Supplementary Data

Synthesis of substituted *t*-butyl 3-methyl-oxindole-3-carboxylates from di-*t*-butyl 2-nitrophenyl-malonates

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1. Figure

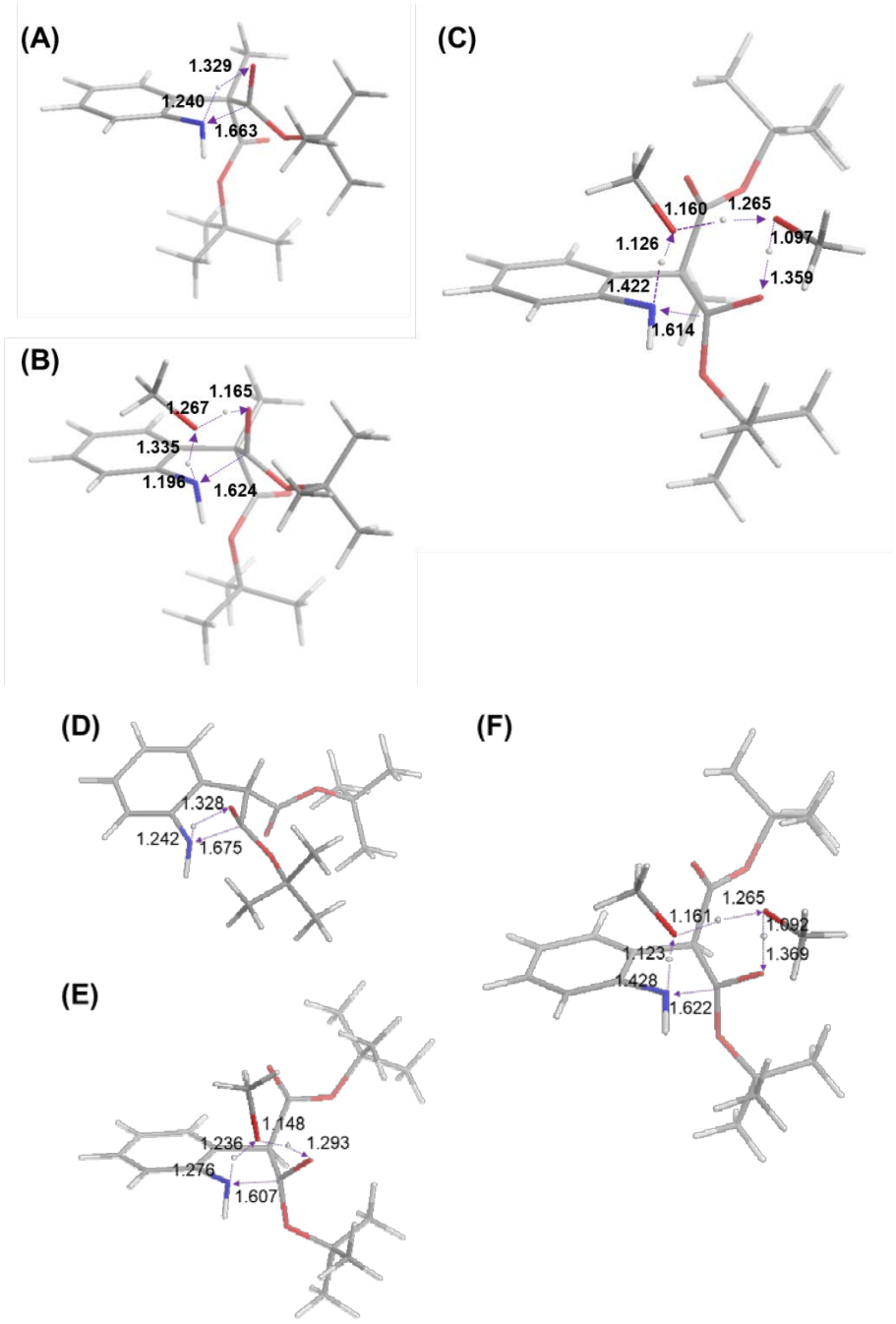
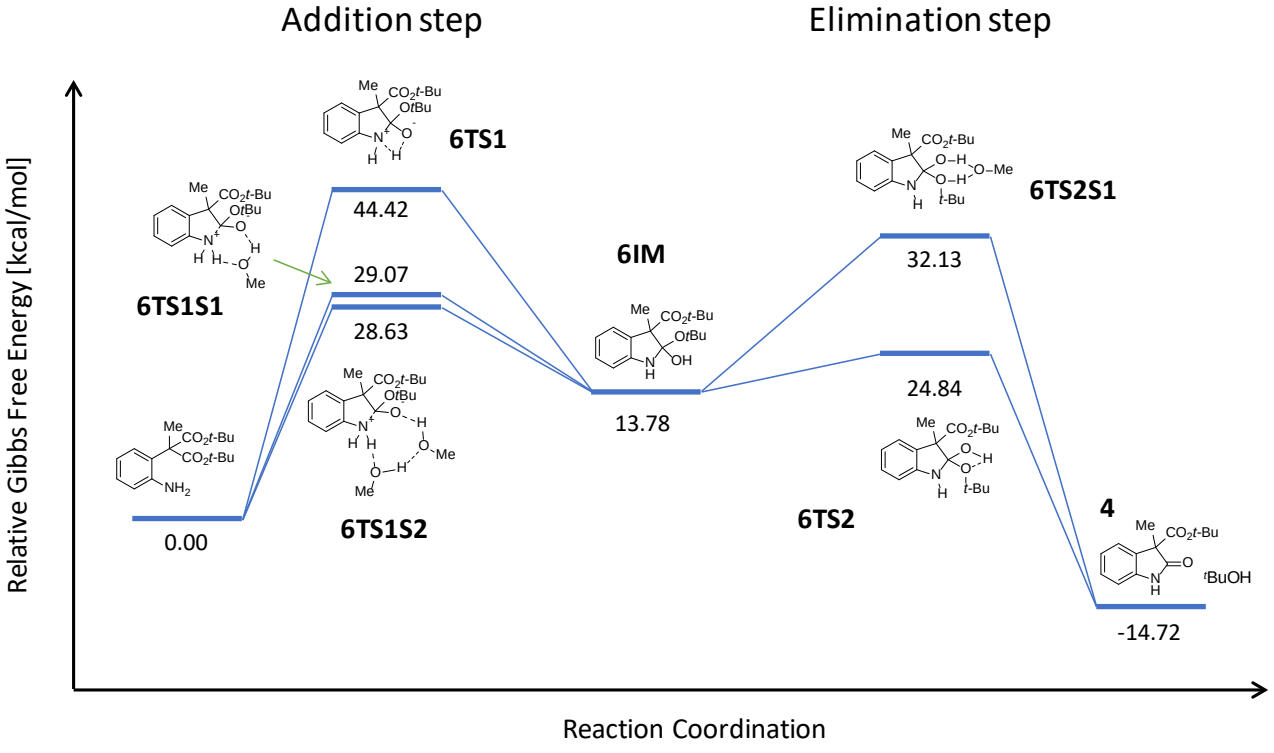
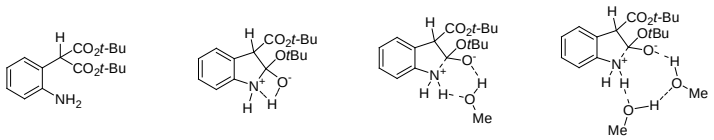


Figure S1. The structures of rate determining steps of cyclization of compounds **5** and **6**. Compound **6** without MeOH (A), with one MeOH (B) and two MeOH (C) and compound **5** without MeOH (D), with one MeOH (E) and two MeOH (F) were shown.

2. Coordinate Information





The cartesian coordination data of all above grand and transition state structures is shown as below.

The cartesian coordination of **6** is as follows:

	0	1	
H	-0.0071361788	2.3177803870	-2.2077956195
C	0.4618114777	2.5287368360	-1.2535779894
C	1.6921797328	3.1114170122	1.1486757126
C	0.4555531437	1.5498599663	-0.2532225875
C	1.0704824161	3.7721951409	-1.0809526071
C	1.7025130535	4.0552867562	0.1277237565
C	1.0641221430	1.8642982219	0.9913659518
H	1.0558643482	4.5006419646	-1.8863344549
H	2.1919023437	5.0131364474	0.2849652429
H	2.1670978325	3.3368649374	2.1017317343
C	-0.1730233884	0.1662377939	-0.5198162465
C	-1.5053162659	0.0283201560	0.2643400596
O	-1.6039132152	0.2608861906	1.4561954842
O	-2.5151084471	-0.3607335257	-0.5170979355
C	0.7253738778	-1.0059596343	-0.0322705152
O	0.2819886968	-1.9779637257	0.5456702862
O	1.9805678433	-0.8401951762	-0.4569133861

C	-3.8699569616	-0.6304413691	0.0211376247
C	3.0360092652	-1.8404578067	-0.1865745032
N	1.1015534750	0.9319498429	2.0337712038
H	1.4577086510	1.3206736063	2.8997459465
H	0.2046452206	0.4728810547	2.1815607367
C	-4.4699069849	0.6589869620	0.5888986810
H	-3.9236324095	0.9946781262	1.4713645780
H	-5.5144572940	0.4804689878	0.8681335461
H	-4.4517235298	1.4539892320	-0.1645779505
C	-4.6309935398	-1.0838978021	-1.2269240718
H	-4.1742113389	-1.9820771907	-1.6548047418
H	-4.6285675022	-0.2981464078	-1.9893728538
H	-5.6703540066	-1.3130859994	-0.9693206090
C	-3.7991171130	-1.7558692492	1.0572792602
H	-3.2736721663	-1.4361681309	1.9580156549
H	-3.2799746739	-2.6247900360	0.6399441931
H	-4.8156747943	-2.0604591533	1.3307684318
C	3.1965494352	-2.0462754893	1.3227114044
H	4.0946974418	-2.6457558140	1.5110050086
H	2.3339171823	-2.5618589977	1.7471868194
H	3.3058212119	-1.0806912846	1.8249312550
C	4.2780121027	-1.1721836884	-0.7802857324
H	5.1503200734	-1.8227125057	-0.6563348618
H	4.4777565534	-0.2199154147	-0.2793399542
H	4.1394154090	-0.9767524691	-1.8486047021
C	2.7060756847	-3.1423064928	-0.9232833685
H	3.5386324944	-3.8466639187	-0.8142016593
H	2.5614377621	-2.9517566697	-1.9925870583
H	1.8032322713	-3.6045286017	-0.5198737392
C	-0.3734480264	-0.1156424816	-2.0305225916
H	0.5741680342	0.0176478111	-2.5571052922
H	-1.1255967526	0.5452015341	-2.4656736216
H	-0.7196245880	-1.1418499325	-2.1747539197

The cartesian coordination of **6TS1** is as follows:

0	1		
H	1.2993306508	0.1179933503	0.4617371179
C	0.7075070870	0.0960655670	1.3728504689
C	-0.8247067931	0.0595069219	3.7338312745
C	0.0670805369	-1.0767772391	1.7675796560
C	0.5716016206	1.2512944762	2.1483136108
C	-0.1941687419	1.2348743590	3.3173299218
C	-0.6853104165	-1.0792523637	2.9464530005
H	1.0645969603	2.1685253403	1.8385100339
H	-0.2936063377	2.1373800010	3.9139197454
H	-1.4033824676	0.0321369768	4.6531712208
C	0.0277543634	-2.4114702446	1.0418116901
N	-1.1842070286	-2.3847764094	3.2571358915
H	-2.1884238577	-2.4539828789	3.4281707720
H	-0.3425640955	-3.1196140605	3.7942097026
C	-0.5226719347	-3.4128947560	2.1300256854
O	0.3627799849	-3.9122031035	2.9944577465
O	-1.4587774589	-4.2489178525	1.5541281636
C	-1.7357777264	-5.5991190289	2.0576835314
C	1.4003608949	-2.8924219601	0.5570686540
H	1.8270176542	-2.1845685986	-0.1595617646
H	1.3057194800	-3.8564545684	0.0514151850
H	2.0690522065	-3.0018269182	1.4124198471
C	-0.9433979510	-2.3187616714	-0.1561180162

O	-0.6693116831	-2.6973712938	-1.2750061139
O	-2.1015108143	-1.7372740723	0.2085908681
C	-3.1921963075	-1.5000812452	-0.7546696398
C	-2.1459335946	-5.5813207206	3.5362135772
H	-1.3088735536	-5.2950309215	4.1750331639
H	-2.4831528715	-6.5800613241	3.8362690384
H	-2.9824053696	-4.8900720548	3.6989989799
C	-0.5273306400	-6.5108011266	1.8121940156
H	0.3313212755	-6.1750463162	2.3941914703
H	-0.2602828366	-6.5006771732	0.7497852682
H	-0.7750859812	-7.5418268317	2.0917682874
C	-2.9198843602	-6.0379361493	1.1889104847
H	-2.6534016358	-5.9914319881	0.1285136708
H	-3.7872285352	-5.3895725498	1.3552528841
H	-3.2066011441	-7.0670882496	1.4310672960
C	-4.2711411818	-0.8571236038	0.1208914665
H	-3.8944028018	0.0591120920	0.5868268230
H	-4.5844964624	-1.5450234788	0.9134480717
H	-5.1487409555	-0.6052113364	-0.4838851951
C	-2.7209094894	-0.5255519303	-1.8393351296
H	-1.9384453045	-0.9714185756	-2.4555324123
H	-2.3349842177	0.3930812918	-1.3839476354
H	-3.5653429266	-0.2574236612	-2.4844750184
C	-3.6858728464	-2.8277913881	-1.3377221467
H	-2.9264026109	-3.2883415027	-1.9710199745
H	-4.5863119965	-2.6509098908	-1.9371211144
H	-3.9398777849	-3.5235413382	-0.5317841244

The cartesian coordination of **6TS1S1** is as follows:

	0	1	
H	0.9914986535	0.2652564598	0.1540130649
C	1.0961244536	0.5387109685	1.2001871142
C	1.3803355428	1.2642010214	3.9105208071
C	0.6854697902	-0.3343057897	2.2038498390
C	1.6435640290	1.7772162074	1.5531136432
C	1.7821764786	2.1393287521	2.8952131374
C	0.8345433963	0.0429641550	3.5385917067
H	1.9671215782	2.4624895343	0.7745558010
H	2.2122950229	3.1021056868	3.1559564335
H	1.4953130832	1.5302438950	4.9574979036
N	0.4026309780	-1.0001277240	4.4445975068
H	1.2560661738	-1.2980897680	5.2281921580
H	-0.5206816137	-0.8158910449	4.8410552684
C	0.0356080228	-1.6999239047	2.0829126812
C	0.2897781326	-2.3293785564	3.5188313146
O	1.4540458126	-2.9624368081	3.6065994005
O	-0.8704211249	-3.0081627556	3.9089872521
C	-0.8940505105	-4.2184224338	4.7367046362
H	1.9882444310	-2.6698943109	4.6002351081
O	2.2669613367	-2.0506121548	5.6701687450
C	3.5541838442	-1.4666167202	5.6470028190
H	3.7856794206	-0.9920215015	4.6796516828
H	4.3216795455	-2.2293135815	5.8395167001
H	3.6414068644	-0.7017638134	6.4316437534
C	-0.3356877488	-3.9495254015	6.1393028809
H	0.7246856265	-3.6908096299	6.1294920372
H	-0.4638434890	-4.8426290690	6.7622599005
H	-0.8868199438	-3.1311780279	6.6190261024
C	-0.1760575508	-5.3831365658	4.0408940051

H	-0.5694977496	-5.5133453497	3.0268009611
H	-0.3584109376	-6.3098265939	4.5980695812
H	0.8976122147	-5.2109749409	3.9753246776
C	-2.3966753648	-4.5159119396	4.8220872930
H	-2.9285665611	-3.6896122927	5.3061792772
H	-2.5697445584	-5.4258918883	5.4066994192
H	-2.8173172409	-4.6579179169	3.8216657262
C	-1.4802957259	-1.5238044994	1.8296656144
O	-2.0825681975	-2.0878828396	0.9426316117
O	-2.0179131605	-0.6355251692	2.6915668325
C	-3.4377900271	-0.2361941718	2.6167699870
C	-3.7023676879	0.4673569538	1.2815058947
H	-3.5918691848	-0.2233856104	0.4440388263
H	-3.0078183557	1.3039003637	1.1471789307
H	-4.7226705243	0.8670466743	1.2732045799
C	-4.3464137684	-1.4509588824	2.8272451598
H	-4.2687813851	-2.1512729562	1.9946874621
H	-5.3866518064	-1.1164474837	2.9131556507
H	-4.0759382017	-1.9722256605	3.7509309328
C	-3.5672584264	0.7480611554	3.7822673680
H	-3.3577999237	0.2502518317	4.7355538829
H	-4.5844988905	1.1511557879	3.8244729233
H	-2.8682094064	1.5823840423	3.6637985930
C	0.6344030525	-2.5867933542	0.9891505618
H	1.7019743310	-2.7199062692	1.1687741232
H	0.4766894360	-2.1405743231	0.0029279785
H	0.1495278150	-3.5659817860	0.9880727479

The cartesian coordination of **6TS1S2** is as follows:

	0	1	
H	-0.3630895838	4.4073825309	0.7417231538
C	0.0003719532	3.6374030673	1.4173660458
C	0.9208046500	1.6546269626	3.1887617192
C	-0.1237095644	2.2921666819	1.0836784826
C	0.5876583520	3.9952100502	2.6360777806
C	1.0418853897	3.0092190313	3.5148973848
C	0.3395481442	1.3155323542	1.9698612900
H	0.6849364116	5.0442370516	2.9016825633
H	1.4910421651	3.2931583567	4.4629177410
H	1.2673941621	0.8853100184	3.8745990502
N	0.1547244626	-0.0047694700	1.4539786713
H	1.3802865397	-0.6039049467	1.0540375063
H	-0.2375744181	-0.6260251899	2.1631341396
C	-0.7355650593	1.6607877893	-0.1509374410
C	-0.9556121826	0.1228897403	0.2896687146
O	-0.8362805405	-0.7830550124	-0.6429188305
O	-2.1832465853	0.1138666518	1.0087031054
C	-3.0788122629	-1.0307558184	1.0277226871
H	1.9309745283	-1.5090080411	-0.3329456311
O	2.2831437331	-1.1916104416	0.7256299514
C	3.4801112322	-0.3941481501	0.7066531178
H	4.2913760567	-1.0083020718	0.3053578531
H	3.7247058871	-0.1120032570	1.7348025242
H	3.3413113820	0.4993306655	0.0949257256
H	0.3454130643	-1.2615590478	-1.1130829535
O	1.2772195418	-1.7757558208	-1.3827657094
C	1.0050495568	-3.1706091223	-1.5111062982
H	0.2685681644	-3.3276267447	-2.3057668073
H	0.6152737396	-3.5999791238	-0.5782740212

H	1.9317532961	-3.6863051491	-1.7810430996
C	0.3240382895	1.6217932338	-1.2660382419
O	1.4738131674	1.2685320738	-1.0723084188
O	-0.1670515221	2.0124514510	-2.4489649461
C	0.6358297890	1.9855313138	-3.6894097647
C	-2.0458054422	2.3216388654	-0.5935385001
H	-1.8635931858	3.3292744019	-0.9803089279
H	-2.7310969688	2.3816816962	0.2527311549
H	-2.5175216065	1.7393822506	-1.3888824924
C	-3.7464408957	-1.2331910756	-0.3410497883
H	-3.0089852369	-1.5167103865	-1.0919168648
H	-4.2306996740	-0.3037954419	-0.6600750800
H	-4.5163086579	-2.0119860328	-0.2738051100
C	-2.3657149502	-2.3108021077	1.4938684180
H	-1.5762821601	-2.5875668359	0.7929926642
H	-3.0825918471	-3.1375957689	1.5604628491
H	-1.9327463787	-2.1738623542	2.4936851002
C	-4.1306042553	-0.6149886822	2.0653577816
H	-3.6631062832	-0.4365007140	3.0396129545
H	-4.8876232743	-1.3990824653	2.1792630585
H	-4.6311839908	0.3076182179	1.7540465739
C	1.0127054474	0.5398400924	-4.0238060367
H	1.5184623159	0.5116382408	-4.9961158879
H	0.1116921041	-0.0791664279	-4.0871494602
H	1.6712130080	0.1087555377	-3.2689389508
C	1.8590930107	2.8983707318	-3.5529973761
H	2.3585272997	2.9828088264	-4.5250301832
H	2.5694735614	2.5059164016	-2.8247409225
H	1.5524879515	3.9034474795	-3.2422937484
C	-0.3423302690	2.5464616039	-4.7250699437
H	0.1284793742	2.5667128558	-5.7137140496
H	-0.6429434096	3.5663382501	-4.4633768217
H	-1.2418475270	1.9253512237	-4.7808274551

The cartesian coordination of **6IM** is as follows:

	0	1	
H	-2.5286550666	0.2224437479	1.1422572635
C	-2.2507193728	0.0466895255	2.1763386819
C	-1.5233075823	-0.4085089195	4.8643791871
C	-1.3559141806	-0.9646623580	2.4998165081
C	-2.7989101676	0.8284629322	3.2025369785
C	-2.4357948118	0.5979245813	4.5308978333
C	-0.9907403352	-1.1832299748	3.8363486469
H	-3.5085070077	1.6148800277	2.9616321718
H	-2.8661694293	1.2071001163	5.3216151711
H	-1.2395033620	-0.5835405812	5.8988358018
C	-0.5446434229	-1.9190623403	1.6289770862
N	-0.0338440255	-2.2098835823	3.9453317867
H	-0.1528541590	-2.7963611684	4.7666535935
C	-0.1053019250	-2.9997813630	2.7078547628
O	1.0989400994	-3.5541903168	2.2665259137
O	-1.0863518131	-3.9797852012	2.9310999972
C	0.6858081880	-1.1726392075	1.0505203259
H	0.3521733125	-0.3319640523	0.4379563802
H	1.3019834229	-1.8425340007	0.4455169162
H	1.2983200301	-0.7926667565	1.8717610787
C	-1.3266300860	-2.5462284976	0.4693222344
O	-1.5568337866	-3.7389220144	0.3367433993
O	-1.6961998540	-1.6103348979	-0.4140337287

C	-2.4449147991	-1.9368867279	-1.6526018110
C	-2.6194519774	-0.5626345220	-2.3030549402
H	-1.6467869594	-0.1003245816	-2.4991273529
H	-3.1958285238	0.1056670840	-1.6551426168
H	-3.1525281442	-0.6648903742	-3.2540477169
C	-1.6004713825	-2.8544763753	-2.5420125431
H	-1.4640659274	-3.8364407291	-2.0869864355
H	-0.6172202666	-2.4082809183	-2.7265206601
H	-2.1009203119	-2.9821418728	-3.5084297242
C	-3.8023018223	-2.5488515596	-1.2950591279
H	-3.6882391345	-3.5303273383	-0.8327608202
H	-4.4010241202	-2.6578538294	-2.2063142579
H	-4.3474704800	-1.8940443654	-0.6068373518
H	-1.2824787467	-4.3596621597	2.0498965137
C	2.0092808987	-4.3290253146	3.0993431966
C	1.3040965665	-5.3111116678	4.0471482106
H	2.0611796961	-5.9408762570	4.5290179454
H	0.6073287285	-5.9535664015	3.5043402296
H	0.7444532557	-4.8071522385	4.8403772173
C	2.9287700891	-3.3708608325	3.8729479669
H	3.4370109302	-2.6945754025	3.1776686960
H	3.6909821728	-3.9362559905	4.4222225643
H	2.3648172690	-2.7614731000	4.5826344597
C	2.8233294198	-5.1153385753	2.0629866837
H	3.2945767620	-4.4293985962	1.3516956109
H	2.1746912292	-5.7969837536	1.5032914825
H	3.6088409135	-5.7014392990	2.5524365913

The cartesian coordination of **6TS2** is as follows:

	0	1	
H	-0.3325294618	0.7890174409	1.7829459020
C	-0.2168712386	0.0755521348	2.5914868754
C	0.1488556302	-1.7731877477	4.7092086982
C	0.0190914394	-1.2636511008	2.3180386253
C	-0.2724662983	0.4938378440	3.9287405770
C	-0.0963269917	-0.4191641639	4.9705406471
C	0.2033742864	-2.1627698302	3.3778378765
H	-0.4486554209	1.5412584027	4.1554329849
H	-0.1417475355	-0.0780999747	6.0009889743
H	0.2950191817	-2.4845968555	5.5170027925
C	0.0506743734	-2.0440626123	1.0163718112
C	0.6136184722	-3.4031547610	1.4946352825
N	0.4390338970	-3.4427723148	2.8414121987
H	0.6883187863	-4.2640365752	3.3755532049
O	0.6444355300	-4.5117728343	0.7920368226
O	2.5294173660	-3.2680288416	0.8930406444
H	1.6884125777	-4.3361388580	0.5090772775
C	3.7323767652	-3.2983135032	1.6423532253
C	3.7579446179	-4.4971785889	2.6143070417
H	4.7243435493	-4.5774695632	3.1266357785
H	3.5823928490	-5.4341510972	2.0722835586
H	2.9875776516	-4.3974167347	3.3874073482
C	4.8929473285	-3.4418929457	0.6378580575
H	5.8611737901	-3.4956992296	1.1512684049
H	4.9111613814	-2.5869104892	-0.0451030580
H	4.7693964959	-4.3544036005	0.0428144153
C	3.8746313538	-1.9747597209	2.4138532745
H	4.8397208970	-1.9165822090	2.9322980233
H	3.0808750025	-1.8701913666	3.1614441944

H	3.7943252521	-1.1309520885	1.7215755457
C	-1.4002126048	-2.3142793220	0.5168939649
H	-1.3826463944	-3.0214722914	-0.3138276656
H	-1.8581527009	-1.3769926861	0.1853718647
H	-2.0093276758	-2.7245720271	1.3278966121
C	0.8609929153	-1.3764231385	-0.1079019016
O	1.4097818184	-0.3015082440	0.0084956971
O	0.7641748004	-2.0992035960	-1.2302064392
C	1.4046212997	-1.6771016576	-2.4938023532
C	2.9185053610	-1.5610926667	-2.3036752056
H	3.1727152062	-0.7187285643	-1.6584481188
H	3.3971444155	-1.4173527230	-3.2792413882
H	3.3084039933	-2.4761370805	-1.8505459150
C	0.7711809913	-0.3687787201	-2.9770308425
H	0.9930941944	0.4515404872	-2.2923067434
H	-0.3157493372	-0.4774274142	-3.0639488263
H	1.1664652798	-0.1150774080	-3.9671826412
C	1.0604941202	-2.8333258337	-3.4357767568
H	1.4740353015	-2.6430802195	-4.4319023013
H	-0.0244912859	-2.9494580970	-3.5274329933
H	1.4764487746	-3.7728370128	-3.0587750520

The cartesian coordination of **6TS2S1** is as follows:

	0	1	
H	0.2036006345	-1.6624326159	0.4635650686
C	-0.1795447087	-1.5968193184	1.4780409600
C	-1.1795573339	-1.4444946069	4.1186488462
C	-0.1412938439	-2.6883767248	2.3382630976
C	-0.7324445193	-0.4075256297	1.9670749453
C	-1.2258531833	-0.3288877635	3.2707254143
C	-0.6288922462	-2.6299653388	3.6519576599
H	-0.7747356351	0.4638170434	1.3193824202
H	-1.6499951855	0.6032626650	3.6325313141
H	-1.5620937970	-1.3778028756	5.1316066314
C	0.3479277484	-4.7705466268	3.2107752777
O	0.3605806845	-6.0501056712	3.0289314322
O	2.0804085072	-4.5034596997	4.1932059610
C	3.3024883822	-4.0219511139	3.6252129171
C	3.2215037978	-2.5005539149	3.4225690927
H	4.1839280024	-2.0973912415	3.0836155050
H	2.9541227260	-2.0126482561	4.3659865066
H	2.4635678438	-2.2309175940	2.6823105373
C	4.4225760537	-4.3342025021	4.6402000006
H	5.3917449751	-3.9632433744	4.2846598216
H	4.5111402223	-5.4148327009	4.7996360704
H	4.2069354623	-3.8613897058	5.6039596732
C	3.6320604032	-4.7372042223	2.2976026063
H	4.6325141008	-4.4613525886	1.9428314030
H	2.9221682307	-4.4686635847	1.5085327340
H	3.6008488760	-5.8232400026	2.4326238945
H	1.0456606029	-6.6182904808	3.7484001341
O	2.0879486889	-6.9171568077	4.4288130112
H	2.2324482229	-5.8331510505	4.5251882380
C	1.9221692729	-7.6345037689	5.6518268331
H	2.8417938217	-7.5612900965	6.2444125162
H	1.7514010475	-8.6885118829	5.4092356223
H	1.0822979675	-7.2478256373	6.2354119331
C	-0.5406330824	-4.0203452599	4.2610975756
N	0.3346251486	-3.9781832599	2.0901723565

H	0.7203606542	-4.3072877474	1.2173585045
C	-1.9371770538	-4.7035557135	4.2203655850
H	-1.8497261599	-5.7384925512	4.5558720305
H	-2.3398586135	-4.6866754609	3.2037240849
H	-2.6326412439	-4.1690160806	4.8754791890
C	-0.0286838686	-4.1445809392	5.7025954021
O	-0.0173737973	-5.2121759861	6.2840831837
O	0.2619498621	-2.9594444120	6.2489539206
C	0.6494312072	-2.8291047906	7.6707287631
C	-0.5249812613	-3.2497475428	8.5602577482
H	-0.7429445806	-4.3133414977	8.4496474036
H	-1.4225512220	-2.6738956707	8.3080945067
H	-0.2790717531	-3.0503404641	9.6093562660
C	0.9233167795	-1.3288951529	7.7996687791
H	1.2159917776	-1.0874919684	8.8270062697
H	0.0306156063	-0.7467949431	7.5486931005
H	1.7315172668	-1.0255235714	7.1267509696
C	1.9171646082	-3.6367822334	7.9601404948
H	1.7284499845	-4.7090291071	7.9008888496
H	2.2767327656	-3.3951767096	8.9669557915
H	2.7010611533	-3.3794612483	7.2423711465

The cartesian coordination of **4** is as follows:

0	1		
H	-1.4002358757	1.4145326491	0.2472026356
C	-1.5789707872	1.2620972496	1.3084739926
C	-2.0545820711	0.8643758779	4.0700066936
C	-1.3195003651	0.0330977018	1.8952941436
C	-2.0790431021	2.3041346925	2.1037164370
C	-2.3113211430	2.1019767891	3.4651116492
C	-1.5615669005	-0.1563377911	3.2661224250
H	-2.2860463617	3.2720354673	1.6569243919
H	-2.6978577741	2.9161073671	4.0721095600
H	-2.2360240284	0.7121668952	5.1302188522
C	-0.7733716066	-1.2585437289	1.3060619294
N	-1.2183917954	-1.4672690769	3.6159438850
H	-1.2942139138	-1.8685141350	4.5403034340
C	-0.7599352514	-2.2041439723	2.5391397947
O	-0.3843566105	-3.3582961800	2.5701744536
C	0.6455410239	-1.1366941269	0.7281594617
H	0.6326285208	-0.5273276653	-0.1782877109
H	1.0266194966	-2.1302998998	0.4757950585
H	1.3156381952	-0.6767484376	1.4607754835
C	-1.7370347742	-1.7978229315	0.2308624405
O	-1.5035512884	-1.7510107391	-0.9577297546
O	-2.8540142932	-2.2692631640	0.8024226364
C	-3.9630154904	-2.8424092270	0.0071334196
C	-4.9706336452	-3.2401715736	1.0877413820
H	-5.2851142103	-2.3642205371	1.6643453848
H	-4.5304657159	-3.9681774198	1.7765127968
H	-5.8567985220	-3.6887825796	0.6266054858
C	-4.5458573548	-1.7698249101	-0.9177293391
H	-3.8298353286	-1.4787191651	-1.6879836513
H	-4.8287840128	-0.8825864637	-0.3409628283
H	-5.4462430932	-2.1603604847	-1.4050597501
C	-3.4648838866	-4.0726974324	-0.7570410605
H	-2.7451255915	-3.7961384947	-1.5292911300
H	-4.3146782908	-4.5746825901	-1.2332922682
H	-2.9909741520	-4.7804819634	-0.0687803341

The cartesian coordination of **5** is as follows:

	0	1	
H	-1.5888426259	4.9219375082	0.4120294659
C	-1.0029594621	4.3673163552	1.1421278223
C	0.4630522322	2.9434434228	3.0081238347
C	-0.8285179363	2.9932814556	0.9546839876
C	-0.4645406250	5.0377432750	2.2401218173
C	0.2649062491	4.3104492294	3.1804479290
C	-0.0655372525	2.2634991209	1.8980485012
H	-0.6204794283	6.1055419022	2.3611550534
H	0.6912476037	4.8072530058	4.0483081645
H	1.0446915059	2.3825025405	3.7371569648
N	0.0987603470	0.8816893085	1.7601668692
H	0.3067970274	0.6006416204	0.8035382629
C	-1.5028711208	2.3243667993	-0.2344502018
C	-2.4133326267	1.1277677126	0.1199257813
O	-2.4520871923	0.1091851451	-0.5398689597
O	-3.1744069116	1.4224809267	1.1759406808
C	-4.1295248913	0.4461844148	1.7454399201
C	-0.5330421830	1.8571200666	-1.3266676457
O	0.4674723140	1.1967486488	-1.1129412795
O	-0.9458989509	2.2776363595	-2.5260706044
C	-0.2610098955	1.8757255121	-3.7775672581
C	-5.2405306086	0.1636262368	0.7295532909
H	-4.8474821876	-0.3433188669	-0.1535361125
H	-5.7220315825	1.0975823193	0.4190911303
H	-6.0038030493	-0.4744656210	1.1893478336
C	-3.3867382719	-0.8232601035	2.1731272618
H	-3.0316243615	-1.3865614914	1.3089340526
H	-4.0632028228	-1.4591887499	2.7555955340
H	-2.5258064273	-0.5639560603	2.7969465617
C	-4.6750044119	1.1956118393	2.9628513246
H	-3.8667366564	1.4334855575	3.6612274540
H	-5.4163327121	0.5787544256	3.4818640825
H	-5.1538175959	2.1319166348	2.6585086208
C	-0.2968671892	0.3509157609	-3.9151560570
H	0.0685817819	0.0675618344	-4.9086770511
H	-1.3227048901	-0.0156590100	-3.8065095434
H	0.3264531054	-0.1322045063	-3.1613745206
C	1.1631998077	2.4385518152	-3.7940843553
H	1.6194731057	2.2443832057	-4.7714217550
H	1.7812947360	1.9779358214	-3.0220173145
H	1.1482042772	3.5226353176	-3.6368297060
C	-1.1247246499	2.5419524817	-4.8508539330
H	-0.7197987703	2.3256022504	-5.8450026642
H	-1.1445220968	3.6279868356	-4.7135758191
H	-2.1526652028	2.1685533847	-4.8059066582
H	-2.1706949602	3.0604613982	-0.6946591718
H	0.7740054564	0.4915829601	2.4079084092

The cartesian coordination of **5TS1** is as follows:

	0	1	
H	0.6921732763	0.4855487916	1.0256656128
C	0.2132826291	0.1998739439	1.9586772211
C	-1.0365220652	-0.5271617529	4.3743428850
C	-0.1854520802	-1.1190232397	2.1674409789
C	-0.0238007896	1.1557324656	2.9489903778

C	-0.6504416334	0.7950124586	4.1460362822
C	-0.7986620400	-1.4674175658	3.3747692961
H	0.2782858377	2.1865105609	2.7867736268
H	-0.8318326750	1.5456978642	4.9101742306
H	-1.5049208456	-0.8179780279	5.3105874973
C	-0.0849134180	-2.2842959021	1.2120556383
N	-1.0399530111	-2.8737967086	3.4633741699
H	-1.9877915284	-3.1521017521	3.7219638647
H	-0.0363903460	-3.5483755873	3.7471251138
C	-0.3776766377	-3.5536508234	2.0826460681
O	0.6594475775	-4.0671923521	2.7424132720
O	-1.2610745882	-4.3795289357	1.4234024644
C	-1.3332796845	-5.8232457980	1.6743889654
C	-1.0688116190	-2.1256319055	0.0506424239
O	-2.2014435779	-1.7109455383	0.1752072464
O	-0.4821535168	-2.4937375224	-1.1039094399
C	-1.2043901866	-2.4488095053	-2.3902019282
C	-1.5701814410	-6.1337013698	3.1584431656
H	-0.7084710848	-5.8490867952	3.7643344868
H	-1.7402497474	-7.2090165131	3.2850133381
H	-2.4643936316	-5.6153585669	3.5264789332
C	-0.0654115524	-6.5042171845	1.1450590642
H	0.8089507202	-6.1797713924	1.7104152560
H	0.0832225974	-6.2461726661	0.0907416918
H	-0.1647522689	-7.5936833862	1.2206276047
C	-2.5561721048	-6.2415583493	0.8510728640
H	-2.4102834394	-5.9970367343	-0.2055569922
H	-3.4553292960	-5.7230471816	1.1998304315
H	-2.7198352369	-7.3212487816	0.9374500278
C	-0.1529286106	-2.9578169539	-3.3793192210
H	0.1645296841	-3.9722158667	-3.1171044780
H	0.7293732457	-2.3095622260	-3.3745563421
H	-0.5661946277	-2.9741270612	-4.3935047967
C	-2.4125952315	-3.3892256159	-2.3480227156
H	-3.1565860880	-3.0443239245	-1.6285747829
H	-2.0953854637	-4.4000653856	-2.0709413369
H	-2.8746665811	-3.4360717455	-3.3407722844
C	-1.6026751099	-1.0045955846	-2.7136810842
H	-2.3417498953	-0.6298517289	-2.0038707868
H	-2.0289748053	-0.9596832290	-3.7222805959
H	-0.7228070653	-0.3520330650	-2.6886118378
H	0.9248879567	-2.4200118602	0.8167645237

The cartesian coordination of **5TS1S1** is as follows:

	0	1	
H	-0.2092710406	1.7121797480	1.8767128772
C	0.2393792800	1.4267886686	2.8246510396
C	1.4030758249	0.6982195355	5.2846522165
C	0.3546537628	0.0822887236	3.1714828789
C	0.7039906937	2.4060181900	3.7066993567
C	1.2802130513	2.0434278818	4.9279446523
C	0.9332059528	-0.2612864265	4.3929435198
H	0.6154832049	3.4559712297	3.4424134664
H	1.6371263337	2.8120123209	5.6078143958
H	1.8514662031	0.4100409073	6.2315517181
N	0.9756786611	-1.6832796972	4.5853535542
H	2.0831855858	-2.3085066492	4.4771964135
H	0.5278964359	-1.9692920442	5.4584666615
C	-0.0734118196	-1.1391470066	2.4020376182

C	0.1082554604	-2.3609890791	3.4140443004
O	0.7229520341	-3.4180857836	2.9213044282
O	-1.1187660776	-2.5784746784	4.0983177878
C	-1.9672174499	-3.7325688978	3.8214053693
H	1.9048881833	-3.5098226609	3.4382685991
O	2.8031300957	-3.2392944856	4.0998847025
C	3.9149840373	-2.8053365858	3.3067191101
H	4.3218855169	-3.6648969852	2.7631490339
H	4.6915871278	-2.4169949236	3.9737113366
H	3.6202600175	-2.0316184020	2.5894343881
H	-1.1221422431	-1.0952035928	2.1031243378
C	0.7852794537	-1.3858679617	1.1653922608
O	1.9687825843	-1.1191613834	1.0911626261
O	0.0431282909	-1.9371684457	0.1920253529
C	0.6448635886	-2.4154309637	-1.0694799657
C	-0.5564299461	-3.0226223303	-1.7983447026
H	-0.2471880069	-3.4129042909	-2.7737546015
H	-1.3335297709	-2.2678317640	-1.9577585959
H	-0.9872448564	-3.8431560159	-1.2158974949
C	1.6994448430	-3.4856309253	-0.7698214423
H	2.0057886470	-3.9684129286	-1.7049502633
H	1.2848303318	-4.2476764597	-0.1025995419
H	2.5800361640	-3.0508673769	-0.2947333169
C	1.2171219592	-1.2306826887	-1.8543805609
H	1.5601678298	-1.5734907317	-2.8373422586
H	2.0588836238	-0.7793788173	-1.3269250354
H	0.4459146787	-0.4684587316	-2.0119203477
C	-2.2564214704	-3.8828783528	2.3214888771
H	-1.3374565065	-4.0619107690	1.7606127484
H	-2.7413135811	-2.9832005380	1.9258036277
H	-2.9365981909	-4.7275230922	2.1606244169
C	-3.2570763609	-3.3847837927	4.5753991929
H	-3.0534396356	-3.2480398529	5.6428337356
H	-3.9931731520	-4.1885812114	4.4640742031
H	-3.6917527583	-2.4573048311	4.1883866929
C	-1.3449023724	-5.0103670987	4.4040930337
H	-0.4261112290	-5.2686946973	3.8771536066
H	-2.0523960540	-5.8449754619	4.3252961796
H	-1.1116969358	-4.8641477934	5.4652778108

The cartesian coordination of **5TS1S2** is as follows:

	0	1	
H	-0.1062341672	4.3561823082	0.7708333769
C	0.1899859668	3.5808949758	1.4731719994
C	0.9325272213	1.5779906654	3.3075722404
C	0.0236068901	2.2384344453	1.1479617829
C	0.7312881332	3.9259208892	2.7163451772
C	1.0967996119	2.9300292904	3.6255370490
C	0.3984283354	1.2498096565	2.0639728453
H	0.8609475037	4.9723335048	2.9780744696
H	1.5101413268	3.2050043227	4.5923091664
H	1.2115022322	0.8031279630	4.0174692404
N	0.1866019427	-0.0631384486	1.5413533049
H	1.4117178107	-0.6848732942	1.1504539525
H	-0.2475236507	-0.6791135020	2.2300894003
C	-0.5491794172	1.6153623009	-0.0982435370
C	-0.8629058693	0.1080334090	0.3164023501
O	-0.7398512165	-0.8200620520	-0.5900445818
O	-2.1309723643	0.1976501879	0.9560290980

C	-3.0782081738	-0.9035609826	0.9716141567
H	1.9986879429	-1.5446657322	-0.2634380661
O	2.3227049303	-1.2466082307	0.8106501402
C	3.4968898557	-0.4129094834	0.8188485006
H	4.3264640360	-0.9920247856	0.4036996064
H	3.7291112191	-0.1519771885	1.8552339512
H	3.3329191936	0.4906860185	0.2282757243
H	0.4510350563	-1.2835630957	-1.0804241315
O	1.3841545938	-1.7870531389	-1.3425635412
C	1.1141431086	-3.1792257851	-1.5081947198
H	0.4168991499	-3.3188975155	-2.3404870772
H	0.6776172916	-3.6216275103	-0.6028172662
H	2.0516111865	-3.6928429970	-1.7417203664
C	0.4355639978	1.6211952774	-1.2565717998
O	1.6008460830	1.2824632804	-1.1568906882
O	-0.1613479298	2.0333270797	-2.3851468913
C	0.5344990455	2.0244806785	-3.6886735240
C	-3.6841709675	-1.1175566720	-0.4240802511
H	-2.9214353660	-1.4538898369	-1.1262620159
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H	-4.4915230942	-1.8590110468	-0.3776954973
C	-2.4528896825	-2.1992907361	1.5138409484
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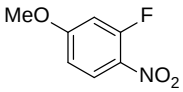
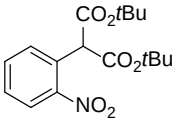
H	-2.0715297861	-2.0506515743	2.5328542832
C	-4.1583074021	-0.4021261344	1.9397808528
H	-3.7333827557	-0.2192556367	2.9326174040
H	-4.9626783427	-1.1404214854	2.0343977584
H	-4.5888452426	0.5365822727	1.5763682240
C	0.8958709754	0.5838461987	-4.0625622347
H	1.3184459749	0.5641832988	-5.0739325223
H	-0.0018102277	-0.0432358069	-4.0520956610
H	1.6211343849	0.1573398956	-3.3680662877
C	1.7568667109	2.9476856320	-3.6468195651
H	2.1773643003	3.0395201152	-4.6548804773
H	2.5254343049	2.5581960048	-2.9783833142
H	1.4674864184	3.9490847217	-3.3088382627
C	-0.5319954057	2.5823365678	-4.6346334173
H	-0.1445592969	2.6187062632	-5.6583906640
H	-0.8223328300	3.5955217813	-4.3375254906
H	-1.4258028110	1.9506335895	-4.6230421158
H	-1.4853886929	2.0755601542	-0.4164793306

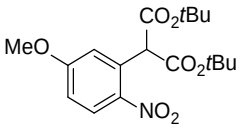
3. Additional Experimental Section



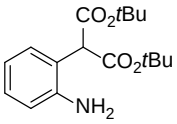
2-Fluoro-4-methoxy-1-nitrobenzene[1] **(17b).** 3-fluoro-4-nitrophenol (1.00 g, 6.37 mmol) was dissolved in DMF (13 mL). K_2CO_3 (1.14 g, 8.28 mmol, 1.3 eq.) and MeI (436 μL, 7.00 mmol, 1.2 eq.) were added to the reaction mixture. The resultant mixture was stirred at room temperature overnight. The reaction mixture was diluted with water and extracted with EtOAc / Hexane = 2 / 1. The combined organic phases were washed with brine, dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Purification using silica gel column chromatography (*n*-hexane/EtOAc = 50/50) afforded title compound (1.18 g, 68%) as a pale yellow solid: ^{1}H NMR (DMSO-d_6) δ: 8.13 (1H, t, *J* = 9.2 Hz), 7.17 (1H, dd, *J* = 13.4, 2.4 Hz), 6.96 (1H, dd, *J* = 9.2, 2.4 Hz), 3.89 (3H, s); ^{13}C NMR (DMSO-d_6) δ: 165.3 (d, *J* = 11.6 Hz), 156.7 (d, *J* = 262.0 Hz), 130.0 (d, *J* = 6.7 Hz), 128.0, 111.3 (d, *J* = 2.9 Hz), 103.4 (d, *J* = 24.1 Hz), 56.8; HRMS (ESI): *m/z* calcd. for $C_7H_7FNO_3$: 172.0404 $[M+H]^+$; found: 172.0405.



Di-*t*-butyl 2-(2-nitrophenyl)malonate[2] **(7)**. See general procedure for di-*t*-butyl 2-(2-nitrophenyl)malonate derivatives in experimental section. Yield: 83% as a pale yellow solid: ^{1}H NMR ($CDCl_3$) δ: 8.04 (1H, d, *J* = 8.0 Hz), 7.63 (1H, dd, *J* = 7.2, 8.0 Hz), 7.55 (1H, d, *J* = 8.0 Hz), 7.49 (1H, dd, *J* = 7.2, 8.0 Hz), 5.11 (1H, s), 1.49 (18H, s); ^{13}C NMR ($CDCl_3$) δ: 166.5, 148.9, 133.3, 130.9, 129.1, 128.8, 125.0, 82.8, 56.3, 27.8; HRMS (ESI): *m/z* calcd. for $C_{17}H_{23}NO_6Na$: 360.1418 $[M+Na]^+$; found: 360.1412.

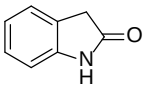


Di-*t*-butyl 2-(5-methoxy-2-nitrophenyl)malonate[3] **(7b)**. See general procedure for di-*t*-butyl 2-(2-nitrophenyl)malonate derivatives in experimental section. Yield: 84% as a colorless solid: ^{1}H NMR (DMSO-d_6) δ: 8.18 (1H, d, *J* = 9.2 Hz), 7.15 (1H, dd, *J* = 9.2, 2.4 Hz), 6.91 (1H, d, *J* = 2.4 Hz), 5.14 (1H, s), 3.87 (3H, s), 1.42 (18H, s); ^{13}C NMR (DMSO-d_6) δ: 165.7, 162.9, 141.2, 131.6, 128.1, 116.8, 113.3, 82.1, 56.9, 56.2, 27.4; HRMS (ESI): *m/z* calcd. for $C_{18}H_{25}NO_7Na$: 390.1523 $[M+Na]^+$; found: 390.1527.

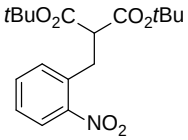


Di-*t*-butyl 2-(2-aminophenyl)malonate[2] **(5)**. See reduction reaction of nitro group of di-*t*-butyl 2-(2-nitrophenyl)malonate (**7**) in experimental section. Yield: 98% as a colorless solid; ^{1}H NMR ($CDCl_3$) δ: 7.17 (1H, d, *J* = 7.6 Hz), 7.11 (1H, t, *J* = 7.6 Hz), 6.76 (1H, t, *J* = 7.6 Hz), 6.71 (1H, d, *J* = 7.6 Hz), 4.47 (1H, s), 4.10 (2H, br s), 1.47 (18H, s); ^{13}C NMR ($CDCl_3$) δ: 167.9, 145.4, 131.1,

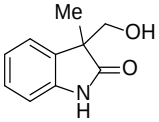
128.8, 119.8, 118.7, 117.3, 82.2, 57.4, 27.9; HRMS (ESI): *m/z* calcd. for $C_{17}H_{26}NO_4$: 308.1856 $[M+H]^+$; found: 308.1854.



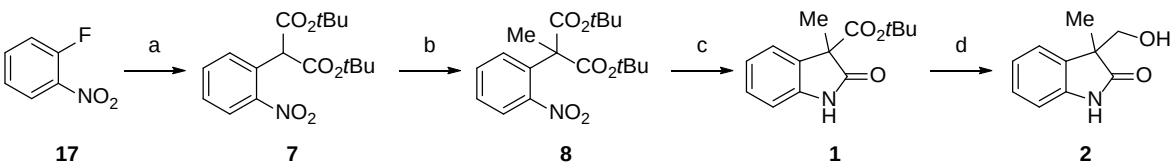
Indolin-2-one. See cyclization reaction of di-*t*-butyl 2-(2-aminophenyl)-2-methylmalonate (**5**) in experimental section. Brown solid; ^{1}H NMR (DMSO-d_6) δ: 10.33 (1H, br s), 7.18 (1H, d, *J* = 7.2 Hz), 7.14 (1H, dd, *J* = 7.2, 7.6 Hz), 6.91 (1H, dd, *J* = 7.6, 8.0 Hz), 6.79 (1H, d, *J* = 8.0 Hz), 3.44 (2H, s); ^{13}C NMR ($CDCl_3$) δ: 178.3, 142.6, 127.9, 125.2, 124.5, 122.3, 109.9, 36.3; HRMS (ESI): *m/z* calcd. for C_8H_8NO: 134.0600 $[M+H]^+$; found: 134.0592.



Di-*t*-butyl 2-(2-nitrobenzyl)malonate[4] **(14)**. To a cooled (0 °C) solution of di-*t*-butyl 2-(2-nitrobenzylidene)malonate **13** (3.18 g, 9.10 mmol) in MeOH (30 mL) was slowly added $NaBH_4$ (448 mg, 11.8 mmol, 1.3 eq.). The reaction mixture was stirred at 0 °C for 1 hour and quenched with 1 N HCl aq. The resultant aqueous phase was extracted with EtOAc. The combined organic phases were washed with brine, dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Purification using silica gel column chromatography (*n*-hexane/EtOAc = 70/30) afforded compound **14** (3.17 g, 99%) as a pale yellow oil: ^{1}H NMR ($CDCl_3$) δ: 8.00 (1H, d, *J* = 8.4 Hz), 7.51 (1H, dd, *J* = 8.4, 7.2 Hz), 7.43–7.37 (2H, m), 3.66 (1H, t, *J* = 8.0 Hz), 3.44 (2H, d, *J* = 8.0 Hz), 1.40 (18H, s); ^{13}C NMR ($CDCl_3$) δ: 167.9, 149.2, 133.6, 133.2, 133.0, 127.9, 125.1, 81.8, 53.8, 32.1, 27.8; HRMS (ESI): *m/z* calcd. for $C_{18}H_{25}NO_6Na$: 374.1574 $[M+Na]^+$; found: 374.1573.



3-(Hydroxymethyl)-3-methylindolin-2-one[5] **(2)**. See synthesis of 3-(hydroxymethyl)-3-methylindolin-2-one (**2**) without column chromatography in experimental section. Yield: 57% as a pale pink solid; ^{1}H NMR (DMSO-d_6) δ: 10.24 (1H, s), 7.23 (1H, d, *J* = 7.3 Hz), 7.13 (1H, t, *J* = 7.3 Hz), 6.92 (1H, t, *J* = 7.3 Hz), 6.79 (1H, d, *J* = 7.3 Hz), 4.81 (1H, t, *J* = 5.5 Hz), 3.60 (1H, dd, *J* = 10.0, 5.5 Hz), 3.55 (1H, dd, *J* = 10.0, 5.5 Hz), 1.13 (3H, s); ^{13}C NMR ($CDCl_3$) δ: 180.6, 142.1, 133.7, 127.4, 123.3, 121.1, 109.0, 66.3, 50.3, 19.1; HRMS (ESI): *m/z* calcd. for $C_{10}H_{12}NO_2$: 178.0863 $[M+H]^+$; found: 178.0859.



17 **7** **8** **1** **2**

Synthesis of 3-(hydroxymethyl)-3-methylindolin-2-one (2) without column chromatography (Scheme 5). a: To a cooled (0 °C) solution of NaH (60% in mineral oil, 11.3 g, 156 mmol, 2.2 eq.) in

DMF (95 mL) was slowly added di-*t*-butyl malonate (17.5 mL, 78.0 mmol, 1.1 eq.). After 15 minutes, 2-fluoro nitrobenzene **17** (10.0 g, 70.9 mmol) was added to the reaction mixture dropwise at 0 °C. The resultant mixture was stirred at room temperature overnight and quenched with 150 mL of 0.1 N HCl aq. The resultant aqueous phase was extracted with EtOAc / *n*-hexane (= 1/1) solution. The combined organic phases were washed with brine. The resultant organic phase was dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Crystallization from *n*-hexane afforded compound **7** (12.9 g, 54%) as a pale yellow solid.

b: Compound **7** (21.9 g, 64.3 mmol) was dissolved in DMF (92 mL, 0.7 M). K_2CO_3 (11.7 g, 1.3 eq.) and MeI (4.84 mL, 1.2 eq.) were added to the reaction mixture. The resultant mixture was stirred at room temperature overnight. The reaction mixture was diluted with water and extracted with EtOAc / *n*-hexane = 2 / 1. The combined organic phases were washed with brine, dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Crystallization of the residue from *n*-hexane afforded compound **8** (21.7 g, 96%).

c: Compound **8** (10.0 g, 28.5 mmol) was dissolved in MeOH (95 mL, 0.3 M). Pd/C (1.00 g, w/w = 1/10) and citric acid (5.47 g, 28.5 mmol) were added to the reaction mixture. The mixture was stirred at room temperature under H_2 atmosphere. The reaction was followed by NMR. The mixture was passed through a pad of Celite with MeOH and the solvent was removed *in vacuo*. The residue was dissolved in EtOAc and washed with sat. $NaHCO_3$ aq., brine, dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Crystallization of the residue from *n*-hexane afforded compound **1** (6.16 g, 88%).

d: To a cooled (0 °C) solution of LAH (308 mg, 8.10 mmol, 2.0 eq.) in THF (14 mL) was slowly added compound **1** (1.00 g, 4.05 mmol) in THF (14 mL). The resultant mixture was stirred at 0 °C for 4 hours and quenched with sat. potassium sodium tartrate aq. The resultant aqueous phase was extracted with EtOAc. The combined organic phases were washed with brine. The resultant organic phase was dried over Na_2SO_4, filtered, and the filtrate was concentrated *in vacuo*. Crystallization from $CHCl_3$/*n*-hexane (= 1/5) afforded 3-(hydroxymethyl)-3-methylindolin-2-one **2** (0.41 g, 57%) as a pale pink solid.

2. References

[1] P. R. Halfpenny, D. C. Horwell, J. Hughes, J. C. Hunter, and D. C. Rees, *J. Med. Chem.*, 1990, **33**, 286.

[2] J. W. Hulshof, H. F. Vischer, M. H. P. Verheij, S. A. Fratantoni, M. J. Smit, I. J. P. de Esch, and R. Leurs, *Bioorg. Med. Chem.*, 2006, **14**, 7213.

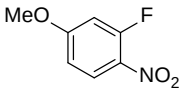
[3] H.-J. Knölker, M. Graf, and U. Mangei, *J. prakt. Chem.*, 1998, **340**, 530.

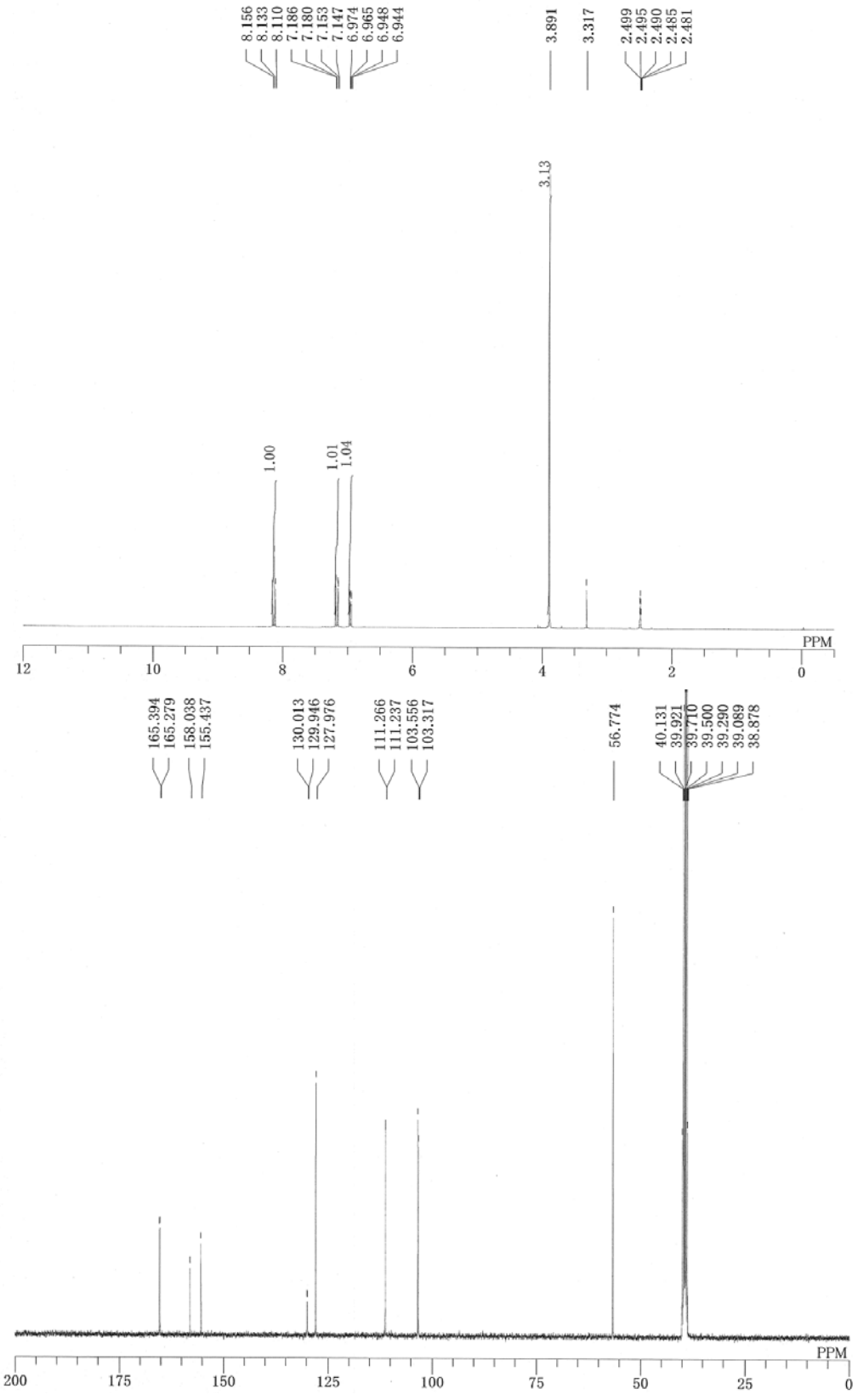
[4] B. Nammalwar, R. A. Bunce, and J. T. Hiett, *Org. Prep. Proced. Int.*, 2015, **47**, 338.

[5] X. Jiang, J. Yang, F. Zhang, P. Yu, P. Yi, Y. Sun, and Y. Wang, *Org. Lett.*, 2016, **18**, 3154.

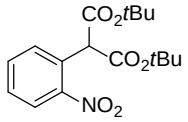
3. ^{1}H NMR and ^{13}C NMR Spectra of The Compounds

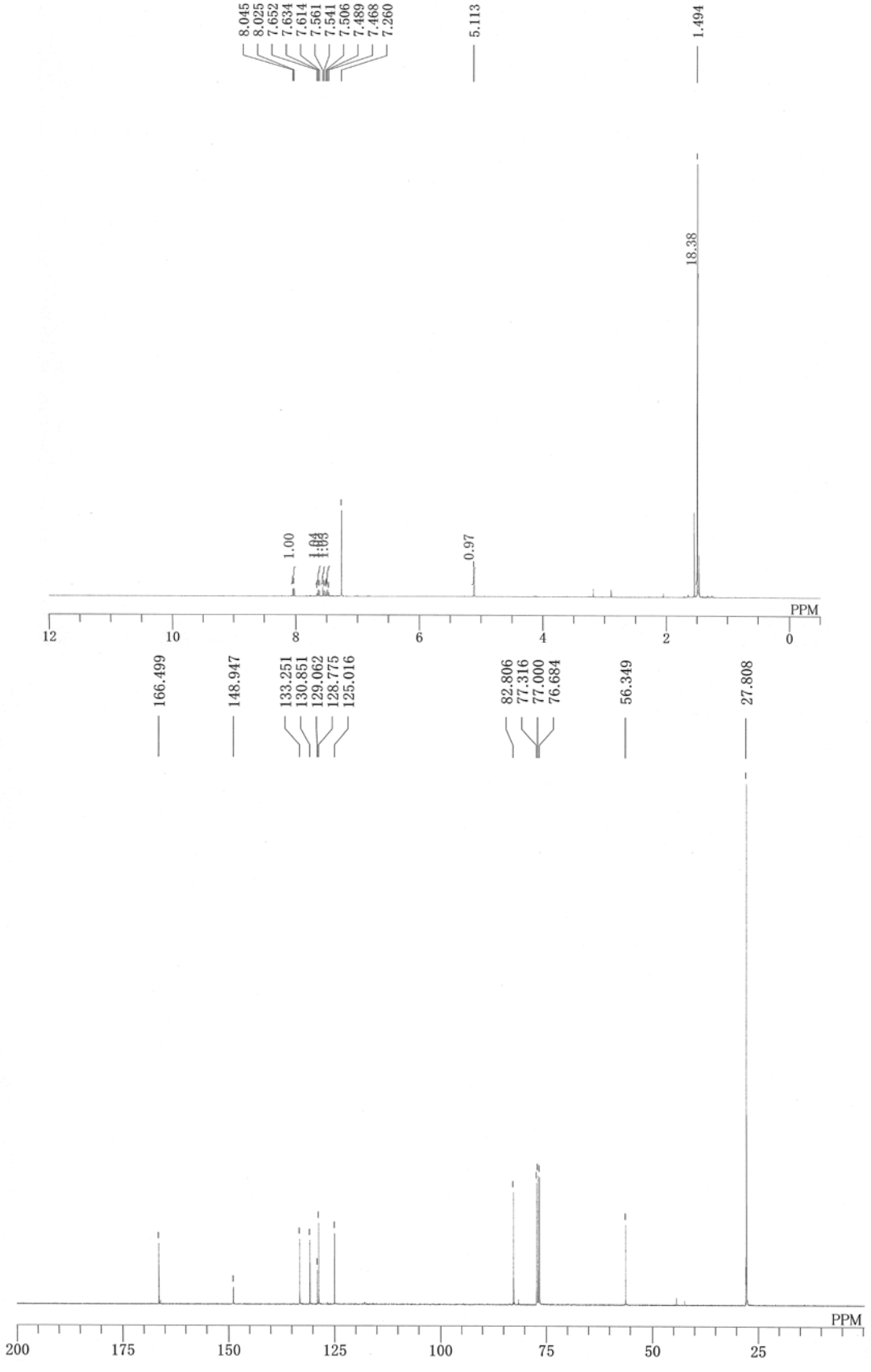
2-Fluoro-4-methoxy-1-nitrobenzene (17b)



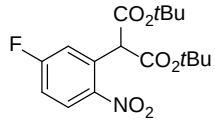


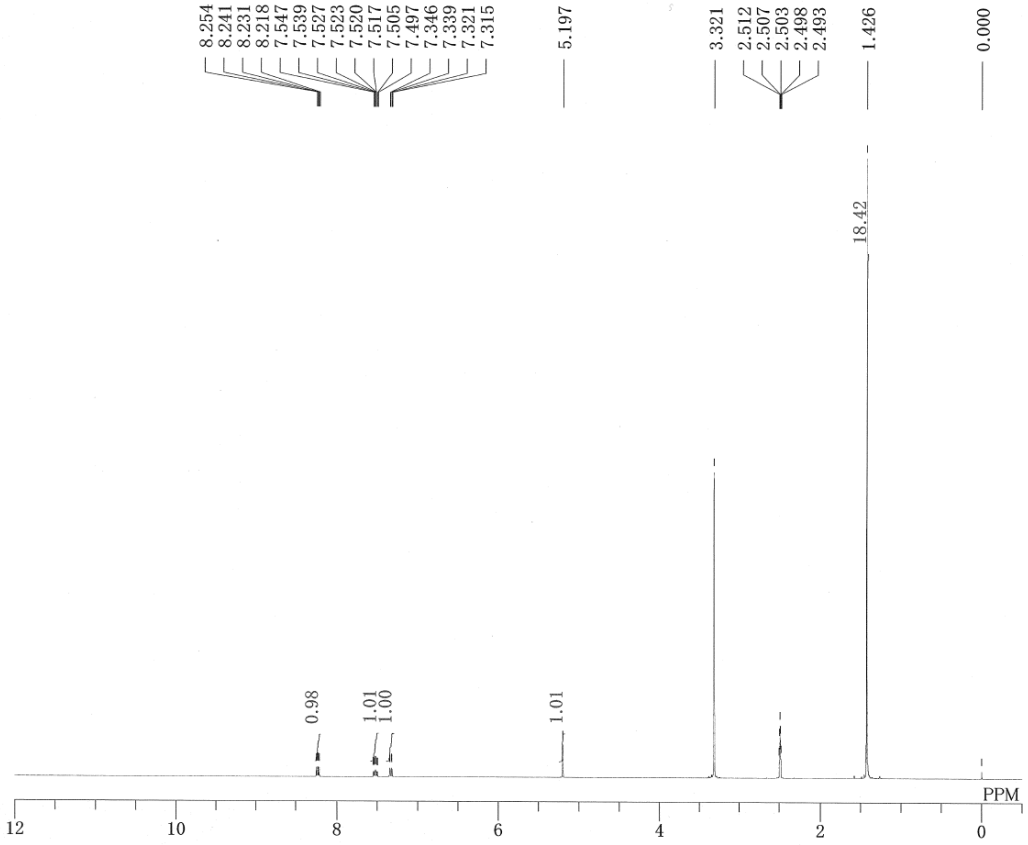
Di-*t*-butyl 2-(2-nitrophenyl)malonate (7)

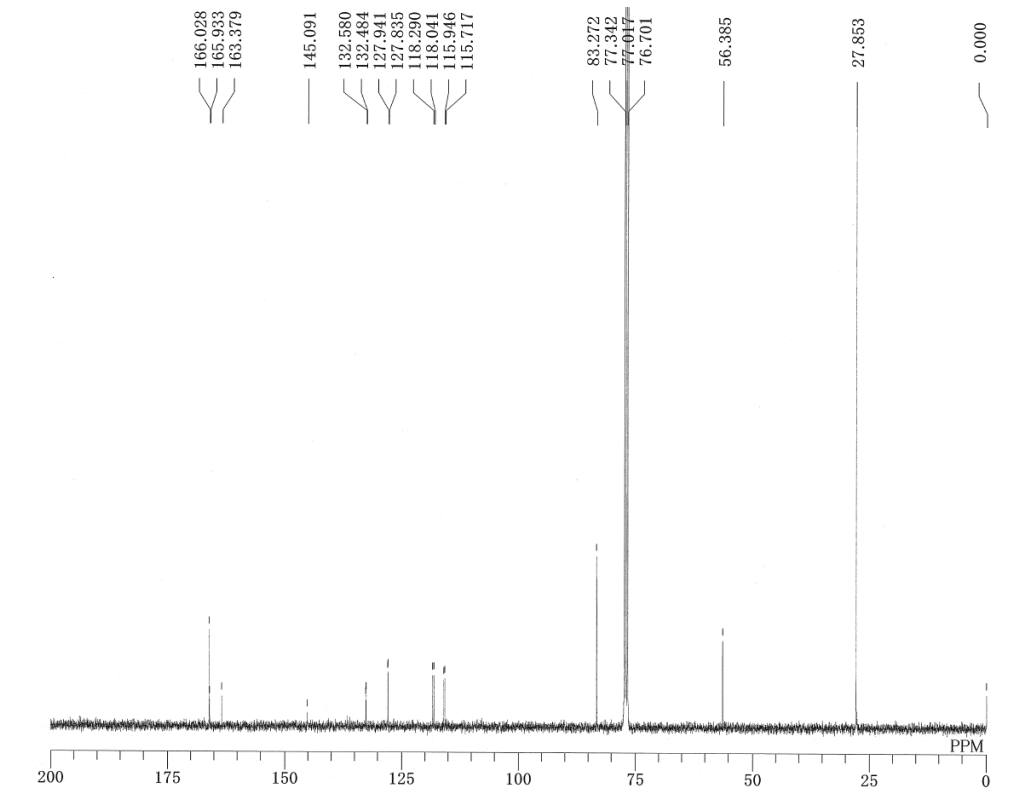




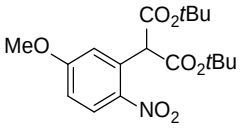
Di-*t*-butyl 2-(5-fluoro-2-nitrophenyl)malonate (7a)

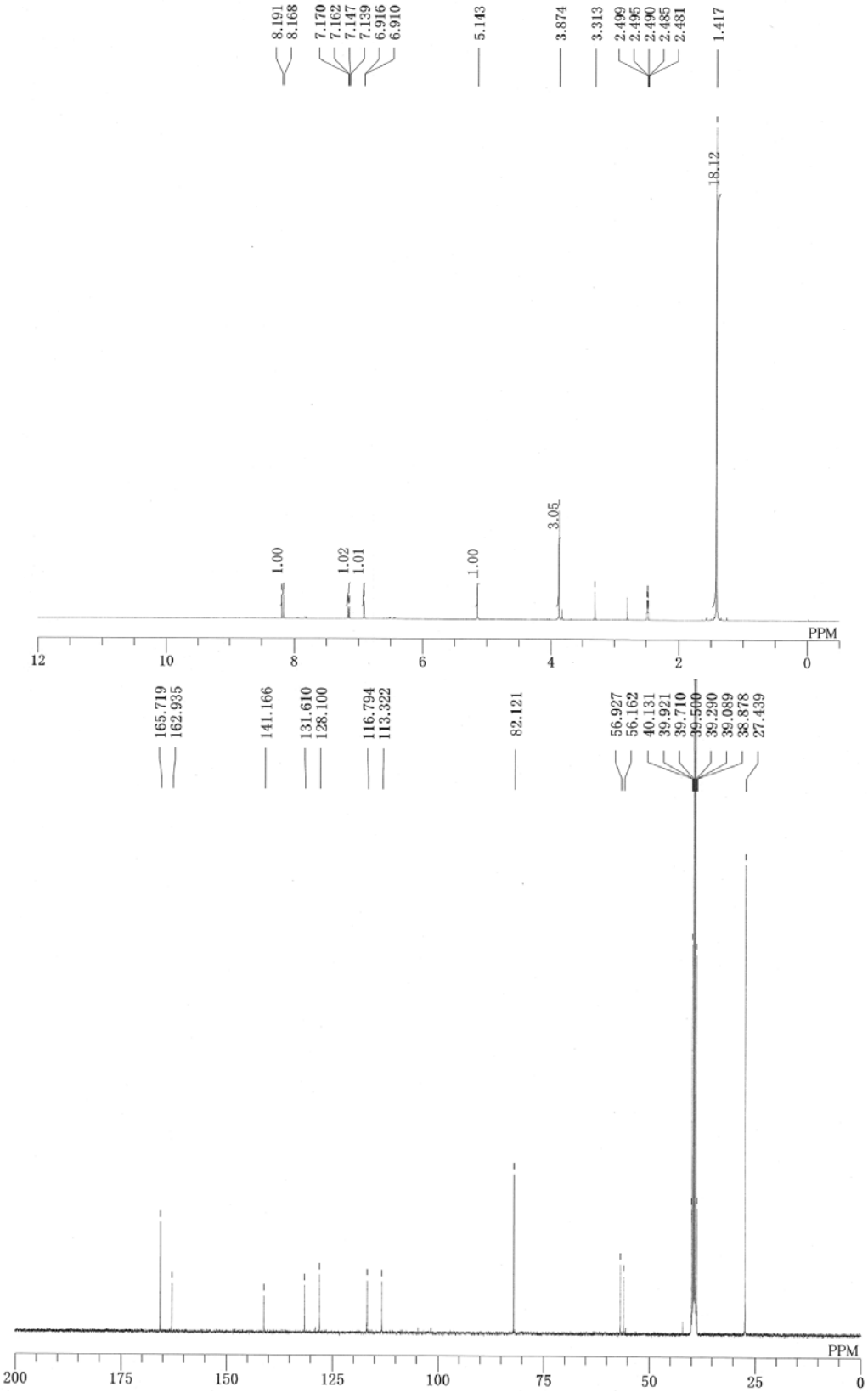




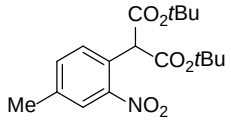


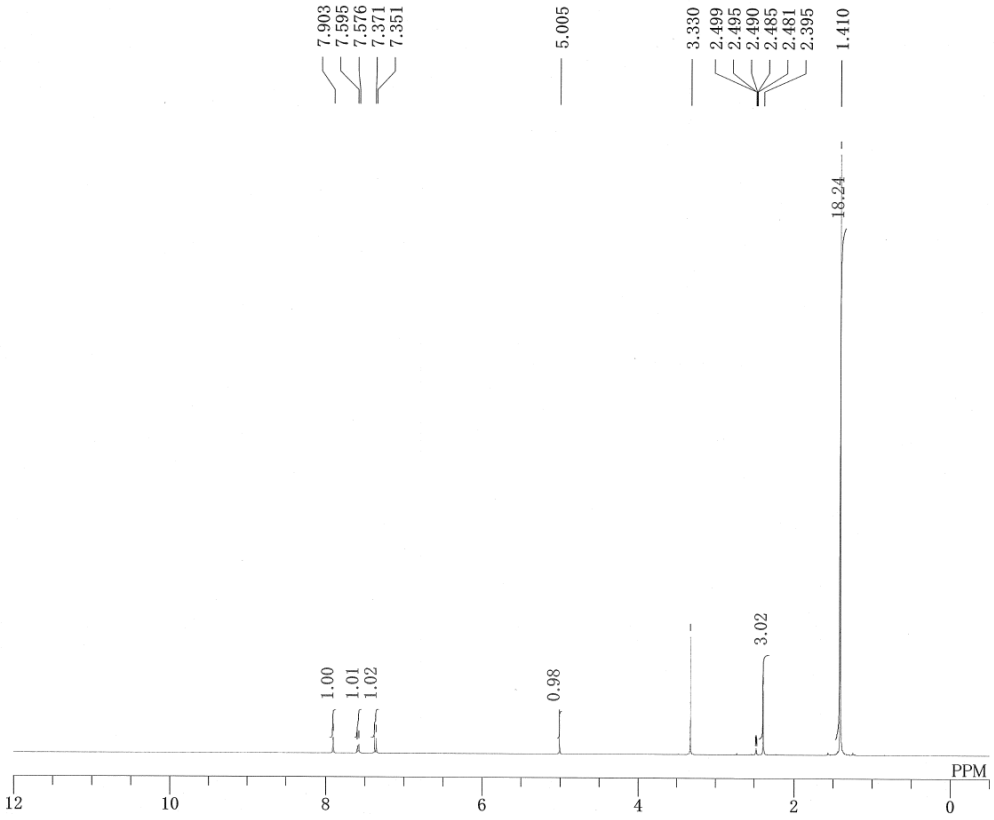
Di-*t*-butyl 2-(5-methoxy-2-nitrophenyl)malonate (7b)

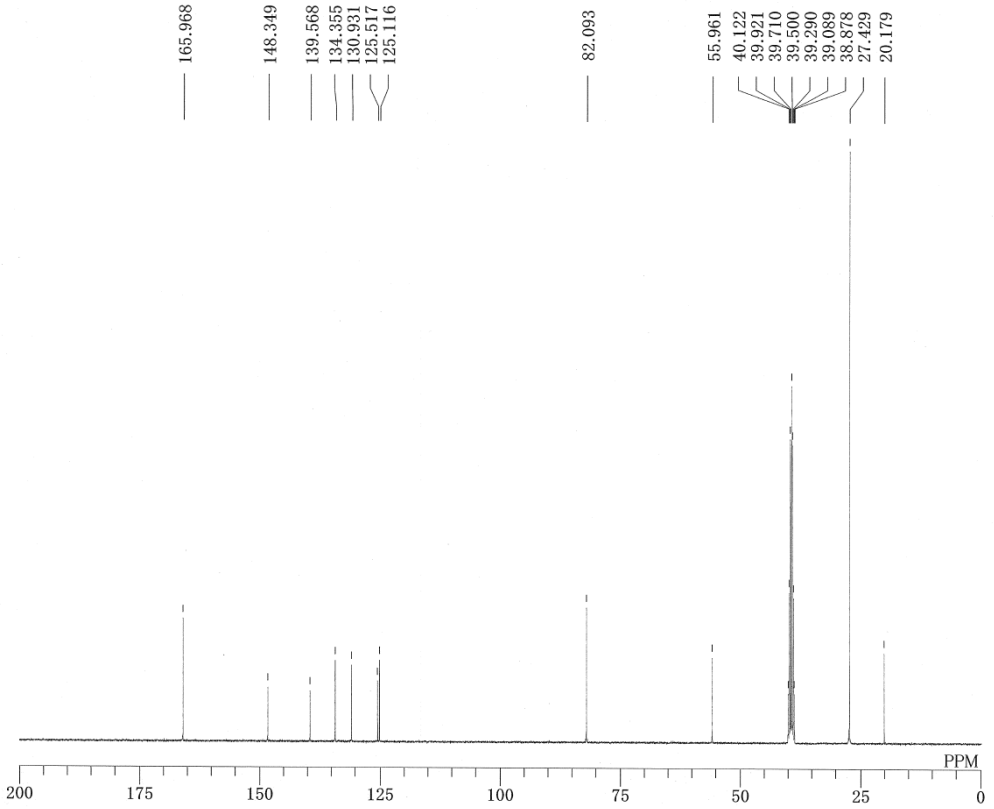




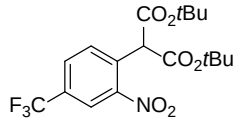
Di-*t*-butyl 2-(4-methyl-2-nitrophenyl)malonate (7c)

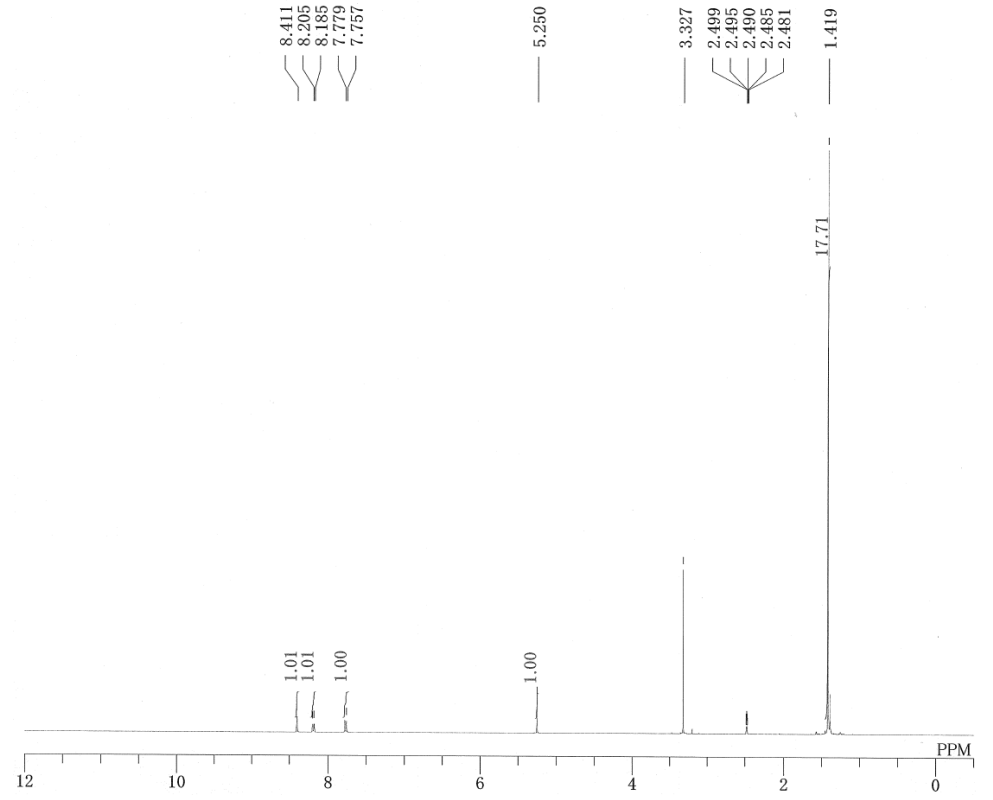


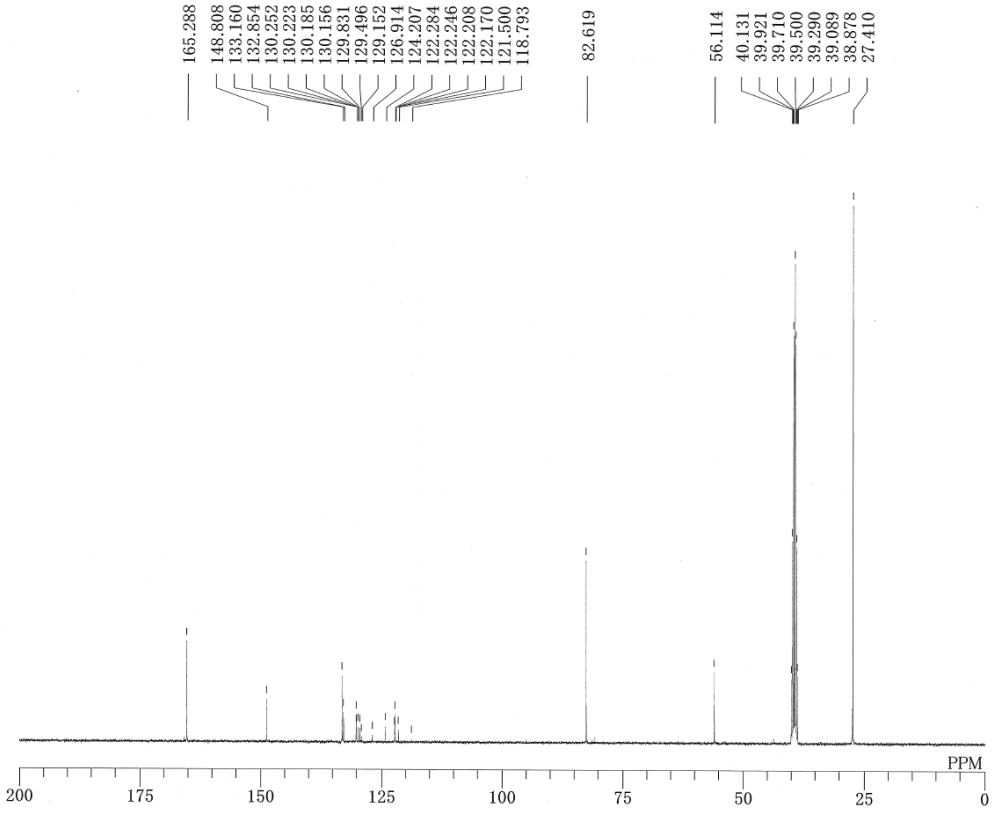




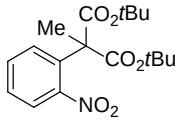
Di-*t*-butyl 2-(2-nitro-4-(trifluoromethyl)phenyl)malonate (7d)

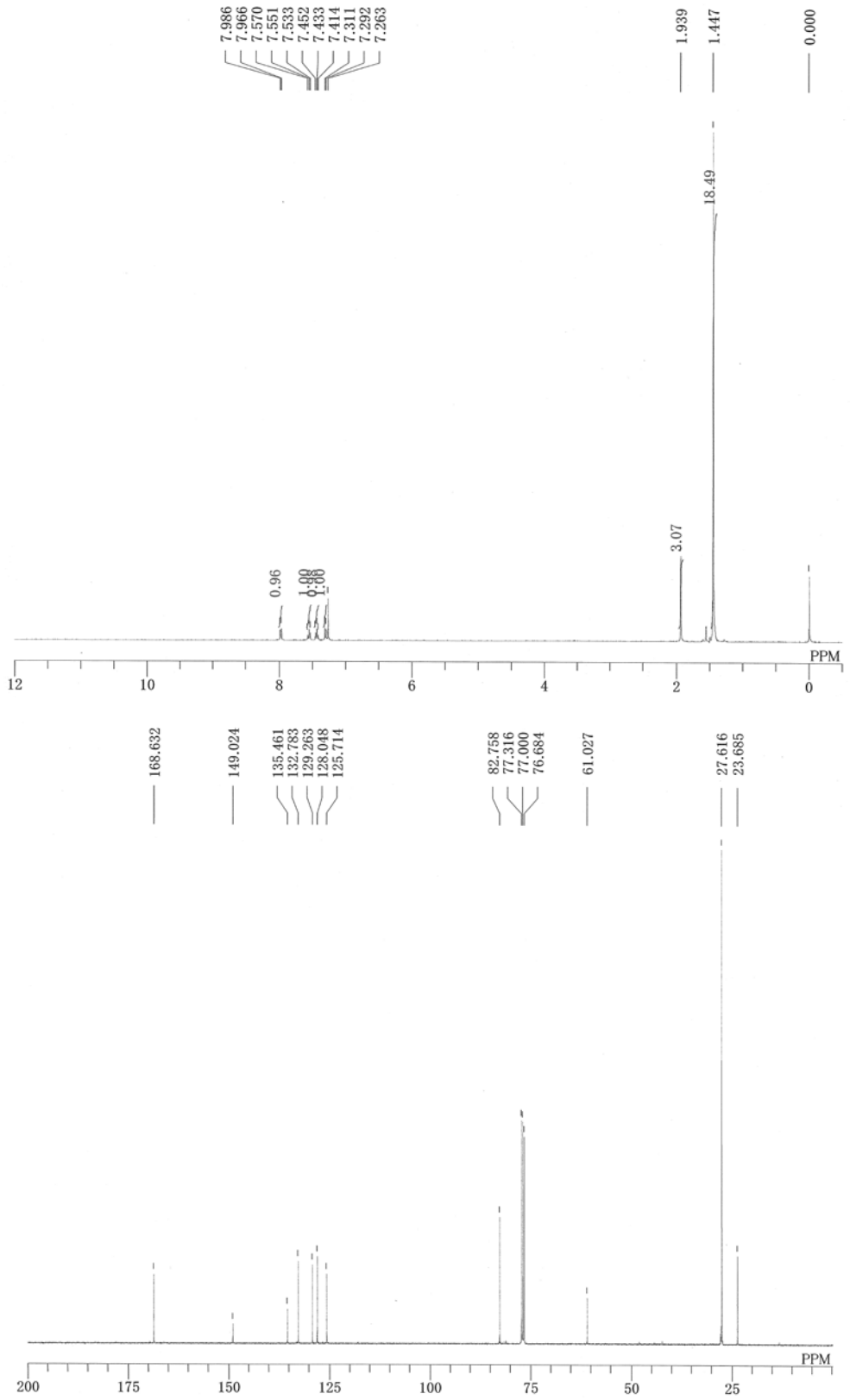




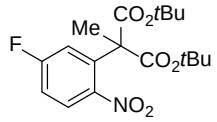


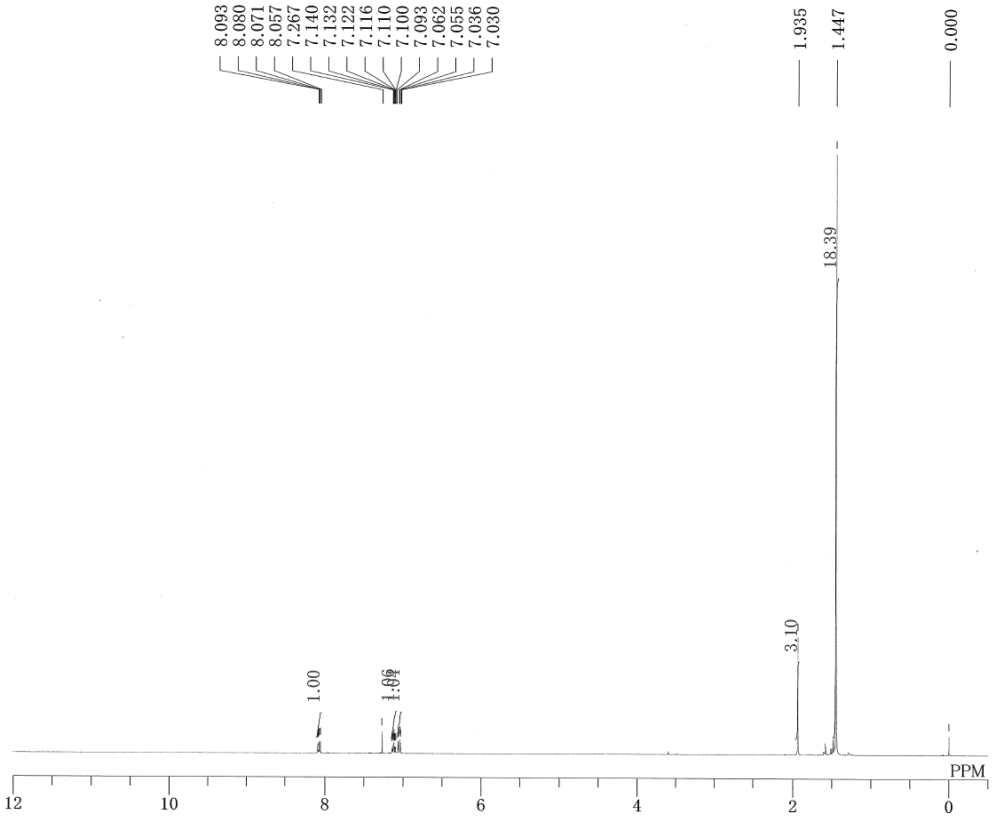
Di-*t*-butyl 2-methyl-2-(2-nitrophenyl)malonate (8)

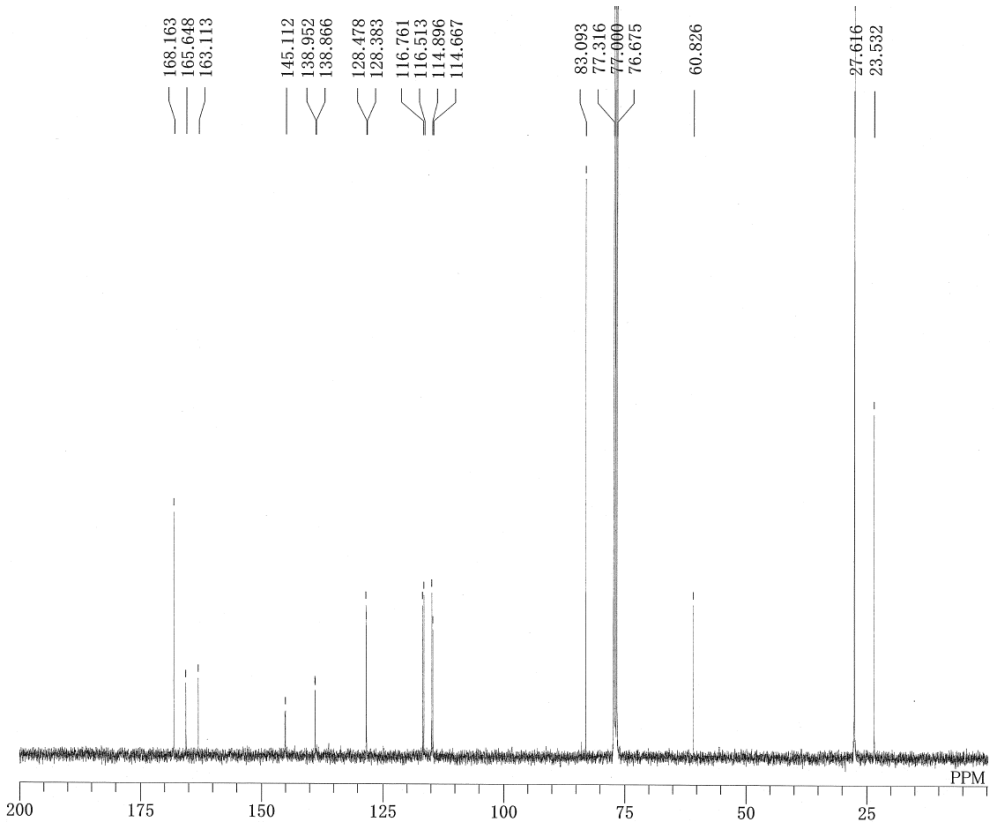




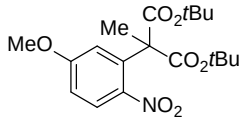
Di-*t*-butyl 2-(5-fluoro-2-nitrophenyl)-2-methylmalonate (8a)

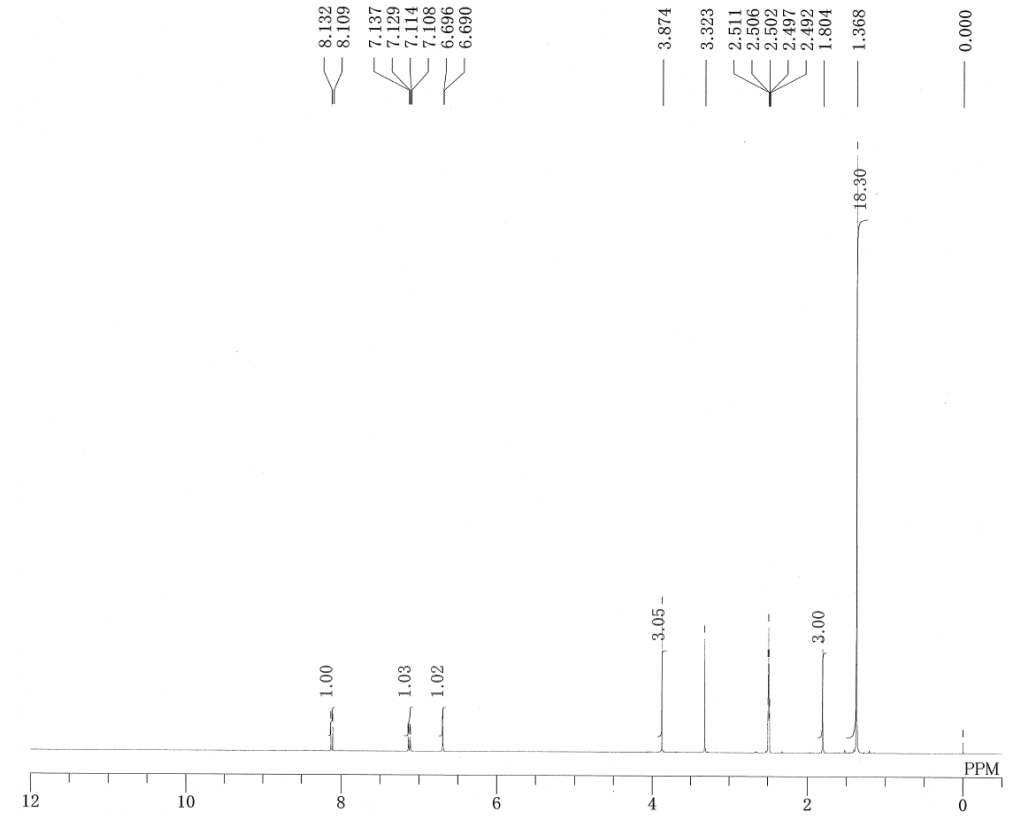


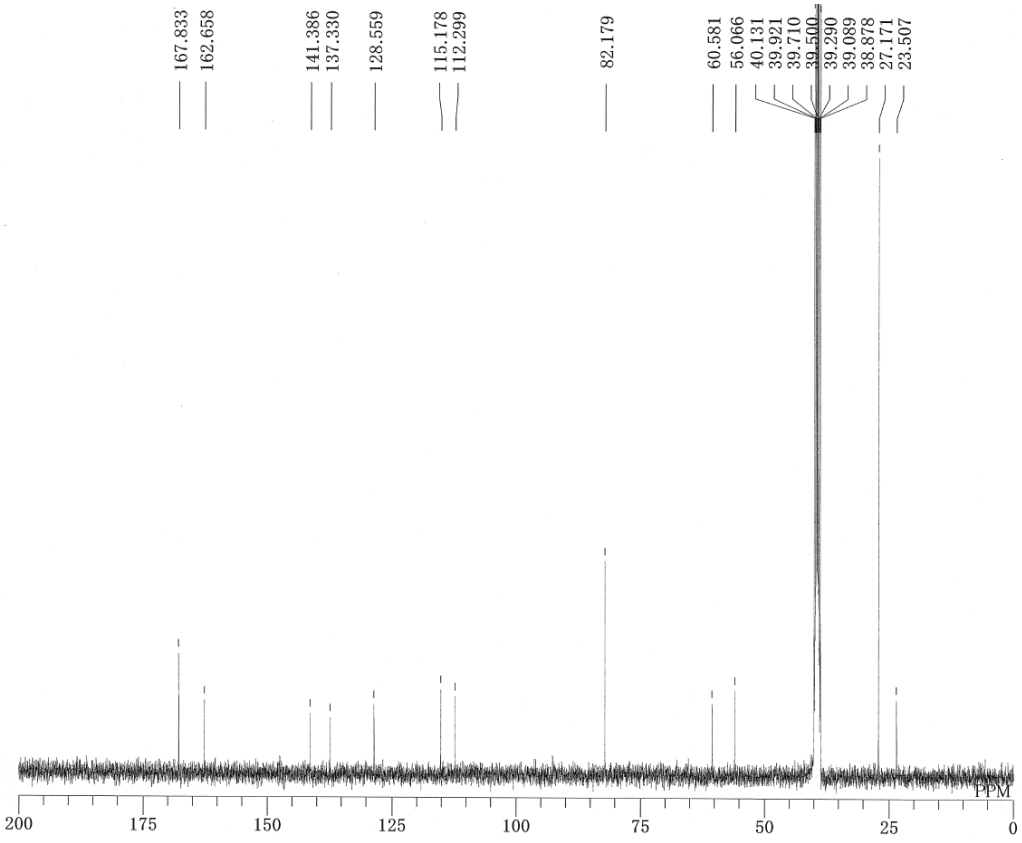




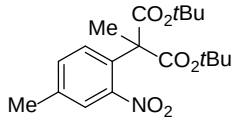
Di-*t*-butyl 2-(5-methoxy-2-nitrophenyl)-2-methylmalonate (8b)

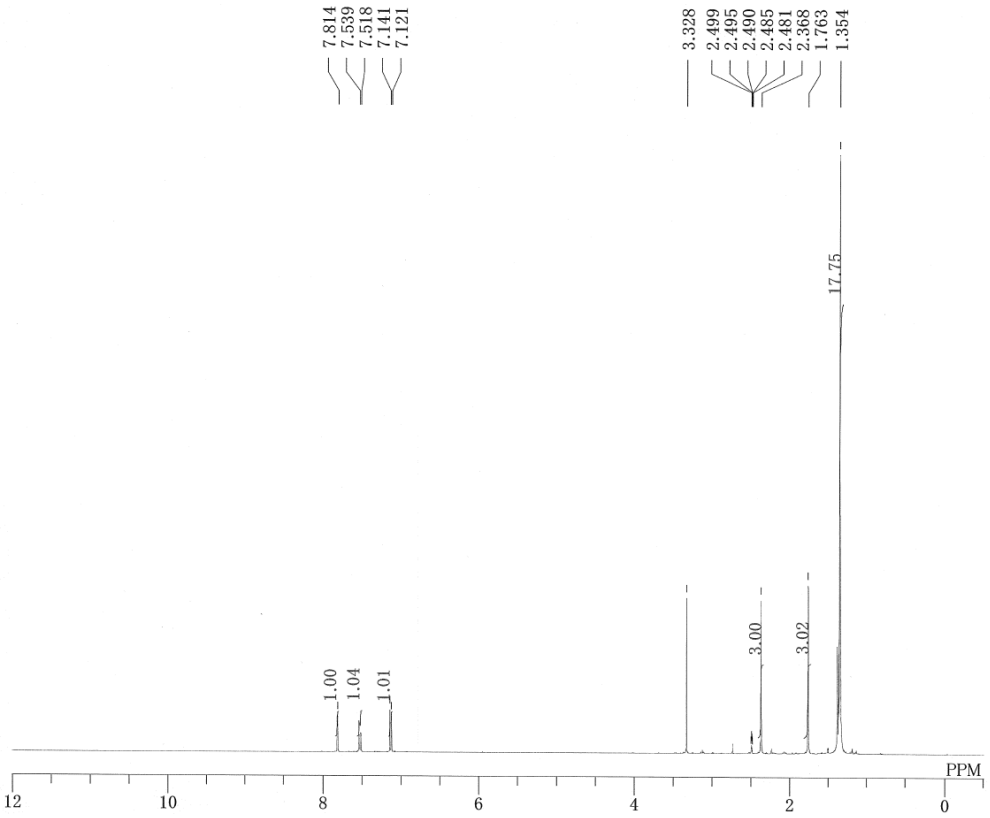


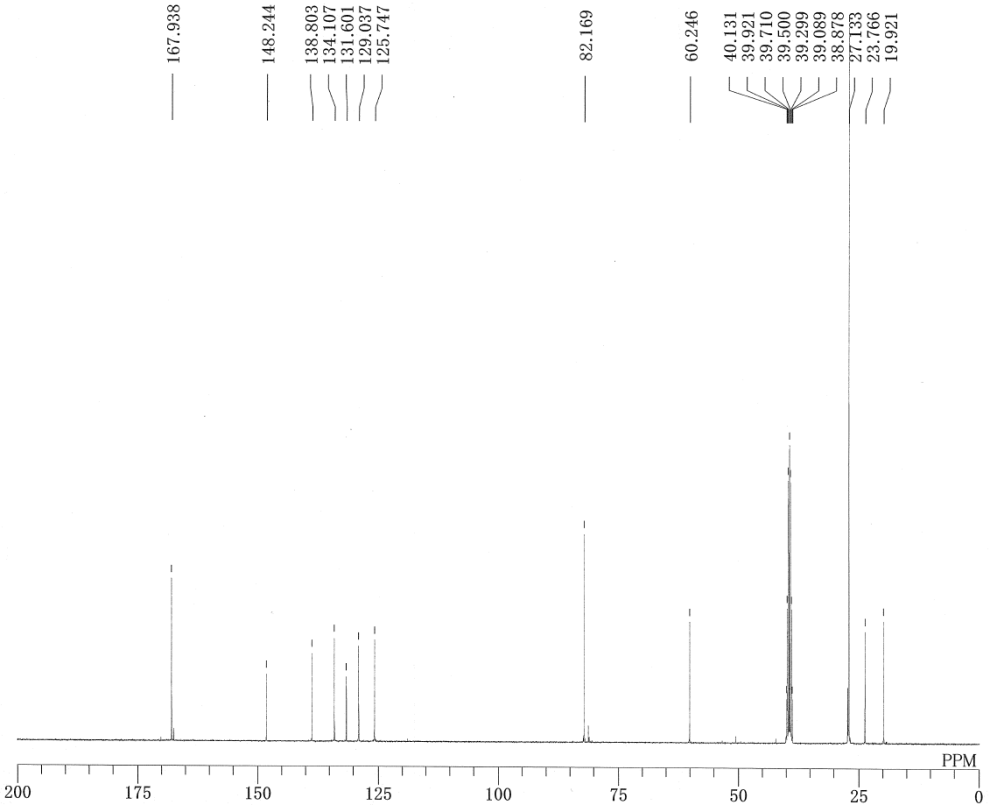




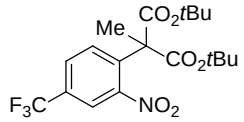
Di-*t*-butyl 2-methyl-2-(4-methyl-2-nitrophenyl)malonate (8c)

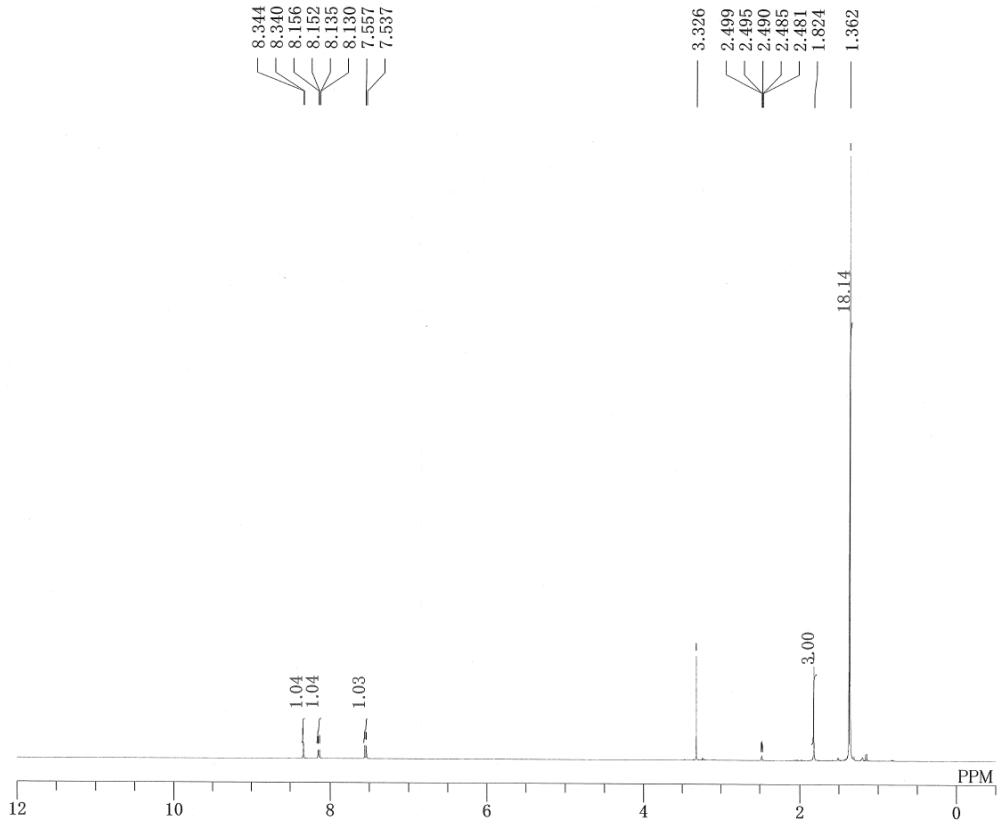


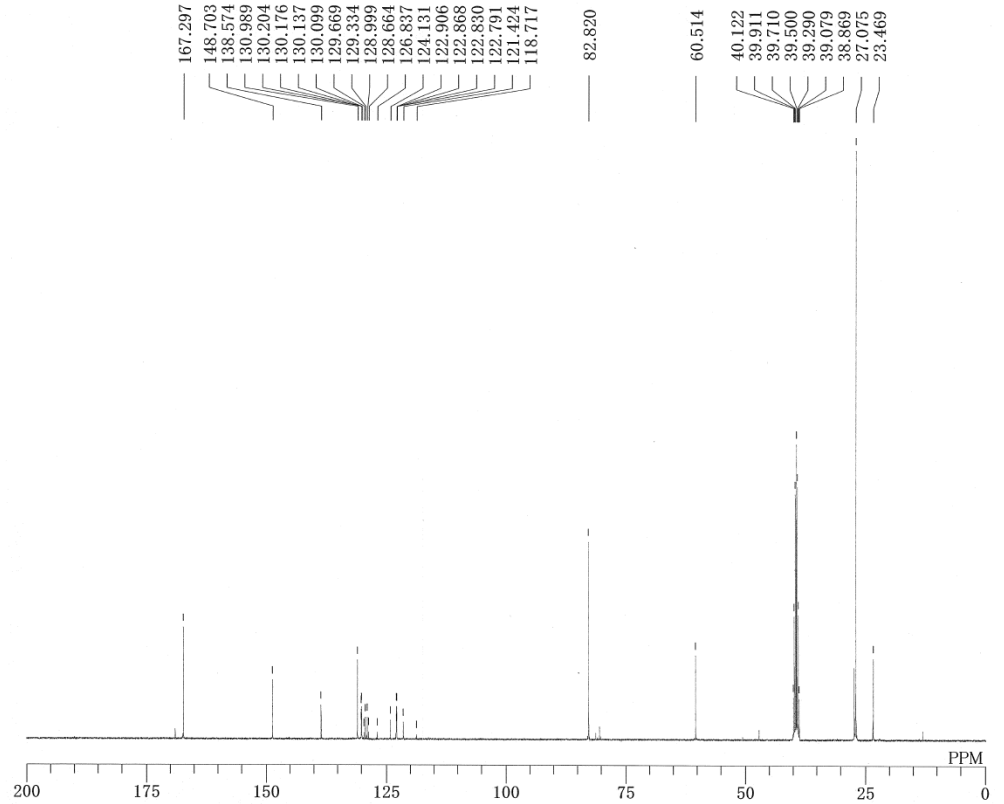




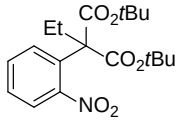
Di-*t*-butyl 2-methyl-2-(2-nitro-4-(trifluoromethyl)phenyl)malonate (8d)

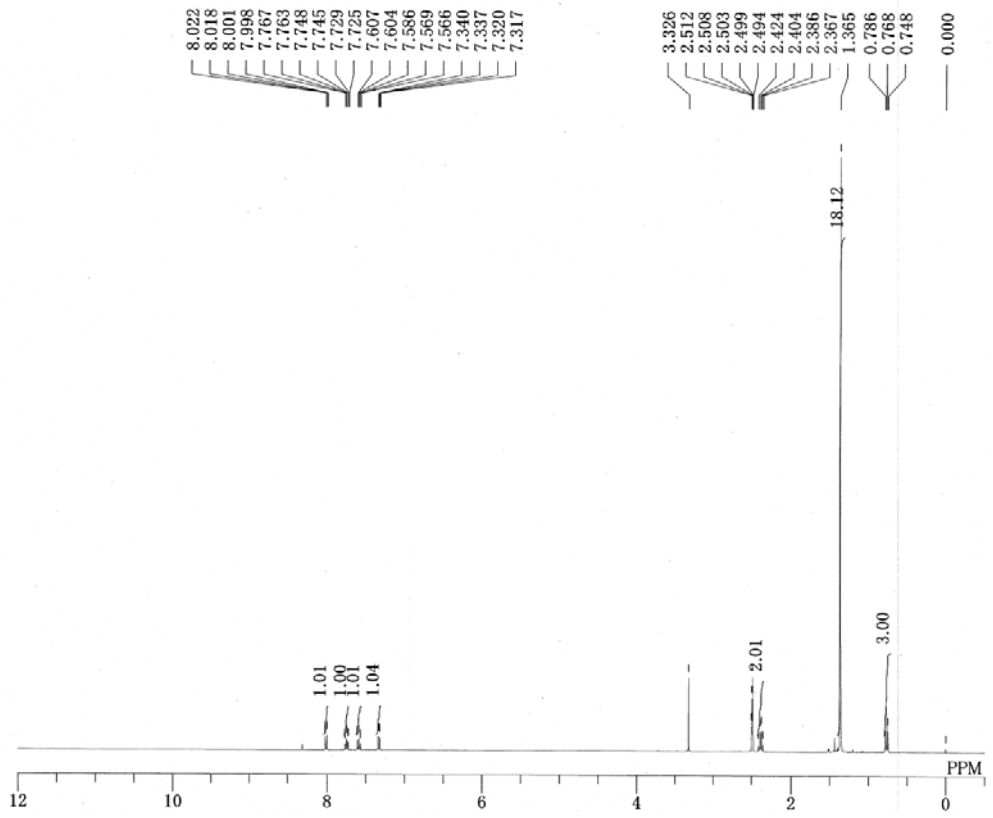


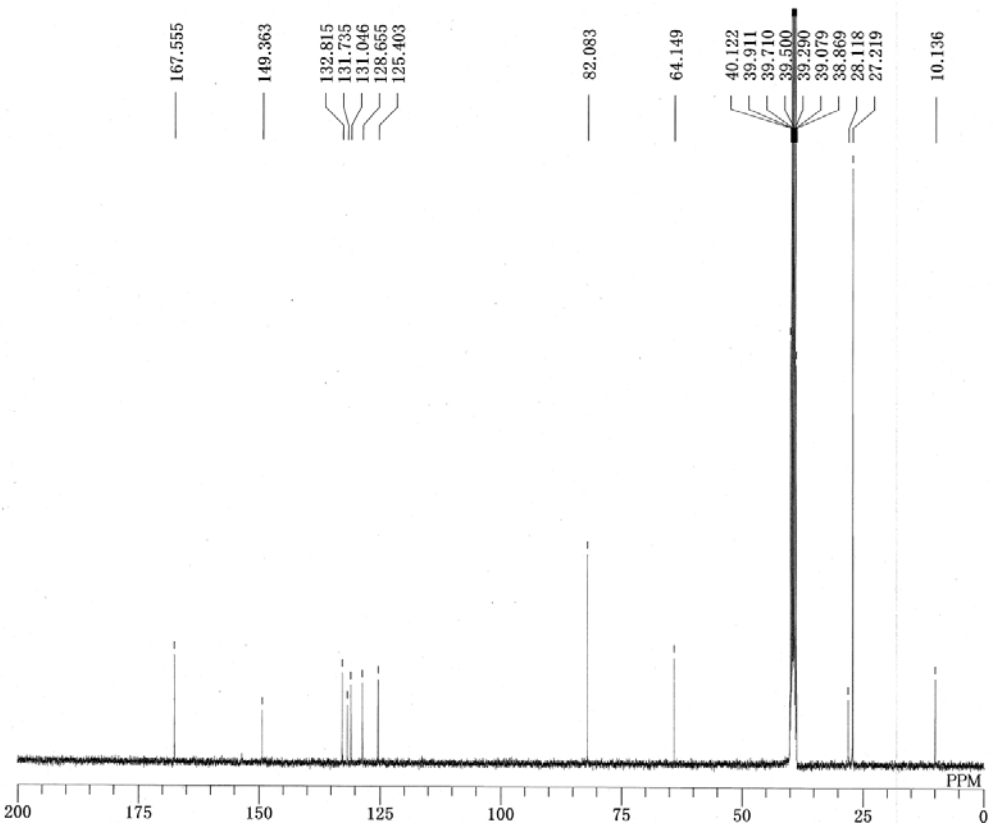




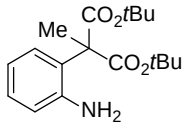
Di-*t*-butyl 2-ethyl-2-(2-nitrophenyl)malonate (8e)

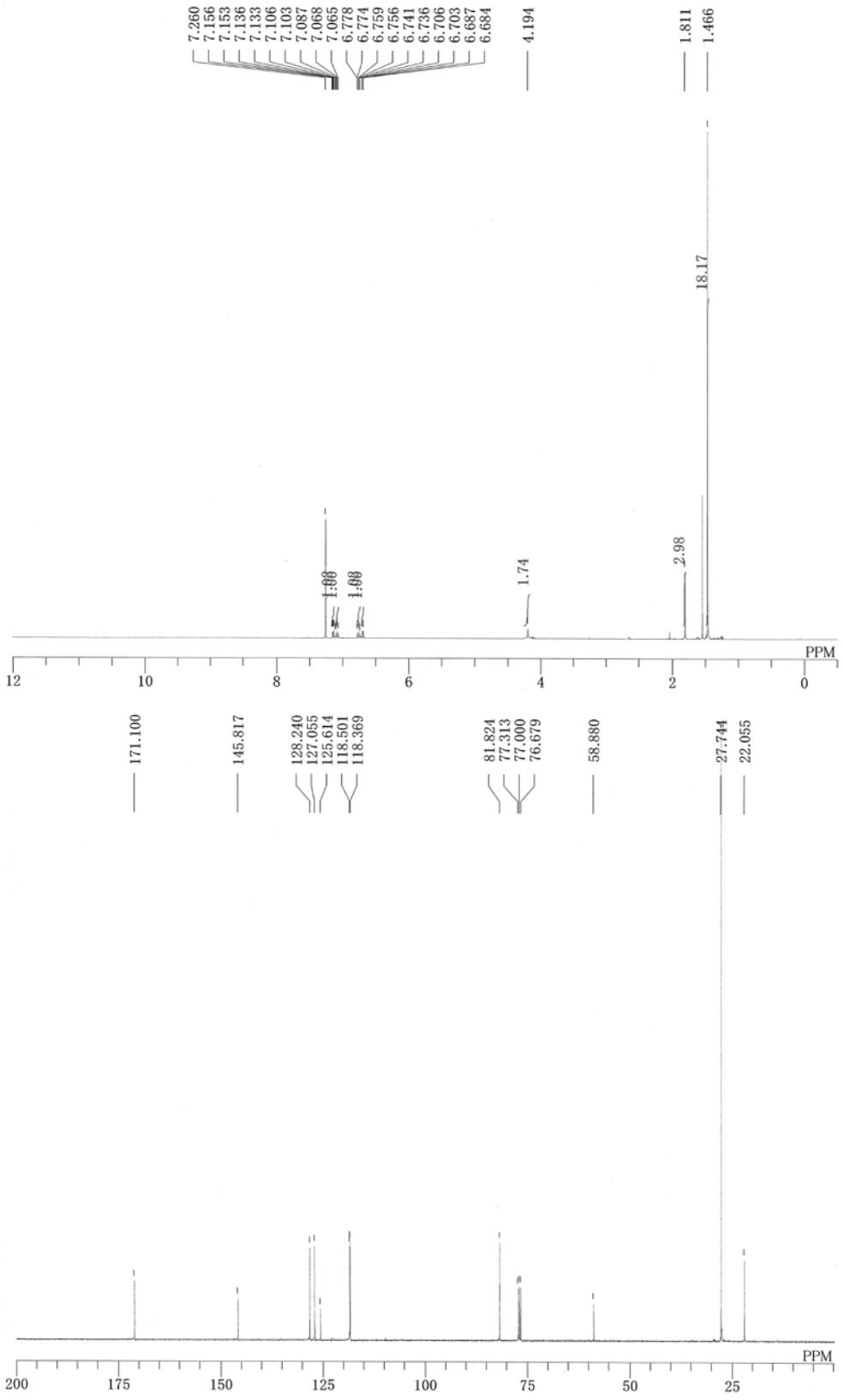




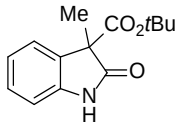


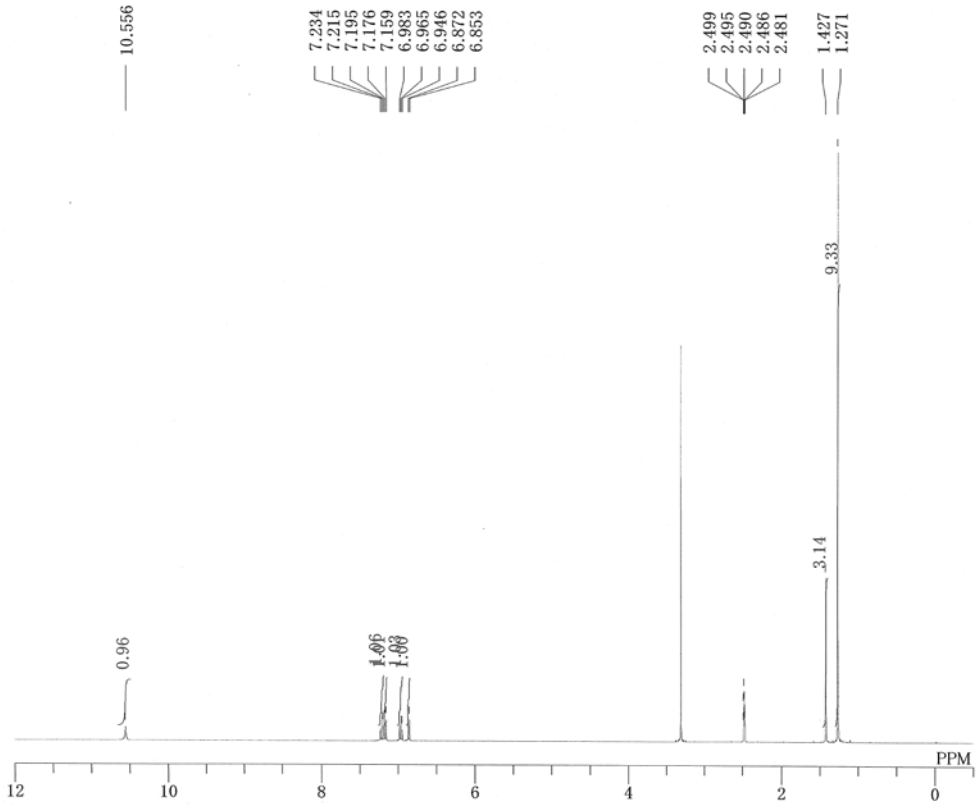
Di-*t*-butyl 2-(2-aminophenyl)-2-methylmalonate (6)

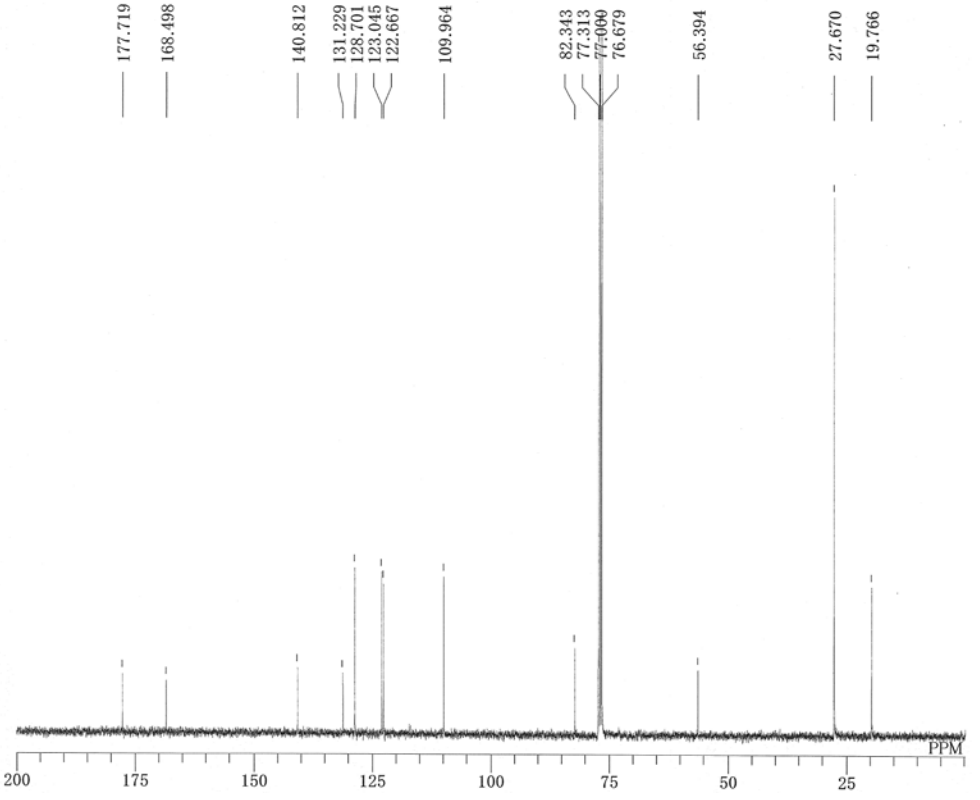




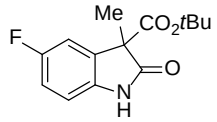
t-Butyl 3-methyl-2-oxoindoline-3-carboxylate (1)

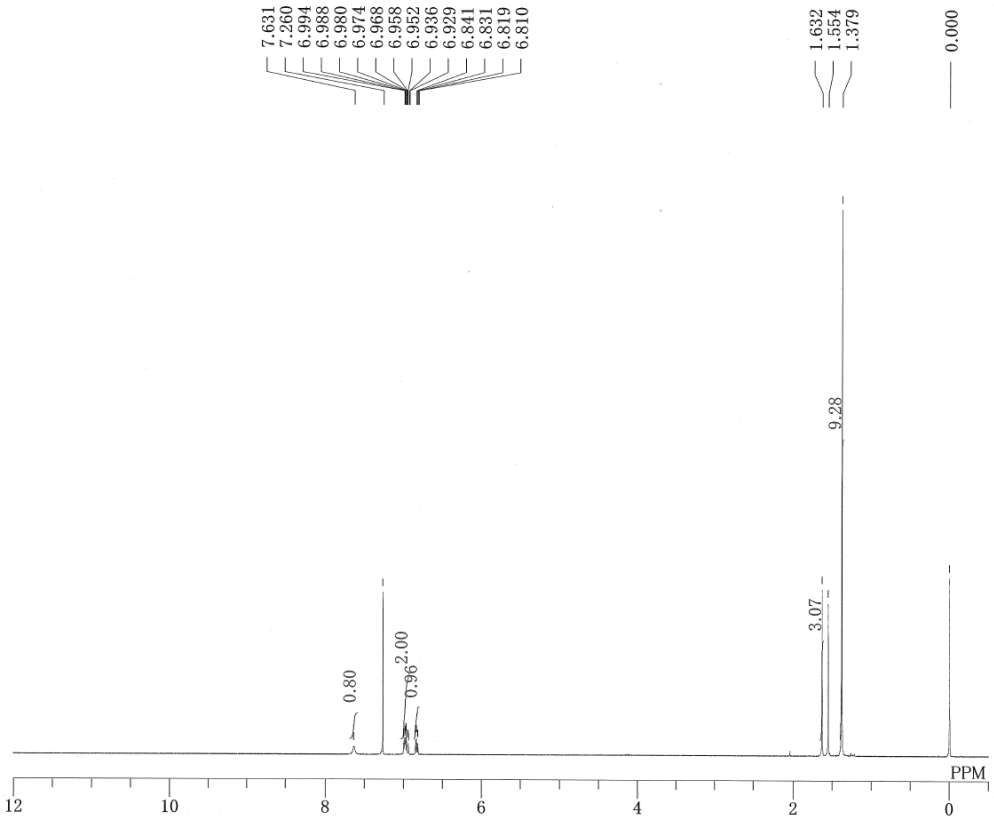


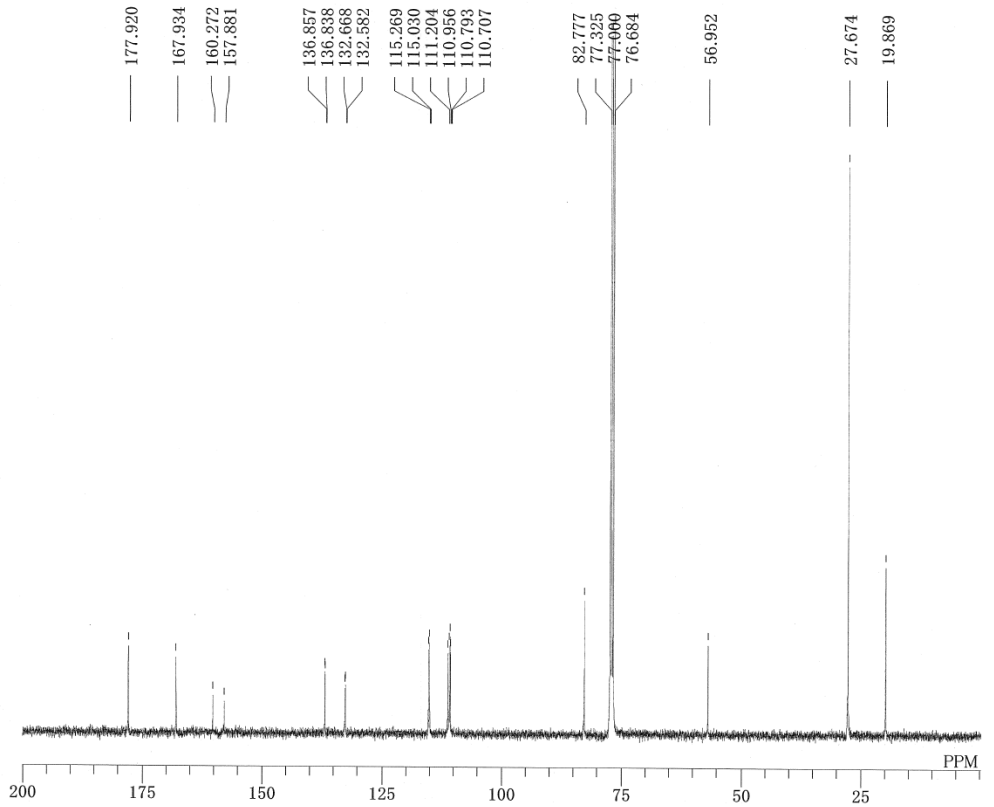




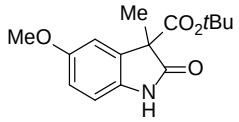
t-Butyl 5-fluoro-3-methyl-2-oxoindoline-3-carboxylate (1a)

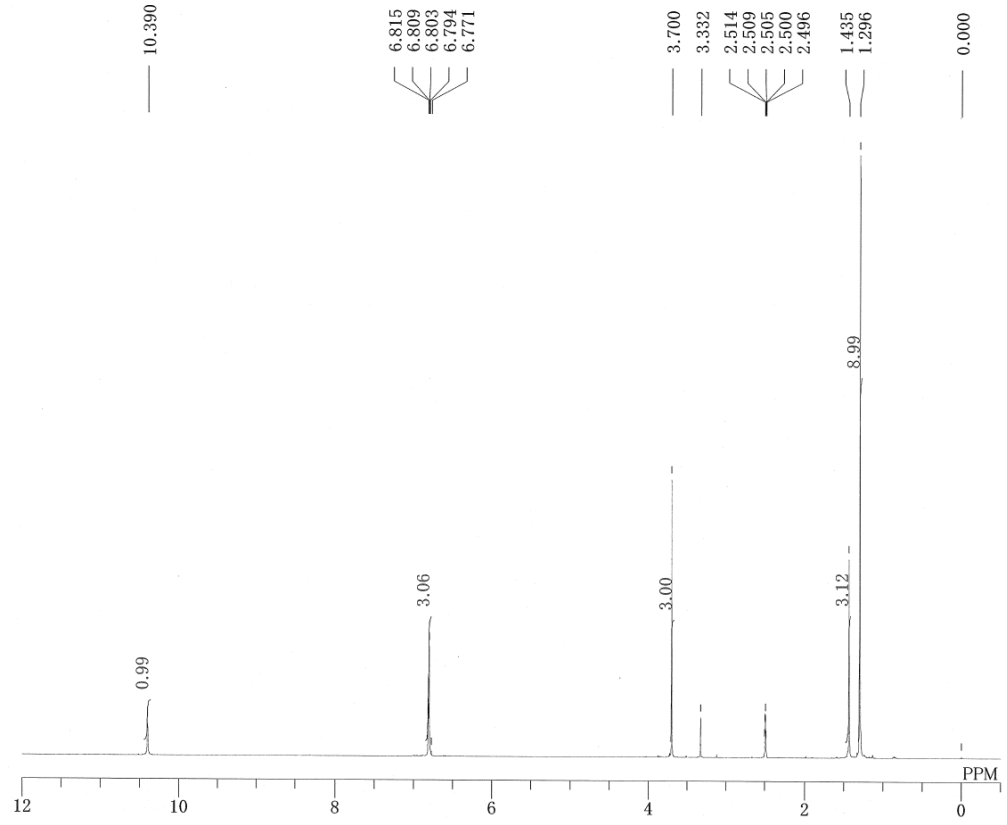


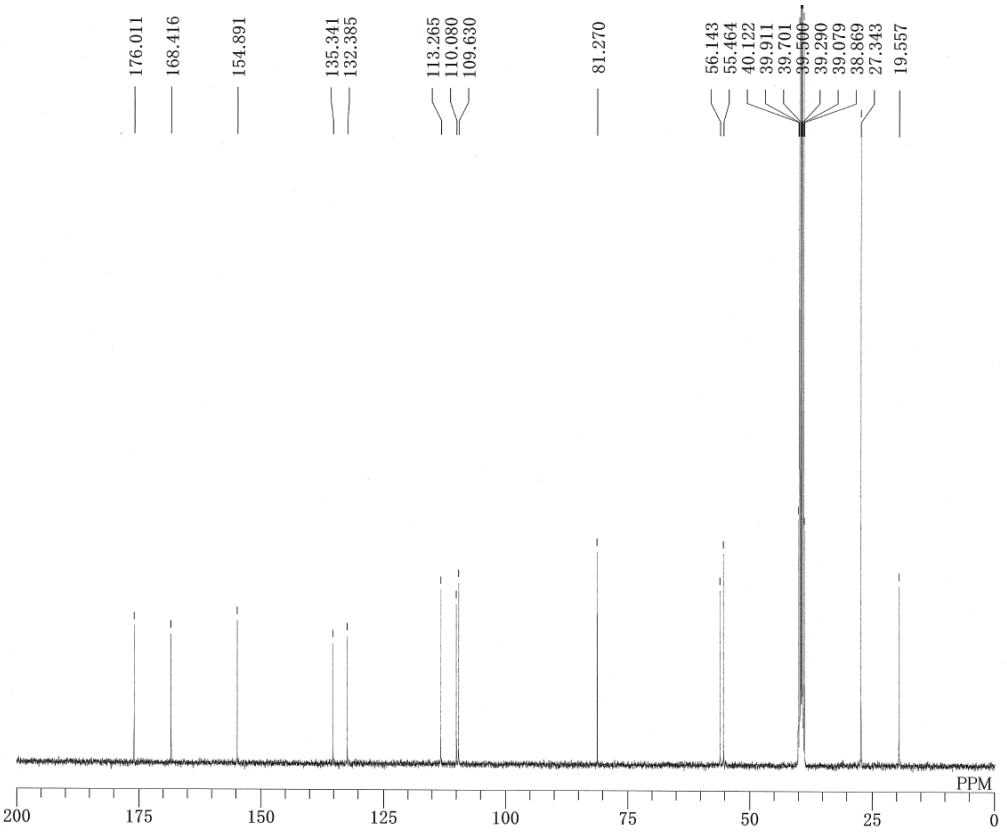




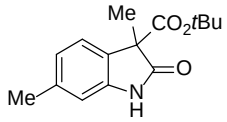
t-Butyl 5-methoxy-3-methyl-2-oxoindoline-3-carboxylate (1b)

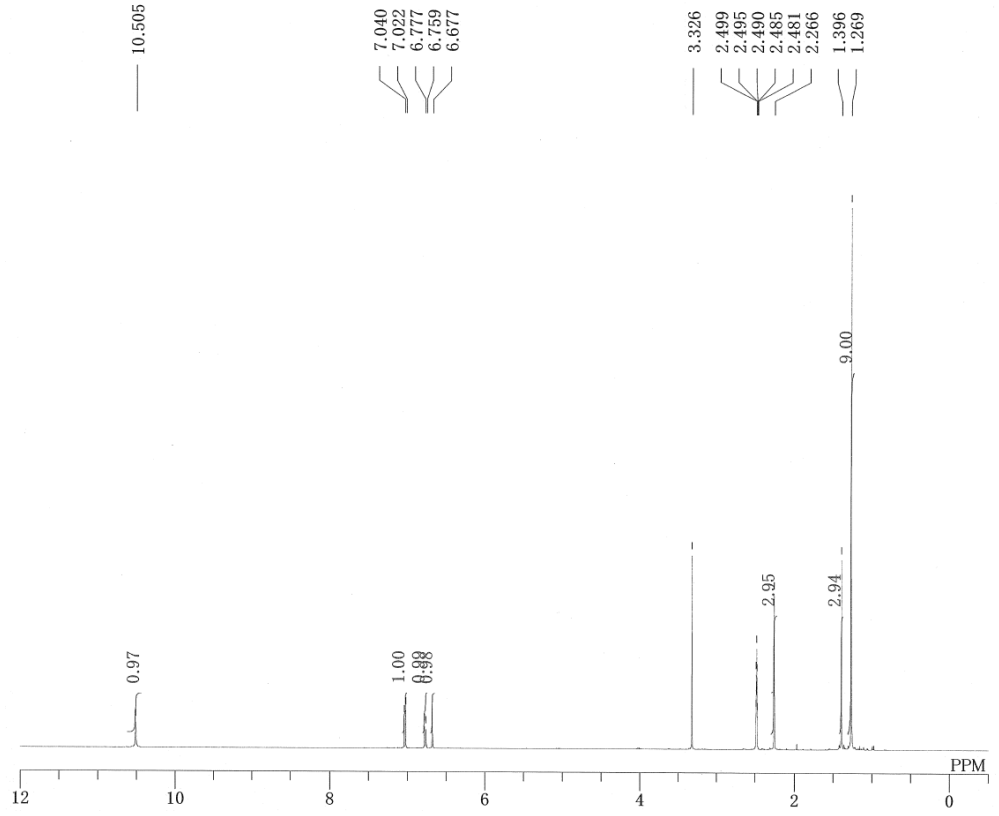


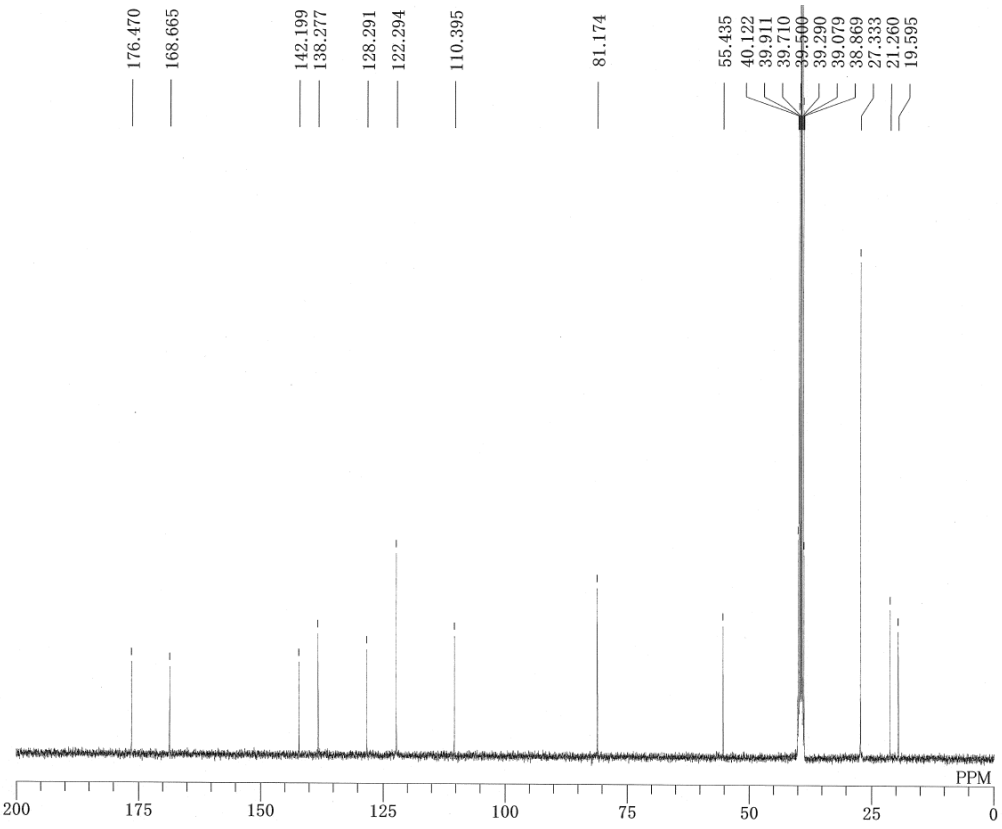




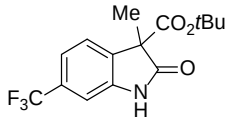
t-Butyl 3,6-dimethyl-2-oxoindoline-3-carboxylate (1c)

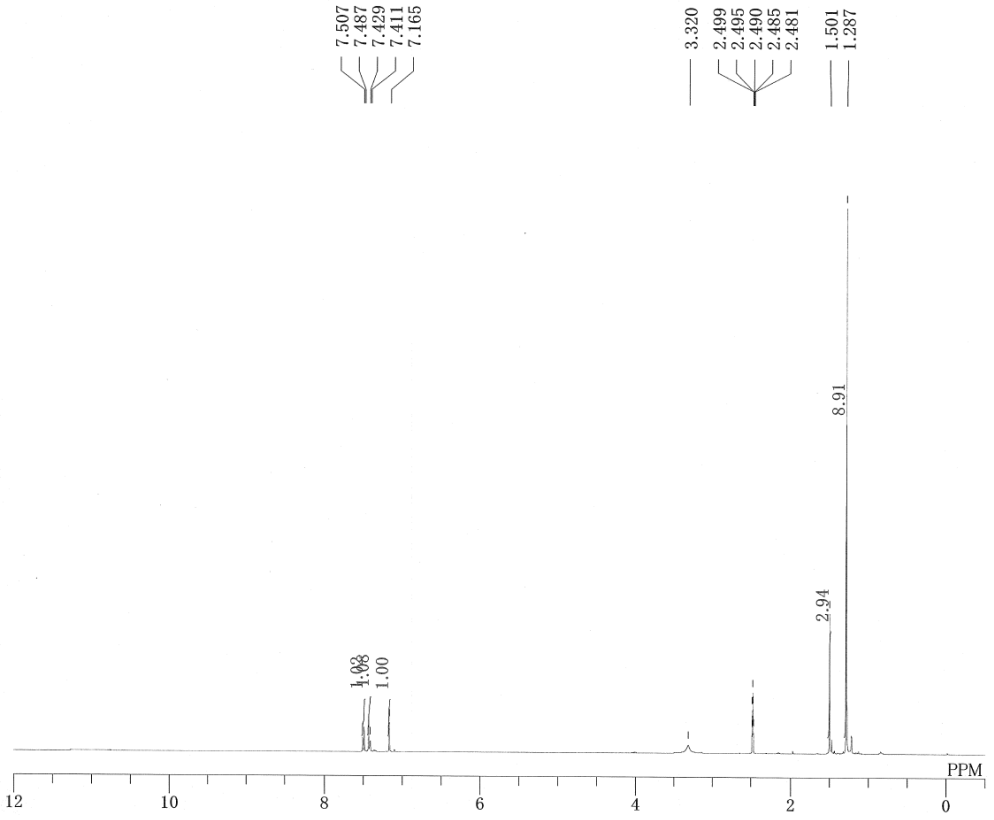


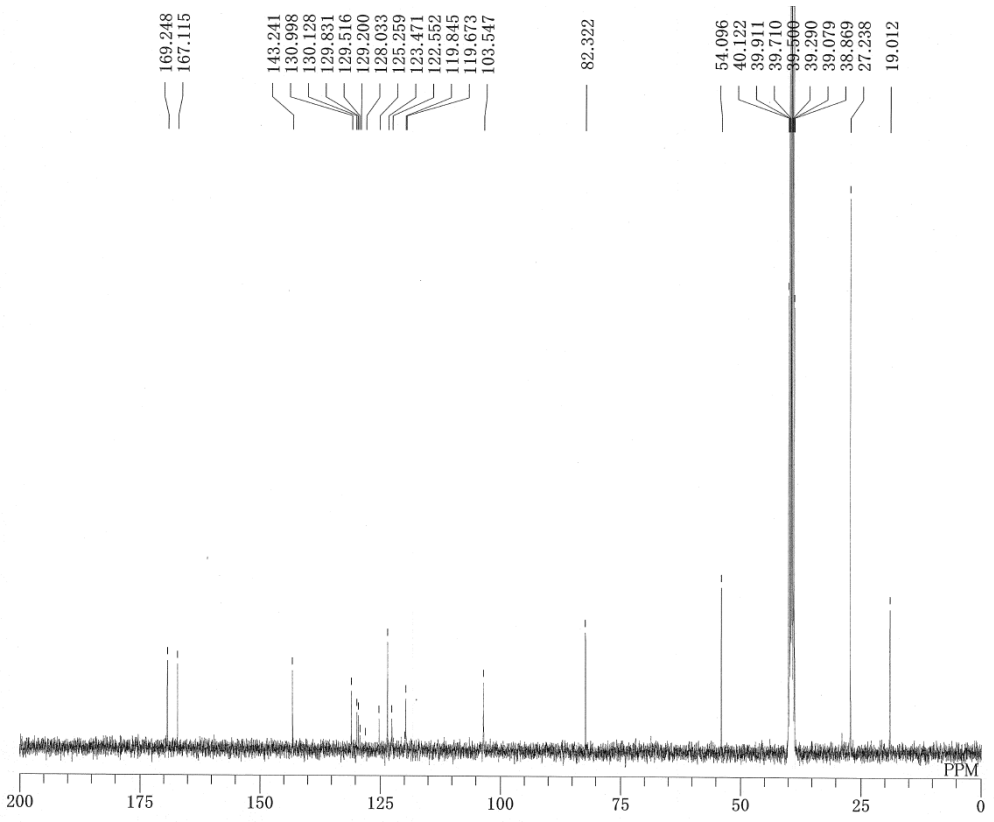




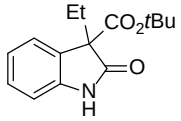
t-Butyl 3-methyl-2-oxo-6-(trifluoromethyl)indoline-3-carboxylate (1d)

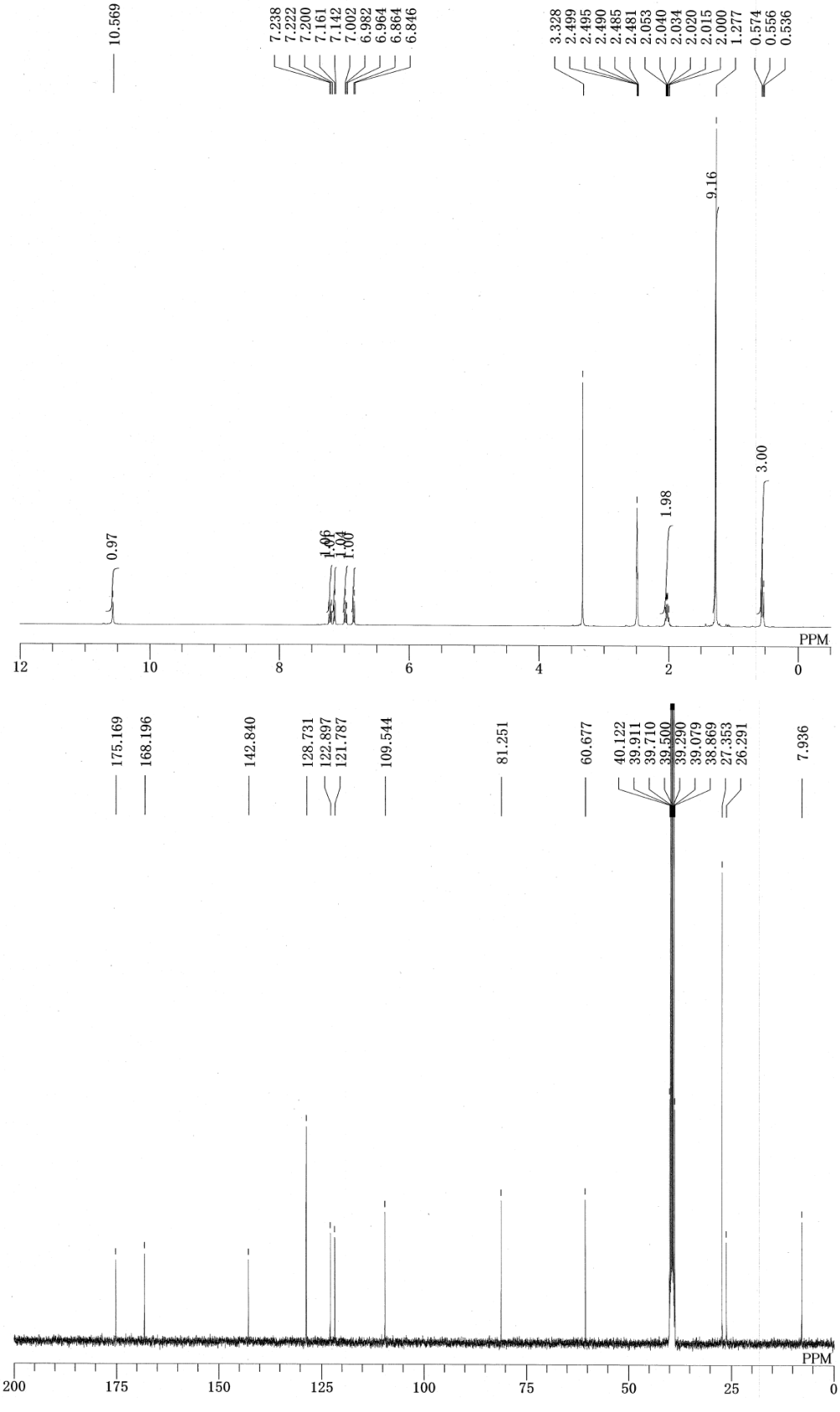




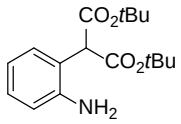


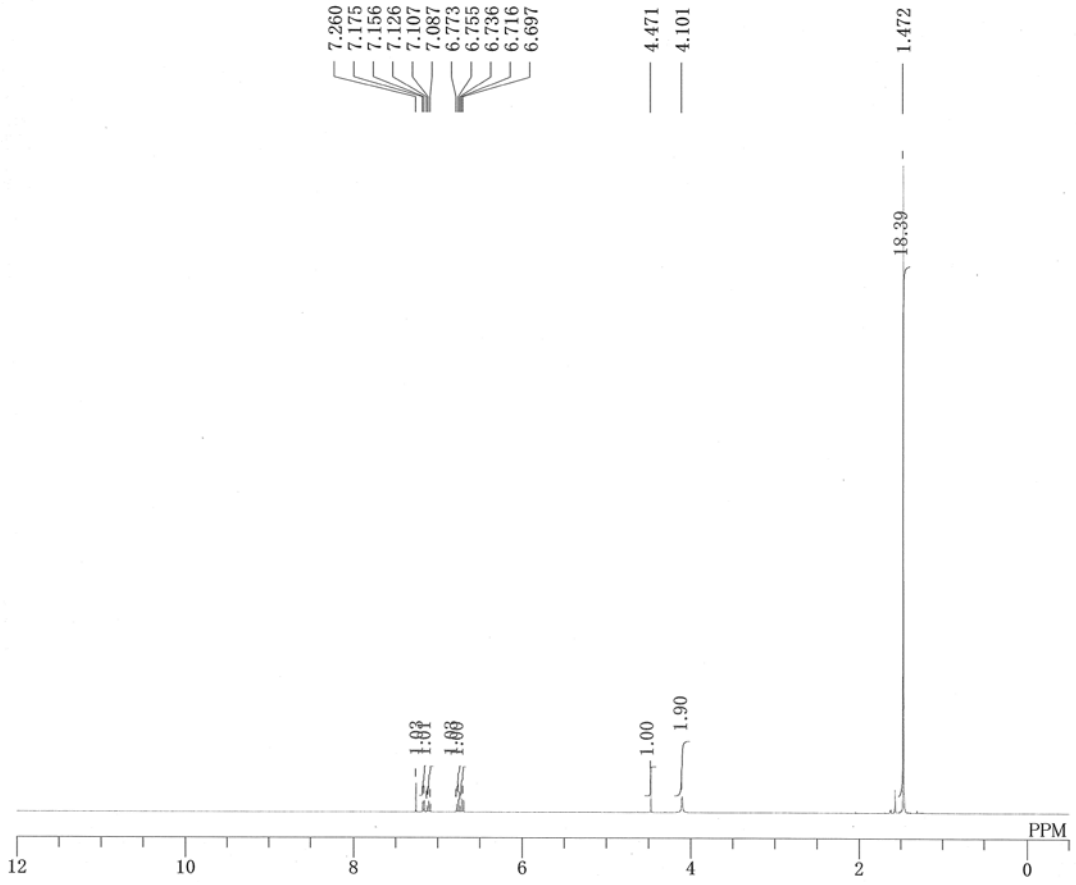
t-Butyl 3-ethyl-2-oxoindoline-3-carboxylate (1e)

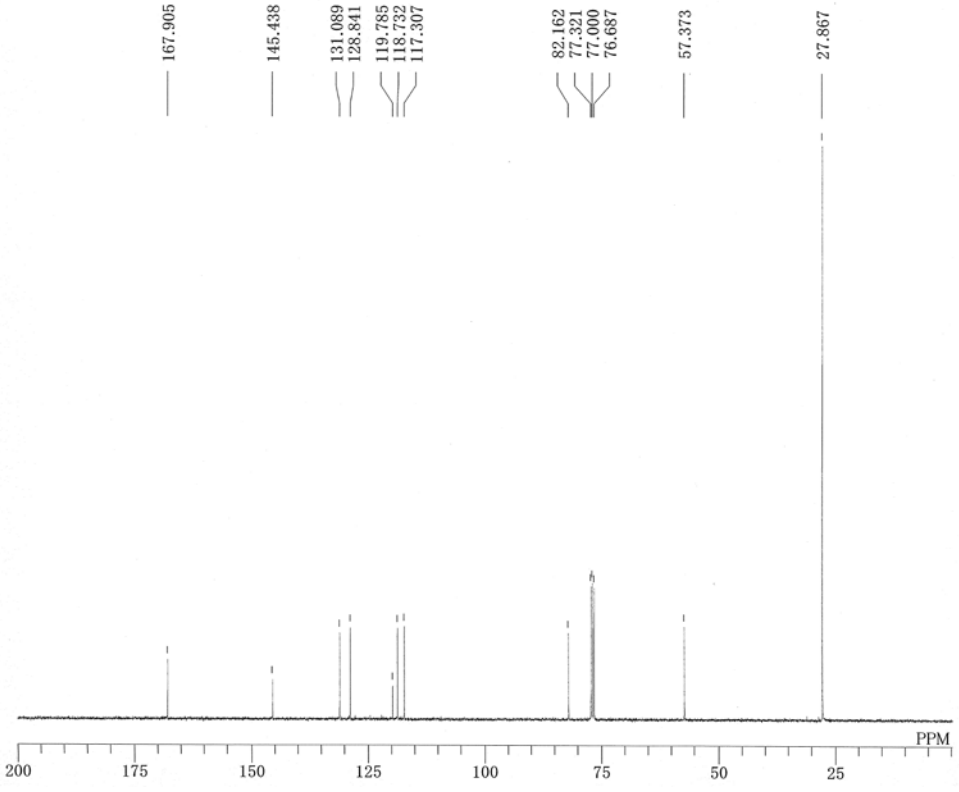




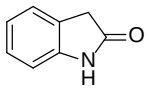
Di-*t*-butyl 2-(2-aminophenyl)malonate (5)

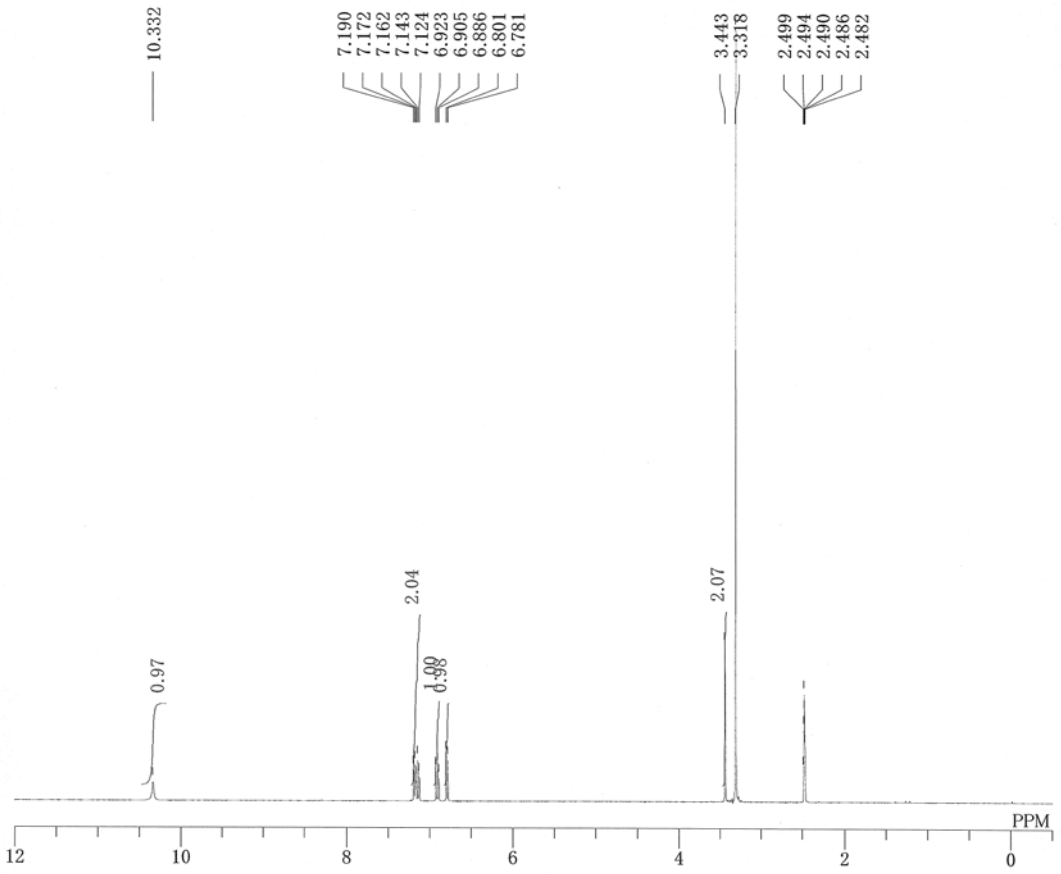






Idolin-2-one


O
N
H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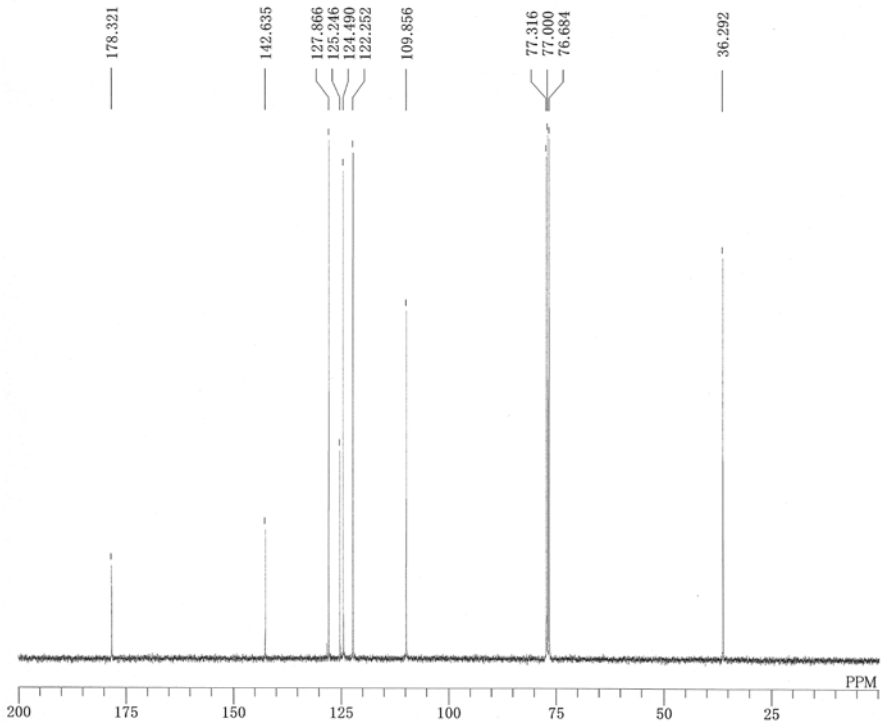
7.190
7.172
7.162
7.143
7.124
6.923
6.905
6.886
6.801
6.781
3.443
3.318
2.499
2.494
2.490
2.486
2.482
2.04
2.07
0.97
1.00
0.98
PPM
12
10
8
6
4
2
0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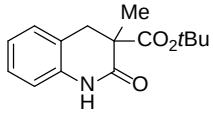
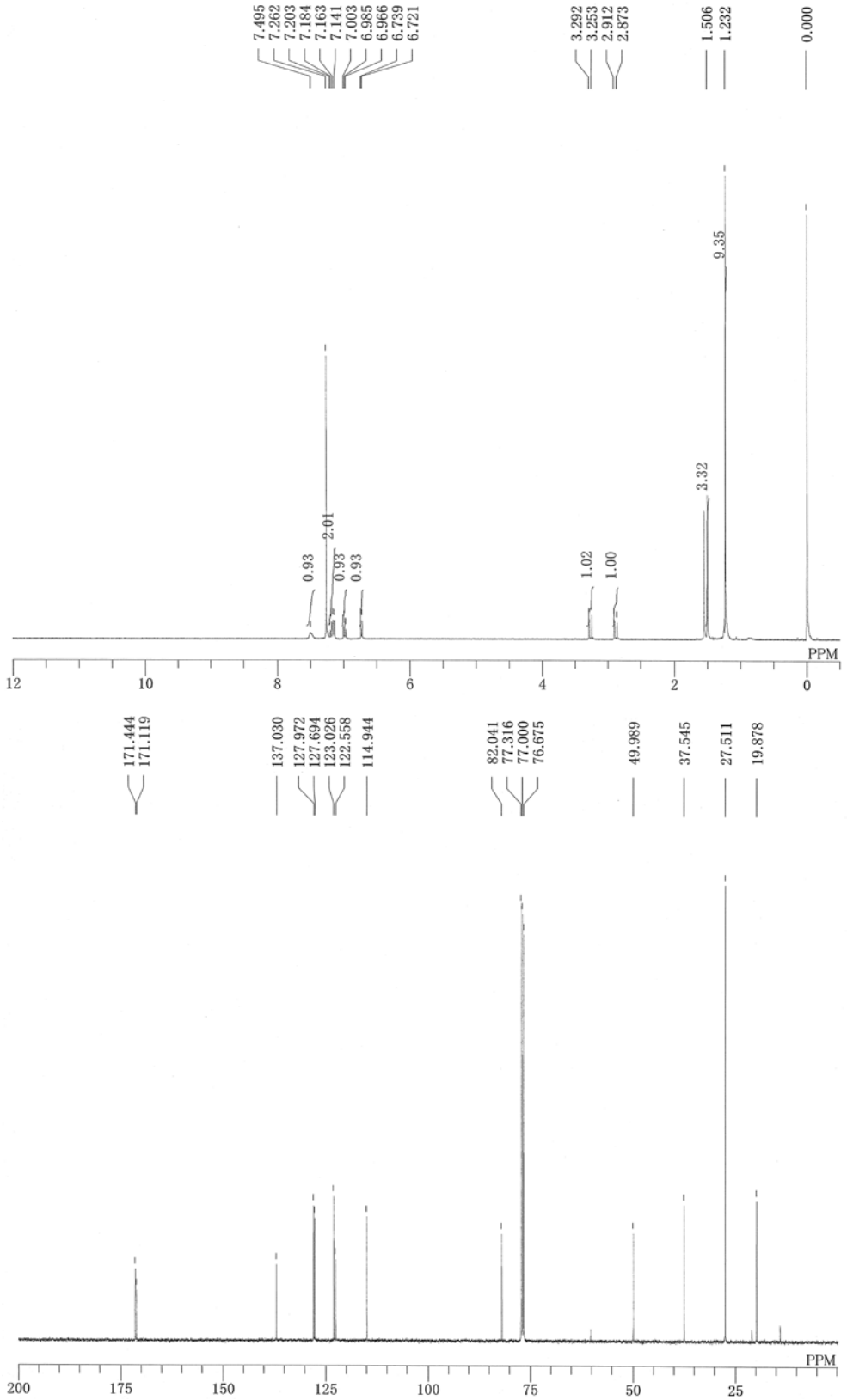
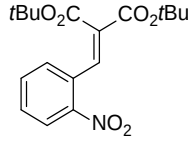
142.635
127.866
125.246
124.490
122.252
109.856
77.316
77.000
76.684
36.292
PPM
200
175
150
125
100
75
50
25

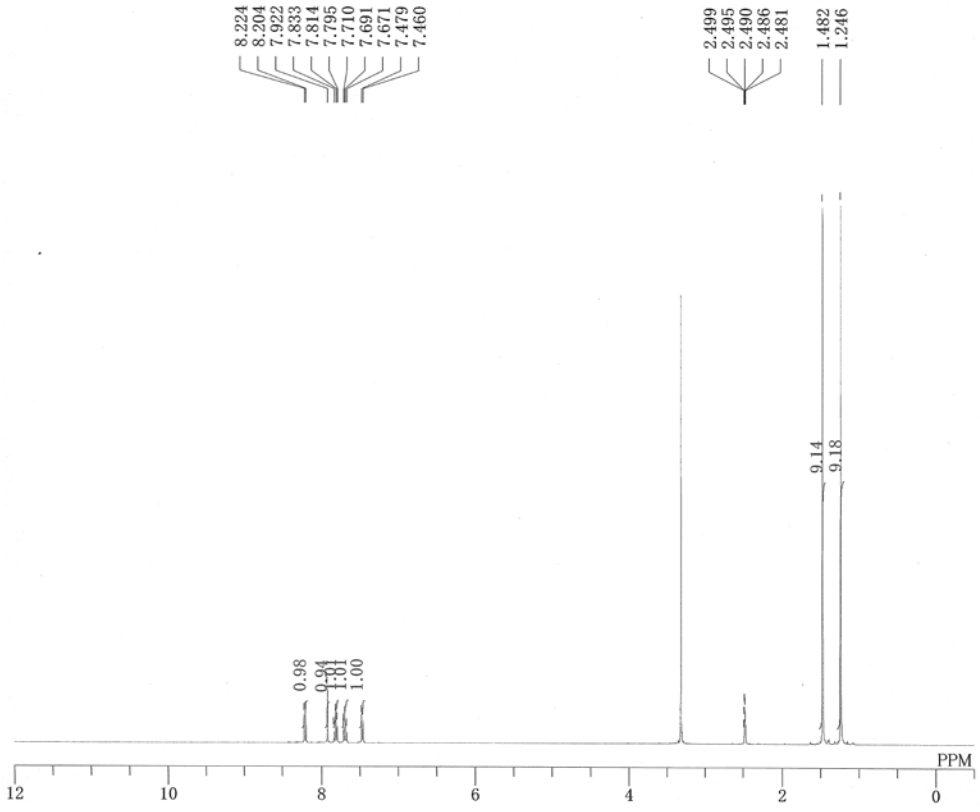
_t_-Butyl 3-methyl-2-oxo-1,2,3,4-tetrahydroquinoline-3-carboxylate (11)

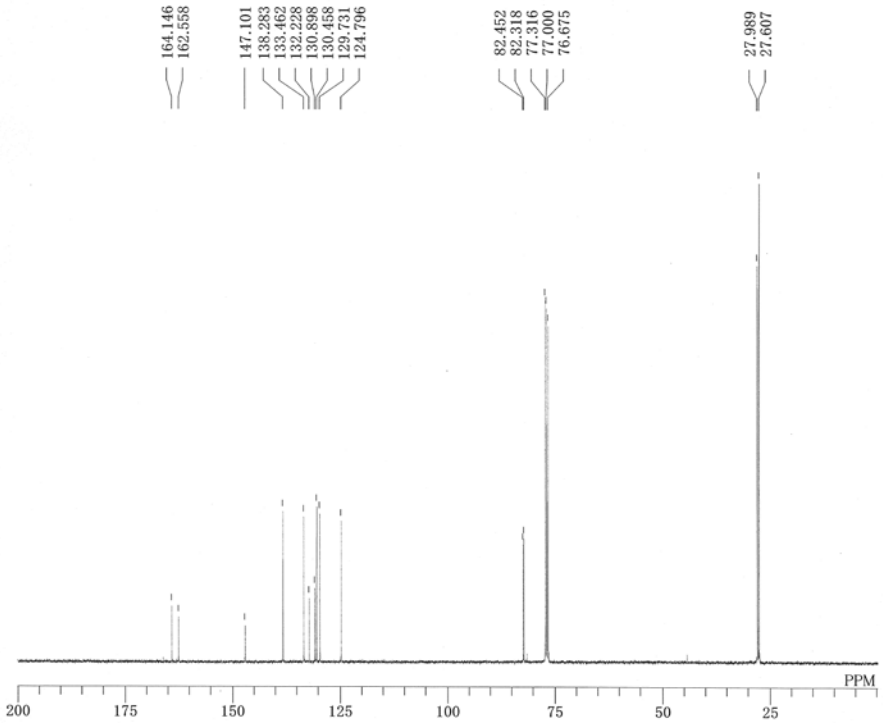




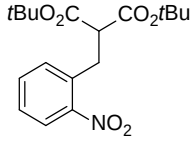
Di-*t*-butyl 2-(2-nitrobenzylidene)malonate (13)

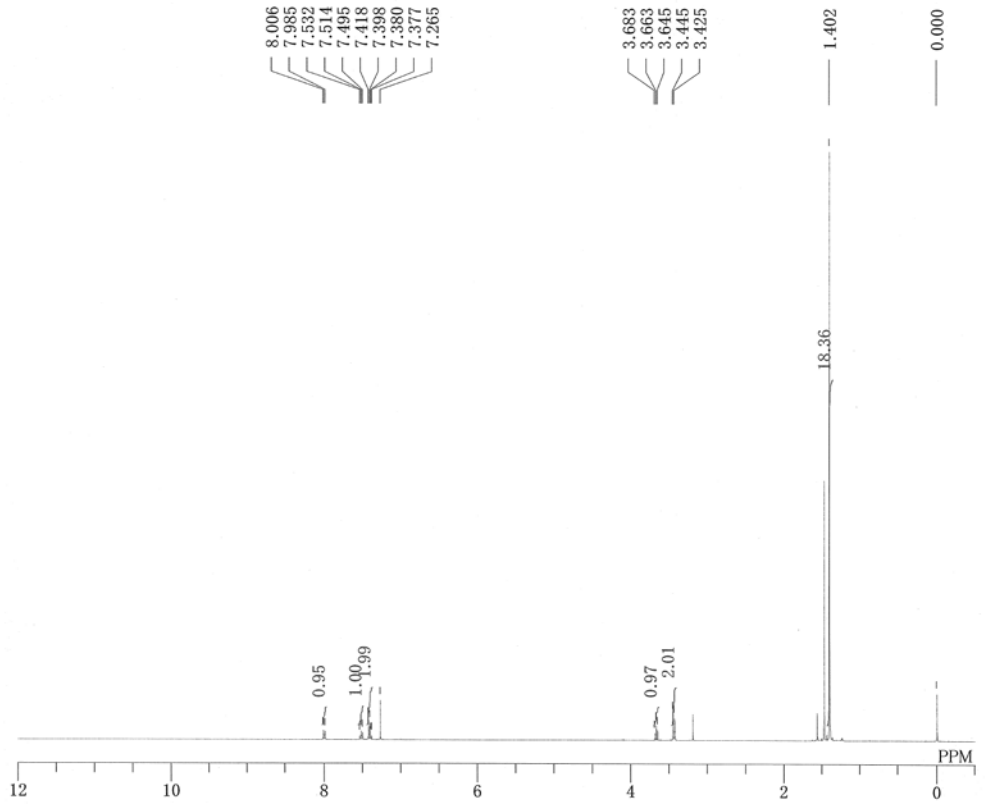


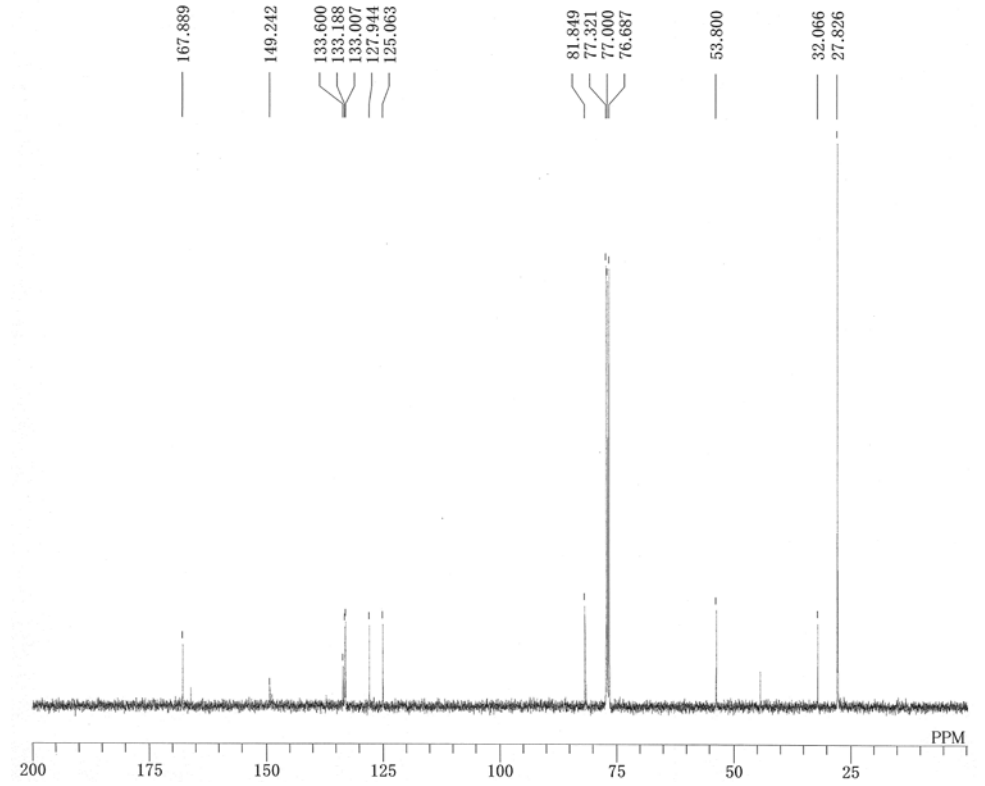




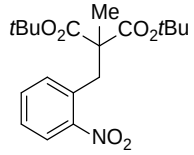
Di-*t*-butyl 2-(2-nitrobenzyl)malonate (14)

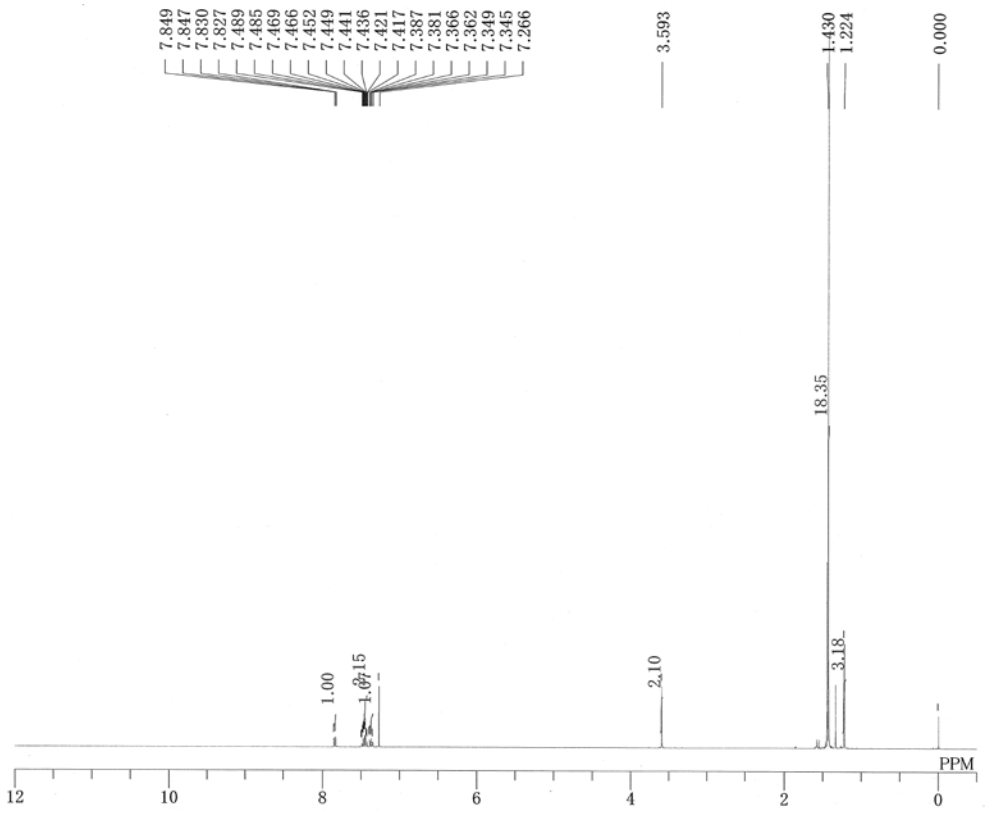


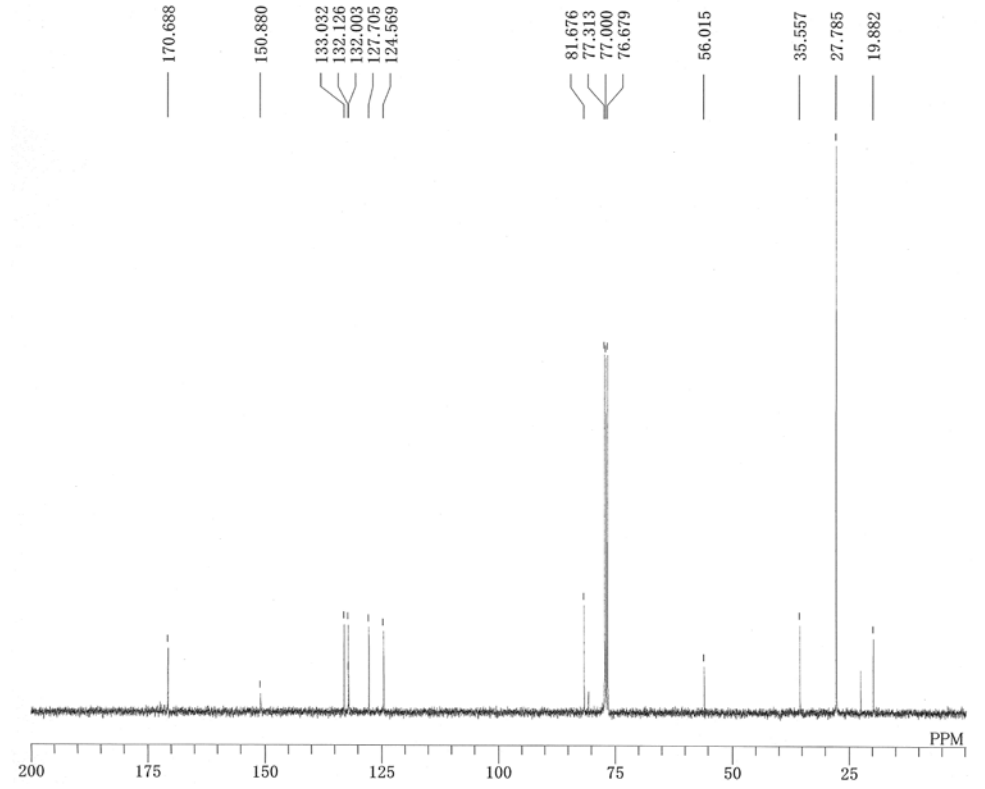




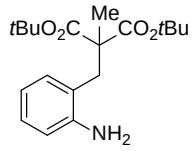
Di-*t*-butyl 2-methyl-2-(2-nitrobenzyl)malonate (15)

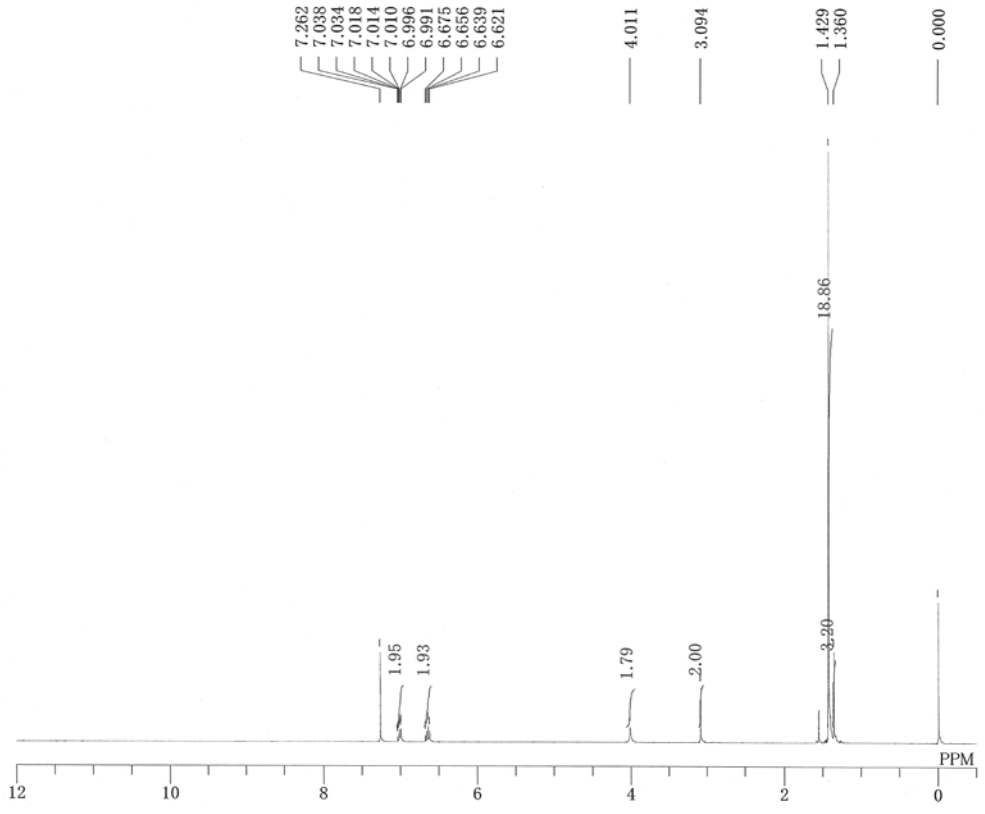


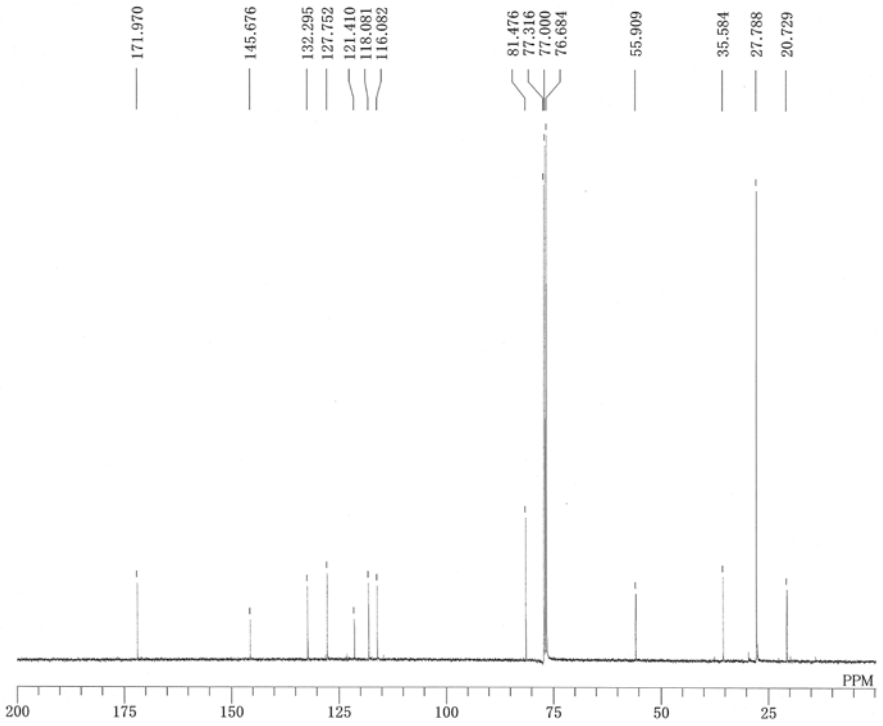




Di-*t*-butyl 2-(2-aminobenzyl)-2-methylmalonate (10)







3-(Hydroxymethyl)-3-methylindolin-2-one (2)