Supporting Information

Design, Synthesis and Bioactivity Investigation of Tetrandrine Derivatives as Potential Anti-cancer Agents

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Content

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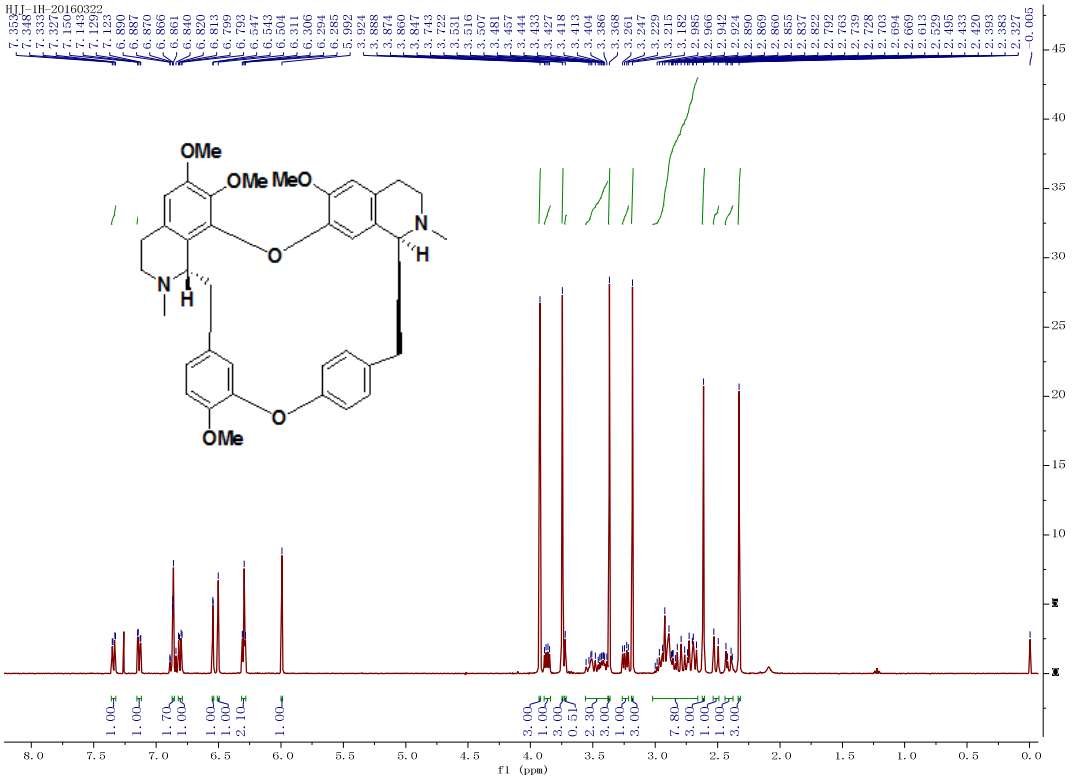
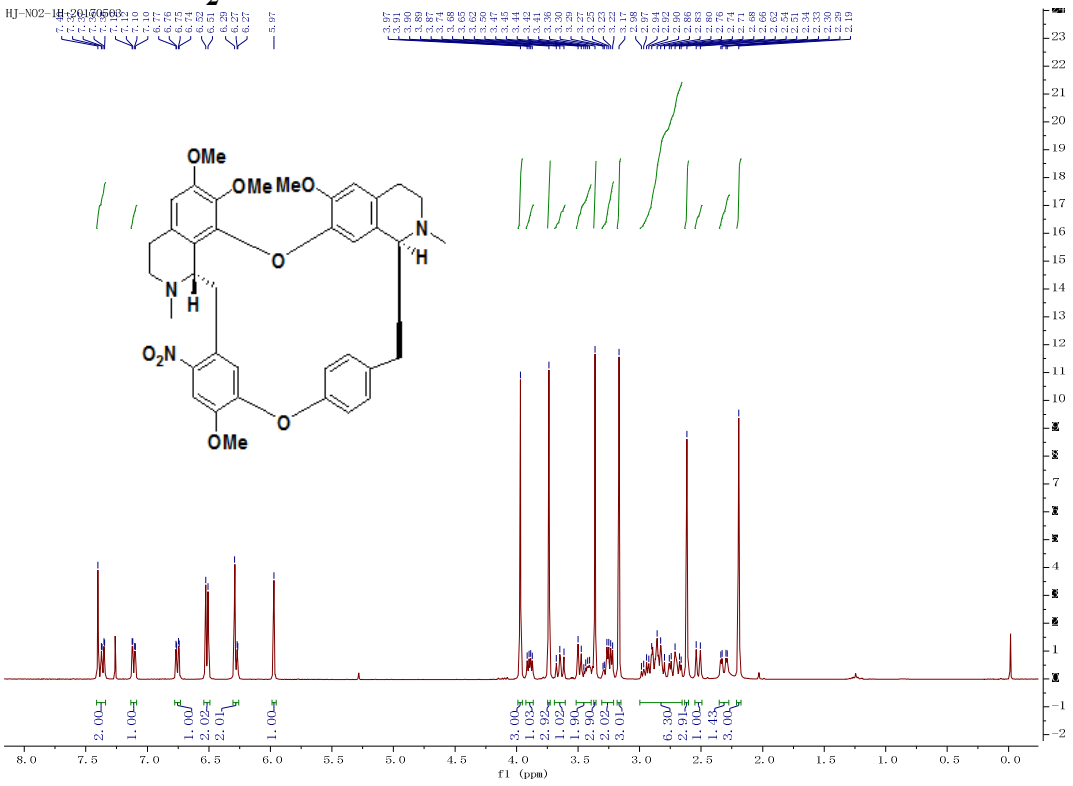
† These authors contributed equally to this work.

1. ^{1}H NMR Spectra

1.1.Tetrandrine



1.2. Tet-NO_2



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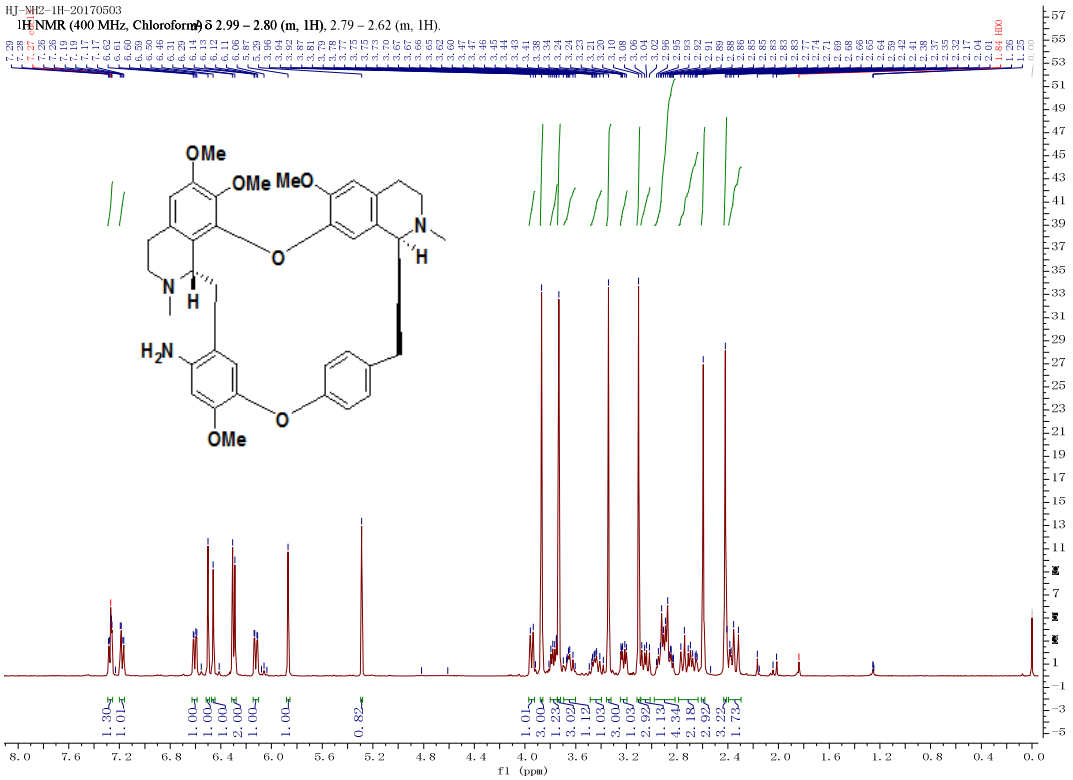
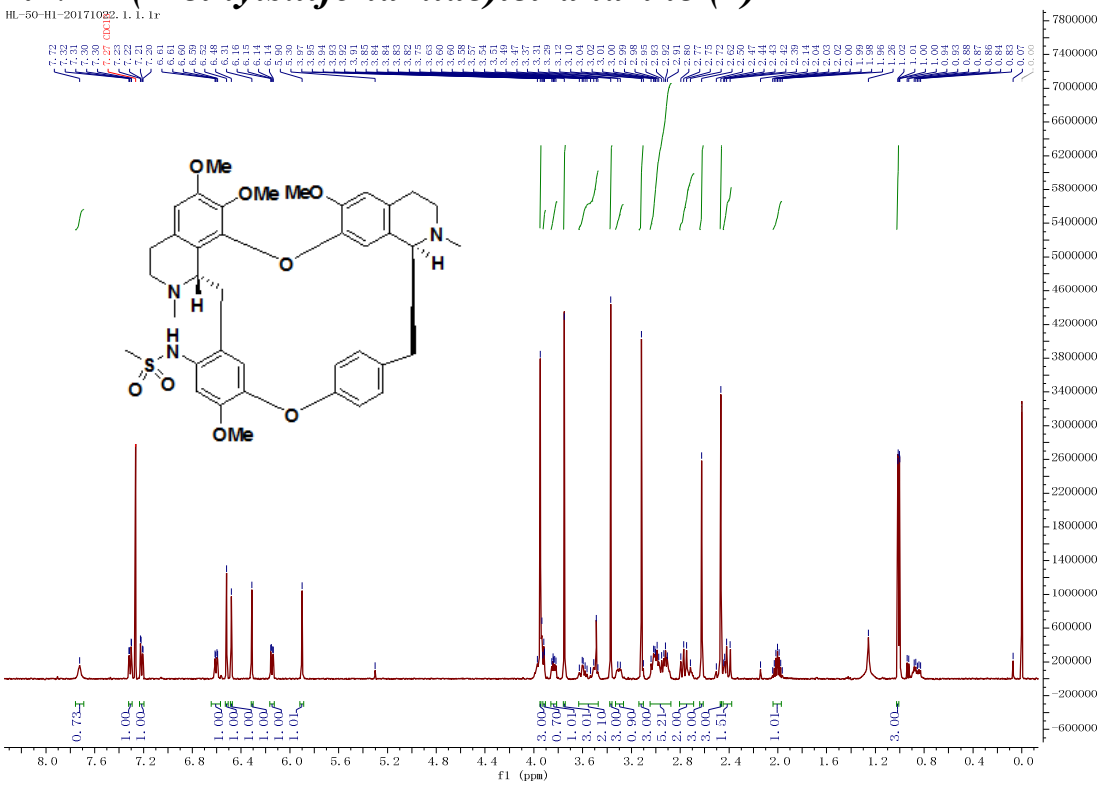
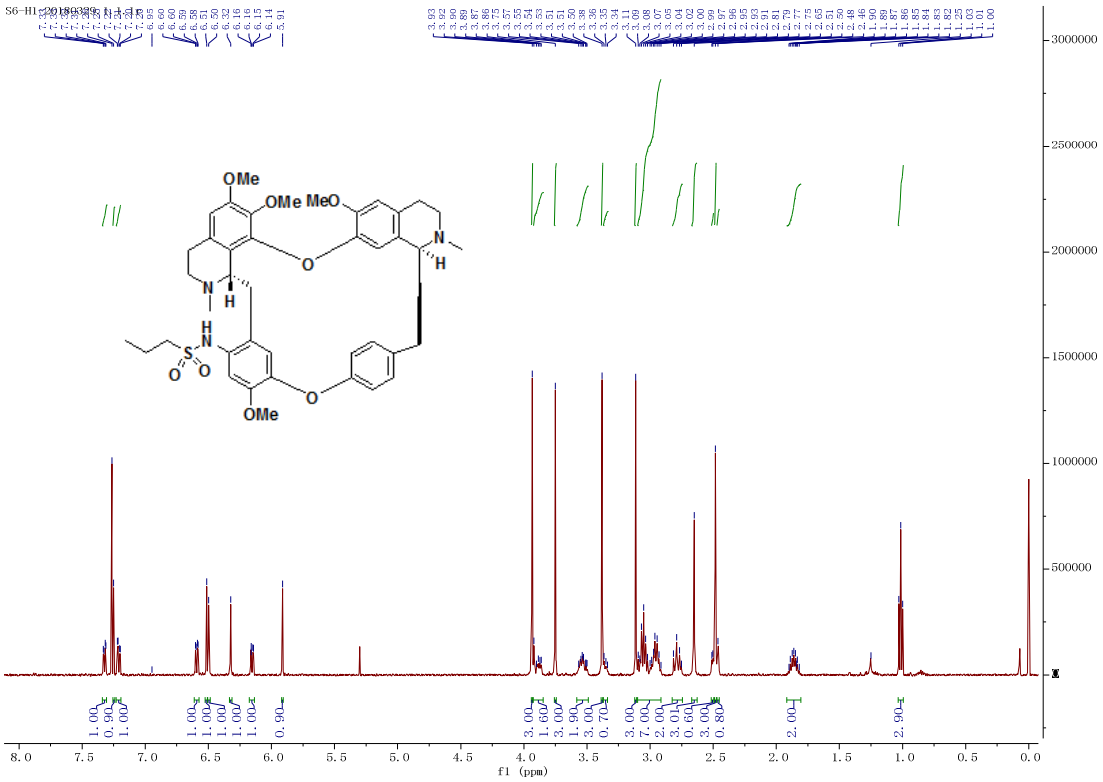


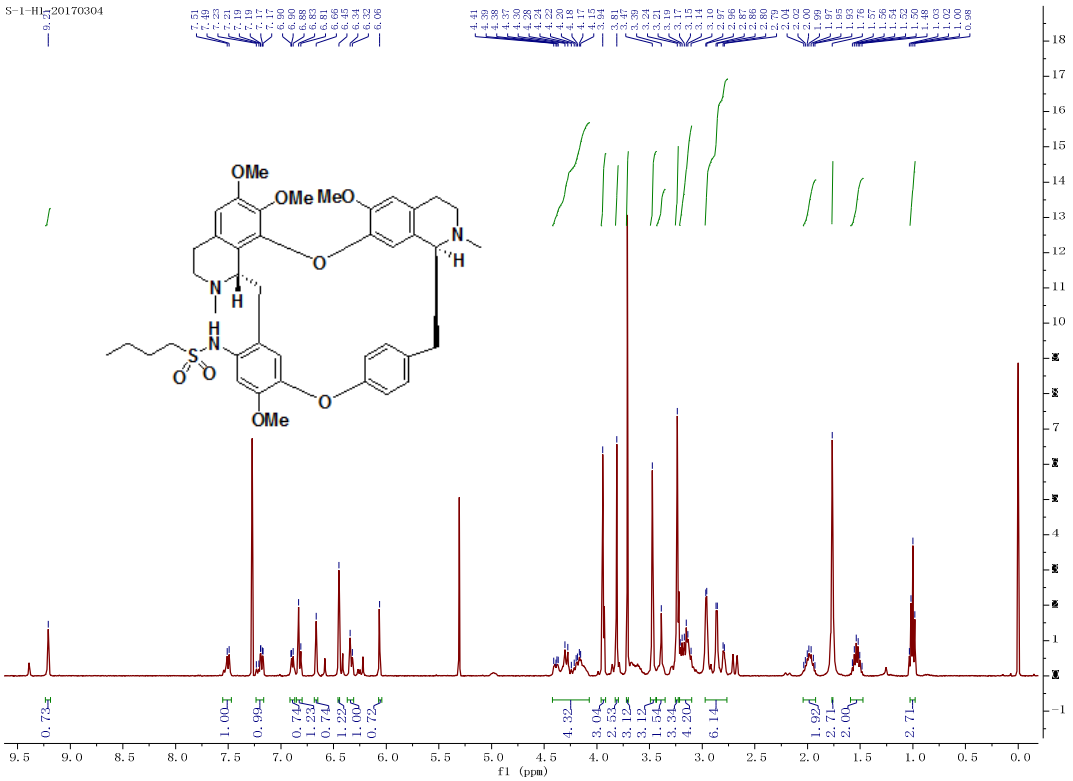
1.4. 14-(Methylsulfonamide)tetrandrine (1)



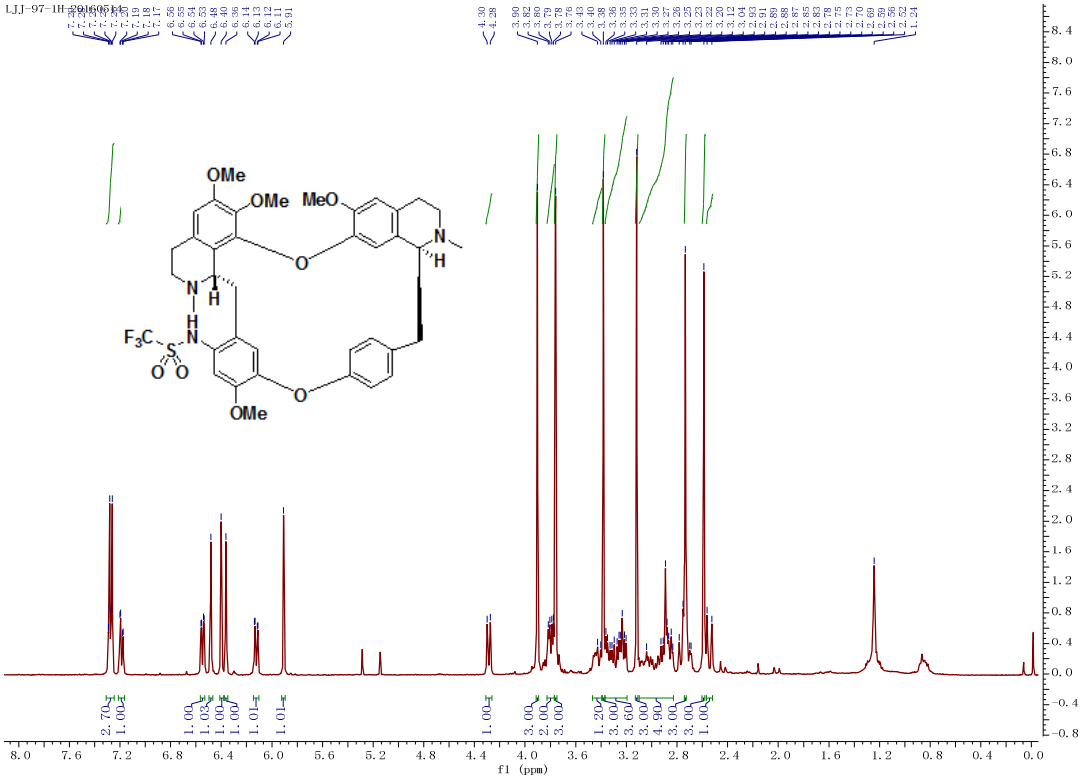
1.5. 14-(Propylsulfonamide)tetrandrine (2)



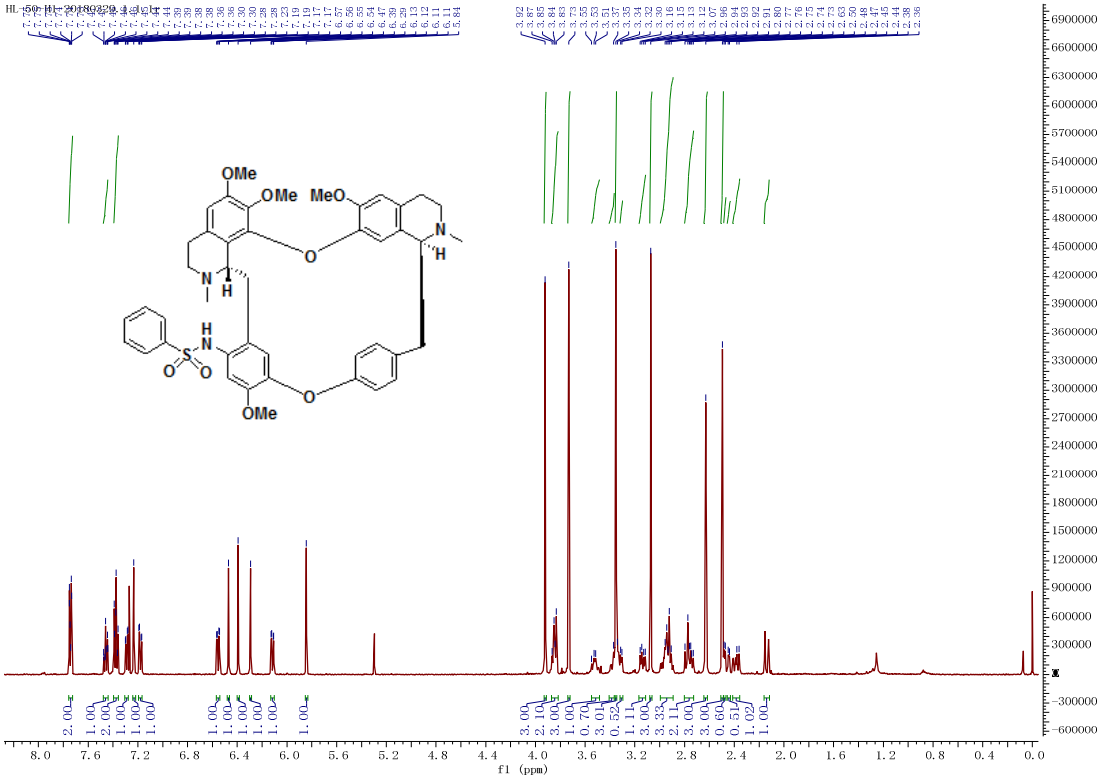
1.6. 14-(Butylsulfonamide)tetrandrine (3)



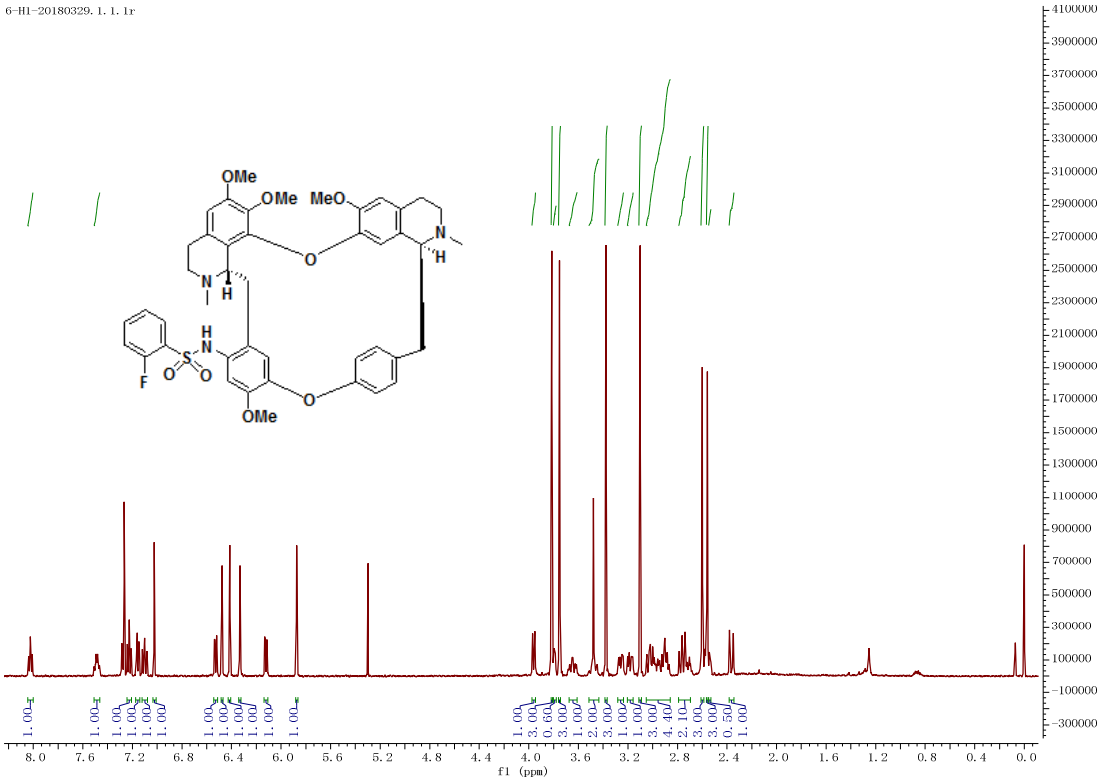
1.7. 14-(Trifluoromethylsulfonamide)tetrandrine (4)



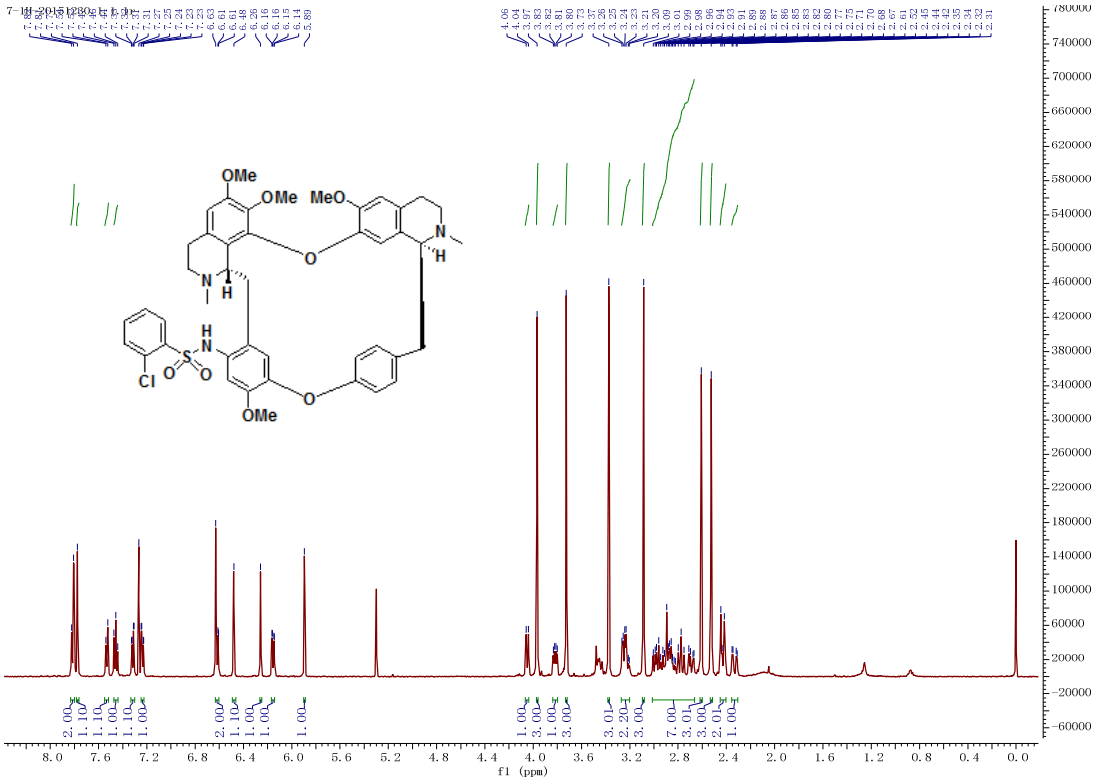
1.8. 14-(Benzenesulfonamide)tetrandrine (5)



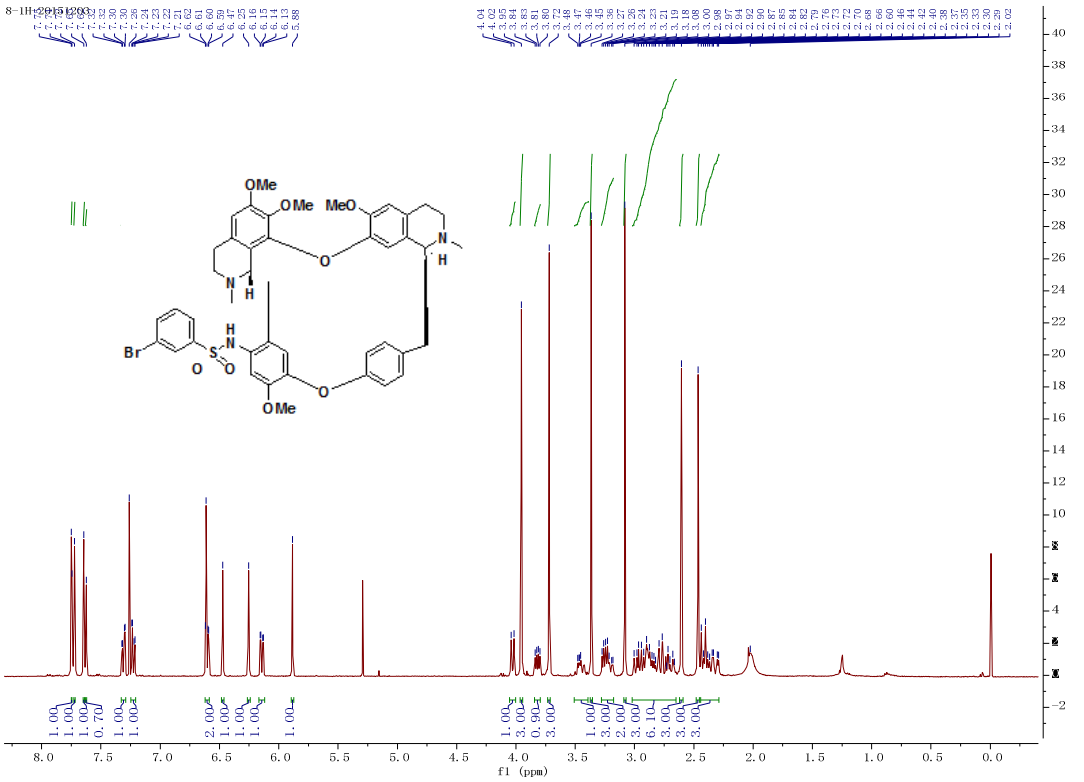
1.9. 14-(2-Fluorobenzenesulfonamide)tetrandrine (6)



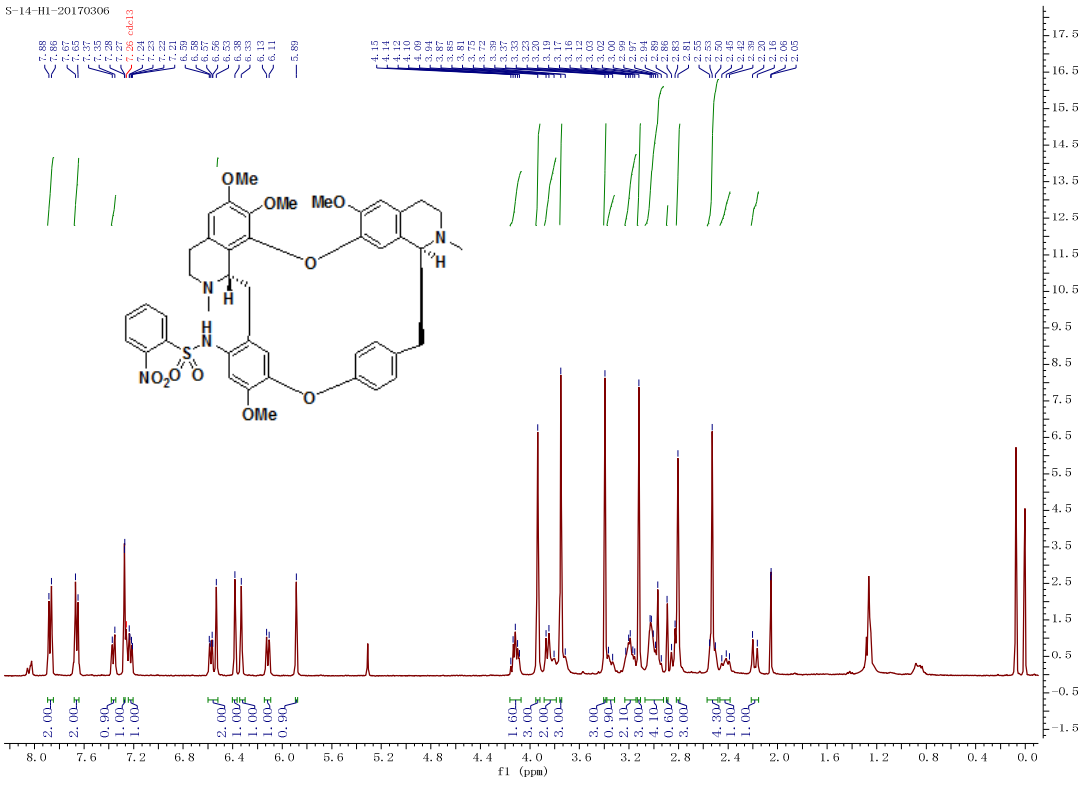
1.10. 14-(2-Chlorobenzenesulfonamide)tetrandrine (7)



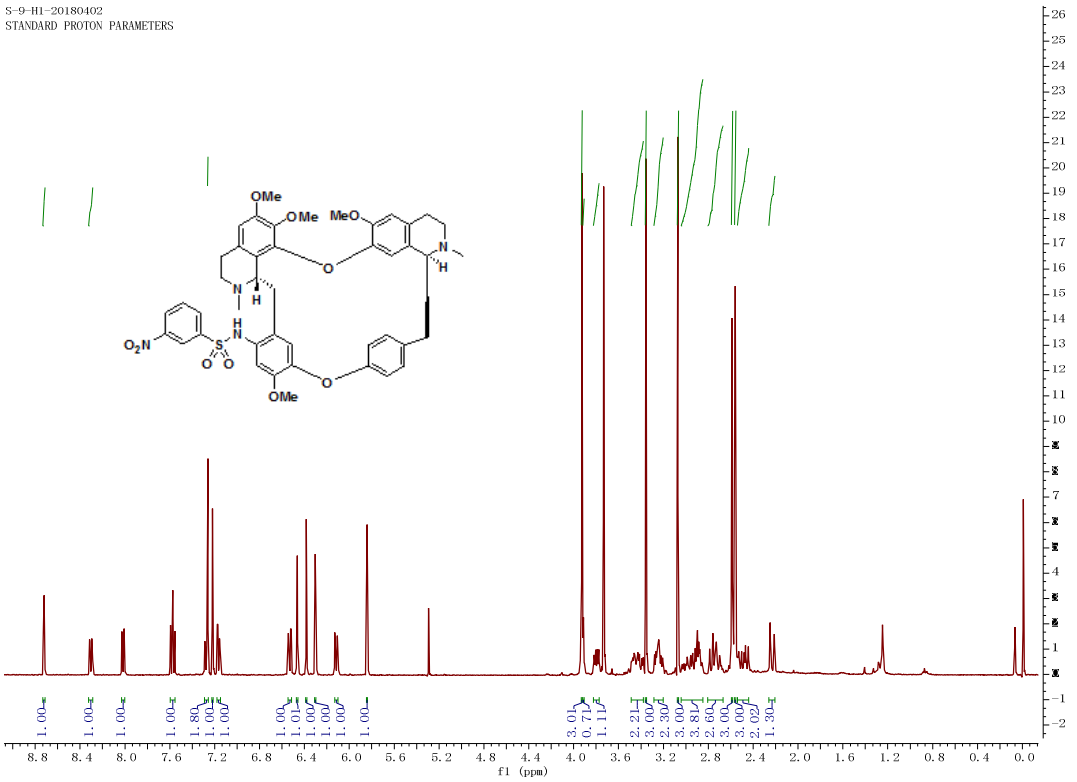
1.11. 14-(3-Bromobenzenesulfonamide)tetrandrine (8)



1.12. 14-(2-Nitrobenzenesulfonamide)tetrandrine (9)



1.13. 14-(3-Nitrobenzenesulfonamide)tetrandrine (10)



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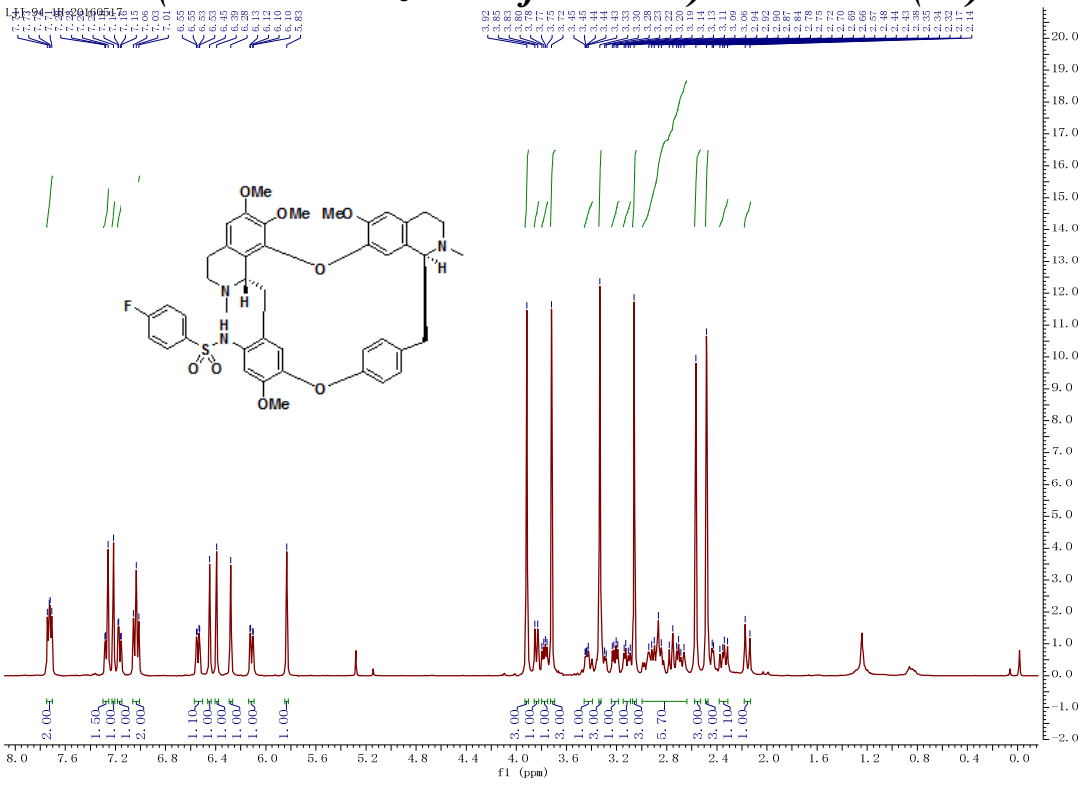
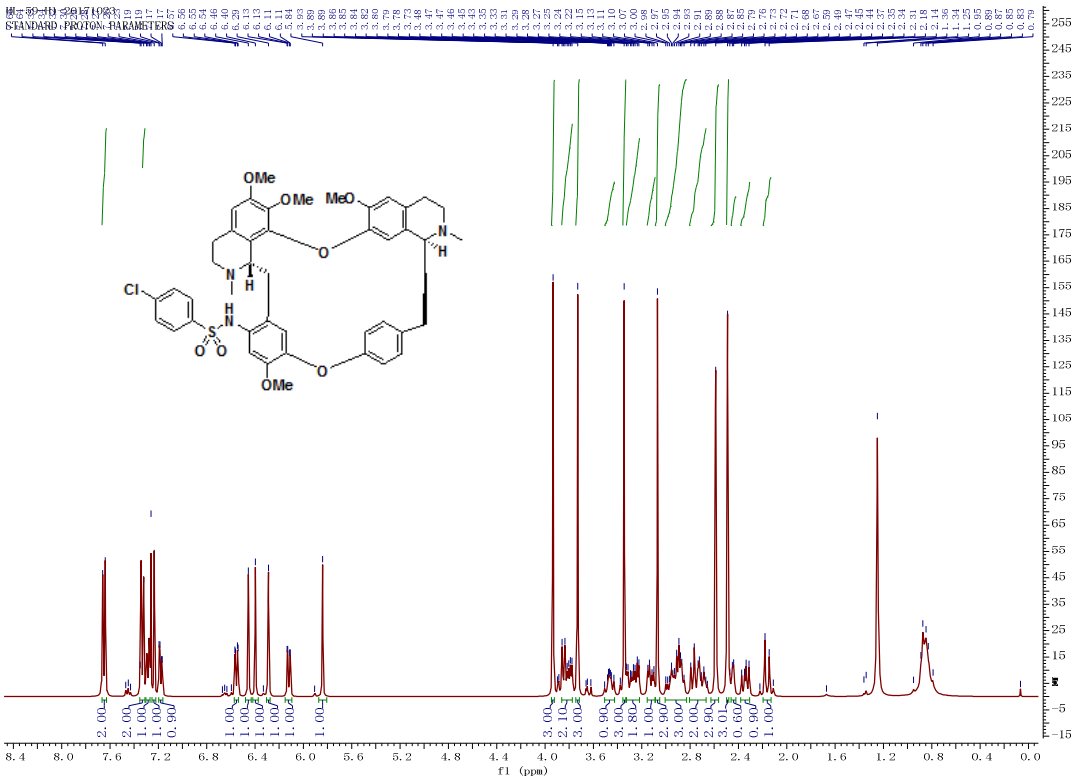


1.15. 14-(4-Chlorobenzenesulfonamide)tetrandrine (12)



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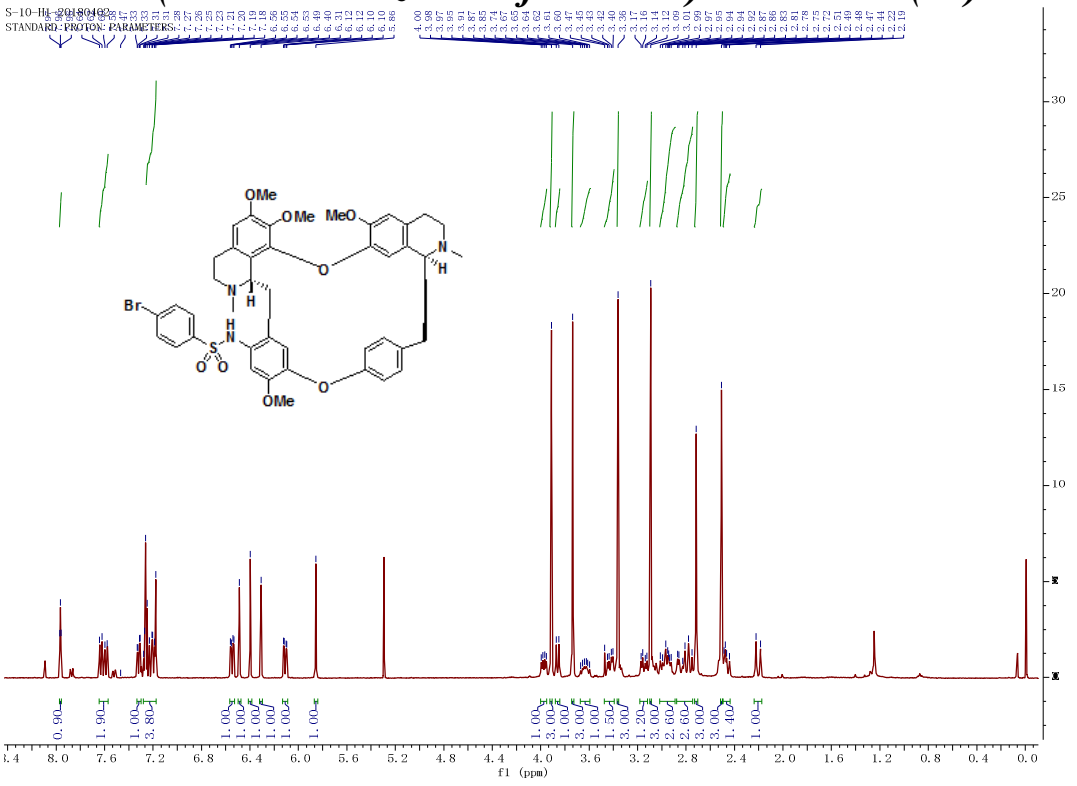

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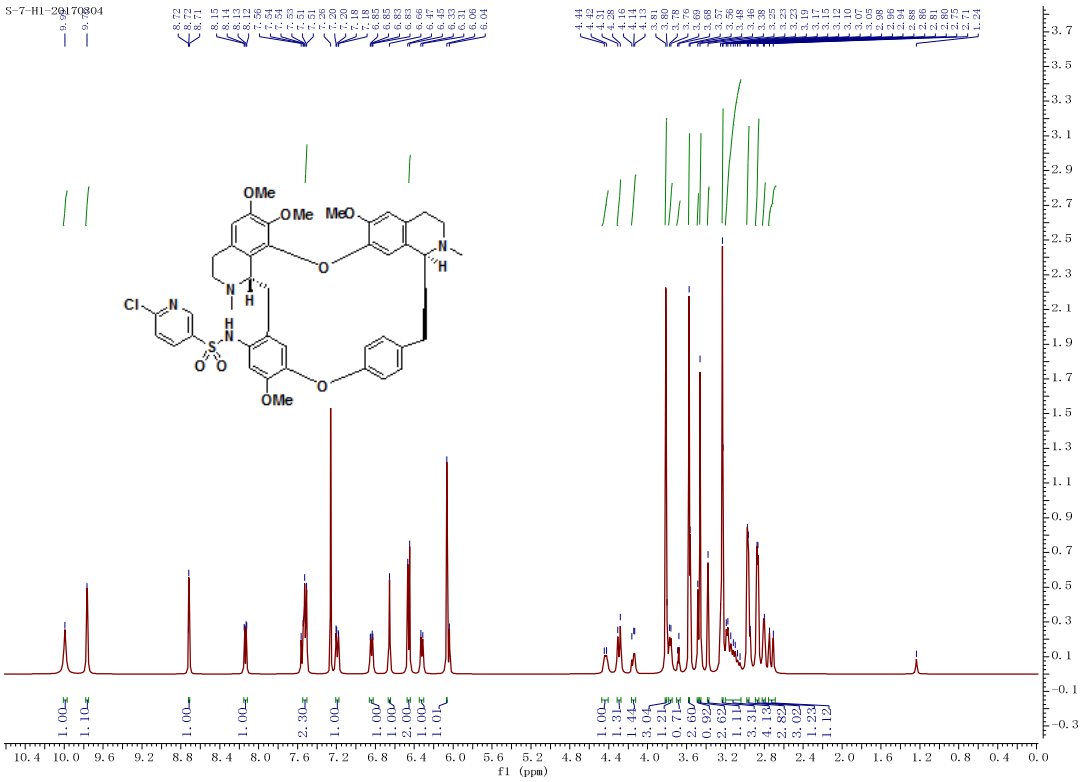

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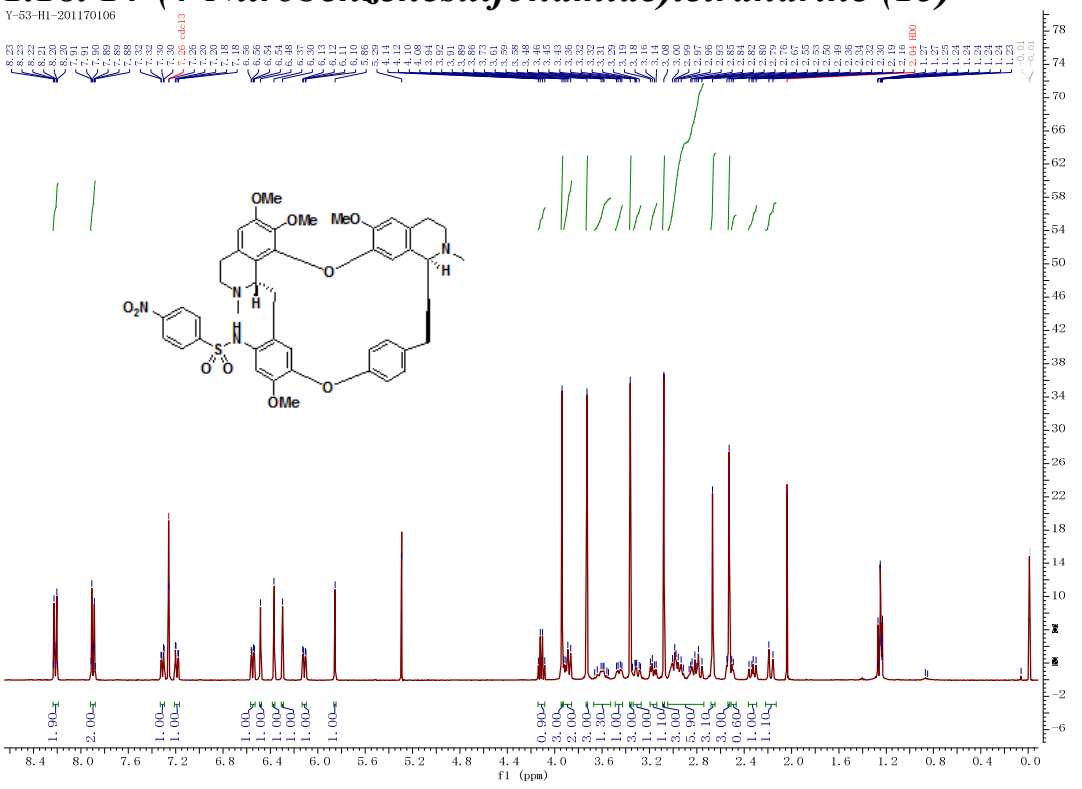
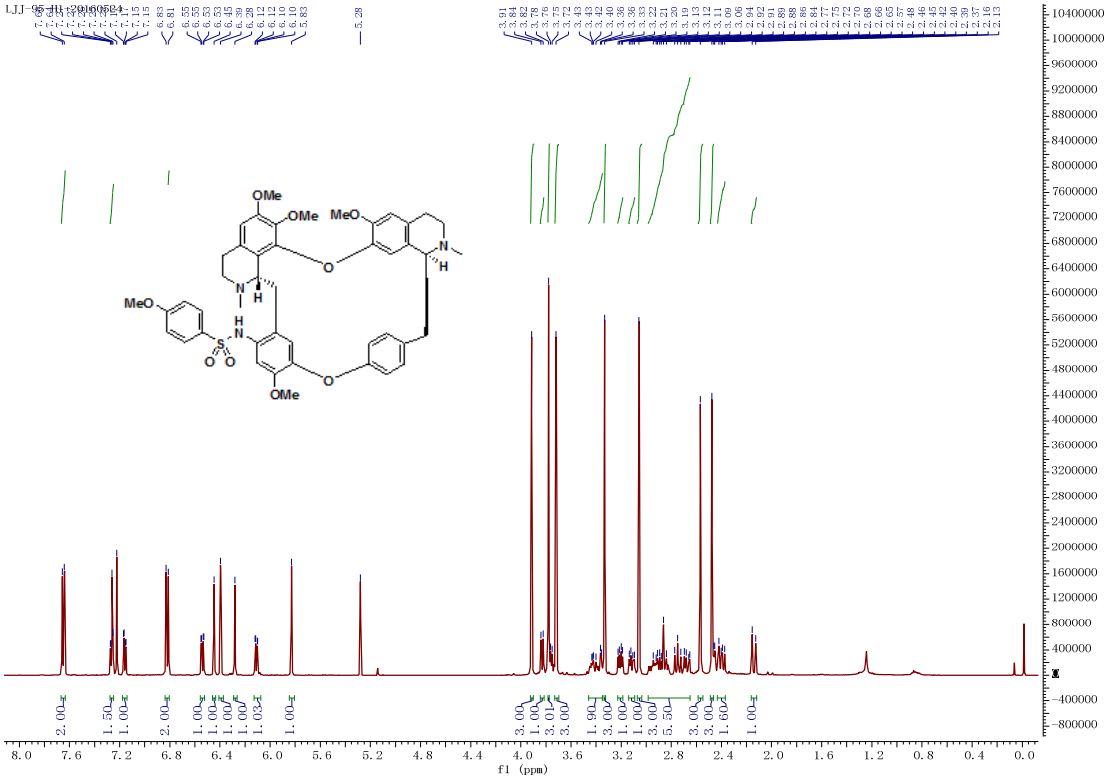


1.19. 14-(3-Methoxybenzenesulfonamide)tetrandrine (16)



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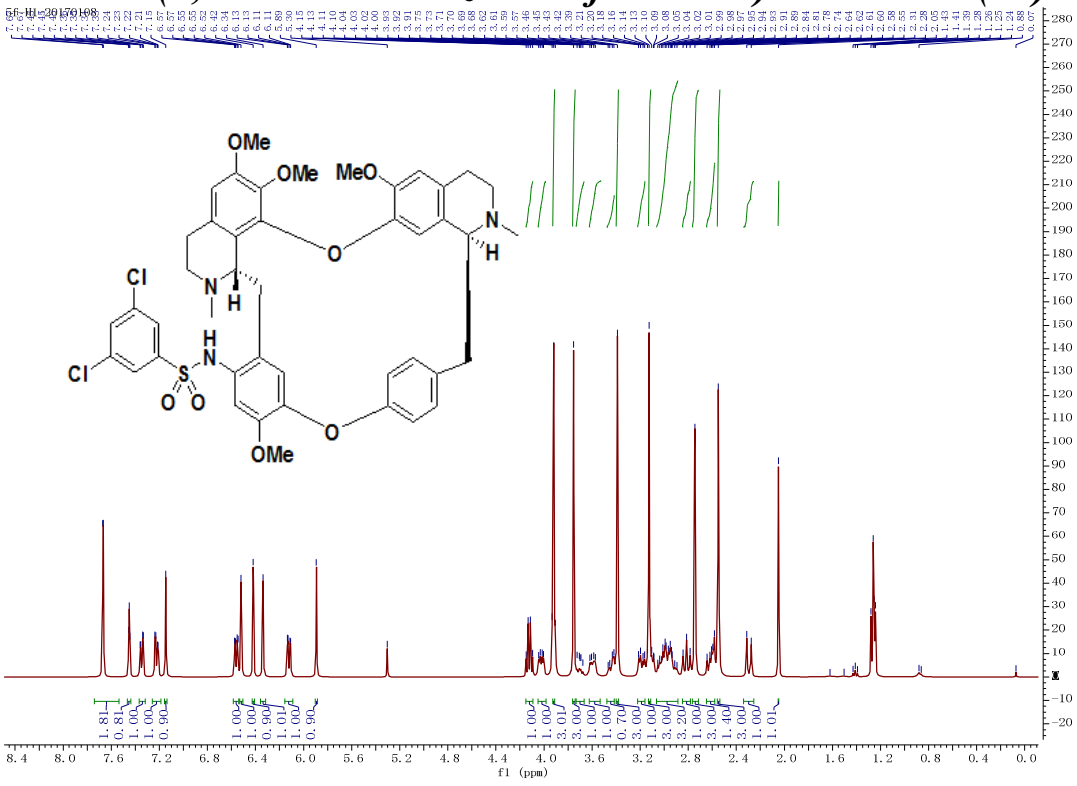
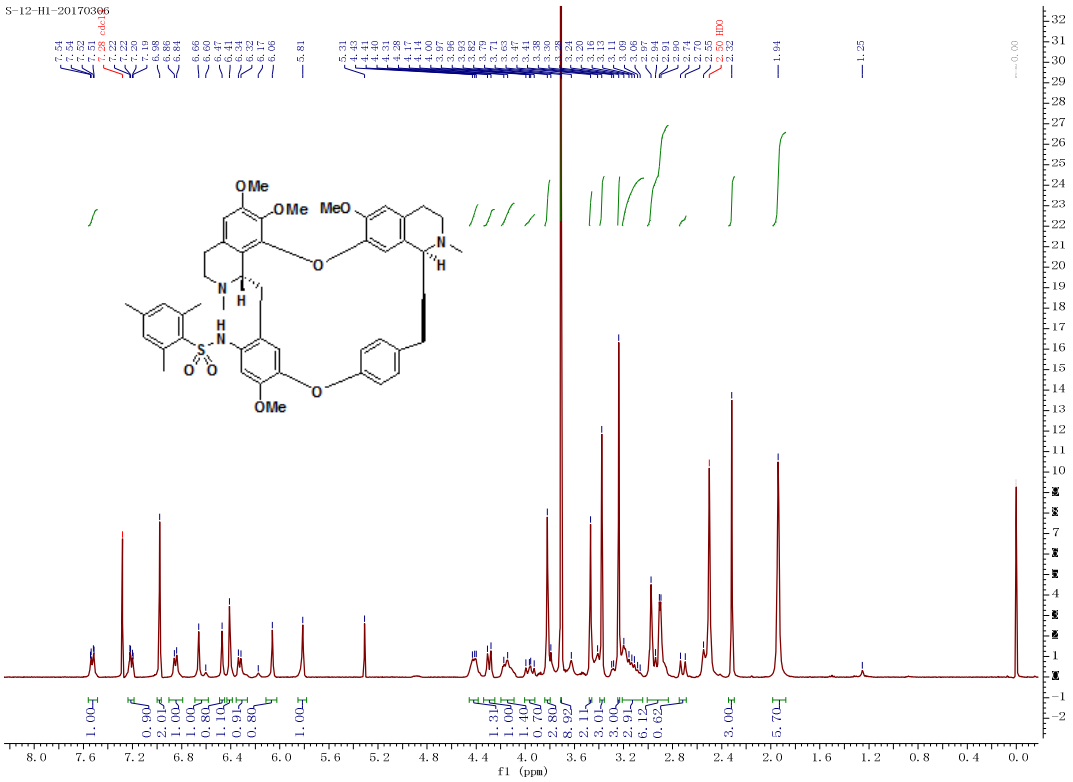
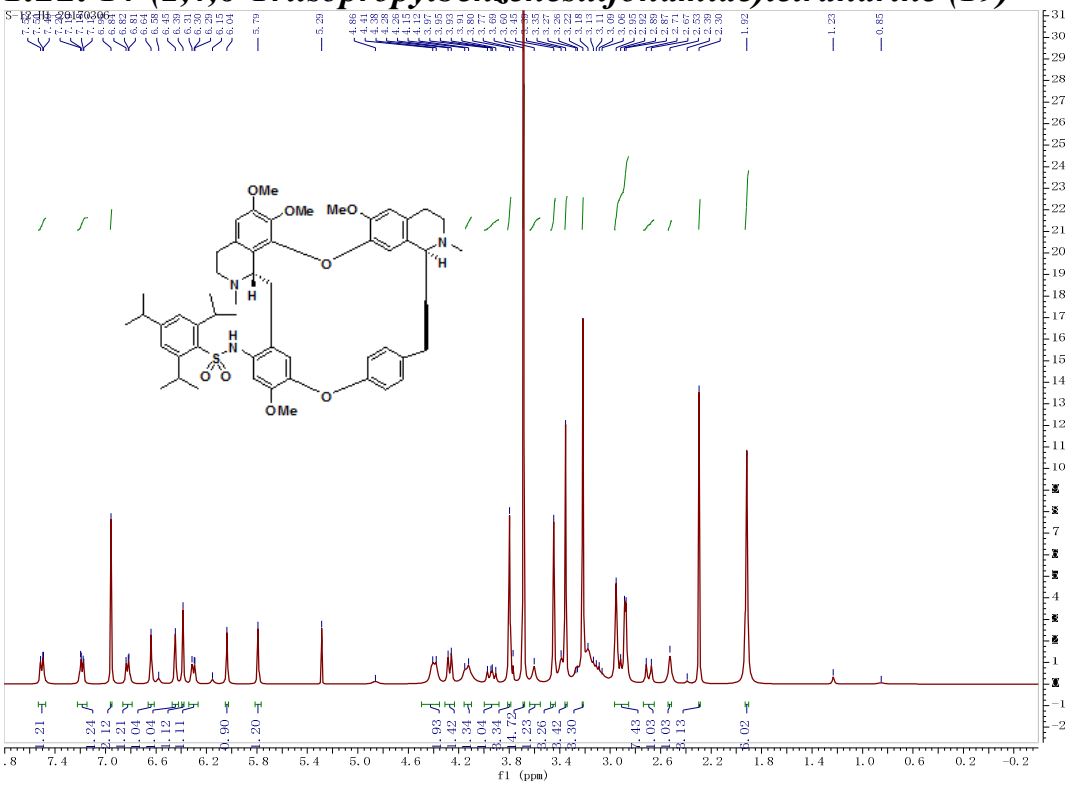


1.21. 14-(2,4,6-Trimethylbenzenesulfonamide)tetrandrine (18)



1.22. 14-(2,4,6-Triisopropylbenzenesulfonamide)tetrandrine (19)



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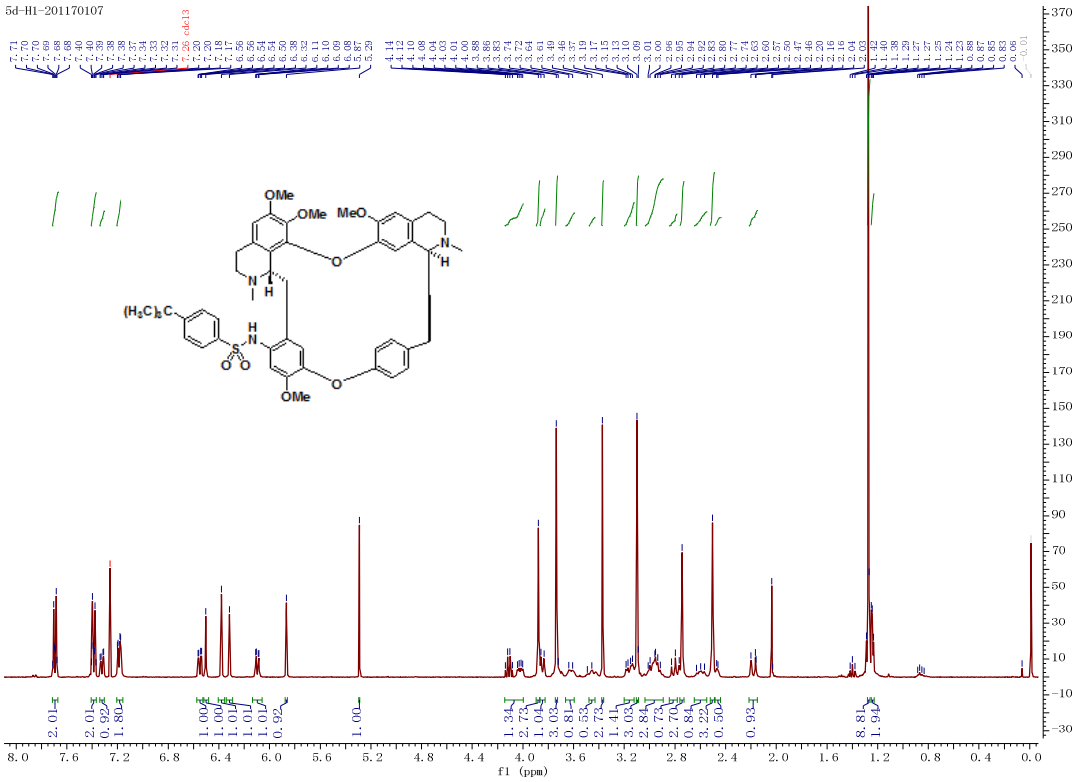

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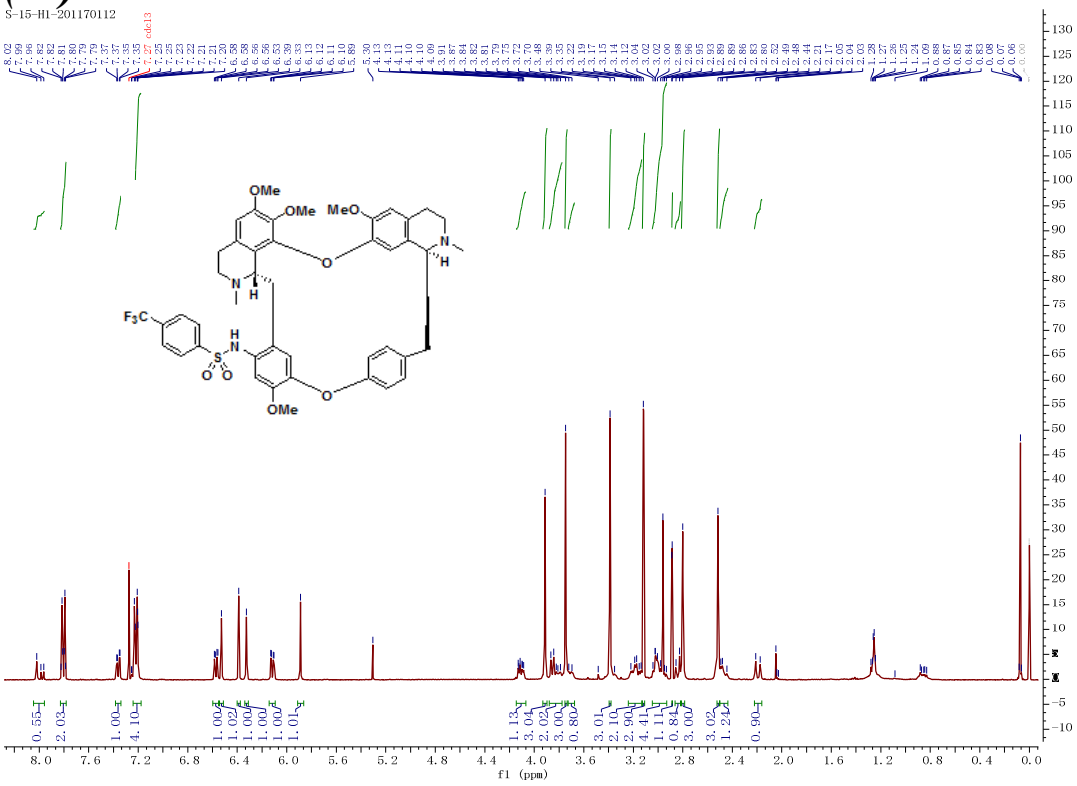

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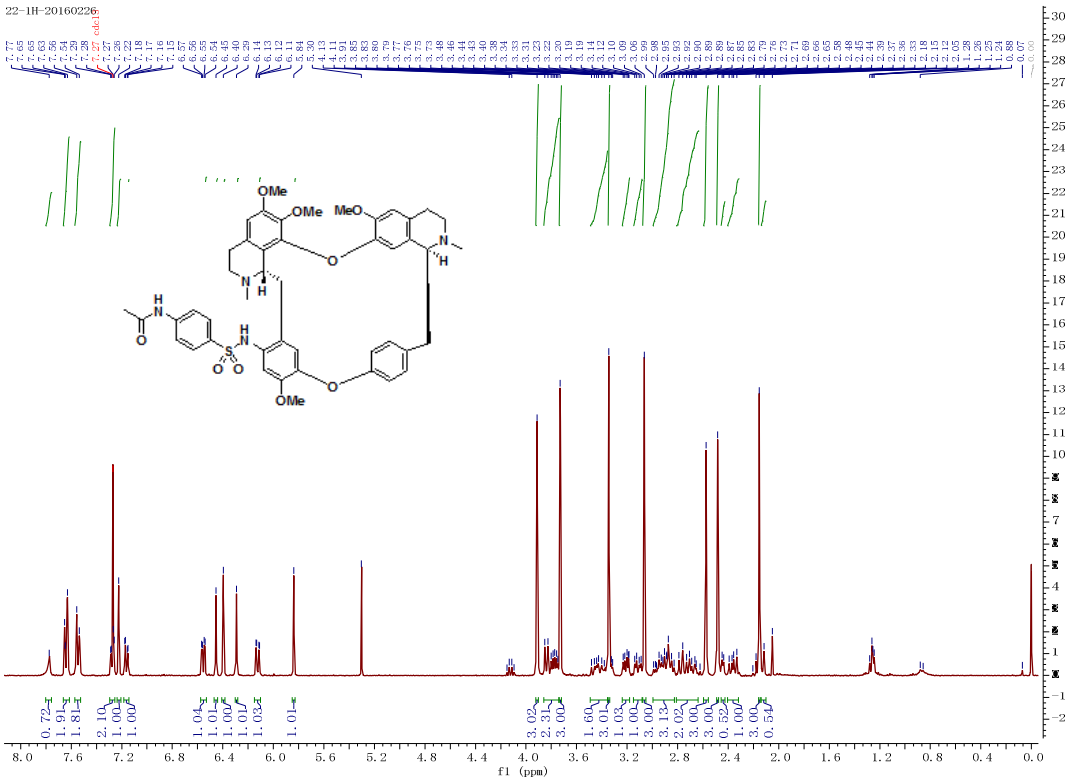

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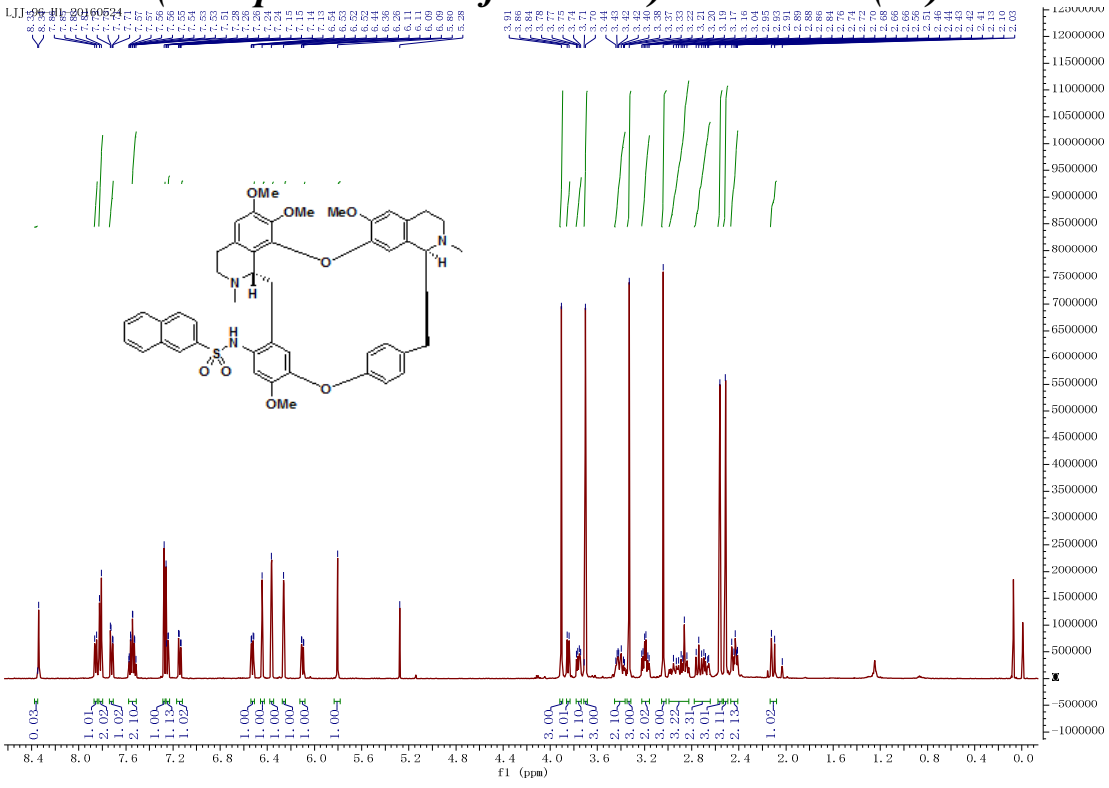
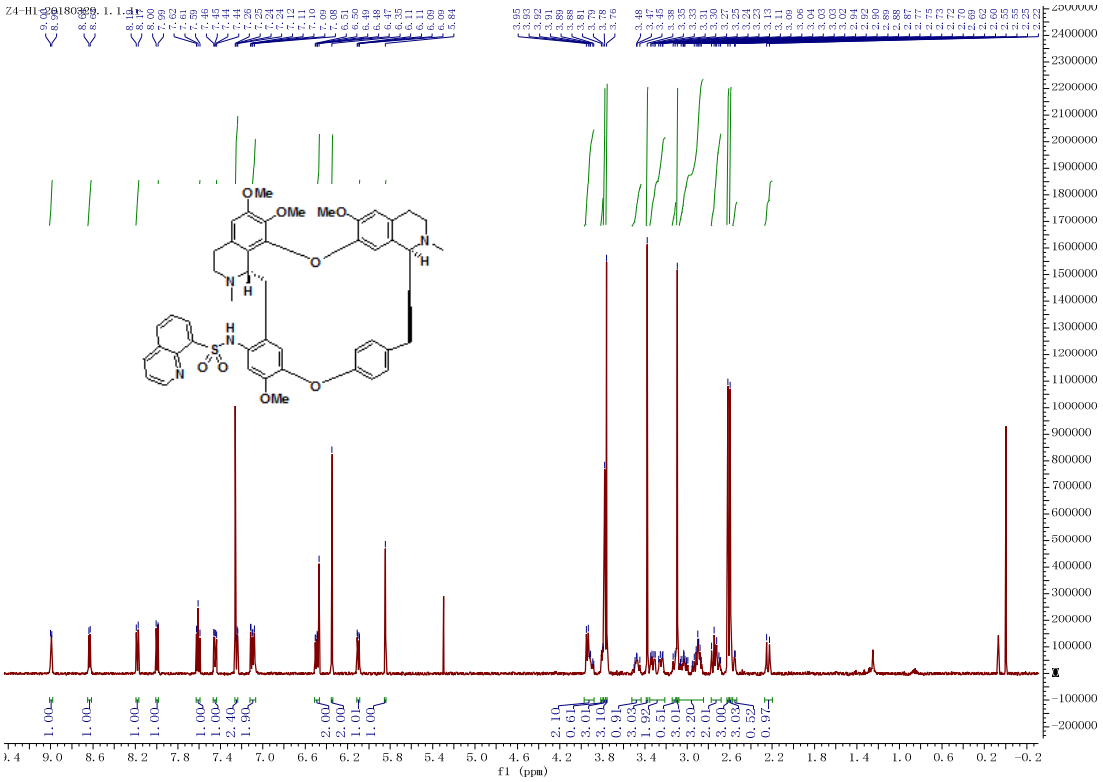
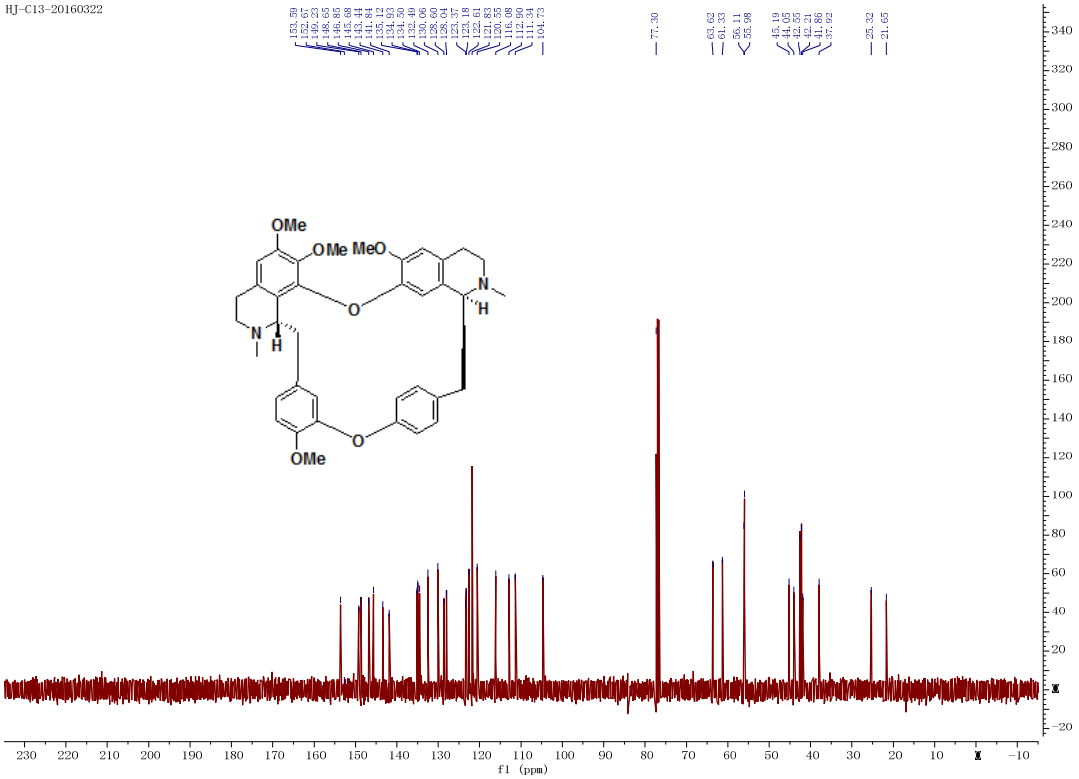


1.27. 14-(Quinoline-8-sulfonamide)tetrandrine (24)



2. ^{13}C NMR Spectra

2.1 Tetrandrine



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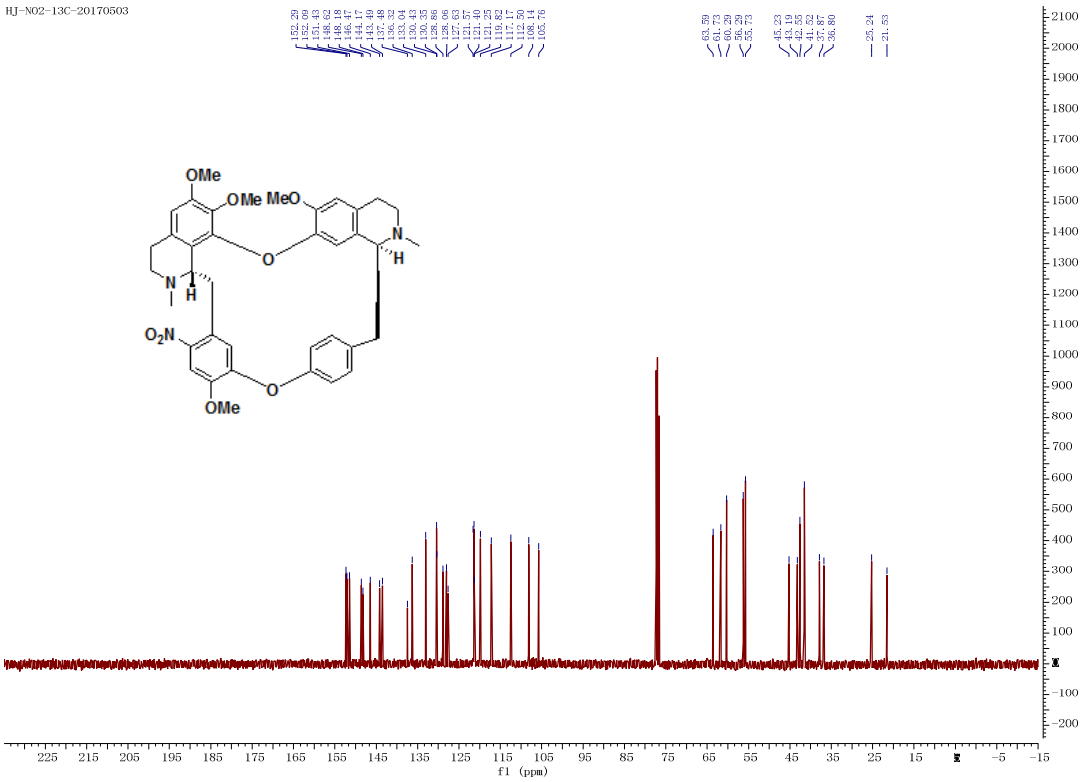

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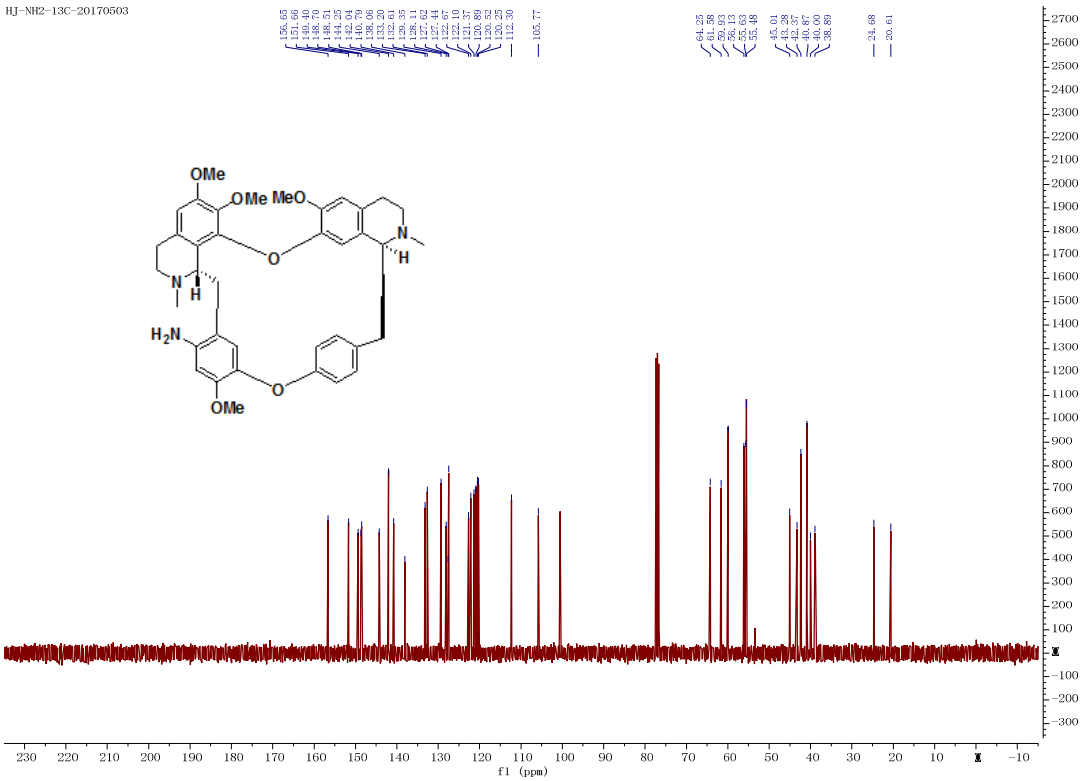
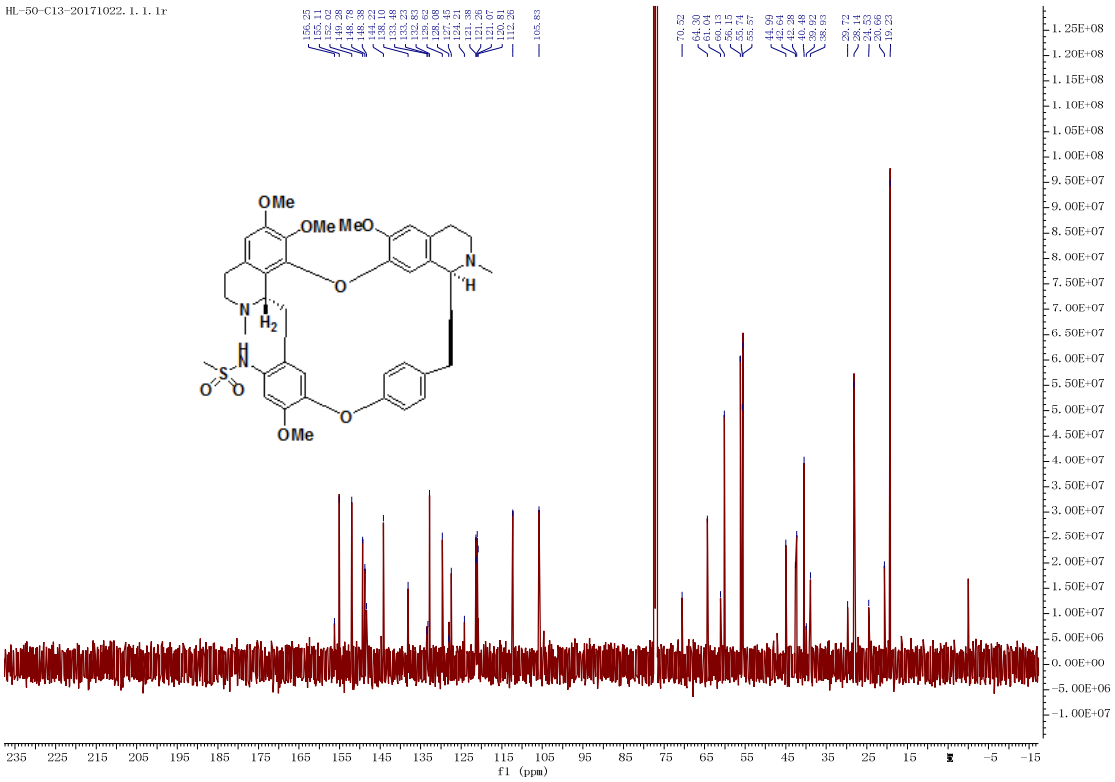
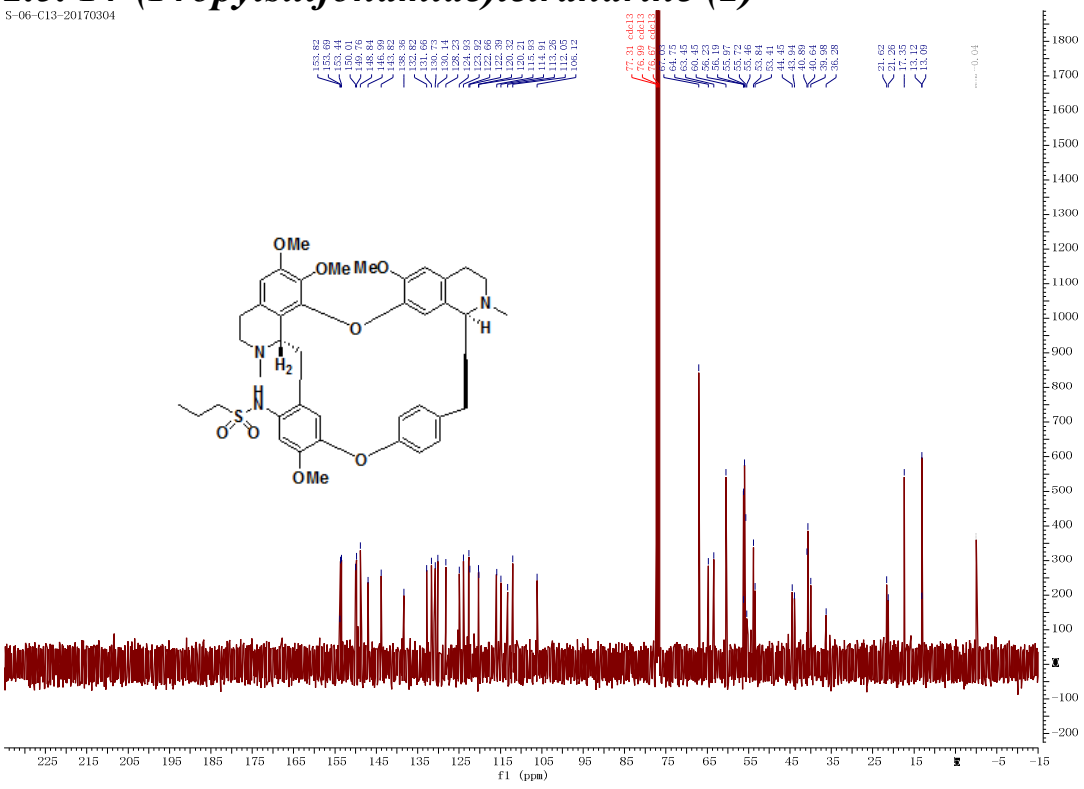


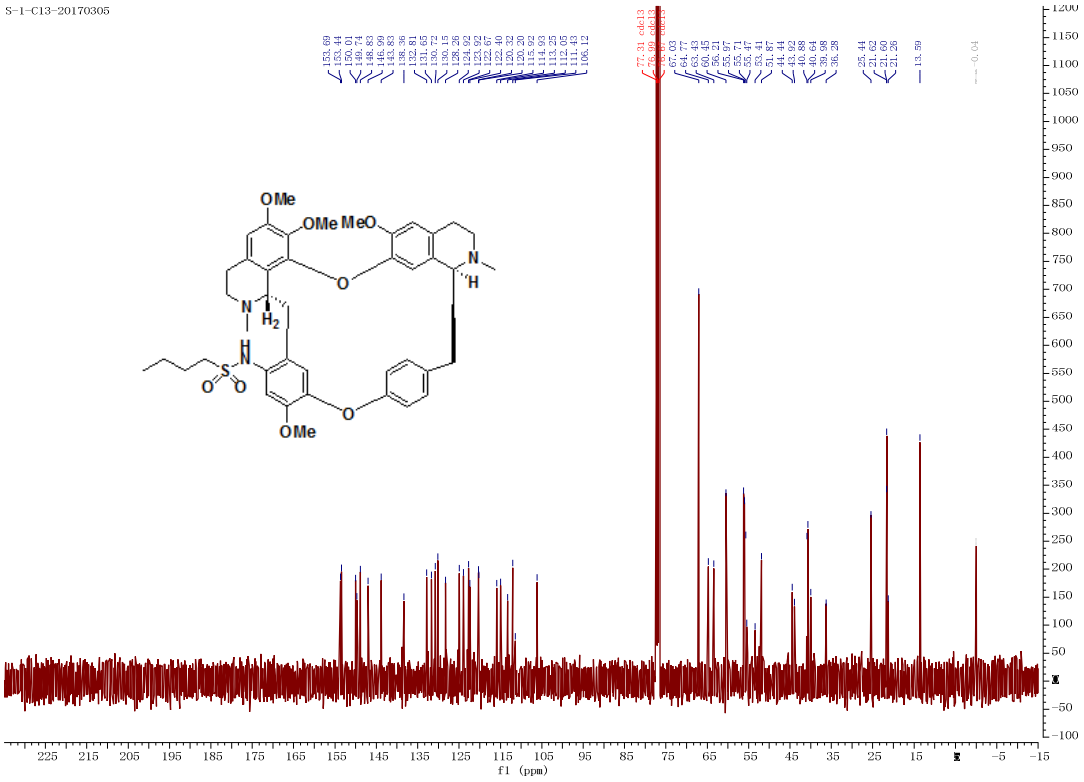
2.4 14-(Methylsulfonamide)tetrandrine (1)



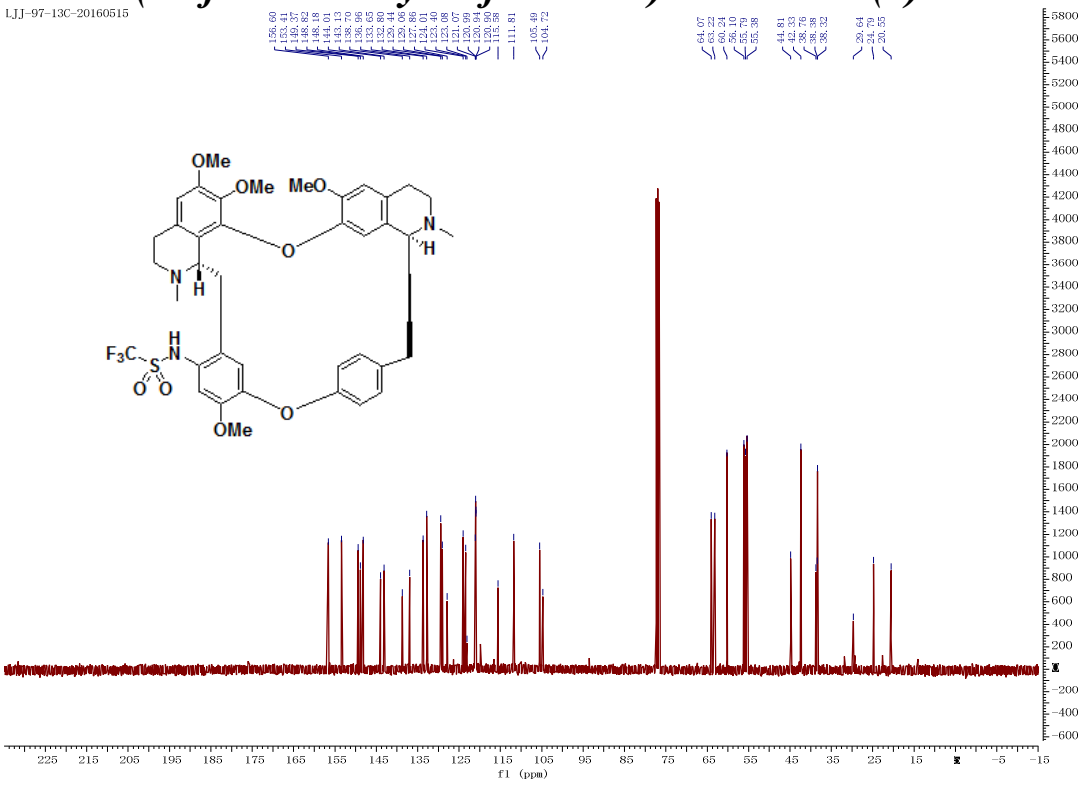
2.5. 14-(Propylsulfonamide)tetrandrine (2)



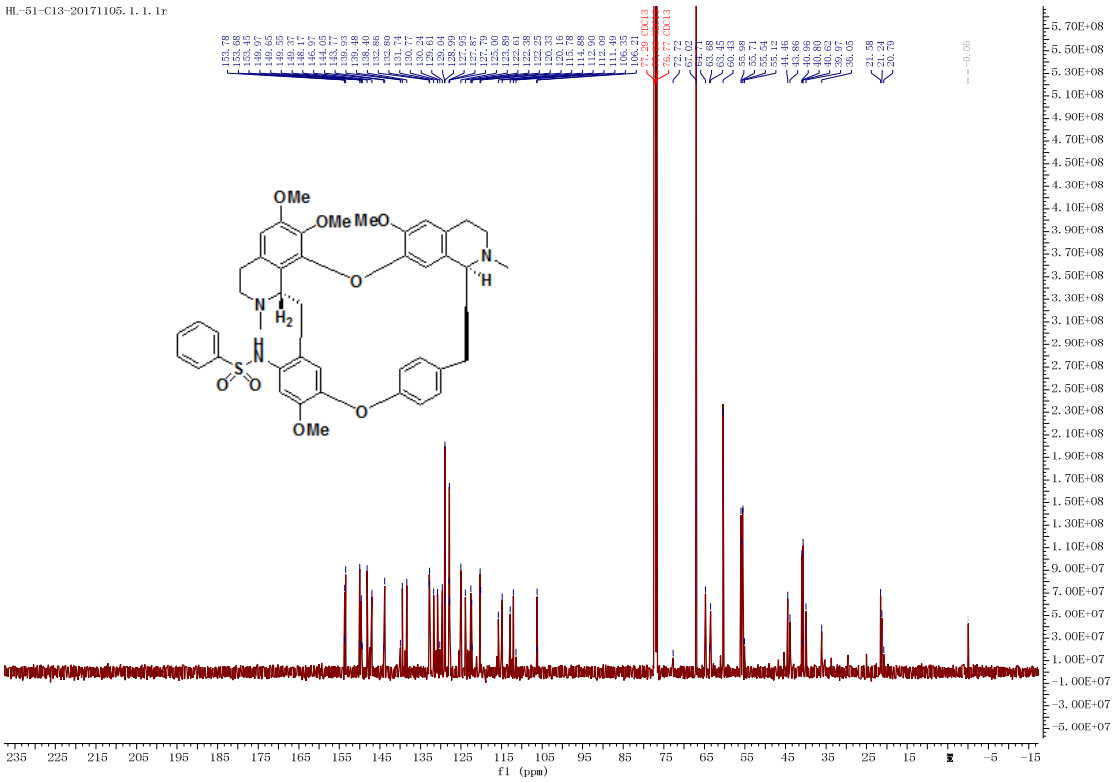
2.6. 14-(Butylsulfonamide)tetrandrine (3)



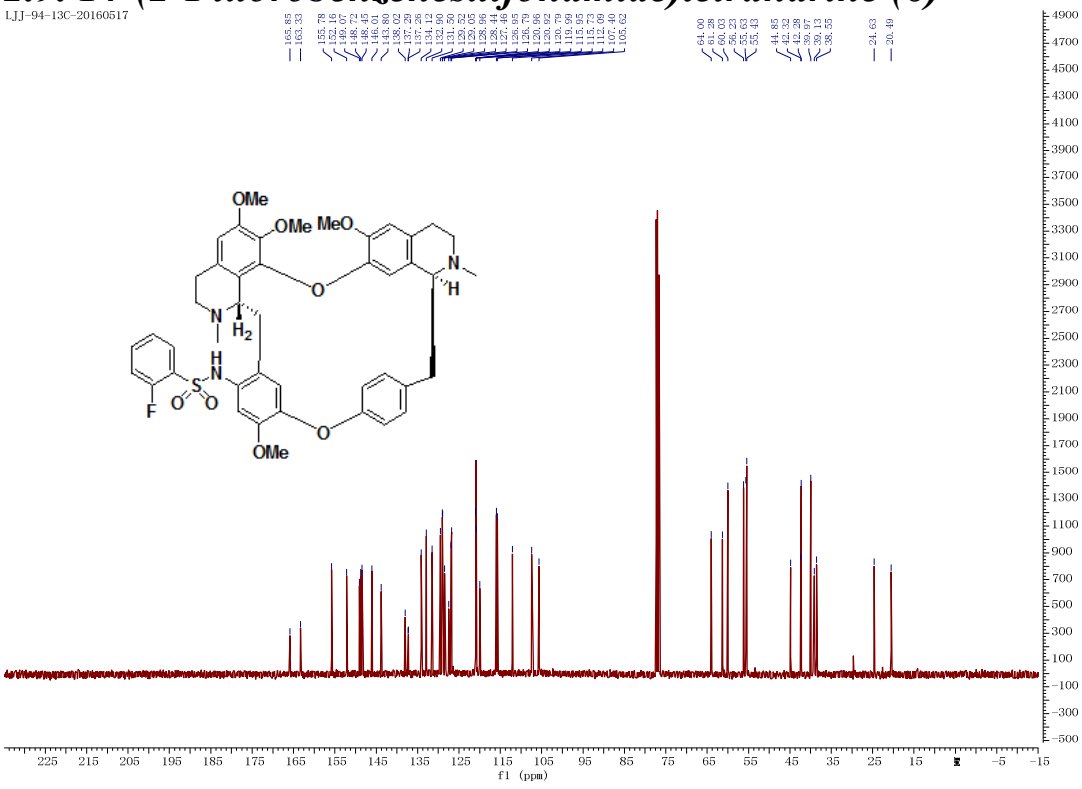
2.7. 14-(Trifluoromethylsulfonamide)tetrandrine (4)



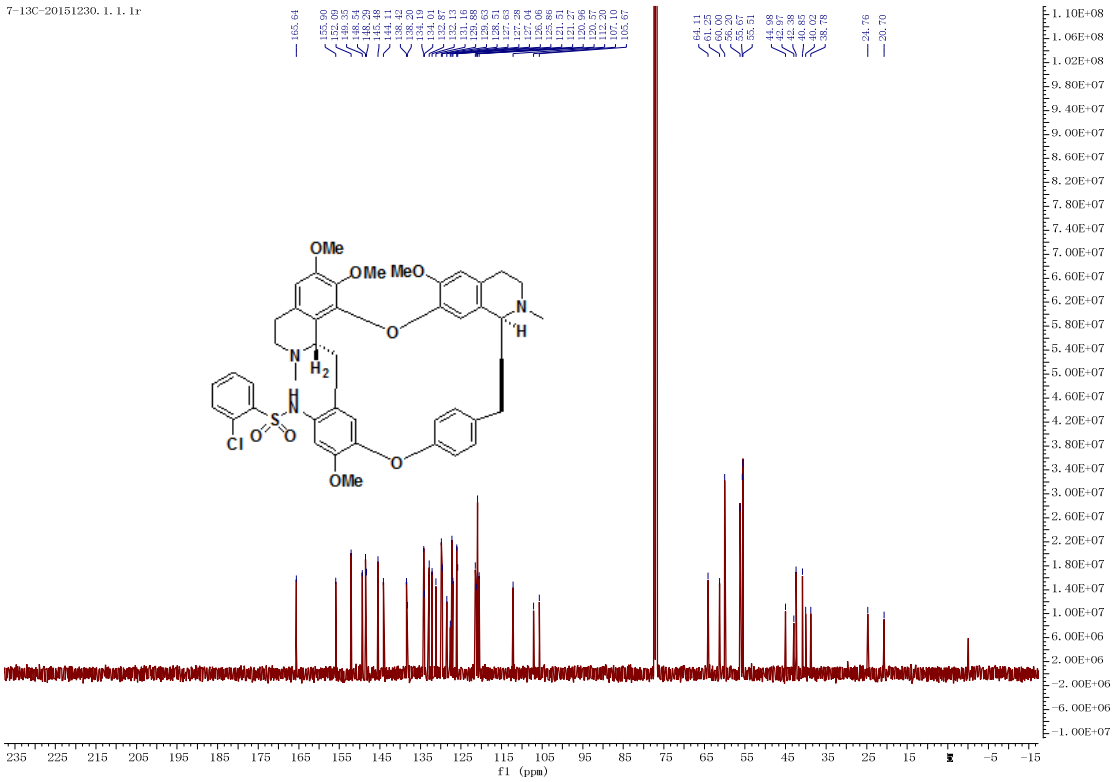
2.8. 14-(Benzenesulfonamide)tetrandrine (5)



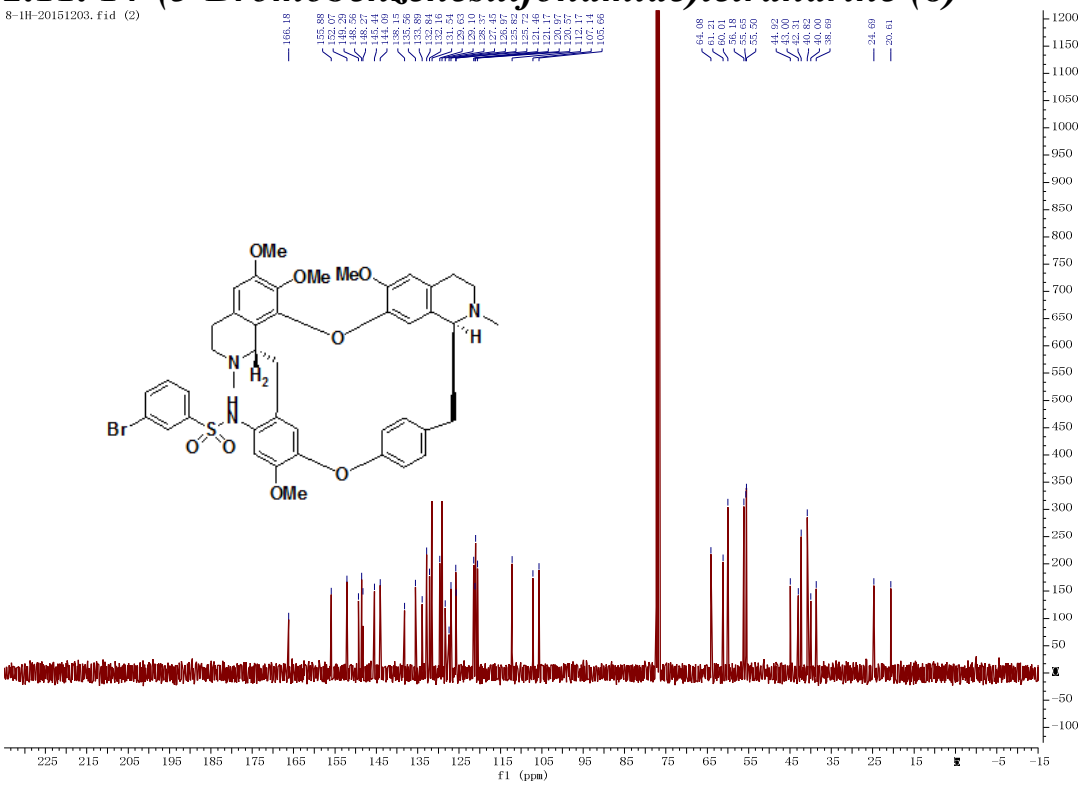
2.9. 14-(2-Fluorobenzenesulfonamide)tetrandrine (6)



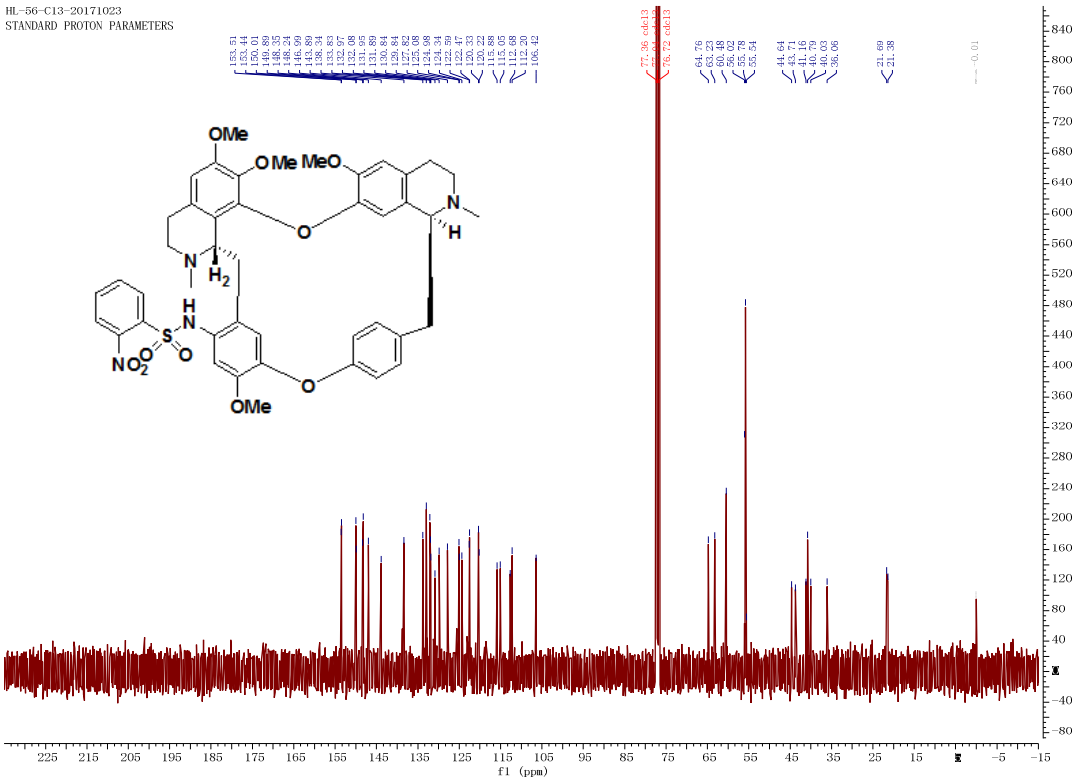
2.10. 14-(2-Chlorobenzenesulfonamide)tetrandrine (7)



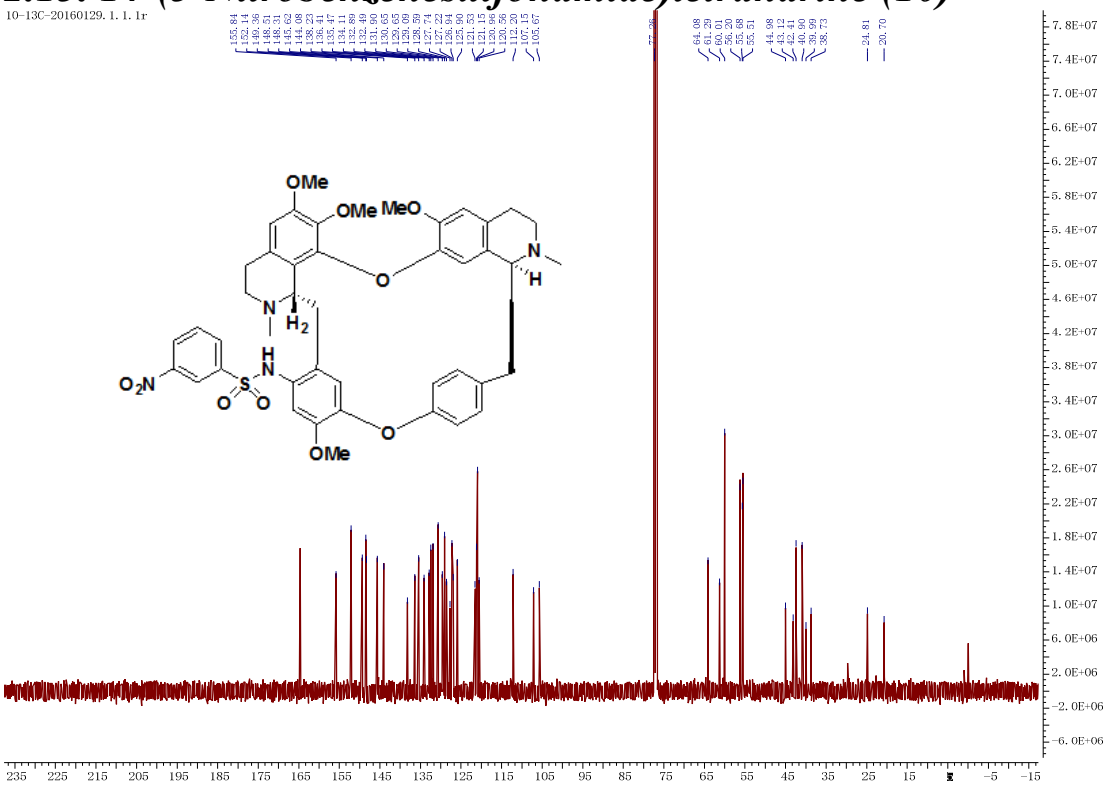
2.11. 14-(3-Bromobenzenesulfonamide)tetrandrine (8)



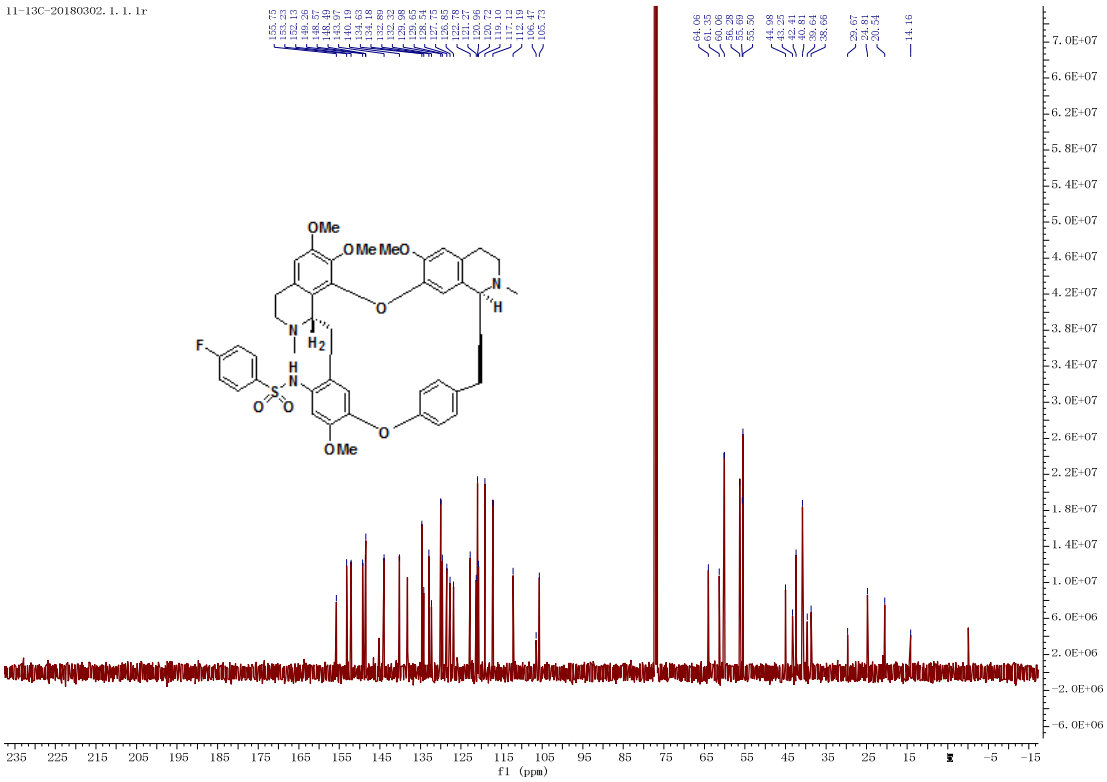
2.12 14-(2-Nitrobenzenesulfonamide)tetrandrine (9)



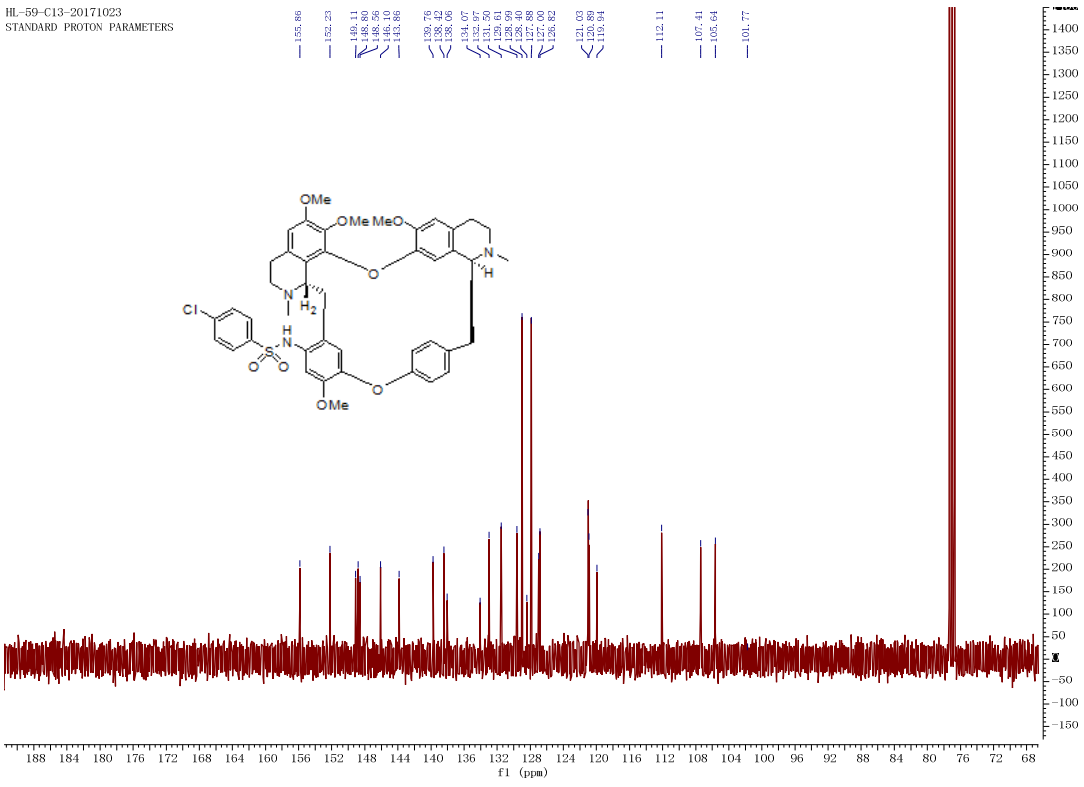
2.13. 14-(3-Nitrobenzenesulfonamide)tetrandrine (10)



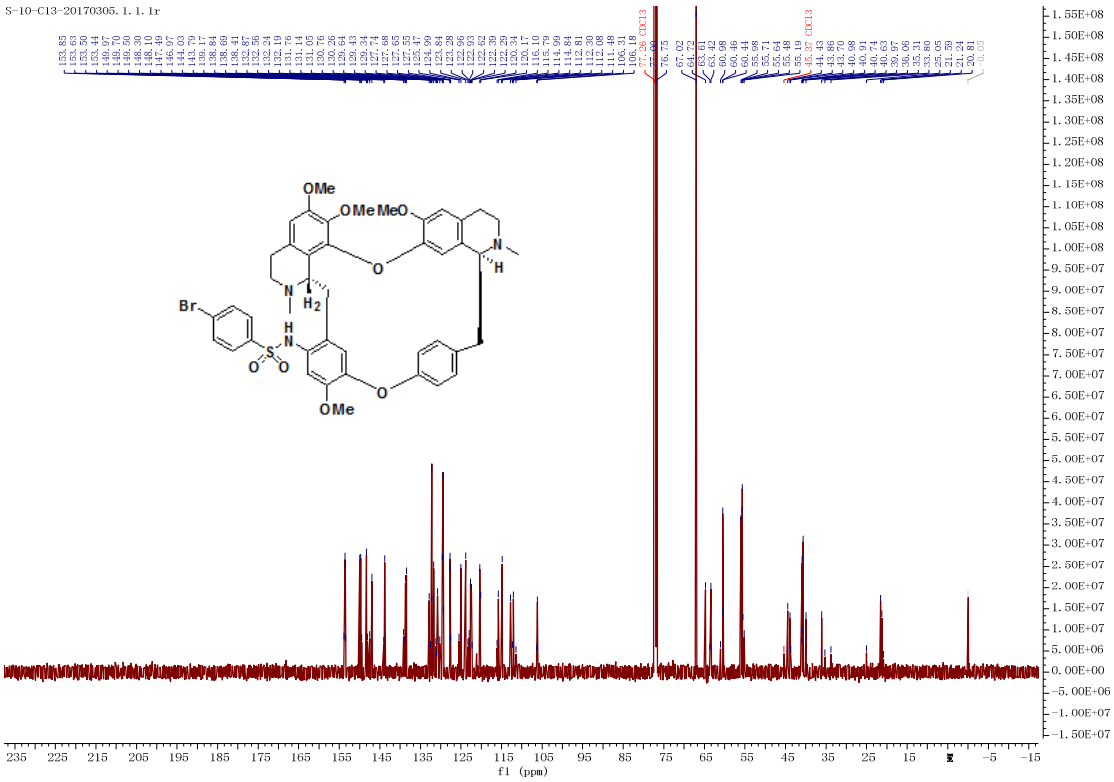
2.14. 14-(4-Fluorobenzenesulfonamide)tetrandrine (11)



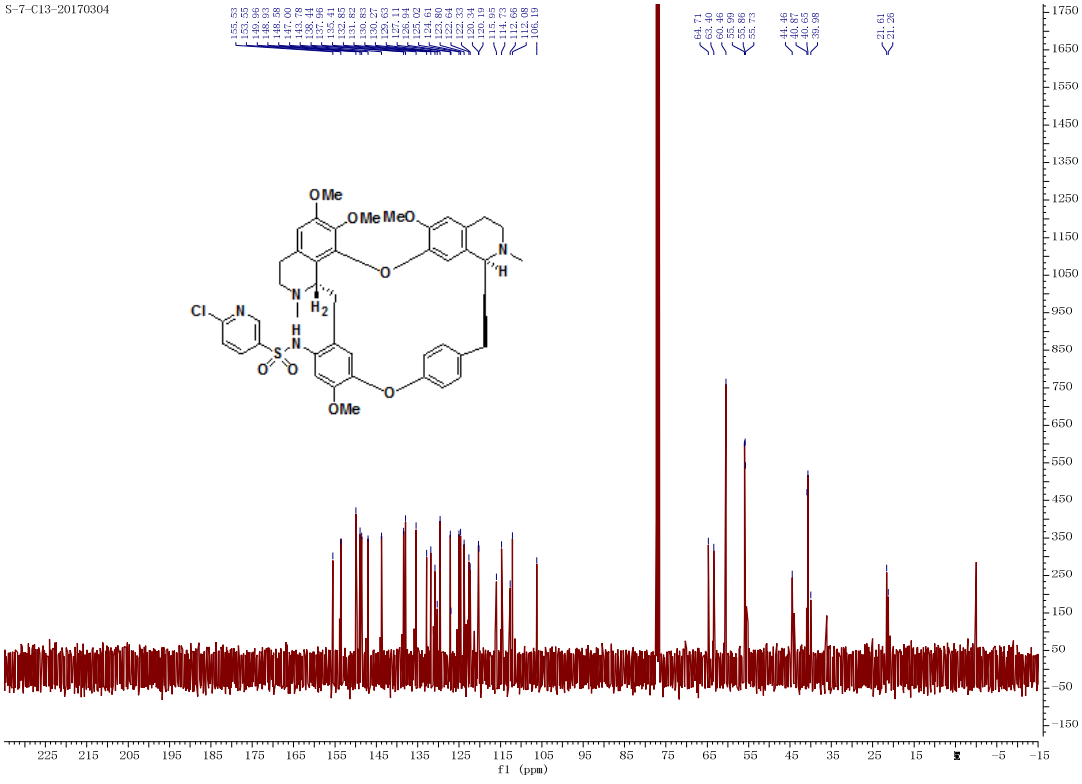
2.15. 14-(4-Chlorobenzenesulfonamide)tetrandrine (12)



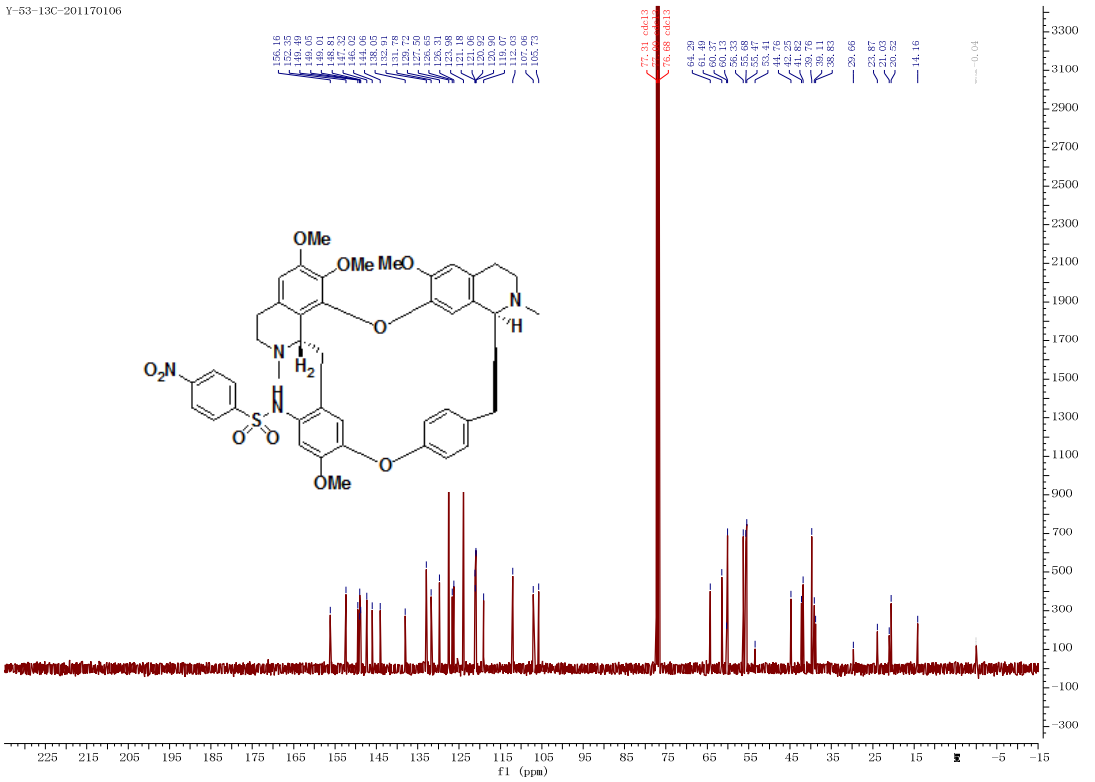
2.16. 14-(4-Bromobenzenesulfonamide)tetrandrine (13)



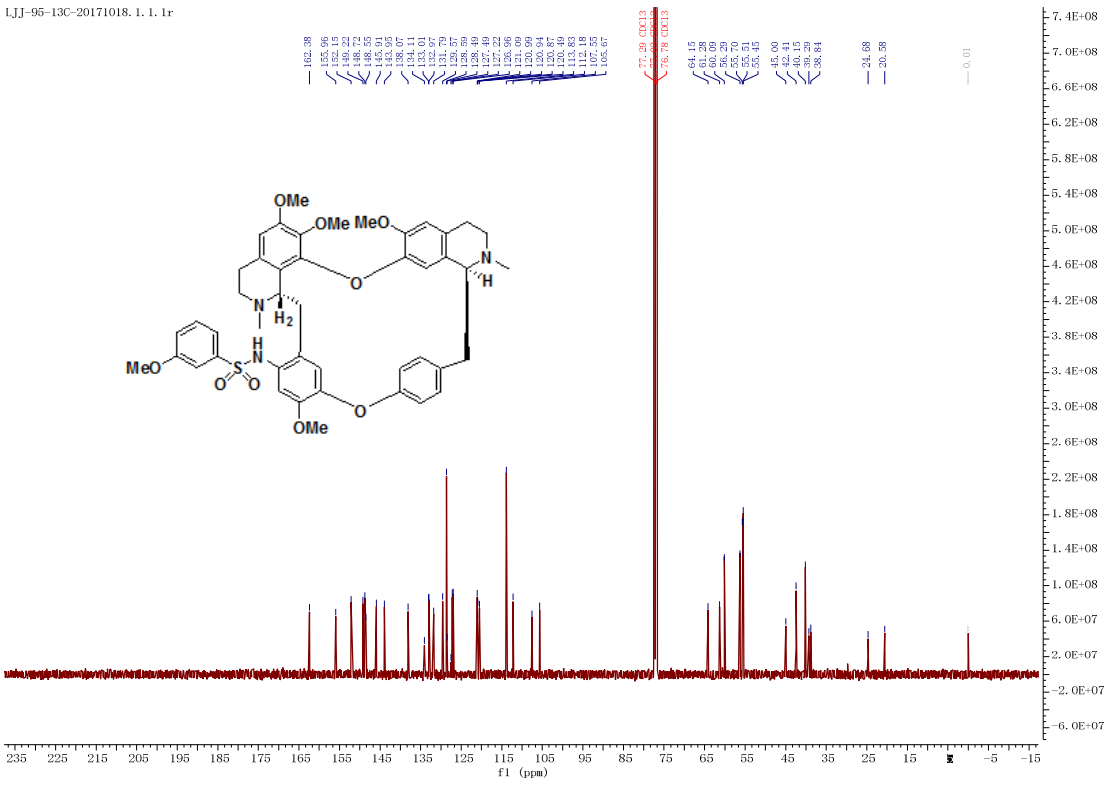
2.17. 14-(6-chloropyridine-3-sulfonamide)tetrandrine (14)



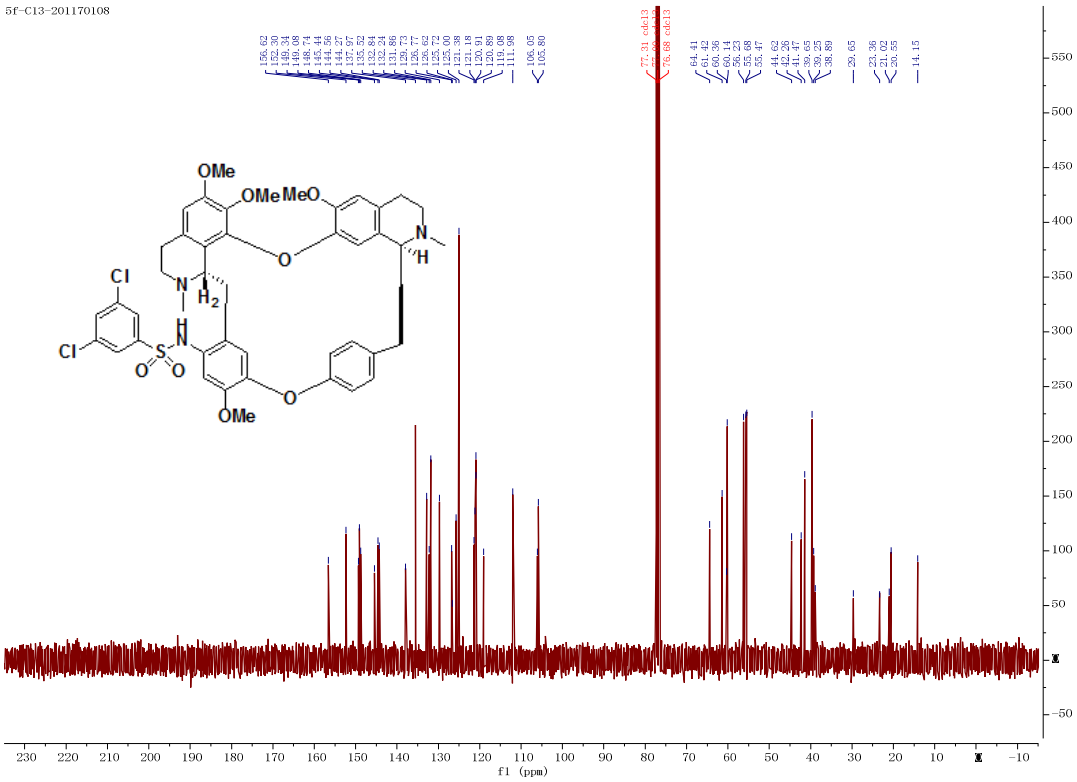
2.18. 14-(4-Nitrobenzenesulfonamide)tetrandrine (15)



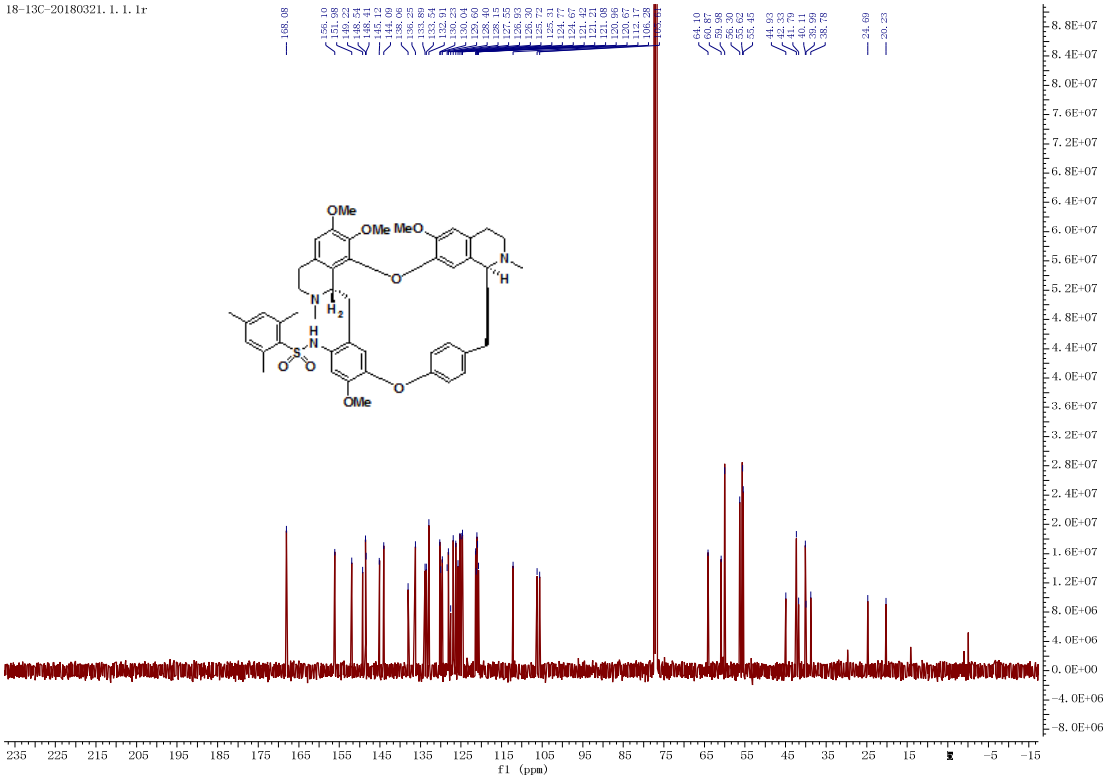
2.19. 14-(3-Methoxybenzenesulfonamide)tetrandrine (16)



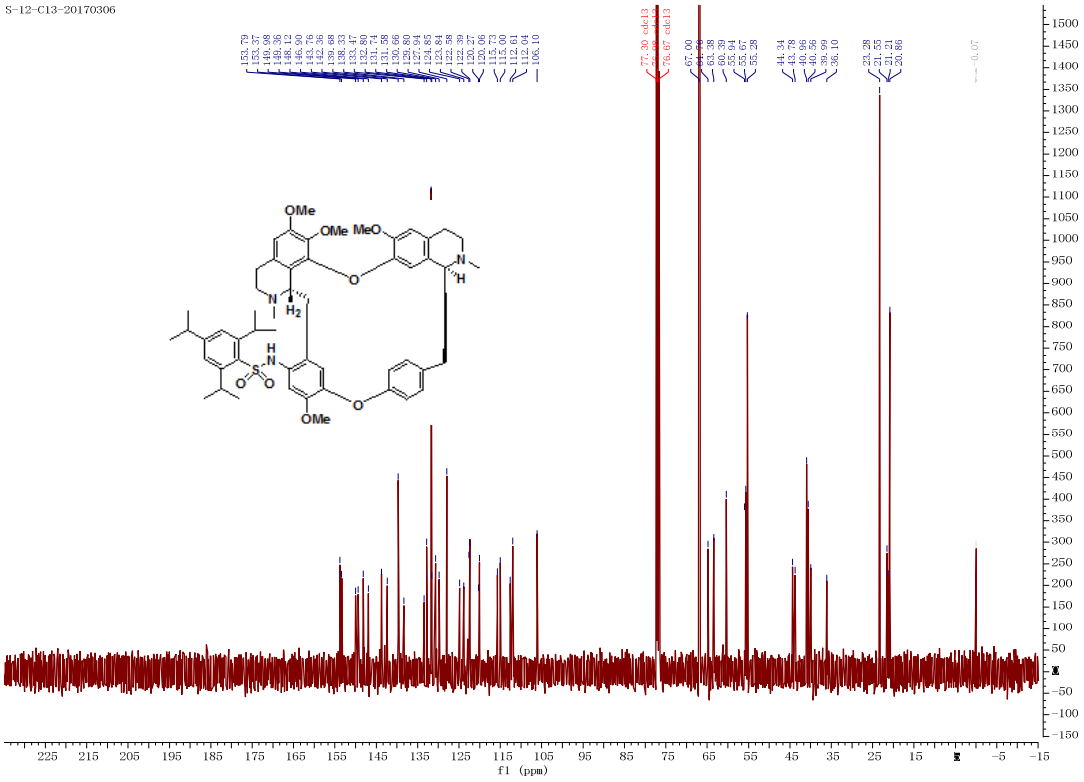
2.20. 14-(3,5-Dichlorobenzenesulfonamide)tetrandrine (17)



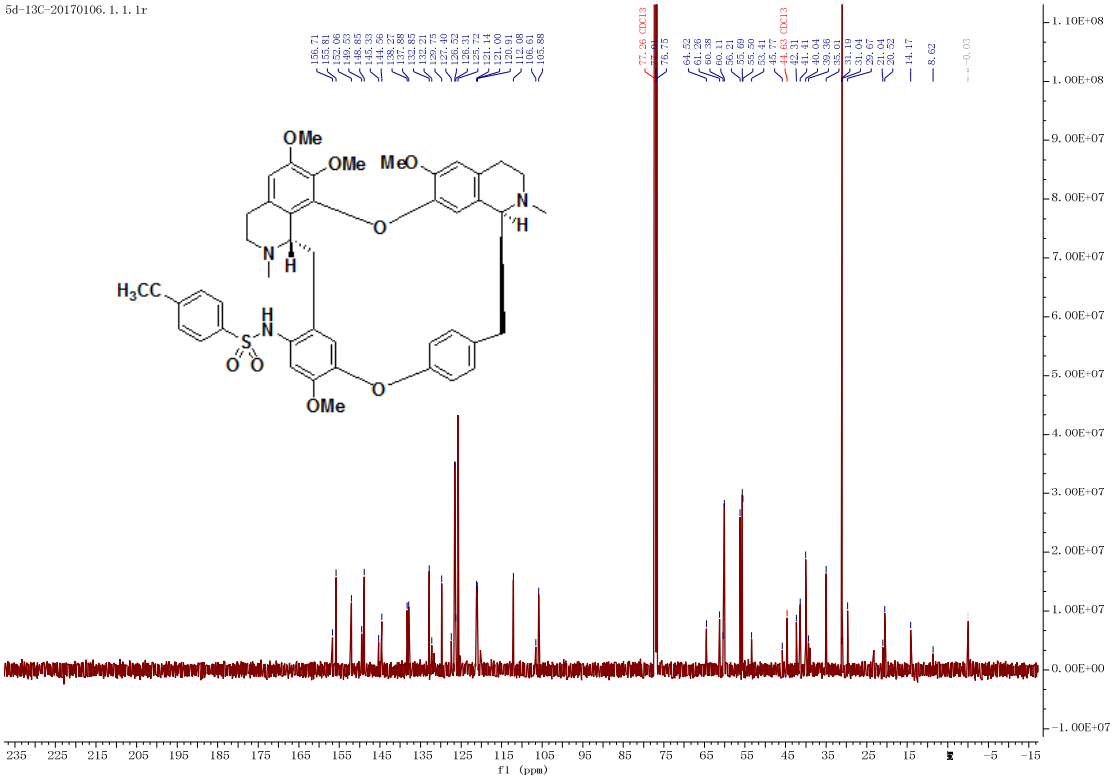
2.21. 14-(2,4,6-Trimethylbenzenesulfonamide)tetrandrine (18)



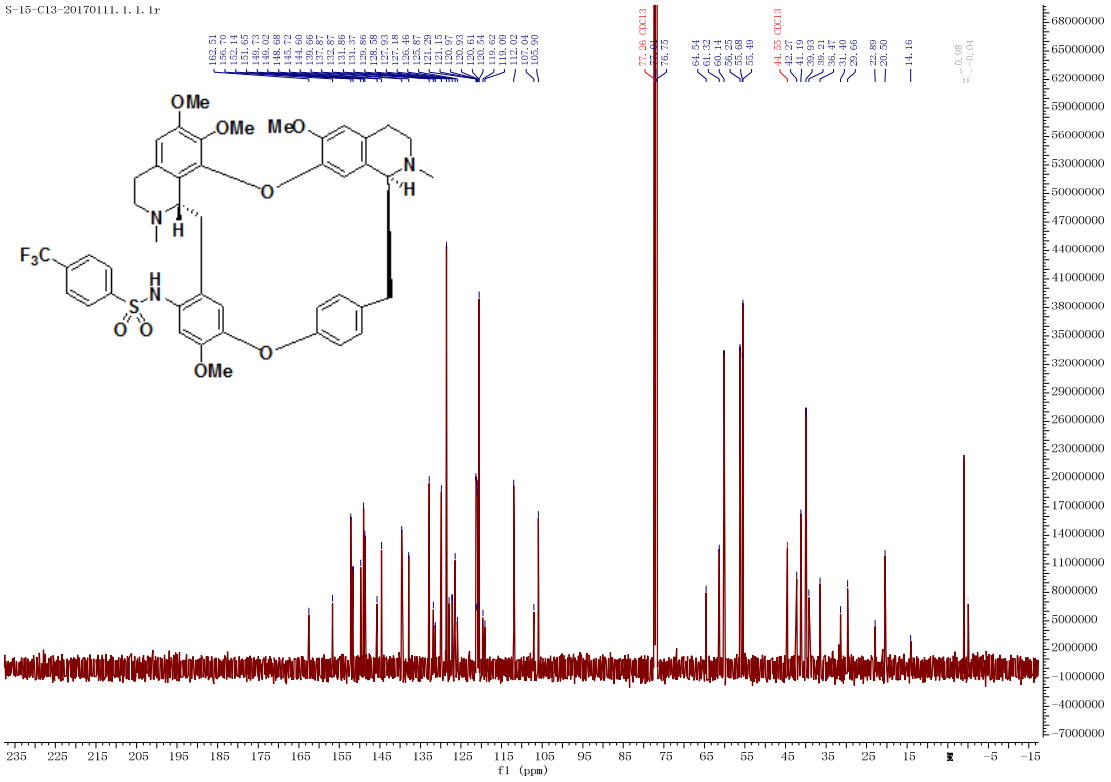
2.22. 14-(2,4,6-Triisopropylbenzenesulfonamide)tetrandrine (19)



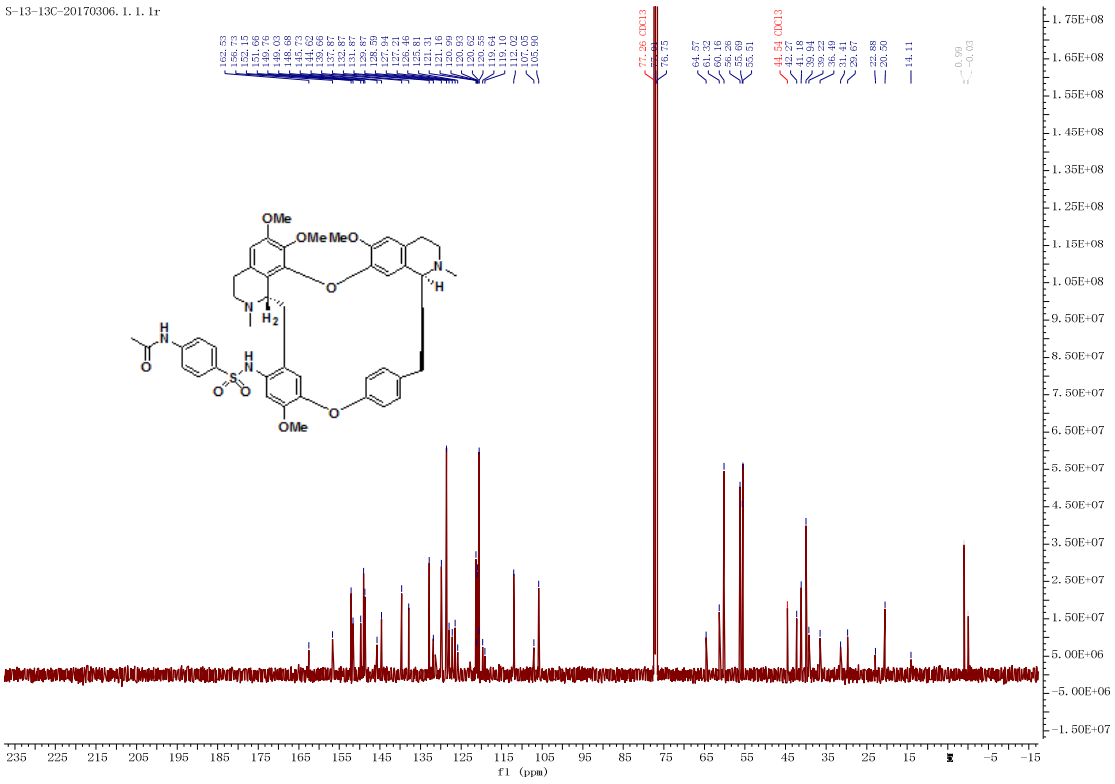
2.23. 14-(4-Tertbutylbenzenesulfonamide)tetrandrine (20)



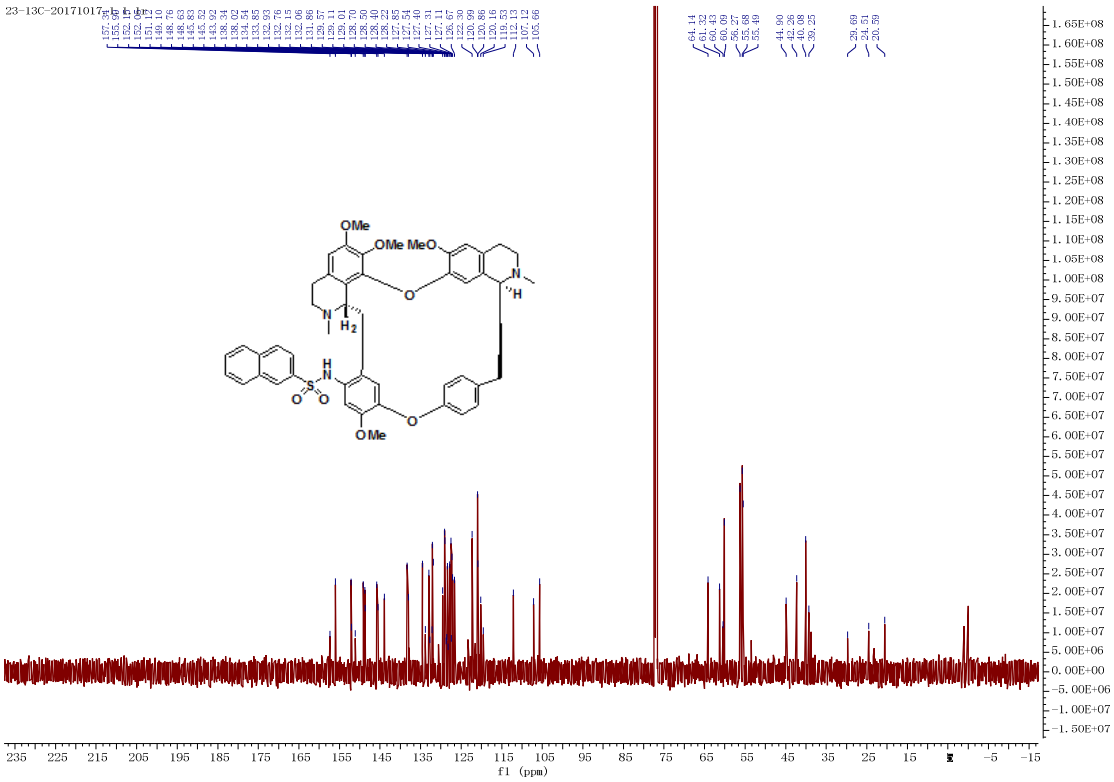
2.24. 14-(4-Trifluoromethylbenzenesulfonamide)tetrandrine (21)



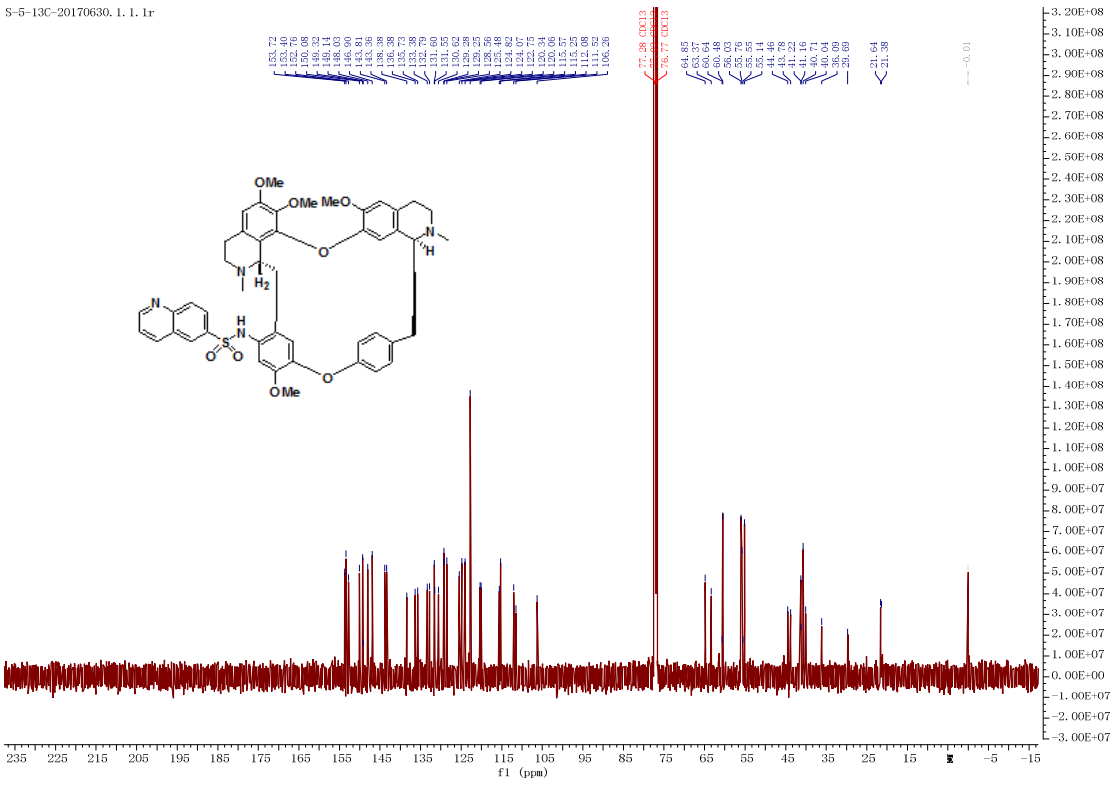
2.25. 14-(4-Acetaminobenzenesulfonamide)tetrandrine (22)



2.26. 14-(2-Naphthalenesulfonamide)tetrandrine (23)



2.27. 14-(Quinoline-8-sulfonamide)tetrandrine (24)



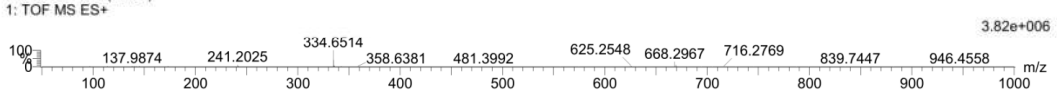
3. HRMS Spectra

3.1. Tet-NO_2

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
420 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10
PWD-NO2 384 (2.134)
1: TOF MS ES+



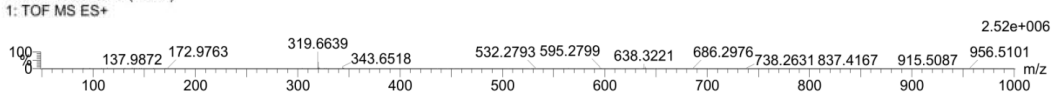
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
668.2967	668.2972	-0.5	-0.7	19.5	582.8	0.024	97.63	C38 H42 N3 O8
	668.2953	1.4	2.1	32.5	586.5	3.741	2.37	C50 H38 N O

3.2. Tet-NH_2

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
438 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10
PWD-HJ-NH2 373 (2.077)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
638.3221	638.3230	-0.9	-1.4	18.5	524.6	0.442	64.26	C38 H44 N3 O6
	638.3190	3.1	4.9	14.5	525.2	1.029	35.74	C33 H44 N5 O8

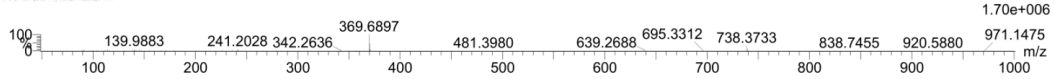
3.3. 14-(Methylsulfonamide)tetrandrine (1)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1719 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 0-10 S: 1-1 Cl: 0-2 Br: 0-1

PWD-1024-HL-50 469 (2.604)
1: TOF MS ES+



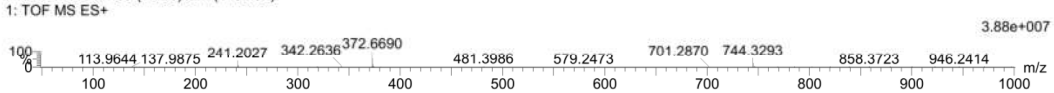
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
738.3733	738.3729	0.4	0.5	23.5	579.1	0.146	86.41	C47 H52 N3 O3 S
	738.3748	-1.5	-2.0	18.5	588.2	9.226	0.01	C46 H57 N O3 S Cl
	738.3707	2.6	3.5	14.5	588.7	9.748	0.01	C41 H57 N3 O5 S Cl
	738.3770	-3.7	-5.0	27.5	581.0	1.997	13.58	C52 H52 N O S

3.4. 14-(Propylsulfonamide)tetrandrine (2)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
837 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-5 O: 0-8 S: 1-1 Cl: 0-2
PWD-1023-S-6 450 (2.496) Cm (446:452)
1: TOF MS ES+



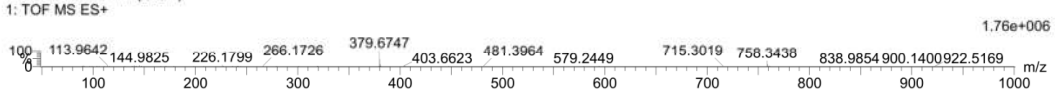
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
744.3293	744.3300	-0.7	-0.9	31.5	1038.9	2.338	9.65	C53 H46 N O S
	744.3278	1.5	2.0	22.5	1047.3	10.723	0.00	C47 H51 N O3 S Cl
	744.3270	2.3	3.1	18.5	1049.8	13.208	0.00	C42 H52 N5 O S Cl2
	744.3319	-2.6	-3.5	18.5	1036.7	0.163	84.95	C41 H50 N3 O8 S
	744.3260	3.3	4.4	27.5	1039.5	2.919	5.40	C48 H46 N3 O3 S
	744.3328	-3.5	-4.7	9.5	1049.7	13.087	0.00	C35 H56 N5 O6 S Cl2
	744.3256	3.7	5.0	13.5	1050.1	13.513	0.00	C41 H56 N O5 S Cl2

3.5. 14-(Butylsulfonamide)tetrandrine (3)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
552 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-5 O: 0-8 S: 0-1
PWD-1024-S-1 471 (2.614)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
758.3438	758.3441	-0.3	-0.4	23.5	634.2	1.524	21.78	C45 H48 N3 O8
	758.3423	1.5	2.0	36.5	637.4	4.703	0.91	C57 H44 N O
	758.3457	-1.9	-2.5	31.5	635.6	2.880	5.61	C54 H48 N O S
	758.3416	2.2	2.9	27.5	633.6	0.939	39.11	C49 H48 N3 O3 S
	758.3475	-3.7	-4.9	18.5	633.8	1.121	32.59	C42 H52 N3 O8 S

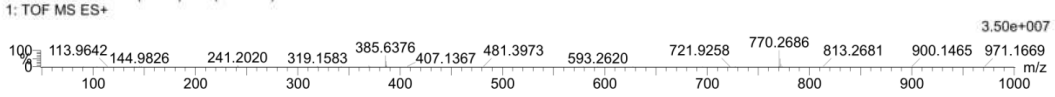
3.6. 14-(Trifluoromethylsulfonamide)tetrandrine (4)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-3 O: 0-8 S: 1-1 F: 3-3

PWD-1023-S-8 473 (2.625) Cm (467:473)
1: TOF MS ES+



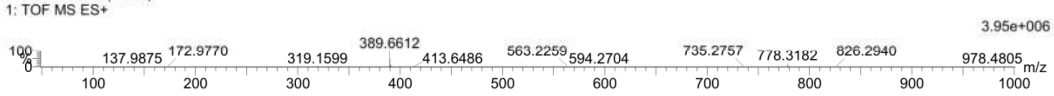
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
770.2686	770.2704	-1.8	-2.3	31.5	1071.6	3.855	2.12	C51 H39 N O S F3
	770.2664	2.2	2.9	27.5	1068.0	0.254	77.55	C46 H39 N3 O3 S F3
	770.2723	-3.7	-4.8	18.5	1069.4	1.593	20.34	C39 H43 N3 O8 S F3

3.7. 14-(Benzenesulfonamide)tetrandrine (5)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
467 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10 S: 0-1
PWD-Y-51 416 (2.310)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
778.3182	778.3202	-2.0	-2.6	26.5	557.0	1.850	15.72	C49 H48 N O6 S
	778.3162	2.0	2.6	22.5	555.4	0.209	81.14	C44 H48 N3 O8 S
	778.3216	-3.4	-4.4	31.5	558.6	3.461	3.14	C50 H44 N5 O2 S

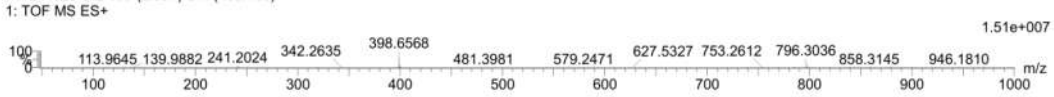
3.8. 14-(2-Fluorobenzenesulfonamide)tetrandrine (6)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
536 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-5 O: 0-8 S: 0-1 F: 1-1

PWD-1023-S-2 460 (2.557) Cm (458:460)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
796.3036	796.3034	0.2	0.3	27.5	984.0	1.001	36.75	C47 H43 N3 O8 F
	796.3049	-1.3	-1.6	35.5	986.4	3.416	3.28	C56 H43 N O S F
	796.3016	2.0	2.5	40.5	988.4	5.449	0.43	C59 H39 N O F
	796.3009	2.7	3.4	31.5	985.0	2.041	12.99	C51 H43 N3 O3 S F
	796.3068	-3.2	-4.0	22.5	983.8	0.788	45.48	C44 H47 N3 O8 S F
	796.3074	-3.8	-4.8	31.5	987.5	4.534	1.07	C52 H43 N O6 F

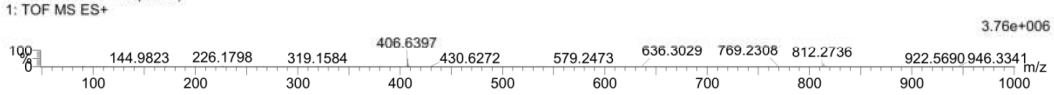
3.9. 14-(2-Chlorobenzenesulfonamide)tetrandrine (7)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
386 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1 Cl: 0-2

PWD-1024-S-3 473 (2.625)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
812.2736	812.2750	-1.4	-1.7	13.5	640.6	3.202	4.07	C38 H52 N3 O10 S Cl12
	812.2772	-3.6	-4.4	22.5	637.5	0.042	95.93	C44 H47 N3 O8 S Cl

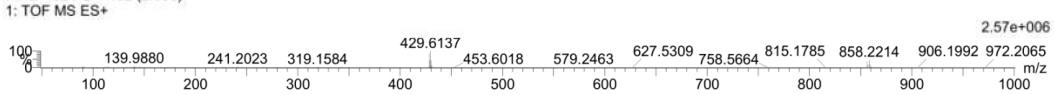
3.10. 14-(3-Bromobenzenesulfonamide)tetrandrine (8)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.1 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
487 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 0-10 S: 1-1 Br: 0-1

PWD-1024-S-4 482 (2.680)
1: TOF MS ES+



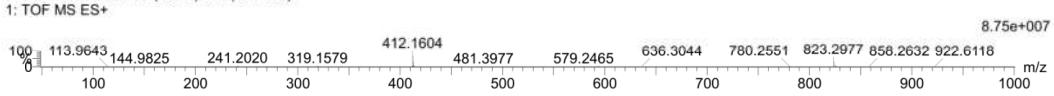
Minimum:				-1.5				
Maximum:		5.0	5.1	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
856.2224	856.2216	0.8	0.9	33.5	747.2	13.303	0.00	C51 H38 N O10 S
	856.2209	1.5	1.8	31.5	734.8	0.884	41.31	C51 H43 N3 O3 S Br
	856.2249	-2.5	-2.9	35.5	737.2	3.276	3.78	C56 H43 N O S Br
	856.2267	-4.3	-5.0	22.5	734.5	0.599	54.91	C44 H47 N3 O8 S Br

3.11. 14-(2-Nitrobenzenesulfonamide)tetrandrine (9)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1
PWD-1023-HL-56 463 (2.572) Cm (462:469)
1: TOF MS ES+



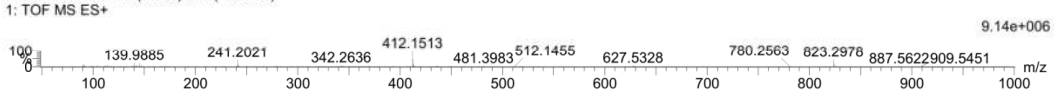
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
823.2977	823.2941	3.6	4.4	27.5	1040.0	2.938	5.30	C50 H47 O9 S
	823.3013	-3.6	-4.4	23.5	1037.1	0.066	93.64	C44 H47 N4 O10 S
	823.3053	-7.6	-9.2	27.5	1041.6	4.542	1.07	C49 H47 N2 O8 S

1.12. 14-(3-Nitrobenzenesulfonamide)tetrandrine (10)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1
PWD-1023-S-9 479 (2.656) Cm (479:492)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
823.2978	823.3013	-3.5	-4.3	23.5	1035.8	0.242	78.52	C44 H47 N4 O10 S
	823.2941	3.7	4.5	27.5	1037.1	1.538	21.48	C50 H47 O9 S

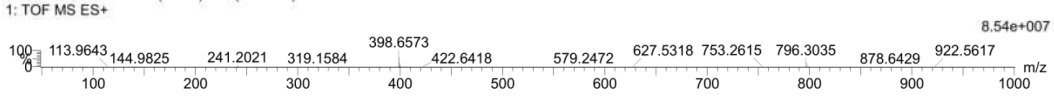
1.13. 14-(4-Fluorobenzenesulfonamide)tetrandrine (11)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
128 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1 F: 1-1

PWD-1023-LJJ-94 463 (2.572) Cm (461:476)
1: TOF MS ES+



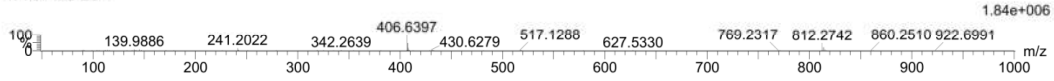
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
796.3035	796.3068	-3.3	-4.1	22.5	1134.2	n/a	n/a	C44 H47 N3 O8 S F

3.14. 14-(4-Chlorobenzenesulfonamide)tetrandrine (12)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
534 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-3 O: 0-8 S: 1-1 Cl: 0-2
PWD-1023-HL-59 481 (2.675)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
812.2742	812.2736	0.6	0.7	40.5	582.8	9.139	0.01	C57 H38 N3 O S
	812.2732	1.0	1.2	26.5	577.2	3.578	2.79	C50 H48 N O3 S Cl2
	812.2754	-1.2	-1.5	35.5	575.9	2.273	10.30	C56 H43 N O S Cl
	812.2714	2.8	3.4	31.5	575.0	1.341	26.16	C51 H43 N3 O3 S Cl
	812.2772	-3.0	-3.7	22.5	574.1	0.499	60.73	C44 H47 N3 O8 S Cl

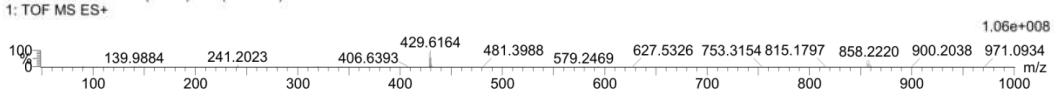
3.15. 14-(4-Bromobenzenesulfonamide)tetrandrine (13)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
258 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1 Br: 0-1

PWD-1023-S-10 476 (2.641) Cm (459:493)
1: TOF MS ES+



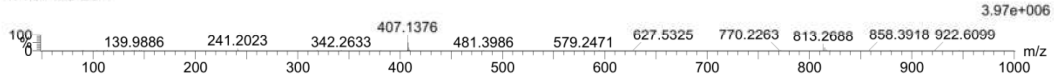
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
856.2230	856.2216	1.4	1.6	33.5	1338.8	13.635	0.00	C51 H38 N O10 S
	856.2267	-3.7	-4.3	22.5	1325.1	0.000	100.00	C44 H47 N3 O8 S Br

3.16. 14-(6-chloropyridine-3-sulfonamide)tetrandrine (14)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
812 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-5 O: 0-8 S: 1-1 Cl: 0-2
PWD-1023-S-7 462 (2.567)
1: TOF MS ES+



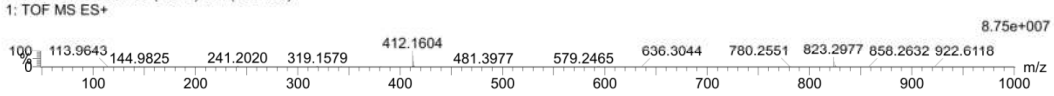
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
813.2688	813.2688	0.0	0.0	40.5	725.8	10.066	0.00	C56 H37 N4 O S
	813.2684	0.4	0.5	26.5	719.8	4.051	1.74	C49 H47 N2 O3 S Cl2
	813.2675	1.3	1.6	35.5	725.7	9.912	0.00	C55 H41 O5 S
	813.2706	-1.8	-2.2	35.5	718.8	2.995	5.01	C55 H42 N2 O S Cl
	813.2666	2.2	2.7	31.5	716.9	1.169	31.08	C50 H42 N4 O3 S Cl
	813.2653	3.5	4.3	26.5	717.7	1.902	14.93	C49 H46 O7 S Cl
	813.2725	-3.7	-4.5	30.5	722.7	6.907	0.10	C54 H47 O S Cl2
	813.2725	-3.7	-4.5	22.5	716.5	0.752	47.14	C43 H46 N4 O8 S Cl

3.17. 14-(4-Nitrobenzenesulfonamide)tetrandrine (15)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1
PWD-1023-HL-56 463 (2.572) Cm (462:469)
1: TOF MS ES+



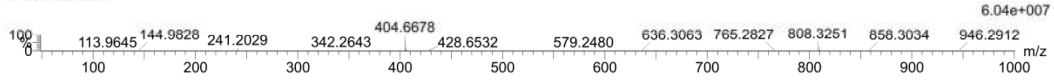
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
823.2977	823.2941	3.6	4.4	27.5	1040.0	2.938	5.30	C50 H47 O9 S
	823.3013	-3.6	-4.4	23.5	1037.1	0.066	93.64	C44 H47 N4 O10 S
	823.3053	-7.6	-9.2	27.5	1041.6	4.542	1.07	C49 H47 N2 O8 S

1.18. 14-(3-Methoxybenzenesulfonamide)tetrandrine (16)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1
PWD-1023-LJJ-95 454 (2.525) Cm (451:459)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
808.3251	808.3268	-1.7	-2.1	22.5	1101.6	n/a	n/a	C45 H50 N3 O9 S

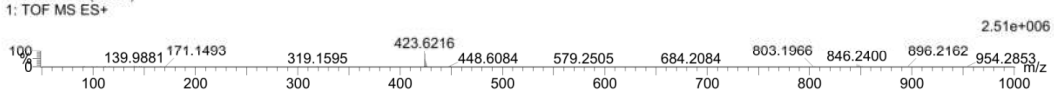
1.19. 14-(3,5-Dichlorobenzenesulfonamide)tetrandrine (17)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
201 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10 S: 0-1

PWD-5f 460 (2.557)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
846.2400	846.2373	2.7	3.2	31.5	486.5	n/a	n/a	C50 H40 N O10 S

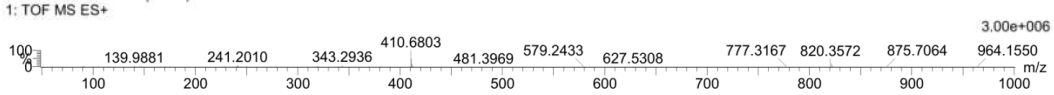
3.20. 14-(2,4,6-Trimethylbenzenesulfonamide)tetrandrine (18)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
264 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 F: 3-3 S: 1-1 Br: 0-1

PWD-1023-S-14 494 (2.743)
1: TOF MS ES+



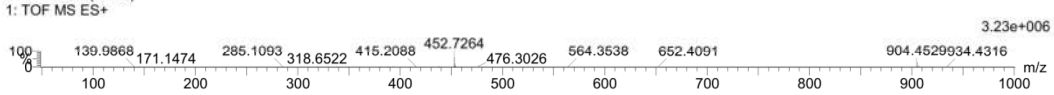
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
820.3572	820.3607	-3.5	-4.3	19.5	610.7	n/a	n/a	C45 H53 N3 O6 F3 S

3.21. 14-(2,4,6-Triisopropylbenzenesulfonamide)tetrandrine (19)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
198 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-60 H: 0-90 N: 0-4 O: 5-10 S: 1-1
S-12-12 443 (2.460)
1: TOF MS ES+



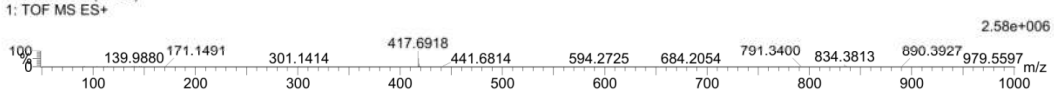
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
904.4529	904.4571	-4.2	-4.6	22.5	554.5	n/a	n/a	C53 H66 N3 O8 S

3.22. 14-(4-Tertbutylbenzenesulfonamide)tetrandrine (20)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
236 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10 S: 0-1
PWD-5d 439 (2.439)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
834.3813	834.3788	2.5	3.0	22.5	450.2	n/a	n/a	C48 H56 N3 O8 S

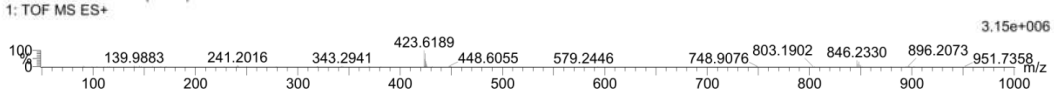
3.23. 14-(4-Trifluoromethylbenzenesulfonamide)tetrandrine (21)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
258 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1 Br: 0-1

PWD-1023-S-16 500 (2.774)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
846.2330	846.2311	1.9	2.2	20.5	686.3	n/a	n/a	C44 H49 N O9 S Br

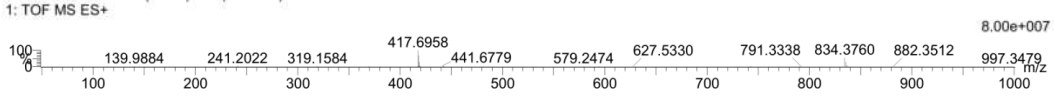
3.24. 14-(4-Acetaminobenzenesulfonamide)tetrandrine (22)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
258 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1 Br: 0-1

PWD-1023-S-15 480 (2.662) Cm (476:484)
1: TOF MS ES+



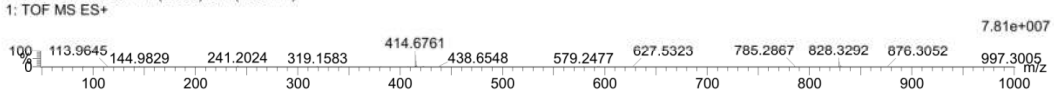
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
834.3760	834.3788	-2.8	-3.4	22.5	986.9	n/a	n/a	C48 H56 N3 O8 S

3.25. 14-(2-Naphthalenesulfonamide)tetrandrine (23)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-4 O: 6-10 S: 1-1
PWD-1023-LJJ-96 474 (2.630) Cm (465:474)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
828.3292	828.3319	-2.7	-3.3	25.5	1087.5	0.010	99.01	C48 H50 N3 O8 S
	828.3359	-6.7	-8.1	29.5	1092.1	4.615	0.99	C53 H50 N O6 S

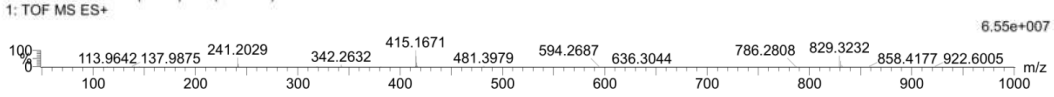
3.26. 14-(Quinoline-8-sulfonamide)tetrandrine (24)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
518 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-5 O: 0-8 S: 1-1 Br: 0-1

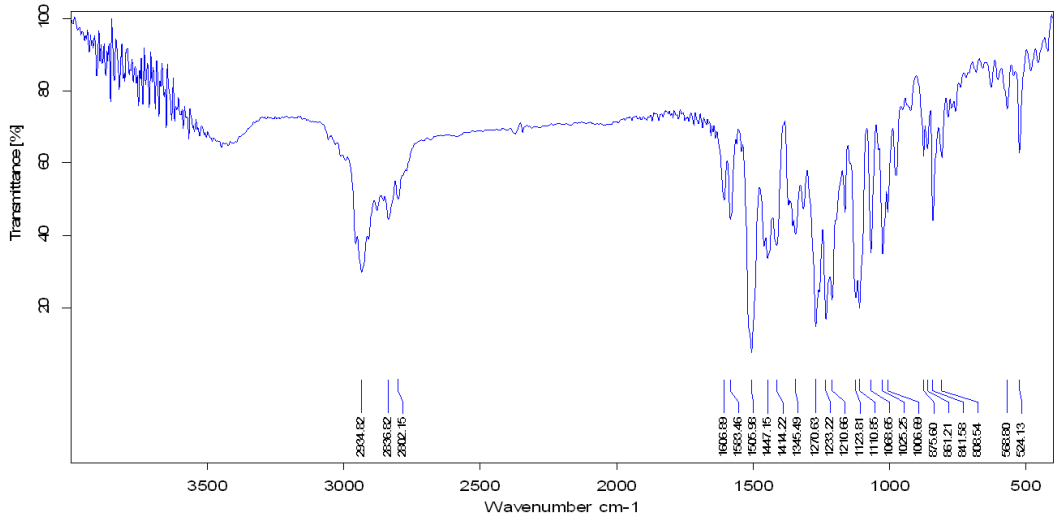
PWD-1023-S-5 449 (2.491) Cm (442:451)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
829.3232	829.3250	-1.8	-2.2	18.5	1138.2	12.968	0.00	C46 H58 N2 O5 S Br
	829.3212	2.0	2.4	34.5	1126.3	1.107	33.04	C54 H45 N4 O3 S
	829.3253	-2.1	-2.5	38.5	1129.0	3.766	2.31	C59 H45 N2 O S
	829.3210	2.2	2.7	14.5	1138.7	13.457	0.00	C41 H58 N4 O7 S Br
	829.3199	3.3	4.0	29.5	1126.9	1.658	19.05	C53 H49 O7 S
	829.3271	-3.9	-4.7	25.5	1126.0	0.785	45.59	C47 H49 N4 O8 S
	829.3191	4.1	4.9	27.5	1138.8	13.589	0.00	C53 H54 N2 S Br

4. IR Spectra

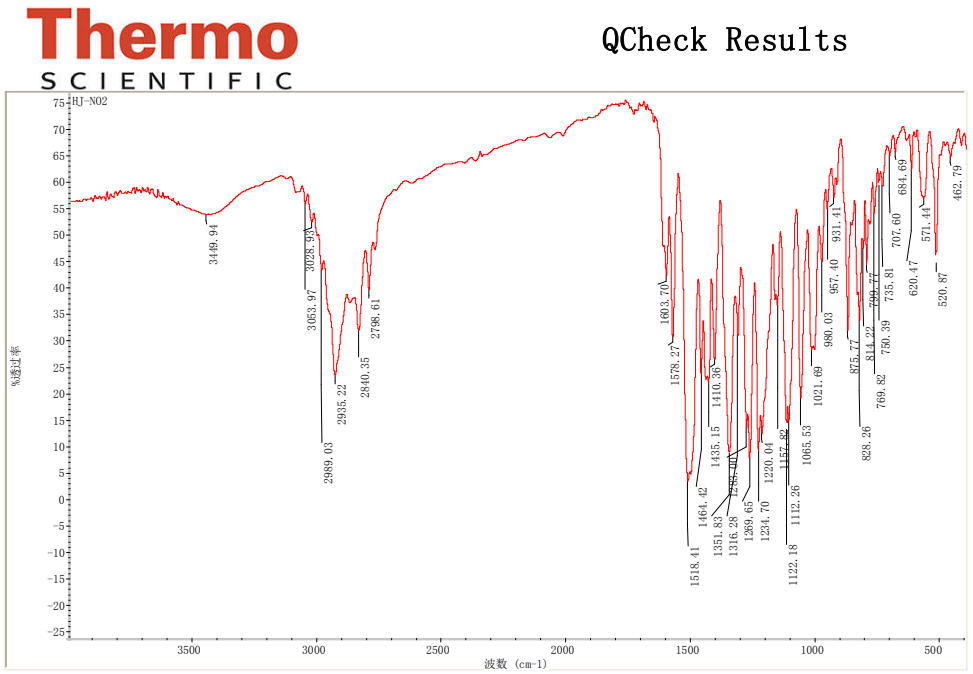
4.1.Tetrandrine



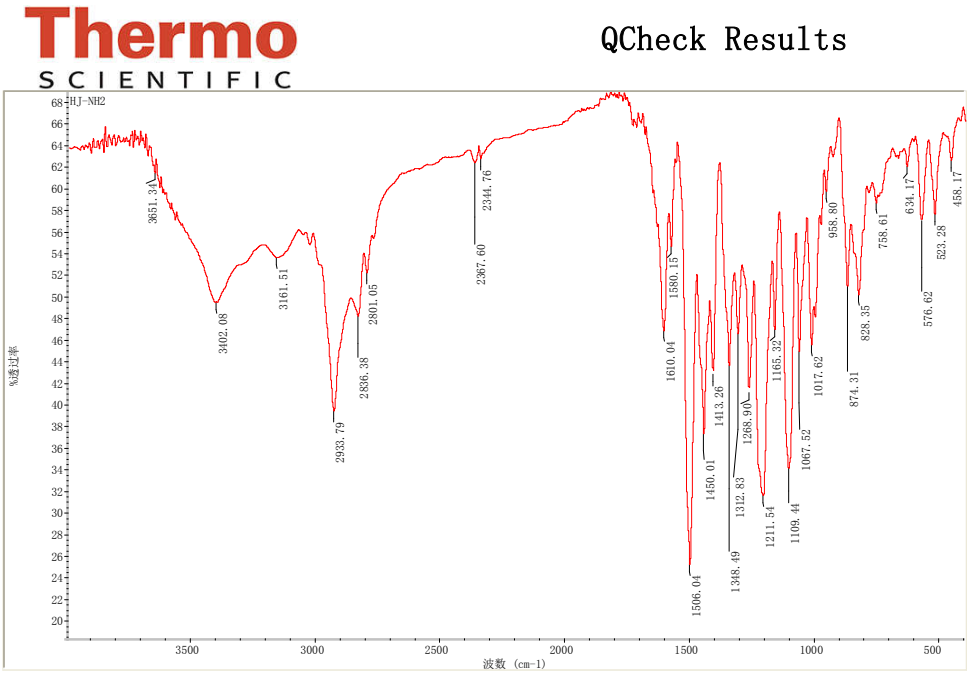
D:\Date\HS\CNHJ-OH.4 HJ S	2017-6-7

Page 1/1

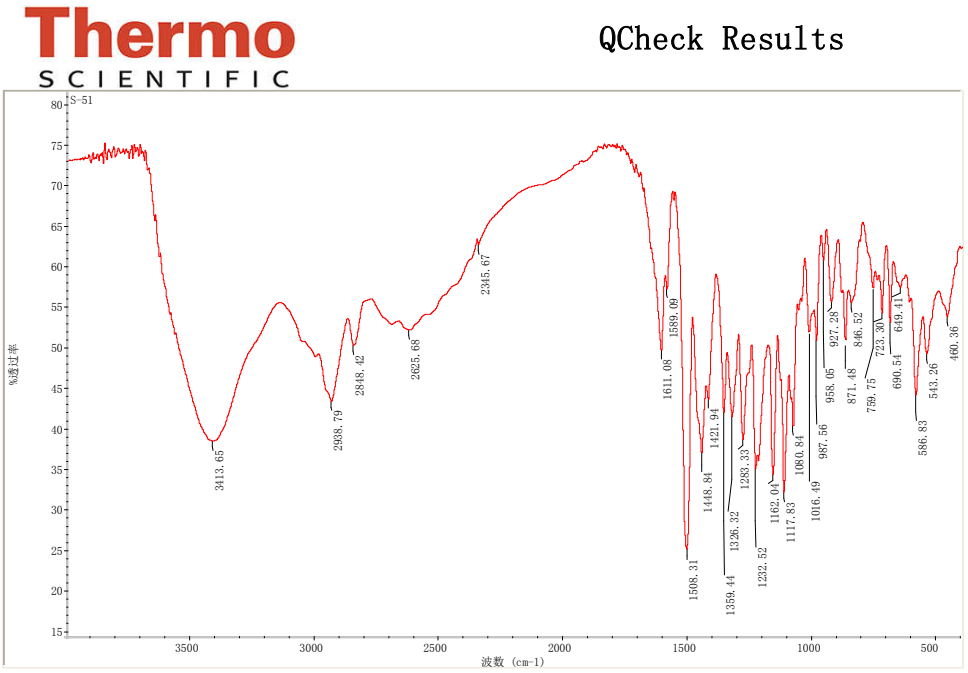
4.2. Tet-NO_2



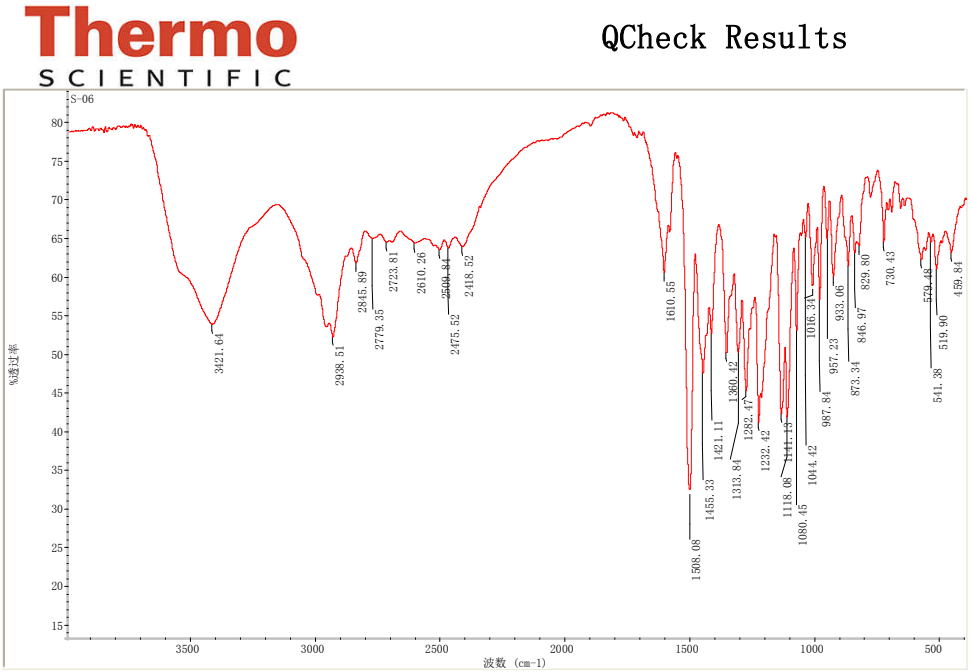
4.3. Tet-NH_2



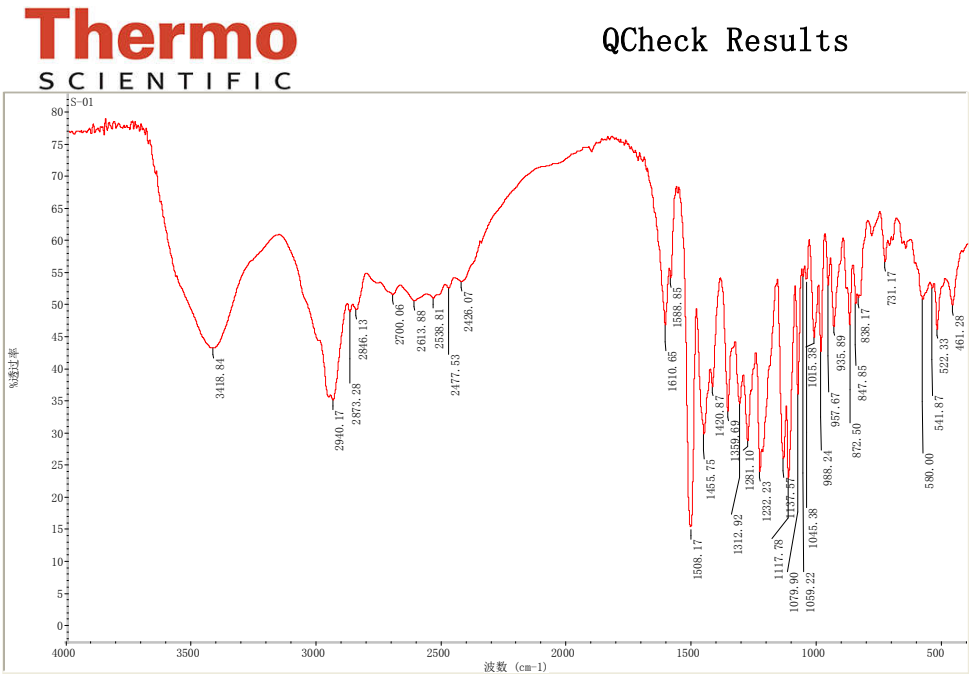
4.4. 14-(Methylsulfonamide)tetrandrine (1)



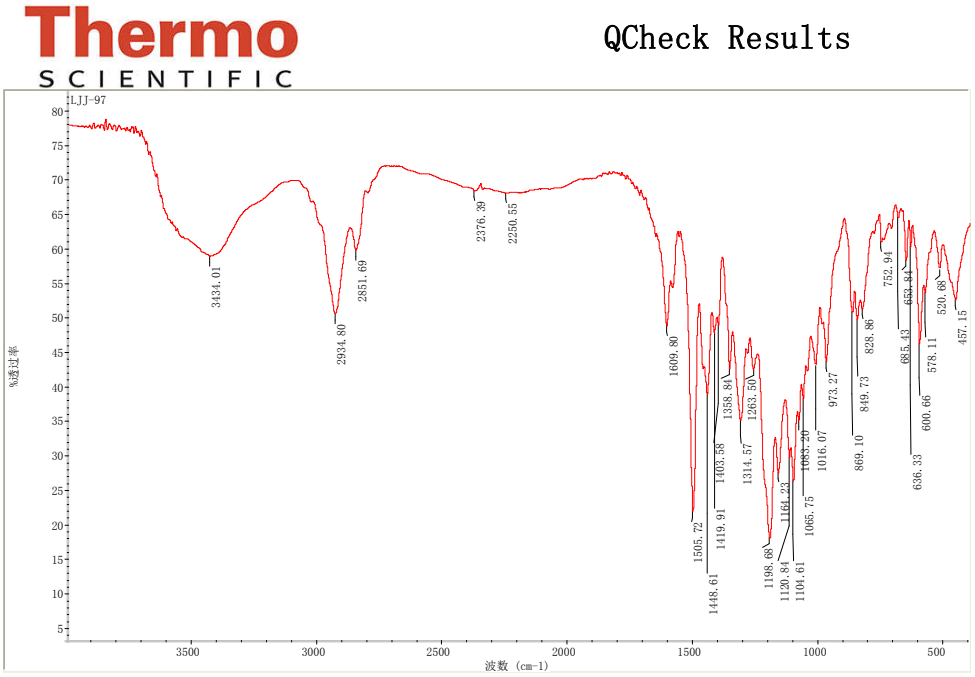
4.5. 14-(Propylsulfonamide)tetrandrine (2)



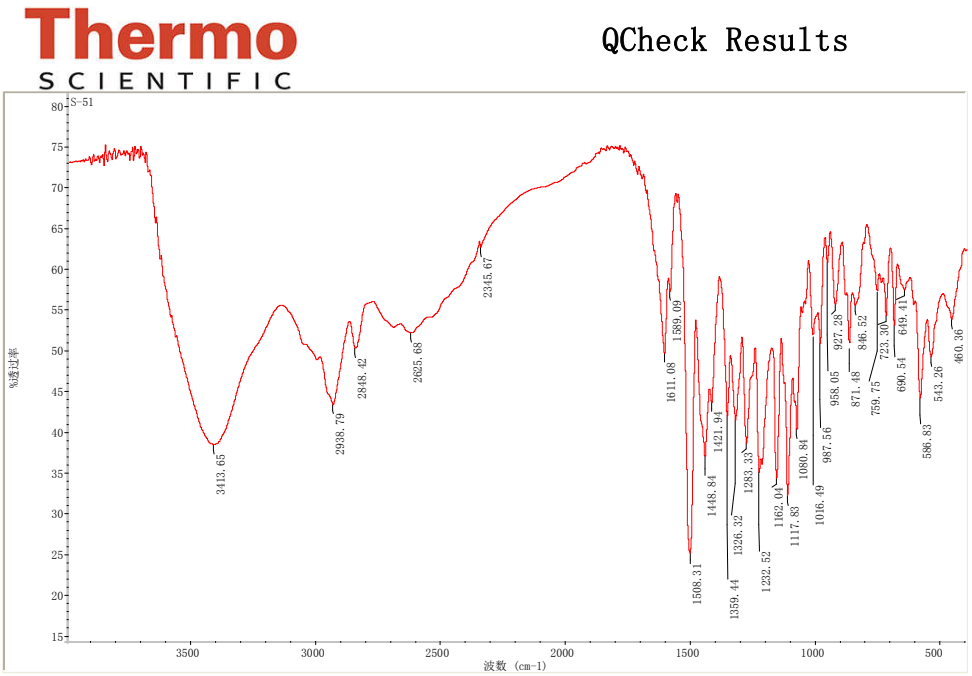
4.6. 14-(Butylsulfonamide)tetrandrine (3)



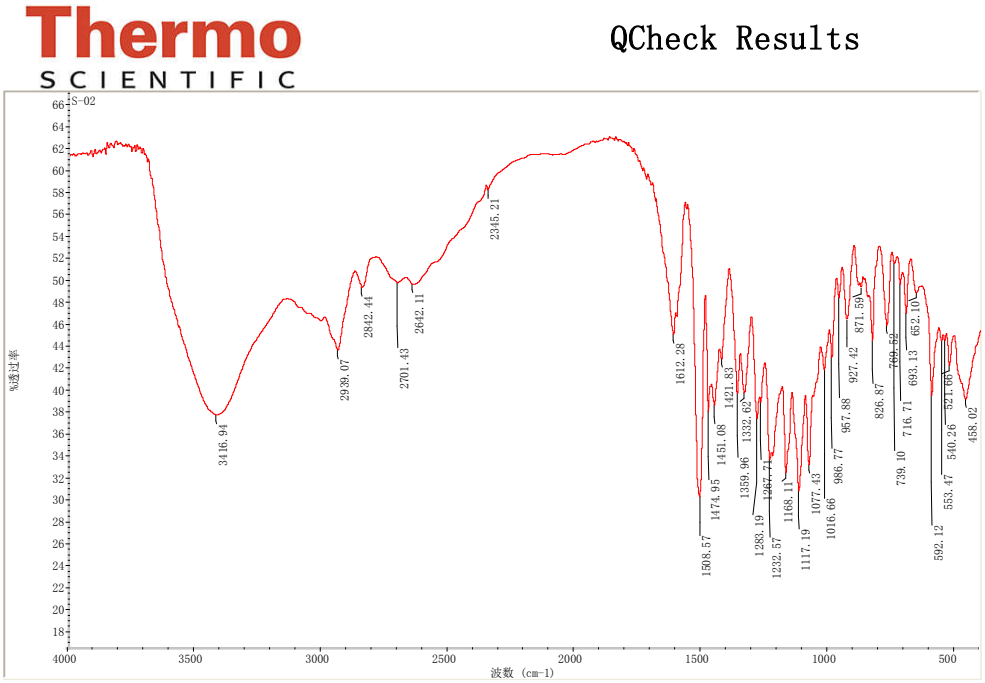
4.7. 14-(Trifluoromethylsulfonamide)tetrandrine (4)



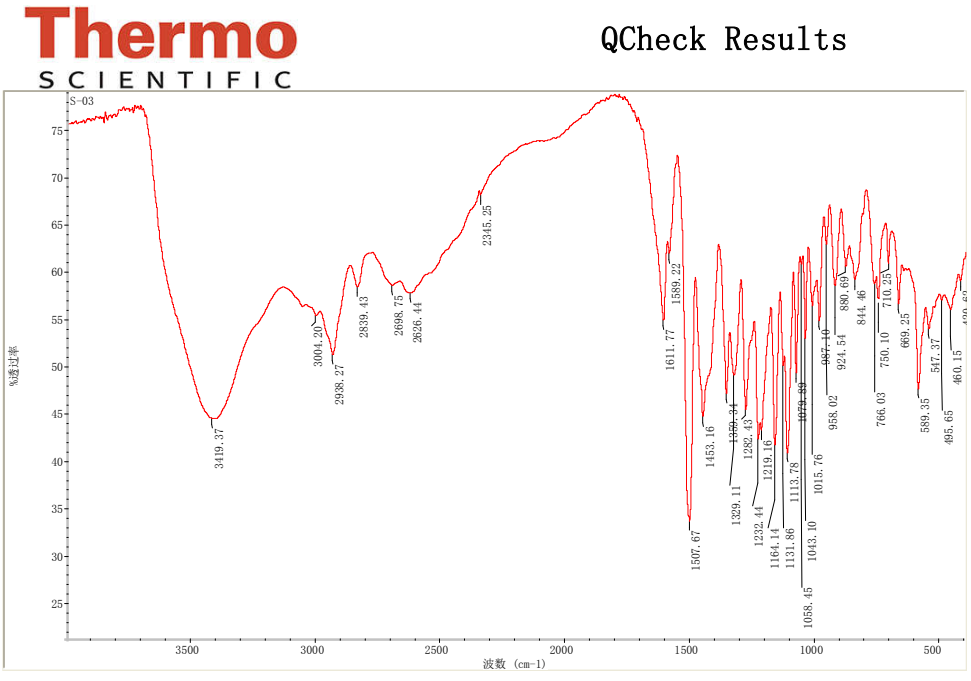
4.8. 14-(Benzenesulfonamide)tetrandrine (5)



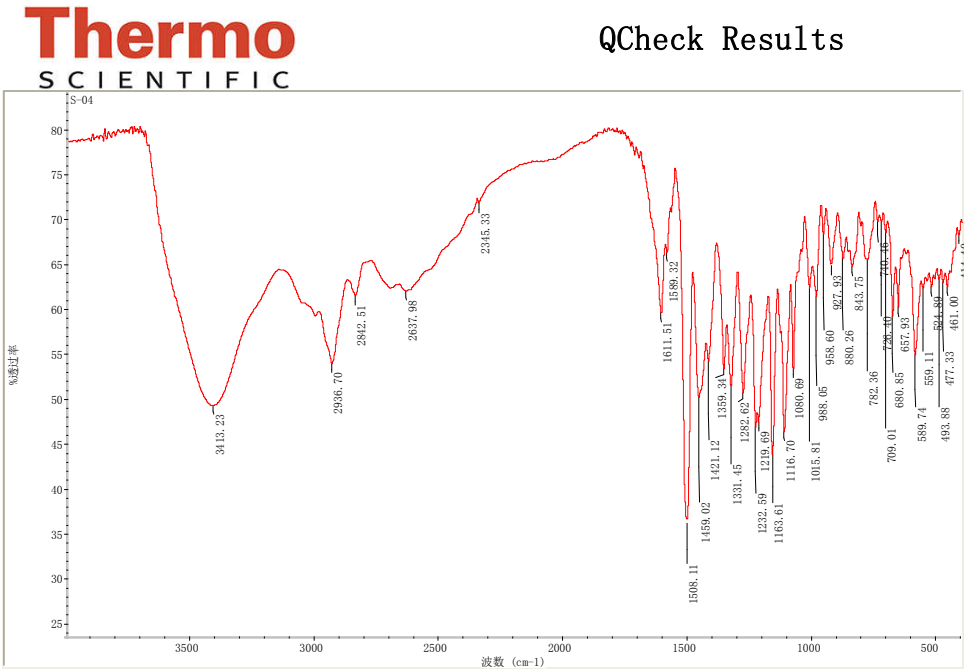
4.9. 14-(2-Fluorobenzenesulfonamide)tetrandrine (6)



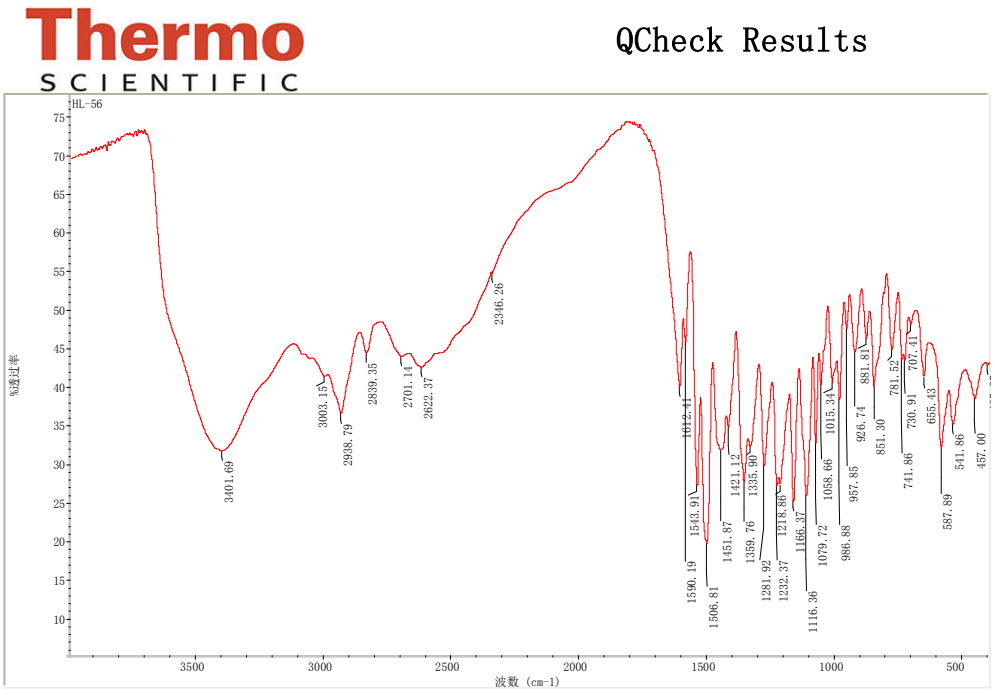
4.10. 14-(2-Chlorobenzenesulfonamide)tetrandrine (7)



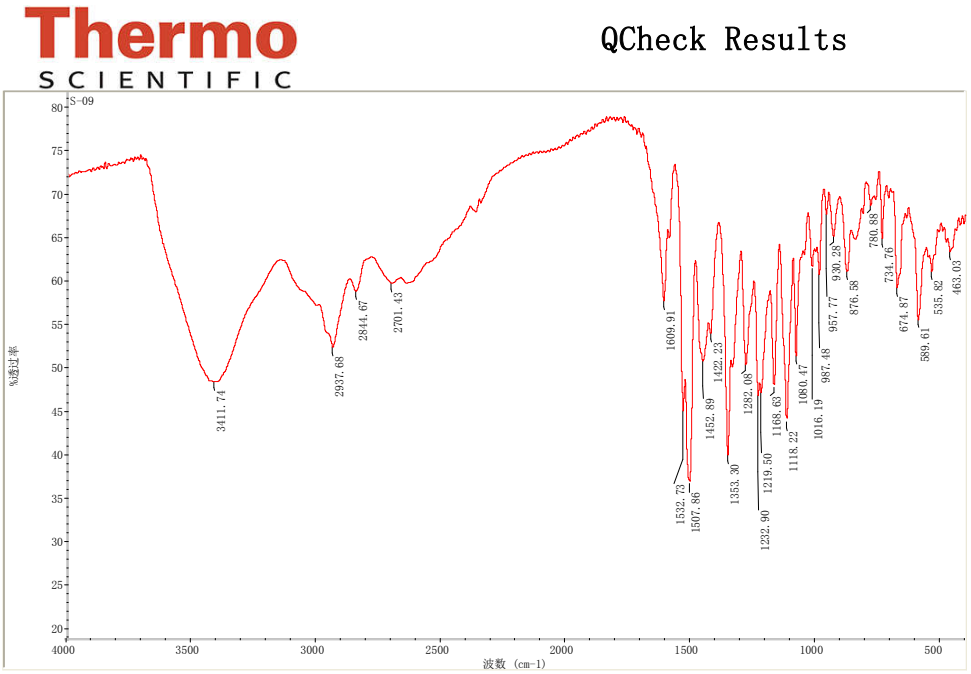
4.11. 14-(3-Bromobenzenesulfonamide)tetrandrine (8)



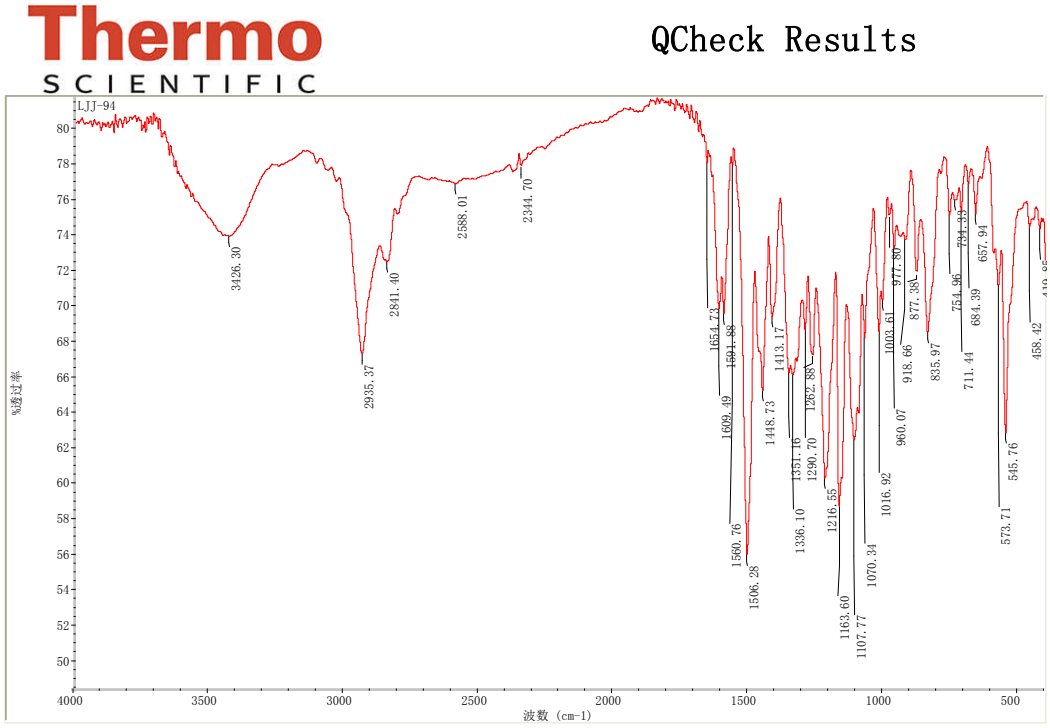
4.12. 14-(2-Nitrobenzenesulfonamide)tetrandrine (9)



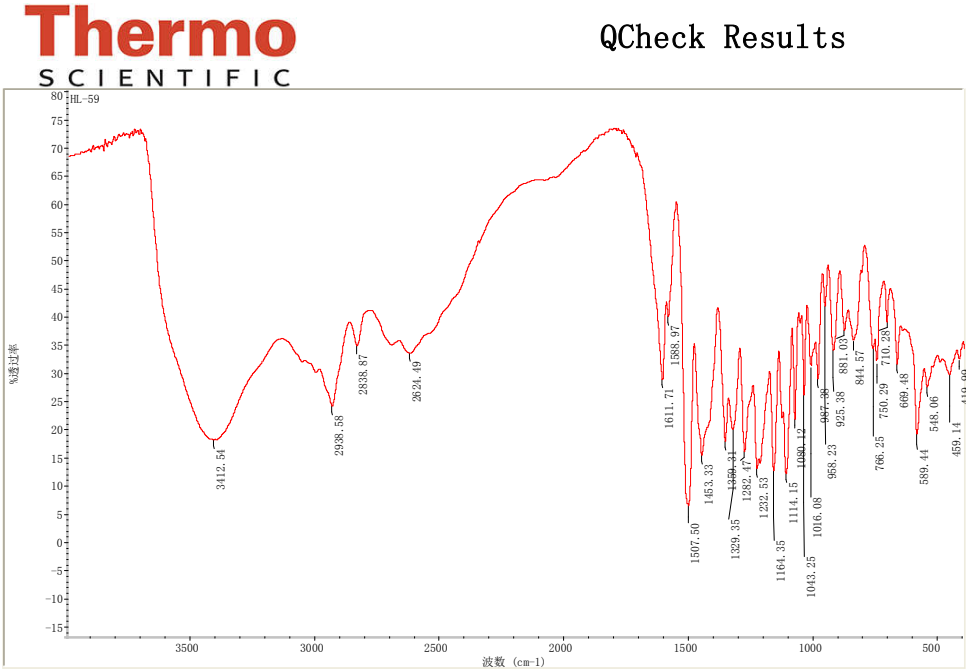
4.13. 14-(3-Nitrobenzenesulfonamide)tetrandrine (10)



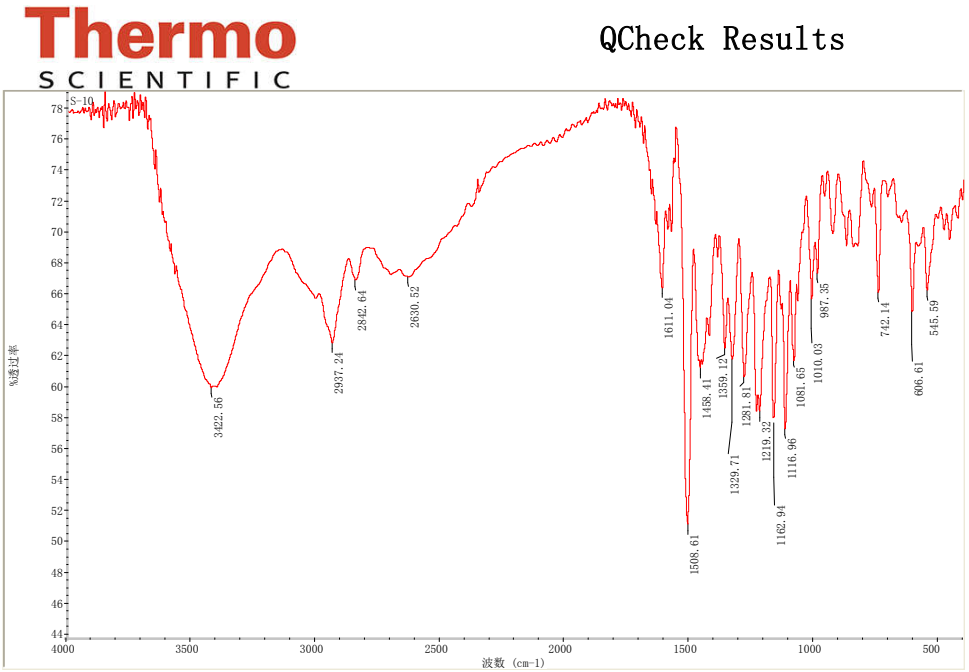
4.14. 14-(4-Fluorobenzenesulfonamide)tetrandrine (11)



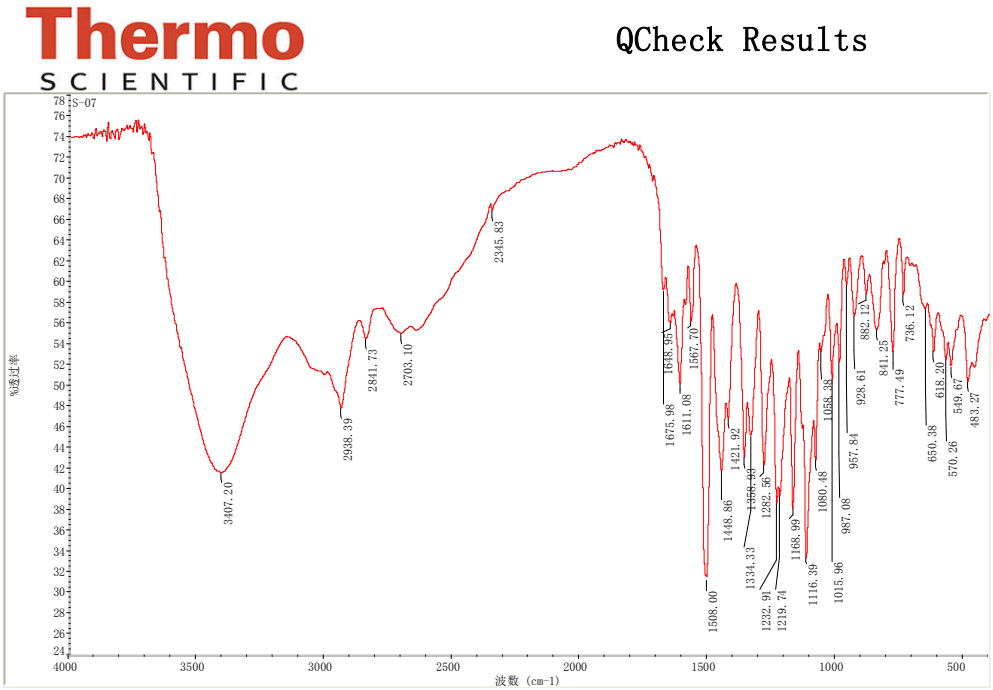
4.15. 14-(4-Chlorobenzenesulfonamide)tetrandrine (12)



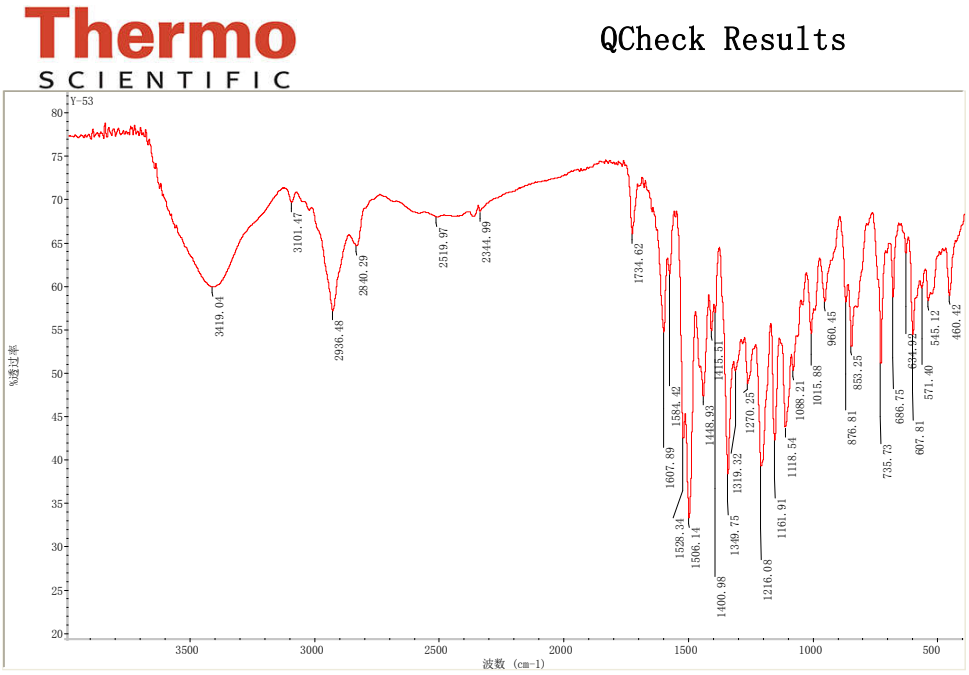
4.16. 14-(4-Bromobenzenesulfonamide)tetrandrine (13)



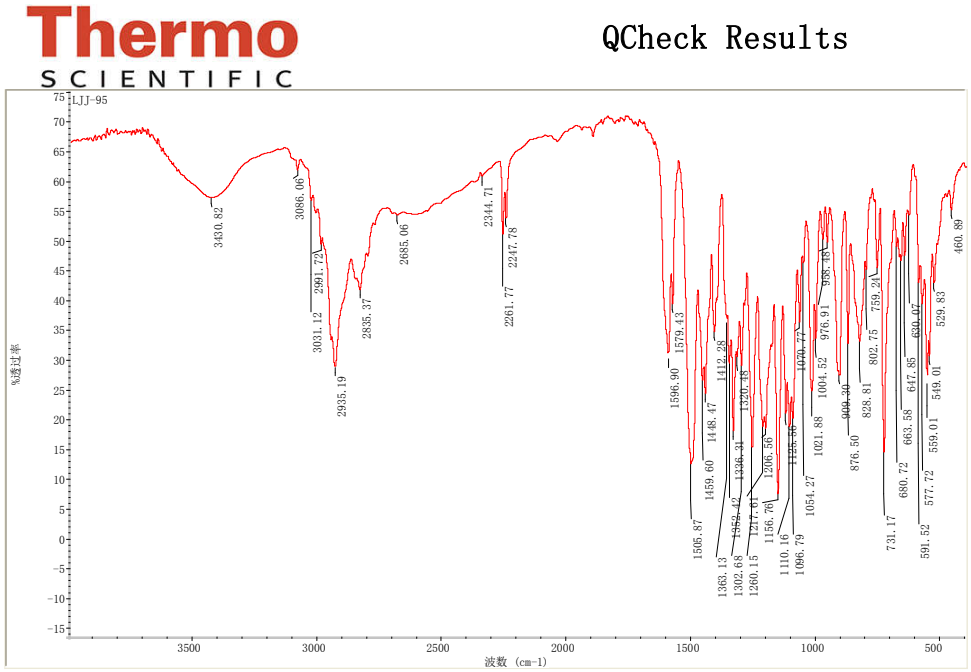
4.17. 14-(6-chloropyridine-3-sulfonamide)tetrandrine (14)



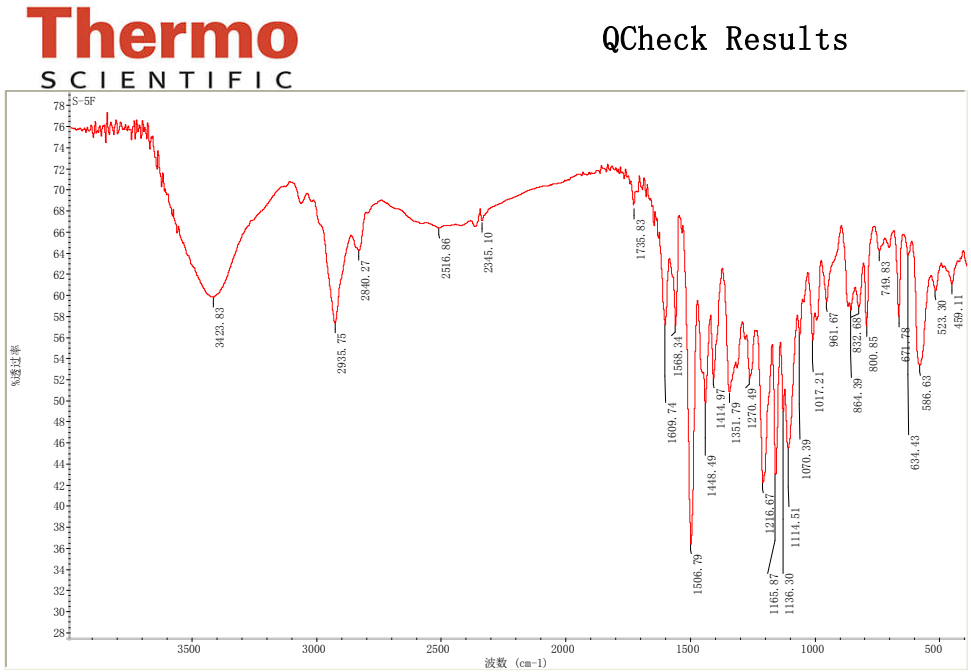
4.18. 14-(4-Nitrobenzenesulfonamide)tetrandrine (15)



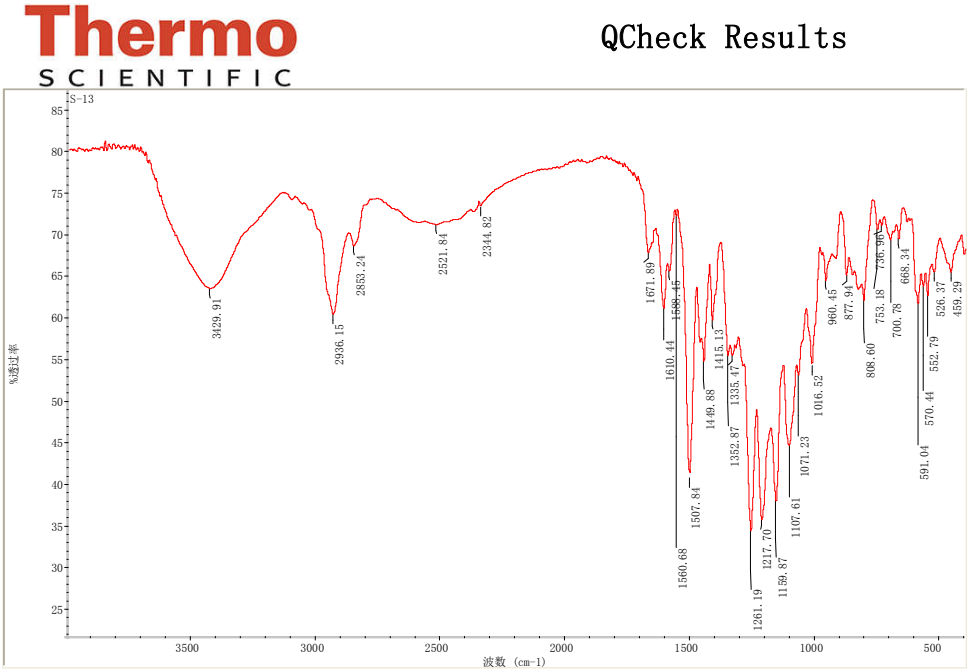
4.19. 14-(3-Methoxybenzenesulfonamide)tetrandrine (16)



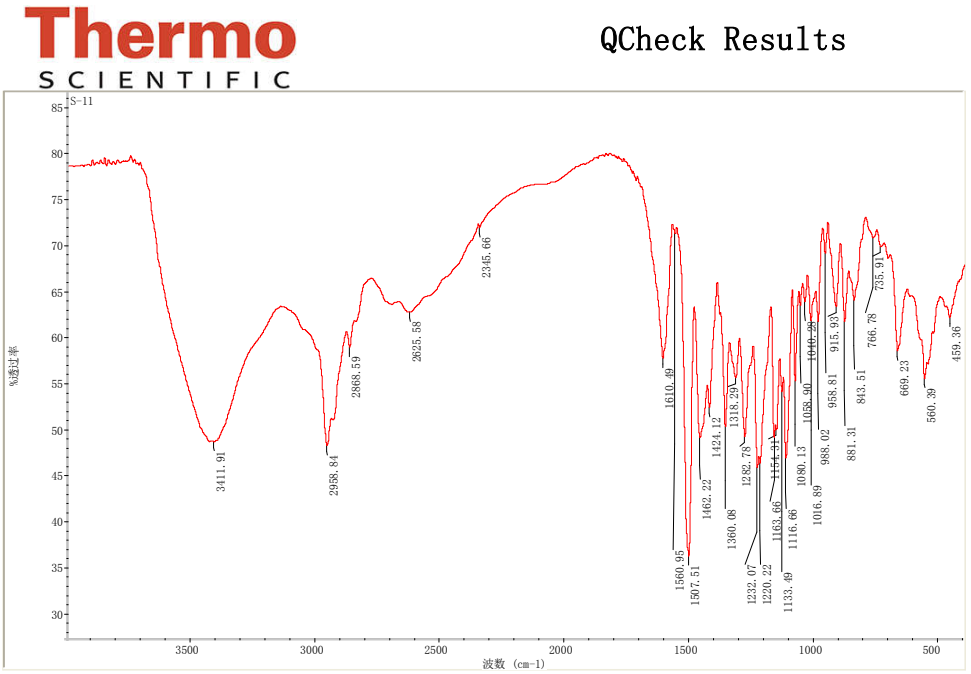
4.20. 14-(3,5-Dichlorobenzenesulfonamide)tetrandrine (17)



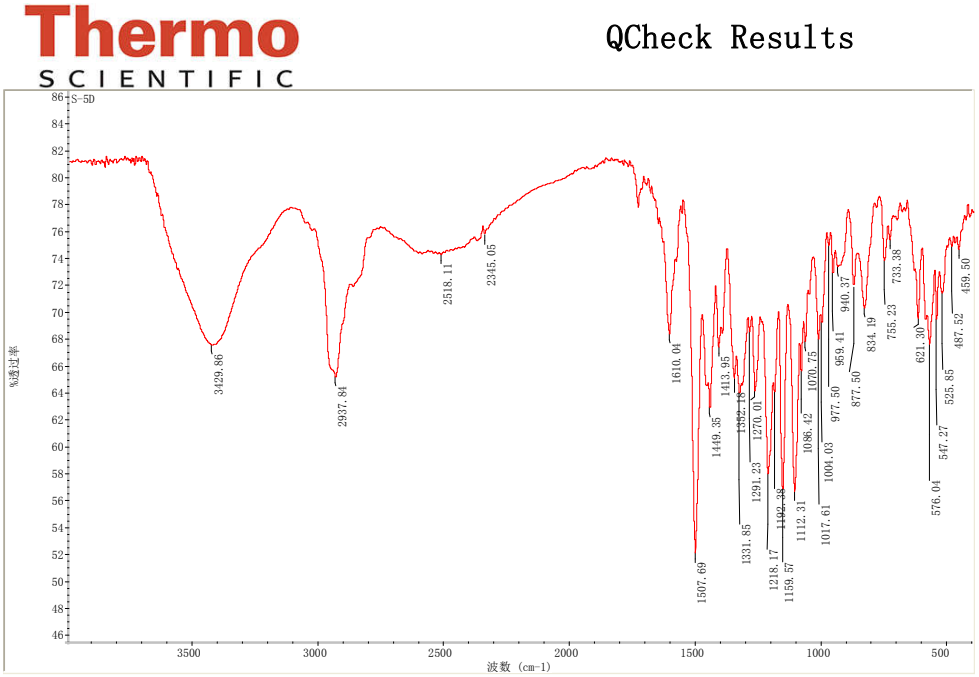
4.21. 14-(2,4,6-Trimethylbenzenesulfonamide)tetrandrine (18)



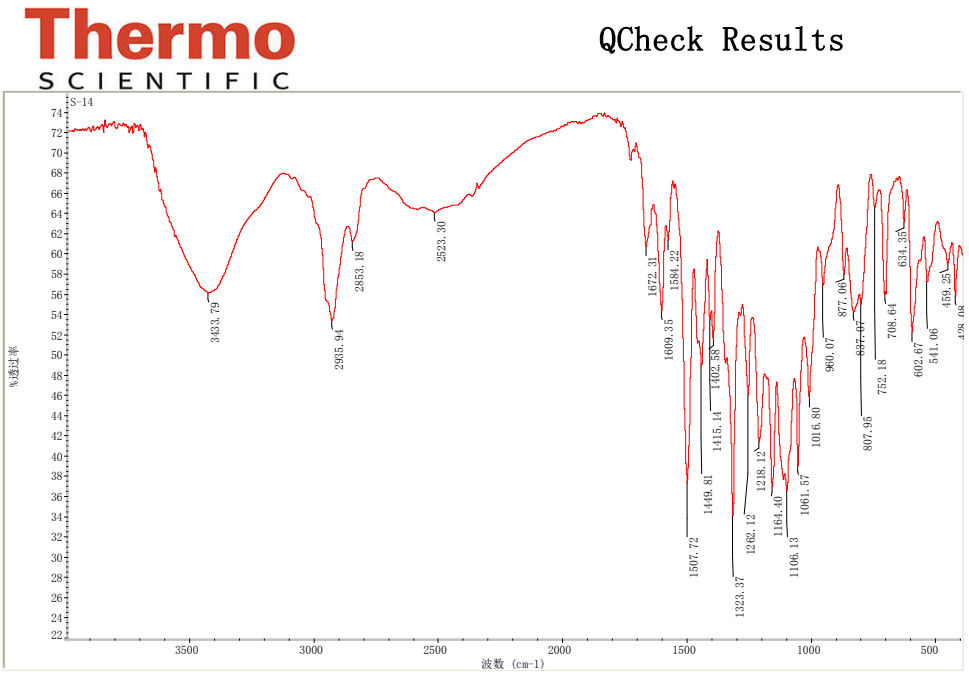
4.22. 14-(2,4,6-Triisopropylbenzenesulfonamide)tetrandrine (19)



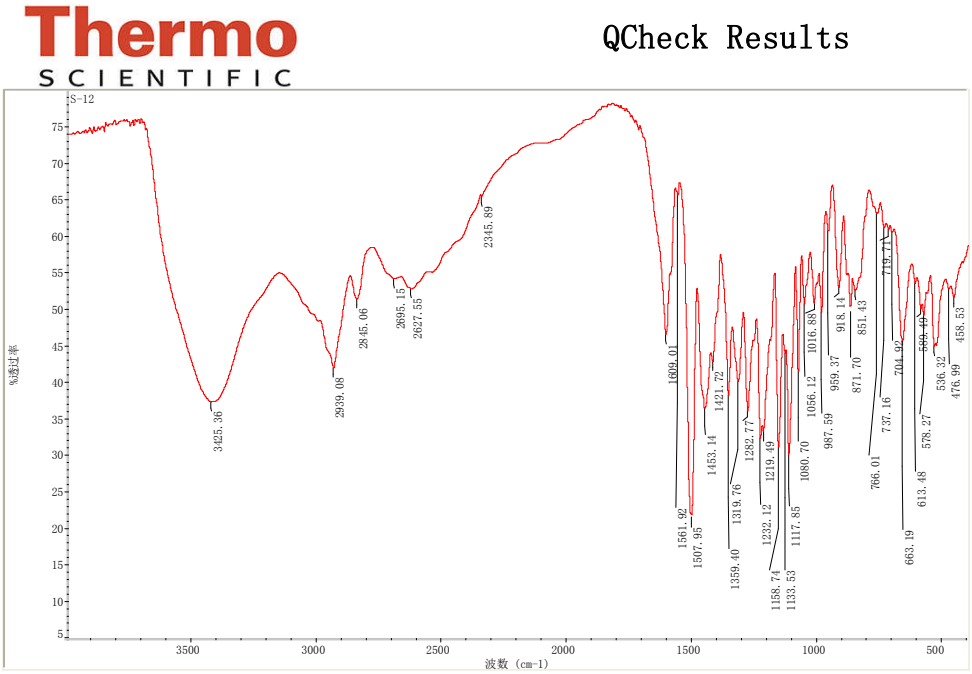
4.23. 14-(4-Tertbutylbenzenesulfonamide)tetrandrine (20)



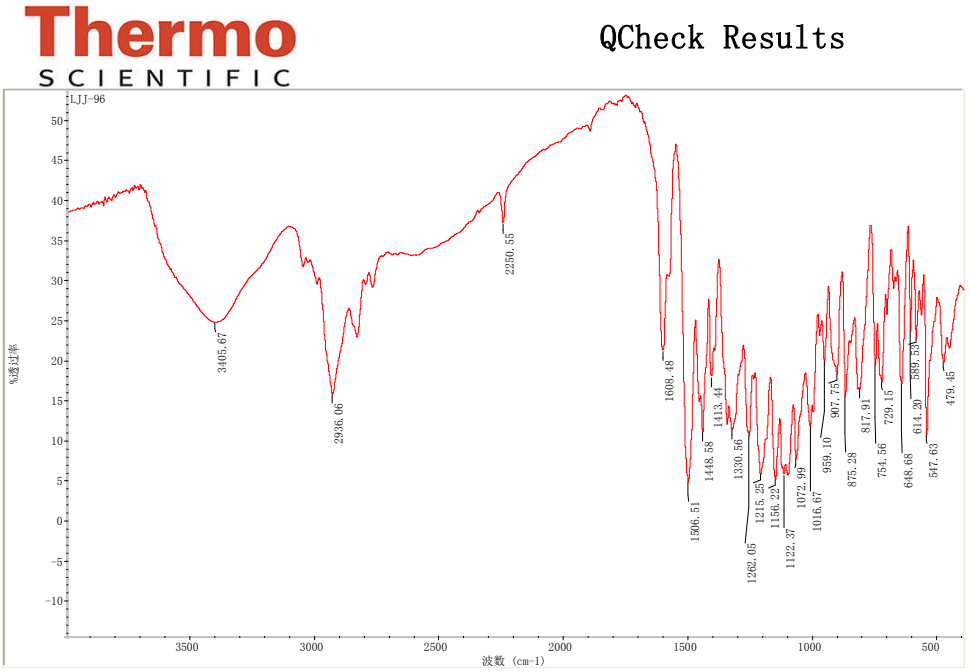
4.24. 14-(4-Trifluoromethylbenzenesulfonamide)tetrandrine (21)



4.25. 14-(4-Acetaminobenzenesulfonamide)tetrandrine (22)



4.26. 14-(2-Naphthalenesulfonamide)tetrandrine (23)



4.27. 14-(Quinoline-8-sulfonamide)tetrandrine (24)