888
129.693
118.035
117.841
117.650
116.865
116.668
116.472
O
O
S
O
CN
D
D
D
OH
D
130
ppm
119
118
117
116
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

XIV. Cartesian Coordinates of the Optimized Geometries at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**,LANL2DZ(Pd) Level of Theory

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(II) Hydroxylation product using N-Formyl-Glycine

Substrate **(1)**

Number of imaginary frequencies : 0

Electronic energy : =-1218.0961336
Zero-point correction= 0.223003
Thermal correction to Energy= 0.239094
Thermal correction to Enthalpy= 0.240038
Thermal correction to Gibbs Free Energy= 0.177894
Sum of electronic and zero-point Energies= -1217.873131
Sum of electronic and thermal Energies= -1217.857040
Sum of electronic and thermal Enthalpies= -1217.856096
Sum of electronic and thermal Free Energies= -1217.918239

.....

Cartesian Coordinates

.....

6	2.396255	1.417286	-0.021171
6	2.451714	0.110423	0.467194
6	3.432837	-0.764415	-0.003253
6	4.353050	-0.332483	-0.952043
6	4.297847	0.973077	-1.433310
6	3.320789	1.848538	-0.965825
1	1.625145	2.093096	0.349187
1	3.473968	-1.783539	0.378757
1	5.116733	-1.016601	-1.315131
1	5.020685	1.311137	-2.172648
1	3.278111	2.869487	-1.338337
6	1.447974	-0.349507	1.475556
1	0.965368	0.477796	2.010786
1	1.866003	-1.048230	2.212183
16	0.094168	-1.267793	0.747080
8	0.573031	-2.415669	-0.005123
8	-0.975330	-1.443078	1.716868
8	-0.399617	-0.137516	-0.351666
6	-1.764793	-0.025466	-0.568497
6	-2.397775	-0.839762	-1.488950
6	-2.465579	0.961124	0.135583
6	-3.759421	-0.657456	-1.717774
1	-1.824030	-1.596584	-2.018290
6	-3.830923	1.137867	-0.106419
6	-4.470467	0.325939	-1.033940

1	-4.267382	-1.290732	-2.440354
1	-4.373952	1.906825	0.436054
1	-5.531639	0.460796	-1.223908
6	-1.754562	1.746570	1.090198
7	-1.140290	2.365846	1.860528

$[Pd(OAc)_2]_3$

Total Energy (SMD/M06/6-31G**)= -1750.60789606

Number of imaginary frequencies : 0

Electronic energy : =-1750.5747527
Zero-point correction= 0.315721
Thermal correction to Energy= 0.349705
Thermal correction to Enthalpy= 0.350649
Thermal correction to Gibbs Free Energy= 0.246602
Sum of electronic and zero-point Energies= -1750.259032
Sum of electronic and thermal Energies= -1750.225048
Sum of electronic and thermal Enthalpies= -1750.224104
Sum of electronic and thermal Free Energies= -1750.328150

Cartesian Coordinates

46	1.559037	0.928514	-0.001488
8	2.288923	0.035247	-1.687034
8	2.647809	-0.307202	1.230488
6	2.237849	-1.316722	1.863936
8	1.167662	-1.961746	1.678836
46	0.023733	-1.809013	-0.005073
6	2.293810	-1.213956	-1.872974
8	1.643990	-2.088612	-1.240602
8	1.121000	1.989958	1.685653
8	0.987212	2.468094	-1.238768
6	-0.097355	2.595324	-1.866543
8	-1.177725	1.970204	-1.674795
46	-1.584818	0.884530	0.004864
6	0.023813	2.584005	1.881424
8	-1.056834	2.431774	1.252415
8	-2.292781	-0.036952	1.684456
8	-2.637838	-0.371229	-1.237573
6	-2.258257	-1.285446	1.868666
6	-2.201320	-1.367910	-1.873886

8	-1.586272	-2.139520	1.230445
8	-1.115966	-1.986972	-1.689102
6	3.211147	-1.714141	-2.954887
1	4.199552	-1.887537	-2.516001
1	2.841563	-2.655565	-3.365126
1	3.317396	-0.959703	-3.737086
6	-0.122286	3.635851	-2.952546
1	-0.414387	4.592792	-2.507050
1	0.869108	3.748845	-3.395060
1	-0.863046	3.373594	-3.710443
6	0.023207	3.615209	2.976519
1	-0.981076	3.739542	3.385116
1	0.731778	3.332597	3.757816
1	0.350769	4.570525	2.552863
6	-3.146918	-1.821609	2.957425
1	-2.653970	-2.649810	3.470838
1	-3.413998	-1.029045	3.658558
1	-4.064063	-2.205104	2.497903
6	-3.092000	-1.901618	-2.962005
1	-3.830496	-2.570373	-2.507229
1	-3.626655	-1.083012	-3.447853
1	-2.508404	-2.473334	-3.685744
6	3.143996	-1.833103	2.947659
1	3.668480	-1.005122	3.428560
1	2.574299	-2.412786	3.676207
1	3.889791	-2.491572	2.489745

N-For-Gly

Number of imaginary frequencies : 0

Electronic energy : =-397.5717136
Zero-point correction= 0.088821
Thermal correction to Energy= 0.096178
Thermal correction to Enthalpy= 0.097122
Thermal correction to Gibbs Free Energy= 0.056113
Sum of electronic and zero-point Energies= -397.482893
Sum of electronic and thermal Energies= -397.475536
Sum of electronic and thermal Enthalpies= -397.474592
Sum of electronic and thermal Free Energies= -397.515600

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Cartesian Coordinates

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7	0.075654	-0.233294	0.062559

1	-0.268678	-1.186697	0.073135
6	-0.884286	0.830975	0.041663
1	-0.816441	1.481019	0.929056
6	-2.271753	0.288369	-0.015970
8	-2.529084	-0.896892	-0.041900
1	-0.748153	1.498169	-0.824122
1	-3.067250	1.060300	-0.031344
6	1.397887	0.014512	0.000651
8	1.899428	1.128317	-0.047066
8	2.113465	-1.125022	0.001051
1	3.049386	-0.874096	-0.039383

AcOH

Number of imaginary frequencies : 0

Electronic energy : =-228.973358
Zero-point correction= 0.061755
Thermal correction to Energy= 0.066344
Thermal correction to Enthalpy= 0.067289
Thermal correction to Gibbs Free Energy= 0.034174
Sum of electronic and zero-point Energies= -228.911603
Sum of electronic and thermal Energies= -228.907014
Sum of electronic and thermal Enthalpies= -228.906069
Sum of electronic and thermal Free Energies= -228.939184

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Cartesian Coordinates

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6	-0.089900	0.118233	-0.000056
8	-0.644338	1.198143	-0.000018
8	-0.767747	-1.038308	0.000092
1	-1.716940	-0.826283	0.000194
6	1.383562	-0.105757	-0.000061
1	1.671047	-0.688063	0.881716
1	1.670927	-0.689146	-0.881153
1	1.909673	0.849956	-0.000651

HFIP (solvent)

Number of imaginary frequencies : 0

Electronic energy : =-789.5311222
Zero-point correction= 0.063551
Thermal correction to Energy= 0.072449
Thermal correction to Enthalpy= 0.073393
Thermal correction to Gibbs Free Energy= 0.028814
Sum of electronic and zero-point Energies= -789.467571
Sum of electronic and thermal Energies= -789.458673
Sum of electronic and thermal Enthalpies= -789.457729
Sum of electronic and thermal Free Energies= -789.502308

.....

Cartesian Coordinates

.....

6	1.274823	-0.144021	-0.040740
6	0.000971	0.547974	-0.501249
6	-1.270207	-0.152131	-0.035530
1	0.001152	0.519453	-1.599841
9	2.330200	0.459895	-0.586831
9	1.296848	-1.426409	-0.407387
9	1.418597	-0.090763	1.283074
9	-1.401520	-1.366127	-0.570712
9	-1.310636	-0.278914	1.291263
9	-2.328133	0.574043	-0.406507
8	0.039308	1.835320	0.027876
1	-0.397338	2.441536	-0.584135

N-H activation

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[a]

Number of imaginary frequencies : 0

Electronic energy : =-981.1028259
Zero-point correction= 0.195257
Thermal correction to Energy= 0.213552
Thermal correction to Enthalpy= 0.214496
Thermal correction to Gibbs Free Energy= 0.147534
Sum of electronic and zero-point Energies= -980.907569
Sum of electronic and thermal Energies= -980.889274
Sum of electronic and thermal Enthalpies= -980.888330
Sum of electronic and thermal Free Energies= -980.955292

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Cartesian Coordinates

.....

46	-0.084926	-0.112912	0.091553
8	2.721618	-0.656196	-1.215826
6	3.182274	-2.844779	-0.402000
6	2.330156	-1.611767	-0.532152
8	1.218713	-1.665523	0.129301
6	0.607233	2.569216	-0.706279
6	-0.875228	2.582928	-0.384417
8	-1.366837	1.466512	0.094026
8	-1.549239	3.575969	-0.589515
1	1.064706	3.511191	-0.385711
1	0.711212	2.503441	-1.793927
1	4.063289	-2.594249	0.199828
1	2.650548	-3.671996	0.072566
1	3.536690	-3.145517	-1.392710
7	1.316111	1.413939	-0.116411
1	2.003136	0.921456	-0.724795
6	1.816542	1.582686	1.204052
8	2.735750	0.935408	1.635045
6	-2.787039	-1.441570	0.105535
6	-3.716349	-2.596767	0.139992
1	-4.428591	-2.523729	-0.687103
1	-3.164532	-3.536018	0.091150
1	-4.290846	-2.557185	1.072294
8	-1.561390	-1.604464	0.237527
8	-3.365880	-0.286215	-0.057062
1	-2.721967	0.472776	-0.039476
1	1.262741	2.352614	1.774963

[a-b] ‡

Number of imaginary frequencies : 1
The smallest frequency is : -1173.4268 cm(-1)

Electronic energy : =-981.0962686
Zero-point correction= 0.190264
Thermal correction to Energy= 0.208116
Thermal correction to Enthalpy= 0.209060
Thermal correction to Gibbs Free Energy= 0.143255
Sum of electronic and zero-point Energies= -980.906005
Sum of electronic and thermal Energies= -980.888152
Sum of electronic and thermal Enthalpies= -980.887208
Sum of electronic and thermal Free Energies= -980.953014
.....

Cartesian Coordinates

46	-0.102869	-0.131229	0.117887
8	2.770138	-0.599517	-0.974746
6	3.075585	-2.922382	-0.638580
6	2.277922	-1.664398	-0.508156
8	1.142490	-1.759421	0.062809
6	0.806489	2.398993	-0.786908
6	-0.669506	2.575611	-0.476604
8	-1.256307	1.538778	0.079480
8	-1.263195	3.603788	-0.748303
1	1.342322	3.331359	-0.573047
1	0.899526	2.209314	-1.862442
1	4.058146	-2.774231	-0.179258
1	2.570141	-3.770830	-0.174705
1	3.240711	-3.126555	-1.701986
7	1.398570	1.267608	-0.058749
1	2.100099	0.468175	-0.608590
6	1.907493	1.565044	1.216492
8	2.473642	0.751358	1.910421
6	-2.887861	-1.272496	0.095717
6	-3.899356	-2.356633	0.138530
1	-4.629266	-2.219481	-0.664282
1	-3.419591	-3.332788	0.059833
1	-4.440058	-2.291571	1.089654
8	-1.677180	-1.524422	0.220628
8	-3.380726	-0.076573	-0.063283
1	-2.682237	0.632517	-0.052851
1	1.766687	2.622983	1.517121

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[b]

Number of imaginary frequencies : 0

Electronic energy : =-981.1041413
Zero-point correction= 0.195010
Thermal correction to Energy= 0.213352
Thermal correction to Enthalpy= 0.214296
Thermal correction to Gibbs Free Energy= 0.146695
Sum of electronic and zero-point Energies= -980.909131
Sum of electronic and thermal Energies= -980.890789
Sum of electronic and thermal Enthalpies= -980.889845
Sum of electronic and thermal Free Energies= -980.957446

Cartesian Coordinates

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46	-0.096343	-0.082998	0.081721
8	2.886624	-0.522076	-1.054558
6	3.310534	-2.766406	-0.503078
6	2.405518	-1.593073	-0.484995
8	1.285616	-1.652493	0.048217
6	0.538354	2.608746	-0.618993
6	-0.960677	2.575980	-0.402266
8	-1.429817	1.434134	0.053867
8	-1.682190	3.525459	-0.653263
1	0.936780	3.555870	-0.230850
1	0.705132	2.610589	-1.705175
1	4.139356	-2.574150	0.187919
1	2.778630	-3.666290	-0.193095
1	3.737750	-2.893181	-1.502029
7	1.191097	1.461910	0.001301
1	2.277267	0.254171	-0.925170
6	2.012171	1.669197	1.060675
8	2.431812	0.802996	1.819752
6	-2.771411	-1.522406	0.105022
6	-3.670849	-2.701204	0.158321
1	-4.377900	-2.663910	-0.676079
1	-3.094200	-3.626290	0.129412
1	-4.255807	-2.659488	1.083700
8	-1.538701	-1.647668	0.165173
8	-3.391554	-0.378272	0.000562
1	-2.766159	0.396096	-0.014579
1	2.337084	2.729478	1.151554

Different Possibilities of Potential Active Catalyst at the SMD/M06/6-31G**

$Pd(OAc)_2$ with Ligand combinations: Active Catalyst

[2a]

Number of imaginary frequencies : 0

Electronic energy : =-981.0986384
Zero-point correction= 0.194720
Thermal correction to Energy= 0.213389
Thermal correction to Enthalpy= 0.214333

Thermal correction to Gibbs Free Energy= 0.145292
Sum of electronic and zero-point Energies= -980.903918
Sum of electronic and thermal Energies= -980.885249
Sum of electronic and thermal Enthalpies= -980.884305
Sum of electronic and thermal Free Energies= -980.953346

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Cartesian Coordinates

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46	1.021675	-0.226759	-0.254224
1	-0.052794	1.846547	1.281234
6	0.975905	2.759744	-0.093310
8	0.382563	2.731923	1.057807
6	1.408536	4.106449	-0.543227
1	1.886183	4.051590	-1.521772
1	0.540426	4.772352	-0.579829
1	2.108039	4.520025	0.191208
8	1.197432	1.762957	-0.807800
6	-3.150322	-0.061015	0.601253
6	-1.662723	0.186041	0.624319
8	-1.014110	-0.196653	-0.411714
8	-1.179878	0.743894	1.623805
1	-3.645382	0.920161	0.622171
1	-3.417428	-0.559164	1.542936
7	-3.578734	-0.834250	-0.538587
1	-2.877580	-1.156621	-1.194904
6	-4.871941	-1.142528	-0.723739
8	-5.778761	-0.797082	0.027224
6	2.622075	-2.018039	0.173255
8	3.012276	-0.824517	-0.051360
6	3.568849	-3.129593	0.389986
1	3.159182	-3.838526	1.114771
1	3.711441	-3.658706	-0.559624
1	4.535535	-2.748081	0.727570
8	1.356319	-2.212949	0.175080
1	-5.042524	-1.745862	-1.634879

[2b]

Number of imaginary frequencies : 0

Electronic energy : =-752.1084531
Zero-point correction= 0.131742
Thermal correction to Energy= 0.144562
Thermal correction to Enthalpy= 0.145506

Thermal correction to Gibbs Free Energy= 0.090919
Sum of electronic and zero-point Energies= -751.976711
Sum of electronic and thermal Energies= -751.963891
Sum of electronic and thermal Enthalpies= -751.962947
Sum of electronic and thermal Free Energies= -752.017534

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Cartesian Coordinates

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46	-0.170506	-0.299151	0.000005
6	2.620945	0.588724	0.000061
6	2.605734	-0.924301	-0.000025
8	1.437563	-1.504843	0.000014
8	3.655799	-1.551328	-0.000070
1	3.170266	0.929804	-0.885896
7	1.259581	1.116360	0.000035
6	1.037512	2.377954	0.000021
8	-0.145751	2.937105	-0.000017
8	-1.996605	0.697286	-0.000113
6	-2.634325	-0.418923	-0.000043
8	-1.944126	-1.481847	0.000037
6	-4.113923	-0.427332	0.000041
1	-4.495083	-1.450334	-0.000500
1	-4.479419	0.108385	-0.882495
1	-4.479329	0.107409	0.883211
1	-0.872704	2.277810	-0.000120
1	3.170148	0.929664	0.886148
1	1.861635	3.095970	0.000039

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[2]

Number of imaginary frequencies : 0

Electronic energy : =-1541.6718995
Zero-point correction= 0.197400
Thermal correction to Energy= 0.220111
Thermal correction to Enthalpy= 0.221055
Thermal correction to Gibbs Free Energy= 0.141693
Sum of electronic and zero-point Energies= -1541.474500
Sum of electronic and thermal Energies= -1541.451788
Sum of electronic and thermal Enthalpies= -1541.450844
Sum of electronic and thermal Free Energies= -1541.530206

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Cartesian Coordinates

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46	-0.995059	-0.016680	-0.271430
6	-2.912384	-2.212945	-0.108610
6	-3.677629	-0.929948	0.130404
8	-2.977450	0.175576	0.094089
8	-4.879502	-0.948756	0.335252
1	-3.340569	-2.689960	-0.999415
1	-3.091880	-2.882465	0.741456
7	-1.482708	-1.971653	-0.292642
6	-0.675392	-2.969844	-0.397897
8	0.603925	-2.878269	-0.584105
8	0.966790	-0.356937	-0.723472
1	0.886976	-1.901330	-0.658798
6	1.920438	0.292524	0.027882
6	3.195899	0.323119	-0.810882
6	2.135714	-0.381926	1.381894
1	1.665993	1.344470	0.245123
9	3.550909	-0.896747	-1.222131
9	2.996142	1.070661	-1.897843
9	4.228630	0.844427	-0.143882
9	2.668412	-1.602209	1.259586
9	2.935371	0.335505	2.172799
9	0.965667	-0.522876	2.015739
8	-0.561069	2.044468	-0.177859
6	-1.365193	2.970015	0.027841
8	-2.642988	2.807203	0.223702
6	-0.910127	4.380250	0.083493
1	-1.534348	4.995812	-0.571272
1	-1.043584	4.752315	1.105478
1	0.139006	4.458994	-0.202476
1	-2.920446	1.850988	0.203088
1	-1.061242	-3.992575	-0.332911

[2d]

Number of imaginary frequencies : 0

Electronic energy : =-2102.2214456
Zero-point correction= 0.200088
Thermal correction to Energy= 0.226948
Thermal correction to Enthalpy= 0.227892
Thermal correction to Gibbs Free Energy= 0.141990
Sum of electronic and zero-point Energies= -2102.021357
Sum of electronic and thermal Energies= -2101.994497
Sum of electronic and thermal Enthalpies= -2101.993553

Sum of electronic and thermal Free Energies= -2102.079455

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Cartesian Coordinates

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46	-0.935606	-0.902121	-0.070506
6	-3.475510	-2.286519	0.050038
6	-2.467378	-3.226708	-0.576629
8	-1.254369	-2.771846	-0.736188
8	-2.807239	-4.346366	-0.931977
1	-3.999227	-2.807385	0.860298
1	-4.216180	-2.039506	-0.721912
7	-2.830824	-1.068898	0.539923
6	-3.470265	-0.251036	1.301210
8	-2.995253	0.857805	1.777191
8	-0.655911	0.971500	0.707062
1	-2.055223	1.026326	1.433328
6	-0.285782	1.951381	-0.188464
6	0.533732	2.981253	0.586312
6	-1.492635	2.574184	-0.890200
1	0.370733	1.581548	-0.996098
9	-0.134557	3.458927	1.636778
9	1.649886	2.407012	1.052415
9	0.900080	4.014250	-0.173175
9	-2.284141	3.238749	-0.043197
9	-1.127969	3.418918	-1.856318
9	-2.231794	1.614377	-1.456983
8	1.113083	-0.869733	-0.809603
1	1.303738	-1.574178	-1.454380
6	2.168616	-0.672955	0.099979
6	3.290345	0.103492	-0.585589
6	2.603673	-2.004219	0.701646
1	1.786888	-0.041839	0.911717
9	3.895077	-0.621989	-1.525803
9	4.201789	0.489896	0.300552
9	2.791064	1.191550	-1.170012
9	3.623528	-1.848663	1.536985
9	2.966705	-2.866786	-0.250724
9	1.587166	-2.544129	1.370892
1	-4.499836	-0.478245	1.596475

[2e]

Number of imaginary frequencies : 0

Electronic energy : =-981.1113991
Zero-point correction= 0.194760
Thermal correction to Energy= 0.212935
Thermal correction to Enthalpy= 0.213880
Thermal correction to Gibbs Free Energy= 0.146560
Sum of electronic and zero-point Energies= -980.916639
Sum of electronic and thermal Energies= -980.898464
Sum of electronic and thermal Enthalpies= -980.897520
Sum of electronic and thermal Free Energies= -980.964839

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Cartesian Coordinates

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46	0.032222	-0.008984	0.117108
6	0.524090	-2.739825	0.684130
6	1.815065	-2.218544	0.077689
8	1.748226	-0.996694	-0.396387
8	2.833243	-2.887835	0.063479
1	0.626902	-2.667619	1.775422
1	0.387576	-3.796366	0.425374
7	-0.594301	-1.917988	0.236621
6	-1.632460	-2.469377	-0.288909
8	-2.623509	-1.865421	-0.860748
8	-1.604461	0.963729	0.865043
8	0.853689	1.925645	-0.032491
6	2.056374	2.208230	-0.162369
8	3.010785	1.330782	-0.297963
6	2.513060	3.619701	-0.188469
1	3.317243	3.758827	0.540740
1	2.928759	3.838603	-1.178204
1	1.685825	4.297358	0.023936
1	2.669004	0.394192	-0.318406
6	-2.575568	1.234649	0.072186
8	-2.750315	0.701909	-1.042762
6	-3.543302	2.272487	0.561536
1	-3.457727	3.157600	-0.078744
1	-4.564767	1.893180	0.459707
1	-3.348987	2.559983	1.596647
1	-2.523588	-0.857633	-0.945303
1	-1.727166	-3.559806	-0.264601

[2f]

Number of imaginary frequencies : 0

Electronic energy : =-2891.7619663
Zero-point correction= 0.266797
Thermal correction to Energy= 0.303754
Thermal correction to Enthalpy= 0.304698
Thermal correction to Gibbs Free Energy= 0.194955
Sum of electronic and zero-point Energies= -2891.495169
Sum of electronic and thermal Energies= -2891.458212
Sum of electronic and thermal Enthalpies= -2891.457268
Sum of electronic and thermal Free Energies= -2891.567011

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Cartesian Coordinates

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46	0.115622	0.199811	-0.115836
8	-0.831714	-1.707142	-0.488215
6	2.457851	3.891617	-0.222037
6	1.342468	2.890838	-0.343055
8	1.400483	1.800660	0.250209
8	0.370114	3.276932	-1.101342
1	2.041846	4.802617	0.219729
1	2.765172	4.148537	-1.244243
7	3.575049	3.435612	0.553757
1	3.697550	3.777532	1.498136
6	4.424851	2.502669	0.077973
8	4.322097	1.981920	-1.026488
8	-1.367831	1.424184	-0.820005
1	-0.399533	2.600330	-1.086651
6	-2.482363	1.607521	-0.032342
6	-3.698286	1.654610	-0.952671
6	-2.341657	2.861097	0.827768
1	-2.670730	0.781411	0.675153
9	-3.795798	0.496544	-1.615662
9	-4.838084	1.828428	-0.280884
9	-3.599818	2.629785	-1.856447
9	-1.265772	2.741233	1.615059
9	-2.168435	3.954524	0.078802
9	-3.395172	3.066775	1.617728
8	1.529677	-1.067059	0.476937
6	2.736466	-0.910612	-0.165702
6	2.909381	-2.015779	-1.199065
6	3.835980	-0.891371	0.889400
1	2.840778	0.043369	-0.714883
9	5.055804	-0.785001	0.356720
9	3.653798	0.161378	1.694542
9	3.816784	-1.987286	1.650203
9	4.046372	-1.904752	-1.888638
9	2.885684	-3.229453	-0.640837
9	1.899163	-1.961446	-2.076530

1	-0.079617	-2.260920	-0.183645
6	-2.051896	-2.110167	0.082773
6	-1.936209	-2.166687	1.604604
6	-2.475848	-3.431445	-0.557667
1	-2.810681	-1.365683	-0.181623
9	-1.726547	-0.939604	2.090809
9	-0.904486	-2.925677	1.975407
9	-3.040418	-2.646968	2.160877
9	-3.702088	-3.776814	-0.181248
9	-2.465826	-3.302795	-1.880020
9	-1.641667	-4.419608	-0.231174
1	5.242794	2.269166	0.783151

[2g]

Number of imaginary frequencies : 0

Electronic energy : =-1933.5908963
Zero-point correction= 0.170651
Thermal correction to Energy= 0.195676
Thermal correction to Enthalpy= 0.196621
Thermal correction to Gibbs Free Energy= 0.114235
Sum of electronic and zero-point Energies= -1933.420246
Sum of electronic and thermal Energies= -1933.395220
Sum of electronic and thermal Enthalpies= -1933.394276
Sum of electronic and thermal Free Energies= -1933.476662

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Cartesian Coordinates

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46	-1.023505	1.082158	0.062691
6	-2.856480	2.705114	0.001378
8	-1.780741	2.961123	0.636160
8	-2.924016	1.568443	-0.583487
8	-0.726316	-0.691370	-0.799165
6	-0.704241	-1.763916	0.056971
6	0.087576	-2.878687	-0.626467
6	-2.125780	-2.194522	0.414750
1	-0.183989	-1.578841	1.016647
9	-0.486830	-3.273226	-1.762870
9	1.316718	-2.440685	-0.926964
9	0.231794	-3.949239	0.155584
9	-2.867135	-2.415307	-0.670846
9	-2.159240	-3.297788	1.166274
9	-2.721788	-1.219594	1.114883
8	0.959411	0.820748	0.879176
1	1.212169	1.511576	1.516939

6	2.008794	0.500782	-0.005665
6	3.046864	-0.350982	0.722128
6	2.576815	1.772698	-0.625335
1	1.576578	-0.114057	-0.805117
9	3.736621	0.363477	1.613476
9	3.905200	-0.885114	-0.140747
9	2.441364	-1.340562	1.373020
9	3.643544	1.515346	-1.372496
9	2.926093	2.651232	0.319269
9	1.654409	2.352936	-1.390404
6	-3.970245	3.674171	-0.063487
1	-4.245597	3.981250	0.950575
1	-3.637724	4.568697	-0.601390
1	-4.833482	3.239319	-0.572168

[2c]

Number of imaginary frequencies : 0

Electronic energy : =-1541.6495692
Zero-point correction= 0.196817
Thermal correction to Energy= 0.220032
Thermal correction to Enthalpy= 0.220976
Thermal correction to Gibbs Free Energy= 0.141307
Sum of electronic and zero-point Energies= -1541.452752
Sum of electronic and thermal Energies= -1541.429537
Sum of electronic and thermal Enthalpies= -1541.428593
Sum of electronic and thermal Free Energies= -1541.508263

Cartesian Coordinates

46	-0.888975	0.055335	-0.200831
8	-3.147658	-1.687187	1.102223
6	-2.639697	-3.833554	0.194861
6	-2.407364	-2.358836	0.373718
8	-1.411480	-1.899072	-0.318520
6	-2.522356	2.177782	0.812746
6	-1.201016	2.798794	0.398621
8	-0.314418	1.985371	-0.108714
8	-0.989452	3.987719	0.578016
1	-3.348863	2.865965	0.609159
1	-2.488494	2.004122	1.893075
1	-3.379976	-3.970972	-0.602236
1	-1.726709	-4.360685	-0.091877
1	-3.051734	-4.258170	1.114209
7	-2.757834	0.868661	0.159584
1	-3.170433	0.116342	0.746886

6	-3.359611	0.908156	-1.131233
8	-4.025394	0.003187	-1.562667
8	1.118628	-0.624986	-0.601974
1	-3.138225	1.846116	-1.675862
1	1.232457	-1.583656	-0.472073
6	2.216306	0.120202	-0.129299
1	1.924362	1.177618	-0.140314
6	3.383697	-0.056465	-1.096061
6	2.531288	-0.266891	1.310959
9	2.989362	0.253459	-2.327468
9	4.401063	0.733455	-0.770558
9	3.819004	-1.317694	-1.108442
9	3.591958	0.386462	1.769825
9	2.764178	-1.577831	1.416028
9	1.489549	0.020138	2.090327

$Pd(OAc)_2$ -Ligand with Substrate at the SMD/M06/6-31G**

[3a]

Number of imaginary frequencies : 0

Electronic energy : =-1970.2242881
Zero-point correction= 0.356704
Thermal correction to Energy= 0.386928
Thermal correction to Enthalpy= 0.387872
Thermal correction to Gibbs Free Energy= 0.294140
Sum of electronic and zero-point Energies= -1969.867584
Sum of electronic and thermal Energies= -1969.837360
Sum of electronic and thermal Enthalpies= -1969.836416
Sum of electronic and thermal Free Energies= -1969.930148

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Cartesian Coordinates

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46	2.778703	-0.248177	0.035529
6	-1.832351	-0.465429	1.153114
1	-0.800076	-0.529394	0.780549
1	-1.864942	-0.887486	2.166627
8	-1.047876	1.877402	2.183677
6	-1.497014	3.043227	-0.390476
6	-0.126808	3.251147	-0.603021
6	-2.394693	4.091335	-0.453722
6	0.345540	4.534238	-0.900052
6	-1.914289	5.365978	-0.746303

1	-3.451283	3.898946	-0.285643
6	-0.556906	5.585913	-0.971536
1	1.407786	4.689396	-1.066480
1	-2.613063	6.196444	-0.802172
1	-0.199161	6.584901	-1.203287
6	0.750227	2.143015	-0.472344
7	1.443227	1.224607	-0.337430
6	5.197604	-0.419490	0.304376
8	4.634624	0.703387	0.073320
6	6.663245	-0.547095	0.421384
1	7.082024	-0.705587	-0.579596
1	7.091780	0.371919	0.829826
1	6.922985	-1.406184	1.045070
8	4.424992	-1.435421	0.401073
6	0.035371	-3.397165	-0.705611
6	0.949371	-2.200204	-0.883384
8	1.279051	-1.607394	0.222077
8	1.337340	-1.900516	-2.008610
1	0.634749	-4.284151	-0.960829
7	-0.546517	-3.503044	0.610102
1	-0.035960	-3.113204	1.393372
6	-1.771439	-4.022392	0.814004
8	-2.482741	-4.506517	-0.058803
8	-1.931159	1.750312	-0.166758
16	-2.125854	1.281304	1.410287
8	-3.503567	1.554272	1.782467
6	-2.835617	-1.086362	0.235154
6	-4.053557	-1.543777	0.742490
6	-2.559848	-1.213978	-1.127410
6	-4.983073	-2.136173	-0.104378
1	-4.264679	-1.439419	1.806409
6	-3.486858	-1.816541	-1.970761
1	-1.608318	-0.851855	-1.519971
6	-4.698080	-2.277180	-1.459929
1	-5.927966	-2.496877	0.295559
1	-3.262789	-1.926992	-3.029371
1	-5.421107	-2.749414	-2.121266
1	-2.078188	-3.969725	1.877259
1	-0.765693	-3.335586	-1.450753

[3b]

Number of imaginary frequencies : 0

Electronic energy : =-1970.2240197
Zero-point correction= 0.356735
Thermal correction to Energy= 0.386859
Thermal correction to Enthalpy= 0.387804
Thermal correction to Gibbs Free Energy= 0.293759
Sum of electronic and zero-point Energies= -1969.867285
Sum of electronic and thermal Energies= -1969.837160
Sum of electronic and thermal Enthalpies= -1969.836216
Sum of electronic and thermal Free Energies= -1969.930260

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Cartesian Coordinates

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46	3.009792	-0.063199	0.499193
6	-3.468026	-0.530266	-0.689733
1	-3.866705	0.391448	-1.131514
1	-3.442735	-1.312803	-1.459571
8	-1.111773	0.220704	-1.664121
6	-1.687706	2.399036	0.033828
6	-0.403775	2.919774	-0.193584
6	-2.812064	3.162035	-0.218294
6	-0.252645	4.221100	-0.682579
6	-2.652174	4.457354	-0.705301
1	-3.796392	2.743054	-0.024609
6	-1.383538	4.984160	-0.936034
1	0.744655	4.614747	-0.856473
1	-3.533157	5.061038	-0.906717
1	-1.275033	5.995717	-1.316413
6	0.711589	2.082495	0.067193
7	1.583701	1.354284	0.289377
6	5.086806	-0.420319	1.737398
8	4.419500	0.658140	1.873444
6	6.369096	-0.637543	2.436881
1	7.183479	-0.290085	1.790150
1	6.396528	-0.062649	3.366089
1	6.519395	-1.701902	2.635430
8	4.603902	-1.296884	0.938769
6	1.211003	-1.855042	-2.916343
6	1.945627	-0.889625	-1.997068
8	1.942076	-1.242648	-0.751874
8	2.527586	0.076012	-2.482756
1	1.980569	-2.491224	-3.375851
7	0.190838	-2.650187	-2.280715
1	0.419260	-3.125764	-1.412527
6	-1.106948	-2.577976	-2.617489
8	-2.022349	-3.135296	-2.016277
8	-1.806240	1.136869	0.584778
16	-1.728214	-0.190849	-0.411654
8	-1.106962	-1.204573	0.415962
6	-4.176373	-0.962911	0.551520

6	-4.078554	-2.290686	0.975282
6	-4.919876	-0.050005	1.300544
6	-4.726084	-2.700946	2.134203
1	-3.491732	-2.994947	0.386515
6	-5.570101	-0.463469	2.458424
1	-4.995663	0.984008	0.965480
6	-5.472544	-1.787924	2.876271
1	-4.651172	-3.736372	2.458430
1	-6.154496	0.249494	3.035567
1	-5.981978	-2.110707	3.781643
1	-1.280365	-1.966333	-3.524800
1	0.756565	-1.268734	-3.722002

[3c]

Number of imaginary frequencies : 0

Electronic energy : =-1970.2216485
Zero-point correction= 0.357030
Thermal correction to Energy= 0.387092
Thermal correction to Enthalpy= 0.388036
Thermal correction to Gibbs Free Energy= 0.294904
Sum of electronic and zero-point Energies= -1969.864619
Sum of electronic and thermal Energies= -1969.834557
Sum of electronic and thermal Enthalpies= -1969.833612
Sum of electronic and thermal Free Energies= -1969.926744

Cartesian Coordinates

46	-2.140785	-0.601879	0.332113
6	1.817219	0.458177	-2.300785
1	0.736737	0.582566	-2.445905
1	2.322249	0.672130	-3.252901
8	1.446076	2.973701	-1.505438
6	2.777278	0.636964	1.075224
6	2.131572	-0.386182	1.791985
6	4.125306	0.884950	1.278755
6	2.854025	-1.197293	2.673926
6	4.832647	0.065774	2.155082
1	4.616432	1.700850	0.761378
6	4.210890	-0.973475	2.843790
1	2.338157	-1.989131	3.210065
1	5.892127	0.255480	2.307576
1	4.782817	-1.599888	3.521999

6	0.743807	-0.569099	1.576008
7	-0.390067	-0.660977	1.356152
6	-4.159314	-1.937523	-0.143275
8	-3.285273	-2.393299	0.659790
6	-5.375090	-2.705337	-0.498357
1	-5.238635	-3.144244	-1.493662
1	-5.546099	-3.507972	0.222807
1	-6.242267	-2.040153	-0.543506
8	-3.944927	-0.786370	-0.663815
8	1.959271	1.405127	0.264894
16	2.335207	1.849947	-1.283386
8	3.774082	2.021718	-1.386285
6	2.158080	-0.883874	-1.737133
6	3.482716	-1.301341	-1.580004
6	1.116826	-1.729673	-1.351794
6	3.757594	-2.543050	-1.017513
1	4.298184	-0.649845	-1.891840
6	1.394265	-2.974125	-0.794539
1	0.084746	-1.403703	-1.492526
6	2.714783	-3.378651	-0.620535
1	4.790111	-2.859706	-0.888577
1	0.574139	-3.622832	-0.492424
1	2.933193	-4.349220	-0.180397
7	-1.535365	1.205071	-0.303102
6	-1.536630	1.425419	-1.619500
8	-1.611030	0.560153	-2.499112
6	-1.580372	2.299899	0.625107
1	-1.039175	2.055999	1.548410
6	-2.988819	2.699932	0.988812
8	-3.995399	2.272274	0.467396
8	-2.988554	3.607613	1.967386
1	-3.910856	3.853757	2.157043
1	-1.419823	2.501292	-1.880291
1	-1.075893	3.186919	0.208300

[3d]

Number of imaginary frequencies : 0

Electronic energy : =-1970.2355041
Zero-point correction= 0.356334
Thermal correction to Energy= 0.386103
Thermal correction to Enthalpy= 0.387047
Thermal correction to Gibbs Free Energy= 0.293628

Sum of electronic and zero-point Energies= -1969.879171
Sum of electronic and thermal Energies= -1969.849401
Sum of electronic and thermal Enthalpies= -1969.848457
Sum of electronic and thermal Free Energies= -1969.941876

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Cartesian Coordinates

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46	2.145783	-0.238008	-0.149457
6	-3.054036	-0.708135	-0.897587
1	-3.760999	-0.184114	-1.550261
1	-2.187237	-1.051410	-1.481972
8	-1.260548	0.054603	0.939663
6	-1.785231	2.940123	-0.576306
6	-0.518301	3.415903	-0.202297
6	-2.868246	3.797383	-0.645059
6	-0.339528	4.770031	0.100473
6	-2.680485	5.143032	-0.340756
1	-3.838647	3.407412	-0.939837
6	-1.427047	5.627251	0.028831
1	0.645320	5.129291	0.384667
1	-3.526934	5.822472	-0.395359
1	-1.297412	6.680512	0.260354
6	0.547402	2.481705	-0.151889
7	1.367769	1.664890	-0.125706
6	1.298820	-2.901262	-0.519312
6	0.391806	-2.054859	-1.394179
8	0.685580	-0.790891	-1.466484
8	-0.576354	-2.552437	-1.962589
1	1.438930	-3.896174	-0.958258
7	2.563553	-2.200681	-0.328956
6	3.677752	-2.795390	-0.572984
8	4.853762	-2.255860	-0.575162
8	-1.910016	1.609850	-0.942050
16	-2.426390	0.539537	0.215735
8	-3.495399	1.184741	0.961811
6	-3.696766	-1.798288	-0.095160
6	-2.935783	-2.870594	0.375655
6	-5.054745	-1.721163	0.222362
6	-3.533171	-3.862090	1.146533
1	-1.880013	-2.932007	0.115368
6	-5.649717	-2.715154	0.990762
1	-5.643402	-0.878694	-0.138931
6	-4.888892	-3.785656	1.454359
1	-2.938518	-4.699515	1.504535
1	-6.709239	-2.654372	1.228737
1	-5.355076	-4.564122	2.054425
8	3.435308	0.280593	1.362087
6	4.666934	0.515413	1.094956
8	5.230807	0.220596	0.021575

6	5.451313	1.183258	2.187367
1	6.285908	0.535109	2.474692
1	5.882291	2.111289	1.796905
1	4.837406	1.404860	3.062436
1	4.859552	-1.254736	-0.405847
1	0.793779	-3.022195	0.450345
1	3.673644	-3.865891	-0.801533

[3f]

Number of imaginary frequencies : 0

Electronic energy : =-1970.2370248
Zero-point correction= 0.354902
Thermal correction to Energy= 0.385089
Thermal correction to Enthalpy= 0.386033
Thermal correction to Gibbs Free Energy= 0.290839
Sum of electronic and zero-point Energies= -1969.882122
Sum of electronic and thermal Energies= -1969.851936
Sum of electronic and thermal Enthalpies= -1969.850992
Sum of electronic and thermal Free Energies= -1969.946186

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Cartesian Coordinates

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46	1.866857	0.208694	-0.299654
6	-2.998943	-2.502432	1.185379
1	-3.613825	-2.280558	2.065858
1	-3.254610	-3.511079	0.835333
8	-5.086227	-1.645421	-0.230225
6	-3.611207	1.130796	-0.089989
6	-2.504292	1.751591	-0.684649
6	-4.881639	1.659854	-0.226493
6	-2.682902	2.926047	-1.424744
6	-5.047863	2.827091	-0.967661
1	-5.720509	1.164227	0.254123
6	-3.957456	3.456304	-1.563321
1	-1.821385	3.403907	-1.882902
1	-6.043203	3.249683	-1.077262
1	-4.100647	4.367463	-2.136945
6	-1.207135	1.190418	-0.532932
7	-0.139179	0.755851	-0.422394
6	3.843337	-1.743811	-0.853626
6	2.684364	-2.033144	-1.788603
8	1.726937	-1.141940	-1.799204

8	2.641423	-3.050940	-2.467141
1	4.791181	-1.959434	-1.364380
7	3.773529	-0.364473	-0.404637
6	4.759052	0.473200	-0.672242
8	4.739179	1.716719	-0.567350
8	-3.400954	-0.004504	0.675687
16	-3.651872	-1.445868	-0.099868
8	-2.827695	-1.446870	-1.297368
6	-1.533930	-2.323445	1.422471
6	-1.084042	-1.488662	2.447644
6	-0.608344	-3.004688	0.629241
6	0.278729	-1.345397	2.684026
1	-1.808475	-0.960471	3.066192
6	0.753406	-2.869222	0.872379
1	-0.960412	-3.655798	-0.169821
6	1.199027	-2.036399	1.897694
1	0.624091	-0.699935	3.488445
1	1.464132	-3.424615	0.262581
1	2.265731	-1.934469	2.093467
8	1.948170	1.429788	1.422818
6	2.280122	2.630122	1.447232
8	3.046814	3.189936	0.568658
6	1.799309	3.523458	2.533585
1	2.658887	3.912970	3.088595
1	1.284371	4.381667	2.088840
1	1.125546	2.991929	3.206451
1	3.585134	2.502498	0.019157
1	5.694632	-0.019429	-1.001603
1	3.764731	-2.438481	-0.004321

[3g]

Number of imaginary frequencies : 0

Electronic energy : =-2759.7825844
Zero-point correction= 0.421751
Thermal correction to Energy= 0.461298
Thermal correction to Enthalpy= 0.462242
Thermal correction to Gibbs Free Energy= 0.349111
Sum of electronic and zero-point Energies= -2759.360834
Sum of electronic and thermal Energies= -2759.321287
Sum of electronic and thermal Enthalpies= -2759.320343

Sum of electronic and thermal Free Energies= -2759.433473

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Cartesian Coordinates

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46	1.829853	0.309431	-1.376262
6	-3.568899	-0.479122	-1.276276
1	-4.504115	0.089593	-1.216785
1	-3.202637	-0.488450	-2.311425
8	-1.052566	-0.157690	-0.463099
6	-2.275135	3.071743	-0.713340
6	-1.022945	3.665079	-0.484792
6	-3.443890	3.740409	-0.405882
6	-0.955078	4.956716	0.049230
6	-3.364445	5.024663	0.125753
1	-4.398271	3.252206	-0.587740
6	-2.129649	5.630716	0.348330
1	0.016085	5.412886	0.219255
1	-4.280011	5.558293	0.366774
1	-2.082405	6.634994	0.759183
6	0.142294	2.910131	-0.780607
7	1.046183	2.222195	-1.013082
6	0.912923	-2.183476	-2.295156
6	0.086381	-1.127764	-3.006180
8	0.528808	0.096161	-2.910411
8	-0.933010	-1.415597	-3.625660
1	1.077726	-3.036474	-2.967502
7	2.167832	-1.598246	-1.849419
6	3.319582	-2.040345	-2.318962
8	4.434493	-1.491468	-2.199443
8	-2.332053	1.822882	-1.316625
16	-2.356065	0.472568	-0.370703
8	-2.835089	0.860278	0.954888
6	-3.639206	-1.842822	-0.663342
6	-2.815712	-2.862493	-1.146264
6	-4.457867	-2.072790	0.443769
6	-2.815789	-4.106287	-0.524938
1	-2.182527	-2.670084	-2.013450
6	-4.456581	-3.318973	1.061488
1	-5.097293	-1.273928	0.817393
6	-3.632003	-4.333301	0.580925
1	-2.175975	-4.900206	-0.903991
1	-5.097862	-3.498242	1.921322
1	-3.628781	-5.305988	1.067965
8	2.981748	0.527498	0.357228
6	4.221888	0.577303	0.463235
8	5.057279	0.188655	-0.441996
6	4.846601	1.104222	1.706647
1	5.368131	0.285094	2.214115
1	5.598305	1.854707	1.443308

1	4.097234	1.531473	2.373020
1	4.647304	-0.382453	-1.198259
1	-1.571032	0.559988	2.399852
8	-0.867692	0.350540	3.040016
6	0.199571	-0.229083	2.367144
6	-0.051905	-1.716551	2.113591
6	1.430064	-0.004915	3.232438
1	0.411764	0.232454	1.388612
9	0.763401	-2.180604	1.160135
9	-1.308860	-1.914580	1.718139
9	0.139090	-2.458544	3.209328
9	2.460606	-0.746455	2.819964
9	1.200955	-0.300706	4.510925
9	1.791155	1.279950	3.178461
1	0.323200	-2.547098	-1.440502
1	3.253196	-3.011312	-2.846924

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[3]

Number of imaginary frequencies : 0

Electronic energy : =-2530.8013909
Zero-point correction= 0.358060
Thermal correction to Energy= 0.392475
Thermal correction to Enthalpy= 0.393419
Thermal correction to Gibbs Free Energy= 0.290078
Sum of electronic and zero-point Energies= -2530.443331
Sum of electronic and thermal Energies= -2530.408916
Sum of electronic and thermal Enthalpies= -2530.407972
Sum of electronic and thermal Free Energies= -2530.511313

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Cartesian Coordinates

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46	-1.137793	0.787899	-0.657357
6	3.633404	1.618929	2.028336
1	4.033087	1.010204	2.847903
1	4.143653	2.590852	2.046608
8	5.725703	0.769517	0.621036
6	3.797414	-1.551946	-0.241869
6	2.711365	-1.741303	-1.107724
6	4.965201	-2.275656	-0.398911
6	2.801745	-2.677712	-2.143825
6	5.045632	-3.202842	-1.435182
1	5.788704	-2.119243	0.292209

6	3.973140	-3.404081	-2.301154
1	1.956265	-2.819809	-2.810987
1	5.959759	-3.776356	-1.563821
1	4.050163	-4.132553	-3.103155
6	1.531528	-0.972297	-0.923732
7	0.567708	-0.346434	-0.783218
6	-2.600077	3.115497	-1.610410
6	-1.201758	3.176351	-2.190020
8	-0.395843	2.191073	-1.908050
8	-0.876952	4.110716	-2.910813
1	-3.296644	2.981600	-2.448814
7	-2.734609	2.018494	-0.655783
6	-3.742244	1.983792	0.144560
8	-3.951672	1.067439	1.039710
8	3.654943	-0.655540	0.804603
16	4.276361	0.858457	0.545114
8	3.664853	1.385160	-0.663896
6	2.143882	1.747932	2.061216
6	1.376126	0.821106	2.769925
6	1.518035	2.816947	1.415891
6	-0.001038	0.985018	2.867528
1	1.868264	-0.017784	3.261026
6	0.139828	2.976952	1.509776
1	2.117626	3.526900	0.847528
6	-0.617507	2.069887	2.248194
1	-0.598049	0.261285	3.418432
1	-0.347822	3.806255	0.999073
1	-1.695686	2.197804	2.330924
8	-1.977716	-0.519993	0.690666
1	-3.234896	0.345719	0.982006
1	-4.500668	2.773113	0.104221
1	-2.830918	4.078855	-1.139044
6	-2.122457	-1.842988	0.355743
1	-1.175667	-2.335953	0.070435
6	-2.625767	-2.570326	1.602099
6	-3.071185	-2.021811	-0.831232
9	-3.868307	-2.189853	1.920077
9	-1.838904	-2.289542	2.641262
9	-2.631547	-3.895477	1.450261
9	-3.424033	-3.294105	-1.024528
9	-4.187491	-1.303843	-0.682053
9	-2.475308	-1.599362	-1.954603

[3h]

Number of imaginary frequencies : 0

Electronic energy : =-2530.8004713
Zero-point correction= 0.360477
Thermal correction to Energy= 0.394414
Thermal correction to Enthalpy= 0.395358
Thermal correction to Gibbs Free Energy= 0.294061
Sum of electronic and zero-point Energies= -2530.439994
Sum of electronic and thermal Energies= -2530.406057
Sum of electronic and thermal Enthalpies= -2530.405113
Sum of electronic and thermal Free Energies= -2530.506410

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Cartesian Coordinates

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46	-1.181053	-0.158309	-1.384015
6	1.482390	2.678294	-0.156856
1	2.080382	3.472696	-0.617982
1	1.043037	2.052834	-0.945644
8	1.999177	0.467011	1.278464
6	4.043887	-0.148427	-0.599844
6	3.263410	-1.252807	-0.976931
6	5.368476	-0.305295	-0.240789
6	3.828278	-2.531826	-0.999008
6	5.923620	-1.583111	-0.271060
1	5.948488	0.567903	0.047180
6	5.162021	-2.686686	-0.648241
1	3.216408	-3.382989	-1.284361
1	6.966413	-1.715628	0.004918
1	5.609899	-3.675976	-0.665917
6	1.894611	-1.029270	-1.275017
7	0.781485	-0.785463	-1.483514
6	-3.041813	2.054385	-1.584345
6	-1.744168	2.487686	-2.236973
8	-0.789007	1.600003	-2.308035
8	-1.613821	3.631321	-2.650179
1	-3.881464	2.319239	-2.238245
7	-3.030140	0.625753	-1.285510
6	-4.125184	-0.006238	-1.050654
8	-4.206537	-1.270564	-0.760642
8	3.479615	1.115247	-0.644359
16	2.652044	1.629718	0.696278
8	3.566067	2.409130	1.514229
6	0.462541	3.190142	0.812235
6	-0.640232	2.397237	1.141425
6	0.618368	4.439770	1.413030
6	-1.590539	2.859466	2.044050
1	-0.748234	1.411478	0.683645
6	-0.334079	4.901861	2.315613

1	1.484450	5.050862	1.162134
6	-1.439280	4.114806	2.629017
1	-2.449189	2.237098	2.289497
1	-0.213148	5.880186	2.775225
1	-2.183841	4.480536	3.332697
8	-1.700932	-1.914297	-0.485131
1	-3.286702	-1.675446	-0.670970
6	-1.093900	-2.152241	0.729676
6	-0.605213	-3.598021	0.723351
6	-2.051435	-1.854159	1.879705
1	-0.202489	-1.527869	0.919184
9	-1.595427	-4.452885	0.462273
9	0.319186	-3.747580	-0.230685
9	-0.050579	-3.958624	1.883227
9	-3.138575	-2.630046	1.837299
9	-1.479432	-2.014809	3.073408
9	-2.464332	-0.582581	1.799129
1	-3.147176	2.634660	-0.656950
1	-5.085146	0.517625	-1.093921

C-H bond activation at the *meta, ortho* and *para* position transition states at the SMD/M06/6-31G** level of theory

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C-H activation Transition states [A to H]

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meta-**A**

Number of imaginary frequencies : 1
The smallest frequency is : -1591.4745 cm(-1)

Electronic energy : =-1801.5891205
Zero-point correction= 0.322012
Thermal correction to Energy= 0.349671
Thermal correction to Enthalpy= 0.350615
Thermal correction to Gibbs Free Energy= 0.262217
Sum of electronic and zero-point Energies= -1801.267109
Sum of electronic and thermal Energies= -1801.239450
Sum of electronic and thermal Enthalpies= -1801.238506
Sum of electronic and thermal Free Energies= -1801.326903

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Cartesian Coordinates

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6	1.087155	-2.565927	1.845154

6	-0.006277	-2.143293	2.593632
6	-1.143337	-1.683840	1.940637
6	-1.210493	-1.667105	0.535398
6	-0.106966	-2.137128	-0.200839
6	1.043423	-2.575830	0.445667
1	1.997146	-2.892417	2.347399
1	0.041563	-2.156892	3.679661
1	-1.998268	-1.332413	2.517817
1	-0.145961	-2.131980	-1.290769
6	2.263331	-2.966711	-0.326181
8	2.316579	-0.793664	-1.925493
6	3.522943	0.669459	0.312404
6	2.487205	1.615243	0.255751
6	4.847111	1.066503	0.318835
6	2.799206	2.979741	0.218434
6	5.144407	2.426544	0.277231
1	5.626917	0.311307	0.370207
6	4.128054	3.377541	0.230526
1	1.993934	3.708083	0.177283
1	6.183844	2.743502	0.285372
1	4.372123	4.435577	0.203240
6	1.130695	1.194744	0.204408
7	0.022611	0.866361	0.130608
46	-1.904727	0.256021	-0.139388
6	-5.752853	-1.599586	-0.766985
6	-4.302635	-1.391470	-0.463829
8	-3.580242	-2.409639	-0.279272
8	-3.881018	-0.195126	-0.423330
1	-2.385821	-1.990232	0.058750
1	-6.306785	-0.660307	-0.729462
1	-5.839943	-2.031536	-1.770106
1	-6.174995	-2.320055	-0.060662
6	-2.952351	4.397558	-0.402527
6	-2.569689	3.029254	0.107957
8	-2.408594	2.156152	-0.833460
8	-2.441622	2.805910	1.315735
1	-3.917788	4.341531	-0.917069
1	-2.217096	4.750472	-1.133145
1	-3.022464	5.110887	0.422242
8	3.204240	-0.675193	0.420398
8	4.489797	-1.904827	-1.365145
16	3.134775	-1.542649	-0.984735
1	3.003308	-3.499496	0.281680
1	2.046339	-3.568198	-1.218569

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meta-**B**

Number of imaginary frequencies : 1
The smallest frequency is : -1683.2556 cm(-1)

Electronic energy : =-1970.2030655
Zero-point correction= 0.350666
Thermal correction to Energy= 0.380819
Thermal correction to Enthalpy= 0.381763
Thermal correction to Gibbs Free Energy= 0.288172
Sum of electronic and zero-point Energies= -1969.852400
Sum of electronic and thermal Energies= -1969.822247
Sum of electronic and thermal Enthalpies= -1969.821302
Sum of electronic and thermal Free Energies= -1969.914893

Cartesian Coordinates

46	1.900586	-0.383885	0.223927
6	-0.072763	-3.672335	1.775954
6	1.015833	-2.991540	1.244842
6	0.897764	-2.270716	0.041076
6	-0.341435	-2.260037	-0.623740
6	-1.434266	-2.938047	-0.097183
6	-1.293311	-3.632002	1.110796
1	-0.445480	-1.709094	-1.558657
1	1.943757	-2.409924	-0.724370
1	1.979498	-3.022904	1.753740
1	-2.157050	-4.149509	1.527099
6	-2.766922	-2.892529	-0.770208
8	-3.610791	-1.295404	1.239795
6	-3.274191	0.966929	-0.538576
6	-2.221717	1.668992	0.067366
6	-4.511263	1.559444	-0.718415
6	-2.418124	2.989607	0.489806
6	-4.700890	2.866412	-0.276148
1	-5.308472	1.008703	-1.209611
6	-3.663801	3.576754	0.322134
1	-1.581561	3.532024	0.926729
1	-5.671749	3.335761	-0.413000
1	-3.823886	4.599374	0.651889
6	-0.957189	1.038415	0.222374
7	0.070062	0.514580	0.331965
6	4.000869	-2.152713	-0.679045
8	3.095824	-2.784187	-1.290529
6	5.423035	-2.568998	-0.880908
1	6.100752	-1.997342	-0.245175
1	5.519267	-3.638892	-0.672796
1	5.688137	-2.414472	-1.932244

1	0.021763	-4.228329	2.705285
8	3.782701	-1.175064	0.103821
6	3.217867	3.700686	0.222451
6	2.659879	2.345782	-0.218042
8	2.827424	1.426795	0.667446
8	2.136249	2.213834	-1.324343
1	4.213809	3.824957	-0.213445
1	3.321865	3.714967	1.312722
7	2.380550	4.791007	-0.222100
1	2.728129	5.467965	-0.888053
6	1.089600	4.830313	0.139446
8	0.566588	4.002531	0.884091
16	-3.787684	-1.542402	-0.181690
8	-3.022908	-0.319895	-0.993568
8	-5.130928	-1.674633	-0.721361
1	-3.377850	-3.779660	-0.561280
1	-2.713419	-2.758522	-1.856997
1	0.537082	5.684652	-0.291198

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meta-**C1**

Number of imaginary frequencies : 1
The smallest frequency is : -1690.8244 cm(-1)

Electronic energy : =-1741.2143863
Zero-point correction= 0.287090
Thermal correction to Energy= 0.311117
Thermal correction to Enthalpy= 0.312061
Thermal correction to Gibbs Free Energy= 0.232674
Sum of electronic and zero-point Energies= -1740.927297
Sum of electronic and thermal Energies= -1740.903270
Sum of electronic and thermal Enthalpies= -1740.902325
Sum of electronic and thermal Free Energies= -1740.981712

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Cartesian Coordinates

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46	2.097879	0.252390	-0.002499
6	0.022501	-2.632394	2.114542
6	1.161256	-2.094001	1.528200
6	1.155785	-1.678156	0.182604
6	-0.031776	-1.822867	-0.558697
6	-1.171243	-2.373223	0.015958
6	-1.137060	-2.771299	1.358624
1	-0.064253	-1.497441	-1.599373

1	2.245877	-2.022787	-0.429704
1	2.083653	-2.010731	2.103073
1	-2.028189	-3.205635	1.809808
6	-2.420209	-2.526335	-0.790227
8	-3.876717	-1.146520	1.016976
6	-3.215657	1.253643	-0.401774
6	-2.191943	2.011825	0.183047
6	-4.509336	1.741895	-0.462285
6	-2.475121	3.277843	0.710075
6	-4.781289	2.994886	0.080503
1	-5.292951	1.156982	-0.936869
6	-3.773415	3.760771	0.662155
1	-1.672003	3.860691	1.152290
1	-5.797061	3.378783	0.037416
1	-4.000089	4.739596	1.074513
6	-0.869738	1.495497	0.205110
7	0.210502	1.077100	0.202506
6	4.979475	0.633624	-0.105221
6	4.359091	2.018893	-0.155368
8	3.064240	2.087273	-0.106901
8	5.085902	3.007522	-0.204753
1	5.484456	0.544951	0.867669
7	3.965620	-0.398706	-0.259649
6	4.255537	-1.597672	-0.687141
8	3.412518	-2.523726	-0.866633
1	0.034035	-2.955505	3.152481
8	-2.860386	0.032216	-0.951086
16	-3.673655	-1.306311	-0.412740
8	-4.821871	-1.511860	-1.279100
1	-2.938935	-3.476960	-0.607735
1	-2.248624	-2.434445	-1.869091
1	5.315319	-1.808693	-0.903039
1	5.751313	0.556657	-0.881302

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meta-**C [4]**

Number of imaginary frequencies : 0

Electronic energy : =-1741.2375988
Zero-point correction= 0.292365
Thermal correction to Energy= 0.316926
Thermal correction to Enthalpy= 0.317870
Thermal correction to Gibbs Free Energy= 0.237367
Sum of electronic and zero-point Energies= -1740.945233

Sum of electronic and thermal Energies= -1740.920673
Sum of electronic and thermal Enthalpies= -1740.919729
Sum of electronic and thermal Free Energies= -1741.000232

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Cartesian Coordinates

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46	-1.943176	0.167854	0.016459
6	-1.331976	-2.189522	-0.309639
6	-1.717140	-1.951881	1.026589
6	-0.731438	-1.919164	2.039461
6	0.586554	-2.166994	1.724926
6	0.967359	-2.447203	0.395232
6	0.021052	-2.424795	-0.614235
1	1.344788	-2.176999	2.506176
1	-1.025692	-1.744531	3.071021
1	-2.768836	-1.982405	1.304265
1	0.308886	-2.646124	-1.640265
6	2.392873	-2.783392	0.087577
1	2.485969	-3.580341	-0.661692
1	2.966143	-3.077509	0.974636
8	2.589056	-0.805553	-1.732921
6	3.485033	0.929420	0.403983
6	2.404803	1.796475	0.188550
6	4.785829	1.394712	0.397455
6	2.640808	3.159200	-0.021526
6	5.010056	2.752782	0.181331
1	5.602230	0.698437	0.568997
6	3.946715	3.628922	-0.023892
1	1.800825	3.827909	-0.186199
1	6.029831	3.128155	0.176201
1	4.136248	4.685639	-0.188812
6	1.090436	1.258815	0.164348
7	0.037016	0.778997	0.135330
6	-4.589281	1.210871	0.220956
6	-3.707748	2.390054	-0.113822
8	-2.442395	2.120519	-0.298857
8	-4.145854	3.532402	-0.165573
1	-5.548774	1.312166	-0.302336
7	-3.928610	-0.040719	-0.114466
6	-4.642204	-1.048332	-0.620747
8	-4.246527	-2.157542	-0.986797
1	-2.106550	-2.327787	-1.061287
8	3.215916	-0.406907	0.662806
8	4.697390	-1.807177	-0.816685
16	3.307510	-1.427283	-0.633494
1	-4.804209	1.275997	1.299561
1	-5.724848	-0.791043	-0.682595

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meta-**C [4-5]**‡

Number of imaginary frequencies : 1
The smallest frequency is : -1635.3265 cm(-1)

Electronic energy : =-1741.2152073
Zero-point correction= 0.286926
Thermal correction to Energy= 0.311012
Thermal correction to Enthalpy= 0.311956
Thermal correction to Gibbs Free Energy= 0.232075
Sum of electronic and zero-point Energies= -1740.928282
Sum of electronic and thermal Energies= -1740.904195
Sum of electronic and thermal Enthalpies= -1740.903251
Sum of electronic and thermal Free Energies= -1740.983132

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Cartesian Coordinates

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46	-1.986766	0.270893	0.055392
6	-1.214749	-1.711838	0.411396
6	-1.151168	-1.933779	1.800848
6	0.008968	-2.414197	2.395139
6	1.124401	-2.670263	1.604460
6	1.084368	-2.483978	0.217824
6	-0.083020	-2.008540	-0.370491
1	2.046858	-3.025587	2.062222
1	0.054196	-2.583024	3.468254
1	-2.030844	-1.727878	2.410579
1	-0.116419	-1.842776	-1.447674
6	2.319628	-2.728633	-0.589011
1	2.130844	-3.250563	-1.536492
1	3.087385	-3.281366	-0.036123
8	2.252759	-0.408398	-1.957407
6	3.454417	0.874257	0.386834
6	2.393448	1.790367	0.443197
6	4.767786	1.305205	0.388119
6	2.668338	3.161445	0.509407
6	5.028345	2.672024	0.450316
1	5.568592	0.571559	0.350935
6	3.986515	3.594299	0.512173
1	1.844232	3.868158	0.552954
1	6.058949	3.016684	0.452826
1	4.202240	4.657682	0.562181
6	1.050364	1.326550	0.402523
7	-0.046285	0.956944	0.344874
6	-4.805113	0.895370	-0.339420

6	-4.057722	2.215101	-0.369260
8	-2.770779	2.173122	-0.210342
8	-4.685780	3.259541	-0.519617
1	-5.448040	0.839836	-1.227316
7	-3.887254	-0.234128	-0.278810
6	-4.291317	-1.451837	-0.514865
8	-3.553078	-2.480205	-0.488460
1	-2.366218	-2.052265	-0.108389
8	3.167394	-0.482311	0.378178
8	4.481536	-1.470936	-1.533459
16	3.117422	-1.209654	-1.105459
1	-5.463676	0.915323	0.540224
1	-5.358197	-1.587925	-0.753580

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meta-**C [5]**

Number of imaginary frequencies : 0

Electronic energy : =-1741.2380436
Zero-point correction= 0.293389
Thermal correction to Energy= 0.317879
Thermal correction to Enthalpy= 0.318823
Thermal correction to Gibbs Free Energy= 0.238454
Sum of electronic and zero-point Energies= -1740.944655
Sum of electronic and thermal Energies= -1740.920165
Sum of electronic and thermal Enthalpies= -1740.919220
Sum of electronic and thermal Free Energies= -1740.999590

Cartesian Coordinates

46	-1.958819	0.417934	0.013085
6	-0.967022	-1.263945	0.478933
6	-1.227281	-1.956286	1.664105
6	-0.327307	-2.923773	2.110187
6	0.842256	-3.178460	1.400198
6	1.083623	-2.517977	0.195374
6	0.150624	-1.597162	-0.283544
1	1.572912	-3.889738	1.781973
1	-0.523987	-3.458606	3.037340
1	-2.116141	-1.731249	2.252804
1	0.344239	-1.073995	-1.218821
6	2.376928	-2.746967	-0.525780
1	2.257574	-3.233109	-1.504459
1	3.081004	-3.340855	0.067096

8	2.611517	-0.506826	-2.016809
6	3.402461	0.935561	0.427536
6	2.406964	1.923367	0.340563
6	4.736982	1.286387	0.534876
6	2.772246	3.275573	0.363972
6	5.085808	2.634317	0.546992
1	5.488522	0.506522	0.619198
6	4.110799	3.624134	0.461717
1	1.996775	4.034252	0.301212
1	6.133775	2.910093	0.629485
1	4.393380	4.672730	0.476209
6	1.033405	1.571279	0.235968
7	-0.092017	1.305425	0.152402
6	-4.851506	0.617510	0.122393
6	-4.381424	2.017924	-0.262899
8	-3.117343	2.192661	-0.403301
8	-5.237730	2.898943	-0.372634
1	-5.789589	0.386899	-0.397009
7	-3.831411	-0.394730	-0.144443
6	-4.187578	-1.539677	-0.590829
8	-3.369426	-2.517603	-0.900153
1	-2.442700	-2.247362	-0.716099
8	3.028337	-0.401766	0.452942
8	4.686609	-1.540844	-1.078548
16	3.268837	-1.247105	-0.950189
1	-5.063722	0.639423	1.200445
1	-5.239370	-1.788518	-0.754510

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meta-**D**

Number of imaginary frequencies : 1
The smallest frequency is : -1741.8994 cm(-1)

Electronic energy : =-1970.1840835
Zero-point correction= 0.350068
Thermal correction to Energy= 0.380084
Thermal correction to Enthalpy= 0.381028
Thermal correction to Gibbs Free Energy= 0.287102
Sum of electronic and zero-point Energies= -1969.834015
Sum of electronic and thermal Energies= -1969.803999
Sum of electronic and thermal Enthalpies= -1969.803055
Sum of electronic and thermal Free Energies= -1969.896982

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Cartesian Coordinates

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46	1.364397	0.784313	0.003653
6	0.982795	-1.300910	-0.368499
6	0.983872	-1.415991	-1.777390
6	-0.081253	-2.001461	-2.447635
6	-1.163310	-2.484802	-1.718885
6	-1.187404	-2.414944	-0.319445
6	-0.126464	-1.812869	0.343620
1	2.084419	-1.629367	0.209645
8	3.088119	-2.353202	0.742434
1	-2.010760	-2.930832	-2.238239
1	-0.078135	-2.081521	-3.531597
1	1.839722	-1.043598	-2.339675
1	-0.142846	-1.731715	1.431328
6	-2.380808	-2.933753	0.418639
8	-2.780445	-0.745292	1.933325
6	-4.094050	0.473046	-0.377227
6	-3.183904	1.539629	-0.326627
6	-5.456068	0.703628	-0.420548
6	-3.658046	2.856411	-0.333361
6	-5.916728	2.018324	-0.423592
1	-6.136793	-0.142501	-0.461363
6	-5.025031	3.087608	-0.383456
1	-2.948679	3.678425	-0.295538
1	-6.986423	2.206427	-0.460812
1	-5.396437	4.108146	-0.390076
6	-1.790385	1.278487	-0.243791
7	-0.654748	1.071002	-0.152723
6	4.906871	-3.702198	0.064814
6	4.058972	-2.471339	-0.092619
8	4.302330	-1.645816	-0.996242
6	3.879631	2.032934	-0.528760
6	2.928218	3.165690	-0.182107
8	1.724568	2.822902	0.166018
8	3.298703	4.329450	-0.278898
1	4.898463	2.289661	-0.221390
1	5.828537	-3.625212	-0.516595
1	5.140844	-3.871910	1.120442
1	4.337668	-4.572806	-0.281919
7	3.455313	0.761059	0.088322
1	3.765349	-0.102499	-0.422491
6	3.707824	0.668864	1.484294
8	4.006038	1.628759	2.152696
8	-3.603315	-0.821792	-0.437279
8	-4.763364	-2.164095	1.354623
16	-3.460614	-1.628255	0.999692
1	-3.014855	-3.579902	-0.198830
1	-2.122608	-3.478693	1.335768
1	3.589402	-0.359714	1.865727

1	3.867236	1.891449	-1.614653

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meta-**E**

Number of imaginary frequencies : 1
The smallest frequency is : -1703.8079 cm(-1)

Electronic energy : =-1801.5763097
Zero-point correction= 0.322567
Thermal correction to Energy= 0.349964
Thermal correction to Enthalpy= 0.350909
Thermal correction to Gibbs Free Energy= 0.263052
Sum of electronic and zero-point Energies= -1801.253743
Sum of electronic and thermal Energies= -1801.226345
Sum of electronic and thermal Enthalpies= -1801.225401
Sum of electronic and thermal Free Energies= -1801.313257

Cartesian Coordinates

46	-2.987113	0.465489	0.006757
6	-0.322013	-0.800266	-0.155235
1	-0.028659	0.022229	-0.809353
8	-0.734454	1.839149	1.591339
8	-1.976475	2.233998	-0.228751
6	-1.340313	-0.597869	0.790552
6	-1.690430	-1.656142	1.652343
6	-1.039830	-2.877334	1.559869
6	-0.037280	-3.062263	0.608257
6	0.336553	-2.022689	-0.247827
1	-1.213880	0.581085	1.293747
1	-2.478921	-1.513480	2.389171
1	-1.311109	-3.695494	2.222238
1	0.459728	-4.027951	0.528865
6	1.446505	-2.190978	-1.234846
8	4.089647	-1.962401	-1.509917
6	3.937166	0.310207	0.179484
6	3.662375	1.557653	-0.393827
6	5.182278	0.027472	0.714574
6	4.663205	2.535244	-0.424134
6	6.171472	1.004618	0.666595
1	5.368463	-0.940173	1.175322
6	5.915330	2.252294	0.101787
1	4.444575	3.504791	-0.863504
1	7.151449	0.788736	1.084256

1	6.694091	3.009271	0.075404
6	2.364391	1.817722	-0.924119
7	1.304916	2.029861	-1.356616
6	-1.127561	2.583051	0.654025
6	-0.606417	3.984135	0.569999
1	-1.237755	4.621022	1.200885
1	0.416380	4.031566	0.950831
1	-0.654099	4.356777	-0.455148
6	-6.571487	-0.963412	-0.914814
6	-5.257832	-0.376329	-0.553702
8	-4.966634	0.826451	-0.830722
8	-4.370659	-1.095875	0.026988
1	-7.324075	-0.178933	-1.026047
1	-6.885349	-1.691792	-0.162187
1	-6.470366	-1.488132	-1.872205
8	2.894064	-0.597466	0.242647
8	3.219295	-3.045231	0.584586
16	3.068279	-2.071461	-0.482606
1	1.439513	-1.419034	-2.013962
1	1.455390	-3.178294	-1.714378

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meta-**F**

Number of imaginary frequencies : 1
The smallest frequency is : -1560.8841 cm(-1)

Electronic energy : =-1970.1895143
Zero-point correction= 0.349461
Thermal correction to Energy= 0.380176
Thermal correction to Enthalpy= 0.381120
Thermal correction to Gibbs Free Energy= 0.284808
Sum of electronic and zero-point Energies= -1969.840053
Sum of electronic and thermal Energies= -1969.809338
Sum of electronic and thermal Enthalpies= -1969.808394
Sum of electronic and thermal Free Energies= -1969.904707

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Cartesian Coordinates

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46	1.265041	0.559159	-0.100776
6	-2.109236	-1.316243	2.361321
1	-3.068261	-1.411184	2.869525
6	-1.028266	-0.749625	3.030048
6	0.180835	-0.594797	2.365346
6	0.322345	-1.015977	1.030281

6	-0.770725	-1.625401	0.386813
6	-1.990741	-1.771787	1.041827
1	-1.142344	-0.417358	4.058993
1	1.028400	-0.134323	2.872420
1	1.489375	-1.575327	0.772350
1	-0.657096	-1.956401	-0.645346
6	-3.202226	-2.394851	0.411139
1	-4.115858	-2.155073	0.968320
1	-3.137393	-3.490412	0.343970
8	-4.956195	-2.195684	-1.549213
6	-3.971263	0.599315	-0.531961
6	-3.174287	1.576464	0.089821
6	-5.348500	0.625929	-0.400541
6	-3.770290	2.588028	0.850553
6	-5.925721	1.631118	0.373557
1	-5.962391	-0.113972	-0.903732
6	-5.149348	2.607077	0.992591
1	-3.142698	3.338895	1.322098
1	-7.007115	1.654110	0.479784
1	-5.620946	3.387191	1.582826
6	-1.764083	1.478830	-0.040101
7	-0.619697	1.334786	-0.149245
6	3.181795	4.188831	-1.267029
6	2.611124	3.038801	-0.473771
8	2.004359	2.160426	-1.205729
8	2.728476	2.978888	0.754153
1	3.885454	3.814641	-2.018293
1	3.691415	4.895874	-0.608270
6	4.901086	-1.785752	0.174685
6	3.470376	-1.333386	0.252952
8	3.200284	-0.152028	-0.101682
8	2.636387	-2.177382	0.676980
1	4.931677	-2.687598	-0.451874
1	5.201667	-2.102460	1.183056
7	5.774265	-0.760036	-0.335713
1	5.377639	0.140067	-0.579421
6	7.091952	-0.980519	-0.473891
8	7.647205	-2.037880	-0.194837
1	2.378680	4.704752	-1.804251
8	-3.284259	-0.306250	-1.322638
8	-2.538307	-2.427454	-2.188303
16	-3.554333	-1.929504	-1.283283
1	7.632686	-0.101364	-0.870907

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meta-**G**

Number of imaginary frequencies : 1
The smallest frequency is : -1342.4979 cm(-1)

Electronic energy : =-1741.1576366
Zero-point correction= 0.285878
Thermal correction to Energy= 0.310319
Thermal correction to Enthalpy= 0.311263
Thermal correction to Gibbs Free Energy= 0.231019
Sum of electronic and zero-point Energies= -1740.871759
Sum of electronic and thermal Energies= -1740.847317
Sum of electronic and thermal Enthalpies= -1740.846373
Sum of electronic and thermal Free Energies= -1740.926617

Cartesian Coordinates

46	-1.978157	0.220291	0.249318
6	-1.133876	-1.690481	0.626893
6	-1.064155	-2.151541	1.950591
6	0.022471	-2.909744	2.374849
6	1.085760	-3.131473	1.505208
6	1.043475	-2.667089	0.186556
6	-0.084125	-1.980893	-0.255210
1	-2.599084	-1.698231	0.184554
1	1.971003	-3.662322	1.852613
1	0.068026	-3.287937	3.393359
1	-1.869231	-1.915029	2.646148
1	-0.117928	-1.605618	-1.278663
6	2.246339	-2.817389	-0.690441
8	2.074357	-0.476990	-2.027059
6	3.323883	0.821778	0.326191
6	2.319230	1.803195	0.351926
6	4.660586	1.176618	0.354222
6	2.675746	3.156270	0.408598
6	5.001067	2.526089	0.404651
1	5.419326	0.399067	0.347106
6	4.016620	3.510277	0.431175
1	1.893374	3.909989	0.431540
1	6.050439	2.807831	0.426256
1	4.294483	4.559449	0.472303
6	0.948727	1.430664	0.321769
7	-0.174193	1.144627	0.305848
6	-4.512986	0.904242	-0.922239
6	-4.370842	-0.607649	-0.834643
8	-3.582260	-1.029269	0.202529
8	-4.942978	-1.388127	-1.549137
1	-5.452041	1.145252	-0.396085

1	-4.684556	1.121852	-1.985883
7	-3.369180	1.618472	-0.387093
6	-3.448867	2.921276	-0.140775
8	-2.561478	3.626155	0.354658
8	2.960239	-0.518897	0.315983
8	4.343562	-1.438572	-1.590217
1	3.059387	-3.368625	-0.204768
1	2.034675	-3.294194	-1.657346
16	2.965550	-1.245134	-1.171257
1	-4.423696	3.376291	-0.440962

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ortho-**A**

Number of imaginary frequencies : 1
The smallest frequency is : -1651.5642 cm(-1)

Electronic energy : =-1801.5823395
Zero-point correction= 0.322244
Thermal correction to Energy= 0.349652
Thermal correction to Enthalpy= 0.350597
Thermal correction to Gibbs Free Energy= 0.264237
Sum of electronic and zero-point Energies= -1801.260095
Sum of electronic and thermal Energies= -1801.232687
Sum of electronic and thermal Enthalpies= -1801.231743
Sum of electronic and thermal Free Energies= -1801.318102

Cartesian Coordinates

46	-1.674634	0.226145	-0.838814
6	-0.814961	-1.741337	-0.596429
1	-1.948617	-1.868368	0.001162
8	-3.038316	-2.139913	0.734275
8	-3.470100	-0.028681	0.124487
6	-0.704332	-2.413950	-1.826317
6	0.453807	-3.100717	-2.166314
6	1.508473	-3.145587	-1.258594
6	1.412413	-2.520604	-0.015052
6	0.270892	-1.797935	0.313797
1	-1.544231	-2.387667	-2.519355
1	0.535647	-3.605130	-3.126031
1	2.416999	-3.688413	-1.509933
1	2.237904	-2.601365	0.688430
6	0.104564	-1.127097	1.649018
1	-0.097262	-1.851829	2.451690

1	-0.716126	-0.396749	1.644002
8	2.667418	-1.077305	2.454239
6	2.929355	0.772392	0.264597
6	2.677366	0.742780	-1.118315
6	4.227595	0.801350	0.741281
6	3.736744	0.734181	-2.029181
6	5.276080	0.781134	-0.176107
1	4.416594	0.849852	1.809341
6	5.037363	0.748633	-1.548500
1	3.526033	0.716513	-3.094531
1	6.298112	0.802425	0.192868
1	5.869846	0.740962	-2.245981
6	1.312406	0.700985	-1.494953
7	0.164258	0.644346	-1.645832
6	-3.763369	-1.108934	0.725643
6	-5.048404	-1.138029	1.492210
1	-5.572128	-2.078917	1.302203
1	-4.809506	-1.102912	2.561122
1	-5.684317	-0.288113	1.239422
6	-1.774602	2.952481	-0.151842
6	-2.169505	4.403419	-0.272969
1	-1.719524	4.992888	0.529347
1	-1.849543	4.799398	-1.242681
1	-3.259730	4.497826	-0.229403
8	-2.266331	2.204240	-1.089274
8	-1.050153	2.552665	0.766161
8	1.821181	0.867140	1.087035
8	1.039399	0.595326	3.395905
16	1.507946	-0.218142	2.292509

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ortho-**B**

Number of imaginary frequencies : 1
The smallest frequency is : -1637.4965 cm(-1)

Electronic energy : =-1970.1935301
Zero-point correction= 0.350304
Thermal correction to Energy= 0.380629
Thermal correction to Enthalpy= 0.381574
Thermal correction to Gibbs Free Energy= 0.286497
Sum of electronic and zero-point Energies= -1969.843226
Sum of electronic and thermal Energies= -1969.812901
Sum of electronic and thermal Enthalpies= -1969.811957
Sum of electronic and thermal Free Energies= -1969.907033

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Cartesian Coordinates

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46	1.250246	-0.577695	-0.004396
6	-0.269826	-1.516660	1.209887
1	0.336635	-2.538037	0.700103
8	0.906289	-3.675744	0.282690
8	2.501711	-2.188317	-0.221453
6	0.048647	-1.235453	2.550924
6	-0.931639	-0.854062	3.457522
6	-2.255866	-0.792367	3.034821
6	-2.609715	-1.116810	1.724219
6	-1.625941	-1.447934	0.799359
1	1.087651	-1.310709	2.870773
1	-0.671655	-0.615008	4.485708
1	-3.035609	-0.504294	3.736388
1	-3.658079	-1.098938	1.437067
6	-1.938683	-1.844582	-0.617310
1	-2.260467	-2.895250	-0.679589
1	-1.063145	-1.729361	-1.270049
8	-4.496636	-0.998469	-0.729237
6	-3.186408	1.567523	-0.712166
6	-2.264316	2.191374	0.145844
6	-4.491647	2.017290	-0.789880
6	-2.657438	3.275915	0.934121
6	-4.875524	3.092371	0.008958
1	-5.192069	1.543967	-1.471289
6	-3.969333	3.720051	0.860930
1	-1.934018	3.751559	1.589825
1	-5.900272	3.450014	-0.046958
1	-4.286499	4.562966	1.467962
6	-0.964739	1.628584	0.178052
7	0.034203	1.044882	0.118961
6	2.068242	-3.377734	-0.105186
6	4.623297	1.665036	-1.373864
6	3.623609	0.915855	-0.493185
8	2.623836	0.471631	-1.174256
8	3.805226	0.772407	0.715362
1	4.067501	2.378238	-1.992635
7	5.647210	2.349916	-0.628605
1	6.544232	1.903578	-0.489356
6	5.348710	3.433250	0.112193
8	4.251428	3.979945	0.129918
16	-3.253439	-0.983509	-1.478036
8	-3.223698	-1.417466	-2.859772
8	-2.692413	0.568372	-1.533842
6	3.029784	-4.478807	-0.424014
1	3.589714	-4.720606	0.486872
1	2.492233	-5.374280	-0.743295

1	3.741775	-4.161690	-1.188875
1	5.089975	0.946059	-2.054021
1	6.212688	3.802403	0.697011

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ortho-**C**

Number of imaginary frequencies : 1
The smallest frequency is : -1642.4016 cm(-1)

Electronic energy : =-1741.2077489
Zero-point correction= 0.286403
Thermal correction to Energy= 0.310656
Thermal correction to Enthalpy= 0.311601
Thermal correction to Gibbs Free Energy= 0.231885
Sum of electronic and zero-point Energies= -1740.921346
Sum of electronic and thermal Energies= -1740.897092
Sum of electronic and thermal Enthalpies= -1740.896148
Sum of electronic and thermal Free Energies= -1740.975863

Cartesian Coordinates

46	-1.583172	-0.333025	-0.436695
6	-1.409885	2.190103	-1.782621
6	-0.536615	2.957412	-2.541588
6	0.677323	3.355977	-1.986038
6	1.008493	3.002636	-0.680706
6	0.152808	2.201717	0.072278
6	-1.078162	1.773370	-0.477903
1	1.941392	3.356166	-0.243829
1	1.365166	3.967543	-2.565708
1	-0.800219	3.255732	-3.553474
1	-2.047579	1.815332	0.393973
6	0.512896	1.910421	1.499502
1	-0.362716	1.639808	2.105346
1	1.009249	2.767072	1.970709
8	1.022490	-0.753400	1.662848
6	3.363100	-0.323730	0.035247
6	2.764713	-1.159485	-0.922470
6	4.659913	-0.541545	0.458139
6	3.491984	-2.220725	-1.469254
6	5.376389	-1.600288	-0.095883
1	5.093786	0.120752	1.202878
6	4.799910	-2.430589	-1.054607
1	3.022889	-2.867511	-2.205085

1	6.398912	-1.776657	0.227343
1	5.371571	-3.251157	-1.478252
6	1.398912	-0.925517	-1.228750
7	0.271750	-0.685380	-1.363335
6	-4.049786	-1.437373	0.658312
6	-3.280060	-2.595817	0.052441
8	-2.134243	-2.327978	-0.495076
8	-3.765597	-3.722961	0.081783
1	-4.312037	-1.697011	1.692299
7	-3.282006	-0.200852	0.601839
6	-3.641043	0.857031	1.275096
8	-3.029522	1.965879	1.268848
1	-2.373517	1.897321	-2.198445
8	2.655013	0.768126	0.509982
8	2.422751	0.823236	3.010159
16	1.656300	0.547505	1.806879
1	-4.552701	0.772050	1.887611
1	-4.989770	-1.341541	0.097472

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ortho-**D**

Number of imaginary frequencies : 1
The smallest frequency is : -1686.2087 cm(-1)

Electronic energy : =-1970.1761744
Zero-point correction= 0.349971
Thermal correction to Energy= 0.379842
Thermal correction to Enthalpy= 0.380786
Thermal correction to Gibbs Free Energy= 0.288610
Sum of electronic and zero-point Energies= -1969.826204
Sum of electronic and thermal Energies= -1969.796333
Sum of electronic and thermal Enthalpies= -1969.795388
Sum of electronic and thermal Free Energies= -1969.887564

Cartesian Coordinates

46	-1.304278	-0.969558	0.138490
6	-0.508753	0.648276	1.325419
1	-1.484065	1.415223	1.030729
6	-0.587348	0.188398	2.660797
6	0.494736	0.274622	3.523685
6	1.671808	0.862555	3.069986
6	1.777825	1.365873	1.770488
6	0.716315	1.232946	0.886531
1	-1.526910	-0.238254	3.012907
1	0.423573	-0.097143	4.542501

1	2.524580	0.949264	3.739526
1	2.701315	1.851355	1.464481
6	0.748929	1.785848	-0.510942
1	0.556456	2.870574	-0.519701
1	-0.004066	1.312182	-1.153948
8	3.390903	2.264892	-0.727457
6	3.524620	-0.601390	-0.761807
6	3.126146	-1.600425	0.143501
6	4.865582	-0.338718	-0.973715
6	4.082364	-2.340243	0.843749
6	5.810139	-1.074409	-0.261814
1	5.166624	0.420737	-1.689121
6	5.426475	-2.067302	0.637501
1	3.759986	-3.113238	1.535135
1	6.865630	-0.871847	-0.423769
1	6.180562	-2.633925	1.175824
6	1.728605	-1.767457	0.302626
7	0.570952	-1.767648	0.348617
8	-2.295741	2.516698	1.035398
6	-2.591825	2.991503	-0.120531
6	-2.819716	4.476391	-0.175629
8	-2.676434	2.300346	-1.157143
6	-3.758771	-1.031929	-1.410496
6	-3.158938	-2.421907	-1.498773
8	-2.031898	-2.612426	-0.882546
8	-3.714314	-3.284413	-2.168431
1	-4.848878	-1.100849	-1.343677
1	-3.504297	-0.494595	-2.331605
1	-3.444546	4.797728	0.663425
1	-1.854150	4.986523	-0.072681
1	-3.278442	4.772037	-1.122006
7	-3.226787	-0.238676	-0.285065
1	-3.048162	0.761396	-0.553164
6	-3.890405	-0.398406	0.954918
8	-4.603922	-1.341844	1.197998
8	2.517728	0.020047	-1.480546
8	1.995596	2.017469	-2.806992
16	2.279449	1.654983	-1.433870
1	-3.670822	0.425529	1.656411

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ortho-**E**

Number of imaginary frequencies : 1
The smallest frequency is : -1649.8461 cm(-1)

Electronic energy : =-1801.5775047
Zero-point correction= 0.322065
Thermal correction to Energy= 0.349606
Thermal correction to Enthalpy= 0.350550
Thermal correction to Gibbs Free Energy= 0.262971
Sum of electronic and zero-point Energies= -1801.255440
Sum of electronic and thermal Energies= -1801.227898
Sum of electronic and thermal Enthalpies= -1801.226954
Sum of electronic and thermal Free Energies= -1801.314534

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Cartesian Coordinates

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46	1.986811	0.807206	0.196631
6	1.772396	-1.189268	0.868935
1	2.672734	-1.363897	-0.029060
8	3.607102	-1.655054	-0.956035
8	3.549593	0.578533	-1.110977
6	2.230092	-1.270341	2.199161
6	1.477063	-1.909044	3.174074
6	0.256423	-2.486577	2.827094
6	-0.204920	-2.443168	1.513282
6	0.536736	-1.791927	0.532455
1	3.192411	-0.829861	2.455178
1	1.835967	-1.964659	4.198795
1	-0.338847	-2.990334	3.585232
1	-1.146952	-2.923253	1.249135
6	0.053709	-1.816167	-0.884514
1	0.881185	-1.773521	-1.606180
1	-0.551364	-2.707286	-1.091434
8	-1.943691	-0.958609	-2.420585
6	-3.152210	0.226654	-0.116775
6	-4.221793	-0.676167	-0.137264
6	-3.356423	1.592780	-0.166901
6	-5.528690	-0.185210	-0.197338
6	-4.663850	2.068832	-0.231669
1	-2.497985	2.260907	-0.147752
6	-5.741775	1.186463	-0.244774
1	-6.361375	-0.882949	-0.210118
1	-4.839872	3.140621	-0.269338
1	-6.757008	1.570112	-0.292632
6	-3.936735	-2.073666	-0.103762
7	-3.671308	-3.206081	-0.074155
6	4.014428	-0.558960	-1.428839
6	5.121214	-0.592164	-2.436992
1	5.981845	-1.112243	-2.004859
1	4.791716	-1.170387	-3.306373
1	5.409128	0.412922	-2.748604
6	-0.263982	3.806510	1.507050

6	0.599037	2.716844	0.986092
8	1.517281	2.949313	0.142687
8	0.440606	1.514004	1.399204
1	0.336669	4.454161	2.155990
1	-1.102408	3.403698	2.080186
1	-0.628721	4.420025	0.677277
8	-1.869769	-0.289612	0.000678
8	-0.309711	0.770179	-1.649269
16	-1.027929	-0.470970	-1.401432

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ortho-**F**

Number of imaginary frequencies : 1
The smallest frequency is : -1634.2989 cm(-1)

Electronic energy : =-1970.188653
Zero-point correction= 0.349342
Thermal correction to Energy= 0.380182
Thermal correction to Enthalpy= 0.381126
Thermal correction to Gibbs Free Energy= 0.283951
Sum of electronic and zero-point Energies= -1969.839311
Sum of electronic and thermal Energies= -1969.808471
Sum of electronic and thermal Enthalpies= -1969.807527
Sum of electronic and thermal Free Energies= -1969.904702

Cartesian Coordinates

46	0.998899	0.787369	0.161787
6	0.121846	-0.659929	1.505920
1	1.223440	-1.246523	1.162975
6	0.122035	-0.107193	2.800272
6	-0.959484	-0.275929	3.653136
6	-2.045232	-1.036989	3.228754
6	-2.055993	-1.631636	1.967069
6	-0.997372	-1.422761	1.088829
1	0.990013	0.464790	3.127015
1	-0.955255	0.168549	4.645181
1	-2.892098	-1.190147	3.893770
1	-2.899232	-2.253152	1.676568
6	-0.931525	-2.088240	-0.256785
1	-0.705773	-3.161770	-0.167017
1	-0.159497	-1.640524	-0.896192
8	-3.563951	-2.601909	-0.538204
6	-3.717193	0.210552	-1.017102

6	-3.405401	1.329883	-0.226441
6	-5.032526	-0.098766	-1.311407
6	-4.423584	2.147178	0.271468
6	-6.039906	0.715291	-0.799004
1	-5.264374	-0.955844	-1.936796
6	-5.742272	1.829913	-0.017505
1	-4.168240	3.013483	0.874784
1	-7.075736	0.477034	-1.026126
1	-6.542986	2.456499	0.364291
6	-2.027059	1.539597	0.025986
7	-0.876102	1.563430	0.155114
6	2.853578	4.299518	-1.374764
6	2.334831	3.201952	-0.478977
8	1.678884	2.282675	-1.113173
8	2.528142	3.216726	0.740765
1	3.437849	3.874761	-2.197331
1	3.469800	5.000239	-0.806150
6	4.507649	-1.749827	0.078664
6	3.133664	-1.200429	0.344698
8	2.894992	-0.008221	-0.003143
8	2.314942	-1.972143	0.907435
1	4.390211	-2.684244	-0.486081
1	4.943057	-2.029831	1.048485
7	5.345649	-0.816682	-0.629903
1	4.992367	0.116174	-0.807550
6	6.578943	-1.162168	-1.034949
8	7.083623	-2.263845	-0.845973
1	2.010630	4.838177	-1.821429
8	-2.647317	-0.485569	-1.552629
8	-2.059418	-2.651289	-2.554076
16	-2.413728	-2.095192	-1.263666
1	7.100114	-0.342330	-1.563622

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para-**A**

Number of imaginary frequencies : 1
The smallest frequency is : -1503.9278 cm(-1)

Electronic energy : =-1801.5866397
Zero-point correction= 0.322406
Thermal correction to Energy= 0.349857
Thermal correction to Enthalpy= 0.350801
Thermal correction to Gibbs Free Energy= 0.263659
Sum of electronic and zero-point Energies= -1801.264234
Sum of electronic and thermal Energies= -1801.236783
Sum of electronic and thermal Enthalpies= -1801.235839

Sum of electronic and thermal Free Energies= -1801.322981

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Cartesian Coordinates

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46	2.133131	0.221566	-0.157693
6	0.747756	-2.046326	1.130428
6	1.396146	-1.801447	-0.094527
6	0.710450	-2.091431	-1.289753
6	-0.603278	-2.531639	-1.262610
6	-1.251456	-2.704057	-0.035949
6	-0.559357	-2.507872	1.163574
1	-1.151895	-2.704749	-2.187326
1	1.204062	-1.925066	-2.246523
1	2.700261	-2.042237	-0.102133
1	-1.065767	-2.670532	2.113482
6	-2.715083	-3.000288	-0.016839
8	-3.240961	-0.963212	1.676796
6	-3.372843	0.801690	-0.568110
6	-2.255765	1.609936	-0.317576
6	-4.644091	1.345693	-0.612619
6	-2.426272	2.983658	-0.101017
6	-4.801494	2.711719	-0.391556
1	-5.495645	0.704276	-0.823666
6	-3.701908	3.526611	-0.133533
1	-1.551091	3.596699	0.100965
1	-5.798869	3.142011	-0.424159
1	-3.839060	4.590014	0.039855
6	-0.940937	1.072220	-0.294063
7	0.162175	0.721643	-0.283435
8	-3.170933	-0.553319	-0.792728
8	-5.093412	-1.832043	0.227231
16	-3.680964	-1.554272	0.424368
1	-3.005743	-3.736806	0.743695
1	-3.106211	-3.325569	-0.987280
8	4.145029	-0.135128	-0.024144
8	2.674781	2.219970	-0.370659
6	4.630747	-1.305535	-0.038148
6	6.119858	-1.438513	-0.000061
1	6.605000	-0.468158	0.115219
1	6.401506	-2.101989	0.823236
1	6.454229	-1.910986	-0.929760
6	2.184647	3.045198	0.498443
6	2.510468	4.489021	0.196358
1	1.950222	4.806832	-0.690679
1	2.238495	5.129548	1.039032
1	3.574227	4.607160	-0.031904
8	3.944717	-2.366105	-0.088846
8	1.501392	2.733142	1.477058
1	1.271997	-1.843914	2.063661

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para-**B**

Number of imaginary frequencies : 1
The smallest frequency is : -1559.4469 cm(-1)

Electronic energy : =-1970.2012183
Zero-point correction= 0.350764
Thermal correction to Energy= 0.380911
Thermal correction to Enthalpy= 0.381855
Thermal correction to Gibbs Free Energy= 0.287701
Sum of electronic and zero-point Energies= -1969.850454
Sum of electronic and thermal Energies= -1969.820307
Sum of electronic and thermal Enthalpies= -1969.819363
Sum of electronic and thermal Free Energies= -1969.913517

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Cartesian Coordinates

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6	-1.268630	-2.696212	-1.253757
6	0.078423	-2.411937	-1.404804
6	0.914569	-2.290713	-0.278261
6	0.372355	-2.532912	0.998096
6	-0.975526	-2.816449	1.153891
6	-1.804192	-2.853990	0.028397
1	-1.926939	-2.748083	-2.119463
1	0.488931	-2.244280	-2.399540
1	2.153130	-2.716884	-0.436145
1	-1.399781	-2.969980	2.144583
6	-3.285340	-2.938900	0.195799
8	-3.342500	-0.782865	1.826007
6	-3.453569	0.880220	-0.580114
6	-2.248655	1.587034	-0.448495
6	-4.660381	1.549232	-0.680017
6	-2.267841	2.988254	-0.427630
6	-4.667560	2.941312	-0.644773
1	-5.579502	0.981718	-0.796918
6	-3.479941	3.656589	-0.522246
1	-1.325521	3.526006	-0.332188
1	-5.614759	3.468531	-0.723681
1	-3.496339	4.742566	-0.503015
6	-0.996677	0.916727	-0.350155
7	0.052419	0.428870	-0.283060
46	1.926789	-0.403754	-0.217895
6	5.627034	-2.635303	-0.314748

6	4.172583	-2.286844	-0.324061
8	3.341822	-3.218756	-0.516355
8	3.860377	-1.070514	-0.146281
1	1.016025	-2.466704	1.874407
1	6.241555	-1.775643	-0.043374
1	5.797428	-3.459084	0.384834
1	5.909136	-2.988439	-1.312425
8	-5.424074	-1.394287	0.569576
8	-3.407397	-0.503886	-0.663897
16	-3.973595	-1.342631	0.642720
1	-3.599521	-3.595217	1.017276
1	-3.814594	-3.236116	-0.716935
6	3.232664	3.460070	1.112327
6	2.755533	2.012986	1.013095
8	2.466286	1.418574	2.055285
8	2.736445	1.523052	-0.174396
1	4.309349	3.450417	1.308265
7	2.984017	4.255838	-0.066005
1	3.754336	4.575480	-0.638433
6	1.728780	4.446160	-0.498794
8	0.734413	4.019317	0.084899
1	1.670483	5.036301	-1.431509
1	2.741998	3.904200	1.986154

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para-**C**

Number of imaginary frequencies : 1
The smallest frequency is : -1564.5696 cm(-1)

Electronic energy : =-1741.2137093
Zero-point correction= 0.287154
Thermal correction to Energy= 0.311158
Thermal correction to Enthalpy= 0.312102
Thermal correction to Gibbs Free Energy= 0.232929
Sum of electronic and zero-point Energies= -1740.926555
Sum of electronic and thermal Energies= -1740.902552
Sum of electronic and thermal Enthalpies= -1740.901607
Sum of electronic and thermal Free Energies= -1740.980780

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Cartesian Coordinates

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46	2.144041	0.169126	-0.024077
6	0.691577	-2.173119	0.970368
6	1.290251	-1.795728	-0.247476

6	0.518262	-1.858996	-1.423365
6	-0.820022	-2.215785	-1.375235
6	-1.411178	-2.521907	-0.145493
6	-0.644983	-2.538827	1.023360
1	-1.428057	-2.221971	-2.278646
1	0.970367	-1.589401	-2.377046
1	2.558842	-2.155557	-0.377381
1	-1.110883	-2.803048	1.971237
6	-2.888713	-2.723412	-0.068837
8	-3.173755	-0.732251	1.737948
6	-3.331336	1.127692	-0.483385
6	-2.190896	1.890894	-0.192614
6	-4.577290	1.721930	-0.581385
6	-2.316868	3.273617	-0.002928
6	-4.688667	3.095446	-0.382187
1	-5.443369	1.111013	-0.821542
6	-3.566536	3.867692	-0.094783
1	-1.429732	3.861602	0.216414
1	-5.665423	3.565444	-0.460645
1	-3.664157	4.939128	0.054197
6	-0.901313	1.295915	-0.106195
7	0.177666	0.877532	-0.040646
6	4.992806	0.756036	0.222682
6	4.261179	2.081481	0.315280
8	2.967346	2.055544	0.227085
8	4.906618	3.113521	0.476883
1	5.537491	0.614201	1.166051
7	4.071642	-0.347433	-0.019838
6	4.510105	-1.553486	-0.248677
8	3.780723	-2.566843	-0.466134
1	1.282639	-2.155912	1.885338
8	-3.180713	-0.232071	-0.715616
8	-5.156322	-1.388398	0.350975
1	-3.193380	-3.476480	0.669273
1	-3.350139	-2.966960	-1.032872
16	-3.717922	-1.232492	0.486405
1	5.601671	-1.698723	-0.252178
1	5.740421	0.833367	-0.577650

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para-**D**

Number of imaginary frequencies : 1
The smallest frequency is : -1792.4581 cm(-1)

Electronic energy : =-1970.1822633
Zero-point correction= 0.350578
Thermal correction to Energy= 0.380374
Thermal correction to Enthalpy= 0.381318
Thermal correction to Gibbs Free Energy= 0.288608
Sum of electronic and zero-point Energies= -1969.831686
Sum of electronic and thermal Energies= -1969.801889
Sum of electronic and thermal Enthalpies= -1969.800945
Sum of electronic and thermal Free Energies= -1969.893656

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Cartesian Coordinates

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46	1.511014	0.696233	0.082525
6	0.455165	-1.698569	1.315435
6	1.092581	-1.411618	0.085455
6	0.402134	-1.718672	-1.110445
6	-0.875783	-2.249344	-1.078144
6	-1.495105	-2.487223	0.154493
6	-0.816808	-2.243597	1.353919
1	0.978426	-1.480826	2.246876
8	3.432900	-2.531622	0.137979
1	-1.418075	-2.458311	-1.998814
1	0.882633	-1.517682	-2.067983
1	2.332962	-1.798686	0.085913
1	-1.300810	-2.459515	2.304629
6	-2.919135	-2.938819	0.186533
8	-3.660392	-0.859435	1.742962
6	-3.986865	0.701048	-0.654068
6	-2.987349	1.644220	-0.375075
6	-5.295332	1.095508	-0.865206
6	-3.316558	3.004785	-0.316782
6	-5.611309	2.450082	-0.794909
1	-6.050694	0.347682	-1.090249
6	-4.629682	3.399548	-0.523479
1	-2.536288	3.731698	-0.109140
1	-6.638571	2.763882	-0.960303
1	-4.887469	4.453570	-0.477079
6	-1.639310	1.245732	-0.166893
7	-0.524747	0.976011	-0.003263
6	5.029074	-3.589478	-1.245875
6	4.147500	-2.415622	-0.926563
8	4.132224	-1.408431	-1.661738
6	4.061541	1.958102	-0.402311
6	3.090307	3.083591	-0.097253
8	1.858997	2.741612	0.130592
8	3.474620	4.246672	-0.128058
1	5.051147	2.193452	0.000897
1	4.405446	-4.459148	-1.481988
1	5.683305	-3.370607	-2.092824

1	5.629937	-3.855117	-0.369785
7	3.597540	0.652109	0.105696
1	3.836061	-0.144105	-0.532044
6	3.856030	0.400153	1.476547
8	4.144334	1.277322	2.254699
16	-4.037372	-1.584357	0.541180
8	-3.629895	-0.636748	-0.750569
8	-5.410566	-2.026812	0.375854
1	-3.126546	-3.662337	0.985447
1	-3.266375	-3.356850	-0.765158
1	3.758481	-0.669021	1.734767
1	4.143843	1.868675	-1.491275

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para-**E**

Number of imaginary frequencies : 1
The smallest frequency is : -1631.1391 cm(-1)

Electronic energy : =-1801.5712219
Zero-point correction= 0.321664
Thermal correction to Energy= 0.349635
Thermal correction to Enthalpy= 0.350579
Thermal correction to Gibbs Free Energy= 0.258429
Sum of electronic and zero-point Energies= -1801.249558
Sum of electronic and thermal Energies= -1801.221587
Sum of electronic and thermal Enthalpies= -1801.220643
Sum of electronic and thermal Free Energies= -1801.312793

Cartesian Coordinates

46	-3.761566	0.371103	-0.163254
6	-0.069421	-0.304730	1.509030
1	0.328273	-0.276624	2.522284
8	-3.451741	-2.767082	-0.374250
8	-5.054981	-1.218505	-0.172717
6	-1.400566	-0.615584	1.278355
6	-1.909026	-0.654796	-0.034858
6	-1.044599	-0.375682	-1.112218
6	0.288546	-0.076579	-0.882444
6	0.773970	-0.026662	0.428726
1	-2.056920	-0.848379	2.115338
1	-2.707367	-1.628041	-0.243394
1	-1.425594	-0.410201	-2.131312
1	0.963634	0.128658	-1.711732

6	2.218667	0.276834	0.673388
1	2.392070	0.812940	1.613891
1	2.673860	0.826357	-0.159992
8	3.092931	-1.970541	-0.450618
6	5.436914	-0.265801	-0.004529
6	5.756927	1.097816	-0.068306
6	5.947899	-1.162513	-0.927821
6	6.597658	1.558759	-1.087211
6	6.774844	-0.686656	-1.941173
1	5.706264	-2.217630	-0.844977
6	7.098835	0.665139	-2.022449
1	6.848475	2.615204	-1.129336
1	7.177089	-1.386616	-2.668946
1	7.750900	1.023350	-2.814086
6	5.232979	2.003463	0.901623
7	4.797908	2.743887	1.686224
6	-4.658715	-2.420102	-0.292905
6	-5.711924	-3.484170	-0.344683
1	-5.638216	-4.005829	-1.304554
1	-5.519379	-4.219206	0.442747
1	-6.712077	-3.064088	-0.228345
6	-4.120672	4.316295	-0.073744
6	-4.034731	2.837629	-0.151187
8	-2.890138	2.260338	-0.138805
8	-5.073106	2.109813	-0.199522
1	-4.081073	4.615149	0.980439
1	-5.065002	4.668028	-0.496575
1	-3.273746	4.778401	-0.588049
16	3.137748	-1.255660	0.811856
8	2.814233	-1.928722	2.053533
8	4.664802	-0.697157	1.067059

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para-**F**

Number of imaginary frequencies : 1
The smallest frequency is : -1405.8683 cm(-1)

Electronic energy : =-1970.1961453
Zero-point correction= 0.350818
Thermal correction to Energy= 0.380979
Thermal correction to Enthalpy= 0.381923
Thermal correction to Gibbs Free Energy= 0.287624
Sum of electronic and zero-point Energies= -1969.845328
Sum of electronic and thermal Energies= -1969.815166

Sum of electronic and thermal Enthalpies= -1969.814222
Sum of electronic and thermal Free Energies= -1969.908521

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Cartesian Coordinates

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6	-0.881144	-2.486704	-0.940633
6	0.332361	-1.826182	-1.043866
6	0.984172	-1.341124	0.105838
6	0.421024	-1.609891	1.367556
6	-0.785860	-2.282436	1.476626
6	-1.460906	-2.676412	0.317461
1	-1.414538	-2.813821	-1.831960
1	0.766277	-1.643376	-2.026070
1	2.317353	-1.410158	0.093121
1	-1.234845	-2.462807	2.451863
6	-2.861764	-3.182005	0.411763
8	-3.667310	-0.997893	1.788661
6	-4.065161	0.334252	-0.770798
6	-3.135272	1.374049	-0.621309
6	-5.398358	0.605437	-1.022238
6	-3.566567	2.703587	-0.728235
6	-5.814139	1.930765	-1.117158
1	-6.097127	-0.216097	-1.153257
6	-4.904724	2.974726	-0.970481
1	-2.841182	3.505276	-0.618563
1	-6.860736	2.146044	-1.315764
1	-5.237659	4.005468	-1.050483
6	-1.755576	1.112444	-0.391888
7	-0.616593	0.975037	-0.228329
46	1.411936	0.752030	-0.062713
8	3.463882	0.683501	0.060602
6	4.098093	-0.407501	0.117032
8	3.581219	-1.554592	0.142590
6	5.606591	-0.268066	0.156048
1	5.865788	0.302587	1.052841
6	6.397808	-2.256327	-0.978715
8	5.945367	-1.913677	-2.063617
7	6.318194	-1.514588	0.144983
8	-3.616217	-0.976529	-0.714456
16	-4.015239	-1.827433	0.646893
8	-5.378376	-2.311646	0.509767
1	-3.205674	-3.700438	-0.490367
1	-3.043179	-3.826484	1.281172
1	0.926967	-1.258003	2.265967
1	6.638431	-1.914970	1.017502
8	1.633981	2.815530	-0.273171
6	1.840334	3.410968	0.856506
8	1.849180	2.855564	1.960063
6	2.104320	4.890739	0.720126

1	3.117292	5.039030	0.328339
1	1.409917	5.347164	0.008326
1	2.025169	5.387173	1.690532
1	6.933136	-3.211360	-0.822421
1	5.892970	0.343180	-0.708149

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para-**H**

Number of imaginary frequencies : 1
The smallest frequency is : -1682.9780 cm(-1)

Electronic energy : =-1970.1847835
Zero-point correction= 0.350336
Thermal correction to Energy= 0.380612
Thermal correction to Enthalpy= 0.381556
Thermal correction to Gibbs Free Energy= 0.285308
Sum of electronic and zero-point Energies= -1969.834447
Sum of electronic and thermal Energies= -1969.804171
Sum of electronic and thermal Enthalpies= -1969.803227
Sum of electronic and thermal Free Energies= -1969.899475

Cartesian Coordinates

46	3.397133	0.034703	-0.007912
6	-0.365586	-0.569656	-1.543553
1	-0.794547	-0.561779	-2.544459
8	2.998379	-3.077377	0.296469
8	4.657845	-1.594098	0.065756
6	0.958154	-0.925858	-1.339811
6	1.507383	-0.937381	-0.041929
6	0.686766	-0.585271	1.047783
6	-0.638737	-0.235501	0.847128
6	-1.160611	-0.210776	-0.450463
1	1.579311	-1.210797	-2.187924
1	2.285682	-1.944927	0.165747
1	1.098238	-0.592180	2.055639
1	-1.276776	0.033317	1.687530
6	-2.595311	0.153823	-0.668434
1	-2.774672	0.613878	-1.647321
1	-2.989494	0.801268	0.124658
8	-3.589465	-1.895775	0.705066
6	-5.857692	-0.174655	0.068356
6	-6.119146	1.201361	0.018718
6	-6.417911	-0.973717	1.050970

6	-6.953376	1.776140	0.983957
6	-7.237183	-0.385669	2.009963
1	-6.215535	-2.040564	1.055898
6	-7.504480	0.980822	1.978247
1	-7.159337	2.842100	0.939511
1	-7.678290	-1.007611	2.784413
1	-8.151815	1.427397	2.727745
6	-5.545799	2.001914	-1.013488
7	-5.073263	2.657331	-1.850347
6	4.218926	-2.777974	0.207867
6	5.227149	-3.882519	0.276440
1	5.115604	-4.405080	1.232029
1	5.020406	-4.606241	-0.518039
1	6.244901	-3.501717	0.178376
6	4.526003	2.650413	-0.686614
6	3.040404	2.832979	-0.417550
8	2.345090	1.778104	-0.111353
8	2.542406	3.944501	-0.546966
1	5.069871	3.531599	-0.332345
1	4.660245	2.573179	-1.770292
7	5.075282	1.424341	-0.083787
1	5.787241	0.948587	-0.640273
6	5.406648	1.485044	1.282554
8	5.004059	2.359758	2.012715
8	-5.093799	-0.723077	-0.953758
8	-3.316801	-2.160758	-1.786630
16	-3.598889	-1.331263	-0.632411
1	6.043597	0.640416	1.599373

Different possibilities of Reductive elimination Transition States
at the SMD/M06/6-31G** Level of Theory

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6 coordination

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conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -290.9417 cm(-1)

Electronic energy : =-2793.1534207
Zero-point correction= 0.350787
Thermal correction to Energy= 0.388886

Thermal correction to Enthalpy= 0.389830
Thermal correction to Gibbs Free Energy= 0.277600
Sum of electronic and zero-point Energies= -2792.802634
Sum of electronic and thermal Energies= -2792.764535
Sum of electronic and thermal Enthalpies= -2792.763591
Sum of electronic and thermal Free Energies= -2792.875821

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Cartesian Coordinates

.....

46	0.951280	-0.541875	0.412424
6	0.955466	2.397390	-2.721234
6	1.496034	1.799860	-1.581225
6	0.568370	1.425592	-0.639712
6	-0.751484	1.786548	-0.587349
6	-1.264857	2.348973	-1.763871
6	-0.413207	2.630261	-2.830034
1	-1.384431	1.615612	0.275099
1	0.823173	-0.871691	-2.420128
1	2.561154	1.627009	-1.473918
1	-0.820009	3.064564	-3.740219
6	-2.736150	2.597429	-1.866084
1	-3.014604	3.017006	-2.839973
1	-3.134075	3.255545	-1.083444
8	-2.995600	-0.085592	-2.202458
6	-4.362861	-0.116674	0.461946
6	-3.525119	-1.039621	1.110860
6	-5.732381	-0.306415	0.438193
6	-4.074475	-2.160997	1.744616
6	-6.266487	-1.431445	1.063371
1	-6.371682	0.425333	-0.046793
6	-5.447337	-2.351546	1.713195
1	-3.416907	-2.863169	2.250049
1	-7.342436	-1.582946	1.048091
1	-5.881740	-3.218786	2.201608
6	-2.124618	-0.829041	1.098624
7	-0.985638	-0.620944	1.076242
6	0.167842	-3.454987	0.347060
6	0.917616	-3.377814	1.685009
8	1.486771	-2.287162	1.980426
8	0.871999	-4.410163	2.369715
1	-0.900427	-3.570925	0.578336
1	0.504493	-4.359345	-0.171601
7	0.364581	-2.303141	-0.528205
6	-0.182170	-2.287697	-1.692789
8	-0.039368	-1.344371	-2.579095
1	1.626206	2.673558	-3.530794
8	-3.784436	1.015694	-0.092620
8	-5.055027	1.350248	-2.248892
16	-3.716197	1.092731	-1.750647

8	2.886584	-0.678484	-0.164662
6	3.228951	-0.856787	-1.381017
8	2.547168	-0.925057	-2.394898
8	1.557298	1.341241	1.151329
6	0.938938	1.916924	2.147572
8	-0.206037	1.800615	2.514760
6	1.916375	2.879437	2.856043
6	4.765421	-0.897202	-1.511070
1	-0.816771	-3.122305	-2.009202
9	5.307862	-1.723644	-0.622799
9	5.246359	0.329467	-1.289469
9	5.134647	-1.278534	-2.725156
9	1.340819	3.447204	3.905020
9	2.302843	3.839100	2.014371
9	3.002768	2.227832	3.267367

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conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -274.6971 cm(-1)

Electronic energy : =-3022.1430582
Zero-point correction= 0.413107
Thermal correction to Energy= 0.457332
Thermal correction to Enthalpy= 0.458276
Thermal correction to Gibbs Free Energy= 0.330435
Sum of electronic and zero-point Energies= -3021.729951
Sum of electronic and thermal Energies= -3021.685726
Sum of electronic and thermal Enthalpies= -3021.684782
Sum of electronic and thermal Free Energies= -3021.812623

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Cartesian Coordinates

.....

46	-0.670872	-0.373993	-0.117894
6	1.634385	-3.983294	-0.507338
6	0.529240	-3.265362	-0.042591
6	0.829408	-2.000082	0.394517
6	2.064408	-1.472071	0.649262
6	3.141613	-2.202222	0.129948
6	2.917316	-3.442732	-0.463581
1	2.223952	-0.536645	1.171563
1	0.268027	-1.769252	-2.407917
1	-0.472951	-3.679400	-0.057229
1	3.757141	-4.004677	-0.865247
6	4.509496	-1.600372	0.189619
1	5.255738	-2.221522	-0.319183

1	4.865428	-1.401321	1.208437
8	3.605049	0.140319	-1.693594
6	3.957459	2.287810	0.330337
6	2.650822	2.773539	0.159478
6	5.041683	3.142571	0.267265
6	2.435208	4.137329	-0.070475
6	4.816102	4.497314	0.031168
1	6.043834	2.749337	0.412470
6	3.524971	4.992696	-0.134504
1	1.420305	4.505241	-0.193436
1	5.664707	5.174432	-0.016324
1	3.365914	6.052234	-0.311983
6	1.565397	1.863949	0.212885
7	0.701335	1.097239	0.287391
6	-1.145160	1.798844	-2.163903
6	-2.223401	2.121753	-1.132543
8	-2.371436	1.362546	-0.143783
8	-2.864567	3.172216	-1.369267
1	-0.367286	2.570466	-2.073409
1	-1.592041	1.883590	-3.160380
7	-0.556978	0.472170	-2.009749
6	0.305562	0.058148	-2.870743
8	0.860779	-1.119135	-2.872539
1	1.470776	-4.977250	-0.916199
8	4.131937	0.940270	0.615393
8	6.001021	0.290010	-0.949898
16	4.612246	-0.013164	-0.656731
8	-2.173867	-1.644704	-0.590030
6	-2.132604	-2.433466	-1.593210
8	-1.242317	-2.634344	-2.408328
8	-0.678429	-1.433889	1.705633
6	-0.241764	-0.898914	2.813732
8	0.524453	0.021362	2.973417
6	-0.844339	-1.657967	4.015322
6	-3.410291	-3.295570	-1.657656
1	0.620588	0.712682	-3.690156
9	-4.508569	-2.564950	-1.496426
9	-3.360098	-4.198133	-0.673049
9	-3.497606	-3.940762	-2.811819
9	-0.457929	-1.113281	5.159375
9	-0.444733	-2.930512	3.995513
9	-2.174480	-1.640460	3.965278
1	-3.984063	3.404714	-0.209275
8	-4.690408	3.533217	0.500085
6	-5.323889	4.675073	0.276713
6	-6.416590	4.921780	1.267307
1	-6.866040	5.903517	1.107214
1	-7.184304	4.146530	1.165127
1	-6.022598	4.851518	2.286491

8	-5.043830	5.427706	-0.641985

5-coordination

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conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -234.5002 cm(-1)

Electronic energy : =-3022.1594918
Zero-point correction= 0.415705
Thermal correction to Energy= 0.459203
Thermal correction to Enthalpy= 0.460148
Thermal correction to Gibbs Free Energy= 0.337244
Sum of electronic and zero-point Energies= -3021.743786
Sum of electronic and thermal Energies= -3021.700288
Sum of electronic and thermal Enthalpies= -3021.699344
Sum of electronic and thermal Free Energies= -3021.822248

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Cartesian Coordinates

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46	1.344499	0.328493	-0.233256
6	0.157688	-2.545925	2.643331
6	1.048212	-1.861853	1.802436
6	0.535120	-1.681826	0.553333
6	-0.573802	-2.190069	-0.049492
6	-1.427215	-2.866362	0.835656
6	-1.061340	-3.021506	2.173348
1	-0.823388	-2.060194	-1.099396
1	2.004514	-1.475823	2.141464
1	-1.732020	-3.548109	2.849145
6	-2.726507	-3.392328	0.318193
1	-3.089324	-4.249801	0.898657
1	-2.689956	-3.681247	-0.738463
8	-4.153843	-1.610102	1.752529
6	-3.930387	0.177881	-0.690642
6	-3.001297	1.200169	-0.949837
6	-5.279915	0.466520	-0.589326
6	-3.436507	2.525452	-1.092505
6	-5.694994	1.789025	-0.725268
1	-6.006782	-0.323313	-0.421271
6	-4.785742	2.813863	-0.975304
1	-2.711109	3.313667	-1.281712

1	-6.754759	2.015584	-0.642345
1	-5.128689	3.838800	-1.079625
6	-1.624388	0.884776	-1.036949
7	-0.496523	0.626219	-1.146441
6	0.877617	3.543856	-1.046718
6	0.331663	3.024506	0.274341
8	0.963299	2.007673	0.828359
8	-0.585605	3.588310	0.846311
1	1.387431	2.764098	-1.619477
1	1.644209	4.287569	-0.785100
7	-0.145269	4.150539	-1.858388
6	-0.740474	5.315025	-1.513745
8	-1.797157	5.713736	-1.985186
1	0.449080	-2.694505	3.680347
8	-3.410572	-1.096802	-0.604569
8	-5.251764	-2.762564	-0.187475
16	-4.063310	-2.205914	0.433255
8	3.055610	0.166967	0.838233
6	3.994073	0.907273	0.358665
8	3.967913	1.629153	-0.620666
8	1.974196	-1.487257	-0.994545
6	1.588117	-1.888103	-2.175883
8	0.852711	-1.340300	-2.962386
6	2.182443	-3.282218	-2.459548
6	5.265350	0.790800	1.222633
1	-0.676300	3.540927	-2.474690
8	-1.682046	0.395349	1.776962
6	-1.241303	0.505387	2.907301
6	-1.910010	-0.025624	4.133285
1	-2.347679	0.812615	4.688196
1	-2.704702	-0.723426	3.860410
1	-1.184130	-0.508289	4.794978
8	-0.102989	1.139245	3.185534
1	0.275042	1.507418	2.345028
1	-0.150343	5.895910	-0.777988
9	5.013176	1.197697	2.467735
9	6.250033	1.529360	0.731599
9	5.677158	-0.476346	1.279597
9	3.504505	-3.284709	-2.315082
9	1.665279	-4.152640	-1.588792
9	1.887738	-3.685005	-3.685643

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conf-5 **[6]**

Number of imaginary frequencies : 0

Electronic energy : =-3251.1797474
Zero-point correction= 0.480497
Thermal correction to Energy= 0.529747
Thermal correction to Enthalpy= 0.530691
Thermal correction to Gibbs Free Energy= 0.395205
Sum of electronic and zero-point Energies= -3250.699250
Sum of electronic and thermal Energies= -3250.650000
Sum of electronic and thermal Enthalpies= -3250.649056
Sum of electronic and thermal Free Energies= -3250.784543

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Cartesian Coordinates

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46	-1.581626	0.033077	-0.150867
6	-0.495620	-3.887001	-1.332449
6	-1.139779	-2.643280	-1.298313
6	-0.841865	-1.878639	-0.200630
6	-0.026293	-2.198893	0.851968
6	0.644375	-3.423715	0.750405
6	0.401486	-4.260514	-0.337871
1	0.144186	-1.552153	1.706415
1	-1.810232	-2.326395	-2.090846
1	0.929502	-5.209528	-0.410396
6	1.696777	-3.728890	1.764841
1	1.911024	-4.801331	1.854883
1	1.478610	-3.331644	2.763426
8	3.596487	-3.266327	-0.089969
6	3.610814	-0.468439	0.790013
6	2.891279	0.561427	0.161880
6	4.993970	-0.477463	0.739791
6	3.563411	1.546771	-0.574192
6	5.652016	0.524842	0.030540
1	5.555466	-1.255276	1.250981
6	4.946639	1.528204	-0.631138
1	2.988808	2.307014	-1.098892
1	6.738076	0.514045	-0.005288
1	5.473595	2.297523	-1.187869
6	1.481279	0.590542	0.230548
7	0.326120	0.661625	0.331359
6	-0.784849	2.715910	-1.837623
6	-0.418846	1.363551	-2.436933
8	-1.091188	0.295021	-2.106187
8	0.448124	1.309639	-3.307290
1	-1.430582	2.640709	-0.956806
1	-1.376707	3.224441	-2.611930
7	0.374825	3.502472	-1.500953
6	1.102062	4.175537	-2.397849
8	2.153857	4.768919	-2.133457

1	-0.699868	-4.550443	-2.169326
8	2.876367	-1.419415	1.470825
8	4.265801	-3.331802	2.331036
16	3.285016	-3.022453	1.306088
8	-3.375463	-0.699694	-0.680623
6	-4.230235	0.263284	-0.795095
8	-4.038076	1.454303	-0.646931
8	-2.094328	-0.312215	1.791662
6	-2.284732	0.806642	2.406359
8	-2.198643	1.936248	1.963936
6	-2.659320	0.548971	3.880207
6	-5.611131	-0.293721	-1.195750
1	0.727145	3.495331	-0.536208
8	1.919382	-1.215250	-1.938117
6	1.762701	-1.796349	-2.998062
6	2.371802	-3.115344	-3.346050
1	3.156526	-2.952372	-4.094536
1	2.816843	-3.580371	-2.463312
1	1.631445	-3.779181	-3.803166
8	1.043570	-1.291240	-3.996889
1	0.759545	-0.373736	-3.746625
1	2.892657	4.701832	-0.591943
8	3.471890	4.632373	0.219024
6	2.843120	4.000648	1.194831
6	3.703058	3.781103	2.393259
1	3.094503	3.485168	3.249422
1	4.415925	2.977426	2.165336
1	4.284804	4.677149	2.627255
8	1.687289	3.603977	1.108045
1	0.682452	4.179340	-3.419199
9	-5.543264	-0.819763	-2.418922
9	-5.996666	-1.250619	-0.354087
9	-6.526878	0.662642	-1.196521
9	-2.824625	1.687027	4.537270
9	-1.698851	-0.152379	4.483628
9	-3.790718	-0.152013	3.953259

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conf-5 **[6-7]**‡

Number of imaginary frequencies : 1
The smallest frequency is : -220.8016 cm(-1)

Electronic energy : =-3251.1577192
Zero-point correction= 0.480012

Thermal correction to Energy= 0.528775
Thermal correction to Enthalpy= 0.529719
Thermal correction to Gibbs Free Energy= 0.395046
Sum of electronic and zero-point Energies= -3250.677707
Sum of electronic and thermal Energies= -3250.628944
Sum of electronic and thermal Enthalpies= -3250.628000
Sum of electronic and thermal Free Energies= -3250.762673

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Cartesian Coordinates

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46	-1.511485	0.445948	0.008905
6	-1.402646	-3.337991	-1.863303
6	-1.986786	-2.249862	-1.197850
6	-1.241645	-1.839819	-0.133828
6	-0.166241	-2.401981	0.483128
6	0.372980	-3.490338	-0.219097
6	-0.238044	-3.934171	-1.392986
1	0.284081	-2.042288	1.404390
1	-2.896574	-1.767165	-1.541024
1	0.189788	-4.779754	-1.927478
6	1.601357	-4.149998	0.317624
1	1.679657	-5.198934	0.006087
1	1.671554	-4.110512	1.410918
8	3.109371	-3.199005	-1.708374
6	3.663187	-0.864926	0.023031
6	2.971773	0.352443	-0.078865
6	5.013903	-0.928752	-0.273617
6	3.640408	1.504537	-0.516706
6	5.667311	0.225573	-0.698863
1	5.557231	-1.863793	-0.164987
6	4.988983	1.436380	-0.824325
1	3.084973	2.434157	-0.616711
1	6.727622	0.173227	-0.931526
1	5.512182	2.328529	-1.156098
6	1.599051	0.430144	0.256513
7	0.484167	0.525013	0.567952
6	-0.278206	3.519660	-0.232999
6	-0.075001	2.561714	-1.397821
8	-0.978894	1.615858	-1.559820
8	0.825968	2.725438	-2.202927
1	-0.848766	3.064881	0.582140
1	-0.895333	4.341458	-0.624168
7	0.965752	4.028030	0.283693
6	1.699586	4.946641	-0.350832
8	2.851144	5.260270	-0.027397
1	-1.892833	-3.707979	-2.760609
8	2.942279	-1.952288	0.478990
8	4.249557	-4.098376	0.339182
16	3.124456	-3.416023	-0.274264

8	-3.378668	0.396655	-0.773087
6	-4.072935	1.435265	-0.460688
8	-3.745693	2.397482	0.208277
8	-2.341290	-0.855054	1.385121
6	-1.880106	-0.864657	2.607839
8	-0.936409	-0.269486	3.070246
6	-2.734476	-1.819143	3.466035
6	-5.498220	1.322192	-1.038839
1	1.425825	3.531509	1.056381
8	1.044617	-0.798748	-2.233061
6	0.456134	-0.914308	-3.292903
6	0.786908	-1.923911	-4.342148
1	1.255750	-1.413028	-5.191361
1	1.481724	-2.665957	-3.943089
1	-0.120857	-2.407452	-4.716627
8	-0.555561	-0.123320	-3.646574
1	-0.688245	0.550916	-2.932888
1	3.744679	4.355758	1.116325
8	4.397893	3.811506	1.641177
6	3.787693	2.837765	2.294169
6	4.737903	1.935446	3.006584
1	4.194393	1.140336	3.519642
1	5.439971	1.502310	2.283468
1	5.331736	2.507938	3.726985
8	2.572433	2.684097	2.300059
1	1.186752	5.439801	-1.195473
9	-5.465892	1.083997	-2.349750
9	-6.142764	0.311165	-0.452285
9	-6.190783	2.433317	-0.832446
9	-2.319954	-1.826303	4.723019
9	-2.639799	-3.057759	2.980344
9	-4.015135	-1.458877	3.442538

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conf-5 **[7]**

Number of imaginary frequencies : 0

Electronic energy : =-3251.2268216
Zero-point correction= 0.483210
Thermal correction to Energy= 0.532003
Thermal correction to Enthalpy= 0.532947
Thermal correction to Gibbs Free Energy= 0.397434
Sum of electronic and zero-point Energies= -3250.743612
Sum of electronic and thermal Energies= -3250.694819

Sum of electronic and thermal Enthalpies= -3250.693874
Sum of electronic and thermal Free Energies= -3250.829388

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Cartesian Coordinates

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46	-1.365901	-0.730169	-0.004551
6	-1.491863	3.660027	1.446395
6	-2.066233	2.649883	0.681837
6	-1.368552	2.219608	-0.432749
6	-0.136563	2.713286	-0.813212
6	0.425588	3.722969	-0.034510
6	-0.252343	4.185281	1.095196
1	0.373223	2.313148	-1.687408
1	-3.018956	2.192588	0.940070
1	0.199745	4.965862	1.704726
6	1.760546	4.285336	-0.396210
1	1.872377	5.332510	-0.086802
1	1.990134	4.220439	-1.466136
8	2.874454	3.228877	1.829317
6	3.753727	0.953320	0.100636
6	3.087168	-0.278855	0.185720
6	5.096323	1.040420	0.431931
6	3.771959	-1.425088	0.617507
6	5.762416	-0.103708	0.865378
1	5.624318	1.985446	0.343428
6	5.110235	-1.331503	0.960112
1	3.233931	-2.369485	0.683443
1	6.815354	-0.030084	1.124588
1	5.646937	-2.216119	1.290107
6	1.724655	-0.402363	-0.172089
7	0.617567	-0.569772	-0.476825
6	0.009334	-3.746760	-0.169597
6	0.089943	-2.969212	1.136072
8	-0.870129	-2.106100	1.387517
8	0.959763	-3.210911	1.957695
1	-0.573237	-3.220193	-0.930510
7	1.314381	-4.065895	-0.690117
6	2.085965	-5.026214	-0.172087
8	3.269144	-5.213831	-0.477849
1	-2.010769	4.029816	2.326564
8	3.024670	2.026517	-0.379570
8	4.368069	4.123872	0.021695
16	3.130990	3.474847	0.421690
8	-3.275380	-0.819387	0.629664
6	-3.913585	-1.874173	0.260905
8	-3.537168	-2.798990	-0.435686
8	-1.850707	1.070366	-1.121297
6	-2.759910	1.040692	-2.122996
8	-3.166126	0.004292	-2.548586

6	-3.195088	2.412825	-2.669385
6	-5.340478	-1.863702	0.844366
1	1.767082	-3.418105	-1.344959
8	0.570697	0.988203	2.102932
6	-0.029820	0.850897	3.153036
6	-0.056757	1.857917	4.255487
1	0.314463	1.402537	5.179930
1	0.559648	2.722299	3.998062
1	-1.087953	2.174315	4.447351
8	-0.747215	-0.233341	3.449633
1	-0.674764	-0.901654	2.724378
1	4.162304	-4.070653	-1.372330
8	4.802196	-3.412988	-1.767693
6	4.158098	-2.411601	-2.339687
6	5.078492	-1.384280	-2.907292
1	4.511010	-0.531257	-3.283747
1	5.787881	-1.057069	-2.138700
1	5.663436	-1.826559	-3.721211
8	2.936768	-2.335199	-2.396262
9	-3.844674	3.092810	-1.731038
9	-2.133335	3.113791	-3.052410
9	-3.991383	2.233613	-3.703858
9	-5.292663	-1.874243	2.178593
9	-6.037316	-2.919123	0.445081
9	-5.996868	-0.763596	0.467988
1	1.571748	-5.678914	0.555469
1	-0.541668	-4.669315	0.064713

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conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -224.6308 cm(-1)

Electronic energy : =-3811.7140304
Zero-point correction= 0.482205
Thermal correction to Energy= 0.535402
Thermal correction to Enthalpy= 0.536346
Thermal correction to Gibbs Free Energy= 0.393230
Sum of electronic and zero-point Energies= -3811.231825
Sum of electronic and thermal Energies= -3811.178629
Sum of electronic and thermal Enthalpies= -3811.177685
Sum of electronic and thermal Free Energies= -3811.320801

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Cartesian Coordinates

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46	1.611662	-0.467881	-0.170215
6	1.475274	3.509250	1.391601
6	2.062037	2.294731	1.005077
6	1.294278	1.226379	1.355122
6	0.188624	1.128469	2.143437
6	-0.373576	2.370355	2.473619
6	0.271575	3.546818	2.088447
1	-0.258793	0.195708	2.474288
1	2.991200	2.235125	0.447520
1	-0.164290	4.505750	2.358813
6	-1.677554	2.394555	3.202672
1	-1.923869	3.395838	3.575721
1	-1.735026	1.688099	4.039541
8	-2.793723	2.370680	0.747566
6	-3.654408	-0.356999	1.229672
6	-2.945010	-0.980950	0.194194
6	-5.033598	-0.445906	1.286098
6	-3.629595	-1.665506	-0.817006
6	-5.705086	-1.148434	0.286512
1	-5.570368	0.026892	2.103579
6	-5.012499	-1.748459	-0.763304
1	-3.061924	-2.111767	-1.631252
1	-6.788466	-1.220356	0.329750
1	-5.550050	-2.282767	-1.541216
6	-1.529529	-0.936219	0.160238
7	-0.371808	-0.947765	0.142554
6	0.785635	-2.645769	-2.429354
6	0.389707	-1.203680	-2.716880
8	1.061640	-0.245220	-2.110601
8	-0.462904	-0.952447	-3.549961
1	1.447942	-2.743264	-1.563870
1	1.362510	-2.976615	-3.304272
7	-0.365767	-3.492939	-2.250286
6	-1.084620	-3.977296	-3.266000
8	-2.145509	-4.599299	-3.134442
1	1.984860	4.428728	1.115674
8	-2.935965	0.333179	2.198622
8	-4.300033	2.378012	2.761838
16	-3.056567	1.987644	2.124080
8	3.463627	0.163076	-0.671829
6	4.271904	-0.808156	-0.924883
8	4.063533	-2.005786	-0.878439
8	2.424102	-0.550614	1.722722
6	1.955579	-1.441837	2.555298
8	1.077979	-2.254230	2.384744
6	2.671354	-1.295717	3.913198
6	5.650234	-0.257722	-1.342457
1	-0.743248	-3.637879	-1.305429

8	0.625329	2.425927	-2.195793
1	0.701936	1.447523	-2.243950
1	-2.881140	-4.793660	-1.608569
8	-3.445169	-4.903210	-0.789705
6	-2.803295	-4.498660	0.291387
6	-3.627048	-4.604807	1.529936
1	-3.016078	-4.400034	2.410696
1	-4.442881	-3.872230	1.476101
1	-4.085225	-5.595675	1.605343
8	-1.661415	-4.054119	0.275381
1	-0.644102	-3.799215	-4.263177
9	5.531870	0.490087	-2.440645
9	6.160484	0.506985	-0.376292
9	6.504318	-1.238820	-1.593961
9	2.283460	-2.236300	4.759856
9	2.365590	-0.102517	4.431418
9	3.992161	-1.363130	3.774829
6	-0.553798	2.782478	-1.561850
1	-0.610994	2.459044	-0.504460
6	-0.611951	4.304436	-1.590357
6	-1.761371	2.174039	-2.282529
9	0.546240	4.825926	-1.189589
9	-1.567066	4.779289	-0.791933
9	-0.850535	4.751318	-2.827838
9	-1.597844	2.190682	-3.603013
9	-2.902585	2.803137	-2.002437
9	-1.902971	0.895119	-1.909755

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conf-6

The smallest frequency is : -211.4531 cm(-1)

Electronic energy : =-4372.2652819
Zero-point correction= 0.484198
Thermal correction to Energy= 0.541902
Thermal correction to Enthalpy= 0.542846
Thermal correction to Gibbs Free Energy= 0.388845
Sum of electronic and zero-point Energies= -4371.781084
Sum of electronic and thermal Energies= -4371.723380
Sum of electronic and thermal Enthalpies= -4371.722436
Sum of electronic and thermal Free Energies= -4371.876437

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Cartesian Coordinates

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46	1.815407	-1.252746	-0.008150

6	4.069564	2.133531	1.328619
6	3.824391	0.787246	1.018978
6	2.568951	0.397166	1.376103
6	1.617940	1.016158	2.130285
6	1.898151	2.367336	2.382128
6	3.113253	2.915573	1.968166
1	0.702078	0.554633	2.488258
1	4.544319	0.156650	0.506840
1	3.322747	3.962511	2.175938
6	0.851091	3.200845	3.045329
1	1.242898	4.167831	3.382082
1	0.359884	2.709245	3.893782
8	-0.005247	3.703760	0.533954
6	-2.325750	2.088604	1.044246
6	-2.111501	1.088362	0.082849
6	-3.456051	2.883924	0.990230
6	-3.016725	0.925622	-0.974560
6	-4.354933	2.708094	-0.059677
1	-3.625053	3.634292	1.757123
6	-4.126083	1.754122	-1.048829
1	-2.828698	0.165851	-1.730436
1	-5.239268	3.337703	-0.109103
1	-4.820991	1.650076	-1.877807
6	-0.985143	0.235879	0.180061
7	-0.098298	-0.504372	0.283715
6	-0.317420	-2.624545	-2.085013
6	0.321613	-1.319358	-2.545767
8	1.435825	-0.923689	-1.966354
8	-0.146597	-0.704735	-3.488025
1	0.147583	-3.043564	-1.188408
1	-0.144192	-3.346338	-2.894268
7	-1.738508	-2.481496	-1.858138
6	-2.653929	-2.468468	-2.836870
8	-3.860295	-2.278662	-2.658859
1	5.027008	2.556355	1.036299
8	-1.377168	2.254719	2.045005
8	-1.236061	4.740523	2.466973
16	-0.469404	3.642526	1.908720
8	3.688037	-1.767187	-0.556637
6	3.769836	-2.985331	-0.969829
8	2.899814	-3.834232	-1.011682
8	2.502794	-1.691029	1.883469
6	1.646699	-2.076753	2.789517
8	0.444756	-2.171995	2.711488
6	2.399203	-2.374643	4.101765
6	5.198265	-3.276941	-1.474793
1	-2.065161	-2.305292	-0.910997
8	2.826996	1.349838	-2.350689
1	2.288767	0.527373	-2.346824

1	-2.237984	-2.654528	-3.841937
9	5.463268	-2.518831	-2.540018
9	6.099613	-2.994022	-0.534327
9	5.337190	-4.548446	-1.819905
9	1.592184	-2.913750	5.001760
9	2.875265	-1.225637	4.588028
9	3.423691	-3.198087	3.900199
6	2.119415	2.371600	-1.741885
1	1.862878	2.166946	-0.686115
6	3.017477	3.603474	-1.765256
6	0.799799	2.644026	-2.474098
9	4.268595	3.282767	-1.441985
9	2.599795	4.527698	-0.898965
9	3.046765	4.156395	-2.982988
9	0.936093	2.482668	-3.787231
9	0.337260	3.875749	-2.257559
9	-0.138251	1.785089	-2.054647
1	-4.434352	-2.275703	-1.029885
8	-4.793477	-2.137563	-0.120602
6	-5.789902	-1.181227	-0.212516
1	-5.557320	-0.371773	-0.924188
6	-7.080341	-1.821639	-0.712057
6	-5.946867	-0.519927	1.149005
9	-8.091848	-0.949712	-0.738259
9	-6.886609	-2.264842	-1.957740
9	-7.453826	-2.864245	0.027895
9	-6.486593	-1.340577	2.052703
9	-6.720485	0.564925	1.062530
9	-4.760638	-0.134883	1.617720

(III) Acetoxylation product using Boc-Ala-OH at the SMD/M06/6-31G Level of Theory**

Boc-Ala-OH

Number of imaginary frequencies : 0

Electronic energy : =-669.2190371
Zero-point correction= 0.234033
Thermal correction to Energy= 0.248915
Thermal correction to Enthalpy= 0.249859
Thermal correction to Gibbs Free Energy= 0.191831
Sum of electronic and zero-point Energies= -668.985004

Sum of electronic and thermal Energies= -668.970122
Sum of electronic and thermal Enthalpies= -668.969178
Sum of electronic and thermal Free Energies= -669.027206

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Cartesian Coordinates

.....

6	-2.026725	0.433524	0.113903
6	-3.120078	-0.607225	0.102895
8	-2.981789	-1.752610	-0.272001
8	-4.270857	-0.108277	0.547239
1	-1.945373	0.806715	1.145348
7	-0.790906	-0.213752	-0.257631
1	-0.835768	-1.127819	-0.692405
6	0.408276	0.295445	0.111935
8	0.540738	1.344607	0.728342
1	-4.945167	-0.808843	0.506691
6	-2.376541	1.600538	-0.805715
1	-2.514085	1.251663	-1.835610
1	-1.558499	2.327316	-0.789613
1	-3.291266	2.101837	-0.475226
8	1.397239	-0.510355	-0.300960
6	2.801970	-0.200515	-0.018731
6	3.531184	-1.363285	-0.665632
1	3.211369	-2.315896	-0.226984
1	4.611507	-1.259183	-0.514566
1	3.334416	-1.393548	-1.743868
6	3.196425	1.105626	-0.683663
1	2.713723	1.966312	-0.213784
1	2.930058	1.086948	-1.747541
1	4.282874	1.235310	-0.609810
6	3.039814	-0.192190	1.479755
1	2.693150	-1.132887	1.924930
1	2.526140	0.639532	1.969669
1	4.114667	-0.099631	1.676754

$PhI(OAc)_2$

Number of imaginary frequencies : 0

Electronic energy : =-699.4835034
Zero-point correction= 0.192310
Thermal correction to Energy= 0.209232
Thermal correction to Enthalpy= 0.210176
Thermal correction to Gibbs Free Energy= 0.144737

Sum of electronic and zero-point Energies= -699.291193
Sum of electronic and thermal Energies= -699.274272
Sum of electronic and thermal Enthalpies= -699.273327
Sum of electronic and thermal Free Energies= -699.338766

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Cartesian Coordinates

.....

6	0.472433	3.588234	1.024559
6	0.535954	2.197719	1.039600
6	-0.061449	1.499593	-0.001014
6	-0.719490	2.133942	-1.046044
6	-0.781366	3.524780	-1.038872
6	-0.185923	4.247633	-0.009257
1	0.937193	4.152704	1.829388
1	1.044379	1.673456	1.844762
1	-1.179577	1.562246	-1.847790
1	-1.293605	4.041272	-1.847060
1	-0.234897	5.333919	-0.012520
53	0.028796	-0.622267	0.010346
8	-2.040138	-2.609693	0.087980
8	2.250363	-2.431838	-0.116321
6	-2.699005	-1.570238	0.108162
8	-2.149803	-0.386320	0.086724
6	2.821029	-1.341763	-0.119701
8	2.176361	-0.207233	-0.064672
6	-4.197566	-1.543568	0.161707
1	-4.595834	-2.559994	0.172597
1	-4.524670	-1.007881	1.058880
1	-4.589878	-0.999467	-0.703458
6	4.311091	-1.189889	-0.185192
1	4.788864	-2.166960	-0.281232
1	4.583214	-0.556940	-1.035828
1	4.670081	-0.690207	0.720529

Different Possibilities of Potential Active Catalyst at the SMD/M06/6-31G** Level of Theory.

(2a')

Number of imaginary frequencies : 0

Electronic energy : =-1252.7277982
Zero-point correction= 0.339244
Thermal correction to Energy= 0.365550
Thermal correction to Enthalpy= 0.366494

Thermal correction to Gibbs Free Energy= 0.281153
Sum of electronic and zero-point Energies= -1252.388554
Sum of electronic and thermal Energies= -1252.362248
Sum of electronic and thermal Enthalpies= -1252.361304
Sum of electronic and thermal Free Energies= -1252.446645

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Cartesian Coordinates

.....

46	-1.820222	0.547486	0.142569
1	-2.186411	-2.004953	-0.898446
6	-3.154907	-2.032151	0.780527
8	-2.945214	-2.471318	-0.420779
6	-4.052244	-2.875377	1.609156
1	-4.204021	-2.429691	2.592588
1	-3.618666	-3.875658	1.709189
1	-5.012745	-2.985450	1.094639
8	-2.669098	-0.984895	1.251011
6	1.559532	-1.851099	-0.939970
6	0.152499	-1.287076	-0.826023
8	-0.011702	-0.385587	0.070787
8	-0.730611	-1.751903	-1.564701
1	1.825471	-1.829896	-2.004907
7	2.495951	-1.017538	-0.214940
1	2.121119	-0.463735	0.541238
6	3.799059	-0.958807	-0.558063
8	4.305305	-1.688368	-1.401546
6	-2.609826	2.734249	-0.595467
8	-3.378857	1.925514	0.024137
6	-3.058760	4.075494	-1.018241
1	-2.492316	4.405975	-1.892820
1	-2.876174	4.781258	-0.199434
1	-4.130510	4.066444	-1.232578
8	-1.413913	2.331879	-0.810210
8	4.582277	-0.075395	0.084984
6	1.560830	-3.294858	-0.449307
1	1.265211	-3.341903	0.605879
1	2.567420	-3.713320	-0.548257
1	0.868114	-3.904197	-1.038355
6	4.154549	1.173201	0.730721
6	5.484722	1.863163	0.978906
1	6.021607	2.009723	0.034796
1	6.113448	1.261492	1.646048
1	5.323541	2.841864	1.444266
6	3.302374	1.998372	-0.216480
1	3.132990	2.986771	0.226905
1	2.321853	1.549239	-0.408414
1	3.818041	2.136982	-1.174071
6	3.464125	0.903026	2.059532
1	2.404802	0.631163	1.969637

1	3.491215	1.815111	2.667169
1	3.987370	0.112922	2.610142

(2b')

Number of imaginary frequencies : 0

Electronic energy : =-1023.74123
Zero-point correction= 0.275800
Thermal correction to Energy= 0.296386
Thermal correction to Enthalpy= 0.297330
Thermal correction to Gibbs Free Energy= 0.226222
Sum of electronic and zero-point Energies= -1023.465430
Sum of electronic and thermal Energies= -1023.444844
Sum of electronic and thermal Enthalpies= -1023.443900
Sum of electronic and thermal Free Energies= -1023.515008

Cartesian Coordinates

46	1.583767	0.205164	-0.056894
6	-0.778463	1.944597	0.004499
6	0.446065	2.793253	-0.299646
8	1.599353	2.186138	-0.370125
8	0.336836	4.005118	-0.435877
1	-1.524804	2.149480	-0.775314
7	-0.397205	0.531584	-0.034700
6	-1.289697	-0.407241	-0.133001
8	-0.982872	-1.683781	-0.143282
8	1.867083	-1.838029	0.240320
6	3.140529	-1.707142	0.127300
8	3.591654	-0.537056	-0.055467
6	4.033693	-2.885598	0.192993
1	4.859935	-2.686328	0.882079
1	4.466487	-3.055401	-0.799558
1	3.484245	-3.776118	0.505644
1	-0.023277	-1.834886	-0.012715
6	-1.328850	2.344047	1.366537
1	-2.231049	1.773206	1.610185
1	-1.581121	3.409114	1.363929
1	-0.578359	2.164834	2.146813
8	-2.546219	-0.082093	-0.251955
6	-3.699764	-1.014371	-0.086025
6	-3.743471	-1.975275	-1.255152
1	-4.688608	-2.529639	-1.216731

1	-2.924981	-2.699849	-1.233965
1	-3.711781	-1.425768	-2.203033
6	-3.608751	-1.698854	1.261590
1	-2.807636	-2.441389	1.304737
1	-4.556582	-2.214469	1.454824
1	-3.457518	-0.960153	2.058467
6	-4.872275	-0.055812	-0.126662
1	-5.807000	-0.618200	-0.027901
1	-4.897007	0.491016	-1.075968
1	-4.814586	0.667896	0.694999

(2d')

Number of imaginary frequencies : 0

Electronic energy : =-1813.2923194
Zero-point correction= 0.341062
Thermal correction to Energy= 0.371944
Thermal correction to Enthalpy= 0.372888
Thermal correction to Gibbs Free Energy= 0.275961
Sum of electronic and zero-point Energies= -1812.951258
Sum of electronic and thermal Energies= -1812.920375
Sum of electronic and thermal Enthalpies= -1812.919431
Sum of electronic and thermal Free Energies= -1813.016358

Cartesian Coordinates

46	1.264691	1.294756	-0.329782
6	1.826088	3.640017	0.053468
8	2.721034	2.728415	-0.034681
6	2.184719	5.060468	0.236679
1	2.311192	5.519549	-0.751142
1	3.128794	5.148670	0.780377
1	1.384484	5.588393	0.761675
8	0.613716	3.257445	-0.054276
6	-2.131811	-1.471671	-0.884927
6	-0.738562	-0.920207	-0.747960
8	-0.556452	0.293605	-0.547236
8	0.198787	-1.796259	-0.889351
1	-2.220178	-2.283734	-0.150261
7	-3.100532	-0.458033	-0.549182
1	-2.938666	0.498746	-0.838757
6	-4.330362	-0.806064	-0.089978
8	-4.653250	-1.953876	0.181863

8	2.310500	-0.418485	-0.619166
1	1.118844	-1.356029	-0.800961
6	3.287635	-0.662742	0.323159
6	2.720617	-1.429969	1.515789
6	4.417689	-1.414134	-0.374697
1	3.734665	0.261952	0.728227
9	1.637540	-0.798358	1.981047
9	3.593775	-1.525168	2.518223
9	2.345102	-2.668189	1.178126
9	4.979979	-0.622626	-1.288995
9	3.977186	-2.504904	-1.003426
9	5.369262	-1.791097	0.482438
6	-2.330045	-2.044954	-2.287161
1	-2.225434	-1.258045	-3.043103
1	-3.338130	-2.465284	-2.359217
1	-1.607196	-2.838998	-2.496478
8	-5.101806	0.282352	0.020275
6	-6.479882	0.192666	0.517359
6	-6.940171	1.637614	0.474028
1	-6.310049	2.266398	1.114254
1	-7.974342	1.711264	0.828831
1	-6.896907	2.030536	-0.548592
6	-7.316039	-0.658896	-0.420017
1	-7.007893	-1.707841	-0.404925
1	-7.240207	-0.282226	-1.447457
1	-8.368390	-0.603551	-0.116331
6	-6.487845	-0.323033	1.944637
1	-5.823597	0.282293	2.573531
1	-6.174096	-1.368475	2.004209
1	-7.502957	-0.243234	2.351968

(2')

Number of imaginary frequencies : 0

Electronic energy : =-1813.3055022
Zero-point correction= 0.339066
Thermal correction to Energy= 0.369292
Thermal correction to Enthalpy= 0.370237
Thermal correction to Gibbs Free Energy= 0.276951
Sum of electronic and zero-point Energies= -1812.966436
Sum of electronic and thermal Energies= -1812.936210
Sum of electronic and thermal Enthalpies= -1812.935266
Sum of electronic and thermal Free Energies= -1813.028552

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Cartesian Coordinates

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46	-0.738791	1.066232	-0.249383
6	1.830499	2.438883	0.050512
6	0.721785	3.438854	0.335709
8	-0.511261	3.016326	0.184885
8	0.976801	4.587379	0.658960
1	2.448221	2.388881	0.959373
7	1.263866	1.120891	-0.239370
6	2.020064	0.040391	-0.242212
8	1.577726	-1.123396	-0.538715
8	-0.795263	-0.943454	-0.748458
1	0.448804	-1.126899	-0.689831
6	-1.568475	-1.802354	0.017929
6	-1.874465	-3.024243	-0.844887
6	-0.882714	-2.178627	1.332350
1	-2.535740	-1.349995	0.284575
9	-0.762491	-3.553856	-1.357813
9	-2.657936	-2.668840	-1.862947
9	-2.502836	-3.978301	-0.155340
9	0.170206	-2.980022	1.143436
9	-1.724349	-2.796968	2.160147
9	-0.440652	-1.080435	1.951490
8	-2.855246	1.079719	-0.183645
6	-3.588658	2.045558	0.084855
8	-3.156261	3.241124	0.373875
6	-5.065898	1.909028	0.091583
1	-5.491579	2.590089	-0.653030
1	-5.455043	2.212111	1.068860
1	-5.359599	0.882805	-0.130509
1	-2.163294	3.306679	0.354885
6	2.669806	2.966204	-1.107309
1	3.510138	2.295549	-1.313254
1	3.064391	3.956506	-0.858715
1	2.057076	3.050220	-2.013384
8	3.285810	0.210297	0.076149
6	4.298158	-0.869973	0.059633
6	3.952215	-1.908649	1.108224
1	3.039882	-2.460863	0.865721
1	3.828754	-1.434179	2.089111
1	4.778417	-2.625997	1.180877
6	4.426166	-1.441821	-1.337958
1	4.550491	-0.635123	-2.071016
1	3.565569	-2.051697	-1.623255
1	5.321150	-2.073867	-1.379341
6	5.557829	-0.118904	0.444452
1	5.790141	0.656145	-0.295915
1	6.402407	-0.814629	0.494452

1 5.443321 0.357117 1.425157

(2e')

Number of imaginary frequencies : 0

Electronic energy : =-1252.7430756
Zero-point correction= 0.338413
Thermal correction to Energy= 0.364770
Thermal correction to Enthalpy= 0.365714
Thermal correction to Gibbs Free Energy= 0.280157
Sum of electronic and zero-point Energies= -1252.404663
Sum of electronic and thermal Energies= -1252.378306
Sum of electronic and thermal Enthalpies= -1252.377361
Sum of electronic and thermal Free Energies= -1252.462919

Cartesian Coordinates

46	-1.082599	-0.012956	0.100052
6	0.945240	-1.976292	0.603429
6	-0.256323	-2.693295	0.010005
8	-1.168846	-1.922305	-0.545368
8	-0.360667	-3.908131	0.034392
1	1.820971	-2.362677	0.064492
7	0.819180	-0.538420	0.375445
6	1.836014	0.193610	-0.094734
8	1.723623	1.332903	-0.581185
8	-1.142296	1.881179	1.020749
8	-3.150880	0.389274	-0.205327
6	-4.026909	-0.422671	-0.539692
8	-3.804141	-1.682470	-0.799928
6	-5.446907	-0.014239	-0.679319
1	-6.069043	-0.634520	-0.025812
1	-5.773846	-0.197834	-1.708221
1	-5.572308	1.039739	-0.429565
1	-2.840510	-1.924118	-0.713460
6	-0.917002	2.958926	0.440531
8	-0.126495	3.073872	-0.581528
6	-1.551922	4.220408	0.898591
1	-2.067886	4.689866	0.054437
1	-0.774600	4.916829	1.230152
1	-2.255151	4.029176	1.709563
1	0.469110	2.252775	-0.669032
6	1.085893	-2.310472	2.079717

1	1.994231	-1.846949	2.479740
1	1.150949	-3.394190	2.223892
1	0.224142	-1.931219	2.643944
8	3.022037	-0.416226	0.039180
6	4.281867	0.182415	-0.418489
6	4.240604	0.434735	-1.914295
1	5.246242	0.702636	-2.260359
1	3.558786	1.246298	-2.179468
1	3.931914	-0.474139	-2.445299
6	4.586611	1.431332	0.386313
1	4.541151	1.212587	1.460093
1	3.895426	2.247413	0.162783
1	5.603443	1.769674	0.153067
6	5.289534	-0.907496	-0.099709
1	6.295659	-0.581295	-0.386178
1	5.055490	-1.826585	-0.650075
1	5.292245	-1.135071	0.972801

(2f')

Number of imaginary frequencies : 0

Electronic energy : =-3163.3938551
Zero-point correction= 0.412095
Thermal correction to Energy= 0.456764
Thermal correction to Enthalpy= 0.457708
Thermal correction to Gibbs Free Energy= 0.332346
Sum of electronic and zero-point Energies= -3162.981760
Sum of electronic and thermal Energies= -3162.937091
Sum of electronic and thermal Enthalpies= -3162.936147
Sum of electronic and thermal Free Energies= -3163.061509

Cartesian Coordinates

46	-0.742656	0.047112	-0.202902
8	-2.409680	-1.329675	-0.375258
6	2.886245	2.346982	-0.987915
6	1.427573	2.001023	-0.826376
8	1.110546	0.976749	-0.195039
8	0.589599	2.811480	-1.377765
1	3.068970	3.205600	-0.320529
7	3.679172	1.217692	-0.553797
1	3.213437	0.358328	-0.289235
6	4.957475	1.371199	-0.120379

8	5.583854	2.418801	-0.182962
8	-1.680479	1.772385	-0.758704
1	-0.370496	2.508460	-1.197591
6	-2.539827	2.317461	0.168702
6	-3.751530	2.853517	-0.589760
6	-1.844814	3.385290	1.010552
1	-2.934447	1.580178	0.891002
9	-4.374245	1.835781	-1.196202
9	-4.636836	3.446766	0.212370
9	-3.402091	3.727379	-1.533260
9	-0.769028	2.858043	1.605322
9	-1.428082	4.412917	0.264943
9	-2.635726	3.868466	1.969126
8	0.143044	-1.662511	0.303970
6	1.211728	-2.010325	-0.483957
6	0.801782	-3.158273	-1.398274
6	2.407778	-2.340872	0.404715
1	1.564231	-1.203688	-1.153425
9	3.519345	-2.555175	-0.304982
9	2.654596	-1.306352	1.218150
9	2.187931	-3.411891	1.167441
9	1.814840	-3.615740	-2.137948
9	0.295487	-4.187553	-0.716775
9	-0.151352	-2.725637	-2.233493
1	-1.933255	-2.157537	-0.155464
6	-3.664322	-1.266727	0.253970
6	-3.507458	-1.453786	1.761215
6	-4.585751	-2.295153	-0.400102
1	-4.090747	-0.273820	0.067177
9	-2.836996	-0.422547	2.279756
9	-2.812944	-2.560635	2.030401
9	-4.682460	-1.531329	2.372419
9	-5.828687	-2.193306	0.055585
9	-4.604543	-2.101882	-1.714598
9	-4.152757	-3.536480	-0.169431
6	3.197575	2.759410	-2.421619
1	4.266514	2.976563	-2.502544
1	2.950632	1.949360	-3.117121
1	2.638635	3.655603	-2.705234
8	5.397543	0.200374	0.357028
6	6.750008	0.037206	0.894917
6	6.758969	-1.424403	1.303940
1	6.571849	-2.071621	0.438688
1	7.732062	-1.689426	1.732375
1	5.984055	-1.620247	2.054721
6	6.940504	0.931499	2.105847
1	6.942927	1.990896	1.835403
1	6.144255	0.756496	2.839688
1	7.899416	0.696483	2.583227

6	7.777491	0.294911	-0.191234
1	7.803972	1.346725	-0.488144
1	8.771940	0.015625	0.177226
1	7.559977	-0.316973	-1.075174

Deprotonation of N-H of the Ligand at the SMD/M06/6-31G** Level of Theory.

(a')

Number of imaginary frequencies : 0

Electronic energy : =-1252.743163
Zero-point correction= 0.338542
Thermal correction to Energy= 0.364708
Thermal correction to Enthalpy= 0.365652
Thermal correction to Gibbs Free Energy= 0.280840
Sum of electronic and zero-point Energies= -1252.404621
Sum of electronic and thermal Energies= -1252.378456
Sum of electronic and thermal Enthalpies= -1252.377511
Sum of electronic and thermal Free Energies= -1252.462323

Cartesian Coordinates

46	-1.072909	0.033316	0.148350
6	0.890394	-1.597667	1.317537
6	0.063933	-2.524308	0.434891
8	-0.804905	-1.914869	-0.347053
8	0.172444	-3.738877	0.469119
1	1.926870	-1.951066	1.303167
7	0.808936	-0.231044	0.793190
6	1.761391	0.245272	-0.037525
8	1.598528	1.239648	-0.767454
6	-3.780306	-0.776068	-0.968086
6	-5.189588	-0.572702	-1.387991
1	-5.844001	-1.181113	-0.754585
1	-5.467738	0.478722	-1.310665
1	-5.316505	-0.923677	-2.417173
8	-3.084820	0.165222	-0.557866
8	-3.364708	-2.009748	-1.069337
1	-2.412137	-2.114765	-0.794522
8	2.917919	-0.416548	0.021319
6	0.358310	-1.667627	2.741564
1	0.404976	-2.696005	3.115576
1	0.956393	-1.028445	3.399236

1	-0.685181	-1.328525	2.784047
6	4.129917	0.036372	-0.677959
6	3.914666	0.009499	-2.179452
6	4.549210	1.399673	-0.163261
6	5.145490	-1.016233	-0.273235
1	3.519822	-0.965573	-2.489886
1	3.228857	0.791359	-2.514211
1	4.878941	0.157407	-2.680559
1	4.634459	1.385651	0.930067
1	5.533507	1.650166	-0.576693
1	3.846562	2.184364	-0.454096
1	6.116003	-0.792437	-0.730132
1	5.272840	-1.036774	0.815449
1	4.828854	-2.011518	-0.606796
8	-1.450532	1.959426	0.895569
6	-1.008973	3.049041	0.489843
6	-1.626750	4.325075	0.935394
1	-0.895126	4.890438	1.522609
1	-1.880644	4.931549	0.060224
1	-2.517421	4.135364	1.535207
8	-0.006250	3.182257	-0.319686
1	0.494376	2.315576	-0.499903

[a'-b']

Total Energy =-1252.742399

Number of imaginary frequencies : 1
The smallest frequency is : -880.7091 cm(-1)

Electronic energy : =-1252.7158242
Zero-point correction= 0.337275
Thermal correction to Energy= 0.362510
Thermal correction to Enthalpy= 0.363454
Thermal correction to Gibbs Free Energy= 0.281913
Sum of electronic and zero-point Energies= -1252.378550
Sum of electronic and thermal Energies= -1252.353314
Sum of electronic and thermal Enthalpies= -1252.352370
Sum of electronic and thermal Free Energies= -1252.433911

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Cartesian Coordinates

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46	-1.000073	0.071837	-0.042423

8	-0.626351	3.077748	0.731432
6	-2.226199	4.147448	-0.645653
6	-1.511174	2.923534	-0.153741
8	-1.853949	1.819881	-0.682619
6	0.895868	0.146752	2.027672
6	0.678062	-1.342518	1.741275
8	-0.135141	-1.587173	0.718585
8	1.167853	-2.211189	2.421951
1	1.937516	0.270012	2.344616
1	-1.538711	4.716793	-1.279760
1	-3.113444	3.883169	-1.222476
1	-2.489804	4.782289	0.204226
7	0.648426	0.953359	0.813961
1	0.105884	2.038093	0.875715
6	1.629345	0.923895	-0.215113
8	1.570001	1.655109	-1.175385
6	-2.856412	-2.181437	-0.772790
6	-4.070816	-2.786046	-1.393165
1	-4.653504	-3.299136	-0.622179
1	-4.673860	-2.017154	-1.875510
1	-3.765472	-3.542418	-2.122472
8	-2.654673	-0.961055	-0.850117
8	-2.083753	-3.042071	-0.178170
1	-1.272523	-2.620706	0.239027
8	2.553068	0.006067	0.045649
6	3.474057	-0.469990	-0.993482
6	2.660388	-1.023529	-2.149959
6	4.414777	0.643239	-1.413633
6	4.220404	-1.580828	-0.278703
1	1.964384	-1.790510	-1.787168
1	2.095100	-0.237466	-2.658628
1	3.335144	-1.490187	-2.877029
1	4.926521	1.059315	-0.538238
1	5.175817	0.233823	-2.088641
1	3.881337	1.445387	-1.928366
1	4.925792	-2.059679	-0.966892
1	4.781505	-1.183183	0.574112
1	3.519148	-2.336170	0.094049
6	-0.035590	0.597498	3.141908
1	0.151924	-0.001210	4.038187
1	0.126410	1.654012	3.379164
1	-1.087473	0.470226	2.853672

[b']

Number of imaginary frequencies : 0

Electronic energy : =-1252.7520843
Zero-point correction= 0.339904
Thermal correction to Energy= 0.366026
Thermal correction to Enthalpy= 0.366971
Thermal correction to Gibbs Free Energy= 0.282395
Sum of electronic and zero-point Energies= -1252.412180
Sum of electronic and thermal Energies= -1252.386058
Sum of electronic and thermal Enthalpies= -1252.385114
Sum of electronic and thermal Free Energies= -1252.469689

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Cartesian Coordinates

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46	-0.923209	0.058553	-0.010039
8	-0.909684	3.031852	1.041083
6	-2.204988	4.094615	-0.661355
6	-1.547274	2.906606	-0.013002
8	-1.703572	1.807081	-0.679318
6	0.951289	-0.114288	2.137932
6	0.698230	-1.547259	1.683726
8	-0.119674	-1.687303	0.667395
8	1.194127	-2.490688	2.274870
1	1.992958	-0.033433	2.469033
1	-1.524144	4.495291	-1.421687
1	-3.136466	3.813955	-1.159603
1	-2.390220	4.874987	0.080953
7	0.718227	0.826570	1.012392
1	0.343049	1.757142	1.285783
6	1.725389	0.970578	0.004753
8	1.765180	1.951209	-0.701886
6	-2.927570	-1.996127	-0.912370
6	-4.157207	-2.467493	-1.594860
1	-4.849450	-2.868947	-0.846998
1	-4.631754	-1.653552	-2.143369
1	-3.901695	-3.286410	-2.274899
8	-2.569697	-0.807813	-0.988576
8	-2.289744	-2.919906	-0.250686
1	-1.457788	-2.580843	0.179619
6	0.005817	0.233706	3.274329
1	0.161881	-0.459834	4.106144
1	0.191290	1.252519	3.631037
1	-1.040320	0.161774	2.949389
8	2.494844	-0.093080	-0.012369
6	3.384571	-0.387961	-1.163526
6	2.529303	-0.475832	-2.410627
6	4.476164	0.657630	-1.248446
6	3.944981	-1.743910	-0.790515

1	1.696848	-1.172518	-2.246143
1	2.125893	0.497517	-2.705955
1	3.137629	-0.857917	-3.238369
1	4.995045	0.749744	-0.287111
1	5.208426	0.342612	-2.001131
1	4.085444	1.637078	-1.537526
1	4.634805	-2.085497	-1.570031
1	4.491718	-1.692698	0.158074
1	3.140419	-2.482788	-0.692493

Different Possibilities of $Pd(OAc)_2$ -Ligand with Substrate at the SMD/M06/6-31G** Level of Theory

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(3a')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8624641
Zero-point correction= 0.501014
Thermal correction to Energy= 0.539162
Thermal correction to Enthalpy= 0.540106
Thermal correction to Gibbs Free Energy= 0.428812
Sum of electronic and zero-point Energies= -2241.361451
Sum of electronic and thermal Energies= -2241.323302
Sum of electronic and thermal Enthalpies= -2241.322358
Sum of electronic and thermal Free Energies= -2241.433653

Cartesian Coordinates

46	-3.315336	-1.061174	-0.141096
6	1.685687	0.609611	-1.215236
1	1.090241	-0.025638	-0.546074
1	1.745065	0.122244	-2.197188
8	-0.618076	1.609814	-2.123974
6	-0.488406	3.438678	0.369863
6	-1.855254	3.219729	0.607230
6	0.053008	4.706791	0.475179
6	-2.681579	4.293402	0.958081
6	-0.780347	5.768275	0.819360
1	1.115731	4.849313	0.299709
6	-2.137160	5.564672	1.060724
1	-3.736967	4.114824	1.143725
1	-0.359377	6.766504	0.905500
1	-2.773444	6.401799	1.332744

6	-2.385214	1.910786	0.466085
7	-2.810065	0.843528	0.322220
6	-5.233721	-2.304546	-1.003185
8	-5.289802	-1.040901	-0.834339
6	-6.390609	-3.083790	-1.486265
1	-6.864002	-3.581593	-0.632029
1	-7.121507	-2.426728	-1.963183
1	-6.055461	-3.857306	-2.183156
8	-4.122481	-2.870178	-0.713586
6	0.248236	-1.864552	2.022986
6	-1.212060	-1.721720	1.610787
8	-1.398761	-1.523217	0.343389
8	-2.083826	-1.742275	2.474575
1	0.320572	-2.761509	2.655443
7	1.096455	-2.002583	0.855087
1	0.643434	-2.082908	-0.047136
6	2.409452	-2.332813	0.937700
8	3.016148	-2.490681	1.987830
8	0.319767	2.349179	0.092267
16	0.630988	2.026115	-1.504447
8	1.347271	3.160382	-2.062849
6	3.027573	0.975583	-0.667432
6	4.060901	1.327202	-1.540043
6	3.256370	0.983847	0.709608
6	5.307965	1.685045	-1.039467
1	3.880695	1.318743	-2.614624
6	4.505633	1.338234	1.208738
1	2.450772	0.713961	1.390141
6	5.530817	1.691765	0.335876
1	6.107825	1.958115	-1.723839
1	4.677947	1.336647	2.282612
1	6.506807	1.970607	0.726952
6	0.592646	-0.631310	2.851893
1	0.403727	0.279587	2.266015
1	-0.028775	-0.598116	3.751884
1	1.643636	-0.653098	3.154369
8	2.923867	-2.430743	-0.298956
6	4.266273	-2.970350	-0.534477
6	4.357384	-4.385475	0.006816
1	4.333105	-4.409297	1.099730
1	3.533254	-4.997858	-0.379100
1	5.299533	-4.838485	-0.324268
6	5.324459	-2.055677	0.052186
1	5.258560	-2.000952	1.142281
1	6.315769	-2.441745	-0.215715
1	5.233304	-1.044589	-0.364620
6	4.353540	-2.972734	-2.049368
1	4.223439	-1.957607	-2.446164
1	5.333923	-3.342942	-2.369907

1	3.580673	-3.617386	-2.484373

(3b')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8623509
Zero-point correction= 0.502356
Thermal correction to Energy= 0.539798
Thermal correction to Enthalpy= 0.540742
Thermal correction to Gibbs Free Energy= 0.433034
Sum of electronic and zero-point Energies= -2241.359995
Sum of electronic and thermal Energies= -2241.322553
Sum of electronic and thermal Enthalpies= -2241.321608
Sum of electronic and thermal Free Energies= -2241.429317

Cartesian Coordinates

46	0.772144	-1.808933	-0.587727
6	-2.883159	-0.306052	1.234545
1	-1.853890	-0.532211	0.929075
1	-2.993267	-0.564021	2.295722
8	-1.840415	2.046966	1.938516
6	-1.953818	2.807075	-0.760037
6	-0.622050	2.554802	-1.120998
6	-2.474905	4.084993	-0.815349
6	0.198234	3.605317	-1.547546
6	-1.652069	5.124742	-1.243066
1	-3.511804	4.251526	-0.533768
6	-0.328035	4.887732	-1.606990
1	1.235081	3.403484	-1.803053
1	-2.053611	6.133430	-1.292219
1	0.300232	5.710559	-1.935517
6	-0.145187	1.222294	-1.011361
7	0.182146	0.117685	-0.889129
6	-0.165542	-3.842450	0.402680
8	-0.824456	-2.747788	0.384337
6	-0.687460	-5.056500	1.061920
1	-0.347651	-5.060549	2.104328
1	-1.780339	-5.055406	1.055032
1	-0.298183	-5.952407	0.571371
8	0.986152	-3.824540	-0.150075
6	4.673184	-0.428593	-1.349222
6	3.576151	-1.396598	-0.871826

8	2.462514	-1.211379	-1.519044
8	3.777490	-2.229675	0.002991
1	4.850480	-0.666981	-2.405971
7	4.180483	0.945584	-1.336001
1	4.170875	1.472215	-2.198797
6	3.507883	1.524633	-0.308419
8	3.039082	2.656308	-0.357360
8	-2.741163	1.731534	-0.390061
16	-2.978756	1.481820	1.232085
8	-4.319379	1.947737	1.540243
6	-3.914351	-0.953822	0.368023
6	-5.208743	-1.153991	0.851850
6	-3.590632	-1.353182	-0.930580
6	-6.170045	-1.753107	0.045948
1	-5.457120	-0.840114	1.864990
6	-4.553043	-1.954651	-1.733943
1	-2.579449	-1.195573	-1.306832
6	-5.842460	-2.153646	-1.246873
1	-7.175782	-1.909631	0.429202
1	-4.295795	-2.268016	-2.743205
1	-6.593727	-2.625504	-1.876391
6	5.965355	-0.593378	-0.573968
1	6.332151	-1.622008	-0.649279
1	6.730456	0.077369	-0.978975
1	5.822147	-0.359314	0.486859
8	3.431860	0.689618	0.732509
6	2.939911	1.088801	2.051658
6	3.170713	-0.168727	2.869076
1	4.235794	-0.431192	2.888185
1	2.829550	-0.016798	3.899433
1	2.616998	-1.013807	2.438963
6	3.773353	2.239408	2.581690
1	3.600263	3.160654	2.018946
1	3.514893	2.423306	3.631222
1	4.840806	1.989773	2.533289
6	1.459528	1.412180	1.992970
1	1.250702	2.276384	1.353664
1	0.901218	0.543907	1.618883
1	1.101708	1.635890	3.005289

(3d')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8592016
Zero-point correction= 0.501995
Thermal correction to Energy= 0.539325
Thermal correction to Enthalpy= 0.540269
Thermal correction to Gibbs Free Energy= 0.433902
Sum of electronic and zero-point Energies= -2241.357207
Sum of electronic and thermal Energies= -2241.319877
Sum of electronic and thermal Enthalpies= -2241.318933
Sum of electronic and thermal Free Energies= -2241.425299

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Cartesian Coordinates

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46	1.279742	1.901073	0.367655
6	-1.534194	-1.347655	-1.797935
1	-0.459009	-1.145118	-1.708631
1	-1.689008	-2.037041	-2.639951
8	-0.820619	-3.210176	-0.033280
6	-3.166174	-0.595133	1.213658
6	-2.966592	0.773167	1.469784
6	-4.418910	-1.159900	1.392592
6	-4.042329	1.586273	1.843053
6	-5.480722	-0.337159	1.759774
1	-4.565253	-2.223444	1.244168
6	-5.303317	1.027491	1.975692
1	-3.868738	2.643462	2.024576
1	-6.464948	-0.780494	1.888349
1	-6.145768	1.650839	2.260555
6	-1.662838	1.306796	1.317834
7	-0.579662	1.694618	1.179670
6	2.781006	3.629117	-0.560910
8	1.650677	3.962532	-0.080437
6	3.693271	4.621545	-1.176617
1	3.583720	4.571079	-2.266205
1	3.445253	5.632744	-0.845536
1	4.732111	4.381373	-0.933421
8	3.102379	2.392006	-0.521042
8	-2.035217	-1.321182	0.883584
16	-1.954880	-2.378927	-0.387360
8	-3.263904	-2.976300	-0.590439
6	-2.331437	-0.085588	-1.908065
6	-3.720648	-0.096126	-2.064461
6	-1.655292	1.133932	-1.843388
6	-4.422618	1.102463	-2.124652
1	-4.253688	-1.043591	-2.128083
6	-2.358721	2.332346	-1.914833
1	-0.570000	1.136946	-1.732600
6	-3.744119	2.317873	-2.047881
1	-5.504784	1.087426	-2.232742
1	-1.818775	3.275977	-1.855340

1	-4.297425	3.253263	-2.095777
7	1.398396	-0.089000	0.606555
6	1.754757	-0.765458	-0.509373
8	1.664658	-0.311225	-1.652840
6	1.843273	-0.536150	1.919460
1	1.742840	0.333924	2.589237
6	3.341545	-0.802689	1.891273
8	4.126541	-0.166787	1.218160
8	3.718417	-1.777919	2.718971
1	4.688722	-1.846990	2.676764
6	1.005731	-1.657068	2.518059
1	1.278289	-1.814159	3.566862
1	-0.055928	-1.386619	2.478190
1	1.149105	-2.598806	1.980248
8	2.156706	-2.014722	-0.218873
6	2.777945	-2.901915	-1.202200
6	3.060259	-4.141088	-0.372051
1	3.571966	-4.897407	-0.978150
1	3.695313	-3.894365	0.488574
1	2.122775	-4.572117	0.002441
6	1.819137	-3.231620	-2.332057
1	0.870220	-3.612316	-1.932835
1	1.616231	-2.364417	-2.965889
1	2.262667	-4.018123	-2.955300
6	4.067720	-2.273331	-1.694183
1	3.877502	-1.369108	-2.280053
1	4.711574	-2.011484	-0.845006
1	4.606336	-2.987801	-2.328267

(3e')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8661439
Zero-point correction= 0.497492
Thermal correction to Energy= 0.535202
Thermal correction to Enthalpy= 0.536146
Thermal correction to Gibbs Free Energy= 0.425944
Sum of electronic and zero-point Energies= -2241.368652
Sum of electronic and thermal Energies= -2241.330942
Sum of electronic and thermal Enthalpies= -2241.329998
Sum of electronic and thermal Free Energies= -2241.440200

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Cartesian Coordinates

.....

46	-1.136885	-1.068199	0.038285
6	3.214207	1.799260	-0.981975
1	3.971517	1.703586	-1.768600
1	2.208756	1.665091	-1.408186
8	2.388737	0.246849	1.047588
6	3.868156	-2.028784	-0.689517
6	2.976601	-3.001491	-0.209397
6	5.204166	-2.332230	-0.880081
6	3.437735	-4.289643	0.084619
6	5.653159	-3.616426	-0.582843
1	5.875747	-1.570735	-1.266155
6	4.778833	-4.588667	-0.102030
1	2.738760	-5.035553	0.452322
1	6.701867	-3.858834	-0.733711
1	5.143694	-5.586685	0.123061
6	1.612186	-2.645628	-0.055931
7	0.509930	-2.306780	0.049469
6	-1.831142	1.681497	-0.332695
6	-0.527962	1.440172	-1.073810
8	-0.064664	0.221046	-1.078791
8	0.074894	2.366728	-1.608803
1	-2.451943	2.333143	-0.959607
7	-2.498319	0.394633	-0.135302
6	-3.811592	0.294154	-0.167957
8	-4.456815	-0.799184	-0.154436
8	3.370986	-0.781667	-1.034890
16	3.488122	0.414617	0.109015
8	4.849803	0.407362	0.621193
6	3.347543	3.065314	-0.191246
6	2.258621	3.552756	0.534450
6	4.570348	3.737149	-0.138330
6	2.386683	4.712268	1.290223
1	1.310746	3.019657	0.492651
6	4.695594	4.898803	0.615903
1	5.421003	3.347629	-0.696120
6	3.604163	5.387352	1.330112
1	1.532343	5.089652	1.848411
1	5.647821	5.423481	0.647391
1	3.702697	6.297141	1.918256
8	-2.060073	-2.405621	1.345981
6	-2.918606	-3.230648	0.924370
8	-3.659724	-3.026823	-0.087972
6	-3.088585	-4.518970	1.657739
1	-4.111358	-4.582137	2.043682
1	-2.958462	-5.345787	0.951213
1	-2.373374	-4.615787	2.475993
1	-3.922762	-1.853790	-0.200274
6	-1.531636	2.382155	0.986754

1	-1.065161	3.357468	0.805232
1	-2.458015	2.541609	1.548740
1	-0.852607	1.773592	1.600340
8	-4.468454	1.445393	-0.207805
6	-5.931933	1.555660	-0.369570
6	-6.364282	0.927593	-1.679934
1	-6.275394	-0.161717	-1.670158
1	-7.414671	1.181838	-1.865923
1	-5.768777	1.326346	-2.509944
6	-6.636410	0.965459	0.836596
1	-7.700863	1.224482	0.787711
1	-6.551703	-0.123121	0.878036
1	-6.228822	1.389074	1.762473
6	-6.127128	3.059544	-0.411059
1	-5.767213	3.523353	0.514763
1	-5.586223	3.500776	-1.256323
1	-7.191936	3.291999	-0.522678

(3f')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8659347
Zero-point correction= 0.499733
Thermal correction to Energy= 0.537712
Thermal correction to Enthalpy= 0.538656
Thermal correction to Gibbs Free Energy= 0.428102
Sum of electronic and zero-point Energies= -2241.366202
Sum of electronic and thermal Energies= -2241.328223
Sum of electronic and thermal Enthalpies= -2241.327279
Sum of electronic and thermal Free Energies= -2241.437833

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Cartesian Coordinates

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46	-0.888123	-1.133358	-0.197258
6	2.822931	2.116924	-0.804038
1	3.542223	2.419136	-1.573296
1	1.934692	1.677652	-1.276940
8	2.726882	0.239149	1.111870
6	4.269818	-1.513166	-0.882623
6	3.451208	-2.599267	-0.532480
6	5.638569	-1.669751	-1.004050
6	4.020877	-3.856768	-0.308488
6	6.195483	-2.925432	-0.774368

1	6.249572	-0.815847	-1.283399
6	5.394165	-4.011559	-0.430487
1	3.381487	-4.693359	-0.041421
1	7.270251	-3.054967	-0.869873
1	5.842464	-4.986061	-0.259235
6	2.055789	-2.377063	-0.396582
7	0.930366	-2.133829	-0.273296
6	-2.122490	1.414364	-0.899899
6	-0.704734	1.406262	-1.422647
8	-0.007515	0.309209	-1.257133
8	-0.218187	2.387502	-1.971203
1	-2.754050	1.659927	-1.764808
7	-2.472131	0.094122	-0.375438
6	-3.740872	-0.318764	-0.401152
8	-4.120358	-1.435138	0.013001
8	3.674253	-0.291100	-1.158895
16	3.608249	0.791840	0.093677
8	4.970444	1.137932	0.470426
6	2.485181	3.216884	0.154100
6	1.306047	3.147866	0.899952
6	3.357768	4.290414	0.334185
6	0.990605	4.159217	1.799233
1	0.644698	2.290272	0.774298
6	3.040593	5.301873	1.235229
1	4.282325	4.330701	-0.240496
6	1.856536	5.238203	1.964858
1	0.067718	4.106742	2.372927
1	3.719978	6.140595	1.368150
1	1.607742	6.031548	2.666264
8	-1.440862	-2.760429	1.078305
6	-2.145005	-2.809939	2.101616
8	-3.224724	-2.111615	2.273452
6	-1.799616	-3.717675	3.226761
1	-1.790024	-3.144654	4.159922
1	-2.577410	-4.482563	3.324262
1	-0.829880	-4.190134	3.066180
1	-3.538371	-1.742588	1.372730
6	-2.285522	2.497265	0.157013
1	-3.336549	2.572543	0.458339
1	-1.688411	2.252475	1.045331
1	-1.960267	3.468036	-0.233779
8	-4.589661	0.581466	-0.911187
6	-6.041971	0.502077	-0.708533
6	-6.355204	0.459513	0.775636
1	-7.435591	0.578305	0.919891
1	-6.051838	-0.484223	1.236508
1	-5.851656	1.284916	1.295600
6	-6.519818	1.810986	-1.310238
1	-6.255062	1.869838	-2.372431

1	-7.609178	1.888469	-1.221205
1	-6.067145	2.664666	-0.790884
6	-6.621440	-0.673844	-1.471828
1	-6.300801	-0.642231	-2.520273
1	-6.322086	-1.632195	-1.040545
1	-7.716338	-0.611570	-1.451757

(3g')

Number of imaginary frequencies : 0

Electronic energy : =-3031.4115565
Zero-point correction= 0.564946
Thermal correction to Energy= 0.613326
Thermal correction to Enthalpy= 0.614270
Thermal correction to Gibbs Free Energy= 0.479569
Sum of electronic and zero-point Energies= -3030.846610
Sum of electronic and thermal Energies= -3030.798231
Sum of electronic and thermal Enthalpies= -3030.797286
Sum of electronic and thermal Free Energies= -3030.931987

Cartesian Coordinates

46	-2.138915	-1.000159	-0.164067
6	1.721160	1.841974	-2.458786
1	2.222683	1.785104	-3.431462
1	0.633154	1.733711	-2.586349
8	1.525234	0.220936	-0.320496
6	2.312822	-2.013774	-2.526652
6	1.618995	-2.994838	-1.800660
6	3.499352	-2.316183	-3.169028
6	2.130670	-4.294557	-1.721210
6	4.001170	-3.611928	-3.080118
1	4.013644	-1.543079	-3.732740
6	3.324151	-4.594281	-2.361027
1	1.585626	-5.050393	-1.163113
1	4.932522	-3.855205	-3.584700
1	3.726445	-5.601485	-2.303060
6	0.396487	-2.634036	-1.177549
7	-0.592239	-2.280207	-0.689097
6	-2.929281	1.742557	-0.319223
6	-1.914253	1.496999	-1.421387
8	-1.494379	0.269645	-1.580645
8	-1.491074	2.416801	-2.116129

1	-3.732090	2.351498	-0.752757
7	-3.462672	0.456858	0.122693
6	-4.772974	0.250002	0.285550
8	-5.311807	-0.868219	0.369646
8	1.752000	-0.747426	-2.643621
16	2.258090	0.395333	-1.565238
8	3.716950	0.324853	-1.512907
6	2.101312	3.049667	-1.658097
6	1.237206	3.521956	-0.668673
6	3.339974	3.664905	-1.849772
6	1.601857	4.611939	0.112687
1	0.276265	3.031590	-0.524984
6	3.702184	4.756370	-1.067424
1	4.016244	3.287332	-2.615769
6	2.834081	5.229558	-0.086143
1	0.921260	4.979814	0.877924
1	4.665390	5.237545	-1.221838
1	3.119034	6.083404	0.524862
8	-2.590815	-2.296401	1.451206
6	-3.397756	-3.240759	1.379932
8	-4.429072	-3.243074	0.590658
6	-3.238478	-4.453767	2.220249
1	-4.084077	-4.521481	2.913217
1	-3.271958	-5.342522	1.581312
1	-2.301020	-4.423806	2.776344
1	-4.646040	-2.291509	0.306469
1	4.873428	0.038581	-0.061911
8	5.209788	-0.105396	0.840392
6	4.115850	-0.181380	1.692088
6	3.717768	1.211126	2.173593
6	4.508702	-1.109262	2.829468
1	3.219953	-0.616496	1.223245
9	2.536087	1.197810	2.793315
9	3.620524	2.034967	1.128298
9	4.617279	1.733593	3.011235
9	3.590579	-1.112093	3.798582
9	5.678113	-0.768901	3.371096
9	4.627225	-2.354886	2.368517
6	-2.275773	2.512771	0.820094
1	-1.909657	3.485965	0.471982
1	-3.007260	2.681527	1.618276
1	-1.431689	1.943298	1.234103
8	-5.471428	1.391328	0.383643
6	-6.936327	1.419375	0.467177
6	-7.231845	2.908171	0.448189
1	-6.881561	3.362436	-0.486326
1	-8.311584	3.076088	0.529695
1	-6.738856	3.414238	1.286649
6	-7.552553	0.747110	-0.745574

1	-7.124508	1.158771	-1.667950
1	-7.402514	-0.335297	-0.739266
1	-8.630906	0.946605	-0.756100
6	-7.394286	0.806961	1.777704
1	-7.200374	-0.267751	1.817489
1	-6.886437	1.290037	2.621411
1	-8.472796	0.968094	1.895242

(3h')

Number of imaginary frequencies : 0

Electronic energy : =-2802.4346333
Zero-point correction= 0.505682
Thermal correction to Energy= 0.546977
Thermal correction to Enthalpy= 0.547922
Thermal correction to Gibbs Free Energy= 0.431517
Sum of electronic and zero-point Energies= -2801.928951
Sum of electronic and thermal Energies= -2801.887656
Sum of electronic and thermal Enthalpies= -2801.886712
Sum of electronic and thermal Free Energies= -2802.003116

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Cartesian Coordinates

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46	-0.629885	-0.212333	-0.919012
6	3.389380	2.126653	-0.601266
1	4.063425	2.472805	-1.393429
1	2.477292	1.702850	-1.047986
8	3.398762	0.135734	1.202349
6	4.507547	-1.581725	-0.862395
6	3.404049	-2.443291	-0.768308
6	5.796773	-2.063553	-0.740195
6	3.602404	-3.811792	-0.561751
6	5.984301	-3.428189	-0.530856
1	6.633066	-1.374013	-0.817986
6	4.897680	-4.296187	-0.445371
1	2.743224	-4.472837	-0.489770
1	6.994682	-3.817126	-0.436100
1	5.061171	-5.357879	-0.284587
6	2.108358	-1.871545	-0.853880
7	1.079070	-1.343719	-0.906655
6	-1.722835	2.468437	-0.907195
6	-0.293678	2.550039	-1.427581
8	0.371071	1.428741	-1.529740

8	0.212539	3.632421	-1.692379
1	-2.347593	3.085728	-1.565728
7	-2.172366	1.075563	-0.947240
6	-3.439182	0.771055	-0.893185
8	-3.866359	-0.456831	-0.861802
8	4.272075	-0.242678	-1.125535
16	4.233190	0.766187	0.190346
8	5.604575	1.109653	0.531853
6	3.091464	3.174385	0.426150
6	1.900735	3.109490	1.154010
6	4.009037	4.192503	0.688304
6	1.626053	4.063590	2.126953
1	1.190920	2.306028	0.949226
6	3.731381	5.147176	1.661219
1	4.937532	4.237994	0.120459
6	2.540947	5.083080	2.380409
1	0.696318	4.012657	2.689877
1	4.446136	5.943091	1.857139
1	2.324874	5.830619	3.140507
8	-1.773218	-1.824836	-0.392012
1	-3.095777	-1.104730	-0.707957
6	-1.541940	-2.356316	0.860698
6	-1.382446	-3.863881	0.699811
6	-2.671057	-1.974599	1.812574
1	-0.612178	-2.000331	1.335613
9	-2.427920	-4.411455	0.078317
9	-0.297614	-4.112805	-0.041123
9	-1.228019	-4.488480	1.869778
9	-3.845355	-2.479097	1.418530
9	-2.447403	-2.384578	3.060390
9	-2.798412	-0.641423	1.840971
6	-1.763419	3.021030	0.512375
1	-1.368721	4.042399	0.532084
1	-2.791433	3.037510	0.890747
1	-1.157032	2.392762	1.179799
8	-4.318003	1.741446	-0.913744
6	-5.733254	1.589782	-0.476476
6	-5.767846	0.990504	0.914785
1	-5.465414	-0.059914	0.925014
1	-5.117443	1.556371	1.593729
1	-6.792540	1.053746	1.298950
6	-6.206208	3.028932	-0.457153
1	-7.258844	3.065101	-0.156239
1	-5.621187	3.622792	0.255168
1	-6.114506	3.483198	-1.450434
6	-6.501921	0.780845	-1.500653
1	-6.373822	1.208376	-2.501999
1	-6.193479	-0.267845	-1.518714
1	-7.568926	0.818843	-1.250919

(3')

Number of imaginary frequencies : 0

Electronic energy : =-2802.4361773
Zero-point correction= 0.504588
Thermal correction to Energy= 0.546062
Thermal correction to Enthalpy= 0.547006
Thermal correction to Gibbs Free Energy= 0.431175
Sum of electronic and zero-point Energies= -2801.931590
Sum of electronic and thermal Energies= -2801.890116
Sum of electronic and thermal Enthalpies= -2801.889172
Sum of electronic and thermal Free Energies= -2802.005002

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Cartesian Coordinates

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46	-0.629290	-0.471104	-1.414331
6	2.347497	2.484399	-0.487614
1	2.937296	3.200014	-1.072328
1	1.785136	1.835863	-1.172832
8	2.897581	0.307590	0.992058
6	4.736497	-0.459674	-1.048624
6	3.861486	-1.513119	-1.350936
6	6.071888	-0.695313	-0.787625
6	4.341060	-2.825639	-1.396310
6	6.541659	-2.006193	-0.839467
1	6.724693	0.142084	-0.555372
6	5.685172	-3.062421	-1.142891
1	3.657846	-3.639124	-1.623980
1	7.591378	-2.202662	-0.637745
1	6.066440	-4.078762	-1.178304
6	2.487966	-1.205490	-1.532791
7	1.373792	-0.904325	-1.627958
6	-2.919054	1.185016	-2.090216
6	-1.801723	1.493276	-3.076589
8	-0.688340	0.819154	-2.965517
8	-1.950784	2.371907	-3.916636
1	-3.833285	1.020880	-2.676137
7	-2.583361	-0.024076	-1.338707
6	-3.495058	-0.692020	-0.687326
8	-3.222150	-1.732728	0.041669
8	4.246342	0.835439	-1.069647
16	3.545820	1.419934	0.311811

8	4.549030	2.192992	1.023014
6	1.481970	3.126627	0.548939
6	1.898900	4.293033	1.192744
6	0.271250	2.529280	0.905590
6	1.101553	4.865561	2.177482
1	2.845919	4.752518	0.913190
6	-0.523834	3.103380	1.892768
1	-0.047474	1.618274	0.390749
6	-0.108243	4.271234	2.527346
1	1.425035	5.778107	2.672703
1	-1.467682	2.637746	2.166958
1	-0.731623	4.721167	3.296781
8	-0.694980	-1.736728	0.206200
1	-2.214140	-1.836935	0.175437
6	-0.038364	-1.266169	1.327129
6	0.810424	-2.401320	1.888994
6	-1.030128	-0.706263	2.343565
1	0.678616	-0.451646	1.122884
9	0.086099	-3.486133	2.167643
9	1.726130	-2.752269	0.980285
9	1.459701	-2.044126	2.999329
9	-1.854350	-1.648281	2.813807
9	-0.422788	-0.133800	3.381523
9	-1.796715	0.230130	1.761855
6	-3.101807	2.381194	-1.164840
1	-3.343876	3.274238	-1.749915
1	-3.913167	2.202588	-0.450563
1	-2.176387	2.572785	-0.603809
8	-4.744901	-0.317689	-0.801307
6	-5.829292	-0.739134	0.126959
6	-5.421176	-0.444049	1.556817
1	-4.650383	-1.125494	1.925996
1	-5.058315	0.587842	1.647886
1	-6.301796	-0.548819	2.201040
6	-6.968708	0.162433	-0.303016
1	-7.858753	-0.059697	0.295750
1	-6.708279	1.217594	-0.157713
1	-7.214168	0.002983	-1.359058
6	-6.168574	-2.194904	-0.117299
1	-6.379674	-2.366013	-1.179453
1	-5.366451	-2.867505	0.197948
1	-7.070951	-2.448890	0.451411

Possibilities of C-H bond activation Transition States at *meta*, *ortho* and *para* positions at the SMD/M06/6-31G** Level of Theory.

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meta-**C' [4'-5']**‡

Number of imaginary frequencies : 1
The smallest frequency is : -1619.6921 cm(-1)

Electronic energy : =-2012.8468083
Zero-point correction= 0.431387
Thermal correction to Energy= 0.463295
Thermal correction to Enthalpy= 0.464239
Thermal correction to Gibbs Free Energy= 0.368060
Sum of electronic and zero-point Energies= -2012.415421
Sum of electronic and thermal Energies= -2012.383513
Sum of electronic and thermal Enthalpies= -2012.382569
Sum of electronic and thermal Free Energies= -2012.478748

.....

Cartesian Coordinates

.....

46	-0.787993	0.843020	0.129068
6	-0.404005	-1.200472	0.692338
6	-0.326921	-1.278017	2.096488
6	0.734409	-1.922144	2.720059
6	1.738860	-2.489606	1.943187
6	1.677587	-2.454001	0.545270
6	0.607425	-1.813115	-0.070841
1	2.589251	-2.973612	2.422324
1	0.791562	-1.975919	3.804495
1	-1.116013	-0.824918	2.696502
1	0.562011	-1.763253	-1.159241
6	2.798877	-3.043330	-0.250233
1	2.462943	-3.631758	-1.114103
1	3.467379	-3.667561	0.353529
8	3.120109	-0.949965	-1.913271
6	4.677328	0.348769	0.193588
6	3.815129	1.455198	0.163289
6	6.046223	0.511897	0.086383
6	4.347785	2.743170	0.032905
6	6.563399	1.798190	-0.047662
1	6.691251	-0.362219	0.116479
6	5.721333	2.906929	-0.072313
1	3.676457	3.597060	0.011541
1	7.638585	1.932184	-0.131136
1	6.137055	3.905147	-0.174817
6	2.407626	1.270123	0.232023
7	1.257298	1.134165	0.257758
6	-3.451827	2.018147	-0.137511
6	-2.434263	3.125304	-0.383772
8	-1.173365	2.820462	-0.316645

8	-2.828916	4.267318	-0.607838
1	-4.132866	2.014880	-1.000589
7	-2.773511	0.727851	-0.040441
6	-3.424811	-0.411136	-0.208504
8	-2.862496	-1.545176	-0.126785
1	-1.629910	-1.325977	0.217492
8	4.138309	-0.915781	0.379863
8	5.109810	-2.389772	-1.420987
16	3.854403	-1.798630	-0.988734
6	-4.240228	2.344962	1.124691
1	-4.730563	3.318442	1.019768
1	-5.007863	1.586192	1.311167
1	-3.569332	2.384090	1.992757
8	-4.718233	-0.293482	-0.480951
6	-5.645600	-1.438042	-0.527604
6	-5.289170	-2.352457	-1.682991
1	-5.222313	-1.779931	-2.615950
1	-4.343058	-2.874970	-1.519783
1	-6.079926	-3.102826	-1.803158
6	-5.658366	-2.147303	0.812435
1	-4.720018	-2.670954	1.013607
1	-5.846947	-1.431434	1.622396
1	-6.469060	-2.885419	0.817085
6	-6.976470	-0.754852	-0.778312
1	-7.773264	-1.504680	-0.834030
1	-7.214186	-0.056632	0.033400
1	-6.958119	-0.199012	-1.722920

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meta-**C' [4']**

Number of imaginary frequencies : 0

Electronic energy : =-2012.8679316
Zero-point correction= 0.436424
Thermal correction to Energy= 0.468999
Thermal correction to Enthalpy= 0.469943
Thermal correction to Gibbs Free Energy= 0.371853
Sum of electronic and zero-point Energies= -2012.431508
Sum of electronic and thermal Energies= -2012.398932
Sum of electronic and thermal Enthalpies= -2012.397988
Sum of electronic and thermal Free Energies= -2012.496079

.....

Cartesian Coordinates

.....

46	-0.738818	1.041817	-0.037567
6	-0.145333	-0.760806	0.618007
6	-0.547914	-1.225038	1.874302
6	0.104282	-2.313020	2.452802
6	1.176089	-2.917793	1.802450
6	1.557469	-2.481305	0.533782
6	0.862470	-1.432952	-0.071238
1	1.722298	-3.728263	2.282393
1	-0.203917	-2.669800	3.433626
1	-1.356350	-0.728593	2.411906
1	1.171271	-1.086184	-1.056360
6	2.755824	-3.092925	-0.126239
1	2.514502	-3.684971	-1.020727
1	3.325545	-3.729845	0.559266
8	3.452622	-1.225339	-1.948870
6	4.598131	0.372221	0.253903
6	3.858359	1.539990	0.002243
6	5.979327	0.413014	0.327948
6	4.529198	2.756589	-0.176395
6	6.632903	1.628315	0.141646
1	6.529535	-0.499102	0.541708
6	5.913865	2.793589	-0.110088
1	3.951609	3.657217	-0.365777
1	7.717506	1.661973	0.200545
1	6.433230	3.737304	-0.249863
6	2.437947	1.501382	-0.050567
7	1.279339	1.477932	-0.085902
6	-3.486677	1.945719	0.272648
6	-2.696152	3.163993	-0.216165
8	-1.467678	2.996115	-0.553725
8	-3.284724	4.249919	-0.231691
1	-4.439568	1.946673	-0.271824
7	-2.756955	0.703603	-0.008620
6	-3.413317	-0.385302	-0.260262
8	-2.815996	-1.524326	-0.541626
1	-1.845327	-1.404034	-0.472300
8	3.921275	-0.819319	0.480691
8	5.263763	-2.523788	-0.815660
16	3.947075	-1.910350	-0.763941
6	-3.756624	2.079088	1.765435
1	-4.288607	3.013341	1.972008
1	-4.365725	1.242262	2.125679
1	-2.810849	2.085725	2.324061
8	-4.722207	-0.381936	-0.245950
6	-5.595026	-1.543180	-0.564542
6	-5.348536	-2.001719	-1.987220
6	-5.389006	-2.633334	0.467086
6	-6.975384	-0.931921	-0.430420
1	-5.391337	-1.151472	-2.678044

1	-4.387504	-2.508490	-2.106297
1	-6.139661	-2.706208	-2.269205
1	-5.496087	-2.227168	1.479873
1	-6.160627	-3.399771	0.328195
1	-4.412330	-3.115931	0.377429
1	-7.735241	-1.694972	-0.630621
1	-7.133233	-0.544164	0.582454
1	-7.111176	-0.112497	-1.145399

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meta-**C' (5')**

Number of imaginary frequencies : 0

Electronic energy : =-2012.8721201
Zero-point correction= 0.436430
Thermal correction to Energy= 0.469045
Thermal correction to Enthalpy= 0.469989
Thermal correction to Gibbs Free Energy= 0.371728
Sum of electronic and zero-point Energies= -2012.435690
Sum of electronic and thermal Energies= -2012.403075
Sum of electronic and thermal Enthalpies= -2012.402131
Sum of electronic and thermal Free Energies= -2012.500392

Cartesian Coordinates

46	-0.782453	0.488674	-0.036752
6	-0.432095	-1.947785	-0.201509
6	-0.779594	-1.568389	1.111181
6	0.208943	-1.577321	2.122235
6	1.484650	-2.007603	1.833602
6	1.821272	-2.431515	0.529996
6	0.881546	-2.365740	-0.482940
1	2.240221	-2.053281	2.616222
1	-0.058153	-1.293704	3.136907
1	-1.826657	-1.458751	1.383107
1	1.137591	-2.694146	-1.488416
6	3.189477	-2.974905	0.260985
1	3.176024	-3.826993	-0.430746
1	3.716114	-3.279841	1.172795
8	3.662730	-1.201003	-1.708217
6	4.708133	0.594812	0.307122
6	3.733426	1.552122	-0.009491
6	6.051968	0.916257	0.307073
6	4.122657	2.859692	-0.319968

6	6.428070	2.220228	-0.007675
1	6.783530	0.153142	0.559003
6	5.471766	3.184856	-0.316536
1	3.364967	3.599792	-0.561041
1	7.482356	2.483814	-0.007964
1	5.778431	4.198684	-0.557193
6	2.366636	1.165007	-0.017025
7	1.263349	0.813167	-0.020666
6	-3.250242	1.938535	0.212071
6	-2.187378	2.938259	-0.194723
8	-0.994482	2.464432	-0.441901
8	-2.427109	4.138863	-0.255558
1	-4.142939	2.161655	-0.386603
7	-2.784779	0.585905	-0.084017
6	-3.650505	-0.422780	-0.306016
8	-3.339050	-1.581521	-0.584670
1	-1.216416	-2.046736	-0.945956
8	4.290263	-0.678637	0.665565
8	5.613891	-2.367835	-0.650851
16	4.278614	-1.807344	-0.540138
6	-3.579184	2.141621	1.687362
1	-3.903608	3.172176	1.869908
1	-4.382182	1.463842	1.995498
1	-2.695070	1.939701	2.307024
8	-4.932990	-0.008352	-0.185131
6	-6.063571	-0.915228	-0.367301
6	-6.094542	-1.451877	-1.786672
6	-6.031081	-2.017871	0.676250
6	-7.253823	-0.003581	-0.124145
1	-6.059802	-0.626287	-2.508171
1	-5.260393	-2.129167	-1.985721
1	-7.030973	-2.000511	-1.946494
1	-5.919954	-1.587203	1.679632
1	-6.977236	-2.572094	0.649704
1	-5.214079	-2.722691	0.504031
1	-8.188139	-0.567161	-0.227505
1	-7.217254	0.421007	0.886708
1	-7.266558	0.821400	-0.846287

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meta-**B'**

Number of imaginary frequencies : 1

The smallest frequency is : -1658.5879 cm(-1)

Electronic energy : =-2241.8419809
Zero-point correction= 0.495699
Thermal correction to Energy= 0.533163
Thermal correction to Enthalpy= 0.534108
Thermal correction to Gibbs Free Energy= 0.426237
Sum of electronic and zero-point Energies= -2241.346282
Sum of electronic and thermal Energies= -2241.308818
Sum of electronic and thermal Enthalpies= -2241.307873
Sum of electronic and thermal Free Energies= -2241.415744

.....

Cartesian Coordinates

.....

46	-0.546683	1.938934	0.021116
6	3.213327	3.046316	1.338518
6	1.941502	3.265086	0.823815
6	1.482949	2.549685	-0.298741
6	2.339845	1.604132	-0.892223
6	3.613063	1.380481	-0.382518
6	4.039448	2.101645	0.739831
1	2.001243	1.031025	-1.755912
1	0.807490	3.309535	-1.116680
1	1.289214	4.009255	1.281326
1	5.035193	1.918265	1.142033
6	4.507040	0.344901	-0.983080
8	4.251649	-1.080175	1.299550
6	2.245896	-2.691700	-0.057840
6	1.007869	-2.364915	0.513564
6	2.737650	-3.983201	0.009747
6	0.246363	-3.355116	1.147510
6	1.982435	-4.955082	0.661546
1	3.690124	-4.225836	-0.453586
6	0.745067	-4.647182	1.222958
1	-0.723560	-3.091263	1.562082
1	2.364704	-5.970860	0.718535
1	0.163798	-5.420024	1.717627
6	0.526296	-1.033415	0.407098
7	0.137702	0.050467	0.291418
6	-0.842711	4.572944	-1.133715
8	0.225023	4.328727	-1.760621
6	-1.592175	5.826264	-1.456225
1	-0.899336	6.671283	-1.496236
1	-2.037005	5.715880	-2.451605
1	-2.383444	6.014076	-0.728731
1	3.562877	3.604390	2.203368
8	-1.338040	3.809258	-0.245557
6	-4.082102	0.264540	1.827372
6	-2.700288	0.907852	1.611125

8	-2.490636	1.280334	0.395467
8	-1.934120	1.067763	2.562954
1	-4.793280	1.101553	1.839494
7	-4.470453	-0.562293	0.694701
1	-5.183673	-0.213706	0.068081
6	-3.590932	-1.448638	0.162929
8	-2.552849	-1.798521	0.709858
16	4.394466	-1.231919	-0.138468
8	2.920658	-1.689363	-0.738514
8	5.398330	-2.141467	-0.665615
1	5.571837	0.598892	-0.903178
1	4.284904	0.124044	-2.033775
6	-4.177344	-0.481466	3.144278
1	-5.183946	-0.895413	3.267223
1	-3.455018	-1.303430	3.182606
1	-3.973178	0.189445	3.983573
8	-4.040085	-1.888943	-1.021046
6	-3.232396	-2.774151	-1.861295
6	-3.097989	-4.135494	-1.204890
1	-2.577332	-4.818158	-1.887607
1	-2.529289	-4.083417	-0.271302
1	-4.087580	-4.558249	-0.992595
6	-1.887001	-2.135606	-2.165556
1	-1.185141	-2.235211	-1.334242
1	-1.445660	-2.621092	-3.044353
1	-2.012792	-1.069094	-2.393526
6	-4.064798	-2.871820	-3.126077
1	-4.161200	-1.890355	-3.606049
1	-3.590559	-3.558892	-3.835721
1	-5.069710	-3.247374	-2.900159

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ortho-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1642.7190 cm(-1)

Electronic energy : =-2241.8305257
Zero-point correction= 0.494825
Thermal correction to Energy= 0.532618
Thermal correction to Enthalpy= 0.533562
Thermal correction to Gibbs Free Energy= 0.424514
Sum of electronic and zero-point Energies= -2241.335701
Sum of electronic and thermal Energies= -2241.297907
Sum of electronic and thermal Enthalpies= -2241.296963
Sum of electronic and thermal Free Energies= -2241.406011

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Cartesian Coordinates

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46	-1.057123	-1.526578	-0.259763
6	-2.576722	-0.862560	1.113464
1	-3.201400	-1.546190	0.214209
8	-3.974441	-2.425315	-0.481489
8	-1.940231	-3.340460	-0.632056
6	-2.367244	-1.572790	2.311873
6	-2.585999	-0.981448	3.547690
6	-3.065567	0.324717	3.599707
6	-3.321363	1.033794	2.429197
6	-3.050144	0.469556	1.184444
1	-2.037380	-2.610160	2.257657
1	-2.404217	-1.536847	4.464404
1	-3.263157	0.793760	4.560894
1	-3.741261	2.035609	2.496433
6	-3.425081	1.210280	-0.066423
1	-4.504944	1.404821	-0.100135
1	-3.146971	0.676591	-0.983418
8	-1.987710	3.291063	0.956086
6	-0.414975	3.287611	-1.330883
6	0.670526	2.572461	-0.801010
6	-0.260117	4.581596	-1.786498
6	1.939190	3.151914	-0.752754
6	1.006681	5.159611	-1.719204
1	-1.114910	5.114998	-2.194885
6	2.095699	4.452137	-1.212890
1	2.773646	2.571085	-0.369583
1	1.144027	6.176802	-2.076641
1	3.076142	4.918446	-1.180007
6	0.357050	1.264470	-0.357116
7	-0.099894	0.245738	-0.049231
6	-3.207607	-3.389960	-0.746622
6	2.854365	-2.315021	-1.776042
6	1.610802	-2.261961	-0.874375
8	0.511586	-2.087187	-1.523668
8	1.722720	-2.389334	0.346794
1	2.721890	-1.574021	-2.572726
7	4.039017	-1.971402	-1.010260
1	4.436877	-2.735569	-0.472845
6	4.011269	-0.781848	-0.335805
8	3.312189	0.165598	-0.667998
16	-2.731689	2.880286	-0.221848
8	-3.746195	3.759285	-0.776953
8	-1.628048	2.624120	-1.431566
6	3.004678	-3.703349	-2.368577
1	3.897188	-3.762057	-3.000568
1	3.093344	-4.451835	-1.570051

1	2.130065	-3.955939	-2.976035
8	4.867250	-0.809892	0.691562
6	4.891599	0.263403	1.690553
6	3.507779	0.440226	2.291139
1	3.569359	1.123058	3.146818
1	2.787231	0.846177	1.575068
1	3.130024	-0.525089	2.651071
6	5.447271	1.532187	1.072912
1	4.792064	1.929100	0.293599
1	5.563604	2.297537	1.849634
1	6.433874	1.341944	0.633183
6	5.849834	-0.277622	2.735528
1	6.835537	-0.471194	2.296082
1	5.970796	0.450769	3.545373
1	5.469720	-1.212271	3.164192
6	-3.793314	-4.671387	-1.248400
1	-3.880750	-4.604294	-2.339044
1	-3.145286	-5.517025	-1.008907
1	-4.792897	-4.819672	-0.833822

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ortho-**C'**

Number of imaginary frequencies : 1
The smallest frequency is : -1688.5000 cm(-1)

Electronic energy : =-2012.8392086
Zero-point correction= 0.430187
Thermal correction to Energy= 0.462527
Thermal correction to Enthalpy= 0.463471
Thermal correction to Gibbs Free Energy= 0.366037
Sum of electronic and zero-point Energies= -2012.409022
Sum of electronic and thermal Energies= -2012.376682
Sum of electronic and thermal Enthalpies= -2012.375738
Sum of electronic and thermal Free Energies= -2012.473171

Cartesian Coordinates

46	-0.403790	0.941508	0.636855
6	-0.250204	-0.971952	2.804872
6	0.632090	-1.656616	3.629467
6	1.592308	-2.488595	3.057806
6	1.662867	-2.641847	1.675983
6	0.804780	-1.927631	0.842500
6	-0.173049	-1.071439	1.401450

1	2.390046	-3.327620	1.243563
1	2.279820	-3.042223	3.693369
1	0.567056	-1.557853	4.710352
1	-1.309681	-1.173876	0.772079
6	0.867061	-2.181853	-0.634652
1	-0.063836	-1.903861	-1.147502
1	1.082539	-3.234870	-0.850943
8	1.758024	0.081605	-1.847834
6	4.286132	-0.285271	-0.514304
6	4.033959	0.930620	0.143163
6	5.489894	-0.511903	-1.152726
6	5.017817	1.923016	0.167259
6	6.463774	0.483934	-1.121302
1	5.654410	-1.461777	-1.655114
6	6.232626	1.689378	-0.462312
1	4.816188	2.863060	0.672920
1	7.415186	0.312969	-1.618246
1	7.002179	2.455763	-0.444293
6	2.737299	1.119612	0.687719
7	1.634509	1.191992	1.039789
6	-2.910468	2.111267	-0.328575
6	-1.848739	3.203427	-0.350813
8	-0.641086	2.888491	0.012236
8	-2.161174	4.342339	-0.688686
1	-3.321689	2.052069	-1.347201
7	-2.306046	0.831792	0.035151
6	-2.928490	-0.315603	-0.186019
8	-2.444175	-1.437514	0.149551
1	-1.022268	-0.342752	3.246437
8	3.335456	-1.291315	-0.456648
8	2.565117	-2.130833	-2.690801
16	2.127864	-1.299070	-1.582318
6	-4.017215	2.513036	0.637917
1	-3.616182	2.613038	1.654844
1	-4.445162	3.474378	0.336056
1	-4.815033	1.762389	0.648497
8	-4.102939	-0.217532	-0.796244
6	-5.040288	-1.348519	-0.931208
6	-6.228833	-0.691782	-1.607220
1	-7.024442	-1.429286	-1.760256
1	-6.625339	0.122755	-0.989123
1	-5.944157	-0.282791	-2.583558
6	-4.448126	-2.422596	-1.823090
1	-4.092479	-1.985056	-2.763742
1	-3.621756	-2.953531	-1.344149
1	-5.229753	-3.152791	-2.064915
6	-5.425593	-1.859498	0.442982
1	-4.586989	-2.336197	0.957864
1	-5.804283	-1.038321	1.064782

1 -6.226504 -2.601394 0.339479

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para-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1543.4182 cm(-1)

Electronic energy : =-2241.8401486
Zero-point correction= 0.496402
Thermal correction to Energy= 0.533606
Thermal correction to Enthalpy= 0.534551
Thermal correction to Gibbs Free Energy= 0.427629
Sum of electronic and zero-point Energies= -2241.343746
Sum of electronic and thermal Energies= -2241.306542
Sum of electronic and thermal Enthalpies= -2241.305598
Sum of electronic and thermal Free Energies= -2241.412519

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Cartesian Coordinates

.....

6	2.843102	1.803052	-1.689062
6	1.536464	2.259126	-1.755895
6	0.919286	2.830630	-0.627008
6	1.677609	2.997997	0.547511
6	2.985597	2.544488	0.618216
6	3.551967	1.904946	-0.488204
1	3.309482	1.317604	-2.545019
1	0.967855	2.137443	-2.676786
1	0.064029	3.809243	-0.864750
1	3.557421	2.638618	1.539751
6	4.866538	1.211229	-0.349955
8	3.973885	-0.255639	1.738105
6	2.933176	-2.172606	-0.179905
6	1.572619	-2.072700	0.147151
6	3.587745	-3.390318	-0.123093
6	0.868522	-3.223339	0.528602
6	2.878784	-4.524728	0.264122
1	4.638457	-3.444649	-0.394215
6	1.526989	-4.443330	0.585829
1	-0.188886	-3.132076	0.770015
1	3.391726	-5.481950	0.306727
1	0.978632	-5.334302	0.879668
6	0.872989	-0.834676	0.075949
7	0.245132	0.137325	0.012231
46	-0.907773	1.829863	-0.105908

6	-2.882959	5.636874	-0.638336
6	-1.843748	4.561372	-0.611139
8	-0.686905	4.846064	-1.031203
8	-2.186899	3.425737	-0.163731
1	1.217163	3.460811	1.419910
1	-3.847020	5.270920	-0.282412
1	-2.547773	6.470214	-0.012393
1	-2.979355	6.015231	-1.660914
8	5.915932	-1.117659	0.405346
8	3.606507	-1.037908	-0.609599
16	4.669055	-0.373958	0.467485
1	5.582116	1.742616	0.290220
1	5.349784	0.984688	-1.307164
6	-3.862589	-0.427036	2.068659
6	-2.649476	0.430080	1.666482
8	-1.859651	0.817938	2.530862
8	-2.598816	0.717917	0.412579
1	-4.691304	0.284376	2.185944
7	-4.267838	-1.330941	1.002269
1	-5.076940	-1.077536	0.450114
6	-3.324595	-2.065888	0.357438
8	-2.192423	-2.246998	0.785565
6	-3.646943	-1.148381	3.385654
1	-4.545133	-1.715738	3.652008
1	-2.803601	-1.843489	3.318030
1	-3.437198	-0.434538	4.186954
8	-3.824717	-2.567003	-0.780101
6	-2.968077	-3.246811	-1.754604
6	-2.482591	-4.569021	-1.190240
1	-1.929811	-5.113945	-1.965340
1	-1.821596	-4.425920	-0.330566
1	-3.333443	-5.188149	-0.880972
6	-1.831054	-2.332630	-2.179806
1	-1.056170	-2.248195	-1.412948
1	-1.369947	-2.729512	-3.092172
1	-2.213754	-1.327237	-2.399367
6	-3.915731	-3.479759	-2.916467
1	-4.277960	-2.526499	-3.319579
1	-3.400963	-4.020477	-3.718564
1	-4.781232	-4.073624	-2.599653

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para-**C'**

Number of imaginary frequencies : 1

The smallest frequency is : -1527.2149 cm(-1)

Electronic energy : =-2012.8447449
Zero-point correction= 0.431793
Thermal correction to Energy= 0.463483
Thermal correction to Enthalpy= 0.464427
Thermal correction to Gibbs Free Energy= 0.369261
Sum of electronic and zero-point Energies= -2012.412952
Sum of electronic and thermal Energies= -2012.381262
Sum of electronic and thermal Enthalpies= -2012.380318
Sum of electronic and thermal Free Energies= -2012.475483

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Cartesian Coordinates

.....

46	-0.938631	0.763382	-0.153569
6	0.120565	-1.819918	-1.088913
6	-0.480855	-1.324852	0.084923
6	0.170622	-1.542126	1.314169
6	1.409964	-2.161792	1.360999
6	2.017904	-2.584271	0.175321
6	1.352830	-2.453522	-1.047961
1	1.935609	-2.286972	2.306450
1	-0.286338	-1.183813	2.235766
1	-1.807313	-1.420014	0.061960
1	1.824340	-2.811711	-1.961771
6	3.427767	-3.075028	0.208422
8	4.234807	-1.257264	-1.620726
6	4.580976	0.634781	0.536053
6	3.636076	1.583038	0.115810
6	5.906657	0.987160	0.716420
6	4.043510	2.902201	-0.125008
6	6.298576	2.299709	0.466725
1	6.616768	0.240931	1.061564
6	5.374341	3.251951	0.045768
1	3.307333	3.634392	-0.445320
1	7.339378	2.578468	0.608676
1	5.689378	4.273933	-0.144108
6	2.261307	1.249732	-0.036374
7	1.123550	1.059953	-0.150815
6	-3.605399	1.959991	-0.091269
6	-2.613978	3.065963	-0.428111
8	-1.351548	2.762086	-0.456700
8	-3.025739	4.208345	-0.616677
1	-4.393531	1.984565	-0.857144
7	-2.933452	0.661227	-0.111195
6	-3.618501	-0.469351	-0.098745
8	-3.067694	-1.611434	-0.034090
1	-0.383869	-1.684022	-2.045291
8	4.155712	-0.658603	0.807688

8	5.937374	-2.227662	-0.057170
1	3.624063	-3.897741	-0.491192
1	3.764020	-3.374406	1.207495
16	4.573234	-1.798848	-0.315104
6	-4.213137	2.268465	1.272946
1	-4.701248	3.248287	1.252653
1	-4.956871	1.512957	1.547721
1	-3.429021	2.284986	2.041165
8	-4.937115	-0.343522	-0.179702
6	-5.869931	-1.459454	0.071641
6	-7.218436	-0.771902	-0.026920
1	-8.019536	-1.499818	0.142777
1	-7.308526	0.022022	0.724275
1	-7.359078	-0.330109	-1.020337
6	-5.729151	-2.515782	-1.006675
1	-5.811635	-2.060675	-2.000980
1	-4.777977	-3.049821	-0.939014
1	-6.541395	-3.245088	-0.901026
6	-5.649617	-2.002733	1.469796
1	-4.693843	-2.525208	1.564504
1	-5.684270	-1.190567	2.206926
1	-6.450767	-2.711952	1.709076

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para-**D'**

Number of imaginary frequencies : 1
The smallest frequency is : -1804.2962 cm(-1)

Electronic energy : =-2241.8285368
Zero-point correction= 0.496104
Thermal correction to Energy= 0.533251
Thermal correction to Enthalpy= 0.534195
Thermal correction to Gibbs Free Energy= 0.427309
Sum of electronic and zero-point Energies= -2241.332433
Sum of electronic and thermal Energies= -2241.295286
Sum of electronic and thermal Enthalpies= -2241.294342
Sum of electronic and thermal Free Energies= -2241.401228

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Cartesian Coordinates

.....

46	0.809999	0.838476	-0.207241
6	-0.040282	-1.801861	0.698183
6	0.513692	-1.275715	-0.492411
6	-0.251100	-1.379805	-1.679855

6	-1.512196	-1.950160	-1.672038
6	-2.038252	-2.444501	-0.472776
6	-1.290305	-2.397656	0.709378
1	0.538353	-1.738924	1.620989
8	2.722818	-2.543007	-0.935936
1	-2.107533	-2.005663	-2.581835
1	0.170148	-1.000394	-2.612202
1	1.727408	-1.686658	-0.672585
1	-1.707523	-2.802878	1.629368
6	-3.434418	-2.977208	-0.451811
8	-4.138194	-1.438952	1.646859
6	-4.719412	0.682538	-0.204391
6	-3.728724	1.582877	0.211840
6	-6.057486	1.028661	-0.163696
6	-4.097969	2.852871	0.672741
6	-6.412431	2.291204	0.304737
1	-6.804781	0.317921	-0.506123
6	-5.440660	3.197504	0.721298
1	-3.326144	3.549573	0.987885
1	-7.462558	2.568807	0.337708
1	-5.730146	4.180757	1.080581
6	-2.354038	1.228704	0.145380
7	-1.221965	0.989469	0.088458
6	4.435449	-3.174129	-2.431453
6	3.475354	-2.148055	-1.893124
8	3.467649	-0.991373	-2.364791
6	3.076308	2.306752	-1.167287
6	2.140737	3.340276	-0.550448
8	1.040663	2.894785	-0.023893
8	2.420283	4.532249	-0.627525
1	4.109981	2.620818	-0.979816
1	5.242992	-3.317001	-1.703166
1	3.939625	-4.141040	-2.559505
1	4.871507	-2.843913	-3.377455
7	2.858816	0.975139	-0.544052
1	3.109438	0.186757	-1.190511
6	3.450885	0.829819	0.750908
8	3.758857	1.783211	1.429403
16	-4.578425	-1.837434	0.320692
8	-4.323194	-0.554645	-0.692106
8	-5.940507	-2.305375	0.133744
1	-3.540433	-3.891204	0.147080
1	-3.842210	-3.164708	-1.451614
6	2.821268	2.215303	-2.661961
1	2.927531	3.209841	-3.106539
1	3.537421	1.541583	-3.141976
1	1.805755	1.849513	-2.866185
8	3.567492	-0.449766	1.029062
6	3.992001	-0.917537	2.367773

6	3.009916	-0.409397	3.404057
1	3.221269	-0.893839	4.364498
1	3.080195	0.672837	3.545229
1	1.981351	-0.663410	3.115888
6	5.417780	-0.478053	2.634297
1	5.769815	-0.958900	3.554528
1	6.076438	-0.790523	1.815286
1	5.499034	0.604729	2.761973
6	3.907214	-2.423895	2.226810
1	4.222048	-2.897914	3.162969
1	2.881331	-2.740988	2.002185
1	4.559647	-2.776634	1.419071

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para-**F'**

Number of imaginary frequencies : 1
The smallest frequency is : -1325.6085 cm(-1)

Electronic energy : =-2241.8317567
Zero-point correction= 0.494132
Thermal correction to Energy= 0.532554
Thermal correction to Enthalpy= 0.533498
Thermal correction to Gibbs Free Energy= 0.420069
Sum of electronic and zero-point Energies= -2241.337625
Sum of electronic and thermal Energies= -2241.299203
Sum of electronic and thermal Enthalpies= -2241.298258
Sum of electronic and thermal Free Energies= -2241.411687

Cartesian Coordinates

6	-1.917144	-2.369694	-1.281435
6	-0.858416	-1.480962	-1.367906
6	-0.227024	-1.002098	-0.204040
6	-0.638462	-1.503544	1.044409
6	-1.686947	-2.406586	1.134755
6	-2.358632	-2.799995	-0.026682
1	-2.442908	-2.700044	-2.176036
1	-0.536971	-1.115472	-2.342384
1	1.099936	-0.817602	-0.327603
1	-2.021170	-2.772702	2.103933
6	-3.626202	-3.581719	0.069526
8	-4.754599	-1.807593	1.769029
6	-5.546929	-0.237350	-0.526989
6	-4.806466	0.929077	-0.283606

6	-6.925855	-0.192100	-0.631080
6	-5.474531	2.153905	-0.147786
6	-7.577000	1.029712	-0.484052
1	-7.477424	-1.105298	-0.837143
6	-6.857025	2.196777	-0.243325
1	-4.895590	3.055401	0.033823
1	-8.659981	1.067030	-0.565744
1	-7.373675	3.145928	-0.134142
6	-3.386288	0.910140	-0.205167
7	-2.230721	0.980967	-0.159107
46	-0.190048	1.140300	-0.184535
8	1.841840	1.447544	-0.209462
6	2.663249	0.499374	-0.341248
8	2.357202	-0.721965	-0.432628
6	4.119220	0.901095	-0.443595
1	4.331093	1.556521	0.410785
6	6.269902	-0.146528	0.013001
8	6.784688	0.904964	0.368501
7	4.967802	-0.263930	-0.347620
8	-4.868529	-1.434120	-0.704894
16	-5.003975	-2.527626	0.531568
8	-6.252070	-3.254338	0.372652
1	-3.925569	-4.049183	-0.875360
1	-3.615997	-4.348035	0.855570
1	-0.147431	-1.153766	1.951627
1	4.629454	-1.152229	-0.696180
6	4.334503	1.681242	-1.738442
1	5.384578	1.982601	-1.805074
1	4.093623	1.057600	-2.607572
1	3.711955	2.580882	-1.763058
8	6.877191	-1.338380	-0.069693
6	8.300459	-1.495090	0.245157
6	8.531301	-2.973788	-0.003993
1	8.312234	-3.231469	-1.046997
1	9.576974	-3.228393	0.202762
1	7.892666	-3.583710	0.645982
6	9.142455	-0.663164	-0.704526
1	8.886728	-0.895471	-1.745495
1	9.009882	0.409110	-0.538885
1	10.201084	-0.906423	-0.553721
6	8.555571	-1.157583	1.702273
1	7.890420	-1.740963	2.350511
1	9.590280	-1.416595	1.957652
1	8.406197	-0.094254	1.907270
8	-0.356663	3.223257	-0.260232
6	-0.263198	3.771465	0.907543
8	-0.129712	3.155763	1.970067
6	-0.316497	5.279688	0.874147
1	-0.356263	5.686178	1.887573

1	0.574367	5.665086	0.365863
1	-1.187293	5.619515	0.304292

Possibilities of RE Transition States for the *meta* Product at the SMD/M06/6-31G** Level of Theory

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conf-2' (6-coordination)

Number of imaginary frequencies : 1
The smallest frequency is : -278.7569 cm(-1)

Electronic energy : =-2698.5139174
Zero-point correction= 0.603858
Thermal correction to Energy= 0.651051
Thermal correction to Enthalpy= 0.651995
Thermal correction to Gibbs Free Energy= 0.525780
Sum of electronic and zero-point Energies= -2697.910059
Sum of electronic and thermal Energies= -2697.862867
Sum of electronic and thermal Enthalpies= -2697.861923
Sum of electronic and thermal Free Energies= -2697.988138

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Cartesian Coordinates

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46	-2.047633	-0.283824	-0.090816
6	-2.811123	3.714983	-1.309385
6	-2.960431	2.324042	-1.341433
6	-1.780766	1.637739	-1.218258
6	-0.504846	2.130904	-1.257631
6	-0.401532	3.526142	-1.196126
6	-1.556502	4.307341	-1.210303
1	0.374423	1.497194	-1.299165
1	-3.937536	1.857781	-1.390122
1	-1.470617	5.390498	-1.165579
6	0.954145	4.151811	-1.099249
1	0.904344	5.247000	-1.117256
1	1.648393	3.829100	-1.884947
8	0.890269	3.627575	1.560492
6	2.942871	1.531494	1.047524
6	2.245903	0.413430	1.530817
6	4.203278	1.839385	1.528292
6	2.832639	-0.414240	2.495536
6	4.766019	1.023709	2.508492
1	4.737101	2.698214	1.131443

6	4.091044	-0.097809	2.985466
1	2.290321	-1.287382	2.849188
1	5.753955	1.264096	2.892240
1	4.550043	-0.732014	3.738109
6	0.938397	0.153084	1.044542
7	-0.127669	-0.019529	0.631780
6	0.464138	-3.663164	0.421934
6	-0.974518	-3.231555	0.053966
8	-1.670089	-2.745065	1.001952
8	-1.309733	-3.329679	-1.137628
1	0.646190	-4.634261	-0.065739
7	1.322819	-2.653458	-0.193132
6	2.667861	-2.760911	-0.278743
8	3.334201	-3.683235	0.173600
1	-3.707683	4.328638	-1.347212
8	2.357554	2.280378	0.034577
8	2.949504	4.672112	0.575017
16	1.803657	3.789992	0.442689
8	-3.868250	-0.806279	-0.701103
6	-4.962961	-0.259100	-0.229243
8	-5.014769	0.721974	0.500330
8	-1.794123	-0.245635	-2.138093
6	-0.657781	-0.615407	-2.720799
8	0.436699	-0.625930	-2.183585
6	-0.900111	-1.027520	-4.141085
1	-1.513429	-0.286683	-4.661775
1	0.055053	-1.164409	-4.652443
1	-1.452682	-1.974057	-4.137945
6	-6.184066	-1.015907	-0.679619
1	-6.246858	-1.944730	-0.100542
1	-7.078095	-0.415664	-0.495161
1	-6.117837	-1.287755	-1.736355
6	0.704883	-3.784140	1.911819
1	1.743828	-4.060864	2.116279
1	0.481265	-2.837632	2.417310
1	0.053895	-4.553999	2.341317
8	3.154400	-1.674260	-0.911302
6	4.539193	-1.605939	-1.370064
6	4.570556	-0.288040	-2.123552
1	5.569910	-0.113698	-2.538680
1	3.846060	-0.297075	-2.946937
1	4.323660	0.549823	-1.457500
6	4.833924	-2.760403	-2.312005
1	5.811166	-2.605536	-2.784998
1	4.856043	-3.720076	-1.788300
1	4.076848	-2.808193	-3.104231
6	5.487931	-1.563813	-0.187309
1	6.516637	-1.447925	-0.550483
1	5.257671	-0.704119	0.454785

1	5.430177	-2.478849	0.409433
1	0.896391	-1.956306	-0.798459
8	-2.613207	0.039634	1.920948
6	-3.433782	-0.668151	2.543835
8	-3.720707	-1.894361	2.240022
6	-4.159396	-0.110206	3.710486
1	-5.235058	-0.187689	3.516347
1	-3.940621	-0.709743	4.599839
1	-3.886031	0.932392	3.875285
1	-3.054196	-2.283536	1.576973

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conf-1' (6-coordination)

Number of imaginary frequencies : 1
The smallest frequency is : -318.4065 cm(-1)

Electronic energy : =-2469.5222936
Zero-point correction= 0.540602
Thermal correction to Energy= 0.581848
Thermal correction to Enthalpy= 0.582792
Thermal correction to Gibbs Free Energy= 0.469318
Sum of electronic and zero-point Energies= -2468.981692
Sum of electronic and thermal Energies= -2468.940446
Sum of electronic and thermal Enthalpies= -2468.939502
Sum of electronic and thermal Free Energies= -2469.052976

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Cartesian Coordinates

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46	-1.620861	-0.570960	0.675565
6	-1.171109	-2.163470	-3.282216
6	-1.840465	-2.008619	-2.068582
6	-1.038508	-1.950573	-0.948290
6	0.300889	-2.255570	-0.910366
6	0.949679	-2.362010	-2.145856
6	0.214836	-2.296283	-3.326961
1	0.850361	-2.362425	0.016992
1	-1.489623	0.761589	-1.805314
1	-2.919458	-1.910232	-2.026200
1	0.725326	-2.380247	-4.283740
6	2.437987	-2.502410	-2.172088
1	2.828343	-2.569020	-3.194396
1	2.816945	-3.361074	-1.603609
8	2.508142	0.145235	-1.565915
6	3.712307	-0.628762	1.041512

6	2.761328	-0.016850	1.874118
6	5.059480	-0.353468	1.189622
6	3.172099	0.881398	2.865572
6	5.456425	0.547411	2.175934
1	5.784075	-0.847941	0.549114
6	4.523020	1.160556	3.008288
1	2.425748	1.344323	3.505752
1	6.514233	0.765589	2.297127
1	4.850757	1.856278	3.775058
6	1.389013	-0.316274	1.684304
7	0.283565	-0.603417	1.494535
6	-1.179967	2.281502	1.650371
6	-1.583942	1.511219	2.924085
8	-2.224228	0.427910	2.781088
8	-1.293431	2.069246	3.995111
1	-0.175054	2.688091	1.828624
7	-1.152269	1.438434	0.454592
6	-0.503905	1.816980	-0.612060
8	-0.551048	1.135111	-1.726373
1	-1.751701	-2.170697	-4.201473
8	3.267329	-1.556464	0.109453
8	4.672660	-1.074334	-1.928669
16	3.291345	-1.076291	-1.479300
8	-3.521293	-0.281982	0.062883
6	-3.846921	0.386682	-0.994845
8	-3.073256	0.796203	-1.870525
8	-2.159662	-2.596913	0.617932
6	-1.563268	-3.504562	1.388872
8	-0.457561	-3.385533	1.880952
6	-2.438335	-4.712767	1.558459
1	-2.602626	-5.186162	0.584407
1	-1.966387	-5.423290	2.240154
1	-3.417150	-4.414940	1.947347
6	-5.323233	0.648080	-1.089664
1	-5.574630	1.471732	-0.411762
1	-5.589191	0.932241	-2.110181
1	-5.897428	-0.226921	-0.774247
6	-2.190896	3.405631	1.459450
1	-1.945520	4.023226	0.587898
1	-3.192885	2.979663	1.314033
1	-2.209735	4.043744	2.348960
8	0.227189	2.902589	-0.569508
6	0.442530	3.777474	-1.761484
6	0.982470	5.043189	-1.127828
1	1.211199	5.775231	-1.910142
1	0.249263	5.486417	-0.444096
1	1.902772	4.836704	-0.569694
6	-0.889054	4.035691	-2.437104
1	-0.749928	4.799266	-3.211144

1	-1.300519	3.141812	-2.915882
1	-1.619162	4.420516	-1.713810
6	1.473680	3.154412	-2.678630
1	1.700818	3.867166	-3.480661
1	2.402500	2.952907	-2.133031
1	1.122091	2.225931	-3.136241

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conf-5' (5- coordination) **[6'-7']**‡

Number of imaginary frequencies : 1
The smallest frequency is : -256.0709 cm(-1)

Electronic energy : =-2927.5280552
Zero-point correction= 0.669286
Thermal correction to Energy= 0.721540
Thermal correction to Enthalpy= 0.722484
Thermal correction to Gibbs Free Energy= 0.584558
Sum of electronic and zero-point Energies= -2926.858769
Sum of electronic and thermal Energies= -2926.806515
Sum of electronic and thermal Enthalpies= -2926.805571
Sum of electronic and thermal Free Energies= -2926.943497

Cartesian Coordinates

46	-1.062094	-1.977571	-0.407049
6	-4.347213	-0.764513	1.951906
6	-3.558034	-1.621898	1.175501
6	-3.008418	-1.022560	0.074077
6	-3.266904	0.219253	-0.441072
6	-4.062212	1.042021	0.364520
6	-4.582926	0.549166	1.562341
1	-2.860052	0.571433	-1.384572
1	-3.363311	-2.651045	1.461096
1	-5.198796	1.196837	2.183440
6	-4.324391	2.446615	-0.073156
1	-5.255990	2.850151	0.343393
1	-4.357237	2.564829	-1.162536
8	-2.721526	3.419795	1.873047
6	-0.537241	3.348198	-0.131754
6	0.391848	2.299382	-0.209382
6	-0.125602	4.628102	0.196832
6	1.744932	2.540917	0.065568
6	1.222344	4.854432	0.465170
1	-0.843578	5.443187	0.230144
6	2.155036	3.821211	0.400559

1	2.457974	1.721363	0.008481
1	1.544538	5.860161	0.721881
1	3.205040	4.012763	0.604265
6	-0.037410	0.999589	-0.576299
7	-0.378708	-0.056865	-0.915477
6	2.304847	-1.760513	-0.599869
6	1.602237	-1.356683	0.697712
8	0.476109	-1.991041	0.958764
8	2.084021	-0.566894	1.494833
1	1.539434	-1.874559	-1.379303
7	3.186821	-0.718092	-1.095564
6	4.293231	-0.218187	-0.503591
8	4.808982	0.847645	-0.865490
1	-4.778398	-1.152297	2.871875
8	-1.843484	3.042079	-0.462488
8	-3.426698	4.938819	0.004497
16	-3.078861	3.611055	0.479766
8	-1.569664	-3.780841	0.319817
6	-0.915751	-4.717503	-0.317520
8	-0.127826	-4.489435	-1.232925
8	-2.738573	-2.299197	-1.551848
6	-2.838316	-1.739272	-2.757892
8	-2.049387	-0.934922	-3.213994
6	-4.072331	-2.216750	-3.463095
6	-1.223472	-6.094388	0.194783
1	2.808230	-0.100544	-1.817209
8	-1.131907	0.633096	2.079381
6	-1.261132	0.002749	3.112844
6	-1.994909	0.492754	4.318417
1	-1.266647	0.751455	5.095949
1	-2.582118	1.380145	4.068772
1	-2.639859	-0.290951	4.727880
8	-0.731038	-1.205718	3.292762
1	-0.224627	-1.455112	2.475512
1	4.129915	1.958998	-1.951434
8	3.745451	2.743548	-2.433849
6	2.573444	2.429865	-2.959302
6	1.878393	3.605276	-3.558212
1	0.966296	3.291582	-4.068417
1	1.629312	4.311122	-2.755395
1	2.542455	4.127854	-4.253831
8	2.101408	1.300421	-2.928985
1	-0.717434	-6.843583	-0.417806
1	-2.303772	-6.269178	0.183747
1	-0.887069	-6.182184	1.233195
1	-4.139528	-3.307973	-3.430013
1	-4.068489	-1.869063	-4.498061
1	-4.950530	-1.816698	-2.942180
6	2.956613	-3.129076	-0.406707

1	3.584390	-3.363230	-1.272769
1	3.576661	-3.164341	0.493886
1	2.178491	-3.895216	-0.327777
8	4.784387	-0.997359	0.447603
6	5.783208	-0.521857	1.414076
6	7.132491	-0.409972	0.733268
6	5.337289	0.783328	2.049503
6	5.779109	-1.637364	2.442577
1	7.410473	-1.364181	0.269945
1	7.129418	0.367974	-0.035451
1	7.897018	-0.157944	1.478162
1	4.295877	0.709733	2.385391
1	5.963702	0.982013	2.927327
1	5.429918	1.632559	1.367334
1	6.503509	-1.423822	3.236528
1	4.784087	-1.735885	2.895514
1	6.047430	-2.594178	1.978496

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[6']

Number of imaginary frequencies : 0

Electronic energy : =-2927.5487524
Zero-point correction= 0.671701
Thermal correction to Energy= 0.724013
Thermal correction to Enthalpy= 0.724957
Thermal correction to Gibbs Free Energy= 0.588894
Sum of electronic and zero-point Energies= -2926.877051
Sum of electronic and thermal Energies= -2926.824739
Sum of electronic and thermal Enthalpies= -2926.823795
Sum of electronic and thermal Free Energies= -2926.959858

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Cartesian Coordinates

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46	-0.868153	-2.158250	-0.309595
6	-3.651614	-0.893563	2.616432
6	-2.684459	-1.658227	1.951618
6	-2.454386	-1.305940	0.645827
6	-3.125015	-0.347721	-0.074989
6	-4.045703	0.431570	0.631691
6	-4.296158	0.158407	1.977096
1	-2.933983	-0.150992	-1.124999
1	-2.145501	-2.453912	2.457443
1	-5.008625	0.773039	2.524359

6	-4.680828	1.587910	-0.069559
1	-5.643969	1.878363	0.369744
1	-4.827356	1.419992	-1.142894
8	-3.275620	3.357899	1.400487
6	-1.160352	3.165351	-0.596471
6	-0.060589	2.293507	-0.552158
6	-0.971743	4.528035	-0.442611
6	1.224944	2.788560	-0.294850
6	0.313662	5.010597	-0.205831
1	-1.814343	5.211348	-0.511492
6	1.407196	4.150852	-0.124174
1	2.060026	2.093605	-0.231713
1	0.457222	6.081007	-0.084188
1	2.401966	4.543004	0.067321
6	-0.245614	0.904824	-0.743818
7	-0.384433	-0.228157	-0.954629
6	2.363367	-1.632706	-0.206283
6	1.538514	-1.143266	0.985002
8	0.426957	-1.796773	1.266231
8	1.929400	-0.241038	1.712052
1	1.690348	-2.026505	-0.978509
7	3.066471	-0.546376	-0.869206
6	4.072403	0.219140	-0.392087
8	4.410191	1.276451	-0.940955
1	-3.869664	-1.122058	3.657389
8	-2.395738	2.598598	-0.843009
8	-4.367561	4.144940	-0.719135
16	-3.710655	3.096505	0.041317
8	-1.369816	-3.920425	0.488749
6	-0.541188	-4.840360	0.054376
8	0.376939	-4.595895	-0.723160
8	-2.146555	-2.559824	-1.823328
6	-1.484418	-2.630799	-2.955774
8	-0.273269	-2.465252	-3.048682
6	-2.377725	-2.941877	-4.121178
6	-0.838558	-6.198734	0.611947
1	2.594971	-0.127723	-1.675016
8	-0.977688	1.203521	2.049664
6	-0.974117	0.835573	3.209812
6	-1.571954	1.595214	4.347339
1	-0.766611	2.064952	4.924167
1	-2.239985	2.372615	3.971227
1	-2.109442	0.922804	5.022789
8	-0.407208	-0.304426	3.605226
1	-0.025854	-0.746685	2.811123
1	3.596888	2.064684	-2.217451
8	3.120390	2.669045	-2.851401
6	2.020921	2.084622	-3.296959
6	1.200145	2.978436	-4.163360

1	0.382268	2.419806	-4.621110
1	0.788372	3.787736	-3.547217
1	1.823117	3.442674	-4.933904
8	1.700578	0.940477	-3.001315
1	-0.119468	-6.923427	0.223972
1	-1.855148	-6.499111	0.338995
1	-0.785765	-6.170311	1.704958
1	-2.841744	-3.923407	-3.978521
1	-1.793738	-2.942140	-5.044184
1	-3.182711	-2.203642	-4.188923
6	3.233910	-2.797112	0.259750
1	3.916702	-3.093772	-0.542985
1	3.820628	-2.538328	1.146087
1	2.593188	-3.651567	0.502476
8	4.675340	-0.294247	0.668841
6	5.565520	0.501398	1.524955
6	6.883929	0.732113	0.813712
6	4.886618	1.794122	1.941326
6	5.745466	-0.411874	2.723490
1	7.323549	-0.222840	0.501707
1	6.759284	1.367802	-0.067235
1	7.586108	1.222411	1.498848
1	3.875535	1.590577	2.314102
1	5.462874	2.252887	2.753569
1	4.823415	2.513682	1.120377
1	6.421132	0.049750	3.452260
1	4.779868	-0.598316	3.210599
1	6.173944	-1.373570	2.416225

[7']

Number of imaginary frequencies : 0

Electronic energy : =-2927.6075267
Zero-point correction= 0.671618
Thermal correction to Energy= 0.724227
Thermal correction to Enthalpy= 0.725171
Thermal correction to Gibbs Free Energy= 0.585909
Sum of electronic and zero-point Energies= -2926.935909
Sum of electronic and thermal Energies= -2926.883300
Sum of electronic and thermal Enthalpies= -2926.882355
Sum of electronic and thermal Free Energies= -2927.021617

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Cartesian Coordinates

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46	-0.862314	-1.951901	-0.326919
6	-4.843629	-0.404218	1.500735
6	-4.182009	-1.301054	0.668856
6	-3.583600	-0.802547	-0.477516
6	-3.610003	0.535232	-0.826281
6	-4.269397	1.424534	0.020522
6	-4.878493	0.949978	1.183475
1	-3.103401	0.869670	-1.730044
1	-4.109729	-2.362137	0.900276
1	-5.383999	1.651552	1.844897
6	-4.307558	2.880848	-0.308034
1	-5.205512	3.376573	0.082444
1	-4.240072	3.091738	-1.381735
8	-2.741385	3.466554	1.816311
6	-0.442390	3.435944	-0.106951
6	0.447989	2.351849	-0.145196
6	0.012728	4.701882	0.224451
6	1.803561	2.545683	0.160937
6	1.359584	4.878643	0.531103
1	-0.669507	5.546764	0.229066
6	2.254131	3.811236	0.498737
1	2.481393	1.694422	0.126742
1	1.712209	5.873822	0.789023
1	3.305007	3.965299	0.727321
6	0.005750	1.054191	-0.502810
7	-0.299116	-0.023329	-0.806948
6	2.480124	-1.773246	-0.665474
6	1.797952	-1.376276	0.644211
8	0.725449	-2.075562	0.954235
8	2.245258	-0.522242	1.395514
1	1.697371	-1.878937	-1.428664
7	3.352511	-0.726558	-1.168909
6	4.449040	-0.218191	-0.565538
8	4.953179	0.858724	-0.910267
1	-5.324625	-0.762793	2.407041
8	-1.749138	3.184668	-0.481963
8	-3.133397	5.221808	0.065994
16	-2.977176	3.823068	0.429010
8	-1.465122	-3.730329	0.343330
6	-0.856247	-4.749821	-0.202887
8	-0.004242	-4.664426	-1.083635
8	-2.790927	-1.663011	-1.258965
6	-3.291474	-2.530086	-2.223149
8	-2.505717	-3.282647	-2.726194
6	-4.737364	-2.388866	-2.523273
6	-1.293972	-6.064558	0.382922
1	2.942235	-0.084026	-1.850954
8	-1.513243	0.459401	1.910702

6	-1.537559	-0.205720	2.930703
6	-2.397487	0.088911	4.116203
1	-1.760894	0.314225	4.979330
1	-3.046515	0.942731	3.911554
1	-2.994962	-0.789904	4.380521
8	-0.786762	-1.289764	3.116609
1	-0.200453	-1.445847	2.331723
1	4.209254	1.993743	-1.919602
8	3.794174	2.787632	-2.361054
6	2.611485	2.474333	-2.859924
6	1.892873	3.653073	-3.423761
1	0.924085	3.351312	-3.825418
1	1.753373	4.401265	-2.633841
1	2.495844	4.120839	-4.209112
8	2.150850	1.339584	-2.844565
1	-0.995975	-6.885711	-0.273295
1	-2.375560	-6.084337	0.543947
1	-0.812575	-6.197683	1.358474
1	-5.337060	-2.639324	-1.641272
1	-4.988353	-3.065226	-3.341111
1	-4.973489	-1.356844	-2.804839
6	3.131126	-3.145892	-0.499296
1	3.755042	-3.365521	-1.372023
1	3.756296	-3.198540	0.397309
1	2.351603	-3.912271	-0.430572
8	4.946629	-1.006014	0.375700
6	5.944257	-0.538593	1.346515
6	7.294370	-0.430637	0.666935
6	5.507494	0.766592	1.988823
6	5.930593	-1.658010	2.370726
1	7.571534	-1.386197	0.205979
1	7.291606	0.345447	-0.104018
1	8.059066	-0.176892	1.411086
1	4.463185	0.702081	2.317460
1	6.129735	0.949974	2.872902
1	5.615242	1.620361	1.314915
1	6.653163	-1.452127	3.168375
1	4.932556	-1.751376	2.818524
1	6.194294	-2.614829	1.904073

Acetoxylation product using Boc-Ala-OH (M06/6-31G)**

$[Pd(OAc)_2]_3$

Number of imaginary frequencies : 0

Electronic energy : =-1750.5747527
Zero-point correction= 0.315721
Thermal correction to Energy= 0.349705
Thermal correction to Enthalpy= 0.350649
Thermal correction to Gibbs Free Energy= 0.246602
Sum of electronic and zero-point Energies= -1750.259032
Sum of electronic and thermal Energies= -1750.225048
Sum of electronic and thermal Enthalpies= -1750.224104
Sum of electronic and thermal Free Energies= -1750.328150

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Cartesian Coordinates

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46	1.559037	0.928514	-0.001488
8	2.288923	0.035247	-1.687034
8	2.647809	-0.307202	1.230488
6	2.237849	-1.316722	1.863936
8	1.167662	-1.961746	1.678836
46	0.023733	-1.809013	-0.005073
6	2.293810	-1.213956	-1.872974
8	1.643990	-2.088612	-1.240602
8	1.121000	1.989958	1.685653
8	0.987212	2.468094	-1.238768
6	-0.097355	2.595324	-1.866543
8	-1.177725	1.970204	-1.674795
46	-1.584818	0.884530	0.004864
6	0.023813	2.584005	1.881424
8	-1.056834	2.431774	1.252415
8	-2.292781	-0.036952	1.684456
8	-2.637838	-0.371229	-1.237573
6	-2.258257	-1.285446	1.868666
6	-2.201320	-1.367910	-1.873886
8	-1.586272	-2.139520	1.230445
8	-1.115966	-1.986972	-1.689102
6	3.211147	-1.714141	-2.954887
1	4.199552	-1.887537	-2.516001
1	2.841563	-2.655565	-3.365126
1	3.317396	-0.959703	-3.737086
6	-0.122286	3.635851	-2.952546
1	-0.414387	4.592792	-2.507050
1	0.869108	3.748845	-3.395060
1	-0.863046	3.373594	-3.710443
6	0.023207	3.615209	2.976519
1	-0.981076	3.739542	3.385116
1	0.731778	3.332597	3.757816

1	0.350769	4.570525	2.552863
6	-3.146918	-1.821609	2.957425
1	-2.653970	-2.649810	3.470838
1	-3.413998	-1.029045	3.658558
1	-4.064063	-2.205104	2.497903
6	-3.092000	-1.901618	-2.962005
1	-3.830496	-2.570373	-2.507229
1	-3.626655	-1.083012	-3.447853
1	-2.508404	-2.473334	-3.685744
6	3.143996	-1.833103	2.947659
1	3.668480	-1.005122	3.428560
1	2.574299	-2.412786	3.676207
1	3.889791	-2.491572	2.489745

HFIP (Solvent)

Number of imaginary frequencies : 0

Electronic energy : =-789.5215432
Zero-point correction= 0.063922
Thermal correction to Energy= 0.072851
Thermal correction to Enthalpy= 0.073796
Thermal correction to Gibbs Free Energy= 0.029116
Sum of electronic and zero-point Energies= -789.457621
Sum of electronic and thermal Energies= -789.448692
Sum of electronic and thermal Enthalpies= -789.447748
Sum of electronic and thermal Free Energies= -789.492427

Cartesian Coordinates

6	-1.283718	-0.135145	-0.030927
6	-0.002832	0.543010	-0.499026
6	1.262325	-0.164874	-0.025539
1	-0.002373	0.474571	-1.600544
9	-1.459539	-0.025204	1.278021
9	-2.325072	0.424648	-0.642096
9	-1.260249	-1.431296	-0.348226
9	1.262895	-0.395792	1.279938
9	1.448777	-1.315253	-0.664941
9	2.307693	0.632968	-0.303658
8	-0.046081	1.843729	-0.018219
1	0.745819	2.307000	-0.312083

AcOH

Number of imaginary frequencies : 0

Electronic energy : =-1218.074667
Zero-point correction= 0.223415
Thermal correction to Energy= 0.239432
Thermal correction to Enthalpy= 0.240376
Thermal correction to Gibbs Free Energy= 0.178912
Sum of electronic and zero-point Energies= -1217.851252
Sum of electronic and thermal Energies= -1217.835235
Sum of electronic and thermal Enthalpies= -1217.834291
Sum of electronic and thermal Free Energies= -1217.895755

Cartesian Coordinates

6	2.352473	1.400784	0.089725
6	2.392458	0.055776	0.460263
6	3.386937	-0.775889	-0.057281
6	4.334099	-0.264588	-0.935584
6	4.294975	1.078569	-1.298512
6	3.304852	1.910499	-0.784547
1	1.569481	2.041772	0.495194
1	3.411347	-1.826965	0.225626
1	5.106512	-0.916529	-1.336362
1	5.039400	1.477673	-1.983742
1	3.273452	2.960322	-1.065773
6	1.364827	-0.479333	1.405383
1	0.842247	0.312888	1.955197
1	1.776372	-1.199250	2.124252
16	0.058387	-1.421536	0.605229
8	0.611352	-2.507433	-0.175005
8	-1.021748	-1.645693	1.545411
8	-0.451760	-0.264870	-0.482674
6	-1.803593	-0.023710	-0.560688
6	-2.611333	-0.809776	-1.365694
6	-2.334794	1.058401	0.152412
6	-3.964203	-0.505286	-1.470276
1	-2.163307	-1.646056	-1.896457
6	-3.694704	1.359020	0.034536
6	-4.503708	0.576735	-0.777504
1	-4.603414	-1.119493	-2.099173
1	-4.102721	2.200663	0.587334
1	-5.561180	0.808412	-0.867954
6	-1.460784	1.807052	0.997427

7	-0.710021	2.380796	1.676910

Different Possibilities of Potential Active Catalyst

$Pd(OAc)_2$ with Ligand combinations (M06/6-31G**)

(2a')

Number of imaginary frequencies : 0

Electronic energy : =-1252.710489
Zero-point correction= 0.339273
Thermal correction to Energy= 0.366055
Thermal correction to Enthalpy= 0.366999
Thermal correction to Gibbs Free Energy= 0.278684
Sum of electronic and zero-point Energies= -1252.371216
Sum of electronic and thermal Energies= -1252.344434
Sum of electronic and thermal Enthalpies= -1252.343490
Sum of electronic and thermal Free Energies= -1252.431805

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Cartesian Coordinates

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46	-2.286097	0.397797	-0.326306
1	-2.041467	-2.074674	1.033737
6	-2.897834	-2.487783	-0.666445
8	-2.685122	-2.737434	0.580342
6	-3.541707	-3.597700	-1.428049
1	-3.719632	-3.302654	-2.461913
1	-2.902235	-4.484464	-1.388584
1	-4.486379	-3.859721	-0.941659
8	-2.617177	-1.424285	-1.251039
6	1.426543	-0.733055	1.428426
6	-0.032890	-0.722344	1.006685
8	-0.323887	0.032753	0.013817
8	-0.832732	-1.413328	1.658096
7	2.240683	0.018364	0.501886
1	1.787005	0.625101	-0.166261
6	3.575092	-0.218415	0.407312
8	4.176389	-1.007421	1.113770
6	-3.689776	2.340799	0.057172
8	-4.155468	1.296841	-0.503134
6	-4.521799	3.551428	0.267122
1	-4.232709	4.046103	1.197573

1	-4.347793	4.251981	-0.556539
1	-5.580434	3.283575	0.280526
8	-2.464575	2.314433	0.413758
8	4.104504	0.545513	-0.567312
6	5.531822	0.491563	-0.849733
6	5.688812	1.494615	-1.979393
1	5.370855	2.492103	-1.656108
1	6.737689	1.547083	-2.292756
1	5.081178	1.200860	-2.842634
6	5.925220	-0.900535	-1.316649
1	5.807505	-1.633833	-0.515280
1	5.305985	-1.201594	-2.170082
1	6.972710	-0.894602	-1.641773
6	6.327986	0.933706	0.367393
1	7.388671	1.013269	0.100144
1	5.986492	1.919423	0.705167
1	6.223057	0.220792	1.188524
6	1.545092	-0.216185	2.859895
1	2.591686	-0.274706	3.171554
1	1.217577	0.828362	2.915479
1	0.931907	-0.818424	3.535909
1	1.749195	-1.784341	1.413027

(2b')

Number of imaginary frequencies : 0

Electronic energy : =-1023.7122798
Zero-point correction= 0.276900
Thermal correction to Energy= 0.297460
Thermal correction to Enthalpy= 0.298404
Thermal correction to Gibbs Free Energy= 0.227350
Sum of electronic and zero-point Energies= -1023.435380
Sum of electronic and thermal Energies= -1023.414820
Sum of electronic and thermal Enthalpies= -1023.413876
Sum of electronic and thermal Free Energies= -1023.484930

Cartesian Coordinates

46	1.582809	0.217312	-0.053443
6	-0.771323	1.963698	-0.041953
6	0.480365	2.811831	-0.284504
8	1.628691	2.177734	-0.323964
8	0.380242	4.014592	-0.397580

1	-1.473783	2.164975	-0.862159
7	-0.396399	0.547199	-0.053380
6	-1.272772	-0.398562	-0.148172
8	-0.959428	-1.677502	-0.124231
8	1.812141	-1.851715	0.191194
6	3.092586	-1.733072	0.121113
8	3.578753	-0.581904	-0.020932
6	3.958456	-2.941596	0.194811
1	4.765445	-2.771006	0.912527
1	4.421478	-3.109118	-0.783057
1	3.376111	-3.820755	0.476959
1	0.006461	-1.818153	-0.003781
6	-1.392857	2.373897	1.284548
1	-2.331167	1.840261	1.470706
1	-1.589629	3.449579	1.265008
1	-0.696725	2.163794	2.105611
8	-2.537791	-0.091200	-0.303891
6	-3.670142	-1.013446	-0.077279
6	-3.701362	-2.075581	-1.159997
1	-4.639689	-2.636675	-1.079889
1	-2.870381	-2.779173	-1.073994
1	-3.670336	-1.608018	-2.150387
6	-3.584157	-1.586872	1.324590
1	-2.746388	-2.279546	1.437731
1	-4.509080	-2.131779	1.544749
1	-3.484236	-0.779755	2.060629
6	-4.860156	-0.080851	-0.204338
1	-5.788838	-0.643126	-0.059821
1	-4.884358	0.382561	-1.196135
1	-4.812014	0.712481	0.549684

(3d')

Number of imaginary frequencies : 0

Electronic energy : =-1813.2693842
Zero-point correction= 0.342261
Thermal correction to Energy= 0.373246
Thermal correction to Enthalpy= 0.374190
Thermal correction to Gibbs Free Energy= 0.276385
Sum of electronic and zero-point Energies= -1812.927123
Sum of electronic and thermal Energies= -1812.896139
Sum of electronic and thermal Enthalpies= -1812.895194
Sum of electronic and thermal Free Energies= -1812.992999

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Cartesian Coordinates

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46	1.197495	1.231589	-0.381653
6	1.790104	3.566056	-0.059034
8	2.670053	2.637813	-0.123026
6	2.187962	4.986423	0.095806
1	2.333585	5.425280	-0.897190
1	3.130947	5.056491	0.642830
1	1.398286	5.543197	0.605181
8	0.573877	3.215494	-0.160153
6	-2.156987	-1.620190	-0.532325
6	-0.767305	-1.043548	-0.501039
8	-0.600847	0.189659	-0.564035
8	0.173517	-1.919734	-0.429860
1	-2.251413	-2.256493	0.361720
7	-3.128761	-0.559039	-0.468023
1	-2.828848	0.399917	-0.575194
6	-4.401875	-0.832201	-0.064299
8	-4.797586	-1.955571	0.186197
8	2.229016	-0.486147	-0.607863
1	1.094531	-1.466233	-0.476017
6	3.352515	-0.574627	0.186725
6	3.001777	-1.106378	1.576252
6	4.364952	-1.453993	-0.547472
1	3.842135	0.404245	0.334794
9	1.969711	-0.409980	2.072481
9	4.016776	-0.988396	2.427761
9	2.631481	-2.386910	1.532808
9	4.788284	-0.819946	-1.638167
9	3.829272	-2.612118	-0.925349
9	5.425121	-1.715327	0.219286
6	-2.333088	-2.506768	-1.765818
1	-2.222813	-1.914995	-2.681212
1	-3.340125	-2.930698	-1.737163
1	-1.601933	-3.319726	-1.771620
8	-5.111985	0.304124	-0.000785
6	-6.513259	0.274934	0.407683
6	-6.908270	1.739878	0.354266
1	-6.288321	2.331834	1.036705
1	-7.957804	1.855712	0.647300
1	-6.783591	2.137470	-0.659053
6	-7.330266	-0.534507	-0.585355
1	-7.048784	-1.589993	-0.565172
1	-7.186087	-0.144679	-1.599938
1	-8.394722	-0.448269	-0.336403
6	-6.635131	-0.257261	1.826024
1	-5.994261	0.320679	2.502416
1	-6.353228	-1.311324	1.882060

1	-7.671923	-0.150182	2.166503

(2')

Number of imaginary frequencies : 0

Electronic energy : =-1813.2842259
Zero-point correction= 0.340864
Thermal correction to Energy= 0.370969
Thermal correction to Enthalpy= 0.371913
Thermal correction to Gibbs Free Energy= 0.278354
Sum of electronic and zero-point Energies= -1812.943361
Sum of electronic and thermal Energies= -1812.913257
Sum of electronic and thermal Enthalpies= -1812.912312
Sum of electronic and thermal Free Energies= -1813.005872

Cartesian Coordinates

46	-0.748180	1.034084	-0.225341
6	1.777318	2.472531	0.052916
6	0.642237	3.460823	0.317051
8	-0.585317	2.966597	0.233910
8	0.858106	4.622202	0.568118
1	2.388834	2.453931	0.967462
7	1.245192	1.136112	-0.211738
6	2.016100	0.065102	-0.207497
8	1.600463	-1.106847	-0.480707
8	-0.756026	-0.972088	-0.749593
1	0.442866	-1.143743	-0.657000
6	-1.540042	-1.844793	-0.013554
6	-1.775563	-3.086013	-0.873724
6	-0.908235	-2.182721	1.338679
1	-2.527122	-1.405277	0.195795
9	-0.628228	-3.583553	-1.328376
9	-2.531086	-2.764520	-1.920970
9	-2.404008	-4.043527	-0.188865
9	0.162132	-2.966938	1.207405
9	-1.779641	-2.790938	2.140697
9	-0.512017	-1.060412	1.948216
8	-2.863666	1.051451	-0.152400
6	-3.582271	2.042434	0.053375
8	-3.155558	3.245635	0.287673
6	-5.068124	1.916105	0.048937
1	-5.488347	2.615010	-0.680302

1	-5.457852	2.203770	1.030280
1	-5.366024	0.895498	-0.190287
1	-2.152534	3.314193	0.303103
6	2.619927	2.995498	-1.103977
1	3.497338	2.360266	-1.260766
1	2.945769	4.015881	-0.881958
1	2.025709	3.009879	-2.025251
8	3.286870	0.268236	0.099798
6	4.304233	-0.793619	0.063316
6	3.989205	-1.849799	1.107714
1	3.068656	-2.391774	0.877884
1	3.890754	-1.386677	2.096337
1	4.817015	-2.567422	1.150927
6	4.416597	-1.359149	-1.340953
1	4.559962	-0.547653	-2.064888
1	3.532631	-1.935546	-1.622274
1	5.292460	-2.016330	-1.392510
6	5.564746	-0.032617	0.432648
1	5.767131	0.756703	-0.300570
1	6.420704	-0.715821	0.454456
1	5.461873	0.429255	1.420478

(2c')

Number of imaginary frequencies : 0

Electronic energy : =-2373.8245906
Zero-point correction= 0.345884
Thermal correction to Energy= 0.380452
Thermal correction to Enthalpy= 0.381396
Thermal correction to Gibbs Free Energy= 0.279021
Sum of electronic and zero-point Energies= -2373.478706
Sum of electronic and thermal Energies= -2373.444139
Sum of electronic and thermal Enthalpies= -2373.443195
Sum of electronic and thermal Free Energies= -2373.545570

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Cartesian Coordinates

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46	-0.022862	-0.940211	-0.224820
6	2.374229	-2.578629	-0.382614
6	1.204587	-3.346180	-1.006502
8	0.026550	-2.755891	-0.993418
8	1.376637	-4.452762	-1.466680
1	3.117728	-2.425512	-1.179033

7	1.918954	-1.272844	0.113790
6	2.760801	-0.341343	0.474521
8	2.393630	0.802607	0.959517
8	-0.085173	0.963772	0.584133
1	1.373757	0.939600	0.904789
6	-0.494671	1.971370	-0.261742
6	-1.181957	3.041202	0.588767
6	0.661555	2.550297	-1.083766
1	-1.250137	1.642108	-1.000244
9	-0.421414	3.443701	1.598799
9	-2.307856	2.529614	1.111340
9	-1.522317	4.106380	-0.134955
9	1.509724	3.252083	-0.326640
9	0.223959	3.340031	-2.060309
9	1.359725	1.556245	-1.645986
8	-2.118970	-0.857519	-0.761916
1	-2.358785	-1.716568	-1.151912
6	-3.041081	-0.481788	0.240344
6	-4.190671	0.280950	-0.409568
6	-3.468917	-1.723206	1.015539
1	-2.528405	0.206539	0.920958
9	-4.950991	-0.532337	-1.141542
9	-4.942330	0.866240	0.511948
9	-3.698297	1.222262	-1.212007
9	-4.514295	-1.483564	1.790771
9	-3.785345	-2.698569	0.154393
9	-2.462099	-2.154771	1.765709
6	2.982557	-3.433176	0.719897
1	3.891560	-2.978108	1.122792
1	3.222415	-4.416574	0.305631
1	2.259907	-3.566683	1.533425
8	4.046569	-0.588675	0.361445
6	5.096024	0.449693	0.460975
6	5.179887	0.980912	1.879471
1	4.305046	1.575614	2.149570
1	6.070528	1.614157	1.966388
1	5.283244	0.153874	2.590873
6	4.836146	1.533263	-0.569737
1	3.936677	2.113028	-0.348028
1	4.737210	1.092189	-1.568571
1	5.691499	2.218374	-0.585955
6	6.344091	-0.338441	0.109424
1	6.502842	-1.151573	0.826331
1	7.217955	0.321400	0.133441
1	6.260339	-0.769904	-0.893655

(2e')

Number of imaginary frequencies : 0

Electronic energy : =-1252.7193173
Zero-point correction= 0.339633
Thermal correction to Energy= 0.366004
Thermal correction to Enthalpy= 0.366948
Thermal correction to Gibbs Free Energy= 0.281314
Sum of electronic and zero-point Energies= -1252.379684
Sum of electronic and thermal Energies= -1252.353314
Sum of electronic and thermal Enthalpies= -1252.352369
Sum of electronic and thermal Free Energies= -1252.438003

Cartesian Coordinates

46	-1.094273	0.018451	0.095838
6	0.895877	-1.998241	0.559241
6	-0.353934	-2.694563	0.033945
8	-1.268896	-1.882310	-0.490283
8	-0.503562	-3.891953	0.083084
1	1.734618	-2.402510	-0.023095
7	0.796334	-0.557950	0.338338
6	1.834328	0.161790	-0.095481
8	1.774053	1.325463	-0.527926
8	-1.115656	1.945892	0.941489
8	-3.165453	0.407914	-0.221380
6	-4.034609	-0.418870	-0.530895
8	-3.831628	-1.684350	-0.746611
6	-5.458875	-0.002103	-0.689994
1	-6.089951	-0.607643	-0.032727
1	-5.780341	-0.202277	-1.716778
1	-5.575800	1.056596	-0.459184
1	-2.861221	-1.938080	-0.656630
6	-0.793131	3.025653	0.422096
8	0.079409	3.164074	-0.520362
6	-1.423342	4.298179	0.884533
1	-1.886136	4.798772	0.028369
1	-0.650180	4.969811	1.269410
1	-2.170681	4.099457	1.652519
1	0.664665	2.323840	-0.607667
6	1.103200	-2.342034	2.026241
1	2.052011	-1.925800	2.378839
1	1.111391	-3.428601	2.157321
1	0.292975	-1.919045	2.633114
8	3.000580	-0.498152	-0.000652
6	4.269555	0.090461	-0.417731

6	4.244688	0.422677	-1.900046
1	5.252332	0.712305	-2.221724
1	3.557184	1.241979	-2.118651
1	3.944107	-0.458194	-2.479535
6	4.600009	1.296047	0.444819
1	4.565492	1.022726	1.505983
1	3.904703	2.118457	0.266777
1	5.616097	1.638666	0.214890
6	5.253351	-1.035859	-0.147714
1	6.268391	-0.720284	-0.413932
1	4.997844	-1.921863	-0.739462
1	5.241234	-1.312851	0.912294

(2f')

Number of imaginary frequencies : 0

Electronic energy : =-3163.3631122
Zero-point correction= 0.412870
Thermal correction to Energy= 0.457678
Thermal correction to Enthalpy= 0.458622
Thermal correction to Gibbs Free Energy= 0.331432
Sum of electronic and zero-point Energies= -3162.950242
Sum of electronic and thermal Energies= -3162.905434
Sum of electronic and thermal Enthalpies= -3162.904490
Sum of electronic and thermal Free Energies= -3163.031680

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Cartesian Coordinates

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46	-0.734096	0.060810	-0.290870
8	-2.432427	-1.259814	-0.373492
6	2.942497	2.335508	-0.932360
6	1.477332	1.995940	-0.852095
8	1.140078	0.906777	-0.345873
8	0.661764	2.868290	-1.329856
1	3.098063	3.186427	-0.245366
7	3.703818	1.190448	-0.495700
1	3.207808	0.394942	-0.111919
6	5.008146	1.342318	-0.111576
8	5.644749	2.368322	-0.254783
8	-1.609438	1.831007	-0.795634
1	-0.307108	2.570325	-1.177497
6	-2.461315	2.367530	0.143382
6	-3.713382	2.852574	-0.583547

6	-1.775172	3.464436	0.954338
1	-2.811001	1.630521	0.889085
9	-4.360511	1.781271	-1.073653
9	-4.551945	3.486700	0.234961
9	-3.423608	3.653959	-1.596751
9	-0.619472	2.988932	1.435476
9	-1.496445	4.526859	0.200662
9	-2.513872	3.857741	1.987491
8	0.038949	-1.694676	0.219495
6	1.104386	-2.142836	-0.523484
6	0.642328	-3.300631	-1.403197
6	2.254623	-2.503918	0.414890
1	1.524612	-1.385450	-1.211463
9	3.300368	-2.992197	-0.253313
9	2.664574	-1.393798	1.048624
9	1.891603	-3.389217	1.332114
9	1.599728	-3.742282	-2.214265
9	0.200009	-4.322591	-0.673857
9	-0.375561	-2.875032	-2.164898
1	-1.916692	-2.052029	-0.097520
6	-3.668126	-1.174876	0.291327
6	-3.445055	-1.312303	1.796263
6	-4.598600	-2.234251	-0.301176
1	-4.100642	-0.190320	0.075530
9	-2.778028	-0.240886	2.242901
9	-2.702784	-2.385780	2.053980
9	-4.584342	-1.398694	2.463209
9	-5.821273	-2.133679	0.202988
9	-4.667316	-2.074278	-1.614855
9	-4.126156	-3.454921	-0.046936
6	3.321103	2.787584	-2.340320
1	4.385252	3.034649	-2.342078
1	3.143364	1.982251	-3.061189
1	2.745352	3.668517	-2.636114
8	5.435128	0.188347	0.417233
6	6.798561	0.039925	0.912734
6	6.814178	-1.401291	1.390660
1	6.613739	-2.084377	0.557893
1	7.792490	-1.647521	1.818356
1	6.045243	-1.559091	2.155217
6	7.039780	0.993862	2.070063
1	7.017163	2.035086	1.739193
1	6.279404	0.848438	2.846474
1	8.021565	0.788384	2.513175
6	7.793787	0.241887	-0.216908
1	7.797657	1.277486	-0.564402
1	8.799792	-0.015403	0.135524
1	7.550078	-0.416970	-1.058568

Different Possibilities of $Pd(OAc)_2$ -Ligand with Substrate at the M06/6-31G** Level of Theory
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(3a')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8174069
Zero-point correction= 0.503322
Thermal correction to Energy= 0.541001
Thermal correction to Enthalpy= 0.541945
Thermal correction to Gibbs Free Energy= 0.431587
Sum of electronic and zero-point Energies= -2241.314085
Sum of electronic and thermal Energies= -2241.276406
Sum of electronic and thermal Enthalpies= -2241.275462
Sum of electronic and thermal Free Energies= -2241.385820

Cartesian Coordinates

46	3.570745	-0.446359	0.137400
6	-2.036196	0.039670	1.639908
1	-1.582294	-0.761382	1.046507
1	-2.157942	-0.316290	2.670191
8	0.456752	0.708832	2.280623
6	-0.310314	2.844717	-0.270564
6	1.020211	3.214657	-0.519551
6	-1.346417	3.732150	-0.509842
6	1.308440	4.486751	-1.024752
6	-1.048101	4.996395	-1.006426
1	-2.365694	3.417986	-0.297324
6	0.269475	5.372842	-1.264821
1	2.340113	4.761256	-1.225043
1	-1.855721	5.698721	-1.195307
1	0.485315	6.362423	-1.657024
6	2.024816	2.245627	-0.255057
7	2.785270	1.407589	-0.017567
6	5.602717	-1.580622	0.848454
8	5.515643	-0.313164	0.909685
6	6.843460	-2.297077	1.240444
1	7.407026	-2.555999	0.337855
1	7.463950	-1.660580	1.874657
1	6.588854	-3.227414	1.754493
8	4.587925	-2.221211	0.415698
6	0.081986	-1.224864	-2.173644

6	1.475653	-0.757857	-1.733868
8	1.773057	-1.090406	-0.510355
8	2.182413	-0.139358	-2.511340
1	0.241921	-2.059823	-2.875950
7	-0.673059	-1.691373	-1.020911
1	-0.116973	-1.863887	-0.190643
6	-1.838159	-2.383354	-1.169574
8	-2.426275	-2.538887	-2.221914
8	-0.558853	1.560602	0.148039
16	-0.768190	1.297945	1.786317
8	-1.298333	2.520215	2.357076
6	-3.311336	0.551496	1.052342
6	-4.353530	0.954491	1.887841
6	-3.475263	0.624925	-0.334355
6	-5.553129	1.405051	1.348557
1	-4.219712	0.911461	2.967951
6	-4.673877	1.079879	-0.871991
1	-2.662022	0.320205	-0.991464
6	-5.715277	1.465519	-0.032361
1	-6.362637	1.708928	2.007684
1	-4.797245	1.119732	-1.951539
1	-6.655419	1.812721	-0.454618
6	-0.623004	-0.099469	-2.913213
1	-0.784679	0.749696	-2.236553
1	0.000557	0.235308	-3.745663
1	-1.588325	-0.445901	-3.292357
8	-2.252330	-2.815400	0.043452
6	-3.480208	-3.590577	0.182266
6	-4.687051	-2.773015	-0.247931
1	-5.599776	-3.344879	-0.040439
1	-4.737671	-1.833445	0.317778
1	-4.651452	-2.541920	-1.315080
6	-3.534249	-3.857995	1.676220
1	-3.586422	-2.912742	2.230400
1	-4.422258	-4.451029	1.922292
1	-2.644594	-4.406333	2.005116
6	-3.360963	-4.893067	-0.591237
1	-2.456504	-5.432796	-0.286524
1	-4.227394	-5.528722	-0.372655
1	-3.319815	-4.710856	-1.667655

(3b')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8158745
Zero-point correction= 0.503825
Thermal correction to Energy= 0.541497
Thermal correction to Enthalpy= 0.542441
Thermal correction to Gibbs Free Energy= 0.433274
Sum of electronic and zero-point Energies= -2241.312049
Sum of electronic and thermal Energies= -2241.274378
Sum of electronic and thermal Enthalpies= -2241.273434
Sum of electronic and thermal Free Energies= -2241.382600

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Cartesian Coordinates

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46	-0.473750	-1.995605	0.474321
6	2.988295	-0.167332	-1.303254
1	2.031203	-0.613174	-1.007463
1	3.161489	-0.398276	-2.362178
8	1.398885	1.889931	-1.889316
6	1.746923	2.835270	0.732326
6	0.449886	2.460789	1.112530
6	2.148019	4.157091	0.804889
6	-0.459713	3.418496	1.571613
6	1.242268	5.106922	1.270847
1	3.156975	4.417852	0.497078
6	-0.048399	4.742724	1.649318
1	-1.472918	3.109892	1.820824
1	1.548559	6.148160	1.331238
1	-0.744788	5.498215	2.001477
6	0.114362	1.087395	0.977185
7	-0.067124	-0.046507	0.830167
6	0.656355	-3.941458	-0.472818
8	1.251340	-2.812716	-0.413341
6	1.305017	-5.119523	-1.103894
1	1.055731	-5.131996	-2.170382
1	2.390669	-5.051551	-1.003706
1	0.928069	-6.041450	-0.655265
8	-0.519303	-4.015083	0.003499
6	-4.535659	-1.218157	1.193580
6	-3.251805	-1.718646	0.501496
8	-2.244805	-1.631360	1.331348
8	-3.208510	-2.092249	-0.656141
1	-4.607323	-1.759611	2.145467
7	-4.358316	0.190030	1.579935
1	-4.004616	0.338024	2.515174
6	-3.850017	1.135719	0.724547
8	-3.255113	2.132459	1.102930
8	2.612240	1.851492	0.317135
16	2.708548	1.606467	-1.333818
8	3.883726	2.312259	-1.800421

6	4.122545	-0.587359	-0.424993
6	5.444126	-0.429396	-0.843687
6	3.855593	-1.135130	0.830619
6	6.489101	-0.820572	-0.015283
1	5.650247	0.009292	-1.818853
6	4.901884	-1.527970	1.656085
1	2.820626	-1.258695	1.148051
6	6.218846	-1.371013	1.234234
1	7.517176	-0.696830	-0.346894
1	4.688739	-1.958640	2.631554
1	7.037490	-1.679579	1.880318
6	-5.780360	-1.485246	0.374688
1	-5.919564	-2.564685	0.257358
1	-6.656476	-1.067253	0.880863
1	-5.696039	-1.049642	-0.622335
8	-4.131605	0.816446	-0.536613
6	-3.545936	1.501760	-1.682369
6	-4.064873	0.673112	-2.845157
1	-5.160578	0.699380	-2.875120
1	-3.680934	1.068188	-3.792667
1	-3.745872	-0.369439	-2.731047
6	-4.057340	2.929352	-1.749427
1	-3.705297	3.515972	-0.896859
1	-3.701322	3.398939	-2.674435
1	-5.153387	2.940340	-1.759853
6	-2.031169	1.430515	-1.620051
1	-1.630022	2.073344	-0.830596
1	-1.709550	0.394092	-1.447235
1	-1.607052	1.765345	-2.573682

(3c')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8127712
Zero-point correction= 0.502806
Thermal correction to Energy= 0.540609
Thermal correction to Enthalpy= 0.541553
Thermal correction to Gibbs Free Energy= 0.431079
Sum of electronic and zero-point Energies= -2241.309966
Sum of electronic and thermal Energies= -2241.272162
Sum of electronic and thermal Enthalpies= -2241.271218
Sum of electronic and thermal Free Energies= -2241.381692

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Cartesian Coordinates

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46	3.405608	0.407107	-0.542182
6	-2.898145	-1.356738	0.015406
1	-3.110007	-1.957661	0.908363
1	-3.247880	-0.325743	0.165874
8	-0.727922	-0.555419	1.305658
6	-0.134407	-3.261075	1.220813
6	1.112278	-2.869443	1.738895
6	-0.871767	-4.245522	1.861687
6	1.598852	-3.466353	2.906949
6	-0.374969	-4.839558	3.016343
1	-1.825746	-4.539968	1.431419
6	0.854723	-4.449554	3.541858
1	2.559795	-3.148541	3.301985
1	-0.955247	-5.613240	3.512321
1	1.234907	-4.913313	4.447289
6	1.871032	-1.870191	1.066139
7	2.495761	-1.075412	0.502995
6	5.535848	0.828956	-1.642205
8	5.331035	-0.275319	-1.044823
6	6.841077	1.136883	-2.282156
1	7.443312	1.738368	-1.593020
1	7.379854	0.213510	-2.505545
1	6.681685	1.723996	-3.189974
8	4.585775	1.679389	-1.655938
6	0.236318	2.854503	0.843920
6	1.574651	2.100877	0.713800
8	1.686297	1.441533	-0.402348
8	2.413629	2.169563	1.596123
1	0.451696	3.896282	0.554290
7	-0.729314	2.272456	-0.079663
1	-0.398071	1.502543	-0.651159
6	-2.065173	2.452044	-0.103261
8	-2.841124	1.675810	-0.656538
8	-0.603363	-2.736466	0.048603
16	-1.115004	-1.130992	0.031091
8	-0.625349	-0.620628	-1.226843
6	-3.409042	-1.949173	-1.255265
6	-3.610252	-1.123289	-2.363543
6	-3.679695	-3.313967	-1.348913
6	-4.088572	-1.665548	-3.549871
1	-3.385597	-0.061111	-2.275257
6	-4.160630	-3.852763	-2.536414
1	-3.520784	-3.955181	-0.481910
6	-4.365182	-3.027299	-3.637591
1	-4.247546	-1.021154	-4.410998
1	-4.376671	-4.916408	-2.602325
1	-4.742737	-3.446448	-4.567509

6	-0.210868	2.821605	2.298958
1	0.632150	3.103318	2.933836
1	-1.043124	3.508123	2.473144
1	-0.523381	1.805140	2.565681
8	-2.432008	3.583078	0.521486
6	-3.829644	3.855234	0.815200
6	-4.419369	2.732615	1.655627
1	-4.562193	1.821804	1.068816
1	-3.757281	2.510814	2.502521
1	-5.391198	3.046531	2.055103
6	-3.758685	5.135578	1.630076
1	-3.258137	5.925610	1.059791
1	-4.768556	5.475897	1.886068
1	-3.199772	4.973621	2.559325
6	-4.605521	4.086829	-0.471070
1	-4.141879	4.894670	-1.049116
1	-4.630093	3.182992	-1.084303
1	-5.633443	4.384940	-0.230456

(3d')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8110682
Zero-point correction= 0.504159
Thermal correction to Energy= 0.541427
Thermal correction to Enthalpy= 0.542371
Thermal correction to Gibbs Free Energy= 0.435610
Sum of electronic and zero-point Energies= -2241.306910
Sum of electronic and thermal Energies= -2241.269641
Sum of electronic and thermal Enthalpies= -2241.268697
Sum of electronic and thermal Free Energies= -2241.375458

Cartesian Coordinates

46	1.294963	1.873648	0.386193
6	-1.550971	-1.407512	-1.780019
1	-0.468245	-1.261549	-1.667399
1	-1.726854	-2.090661	-2.622734
8	-1.027650	-3.317852	0.003595
6	-3.213405	-0.552330	1.188985
6	-2.978911	0.810396	1.445335
6	-4.490065	-1.074965	1.357216

6	-4.033000	1.652744	1.815577
6	-5.527550	-0.223680	1.720718
1	-4.662325	-2.131206	1.189538
6	-5.310845	1.134957	1.943281
1	-3.829345	2.704567	1.997203
1	-6.525698	-0.637295	1.841499
1	-6.134836	1.782651	2.227564
6	-1.659394	1.312627	1.304978
7	-0.571247	1.691212	1.185507
6	2.812457	3.551124	-0.549290
8	1.686895	3.916363	-0.084169
6	3.754298	4.527757	-1.162400
1	3.670689	4.467796	-2.252676
1	3.509846	5.543271	-0.843636
1	4.782466	4.272871	-0.893179
8	3.115138	2.314741	-0.498803
8	-2.111859	-1.305077	0.871248
16	-2.079518	-2.409294	-0.383873
8	-3.433421	-2.878789	-0.616156
6	-2.273861	-0.101923	-1.912615
6	-3.663349	-0.036804	-2.055448
6	-1.524059	1.074737	-1.884701
6	-4.294502	1.198293	-2.139608
1	-4.246940	-0.955882	-2.078140
6	-2.160303	2.309729	-1.974863
1	-0.438281	1.005755	-1.795597
6	-3.545124	2.372468	-2.095058
1	-5.376414	1.245475	-2.240761
1	-1.565246	3.220617	-1.941143
1	-4.042946	3.337422	-2.162372
7	1.381328	-0.116766	0.636348
6	1.709060	-0.786866	-0.493377
8	1.510110	-0.357878	-1.629219
6	1.806432	-0.589629	1.939691
1	1.673741	0.259846	2.631565
6	3.306996	-0.850600	1.963555
8	4.121078	-0.304456	1.261237
8	3.654113	-1.729654	2.923449
1	4.621448	-1.783387	2.886443
6	0.951784	-1.736541	2.471182
1	1.223304	-1.970877	3.504854
1	-0.104792	-1.447300	2.435153
1	1.078724	-2.635097	1.861200
8	2.205502	-2.008688	-0.220612
6	2.843951	-2.823523	-1.241642
6	3.303891	-4.029498	-0.440771
1	3.825175	-4.743251	-1.088916
1	3.987442	-3.717066	0.358461
1	2.441874	-4.530802	0.016387

6	1.843175	-3.246069	-2.306020
1	0.959412	-3.696375	-1.835506
1	1.535187	-2.394191	-2.917858
1	2.304074	-3.998553	-2.958083
6	4.027693	-2.066971	-1.819755
1	3.694336	-1.190019	-2.381615
1	4.686498	-1.729933	-1.010577
1	4.595506	-2.724238	-2.489837

(3e')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8262095
Zero-point correction= 0.500609
Thermal correction to Energy= 0.538831
Thermal correction to Enthalpy= 0.539775
Thermal correction to Gibbs Free Energy= 0.426459
Sum of electronic and zero-point Energies= -2241.325601
Sum of electronic and thermal Energies= -2241.287378
Sum of electronic and thermal Enthalpies= -2241.286434
Sum of electronic and thermal Free Energies= -2241.399750

Cartesian Coordinates

46	-1.216438	-1.041633	0.017394
6	3.234058	1.742503	-0.975389
1	3.948124	1.595518	-1.793039
1	2.197925	1.682472	-1.346994
8	2.391880	0.171108	1.041700
6	3.771156	-2.095541	-0.749612
6	2.851987	-3.062076	-0.310568
6	5.112769	-2.424972	-0.883569
6	3.283088	-4.362379	-0.021466
6	5.531191	-3.717553	-0.591874
1	5.806980	-1.655930	-1.207225
6	4.622687	-4.685402	-0.164934
1	2.560463	-5.101109	0.314091
1	6.582223	-3.973465	-0.697801
1	4.962375	-5.692797	0.057565
6	1.489258	-2.684815	-0.170849
7	0.382863	-2.361886	-0.064496
6	-1.772000	1.750016	-0.211957

6	-0.470792	1.472835	-0.947144
8	-0.099599	0.222124	-1.044190
8	0.210655	2.386611	-1.389987
1	-2.363991	2.430793	-0.835738
7	-2.487650	0.491021	-0.032385
6	-3.807214	0.399056	-0.179411
8	-4.457060	-0.660839	-0.249106
8	3.312911	-0.850194	-1.087062
16	3.481287	0.335866	0.101107
8	4.858337	0.260556	0.554246
6	3.496502	2.990125	-0.186166
6	2.450816	3.607283	0.500835
6	4.787661	3.512343	-0.092767
6	2.694190	4.744692	1.261334
1	1.448847	3.194714	0.408317
6	5.028153	4.650803	0.666256
1	5.605070	3.017129	-0.615083
6	3.980795	5.267902	1.344545
1	1.873625	5.225744	1.789065
1	6.035223	5.055846	0.731840
1	4.169509	6.159149	1.938878
8	-2.173191	-2.419377	1.317510
6	-3.084488	-3.222076	1.062045
8	-3.982799	-3.059631	0.149768
6	-3.207012	-4.489773	1.844444
1	-4.156494	-4.488636	2.388541
1	-3.235605	-5.337706	1.153293
1	-2.375374	-4.594751	2.541232
1	-4.046041	-2.064974	-0.130249
6	-1.461295	2.430293	1.115224
1	-0.955306	3.386288	0.939447
1	-2.388802	2.615111	1.666407
1	-0.809209	1.792474	1.727525
8	-4.414404	1.597913	-0.233547
6	-5.849103	1.735090	-0.457094
6	-6.235656	1.149244	-1.804630
1	-6.107562	0.064811	-1.821367
1	-7.286348	1.383586	-2.014583
1	-5.623917	1.592705	-2.599054
6	-6.626773	1.113857	0.691394
1	-7.690648	1.357754	0.583915
1	-6.512911	0.028096	0.708354
1	-6.278944	1.523057	1.647298
6	-6.035321	3.243153	-0.463962
1	-5.715774	3.674934	0.491016
1	-5.445225	3.701862	-1.265150
1	-7.090945	3.490818	-0.622941

(3f')

Number of imaginary frequencies : 0

Electronic energy : =-2241.8256832
Zero-point correction= 0.500823
Thermal correction to Energy= 0.538748
Thermal correction to Enthalpy= 0.539692
Thermal correction to Gibbs Free Energy= 0.428488
Sum of electronic and zero-point Energies= -2241.324860
Sum of electronic and thermal Energies= -2241.286935
Sum of electronic and thermal Enthalpies= -2241.285991
Sum of electronic and thermal Free Energies= -2241.397195

Cartesian Coordinates

46	-0.894858	-1.097242	-0.133344
6	2.813286	2.100774	-0.795357
1	3.505226	2.439724	-1.573727
1	1.918592	1.659791	-1.257670
8	2.859302	0.161688	1.072054
6	4.270726	-1.505724	-0.963154
6	3.441814	-2.554274	-0.532093
6	5.632875	-1.713492	-1.121866
6	3.988304	-3.817716	-0.282626
6	6.166227	-2.972127	-0.868032
1	6.250287	-0.878291	-1.438683
6	5.349070	-4.022266	-0.453401
1	3.337630	-4.623201	0.046616
1	7.233639	-3.134287	-0.993287
1	5.775970	-5.002298	-0.260640
6	2.054593	-2.301356	-0.345667
7	0.928195	-2.084075	-0.196278
6	-2.119186	1.448989	-0.874928
6	-0.670880	1.459079	-1.315909
8	0.019290	0.357390	-1.115215
8	-0.154476	2.443521	-1.812127
1	-2.709616	1.661848	-1.776517
7	-2.476884	0.136845	-0.334839
6	-3.750197	-0.257626	-0.359040
8	-4.175094	-1.334453	0.107285
8	3.716527	-0.284887	-1.251425
16	3.675356	0.784024	0.047998
8	5.048001	1.156522	0.335323
6	2.489993	3.170678	0.202359

6	1.359326	3.047848	1.012490
6	3.327569	4.274811	0.351594
6	1.056560	4.035680	1.939698
1	0.727762	2.165798	0.913478
6	3.023244	5.264288	1.280003
1	4.220824	4.353877	-0.266705
6	1.885079	5.147277	2.071013
1	0.168508	3.938714	2.560461
1	3.676267	6.127254	1.385503
1	1.644376	5.922822	2.794605
8	-1.482541	-2.772306	1.058075
6	-2.236091	-2.913208	2.033243
8	-3.321514	-2.247460	2.237953
6	-1.927071	-3.938537	3.077779
1	-2.019641	-3.486258	4.069395
1	-2.668864	-4.741534	3.019702
1	-0.926775	-4.347747	2.935185
1	-3.621111	-1.782298	1.356435
6	-2.351414	2.560380	0.139808
1	-3.418677	2.648530	0.371426
1	-1.812840	2.337180	1.070363
1	-1.985663	3.512320	-0.259206
8	-4.574876	0.628564	-0.939103
6	-6.025521	0.546010	-0.810900
6	-6.422736	0.566465	0.655593
1	-7.509970	0.682018	0.737517
1	-6.132073	-0.353933	1.166752
1	-5.951701	1.419237	1.161117
6	-6.481731	1.822370	-1.497304
1	-6.154644	1.834754	-2.542768
1	-7.574830	1.894686	-1.473151
1	-6.060961	2.700437	-0.993275
6	-6.556893	-0.673055	-1.544660
1	-6.205873	-0.670440	-2.583129
1	-6.232674	-1.598600	-1.064574
1	-7.653193	-0.640951	-1.555965

(3g')

Number of imaginary frequencies : 0

Electronic energy : =-3031.3688687
Zero-point correction= 0.564992
Thermal correction to Energy= 0.613054

Thermal correction to Enthalpy= 0.613999
Thermal correction to Gibbs Free Energy= 0.479332
Sum of electronic and zero-point Energies= -3030.803876
Sum of electronic and thermal Energies= -3030.755814
Sum of electronic and thermal Enthalpies= -3030.754870
Sum of electronic and thermal Free Energies= -3030.889537

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Cartesian Coordinates

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46	-2.253519	-1.043630	-0.170573
6	1.698960	1.815552	-2.393841
1	2.094437	1.710982	-3.410394
1	0.596982	1.766216	-2.392168
8	1.599761	0.148512	-0.270972
6	2.277580	-2.047089	-2.454555
6	1.551979	-3.005892	-1.729640
6	3.492585	-2.381815	-3.032454
6	2.054631	-4.305186	-1.593742
6	3.983958	-3.674393	-2.888917
1	4.038543	-1.618633	-3.577943
6	3.270153	-4.633722	-2.173205
1	1.484276	-5.040035	-1.032611
1	4.938243	-3.934468	-3.339015
1	3.664894	-5.639772	-2.065982
6	0.306416	-2.632632	-1.155454
7	-0.706762	-2.307115	-0.701251
6	-2.934627	1.733522	-0.219976
6	-1.822895	1.504739	-1.230214
8	-1.464400	0.268748	-1.451127
8	-1.277556	2.451357	-1.781927
1	-3.668357	2.398458	-0.691680
7	-3.559910	0.450475	0.100895
6	-4.866445	0.355179	0.279233
8	-5.518089	-0.715073	0.396253
8	1.745491	-0.788284	-2.621205
16	2.278868	0.362537	-1.533453
8	3.737922	0.288867	-1.566181
6	2.227113	3.016007	-1.667911
6	1.466318	3.601372	-0.655404
6	3.500097	3.512214	-1.955411
6	1.975076	4.680655	0.056921
1	0.472548	3.207937	-0.452045
6	4.004031	4.592507	-1.243398
1	4.097521	3.041298	-2.734951
6	3.242202	5.175538	-0.234301
1	1.379669	5.136215	0.844446
1	4.995232	4.977126	-1.470836
1	3.639230	6.018361	0.326709
8	-2.815319	-2.442304	1.275349

6	-3.801808	-3.212869	1.207648
8	-4.864663	-2.990967	0.542949
6	-3.756190	-4.497409	1.977333
1	-4.520420	-4.470990	2.760359
1	-4.011558	-5.325455	1.309421
1	-2.773387	-4.654685	2.422700
1	-5.060091	-1.884396	0.375867
1	4.920776	0.049797	-0.117855
8	5.282472	-0.192222	0.750309
6	4.228067	-0.231374	1.646666
6	3.877962	1.171620	2.138796
6	4.637086	-1.169583	2.770437
1	3.296664	-0.638580	1.220011
9	2.713952	1.183142	2.789244
9	3.768550	1.988938	1.087692
9	4.810727	1.673598	2.947124
9	3.739949	-1.153286	3.760414
9	5.823491	-0.860560	3.280529
9	4.705225	-2.418211	2.301745
6	-2.364379	2.420592	1.013735
1	-1.905309	3.373571	0.729744
1	-3.158876	2.611129	1.742124
1	-1.601987	1.788248	1.487240
8	-5.499537	1.530210	0.342496
6	-6.954829	1.651692	0.441622
6	-7.152658	3.157475	0.401516
1	-6.777047	3.572396	-0.540473
1	-8.218308	3.397679	0.486688
1	-6.619621	3.638755	1.228892
6	-7.628431	0.998613	-0.752904
1	-7.198702	1.380775	-1.686391
1	-7.525176	-0.088163	-0.732507
1	-8.695785	1.249547	-0.744389
6	-7.440453	1.089165	1.766026
1	-7.304358	0.007019	1.817654
1	-6.900976	1.557462	2.597508
1	-8.507096	1.314890	1.884051

(3')

Number of imaginary frequencies : 0

Electronic energy : =-2802.394762
Zero-point correction= 0.505418

Thermal correction to Energy= 0.546941
Thermal correction to Enthalpy= 0.547885
Thermal correction to Gibbs Free Energy= 0.430074
Sum of electronic and zero-point Energies= -2801.889344
Sum of electronic and thermal Energies= -2801.847821
Sum of electronic and thermal Enthalpies= -2801.846877
Sum of electronic and thermal Free Energies= -2801.964688

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Cartesian Coordinates

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46	0.616158	0.254611	-0.920872
6	-3.370049	-2.125610	-0.571582
1	-4.029441	-2.515224	-1.354618
1	-2.467409	-1.688936	-1.024524
8	-3.478480	-0.091949	1.183089
6	-4.533916	1.545872	-0.933736
6	-3.447869	2.424821	-0.797449
6	-5.832397	2.022497	-0.848142
6	-3.668341	3.791470	-0.599857
6	-6.043180	3.382755	-0.646298
1	-6.652330	1.315974	-0.941113
6	-4.969960	4.265002	-0.527792
1	-2.817308	4.459774	-0.498042
1	-7.060348	3.760115	-0.580568
1	-5.150158	5.324853	-0.373536
6	-2.139610	1.873084	-0.833613
7	-1.093733	1.378094	-0.849746
6	1.715246	-2.422986	-1.066472
6	0.241798	-2.491766	-1.471903
8	-0.420588	-1.354305	-1.494795
8	-0.284990	-3.559502	-1.704222
1	2.287856	-2.981745	-1.818242
7	2.154738	-1.026303	-1.040376
6	3.417510	-0.711663	-0.993669
8	3.850840	0.506636	-0.897314
8	-4.283187	0.222692	-1.181973
16	-4.272012	-0.773475	0.178745
8	-5.649634	-1.132580	0.452303
6	-3.046178	-3.130331	0.489515
6	-1.853495	-3.013664	1.204247
6	-3.941288	-4.152949	0.800851
6	-1.551386	-3.924399	2.207883
1	-1.172503	-2.196743	0.963863
6	-3.637527	-5.064699	1.805197
1	-4.878456	-4.230765	0.251259
6	-2.441649	-4.952106	2.507312
1	-0.618623	-3.832179	2.759950
1	-4.335929	-5.864204	2.040074
1	-2.203274	-5.666376	3.292080

8	1.797283	1.834460	-0.355683
1	3.084400	1.161095	-0.680952
6	1.553885	2.356247	0.894320
6	1.640615	3.877937	0.791559
6	2.519322	1.769257	1.923221
1	0.539144	2.135973	1.271268
9	2.802743	4.272939	0.281955
9	0.665449	4.317274	-0.010177
9	1.482962	4.469688	1.978124
9	3.787676	2.065443	1.622333
9	2.272533	2.196946	3.158875
9	2.411261	0.433596	1.932419
6	1.878323	-3.081776	0.297809
1	1.448192	-4.087842	0.272846
1	2.936531	-3.146730	0.573515
1	1.357232	-2.491061	1.064104
8	4.301908	-1.683525	-1.085324
6	5.679935	-1.568595	-0.569095
6	5.648143	-1.062306	0.862408
1	5.370262	-0.007230	0.925183
1	4.937142	-1.648902	1.458532
1	6.642728	-1.182751	1.306865
6	6.154645	-3.008987	-0.618895
1	7.194052	-3.070230	-0.278657
1	5.538640	-3.644071	0.028033
1	6.099568	-3.398414	-1.641026
6	6.507705	-0.694909	-1.492034
1	6.452239	-1.070036	-2.520118
1	6.172927	0.344609	-1.474903
1	7.556233	-0.729561	-1.173355

Possibilities of C-H Bond Activation Transition States at *meta*, *ortho* and *para* Positions at the /M06/6-31G** Level of Theory

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C-H activation **[A'-to-F']**

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meta-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1523.7765 cm(-1)

Electronic energy : =-2241.7935358
Zero-point correction= 0.496579

Thermal correction to Energy= 0.534385
Thermal correction to Enthalpy= 0.535329
Thermal correction to Gibbs Free Energy= 0.425779
Sum of electronic and zero-point Energies= -2241.296957
Sum of electronic and thermal Energies= -2241.259151
Sum of electronic and thermal Enthalpies= -2241.258207
Sum of electronic and thermal Free Energies= -2241.367757

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Cartesian Coordinates

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46	-0.538519	1.965150	-0.051652
6	3.170775	2.849258	1.486961
6	1.952010	3.173118	0.901744
6	1.537473	2.571104	-0.298712
6	2.399611	1.642222	-0.905320
6	3.622922	1.312727	-0.331731
6	3.997811	1.916705	0.874013
1	2.095925	1.154510	-1.832786
1	0.866510	3.381157	-1.079008
1	1.296903	3.902090	1.378993
1	4.945541	1.642389	1.335241
6	4.515527	0.296097	-0.966713
8	4.372347	-1.250879	1.239524
6	2.191793	-2.683071	-0.075681
6	0.930826	-2.361823	0.445104
6	2.691664	-3.971344	0.027663
6	0.150633	-3.350146	1.057286
6	1.919548	-4.940572	0.660783
1	3.668925	-4.199558	-0.389490
6	0.656477	-4.637404	1.165308
1	-0.840303	-3.079131	1.414158
1	2.309060	-5.951584	0.749051
1	0.061253	-5.410063	1.643472
6	0.461264	-1.025744	0.320148
7	0.116273	0.068586	0.181552
6	-0.780390	4.632551	-1.103388
8	0.323290	4.434966	-1.677813
6	-1.524645	5.900216	-1.410619
1	-0.825005	6.737283	-1.468071
1	-1.995692	5.793978	-2.393423
1	-2.298849	6.086624	-0.665270
1	3.474993	3.312869	2.421802
8	-1.331047	3.832776	-0.287788
6	-3.906725	0.322626	1.924920
6	-2.553324	0.979531	1.590065
8	-2.433053	1.270368	0.331735
8	-1.740982	1.210865	2.473809
1	-4.622188	1.151477	2.019910
7	-4.406565	-0.499988	0.829862

1	-5.052083	-0.069975	0.183465
6	-3.592135	-1.428180	0.258039
8	-2.569697	-1.862518	0.762492
16	4.410417	-1.330589	-0.205361
8	2.874688	-1.683422	-0.737704
8	5.331585	-2.226909	-0.875653
1	5.582098	0.536858	-0.874447
1	4.295732	0.121783	-2.025855
6	-3.855670	-0.438725	3.236038
1	-4.847770	-0.832291	3.481062
1	-3.151974	-1.271741	3.157222
1	-3.513831	0.220171	4.037489
8	-4.108440	-1.810043	-0.924460
6	-3.404618	-2.745320	-1.783916
6	-3.338035	-4.115976	-1.129598
1	-2.904023	-4.836934	-1.833211
1	-2.723897	-4.094989	-0.225040
1	-4.345078	-4.459523	-0.865803
6	-2.025999	-2.210583	-2.140382
1	-1.332043	-2.311409	-1.303553
1	-1.627516	-2.767779	-2.996839
1	-2.090087	-1.150374	-2.414274
6	-4.286166	-2.789393	-3.020529
1	-4.340647	-1.800179	-3.488664
1	-3.879758	-3.499402	-3.749686
1	-5.302232	-3.102767	-2.756610

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meta-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1556.2727 cm(-1)

Electronic energy : =-2241.7879468
Zero-point correction= 0.496487
Thermal correction to Energy= 0.534604
Thermal correction to Enthalpy= 0.535548
Thermal correction to Gibbs Free Energy= 0.422905
Sum of electronic and zero-point Energies= -2241.291460
Sum of electronic and thermal Energies= -2241.253343
Sum of electronic and thermal Enthalpies= -2241.252398
Sum of electronic and thermal Free Energies= -2241.365042

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Cartesian Coordinates

.....

46	-0.097198	1.203743	0.115420
6	3.194766	2.936829	1.911187
6	1.913178	2.959293	1.372345
6	1.662793	2.485105	0.072956
6	2.750218	1.997894	-0.676297
6	4.034743	1.964608	-0.147407
6	4.245984	2.434748	1.155379
1	2.577452	1.613430	-1.682648
1	0.751296	3.174845	-0.549473
1	1.083303	3.354429	1.958423
1	5.248480	2.394324	1.579192
6	5.178851	1.408117	-0.932710
8	5.562413	-0.433728	0.998414
6	4.014200	-2.265883	-0.580920
6	2.729403	-2.378739	-0.039183
6	4.866847	-3.356753	-0.599240
6	2.279877	-3.596324	0.482514
6	4.418796	-4.562982	-0.066940
1	5.860497	-3.252955	-1.027572
6	3.137015	-4.687200	0.467598
1	1.271844	-3.645529	0.889839
1	5.083208	-5.423130	-0.076001
1	2.805806	-5.639229	0.871862
6	1.883107	-1.242818	-0.033950
7	1.169188	-0.336412	-0.030634
6	-1.215072	3.812824	-0.357807
8	-0.138025	4.094498	-0.944365
6	-2.347162	4.798114	-0.411557
1	-2.952770	4.733003	0.494351
1	-1.964419	5.809403	-0.559087
1	-2.986267	4.540521	-1.262708
1	3.377140	3.301887	2.918564
8	-1.440955	2.734741	0.274825
6	-3.078325	-1.928456	0.607762
6	-1.728236	-1.206015	0.713837
8	-1.742145	-0.018008	0.194332
8	-0.792742	-1.790845	1.242274
1	-3.370106	-2.183742	1.638056
7	-4.088940	-1.073189	0.022314
1	-3.798000	-0.155608	-0.287465
6	-5.406872	-1.362271	0.141642
8	-5.846810	-2.383657	0.640285
16	5.655180	-0.256840	-0.435444
8	4.363088	-1.046632	-1.126542
8	6.847349	-0.644843	-1.160716
1	6.109522	1.973440	-0.797809
1	4.978322	1.335607	-2.007313
6	-2.902227	-3.223149	-0.176127
1	-3.851089	-3.766729	-0.196091

1	-2.600156	-3.003862	-1.207500
1	-2.135839	-3.844909	0.295344
8	-6.141730	-0.354782	-0.380612
6	-7.590812	-0.439597	-0.411623
6	-8.150771	-0.507471	1.000079
1	-9.244662	-0.434157	0.963803
1	-7.873489	-1.443931	1.488790
1	-7.772185	0.331198	1.596515
6	-8.034640	-1.620819	-1.260104
1	-7.752637	-2.568489	-0.795458
1	-9.124379	-1.595645	-1.382675
1	-7.577836	-1.561888	-2.255331
6	-7.990097	0.867428	-1.075851
1	-7.552099	0.939383	-2.077792
1	-9.080728	0.928683	-1.166179
1	-7.640664	1.721223	-0.484302

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meta-**C'**

Number of imaginary frequencies : 1
The smallest frequency is : -1443.1205 cm(-1)

Electronic energy : =-2012.8022092
Zero-point correction= 0.432409
Thermal correction to Energy= 0.464347
Thermal correction to Enthalpy= 0.465291
Thermal correction to Gibbs Free Energy= 0.368806
Sum of electronic and zero-point Energies= -2012.369800
Sum of electronic and thermal Energies= -2012.337862
Sum of electronic and thermal Enthalpies= -2012.336918
Sum of electronic and thermal Free Energies= -2012.433403

Cartesian Coordinates

46	-0.804742	0.819640	0.144382
6	-0.420392	-1.272750	0.680203
6	-0.374080	-1.359084	2.082713
6	0.692476	-1.966070	2.735829
6	1.732557	-2.502981	1.986752
6	1.701765	-2.468055	0.589349
6	0.626234	-1.857461	-0.051664
1	2.585571	-2.959853	2.488207
1	0.724144	-2.015080	3.821600
1	-1.192259	-0.931342	2.662366

1	0.620077	-1.793231	-1.140540
6	2.849569	-3.038063	-0.181522
1	2.538859	-3.652729	-1.036176
1	3.529233	-3.631427	0.439646
8	3.140593	-0.987814	-1.892465
6	4.671942	0.385480	0.176207
6	3.790736	1.474754	0.118447
6	6.037974	0.574286	0.045159
6	4.298500	2.767123	-0.055489
6	6.530746	1.863558	-0.131411
1	6.692157	-0.292118	0.083363
6	5.667331	2.955700	-0.178305
1	3.608696	3.605438	-0.099184
1	7.602020	2.015095	-0.233837
1	6.062756	3.957999	-0.314768
6	2.386368	1.262838	0.209146
7	1.240390	1.109652	0.259072
6	-3.443014	2.041348	-0.121009
6	-2.389060	3.141448	-0.279699
8	-1.131576	2.776996	-0.228778
8	-2.738502	4.296292	-0.423817
1	-4.071438	2.070550	-1.022918
7	-2.787441	0.739309	-0.023585
6	-3.430503	-0.394299	-0.228985
8	-2.875143	-1.532918	-0.169521
1	-1.652925	-1.340450	0.171255
8	4.163376	-0.876257	0.403107
8	5.155209	-2.397629	-1.348893
16	3.895283	-1.798472	-0.958783
6	-4.299649	2.352151	1.097958
1	-4.720398	3.356666	0.992893
1	-5.113641	1.627388	1.204788
1	-3.683992	2.327542	2.005892
8	-4.725951	-0.271808	-0.511906
6	-5.635930	-1.413848	-0.594202
6	-5.264358	-2.303227	-1.767174
1	-5.212057	-1.711285	-2.688159
1	-4.303601	-2.797614	-1.608360
1	-6.037540	-3.069726	-1.899192
6	-5.655314	-2.161436	0.727739
1	-4.705286	-2.664836	0.921351
1	-5.867039	-1.467266	1.550387
1	-6.451787	-2.914554	0.705452
6	-6.973857	-0.737735	-0.839094
1	-7.764840	-1.491045	-0.924734
1	-7.221185	-0.062900	-0.011507
1	-6.946846	-0.152792	-1.764795

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ortho-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1527.3965 cm(-1)

Electronic energy : =-2241.7802871
Zero-point correction= 0.495255
Thermal correction to Energy= 0.533879
Thermal correction to Enthalpy= 0.534823
Thermal correction to Gibbs Free Energy= 0.417959
Sum of electronic and zero-point Energies= -2241.285032
Sum of electronic and thermal Energies= -2241.246408
Sum of electronic and thermal Enthalpies= -2241.245464
Sum of electronic and thermal Free Energies= -2241.362328

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Cartesian Coordinates

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46	-0.184884	1.152450	-0.379290
6	-2.250243	1.888609	-0.482433
1	-1.650271	2.736397	0.290631
8	-1.184858	3.718430	1.067188
8	0.713759	2.884044	0.215295
6	-2.422430	2.240775	-1.831537
6	-3.578429	1.900409	-2.523259
6	-4.601247	1.240104	-1.851288
6	-4.482688	0.924959	-0.497710
6	-3.305615	1.221444	0.183519
1	-1.617641	2.767138	-2.344481
1	-3.685612	2.153520	-3.574985
1	-5.516644	0.979599	-2.378185
1	-5.309416	0.442566	0.018206
6	-3.139103	0.956184	1.655539
1	-3.631851	1.725115	2.268372
1	-2.081621	0.936607	1.947264
8	-5.221557	-0.714801	1.992105
6	-3.527579	-2.447361	0.459244
6	-2.894457	-2.396920	-0.795326
6	-4.610468	-3.289691	0.660154
6	-3.344562	-3.199686	-1.846819
6	-5.057683	-4.074149	-0.398248
1	-5.088792	-3.326608	1.633386
6	-4.430223	-4.037134	-1.642591
1	-2.841156	-3.152023	-2.808223
1	-5.906367	-4.734916	-0.242661

1	-4.788628	-4.664973	-2.452922
6	-1.833883	-1.461781	-0.920838
7	-1.030543	-0.629315	-0.884528
6	0.057597	3.754339	0.864030
6	0.846536	4.919779	1.387594
1	0.302176	5.420266	2.189846
1	1.829151	4.586429	1.727372
1	1.000035	5.630333	0.568715
6	3.581273	-0.108700	-1.810038
6	2.160365	0.426431	-1.633366
8	1.699684	0.350096	-0.421452
8	1.555204	0.870350	-2.600705
1	4.189901	0.748485	-2.137567
7	4.111322	-0.612752	-0.559260
1	3.499374	-0.612923	0.245083
6	5.448060	-0.749142	-0.376941
8	6.282633	-0.583586	-1.248862
16	-3.818747	-0.565917	2.325924
8	-3.344623	-0.699983	3.680691
8	-2.960037	-1.703287	1.462412
6	3.606093	-1.162405	-2.909238
1	4.636333	-1.489514	-3.076499
1	3.004138	-2.030934	-2.615992
1	3.200233	-0.747357	-3.835602
8	5.697110	-1.101656	0.903520
6	7.060081	-1.322726	1.354084
6	7.869085	-0.040598	1.237911
1	8.856198	-0.186197	1.693885
1	8.000443	0.248157	0.192501
1	7.363525	0.773380	1.771254
6	7.695973	-2.471522	0.587111
1	7.840574	-2.213415	-0.464361
1	8.669544	-2.712552	1.031423
1	7.062151	-3.364097	0.650210
6	6.873944	-1.701586	2.813629
1	6.260429	-2.605388	2.900191
1	7.846472	-1.892503	3.281728
1	6.375596	-0.892828	3.359846

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ortho-**C'**

Number of imaginary frequencies : 1
The smallest frequency is : -1451.0848 cm(-1)

Electronic energy : =-2012.7943168
Zero-point correction= 0.432096
Thermal correction to Energy= 0.464138
Thermal correction to Enthalpy= 0.465082
Thermal correction to Gibbs Free Energy= 0.368841
Sum of electronic and zero-point Energies= -2012.362221
Sum of electronic and thermal Energies= -2012.330179
Sum of electronic and thermal Enthalpies= -2012.329235
Sum of electronic and thermal Free Energies= -2012.425476

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Cartesian Coordinates

.....

46	-0.416895	0.979086	0.663765
6	-0.220491	-0.866539	2.903598
6	0.696654	-1.475325	3.750494
6	1.673467	-2.309532	3.212646
6	1.720452	-2.541185	1.842605
6	0.818758	-1.905692	0.989358
6	-0.166891	-1.040307	1.509051
1	2.467730	-3.218812	1.431614
1	2.391382	-2.800053	3.866196
1	0.648614	-1.311467	4.824456
1	-1.307202	-1.136355	0.830086
6	0.846480	-2.242450	-0.471878
1	-0.111739	-2.011340	-0.956781
1	1.084804	-3.298000	-0.644822
8	1.657343	-0.014620	-1.798669
6	4.230399	-0.308773	-0.567229
6	3.983545	0.939386	0.029936
6	5.416527	-0.541483	-1.243402
6	4.950047	1.946466	-0.043051
6	6.373222	0.466811	-1.305754
1	5.567614	-1.512860	-1.706546
6	6.145338	1.702758	-0.704250
1	4.747592	2.911875	0.412117
1	7.306227	0.285480	-1.832840
1	6.898103	2.483503	-0.761472
6	2.709755	1.150631	0.625190
7	1.629515	1.243455	1.034390
6	-2.898210	2.113618	-0.393584
6	-1.837738	3.218178	-0.359609
8	-0.632422	2.878501	0.025493
8	-2.137136	4.352248	-0.675660
1	-3.230127	2.030721	-1.438983
7	-2.304678	0.848358	0.032510
6	-2.873829	-0.315189	-0.206607
8	-2.368284	-1.424564	0.157037
1	-0.995563	-0.226361	3.323382
8	3.314489	-1.324958	-0.430186

8	2.448177	-2.267271	-2.593306
16	2.047426	-1.380985	-1.520463
6	-4.078684	2.514669	0.477132
1	-3.763747	2.598753	1.524433
1	-4.451193	3.489353	0.148146
1	-4.883505	1.774170	0.409068
8	-4.025815	-0.268481	-0.871141
6	-4.930979	-1.413846	-0.975367
6	-6.111908	-0.820219	-1.723324
1	-6.886537	-1.581670	-1.866848
1	-6.543637	0.016023	-1.161795
1	-5.798933	-0.451216	-2.706005
6	-4.296000	-2.529743	-1.786236
1	-3.933550	-2.141356	-2.745023
1	-3.463464	-2.994073	-1.253397
1	-5.051829	-3.296644	-1.994209
6	-5.349284	-1.861613	0.413652
1	-4.509676	-2.286356	0.969721
1	-5.759523	-1.013843	0.976412
1	-6.131917	-2.624902	0.330233

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ortho-**F'**

Number of imaginary frequencies : 1
The smallest frequency is : -1493.9133 cm(-1)

Electronic energy : =-2241.7785293
Zero-point correction= 0.495707
Thermal correction to Energy= 0.534141
Thermal correction to Enthalpy= 0.535085
Thermal correction to Gibbs Free Energy= 0.420838
Sum of electronic and zero-point Energies= -2241.282823
Sum of electronic and thermal Energies= -2241.244389
Sum of electronic and thermal Enthalpies= -2241.243445
Sum of electronic and thermal Free Energies= -2241.357691

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Cartesian Coordinates

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46	-0.173231	0.903367	0.245049
6	-1.263636	-0.504997	1.534092
1	-0.119655	-1.099008	1.311934
6	-1.409754	0.195706	2.742621
6	-2.608887	0.182758	3.444412
6	-3.667707	-0.579790	2.963041

6	-3.536406	-1.329830	1.794591
6	-2.352328	-1.275873	1.063203
1	-0.569795	0.783392	3.114107
1	-2.715726	0.754199	4.363045
1	-4.607191	-0.611352	3.510556
1	-4.364585	-1.949117	1.458287
6	-2.129100	-2.099827	-0.176299
1	-1.873627	-3.142364	0.063411
1	-1.311446	-1.696020	-0.786717
8	-4.694712	-2.753054	-0.674724
6	-4.814992	0.017351	-1.366305
6	-4.543069	1.227978	-0.705357
6	-6.124456	-0.350361	-1.636766
6	-5.588343	2.072483	-0.321387
6	-7.156794	0.492622	-1.238877
1	-6.322426	-1.285857	-2.149921
6	-6.895967	1.698531	-0.589978
1	-5.361600	3.006694	0.184462
1	-8.183609	0.205460	-1.449617
1	-7.715577	2.347127	-0.295252
6	-3.177849	1.496565	-0.423904
7	-2.040093	1.564094	-0.220852
6	1.788124	4.441115	-0.779880
6	1.053760	3.328644	-0.065308
8	0.712890	2.360022	-0.869749
8	0.823326	3.355016	1.137681
1	2.739580	4.063184	-1.167533
1	1.973602	5.264936	-0.087903
6	3.325121	-1.512047	1.019844
6	1.900140	-1.006944	0.926142
8	1.726745	0.197940	0.586761
8	0.983782	-1.816193	1.230801
1	3.371892	-2.448105	0.444840
7	4.234764	-0.557200	0.436989
1	3.906371	0.379935	0.247500
6	5.448407	-0.961941	-0.024606
8	5.864422	-2.101968	0.077548
1	1.206210	4.790223	-1.637946
8	-3.732478	-0.707886	-1.794907
8	-2.974091	-2.940876	-2.512171
16	-3.488985	-2.290789	-1.332973
6	3.657951	-1.824653	2.477452
1	4.673453	-2.227217	2.526348
1	3.611281	-0.911921	3.082557
1	2.958692	-2.561032	2.884051
8	6.088874	0.077527	-0.587807
6	7.420941	-0.094664	-1.151478
6	7.378225	-1.080228	-2.307603
1	8.357829	-1.108406	-2.800061

1	7.128027	-2.085920	-1.962143
1	6.634349	-0.761724	-3.047418
6	8.399734	-0.518724	-0.068565
1	9.417577	-0.519461	-0.476868
1	8.368494	0.190163	0.767400
1	8.167815	-1.519047	0.304831
6	7.754965	1.299140	-1.653505
1	7.743968	2.018823	-0.827418
1	8.751676	1.306015	-2.109126
1	7.025566	1.623577	-2.403990

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para-**B'**

Number of imaginary frequencies : 1
The smallest frequency is : -1424.9956 cm(-1)

Electronic energy : =-2241.7891359
Zero-point correction= 0.496583
Thermal correction to Energy= 0.534663
Thermal correction to Enthalpy= 0.535607
Thermal correction to Gibbs Free Energy= 0.422875
Sum of electronic and zero-point Energies= -2241.292553
Sum of electronic and thermal Energies= -2241.254473
Sum of electronic and thermal Enthalpies= -2241.253529
Sum of electronic and thermal Free Energies= -2241.366261

Cartesian Coordinates

6	3.670936	2.161311	-1.154033
6	2.331472	2.479951	-1.310654
6	1.494772	2.662282	-0.192761
6	2.075265	2.590506	1.087606
6	3.416859	2.281028	1.252091
6	4.208609	2.025172	0.128972
1	4.300493	1.965144	-2.020905
1	1.905828	2.544952	-2.310962
1	0.496491	3.513163	-0.322608
1	3.845528	2.184564	2.247887
6	5.605957	1.522476	0.293958
8	4.842858	-0.452218	1.955370
6	4.287280	-2.067431	-0.373173
6	2.895896	-2.165293	-0.254258
6	5.077840	-3.203300	-0.370853
6	2.282483	-3.420347	-0.152952

6	4.463449	-4.448031	-0.255831
1	6.155627	-3.097423	-0.459479
6	3.078380	-4.557326	-0.152130
1	1.196686	-3.457542	-0.078994
1	5.078473	-5.344280	-0.252818
1	2.615191	-5.536418	-0.069684
6	2.075530	-1.006291	-0.240834
7	1.317821	-0.135405	-0.236369
46	-0.153666	1.240082	-0.261167
6	-2.788824	4.656867	-0.382760
6	-1.546674	3.813041	-0.346190
8	-0.434677	4.405063	-0.395381
8	-1.711591	2.559976	-0.278495
1	1.449047	2.748355	1.964629
1	-3.674290	4.060065	-0.161753
1	-2.689051	5.479777	0.329612
1	-2.884264	5.097713	-1.380097
6	-2.990661	-2.097440	-0.315292
6	-1.613629	-1.420755	-0.247357
8	-1.683391	-0.130396	-0.305261
8	-0.622137	-2.134451	-0.174193
1	-3.048919	-2.765890	0.556319
7	-4.060173	-1.126458	-0.238028
1	-3.806396	-0.148468	-0.283071
6	-5.309747	-1.489371	0.137362
8	-5.662410	-2.637402	0.344302
8	7.029150	-0.679787	0.722138
8	4.846569	-0.811133	-0.532748
16	5.659979	-0.211380	0.784207
1	6.158816	2.021317	1.099742
1	6.200876	1.578369	-0.623962
6	-3.072624	-2.942611	-1.580967
1	-4.026603	-3.477469	-1.602764
1	-3.009004	-2.301803	-2.468747
1	-2.251897	-3.665127	-1.605468
8	-6.090266	-0.389855	0.236957
6	-7.483683	-0.508949	0.626242
6	-7.598303	-1.094949	2.024607
1	-8.643613	-1.054505	2.354795
1	-7.259679	-2.133172	2.045715
1	-6.995098	-0.509530	2.728845
6	-8.255498	-1.323000	-0.400211
1	-7.924004	-2.363588	-0.408913
1	-9.325840	-1.293434	-0.161740
1	-8.116999	-0.896279	-1.400811
6	-7.958437	0.934483	0.619098
1	-7.839613	1.373441	-0.378026
1	-9.016745	0.986338	0.899813
1	-7.378311	1.532558	1.330984

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para-**C'**

Number of imaginary frequencies : 1
The smallest frequency is : -1277.6530 cm(-1)

Electronic energy : =-2012.8012287
Zero-point correction= 0.432427
Thermal correction to Energy= 0.464348
Thermal correction to Enthalpy= 0.465293
Thermal correction to Gibbs Free Energy= 0.368781
Sum of electronic and zero-point Energies= -2012.368802
Sum of electronic and thermal Energies= -2012.336880
Sum of electronic and thermal Enthalpies= -2012.335936
Sum of electronic and thermal Free Energies= -2012.432448

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Cartesian Coordinates

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46	-0.955899	0.742962	-0.107035
6	0.123607	-1.874869	-1.024735
6	-0.498378	-1.384836	0.137320
6	0.156531	-1.582393	1.365644
6	1.413712	-2.166054	1.421936
6	2.038393	-2.585645	0.245162
6	1.373582	-2.474936	-0.978709
1	1.940296	-2.261656	2.371038
1	-0.310876	-1.228124	2.283640
1	-1.845595	-1.430500	0.082282
1	1.860794	-2.812816	-1.891796
6	3.455169	-3.053721	0.291457
8	4.258629	-1.323236	-1.614497
6	4.578670	0.664444	0.470422
6	3.615405	1.600245	0.067042
6	5.911914	1.027232	0.583322
6	4.006532	2.916017	-0.213245
6	6.287526	2.334363	0.291991
1	6.634952	0.281465	0.901120
6	5.340788	3.276338	-0.103513
1	3.252141	3.636940	-0.516465
1	7.332499	2.619703	0.379228
1	5.642410	4.296051	-0.324170
6	2.238981	1.248396	-0.036278
7	1.102154	1.042225	-0.112937
6	-3.596839	1.984797	-0.065069

6	-2.561005	3.079900	-0.334231
8	-1.304238	2.713482	-0.384206
8	-2.920670	4.234188	-0.456230
1	-4.338833	2.034384	-0.874585
7	-2.946472	0.675403	-0.070317
6	-3.627862	-0.452013	-0.105144
8	-3.087049	-1.599809	-0.047832
1	-0.377287	-1.752849	-1.984838
8	4.169500	-0.613414	0.792934
8	5.961715	-2.215622	0.012918
1	3.664154	-3.902297	-0.372232
1	3.799900	-3.305963	1.300043
16	4.607715	-1.799112	-0.292088
6	-4.278120	2.283264	1.264075
1	-4.704726	3.290115	1.230365
1	-5.072362	1.558210	1.470721
1	-3.543147	2.244345	2.077942
8	-4.948175	-0.322702	-0.218952
6	-5.874472	-1.441243	-0.036144
6	-7.226928	-0.758764	-0.146258
1	-8.028439	-1.496210	-0.026966
1	-7.338633	0.006660	0.630277
1	-7.338353	-0.277946	-1.124120
6	-5.701032	-2.462352	-1.146022
1	-5.779554	-1.974434	-2.124331
1	-4.736160	-2.969098	-1.078257
1	-6.498921	-3.211216	-1.074102
6	-5.693937	-2.040124	1.347643
1	-4.731032	-2.546773	1.447058
1	-5.764645	-1.254489	2.110237
1	-6.491556	-2.768724	1.534652

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para-**D'**

Number of imaginary frequencies : 1
The smallest frequency is : -1587.6564 cm(-1)

Electronic energy : =-2241.7744668
Zero-point correction= 0.497566
Thermal correction to Energy= 0.534643
Thermal correction to Enthalpy= 0.535587
Thermal correction to Gibbs Free Energy= 0.428942
Sum of electronic and zero-point Energies= -2241.276901
Sum of electronic and thermal Energies= -2241.239824

Sum of electronic and thermal Enthalpies= -2241.238880
Sum of electronic and thermal Free Energies= -2241.345525

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Cartesian Coordinates

.....

46	0.803965	0.807730	-0.210172
6	-0.021865	-1.863772	0.675440
6	0.561016	-1.369743	-0.510241
6	-0.200042	-1.462205	-1.696485
6	-1.484205	-1.983111	-1.692308
6	-2.037458	-2.451303	-0.496063
6	-1.296565	-2.408946	0.688817
1	0.551536	-1.809972	1.602063
8	2.822569	-2.493974	-0.974142
1	-2.075237	-2.022393	-2.606662
1	0.246753	-1.111638	-2.628187
1	1.792033	-1.686099	-0.674469
1	-1.738477	-2.774471	1.614084
6	-3.440085	-2.967453	-0.485982
8	-4.151103	-1.463540	1.628216
6	-4.726767	0.675518	-0.205327
6	-3.732594	1.576774	0.197882
6	-6.066565	1.018943	-0.129994
6	-4.094969	2.845347	0.666299
6	-6.415177	2.277990	0.348604
1	-6.813327	0.296231	-0.447038
6	-5.436724	3.188397	0.742188
1	-3.316860	3.541995	0.966102
1	-7.465049	2.551807	0.409645
1	-5.720827	4.170675	1.107930
6	-2.360372	1.208893	0.119683
7	-1.235096	0.947434	0.054177
6	4.555006	-3.001182	-2.490745
6	3.572948	-2.022312	-1.891367
8	3.563323	-0.840000	-2.292176
6	3.040037	2.368109	-1.085462
6	2.010447	3.352030	-0.530796
8	0.929915	2.820709	-0.007878
8	2.178603	4.547384	-0.643535
1	4.035259	2.731719	-0.804699
1	5.373795	-3.158546	-1.779217
1	4.078890	-3.971629	-2.654936
1	4.970025	-2.610489	-3.422288
7	2.844715	1.015043	-0.497693
1	3.120096	0.239224	-1.167897
6	3.440566	0.847009	0.795433
8	3.780087	1.772975	1.486898
16	-4.600584	-1.846361	0.305703
8	-4.337700	-0.549309	-0.706346

8	-5.952256	-2.318456	0.088203
1	-3.559016	-3.890474	0.095600
1	-3.847183	-3.135054	-1.489006
6	2.907065	2.286921	-2.596920
1	3.036242	3.289233	-3.014952
1	3.649442	1.607899	-3.026400
1	1.910870	1.920225	-2.880160
8	3.532256	-0.448886	1.048169
6	3.989219	-0.932131	2.355758
6	3.033081	-0.442933	3.429002
1	3.299177	-0.901509	4.388420
1	3.072846	0.643921	3.539921
1	2.003435	-0.737086	3.186715
6	5.420208	-0.488142	2.605352
1	5.792669	-0.975731	3.513944
1	6.061722	-0.792808	1.770447
1	5.493926	0.594098	2.734703
6	3.915286	-2.438945	2.197528
1	4.230635	-2.923824	3.128382
1	2.896252	-2.760389	1.955656
1	4.565477	-2.773795	1.382509

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para-**F'**

Number of imaginary frequencies : 1
The smallest frequency is : -1059.6758 cm(-1)

Electronic energy : =-2241.7852515
Zero-point correction= 0.496402
Thermal correction to Energy= 0.534514
Thermal correction to Enthalpy= 0.535458
Thermal correction to Gibbs Free Energy= 0.423439
Sum of electronic and zero-point Energies= -2241.288850
Sum of electronic and thermal Energies= -2241.250738
Sum of electronic and thermal Enthalpies= -2241.249793
Sum of electronic and thermal Free Energies= -2241.361813

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Cartesian Coordinates

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6	1.804596	-2.250847	1.763126
6	0.737425	-1.366760	1.802154
6	0.070044	-0.983700	0.624248
6	0.460564	-1.591172	-0.582772
6	1.517670	-2.487536	-0.629467

6	2.221443	-2.784921	0.541197
1	2.353576	-2.497452	2.671236
1	0.447666	-0.917200	2.751026
1	-1.258230	-0.713481	0.717859
1	1.846158	-2.910300	-1.577052
6	3.471395	-3.601255	0.482460
8	4.414708	-2.274141	-1.657212
6	5.461070	-0.291702	0.104695
6	4.633637	0.815480	-0.113737
6	6.808597	-0.235568	-0.208596
6	5.159124	1.995076	-0.658417
6	7.325268	0.938893	-0.749527
1	7.430557	-1.108599	-0.029982
6	6.509252	2.045475	-0.974891
1	4.477280	2.827035	-0.834128
1	8.381911	0.986092	-1.000050
1	6.927367	2.952278	-1.402462
6	3.249446	0.783924	0.200611
7	2.123443	0.894142	0.433484
46	0.127179	1.177730	0.381067
8	-1.888265	1.536795	0.201742
6	-2.745767	0.640993	0.409085
8	-2.496688	-0.559607	0.726795
6	-4.193932	1.071155	0.290547
1	-4.310274	1.540818	-0.696694
6	-6.293335	-0.049468	-0.212260
8	-6.767983	0.938022	-0.742175
7	-5.060328	-0.080915	0.362103
8	4.903023	-1.430603	0.658431
16	4.822012	-2.748487	-0.351126
8	6.037274	-3.518747	-0.184769
1	3.863815	-3.864831	1.470449
1	3.371358	-4.521181	-0.107870
1	-0.054346	-1.322655	-1.504725
1	-4.687495	-0.955406	0.704252
6	-4.513381	2.113174	1.359659
1	-5.549246	2.439246	1.231149
1	-4.402590	1.679620	2.360320
1	-3.848376	2.976464	1.267741
8	-6.878339	-1.254980	-0.091583
6	-8.218151	-1.480283	-0.619295
6	-8.482247	-2.930586	-0.254143
1	-8.442540	-3.067877	0.832204
1	-9.474399	-3.233487	-0.607593
1	-7.733801	-3.586265	-0.713010
6	-9.217806	-0.567943	0.072285
1	-9.146379	-0.686212	1.159997
1	-9.041237	0.479167	-0.183381
1	-10.234606	-0.841837	-0.233929

6	-8.224232	-1.302676	-2.128582
1	-7.469976	-1.951849	-2.588912
1	-9.205902	-1.587968	-2.525768
1	-8.019418	-0.266286	-2.406745
8	0.290251	3.209320	0.234321
6	1.267600	3.810521	-0.375481
8	2.213167	3.296679	-0.961641
6	1.113074	5.319053	-0.293271
1	1.078590	5.635244	0.753770
1	1.944999	5.807140	-0.805518
1	0.166032	5.619592	-0.751401

Possibilities of Reductive Elimination Transition States of *meta* product at the M06/6-31G**Level of Theory

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Reductive Elimination

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conf-4 (5-coordination)

Number of imaginary frequencies : 1
The smallest frequency is : -330.5492 cm(-1)

Electronic energy : =-2698.4547193
Zero-point correction= 0.604755
Thermal correction to Energy= 0.652277
Thermal correction to Enthalpy= 0.653221
Thermal correction to Gibbs Free Energy= 0.524259
Sum of electronic and zero-point Energies= -2697.849964
Sum of electronic and thermal Energies= -2697.802443
Sum of electronic and thermal Enthalpies= -2697.801498
Sum of electronic and thermal Free Energies= -2697.930460

Cartesian Coordinates

46	2.009543	-0.527276	0.111626
6	3.642808	3.220344	1.000792
6	3.480928	1.837279	1.111638
6	2.177164	1.388089	1.131520
6	1.062504	2.194131	1.216274
6	1.255181	3.568338	1.077760
6	2.548658	4.077457	0.960157
1	0.074656	1.769272	1.348952

1	4.334796	1.170079	1.065948
1	2.700866	5.148946	0.846388
6	0.059585	4.466978	1.037381
1	0.331689	5.524970	0.949242
1	-0.607864	4.357893	1.900583
8	-0.292980	3.799817	-1.570516
6	-2.616483	2.168642	-0.660846
6	-2.197885	0.927302	-1.162823
6	-3.861912	2.678478	-0.992657
6	-3.054491	0.176826	-1.974083
6	-4.691964	1.939002	-1.830626
1	-4.163068	3.641728	-0.591749
6	-4.294349	0.694879	-2.316354
1	-2.731459	-0.802546	-2.319658
1	-5.666644	2.337815	-2.099546
1	-4.956265	0.122049	-2.959821
6	-0.892327	0.458160	-0.854941
7	0.185109	0.129650	-0.599002
6	-0.954222	-3.409301	-0.544364
6	0.428697	-2.994711	-0.004028
8	1.278751	-2.593019	-0.878111
8	0.567759	-2.965582	1.218573
1	-1.213381	-4.379523	-0.093135
7	-1.868296	-2.385448	-0.026364
6	-3.213704	-2.612550	-0.002324
8	-3.771484	-3.572732	-0.498263
1	4.650742	3.619078	0.917912
8	-1.786327	2.842698	0.212805
8	-1.992391	5.274058	-0.429821
16	-1.019910	4.200612	-0.385523
8	3.620256	-1.467209	0.767086
6	4.839600	-1.237100	0.350925
8	5.211948	-0.310353	-0.350944
8	1.783916	-0.281411	2.183999
6	0.565191	-0.539811	2.671215
8	-0.490792	-0.197205	2.177082
6	0.678189	-1.349817	3.930895
1	1.571133	-1.096055	4.505704
1	-0.227968	-1.224722	4.527364
1	0.759567	-2.391376	3.598089
6	5.770398	-2.325214	0.838767
1	5.684995	-3.174326	0.151868
1	6.797398	-1.954282	0.822197
1	5.493905	-2.673246	1.836086
6	-1.037182	-3.495488	-2.053392
1	-2.061848	-3.726342	-2.362161
1	-0.712723	-2.547454	-2.498642
1	-0.372112	-4.278978	-2.431117
8	-3.820939	-1.572775	0.611626

6	-5.232253	-1.628937	0.951981
6	-5.475630	-0.262050	1.568753
1	-6.518276	-0.171838	1.894637
1	-4.820451	-0.108274	2.433168
1	-5.267543	0.527591	0.834345
6	-5.462046	-2.733855	1.969254
1	-6.502195	-2.710696	2.315903
1	-5.263934	-3.716045	1.530745
1	-4.807048	-2.591687	2.836585
6	-6.103074	-1.810402	-0.282414
1	-7.157613	-1.716217	0.005387
1	-5.883512	-1.027463	-1.018398
1	-5.942359	-2.786400	-0.744616
1	-1.515346	-1.804577	0.730591
8	2.747522	-0.213257	-1.906493
6	3.426943	-1.057998	-2.510307
8	3.390456	-2.337534	-2.288783
6	4.399616	-0.617810	-3.548440
1	5.342527	-0.417011	-3.026508
1	4.561151	-1.396079	-4.296533
1	4.060493	0.312626	-4.006578
1	2.636384	-2.570519	-1.656298

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conf-1 (6-coordination)

Number of imaginary frequencies : 1
The smallest frequency is : -323.1206 cm(-1)

Electronic energy : =-2469.4590197
Zero-point correction= 0.540993
Thermal correction to Energy= 0.582282
Thermal correction to Enthalpy= 0.583227
Thermal correction to Gibbs Free Energy= 0.469664
Sum of electronic and zero-point Energies= -2468.918027
Sum of electronic and thermal Energies= -2468.876737
Sum of electronic and thermal Enthalpies= -2468.875793
Sum of electronic and thermal Free Energies= -2468.989356

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Cartesian Coordinates

.....

46	-1.702041	-0.540327	0.665392
6	-1.515444	-1.085842	-3.550776
6	-2.143078	-1.178919	-2.309662
6	-1.346970	-1.527250	-1.233849

6	-0.053925	-1.996624	-1.364117
6	0.570716	-1.834115	-2.601398
6	-0.157703	-1.363357	-3.692581
1	0.476238	-2.431478	-0.526632
1	-1.787934	1.387577	-1.511830
1	-3.188895	-0.923294	-2.183858
1	0.327791	-1.235573	-4.658067
6	2.033054	-2.130574	-2.702012
1	2.417517	-2.023180	-3.722551
1	2.313048	-3.124080	-2.331378
8	2.461206	0.295658	-1.538015
6	3.568757	-1.145590	0.789356
6	2.670143	-0.703119	1.770784
6	4.928424	-0.944831	0.949940
6	3.118217	-0.048634	2.922786
6	5.374293	-0.296583	2.101264
1	5.614745	-1.294249	0.184155
6	4.484081	0.148853	3.076804
1	2.373106	0.303767	3.640098
1	6.441417	-0.137660	2.235086
1	4.857848	0.655014	3.962113
6	1.288046	-0.889703	1.536448
7	0.174947	-1.047842	1.271829
6	-0.459036	1.883351	2.029472
6	-0.707422	0.801951	3.123693
8	-1.741452	0.092500	2.949871
8	0.119399	0.772955	4.040992
1	0.621580	2.079944	2.017121
7	-0.885504	1.417505	0.715210
6	-0.394004	1.947718	-0.366660
8	-0.794137	1.609823	-1.560005
1	-2.098761	-0.766530	-4.410913
8	3.051152	-1.817159	-0.306152
8	4.436784	-1.082801	-2.279147
16	3.087016	-0.993210	-1.758513
8	-3.590925	0.078160	0.389994
6	-3.974941	0.976201	-0.444829
8	-3.304784	1.488345	-1.352723
8	-2.485113	-2.438664	0.156201
6	-1.952717	-3.555101	0.662150
8	-0.782895	-3.732354	0.917973
6	-3.028293	-4.593133	0.862053
1	-3.570654	-4.763102	-0.072513
1	-2.576720	-5.521932	1.215247
1	-3.751734	-4.226804	1.596896
6	-5.408402	1.391976	-0.234603
1	-5.442991	2.099651	0.600356
1	-5.789924	1.880440	-1.133188
1	-6.025393	0.532995	0.038192

6	-1.222266	3.140619	2.415509
1	-1.029442	3.955053	1.705170
1	-2.297335	2.924679	2.430694
1	-0.916015	3.464051	3.416065
8	0.546708	2.861878	-0.257476
6	0.799257	3.885449	-1.288536
6	1.768642	4.810584	-0.576296
1	2.037718	5.646676	-1.231108
1	1.316533	5.211710	0.338211
1	2.682550	4.271723	-0.304752
6	-0.495900	4.611593	-1.607052
1	-0.279204	5.456895	-2.270421
1	-1.220979	3.963525	-2.107122
1	-0.948050	5.009634	-0.690108
6	1.447011	3.261113	-2.509660
1	1.762321	4.061358	-3.190449
1	2.328858	2.680681	-2.218743
1	0.757508	2.598353	-3.038373

(IV) Hydrolysis of Trifluoroacetoxy and Acetoxy Products

(R=CF_3) Trifluoro Acetoxylation leads to hydrolysis [8b-9]

[8b]

Number of imaginary frequencies : 0

Electronic energy : =-1820.3378601
Zero-point correction= 0.280400
Thermal correction to Energy= 0.305204
Thermal correction to Enthalpy= 0.306148
Thermal correction to Gibbs Free Energy= 0.225382
Sum of electronic and zero-point Energies= -1820.057460
Sum of electronic and thermal Energies= -1820.032656
Sum of electronic and thermal Enthalpies= -1820.031712
Sum of electronic and thermal Free Energies= -1820.112478

.....

Cartesian Coordinates

.....

6	0.694967	-2.975250	1.961293
6	1.671633	-1.993539	1.831662
6	1.615489	-1.180718	0.717167
6	0.647536	-1.276054	-0.264136

6	-0.327106	-2.260439	-0.112165
6	-0.298819	-3.104681	0.999652
1	0.646194	-0.603769	-1.119591
1	2.454557	-1.855123	2.571656
1	-1.067608	-3.866851	1.111222
6	-1.426856	-2.376785	-1.115379
1	-1.766074	-3.410818	-1.256465
1	-1.176000	-1.959850	-2.097650
8	-3.207015	-1.731271	0.800952
6	-3.013227	1.068376	-0.190431
6	-2.214354	2.136922	0.240388
6	-4.391469	1.120082	-0.058135
6	-2.815235	3.261470	0.818704
6	-4.969920	2.236889	0.535703
1	-5.015119	0.308643	-0.422975
6	-4.191141	3.304238	0.973415
1	-2.187628	4.088295	1.139450
1	-6.050443	2.273083	0.644227
1	-4.658127	4.172878	1.427876
6	-0.802777	2.097235	0.059413
7	0.348655	2.088895	-0.094768
1	0.708866	-3.635384	2.823637
8	-2.346904	0.016271	-0.795634
8	-3.960038	-1.742350	-1.593233
16	-2.916748	-1.524193	-0.606308
8	2.569181	-0.125371	0.656420
6	3.460763	-0.073235	-0.258682
8	3.713881	-1.100328	-0.974862
6	4.518209	1.008746	0.000470
8	2.435200	1.053345	-1.665636
1	1.825151	1.655734	-1.186160
1	2.919219	1.597198	-2.304728
9	3.961893	2.125436	0.418070
9	5.222322	1.231012	-1.097473
9	5.323059	0.538479	0.944490
1	4.448326	-0.975437	-1.609651

[8b-8c]‡

Number of imaginary frequencies : 1
The smallest frequency is : -60.6468 cm(-1)

Electronic energy : =-1820.3378569
Zero-point correction= 0.279861

Thermal correction to Energy= 0.303966
Thermal correction to Enthalpy= 0.304910
Thermal correction to Gibbs Free Energy= 0.226069
Sum of electronic and zero-point Energies= -1820.057996
Sum of electronic and thermal Energies= -1820.033891
Sum of electronic and thermal Enthalpies= -1820.032947
Sum of electronic and thermal Free Energies= -1820.111787

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Cartesian Coordinates

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6	0.704281	-2.994062	1.940120
6	1.675969	-2.006994	1.813301
6	1.610748	-1.184317	0.706299
6	0.638162	-1.277416	-0.270730
6	-0.331672	-2.267017	-0.121834
6	-0.294348	-3.119915	0.983026
1	0.629353	-0.598311	-1.120618
1	2.461874	-1.871281	2.550648
1	-1.059963	-3.885662	1.092586
6	-1.437731	-2.378270	-1.118617
1	-1.780134	-3.411094	-1.260619
1	-1.192936	-1.958576	-2.101274
8	-3.199279	-1.728993	0.813929
6	-3.009622	1.071811	-0.186572
6	-2.205405	2.143907	0.225394
6	-4.386036	1.124678	-0.036561
6	-2.798689	3.273344	0.801959
6	-4.956688	2.246460	0.555498
1	-5.014557	0.310484	-0.386478
6	-4.172467	3.317503	0.973980
1	-2.167075	4.102699	1.107976
1	-6.035697	2.283396	0.678129
1	-4.633619	4.189857	1.427271
6	-0.796224	2.102270	0.027448
7	0.353132	2.092359	-0.140484
1	0.725654	-3.661349	2.796795
8	-2.350310	0.015784	-0.791984
8	-3.974944	-1.739733	-1.572962
16	-2.921832	-1.523401	-0.596113
8	2.556413	-0.123025	0.649850
6	3.450726	-0.064295	-0.265773
8	3.721007	-1.099882	-0.967107
6	4.508207	1.013111	0.011435
8	2.450148	1.029947	-1.658503
1	1.837235	1.641857	-1.192232
1	2.943840	1.558635	-2.303592
9	3.948927	2.129490	0.427626
9	5.225697	1.240675	-1.077164
9	5.301369	0.537014	0.962067

1	4.459944	-0.974942	-1.596165

[8c]

Number of imaginary frequencies : 0

Electronic energy : =-1820.3446165
Zero-point correction= 0.279072
Thermal correction to Energy= 0.302590
Thermal correction to Enthalpy= 0.303534
Thermal correction to Gibbs Free Energy= 0.225693
Sum of electronic and zero-point Energies= -1820.065545
Sum of electronic and thermal Energies= -1820.042027
Sum of electronic and thermal Enthalpies= -1820.041083
Sum of electronic and thermal Free Energies= -1820.118924

Cartesian Coordinates

6	0.654908	-3.036982	1.902165
6	1.614025	-2.041424	1.755762
6	1.540831	-1.195856	0.659881
6	0.546334	-1.323546	-0.298378
6	-0.418341	-2.316362	-0.133992
6	-0.364052	-3.170817	0.967408
1	0.501850	-0.665050	-1.162432
1	2.410857	-1.903806	2.481571
1	-1.127175	-3.937180	1.090485
6	-1.550540	-2.411992	-1.103235
1	-1.939300	-3.432753	-1.209132
1	-1.318473	-2.027107	-2.103184
8	-3.244550	-1.649540	0.851541
6	-2.904604	1.127480	-0.174858
6	-2.020170	2.187307	0.092697
6	-4.246521	1.250936	0.142941
6	-2.484269	3.368781	0.688204
6	-4.689496	2.422327	0.749942
1	-4.950214	0.456165	-0.085541
6	-3.821669	3.476927	1.023868
1	-1.784205	4.177210	0.877404
1	-5.742572	2.510933	1.002743
1	-4.192311	4.383765	1.491343
6	-0.659976	2.058166	-0.267731
7	0.449298	1.955818	-0.575358
1	0.700385	-3.705872	2.757114

8	-2.352238	0.033697	-0.801698
8	-4.071081	-1.655563	-1.519539
16	-2.989007	-1.484913	-0.567058
8	2.451768	-0.135691	0.638185
6	3.249683	0.073283	-0.438305
8	3.654171	-1.079480	-1.003595
6	4.417839	0.956964	0.048832
8	2.476307	0.863599	-1.393748
1	1.568822	1.511174	-0.975949
1	2.982316	1.245136	-2.135929
9	3.968993	2.082481	0.587018
9	5.202048	1.262675	-0.987341
9	5.135507	0.301543	0.946500
1	4.311199	-0.932354	-1.704014

[8d]

Number of imaginary frequencies : 0

Electronic energy : =-1896.7730984
Zero-point correction= 0.309765
Thermal correction to Energy= 0.335635
Thermal correction to Enthalpy= 0.336580
Thermal correction to Gibbs Free Energy= 0.254258
Sum of electronic and zero-point Energies= -1896.463334
Sum of electronic and thermal Energies= -1896.437463
Sum of electronic and thermal Enthalpies= -1896.436519
Sum of electronic and thermal Free Energies= -1896.518840

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Cartesian Coordinates

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6	-1.365332	2.866722	1.591998
6	-2.010995	1.640882	1.490173
6	-1.545840	0.707683	0.572713
6	-0.467070	0.975651	-0.255488
6	0.171754	2.210746	-0.148715
6	-0.271442	3.149567	0.782134
1	-0.114850	0.236931	-0.968483
1	-2.871309	1.397104	2.110322
1	0.242582	4.104838	0.868321
6	1.372099	2.505229	-0.988765
1	1.602242	3.577255	-1.028900
1	1.304570	2.129734	-2.016627
8	2.884820	1.781828	1.125607

6	3.316245	-0.809223	-0.268673
6	2.640947	-2.036322	-0.191237
6	4.629573	-0.701968	0.160789
6	3.294255	-3.156982	0.336424
6	5.257996	-1.821749	0.695664
1	5.167621	0.237604	0.071626
6	4.598865	-3.044510	0.787110
1	2.762110	-4.102855	0.384531
1	6.286075	-1.733241	1.036451
1	5.105471	-3.910582	1.202242
6	1.304409	-2.155457	-0.666488
7	0.216741	-2.275551	-1.057132
1	-1.718264	3.603254	2.308743
8	2.613390	0.234013	-0.842447
8	4.024361	2.302034	-1.050546
16	2.875730	1.786374	-0.326341
8	-2.146871	-0.553569	0.579963
6	-2.929288	-1.028002	-0.539013
8	-2.247281	-0.964741	-1.704132
6	-4.185540	-0.147952	-0.681975
8	-3.369660	-2.266735	-0.163477
1	-2.635136	-2.899439	-0.219664
1	-3.910214	-2.020254	2.554796
9	-4.833184	-0.076419	0.481762
9	-5.006075	-0.660489	-1.590456
9	-3.861539	1.086398	-1.054438
1	-2.701785	-1.107966	1.960273
8	-3.203504	-1.391229	2.802444
1	-1.448215	-1.535143	-1.641333
1	-2.598432	-1.834465	3.428079

[8d-9]‡

Number of imaginary frequencies : 1
The smallest frequency is : -213.1534 cm(-1)

Electronic energy : =-1896.7627334
Zero-point correction= 0.306843
Thermal correction to Energy= 0.332800
Thermal correction to Enthalpy= 0.333744
Thermal correction to Gibbs Free Energy= 0.250645
Sum of electronic and zero-point Energies= -1896.455890
Sum of electronic and thermal Energies= -1896.429933
Sum of electronic and thermal Enthalpies= -1896.428989

S300

Sum of electronic and thermal Free Energies= -1896.512088

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Cartesian Coordinates

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6	-1.379305	3.114368	1.371374
6	-2.014036	1.880057	1.427009
6	-1.510032	0.837263	0.658232
6	-0.425996	1.008098	-0.188493
6	0.196853	2.254037	-0.241447
6	-0.272015	3.301445	0.550791
1	-0.065087	0.179531	-0.790836
1	-2.882398	1.717559	2.061468
1	0.229156	4.266457	0.516321
6	1.401380	2.454472	-1.103523
1	1.655678	3.514547	-1.225007
1	1.320089	2.006308	-2.100993
8	2.890807	1.819865	1.055045
6	3.300255	-0.849294	-0.218379
6	2.620514	-2.073655	-0.122905
6	4.602755	-0.734834	0.240324
6	3.256287	-3.182028	0.450632
6	5.213642	-1.841737	0.820590
1	5.147348	0.199668	0.140313
6	4.549603	-3.060478	0.929370
1	2.718906	-4.124162	0.512260
1	6.233115	-1.746128	1.184529
1	5.043513	-3.915486	1.380917
6	1.294515	-2.199525	-0.620564
7	0.213434	-2.319688	-1.026404
1	-1.752155	3.936730	1.975937
8	2.611759	0.176817	-0.835552
8	4.051655	2.211669	-1.137461
16	2.891536	1.751091	-0.394920
8	-2.076784	-0.425628	0.748500
6	-2.984844	-1.253450	-0.599062
8	-2.174490	-1.186255	-1.598866
6	-4.182263	-0.305098	-0.734346
8	-3.299711	-2.358872	0.018842
1	-2.607027	-3.042456	-0.050176
1	-4.025945	-1.576879	2.695350
9	-4.816303	-0.172743	0.420903
9	-5.016610	-0.822792	-1.627337
9	-3.781383	0.883132	-1.152896
1	-2.582424	-0.579487	1.634640
8	-3.428271	-0.836070	2.871207
1	-1.378508	-1.788996	-1.508149
1	-2.887801	-1.125273	3.619605

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[9]

Number of imaginary frequencies : 0

Electronic energy : =-1896.767337
Zero-point correction= 0.305191
Thermal correction to Energy= 0.331822
Thermal correction to Enthalpy= 0.332766
Thermal correction to Gibbs Free Energy= 0.248316
Sum of electronic and zero-point Energies= -1896.462146
Sum of electronic and thermal Energies= -1896.435515
Sum of electronic and thermal Enthalpies= -1896.434571
Sum of electronic and thermal Free Energies= -1896.519021

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Cartesian Coordinates

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6	-0.683924	3.302797	1.655329
6	-1.549825	2.220808	1.760668
6	-1.443120	1.160786	0.859105
6	-0.486820	1.200547	-0.154629
6	0.379564	2.285896	-0.247061
6	0.288249	3.340577	0.662450
1	-0.419629	0.381566	-0.867345
1	-2.312956	2.186829	2.536343
1	0.975953	4.180660	0.588325
6	1.441538	2.300249	-1.297926
1	1.739635	3.316232	-1.587022
1	1.179708	1.747615	-2.208372
8	3.276025	1.900375	0.643869
6	3.199430	-0.989693	-0.131454
6	2.470465	-2.146609	0.197257
6	4.548601	-0.913463	0.174466
6	3.096897	-3.221526	0.843666
6	5.152618	-1.983499	0.826926
1	5.137208	-0.041536	-0.095646
6	4.438999	-3.131385	1.164388
1	2.515502	-4.107525	1.082305
1	6.210292	-1.916500	1.067091
1	4.933408	-3.955050	1.669786
6	1.104084	-2.230199	-0.157180
7	-0.009742	-2.312365	-0.456381
1	-0.769096	4.124791	2.362059
8	2.492989	-0.014856	-0.794848
8	4.007803	1.745692	-1.753162
16	2.982365	1.574552	-0.739211

8	-2.235325	0.067478	0.943432
6	-3.179981	-1.493197	-0.636978
8	-2.174949	-1.621855	-1.347209
6	-4.203937	-0.427260	-1.050610
8	-3.552466	-2.234364	0.344080
1	-2.905499	-2.939766	0.551437
1	-4.638098	-0.683493	2.723854
1	-2.837021	0.107052	1.734280
8	-3.998099	0.004941	2.948053
1	-1.201935	-2.095926	-0.909569
1	-3.591779	-0.306048	3.767455
9	-4.960761	-0.065357	-0.029914
9	-4.976722	-0.945512	-2.000154
9	-3.576982	0.629377	-1.534062

(R=CH_3) Acetoxy product leads to Hydrolysis

[8b']

Number of imaginary frequencies : 0

Electronic energy : =-1522.720254
Zero-point correction= 0.301693
Thermal correction to Energy= 0.325180
Thermal correction to Enthalpy= 0.326125
Thermal correction to Gibbs Free Energy= 0.249230
Sum of electronic and zero-point Energies= -1522.418561
Sum of electronic and thermal Energies= -1522.395074
Sum of electronic and thermal Enthalpies= -1522.394129
Sum of electronic and thermal Free Energies= -1522.471024

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Cartesian Coordinates

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6	1.903819	-2.544304	1.887894
6	2.612203	-1.350509	1.804320
6	2.338701	-0.514604	0.735932
6	1.405450	-0.798536	-0.244217
6	0.696792	-1.994109	-0.137274
6	0.947223	-2.858598	0.929481
1	1.239063	-0.108737	-1.067820
1	3.353012	-1.064112	2.545453
1	0.384974	-3.787259	1.005440
6	-0.364543	-2.319217	-1.136613
1	-0.500532	-3.399596	-1.273698

1	-0.201958	-1.865702	-2.121138
8	-2.215490	-2.027705	0.792965
6	-2.558599	0.760522	-0.165652
6	-1.973788	1.985259	0.185160
6	-3.901134	0.523450	0.084368
6	-2.748405	2.967119	0.814648
6	-4.651580	1.504824	0.723965
1	-4.369618	-0.408087	-0.220301
6	-4.082618	2.719837	1.093478
1	-2.285456	3.914506	1.076751
1	-5.701811	1.312746	0.926433
1	-4.681671	3.477890	1.589010
6	-0.610712	2.251966	-0.130804
7	0.492657	2.499879	-0.398259
1	2.094935	-3.226332	2.711159
8	-1.729669	-0.144229	-0.807920
8	-2.976839	-2.179037	-1.594284
16	-1.985929	-1.766053	-0.616293
8	2.989720	0.744117	0.699717
6	4.066357	0.930935	0.015402
8	4.686776	-0.007378	-0.592143
6	4.699520	2.247673	0.114459
8	2.773645	1.581183	-1.961954
1	2.067859	2.118397	-1.561858
1	3.203810	2.168020	-2.595629
1	5.298139	2.447246	-0.775229
1	5.364000	2.228301	0.988070
1	3.940305	3.016139	0.268700
1	4.223982	-0.871591	-0.585160

[8b'-8c']‡

Number of imaginary frequencies : 1
The smallest frequency is : -253.9562 cm(-1)

Electronic energy : =-1522.7142822
Zero-point correction= 0.303705
Thermal correction to Energy= 0.325321
Thermal correction to Enthalpy= 0.326265
Thermal correction to Gibbs Free Energy= 0.253232
Sum of electronic and zero-point Energies= -1522.410577
Sum of electronic and thermal Energies= -1522.388962
Sum of electronic and thermal Enthalpies= -1522.388017
Sum of electronic and thermal Free Energies= -1522.461050

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Cartesian Coordinates

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6	2.212657	-2.728547	1.575201
6	2.806839	-1.471786	1.550983
6	2.334738	-0.534807	0.644148
6	1.308789	-0.811266	-0.245190
6	0.717975	-2.073467	-0.207466
6	1.165732	-3.024573	0.709748
1	0.958122	-0.058563	-0.946734
1	3.616511	-1.205608	2.225332
1	0.691212	-4.003310	0.740722
6	-0.425087	-2.383212	-1.118082
1	-0.585392	-3.461812	-1.241890
1	-0.334586	-1.934895	-2.114145
8	-2.100261	-1.985222	0.952867
6	-2.576972	0.743489	-0.166903
6	-1.989786	1.994400	0.074008
6	-3.903299	0.514612	0.164067
6	-2.745030	3.013892	0.667022
6	-4.633386	1.533457	0.767542
1	-4.375284	-0.439869	-0.051638
6	-4.062956	2.777285	1.020998
1	-2.280097	3.980367	0.841203
1	-5.671038	1.347868	1.031394
1	-4.647791	3.564065	1.487680
6	-0.640277	2.241498	-0.305052
7	0.454551	2.464161	-0.621595
1	2.564353	-3.476332	2.280409
8	-1.772791	-0.193560	-0.790137
8	-3.069201	-2.272919	-1.346160
16	-1.997928	-1.805643	-0.484015
8	2.862477	0.763507	0.708369
6	3.843119	1.150578	-0.107792
8	4.689445	0.270429	-0.593618
6	4.444978	2.447091	0.289230
8	2.902704	1.560148	-1.557076
1	2.105352	2.089269	-1.289316
1	3.427579	2.097388	-2.176152
1	5.095132	2.822190	-0.503844
1	5.041817	2.276179	1.191041
1	3.656946	3.169541	0.513773
1	4.274967	-0.596231	-0.761161

[8c']

Number of imaginary frequencies : 0

Electronic energy : =-1522.7163264
Zero-point correction= 0.302859
Thermal correction to Energy= 0.324274
Thermal correction to Enthalpy= 0.325218
Thermal correction to Gibbs Free Energy= 0.253495
Sum of electronic and zero-point Energies= -1522.413468
Sum of electronic and thermal Energies= -1522.392053
Sum of electronic and thermal Enthalpies= -1522.391108
Sum of electronic and thermal Free Energies= -1522.462832

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Cartesian Coordinates

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6	1.575871	-1.216472	2.607270
6	2.641090	-0.617622	1.945465
6	2.738403	-0.726920	0.560666
6	1.791662	-1.437910	-0.166257
6	0.713301	-2.019094	0.501638
6	0.605096	-1.903438	1.888080
1	1.897610	-1.542542	-1.244542
1	3.411522	-0.072969	2.486889
1	-0.239863	-2.360418	2.399474
6	-0.357257	-2.711456	-0.277733
1	-0.965592	-3.395520	0.324768
1	0.022118	-3.258191	-1.150419
8	-2.647545	-2.250938	-1.585974
6	-2.796776	0.264662	0.347020
6	-2.160416	1.518164	0.399272
6	-4.171357	0.184073	0.257512
6	-2.919448	2.697503	0.380738
6	-4.917013	1.361071	0.235903
1	-4.642168	-0.794220	0.216096
6	-4.298992	2.607959	0.302160
1	-2.416509	3.658887	0.424913
1	-5.999633	1.298781	0.170236
1	-4.895967	3.514514	0.290192
6	-0.754733	1.604476	0.436114
7	0.390873	1.712971	0.462143
1	1.499358	-1.139990	3.688686
8	-2.033063	-0.880276	0.441996
8	-0.862026	-0.495281	-1.736378
16	-1.524171	-1.552931	-0.988473
8	3.829017	-0.162893	-0.069828
6	3.674738	1.100484	-0.695917
8	2.962239	1.975118	0.171806

6	2.931131	1.052753	-2.002333
8	4.943071	1.561650	-0.919934
1	5.482700	1.371056	-0.136098
1	3.436809	0.352908	-2.672490
1	2.936154	2.048998	-2.453544
1	1.893573	0.733121	-1.868197
1	1.461874	1.817730	0.377224
1	3.463308	2.095512	0.996296

[8d']

Number of imaginary frequencies : 0

Electronic energy : =-1599.1409438
Zero-point correction= 0.330309
Thermal correction to Energy= 0.354112
Thermal correction to Enthalpy= 0.355056
Thermal correction to Gibbs Free Energy= 0.278267
Sum of electronic and zero-point Energies= -1598.810635
Sum of electronic and thermal Energies= -1598.786832
Sum of electronic and thermal Enthalpies= -1598.785888
Sum of electronic and thermal Free Energies= -1598.862677

Cartesian Coordinates

6	-1.196415	1.681697	2.811756
6	-2.250986	0.855804	2.454002
6	-2.516640	0.601549	1.108041
6	-1.736682	1.192921	0.117933
6	-0.657905	1.996756	0.490812
6	-0.382694	2.242124	1.833925
1	-1.940440	1.040796	-0.936949
1	-2.883290	0.387692	3.204319
1	0.468084	2.863747	2.105456
6	0.248323	2.556874	-0.558250
1	0.844827	3.404756	-0.202157
1	-0.271622	2.859006	-1.477050
8	2.503001	2.010304	-1.905899
6	2.901717	-0.172082	0.364671
6	2.370312	-1.431453	0.674462
6	4.256798	0.011033	0.166939
6	3.237064	-2.523096	0.794592
6	5.105283	-1.086192	0.285363
1	4.632708	1.004131	-0.063500

6	4.599515	-2.343968	0.600459
1	2.828791	-3.499959	1.037877
1	6.172787	-0.952251	0.133805
1	5.271297	-3.191881	0.695614
6	0.963743	-1.602159	0.834648
7	-0.183548	-1.752536	0.938993
1	-0.996629	1.874517	3.862716
8	2.047712	0.927596	0.325426
8	0.828466	0.173322	-1.705973
16	1.457635	1.365617	-1.133966
8	-3.579715	-0.234160	0.890304
6	-3.744125	-1.037629	-0.267298
8	-2.494840	-1.525842	-0.703048
6	-4.413398	-0.311212	-1.403211
8	-4.569769	-2.064434	0.118718
1	-4.211717	-2.459926	0.928796
1	-0.543498	-0.321278	-2.572047
8	-1.405709	-0.739793	-2.837157
1	-1.891646	-1.764332	0.036030
1	-5.387706	0.046436	-1.061315
1	-4.562512	-1.002608	-2.238232
1	-3.823337	0.542947	-1.743812
1	-1.225295	-1.458055	-3.470842
1	-1.854752	-1.117609	-1.980229

[8d'-9']‡

Number of imaginary frequencies : 1
The smallest frequency is : -360.8280 cm(-1)

Electronic energy : =-1599.1336308
Zero-point correction= 0.327424
Thermal correction to Energy= 0.351438
Thermal correction to Enthalpy= 0.352382
Thermal correction to Gibbs Free Energy= 0.274649
Sum of electronic and zero-point Energies= -1598.806207
Sum of electronic and thermal Energies= -1598.782193
Sum of electronic and thermal Enthalpies= -1598.781249
Sum of electronic and thermal Free Energies= -1598.858981

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Cartesian Coordinates

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6	-1.990340	2.920041	1.347125
6	-2.614770	1.680189	1.275023

6	-2.086011	0.714549	0.426531
6	-0.980078	0.969009	-0.369455
6	-0.365614	2.217170	-0.292020
6	-0.864481	3.187144	0.576733
1	-0.591592	0.202918	-1.032876
1	-3.496263	1.459922	1.872854
1	-0.368855	4.153461	0.645337
6	0.872237	2.488615	-1.083881
1	1.110007	3.558156	-1.135990
1	0.851496	2.090941	-2.105416
8	2.268721	1.813712	1.120166
6	2.739480	-0.820689	-0.170610
6	2.051970	-2.042474	-0.115736
6	4.016106	-0.708475	0.356739
6	2.655577	-3.151306	0.490432
6	4.593370	-1.815660	0.969467
1	4.566151	0.225554	0.285599
6	3.920759	-3.032150	1.041014
1	2.115415	-4.093420	0.520845
1	5.591717	-1.721847	1.388358
1	4.387301	-3.888728	1.518199
6	0.756096	-2.168824	-0.691485
7	-0.298739	-2.290423	-1.163121
1	-2.386120	3.680763	2.014474
8	2.089810	0.213369	-0.819032
8	3.523697	2.266007	-1.007200
16	2.335569	1.777523	-0.329665
8	-2.643896	-0.563256	0.398532
6	-3.531849	-1.064186	-0.902121
8	-2.698138	-0.988480	-1.936383
6	-4.676268	-0.115252	-1.002165
8	-3.915812	-2.282161	-0.481366
1	-3.197457	-2.931414	-0.565671
1	-4.416894	-1.989320	2.219324
1	-3.209236	-0.819139	1.297499
8	-3.989082	-1.131806	2.366091
1	-1.936240	-1.603551	-1.828157
1	-3.470033	-1.232761	3.178440
1	-5.269057	-0.136944	-0.083589
1	-5.305060	-0.425343	-1.842288
1	-4.312730	0.898061	-1.190445

[9']

Number of imaginary frequencies : 0

Electronic energy : =-1599.1492526
Zero-point correction= 0.328950
Thermal correction to Energy= 0.354536
Thermal correction to Enthalpy= 0.355480
Thermal correction to Gibbs Free Energy= 0.272974
Sum of electronic and zero-point Energies= -1598.820302
Sum of electronic and thermal Energies= -1598.794717
Sum of electronic and thermal Enthalpies= -1598.793772
Sum of electronic and thermal Free Energies= -1598.876278

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Cartesian Coordinates

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6	-1.966460	3.214754	1.115844
6	-2.568766	1.974656	1.288633
6	-2.036008	0.856145	0.643209
6	-0.935606	0.996023	-0.200744
6	-0.335279	2.241418	-0.361913
6	-0.842400	3.355450	0.307691
1	-0.555545	0.120594	-0.721226
1	-3.444609	1.859927	1.924787
1	-0.365157	4.325656	0.186395
6	0.877203	2.379240	-1.226342
1	1.129852	3.426541	-1.433388
1	0.811721	1.849287	-2.184307
8	2.351523	1.928399	0.987951
6	2.784692	-0.837663	-0.075201
6	2.128794	-2.072857	0.049811
6	4.061358	-0.669870	0.436692
6	2.763433	-3.138313	0.700165
6	4.669931	-1.733751	1.094750
1	4.588388	0.272616	0.318716
6	4.030691	-2.963149	1.229632
1	2.245605	-4.089922	0.781451
1	5.668994	-1.595919	1.499711
1	4.524016	-3.784341	1.740602
6	0.829451	-2.253371	-0.498109
7	-0.228675	-2.419410	-0.945411
1	-2.378022	4.083379	1.624465
8	2.099657	0.137187	-0.770484
8	3.530274	2.149177	-1.218442
16	2.364162	1.744240	-0.451813
8	-2.544725	-0.385116	0.804034
6	-3.592252	-1.521669	-1.139868
8	-2.544075	-1.396521	-1.851223
6	-4.657548	-0.524146	-1.297149
8	-3.828972	-2.528259	-0.373423
1	-3.107621	-3.185794	-0.326733

1	-5.098716	-1.490339	2.108446
1	-3.350628	-0.374993	1.381438
8	-4.902283	-0.544587	2.074081
1	-1.757311	-1.973369	-1.605338
1	-4.924145	-0.264087	2.998498
1	-5.306721	-0.513965	-0.419421
1	-5.251644	-0.795901	-2.178778
1	-4.212934	0.459036	-1.470973

H_2O

Number of imaginary frequencies : 0

Electronic energy : =-76.3979104
Zero-point correction= 0.021513
Thermal correction to Energy= 0.024349
Thermal correction to Enthalpy= 0.025293
Thermal correction to Gibbs Free Energy= 0.003859
Sum of electronic and zero-point Energies= -76.376397
Sum of electronic and thermal Energies= -76.373561
Sum of electronic and thermal Enthalpies= -76.372617
Sum of electronic and thermal Free Energies= -76.394052

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Cartesian Coordinates

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8	0.000000	0.000000	0.119899
1	0.000000	0.754451	-0.479597
1	0.000000	-0.754451	-0.479597

----------End----------