Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information for:

Synthesis of Chiral Lactams via Asymmetric Hydrogenation of α,β-Unsaturated Nitriles

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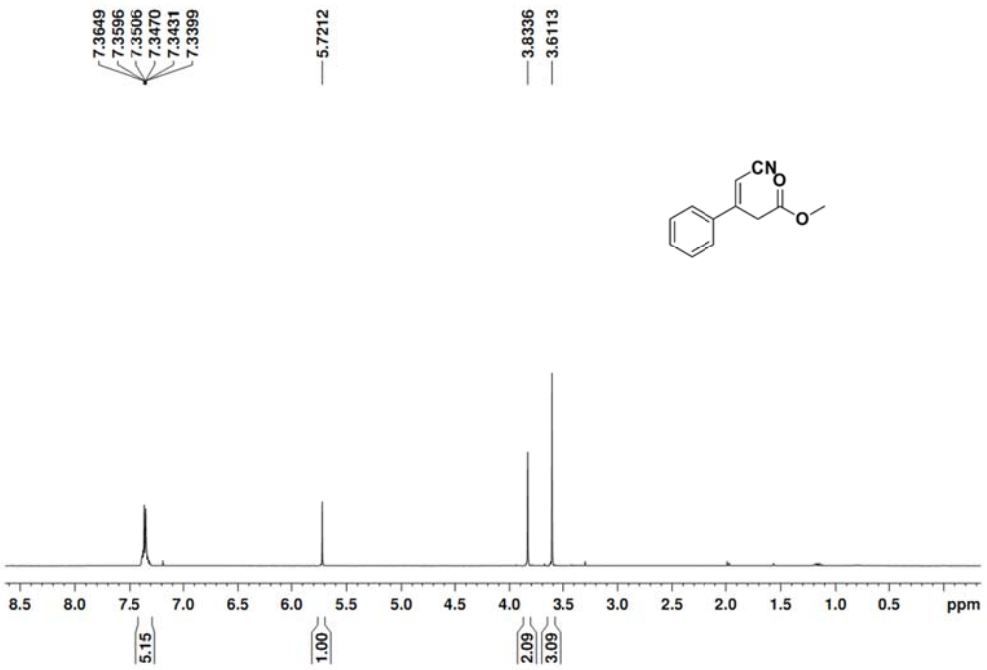
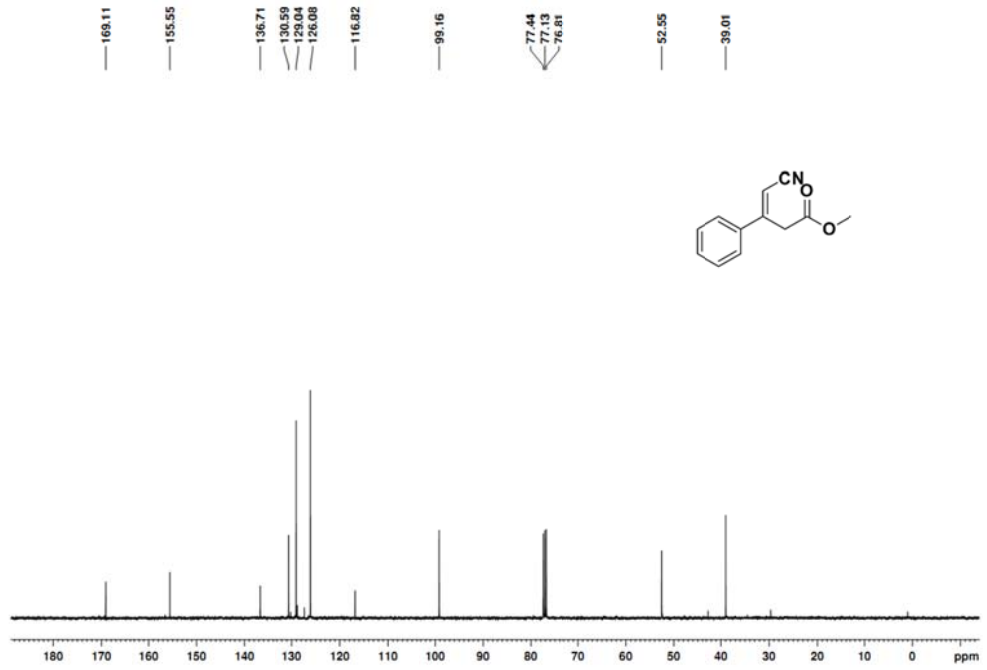
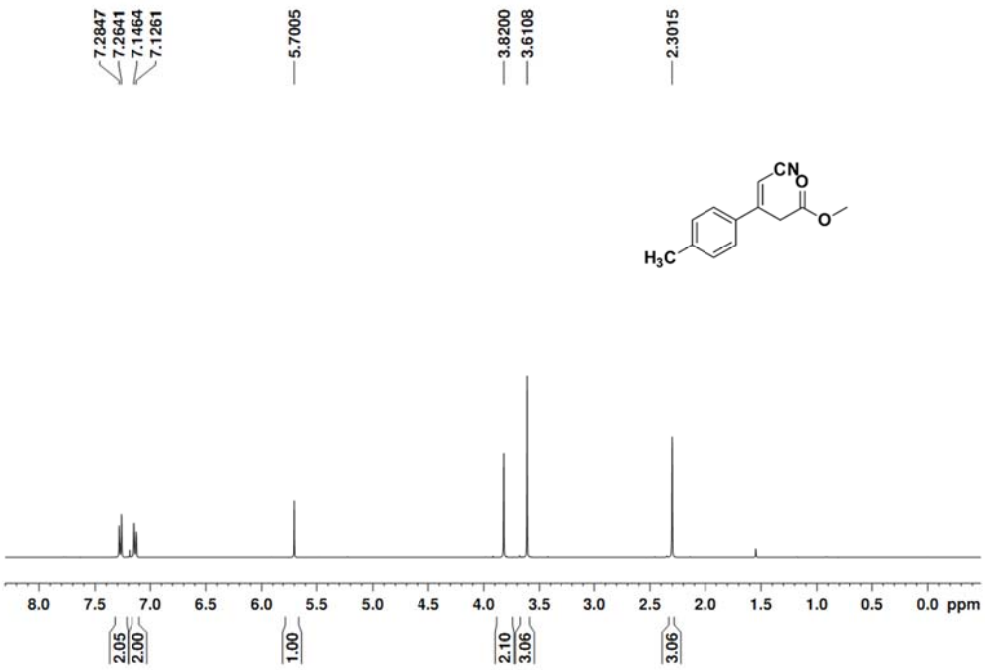
Key Laboratory of Radiopharmaceuticals, College of Chemistry, Beijing Normal University, Beijing 100875, China

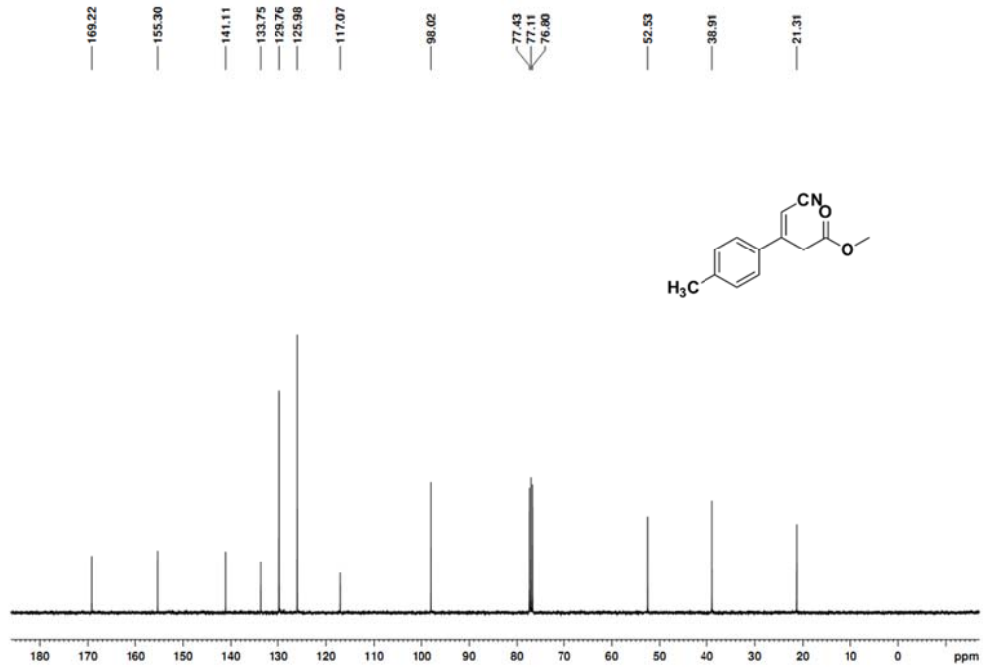
NMR, GC and HPLC spectra of compounds 1-10.
(*E*)-methyl 4-cyano-3-phenylbut-3-enoate (1a)



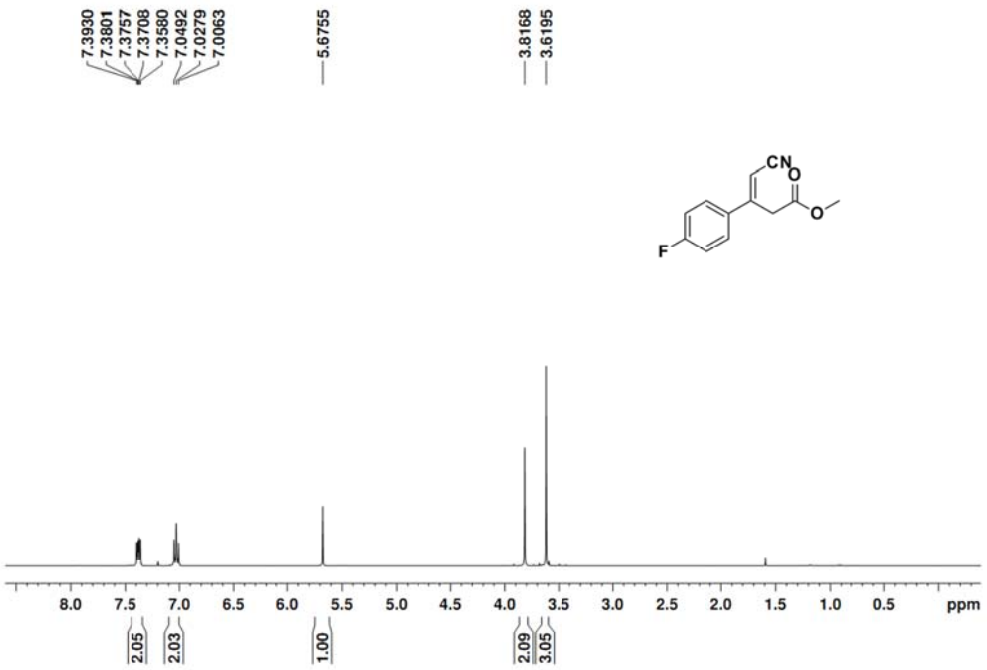


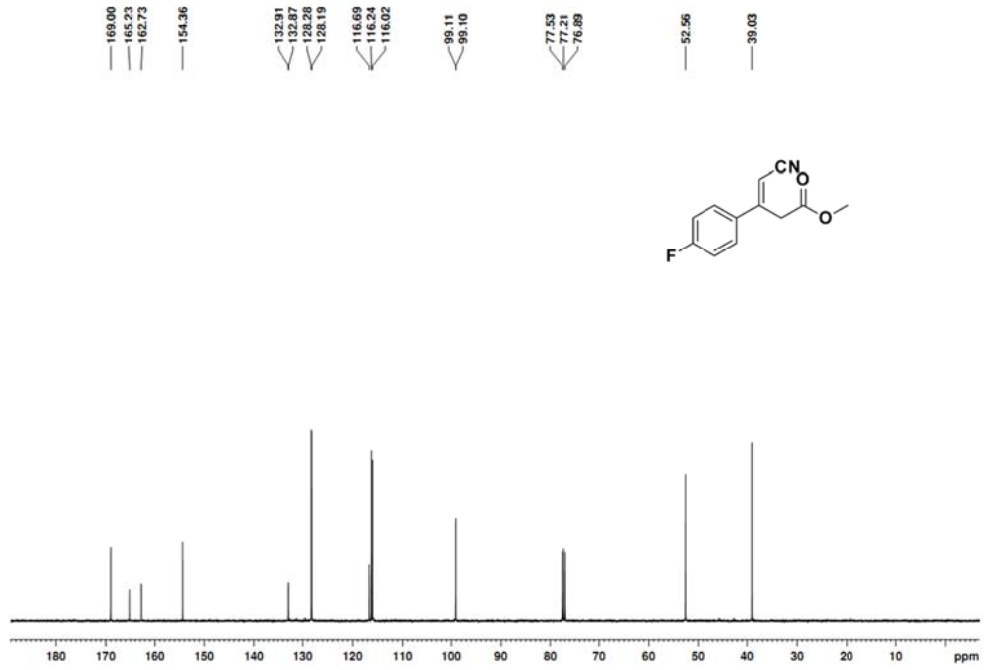
(*E*)-methyl 4-cyano-3-(*p*-tolyl)but-3-enoate (1b)

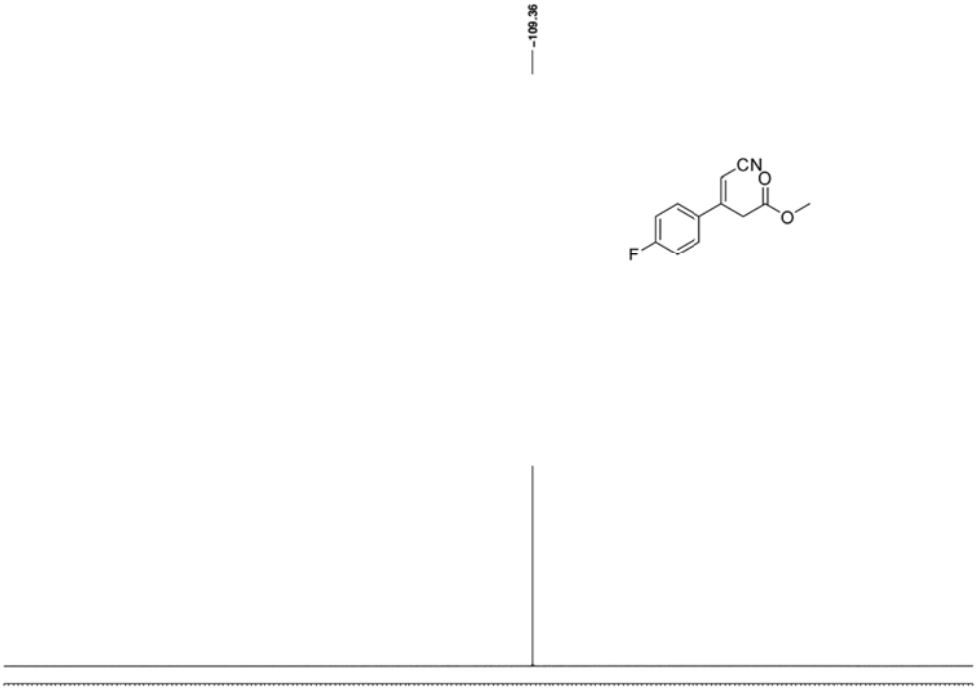




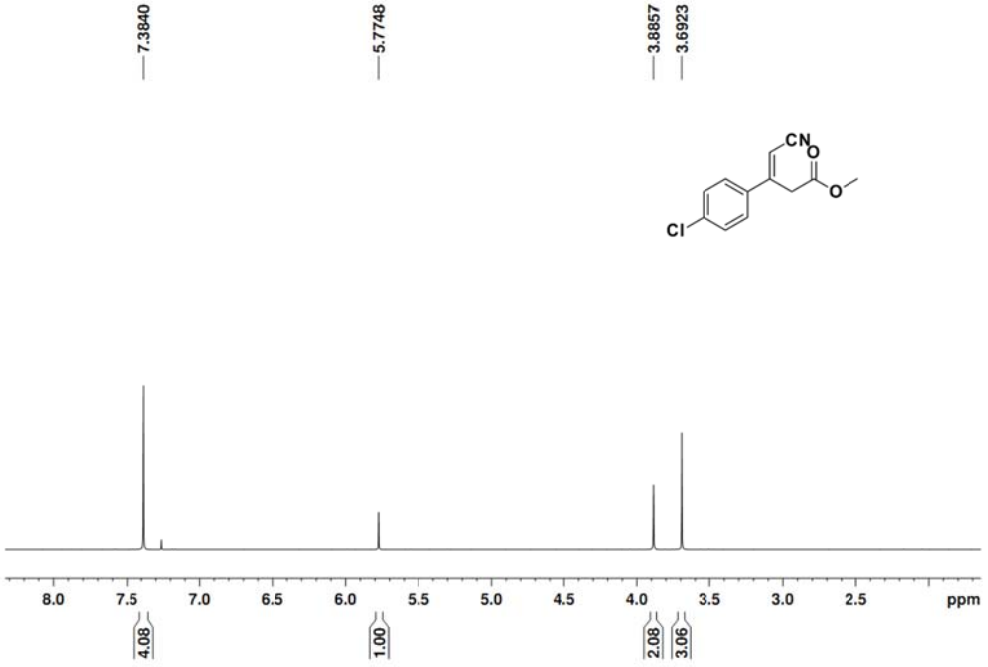
(*E*)-methyl 4-cyano-3-(4-fluorophenyl)but-3-enoate (1c)

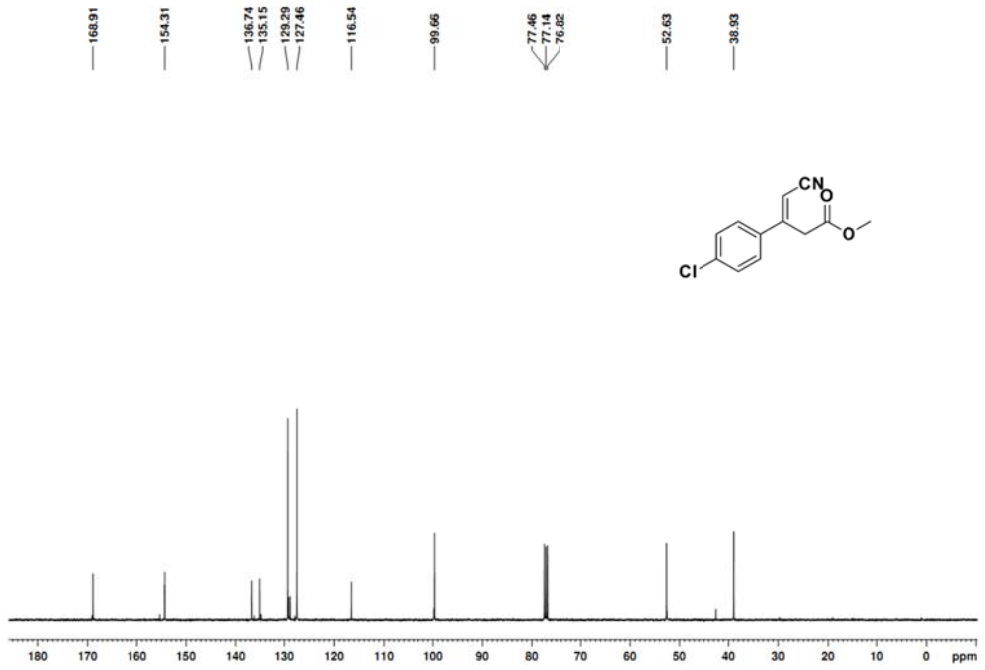






(*E*)-methyl 3-(4-chlorophenyl)-4-cyanobut-3-enoate (1d)





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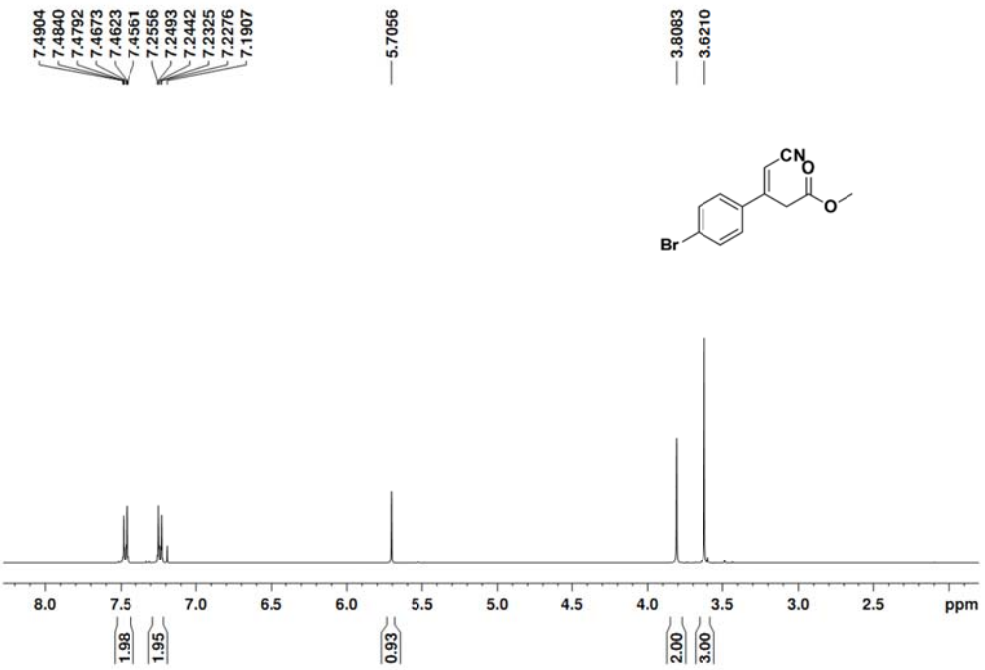

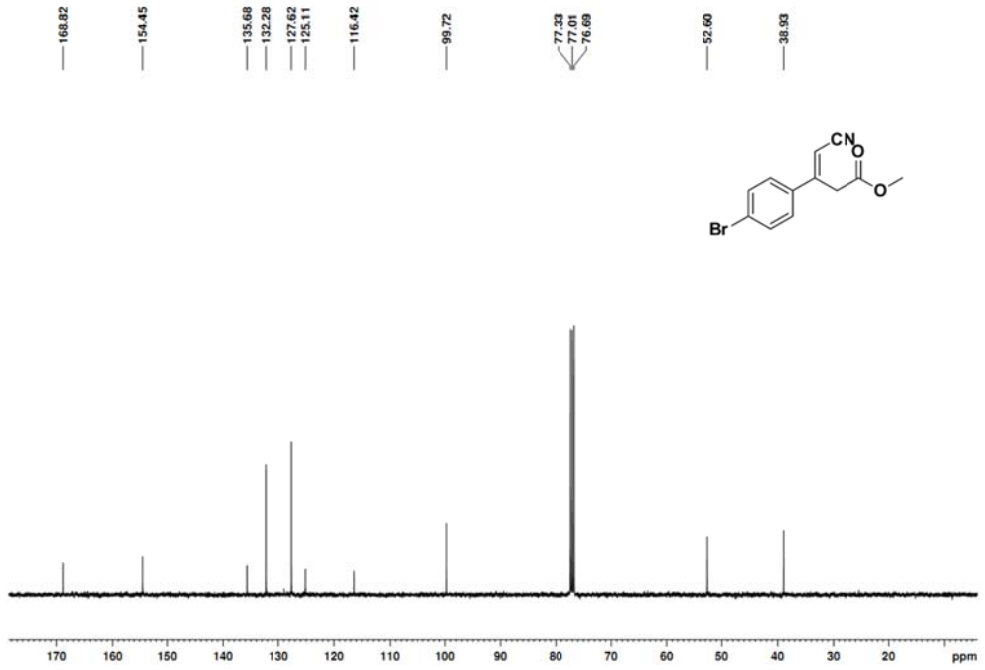

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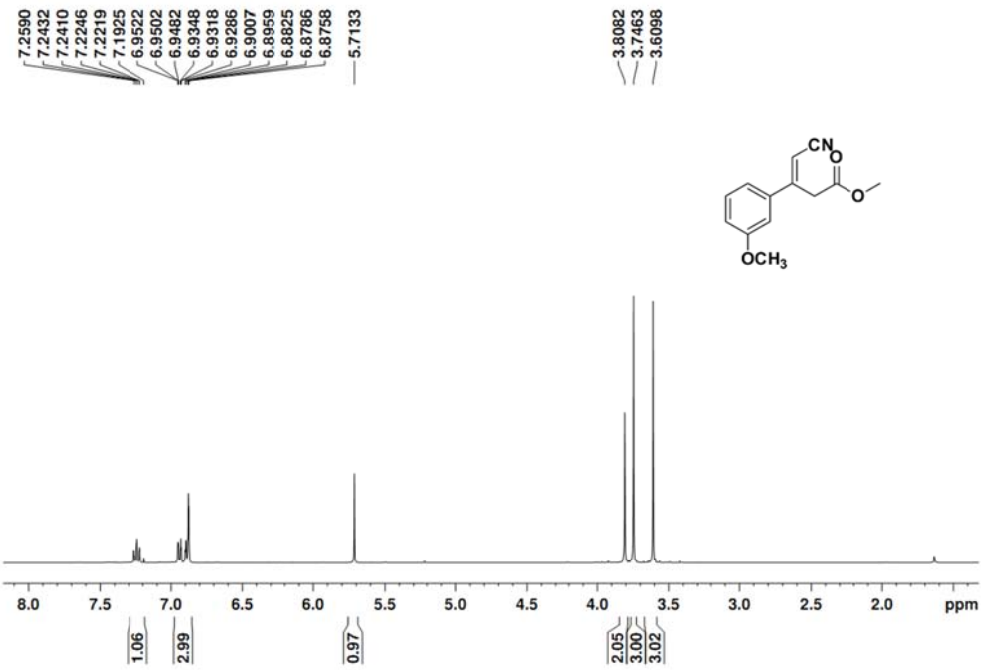

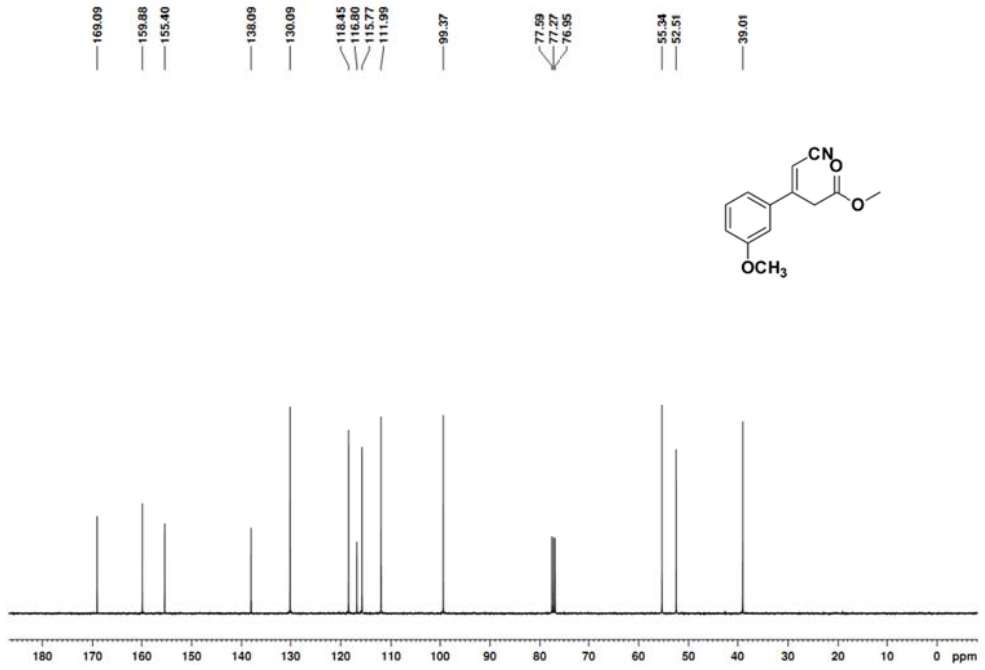

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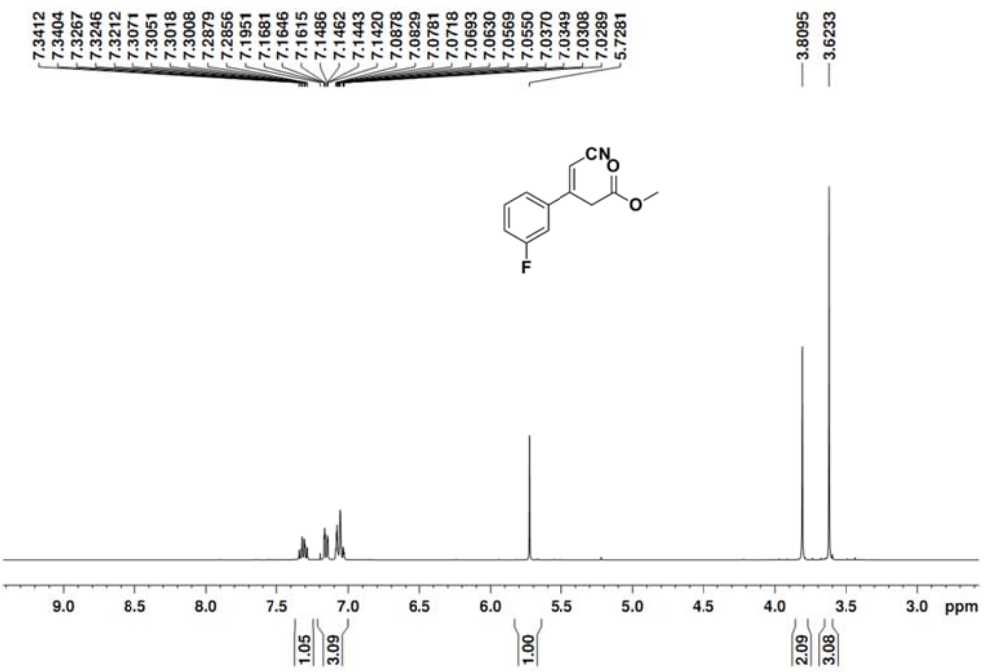

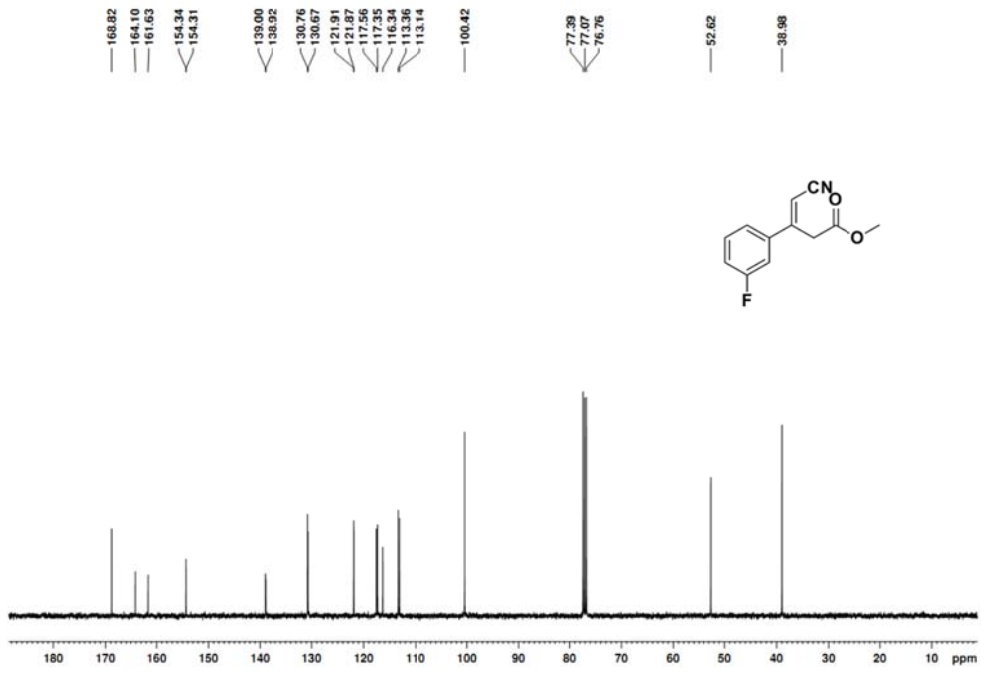
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113.14
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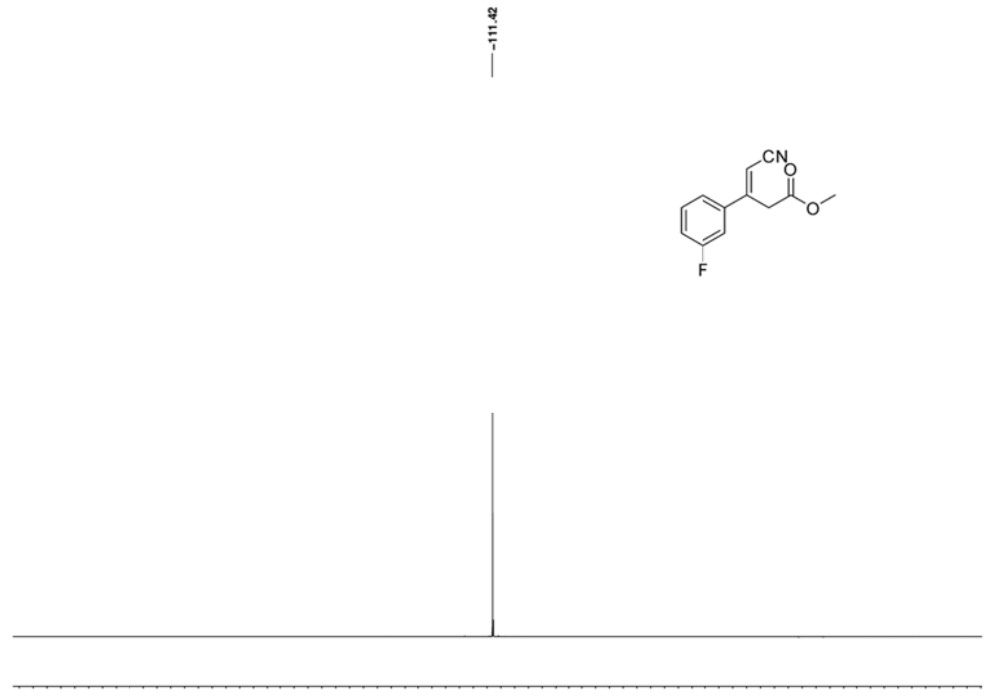
ppm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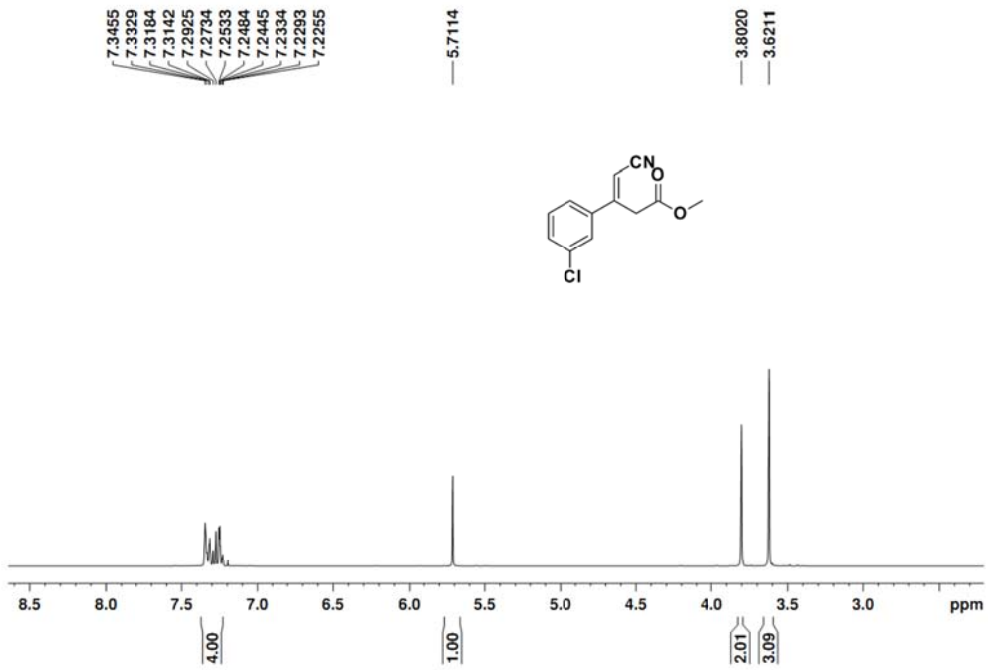
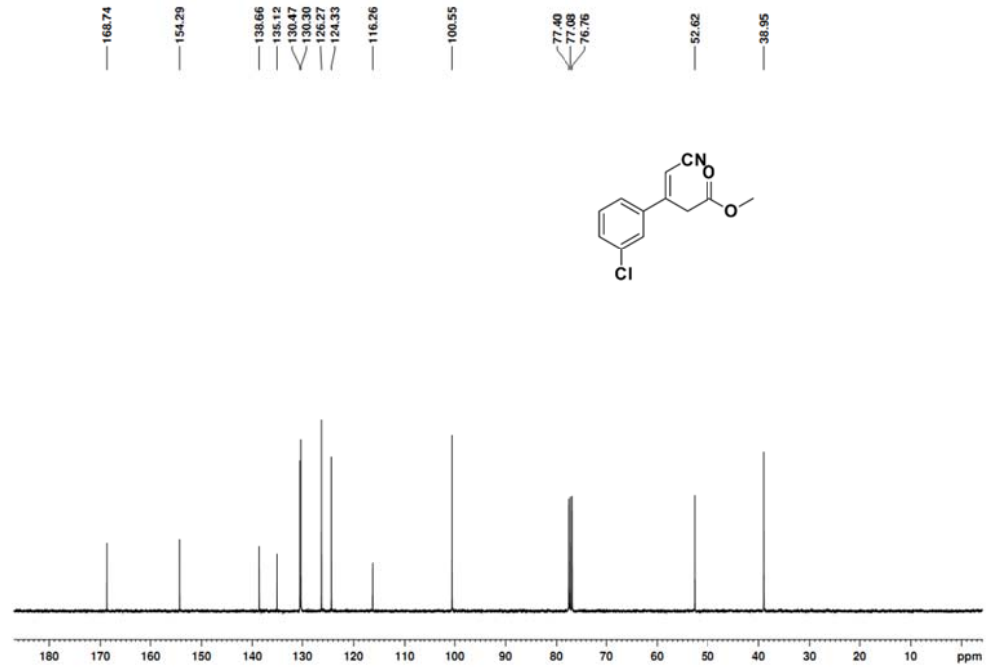
(*E*)-methyl 3-(3-chlorophenyl)-4-cyanobut-3-enoate (1h)





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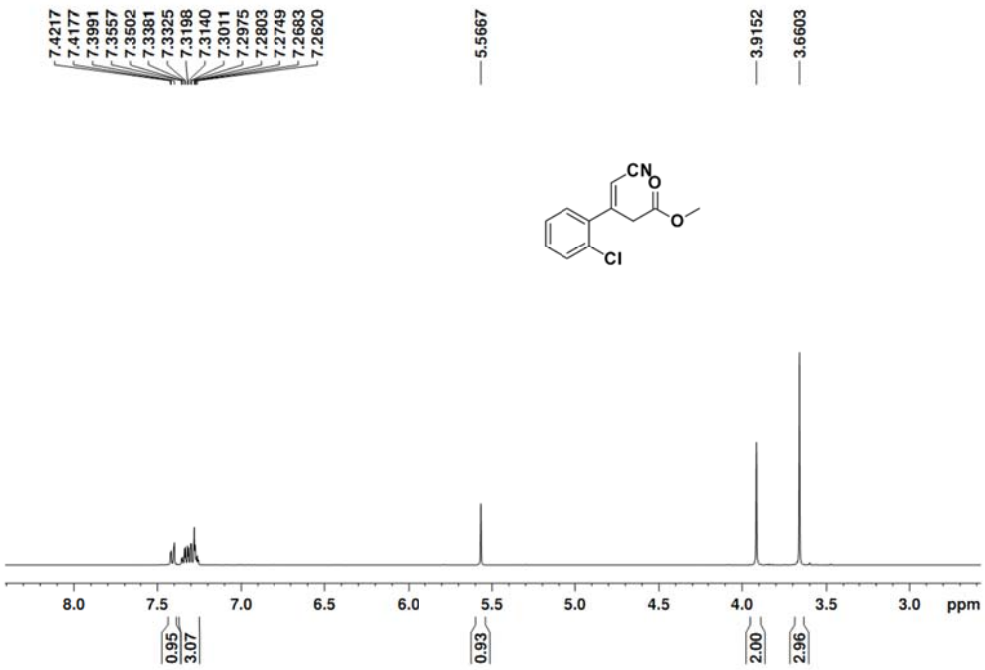
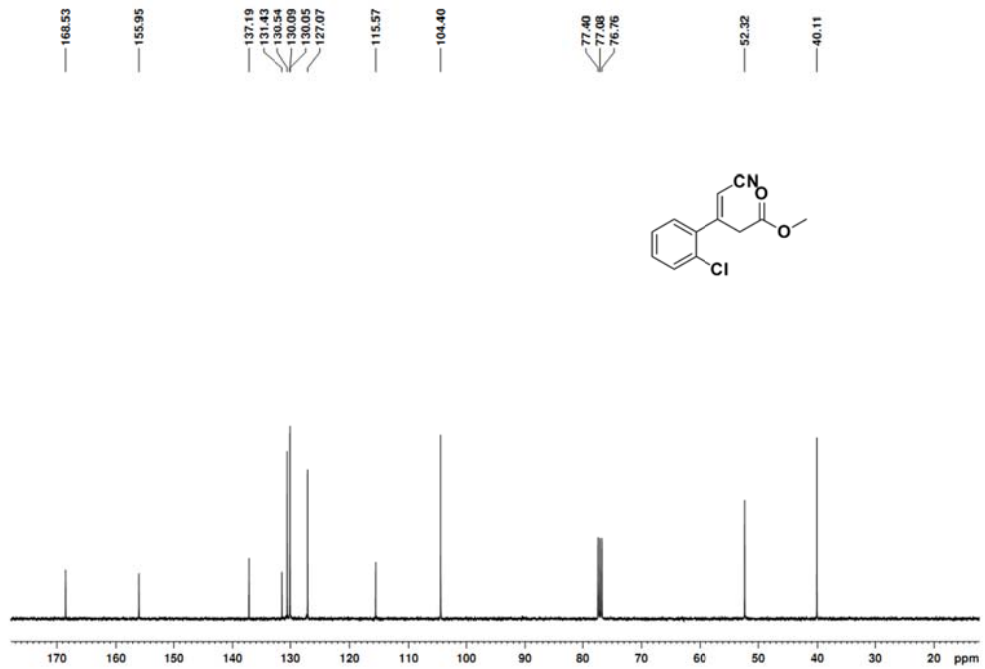
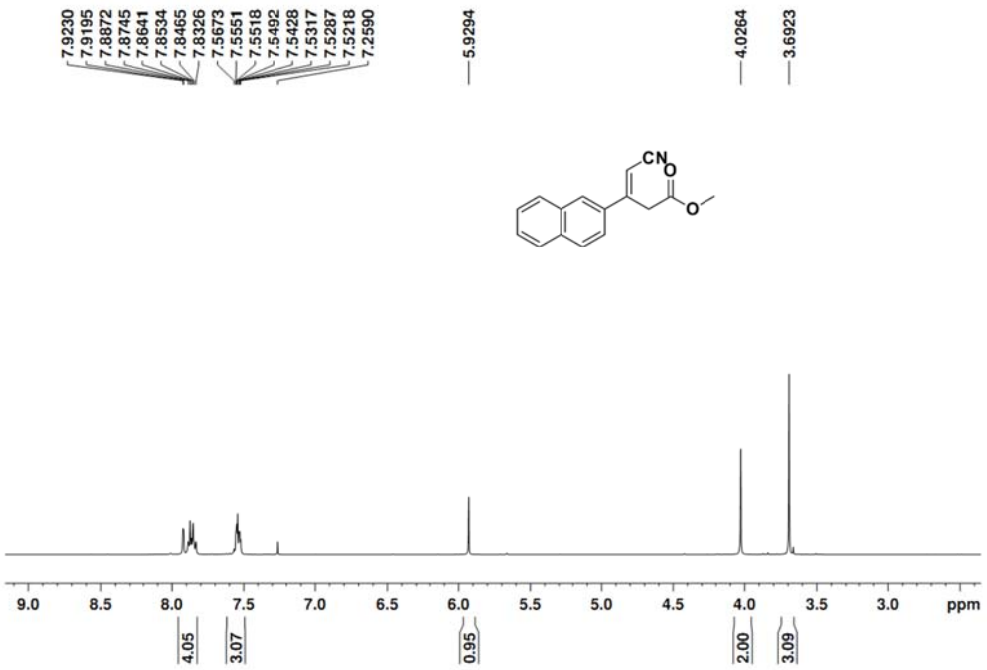
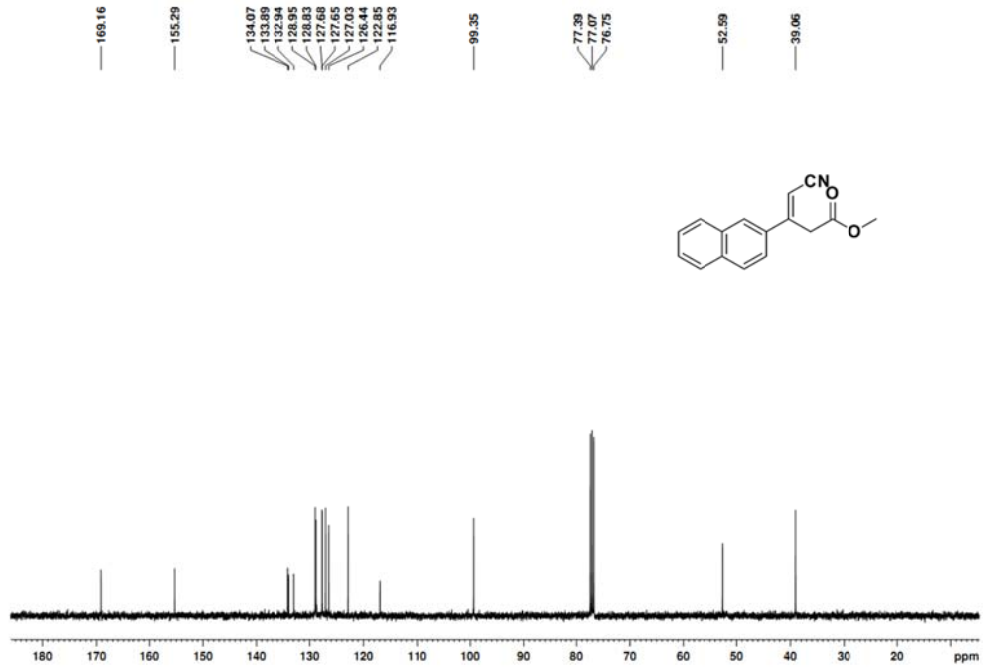


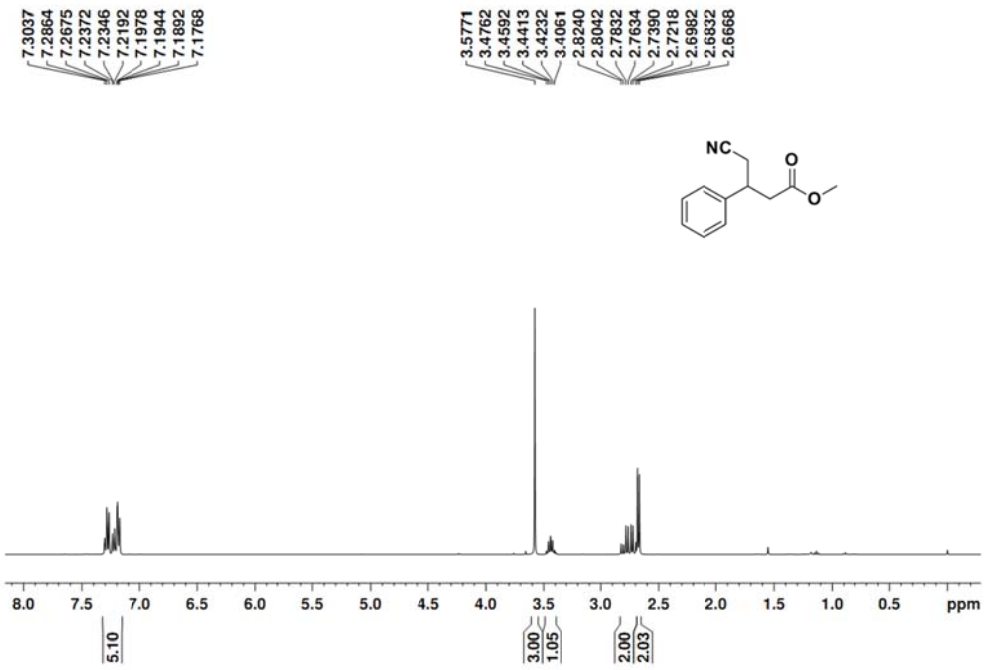


(*E*)-methyl 4-cyano-3-(naphthalen-2-yl)but-3-enoate (1j)

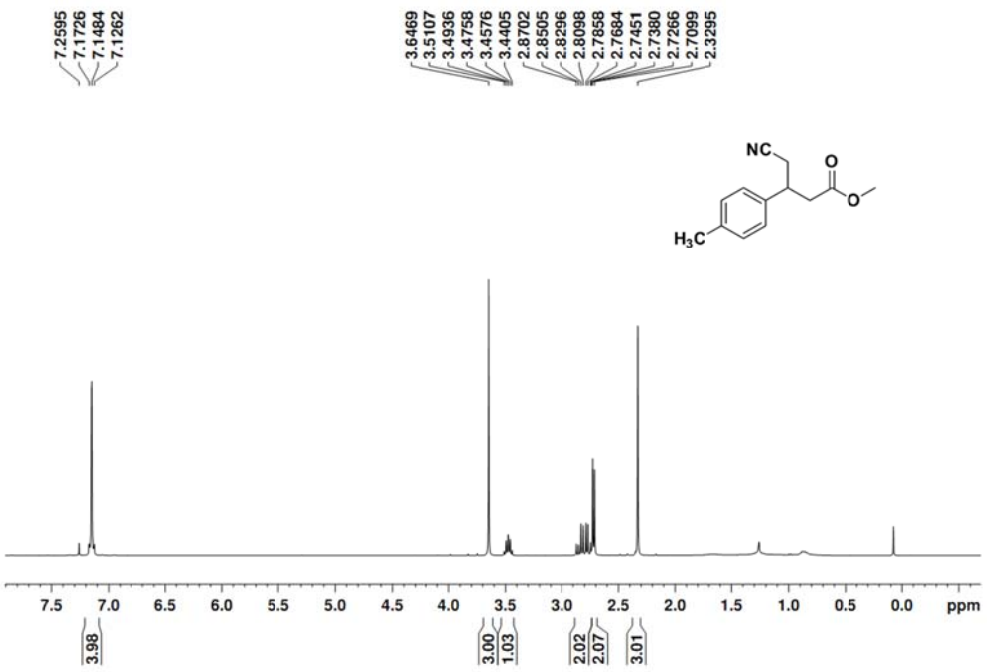


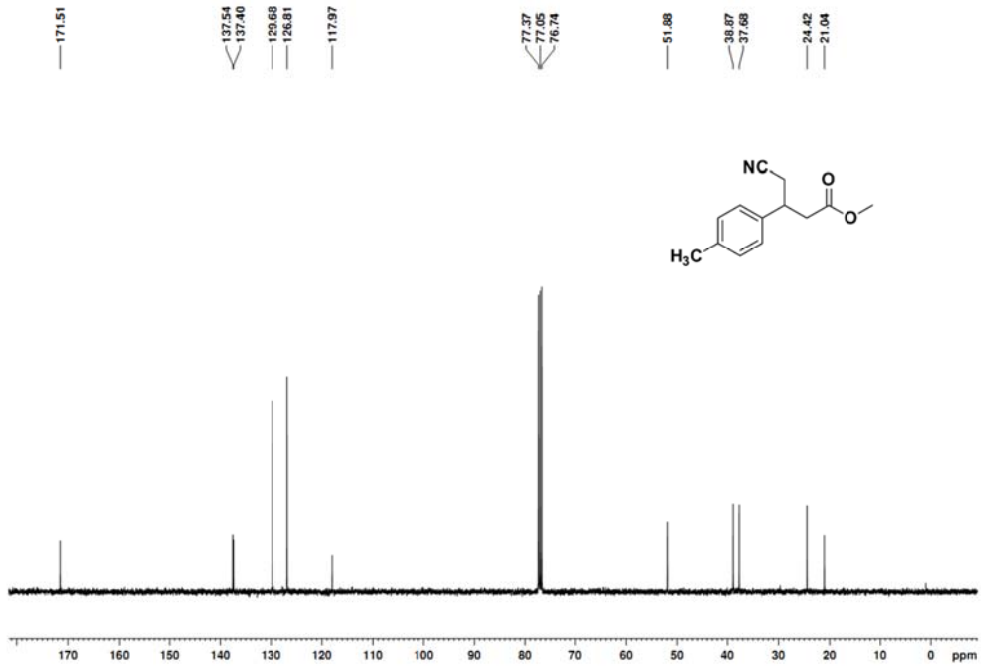


methyl 4-cyano-3-phenylbutanoate (2a)

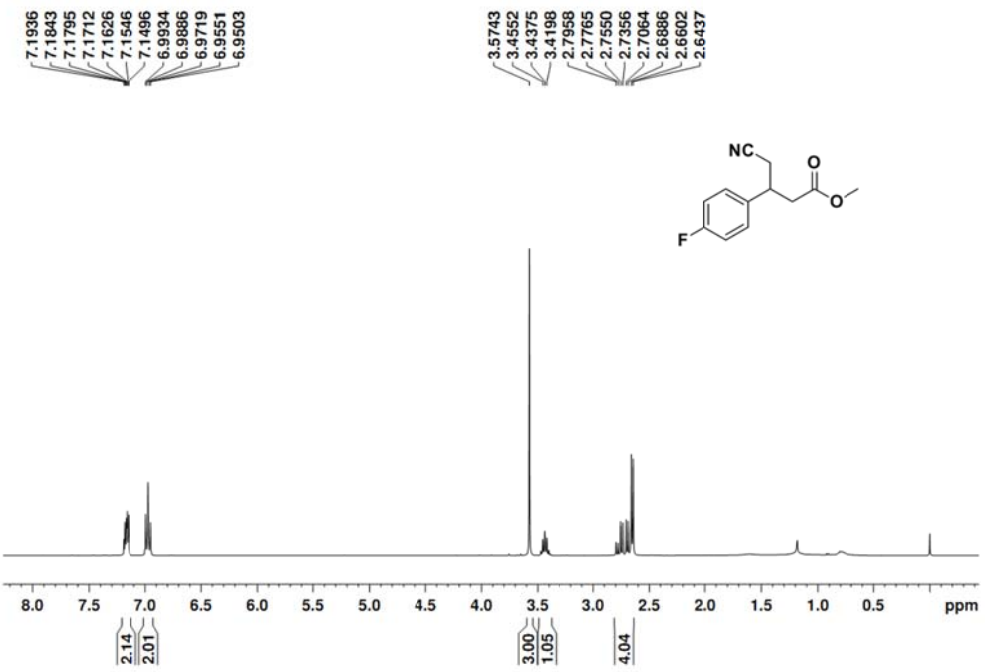


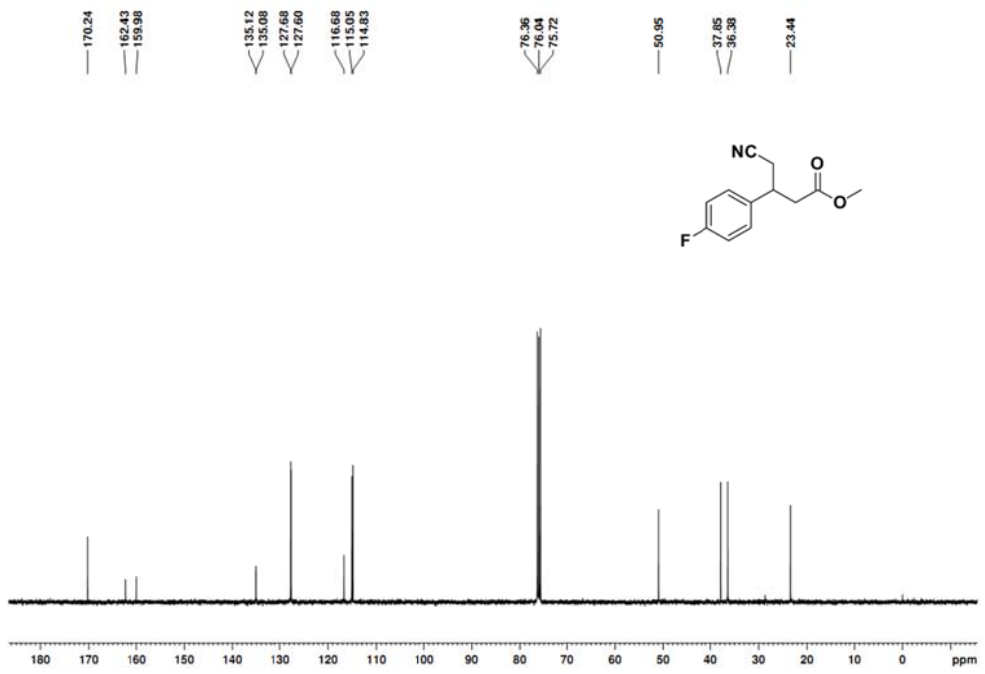
methyl 4-cyano-3-(*p*-tolyl)butanoate (2b)





methyl 4-cyano-3-(4-fluorophenyl)butanoate (2c)

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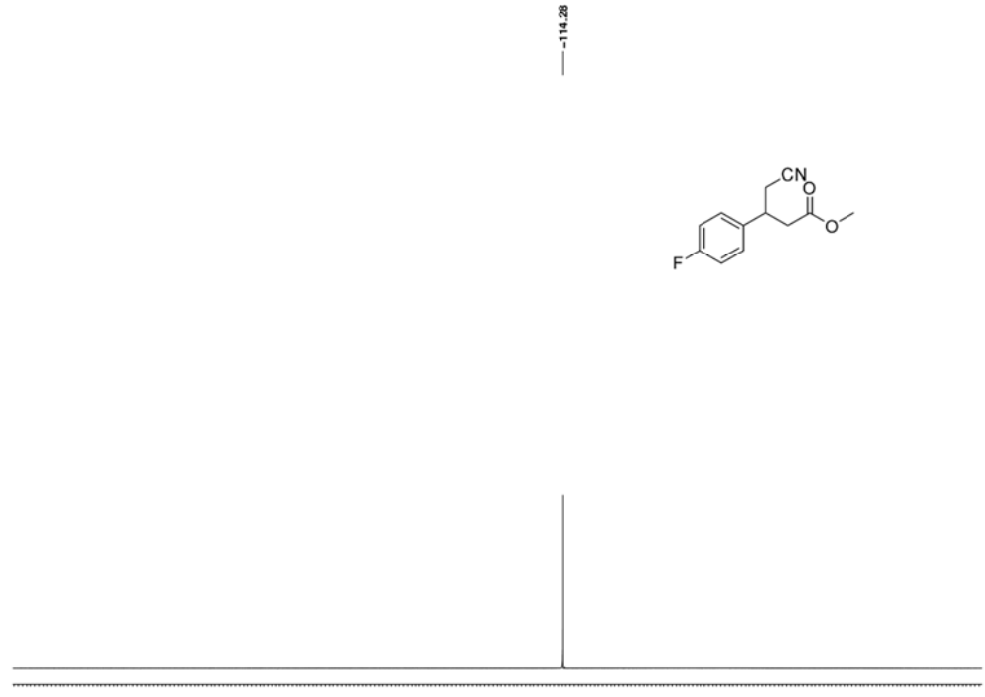
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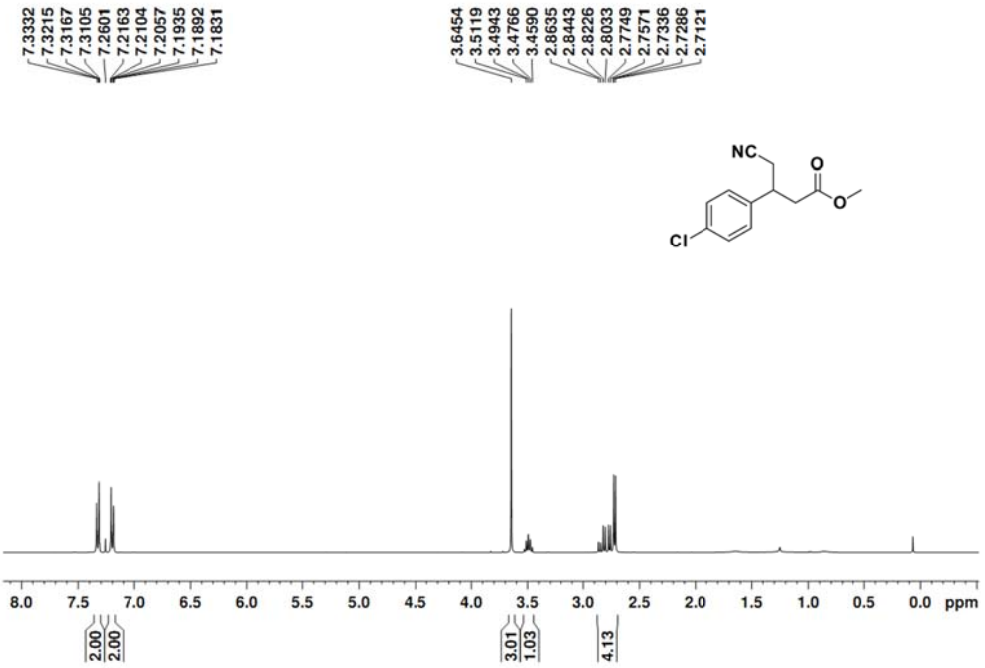
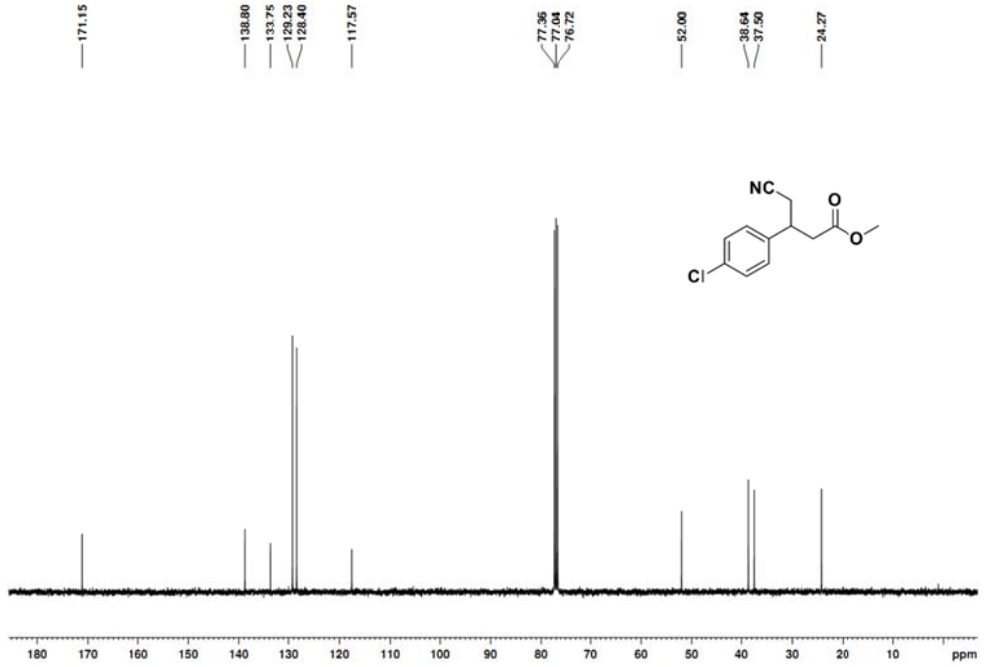
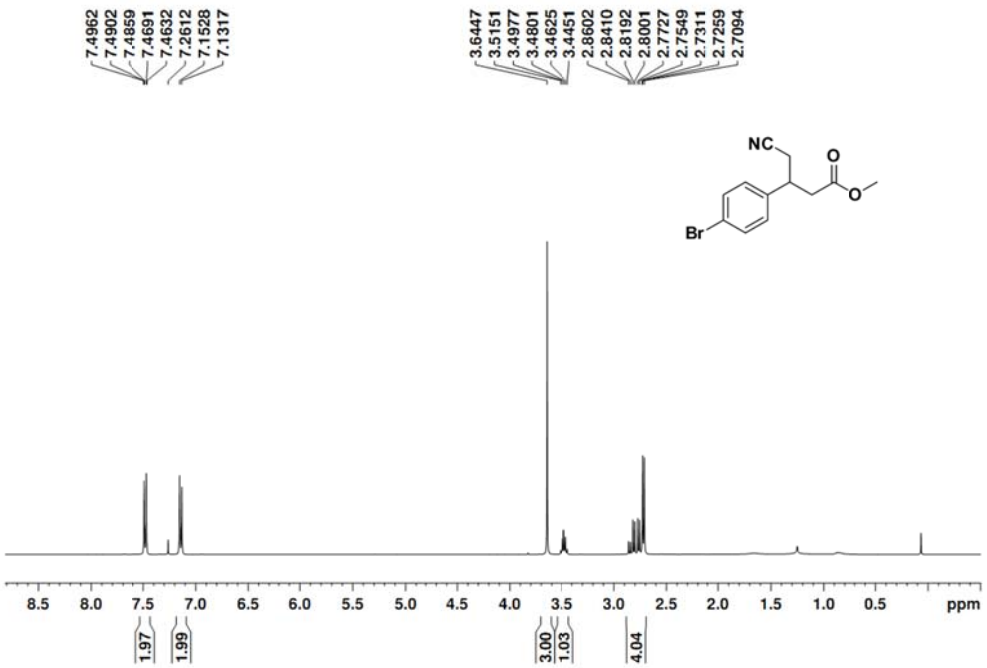
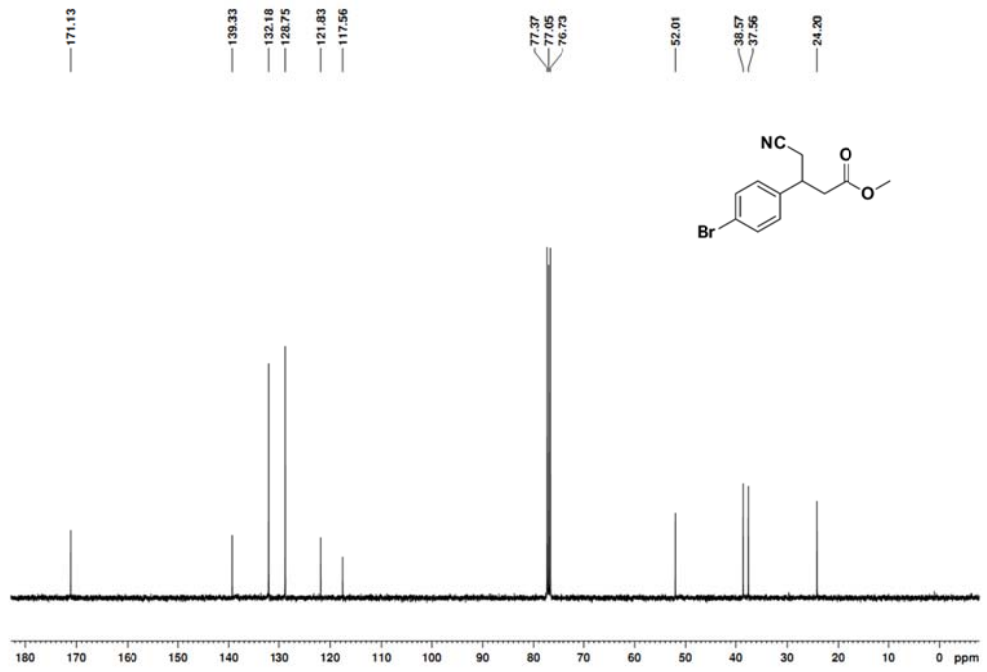
methyl 3-(4-chlorophenyl)-4-cyanobutanoate (2d)



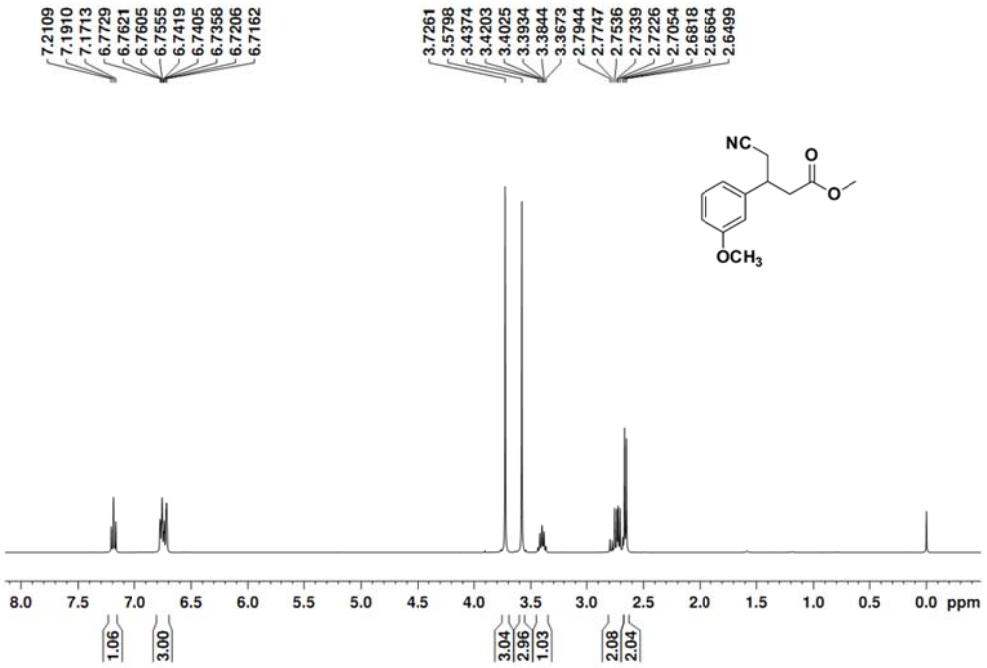


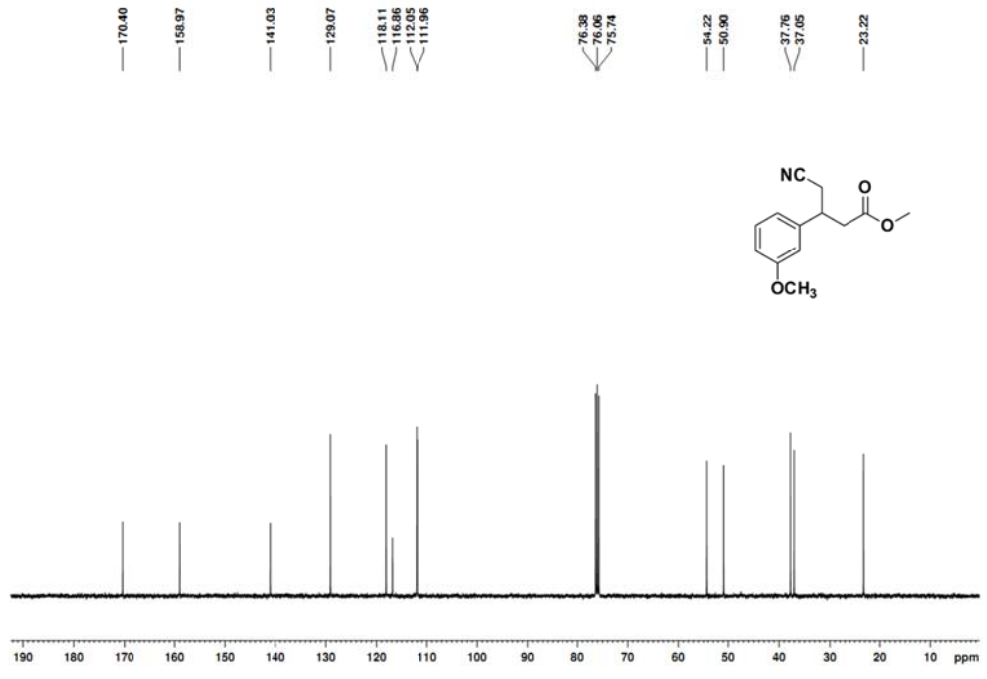
methyl 3-(4-bromophenyl)-4-cyanobutanoate (2e)



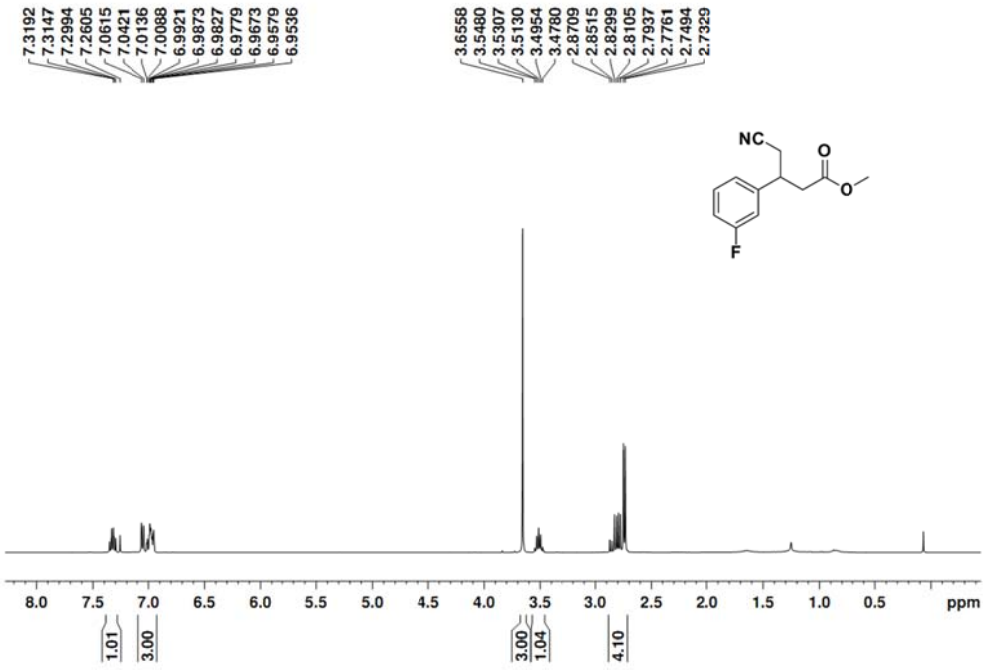


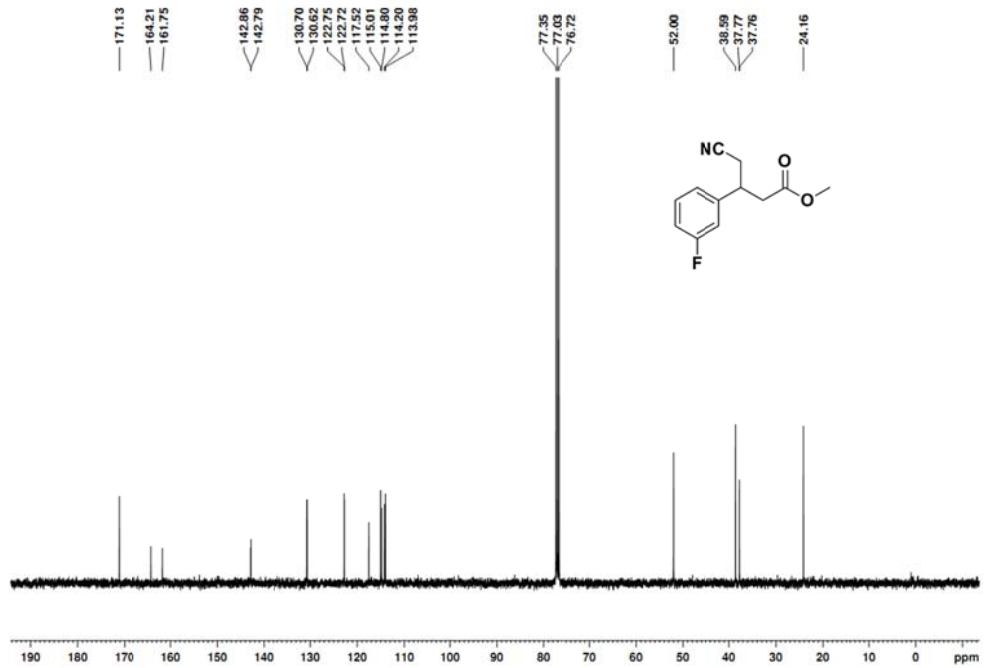
methyl 4-cyano-3-(3-methoxyphenyl)butanoate (2f)

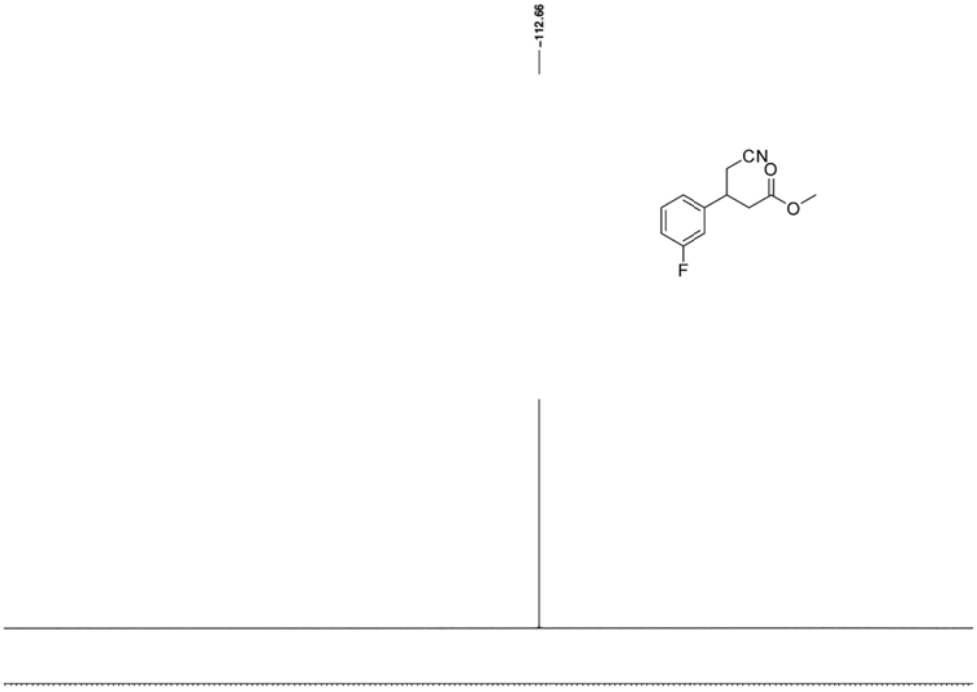




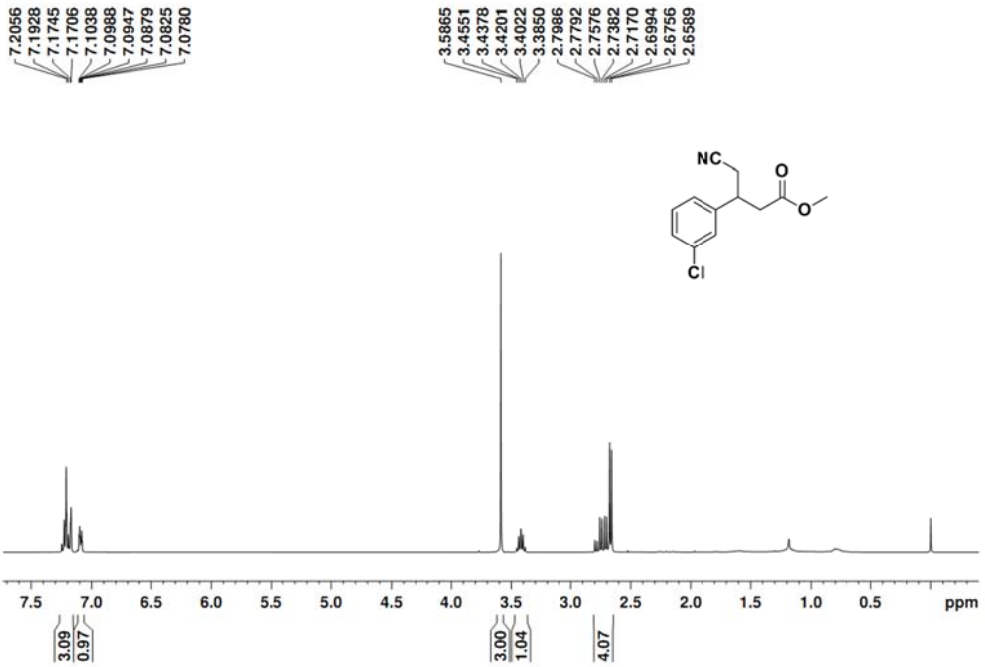
methyl 4-cyano-3-(3-fluorophenyl)butanoate (2g)

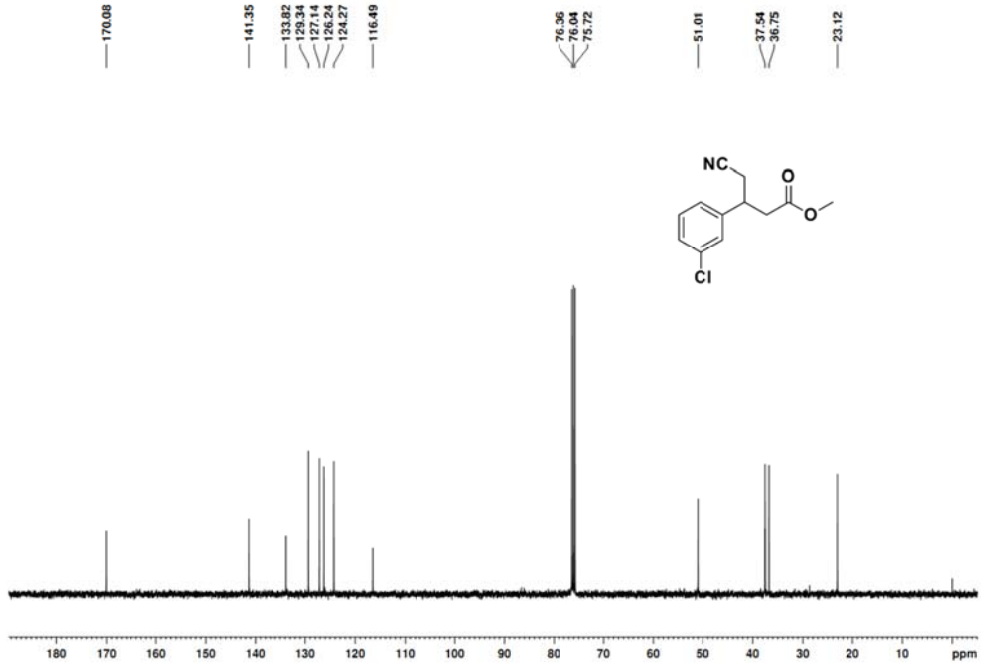




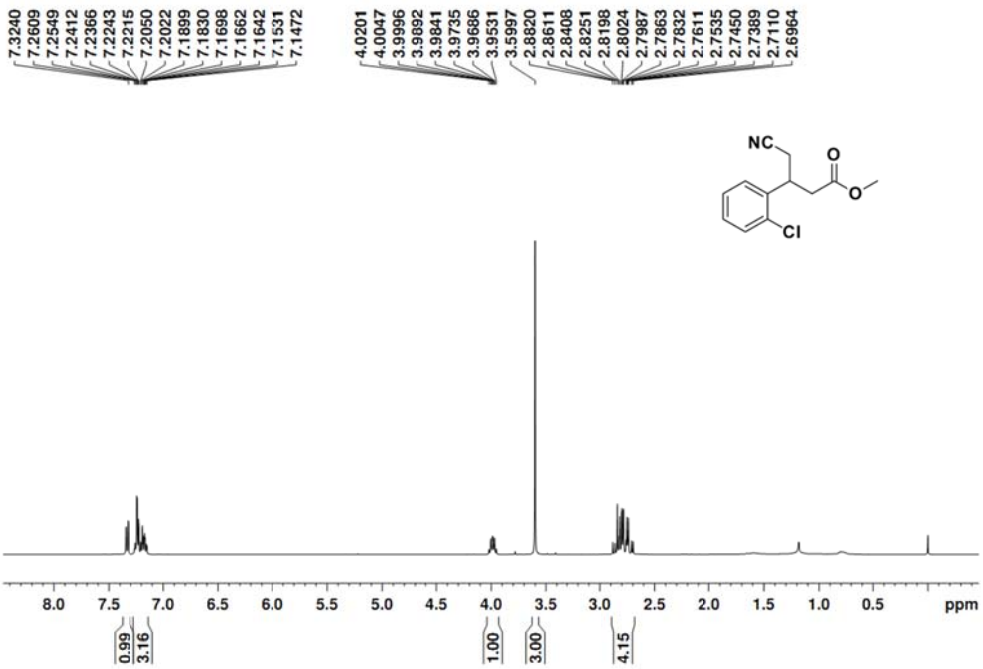


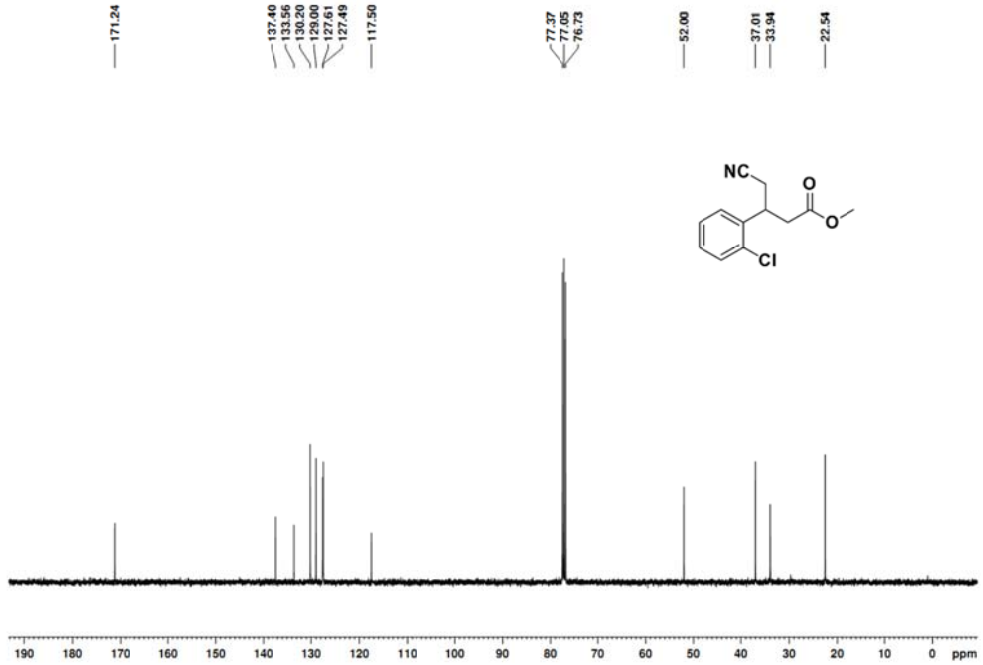
methyl 3-(3-chlorophenyl)-4-cyanobutanoate (2h)



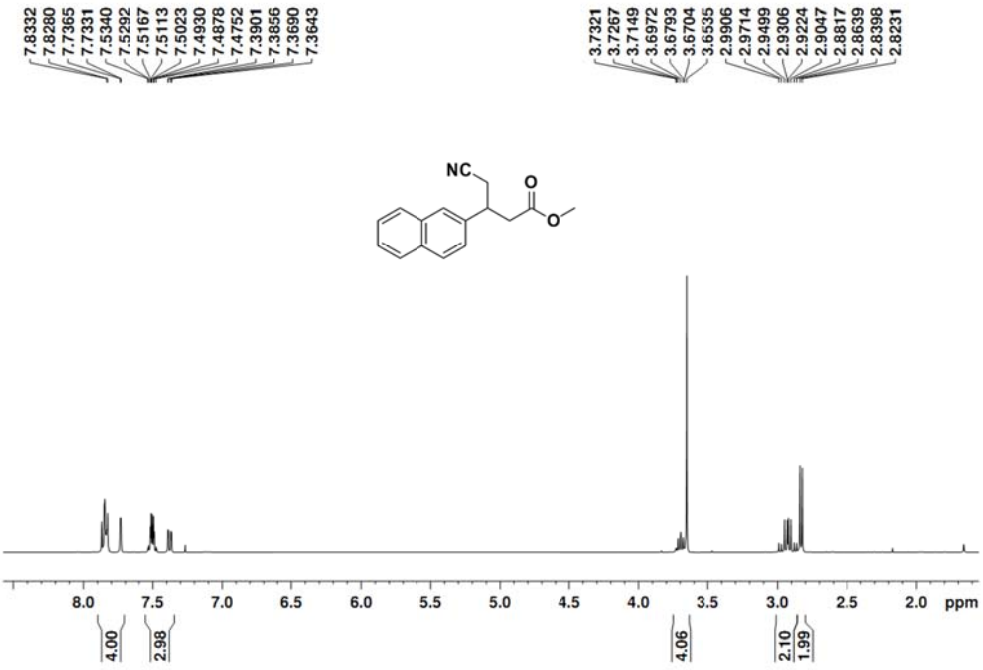


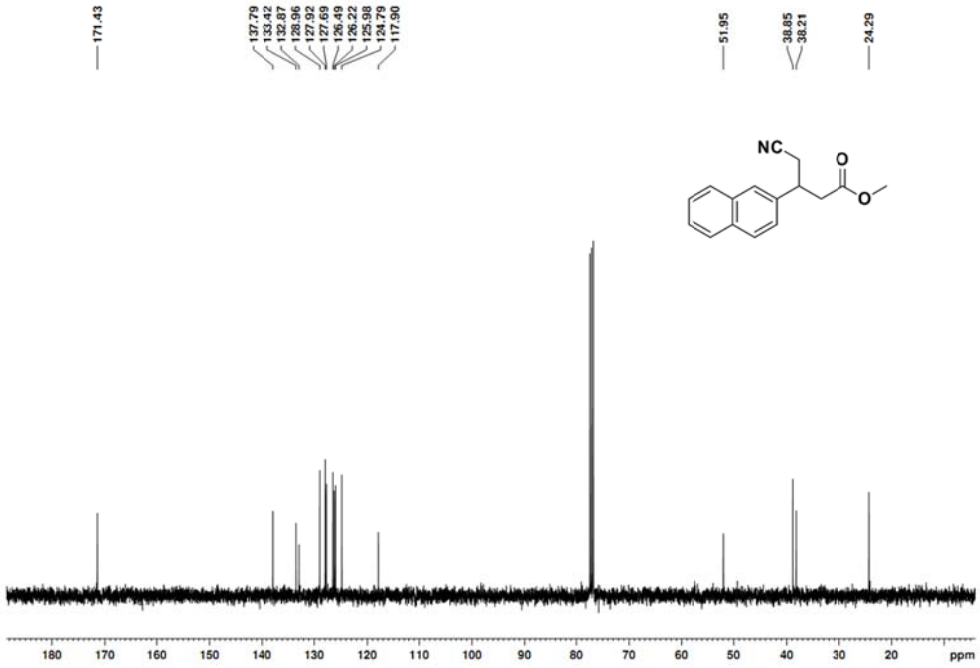
methyl 3-(2-chlorophenyl)-4-cyanobutanoate (2i)



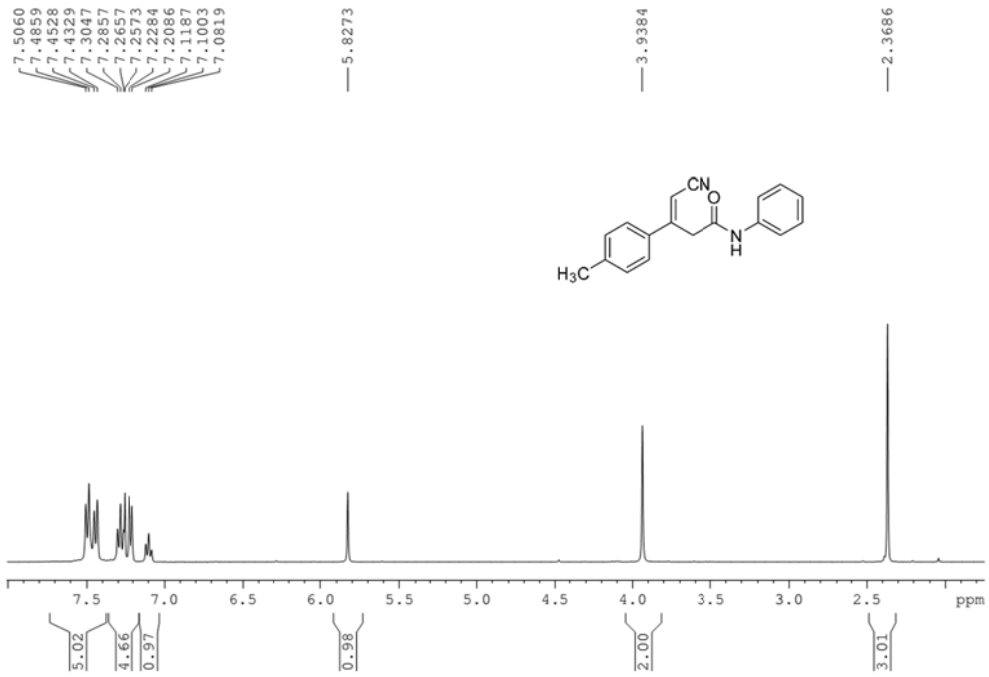


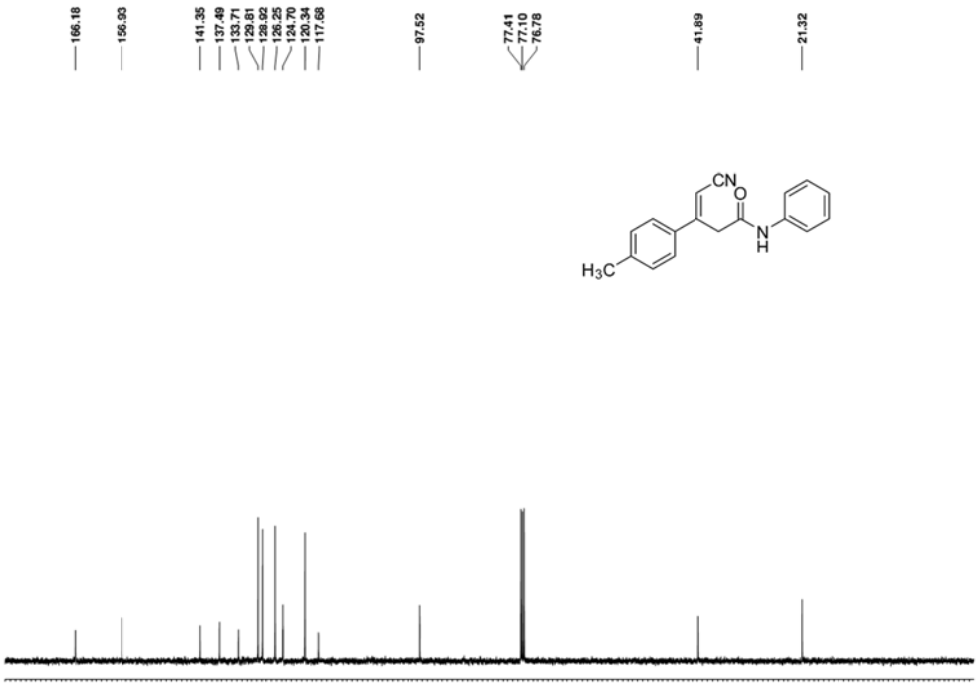
methyl 4-cyano-3-(naphthalen-2-yl)butanoate (2j)



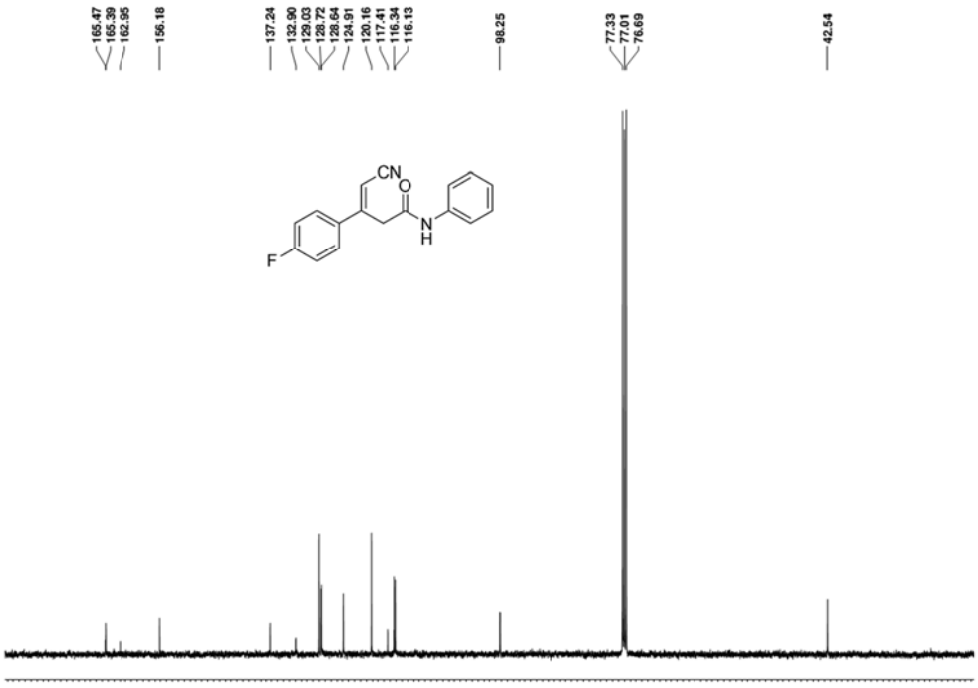


(*E*)-4-cyano-*N*-phenyl-3-(*p*-tolyl)but-3-enamide (3a)





(*E*)-4-cyano-3-(4-fluorophenyl)-*N*-phenylbut-3-enamide (3b)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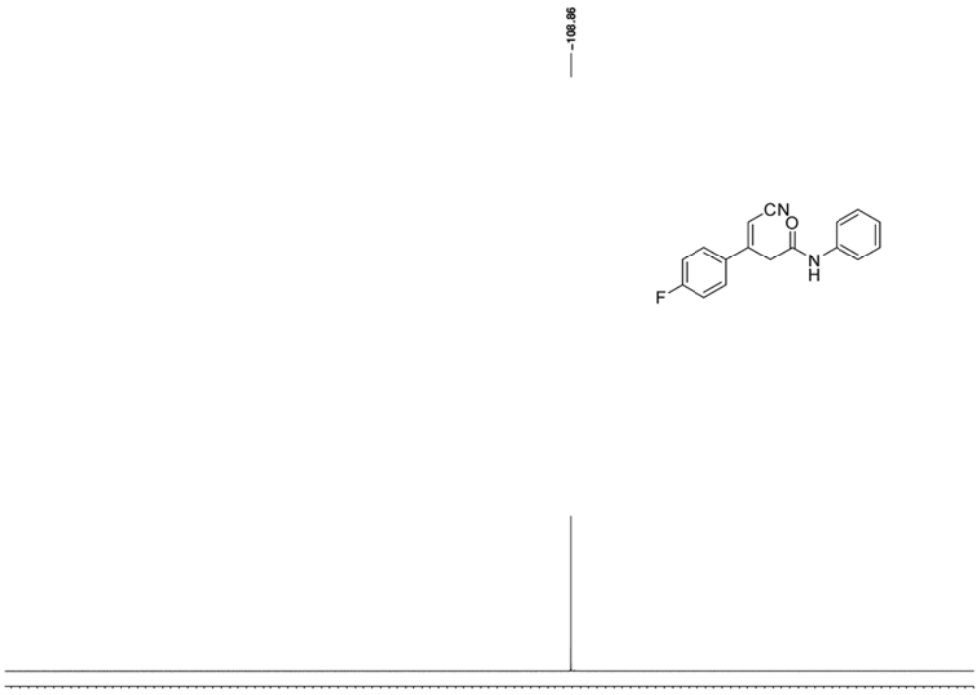
H
F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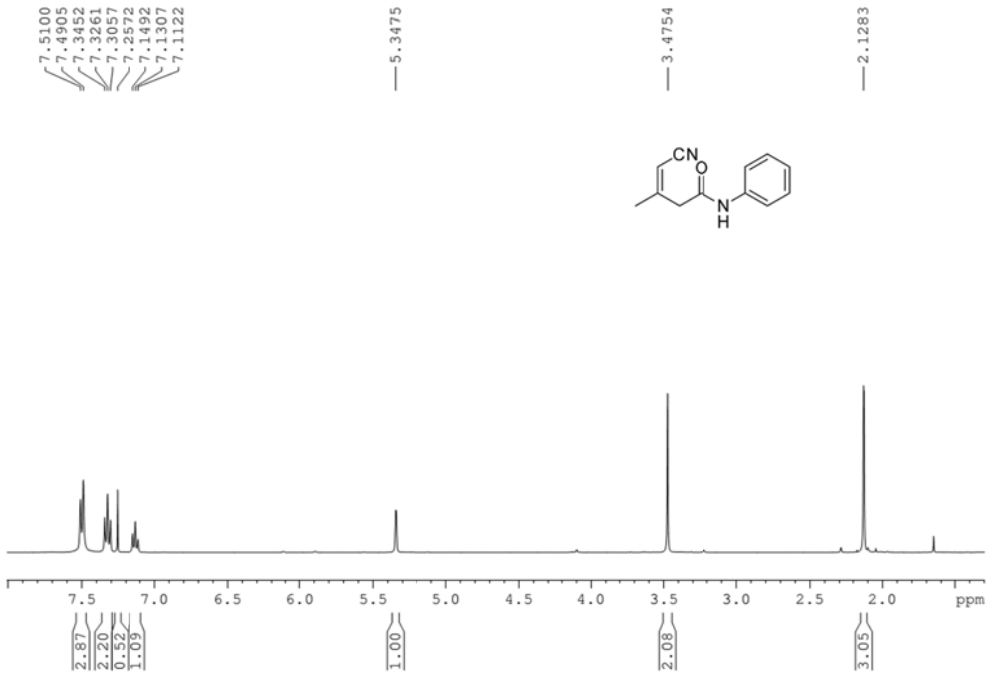
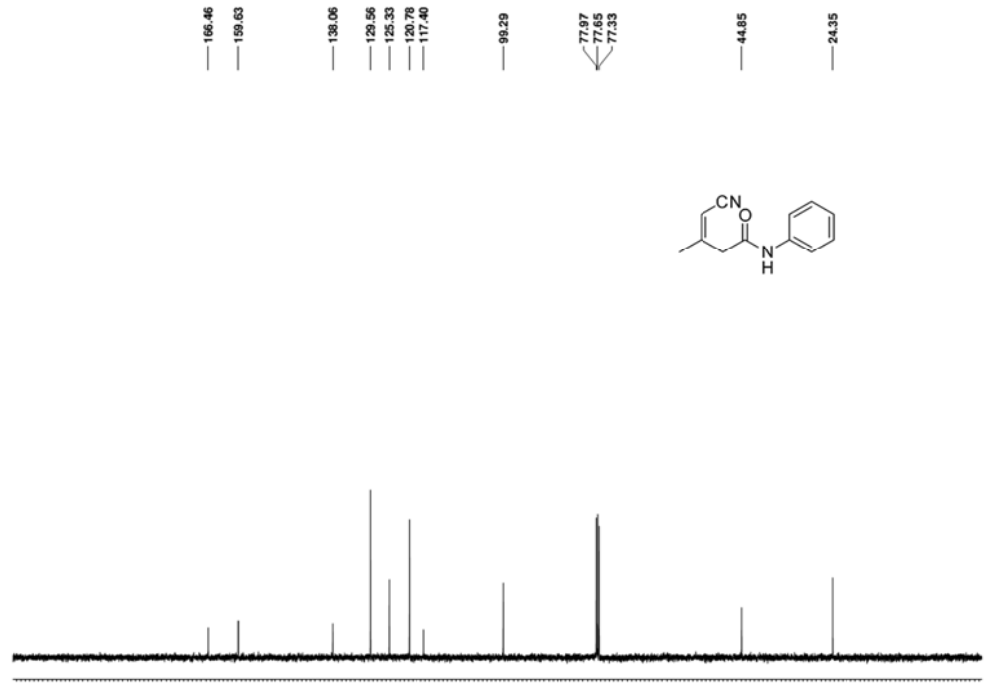
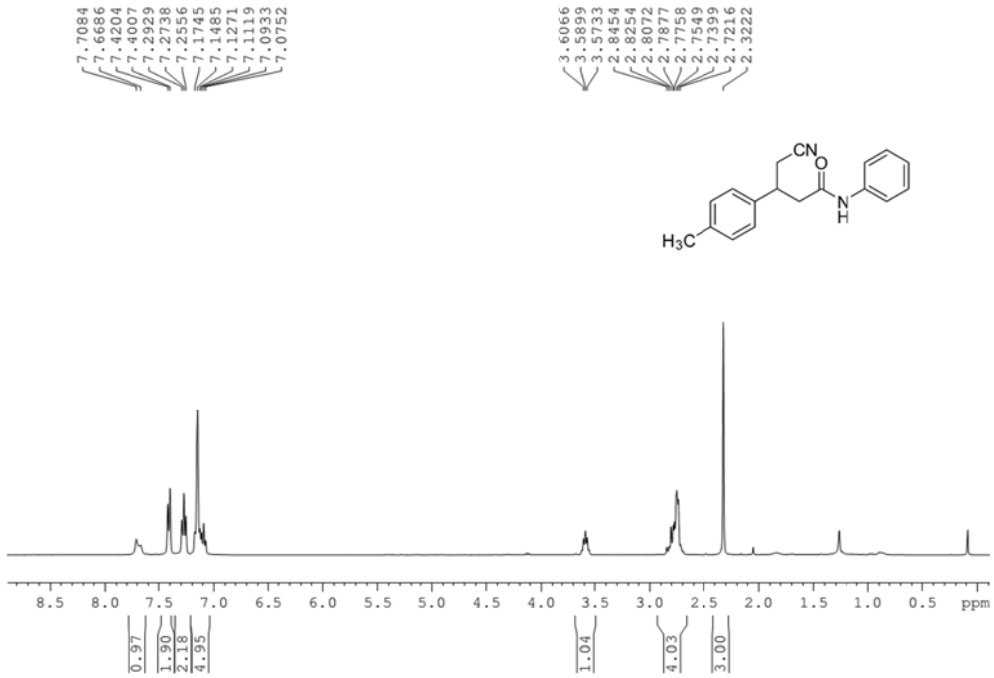
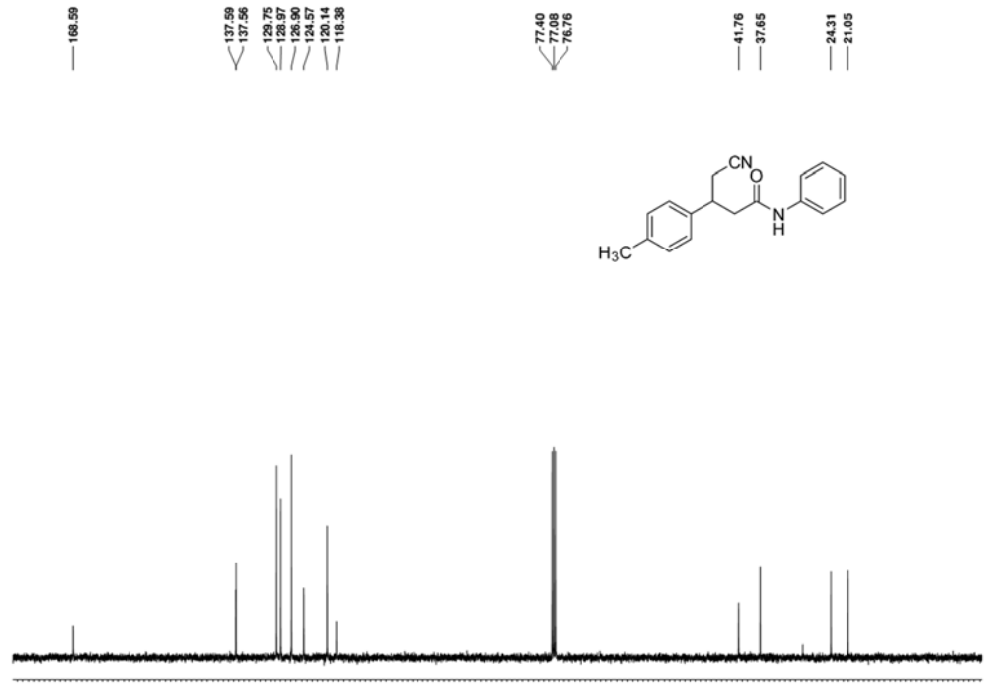
(*Z*)-4-cyano-3-methyl-N-phenylbut-3-enamide (3c)



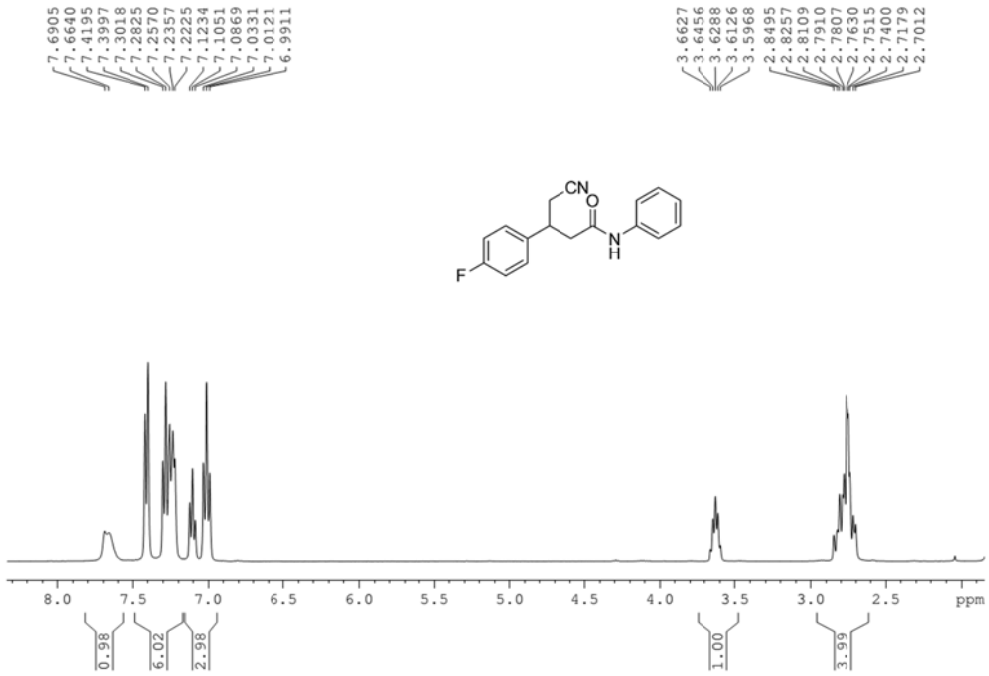


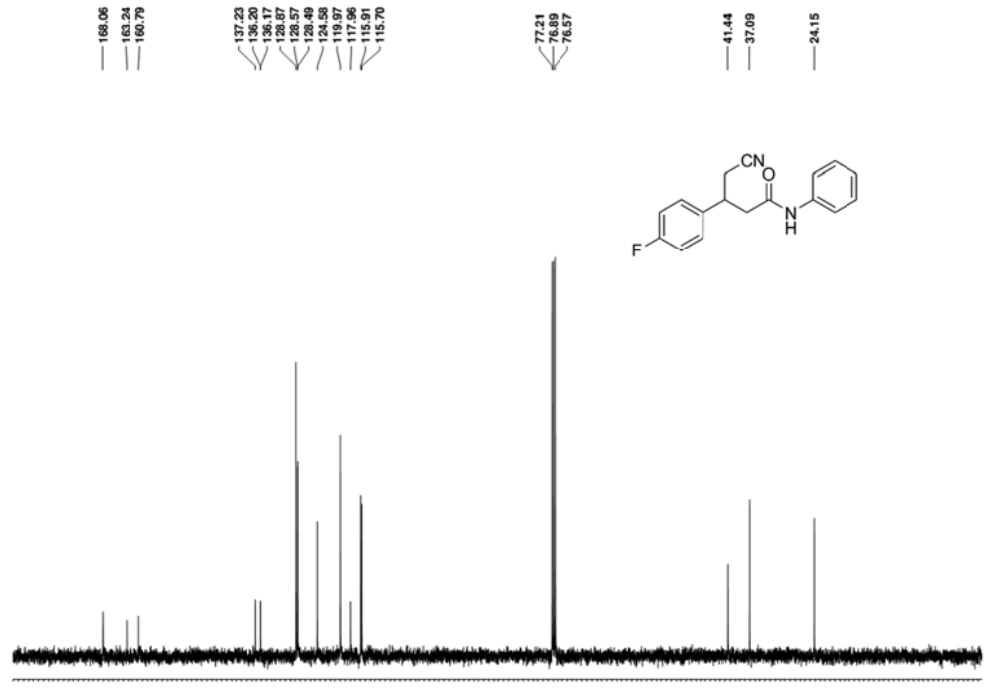
4-cyano-*N*-phenyl-3-(*p*-tolyl)butanamide (4a)

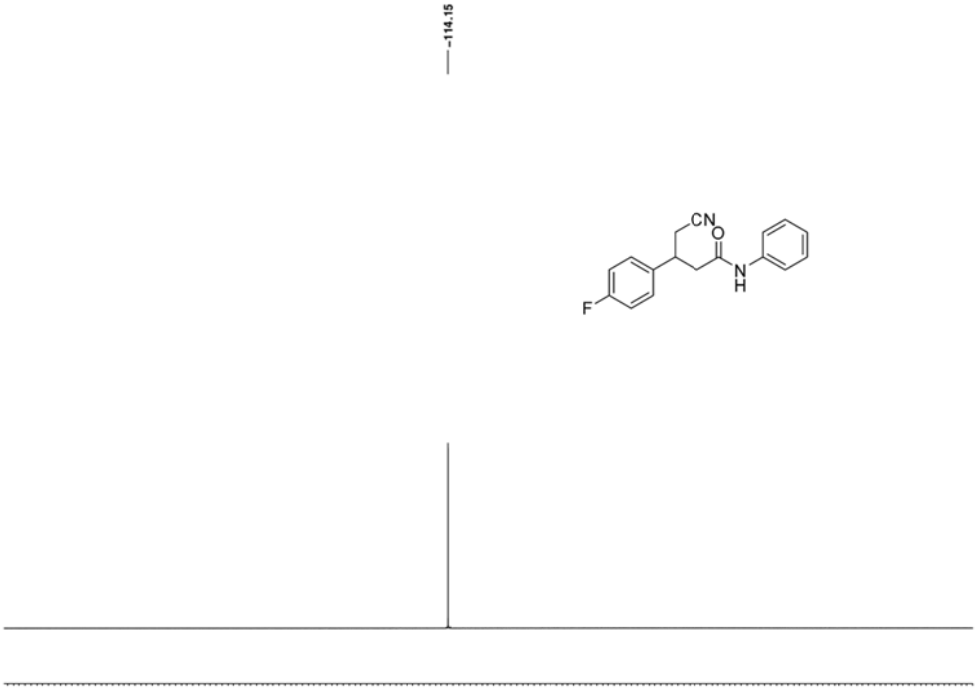




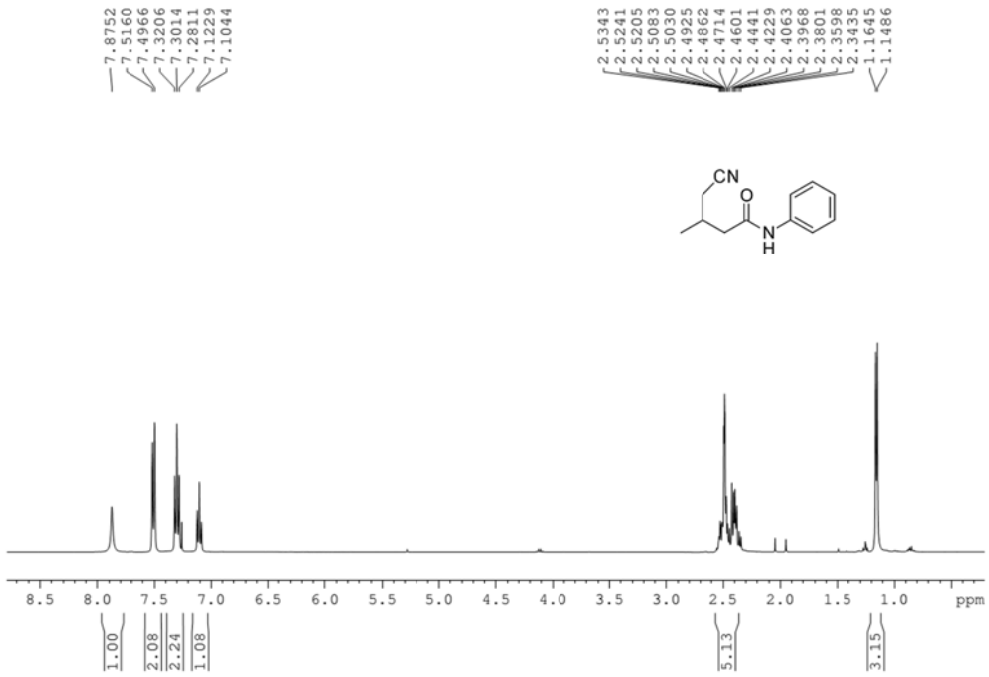
4-cyano-3-(4-fluorophenyl)-*N*-phenylbutanamide (4b)

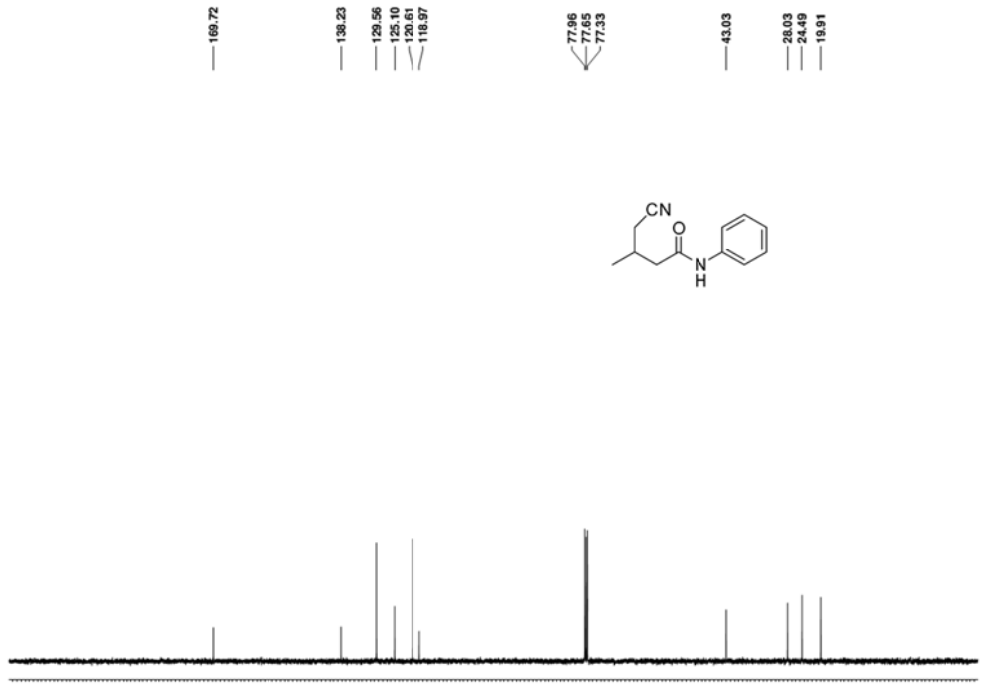




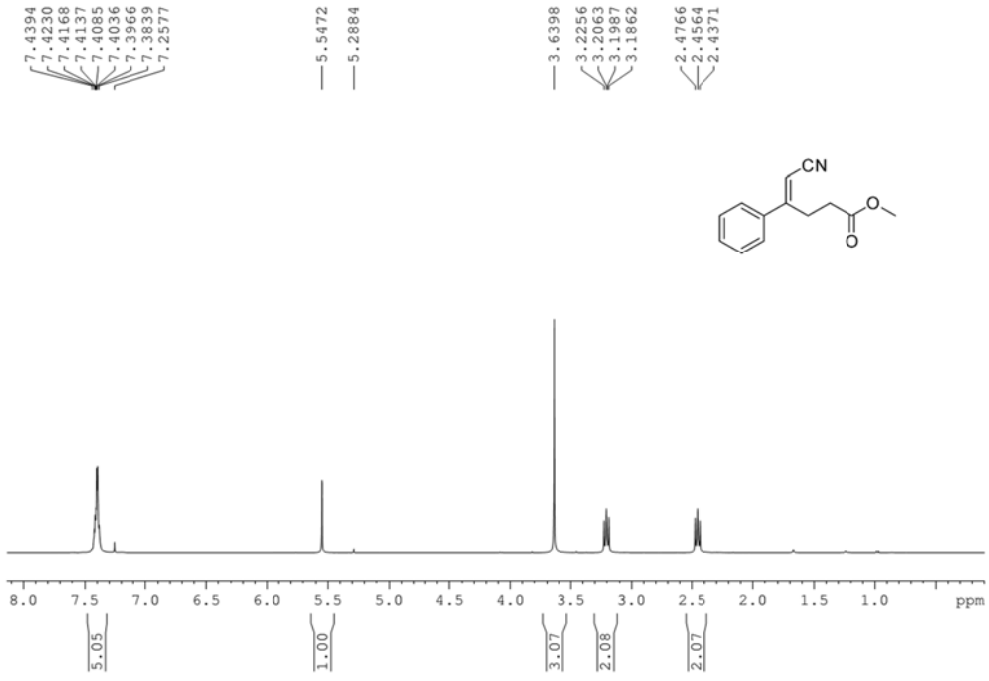


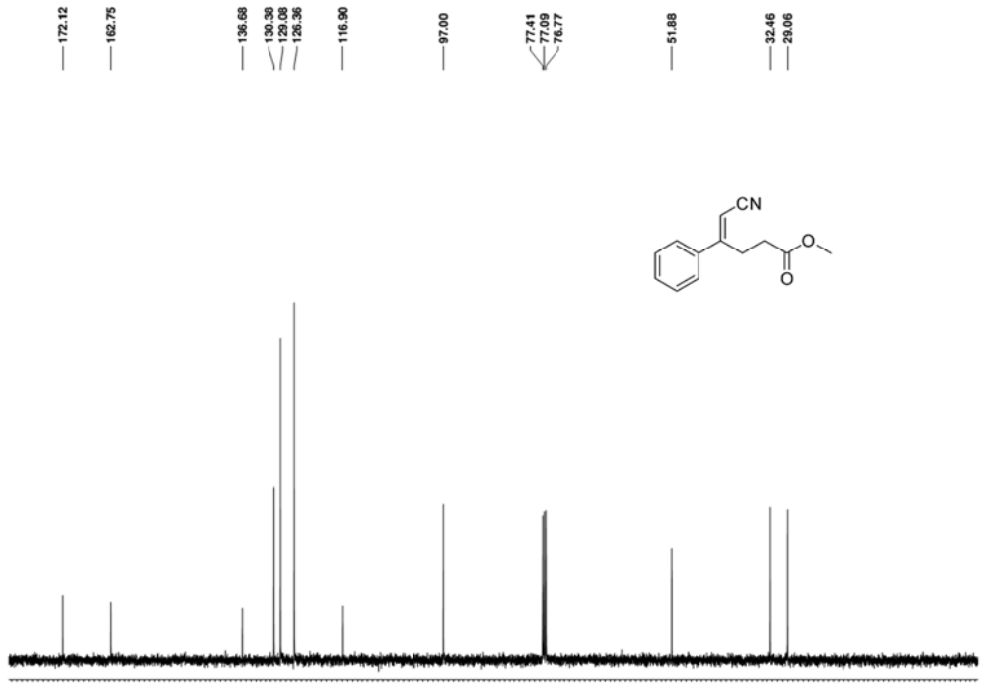
4-cyano-3-methyl-N-phenylbutanamide (4c)



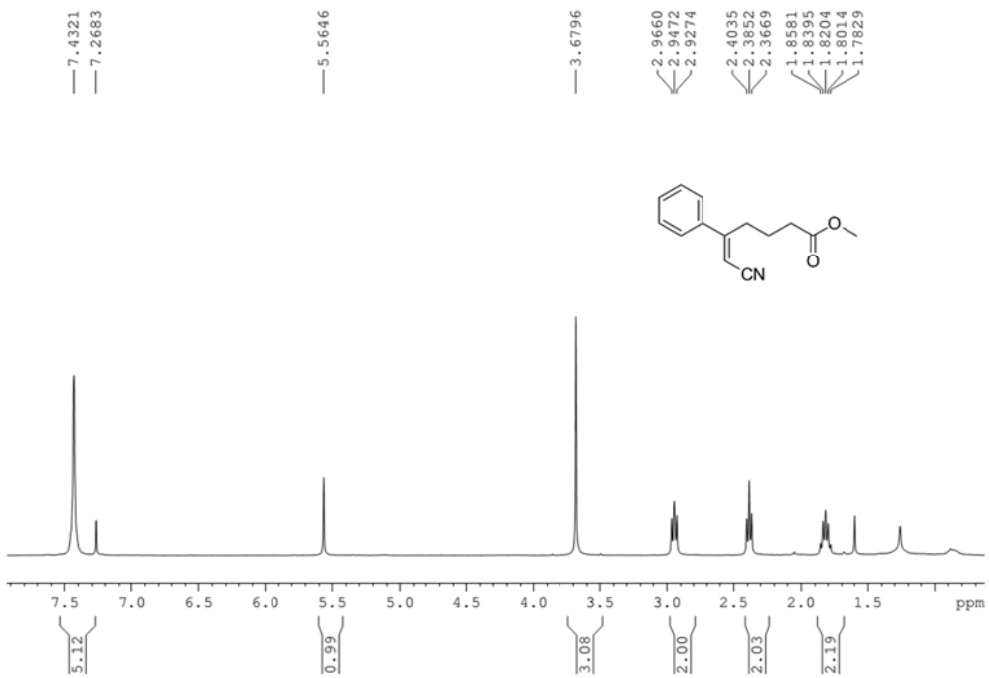


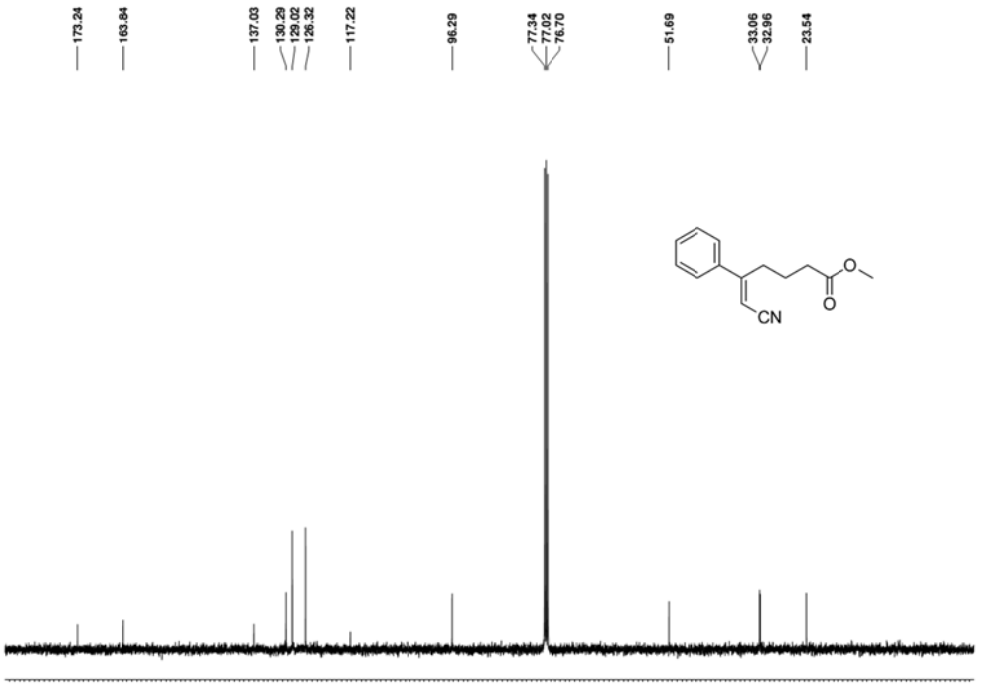
(*E*)-methyl 5-cyano-4-phenylpent-4-enoate (5a)



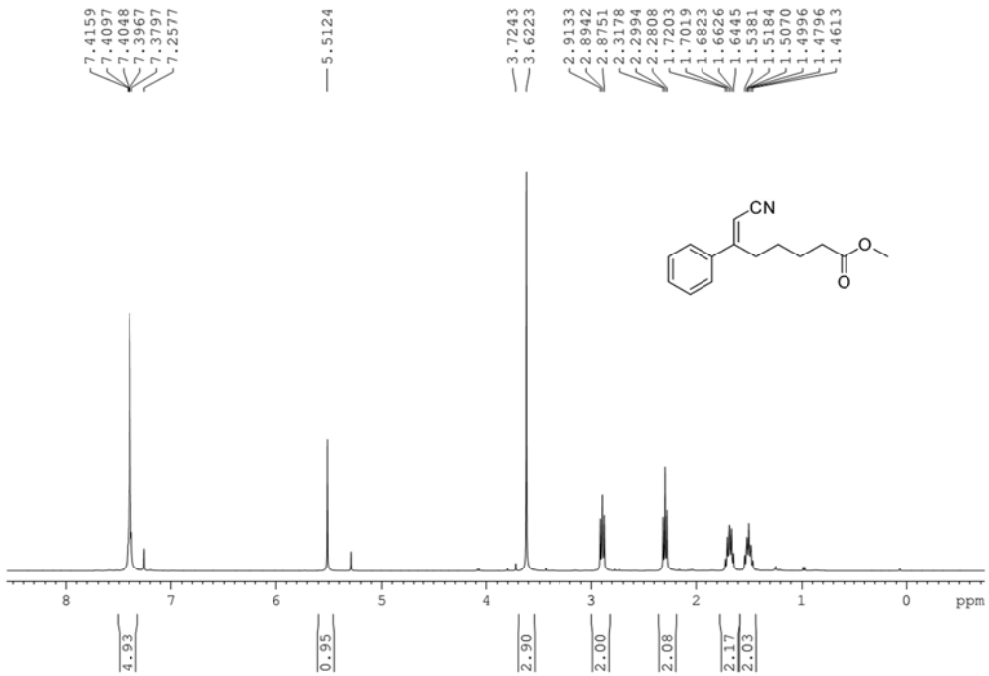


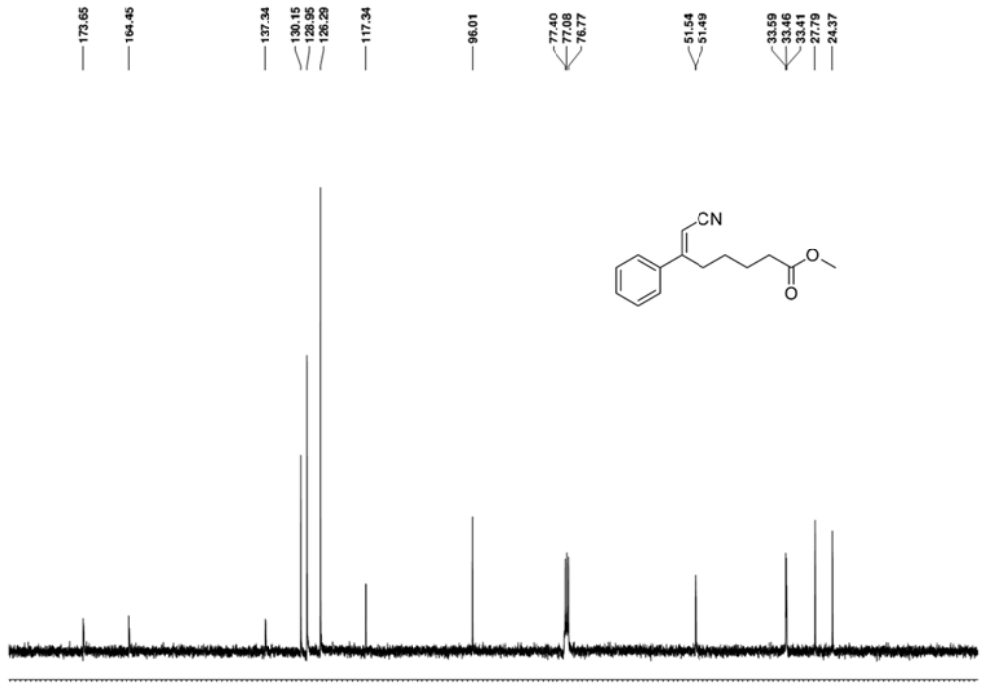
(*E*)-methyl 6-cyano-5-phenylhex-5-enoate (5b)



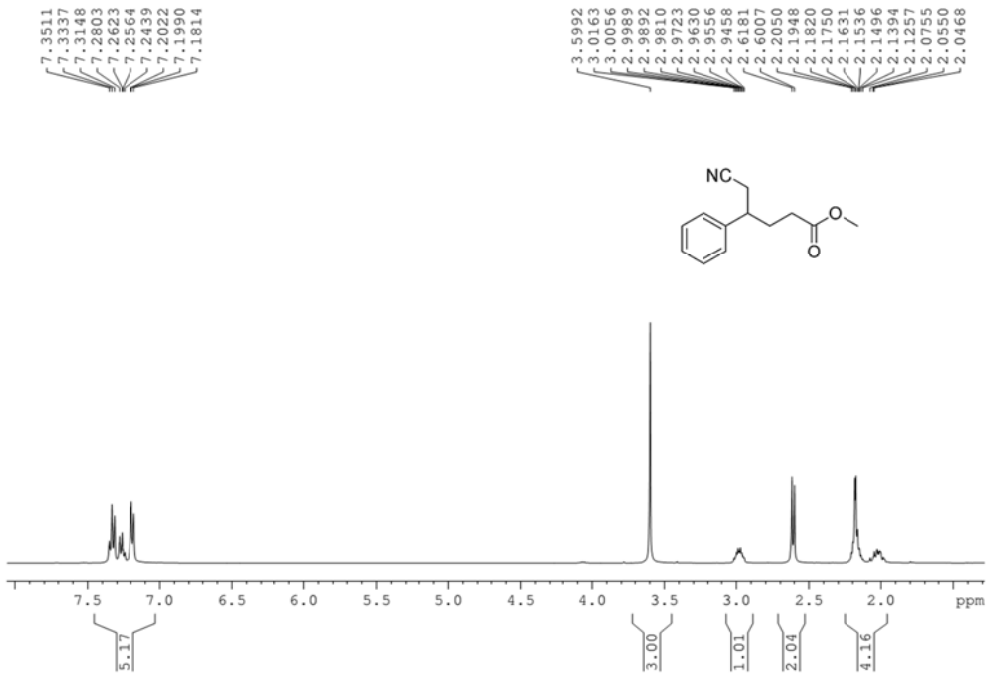


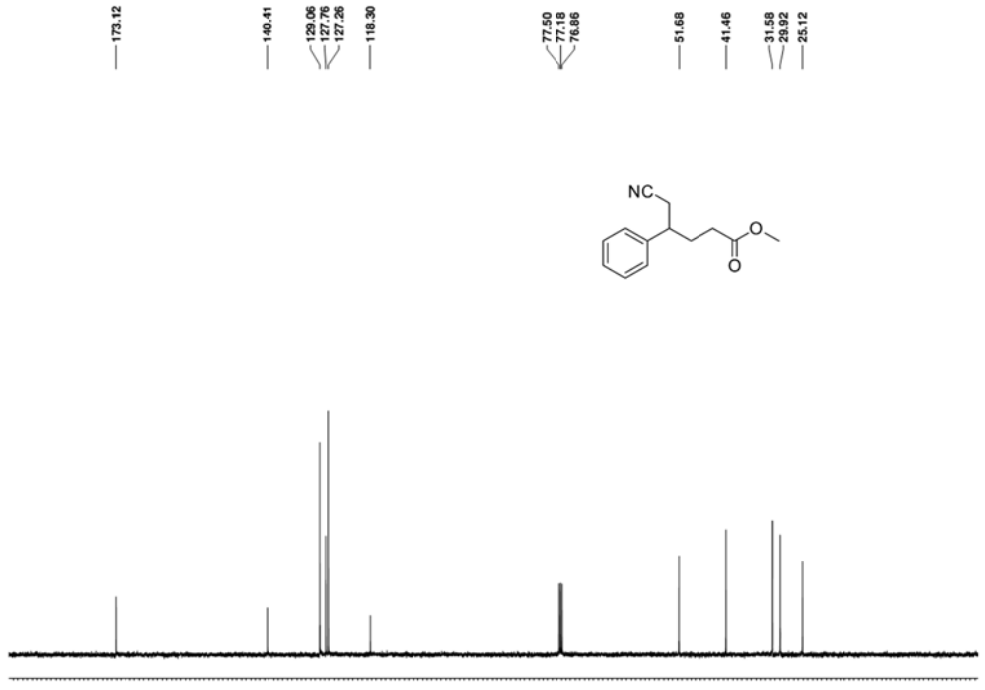
(*E*)-methyl 7-cyano-6-phenylhept-6-enoate (5c)



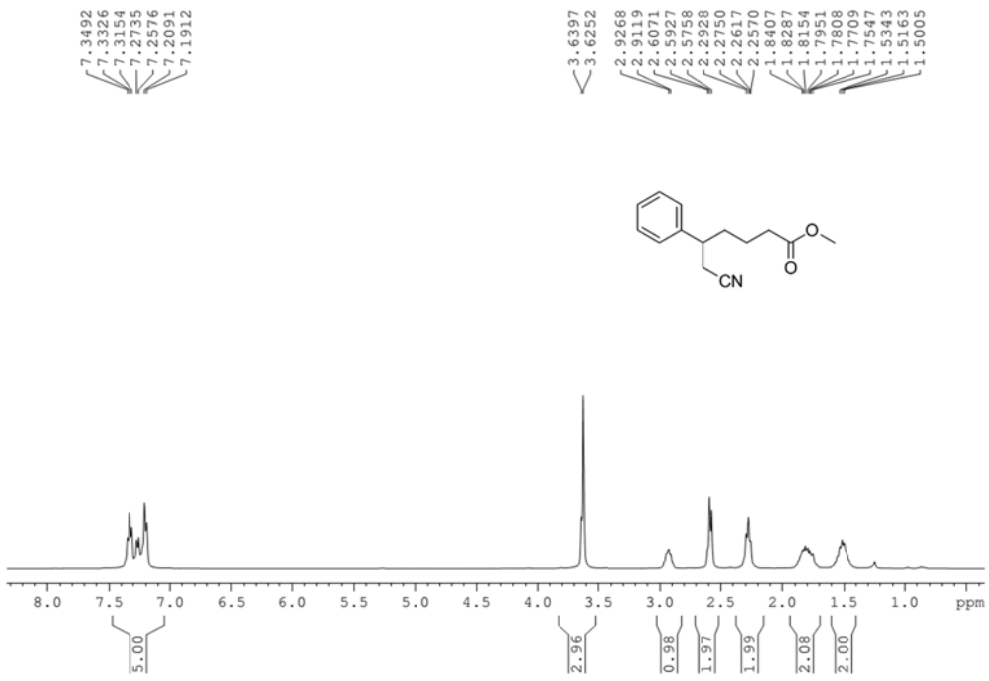


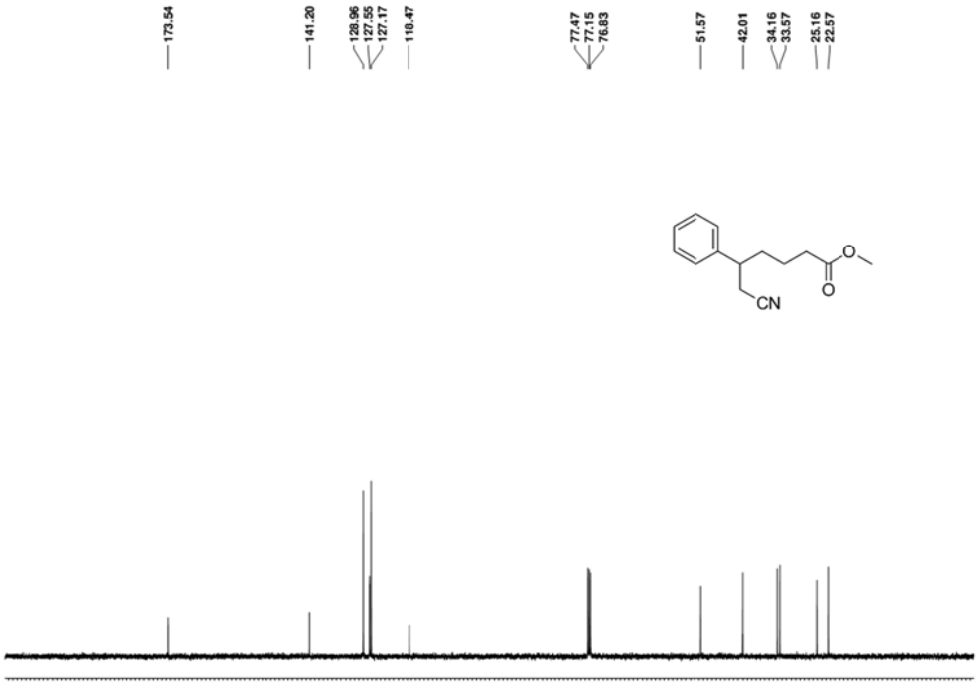
methyl 5-cyano-4-phenylpentanoate (6a)



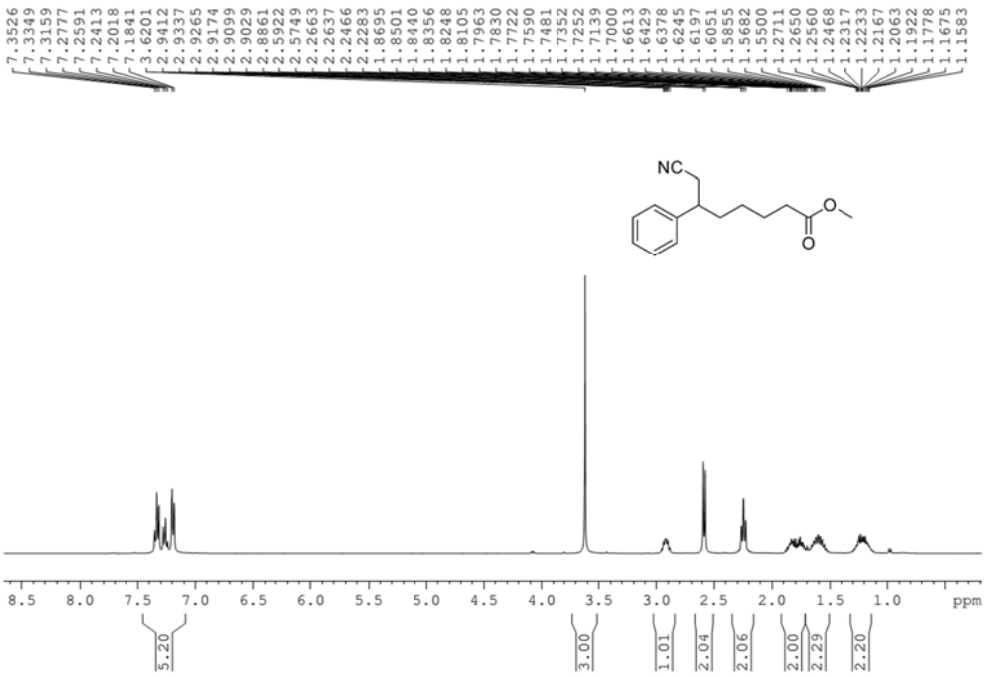


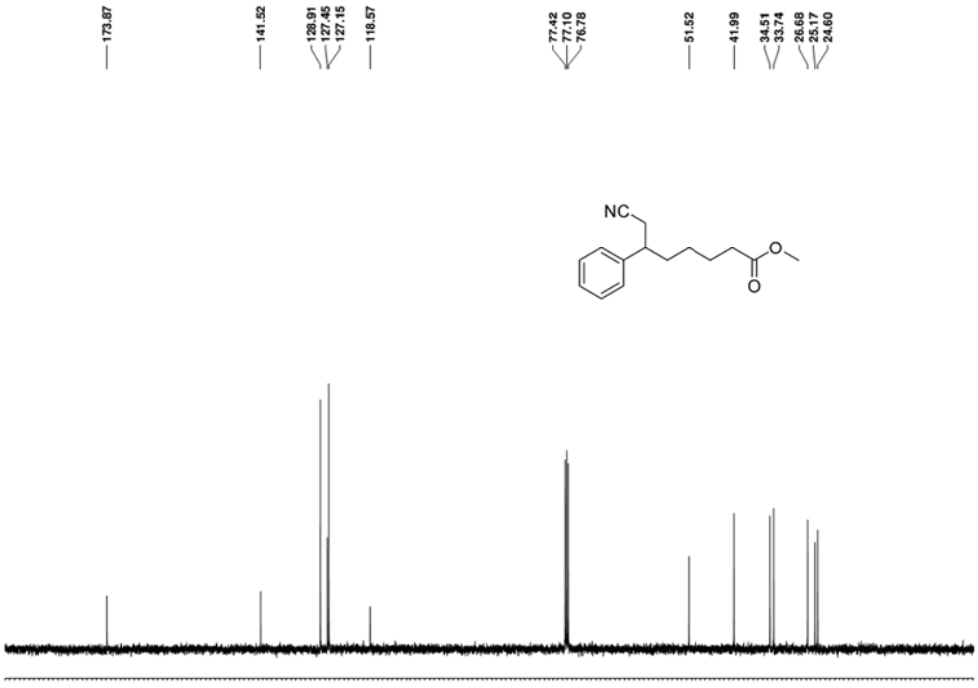
methyl 6-cyano-5-phenylhexanoate (6b)



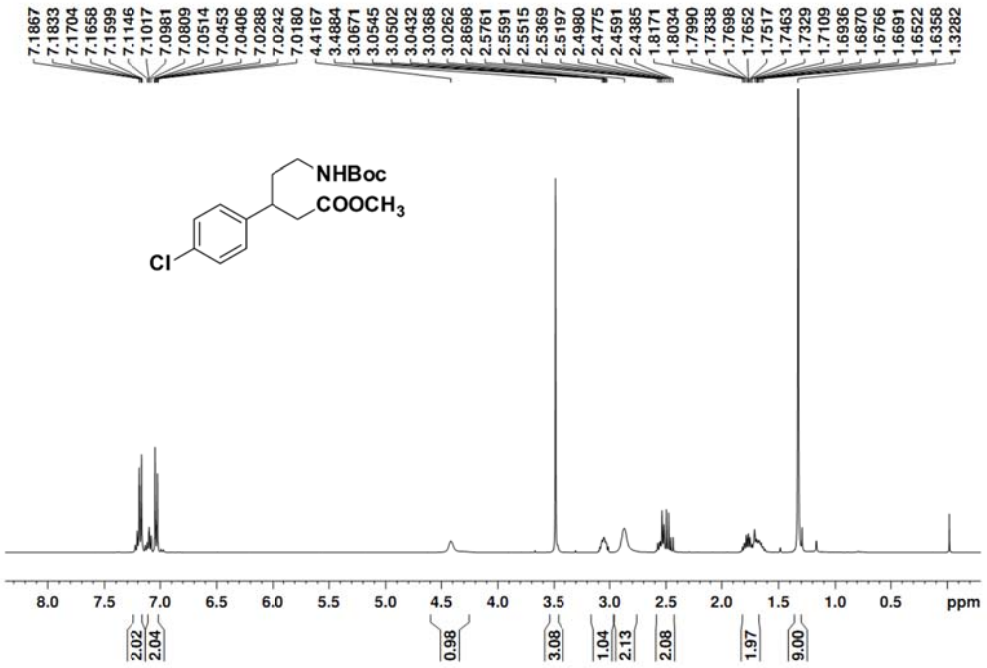


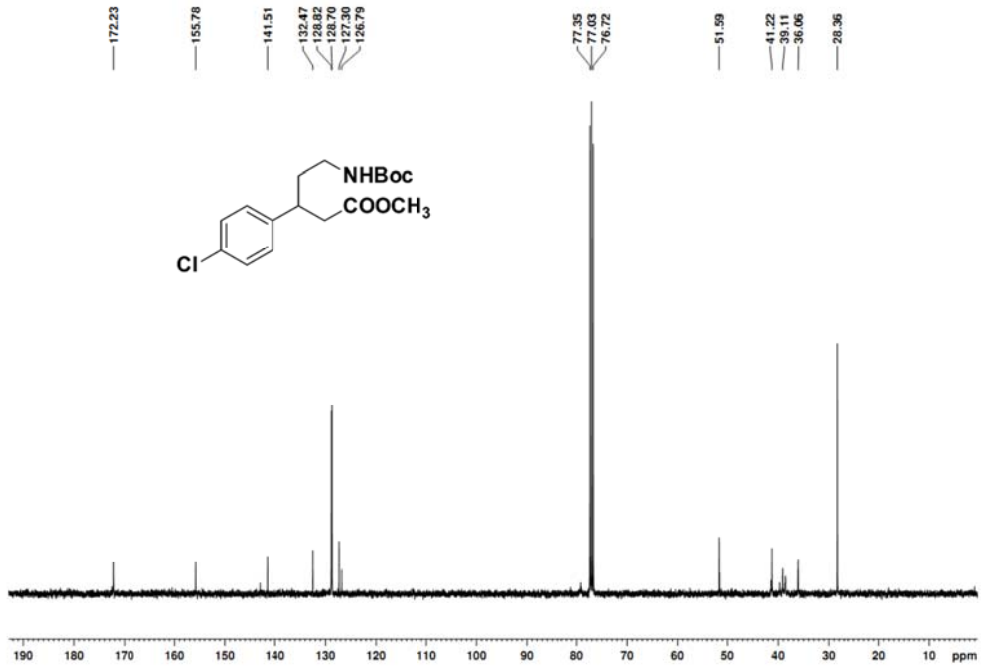
methyl 7-cyano-6-phenylheptanoate (6c)



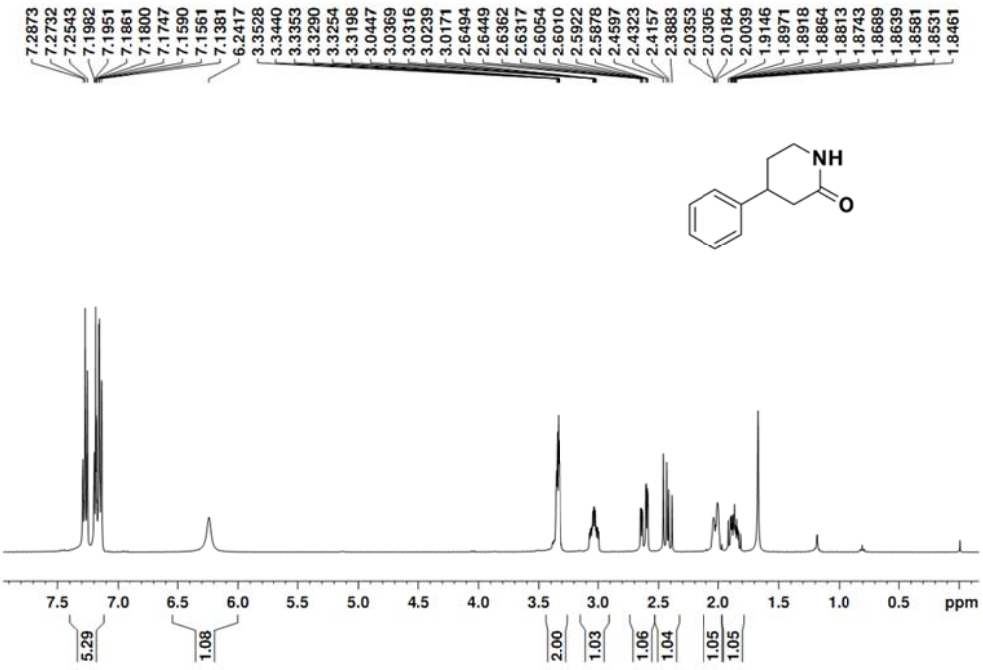


methyl 5-((*tert*-butoxycarbonyl)amino)-3-(4-chlorophenyl)pentanoate (7)

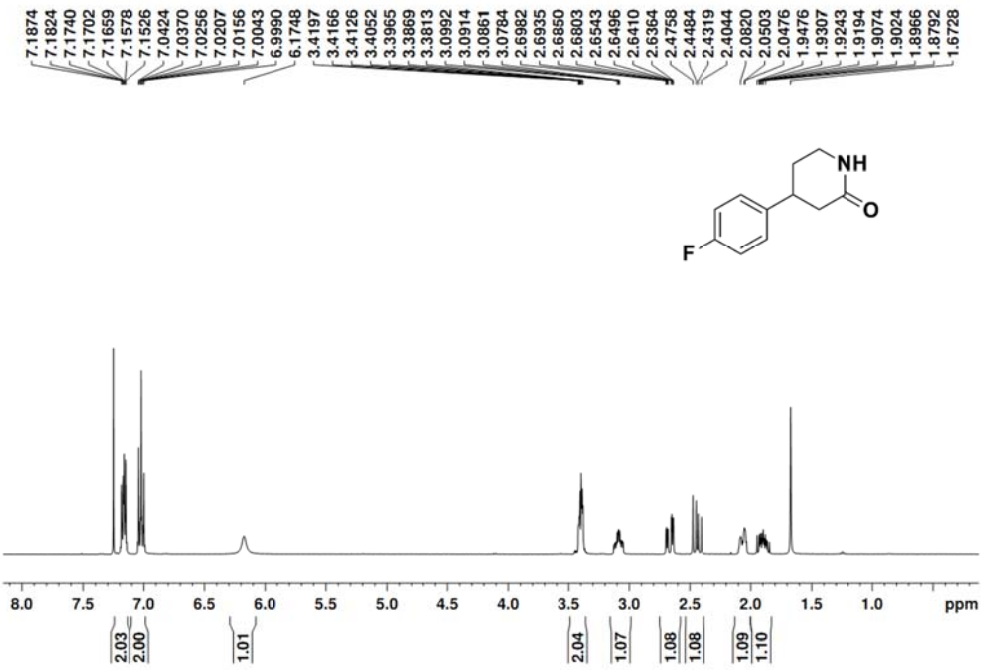


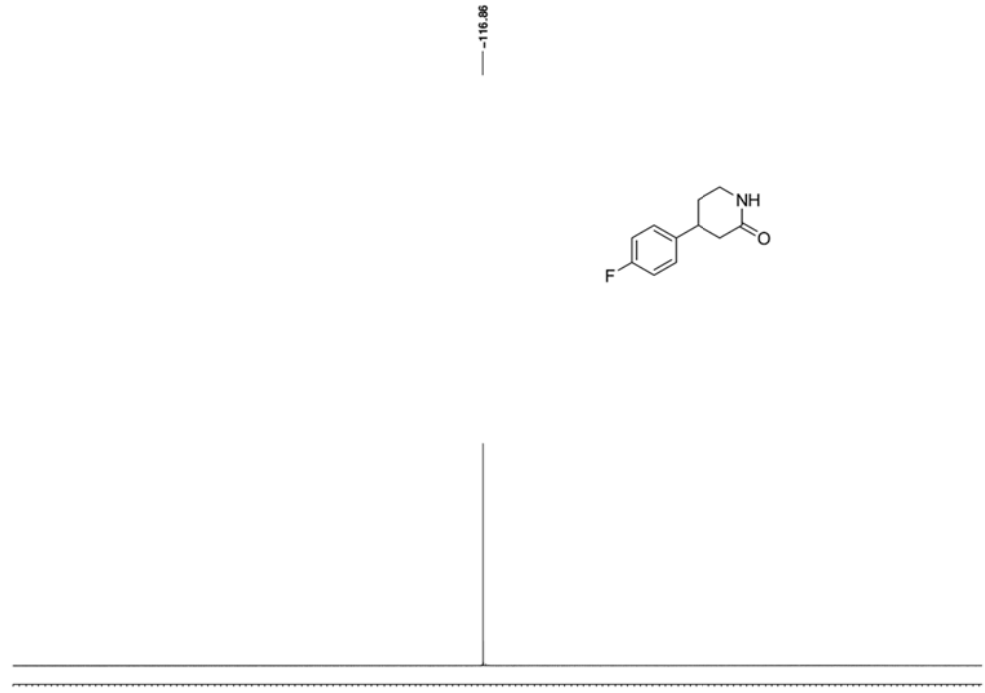


4-phenylpiperidin-2-one (8a)

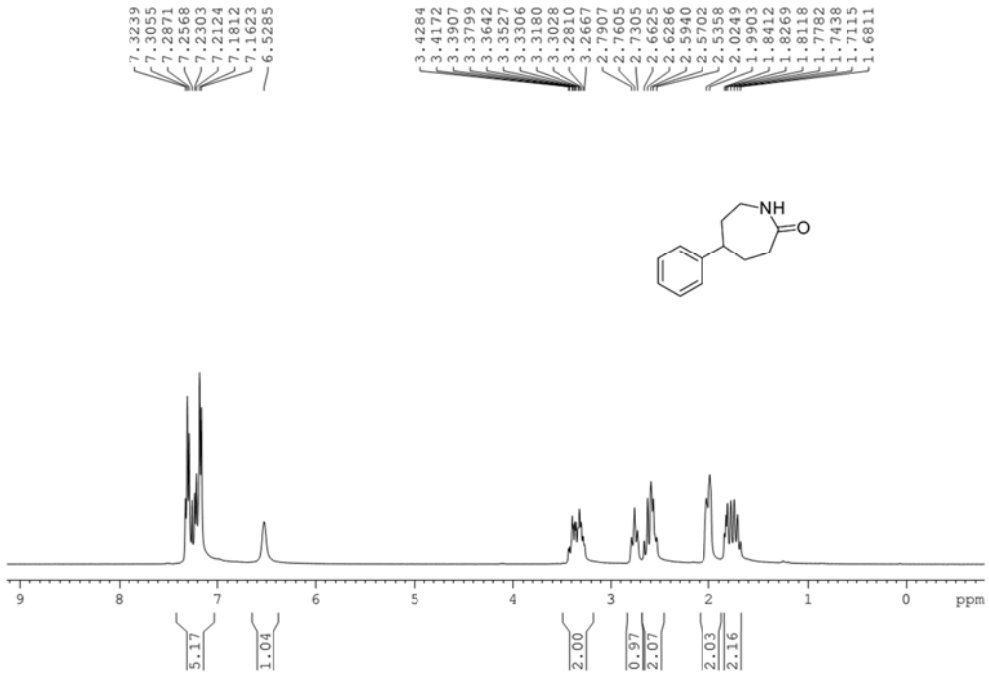


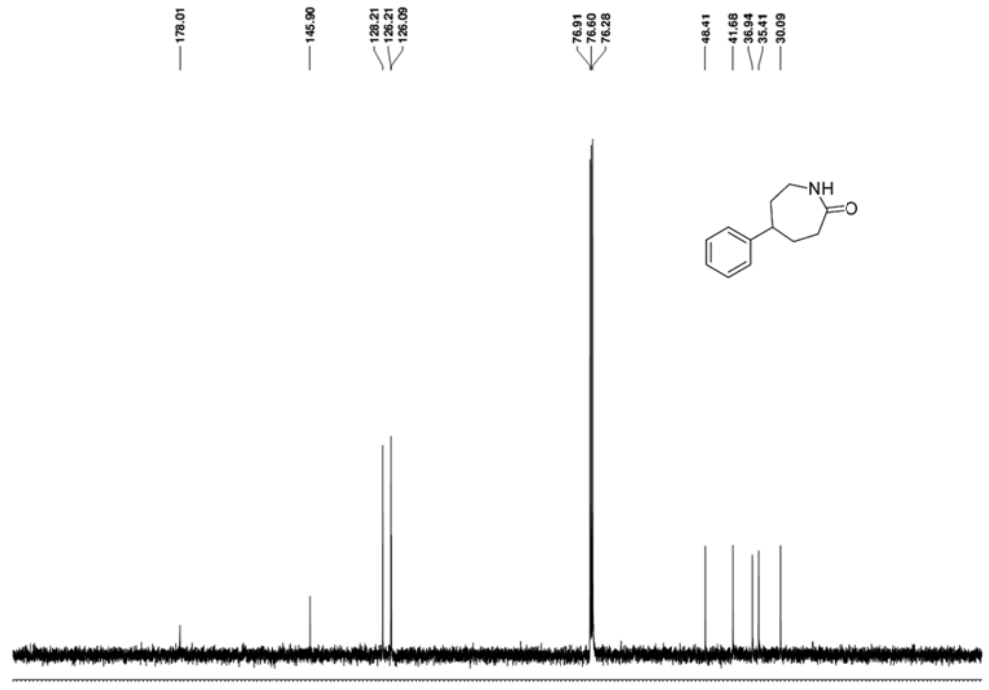
4-(4-fluorophenyl)piperidin-2-one (8b)



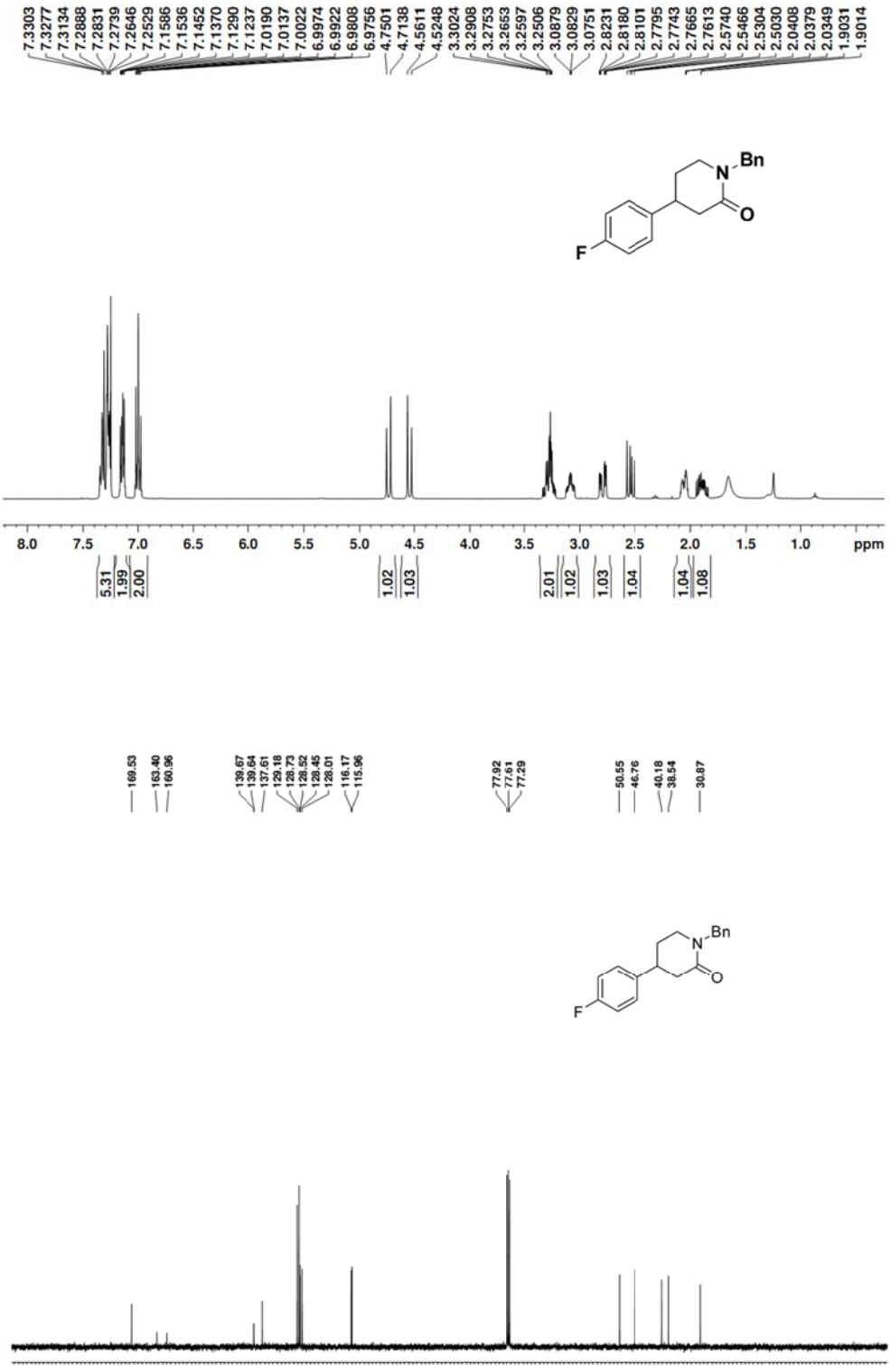


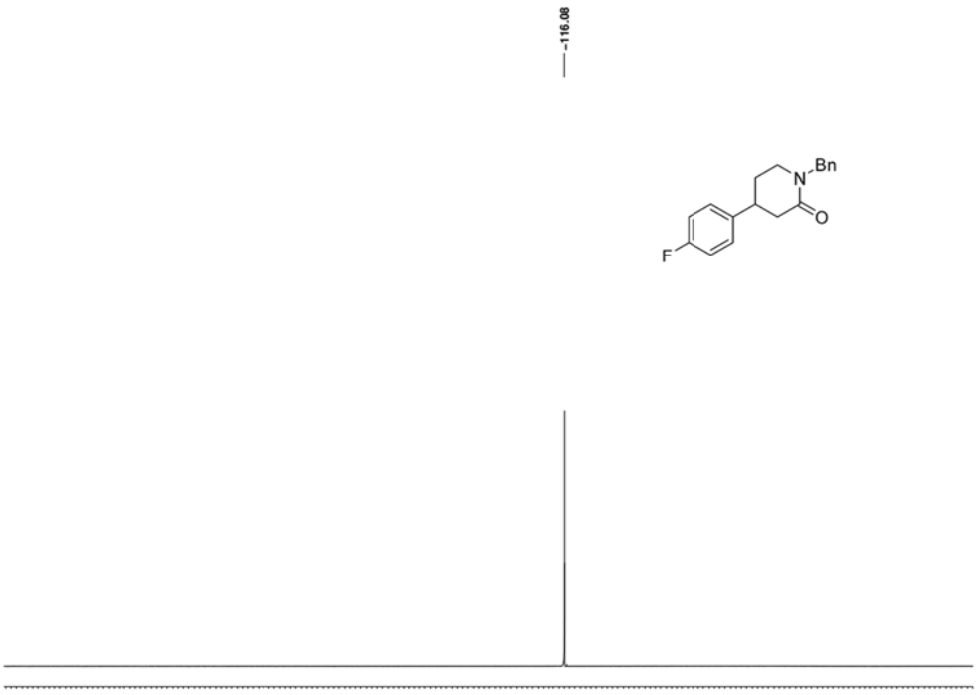
5-phenylazepan-2-one (8c)



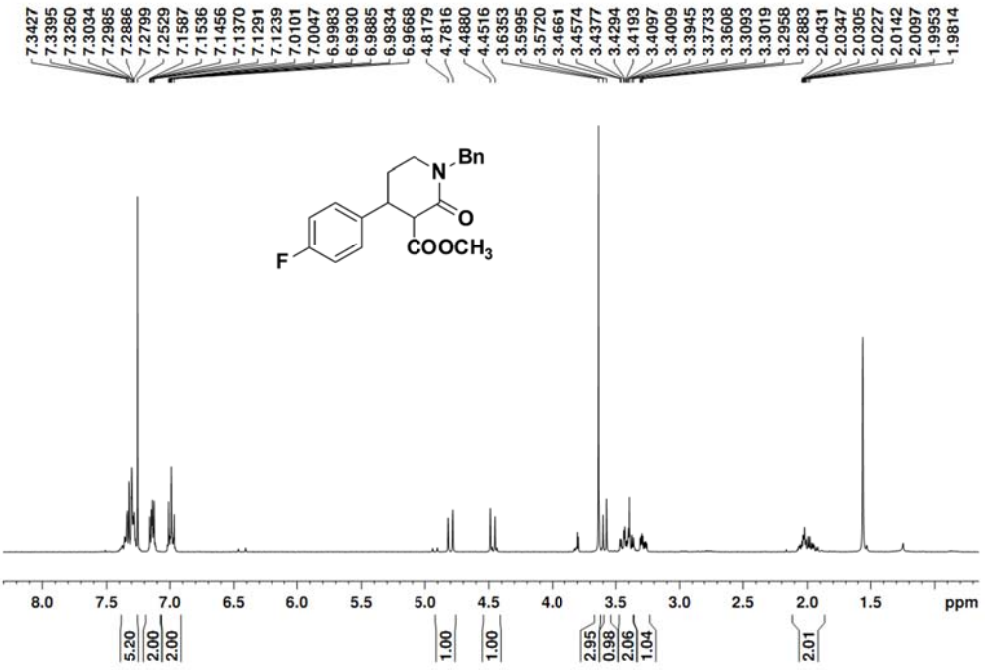


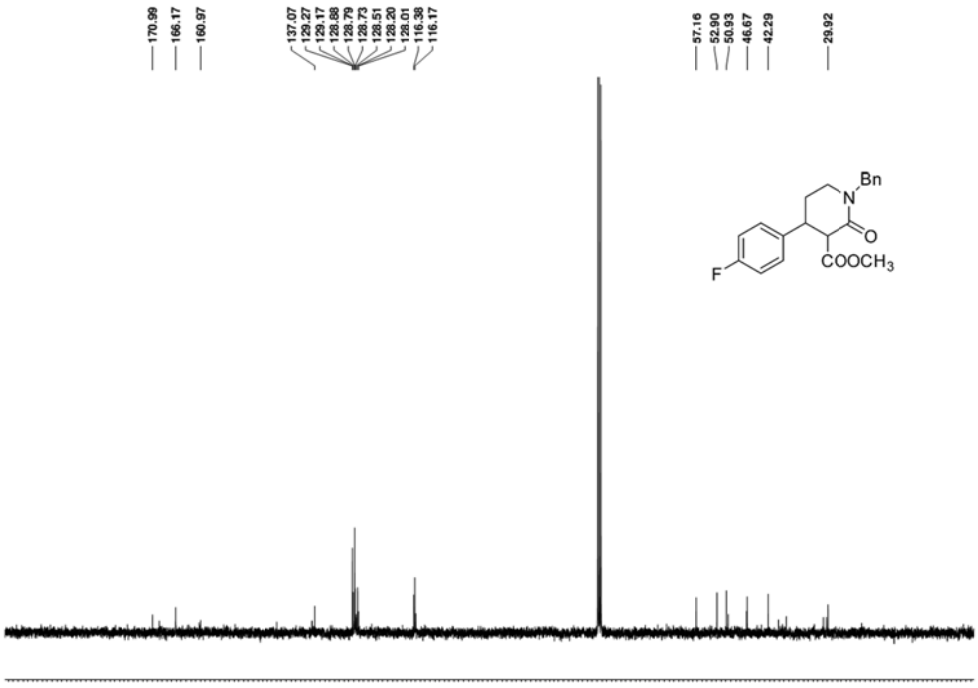
1-benzyl-4-(4-fluorophenyl)piperidin-2-one (9b)

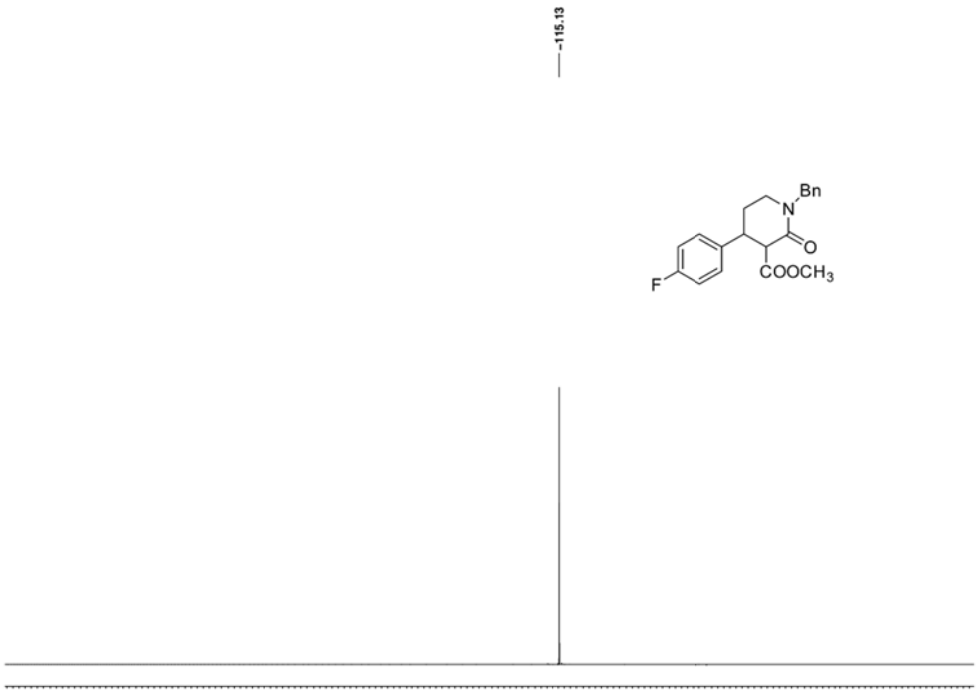


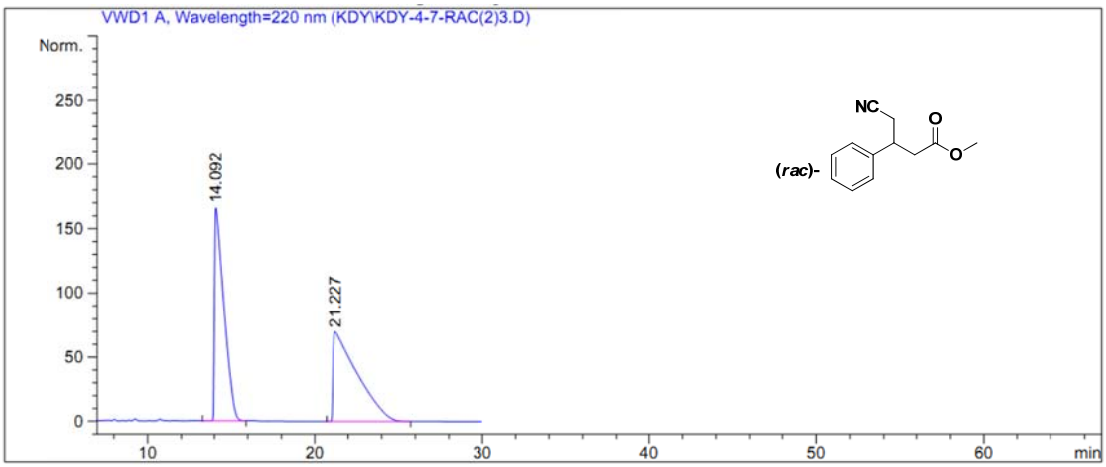


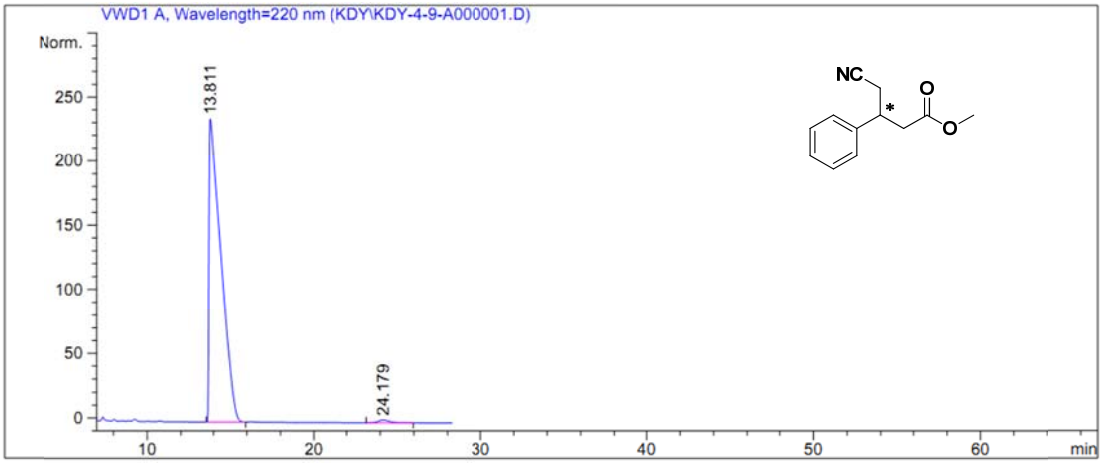
(*3R,4S*)-methyl 1-benzyl-4-(4-fluorophenyl)-2-oxopiperidine-3-carboxylate (10)



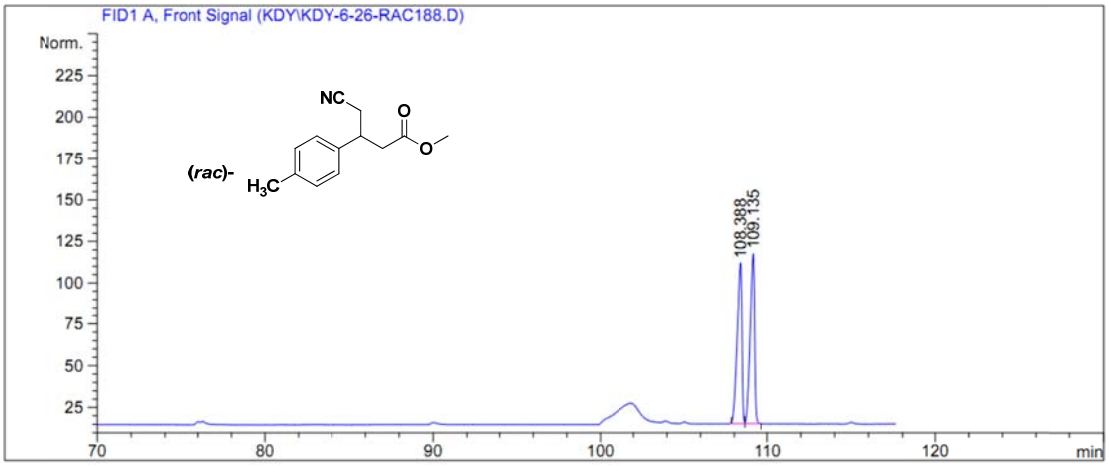

170.99
166.17
160.97
137.07
129.27
129.17
128.88
128.79
128.73
128.51
128.20
128.01
116.38
116.17
57.16
52.90
50.93
46.67
42.29
29.92
Bn
N
O
COOCH3
F

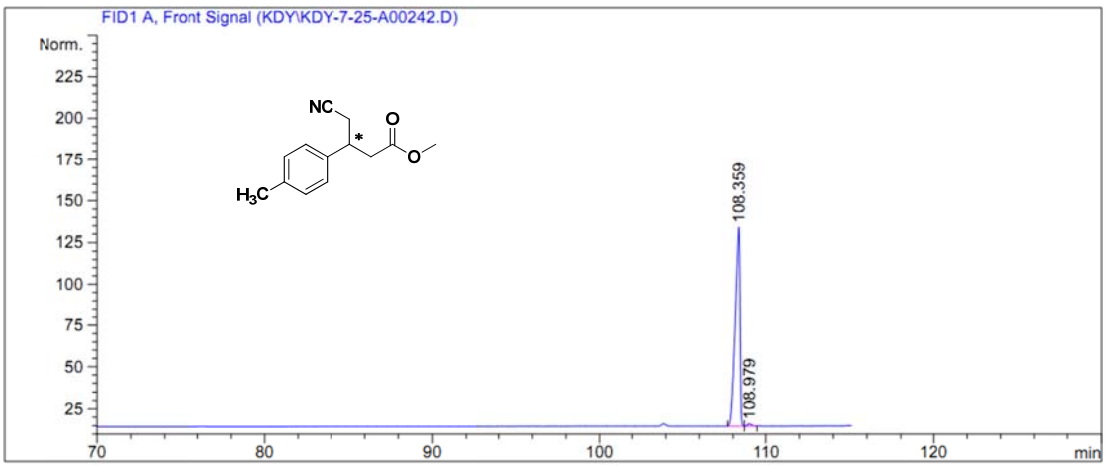

115.13
Bn
N
O
COOCH3
F



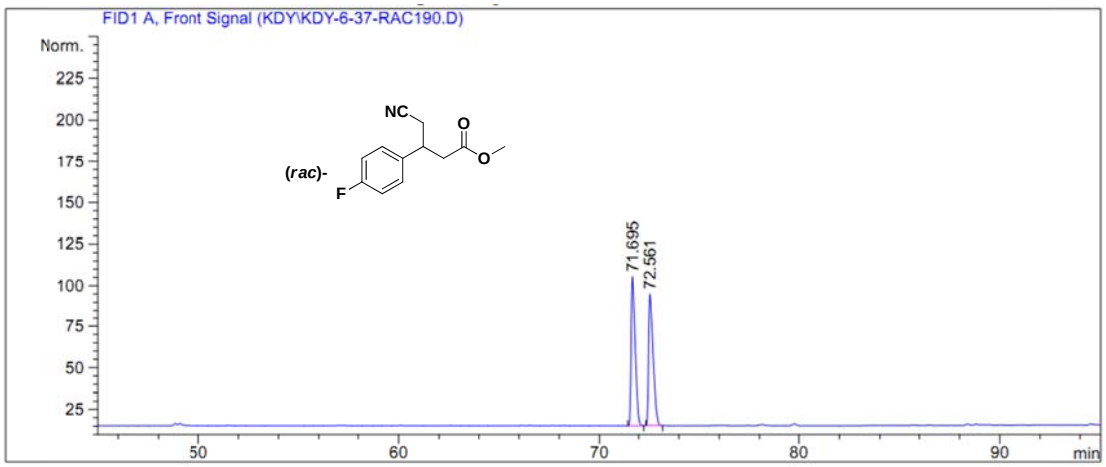


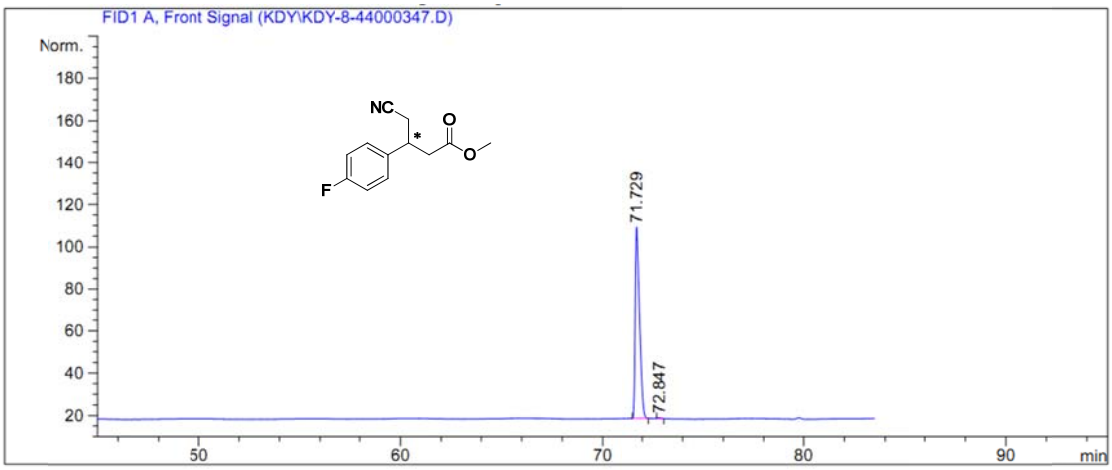
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.811	BB	0.6759	1.16026e4	235.85532	99.1349
2	24.179	BB	0.7020	101.25501	2.21223	0.8651
Totals :				1.17039e4	238.06754	



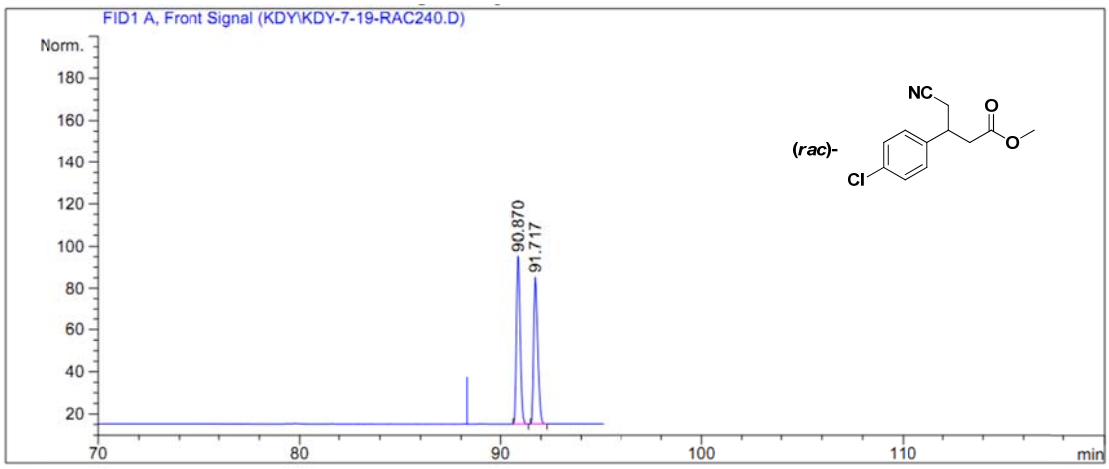


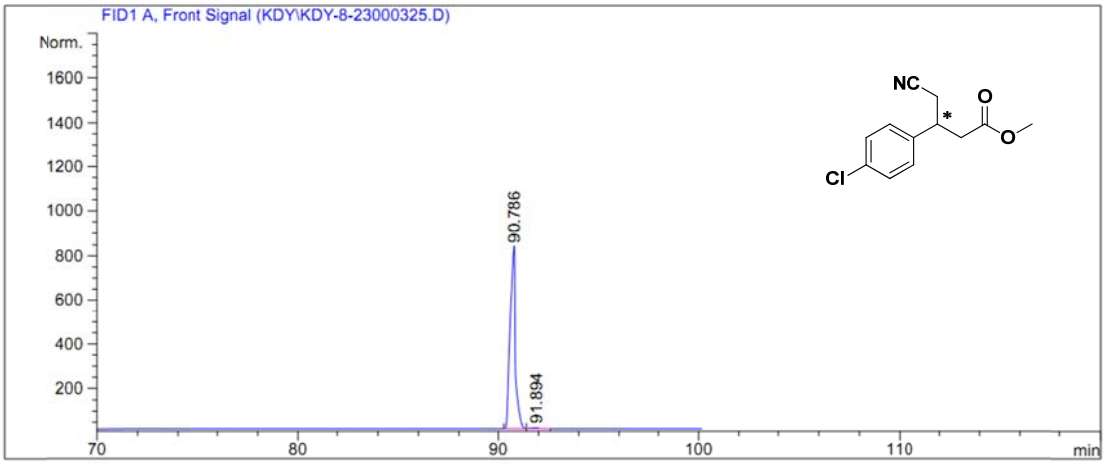
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	108.359	BV	0.2594	2359.98853	119.39586	99.00014
2	108.979	VB	0.2261	23.83479	1.27049	0.99986
Totals :				2383.82332	120.66635	



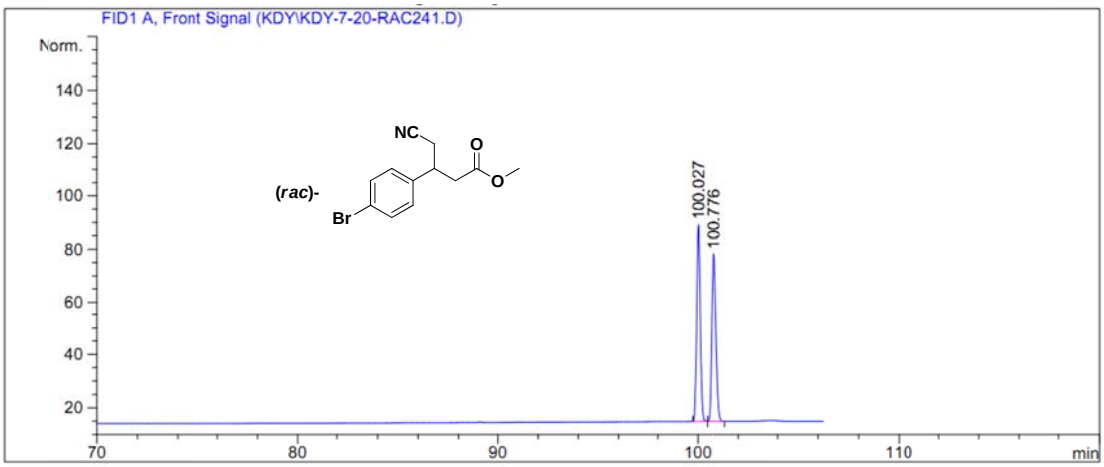


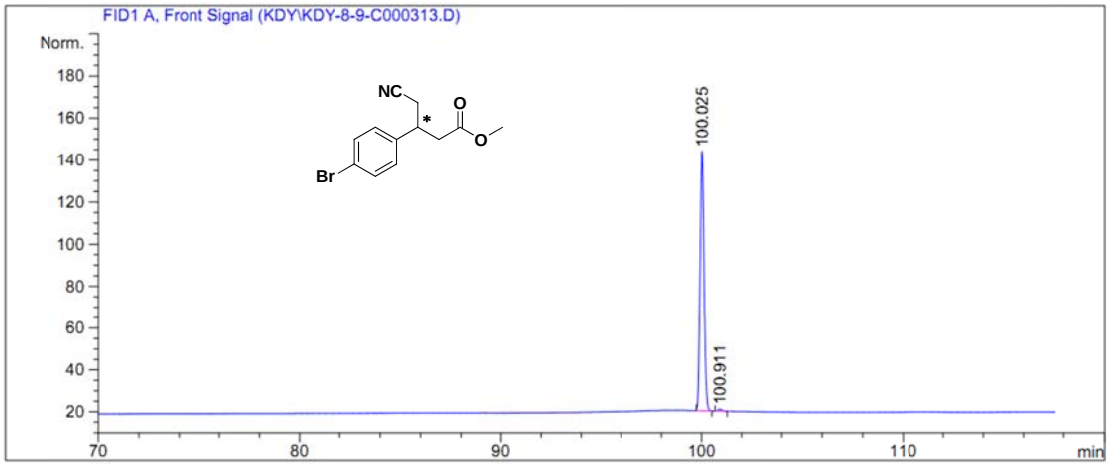
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	71.729	BB	0.1996	1330.31763	90.45253	99.71314
2	72.847	BB	0.1353	3.82719	3.46400e-1	0.28686
Totals :				1334.14482	90.79893	



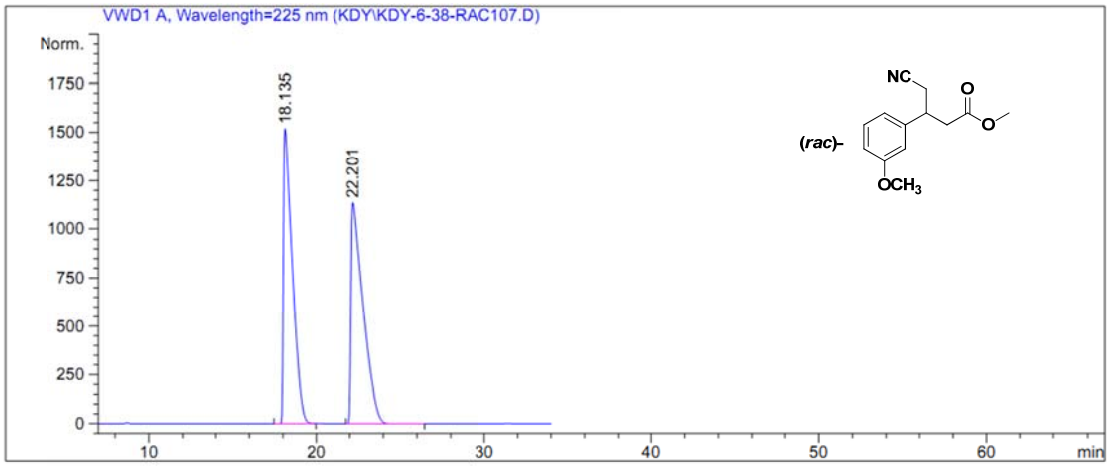


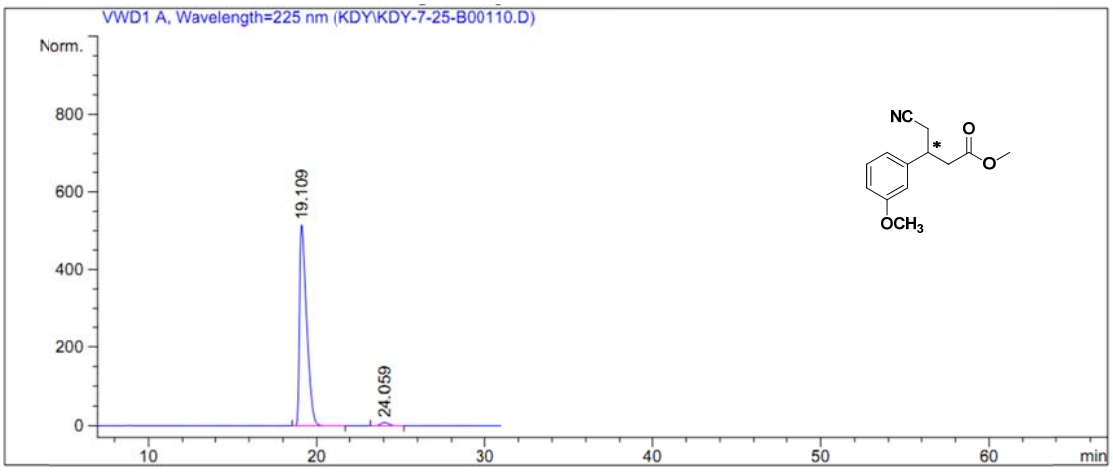
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	90.786	BV	0.2424	1.50921e4	818.21753	99.27309
2	91.894	VB	0.4016	110.50980	3.56575	0.72691
Totals :				1.52026e4	821.78328	



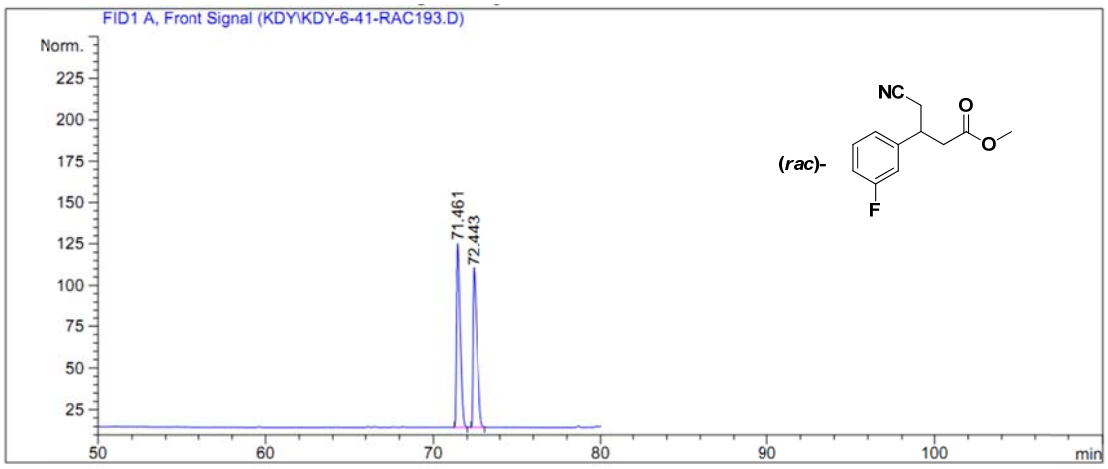


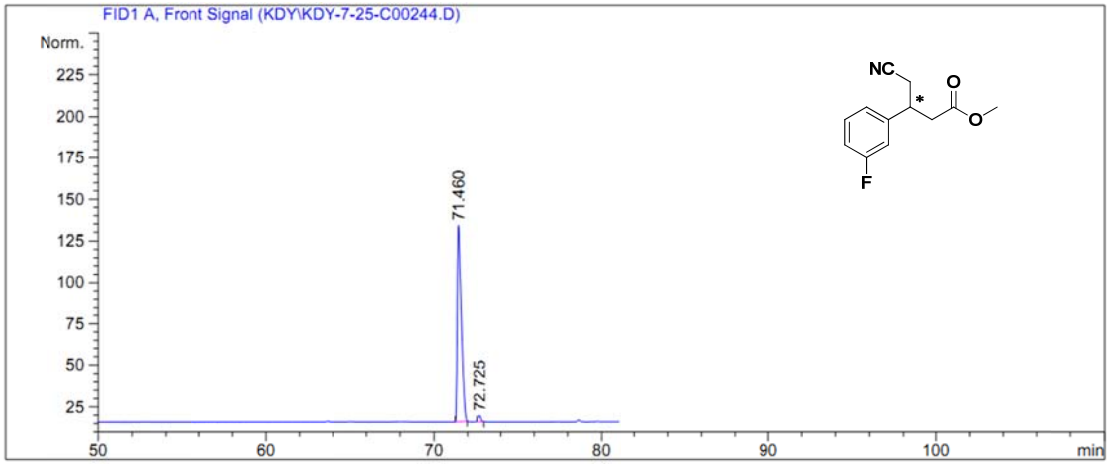
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	100.025	BB	0.2165	1715.52808	123.48541	99.29174
2	100.911	BB	0.2109	12.23703	9.12483e-1	0.70826
Totals :				1727.76510	124.39790	



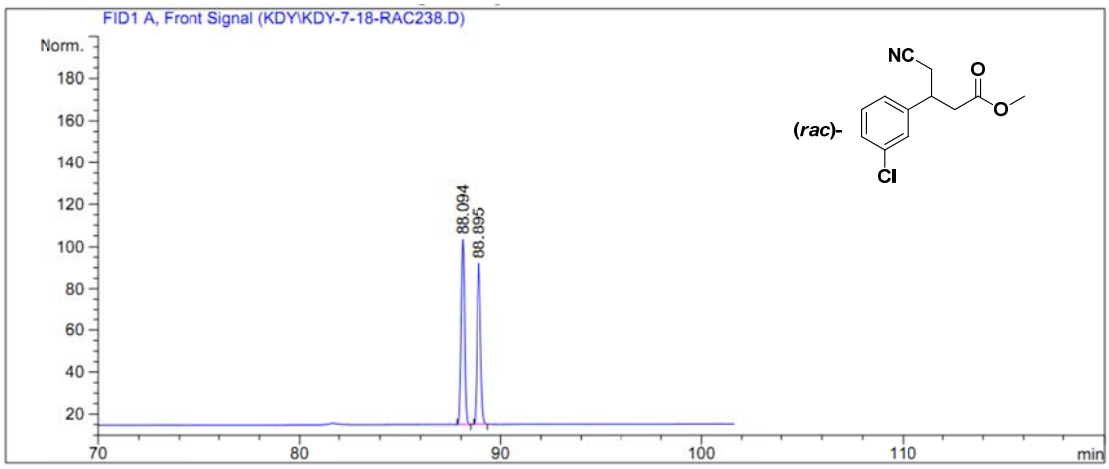


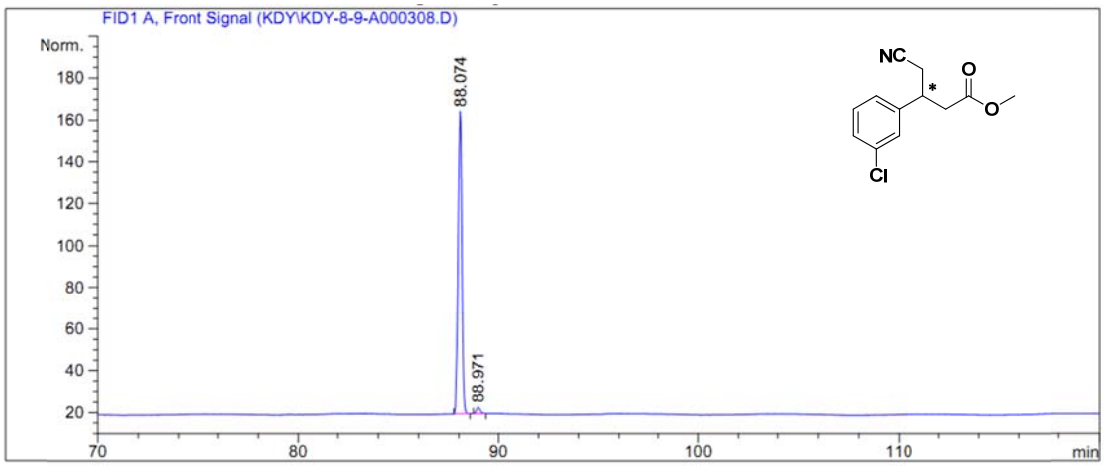
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.109	BB	0.4321	1.48467e4	515.29663	98.1755
2	24.059	BB	0.5030	275.90677	8.53712	1.8245
Totals :				1.51226e4	523.83375	



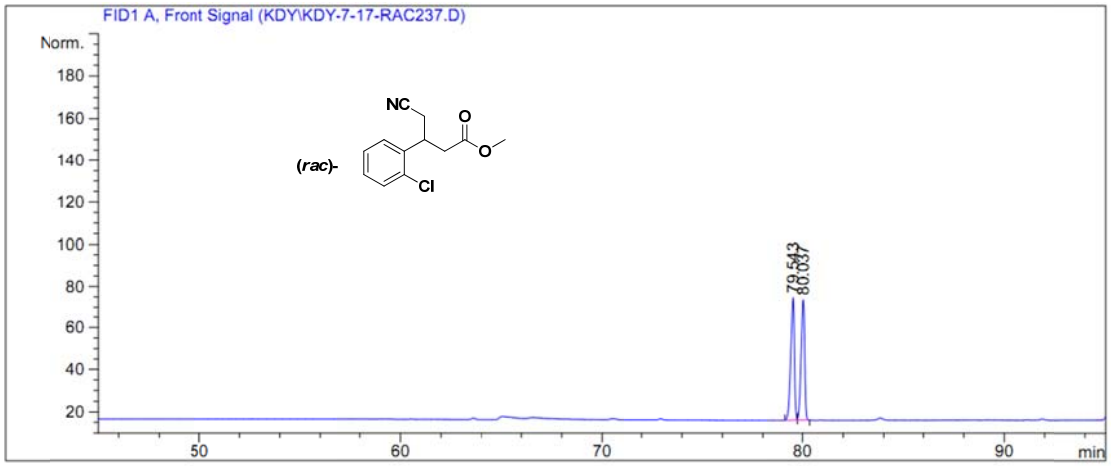


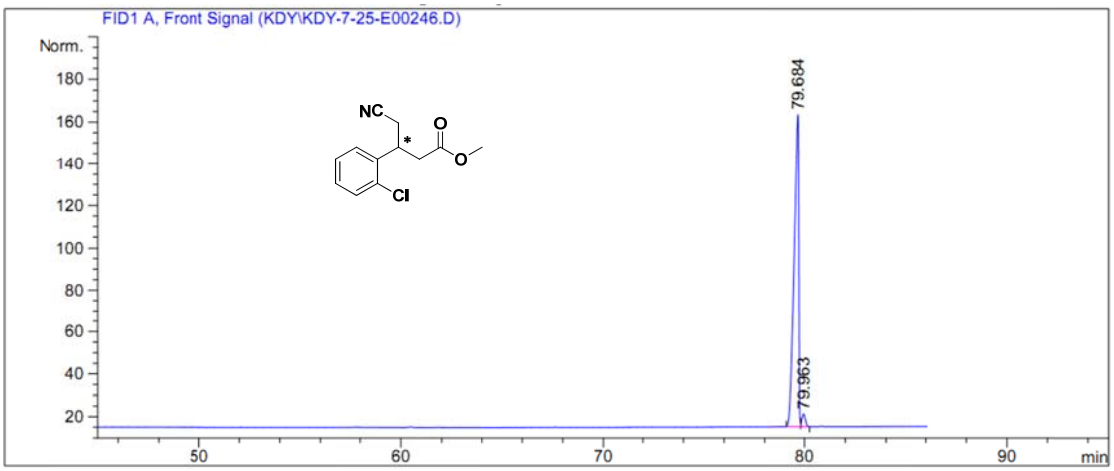
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	71.460	BB	0.2046	1967.55530	118.17234	97.85204
2	72.725	BB	0.1359	43.18992	3.75328	2.14796
Totals :				2010.74522	121.92562	



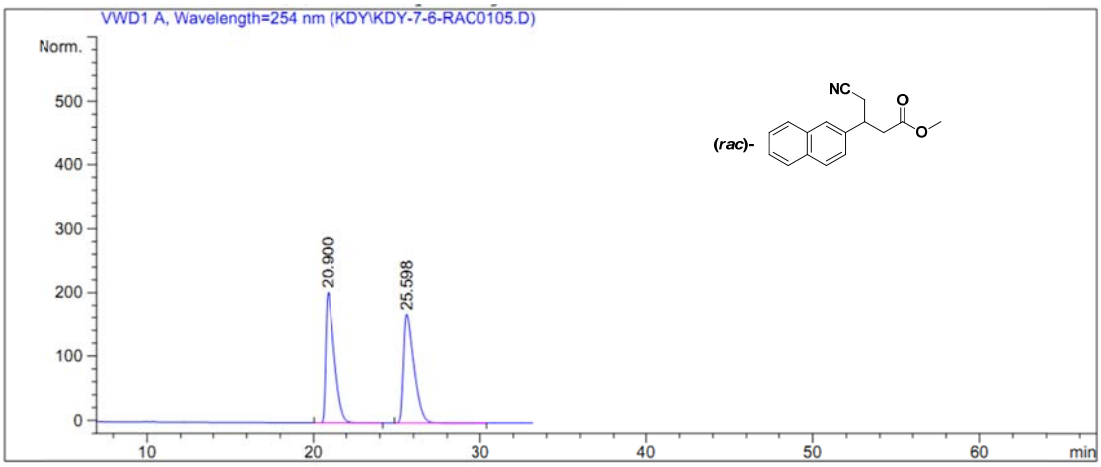


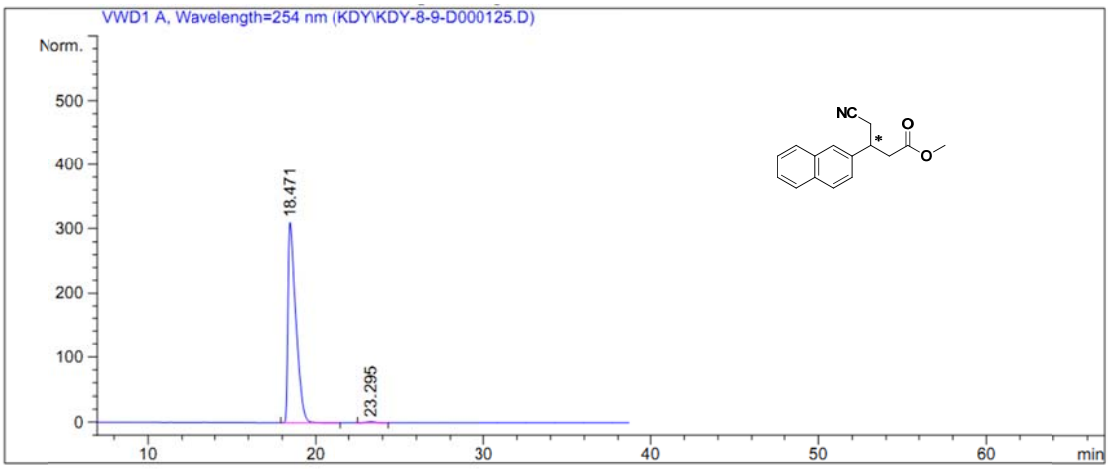
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	88.074	BB	0.2002	1888.25818	144.77686	97.80037
2	88.971	BB	0.2113	42.46884	3.09498	2.19963
Totals :				1930.72702	147.87184	



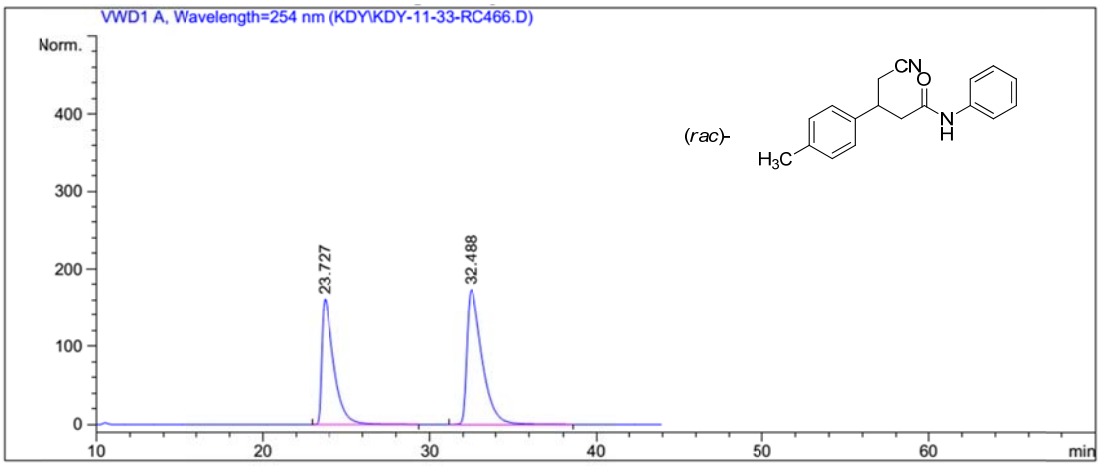


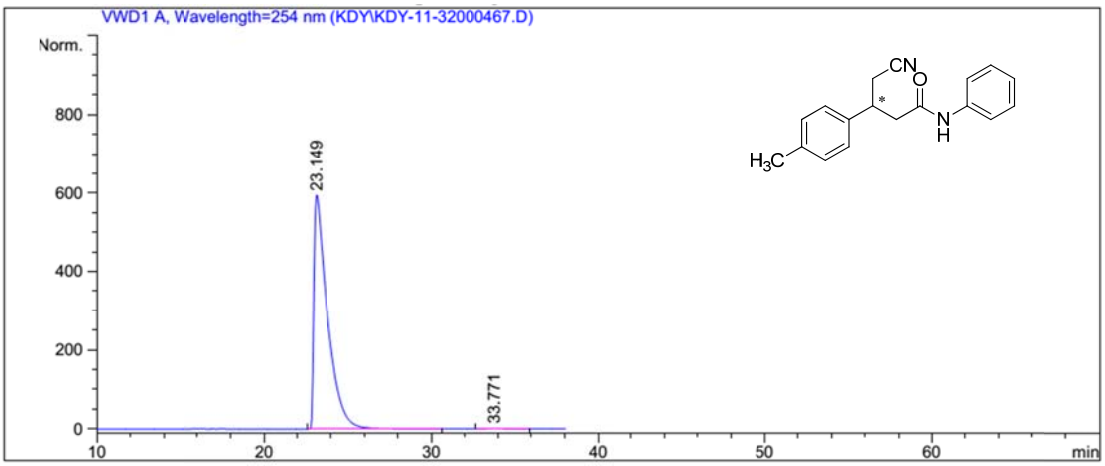
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	79.684	BV	0.2080	2306.87427	148.18503	97.07385
2	79.963	VB	0.1465	69.53731	6.02962	2.92615
Totals :				2376.41158	154.21465	



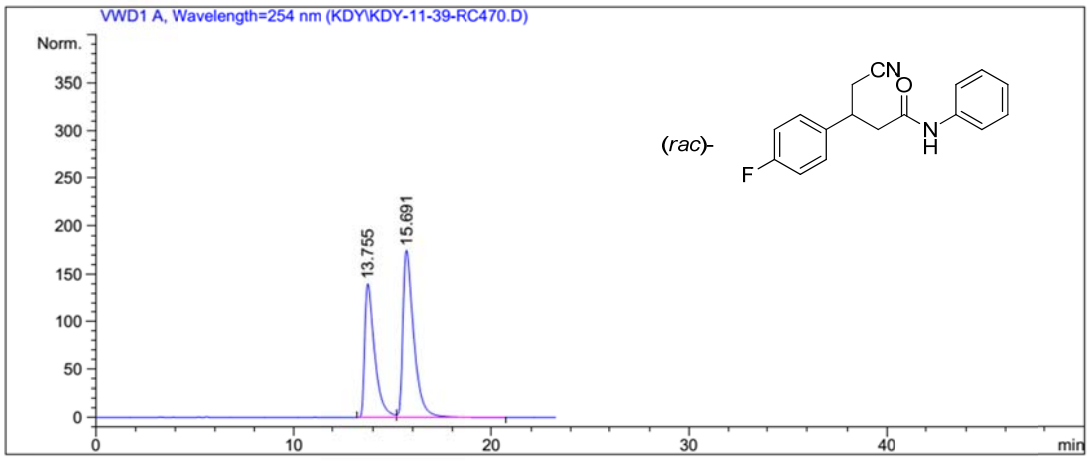


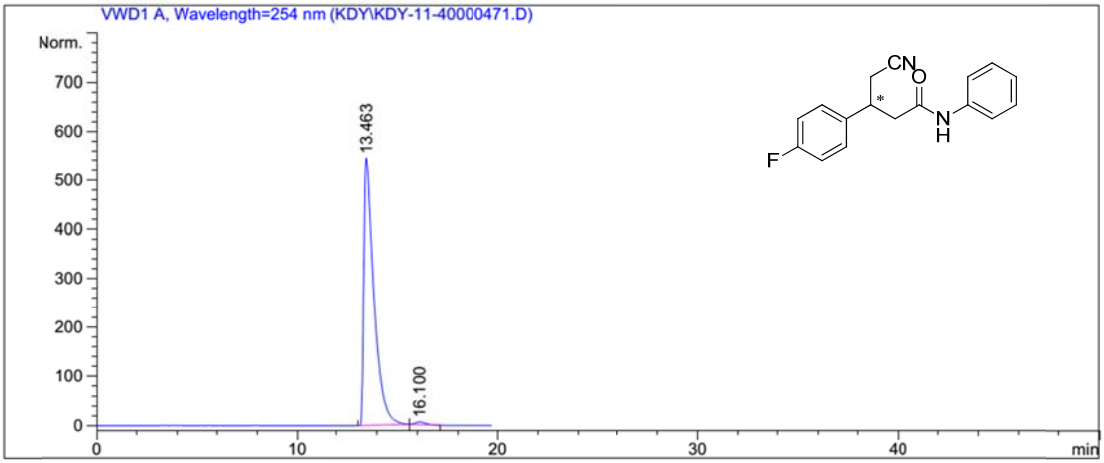
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.471	BB	0.4778	1.00349e4	309.85907	99.5136
2	23.295	BB	0.5281	49.04557	1.40219	0.4864
Totals :				1.00840e4	311.26126	



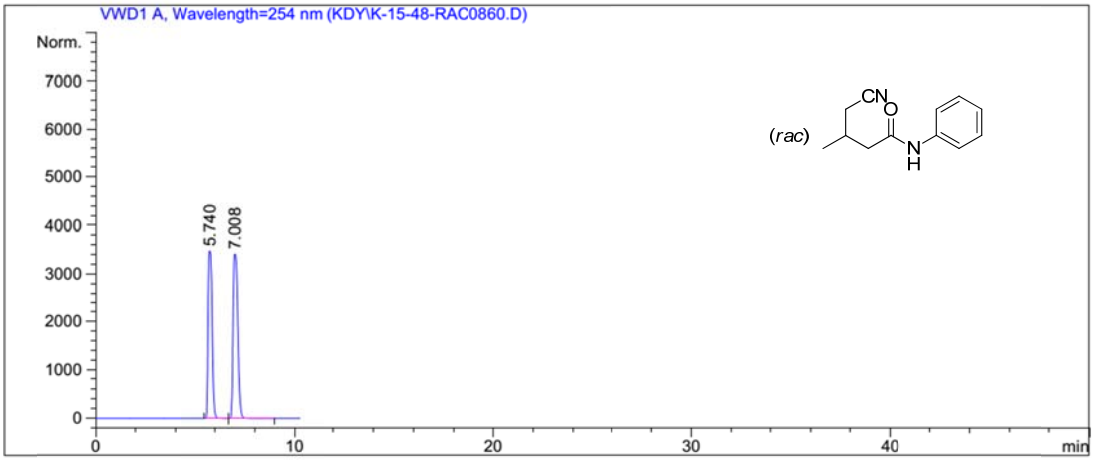


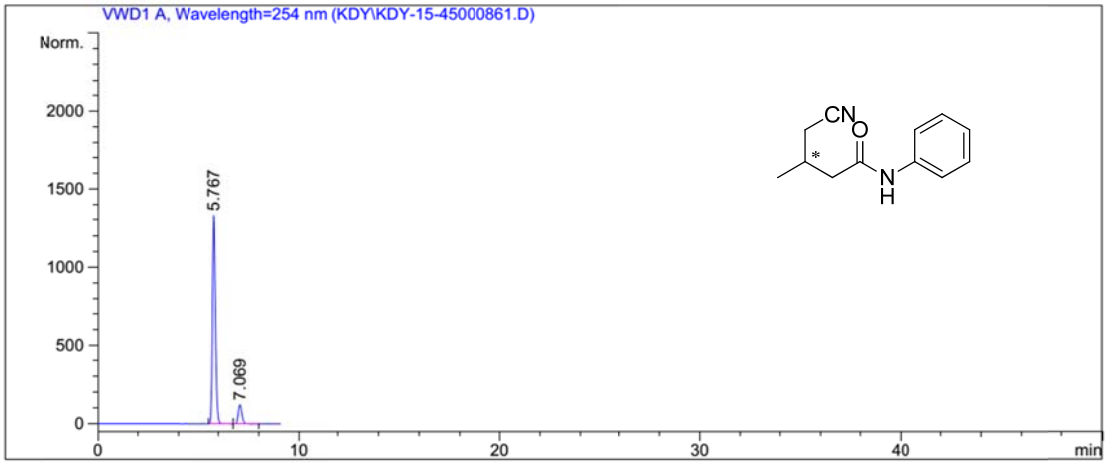
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.149	BB	0.8047	3.41266e4	594.53009	99.8275
2	33.771	BB	0.7783	58.98265	8.94443e-1	0.1725
Totals :				3.41856e4	595.42453	



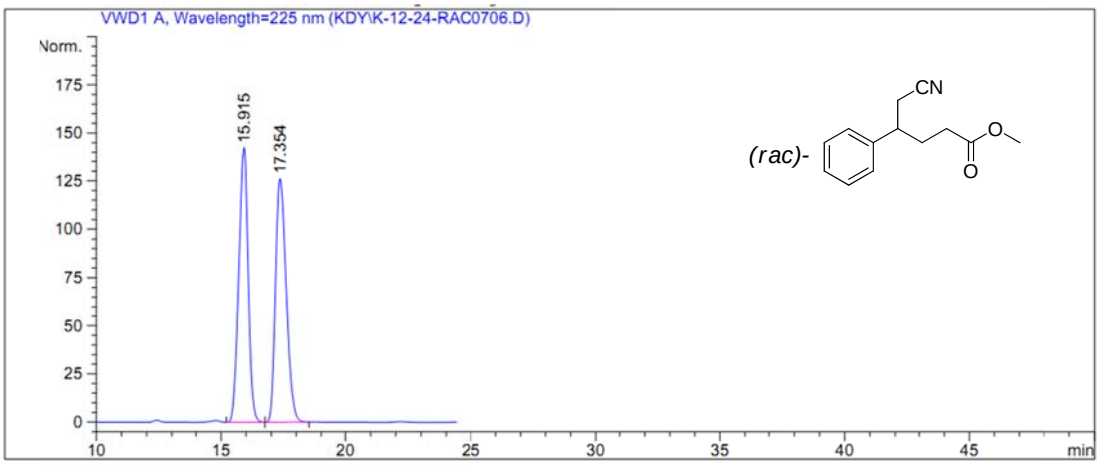


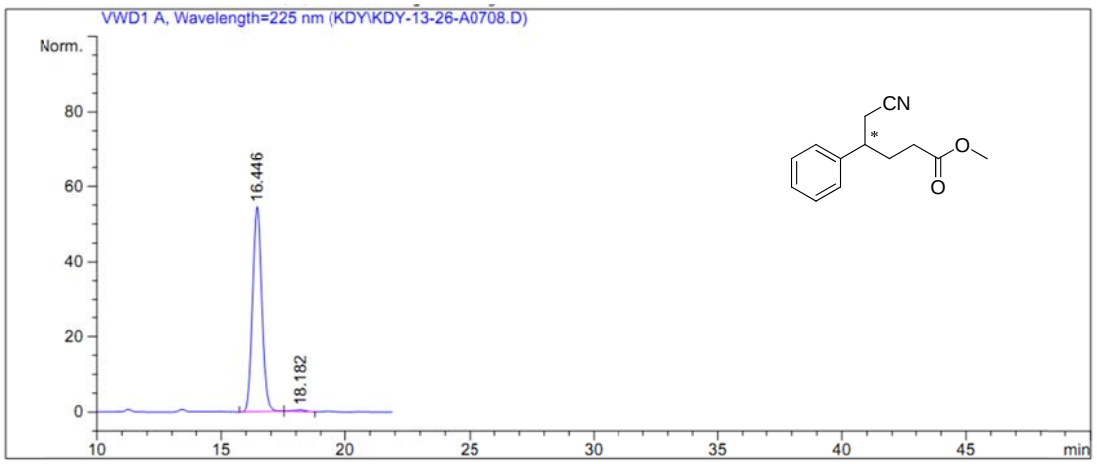
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.463	BB	0.5006	1.88723e4	544.17126	99.0256
2	16.100	BBA	0.5559	185.69261	5.20840	0.9744
Totals :				1.90579e4	549.37966	



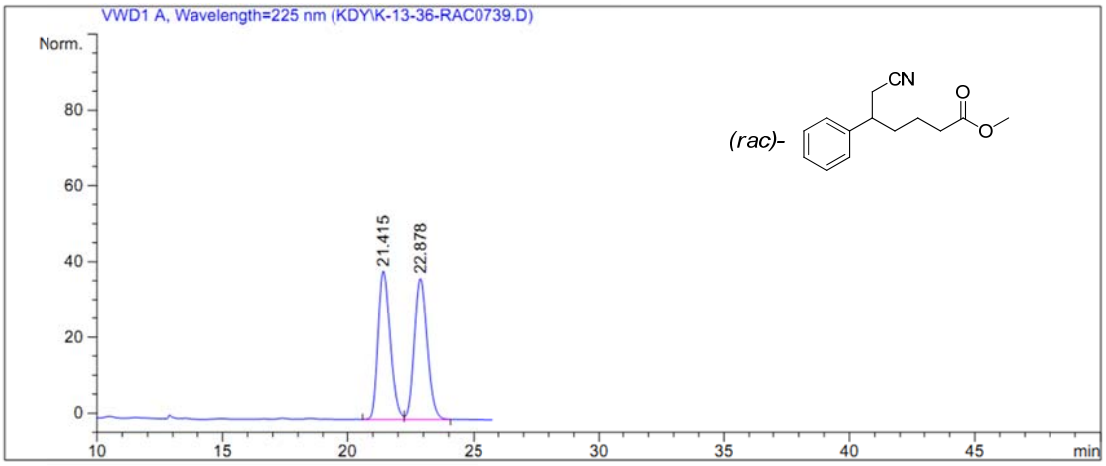


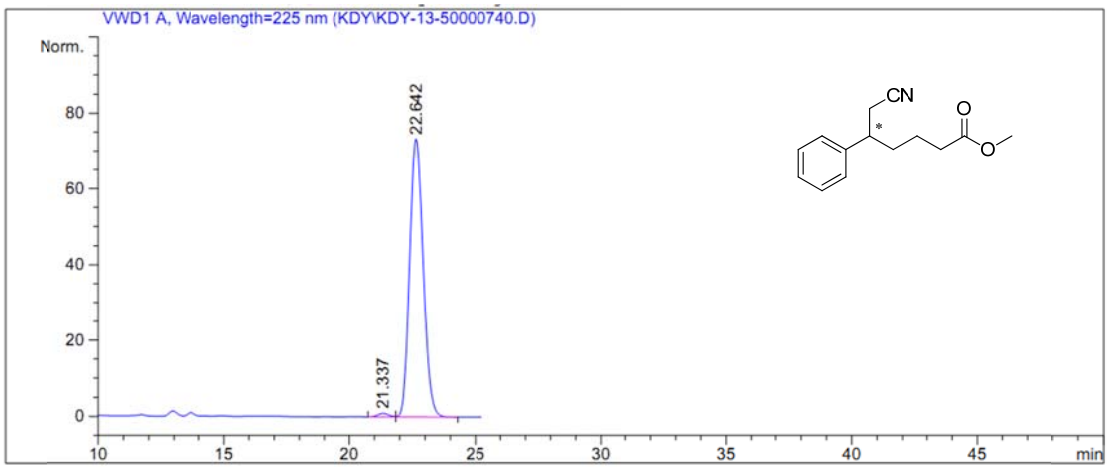
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.767	BB	0.1589	1.36614e4	1329.63123	89.8571
2	7.069	BBA	0.1962	1542.06885	121.36263	10.1429
Totals :				1.52034e4	1450.99385	



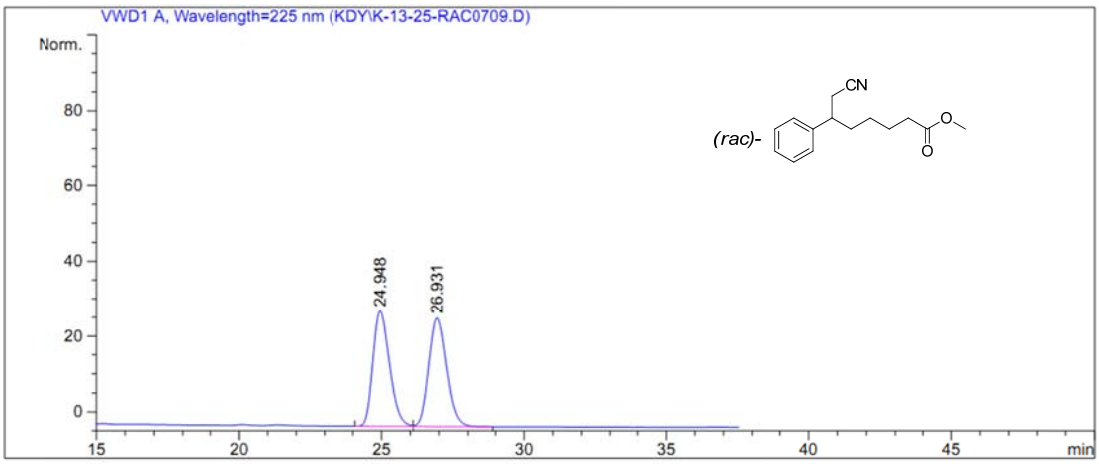


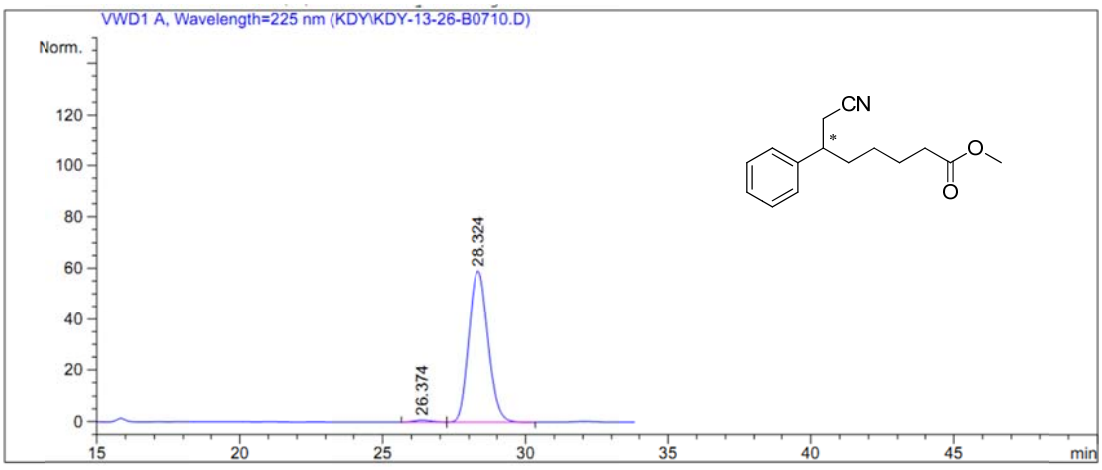
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.446	BB	0.3978	1398.73303	54.43036	99.1479
2	18.182	BB	0.4033	12.02149	3.64032e-1	0.8521
Totals :				1410.75453	54.79439	



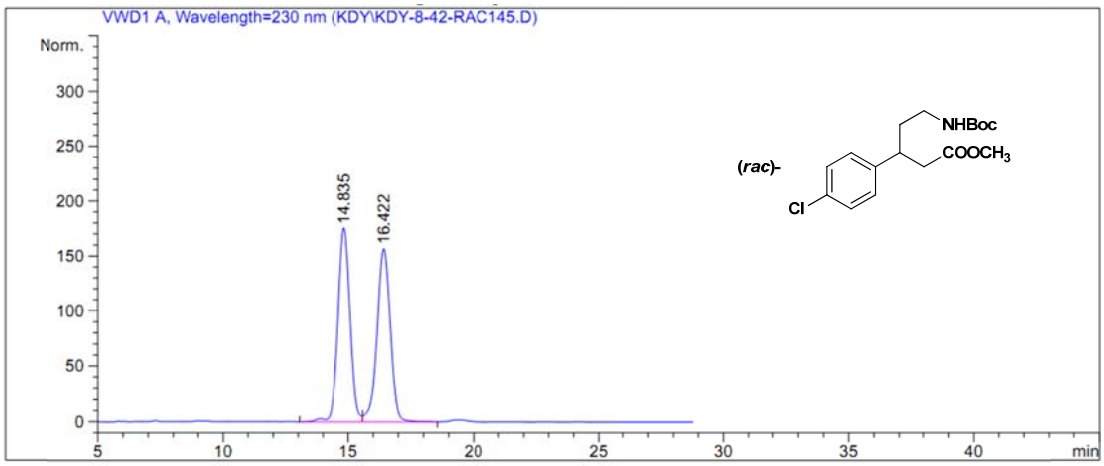


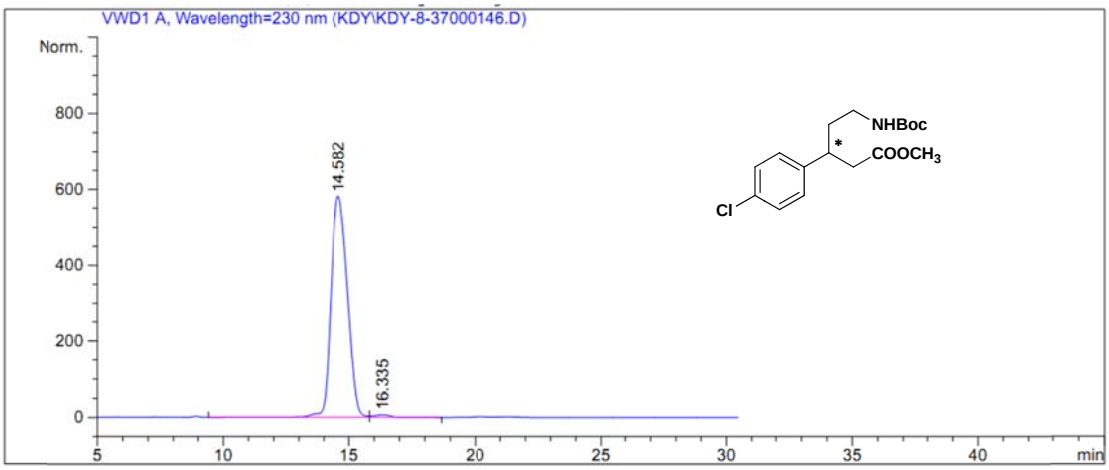
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.337	BV	0.4412	27.06177	8.91470e-1	0.9823
2	22.642	VB	0.5828	2727.88135	73.36728	99.0177
Totals :				2754.94312	74.25875	



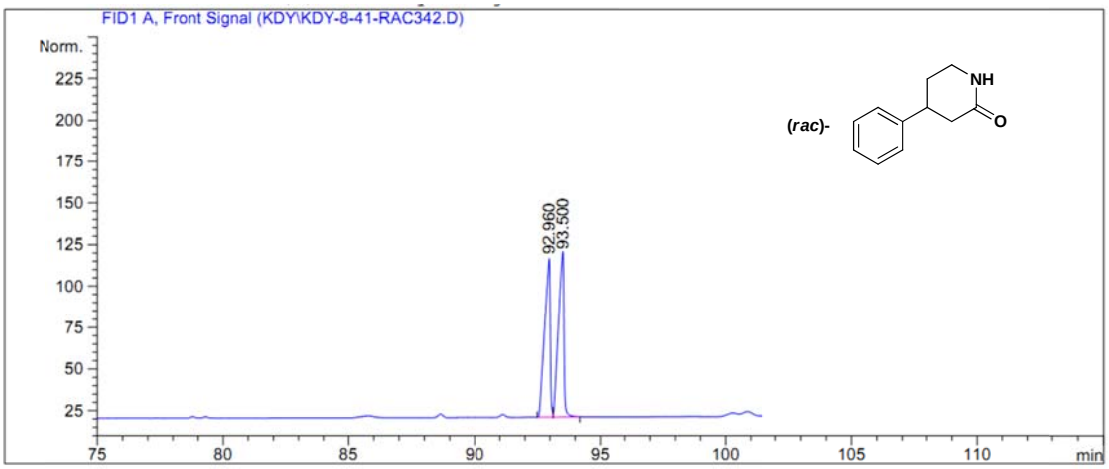


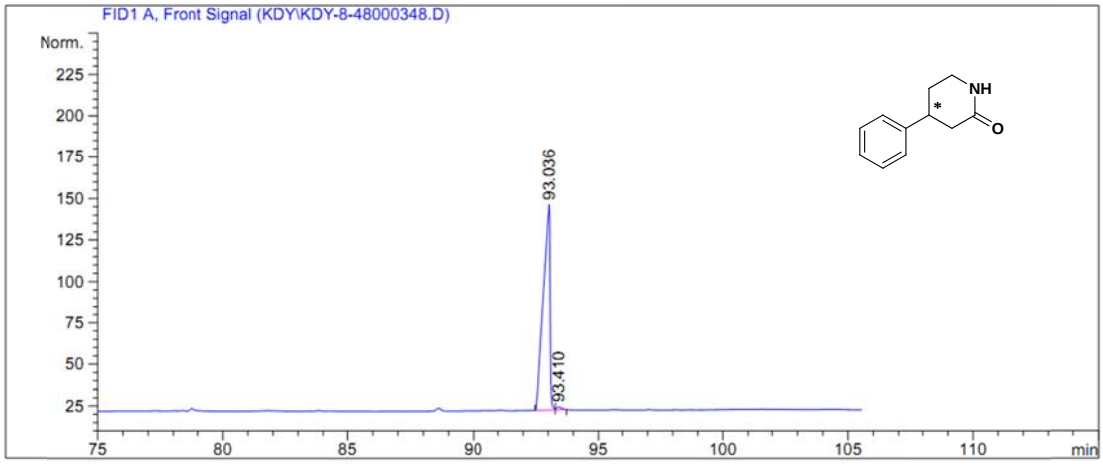
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.374	BB	0.4854	27.09231	7.16018e-1	0.9654
2	28.324	BB	0.7370	2779.30127	59.06083	99.0346
Totals :				2806.39358	59.77685	



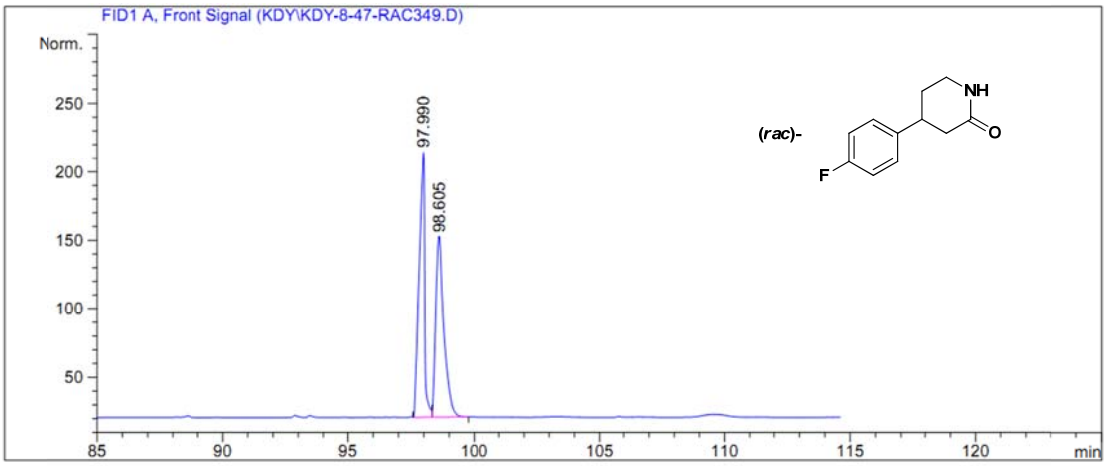


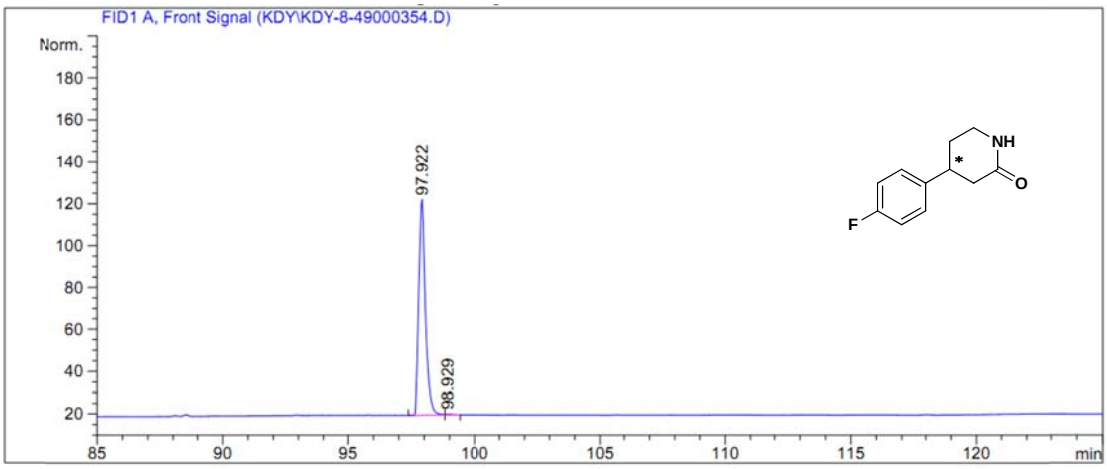
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.582	BV	0.7419	2.65455e4	580.07733	98.9062
2	16.335	VB	0.6744	293.57623	6.65788	1.0938
Totals :				2.68391e4	586.73521	



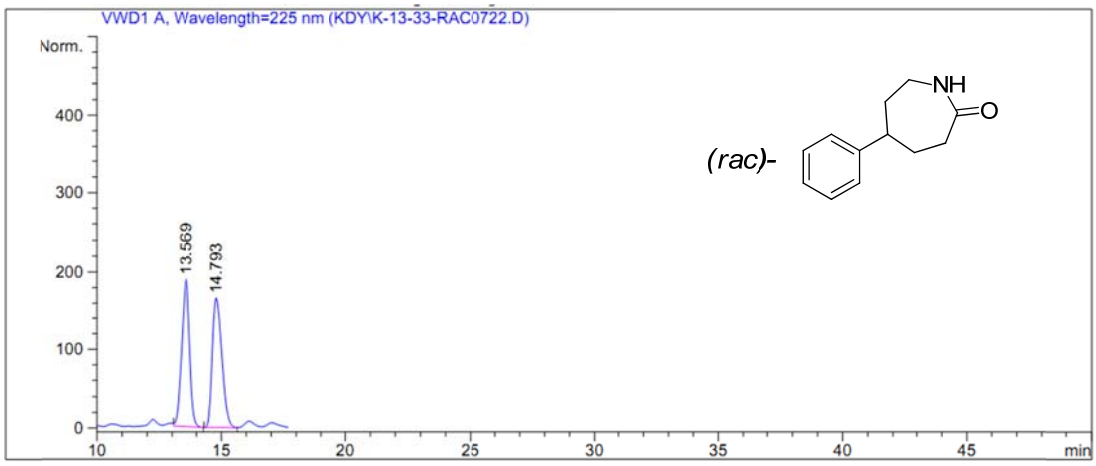


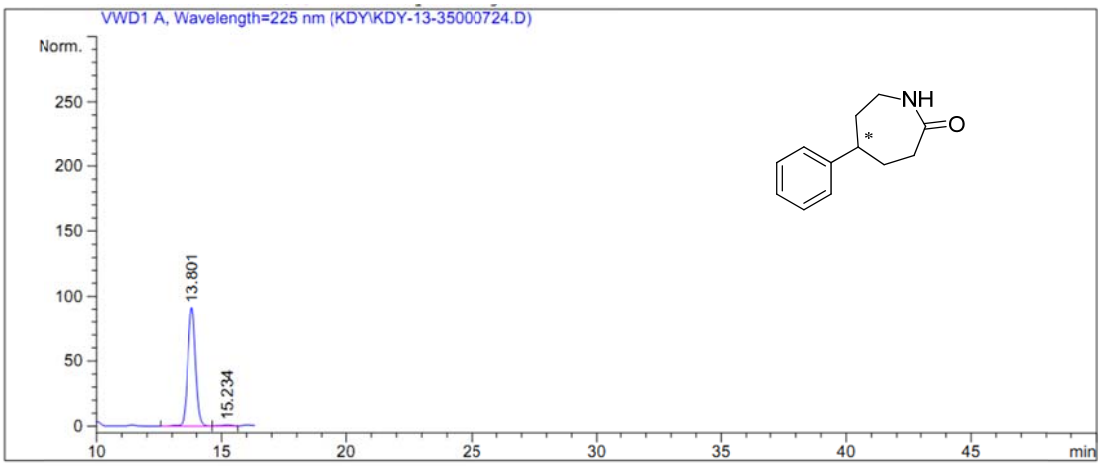
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	93.036	BV	0.2338	2322.68091	123.71865	98.94299
2	93.410	VB	0.1763	24.81335	1.66098	1.05701
Totals :				2347.49426	125.37963	



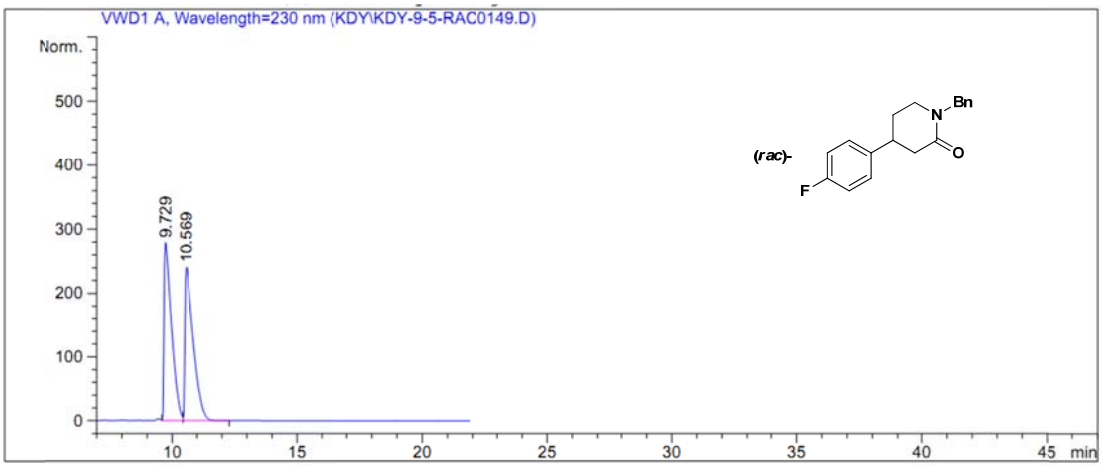


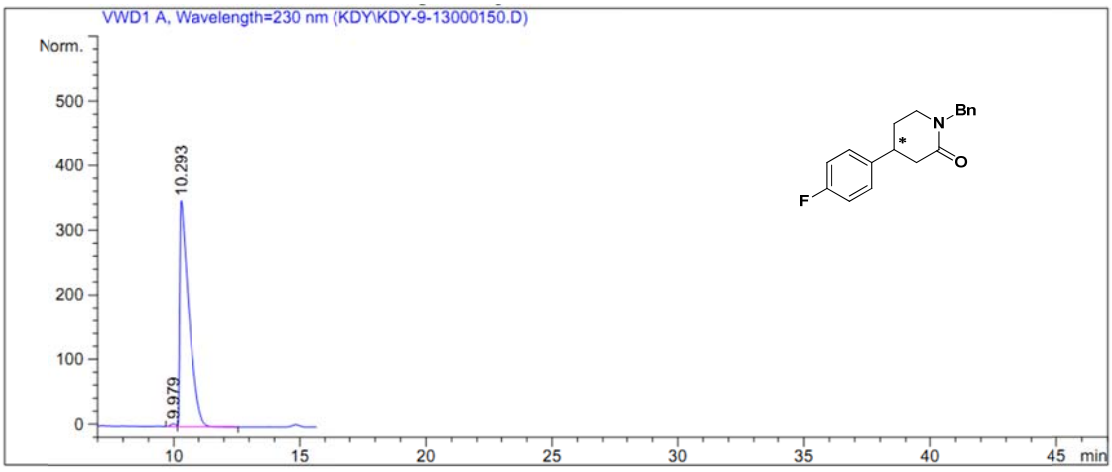
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	97.922	BB	0.2254	1887.79272	102.45014	99.74262
2	98.929	BB	0.2141	4.87142	2.68521e-1	0.25738
Totals :				1892.66415	102.71866	



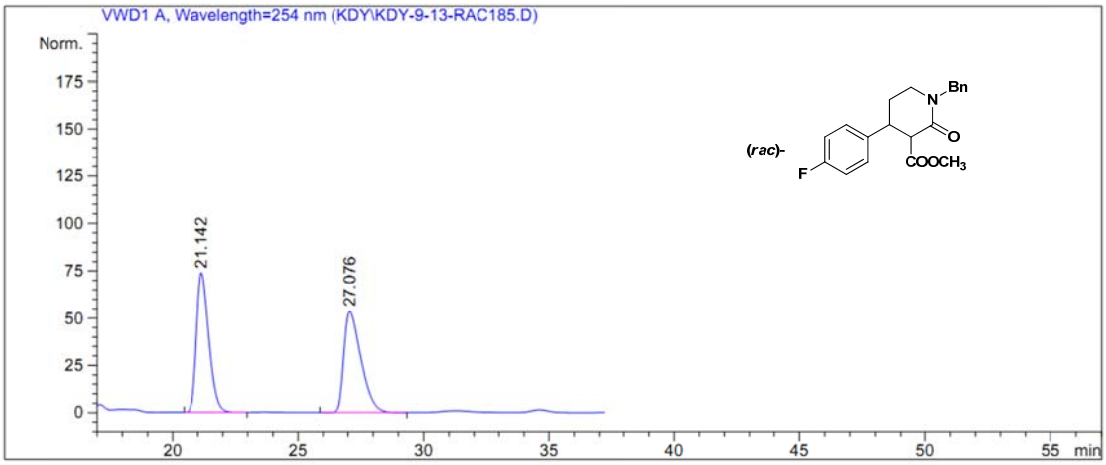


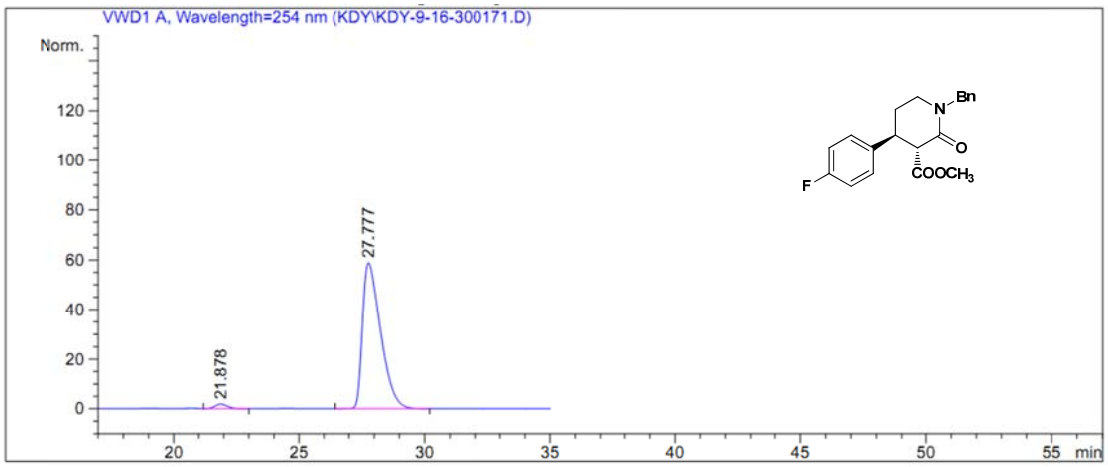
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.801	BB	0.3452	2034.67407	91.23942	99.0083
2	15.234	BB	0.3748	20.37996	7.82746e-1	0.9917
Totals :				2055.05403	92.02216	





Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.979	VV	0.2333	61.58818	4.26880	0.6926
2	10.293	VB	0.3551	8830.53516	349.16031	99.3074
Totals :				8892.12333	353.42911	





Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.878	BB	0.5145	63.44689	1.83883	2.1198
2	27.777	BB	0.7617	2929.61255	58.75462	97.8802
Totals :				2993.05944	60.59345	