Supplementary Materials:

Understanding the Photo- and Electro-carboxylation of Methyl Benzophenone with Carbon Dioxide

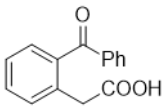
Keyi Tian,[a] Ruonan Chen,[a] Jiafang Xu,[a] Ge Yang,[a] Xintong Xu,[a] and Yanhua Zhang*[a]

[a] Institute of Advanced Synthesis and School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, Jiangsu, P. R. China.
E-mail: tiankeyi@njtech.edu.cn (K. T); rnchen@njtech.edu.cn (R. C); 201761100557@njtech.edu.cn (J. X); yangge05@njtech.edu.cn (G. Y); 201961105031@njtech.edu.cn (X. X).
*Correspondence: ias_yhzhang@njtech.edu.cn (Y. Z)

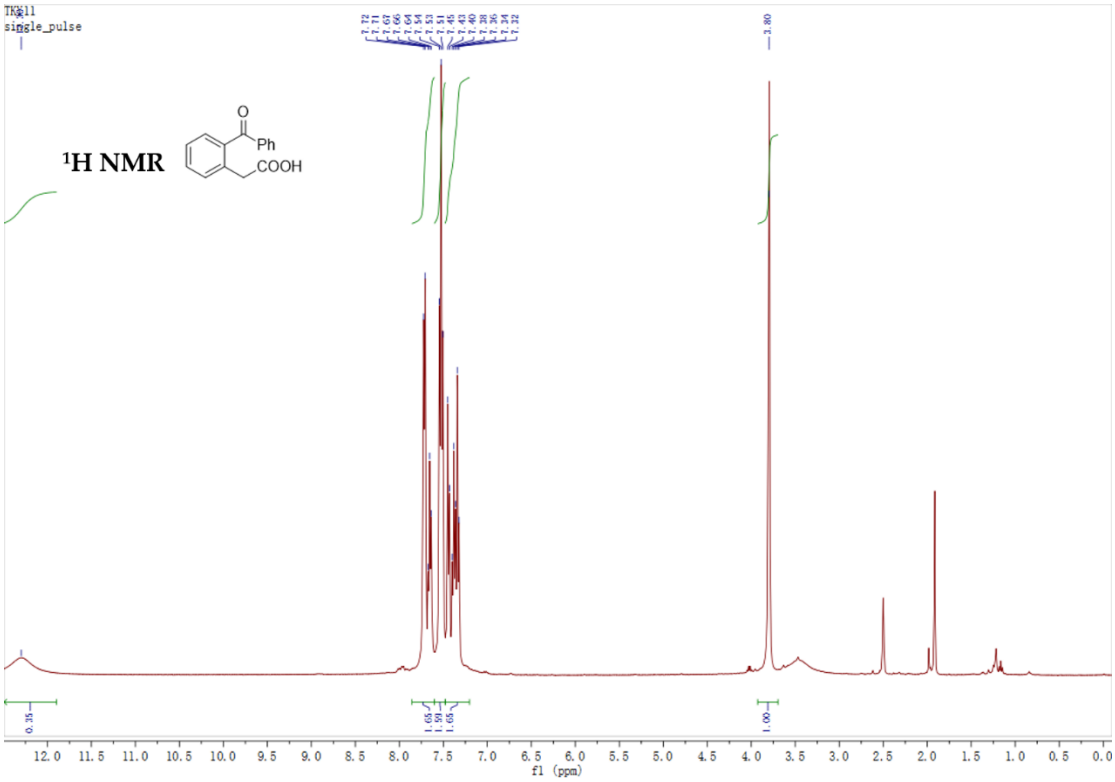
Equipments.

Photoreactions were carried out under a LED lamp (customized by Shanghai Guige, 365 nm) irradiation. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL (100 MHz) or Bruker (400 MHz) in DMSO-d_6. Proton chemical shifts were referenced to the residual proton signal of the solvent at 7.26 ppm ($CHCl_3$) and 2.50 ppm (DMSO-d_6). High-resolution mass spectra were recorded on a Waters (Acquity UPLC/XEVO G2-XS QTOF) spectrometer. IR measurements were performed on a FTIR (Nicolet is10) spectrometer fitted with a Pike Technologies MIRacle Single Reflection ATR adapter. Liquid chromatograph-mass spectra were recorded on a Thermo Scientific Exactive (MSQ PLUS/U3000) spectrometer. Conversion yield is measured by HPLC (ACQUITY Arc, Waters).

Supplementary data.



^{1}H NMR (100 MHz, DMSO-d_6): δ = 12.30 (s, 1H), 7.68 (dd, *J* = 27.3, 7.5 Hz, 3H), 7.53 (t, *J* = 7.8 Hz, 3H), 7.48 – 7.20 (m, 3H), 3.80 (s, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ = 197.94, 172.76, 138.51, 137.77, 135.02, 133.64, 132.55, 131.28, 130.49, 129.85, 128.99, 126.90, 39.94, 38.78, 21.61; **HRMS** (ESI+) *m*/*z***:** calcd. For $C_{15}H_{13}O_3$ $(M+H)^+$ 241.0859, found 241.0851.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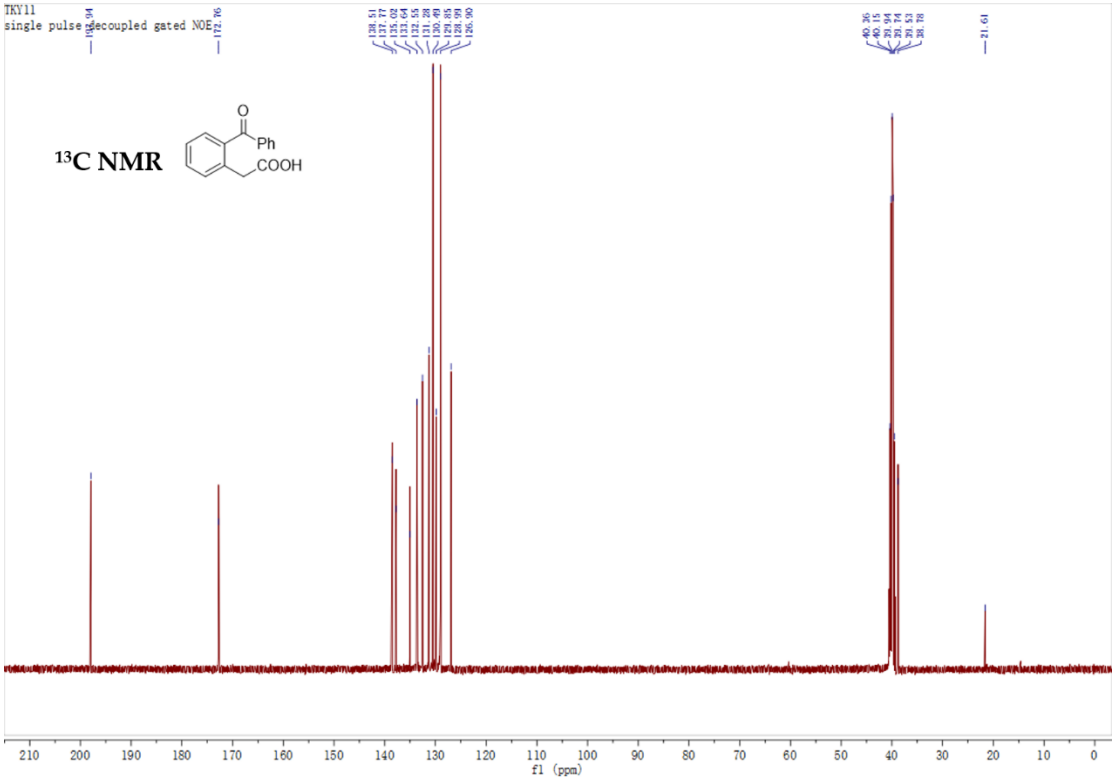
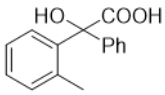
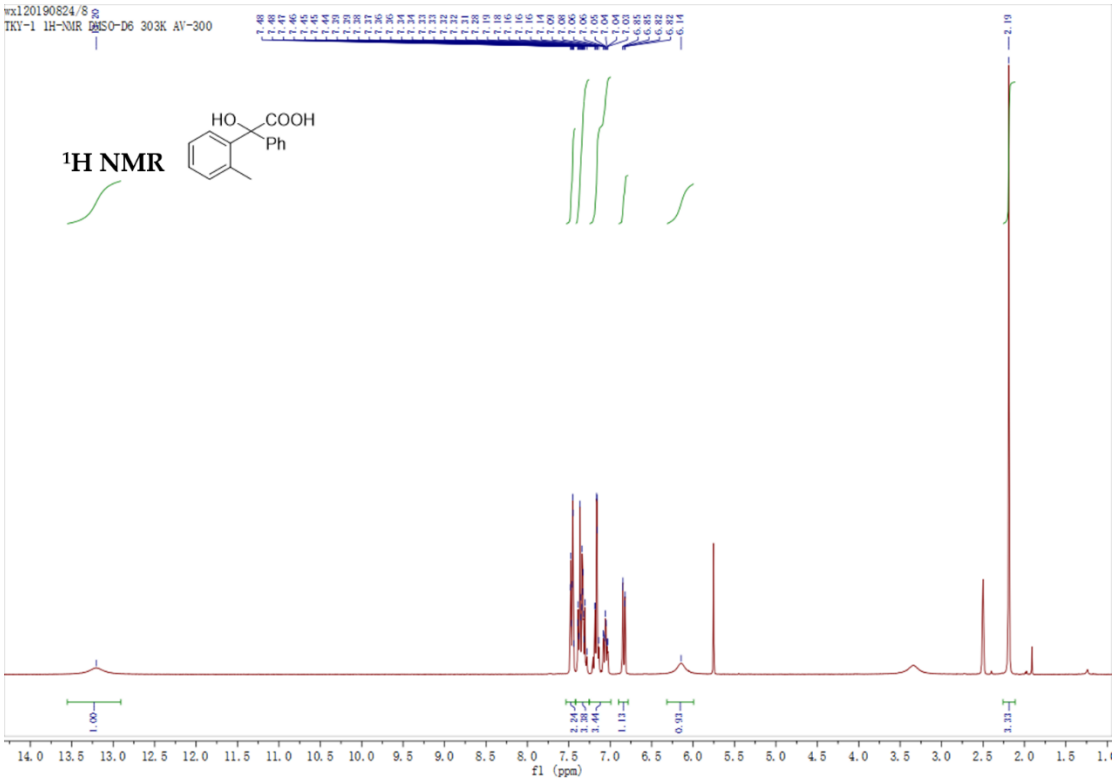
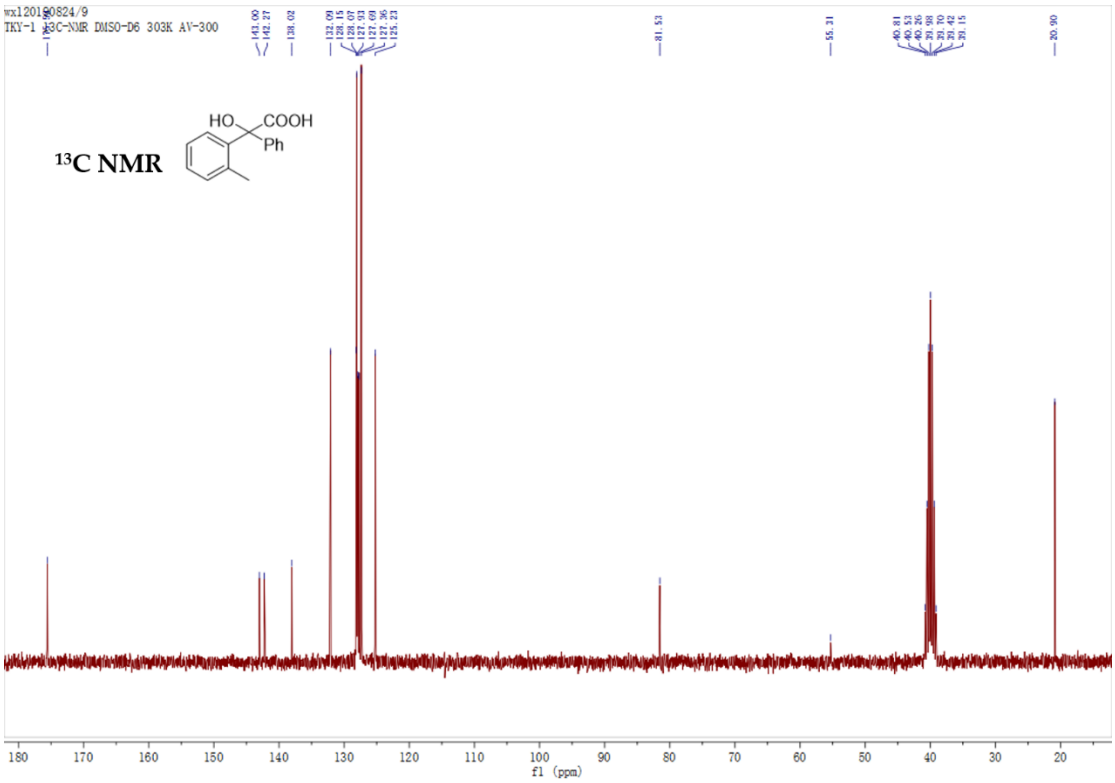
single_pulse
7.72
7.71
7.67
7.66
7.54
7.54
7.53
7.51
7.45
7.43
7.40
7.38
7.35
7.34
7.32
3.80
0.35
1.65
1.59
1.65
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
^{1}H NMR
O
Ph
COOH

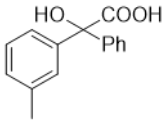

TKY11
single pulse decoupled gated NOE
197.94
172.76
138.51
137.77
133.03
131.64
132.55
131.28
129.49
129.35
126.99
126.90
40.36
40.15
39.94
39.74
39.53
38.78
21.61
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
^{13}C NMR
O
Ph
COOH



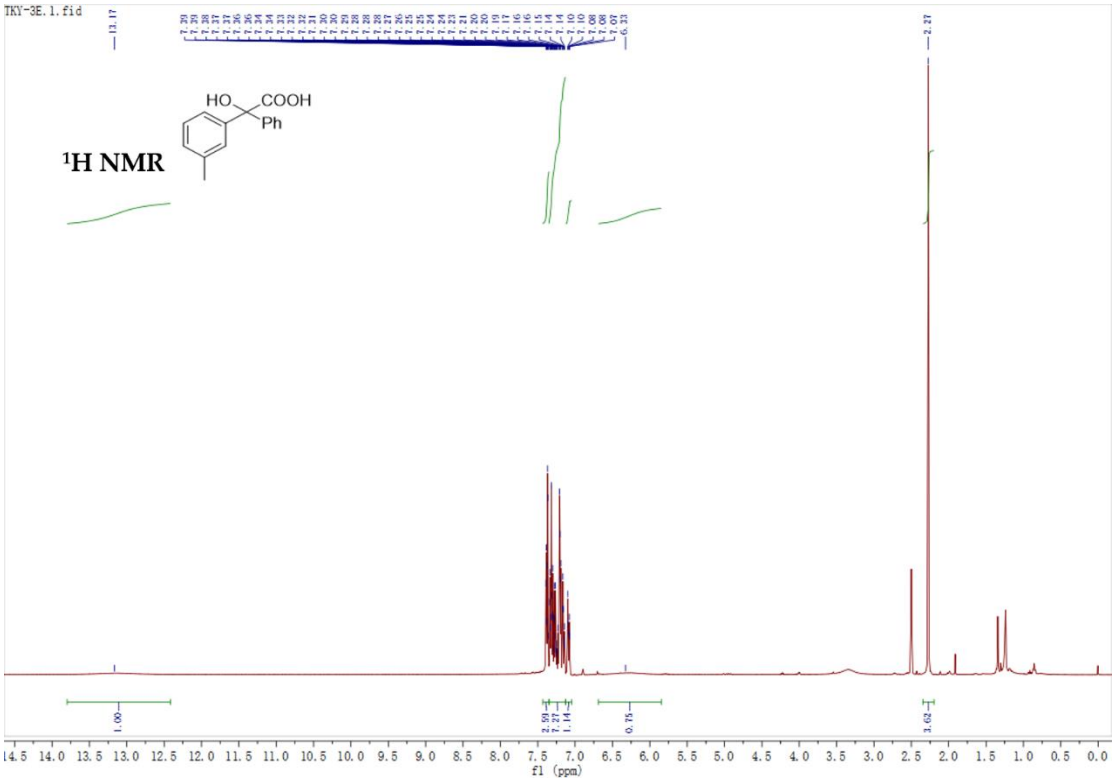
^{1}H NMR (400MHz, DMSO-d_6): δ =13.20 (s, 1H), 7.53 – 7.42 (m, 2H), 7.42 – 7.26 (m, 3H), 7.24 – 7.11 (m, 2H), 7.06 (td, *J* = 7.1, 2.2 Hz, 1H), 6.85 (d, *J* = 1.3 Hz, 1H), 6.14 (s, 1H), 2.19 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ=175.75, 143.10, 142.40, 138.15, 132.21, 128.27, 128.20, 128.06, 127.82, 127.48, 125.35, 81.64, 56.43, 40.05, 21.01; **HRMS**(ESI+) *m*/*z*: calcd. For $C_{15}H_{14}O_3$ $(M+H)^+$ 243.1021, found 243.1011.

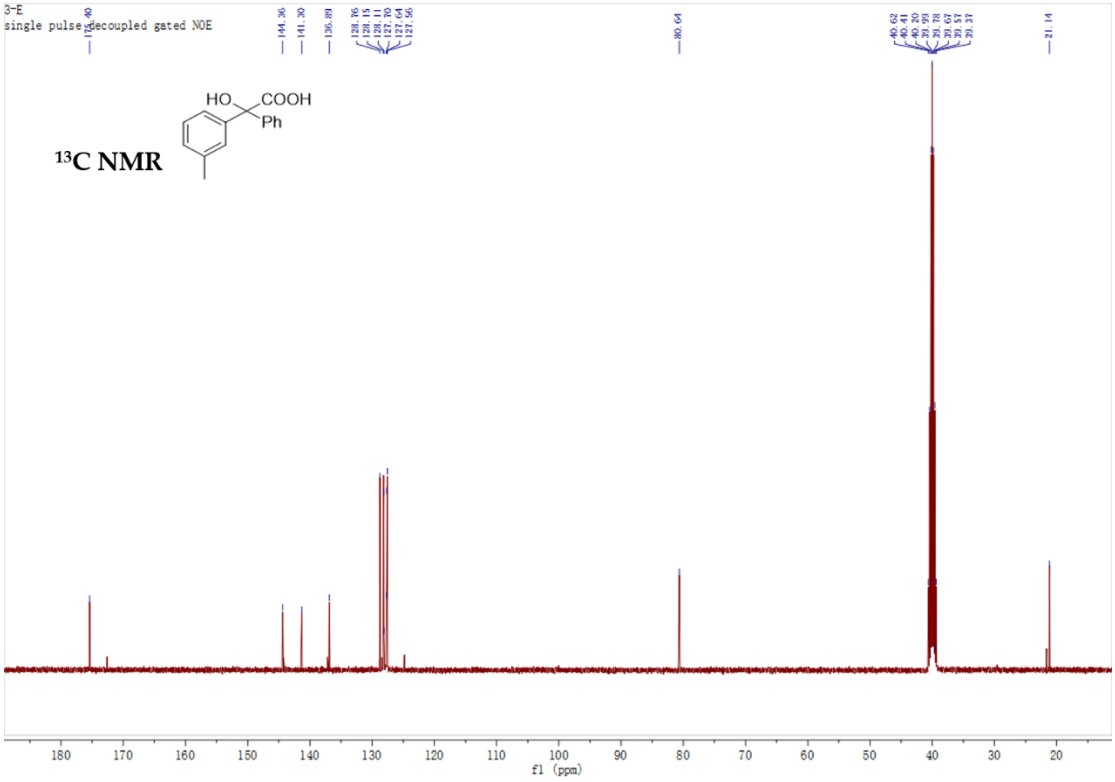


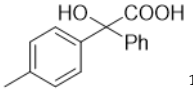




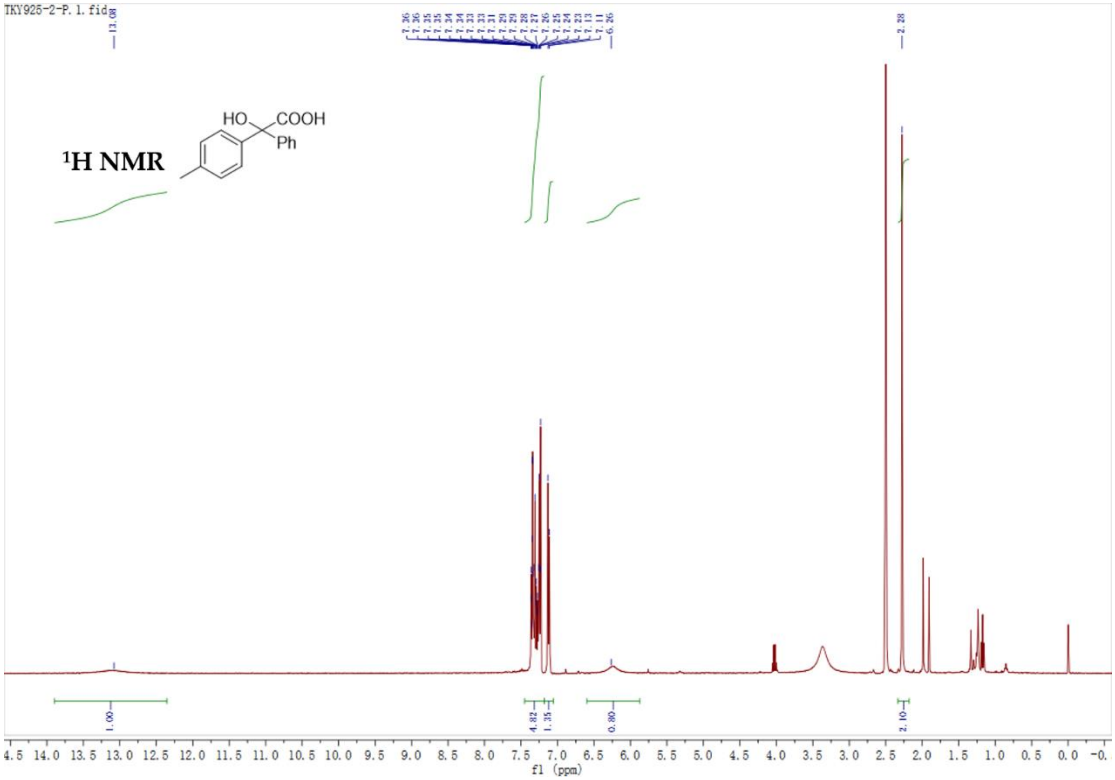
^{1}H NMR (400 MHz, DMSO-d_6): δ = 13.26 (s, 1H), 7.46 – 7.35 (m, 2H), 7.35 – 7.24 (m, 3H), 7.23 – 7.12 (m, 3H), 7.12 – 7.06 (m, 1H), 6.26 (s, 1H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ = 175.40, 175.30, 144.36, 141.30, 136.89, 128.76, 128.15, 128.11, 127.70, 127.64, 127.56, 124.82, 80.64, 39.99, 21.14; **HRMS**(ESI+) *m/z*: calcd. For $C_{15}H_{14}O_3$ $(M+H)^+$ 243.1021, found 243.1017.

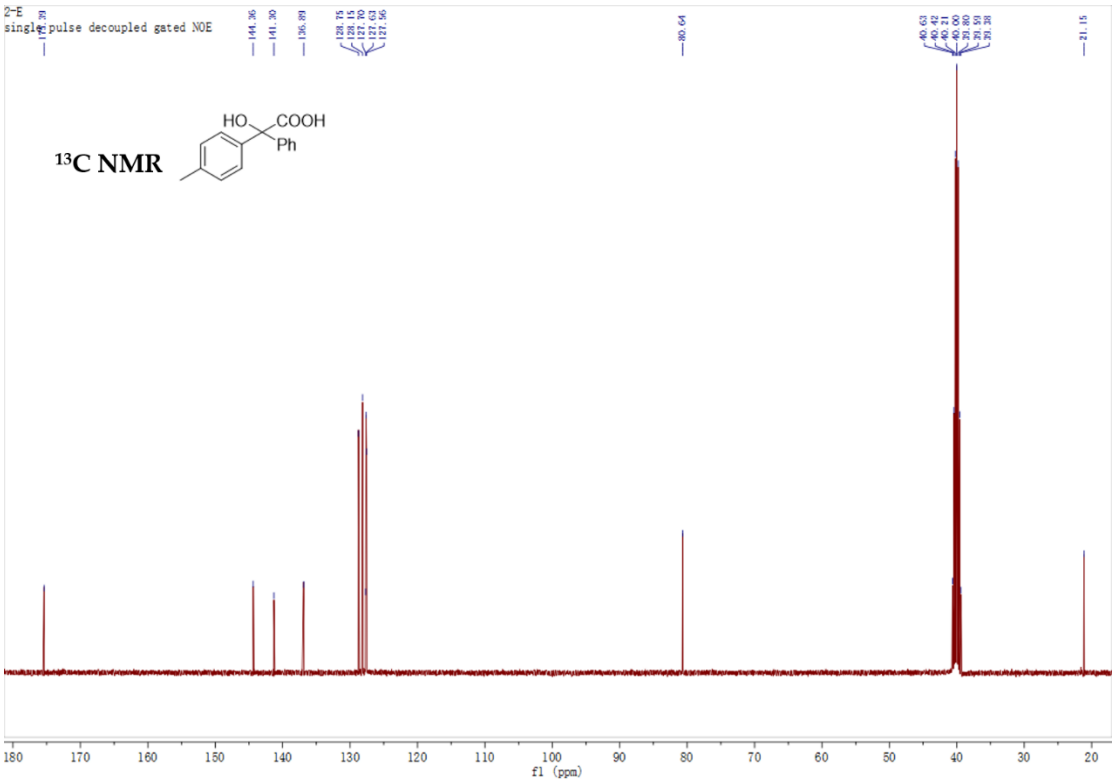


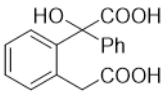




^{1}H NMR (400 MHz, DMSO-d_6): δ = 13.08 (s, 1H), 7.40 – 7.20 (m, 7H), 7.07-7.17 (d, *J* = 7.9 Hz, 2H), 6.22 (s, 1H), 2.28 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ =175.39, 144.36, 141.30, 136.89, 128.75, 128.15, 127.70, 127.63, 127.56, 80.54, 40.00, 21.15; **HRMS**(ESI+) *m*/*z*: calcd. For $C_{15}H_{14}O_3$ $(M+H)^+$ 243.1021, found 243.1023.







LC-MS *m/z*: calcd. For $C_{16}H_{14}O_5$ $(M+Na)^+$ 309.27, found 309.21.

Supplementary figures and tables.

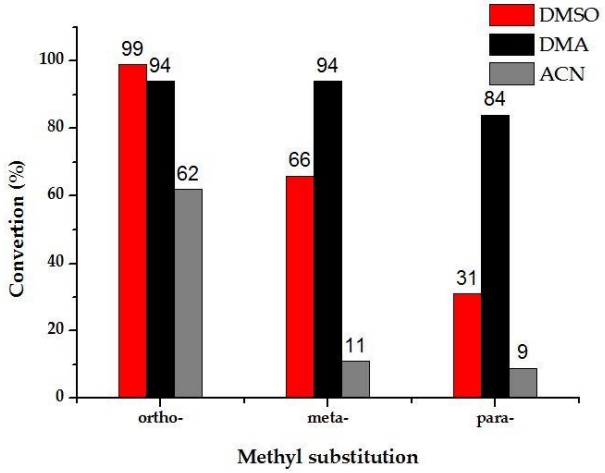


Figure S1. Photocarboxylation of *o-*, *m-* and *p*-methyl benzophenone with CO_2 in different solvent.

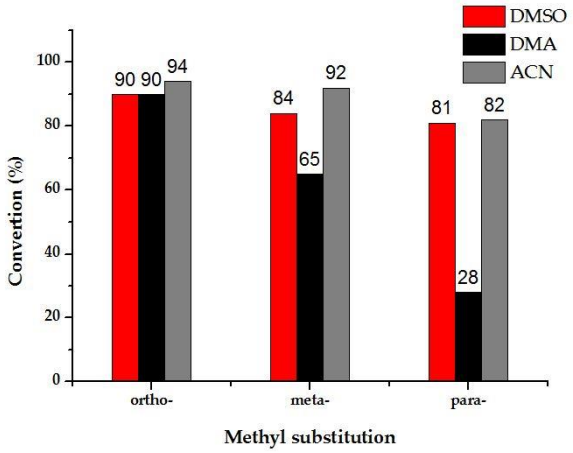


Figure S2. Electrocarboxylation of *o-*, *m-* and *p*-methyl benzophenone with CO_2 in different solvent.

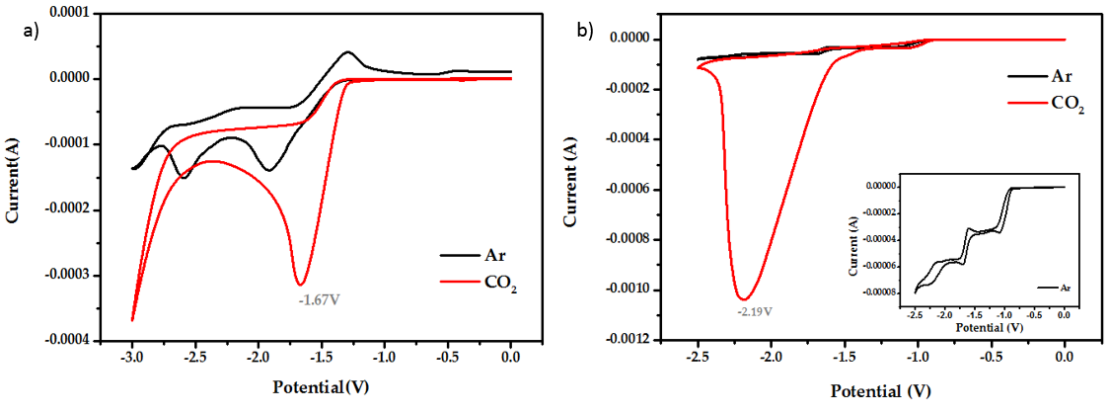


Figure S3. Cyclic voltammogram of a) *o*-methyl benzophenone and b) *o*-acylphenylacetic acid on glassy carbon electrode under argon (black trace) or with CO_2 bubbling (red trace). The reaction solution consists of supporting electrolyte (0.1 M of Bu_4NBr) and substrate (0.08 mM) in 20 mL of **DMSO** by using Ag/AgBr as the reference electrode and Al as the counter electrode.

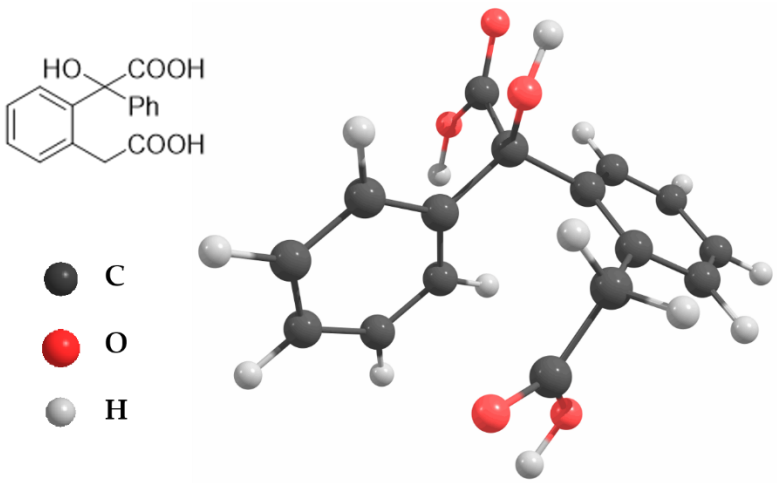
Quantum chemical computational details.

All calculations in this work were performed using Gaussian 09 program package [1]. Full geometry optimizations in DMSO solvent were performed to locate all the stationary points, using the M062X [2] method with the 6-311+G(d) [3] basis, namely M062X/6-311+G(d) at 298.25 K. The self-consistent reaction field (SCRF) method based on the universal solvation model SMD was adopted to evaluate the effect of the solvent [4]. The intrinsic reaction coordinate (IRC) path was traced to check the energy profiles connecting each transition state to two associated minima of the proposed mechanism [5]. The solvation free energies of the proton $\Delta G_{sol}(H^+)$ [6] is defined analogously as followed:

$$\Delta G_{\mathrm{sol}}(\mathrm{H}^+) = G(\mathrm{S}-\mathrm{H})^+_{\mathrm{sol}} - G(\mathrm{S}_{\mathrm{sol}}) - G(\mathrm{H}^+_{\mathrm{gas}})$$

Wherein, S represents the solvent molecule, DMSO in this work; The value of $G(\mathrm{H}^+_{\mathrm{gas}})$ was referenced from the literatures [7,8].

Unless specified, the Gibbs free energies at 298.25 K were used in the discussion.



Structure of 2-(2-(carboxymethyl)-phenyl)-2-hydroxy-2-phenylacetic acid.

Energies optimized at M062X/6-311+G(d) level

	E	H	G
CO_2	-188.565	-188.561557	-188.58582
Im1	-992.745	-992.725734	-992.809
Im2	-992.838	-992.818457	-992.904
Im3	-992.845	-992.825355	-992.896
Ts1	-992.840	-992.821303	-992.889
Im4	-992.848	-992.830033	-992.894
Im5-tri	-992.889	-992.869853	-992.938
Im5	-992.951	-992.933257	-992.996
Im6	-992.955	-992.936065	-992.987
Ts2	-992.955	-992.937251	-992.983
Im7	-992.995	-992.977578	-993.023
Im8	-993.459	-993.0211386	-993.079
Ts3	-993.447	-993.0084776	-993.067
Im9	-993.470	-993.0309856	-993.093
Im10	-993.902	-993.0431033	-993.131

Cartesian coordinates of structures optimized at M062X/6-311+G(d) level

CO_2

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.154894
O	0.000000	0.000000	-1.154894

DMSO

S	-0.000024	0.217595	-0.447148
C	-1.349590	-0.795795	0.189115
H	-2.282360	-0.282599	-0.043025
H	-1.332116	-1.768350	-0.304812
H	-1.233865	-0.905483	1.268373
C	1.349912	-0.795300	0.189132
H	1.332576	-1.767994	-0.304537
H	2.282525	-0.281951	-0.043267
H	1.234336	-0.904749	1.268427
O	-0.000330	1.497023	0.380467

DMSO-H

S	-0.000013	-0.081776	-0.497129
C	1.380664	0.779936	0.231655
H	2.287480	0.250319	-0.056294
H	1.384401	1.787768	-0.187241
H	1.249344	0.805673	1.312787
C	-1.380460	0.780290	0.231670
H	-1.383229	1.788482	-0.186392
H	-2.287540	0.251597	-0.057213
H	-1.249584	0.804887	1.312866
O	-0.000194	-1.438467	0.399831

H	-0.000346	-2.233936	-0.163043

im1

C	3.760213	0.308844	0.593581
C	2.810847	1.026390	-0.125027
C	1.603670	0.441443	-0.509929
C	1.375996	-0.899403	-0.174083
C	2.341043	-1.629798	0.521687
C	3.527850	-1.025350	0.917445
H	4.687116	0.788144	0.889164
H	3.008184	2.057862	-0.400546
H	2.148662	-2.670116	0.763306
H	4.269112	-1.592567	1.469198
C	0.102625	-1.604183	-0.551786
C	-2.377155	-1.347509	-0.681912
C	-3.580938	-0.869829	-0.182695
C	-3.599616	-0.120724	0.994863
C	-2.413403	0.155908	1.667491
C	-1.202600	-0.304358	1.158451
C	-1.181465	-1.060256	-0.016155
H	-2.352131	-1.936687	-1.592042
H	-4.506456	-1.080718	-0.706916
H	-4.542150	0.247848	1.385368
H	-2.428146	0.734018	2.584831
H	-0.278355	-0.086162	1.683161
O	0.127945	-2.600192	-1.244370
C	0.620213	1.238583	-1.335997
H	0.025372	0.608854	-1.998386
H	1.178665	1.922892	-1.985018
C	-0.348561	2.120749	-0.580318
O	-1.413708	2.474352	-1.015723
O	0.123205	2.539056	0.600673
H	-0.541736	3.117857	1.009556

im2

C	3.588475	-1.428159	0.461568
C	3.295777	-0.072234	0.319415
C	2.063981	0.345734	-0.178872
C	1.099209	-0.608519	-0.550037
C	1.397137	-1.963901	-0.384746
C	2.631553	-2.376329	0.113628
H	4.553457	-1.739223	0.847460
H	4.030881	0.671806	0.613400
H	0.653002	-2.706214	-0.660569
H	2.845177	-3.434544	0.224510
C	-0.195301	-0.160579	-1.168140
C	-2.668654	-0.047073	-1.100873
C	-3.881255	-0.263255	-0.468702
C	-3.944565	-0.860820	0.798184
C	-2.738615	-1.226358	1.422287
C	-1.518722	-1.017513	0.805959

C	-1.431995	-0.429631	-0.493531
H	-2.635138	0.418413	-2.079695
H	-4.799704	0.037743	-0.966054
H	-4.897231	-1.026113	1.288902
H	-2.761571	-1.674623	2.411890
H	-0.608917	-1.291953	1.329289
O	-0.133223	0.456964	-2.278855
C	1.731436	1.813533	-0.276388
H	1.529723	2.109009	-1.305920
H	2.566991	2.416944	0.093552
C	0.518258	2.219679	0.529718
O	-0.242111	3.107315	0.233413
O	0.405729	1.540039	1.681940
C	-0.400142	1.836747	2.134427

im3

C	2.784162	-0.160736	2.434206
C	2.720098	0.718014	1.354658
C	1.676236	0.656794	0.433145
C	0.663979	-0.315147	0.585088
C	0.734712	-1.181553	1.684388
C	1.778973	-1.110641	2.600795
H	3.606302	-0.099480	3.139223
H	3.489772	1.474928	1.231591
H	-0.030994	-1.942251	1.805728
H	1.814213	-1.803658	3.435262
C	-0.392794	-0.464886	-0.462757
C	-2.762885	-0.702567	-1.120799
C	-4.118736	-0.701613	-0.838760
C	-4.587570	-0.484259	0.463190
C	-3.646305	-0.253331	1.479118
C	-2.288312	-0.248871	1.212980
C	-1.787380	-0.486187	-0.101455
C	-2.412106	-0.869322	-2.132969
H	-4.829345	-0.871841	-1.643196
H	-5.650014	-0.484535	0.679737
H	-3.986360	-0.065406	2.493730
H	-1.597375	-0.040855	2.022970
O	-0.012180	-0.574232	-1.676132
C	1.607544	1.660620	-0.690587
H	1.609307	1.170381	-1.662466
H	2.470766	2.333586	-0.643077
C	0.388419	2.552094	-0.664417
O	-0.137926	3.025857	-1.639959
O	-0.021509	2.855106	0.578197
H	-0.784331	3.451666	0.509825
C	2.283356	-1.865019	-1.699896
O	2.851676	-0.992893	-2.204782
O	1.817337	-2.805025	-1.213540

im4

C	-2.748428	-2.497514	0.886508
C	-1.691387	-2.527353	-0.015781
C	-0.902104	-1.400756	-0.252131
C	-1.178462	-0.213459	0.453087
C	-2.279729	-0.179494	1.324680
C	-3.053185	-1.308993	1.548831
H	-3.344886	-3.387733	1.054265
H	-1.484491	-3.437580	-0.571019
H	-2.509423	0.748105	1.839467
H	-3.889089	-1.265225	2.238911
C	-0.392276	1.017944	0.292751
C	1.735856	2.263991	0.101779
C	3.109544	2.337478	0.265824
C	3.824545	1.262179	0.801536
C	3.135653	0.110197	1.185882
C	1.761733	0.023611	1.026530
C	1.025385	1.092698	0.462801
H	1.191606	3.101376	-0.319285
H	3.634928	3.240547	-0.028070
H	4.899730	1.326255	0.926515
H	3.674721	-0.724790	1.622422
H	1.240122	-0.864927	1.365389
O	-1.060731	2.179002	0.172541
C	0.126150	-1.443516	-1.356514
H	0.348868	-0.444090	-1.729251
H	-0.295333	-2.000061	-2.202626
C	1.446657	-2.125310	-1.084380
O	2.443810	-1.938950	-1.734122
O	1.396917	-3.028862	-0.095176
H	2.272029	-3.443826	-0.017242
C	-2.099917	2.279782	-0.877467
O	-1.971348	1.480879	-1.800578
O	-2.891022	3.183312	-0.638050

im5

C	1.884414	-3.389253	-0.623292
C	0.714969	-3.042815	0.046831
C	0.301482	-1.719790	0.208464
C	1.067945	-0.653772	-0.364359
C	2.309544	-1.033985	-0.959173
C	2.697428	-2.353324	-1.099027
H	2.177558	-4.427718	-0.729761
H	0.113974	-3.826600	0.503027
H	2.951012	-0.246769	-1.339682
H	3.640269	-2.582000	-1.588242
C	0.736915	0.740620	-0.300061
C	-0.709295	2.747050	-0.185528
C	-1.951941	3.350398	-0.276696
C	-3.103107	2.624537	-0.616272
C	-2.945317	1.262036	-0.906126
C	-1.712659	0.639288	-0.821300

C	-0.531328	1.339162	-0.405852
H	0.156119	3.342679	0.083835
H	-2.031752	4.416103	-0.075044
H	-4.072464	3.105459	-0.682753
H	-3.805338	0.676227	-1.223721
H	-1.625103	-0.395362	-1.132139
O	1.823511	1.618439	-0.400987
O	-0.828556	-1.463600	1.177079
H	-0.859191	-0.418161	1.487106
H	-0.637160	-2.039020	2.091364
C	-2.242801	-1.849596	0.809076
O	-3.202288	-1.609079	1.501109
O	-2.353397	-2.564859	-0.321443
H	-3.290979	-2.784661	-0.447157
C	2.635624	1.851924	0.737283
O	2.244063	1.412565	1.827302
O	3.656004	2.503750	0.459881

im6

C	3.083531	2.361164	1.396134
C	2.158458	2.568623	0.377342
C	1.375383	1.542564	-0.152739
C	1.474990	0.215459	0.379255
C	2.500355	0.015733	1.354789
C	3.264993	1.051278	1.857416
H	3.677616	3.181222	1.783804
H	2.064417	3.561090	-0.058690
H	2.656015	-0.990863	1.727503
H	4.011053	0.842738	2.619484
C	0.714517	-0.918653	-0.054753
C	-1.216112	-2.163225	-0.980137
C	-2.550826	-2.235606	-1.338068
C	-3.420813	-1.147702	-1.170003
C	-2.895912	0.015631	-0.592623
C	-1.564643	0.106852	-0.223639
C	-0.640825	-0.967174	-0.434218
H	-0.574901	-3.026575	-1.122963
H	-2.930030	-3.162875	-1.761582
H	-4.463963	-1.211109	-1.458849
H	-3.548471	0.865329	-0.404154
H	-1.225585	0.992462	0.301087
O	1.305964	-2.166030	0.179182
C	0.619077	1.844390	-1.424704
H	0.321539	0.930596	-1.941091
H	1.295502	2.365900	-2.113121
C	-0.598928	2.739226	-1.387777
O	-1.274930	2.985852	-2.357421
O	-0.834761	3.320289	-0.200976
H	-1.615904	3.889360	-0.295651
C	2.354713	-2.614356	-0.660937
O	2.610069	-1.952430	-1.676675

O	2.878443	-3.658809	-0.237784
C	-2.952009	-0.495653	2.498049
O	-3.281844	0.610114	2.573210
O	-2.640814	-1.607557	2.478452

im7

C	-1.702240	3.454403	-0.664448
C	-0.759015	3.062828	0.273648
C	-0.390327	1.721036	0.428571
C	-0.996391	0.735464	-0.372192
C	-1.959326	1.145170	-1.300430
C	-2.307611	2.481023	-1.455631
H	-1.969039	4.500910	-0.769494
H	-0.289254	3.809405	0.907745
H	-2.440390	0.392487	-1.907048
H	-3.061406	2.760115	-2.185239
C	-0.643134	-0.749124	-0.170782
C	1.520594	-1.943994	0.423728
C	2.870720	-2.213116	0.216823
C	3.584438	-1.524637	-0.761477
C	2.931843	-0.567125	-1.532995
C	1.581005	-0.300961	-1.326841
C	0.859652	-0.980491	-0.342427
H	0.966951	-2.476589	1.187446
H	3.367760	-2.962776	0.824632
H	4.637812	-1.731467	-0.919868
H	3.475052	-0.022345	-2.298978
H	1.083662	0.445725	-1.936174
O	-0.953544	-1.139413	1.155777
C	0.642529	1.414313	1.492067
H	0.533700	0.412493	1.900896
H	0.504723	2.112179	2.326949
C	2.091428	1.583421	1.096274
O	3.011998	1.059111	1.671291
O	2.284217	2.451295	0.091939
H	3.238021	2.500135	-0.082836
C	-2.313394	-1.241039	1.537554
O	-3.159258	-0.776019	0.764008
O	-2.445288	-1.764876	2.655514
C	-1.252494	-1.771456	-1.230566
O	-1.240287	-1.394673	-2.422175
O	-1.572495	-2.882244	-0.780515

im8

C	-1.938372	3.254456	-0.869758
C	-0.978380	2.992551	0.097261
C	-0.508354	1.697373	0.333099
C	-1.031755	0.630686	-0.420320
C	-2.015814	0.902600	-1.374182
C	-2.460826	2.198165	-1.607833
H	-2.283697	4.269389	-1.034925

H	-0.575949	3.808052	0.690589
H	-2.454521	0.091930	-1.936147
H	-3.226185	2.374318	-2.356142
C	-0.560445	-0.798838	-0.122356
C	1.701712	-1.741498	0.589109
C	3.068735	-1.911907	0.392589
C	3.708243	-1.288393	-0.675135
C	2.972225	-0.494311	-1.550053
C	1.604699	-0.325313	-1.357957
C	0.962790	-0.940944	-0.282912
H	1.212751	-2.219579	1.429627
H	3.636331	-2.529365	1.080667
H	4.774966	-1.418804	-0.823540
H	3.462251	-0.001123	-2.382906
H	1.036908	0.296258	-2.042490
O	-0.880434	-1.162059	1.207946
C	0.538319	1.528101	1.412293
H	0.490954	0.555936	1.897422
H	0.358666	2.274245	2.195011
C	1.973569	1.755677	0.992816
O	2.924838	1.349394	1.609869
O	2.103678	2.531762	-0.091987
H	3.051086	2.632794	-0.280013
C	-2.290589	-1.080364	1.588696
O	-3.083127	-1.158614	0.648389
O	-2.427359	-0.982733	2.802315
C	-1.083731	-1.886375	-1.096347
O	-1.210879	-1.745616	-2.282279
O	-1.216132	-3.091889	-0.538843
H	-1.140414	-3.006014	0.425505

im9

C	-2.740535	1.637960	-1.855055
C	-1.879644	2.062481	-0.849346
C	-0.972191	1.188377	-0.247404
C	-0.945796	-0.161109	-0.648158
C	-1.814354	-0.574561	-1.660938
C	-2.700885	0.310980	-2.266512
H	-3.436245	2.336847	-2.307295
H	-1.905408	3.097495	-0.520576
H	-1.801887	-1.608396	-1.984657
H	-3.365662	-0.042220	-3.047802
C	-0.062550	-1.166106	0.100987
C	2.238275	-1.047145	1.150886
C	3.602830	-0.776975	1.090241
C	4.165111	-0.259713	-0.073655
C	3.350813	-0.019177	-1.177787
C	1.987782	-0.292632	-1.116452
C	1.415804	-0.805448	0.049529
H	1.801754	-1.439887	2.061961
H	4.227094	-0.968206	1.957344

H	5.227270	-0.042988	-0.119178
H	3.776427	0.386804	-2.090068
H	1.362254	-0.099747	-1.981269
O	-0.515171	-1.212819	1.447850
C	-0.069970	1.741775	0.832440
H	0.169167	1.002122	1.593685
H	-0.589762	2.558215	1.346148
C	1.233326	2.351890	0.367916
O	2.184896	2.527505	1.085625
O	1.213109	2.768297	-0.906320
H	2.081390	3.151867	-1.111417
C	-2.945576	0.082393	1.947932
O	-3.527497	-0.690595	1.316318
O	-2.430749	0.873242	2.615942
C	-0.201541	-2.631451	-0.492892
O	0.228231	-2.828283	-1.636167
O	-0.737707	-3.443192	0.296648
H	-0.832671	-2.134369	1.533563

dicarboxylated product

C	3.450341	-1.654037	-0.606739
C	2.353578	-2.081836	0.133784
C	1.333143	-1.206230	0.502512
C	1.430858	0.146058	0.122892
C	2.539280	0.569043	-0.612422
C	3.544130	-0.321029	-0.980968
H	4.228227	-2.358135	-0.880663
H	2.284537	-3.121670	0.438156
H	2.647825	1.606932	-0.909497
H	4.394910	0.033945	-1.551667
C	0.341180	1.137658	0.559546
C	-2.182474	1.116344	0.743514
C	-3.442679	0.836901	0.228764
C	-3.575229	0.217496	-1.012683
C	-2.439666	-0.124029	-1.737435
C	-1.174042	0.144598	-1.220097
C	-1.038988	0.764547	0.023895
H	-2.080197	1.598497	1.708106
H	-4.325604	1.105053	0.798888
H	-4.560763	0.001861	-1.410745
H	-2.531751	-0.611035	-2.702151
H	-0.294762	-0.153562	-1.784412
O	0.278751	1.211192	1.967444
C	0.179115	-1.758119	1.309428
H	-0.253043	-1.021357	1.982038
H	0.552575	-2.573607	1.939571
C	-0.960459	-2.369339	0.524077
O	-2.085172	-2.469330	0.941854
O	-0.588130	-2.868260	-0.662454
H	-1.371974	-3.250992	-1.090086
C	0.700827	2.563022	0.058371

O	0.410737	2.880577	-1.199507
O	1.244330	3.351945	0.781440
H	0.964343	1.829306	2.260513
H	-0.091936	2.179478	-1.646897

ts1

C	-2.436760	2.677843	-0.877389
C	-1.336135	2.621919	-0.031234
C	-0.635768	1.433476	0.192147
C	-1.051553	0.253199	-0.462907
C	-2.198469	0.318206	-1.280029
C	-2.876463	1.507125	-1.497678
H	-2.958828	3.615794	-1.032404
H	-1.020888	3.518999	0.494650
H	-2.538085	-0.595478	-1.756922
H	-3.745442	1.524579	-2.147742
C	-0.436317	-1.083996	-0.283889
C	1.551869	-2.539304	-0.020938
C	2.913990	-2.770192	-0.121631
C	3.778894	-1.779258	-0.602125
C	3.237575	-0.552030	-0.999134
C	1.876781	-0.308595	-0.900385
C	0.988409	-1.287002	-0.383737
H	0.890894	-3.313105	0.352272
H	3.314231	-3.733800	0.180156
H	4.844569	-1.964437	-0.677545
H	3.887535	0.220869	-1.399495
H	1.481451	0.634540	-1.262050
O	-1.223312	-2.099122	-0.157098
C	0.444909	1.438118	1.247324
H	0.687776	0.430557	1.585572
H	0.070274	1.971550	2.129413
C	1.758162	2.120313	0.937729
O	2.732980	2.036685	1.642227
O	1.735918	2.896813	-0.154902
H	2.608025	3.315008	-0.247461
C	-2.904080	-1.856378	0.974958
O	-2.527533	-1.154584	1.837214
O	-3.664523	-2.528010	0.386942

ts2

C	-2.934305	2.836207	0.290000
C	-3.162053	1.473242	0.471141
C	-2.156338	0.514014	0.341901
C	-0.828965	0.919044	0.002229
C	-0.629450	2.309497	-0.181124
C	-1.643638	3.245518	-0.037432
H	-3.741182	3.552265	0.401981
H	-4.161146	1.139444	0.740218
H	0.346195	2.651216	-0.498568
H	-1.426743	4.297198	-0.201684

C	0.282134	0.003017	-0.179219
C	2.506987	-0.905871	0.411848
C	3.762682	-0.799798	0.989052
C	4.165352	0.359652	1.661450
C	3.240345	1.403998	1.754324
C	1.980395	1.316638	1.179789
C	1.557272	0.163151	0.449349
H	2.229309	-1.814741	-0.105920
H	4.446142	-1.642267	0.915613
H	5.150146	0.439644	2.108363
H	3.501352	2.307066	2.300438
H	1.301610	2.148427	1.318908
O	-0.033602	-1.346301	-0.405336
C	-2.563660	-0.918718	0.605973
H	-2.525378	-1.542512	-0.288569
H	-3.609742	-0.931281	0.932367
C	-1.822861	-1.674888	1.679290
O	-1.939615	-2.860916	1.871605
O	-1.089987	-0.898630	2.488876
H	-0.672781	-1.469080	3.153863
C	-0.597851	-1.744696	-1.637956
O	-0.991711	-0.852756	-2.405837
O	-0.654083	-2.978393	-1.757754
C	1.275889	0.484868	-2.414879
O	0.924186	1.580357	-2.636665
O	1.856139	-0.523940	-2.541319

ts3

C	-2.456320	2.460334	-1.490248
C	-1.549620	2.564406	-0.441627
C	-0.820861	1.460950	0.005577
C	-1.019828	0.208417	-0.605117
C	-1.935678	0.116105	-1.655586
C	-2.646372	1.226737	-2.101936
H	-3.011099	3.332462	-1.819685
H	-1.398488	3.524089	0.044408
H	-2.110401	-0.838033	-2.136982
H	-3.354543	1.120544	-2.916927
C	-0.300608	-1.026217	-0.029216
C	2.042006	-1.405966	0.854639
C	3.428336	-1.336003	0.751783
C	4.019002	-0.741318	-0.360455
C	3.212812	-0.224145	-1.371414
C	1.826154	-0.302474	-1.270314
C	1.228978	-0.887511	-0.152992
H	1.572385	-1.849001	1.725229
H	4.049440	-1.738468	1.545670
H	5.099569	-0.678659	-0.437798
H	3.663653	0.244648	-2.240292
H	1.206845	0.106442	-2.062060
O	-0.688287	-1.275099	1.274199

C	0.149149	1.658747	1.147009
H	0.256211	0.753290	1.741957
H	-0.238510	2.433124	1.818861
C	1.534921	2.130364	0.769499
O	2.495966	2.033932	1.490501
O	1.597897	2.750537	-0.417907
H	2.519796	3.015445	-0.568921
C	-2.508194	-0.523291	1.901006
O	-3.260667	-1.067615	1.184141
O	-2.160114	0.163885	2.783518
C	-0.631977	-2.322211	-0.851304
O	-0.421955	-2.497483	-2.028859
O	-1.131208	-3.238950	-0.050425
H	-1.139307	-2.721076	0.829357

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