

Supporting information

One pot synthesis of tetrasubstituted thiophenes: [3+2]

Annulation Strategy

Satya Narayan Sahu,^a Maneesh Kumar Gupta,^a SurjeetSingh,^a Pratik Yadav,^a Rahul Panwar,^a

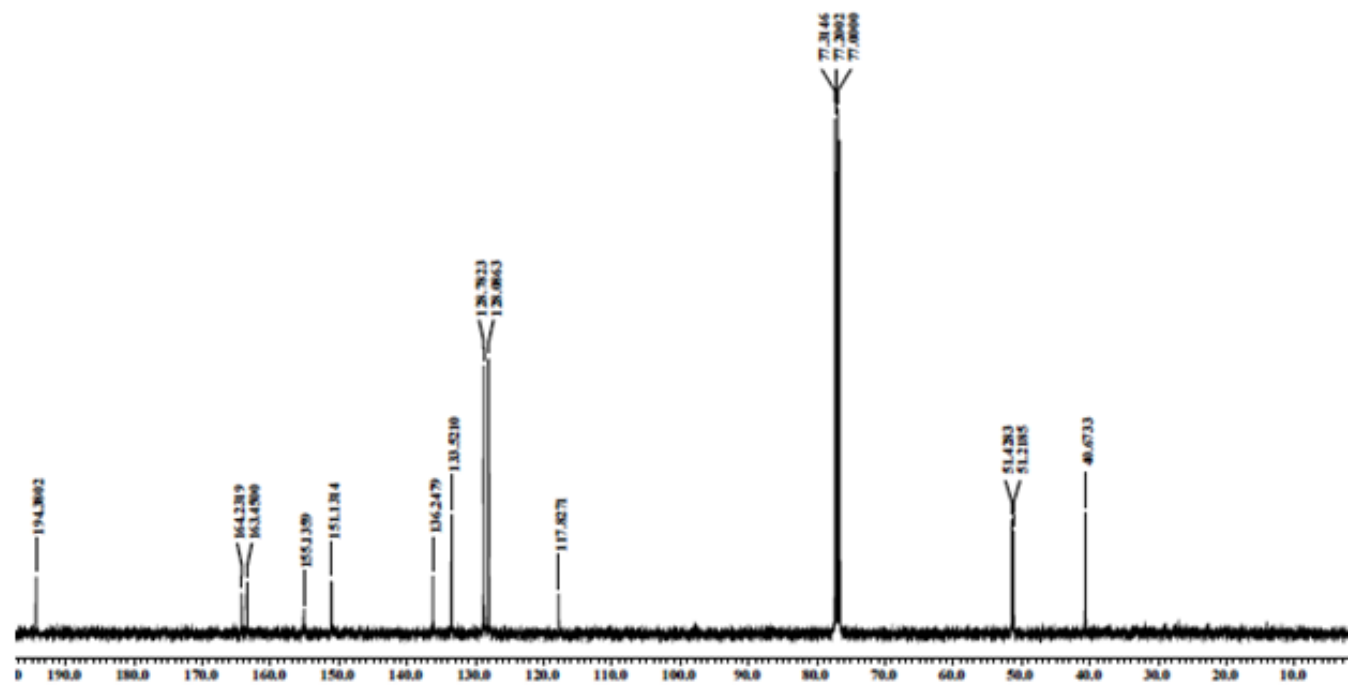
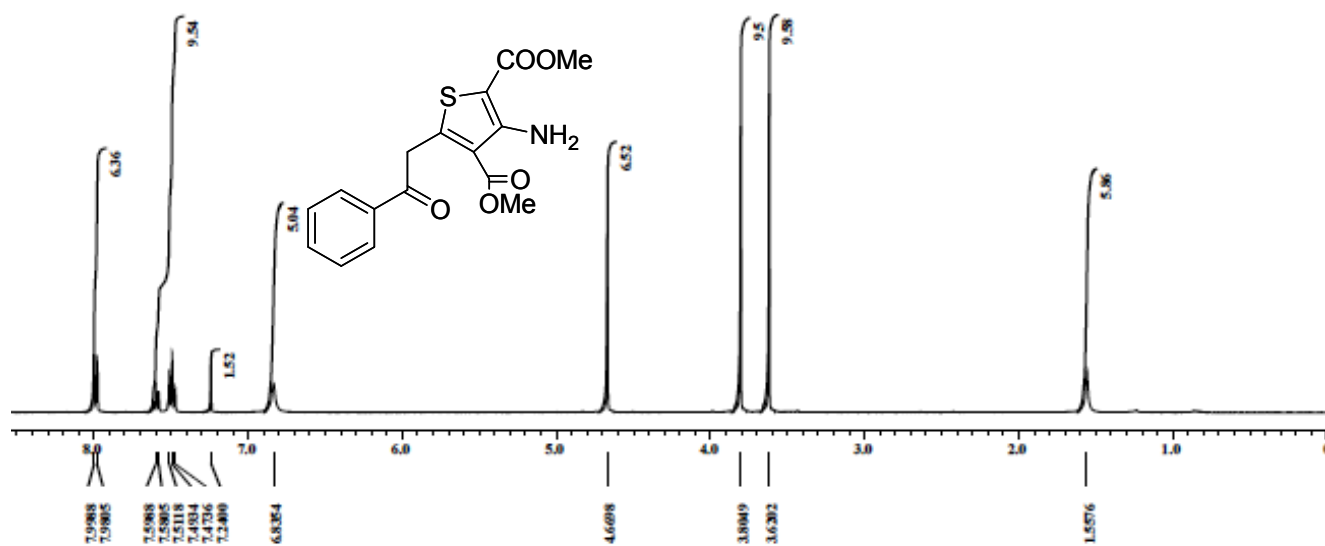
Abhinav Kumar,^b Vishnu Ji Ram,^b Brijesh Kumar^c and Ramendra Pratap^{a,}*

^aDepartment of Chemistry, University of Delhi, North Campus, Delhi, India-110007

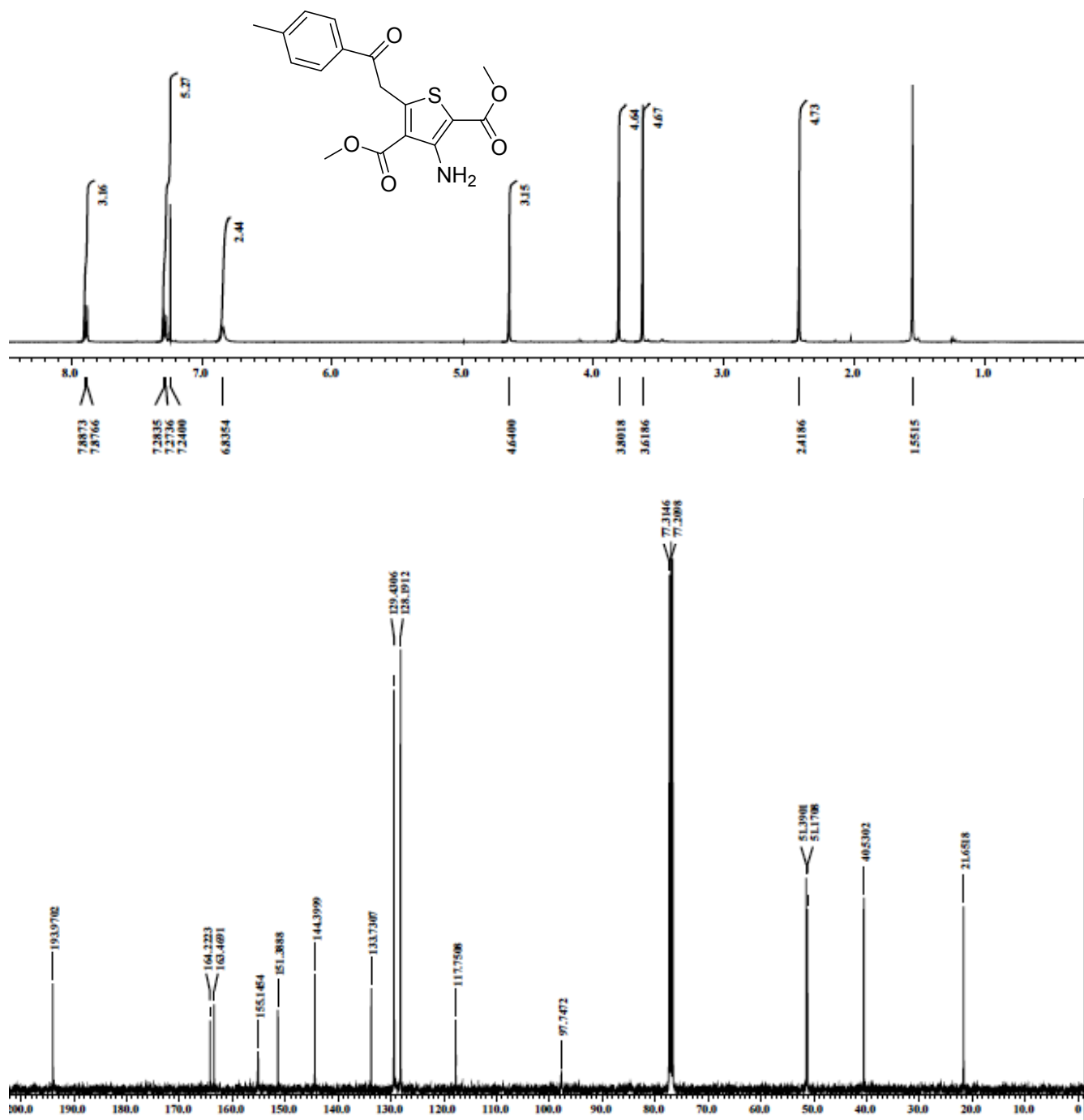
^bDepartment of Chemistry, University of Lucknow, Lucknow, Uttar Pradesh, India-226009.

^cDivision of SAIF, Central Drug Research Institute, Lucknow, Uttar Pradesh, India-226001

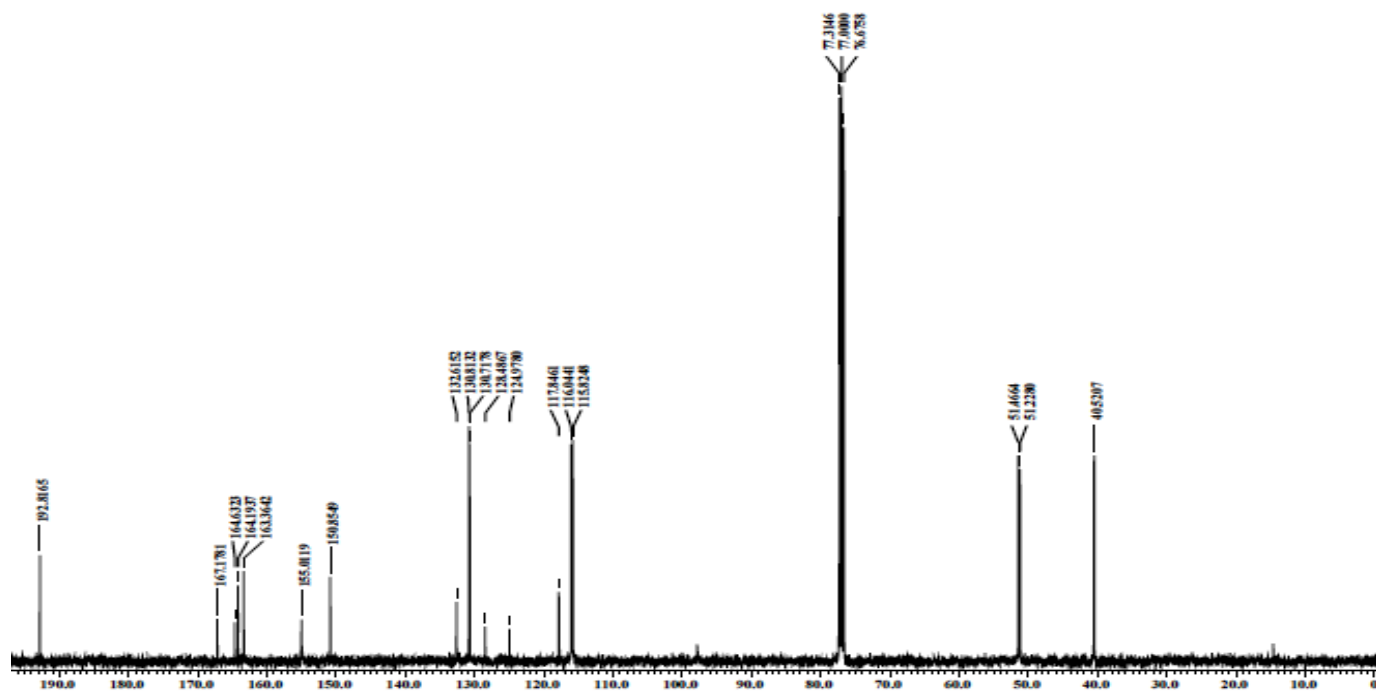
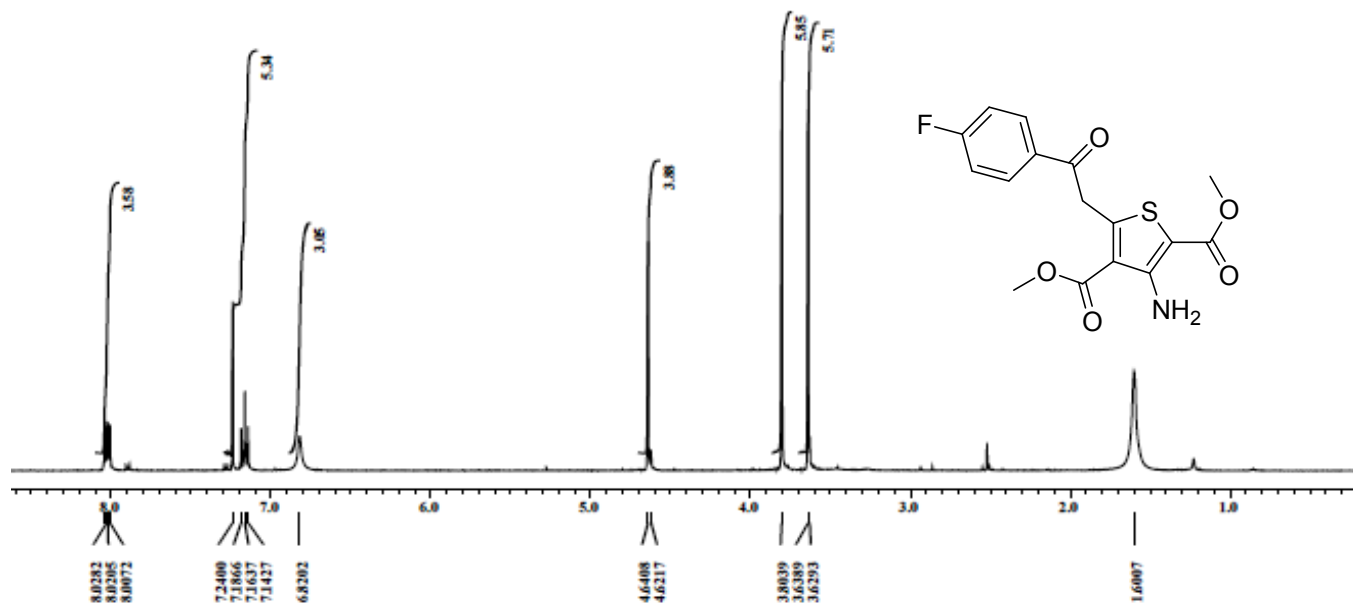
Contents	Page No.
¹ H and ¹³ C spectra of compound 10a-10o	2-16
XYZ Coordinates Monomer	17-22



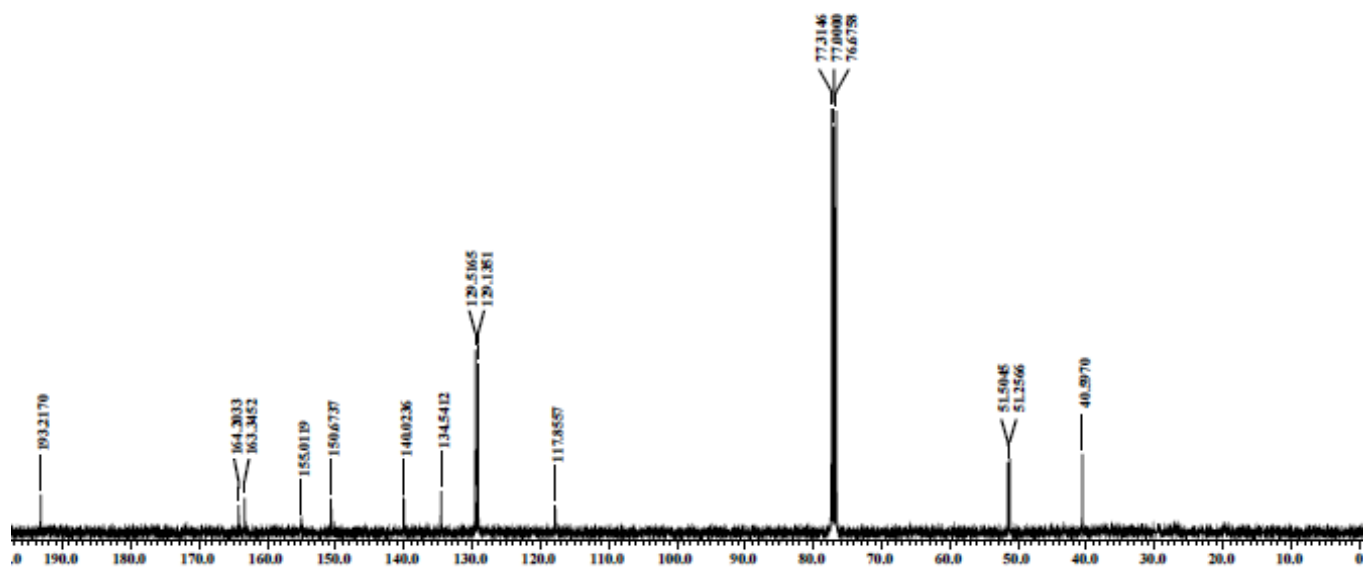
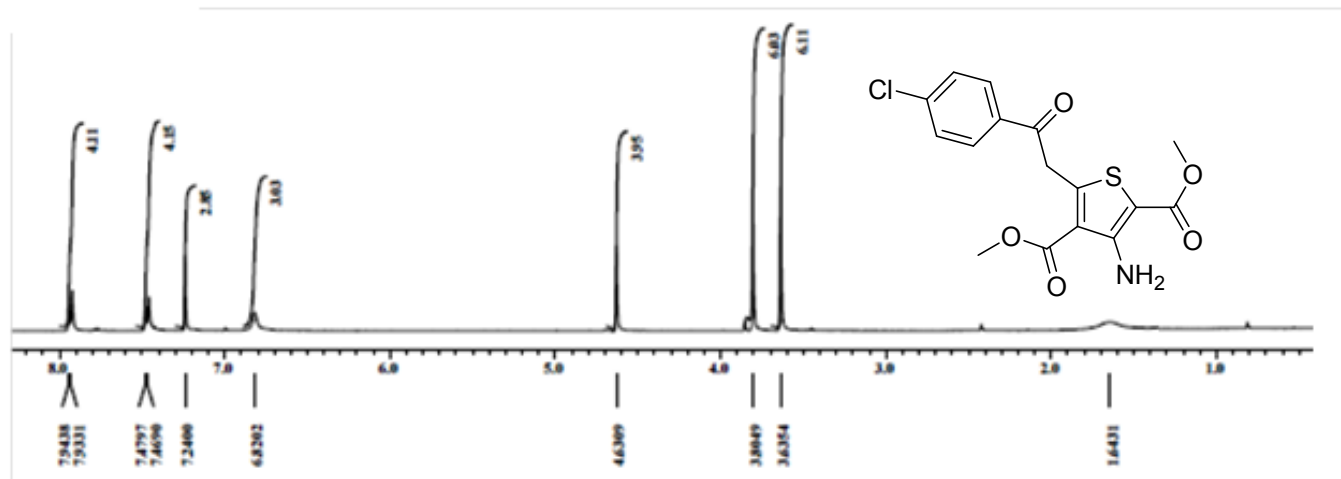
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-oxo-2-phenylethyl)thiophene-2,4-dicarboxylate(10a)



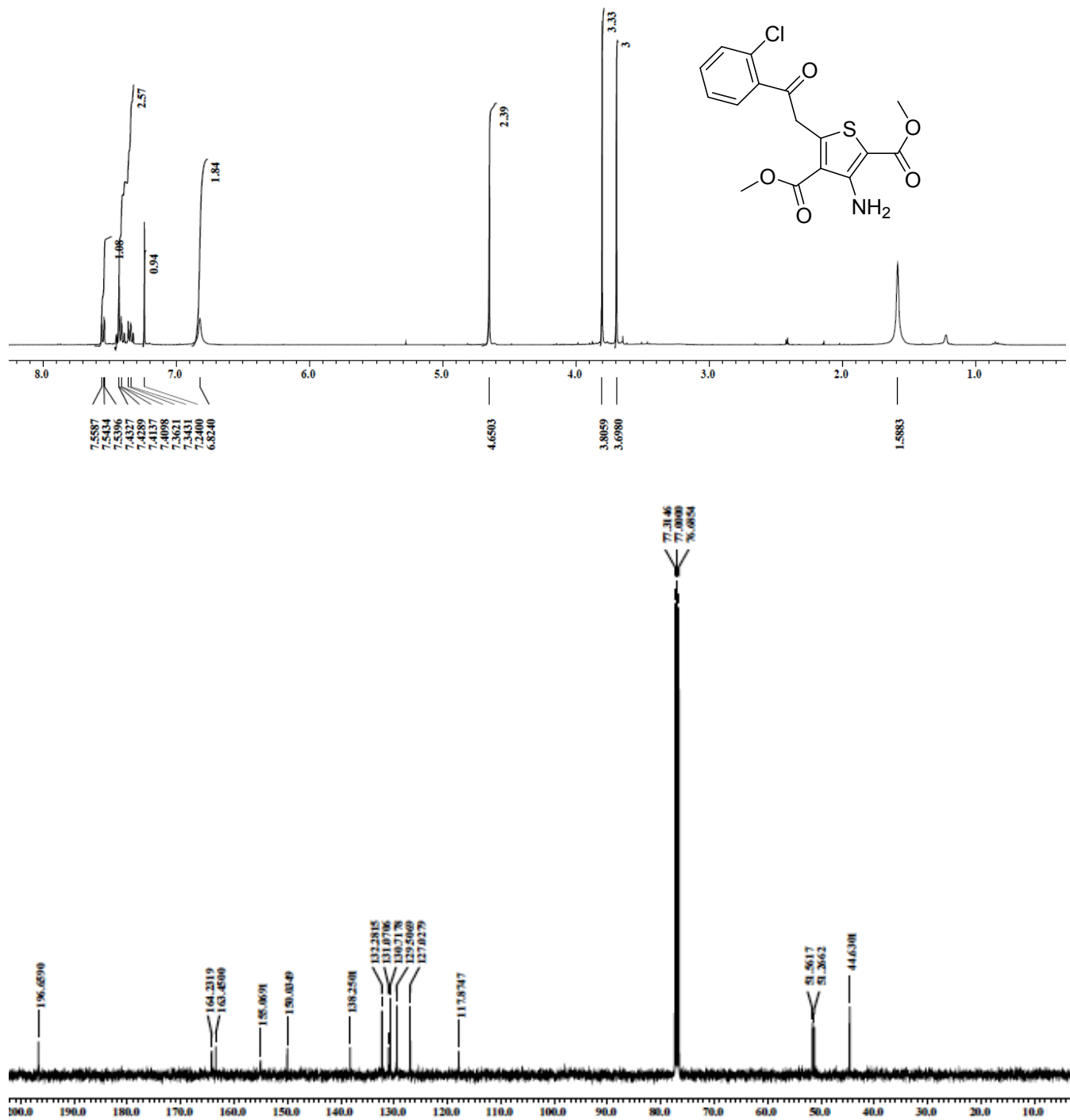
¹H and ¹³C spectra of dimethyl 3-amino-5-(2-oxo-2-(p-tolyl)ethyl)thiophene-2,4-dicarboxylate (10b)



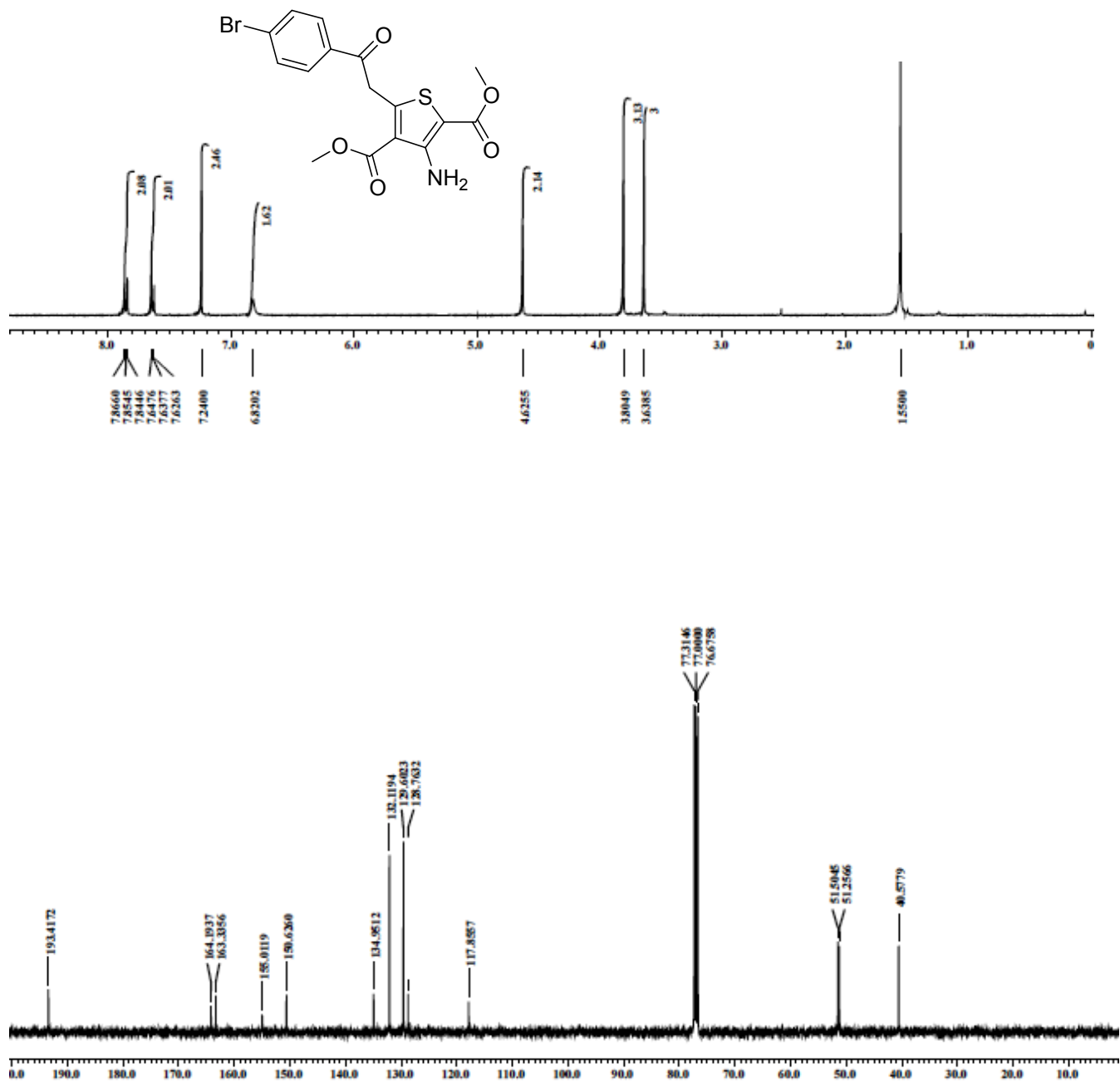
^1H and ^{13}C spectra of spectra of dimethyl 3-amino-5-(2-(4-fluorophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate(10c)



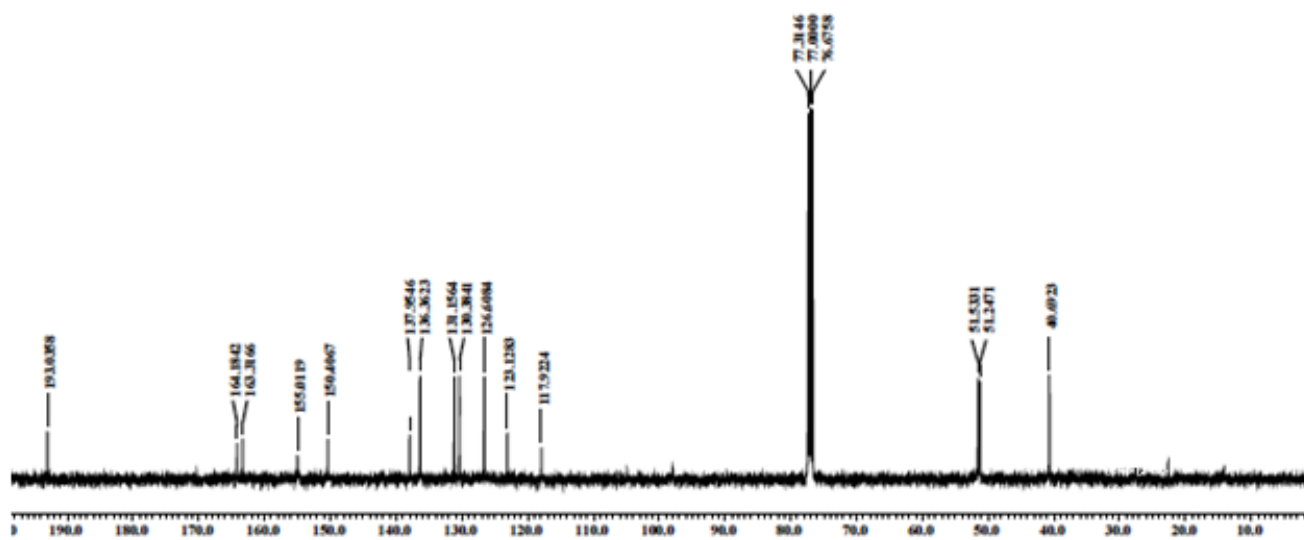
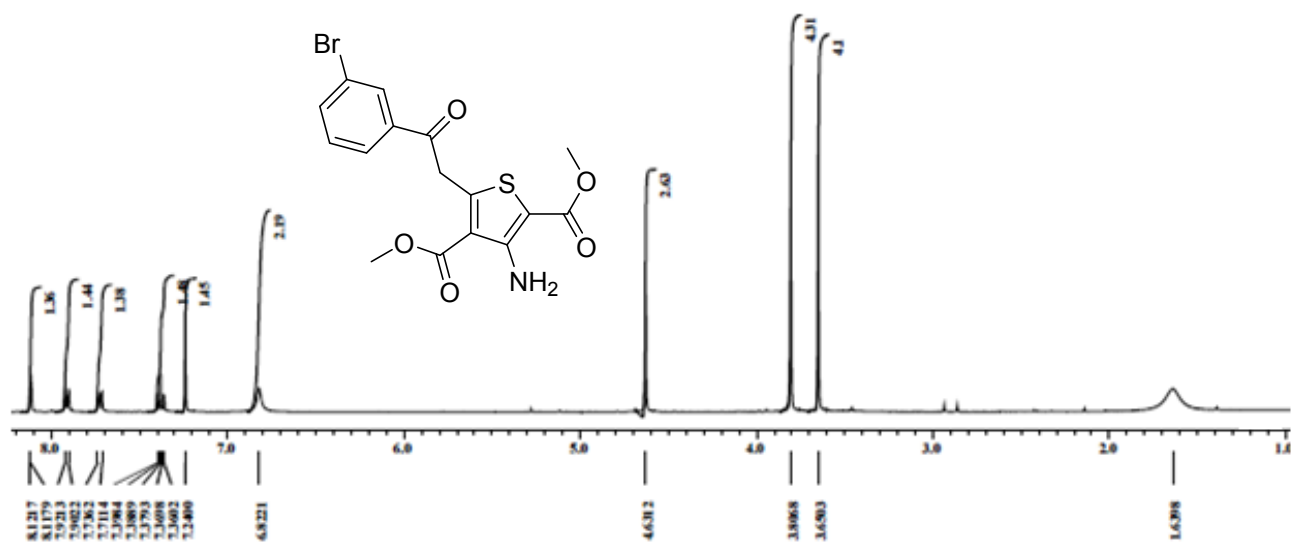
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(4-chlorophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10d**)



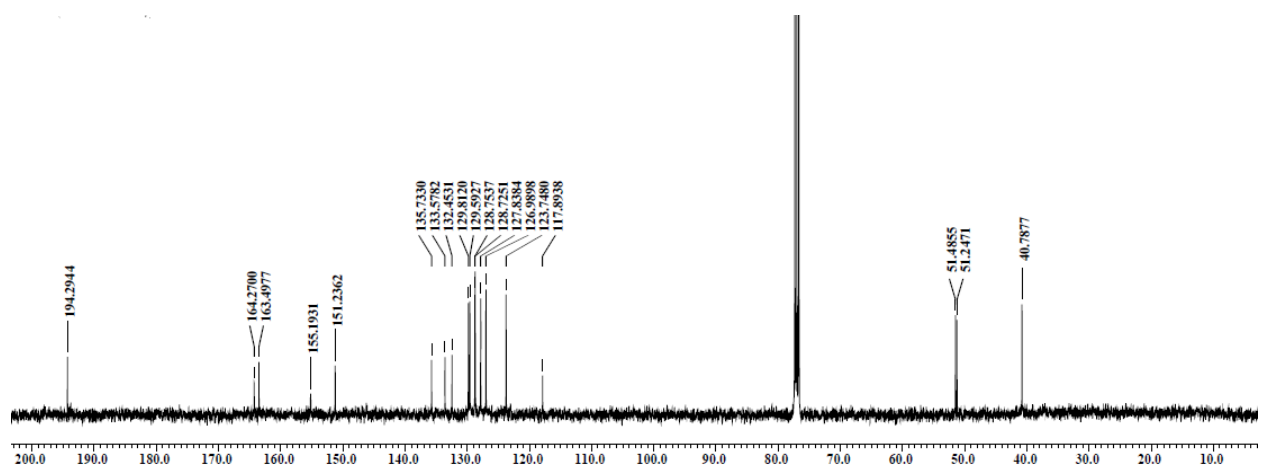
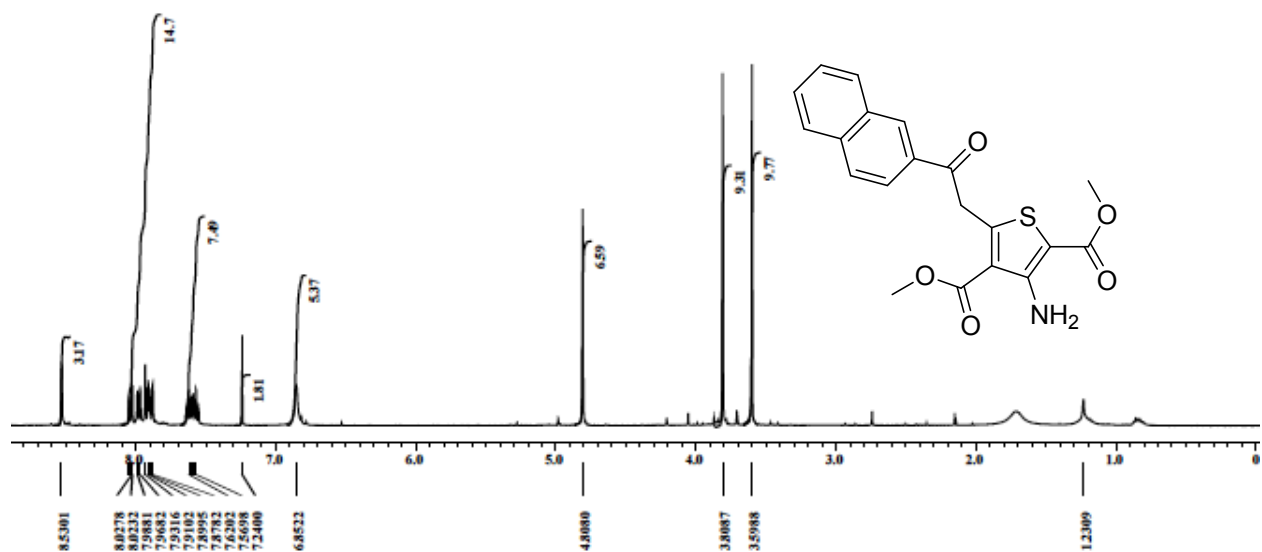
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(2-chlorophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10e**)



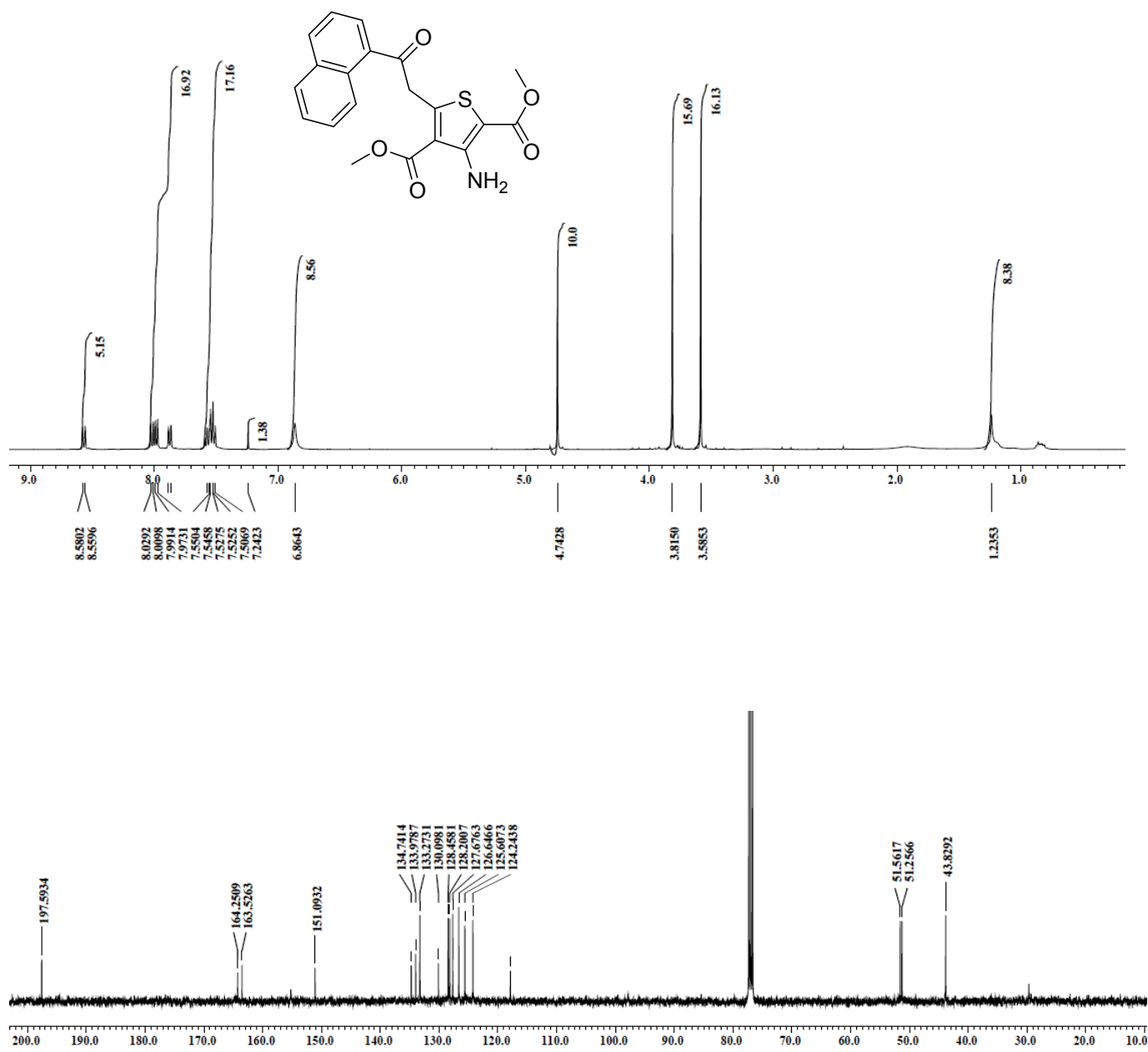
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(4-bromophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10f**)



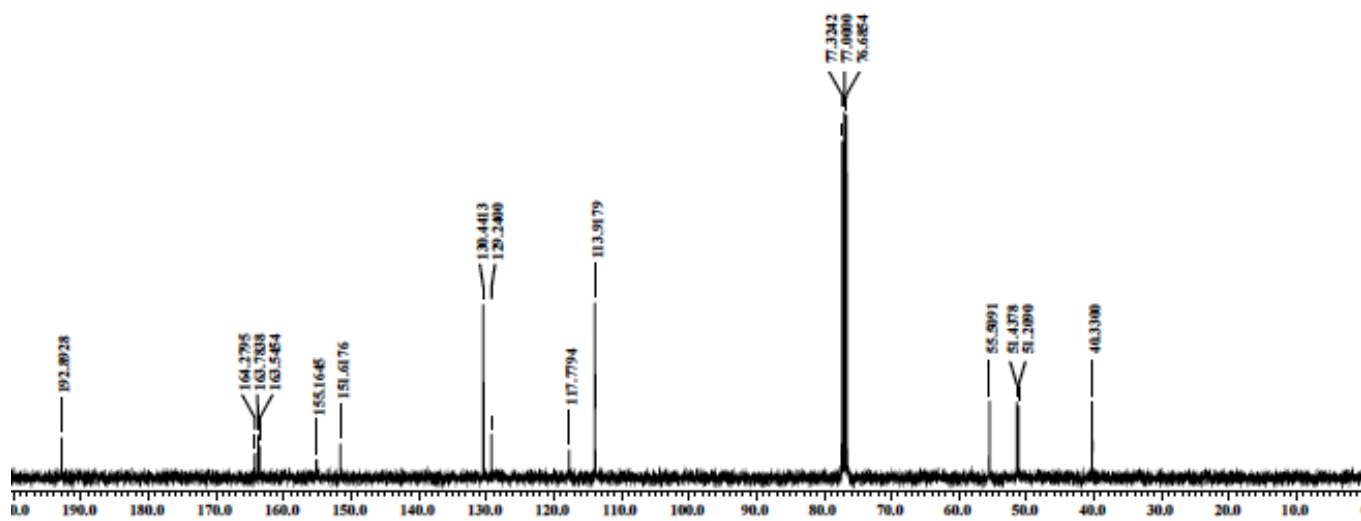
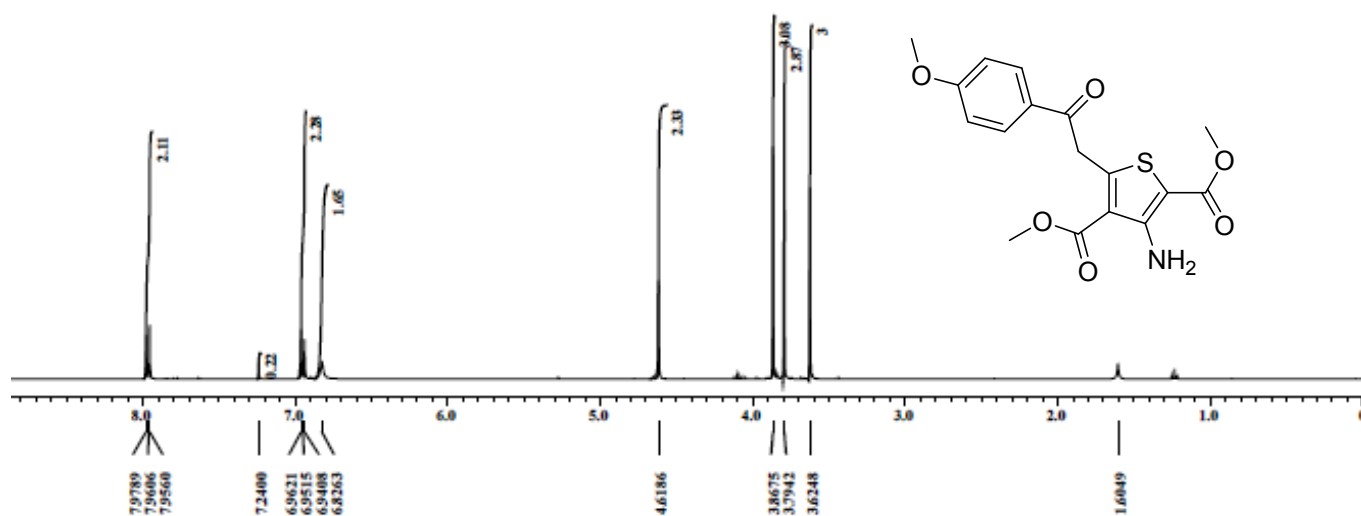
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(3-bromophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10g**)



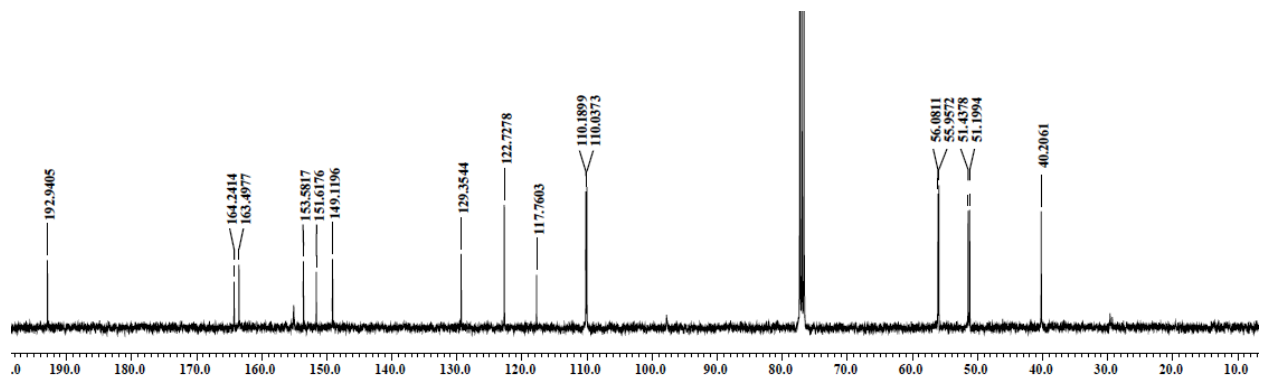
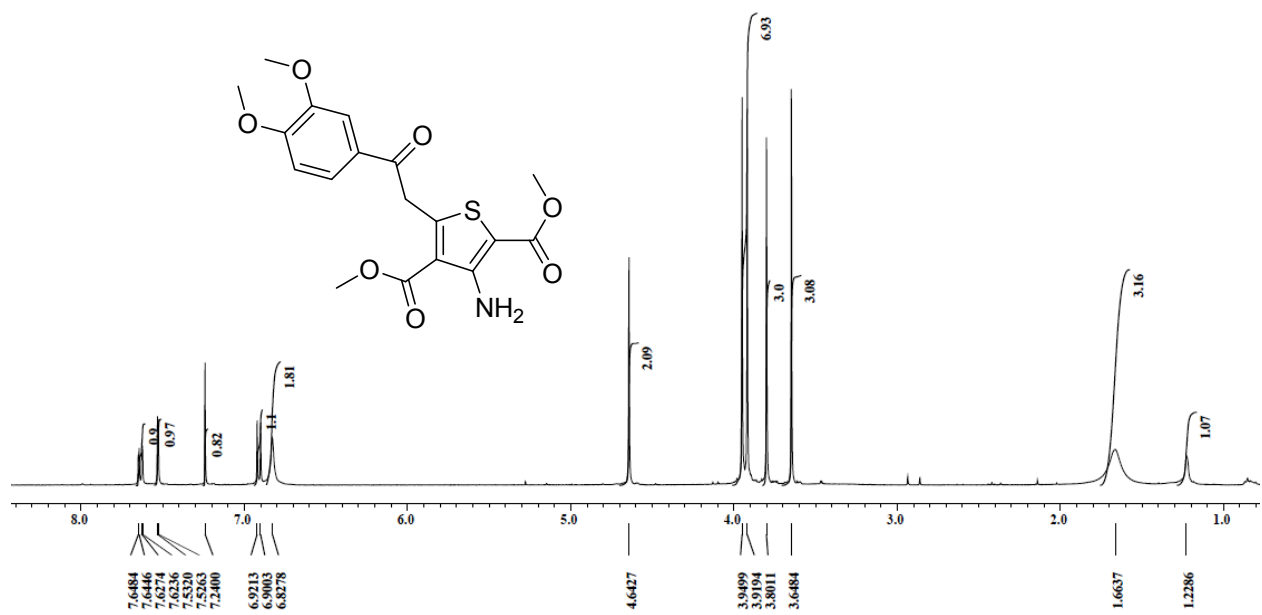
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(naphthalen-2-yl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10h**)



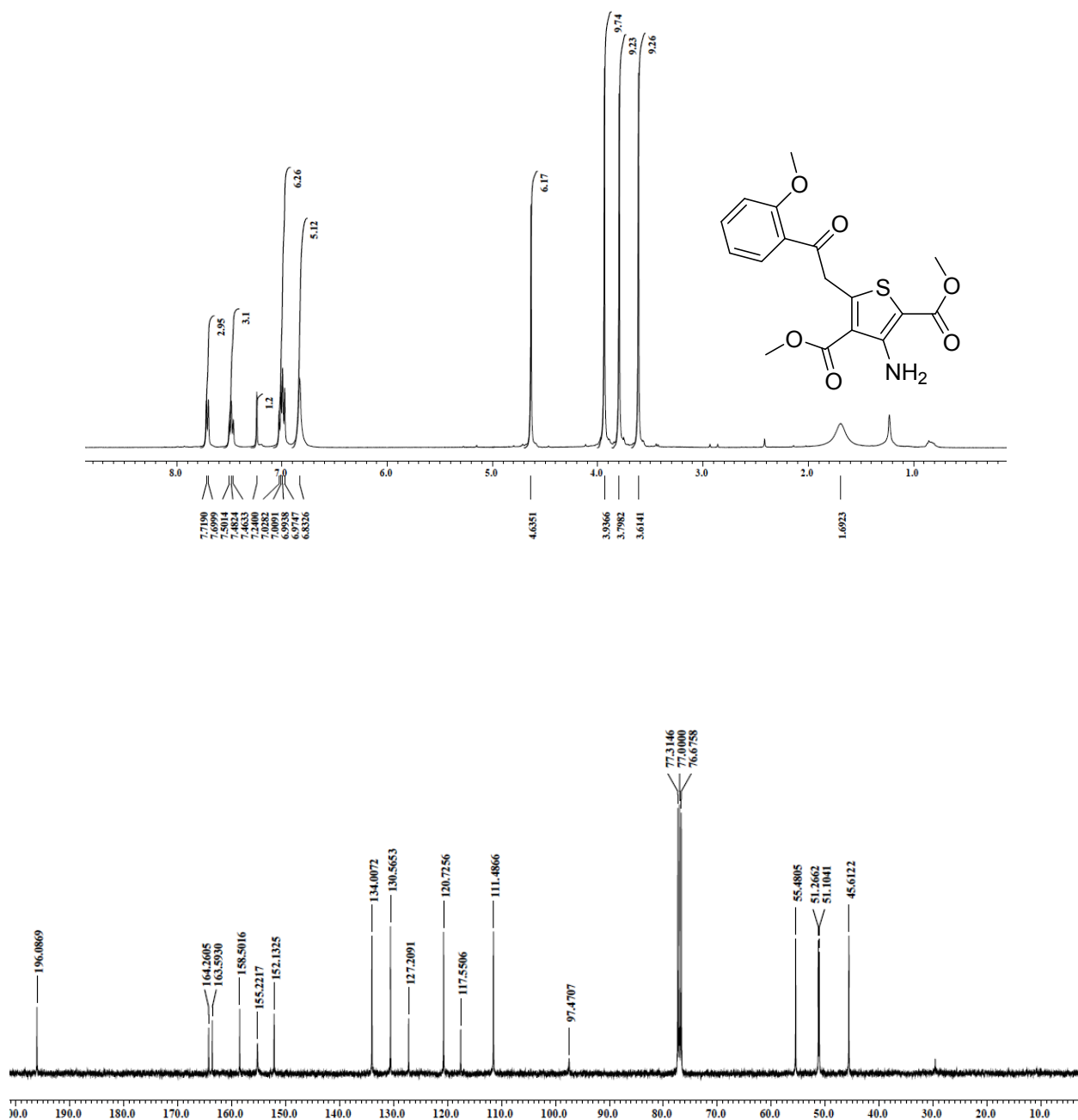
¹H and ¹³C spectra of spectra of dimethyl 3-amino-5-(2-(naphthalen-1-yl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10i**)



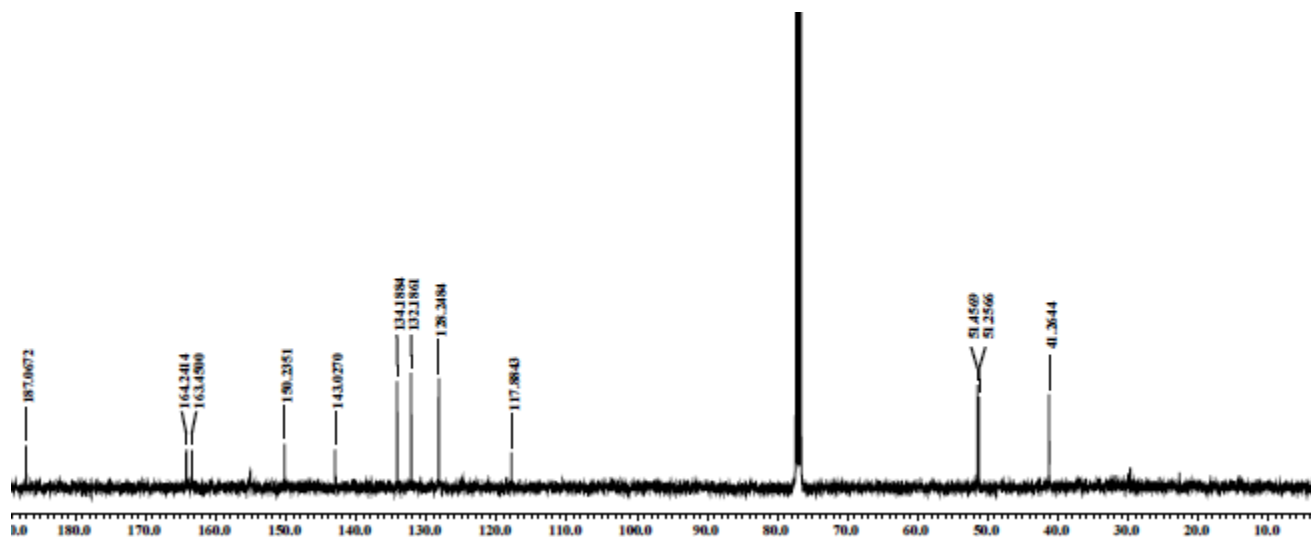
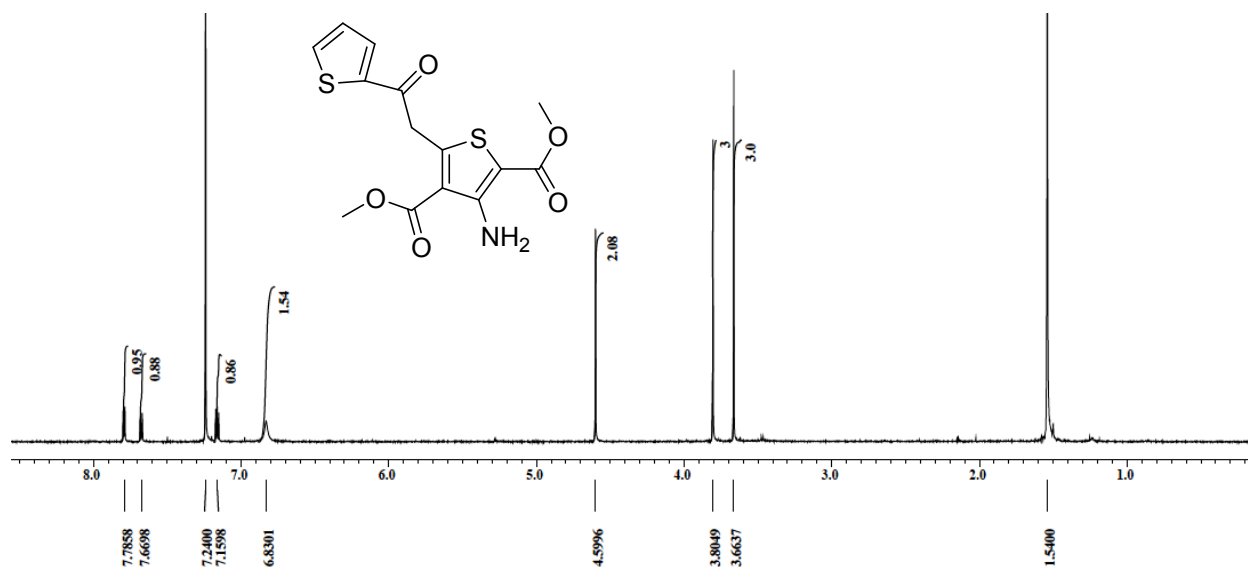
^1H and ^{13}C spectra of spectra of dimethyl 3-amino-5-(2-(4-methoxyphenyl)acetyl)thiophene-2,4-dicarboxylate (**10j**)



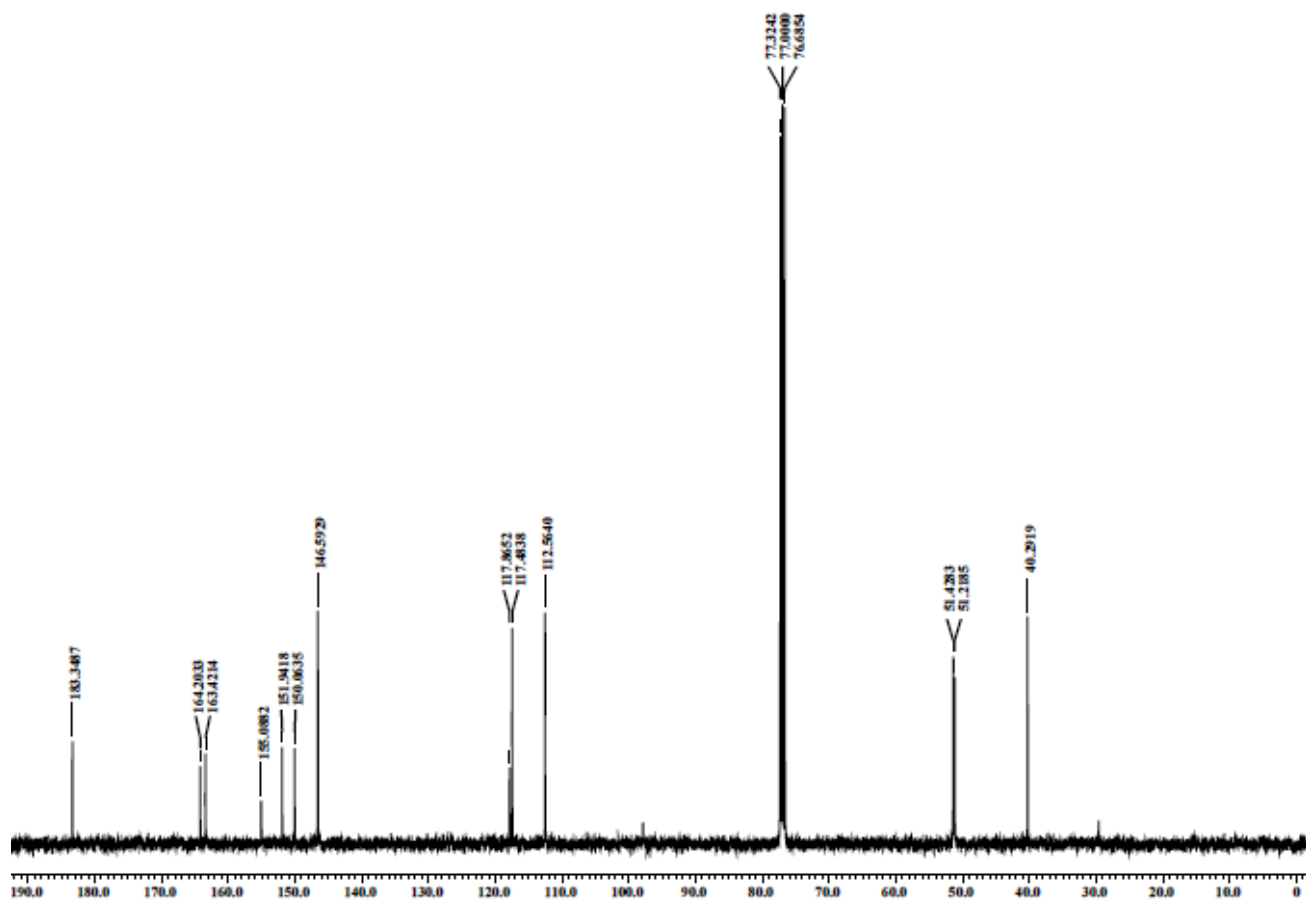
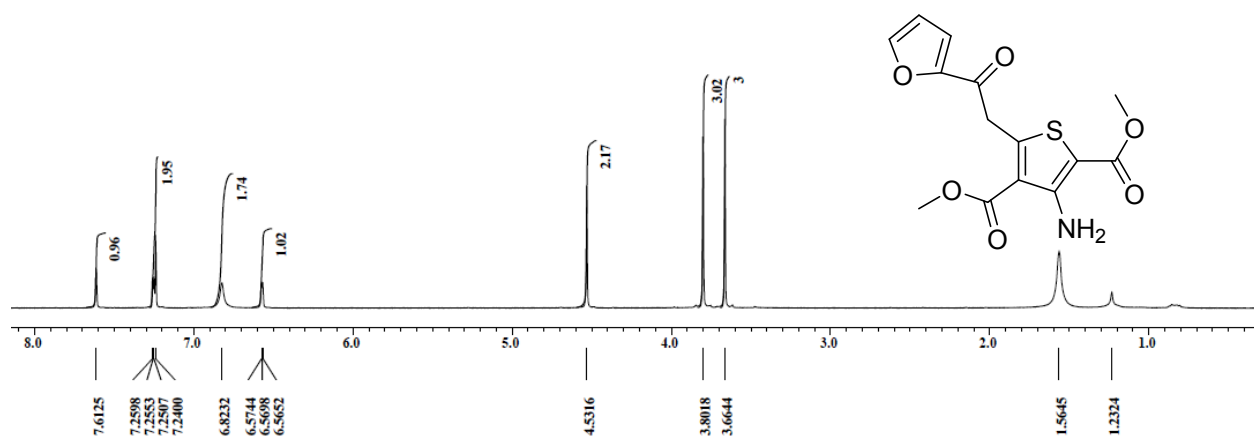
¹H and ¹³C spectra of dimethyl 3-amino-5-(2-(3,4-dimethoxyphenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10k**)



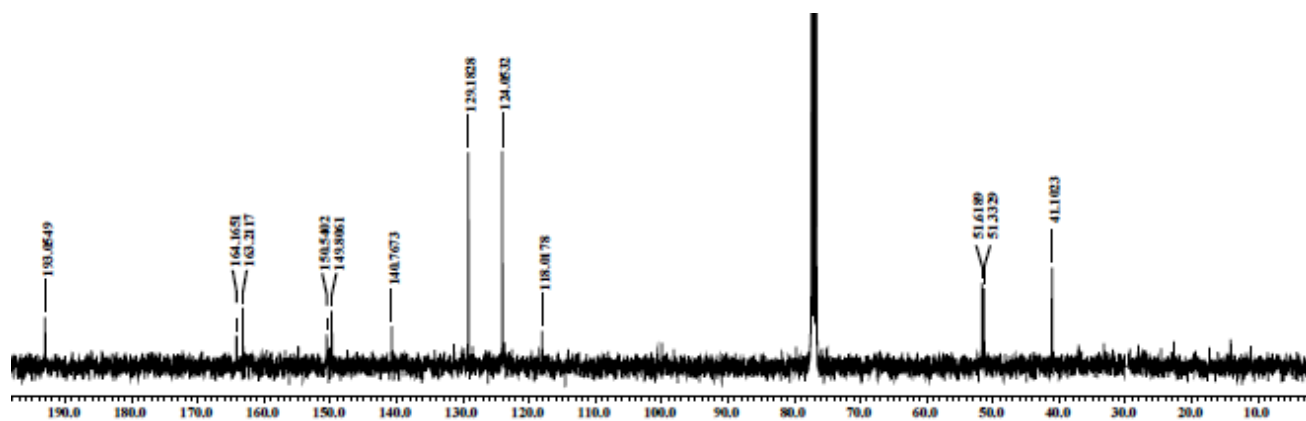
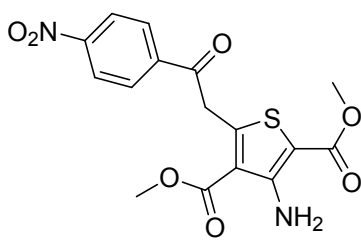
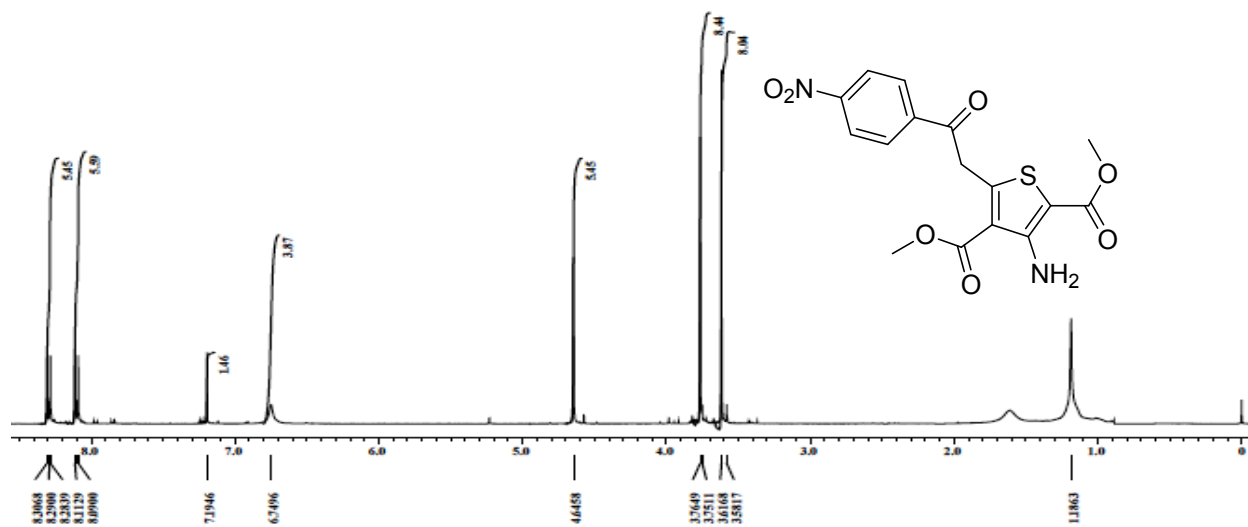
¹H and ¹³C spectra of dimethyl 3-amino-5-(2-(2-methoxyphenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10**)



¹H and ¹³C spectra of dimethyl 3-amino-5-(2-oxo-2-(thiophen-2-yl)ethyl)thiophene-2,4-dicarboxylate (**10m**)



¹H and ¹³C spectra of dimethyl 3-amino-5-(2-(furan-2-yl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10n**)



¹H and ¹³C spectra of dimethyl 3-amino-5-(2-(4-nitrophenyl)-2-oxoethyl)thiophene-2,4-dicarboxylate (**10o**)

XYZ Coordinates Monomer

E = -1447.8510683

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-1.594477	-1.438687	-0.490186
2	8	0	-4.461386	-2.005860	-0.046557
3	8	0	1.482311	-0.346821	1.537224
4	8	0	1.103034	2.225389	-0.460077
5	7	0	-3.124439	2.070865	0.320389
6	6	0	1.931008	-0.553002	0.424649
7	8	0	-0.717310	3.391074	0.172735
8	8	0	-5.138492	0.112252	0.417377
9	6	0	3.392154	-0.817108	0.215625
10	6	0	-0.402978	-0.195063	-0.521212
11	6	0	-0.938239	1.050170	-0.227917
12	6	0	1.017176	-0.573088	-0.815819
13	1	0	1.435734	0.106439	-1.562945
14	1	0	1.056010	-1.581783	-1.244945
15	6	0	6.140945	-1.300631	-0.038665
16	1	0	7.206153	-1.488060	-0.137896
17	6	0	5.322693	-1.313817	-1.169233
18	1	0	5.748871	-1.511808	-2.148060
19	6	0	3.954749	-1.073160	-1.044166

20	1	0	3.333871	-1.088205	-1.933673
21	6	0	-0.209460	2.323436	-0.143935
22	6	0	-2.367153	0.996318	0.028236
23	6	0	-2.864826	-0.306256	-0.081860
24	6	0	5.588937	-1.047678	1.220539
25	1	0	6.224348	-1.038487	2.101115
26	6	0	4.224522	-0.808742	1.346591
27	1	0	3.772242	-0.611821	2.312527
28	6	0	-4.242228	-0.675318	0.121613
29	6	0	-5.814970	-2.435576	0.151292
30	1	0	-5.808932	-3.511795	-0.021336
31	1	0	-6.486727	-1.939226	-0.553646
32	1	0	-6.147504	-2.213855	1.168527
33	6	0	1.854220	3.447125	-0.353567
34	1	0	2.878271	3.181558	-0.614429
35	1	0	1.806326	3.838168	0.664912
36	1	0	1.463741	4.200370	-1.041709
37	1	0	-4.101516	1.908035	0.523967
38	1	0	-2.662727	2.959477	0.449206

XYZ Coordinates Dimer

E = -2895.7100653

Center	Atomic	Atomic	Coordinates (Angstroms)
--------	--------	--------	-------------------------

Number	Number	Type	X	Y	Z
1	16	0	4.559151	-2.202241	-0.575609
2	8	0	1.916666	-3.421614	-0.308693
3	8	0	7.093082	-0.229788	1.534383
4	8	0	6.331945	1.973782	-0.774183
5	7	0	2.197788	0.910742	-0.286924
6	6	0	7.678978	-0.415506	0.483751
7	8	0	4.243490	2.743580	-0.436000
8	8	0	0.675769	-1.527800	-0.145065
9	6	0	9.174316	-0.326257	0.406256
10	6	0	5.426344	-0.718170	-0.660205
11	6	0	4.592009	0.383944	-0.554460
12	6	0	6.917488	-0.772660	-0.806333
13	1	0	7.239337	-0.090106	-1.597036
14	1	0	7.227577	-1.780415	-1.109413
15	6	0	11.970622	-0.134271	0.398051
16	1	0	13.054220	-0.059985	0.394222
17	6	0	11.289997	-0.458923	-0.776313
18	1	0	11.841765	-0.638230	-1.694148
19	6	0	9.898643	-0.554147	-0.773827
20	1	0	9.386543	-0.807586	-1.696070
21	6	0	5.003499	1.794201	-0.574407
22	6	0	3.190607	0.016189	-0.400465
23	6	0	3.024211	-1.375986	-0.399311

24	6	0	11.257278	0.093824	1.578482
25	1	0	11.785634	0.345242	2.493304
26	6	0	9.869763	-0.002958	1.582507
27	1	0	9.293984	0.166870	2.485868
28	6	0	1.771681	-2.068958	-0.272557
29	6	0	0.705115	-4.176646	-0.185580
30	1	0	1.005118	-5.223271	-0.238187
31	1	0	0.013692	-3.938240	-0.998035
32	1	0	0.213227	-3.970444	0.768706
33	6	0	6.774239	3.341390	-0.769747
34	1	0	7.852594	3.298320	-0.920814
35	1	0	6.539243	3.817349	0.184723
36	1	0	6.294598	3.904383	-1.573860
37	1	0	1.239599	0.611943	-0.159516
38	1	0	2.445297	1.889003	-0.262598
39	16	0	-4.557729	2.204155	0.566583
40	8	0	-1.915953	3.422935	0.288066
41	8	0	-7.099739	0.224955	-1.529342
42	8	0	-6.329331	-1.971503	0.782244
43	7	0	-2.197321	-0.909343	0.275653
44	6	0	-7.681526	0.413456	-0.476925
45	8	0	-4.242393	-2.741942	0.436216
46	8	0	-0.675832	1.528591	0.124511
47	6	0	-9.176486	0.323521	-0.393173
48	6	0	-5.424538	0.720220	0.657495

49	6	0	-4.590535	-0.382075	0.551082
50	6	0	-6.915133	0.774926	0.809050
51	1	0	-7.233843	0.094927	1.603227
52	1	0	-7.224271	1.783615	1.110003
53	6	0	-11.972607	0.129674	-0.373109
54	1	0	-13.056130	0.054666	-0.364688
55	6	0	-11.287508	0.458770	0.797411
56	1	0	-11.835718	0.640827	1.716836
57	6	0	-9.896244	0.554914	0.789020
58	1	0	-9.380635	0.811830	1.708337
59	6	0	-5.001837	-1.792310	0.575949
60	6	0	-3.189743	-0.014593	0.391103
61	6	0	-3.023406	1.377585	0.386512
62	6	0	-11.263841	-0.101933	-1.555611
63	1	0	-11.795686	-0.356816	-2.467447
64	6	0	-9.876420	-0.004215	-1.565533
65	1	0	-9.304146	-0.176719	-2.470613
66	6	0	-1.771260	2.070206	0.254289
67	6	0	-0.704693	4.177571	0.159735
68	1	0	-1.004535	5.224350	0.210108
69	1	0	-0.011253	3.941509	0.971163
70	1	0	-0.215193	3.968589	-0.795167
71	6	0	-6.771613	-3.339117	0.782832
72	1	0	-7.849283	-3.295707	0.938618
73	1	0	-6.540887	-3.817215	-0.171613

74	1	0	-6.288381	-3.900307	1.586056
75	1	0	-1.239629	-0.610688	0.144225
76	1	0	-2.444884	-1.887660	0.254194
