Electronic Supplementary Information for

Solvent-Free Aerobic Photocatalytic Oxidation of Alcohols to Aldehydes over ZnO/C_3N_4

Xulu Jiang, [a] Weitao Wang, [*,a] Huan Wang, [a] Zhen-Hong He, [a] Yang Yang, [a] Kuan Wang, [a] Zhao-Tie Liu [*,a, b] and Buxing Han [*,c]

[a] *Shaanxi Key Laboratory of Chemical Additives for Industry, College of Chemistry and Chemical Engineering, Shaanxi University of Science & Technology, Xi'an 710021, China.*

[b] *School of Chemistry & Chemical Engineering, Shaanxi Normal University, Xi'an 710119, China.*

[c] *Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Colloid and Interface and Thermodynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.*

**E-mails: wangweitao@sust.edu.cn (W. Wang), ztliu@snnu.edu.cn (Z.-T. Liu), hanbx@iccas.ac.cn (B. Han)*

1. TABLES

Table S1 The textural properties of catalysts

Catalysts	BET surface area (m^2/g)	BJH adsorption average pore diameter (nm)	BJH pore cumulative volume ($\times 10^3$ cm^3/g)
ZnO-C	45	1.01	8.0
ZnO-A	11	1.0	2.6
ZnO/C_3N_4-500	36	1.2	7.8
ZnO/C_3N_4-600	41	1.2	8.6
ZnO/C_3N_4-700	12	0.51	1.0
ZnO/C_3N_4-800	10	0.36	0.6

Table S2 The effects of the ZnO loading on the catalytic performance

Entry	Catalyst	Catalyst loading (mg)	Time (h)	Conversion (%)	Fr [a] ($\mu mol \cdot g^{-1} \cdot h^{-1}$)
1	ZnO/C_3N_4-600-2.6%	100	12	68.7	11450
2	ZnO/C_3N_4-600-5.5%	100	12	74.6	12433
3	ZnO/C_3N_4-600-7.8%	100	12	73.1	12183
4	ZnO/C_3N_4-600-10.4%	100	12	73.3	12216

Reaction conditions: catalyst 100 mg, benzyl alcohol 20 mmol, 25 °C, 0.1 MPa O_2, light source (λ=400-405 nm) stirred speed 1500 rpm. [a] Formation rate (Fr) = $\mu mol_{BAD} \cdot g_{catalyst}^{-1} \cdot h_{reaction\ time}^{-1}$.

Table S3 Photocatalytic oxidation of benzyl alcohol to benzaldehyde over different catalysts.

Catalysts	Benzyl alcohol (mmol)	Solvent	Oxidant	Catalyst loading (mg)	Light source	Tem. (°C)	Time (h)	Conv. (%)	Sel. (%)	Fr (×μmol·g⁻¹·h⁻¹)	Ref.
1%Pd/$H_2Ti_3O_7$	96.2	-	0.1 MPa O_2	100	Halogen lamp (150 W)	90	6	89	69	98318	[1]
Ir/TiO_2-p	300	-	0.1 MPa O_2	300	Hg lamp (315 – 420 nm)	80	6	11	78	17203	[2]
Pd/TiO_2 (B)	96.2	-	0.1 MPa O_2	100	Halogen lamp (150 W)	90	4	82	69.7	2016	[3]
Cu/Nb_2O_5	96.2	-	0.1 MPa O_2	100	Hg lamp (500 W)	RT	24	36	99	14286	[4]
Pt-TiO_2	0.05	-	0.5 mL/min O_2	50	λ= 366 nm	RT	1	71	62	440	[5]
50% CAO/CdS	0.57	Benzotrifluoride	0.1 MPa O_2	100	λ > 420 nm	80	4	52.1	99	735	[6]
mp-CN	0.1	Acetonitrile	0.1 MPa O_2	20	λ > 420 nm	RT	8	70	99	438	[7]
$CsPbCl_3/W_{18}O_{49}$	1	Hexane	0.1 MPa O_2	10	Xe lamp (150 W)	RT	7	40	99	5714	[8]
0.5 mol% Zr_6-Cu/Fe-1 MOF	0.05	Dimethylsulfoxide	0.1 MPa O_2	10	350−700 nm (13.9 W)	RT	48	80	98	83	[9]
CdS/NiAl-LDH	0.2	H_2O	0.1 MPa Air	1	λ > 400 nm	RT	3	99	99	22000	[10]
$W_{18}O_{49}$/HU-CNS	0.1	H_2O	0.1 MPa O_2	20	Xe lamp (150 W)	RT	1	39.8	99	1990	[11]
TiO_2/Ti_3C- 550	0.02	Hexane	0.1 MPa O_2	30	UV–vis light irradiation	15	5	97	98	13	[12]
CNNA (0.9)	1	Acetonitrile	0.1 MPa O_2	20	Xe lamp (300 W)	RT	9	68.3	100	3794	[13]
CdS-CD	1	H_2O	0.1 MPa Air	1 μM	LED λ=450 nm	RT	180	77.1	98	0.5	[14]
La/$NiWO_4$	0.51	Ethanol	Tert-butyl hydroperoxide	4.5	Bule LED light (3 W)	RT	12	90	99	833	[15]
thioxanthene-9-one	0.2	Dimethylsulfoxide	0.1 MPa Air	8.5	Bule household lamps irradiation (2 × 80 W)	RT	14	82	99	1378	[16]
AgI/$BiVO_4$	1	H_2O	0.1 MPa O_2	15	White LED (16 W)	RT	12	48	99	2667	[17]
mpg-CN	0.8	H_2O	0.8 MPa O_2	50	λ>420 nm	60	3	10	99	533	[18]
$BiVO_4$/g-C_3N_4	0.35	Acetonitrile	0.1 MPa O_2	20	Hg Lamp (250 W)	25	16	68.1	65.5	687	[19]
ZnS-Ni_xS_y	0.5	H_2O	0.1 MP O_2	50	λ > 200 nm	RT	3	42.1	90.5	2943	[20]
ZnO/C_3N_4-600	20	-	0.1 MPa O_2	100	10 W, λ=400-405 nm	RT	20	88.3	>99	8883	This work
ZnO/C_3N_4-600 [a]	20	-	0.1 MPa O_2	100	10 W, λ=400-405 nm	RT	12	99.8	>99	16633	This work

[a] 1 mmol EDTA-2Na.

Table S4 The amount of generated water and benzaldehyde

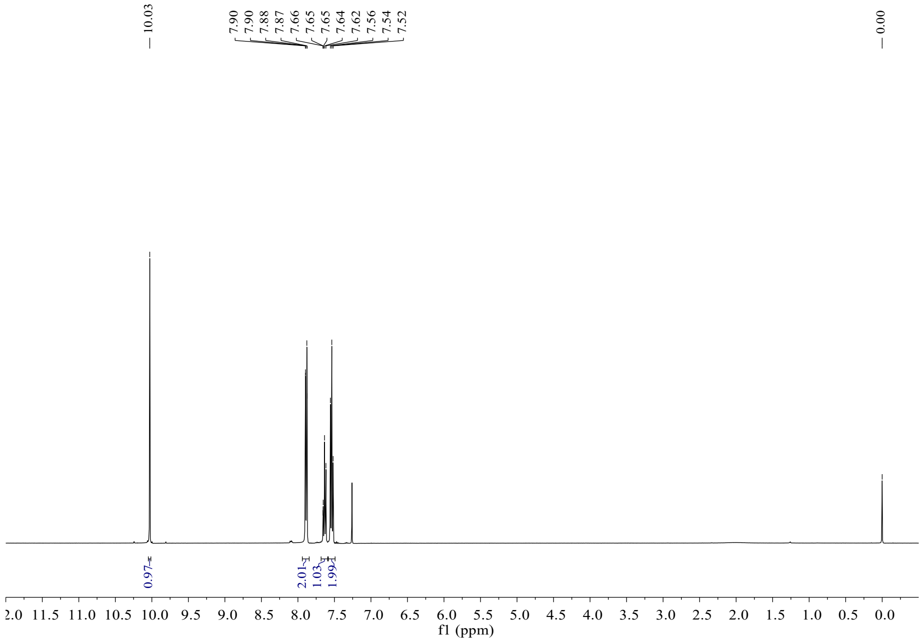
Benzyl alcohol	Conversion (%)	Generated water (mmol)	Water/Benzaldehyde (mmol/mmol)
20.027 mmol	98.9	19.389	0.968/1

Reaction conditions: benzyl alcohol 20.167 g (20.027 mmol), ZnO/C_3N_4-600 100 mg, blue light (10 W, λ=400-405 nm), 1500 rpm, room temperature, 12 h, 2 mmol phenol as hole scavenger.

After the reaction, the catalyst is removed by centrifugation. In the process of centrifugation, dichloromethane is used to wash the catalyst several times, and the washing solution is collected. 2.0227 g of anhydrous sodium sulfate was added in the obtained solution. After it was stirred for 5 minutes, the solution was transferred to the 50 mL volumetric flask and set the volume. The concentration of benzyl alcohol and benzaldehyde can be determined by the HPLC to calculate the amount of the yield benzaldehyde and the conversion of benzyl alcohol. Solid sodium sulfate was weighed to determine the generated water.

2. FIGURES

Figure S1 The MS of benzaldehyde product detected by GC-MS.



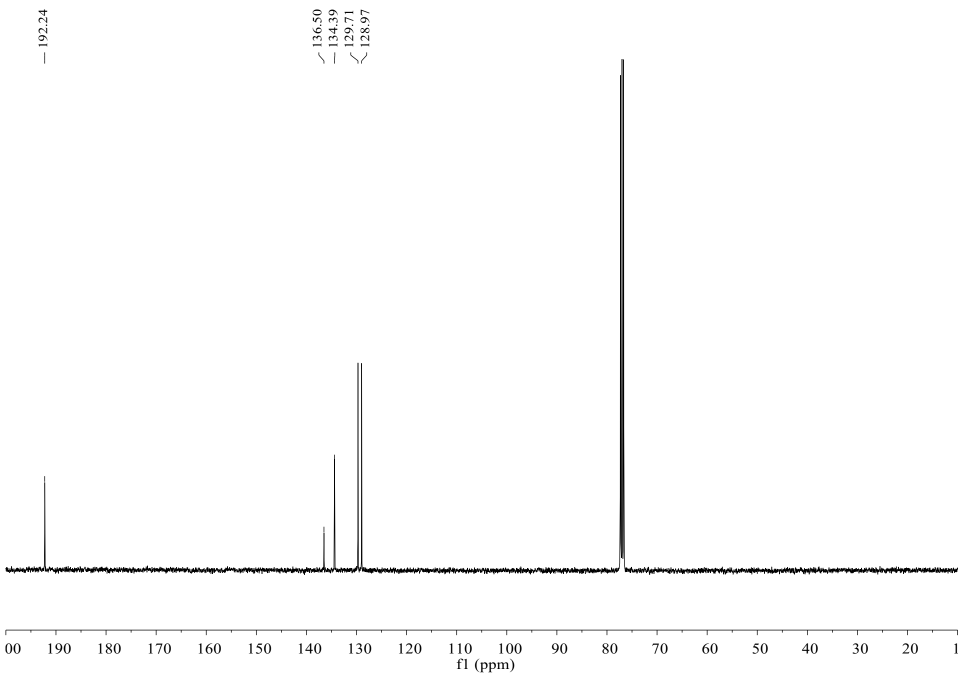


Figure S2 NMR spectra of benzaldehyde

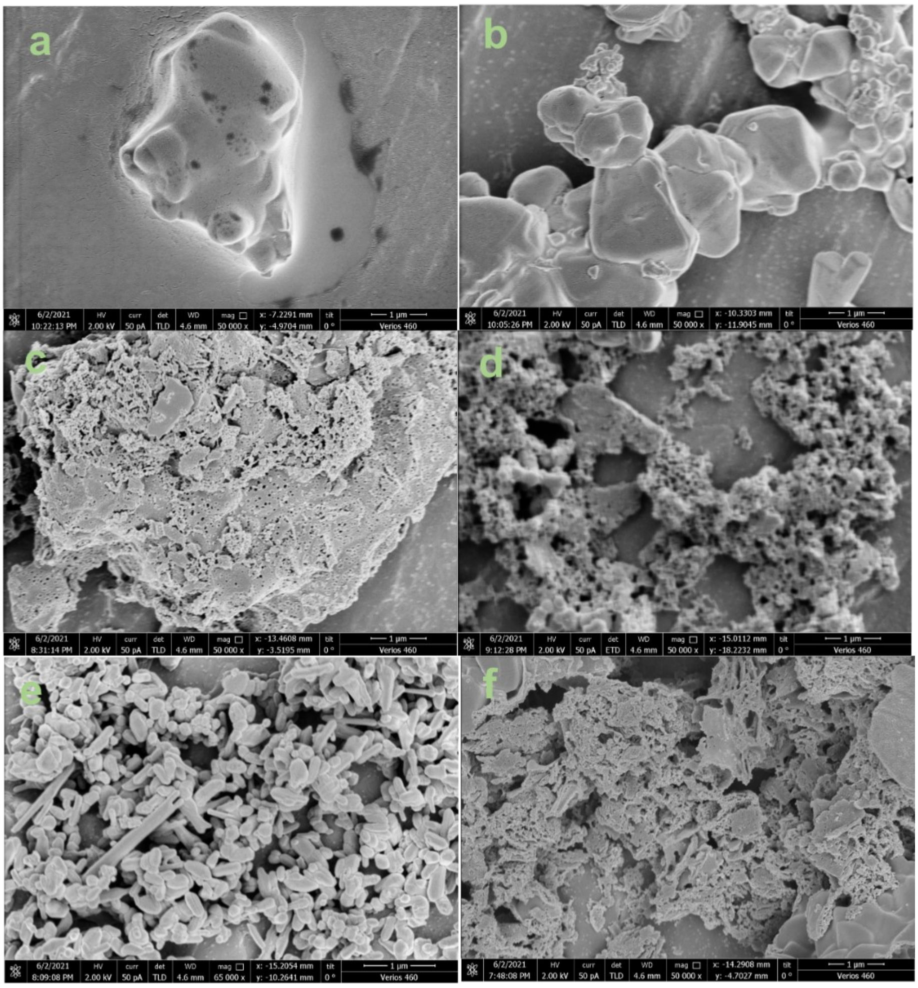


Figure S3 SEM images of (a) ZnO/C_3N_4-800, (b) ZnO/C_3N_4-700, (c) ZnO/C_3N_4-600, (d) ZnO/C_3N_4-500, (e) ZnO-C, (f) ZnO-A.

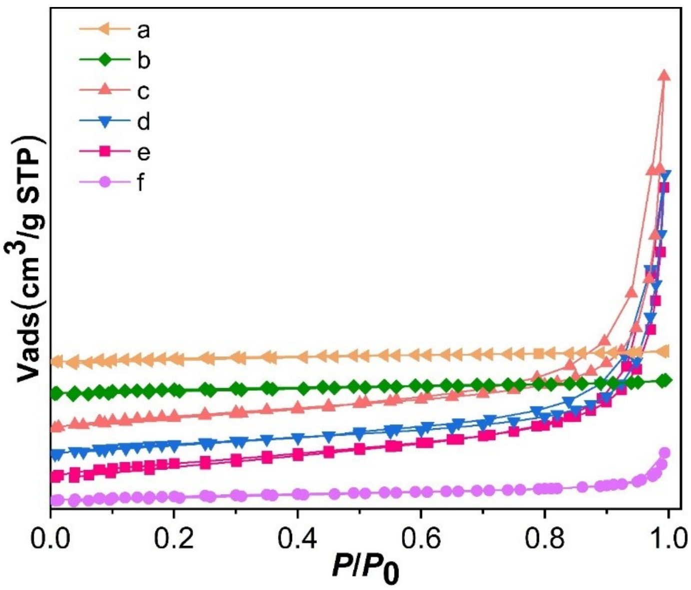


Figure S4 The N_2 adsorption/desorption isotherms of the (a) ZnO/C_3N_4-800, (b) ZnO/C_3N_4-700, (c) ZnO/C_3N_4-600, (d) ZnO/C_3N_4-500, (e) ZnO-C, (f) ZnO-A.

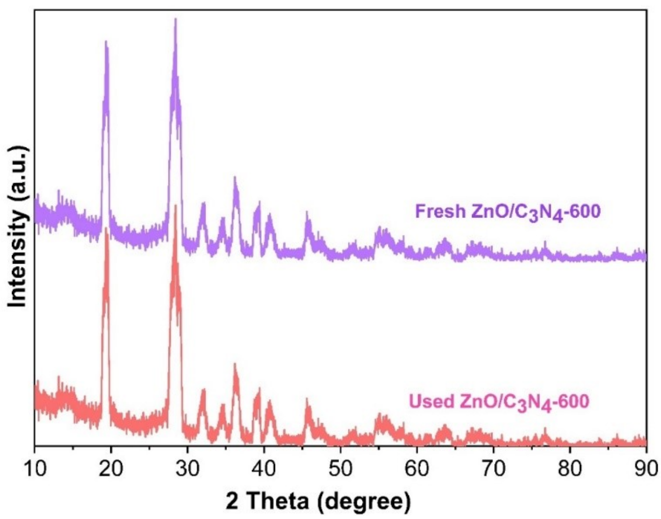


Figure S5 XRD patterns of fresh and used ZnO/C_3N_4-600

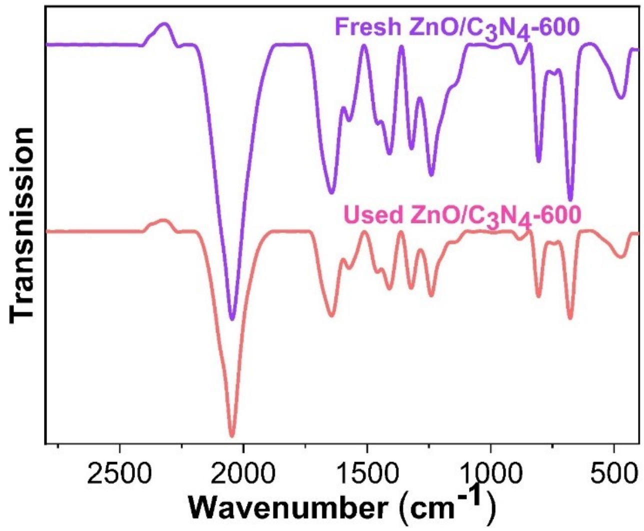


Figure S6 FT-IR spectra of fresh and used ZnO/C_3N_4-600

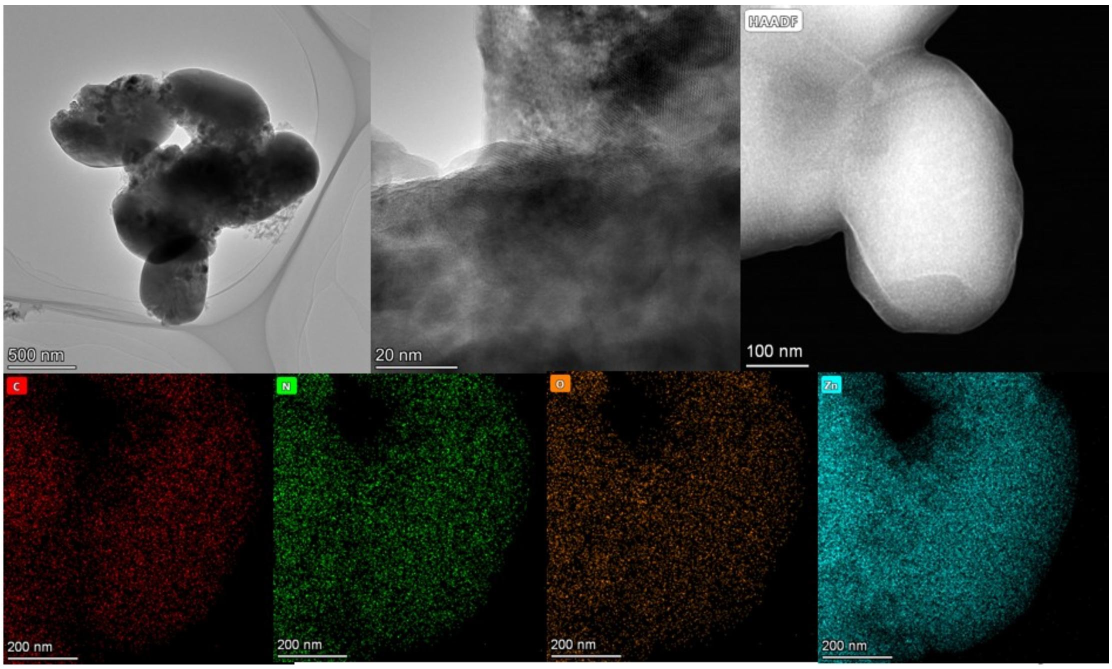


Figure S7 TEM images and the EDX mapping images of used ZnO/C_3N_4-600 catalyst.

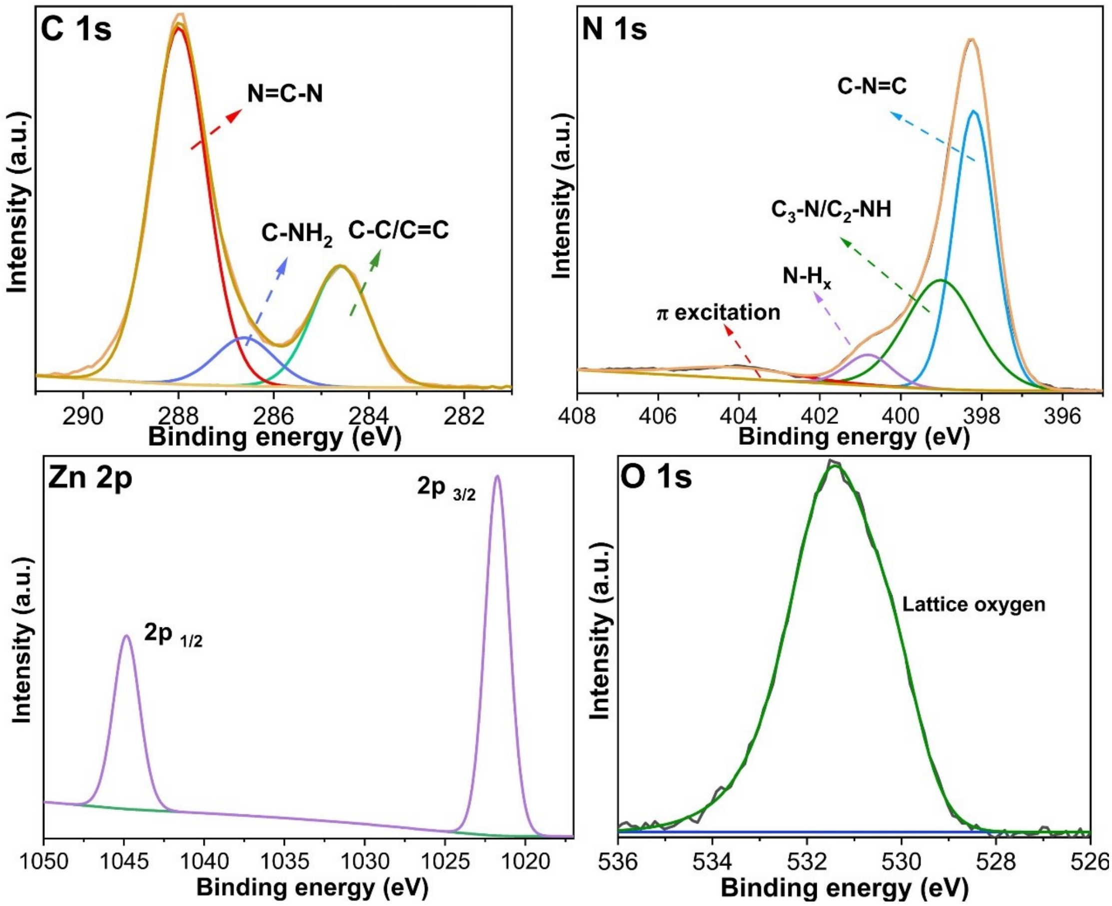


Figure S8 XPS spectra of used ZnO/C_3N_4-600 catalyst.

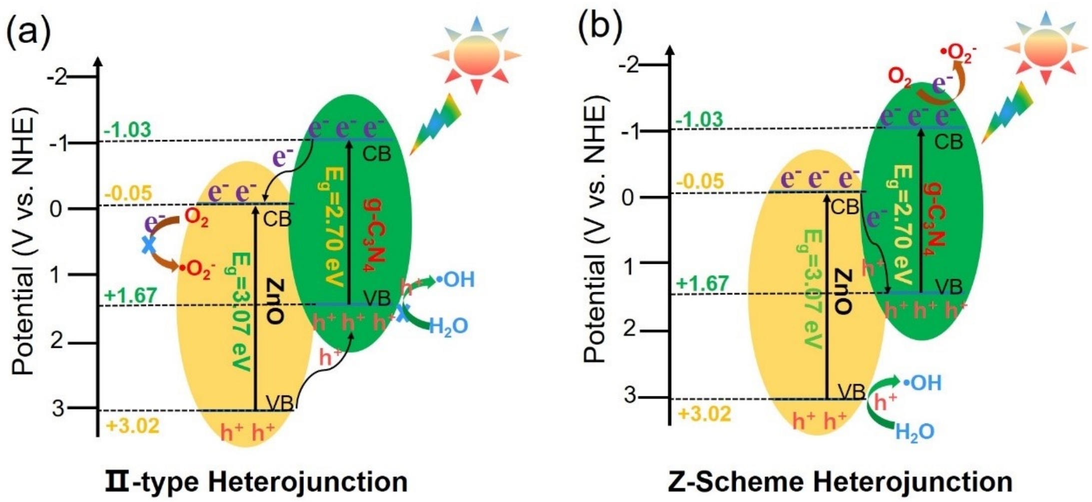


Figure S9. Scheme of the heterojunction type of ZnO/C_3N_4 photocatalysts.

References

[1] M. Du, G. Zeng, J. Huang, D. Sun, Q. Li, G. Wang, X. Li, *ACS Sustainable Chemistry Engineering*, 2019, **7(10)**, 9717-9726.

[2] W. Feng, G. Wu, L. Li, N. Guan, S, *Green Chemistry*, 2011, **13(11)**, 3265-3272.

[3] M. Du, G. Zeng, C. Ye, H. Jin, J. Huang, D. Sun, Q. Li, B. Chen, X. Li, *Molecular. Catalysis*, 2020, **483**, 110771.

[4] S. Furukawa, A. Tamura, T. Shishido, K. Teramura, T. Tanaka, *Applied Catalysis B: Environmental*, 2011, **110**, 216-220.

[5] K. Imamura, H. Tsukahara, K. Hamamichi, N. Seto, K. Hashimoto, H. Kominami, *Applied Catalysis A: General*, 2013, **450**, 28-33.

[6] S. Meng, S. Chang, S. Chen, *ACS Applied Materials Interfaces*, 2020, **12(2)**, 2531-2538.

[7] B. Zhang, T.J. Zhao, H.H. Wang, *ACS Applied Materials Interfaces*, 2019, **11(38)**, 34922-34929.

[8] R. Cheng, J.A. Steele, M.B.J. Roeffaers, J. Hofkens, E. Debroye, *ACS Applied. Energy Materials*, 2021, **4(4)**, 3460-3468.

[9] X. Feng, Y. Pi, Y. Song, Z. Xu, Z. Li, W. Lin, *ACS Catalysis*, 2021, **11(3)**, 1024-1032.

[10] L. Jiao, D. Zhang, Z. Hao, F. Yu, X.-J. Lv, *ACS Catalysis*, 2021, **11(14)**, 8727-8735.

[11] C. Xiao, L. Zhang, H. Hao, W. Wang, *ACS Sustainable Chemistry Engineering*, 2019, **7(7)**, 7268-7276.

[12] X. Bao, H. Li, Z. Wang, F. Tong, M. Liu, Z. Zheng, P. Wang, H. Cheng, Y. Liu, Y. Dai, Y. Fan, Z. Li, B. Huang, *Applied Catalysis B: Environmental*, 2021, **286**, 119885.

[13] J. Ding, W. Xu, H. Wan, D. Yuan, C. Chen, L. Wang, G. Guan, W. L. Dai, N, *Applied Catalysis B: Environm ental*, 2018, **221**, 626-634.

[14] J. Wang, Y. X. Feng, M. Zhang, C. Zhang, M. Li, S. J. Li, W. Zhang, T. B. Lu, *CCS Chemistry*, 2020, **2(3)**, 81-88.

[15] R. Abinaya, K. Mani Rahulan, S. Srinath, A. Rahman, P. Divya, K.K. Balasubramaniam, R. Sridhar, B. Baskar, *Green Chemistry*, 2021, **23(16)**, 5990-6007.

[16] N.F. Nikitas, D.I. Tzaras, I. Triandafillidi, C.G. Kokotos, *Green Chemistry*, 2020, **22(2)**,471-477.

[17] L.-Y. Jiang, J. J. Ming, L. Y. Wang, Y. Y. Jiang, L. H. Ren, Z. C. Wang, W. C. Cheng, *Green Chemistry*, 2020, **22(4)**, 1156-1163

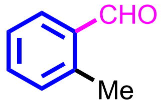
[18] B. Long, Z. Ding, X. Wang, *ChemSusChem*, 2013, **6(11)**, 2074-8.

[19] S. Samanta, S. Khilari, D. Pradhan, R. Srivastava, *ACS Sustainable Chemistry Engineering*, 2017, **5(3)**, 2562-2577.

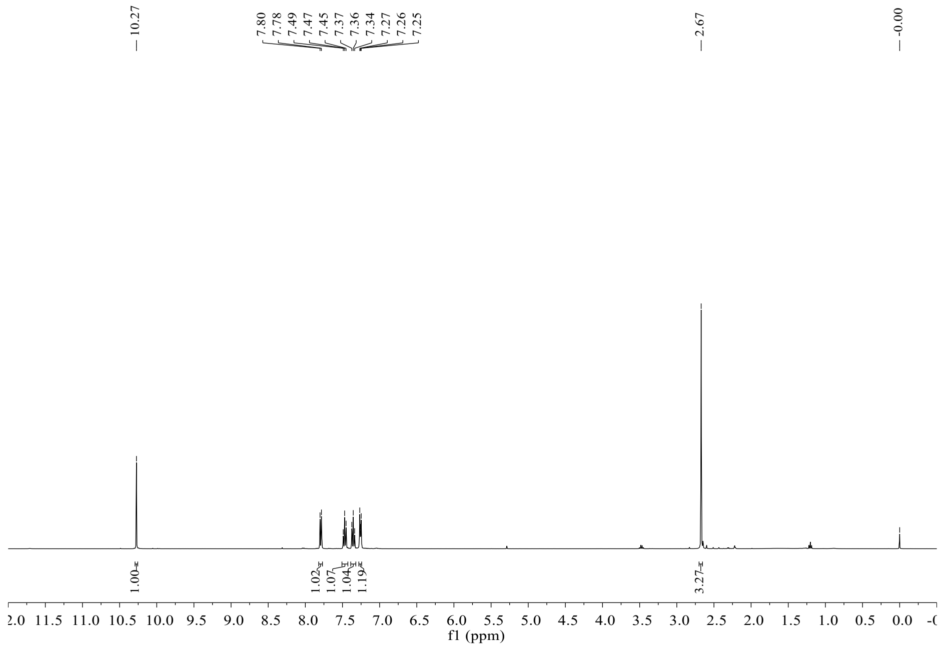
[20] H. Hao, L. Zhang, W. Wang, S. Qiao, X. Liu, *ACS Sustainable Chemistry Engineering*, 2019, **7(12)**, 10501-1 0508.

3. NMR DATA

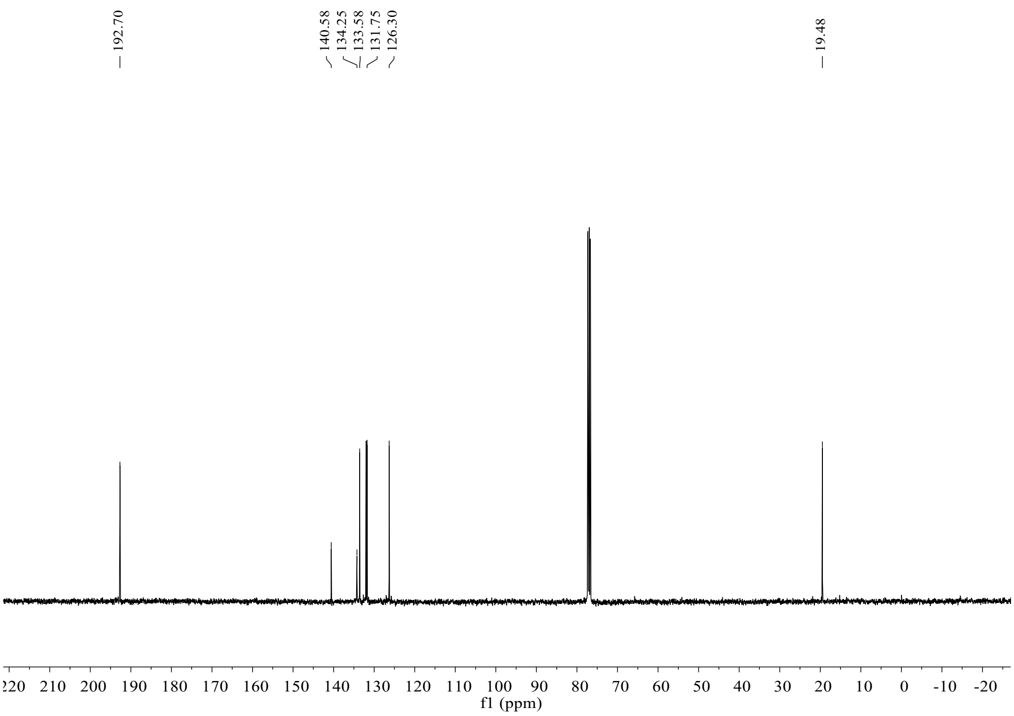
2-Methylbenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.27 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.28-7.24 (m, 1H), 2.67 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 192.70, 140.58, 134.25, 133.58, 131.75, 126.30, 19.48.

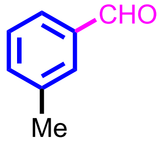


^{1}H NMR spectrogram of 2-methylbenzaldehyde

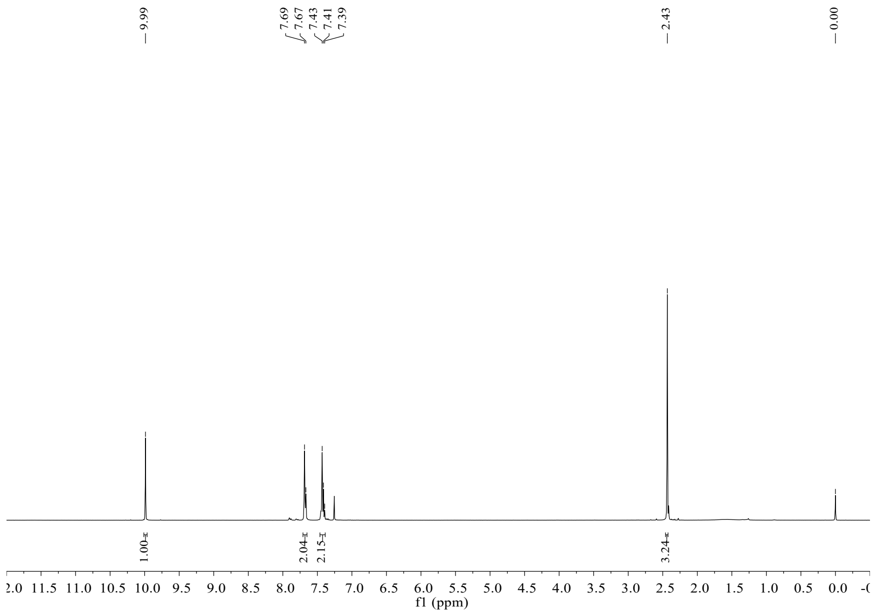


^{13}C NMR spectrogram of 2-methylbenzaldehyde

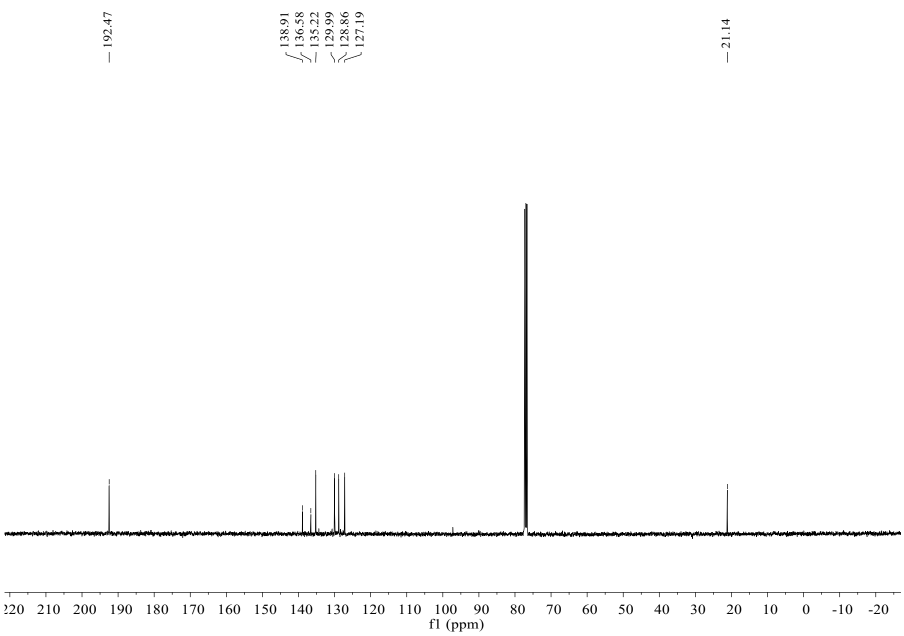
3-Methylbenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.99 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 2.43 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 192.47, 138.91, 136.58, 135.22, 129.99, 128.86, 127.19, 21.14.

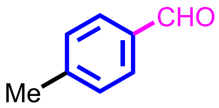


^{1}H NMR spectrogram of 3-methylbenzaldehyde

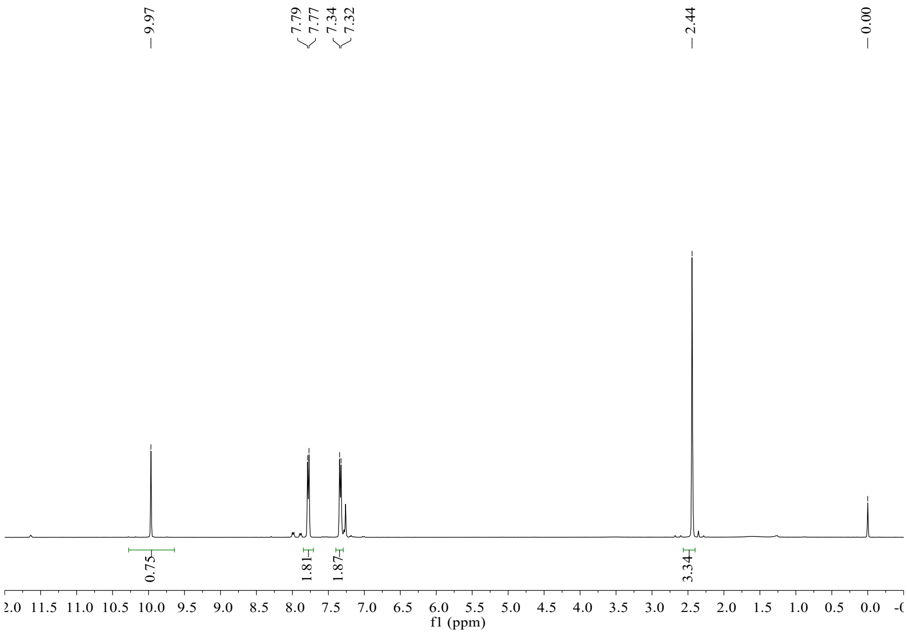


^{13}C NMR spectrogram of 3-methylbenzaldehyde

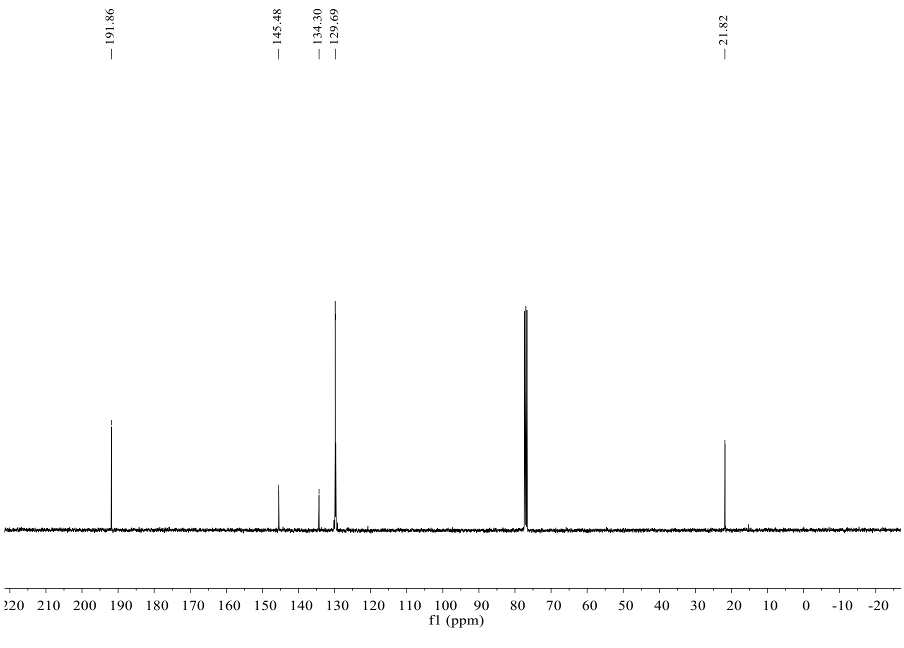
4-Methylbenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.97 (s, 1H), 7.85 – 7.72 (m, 2H), 7.39 – 7.29 (m, 2H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 191.86, 145.48, 134.30, 129.69, 21.82.

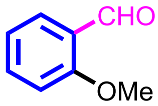


^{1}H NMR spectrogram of 4-methylbenzaldehyde

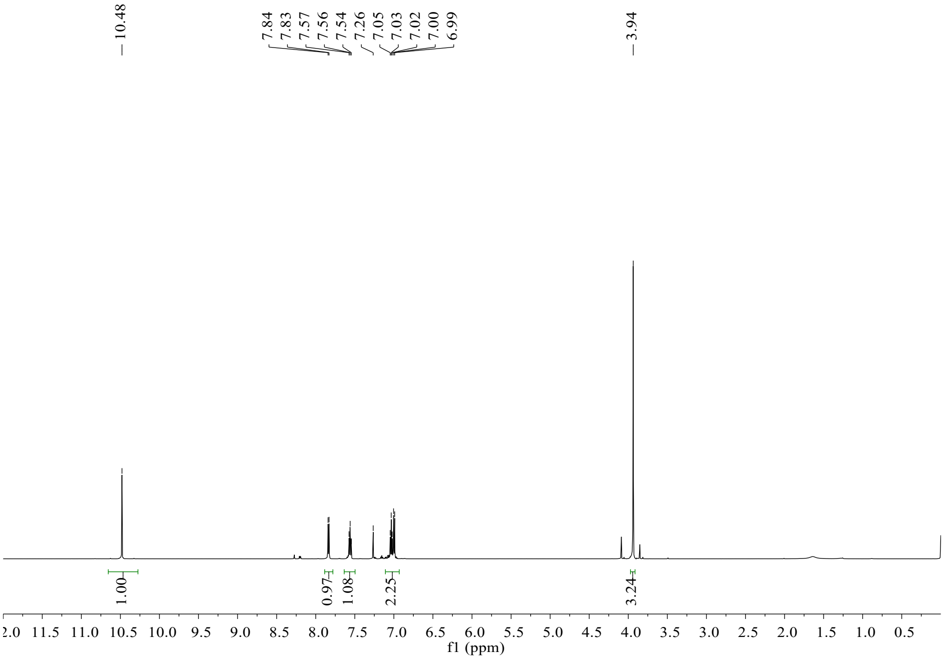


^{13}C NMR spectrogram of 4-methylbenzaldehyde

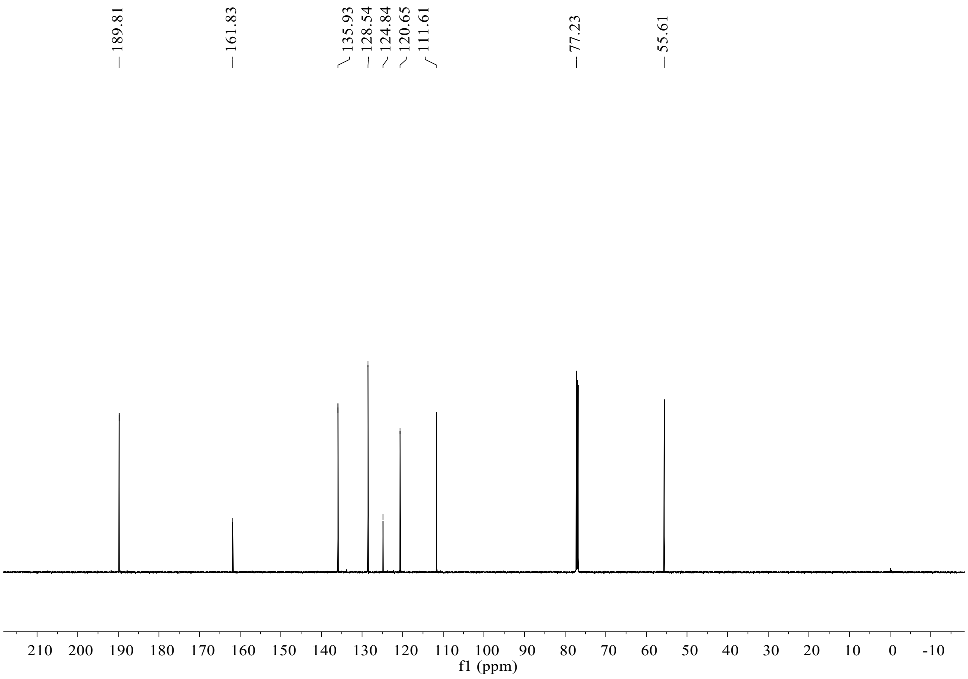
2-Methoxybenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.48 (s, 1H), 7.83 (d, J = 7.7 Hz, 1H), 7.56 (s, 1H), 7.11 – 6.88 (m, 2H), 3.93 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 189.81, 161.83, 135.93, 128.54, 124.84, 120.65, 111.61, 55.61.

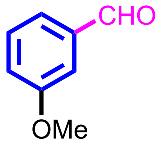


^{1}H NMR spectrogram of 2-methoxybenzaldehyde

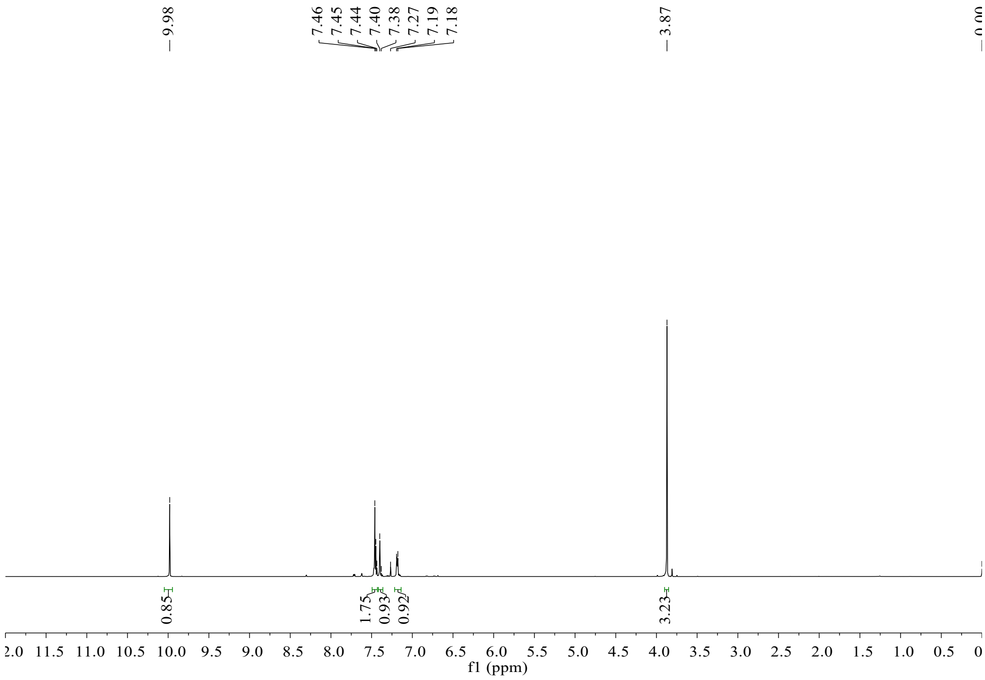


^{13}C NMR spectrogram of 2-methoxybenzaldehyde

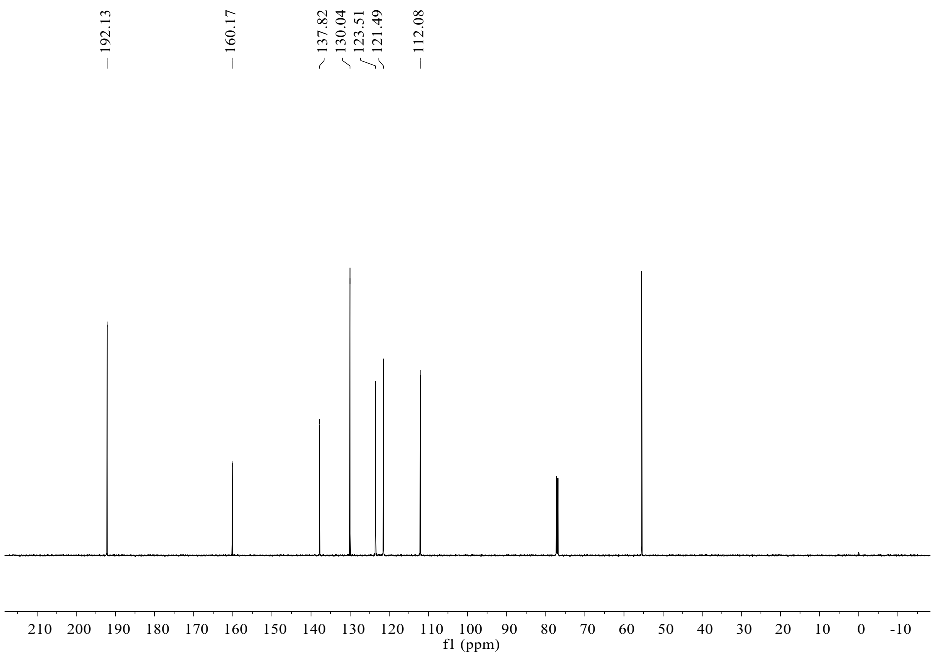
3-Methoxybenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.98 (s, 1H), 7.45 (d, *J* = 7.4 Hz, 2H), 7.40 (s, 1H), 7.19 (d, *J* = 9.3 Hz, 1H), 3.87 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 192.13, 160.17, 137.82, 130.04, 123.51, 121.49, 112.08, 55.45.

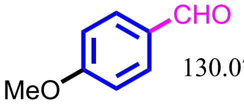


^{1}H NMR spectrogram of 3-methoxybenzaldehyde

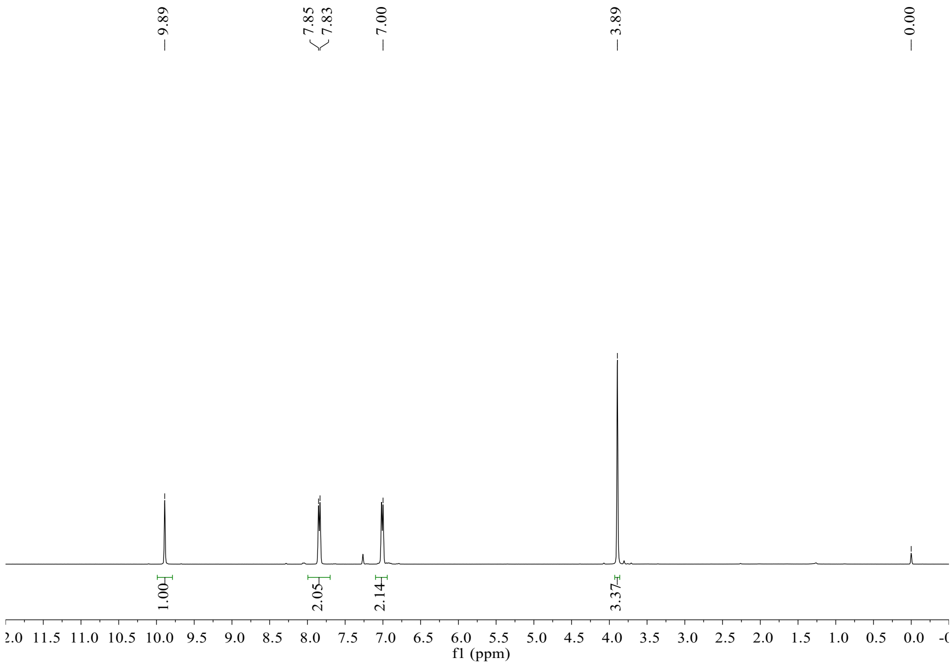


^{13}C NMR spectrogram of 3-methoxybenzaldehyde

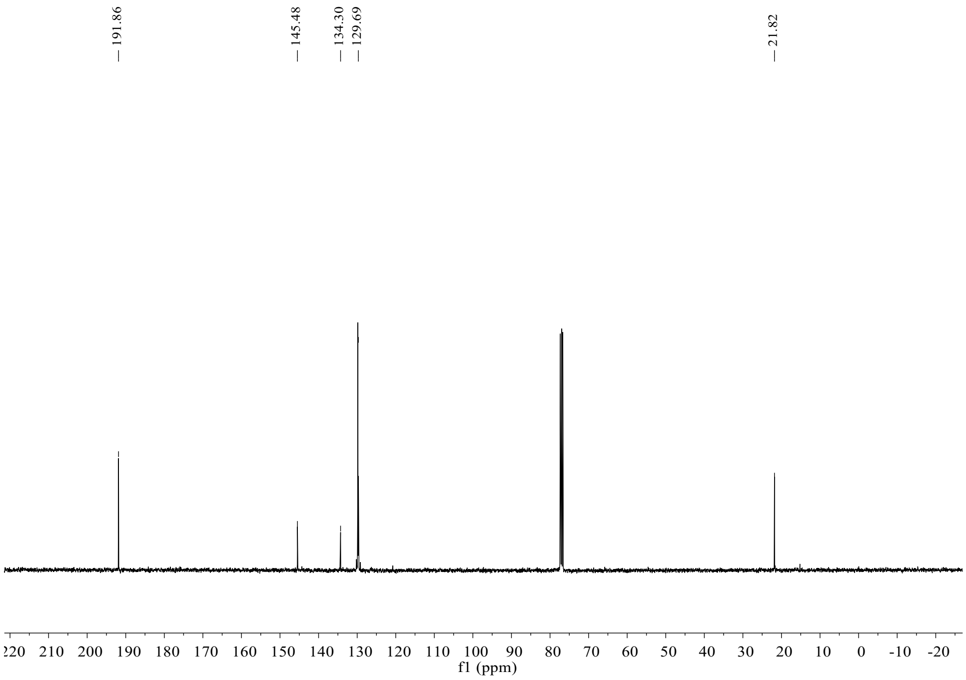
4-Methoxybenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.89 (s, 1H), 7.96 – 7.69 (m, 2H), 7.00 (s, 2H), 3.89 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.65, 164.63, 131.92, 130.07, 114.33, 55.54.

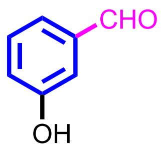


^{1}H NMR spectrogram of 4-methoxybenzaldehyde

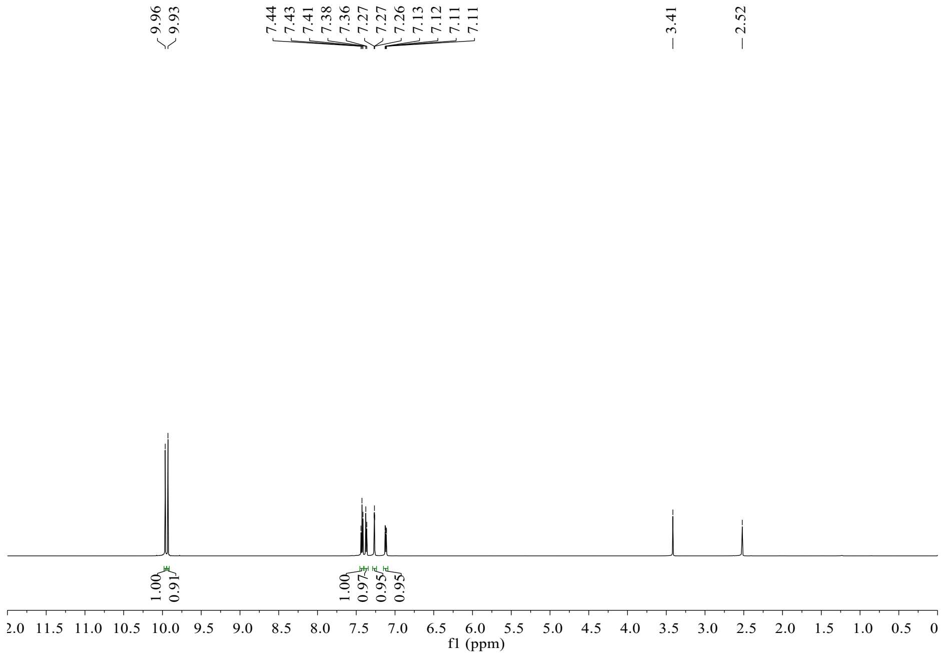


^{13}C NMR spectrogram of 4-methoxybenzaldehyde

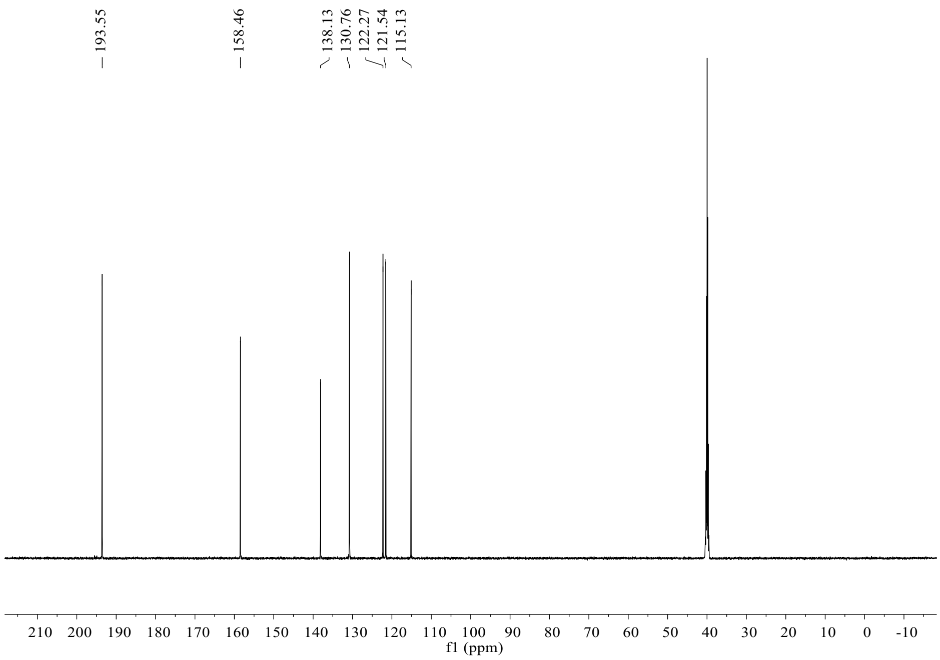
3- Hydroxybenzaldehyde



^{1}H NMR (400 MHz, DMSO-d_6) δ 9.96 (s, 1H), 9.93 (s, 1H), 7.43 (t, J = 7.7 Hz, 1H), 7.37 (d, J = 7.5 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.12 (dd, J = 8.0, 2.5 Hz, 1H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 193.55, 158.46, 138.13, 130.76, 122.27, 121.54, 115.13.

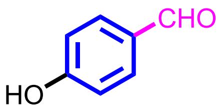


^{1}H NMR spectrogram of 3-hydroxybenzaldehyde

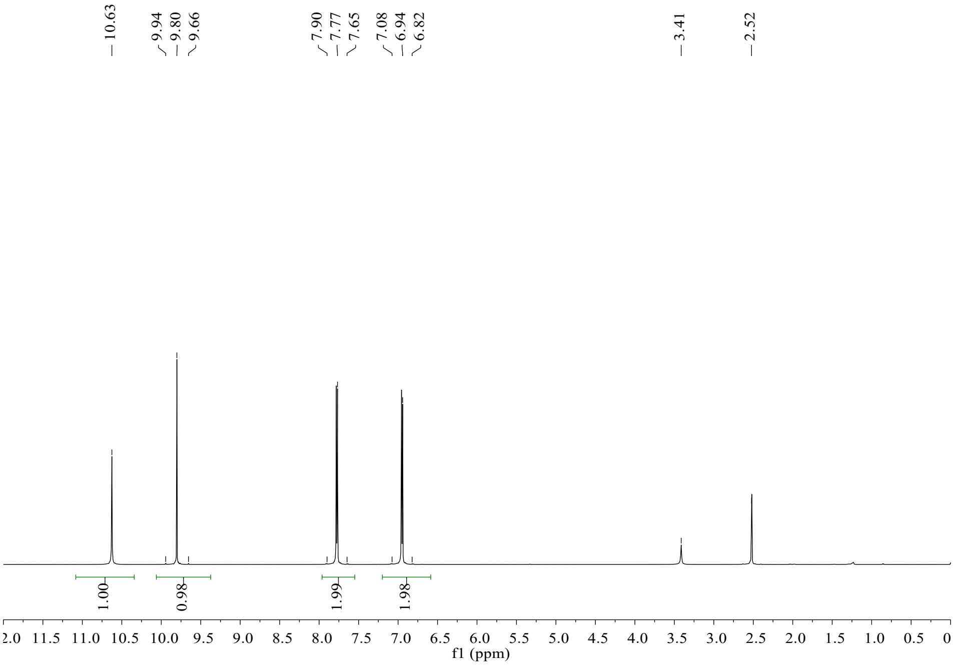


^{13}C NMR spectrogram of 3-hydroxybenzaldehyde

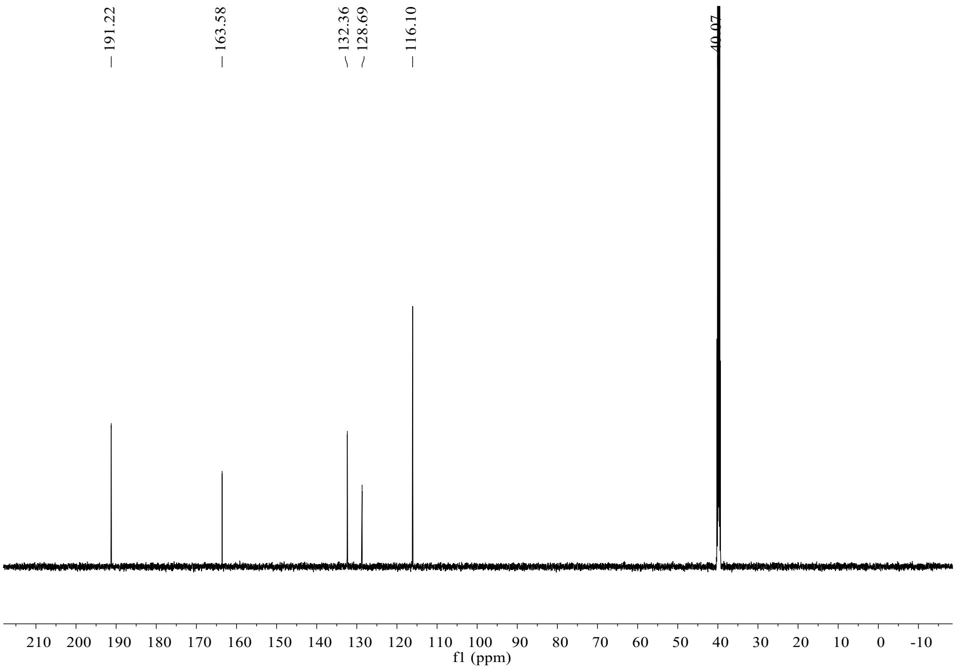
4-Hydroxybenzaldehyde



^{1}H NMR (400 MHz, DMSO-d_6) δ 10.63 (s, 1H), 9.80 (s, 1H), 7.77 (s, 2H), 6.94 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 191.22, 163.58, 132.36, 128.69, 116.10.

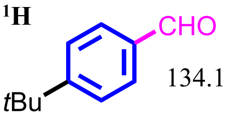


^{1}H NMR spectrogram of 4-hydroxybenzaldehyde

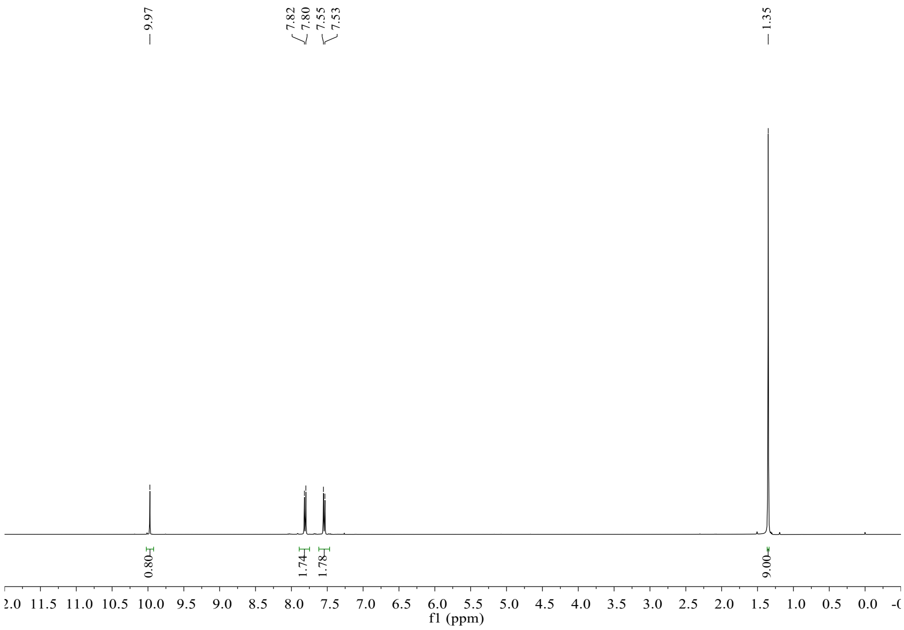


^{13}C NMR spectrogram of 4-hydroxybenzaldehyde

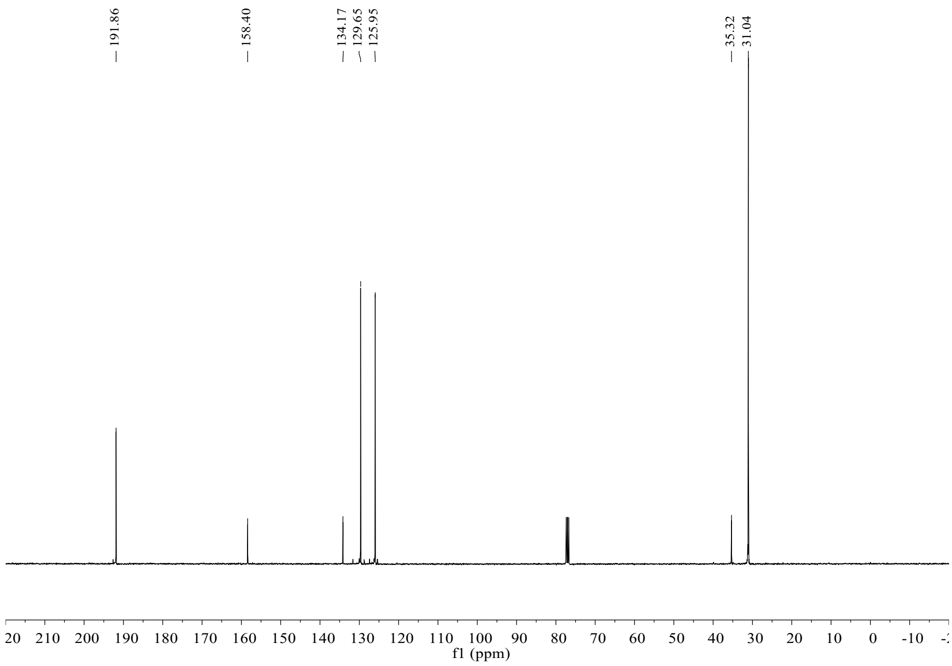
4-Tert-Butylbenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.97 (s, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.47 (m, 2H), 1.35 (s, 9H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 191.86, 158.40, 134.17, 129.65, 125.95, 35.32, 31.04.

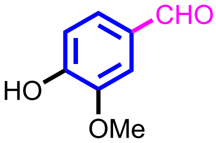


^{1}H NMR spectrogram of 4-tert-butylbenzaldehyde

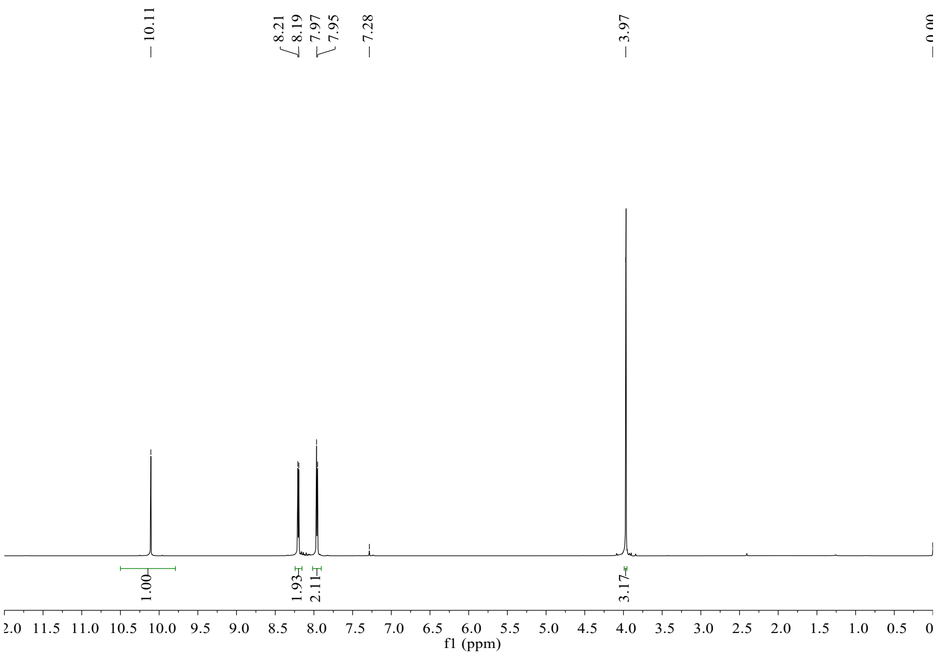


^{13}C NMR spectrogram of 4-tert-nutylbenzaldehyde

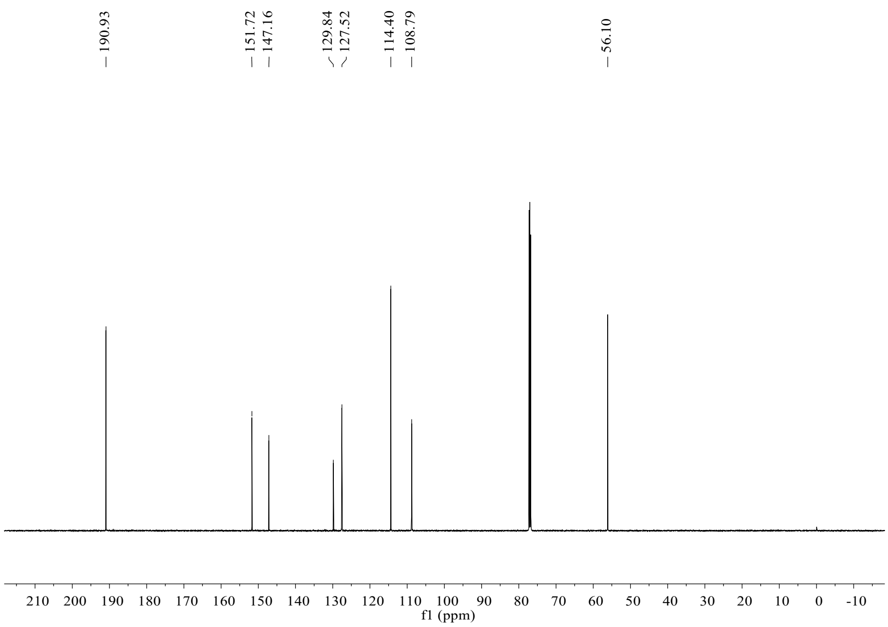
3-Methoxy-4-Hydroxybenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.83 (s, 1H), 7.42 (s, 2H), 7.06 (s, 1H), 6.17 (s, 1H), 3.97 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.93, 151.72, 147.16, 129.84, 127.52, 114.40, 108.79, 56.10.

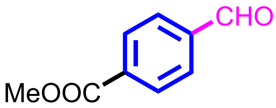


^{1}H NMR spectrogram of 3-methoxy-4-hydroxybenzaldehyde

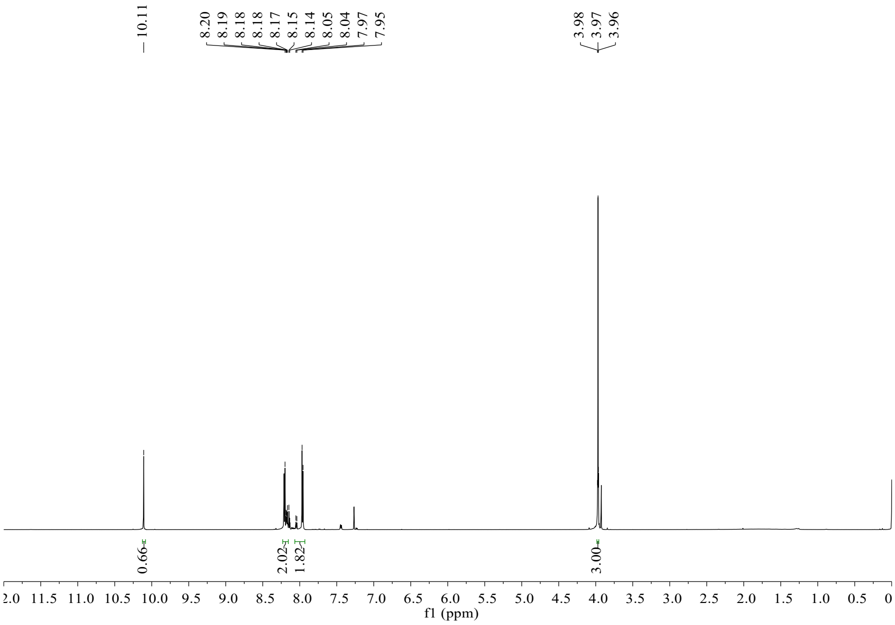


^{13}C NMR spectrogram of 3-methoxy-4-hydroxybenzaldehyde

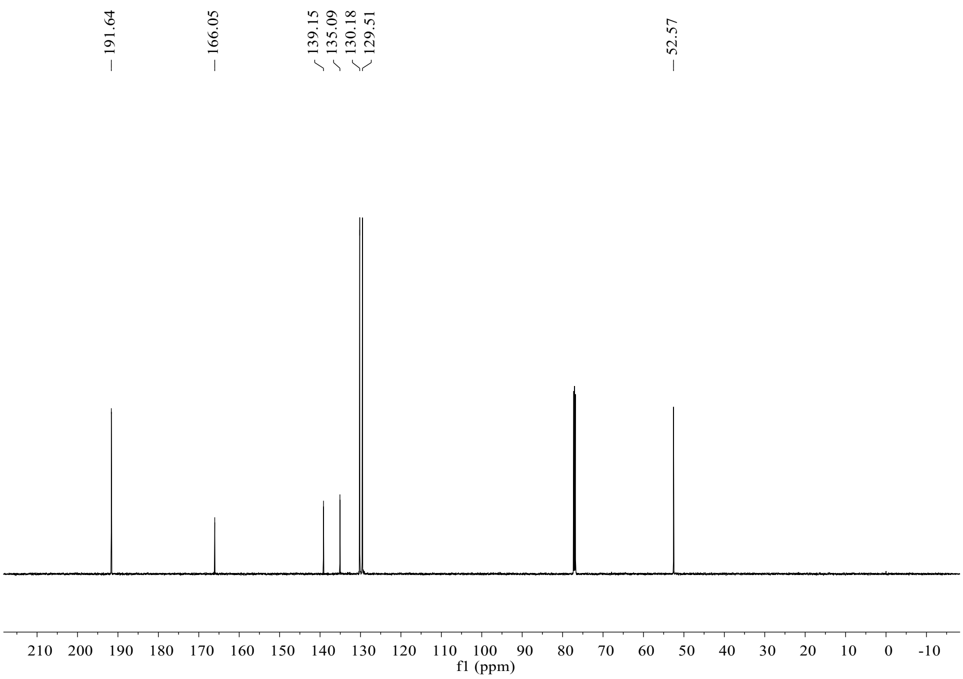
Methyl 4-formylbenzoate



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.11 (s, 1H), 8.20 (d, *J* = 8.1 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 3.97 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 191.64, 166.05, 139.15, 135.09, 130.18, 129.51, 52.57.

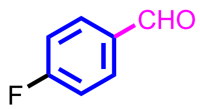


^{1}H NMR spectrogram of methyl 4-formylbenzoate

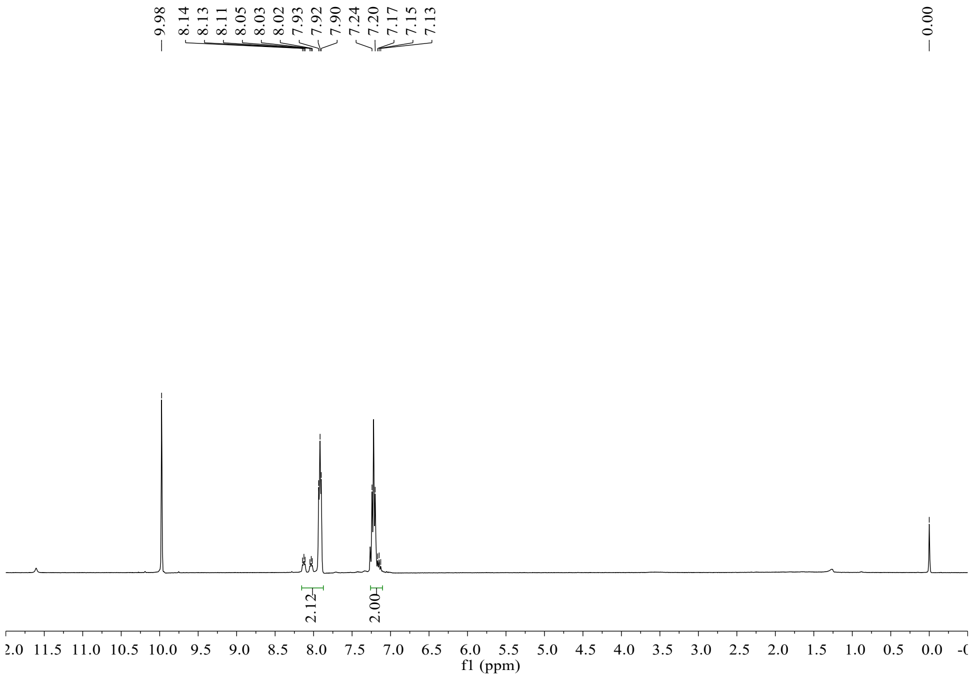


^{13}C NMR spectrogram of methyl 4-formylbenzoate

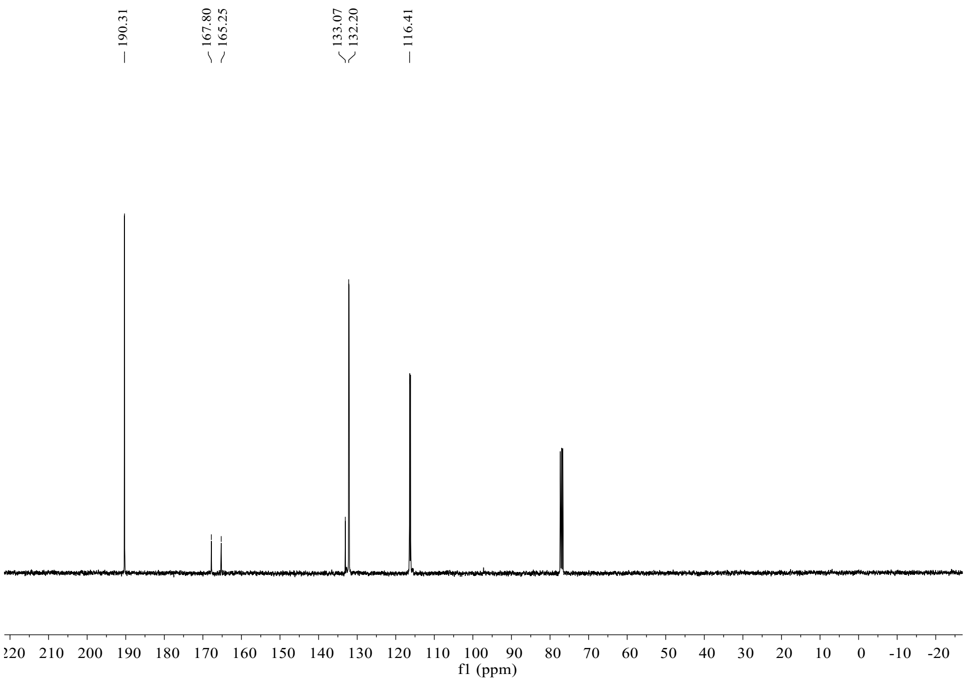
4-Fluorobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.02 – 9.85 (m, 1H), 7.91 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.25 – 7.12 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.31, 166.53 (d, *J* = 253.2 Hz), 133.07, 132.20 (d, *J* = 9.6 Hz), 116.41 (d, *J* = 22.1 Hz).

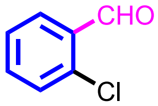


^{1}H NMR spectrogram of 4-fluorobenzaldehyde

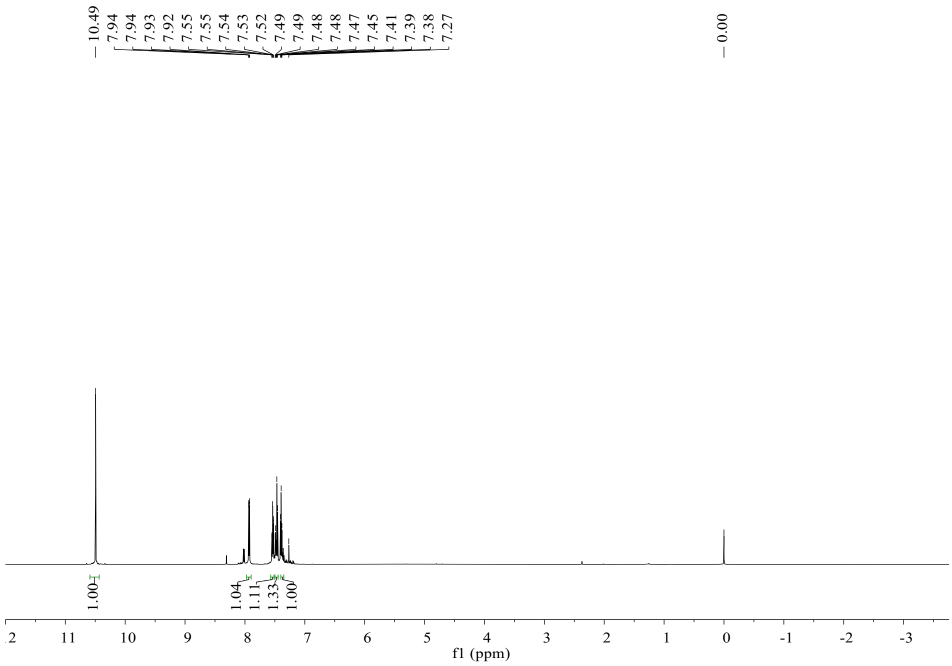


^{13}C NMR spectrogram of 4-fluorobenzaldehyde

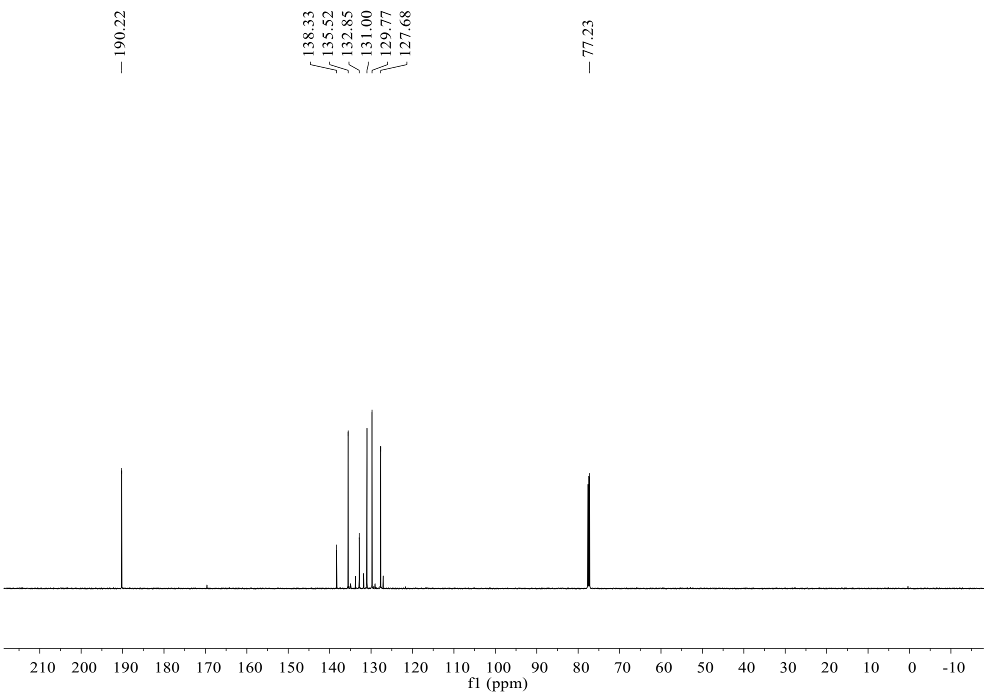
2-Chlorobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.49 (s, 1H), 7.93 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.50 – 7.45 (m, 1H), 7.40 (t, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.22, 138.33, 135.52, 132.85, 131.00, 129.77, 127.68.

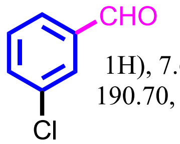


^{1}H NMR spectrogram of 2-chlorobenzaldehyde

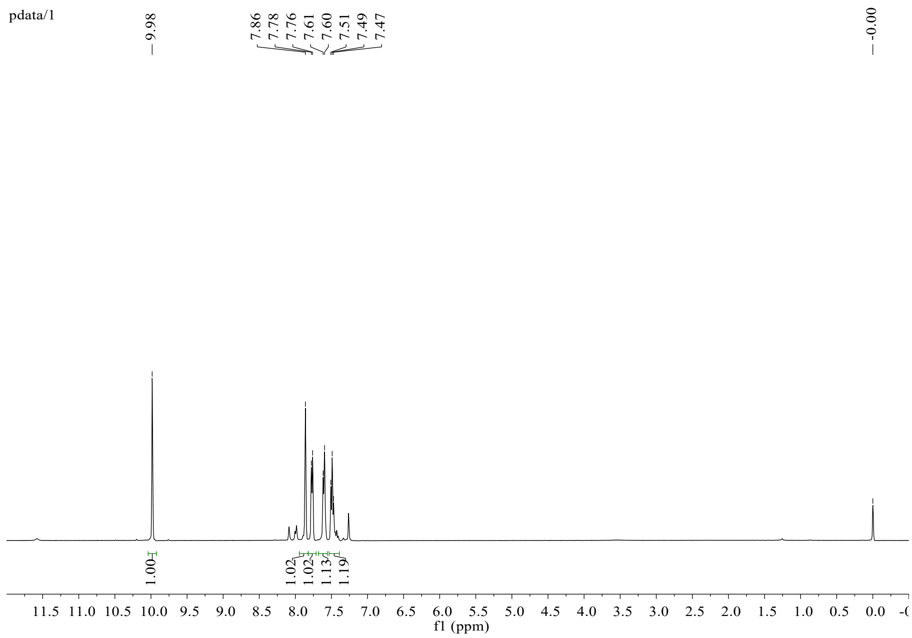


^{13}C NMR spectrogram of 2-chlorobenzaldehyde

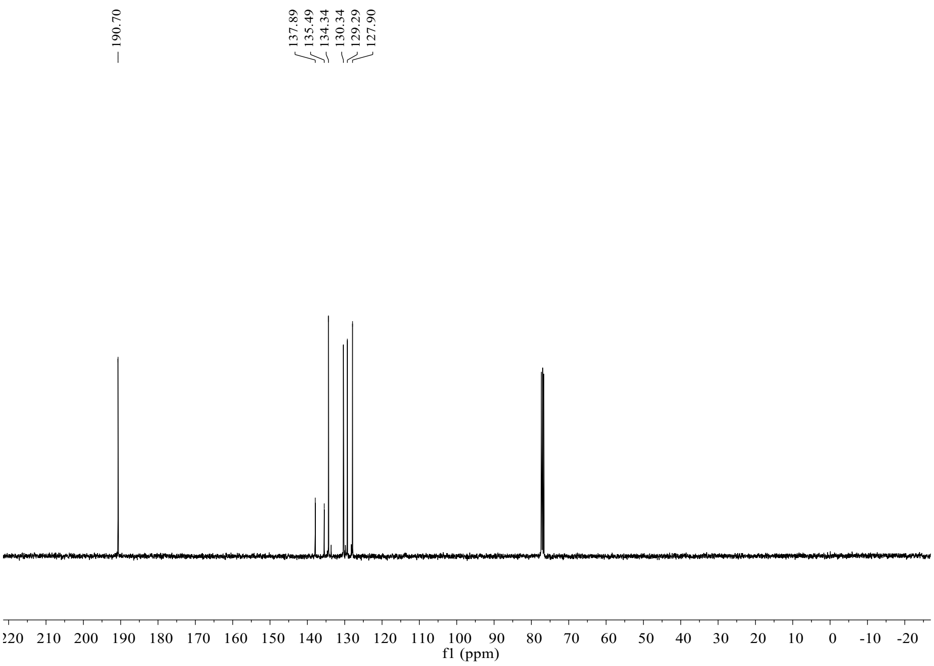
3-Chlorobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.98 (s, 1H), 7.86 (s, 1H), 7.77 (d, J = 7.3 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.70, 137.89, 135.49, 134.34, 130.34, 129.29, 127.90.

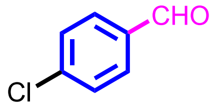


^{1}H NMR spectrogram of 3-chlorobenzaldehyde

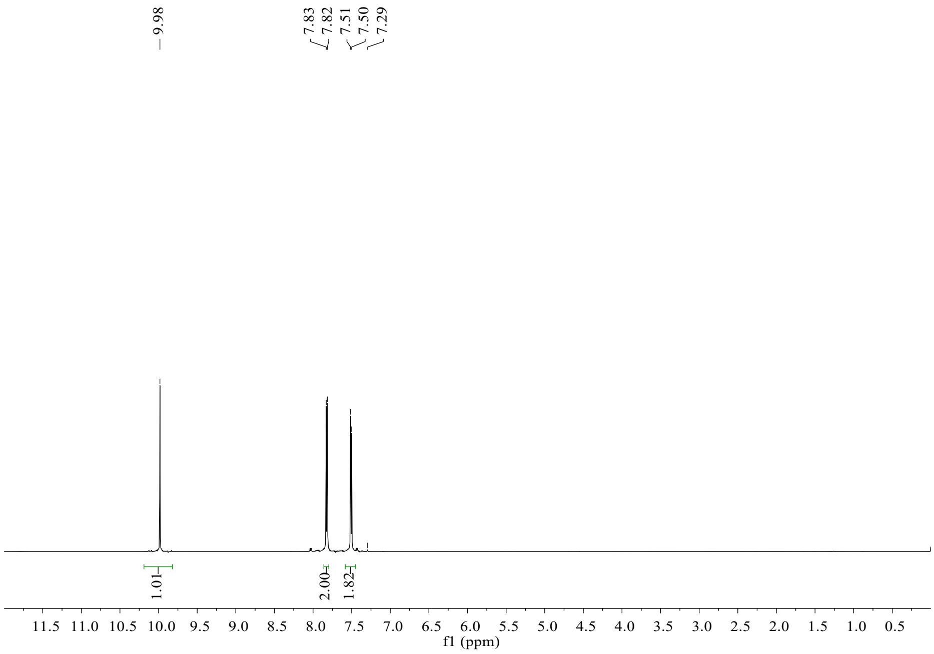


^{13}C NMR spectrogram of 3-chlorobenzaldehyde

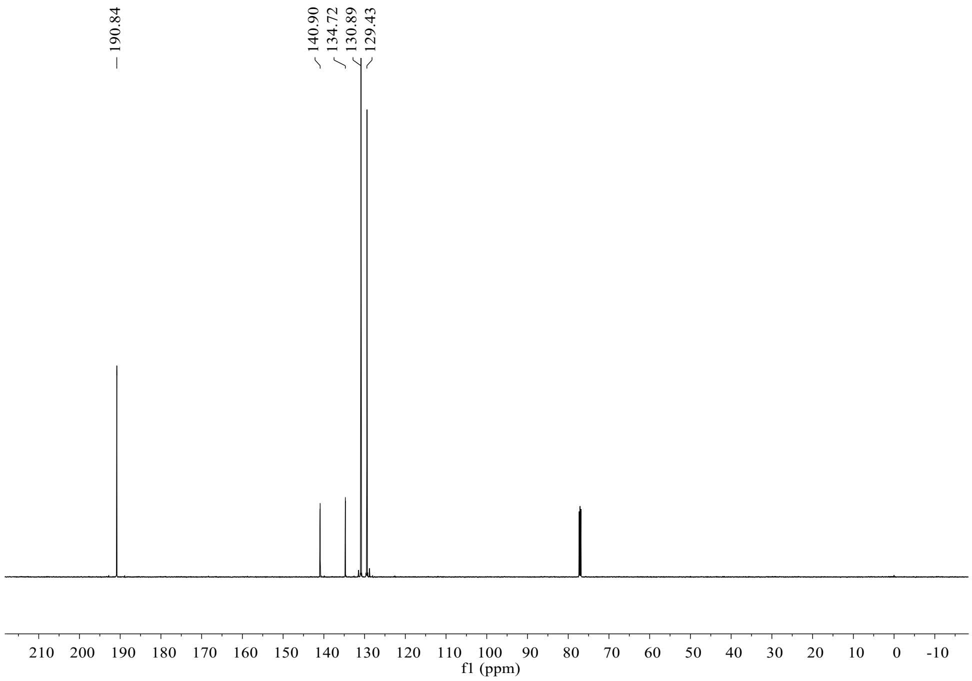
4-Chlorobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.98 (s, 1H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.84, 140.90, 134.72, 130.89, 129.43.

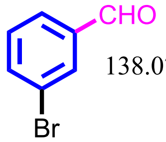


^{1}H NMR spectrogram of 4-chlorobenzaldehyde

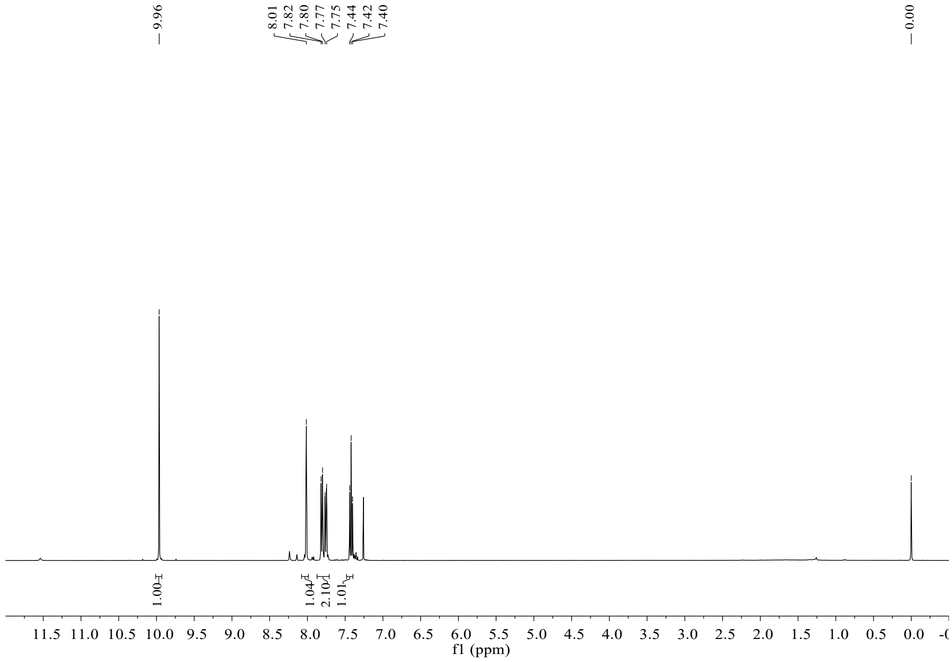


^{13}C NMR spectrogram of 4-chlorobenzaldehyde

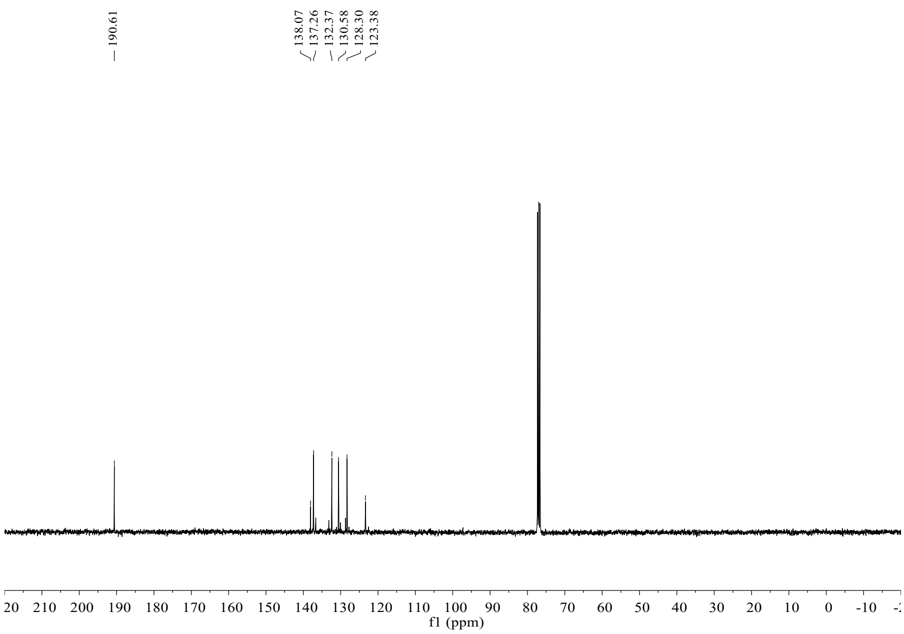
3-Bromobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.96 (s, 1H), 8.01 (s, 1H), 7.78 (dd, *J* = 21.5, 7.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.61, 138.07, 137.26, 132.37, 130.58, 128.30, 123.38.

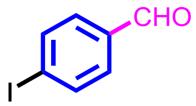


^{1}H NMR spectrogram of 3-bromobenzaldehyde

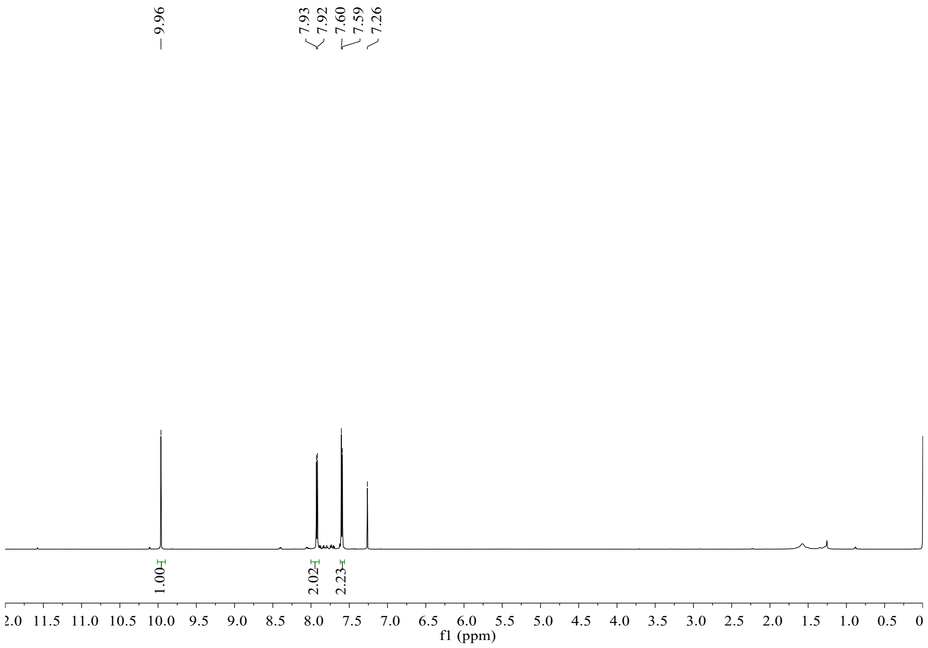


^{13}C NMR spectrogram of 3-bromobenzaldehyde

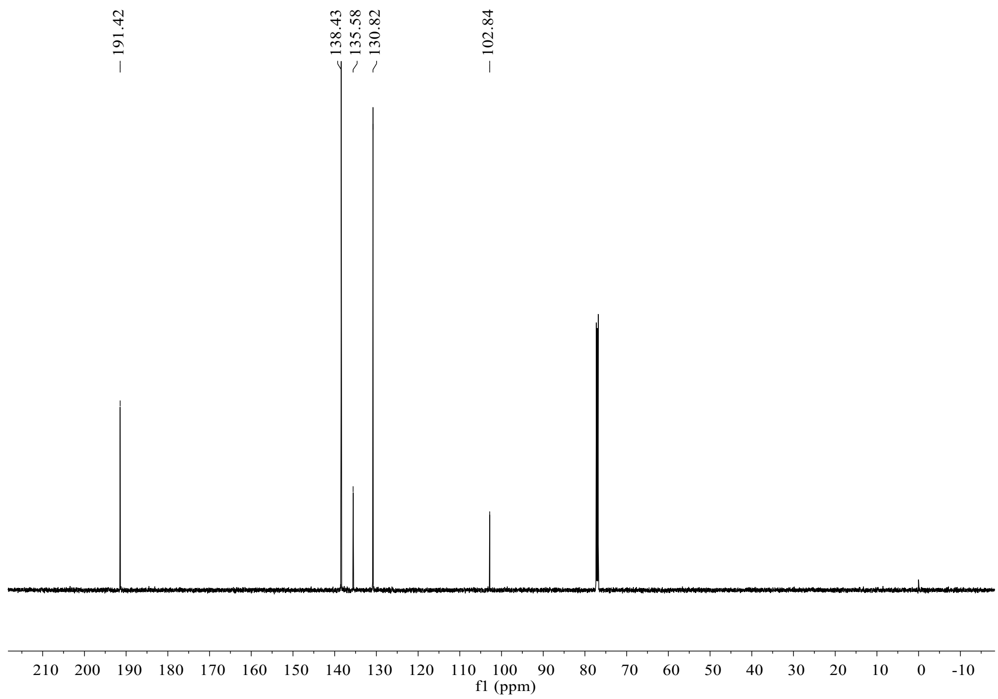
4-Iodobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.96 (s, 1H), 7.92 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 191.42, 138.43, 135.58, 130.82, 102.84.

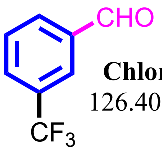


^{1}H NMR spectrogram of 4-iodobenzaldehyde

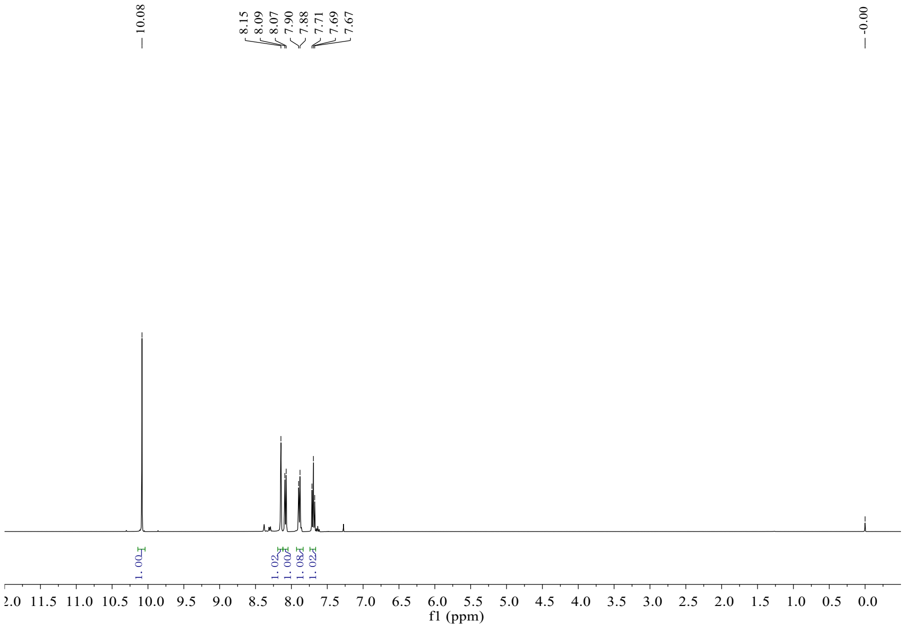


^{13}C NMR spectrogram of 4-iodobenzaldehyde

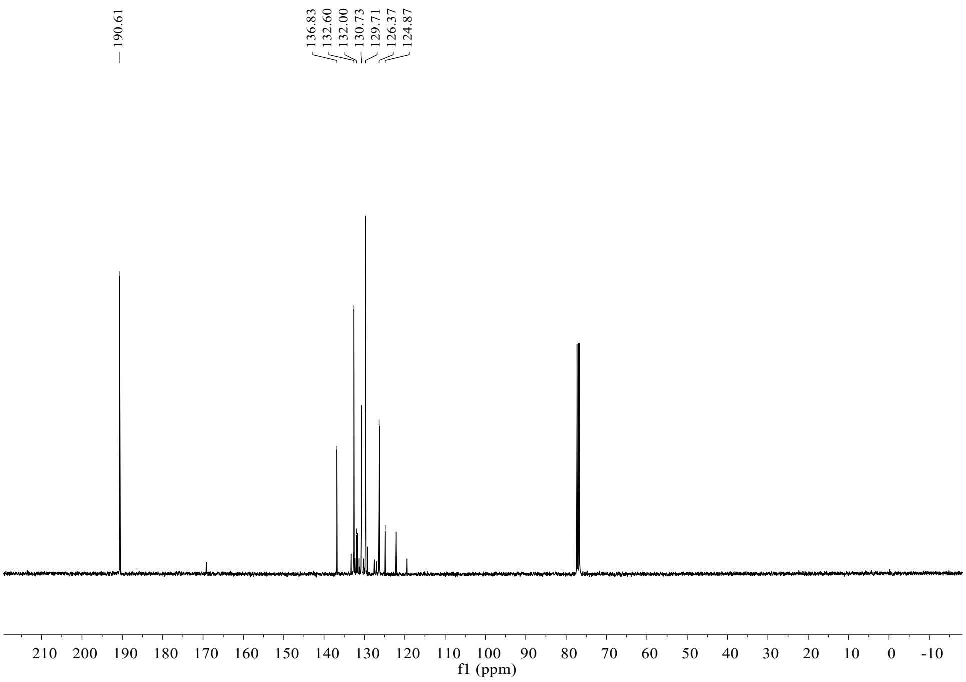
3-Trifluoromethyl Benzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.08 (s, 1H), 8.15 (s, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.7 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.60 136.80 132.60 132.00 (q, *J* = 33.0 Hz), 130.70 (q, *J* = 3.2 Hz), 129.70 126.40 (q, *J* = 3.5 Hz), 124.90 (q, *J* = 270.8 Hz).

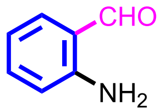


^{1}H NMR spectrogram of 3-trifluoromethyl Benzaldehyde

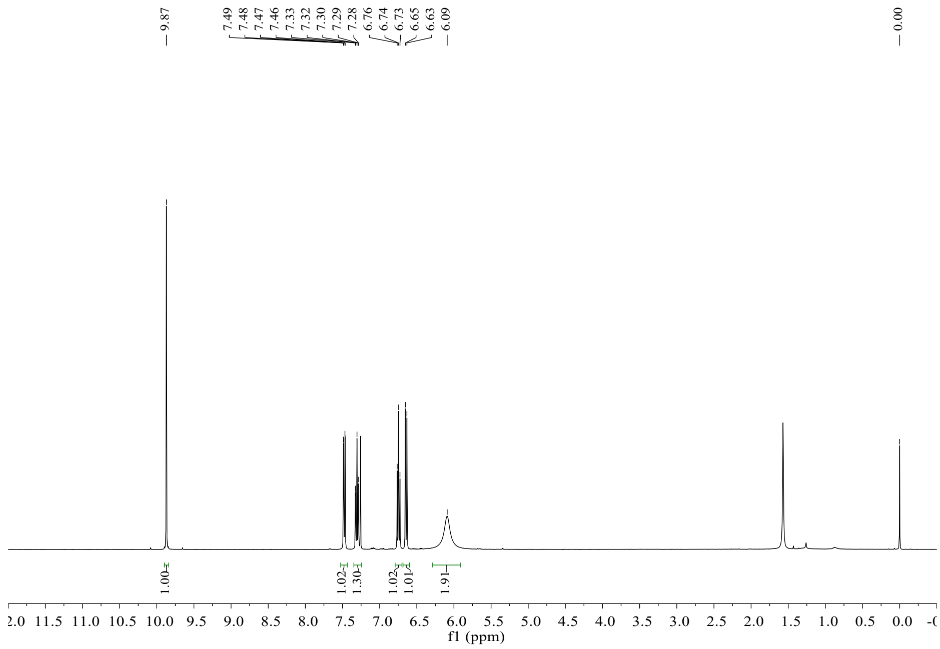


^{13}C NMR spectrogram of 3-trifluoromethyl Benzaldehyde

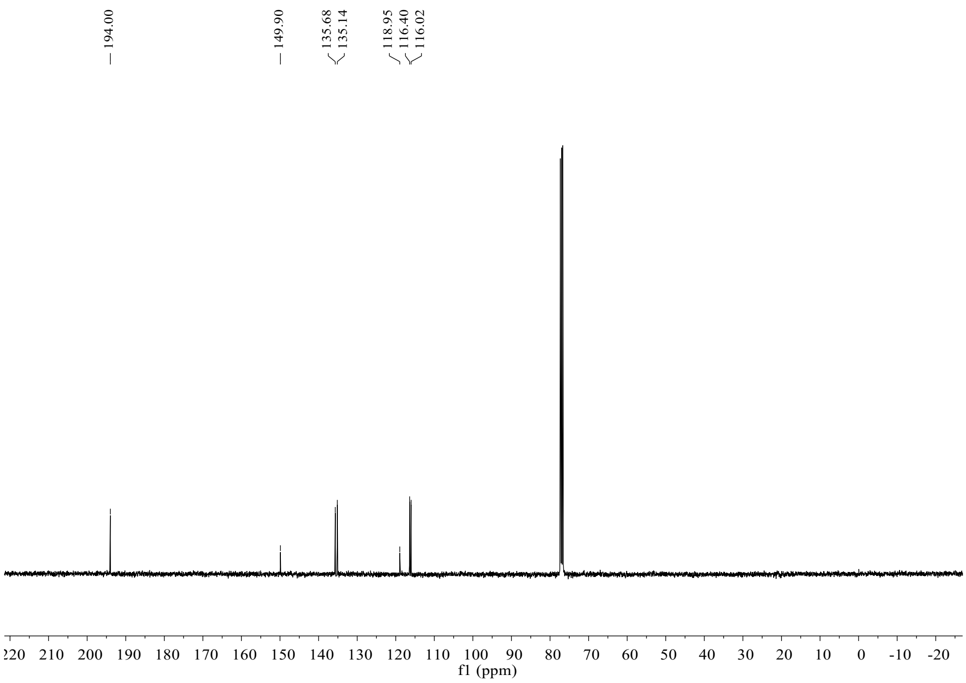
2-Aminobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.87 (s, 1H), 7.52 – 7.44 (m, 1H), 7.35 – 7.24 (m, 1H), 6.74 (t, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 8.3 Hz, 1H), 6.09 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 194.00, 149.90, 135.68, 135.14, 118.95, 116.40, 116.02.

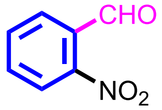


^{1}H NMR spectrogram of 2-aminobenzaldehyde

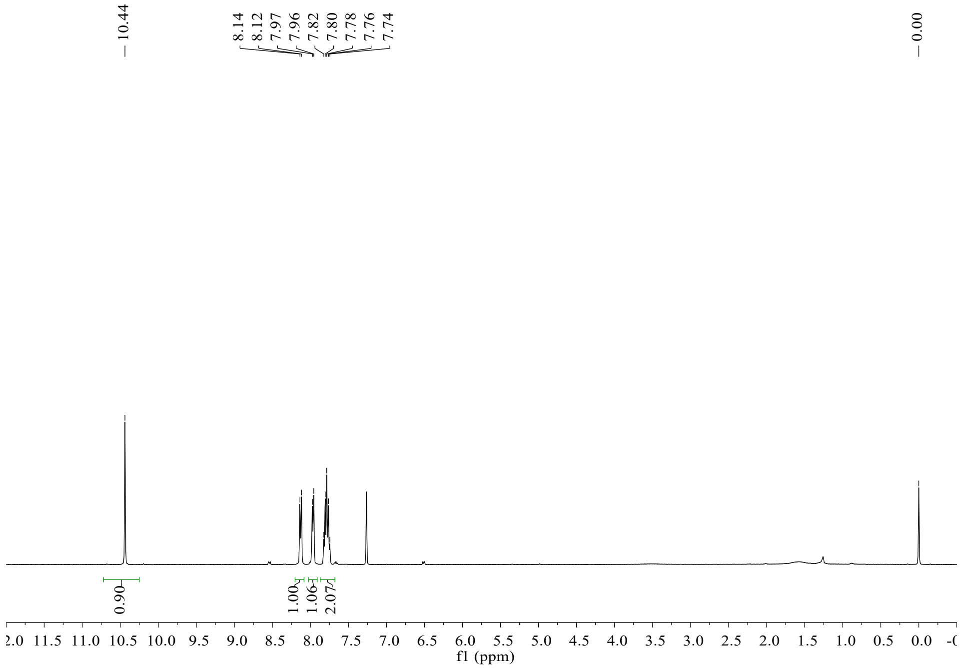


^{13}C NMR spectrogram of 2-aminobenzaldehyde

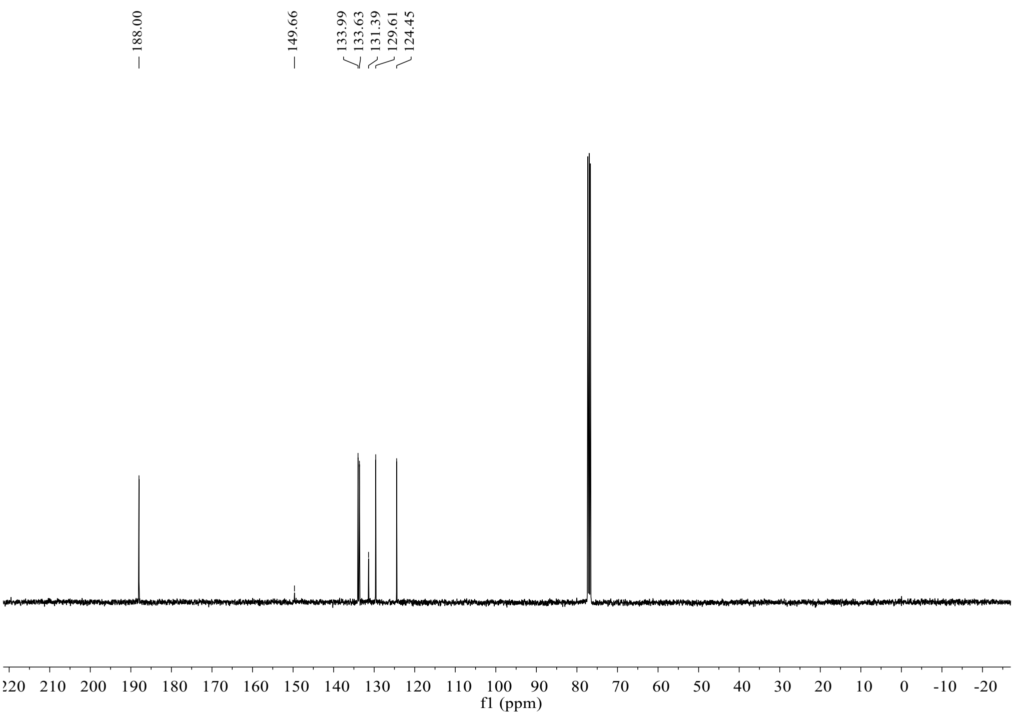
2-Nitrobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.44 (s, 1H), 8.32 – 8.07 (m, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.89 – 7.62 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 188.00, 149.66, 133.99, 133.63, 131.39, 129.61, 124.45.

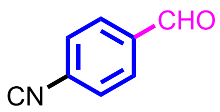


^{1}H NMR spectrogram of 2-nitrobenzaldehyde

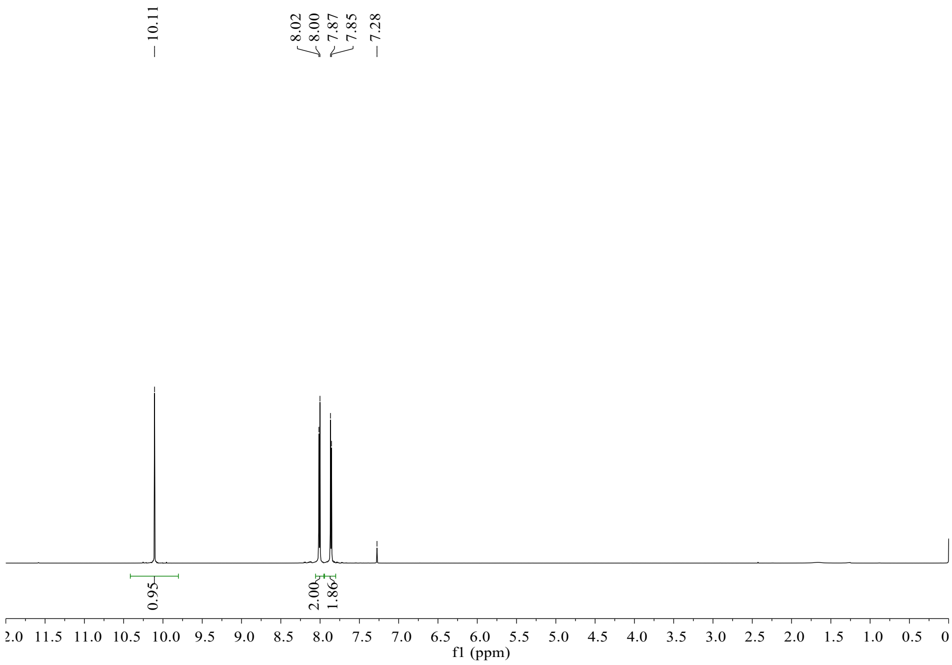


^{13}C NMR spectrogram of 2-nitrobenzaldehyde

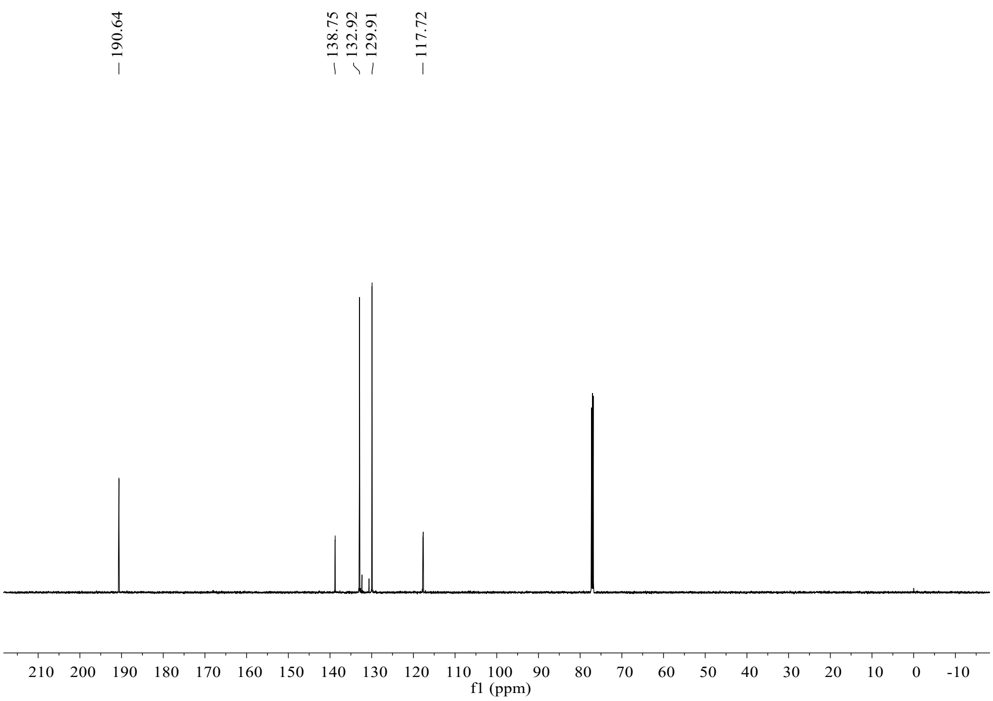
4-Cyanobenzaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.11 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 190.64, 138.75, 132.92, 129.91, 117.72.

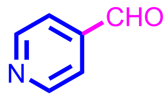


^{1}H NMR spectrogram of 4-cyanobenzaldehyde

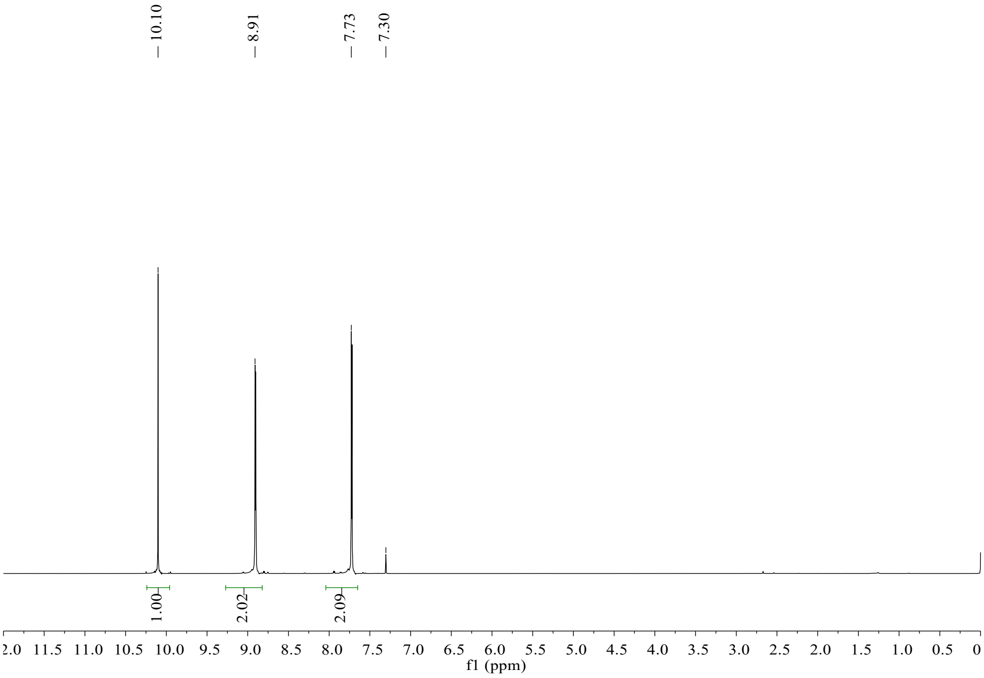


^{13}C NMR spectrogram of 4-cyanobenzaldehyde

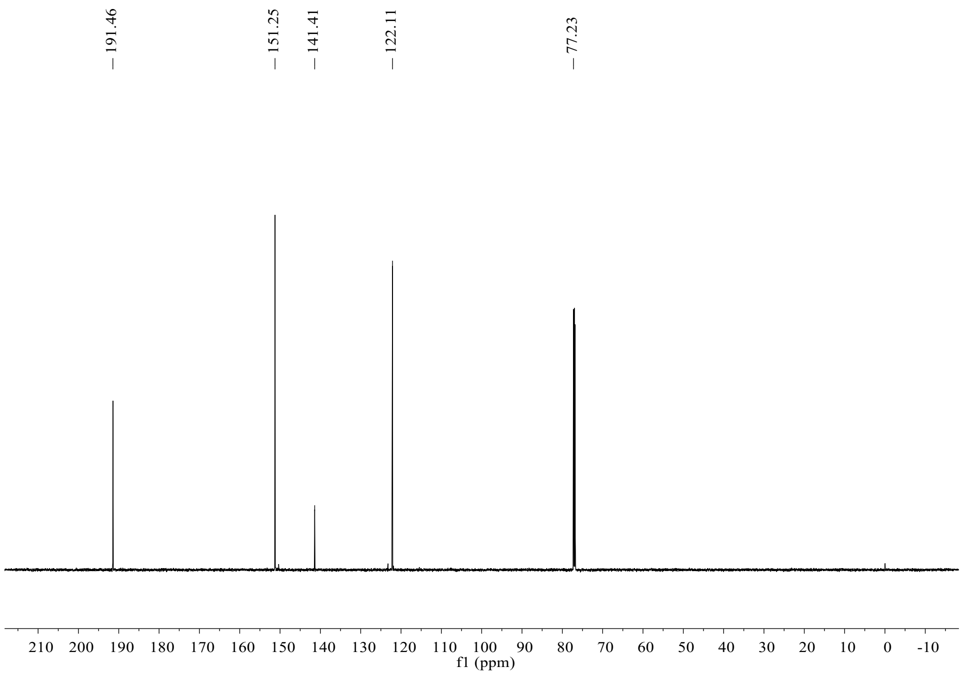
4-Pyridineformaldehyde



[1]H NMR (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H), 8.91 (s, 2H), 7.73 (s, 2H). **[13]C NMR (100 MHz, Chloroform-*d*)** δ 191.46, 151.25, 141.41, 122.11.

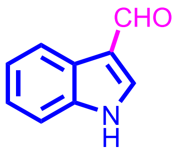


[1]H NMR spectrogram of 4-pyridineformaldehyde

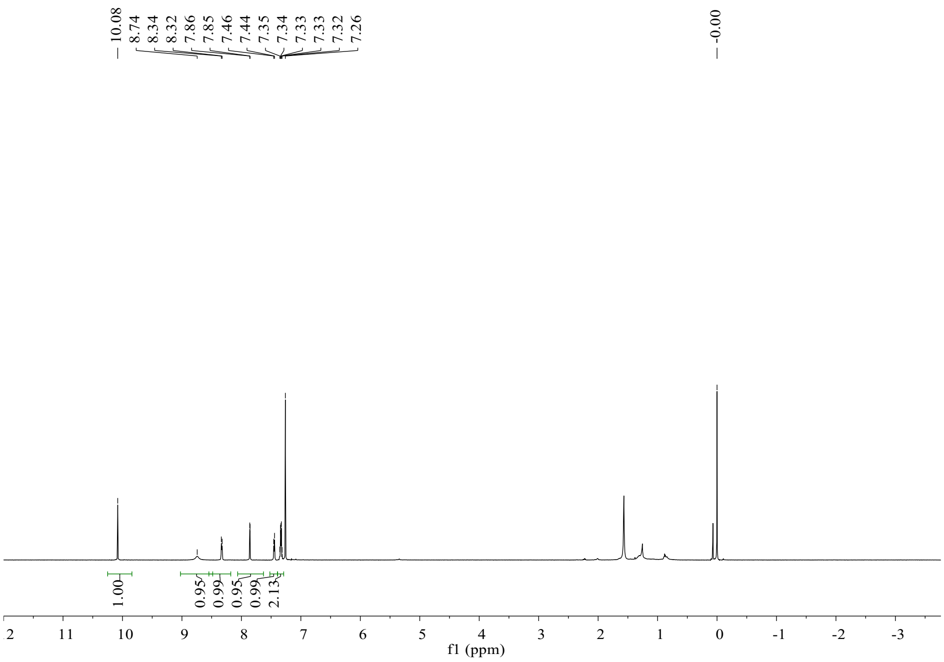


[13]C NMR spectrogram of 4-pyridineformaldehyde

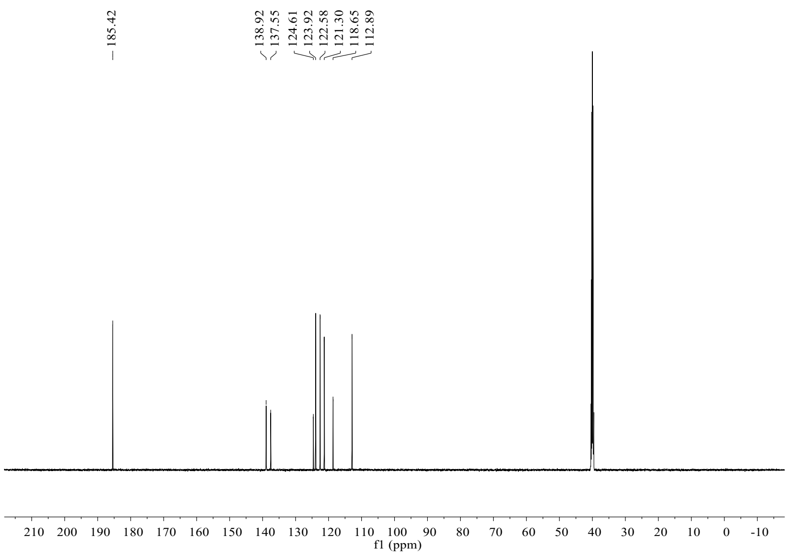
3-Indolealdehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.08 (s, 1H), 8.74 (s, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 7.86 (d, *J* = 2.9 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.40 – 7.28 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*) δ** 185.42, 138.92, 137.55, 124.61, 123.92, 122.58, 121.30, 118.65, 112.89.

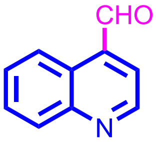


^{1}H NMR spectrogram of 3-indolealdehyde

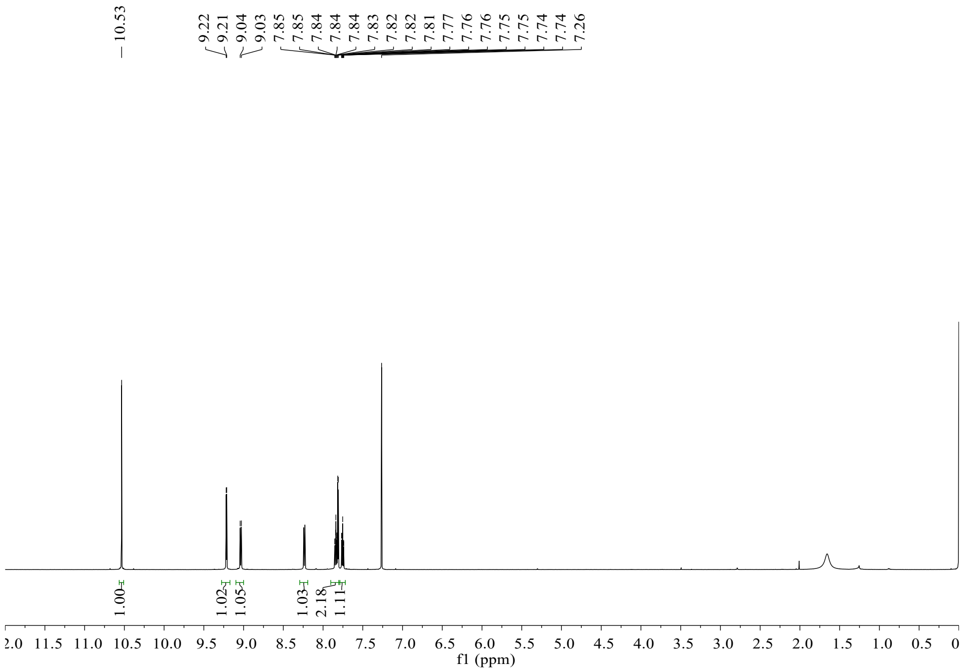


^{13}C NMR spectrogram of 3-indolealdehyde

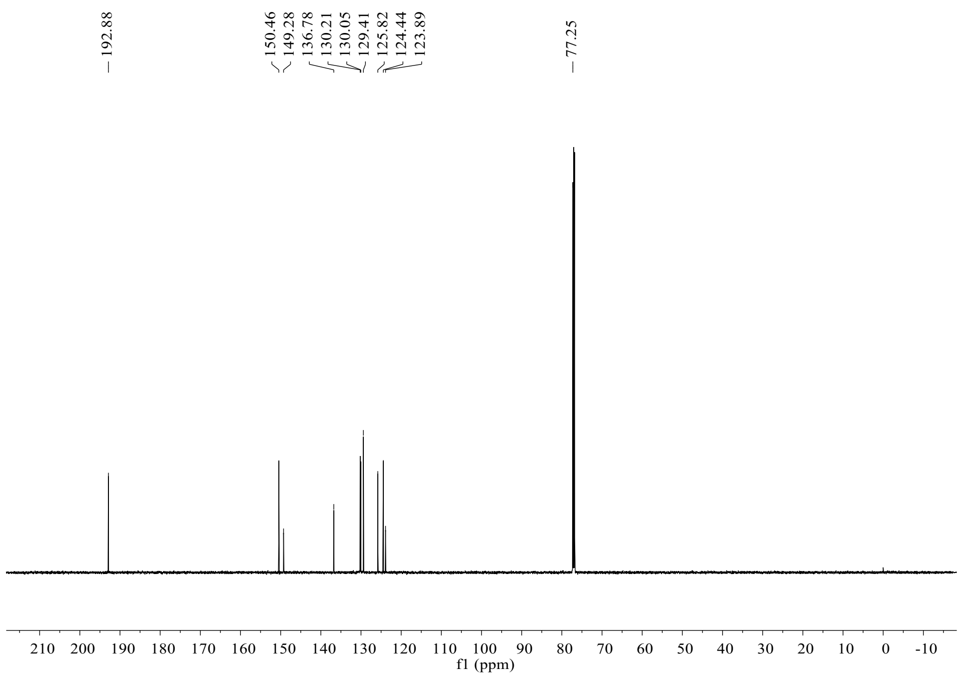
4-Quinolineformaldehyde



¹H NMR (400 MHz, Chloroform-*d*) δ 10.53 (s, 1H), 9.22 (d, *J* = 4.2 Hz, 1H), 9.04 (d, *J* = 9.2 Hz, 1H), 8.24 (dt, *J* = 8.4, 0.9 Hz, 1H), 7.90 – 7.79 (m, 2H), 7.75 (ddd, *J* = 8.3, 6.9, 1.2 Hz, 1H). **¹³C NMR (100 MHz, Chloroform-*d*)** δ 192.88, 150.46, 149.28, 136.78, 130.21, 130.05, 129.41, 125.82, 124.44, 123.89.

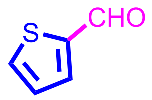


¹H NMR spectrogram of 4-quinolineformaldehyde

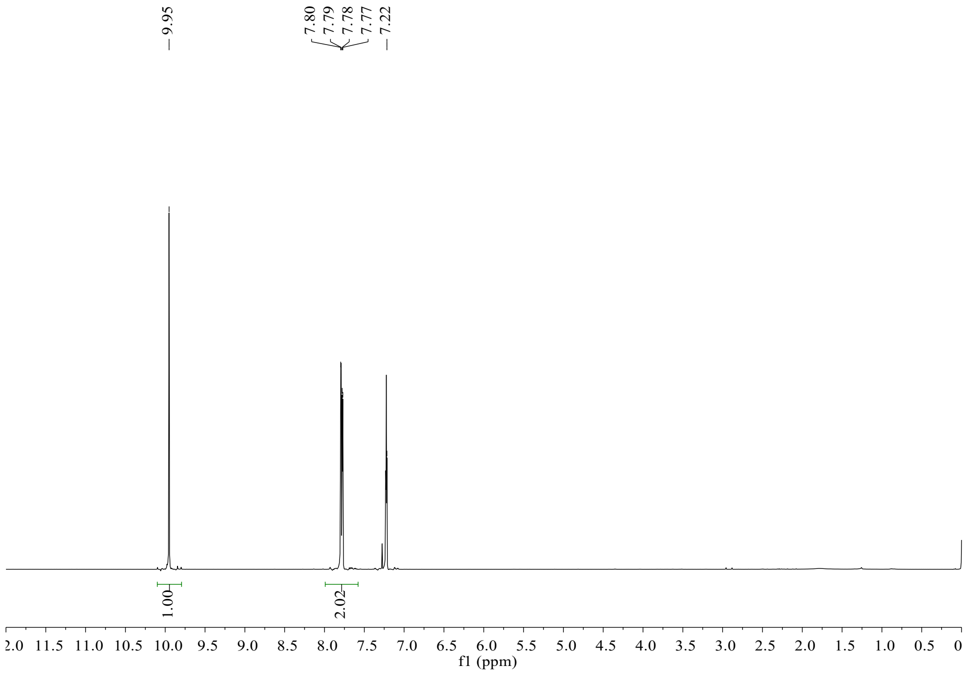


¹³C NMR spectrogram of 4-quinolineformaldehyde

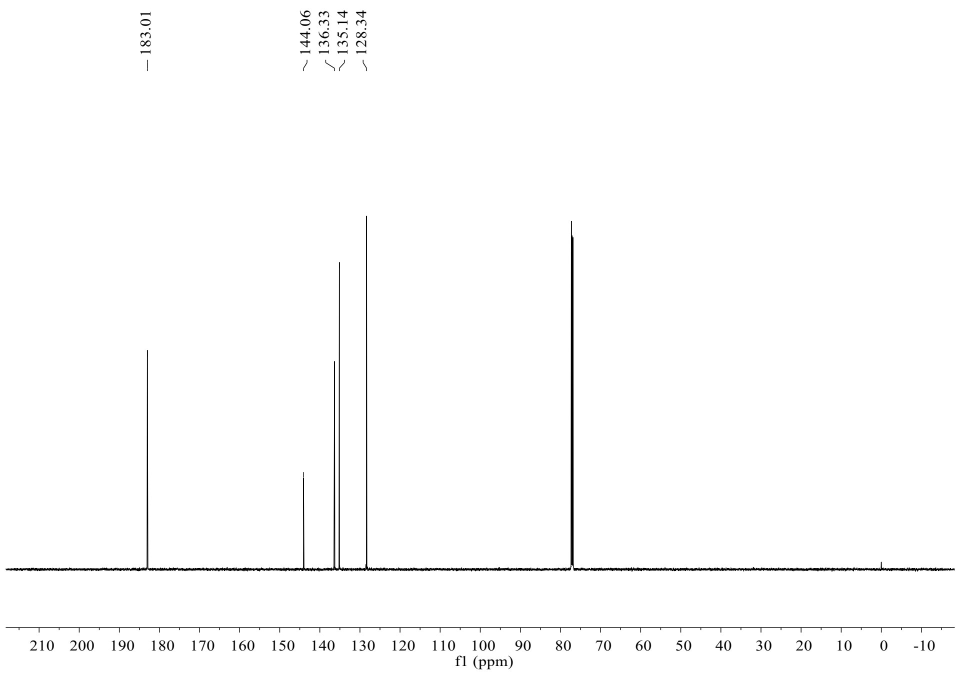
4-Thiopheneformaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.95 (s, 1H), 7.78 (dd, *J* = 11.8, 4.2 Hz, 2H), 7.22 (t, *J* = 4.3 Hz, 1H).**^{13}C NMR (100 MHz, Chloroform-*d*)** δ 183.01, 144.06, 136.33, 135.14, 128.34.

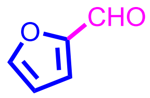


^{1}H NMR spectrogram of 4-thiopheneformaldehyde

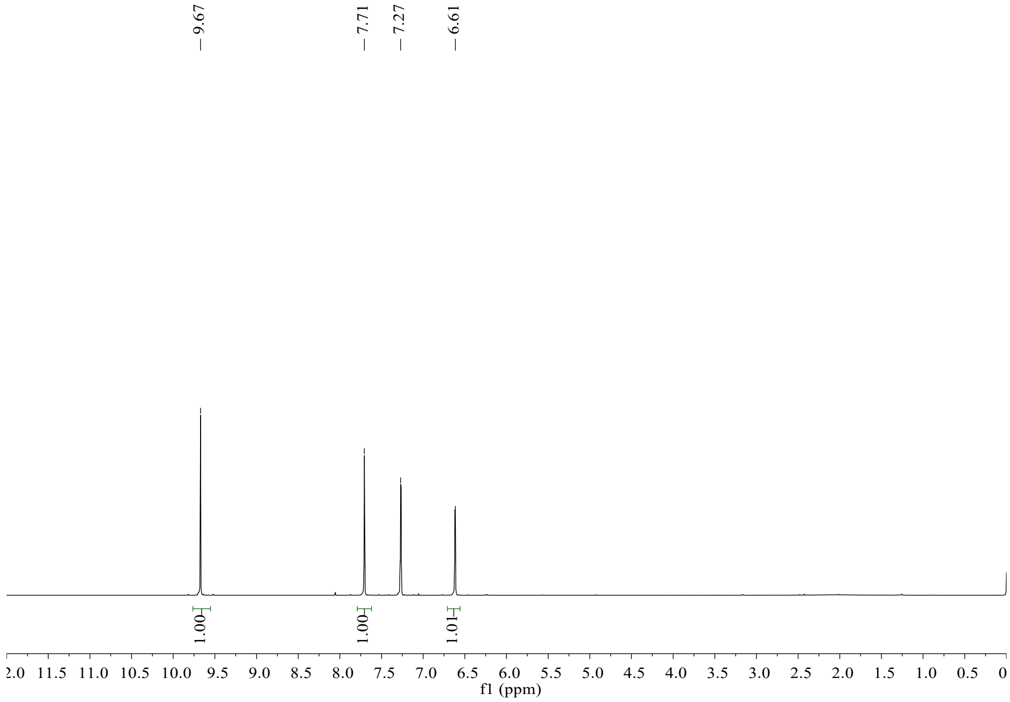


^{13}C NMR spectrogram of 4-thiopheneformaldehyde

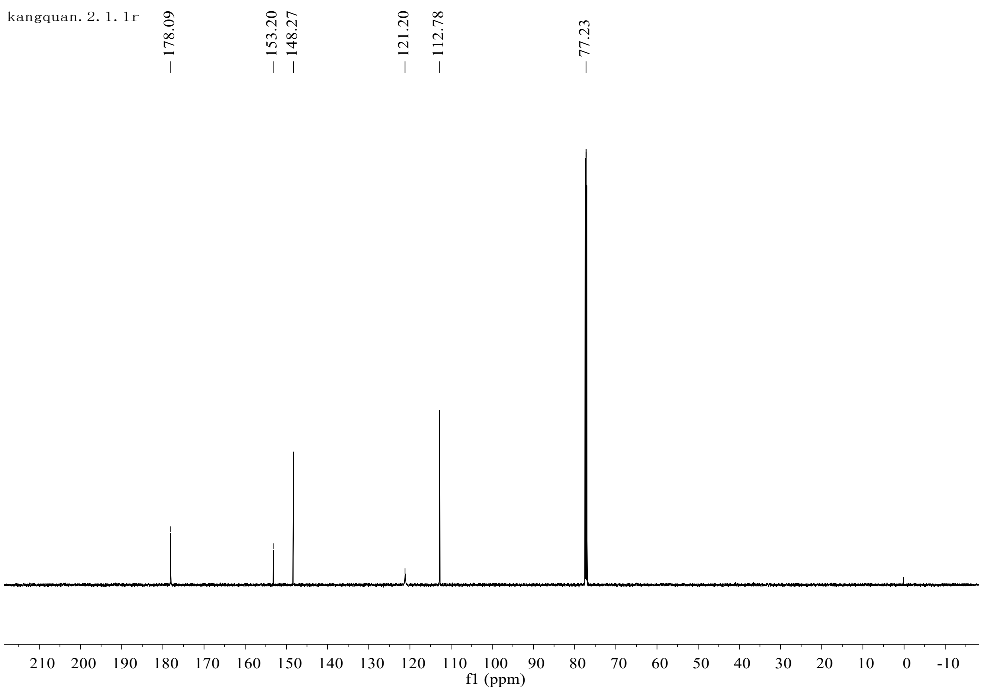
2-Furaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 7.71 (s, 1H), 6.61 (s, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 178.09, 153.20, 148.27, 121.20, 112.78.

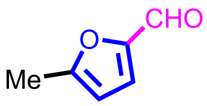


^{1}H NMR spectrogram of 2-furaldehyde

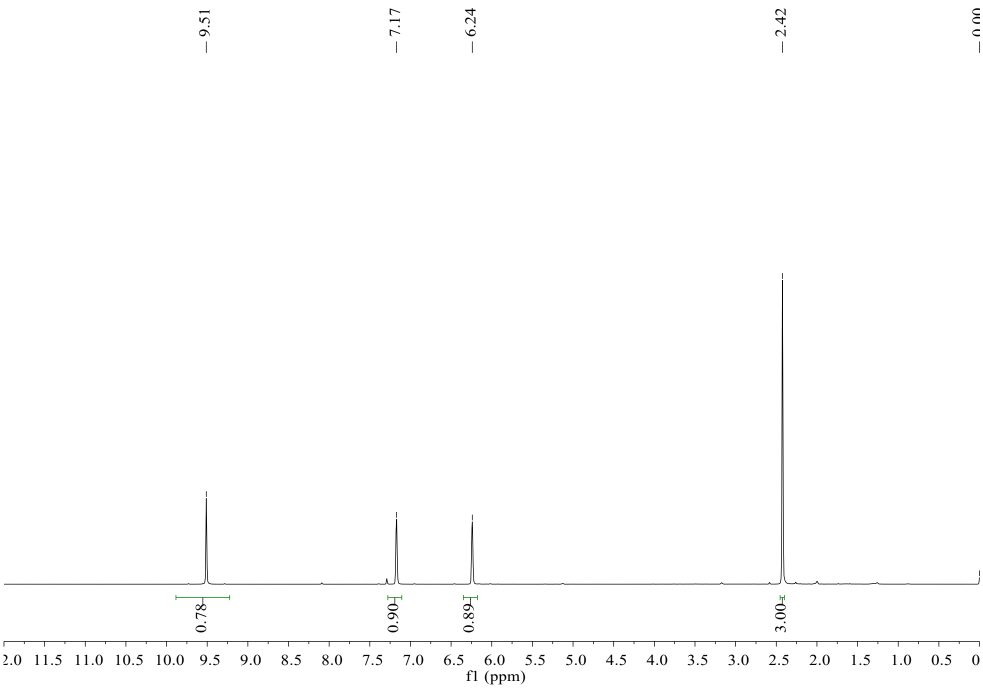


^{13}C NMR spectrogram of 2-furaldehyde

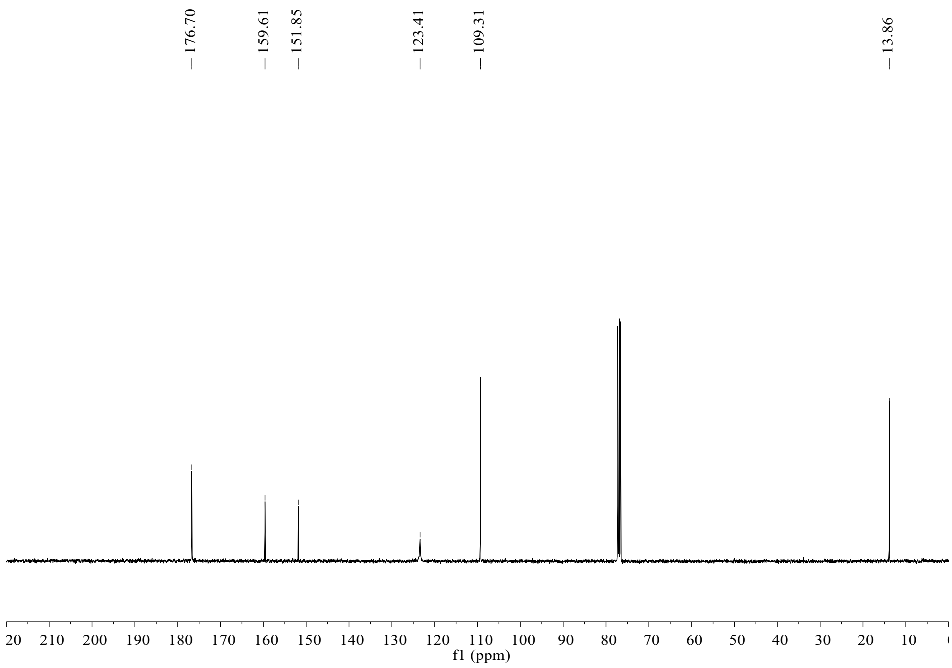
4-Methylfurfural



[1]H NMR (400 MHz, Chloroform-*d*) δ 9.51 (s, 1H), 7.17 (s, 13H), 6.24 (s, 1H), 2.42 (s, 22H). **[13]C NMR (100 MHz, Chloroform-*d*)** δ 176.70, 159.61, 151.85, 109.31, 13.86.

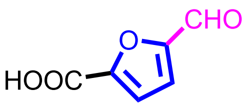


[1]H NMR spectrogram of 4-methylfurfural

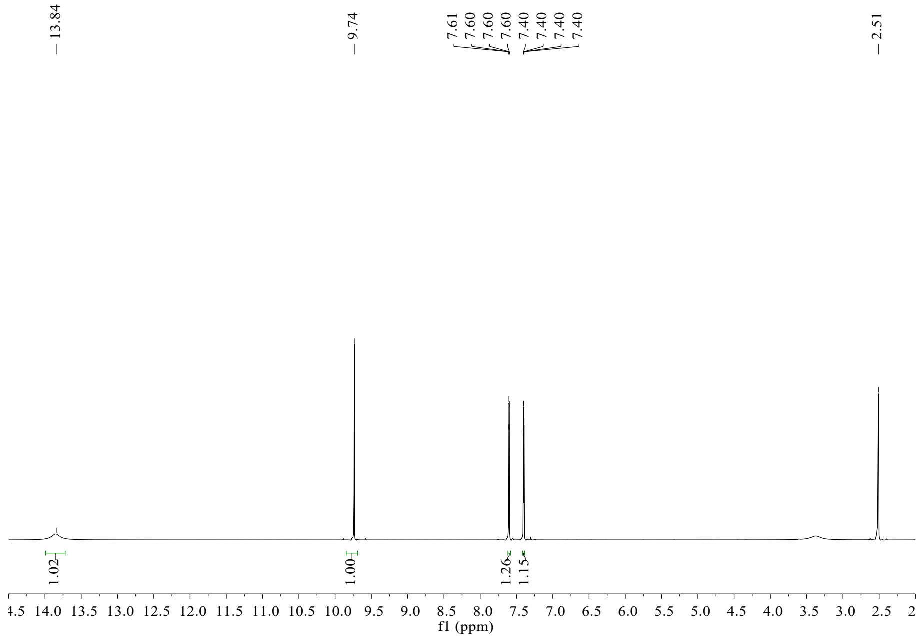


[13]C NMR spectrogram of 4-methylfurfural

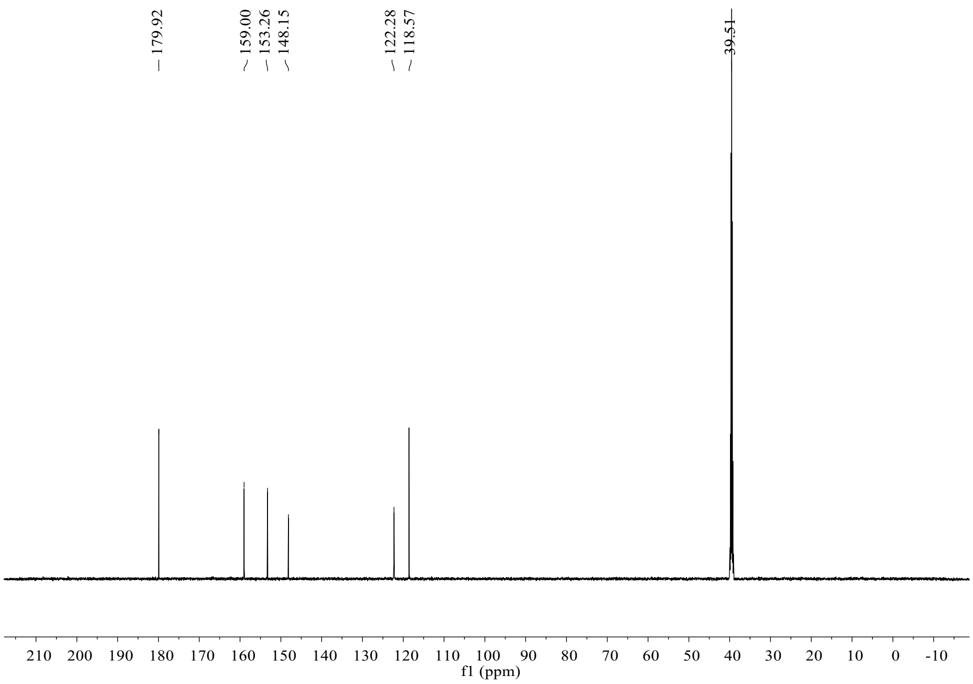
5-Formylfuran-2-Carboxylicacid



^{1}H NMR (400 MHz, DMSO-d_6) δ 13.84 (s, 1H), 9.74 (s, 1H), 7.60 (dd, *J* = 3.7, 0.9 Hz, 1H), 7.42 – 7.38 (m, 1H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 179.92, 159.00, 153.26, 148.15, 122.28, 118.57.

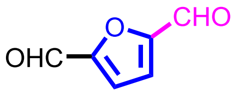


^{1}H NMR spectrogram of 5-Formylfuran-2-carboxylicacid

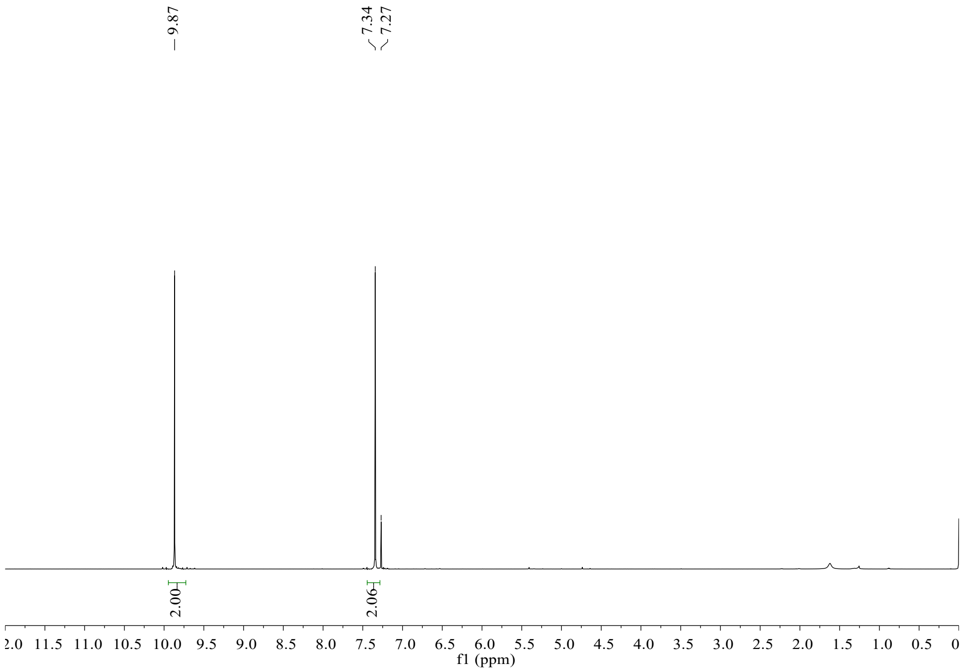


^{13}C NMR spectrogram of 5-Formylfuran-2-carboxylicacid

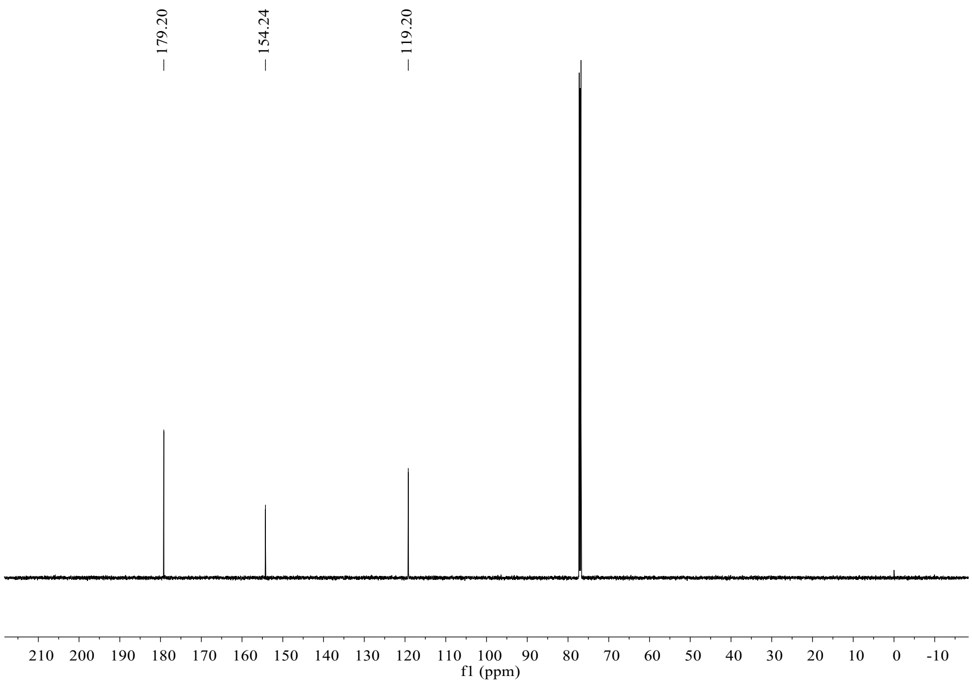
2, 5-Diformylfuran



¹H NMR (400 MHz, Chloroform-*d*) δ 9.87 (s, 2H), 7.34 (s, 2H). **¹³C NMR (100 MHz, Chloroform-*d*)** δ 179.20, 154.24, 119.20.

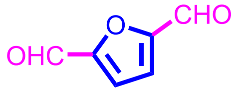


¹H NMR spectrogram of 2, 5-diformylfuran

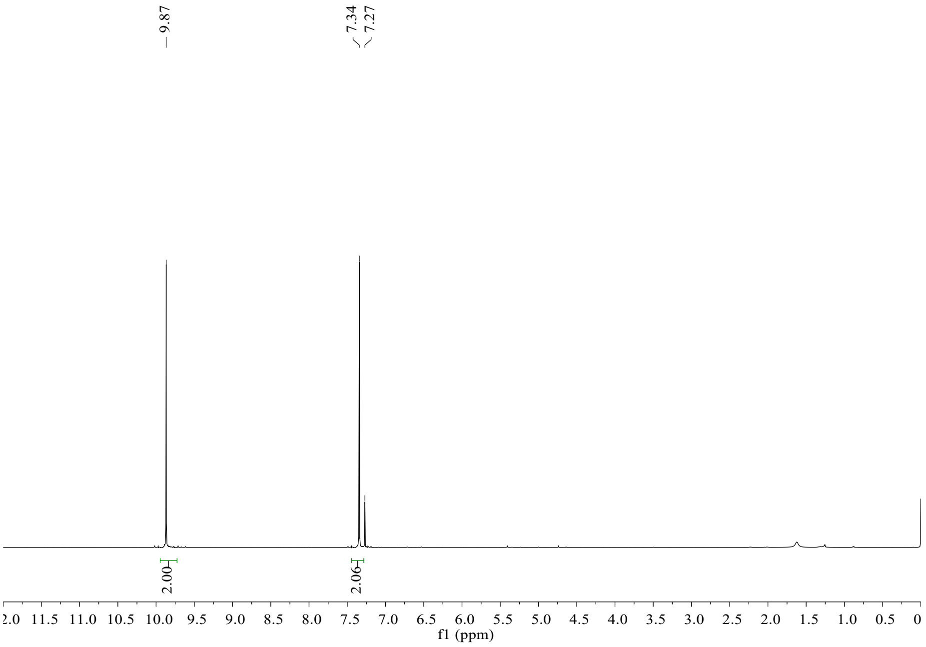


¹³C NMR spectrogram of 2, 5-diformylfuran

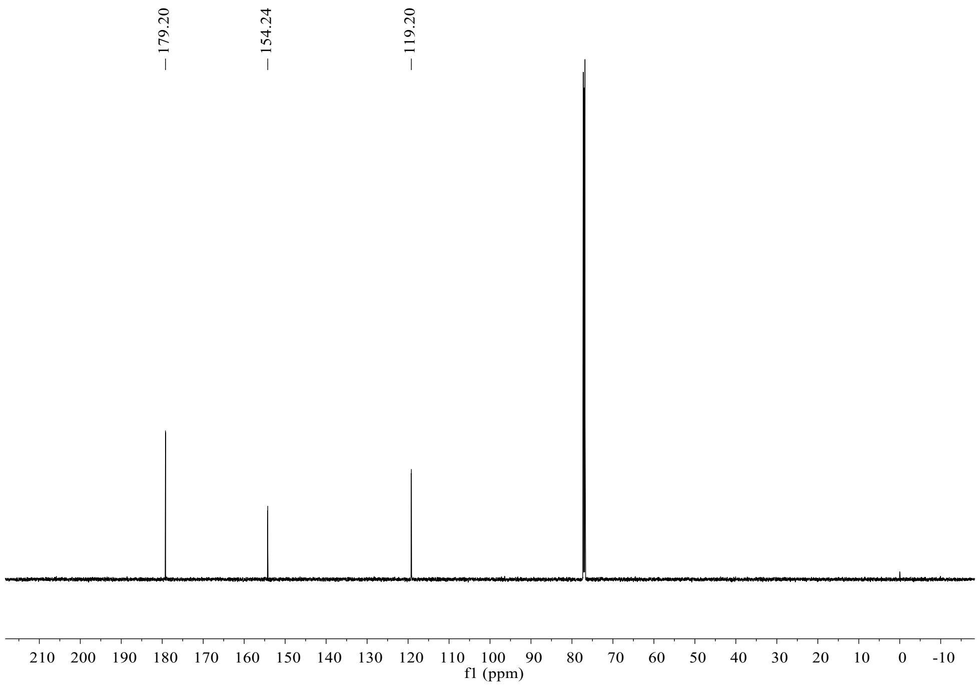
2, 5-Diformylfuran



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.87 (s, 2H), 7.34 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 179.20, 154.24, 119.20.

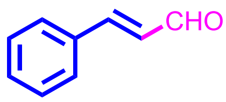


^{1}H NMR spectrogram of 2, 5-diformylfuran

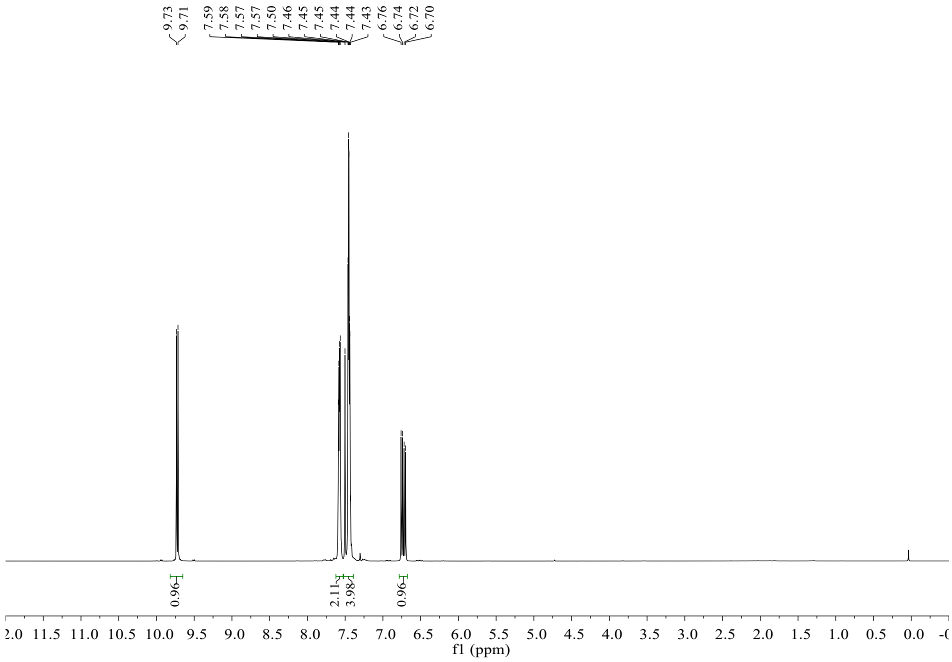


^{13}C NMR spectrogram of 2, 5-diformylfuran

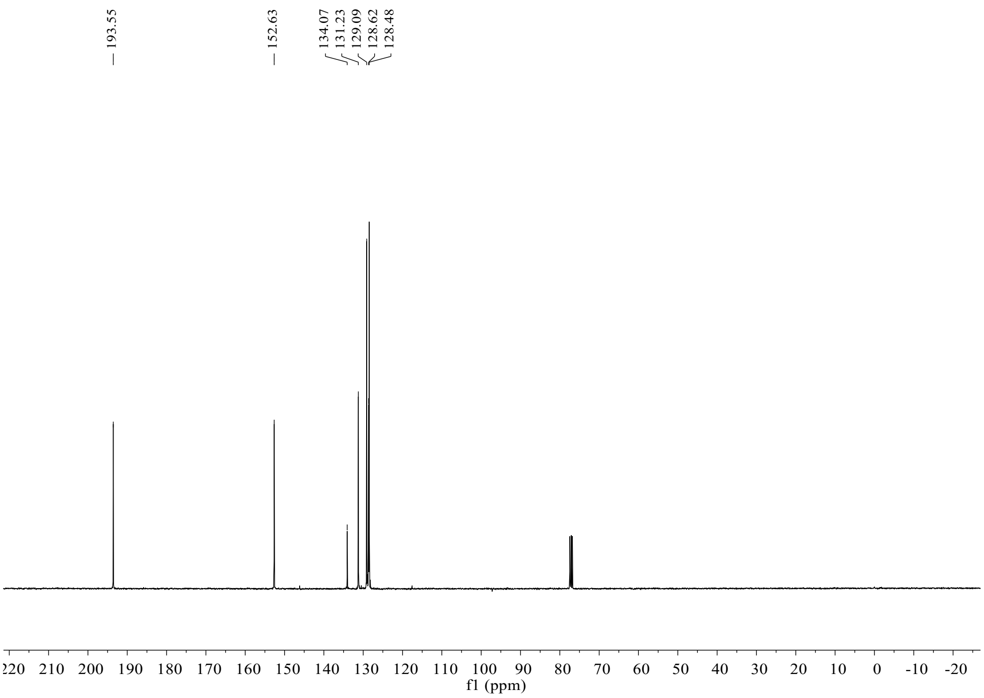
Cinnamaldehyde



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.72 (d, *J* = 7.6 Hz, 1H), 7.58 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.52 – 7.39 (m, 4H), 6.73 (dd, *J* = 15.9, 7.6 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 193.55, 152.63, 134.07, 131.23, 129.09, 128.62, 128.48.



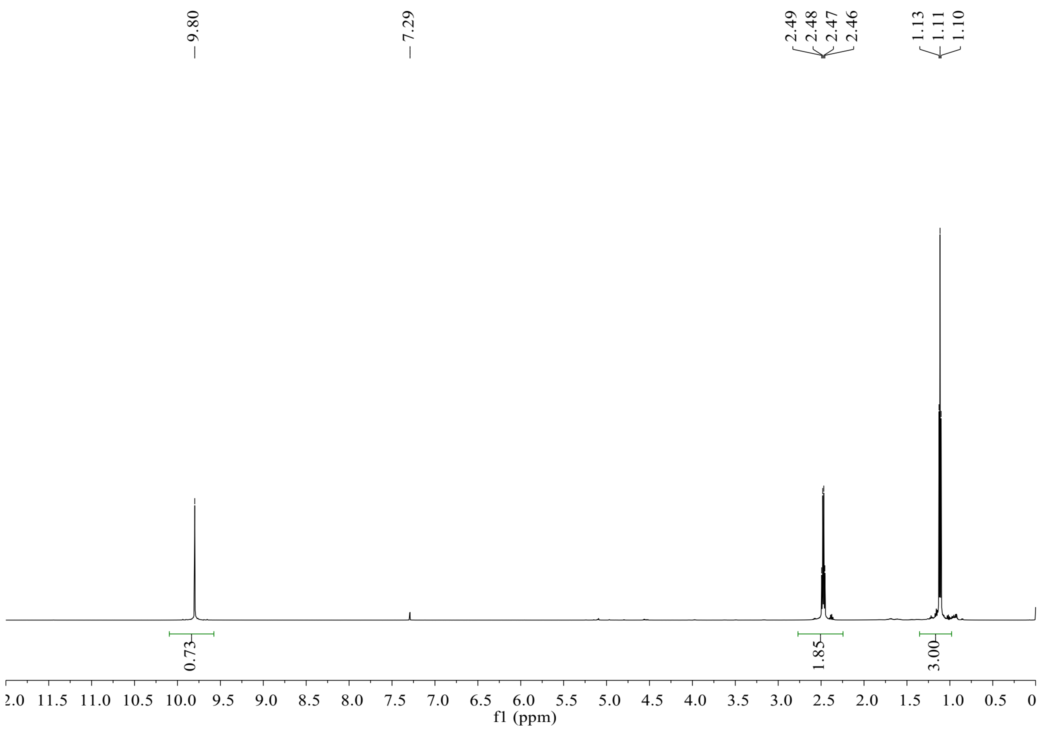
^{1}H NMR spectrogram of cinnamaldehyde



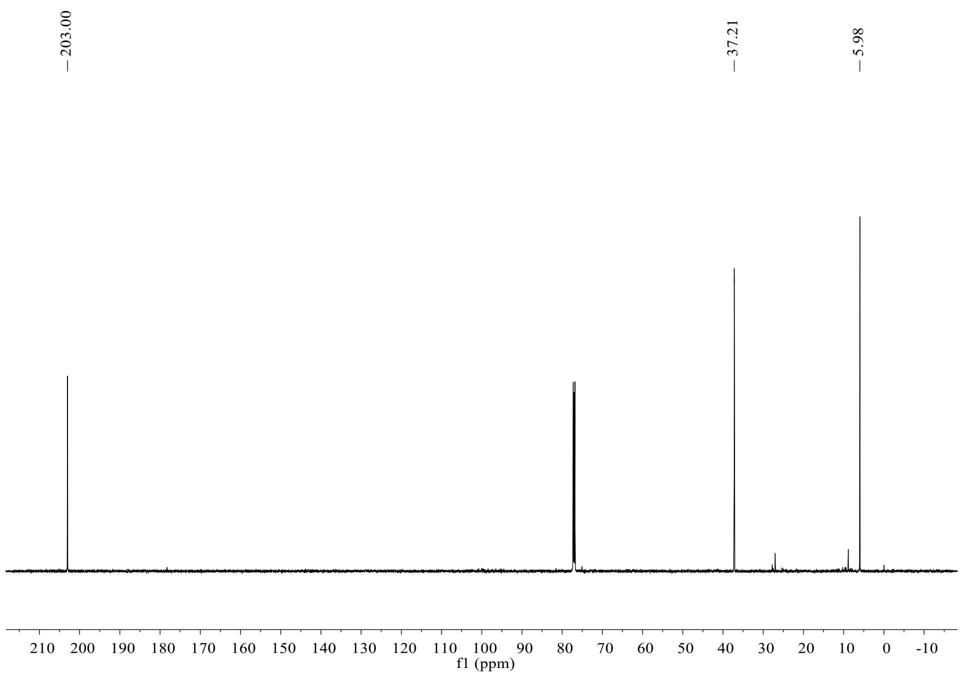
^{13}C NMR spectrogram of cinnamaldehyde

1-Propanal

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.80 (s, 1H), 2.48 (q, *J* = 7.4 Hz, 2H), 1.11 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 203.00, 37.21, 5.98.

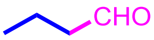


^{1}H NMR spectrogram of 1-propanal

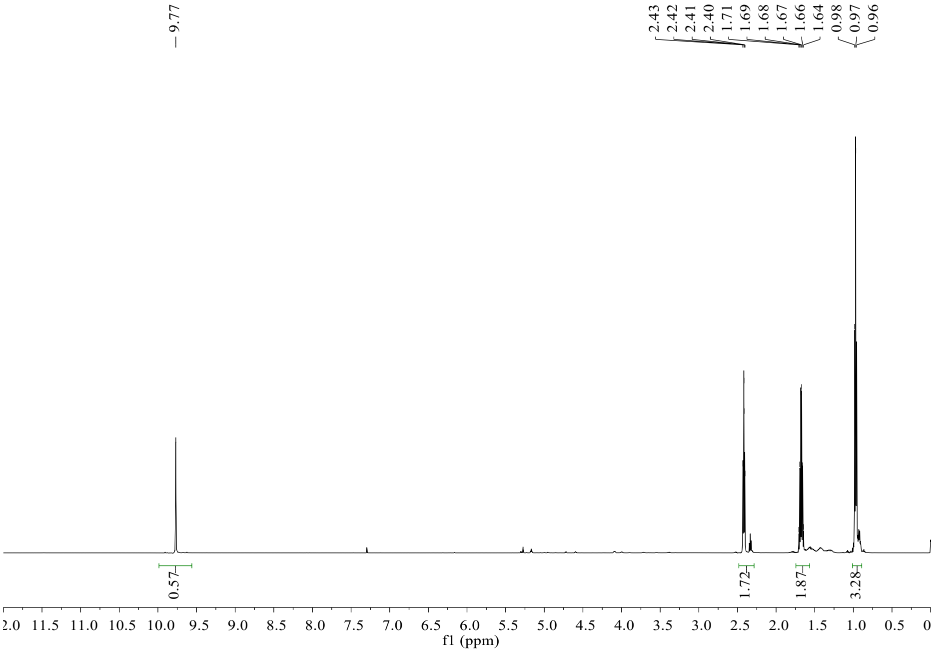


^{13}C NMR spectrogram of 1-propanal

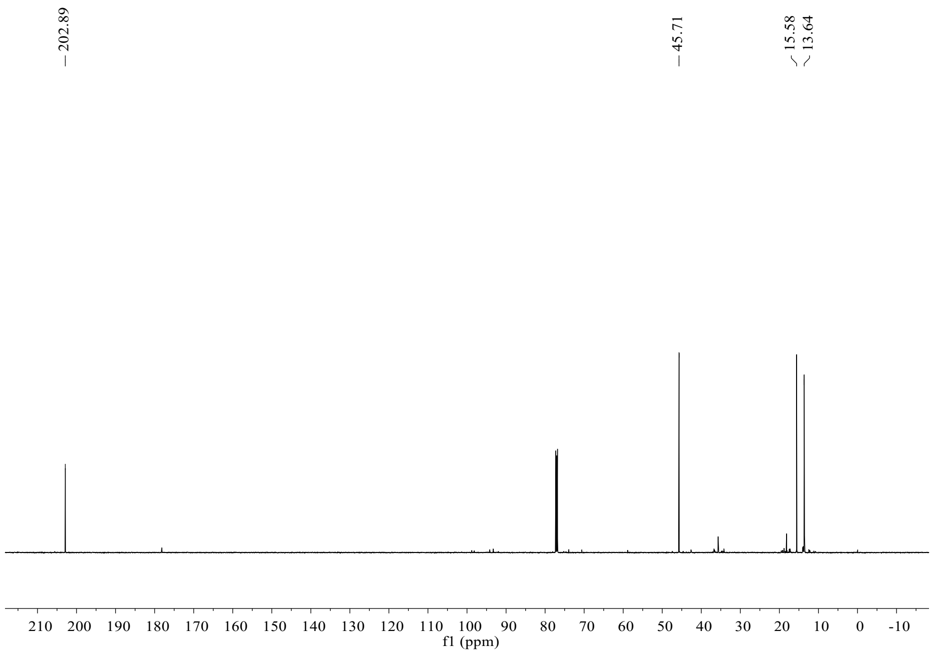
1-**Butyraldehyde**



^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 2.42 (d, *J* = 0.9 Hz, 2H), 1.85 – 1.46 (m, 2H), 0.97 (t, *J* = 7.9 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 202.89, 45.71, 15.58, 13.64.



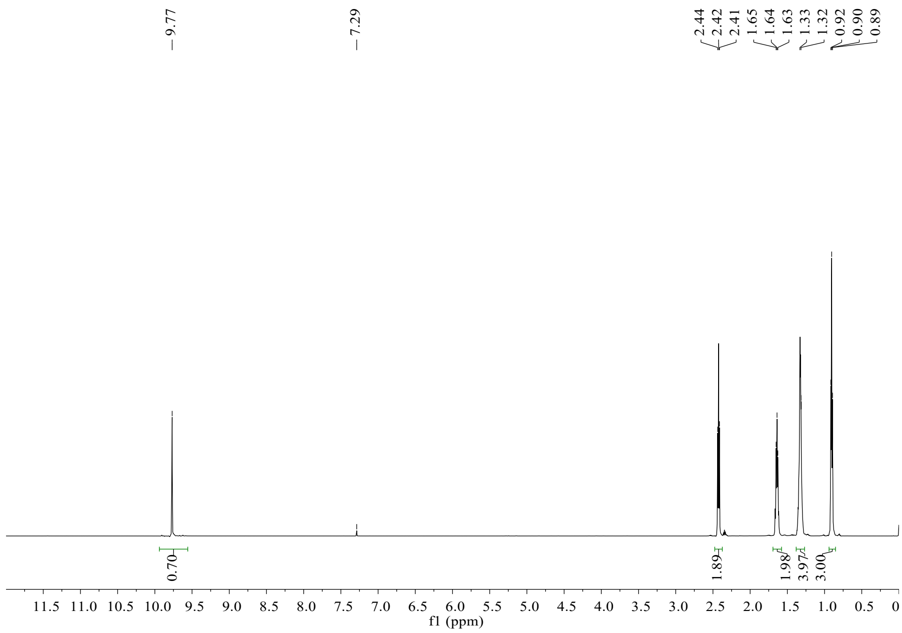
^{1}H NMR spectrogram of 1-Butyraldehyde



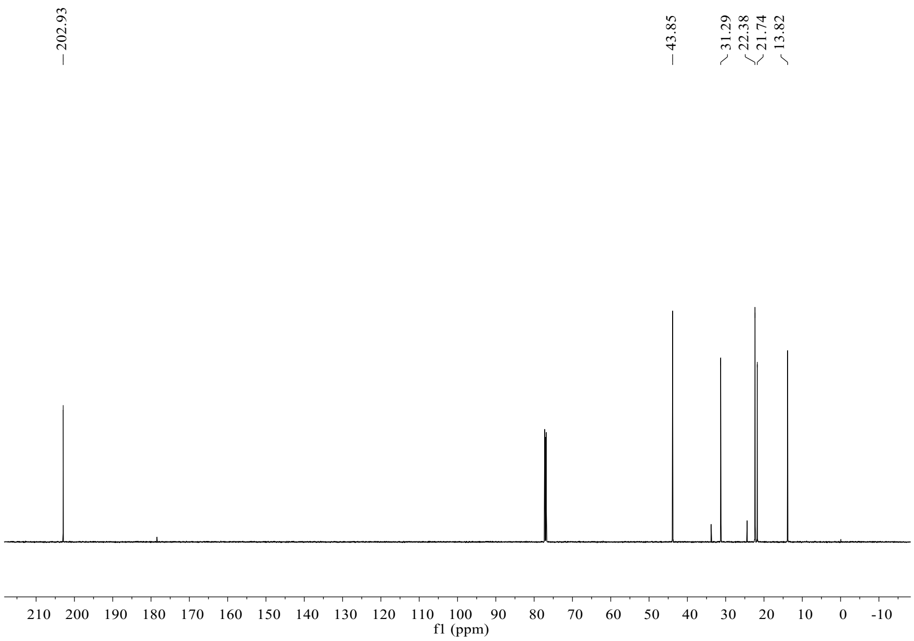
^{13}C NMR spectrogram of 1-Butyraldehyde

1-Pentanecarbaldehyde

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 2.48 – 2.37 (m, 2H), 1.69 – 1.58 (m, 2H), 1.32 (d, J = 9.1 Hz, 4H), 0.90 (t, J = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 202.93, 43.85, 31.29, 22.38, 21.74, 13.82.

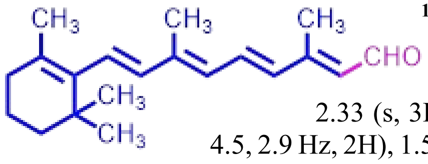


^{1}H NMR spectrogram of 1-pentanecarbaldehyde

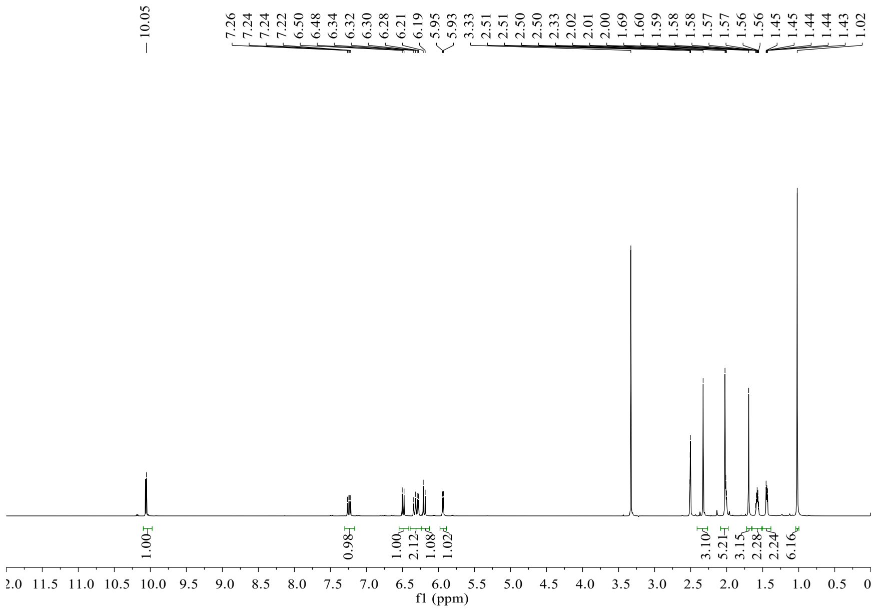


^{13}C NMR spectrogram of 1-pentanecarbaldehyde

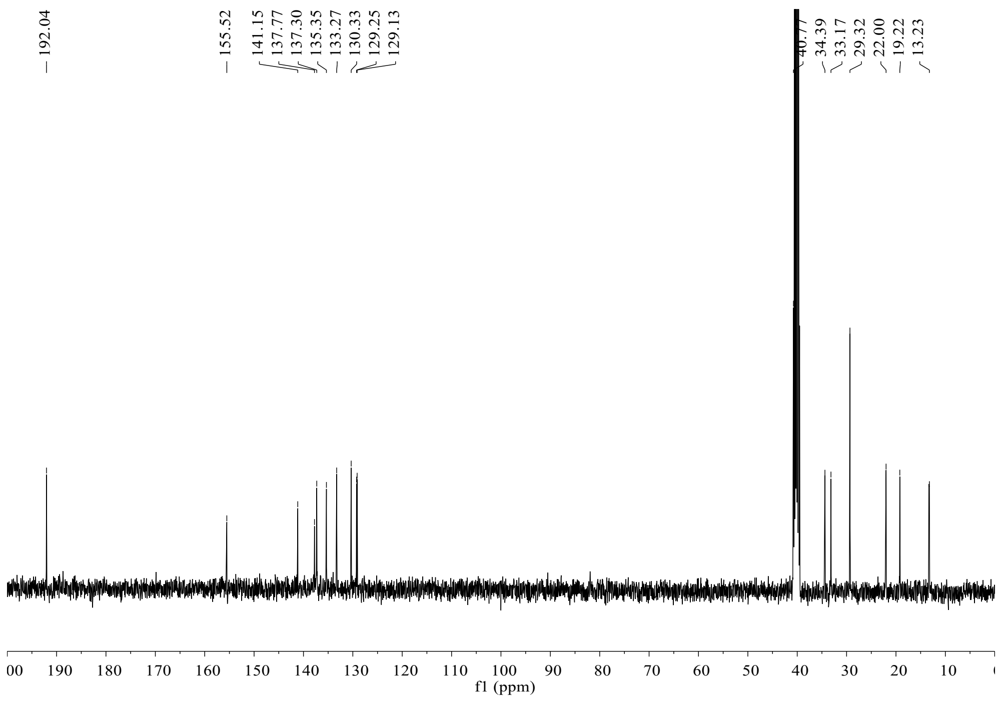
all trans retinoic aldehyde



^{1}H NMR (400 MHz, DMSO-d_6) δ 10.05 (s, 1H), 7.24 (dd, J = 15.1, 11.5 Hz, 1H), 6.49 (d, J = 15.1 Hz, 1H), 6.40 – 6.24 (m, 2H), 6.20 (d, J = 16.1 Hz, 1H), 5.94 (d, J = 8.2 Hz, 1H), 2.33 (s, 3H), 2.02 (d, J = 6.4 Hz, 5H), 1.69 (s, 3H), 1.57 (dp, J = 6.3, 4.5, 2.9 Hz, 2H), 1.50 – 1.38 (m, 2H), 1.02 (s, 6H). **^{13}C NMR (100 MHz, DMSO-*d6*)** δ 192.04, 155.52, 141.15, 137.77, 137.30, 135.35, 133.27, 130.35, 129.19 (d, J = 12.2 Hz), 34.39, 33.17, 29.32, 22.00, 19.22, 13.28 (d, J = 10.3 Hz).

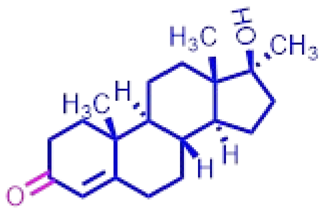


^{1}H NMR spectrogram of all trans retinoic aldehyde

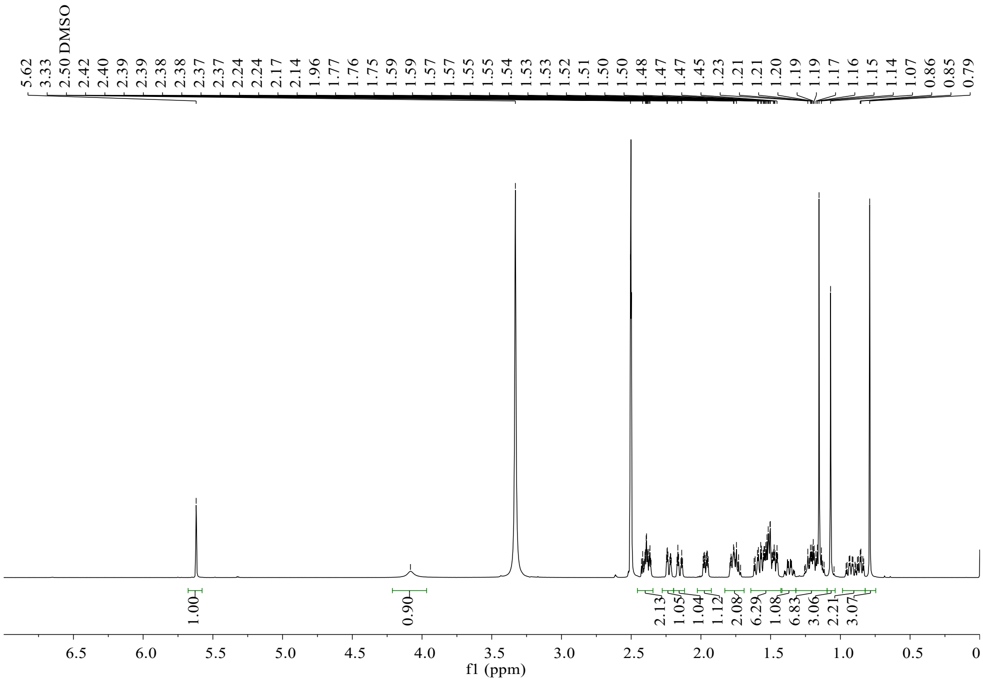


^{13}C NMR spectrogram of all trans retinoic aldehyde

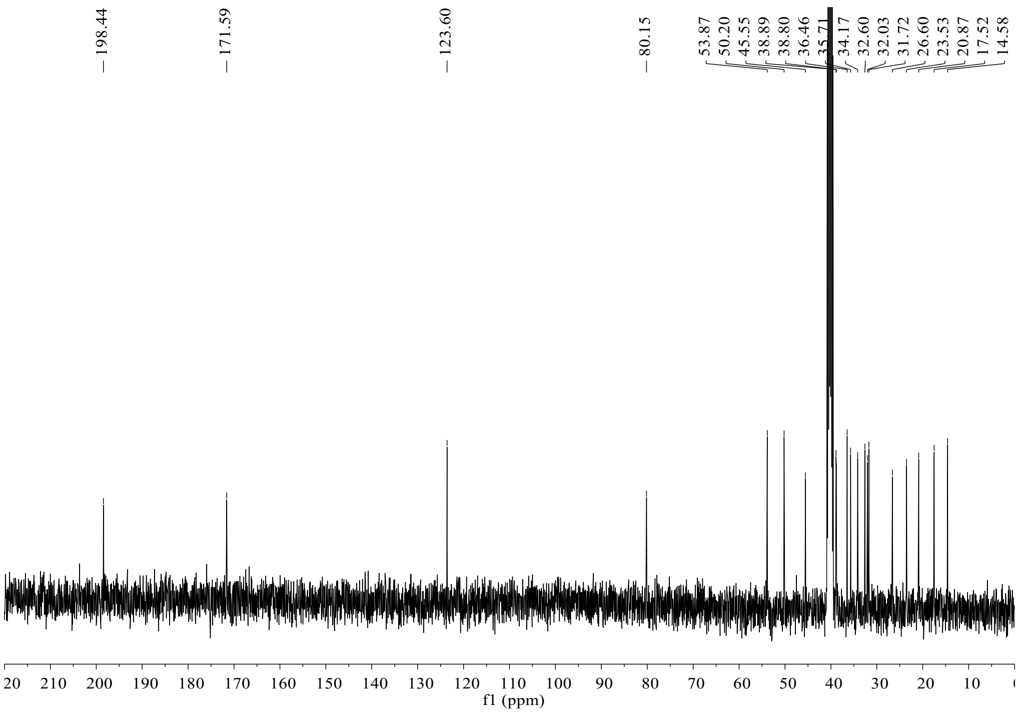
Methyltestosterone



^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 5.62 (s, 1H), 4.08 (s, 1H), 2.39 (dddd, *J* = 14.0, 9.2, 7.8, 4.1 Hz, 0H), 2.23 (ddd, *J* = 14.4, 3.8, 2.4 Hz, 2H), 2.15 (dt, *J* = 16.7, 3.5 Hz, 1H), 1.97 (ddd, *J* = 13.3, 5.0, 3.1 Hz, 1H), 1.76 (ddq, *J* = 17.8, 9.4, 5.2, 3.9 Hz, 2H), 1.64 – 1.42 (m, 6H), 1.37 (qd, *J* = 12.9, 3.9 Hz, 1H), 1.32 – 1.10 (m, 7H), 1.07 (s, 3H), 0.99 – 0.82 (m, 2H), 0.79 (s, 3H). **^{13}C NMR (100 MHz, DMSO-*d6*)** δ 198.44, 171.58, 123.60, 80.15, 53.87, 50.20, 45.55, 38.85 (d, J = 8.3 Hz), 36.46, 35.71, 34.17, 32.60, 32.03, 31.72, 26.60, 23.53.

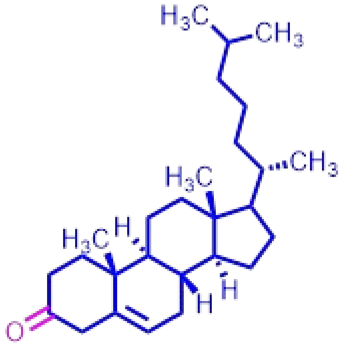


^{1}H NMR spectrogram of Methyltestosterone

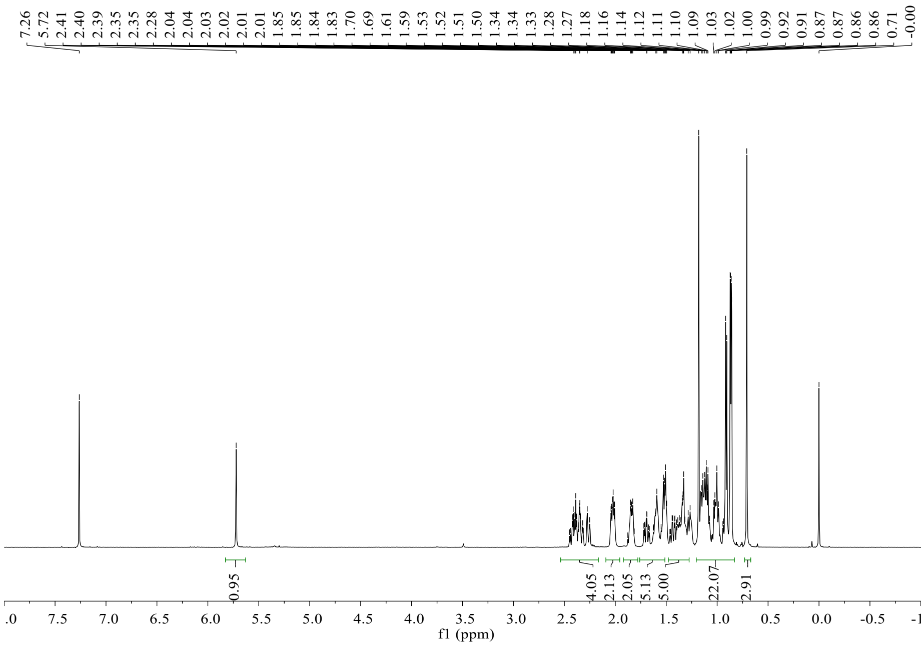


^{13}C NMR spectrogram of Methyltestosterone

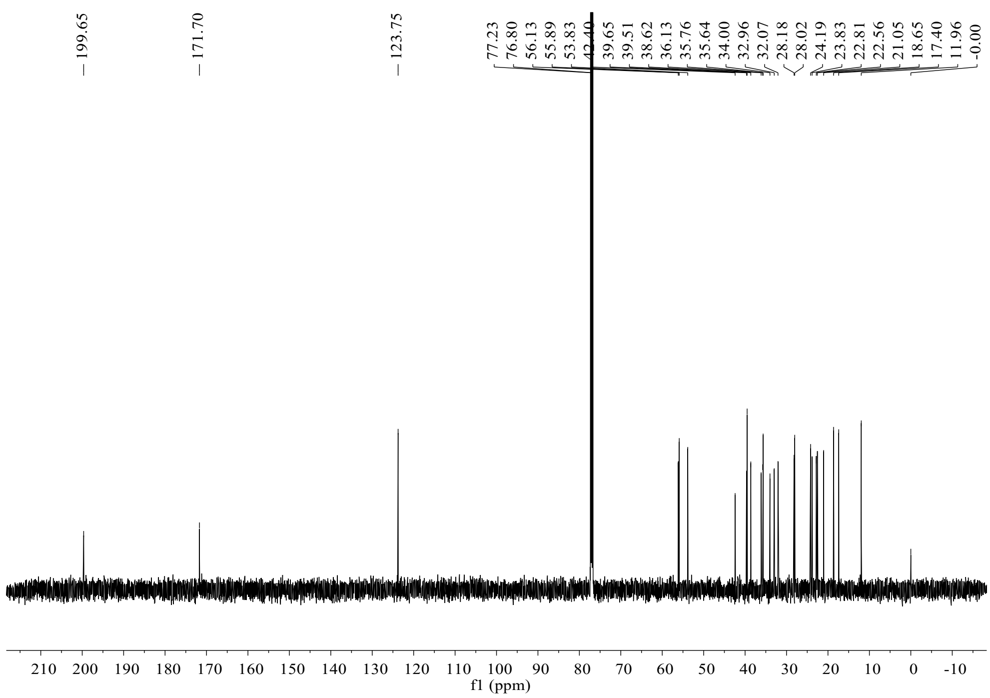
4-Cholesten-3-one



^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.72 (s, 1H), 2.51 – 2.17 (m, 4H), 2.02 (td, *J* = 8.8, 3.9 Hz, 2H), 1.90 – 1.77 (m, 2H), 1.76 – 1.48 (m, 5H), 1.47 – 1.24 (m, 5H), 1.20 – 0.83 (m, 22H), 0.71 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 171.70, 123.75, 56.01 (d, *J* = 34.9 Hz), 53.83, 42.40, 39.58 (d, *J* = 21.5 Hz), 38.62, 37.22 – 34.96 (m), 34.00, 32.96, 32.07, 28.10 (d, *J* = 25.0 Hz), 24.01 (d, *J* = 54.8 Hz), 22.69 (d, *J* = 38.7 Hz), 21.05, 18.65, 17.40, 11.96.

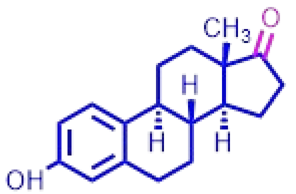


^{1}H NMR spectrogram of 4-Cholesten-3-one

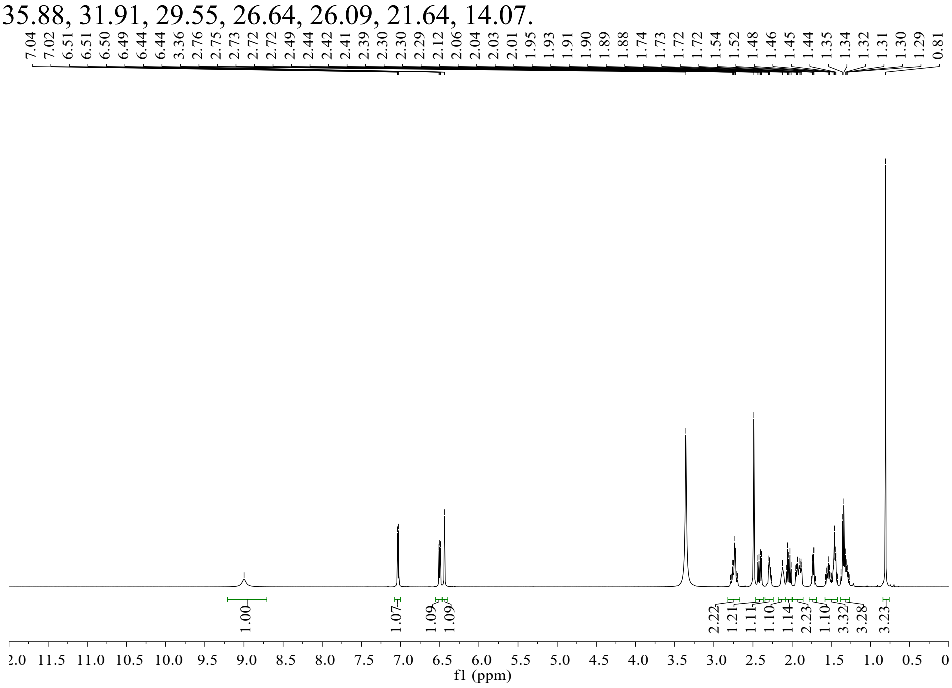


^{13}C NMR spectrogram of 4-Cholesten-3-one

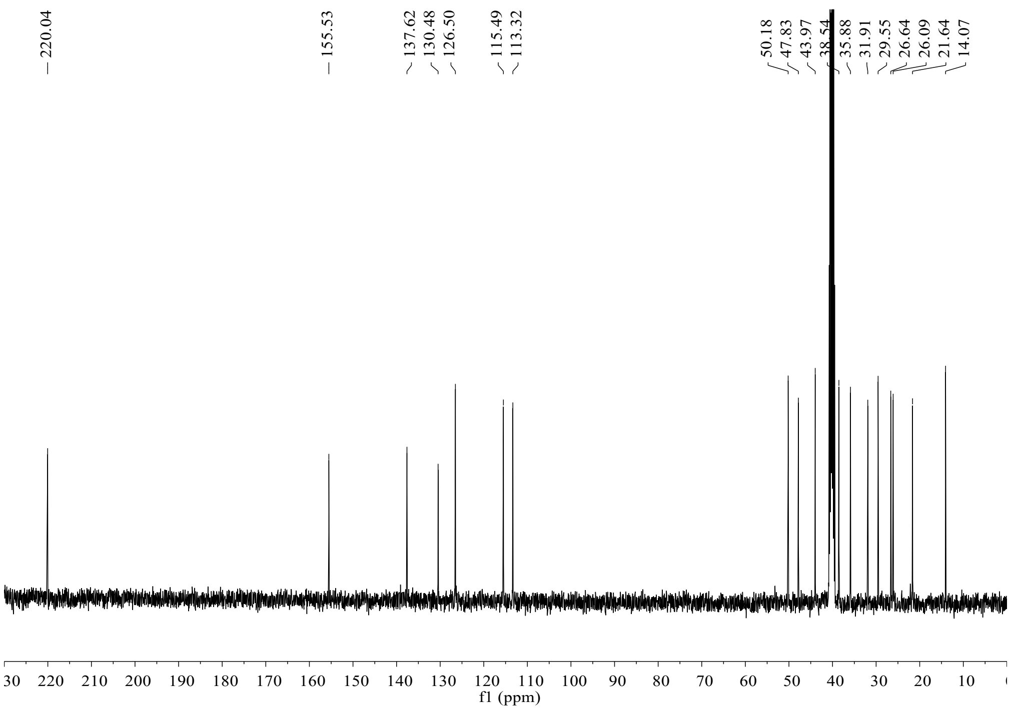
Estrone



^{1}H NMR (400 MHz, DMSO-d_6) δ 9.00 (s, 1H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.50 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.44 (d, *J* = 2.5 Hz, 1H), 2.82-2.67 (m, *J* = 17.1, 6.2 Hz, 4H), 2.41 (dd, *J* = 19.0, 8.4 Hz, 1H), 2.35 – 2.24 (m, 1H), 2.12 (s, 1H), 2.04 (dt, *J* = 18.7, 8.9 Hz, 1H), 1.99 – 1.84 (m, 2H), 1.73 (dd, *J* = 8.7, 2.5 Hz, 1H), 1.58 – 1.41 (m, 3H), 1.38 – 1.25 (m, 3H), 0.81 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 220.04, 155.53, 137.62, 130.48, 126.50, 115.49, 113.32, 50.18, 47.83, 43.97, 38.54, 35.88, 31.91, 29.55, 26.64, 26.09, 21.64, 14.07.

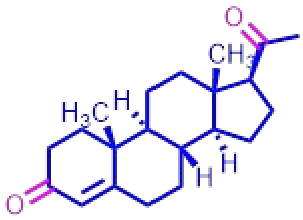


^{1}H NMR spectrogram of Estrone

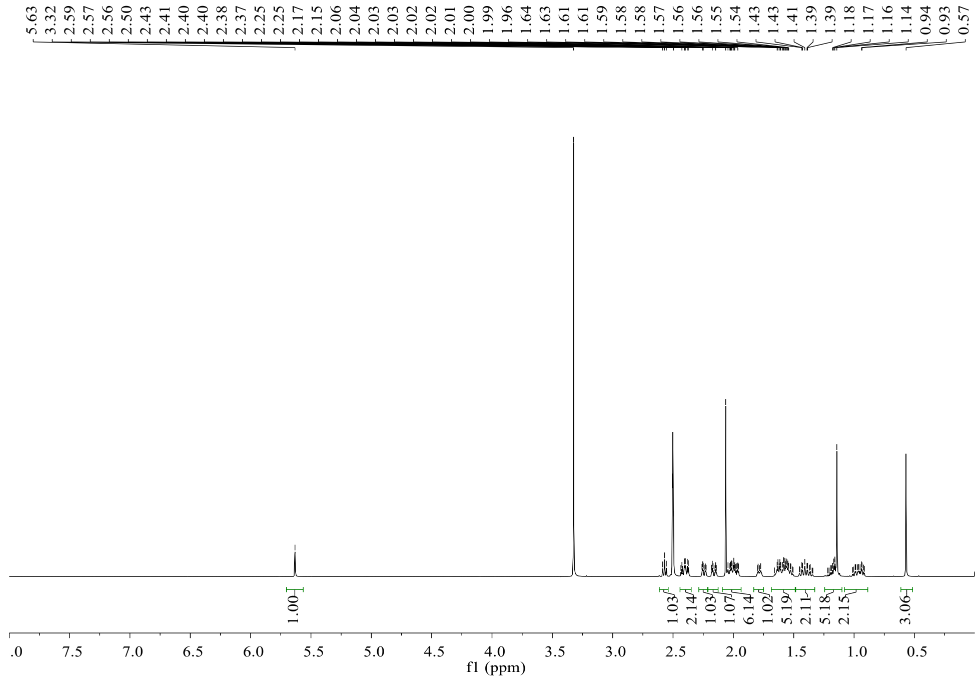


^{13}C NMR spectrogram of Estrone

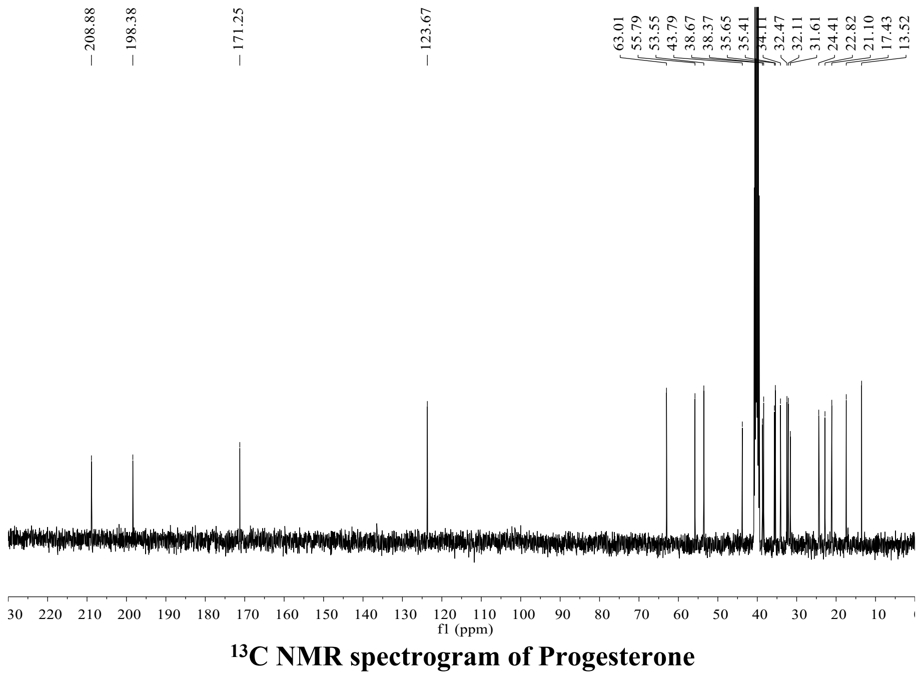
Progesterone



^{1}H NMR (400 MHz, DMSO-d_6) δ 5.63 (s, 1H), 2.57 (t, J = 9.1 Hz, 1H), 2.41 (ddd, J = 19.8, 11.7, 5.1 Hz, 2H), 2.30 – 2.20 (m, 1H), 2.16 (dt, J = 16.2, 3.4 Hz, 1H), 2.08 – 1.93 (m, 6H), 1.79 (dd, J = 10.9, 4.2 Hz, 1H), 1.69 – 1.49 (m, 5H), 1.48 – 1.33 (m, 2H), 1.25 – 1.10 (m, 5H), 1.08 – 0.88 (m, 2H), 0.57 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 208.88, 198.38, 171.25, 123.67, 63.01, 55.79, 53.55, 43.79, 38.67, 38.37, 35.65, 35.41, 34.11, 32.47, 32.11, 31.61, 24.41, 22.82, 21.10, 17.43, 13.52.

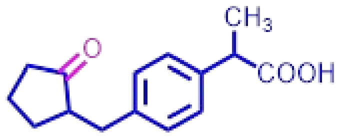


^{1}H NMR spectrogram of Progesterone

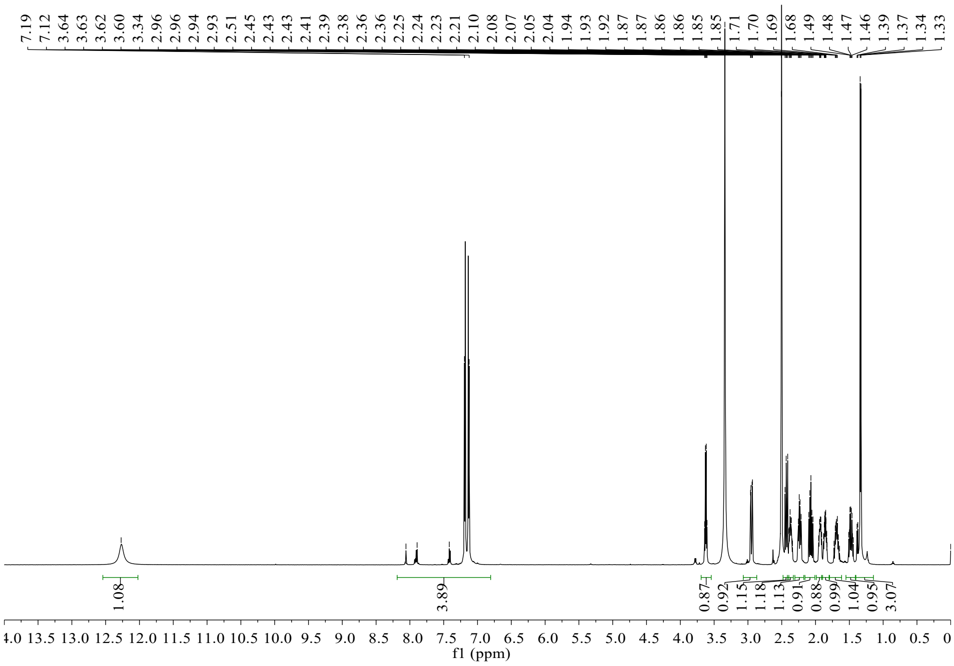


^{13}C NMR spectrogram of Progesterone

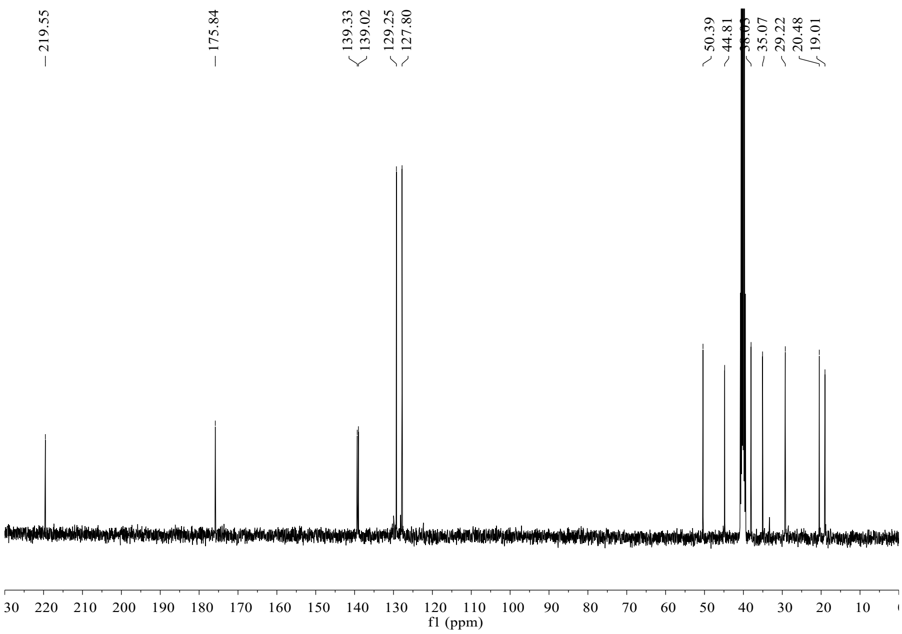
Loxoprofen



^{1}H NMR (400 MHz, DMSO-d_6) δ 12.27 (s, 1H), 8.18 – 6.73 (m, 4H), 3.62 (q, *J* = 7.1 Hz, 1H), 2.95 (dd, *J* = 13.6, 4.0 Hz, 1H), 2.43 (dd, *J* = 13.6, 9.7 Hz, 1H), 2.40 – 2.31 (m, 1H), 2.30 – 2.18 (m, 1H), 2.07 (dt, *J* = 18.8, 9.5 Hz, 1H), 1.93 (dt, *J* = 12.4, 7.4 Hz, 1H), 1.79 – 1.61 (m, 1H), 1.55 – 1.42 (m, 1H), 1.33 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR (100 MHz, DMSO-*d6*)** δ 219.55, 175.84, 139.33, 139.02, 129.25, 127.80, 50.39, 44.81, 38.03, 35.07, 29.22, 20.48, 19.01.



^{1}H NMR spectrogram of Loxoprofen



^{13}C NMR spectrogram of Loxoprofen