

Synthesis of 2-arylindole derivatives and evaluation as nitric oxide synthase and NFκB inhibitors

Xufen Yu, Eun-Jung Park, Tamara P. Kondratyuk, John M. Pezzuto, and Dianqing Sun*

Department of Pharmaceutical Sciences, College of Pharmacy, University of Hawai'i at Hilo, Hilo, HI 96720, USA

dianqing@hawaii.edu.

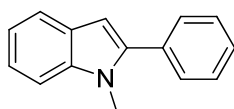
Supporting Information

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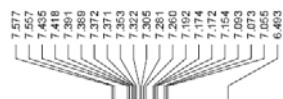
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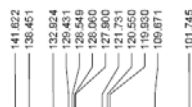
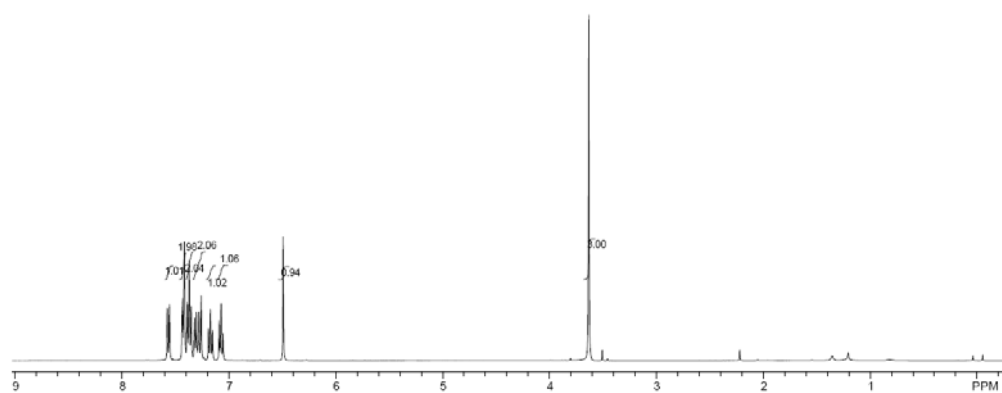
^1H NMR, ^{13}C NMR and HPLC spectra of compound 2a



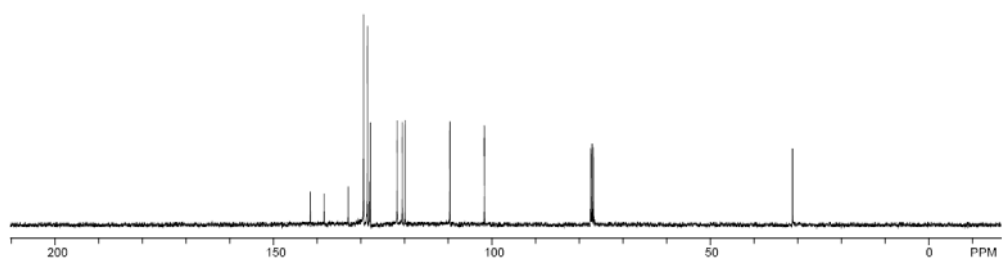
2a



YXF-1-1-I-P



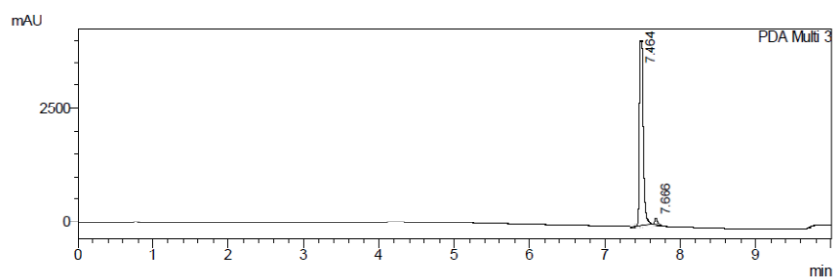
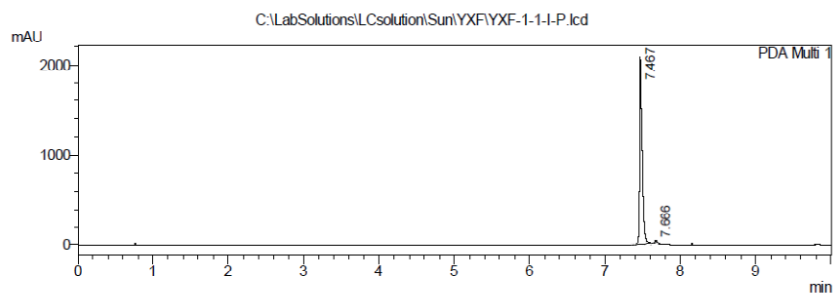
YXF-1-1-P-C13



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PeakTable

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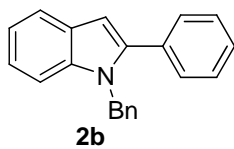
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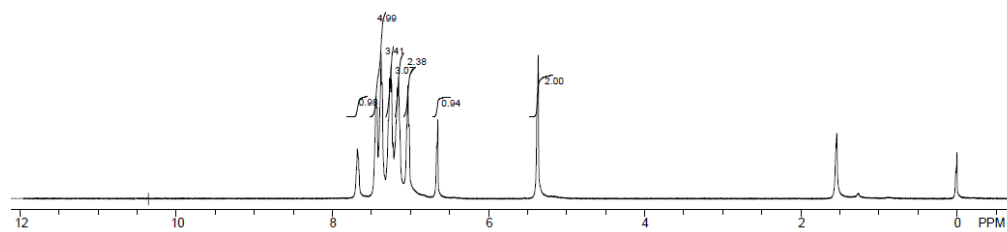
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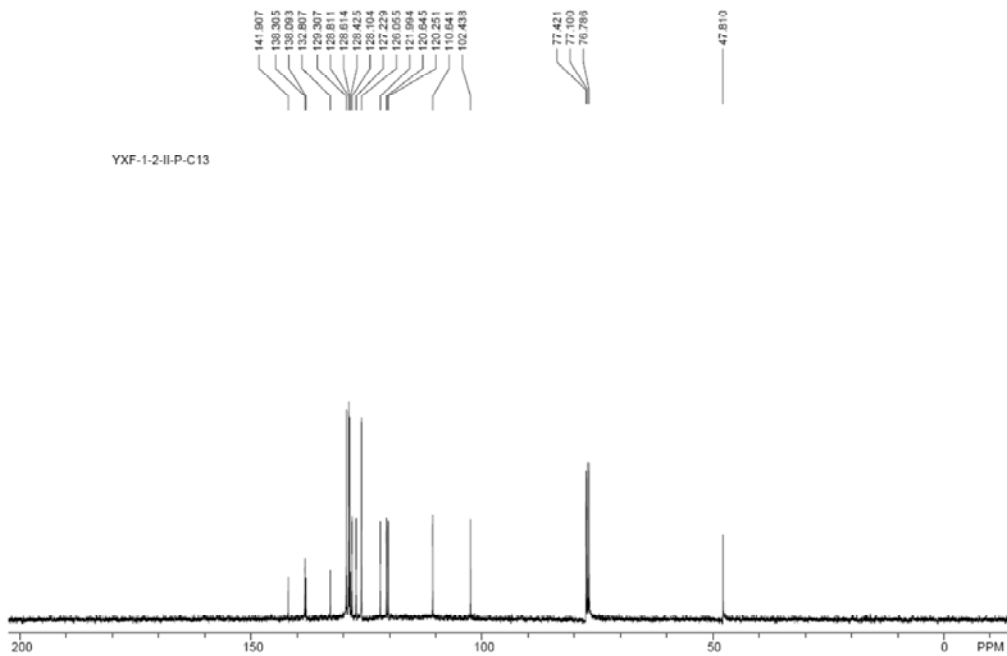
¹H NMR, ¹³C NMR and HPLC spectra of compound 2b



YXF-1-2-II-P(2b)



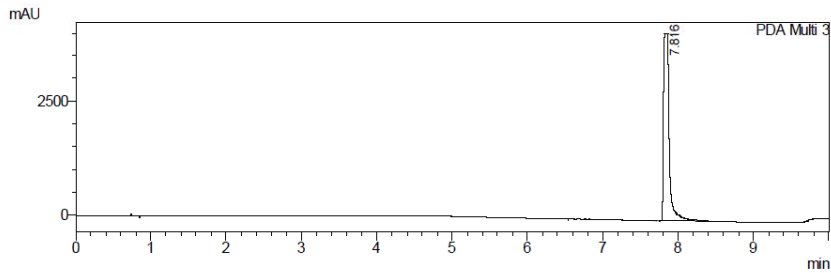
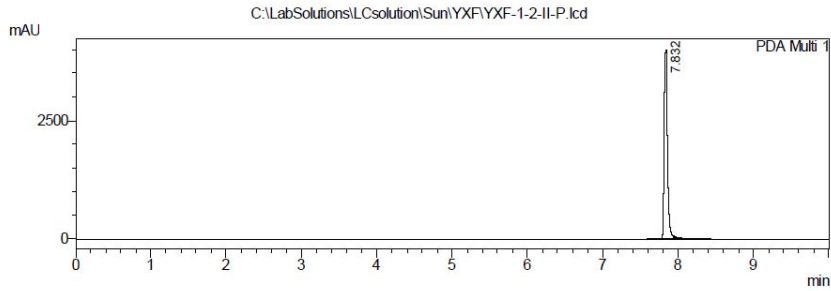
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PeakTable

PDA Ch1 254nm 4nm

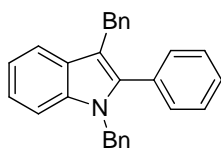
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PeakTable

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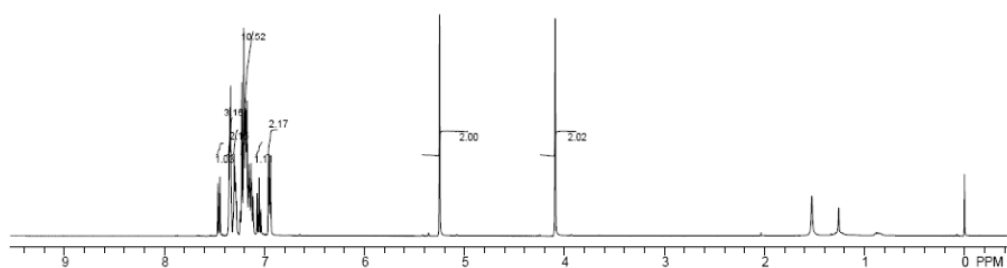
¹H NMR, ¹³C NMR and HPLC spectra of compound 2b'



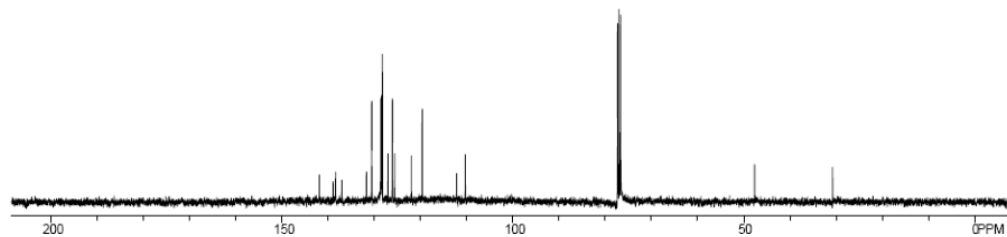
2b'



YXF-1-2-II-P1



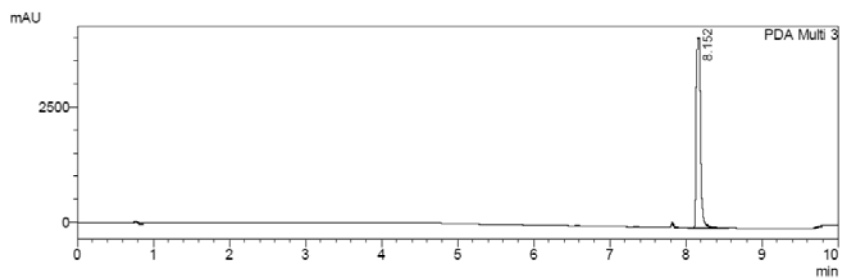
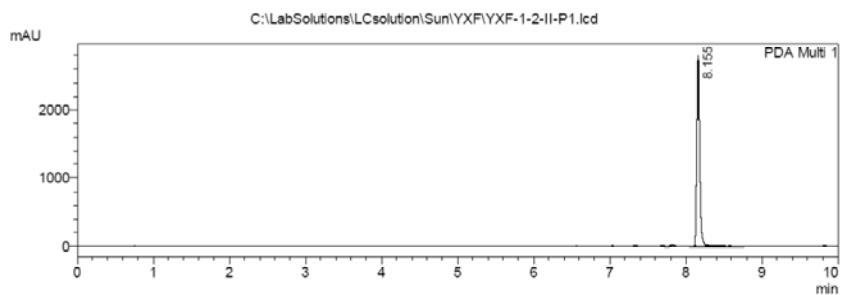
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PeakTable

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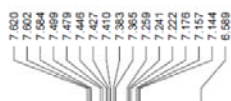
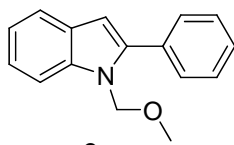
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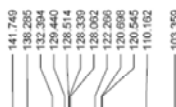
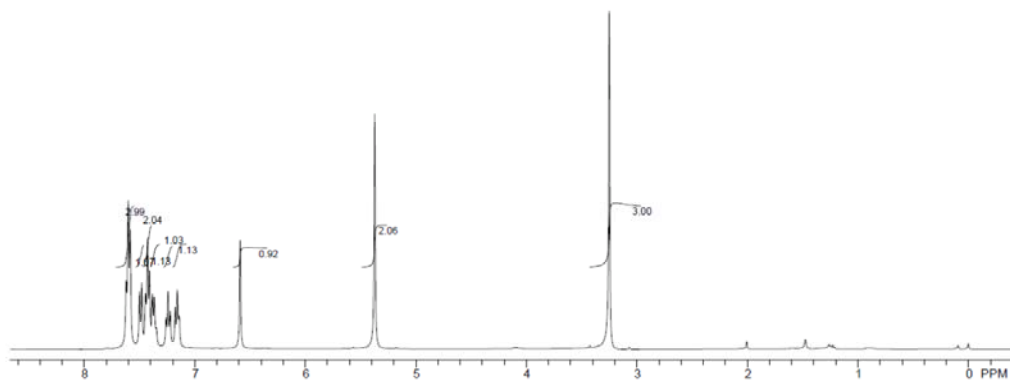
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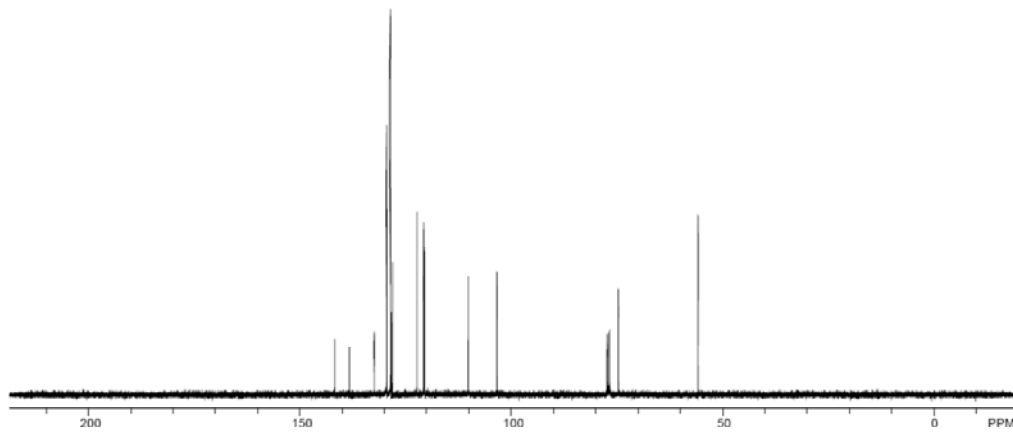
^1H NMR, ^{13}C NMR and HPLC spectra of compound 2c



YXF-1-6-P



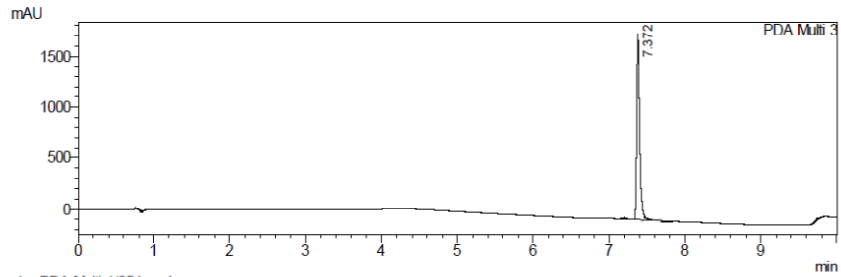
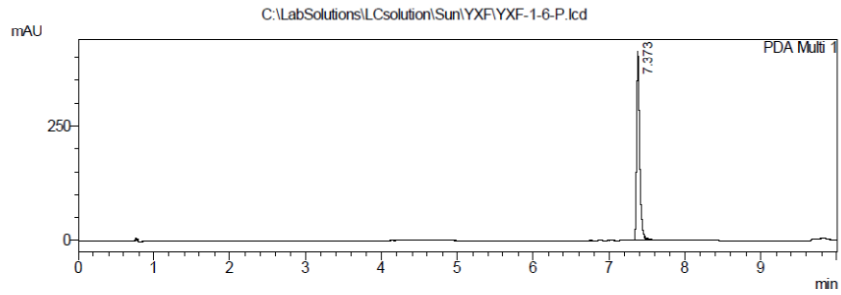
YXF-1-6-P-C13



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PeakTable

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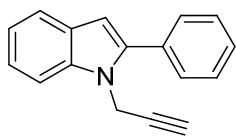
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PeakTable

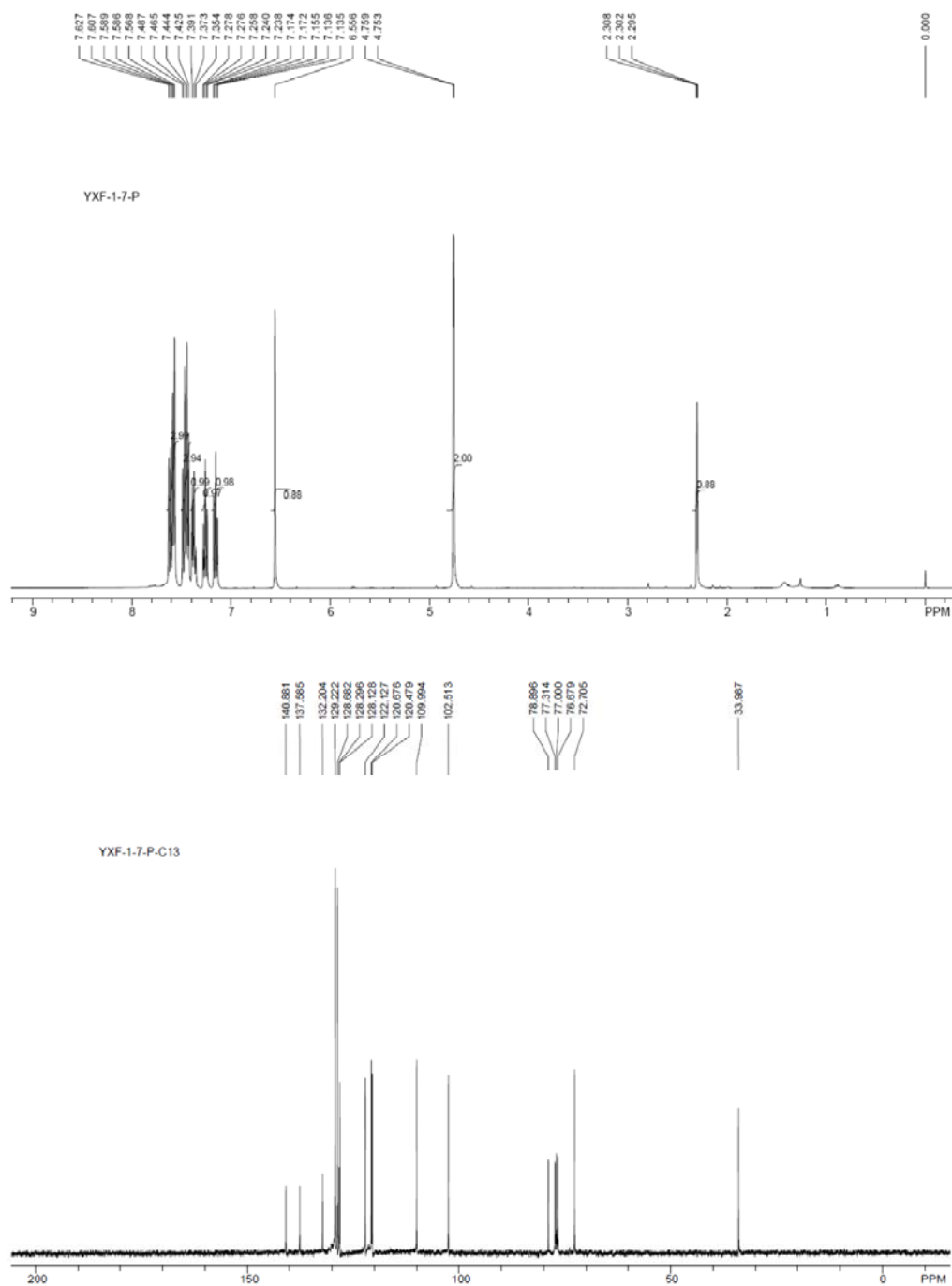
PDA Ch3 220nm 4nm

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¹H NMR, ¹³C NMR and HPLC spectra of compound 2d



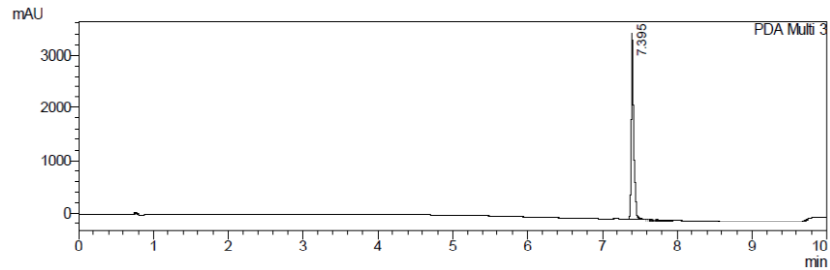
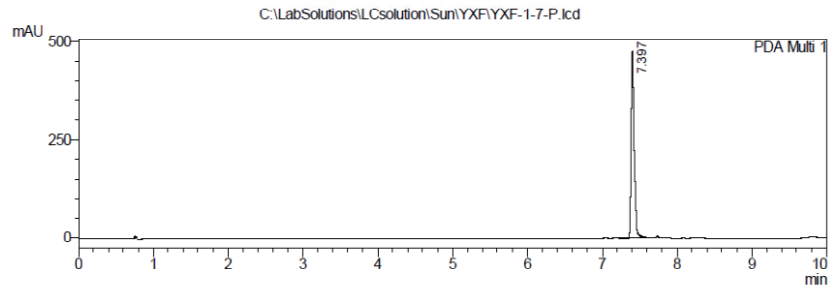
2d



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PeakTable

PDA Ch1 254nm 4nm

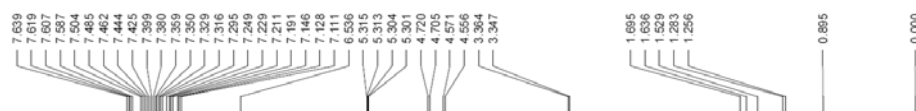
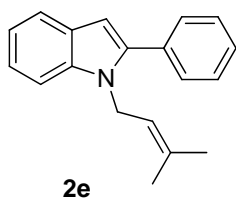
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PeakTable

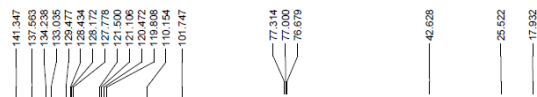
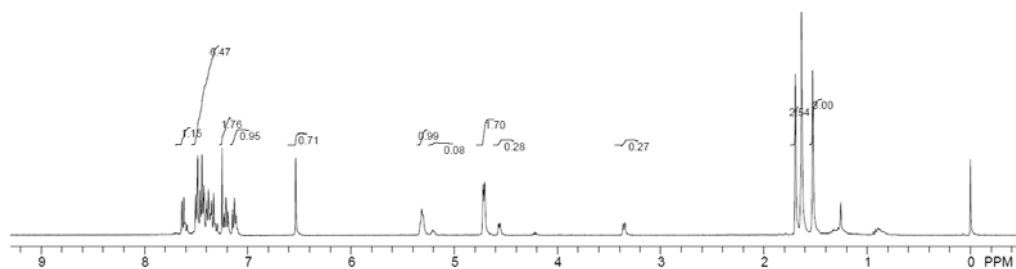
PDA Ch3 220nm 4nm

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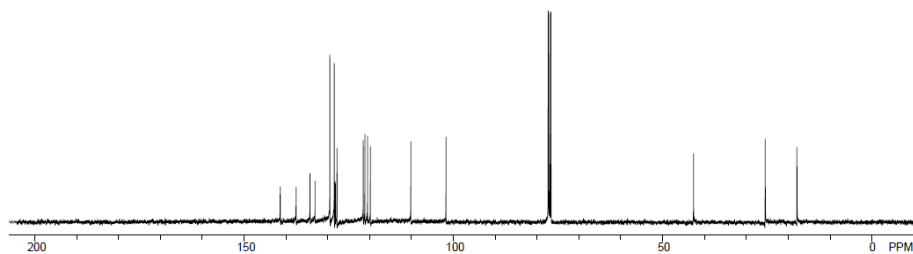
¹H NMR, ¹³C NMR and HPLC spectra of compound 2e



YXF-1-8-P1



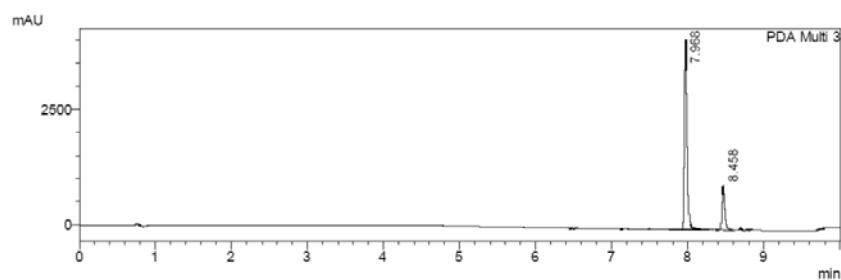
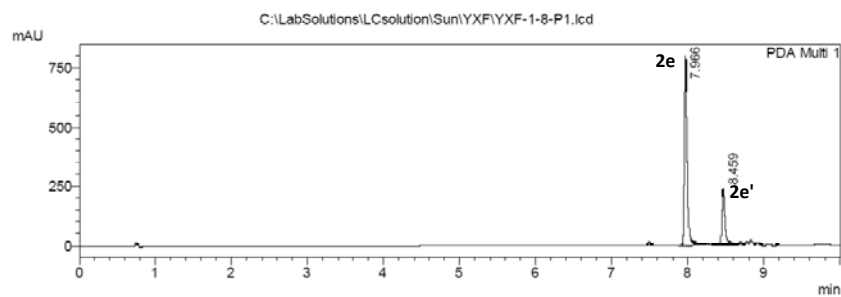
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- 1 PDA Multi 1/254nm 4nm
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PeakTable

PDA Ch1 254nm 4nm

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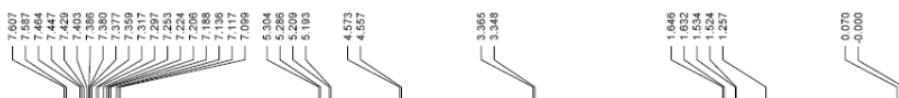
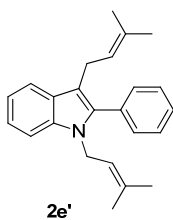
PeakTable

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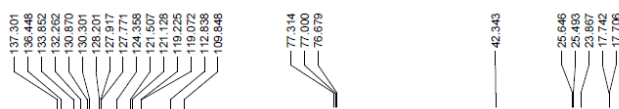
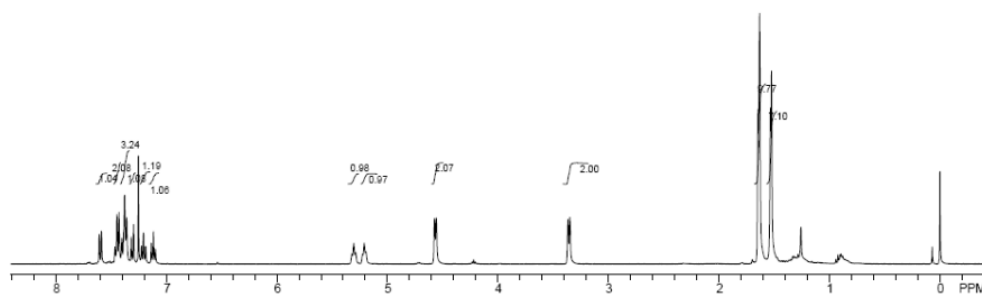
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2	8.458	2480684	963271	18.866	19.023
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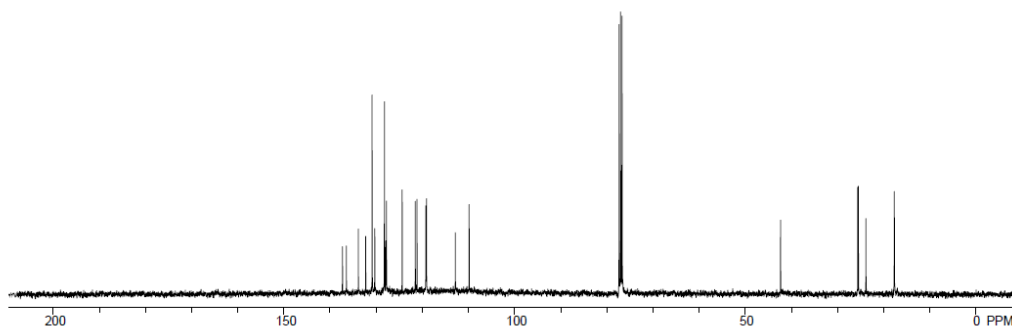
¹H NMR, ¹³C NMR and HPLC spectra of compound 2e'



YXF-1-8-P2



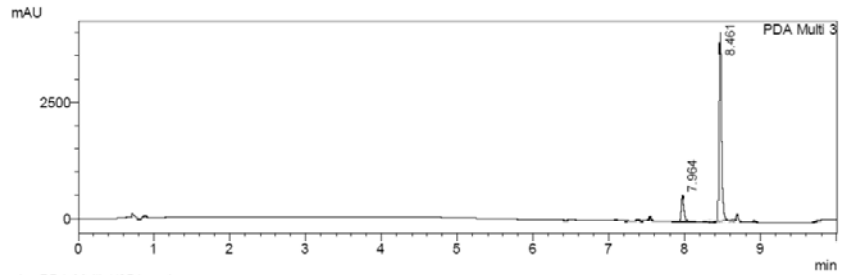
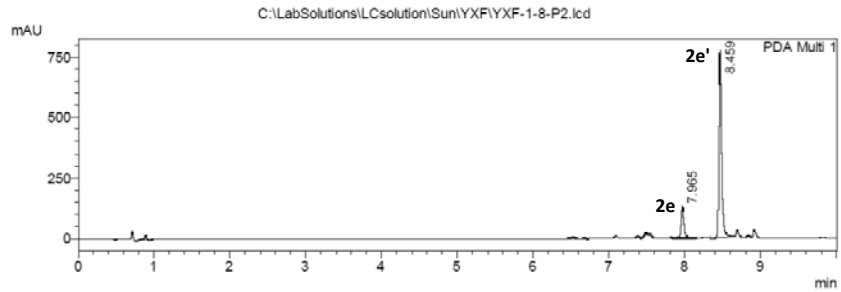
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==== Shimadzu LCsolution Analysis Report ====

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- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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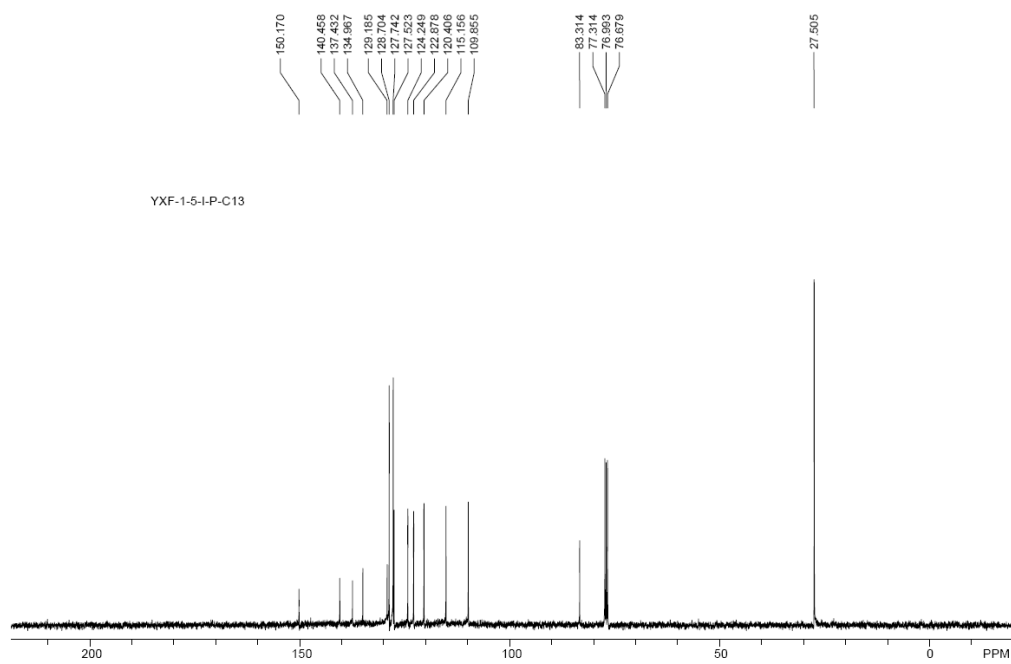
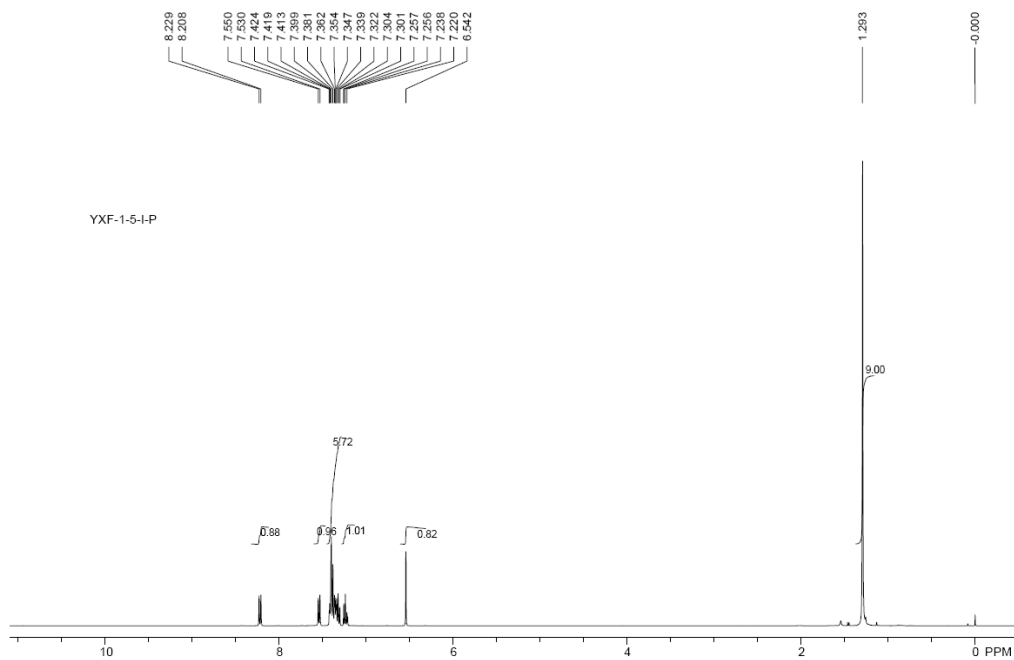
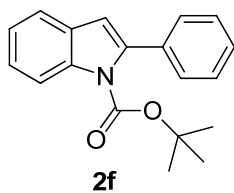
PeakTable

PDA Ch3 220nm 4nm

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Total		10866614	4613407	100.000	100.000

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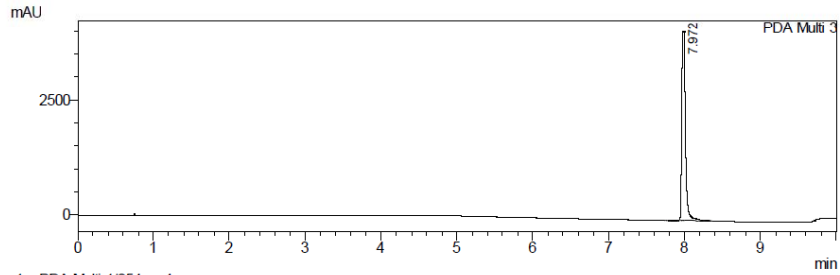
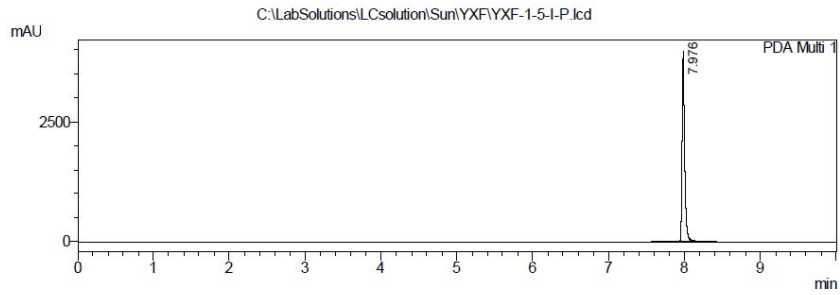
¹H NMR, ¹³C NMR and HPLC spectra of compound 2f



==== Shimadzu LCsolution Analysis Report ====

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- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

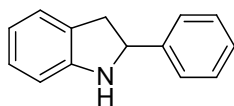
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Total		10652806	3843756	100.000	100.000

PeakTable

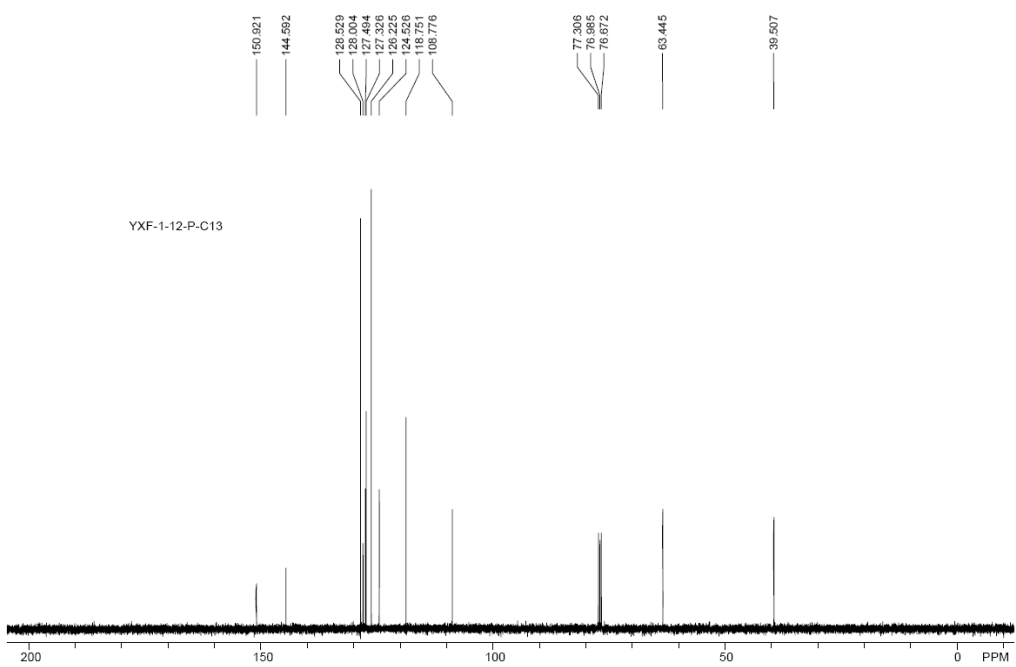
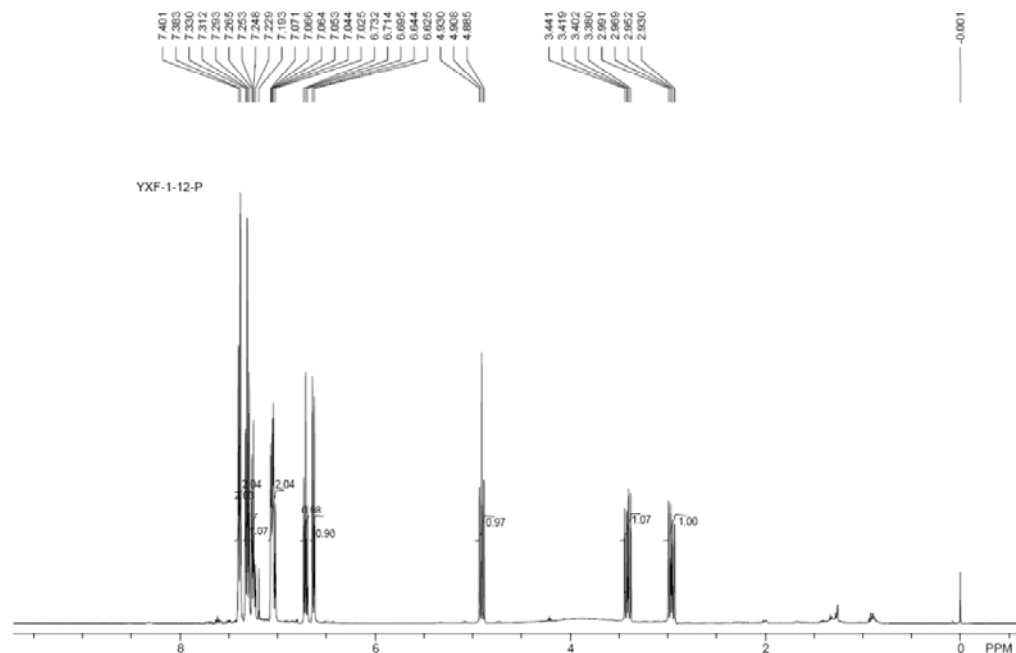
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.972	15700617	4119156	100.000	100.000
Total		15700617	4119156	100.000	100.000

¹H NMR, ¹³C NMR and HPLC spectra of compound 3



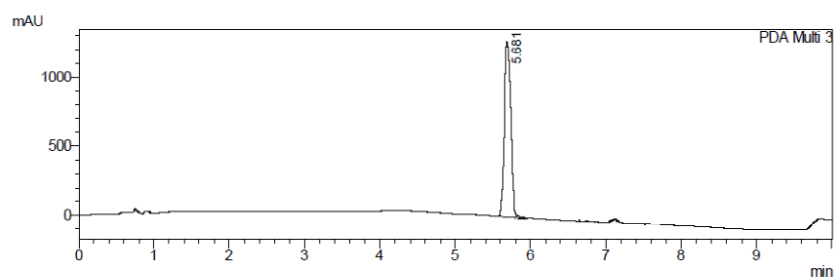
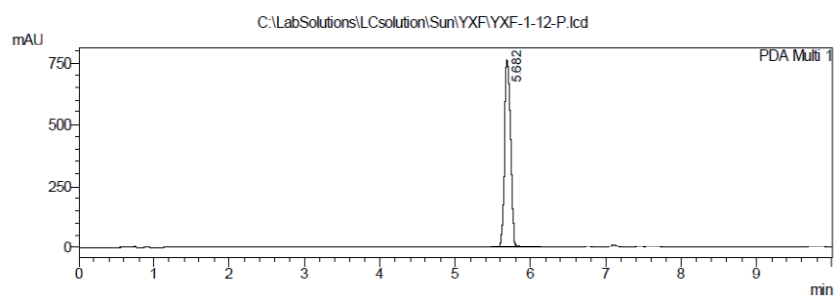
3



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-12-P.lcd
 Sample Name : YXF-1-12-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-12-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name :
 Data Acquired : 3/2/2012 11:01:52 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.682	4263748	761957	100.000	100.000
Total		4263748	761957	100.000	100.000

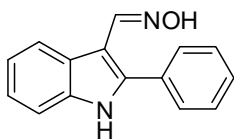
PeakTable

PDA Ch3 220nm 4nm

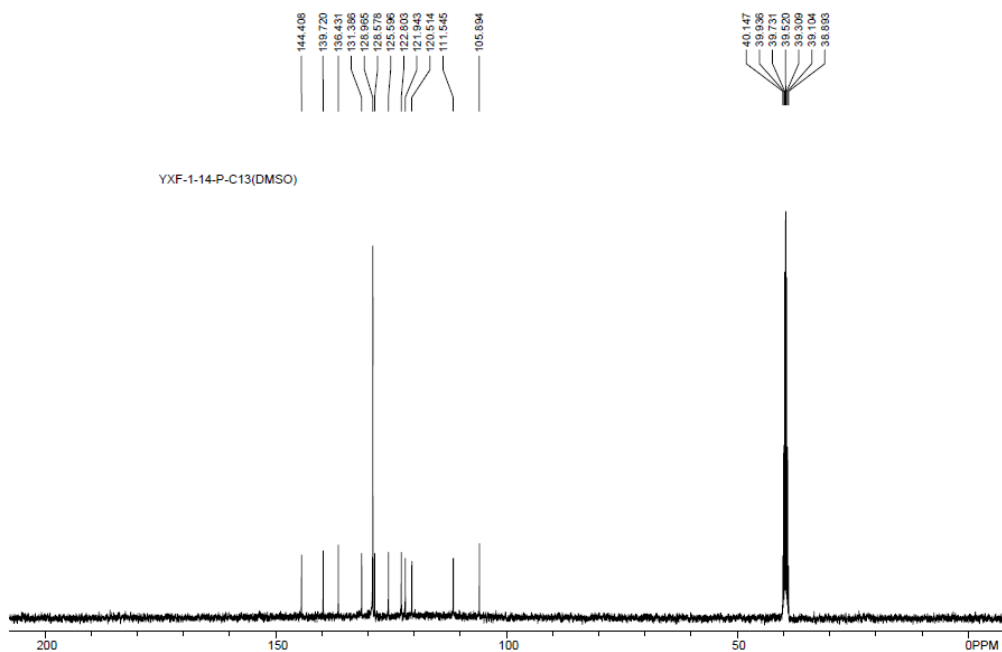
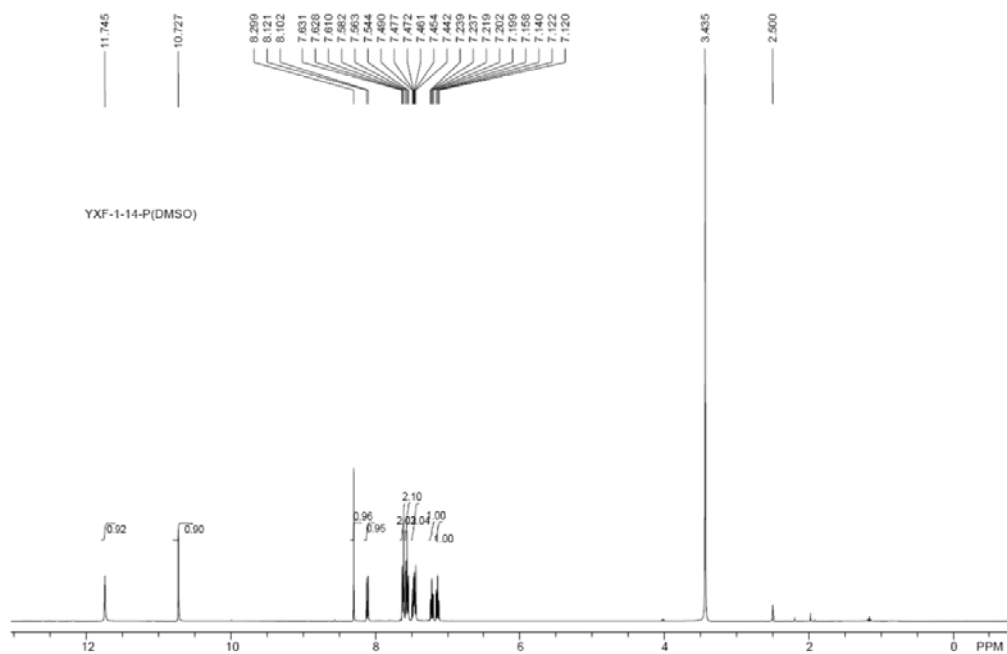
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.681	7602791	1276296	100.000	100.000
Total		7602791	1276296	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-12-P.lcd

¹H NMR, ¹³C NMR and HPLC spectra of compound 5



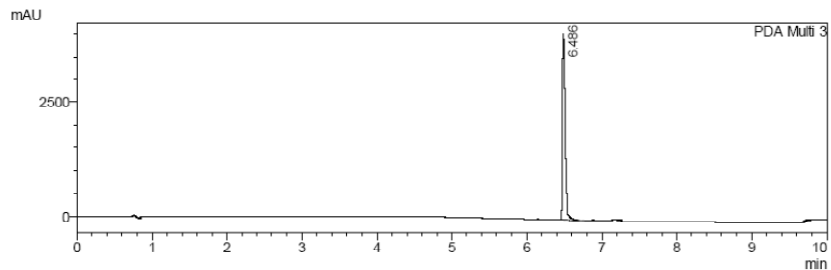
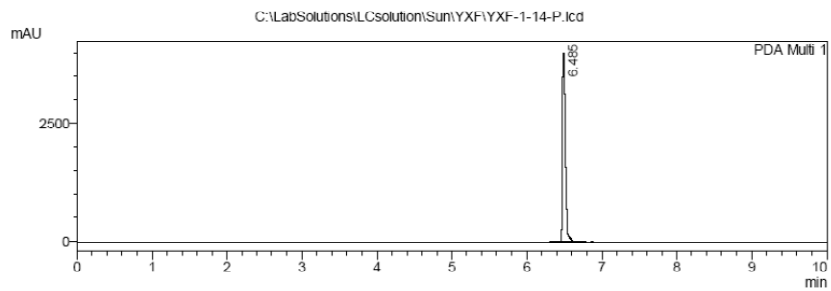
5



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-14-P.lcd
 Sample Name : YXF-1-14-P
 Tray# : 1
 Vial # : 16
 Injection Volume : 5 uL
 Data File Name : YXF-1-14-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name :
 Data Acquired : 9/27/2011 12:48:47 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

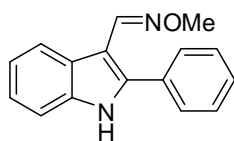
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.485	10483899	3934865	100.000	100.000
Total		10483899	3934865	100.000	100.000

PeakTable

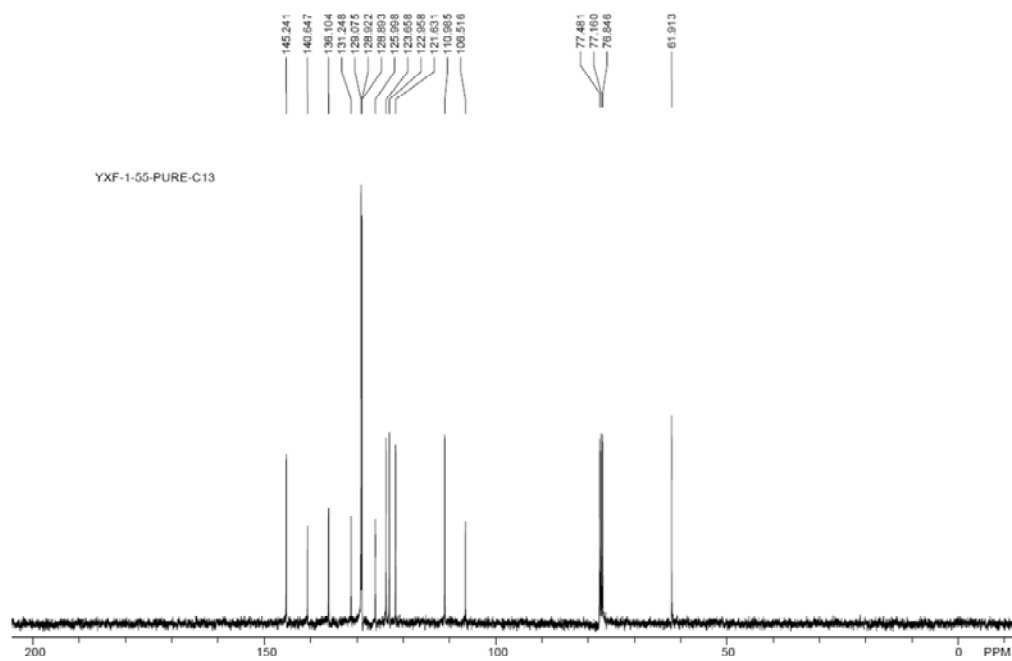
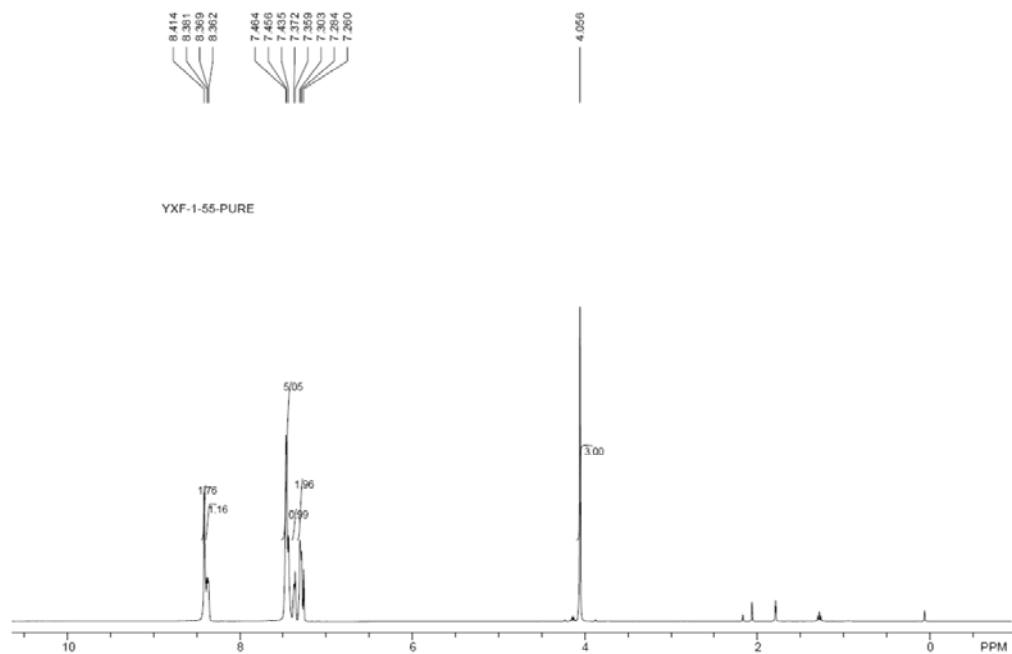
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.486	9798412	4068656	100.000	100.000
Total		9798412	4068656	100.000	100.000

¹H NMR, ¹³C NMR and HPLC spectra of compound 6a



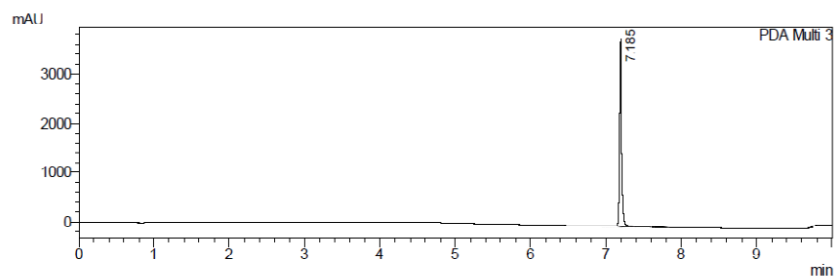
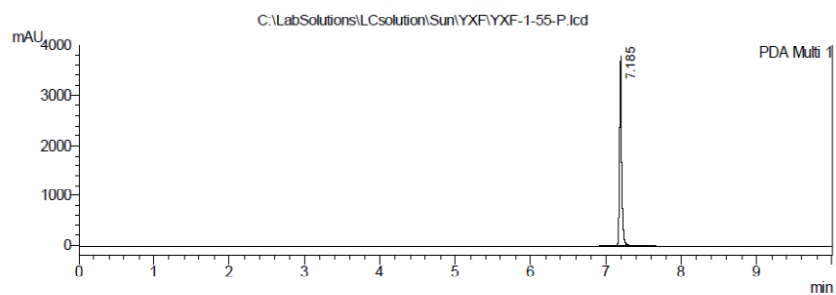
6a



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-55-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-55-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/22/2011 9:14:02 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

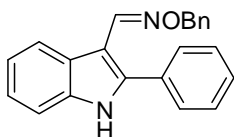
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.185	8329315	3597285	100.000	100.000
Total		8329315	3597285	100.000	100.000

PeakTable

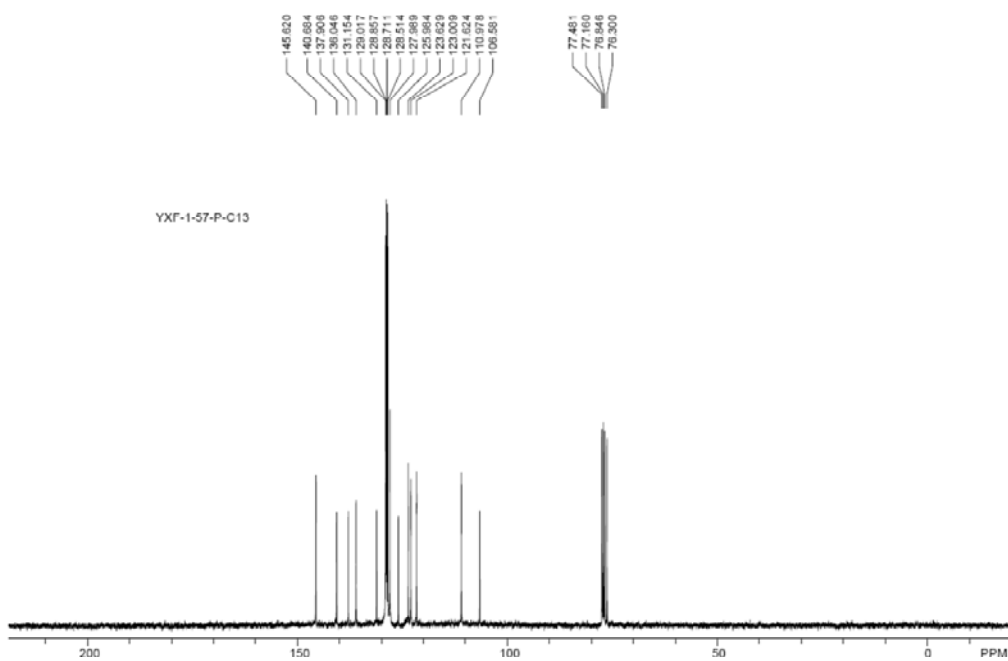
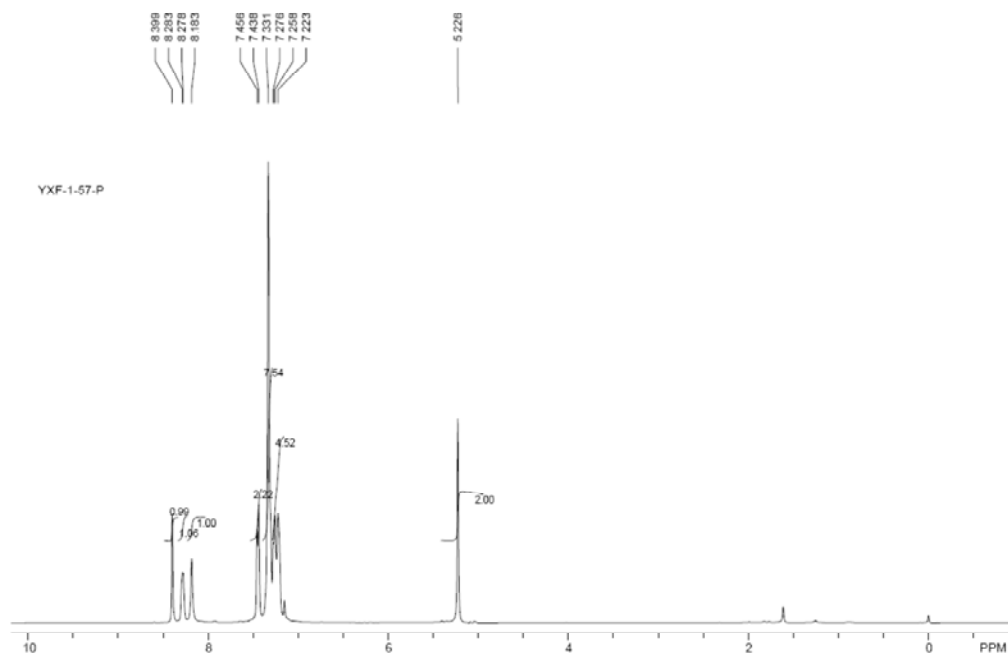
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.185	7919980	3802382	100.000	100.000
Total		7919980	3802382	100.000	100.000

¹H NMR, ¹³C NMR and HPLC spectra of compound 6b



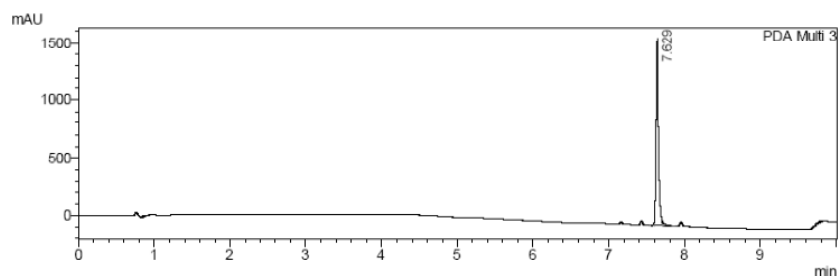
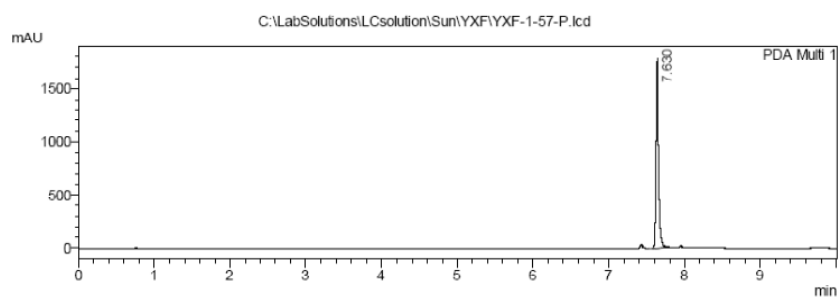
6b



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-57-P.lcd
 Sample Name : YXF-1-57-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-57-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/22/2011 5:49:28 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.630	4221511	1751041	100.000	100.000
Total		4221511	1751041	100.000	100.000

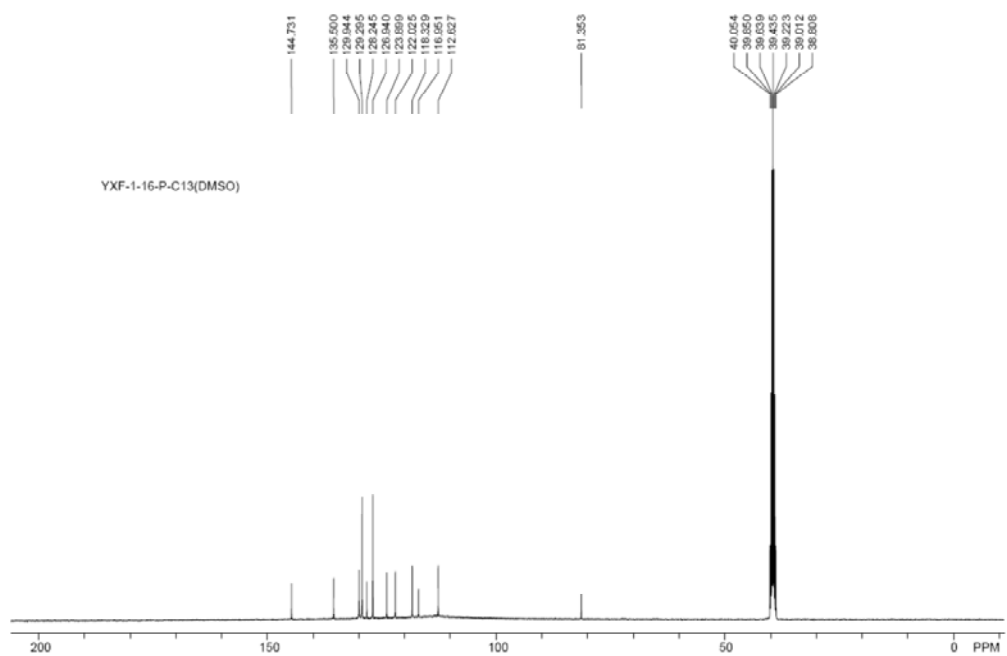
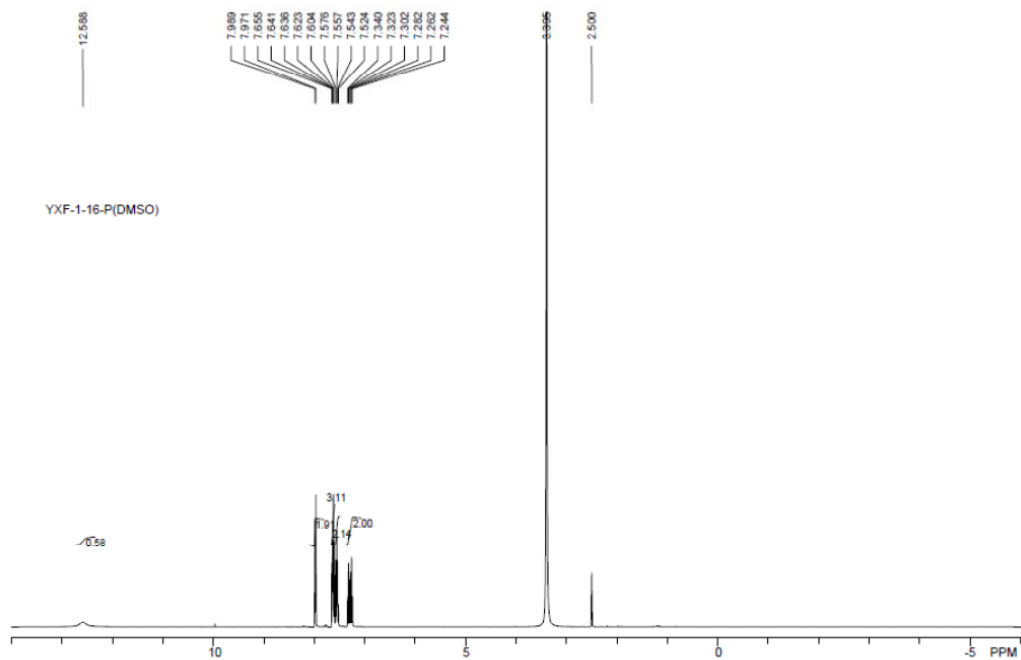
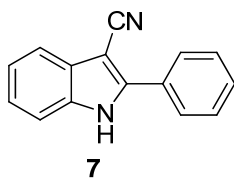
PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.629	3787329	1619584	100.000	100.000
Total		3787329	1619584	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-57-P.lcd

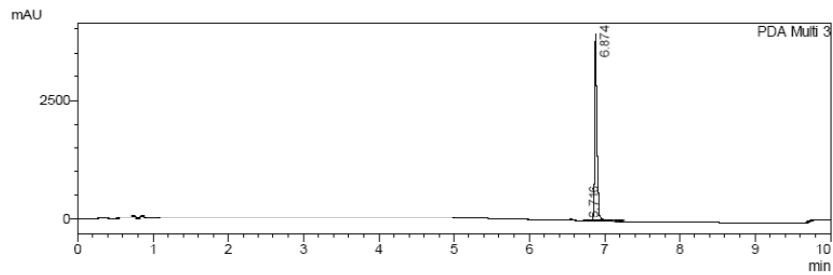
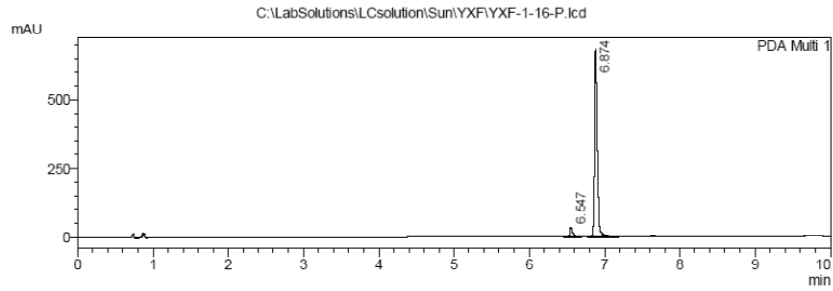
¹H NMR, ¹³C NMR and HPLC spectra of compound 7



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-16-P.lcd
 Sample Name : YXF-1-16-P
 Tray# : 1
 Vial # : 17
 Injection Volume : 5 uL
 Data File Name : YXF-1-16-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 9/28/2011 4:02:54 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

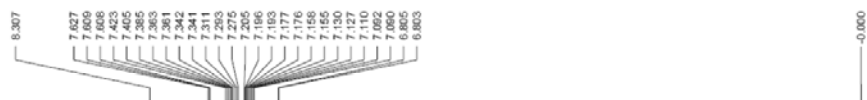
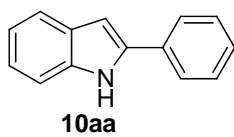
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.547	85904	34808	4.661	4.940
2	6.874	1757011	669820	95.339	95.060
Total		1842914	704628	100.000	100.000

PeakTable

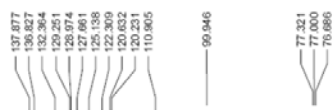
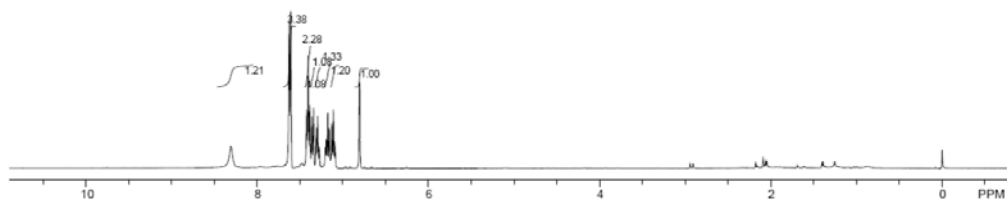
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.716	118	0	0.001	0.000
2	6.874	8643545	3930576	99.999	100.000
Total		8643663	3930576	100.000	100.000

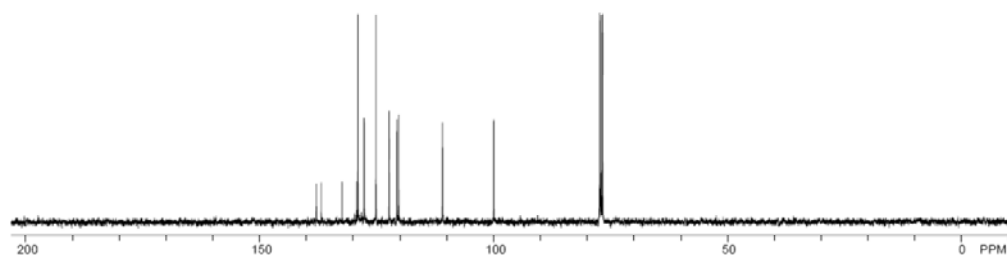
¹H NMR, ¹³C NMR and HPLC spectra of compound 10aa



YXF-1-23-Pure



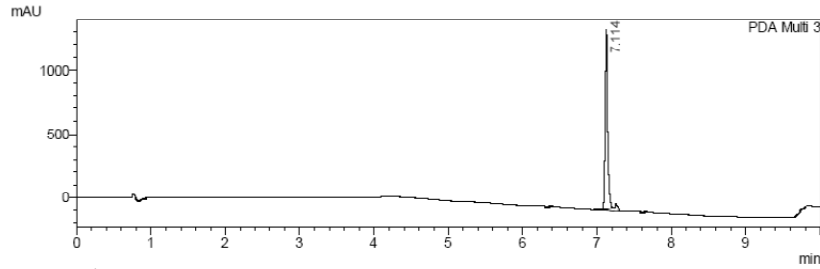
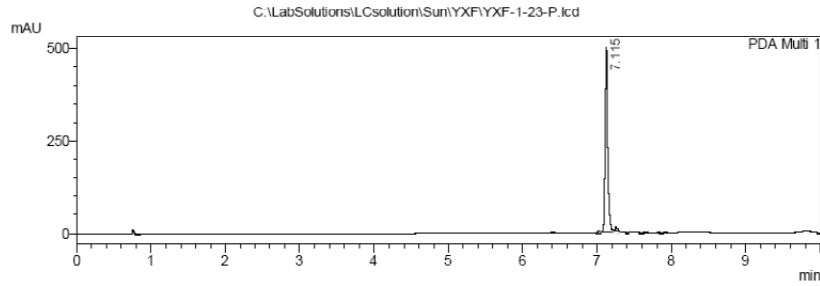
YXF-1-23-Pure-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-23-P
 Tray# : 1
 Vial # : 1
 Injection Volume : 5 uL
 Data File Name : YXF-1-23-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/12/2011 12:11:08 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

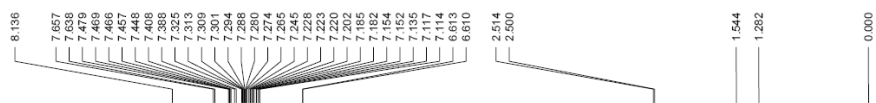
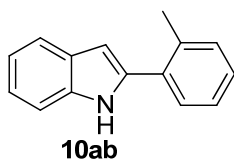
PeakTable

PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.115	1279880	490263	100.000	100.000
Total		1279880	490263	100.000	100.000

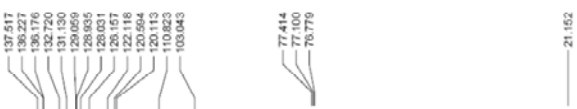
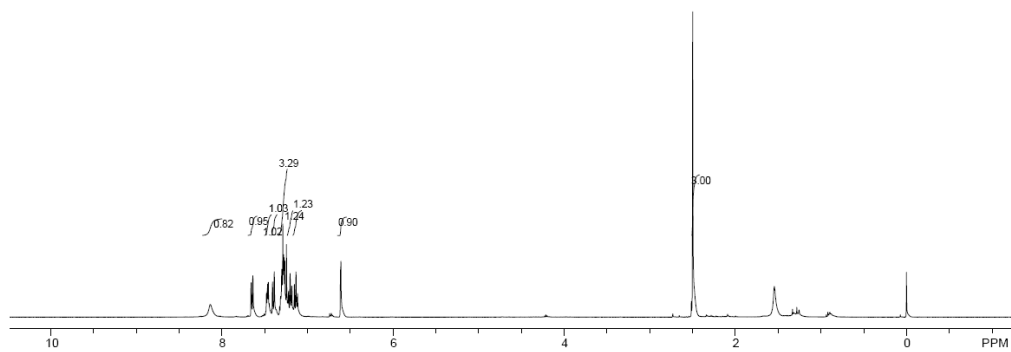
PeakTable

PDA Ch3 220nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.114	3593907	1405153	100.000	100.000
Total		3593907	1405153	100.000	100.000

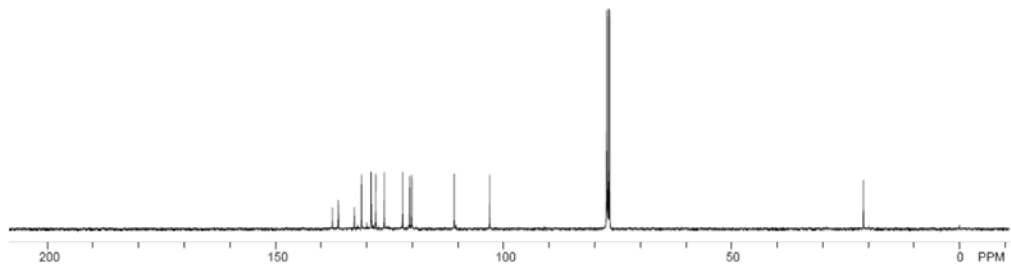
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ab



YXF-1-17-P



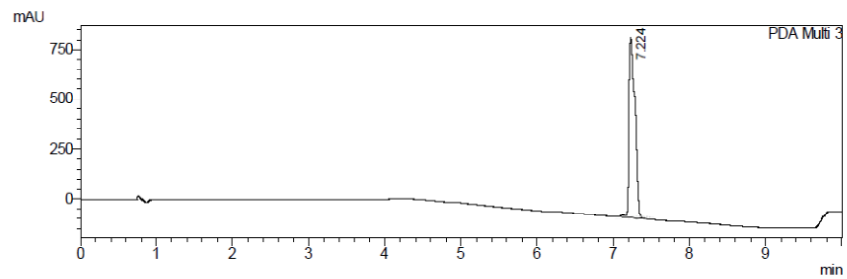
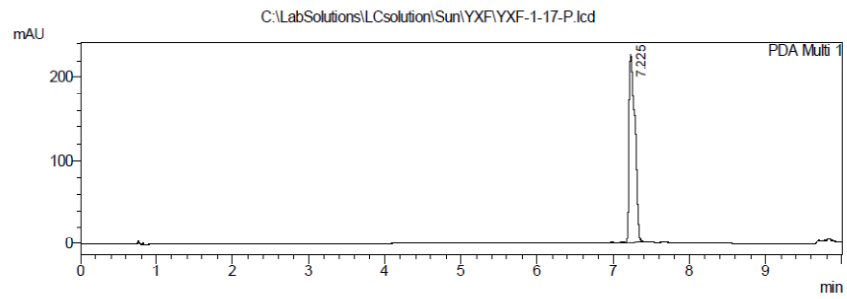
YXF-1-17-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-17-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-17-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 3/12/2012 12:14:54 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

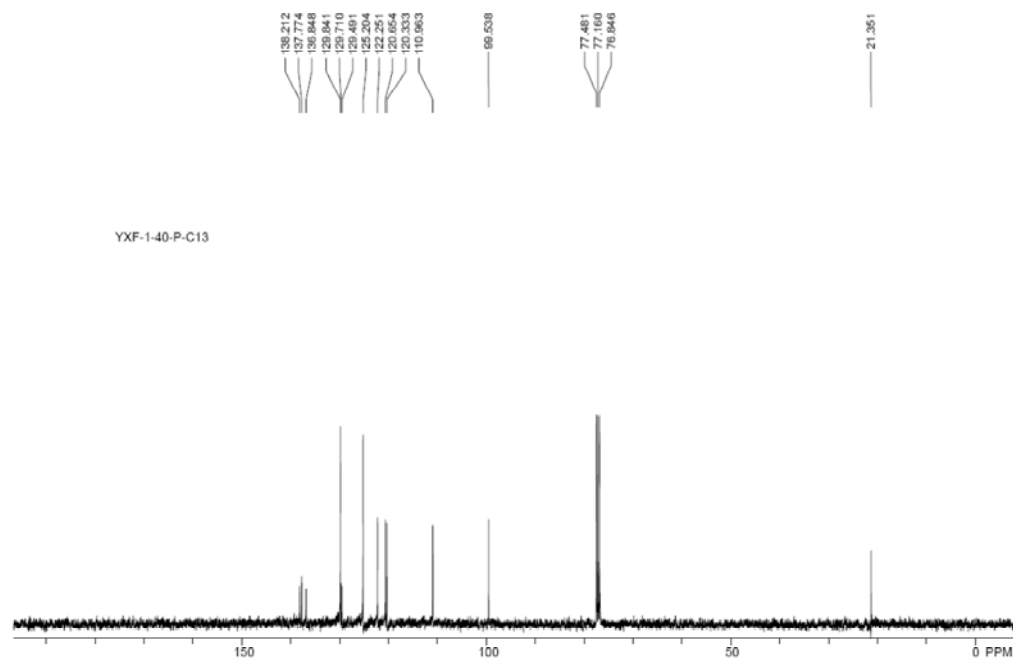
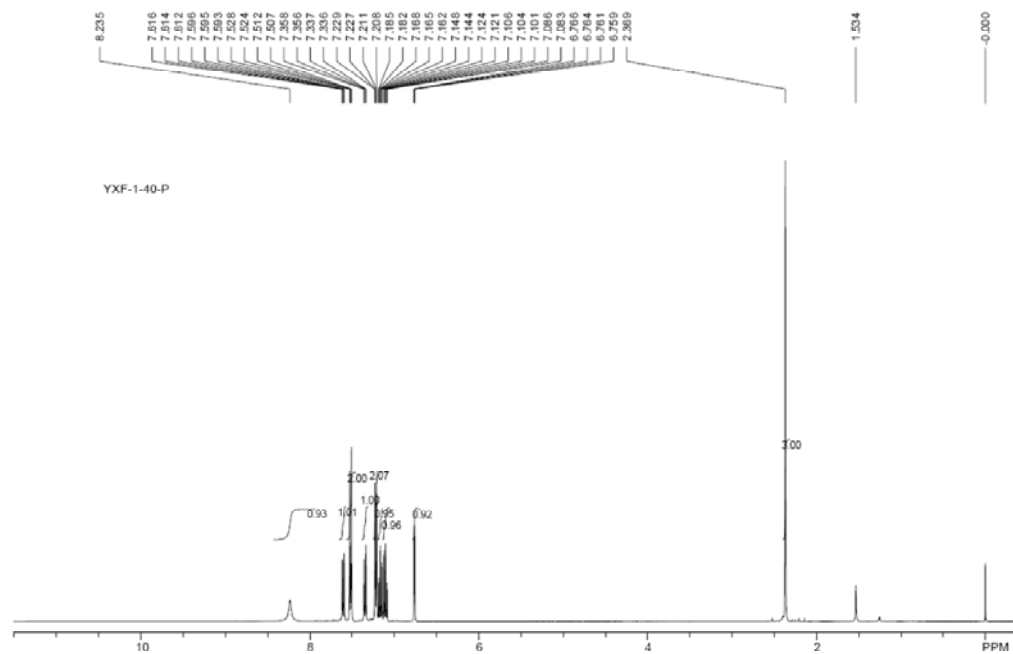
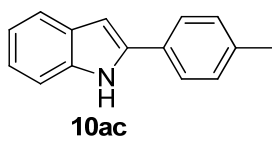
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.225	1210878	225239	100.000	100.000
Total		1210878	225239	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.224	4855657	904691	100.000	100.000
Total		4855657	904691	100.000	100.000

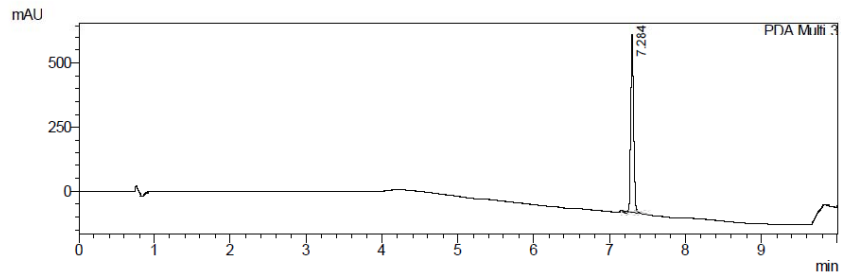
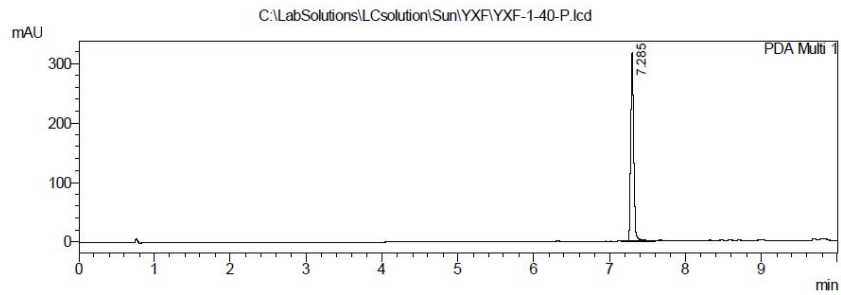
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ac



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-40-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-40-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name :
 Data Acquired : 11/7/2011 12:47:28 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

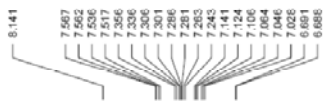
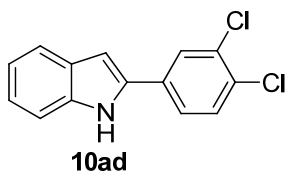
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.285	797835	316154	100.000	100.000
Total		797835	316154	100.000	100.000

PeakTable

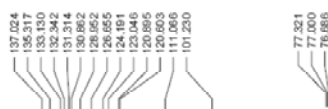
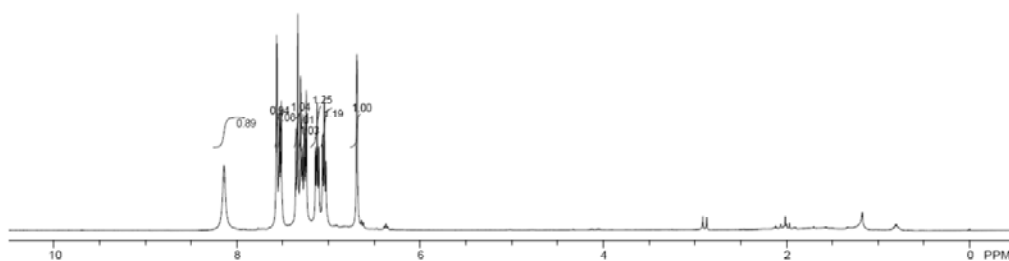
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.284	1658359	694052	100.000	100.000
Total		1658359	694052	100.000	100.000

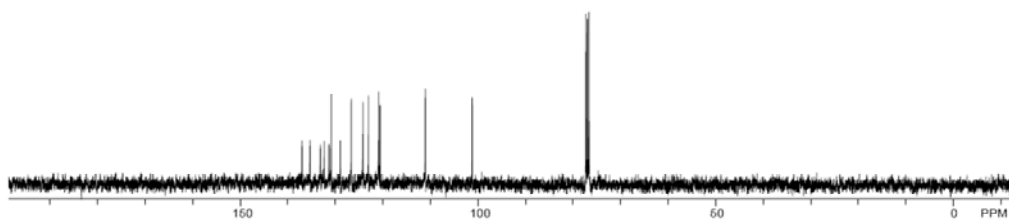
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ad



YXF-1-18-P



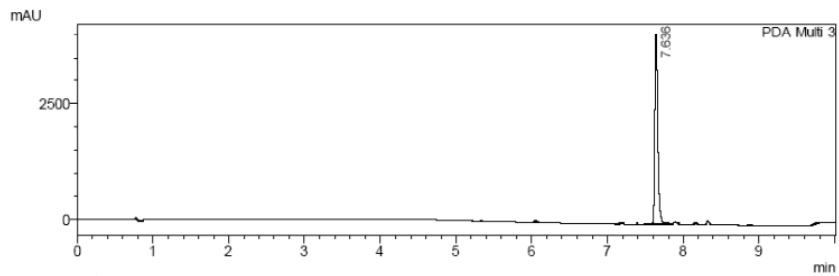
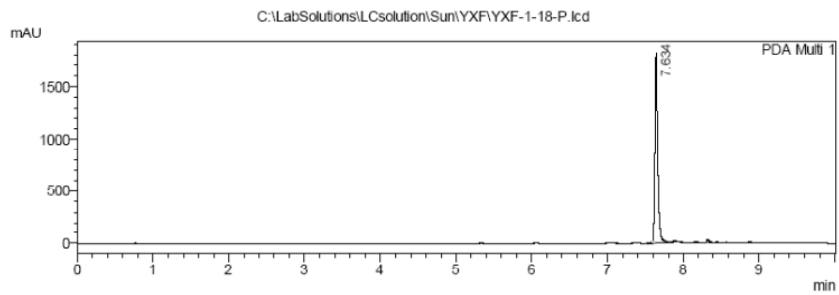
YXF-1-18-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-18-P
 Tray# : 1
 Vial # : 17
 Injection Volume : 3 uL
 Data File Name : YXF-1-18-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/3/2011 4:23:41 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

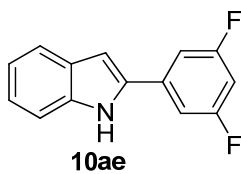
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.634	4661829	1780432	100.000	100.000
Total		4661829	1780432	100.000	100.000

PeakTable

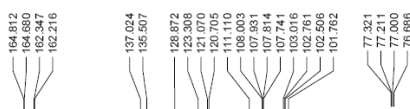
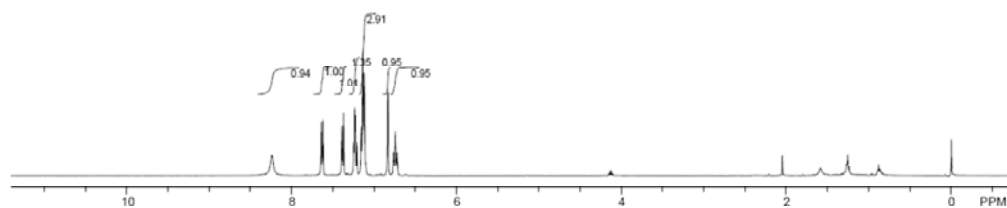
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.636	11303408	4091729	100.000	100.000
Total		11303408	4091729	100.000	100.000

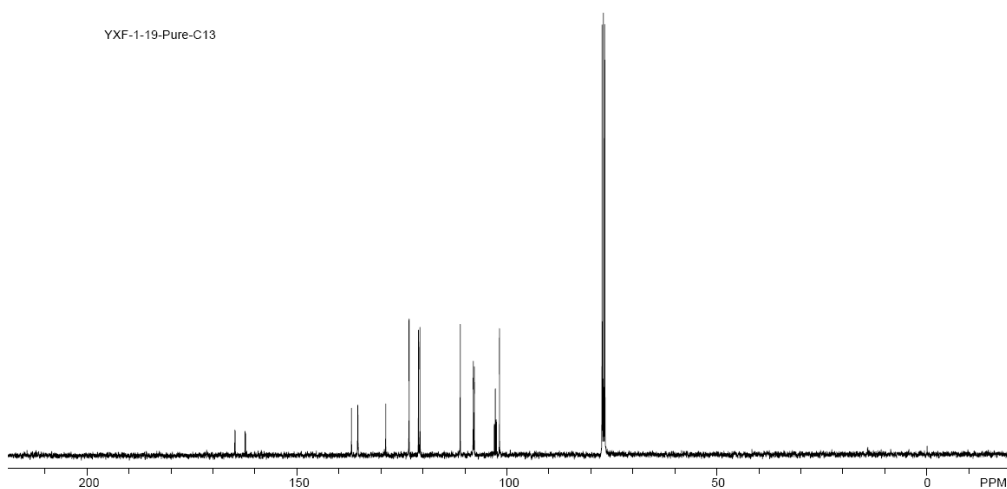
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ae



YXF-1-19-Pure



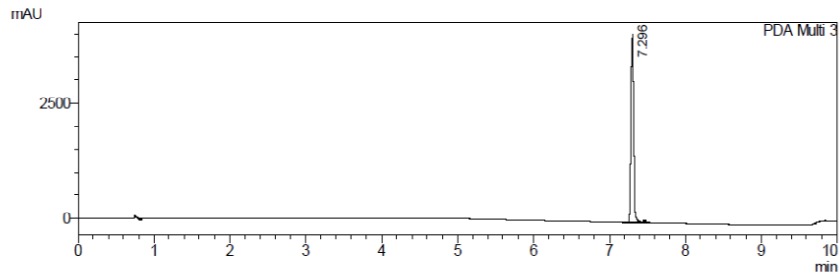
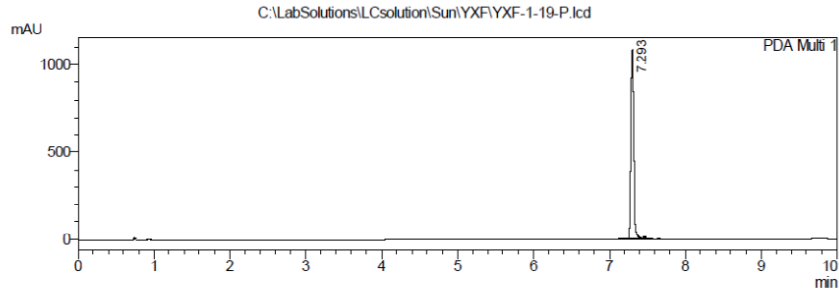
YXF-1-19-Pure-C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-19-P.lcd
 Sample Name : YXF-1-19-P
 Tray# : 1
 Vial # : 16
 Injection Volume : 5 uL
 Data File Name : YXF-1-19-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/11/2011 3:31:35 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

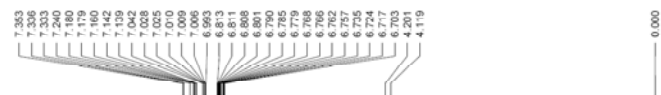
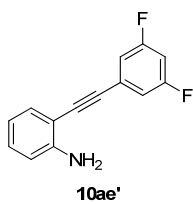
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.293	2763204	1082975	100.000	100.000
Total		2763204	1082975	100.000	100.000

PeakTable

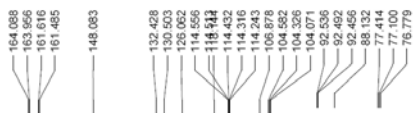
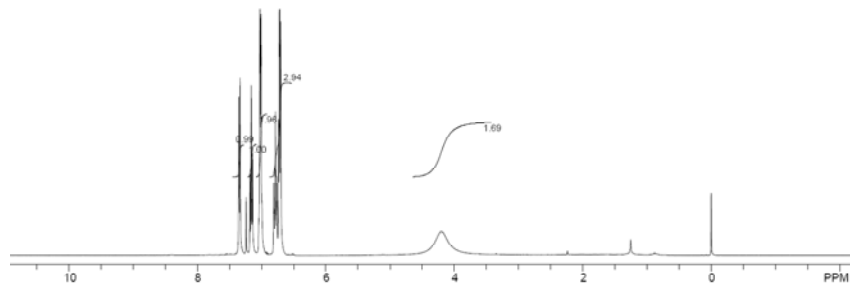
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.296	9535136	4068002	100.000	100.000
Total		9535136	4068002	100.000	100.000

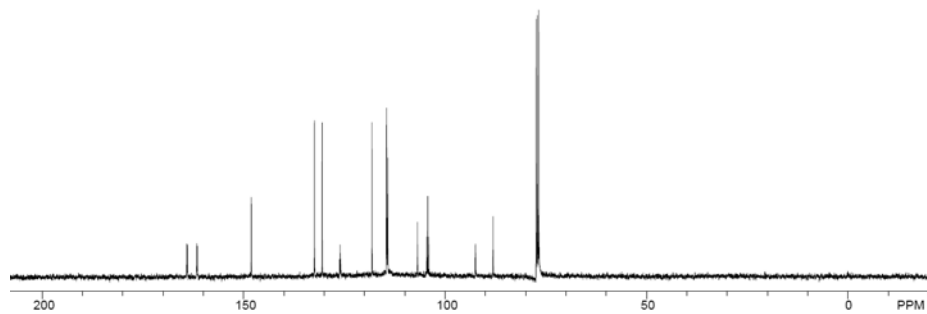
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ae'



YXF-2-49-II-P



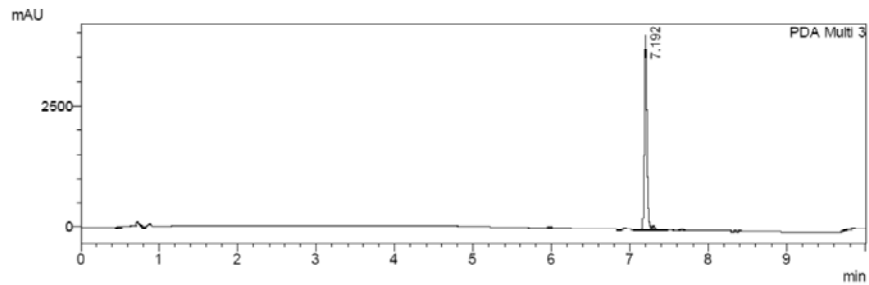
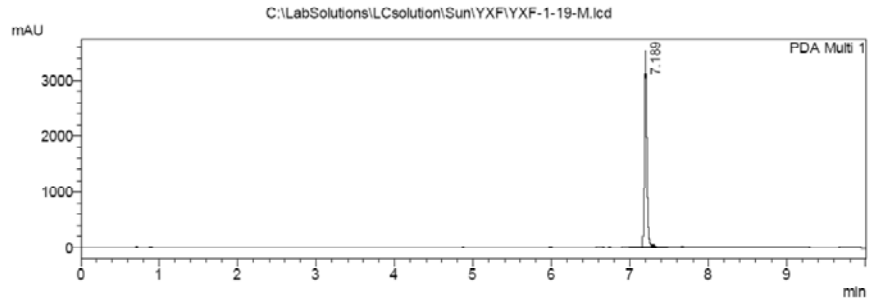
YXF-2-49-II-P-C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-19-M.lcd
 Sample Name : YXF-1-19-M
 Tray# : 1
 Vial# : 3
 Injection Volume : 10 uL
 Data File Name : YXF-1-19-M.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 10/7/2011 9:30:42 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

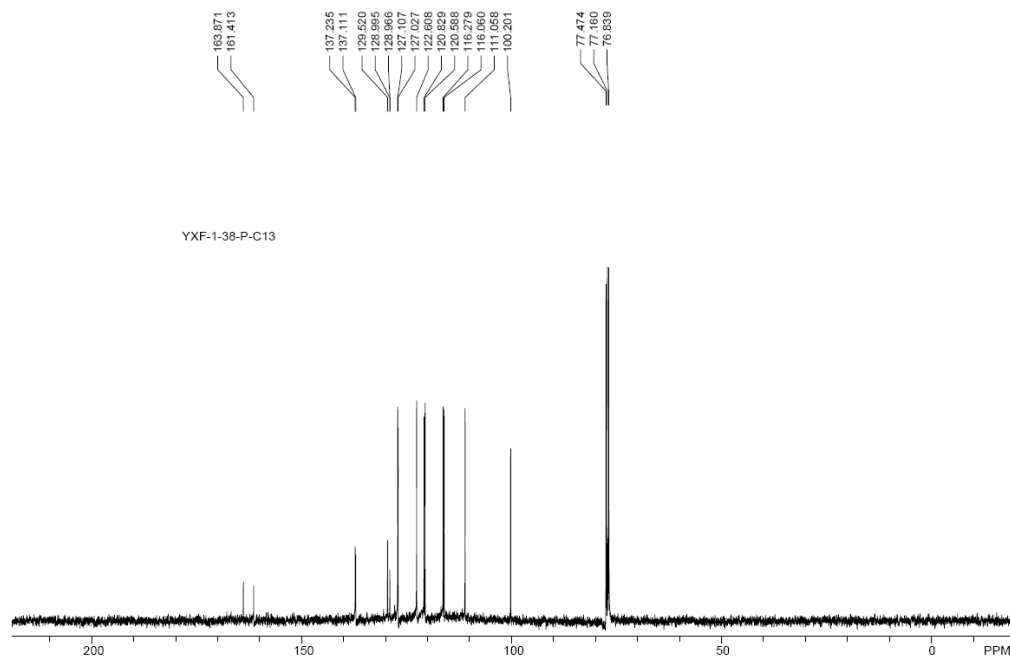
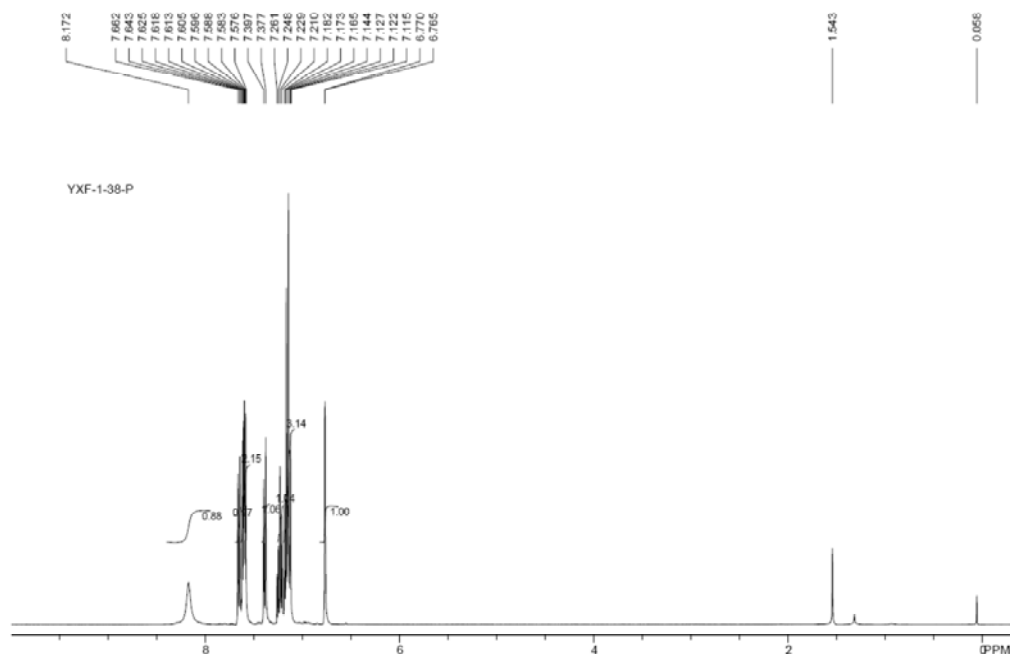
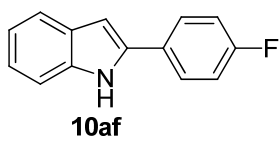
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.189	7326546	3411179	100.000	100.000
Total		7326546	3411179	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.192	9080215	3967240	100.000	100.000
Total		9080215	3967240	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-19-M.lcd

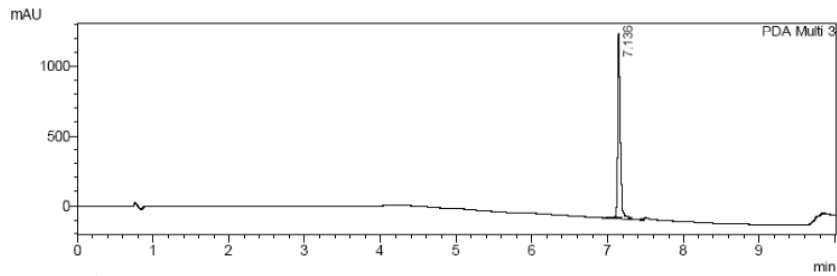
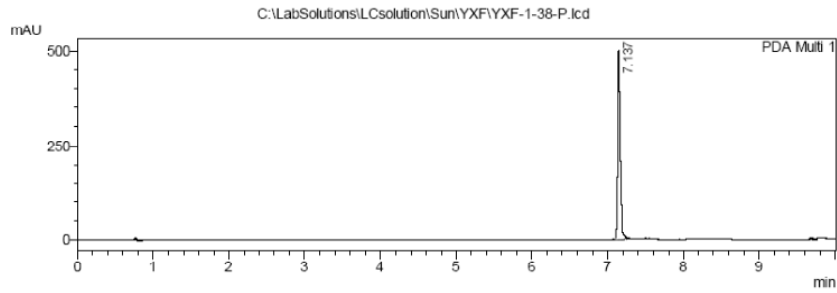
¹H NMR, ¹³C NMR and HPLC spectra of compound 10af



==== Shimadzu LCsolution Analysis Report ====

Sample Name : YXF-1-38-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-38-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/3/2011 12:07:32 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

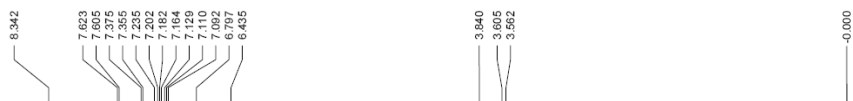
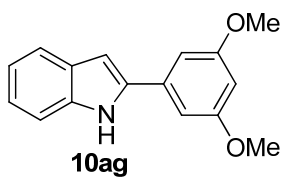
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.137	1256218	488189	100.000	100.000
Total		1256218	488189	100.000	100.000

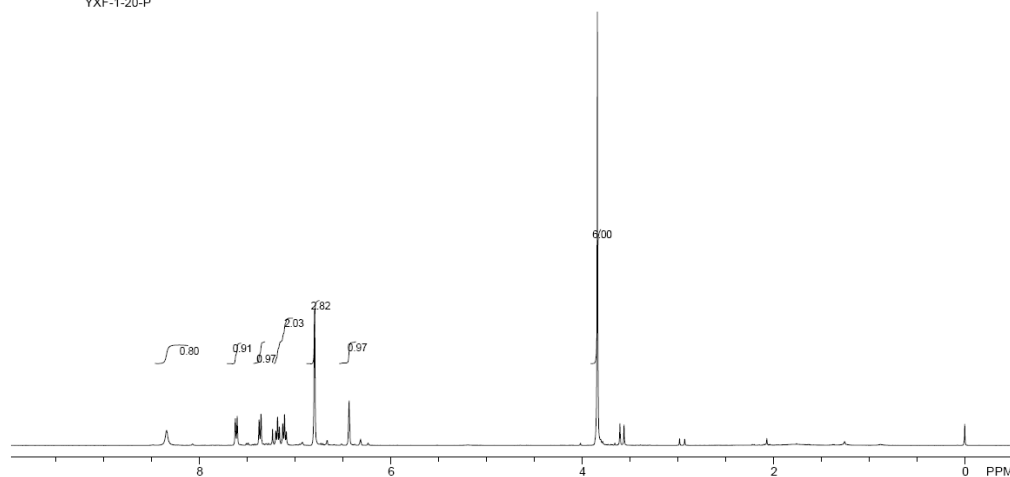
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.136	3266849	1314428	100.000	100.000
Total		3266849	1314428	100.000	100.000

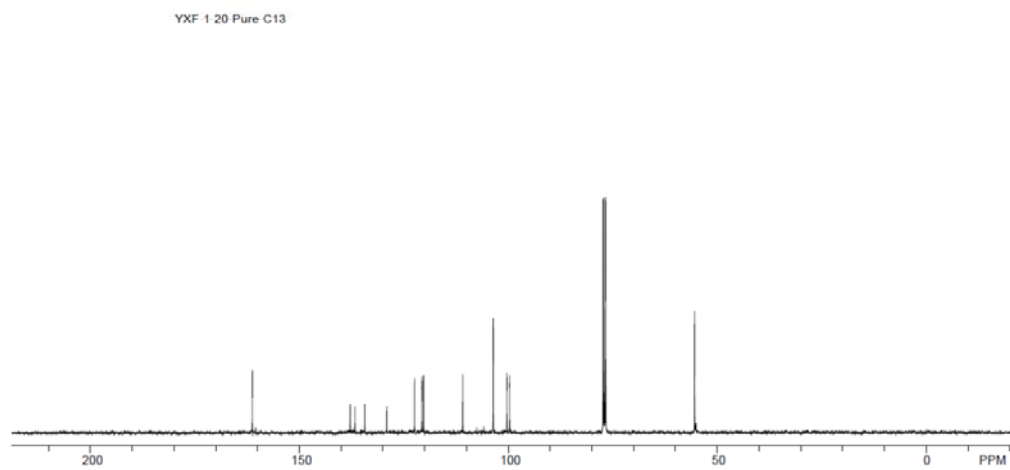
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ag



YXF-1-20-P



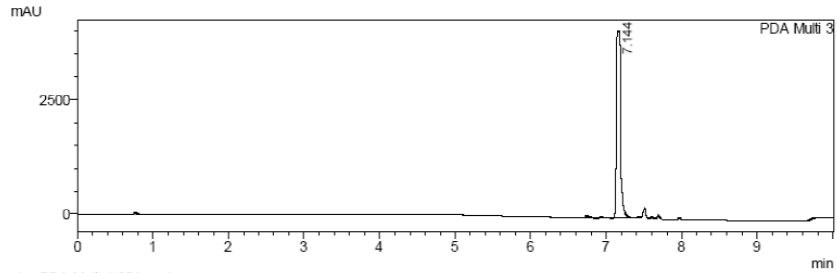
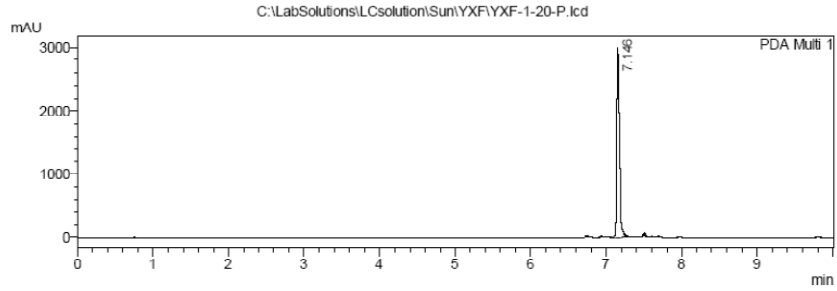
YXF-1-20 Pure C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-20-P.lcd
 Sample Name : YXF-1-20-P
 Tray# : 1
 Vail # : 1
 Injection Volume : 5 uL
 Data File Name : YXF-1-20-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 10/11/2011 12:15:28 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

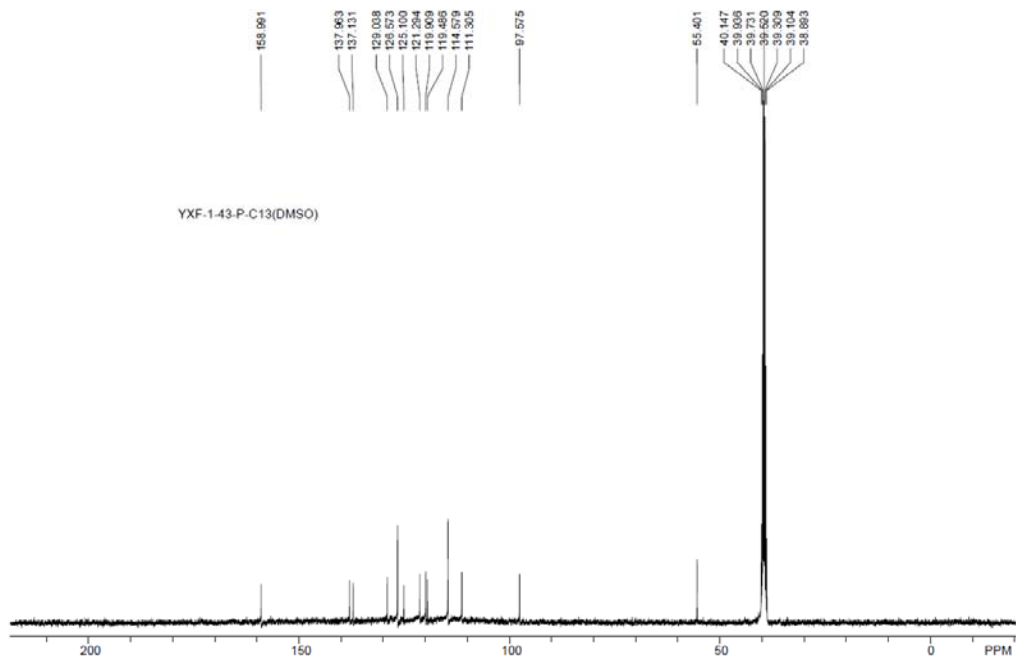
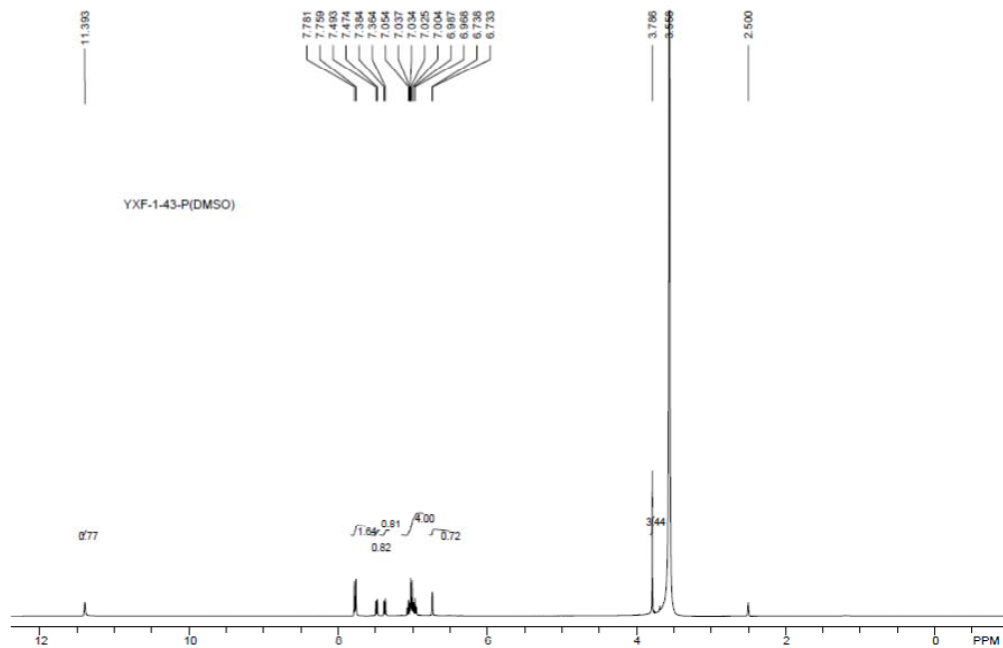
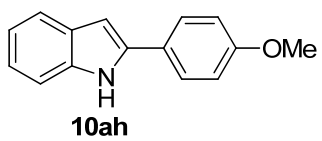
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.146	7233514	2885804	100.000	100.000
Total		7233514	2885804	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.144	16629064	4079232	100.000	100.000
Total		16629064	4079232	100.000	100.000

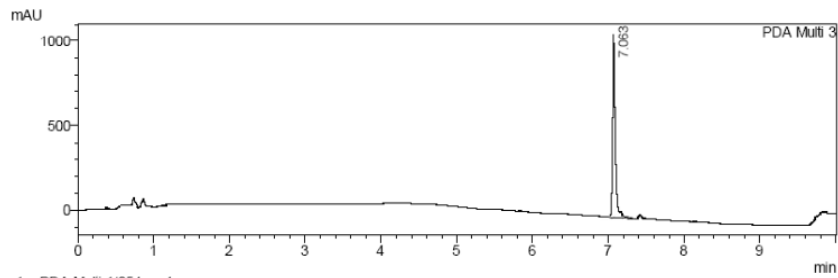
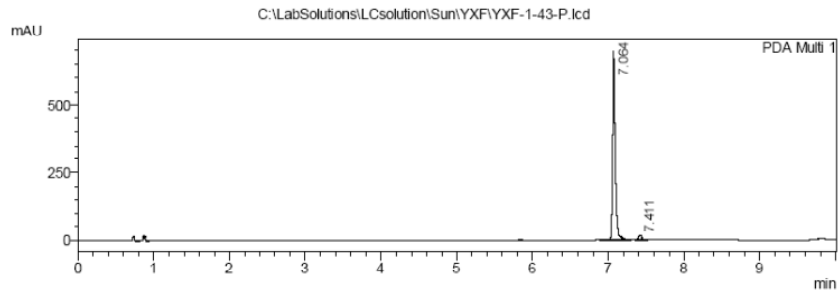
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ah



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-43-P.lcd
 Sample Name : YXF-1-43-P
 Tray# : 1
 Vial # : 32
 Injection Volume : 5 uL
 Data File Name : YXF-1-43-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 11/9/2011 2:20:58 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

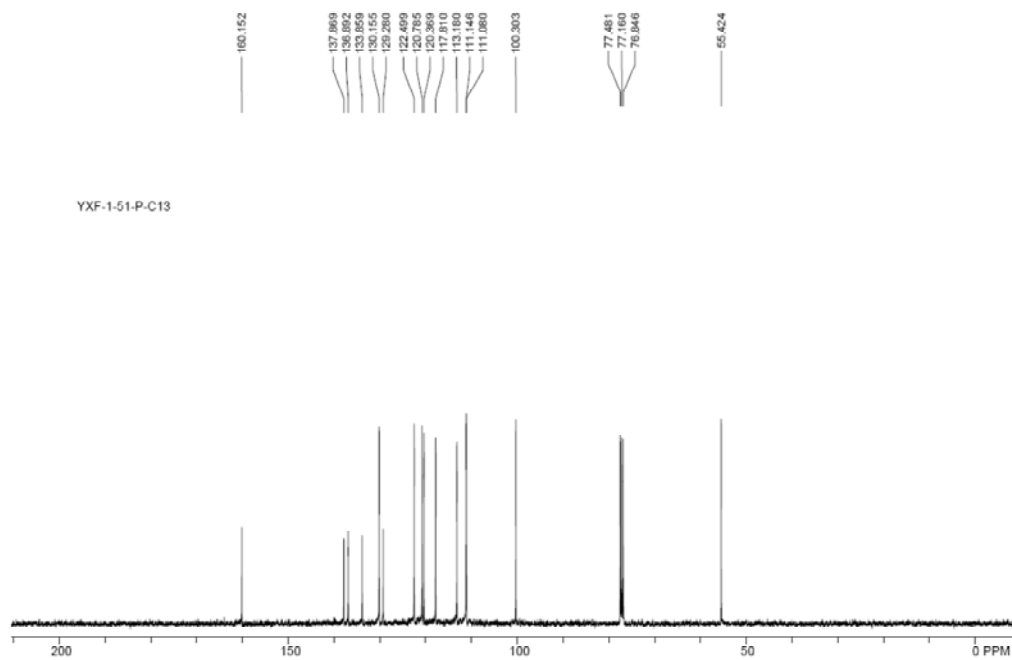
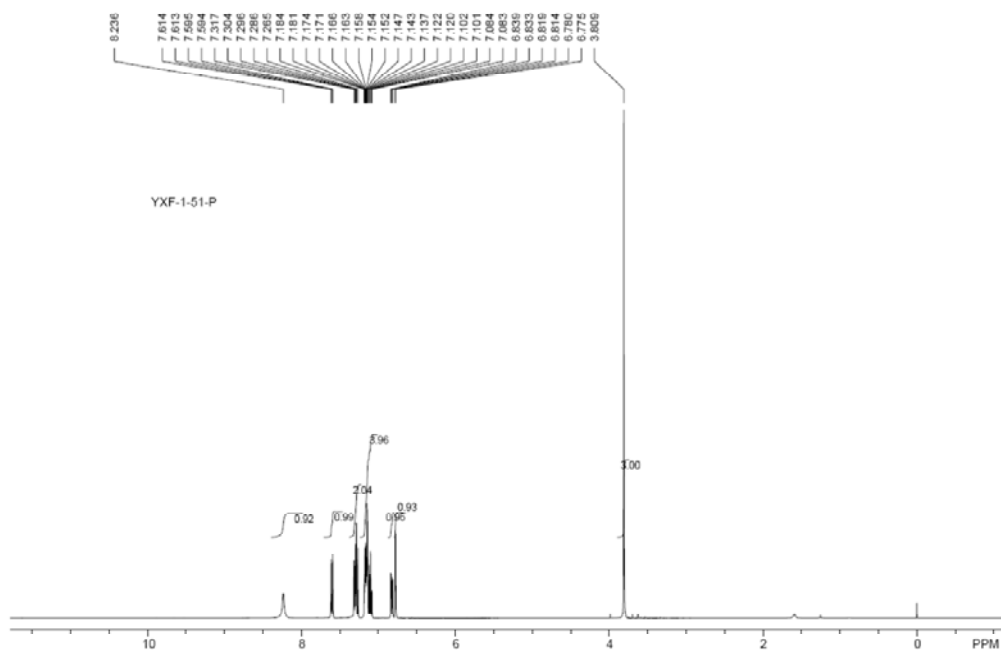
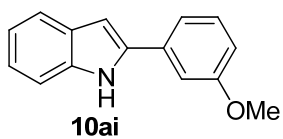
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.064	1756966	675327	97.761	97.631
2	7.411	40232	16389	2.239	2.369
Total		1797198	691716	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.063	2750751	1078590	100.000	100.000
Total		2750751	1078590	100.000	100.000

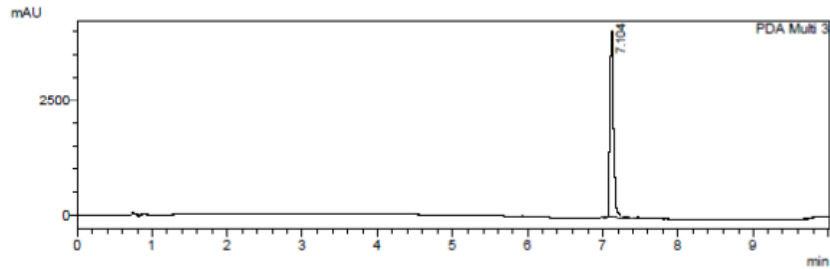
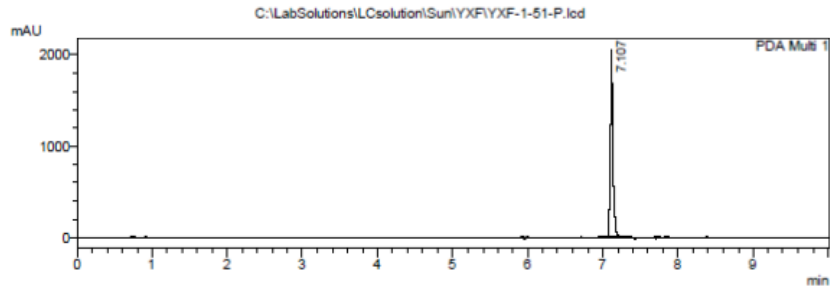
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ai



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-51-P.lcd
 Sample Name : YXF-1-51-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-51-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/17/2011 4:29:29 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

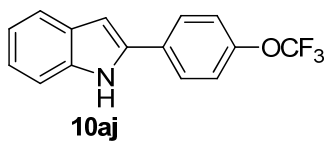
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.107	5088913	2020372	100.000	100.000
Total		5088913	2020372	100.000	100.000

PeakTable

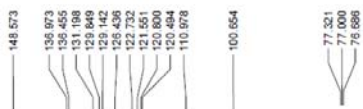
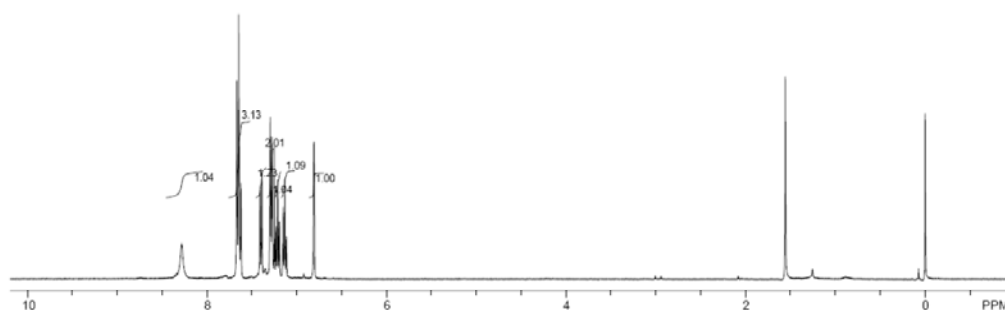
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.104	14076706	4050339	100.000	100.000
Total		14076706	4050339	100.000	100.000

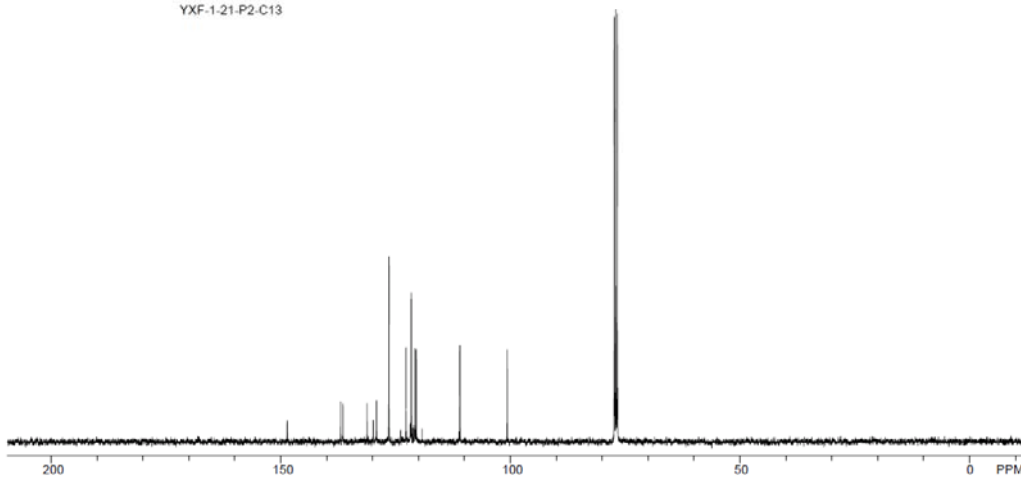
¹H NMR, ¹³C NMR and HPLC spectra of compound 10aj



YXF-1-21-P1



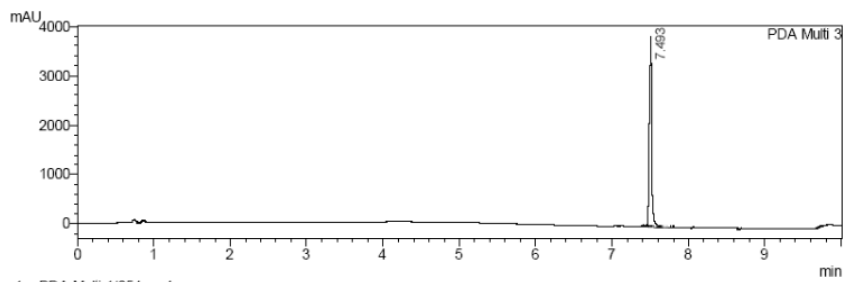
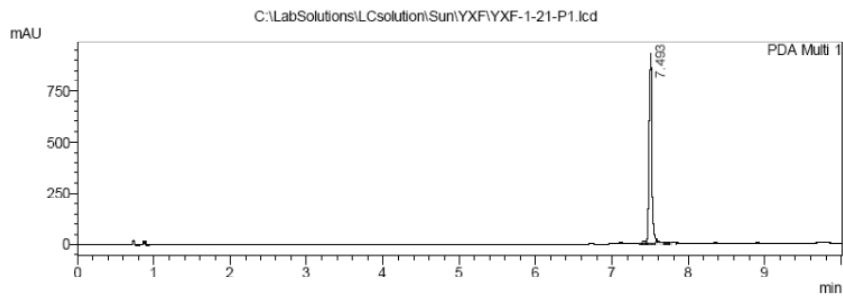
YXF-1-21-P2-C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-21-P1.lcd
 Sample Name : YXF-1-21-P1
 Tray# : 1
 Vial # : 2
 Injection Volume : 5 uL
 Data File Name : YXF-1-21-P1.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 10/11/2011 12:25:56 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

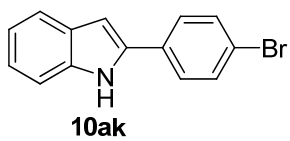
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.493	2306778	917006	100.000	100.000
Total		2306778	917006	100.000	100.000

PeakTable

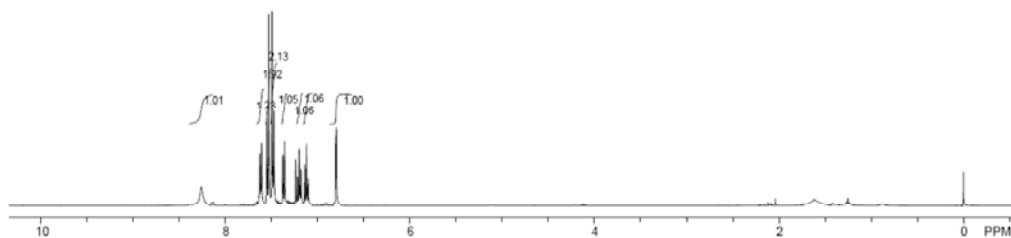
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.493	7768328	3837394	100.000	100.000
Total		7768328	3837394	100.000	100.000

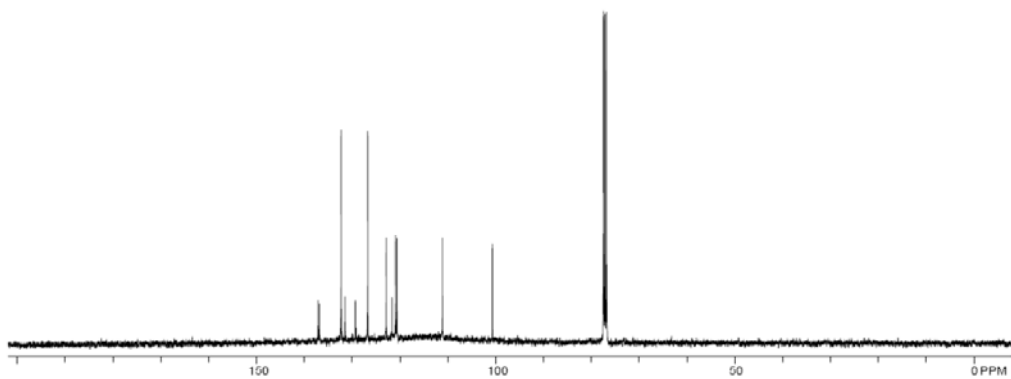
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ak



YXF-1-29-Pure



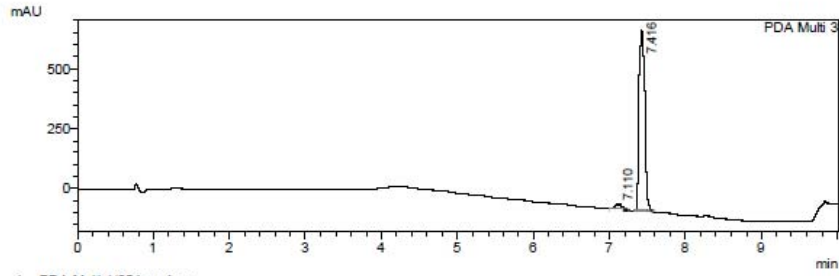
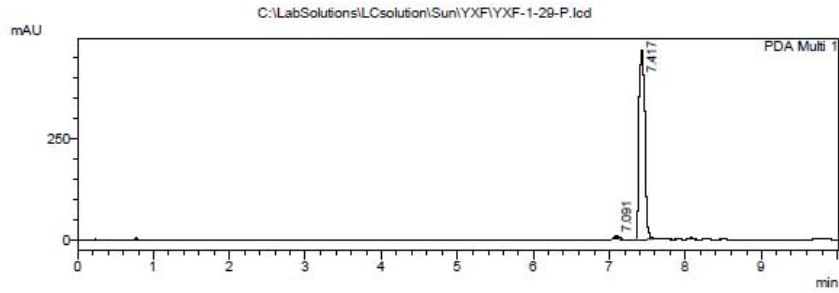
YXF-1-29-Pure-C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-29-P.lcd
 Sample Name : YXF-1-29-P
 Tray# : 1
 Vail # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-29-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 3/1/2012 5:08:00 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

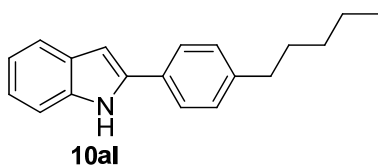
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.091	28183	6219	1.125	1.319
2	7.417	2477413	465286	98.875	98.681
Total		2505596	471505	100.000	100.000

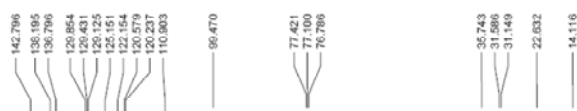
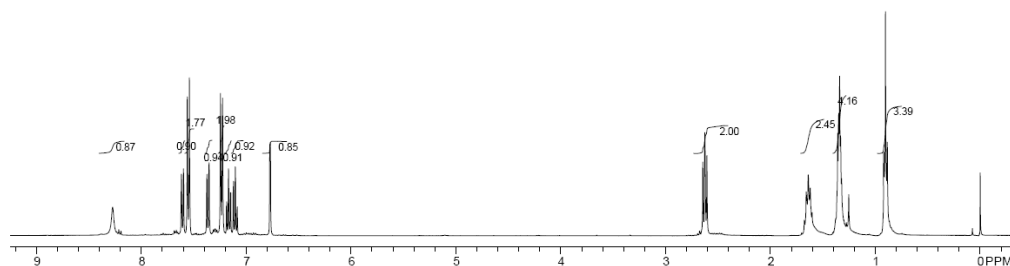
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.110	139509	21795	3.420	2.822
2	7.416	3940148	750546	96.580	97.178
Total		4079657	772342	100.000	100.000

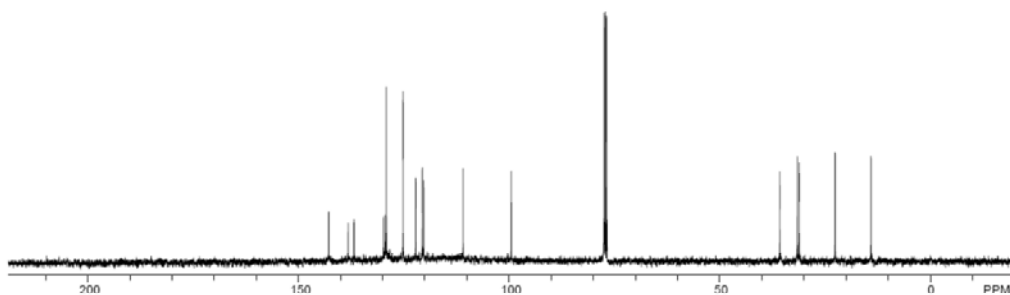
¹H NMR, ¹³C NMR and HPLC spectra of compound 10al



yxf-1-30-P-P



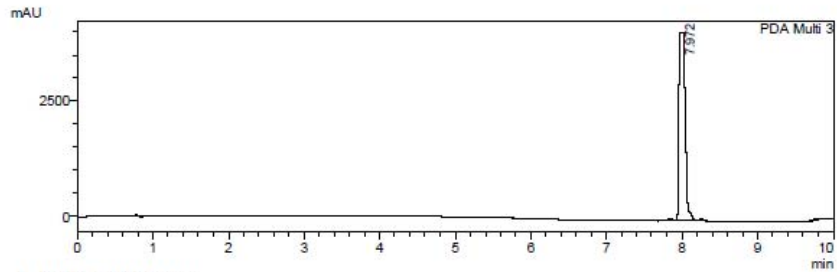
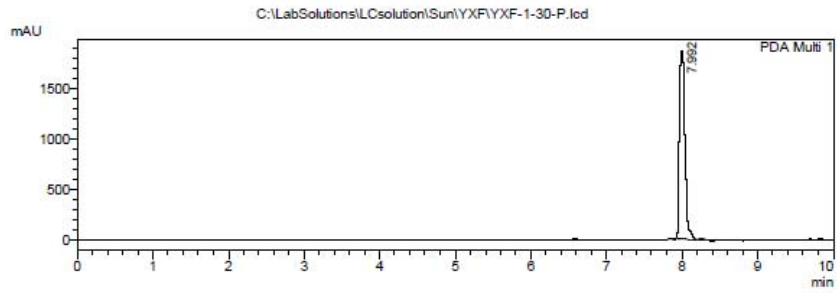
YXF-1-30-Pure-C13



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-30-P.lcd
 Sample Name : YXF-1-30-P
 Tray# : 1
 Vial# : 31
 Injection Volume : 3 uL
 Data File Name : YXF-1-30-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 2/29/2012 1:52:43 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.992	9715937	1859521	100.000	100.000
Total		9715937	1859521	100.000	100.000

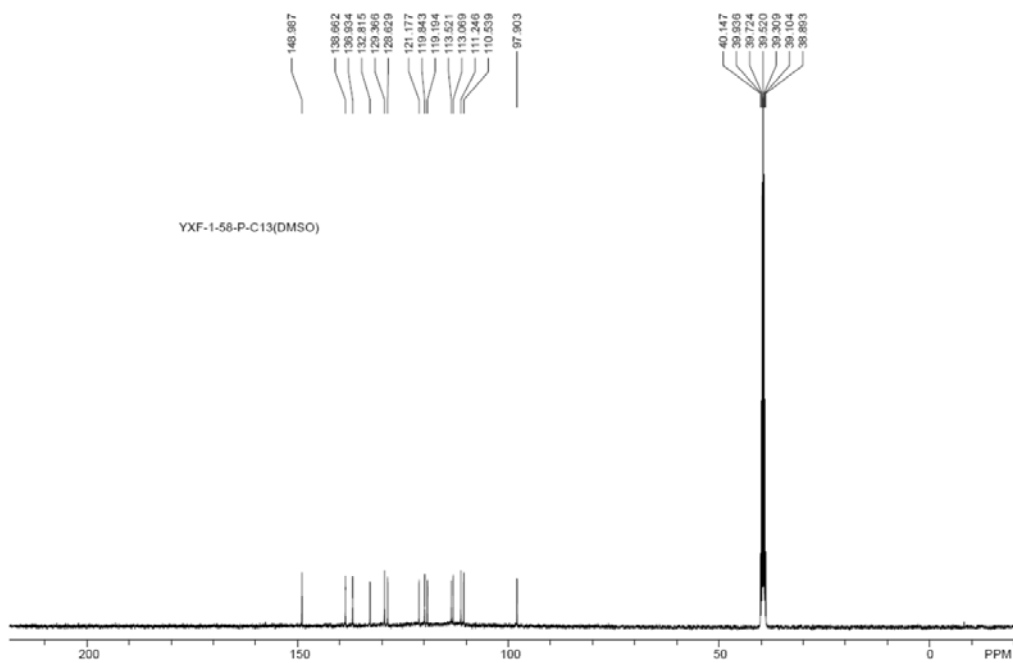
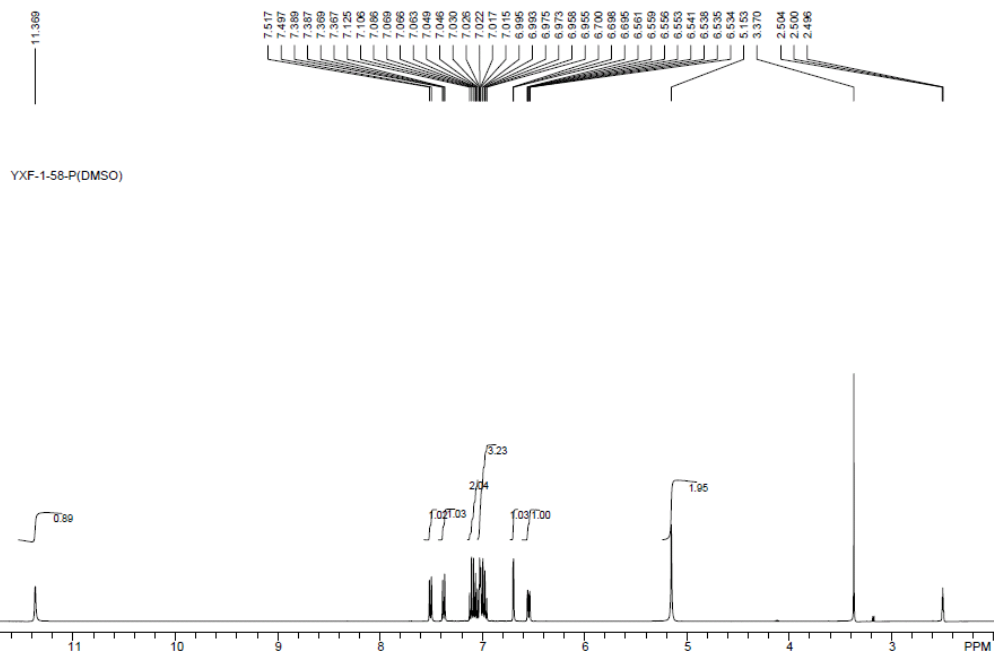
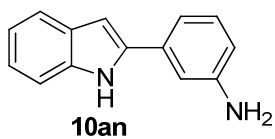
PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.972	23808674	4075838	100.000	100.000
Total		23808674	4075838	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-30-P.lcd

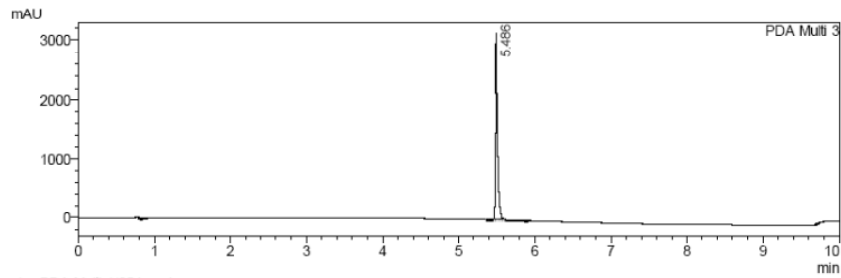
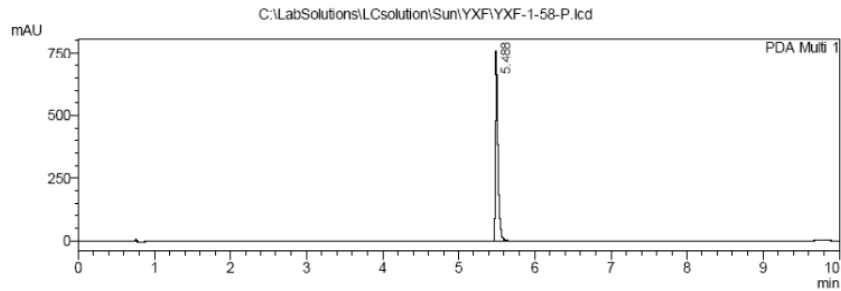
¹H NMR, ¹³C NMR and HPLC spectra of compound 10an



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-58-P.lcd
 Sample Name : YXF-1-58-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-58-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/28/2011 4:58:27 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

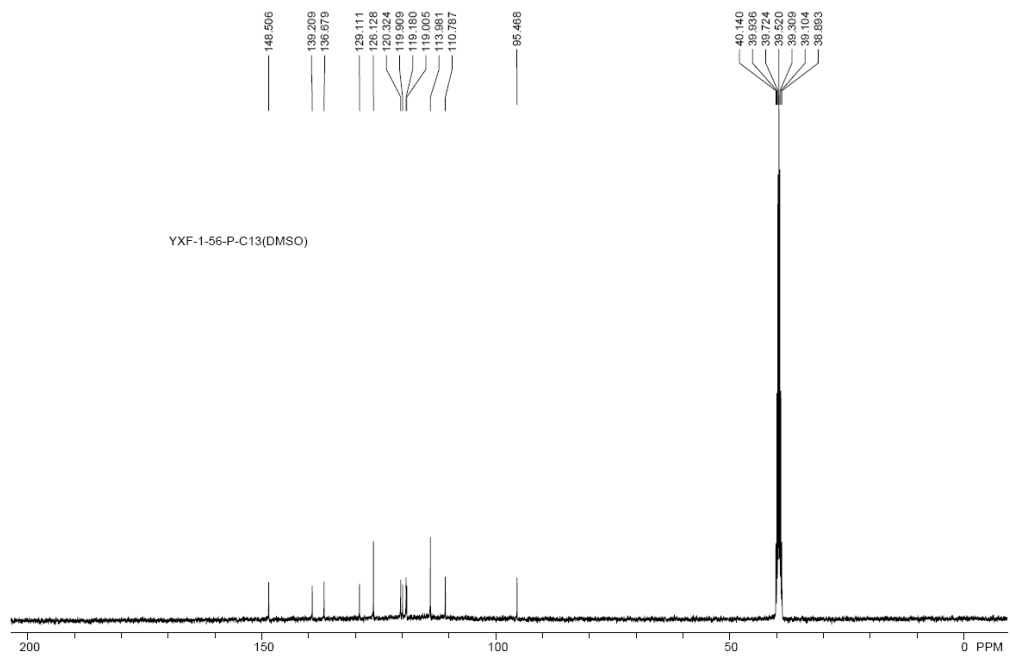
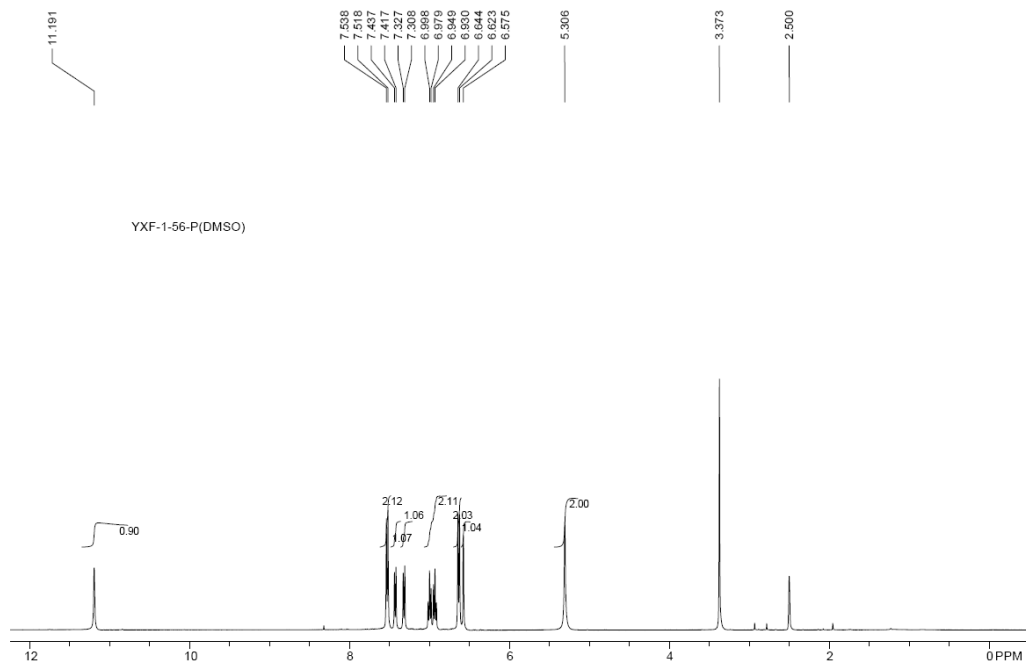
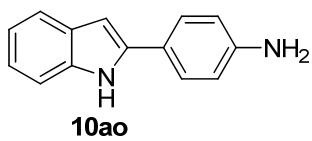
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.488	1839902	733349	100.000	100.000
Total		1839902	733349	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.486	5740944	3141286	100.000	100.000
Total		5740944	3141286	100.000	100.000

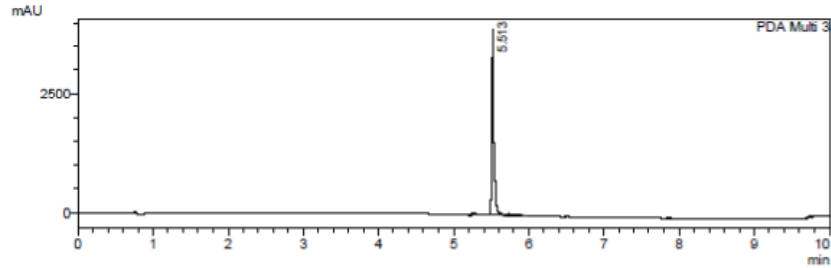
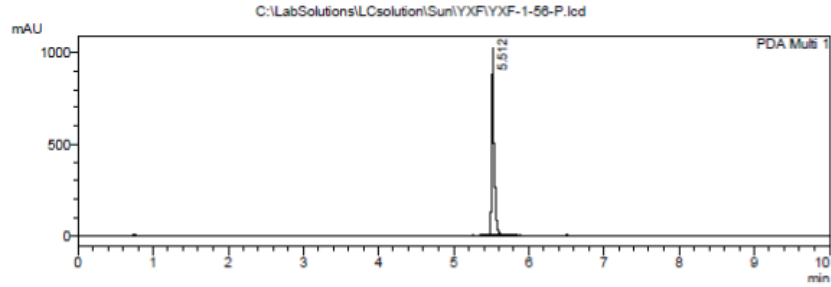
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ao



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-56-P
 Tray# : 1
 Vail # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-56-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/25/2011 11:06:38 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

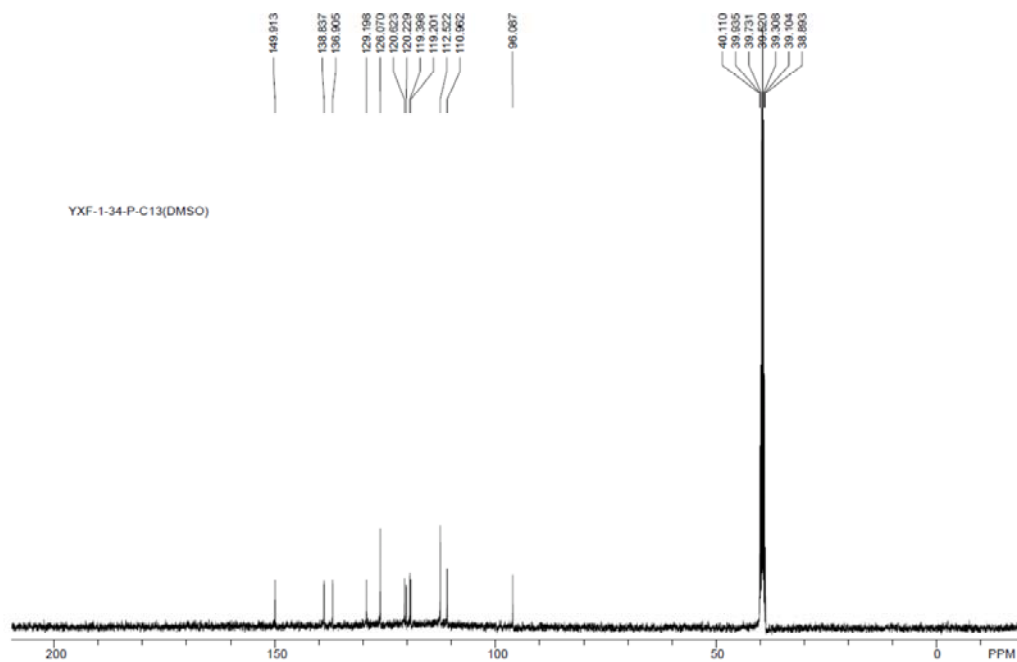
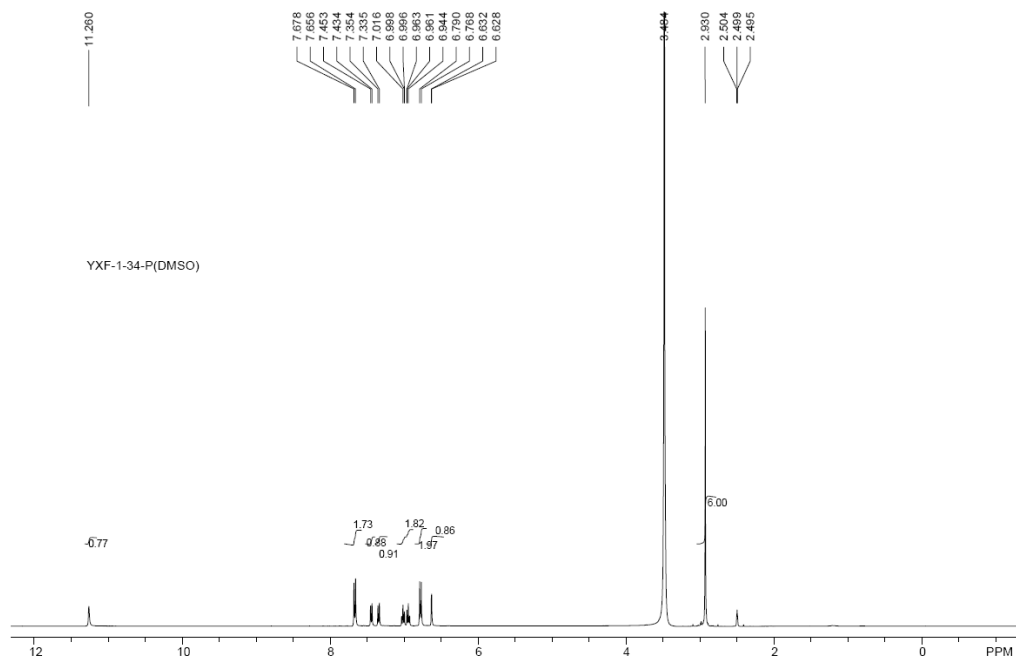
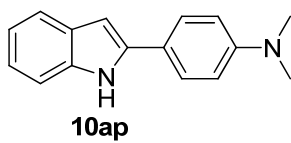
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.512	2556906	986066	100.000	100.000
Total		2556906	986066	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.513	8245465	3892024	100.000	100.000
Total		8245465	3892024	100.000	100.000

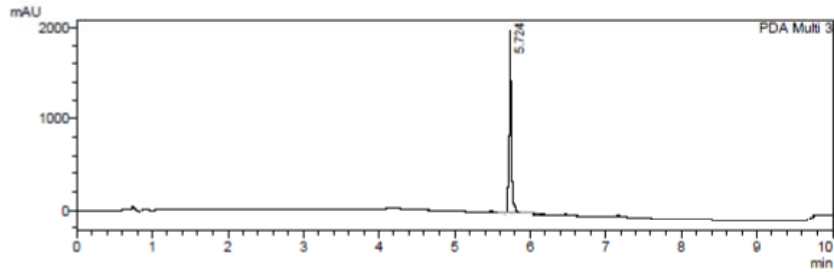
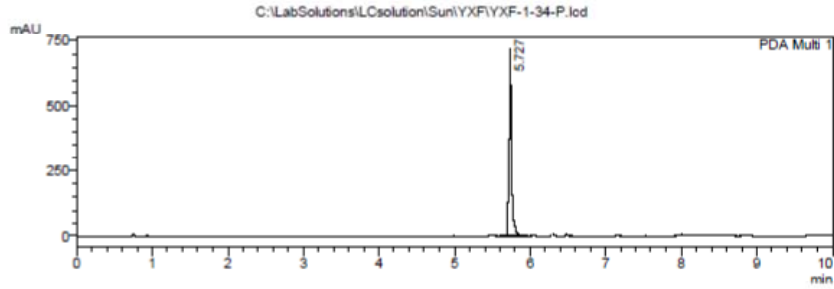
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ap



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-34-P.lcd
 Sample Name : YXF-1-34-P
 Tray# : 1
 Vial # : 16
 Injection Volume : 5 uL
 Data File Name : YXF-1-34-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/28/2011 5:39:33 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

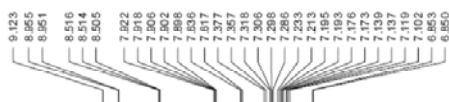
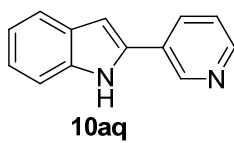
Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.727	1744930	701.796	100.000	100.000
Total		1744930	701.796	100.000	100.000

PeakTable

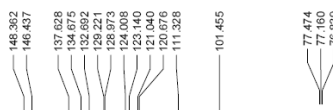
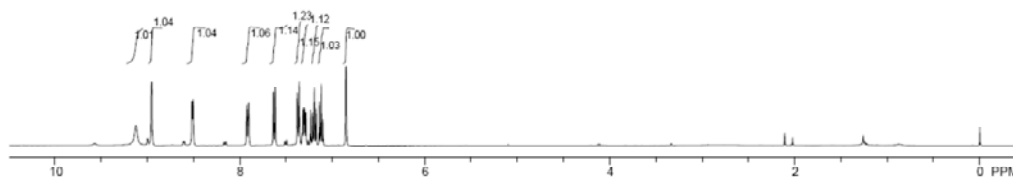
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.724	4329639	1985647	100.000	100.000
Total		4329639	1985647	100.000	100.000

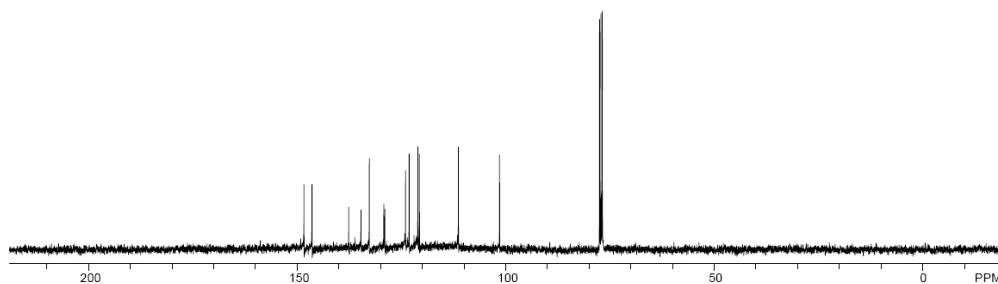
¹H NMR, ¹³C NMR and HPLC spectra of compound 10aq



YXF-1-35-P



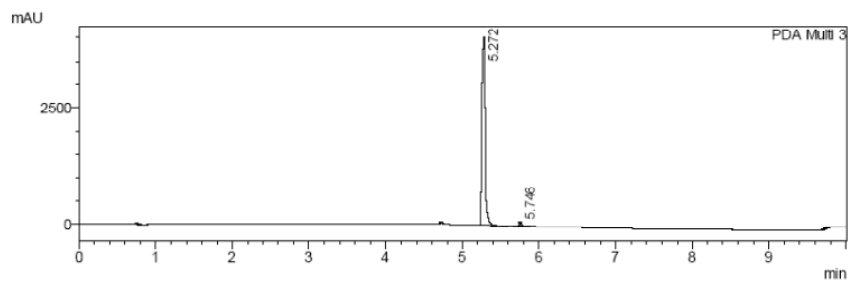
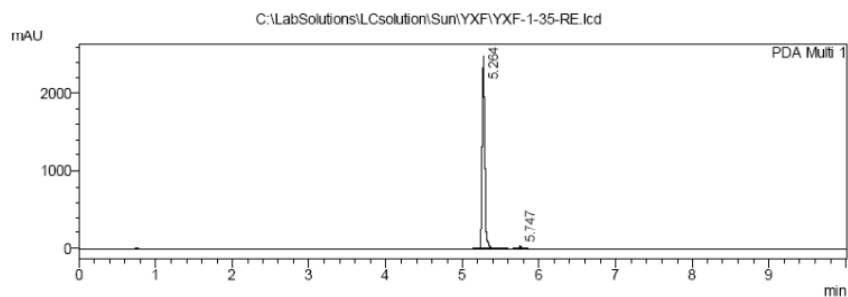
YXF-1-35-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-35-RE
 Tray# : 1
 Vial # : 31
 Injection Volume : 10 uL
 Data File Name : YXF-1-35-RE.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/4/2011 8:58:55 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.264	5223591	2336958	98.643	98.716
2	5.747	71854	30402	1.357	1.284
Total		5295445	2367360	100.000	100.000

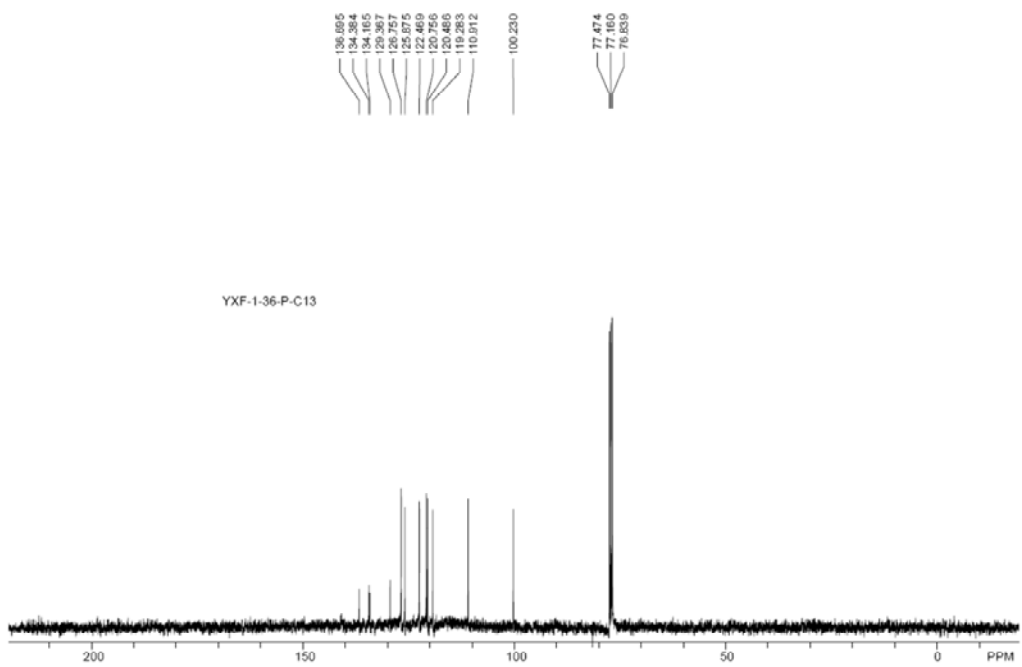
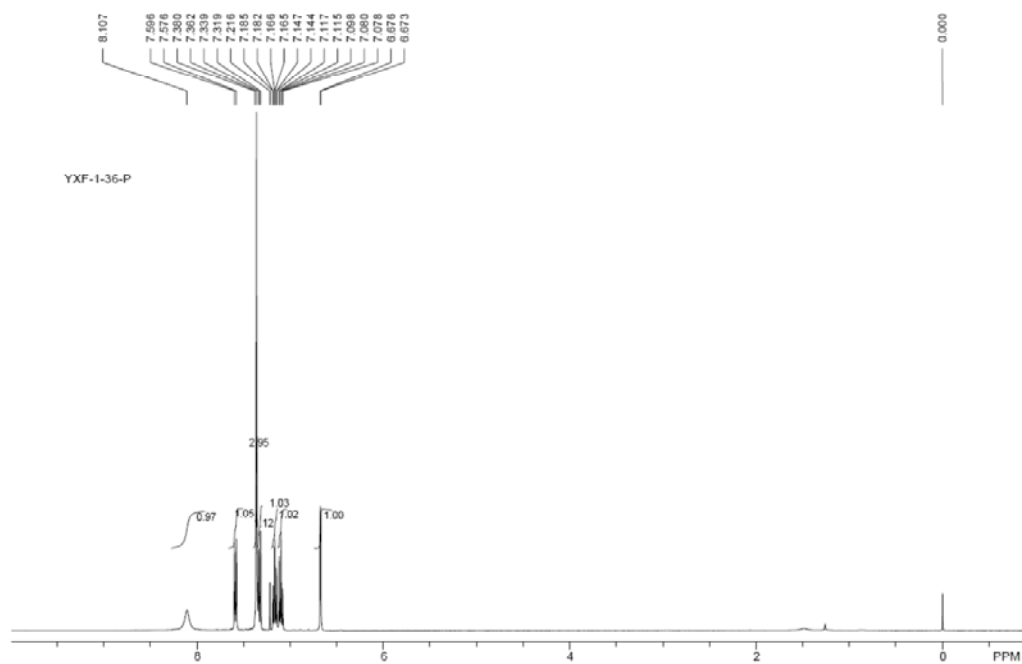
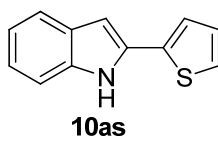
PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.272	11134909	4030522	98.175	97.866
2	5.746	206951	87877	1.825	2.134
Total		11341861	4118399	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-35-RE.lcd

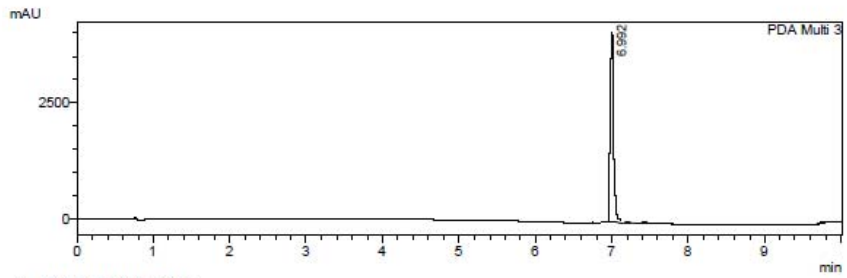
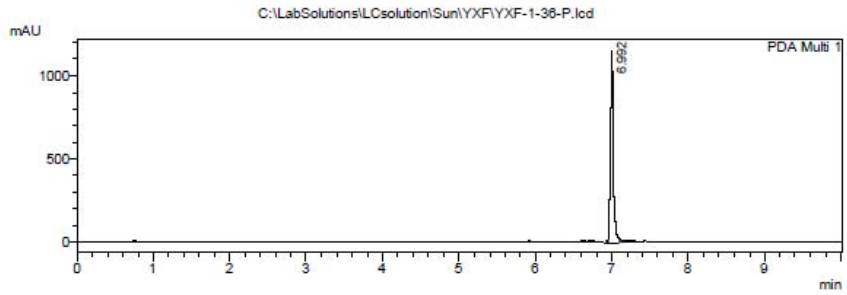
¹H NMR, ¹³C NMR and HPLC spectra of compound 10as



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-36-P.lcd
 Sample Name : YXF-1-36-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-36-P.lcd
 Method File Name : SDQ gradient.lom
 Batch File Name :
 Data Acquired : 11/2/2011 9:32:59 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

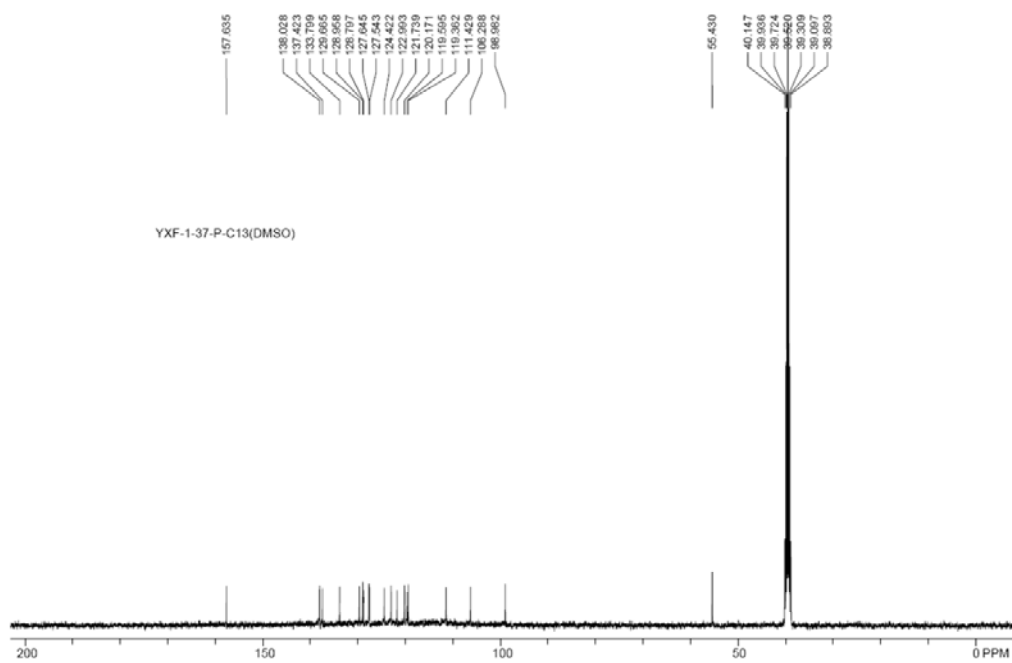
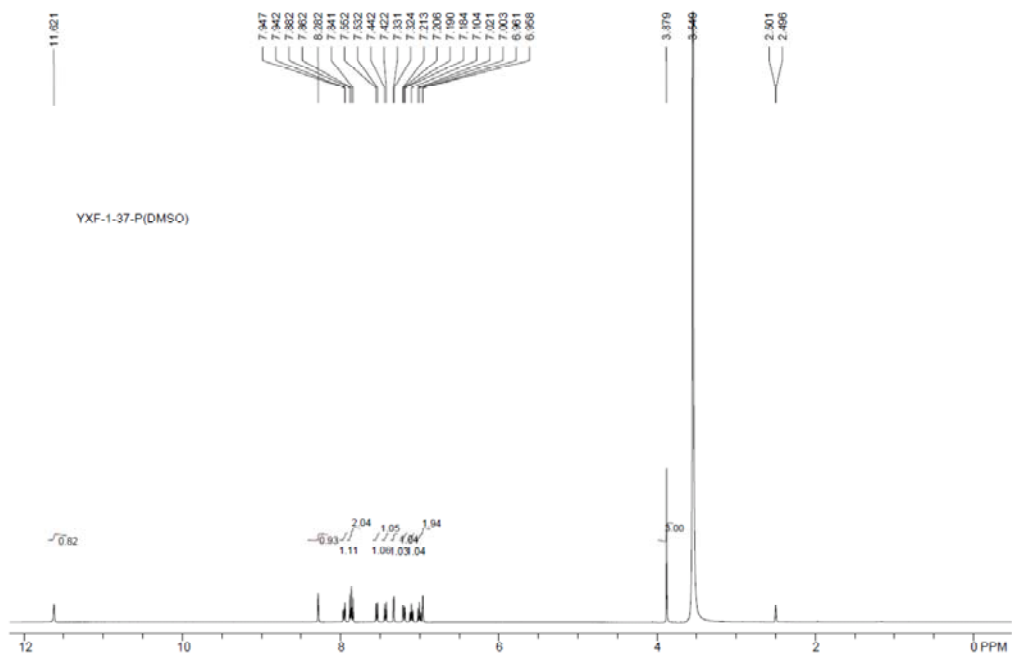
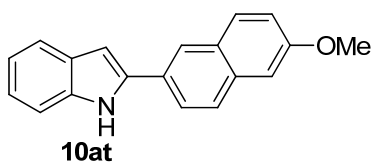
PeakTable

PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.992	2960666	1109863	100.000	100.000
Total		2960666	1109863	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.992	13002716	4075365	100.000	100.000
Total		13002716	4075365	100.000	100.000

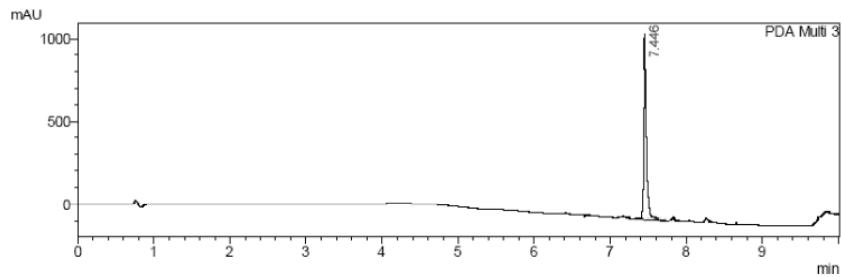
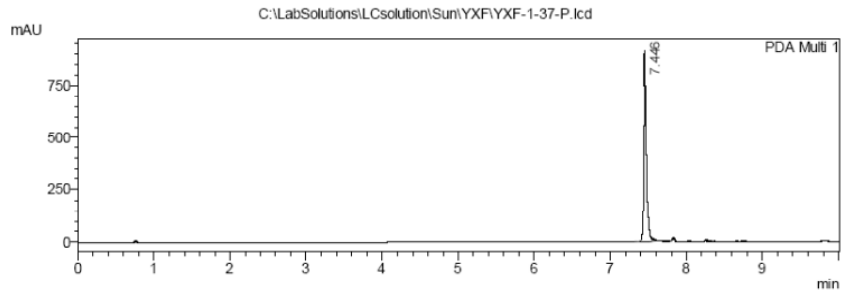
¹H NMR, ¹³C NMR and HPLC spectra of compound 10at



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-37-P
 Tray# : 1
 Vial# : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-37-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/3/2011 3:08:17 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

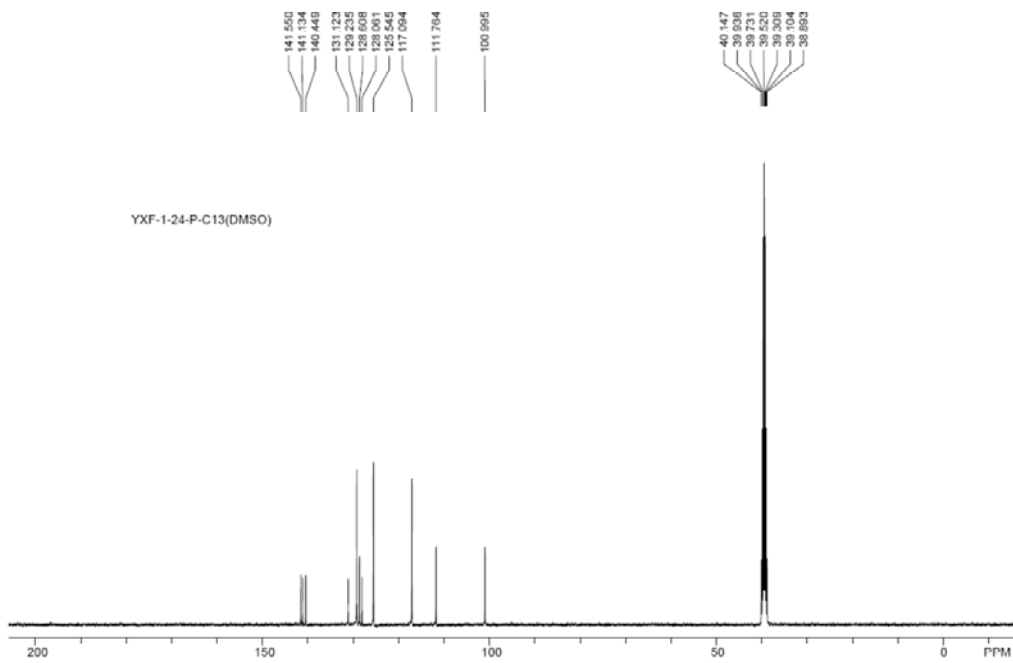
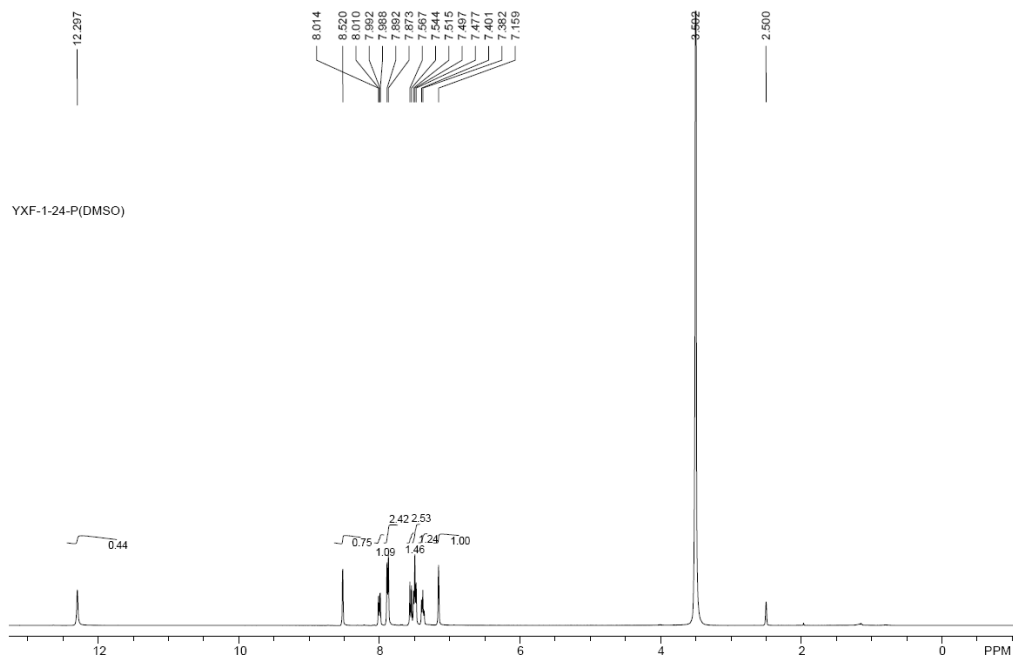
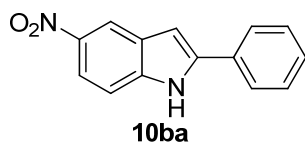
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.446	2313370	899173	100.000	100.000
Total		2313370	899173	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.446	2795756	1113262	100.000	100.000
Total		2795756	1113262	100.000	100.000

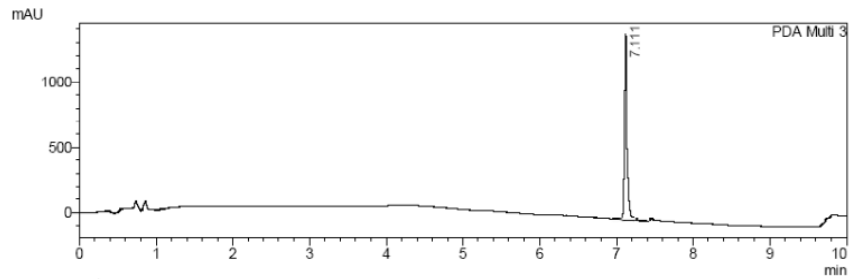
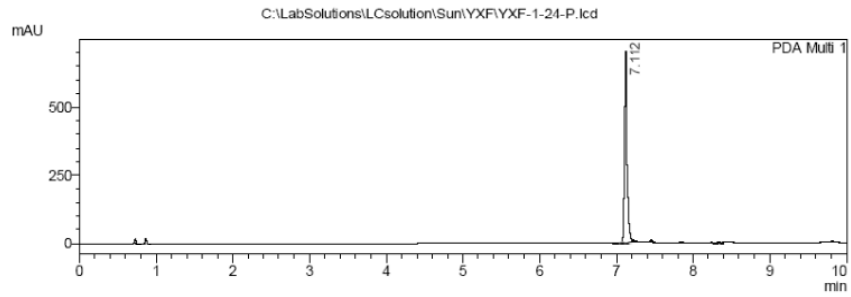
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ba



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-24-P
 Tray# : 1
 Vial # : 2
 Injection Volume : 5 uL
 Data File Name : YXF-1-24-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 10/13/2011 10:30:57 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

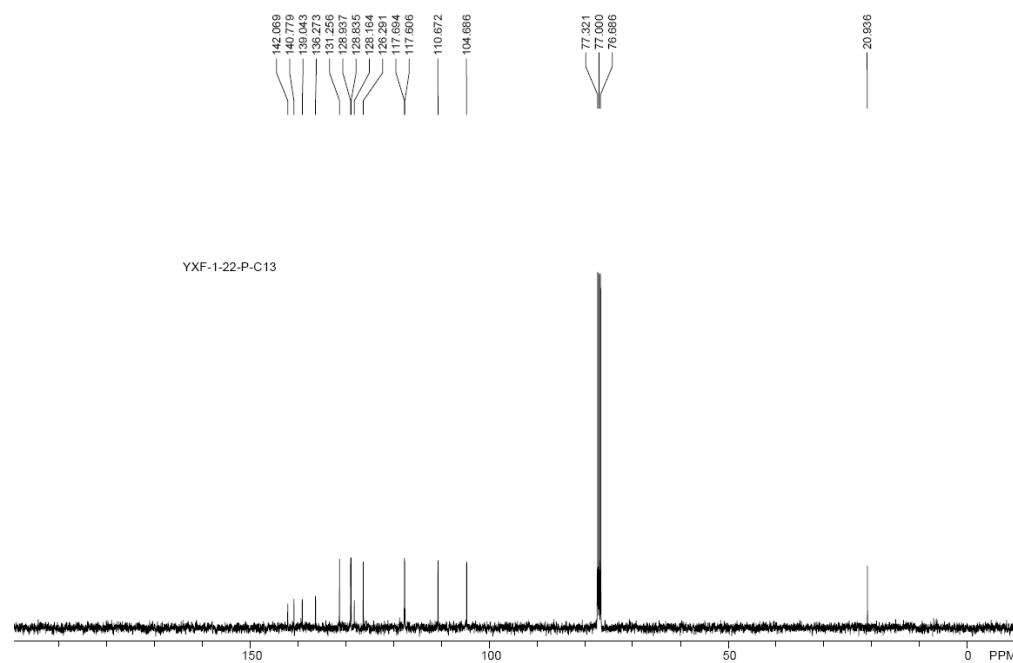
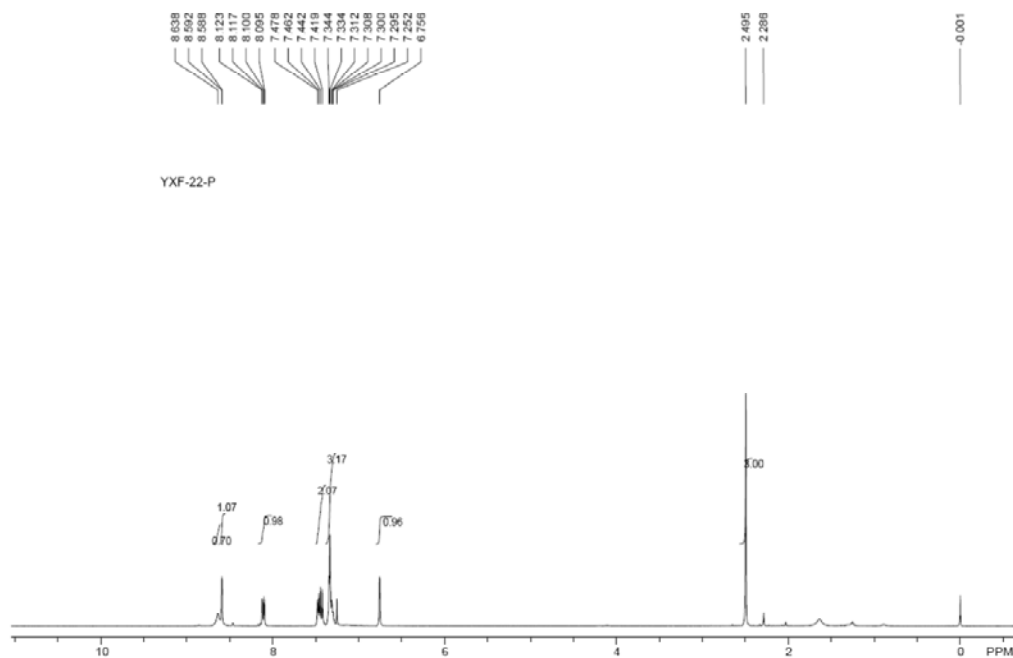
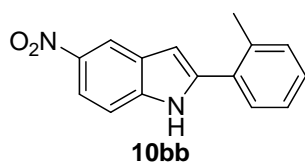
PDA Ch1 254nm 4nm						
Peak#	Ret. Time	Area	Height	Area %	Height %	
1	7.112	1788630	677180	100.000	100.000	
Total		1788630	677180	100.000	100.000	

PeakTable

PDA Ch3 220nm 4nm						
Peak#	Ret. Time	Area	Height	Area %	Height %	
1	7.111	3499548	1412401	100.000	100.000	
Total		3499548	1412401	100.000	100.000	

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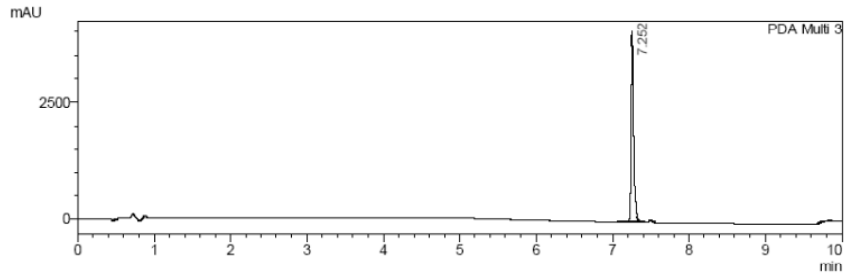
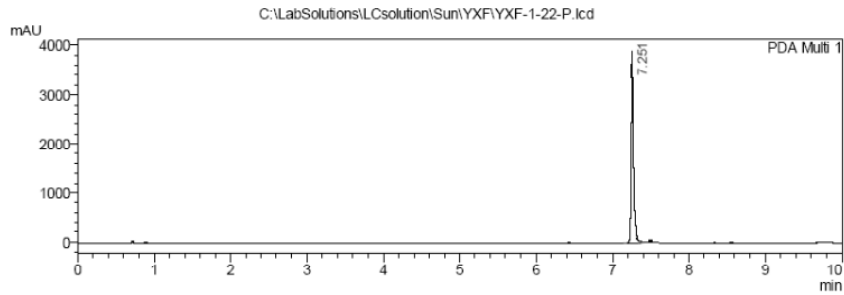
¹H NMR, ¹³C NMR and HPLC spectra of compound 10bb



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-22-P.lcd
 Sample Name : YXF-1-22-P
 Tray# : 1
 Vial # : 4
 Injection Volume : 10 uL
 Data File Name : YXF-1-22-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 10/7/2011 9:41:11 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

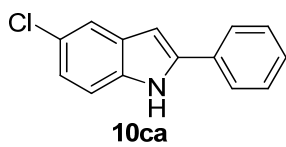
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.251	9249252	3859024	100.000	100.000
Total		9249252	3859024	100.000	100.000

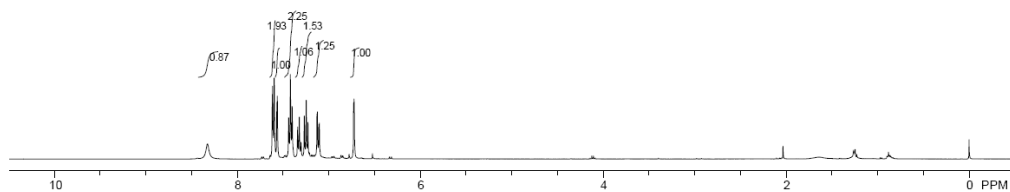
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.252	10459178	4044788	100.000	100.000
Total		10459178	4044788	100.000	100.000

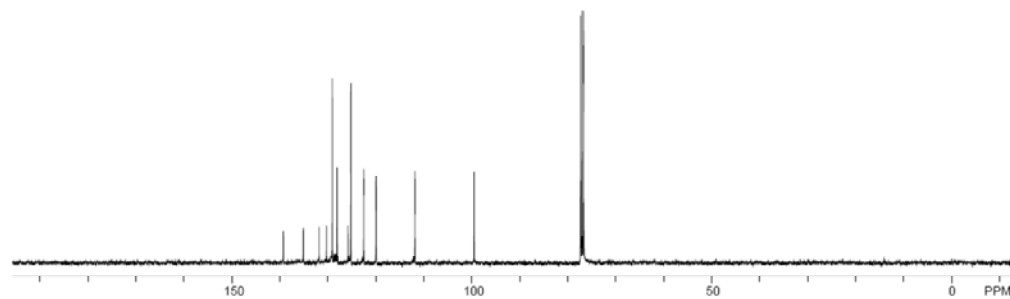
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ca



YXF-1-25-P



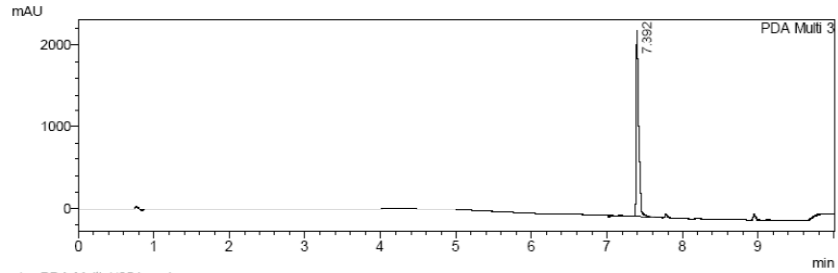
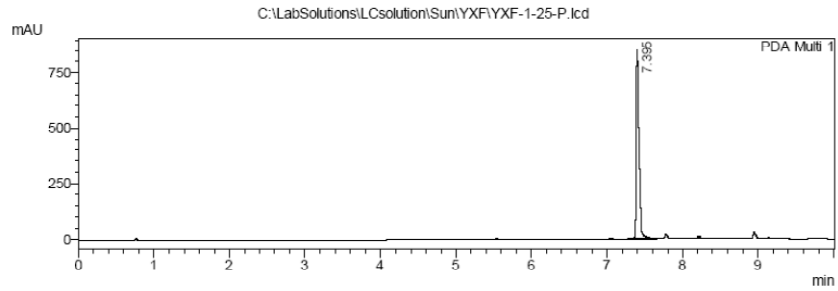
YXF-1-25-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-25-P
 Tray# : 1
 Vial # : 46
 Injection Volume : 5 uL
 Data File Name : YXF-1-25-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/14/2011 1:00:34 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

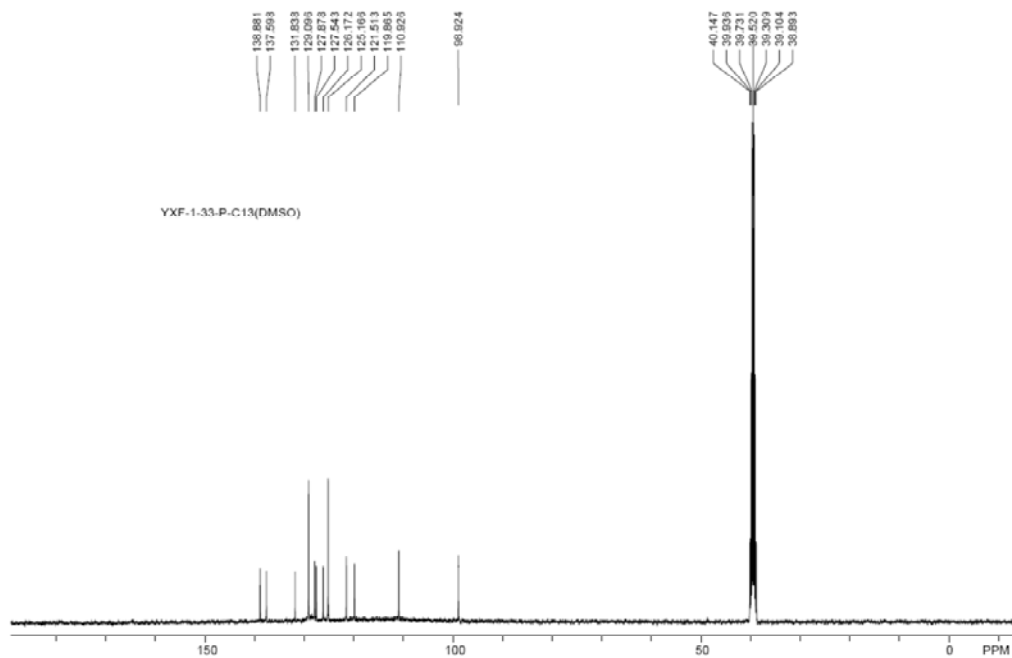
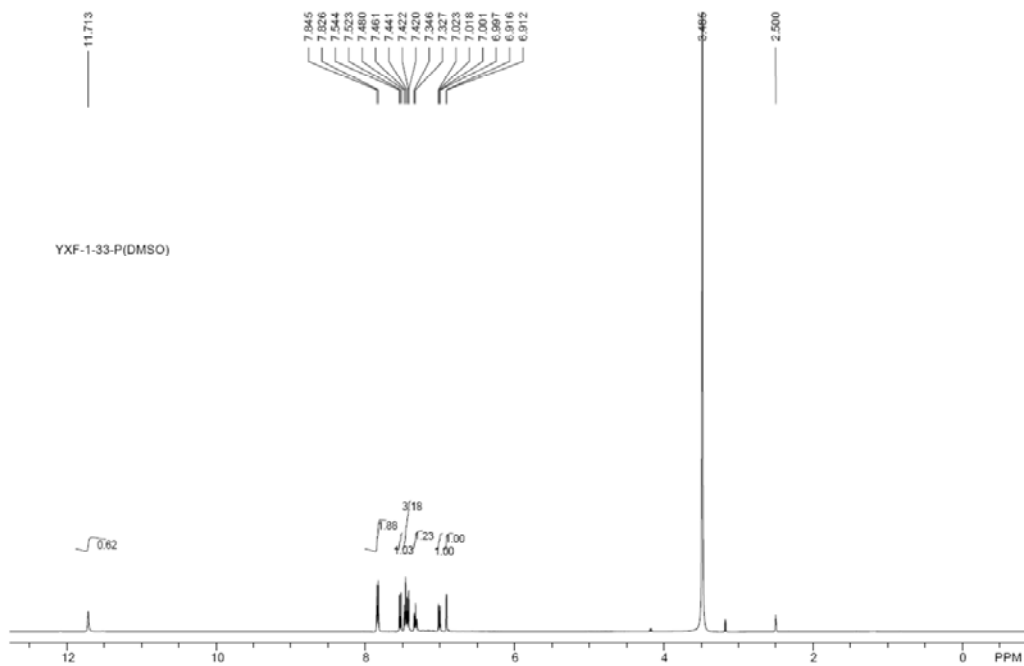
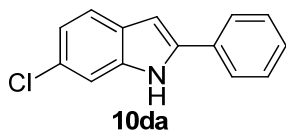
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.395	2156402	839166	100.000	100.000
Total		2156402	839166	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.392	5060669	2272048	100.000	100.000
Total		5060669	2272048	100.000	100.000

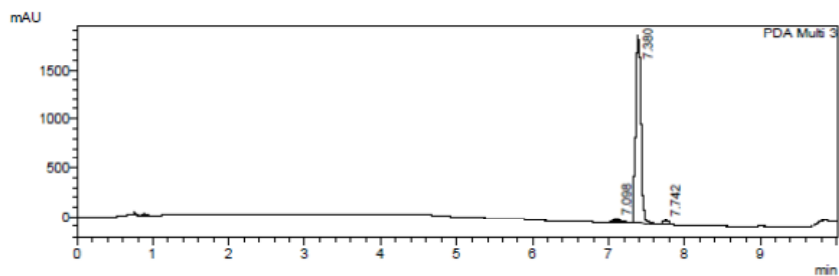
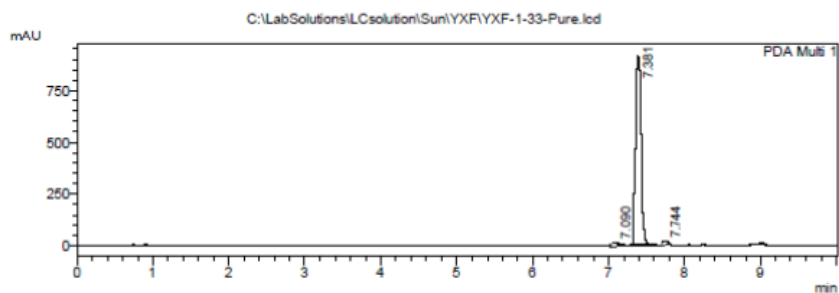
¹H NMR, ¹³C NMR and HPLC spectra of compound 10da



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-33-Pure
 Tray# : 1
 Vial # : 31
 Injection Volume : 3 uL
 Data File Name : YXF-1-33-Pure.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 2/29/2012 11:54:23 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.090	71624	14268	1.466	1.506
2	7.381	4731715	916578	96.845	96.728
3	7.744	82514	16739	1.689	1.766
Total		4885853	947585	100.000	100.000

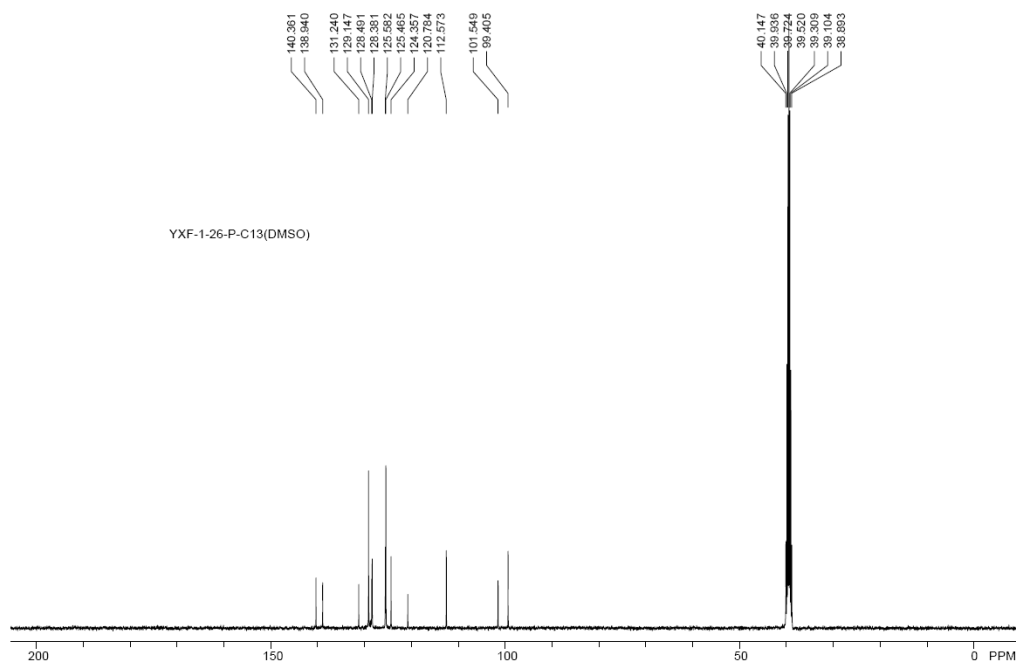
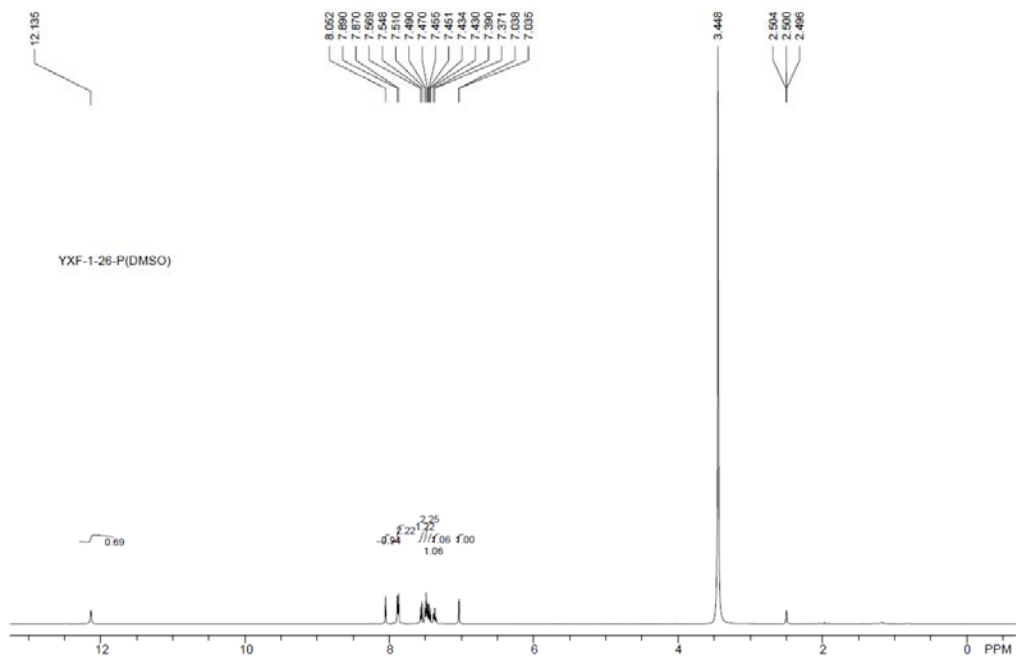
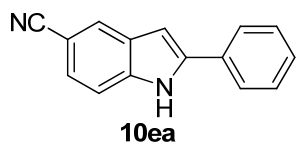
PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.098	177928	35004	1.831	1.776
2	7.380	9366588	1903411	96.406	96.554
3	7.742	171270	32936	1.763	1.671
Total		9715786	1971351	100.000	100.000

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-33-Pure.lcd

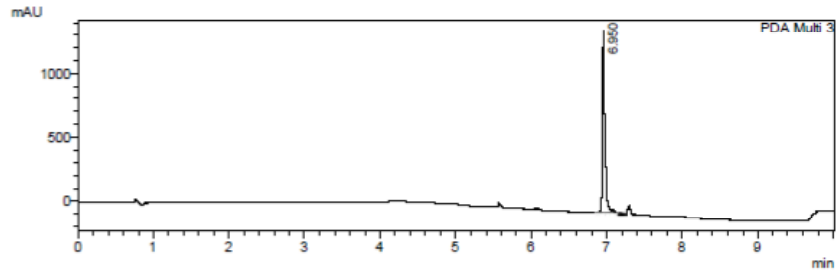
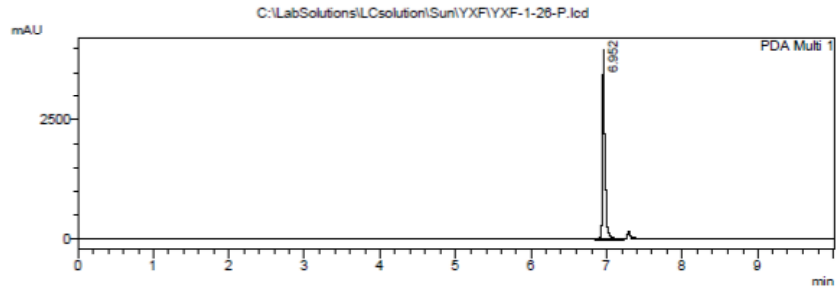
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ea



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-26-P
 Tray# : 1
 Vial # : 16
 Injection Volume : 5 uL
 Data File Name : YXF-1-26-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 10/17/2011 11:28:04 AM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

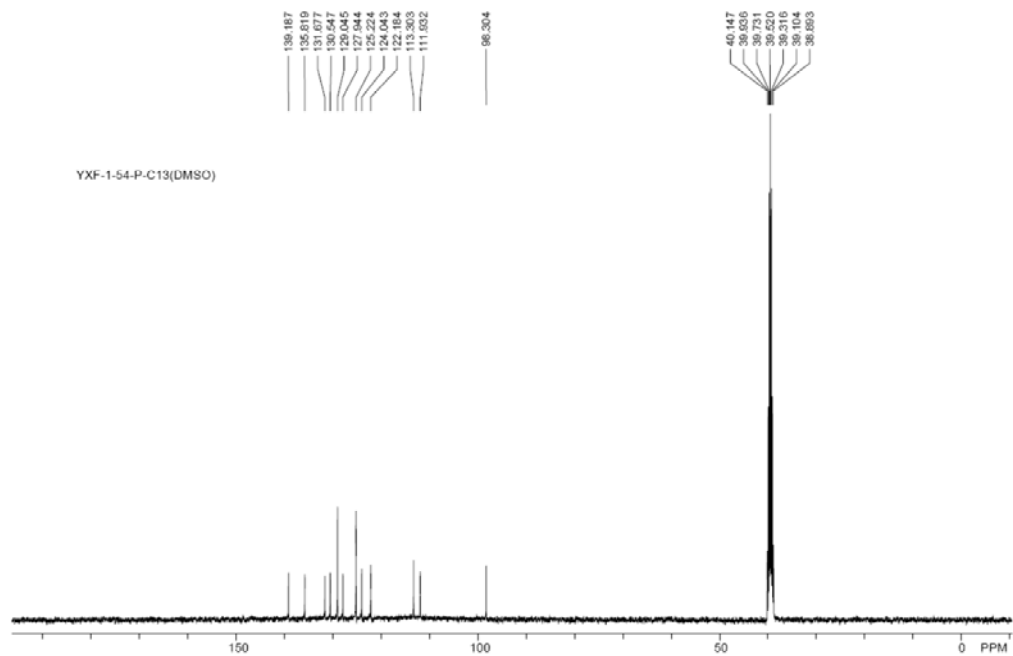
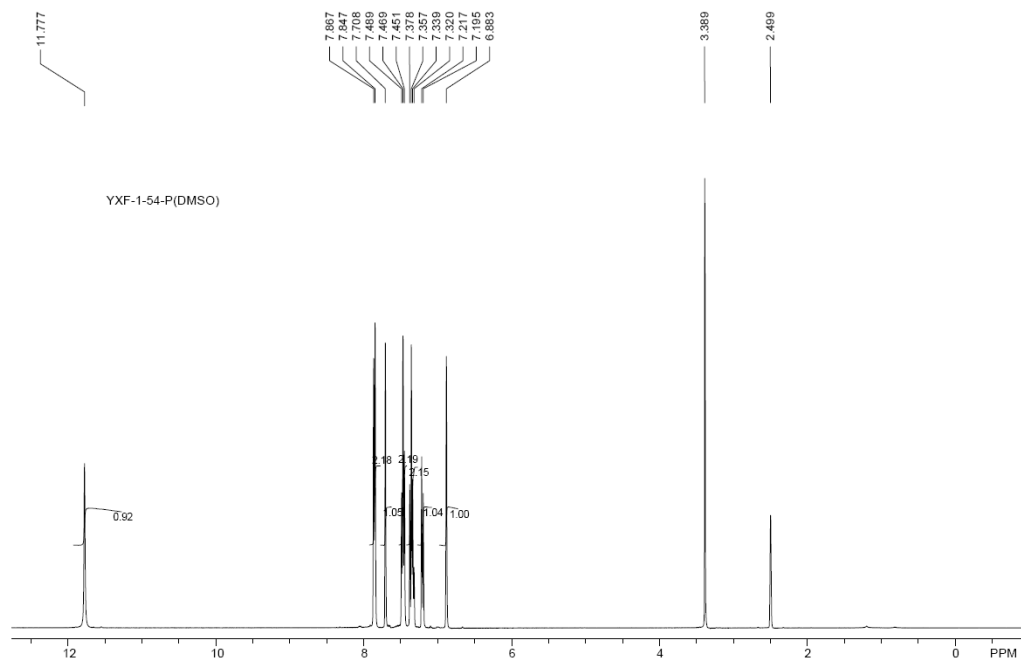
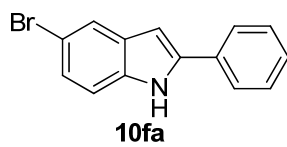
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.952	9777743	3791031	100.000	100.000
Total		9777743	3791031	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.950	3588053	1425354	100.000	100.000
Total		3588053	1425354	100.000	100.000

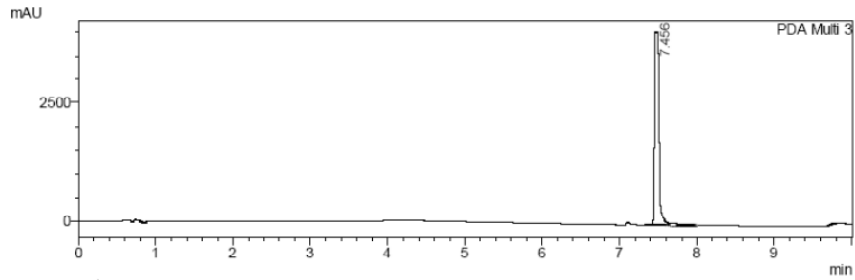
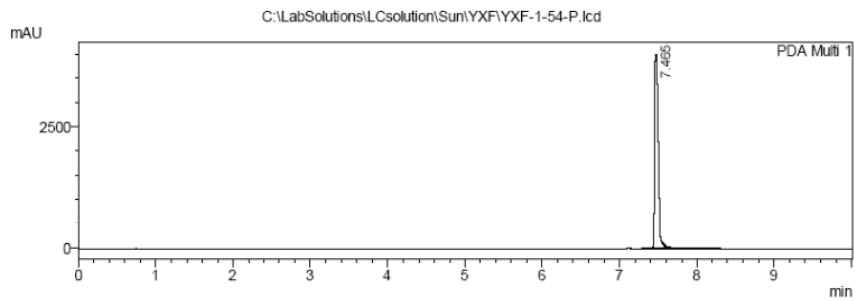
¹H NMR, ¹³C NMR and HPLC spectra of compound 10fa



==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\LCsolution\Sun\YXF\YXF-1-54-P.lcd
 Sample Name : YXF-1-54-P
 Tray# : 1
 Vail # : 31
 Injection Volume : 10 uL
 Data File Name : YXF-1-54-P.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name :
 Data Acquired : 11/22/2011 3:05:28 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

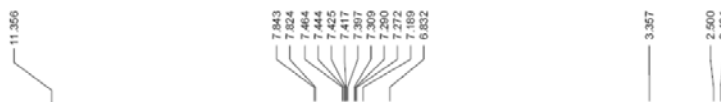
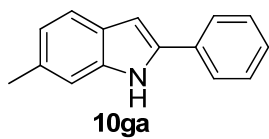
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.465	13537938	3998146	100.000	100.000
Total		13537938	3998146	100.000	100.000

PeakTable

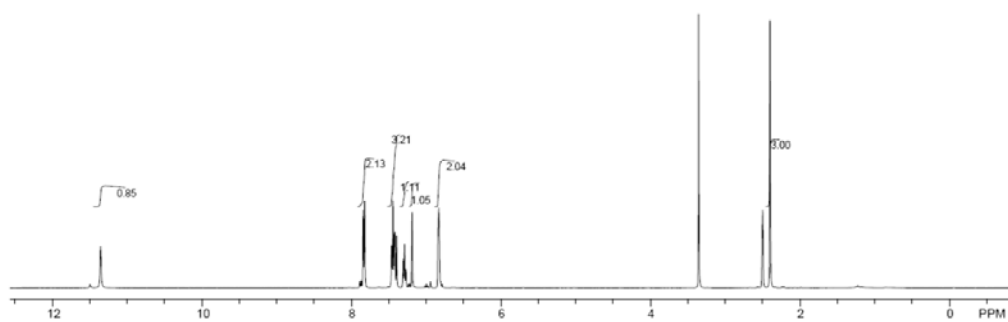
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.456	17386343	4085725	100.000	100.000
Total		17386343	4085725	100.000	100.000

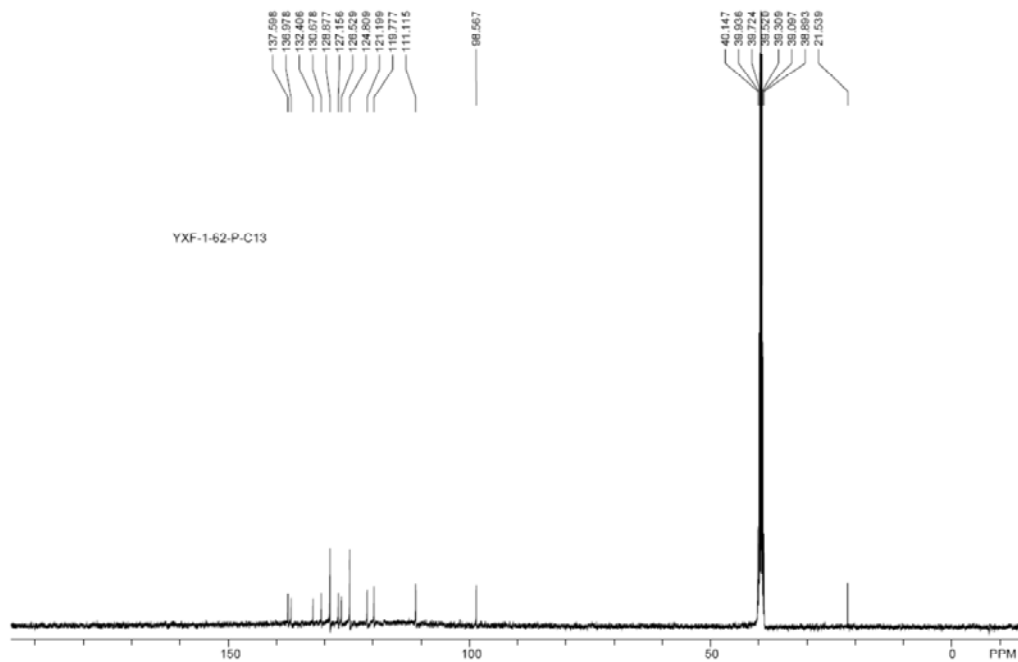
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ga



YXF-1-62-P(DMSO)



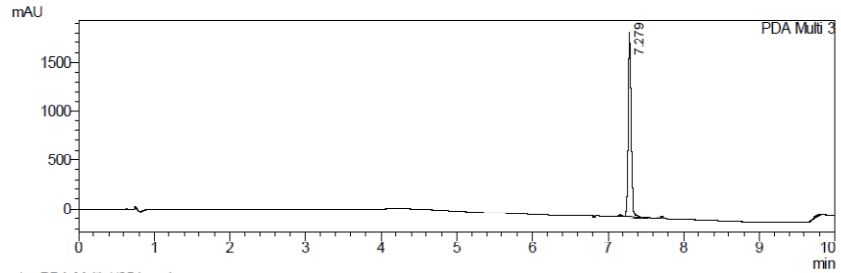
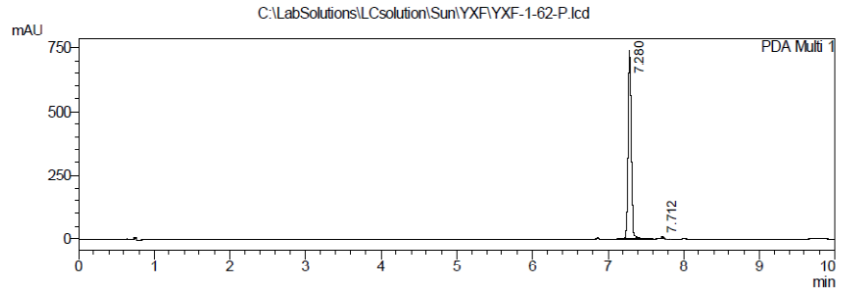
YXF-1-62-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-62-P
 Tray# : 1
 Vial # : 31
 Injection Volume : 5 uL
 Data File Name : YXF-1-62-P.lcd
 Method File Name : SDQ.gradient.lcm
 Batch File Name :
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<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

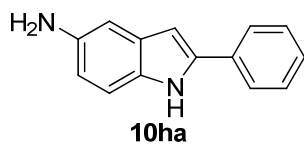
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.280	1998208	715790	98.850	98.465
2	7.712	23249	11159	1.150	1.535
Total		2021456	726949	100.000	100.000

PeakTable

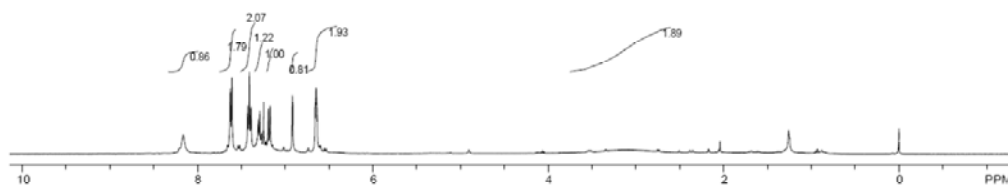
PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.279	4662707	1896352	100.000	100.000
Total		4662707	1896352	100.000	100.000

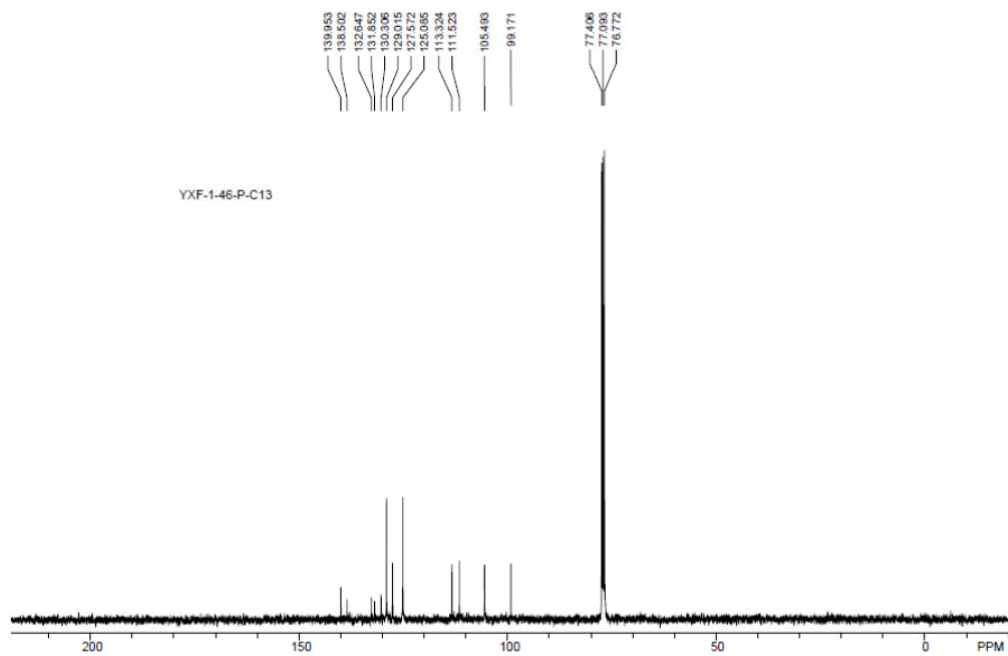
¹H NMR, ¹³C NMR and HPLC spectra of compound 10ha



YXF-1-46-P



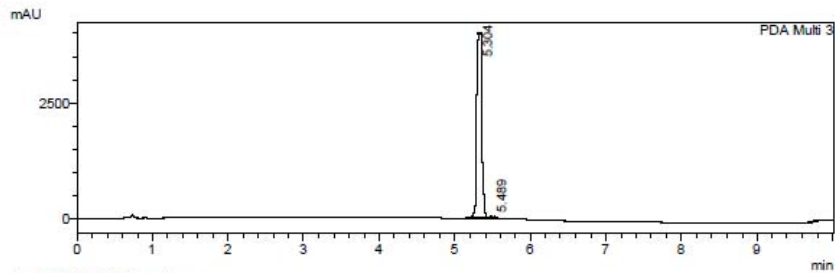
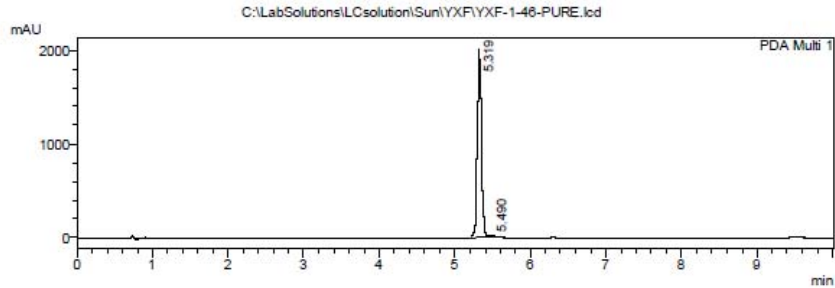
YXF-1-46-P-C13



==== Shimadzu LCsolution Analysis Report ====

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 Sample Name : YXF-1-46-P
 Tray# : 1
 Vial # : 32
 Injection Volume : 10 uL
 Data File Name : YXF-1-46-PURE.lcd
 Method File Name : SDQ gradient.lcm
 Batch File Name : Batch 1.lcb
 Data Acquired : 2/25/2012 1:45:45 PM

<Chromatogram>



- 1 PDA Multi 1/254nm 4nm
- 2 PDA Multi 3/220nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.319	8165117	1999113	99.237	98.940
2	5.490	62785	21421	0.763	1.060
Total		8227903	2020534	100.000	100.000

PeakTable

PDA Ch3 220nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.304	19503880	3982112	99.085	98.683
2	5.489	180134	53153	0.915	1.317
Total		19684014	4035264	100.000	100.000