HPLC Data and Profiles
For

Synthesis and anticancer activity studies of α-aminoalkylated conjugated nitroalkenes

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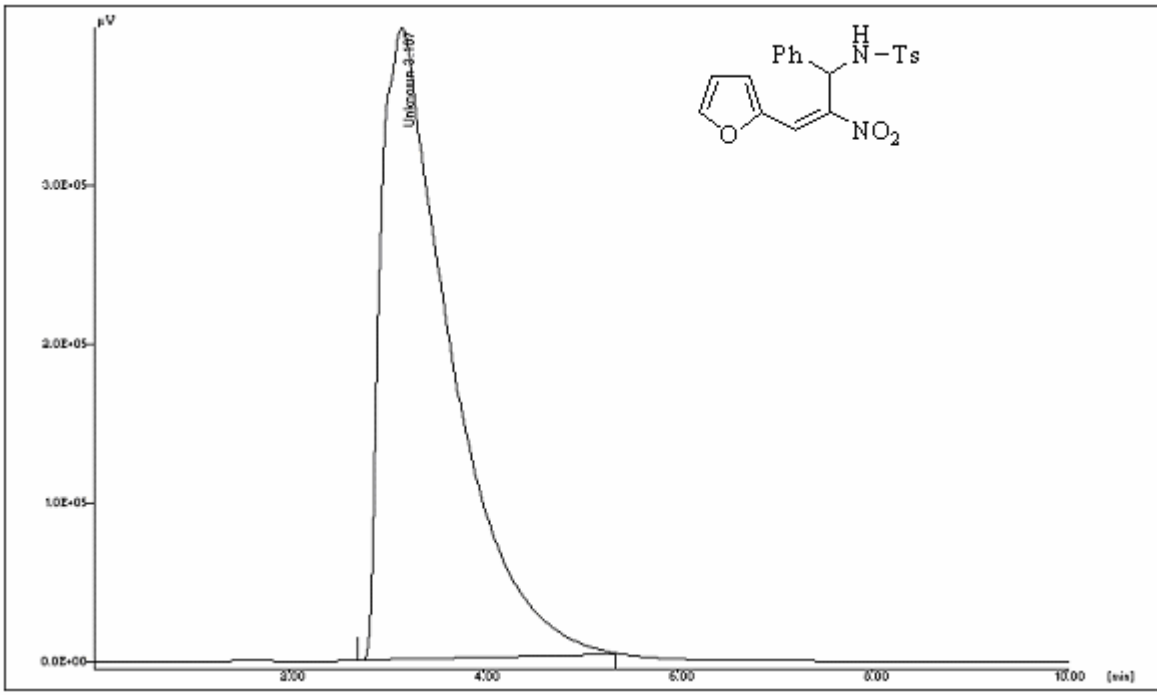
Table S1. HPLC data for MBH adducts **3a-k**.

Entry	Compd	HPLC			
		AcCN/H_2O (90:10)		MeOH/H_2O (40:60)	
		Retention Time (min)	% Purity	Retention Time (min)	% Purity
1	**3a**	3.167	100.0	4.450	100.0
2	**3b**	3.108	100.0	7.333	100.0
3	**3c**	2.925	100.0	8.867	95.1
4	**3d**	3.200	99.8	4.625	100.0
5	**3e**	3.050	100.0	4.625	98.8
6	**3f**	3.325	100.0	7.075	100.0
7	**3g**	5.767	100.0	6.750	99.3
8	**3h**	3.267	100.0	5.367	100.0
9	**3i**	3.333	100.0	5.475	100.0
10	**3j**	7.758	100.0	6.458	95.2
11	**3k**	7.867	99.9	6.983	100.0



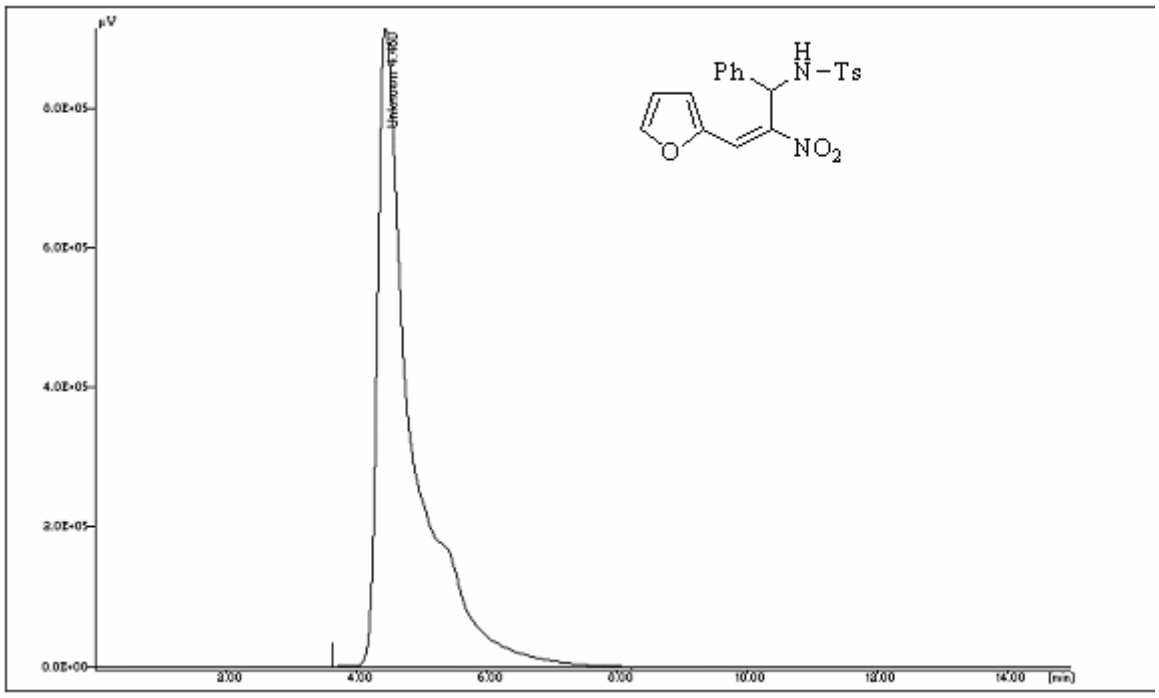
File name: NR-152

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: μV
Acquisition Time: 10.03 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3a**	3.167	19446643.750	100.000

Total Area of Peak = 19446643.750 [μV.Sec]
Injection Volume = 20.00 μl



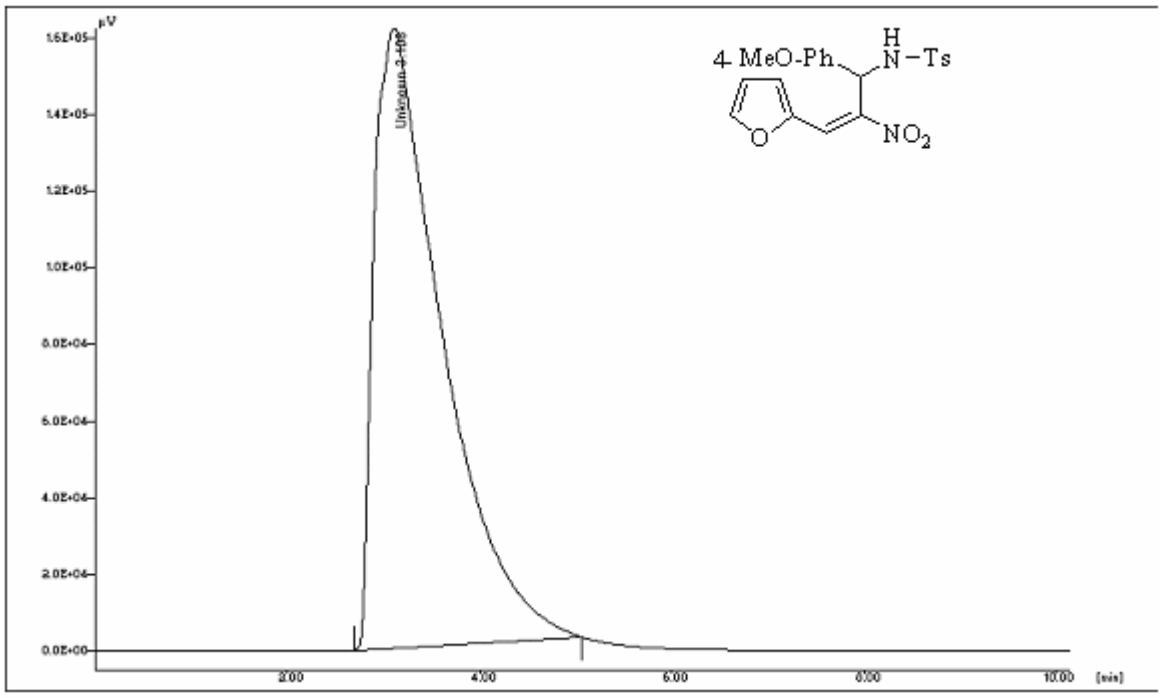
File name: NR-152

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: μV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3a**	4.450	32919955.000	100.000

Total Area of Peak = 32919955.000 [μV.Sec]
Injection Volume = 20.00 μl



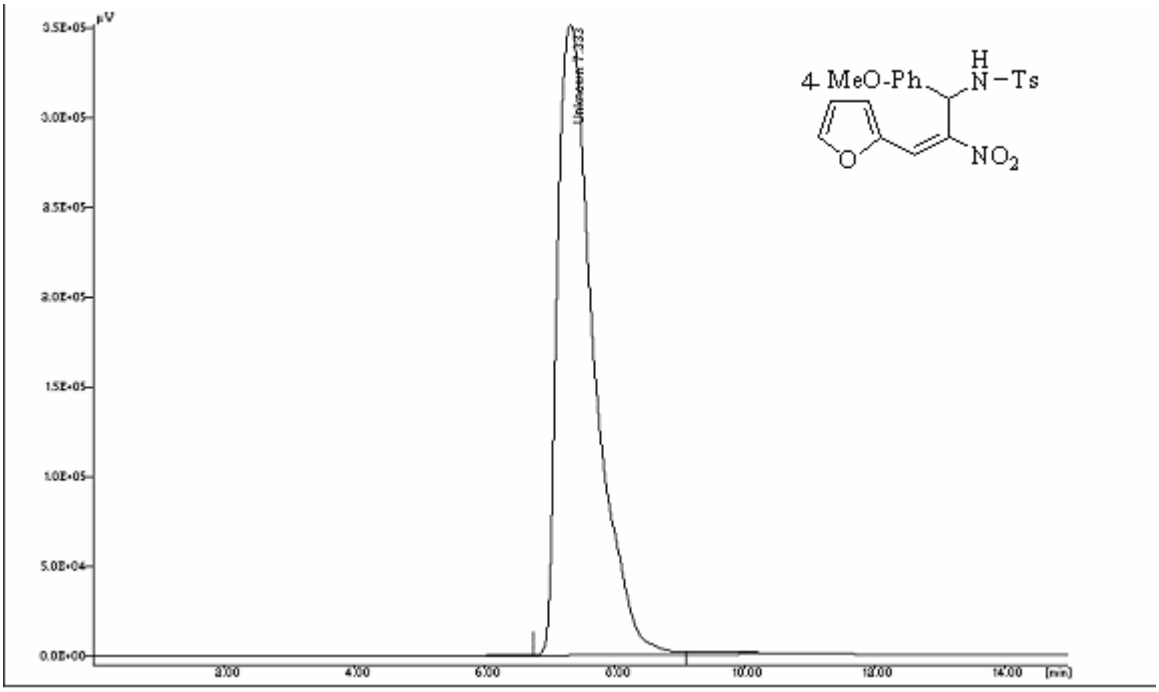
File name: NR-142

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 10.15 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3b**	3.108	7830377.500	100.000

Total Area of Peak = 7830377.500 [µV.Sec]
Injection Volume = 20.00 µl



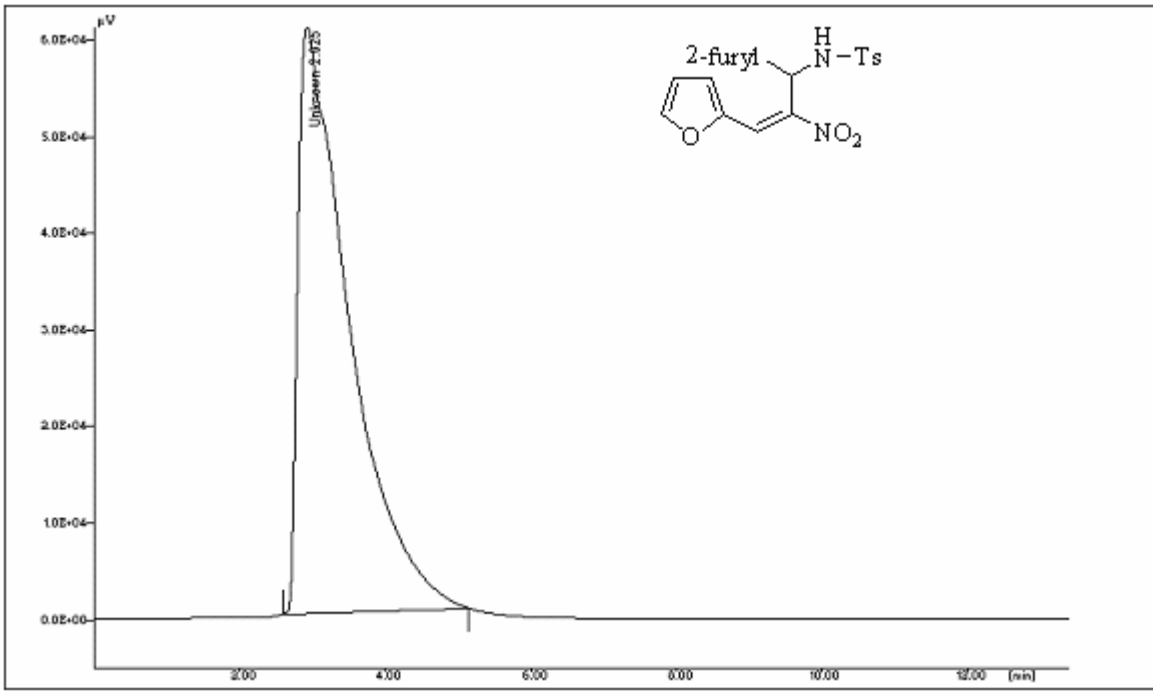
File name: NR-142

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3b**	7.333	13207397.658	100.000

Total Area of Peak = 13207397.658 [µV.Sec]
Injection Volume = 20.00 µl



File name: NR-162

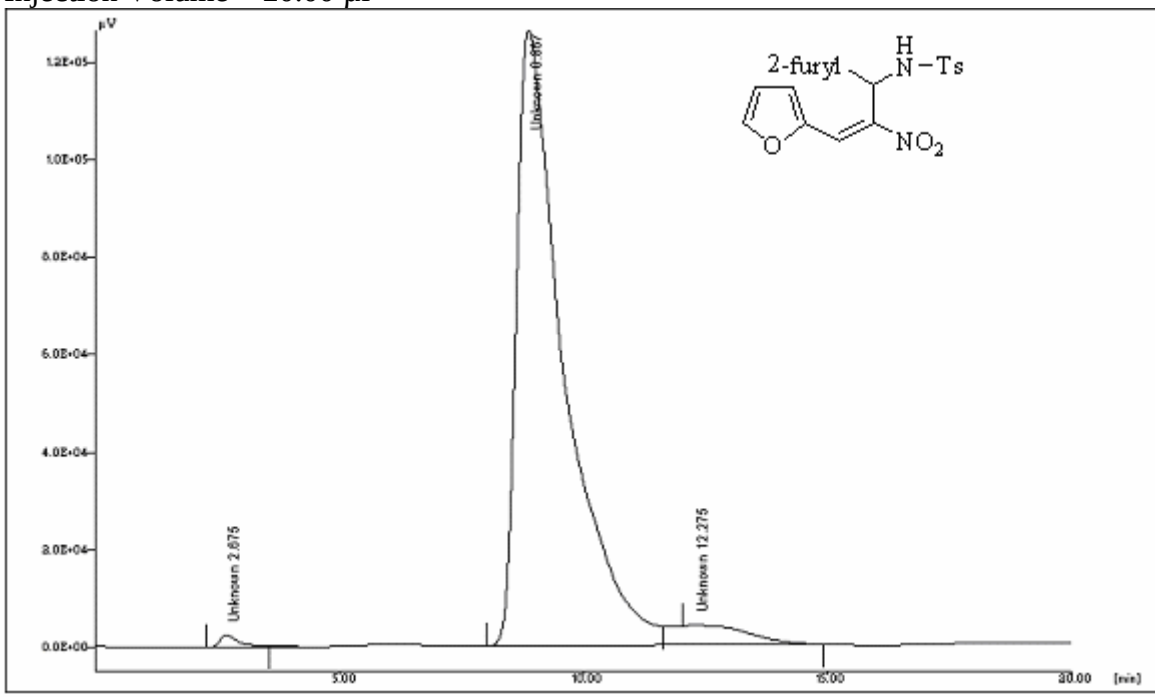
Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 13.40 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3c**	2.925	2892594.750	100.000

Total Area of Peak = 2892594.750 [µV.Sec]
Injection Volume = 20.00 µl

Injection Volume = 20.00 µl



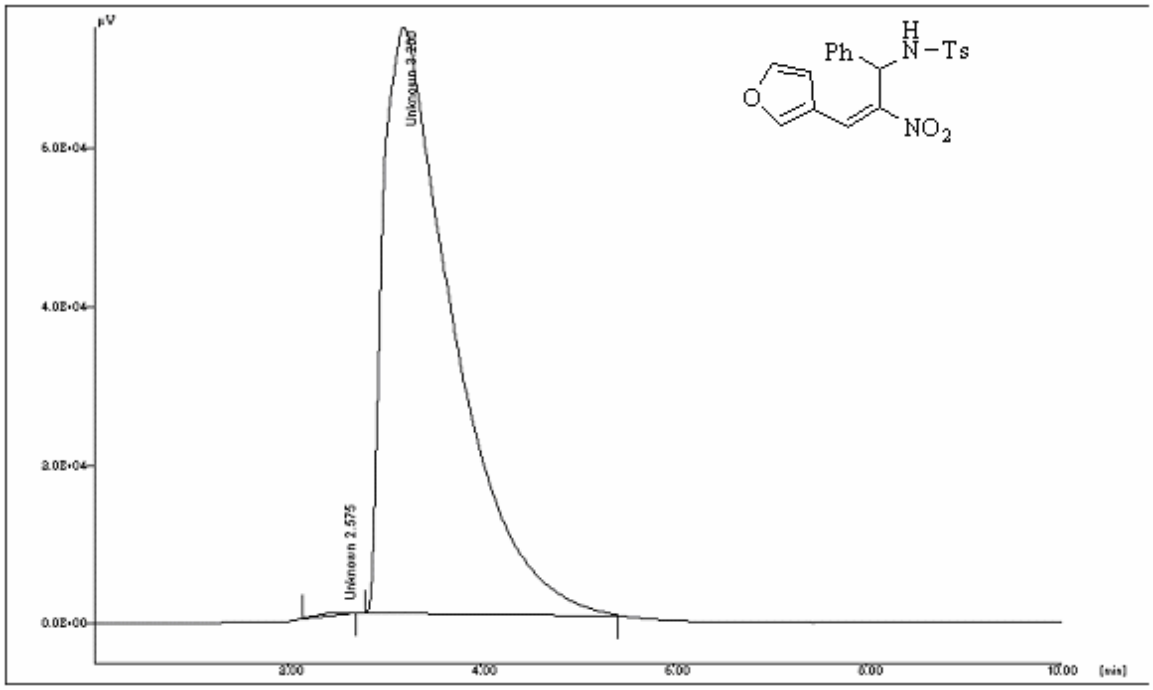
File name: NR-162

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 20.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1		2.675	63498.571	0.727
2	**3c**	8.867	8311510.735	95.110
3		12.275	363830.333	4.163

Total Area of Peak = 8738839.639 [µV.Sec]
Injection Volume = 20.00 µl



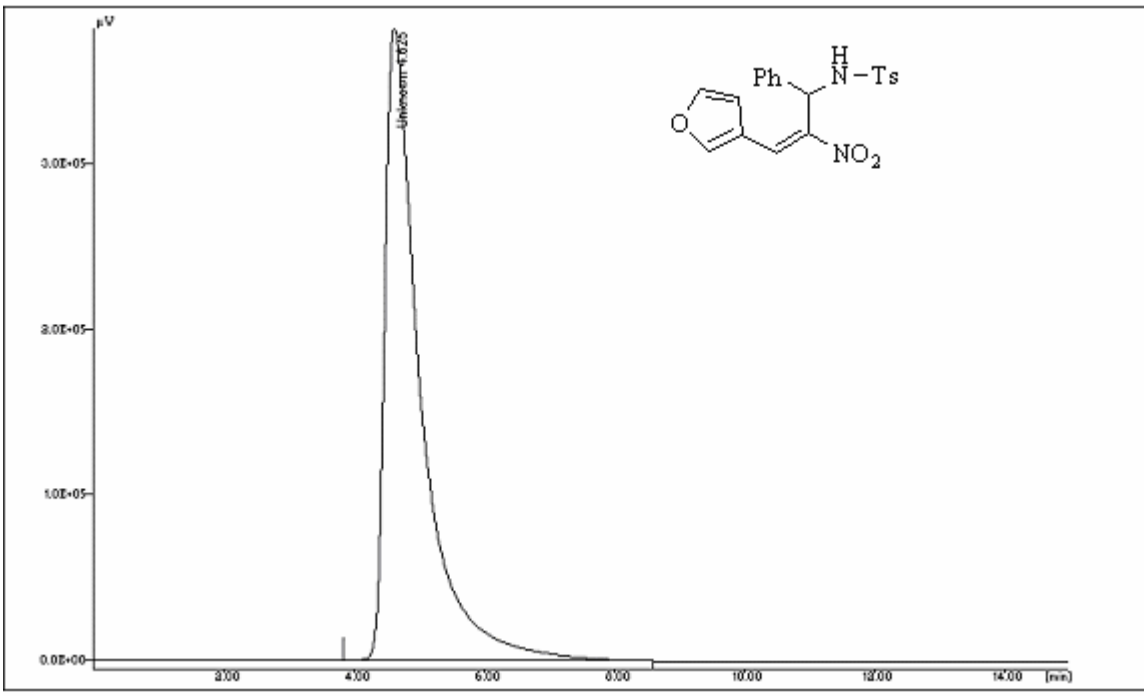
File name: NR-176

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 10.03 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1		2.575	6215.000	0.169
2	**3d**	3.200	3662570.000	99.831

Total Area of Peak = 3668785.000 [µV.Sec]
Injection Volume = 20.00 µl



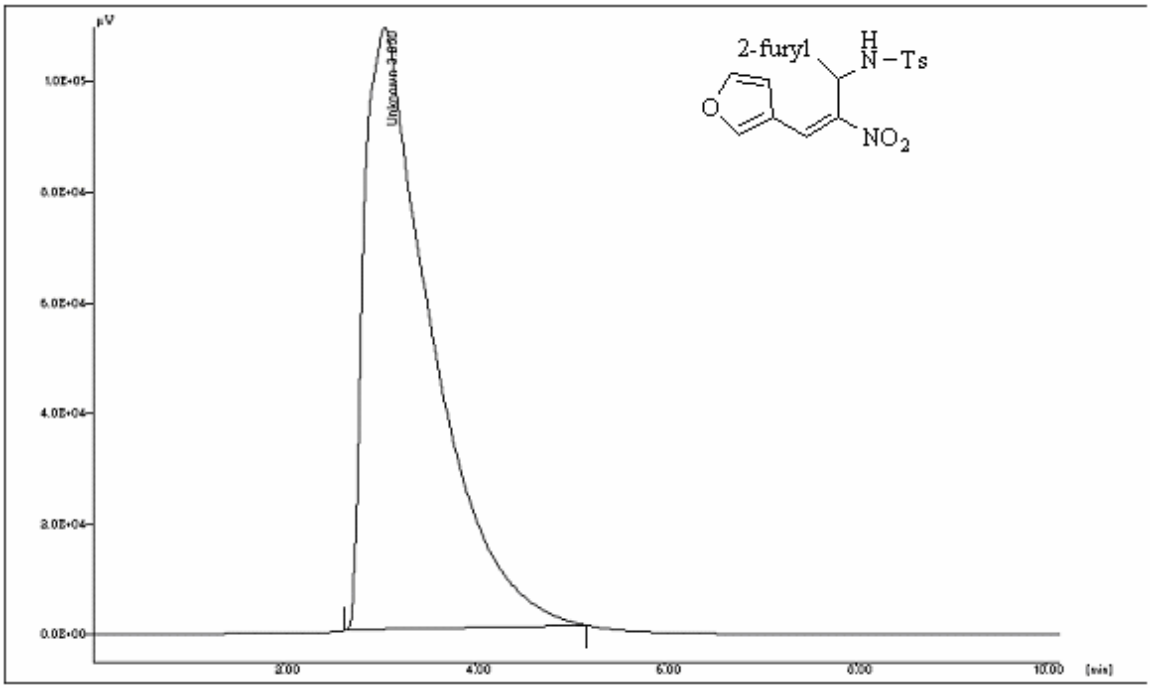
File name: NR-176

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3d**	4.625	14076723.250	100.000

Total Area of Peak = 14076723.250 [µV.Sec]
Injection Volume = 20.00 µl



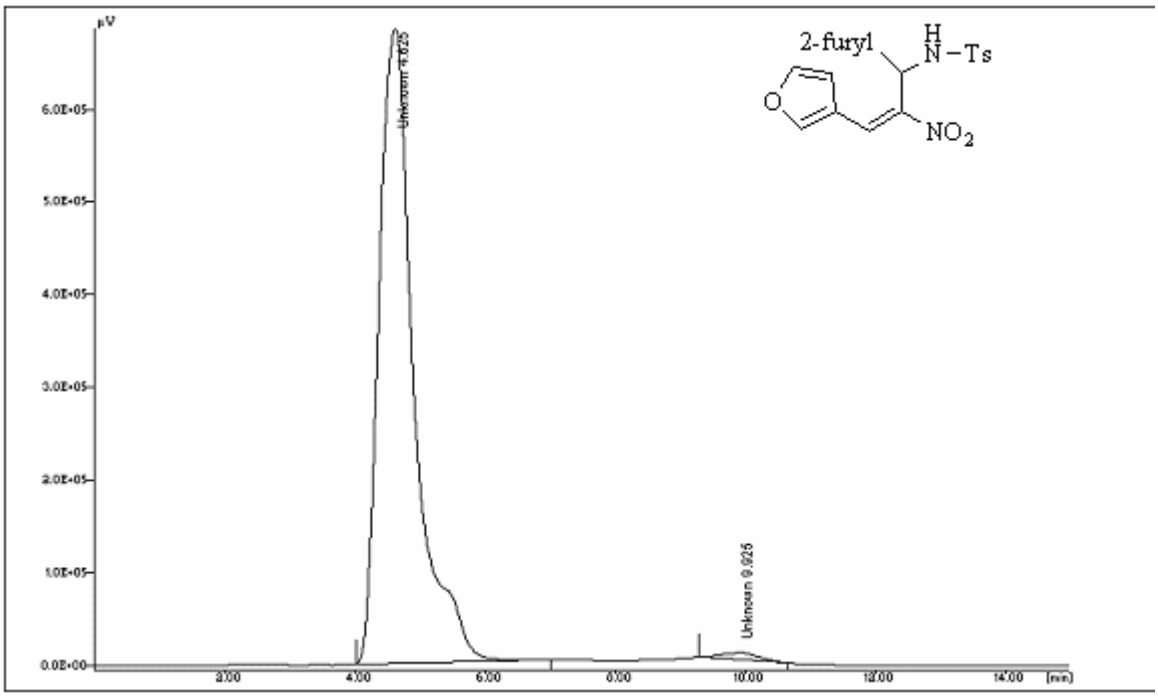
File name: NR-184

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 10.15 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3e**	3.050	5250335.500	100.000

Total Area of Peak = 5250335.500 [µV.Sec]
Injection Volume = 20.00 µl



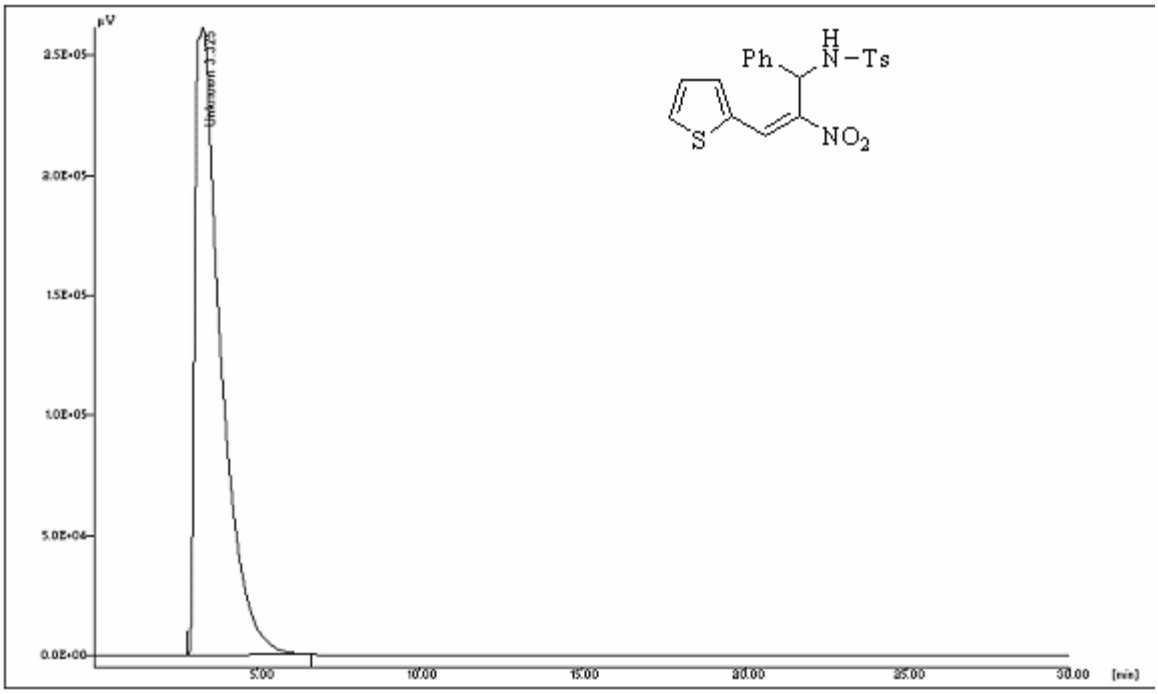
File name: NR-184

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: μV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3e**	4.625	24651739.000	98.840
2		9.925	289343.750	1.160

Total Area of Peak = 24941082.750 [μV.Sec]
Injection Volume = 20.00 μl



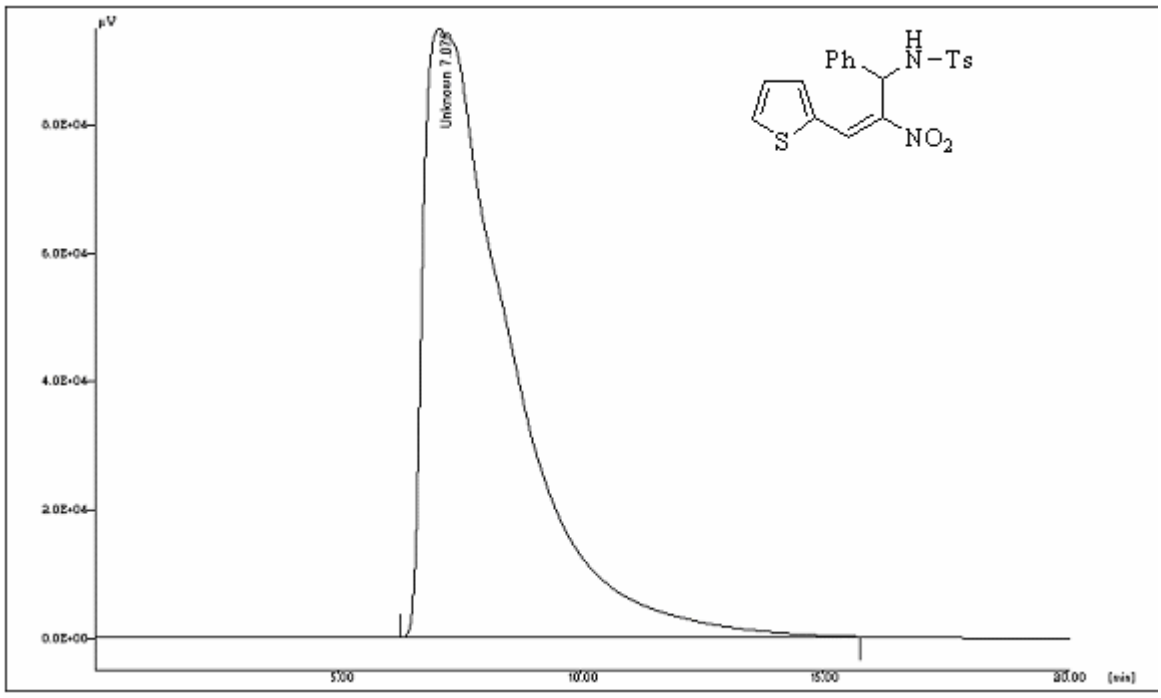
File name: NR-178

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 30.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3f**	3.325	13673017.750	100.000

Total Area of Peak = 13673017.750 [µV.Sec]
Injection Volume = 20.00 µl



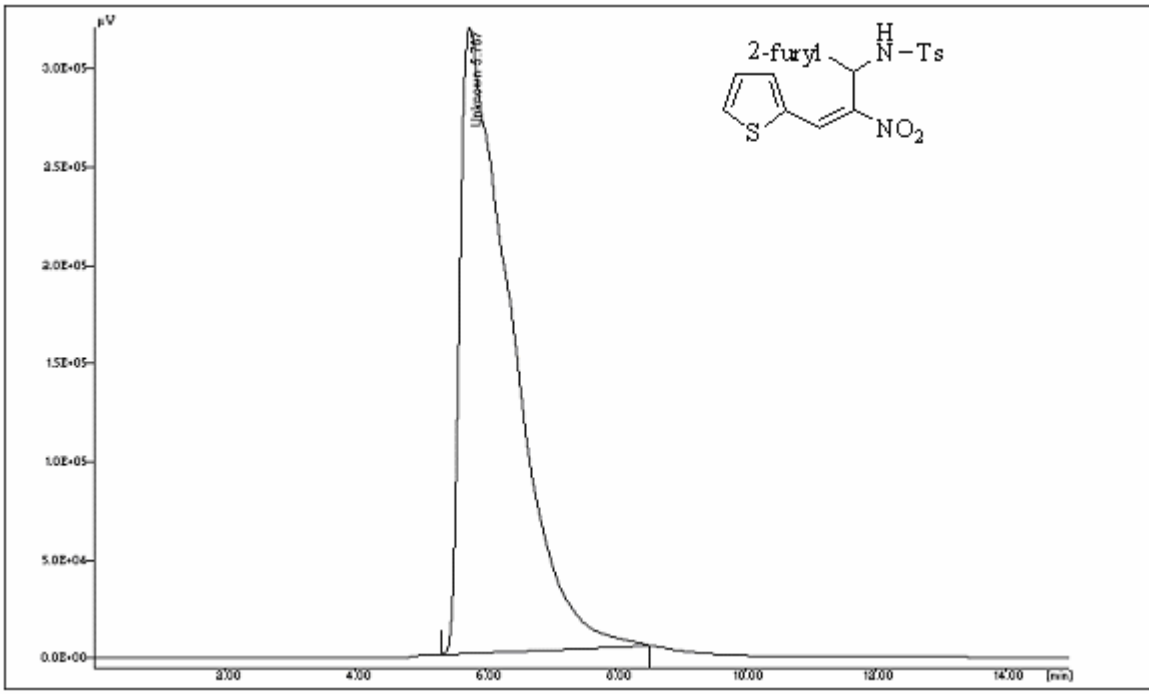
File name: NR-178

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: μV
Acquisition Time: 20.10 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3f**	7.075	11686434.500	100.000

Total Area of Peak = 11686434.500 [μV.Sec]
Injection Volume = 20.00 μl



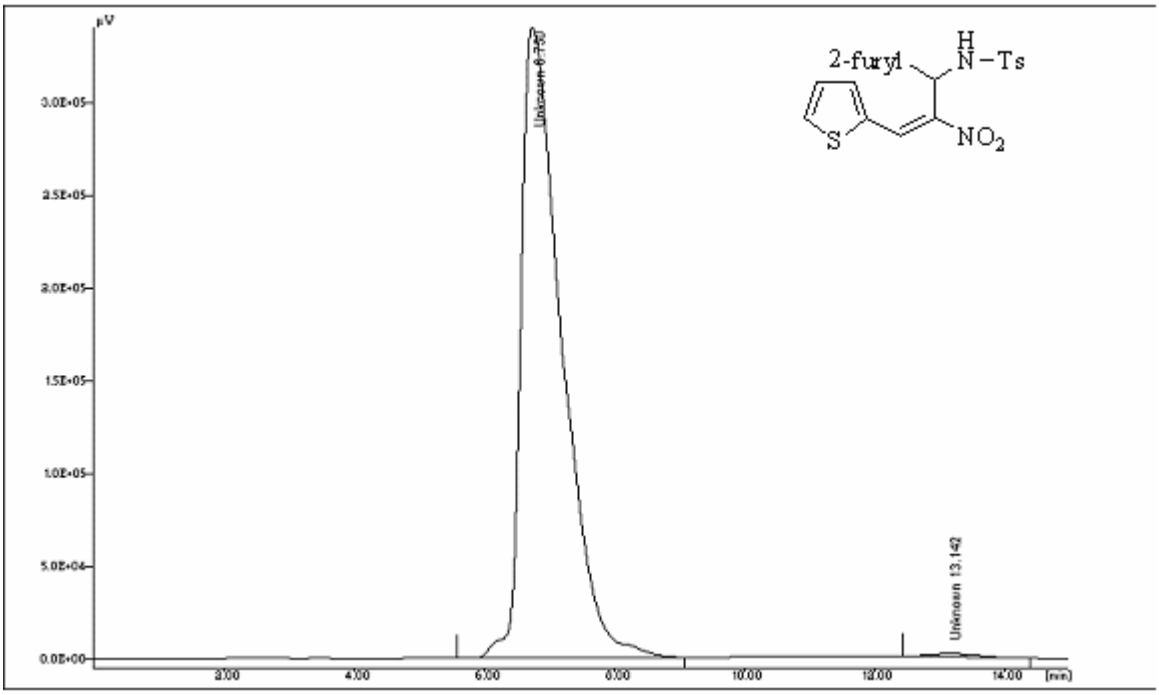
File name: NR-180

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3g**	5.767	16969436.750	100.000

Total Area of Peak = 16969436.750 [µV.Sec]
Injection Volume = 20.00 µl



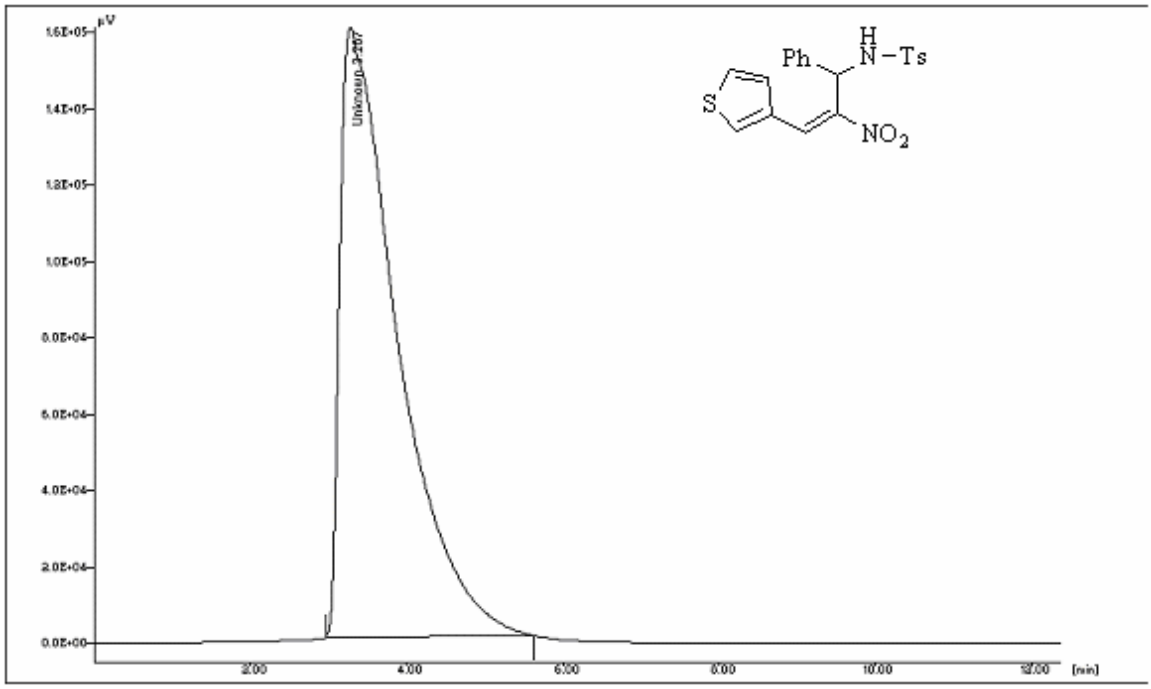
File name: NR-180

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3g**	6.750	14282963.750	99.304
2		13.142	100061.407	0.696

Total Area of Peak = 14383025.157 [µV.Sec]
Injection Volume = 20.00 µl



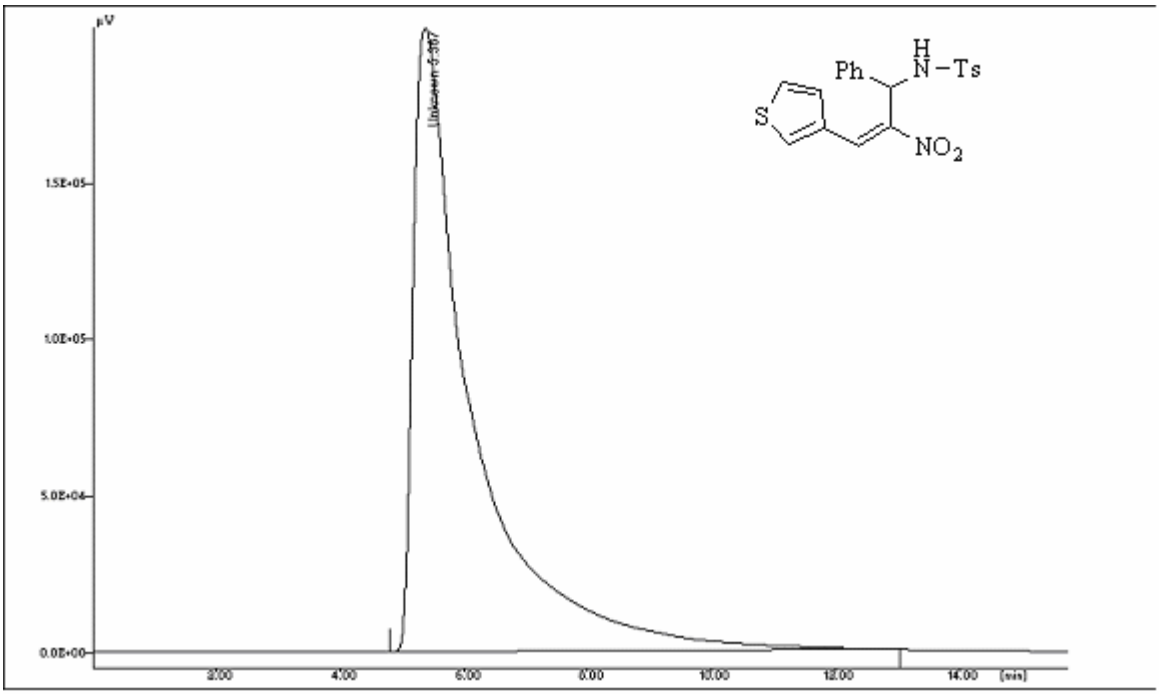
File name: NR-179

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 12.38 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3h**	3.267	7998569.250	100.000

Total Area of Peak = 7998569.250 [µV.Sec]
Injection Volume = 20.00 µl



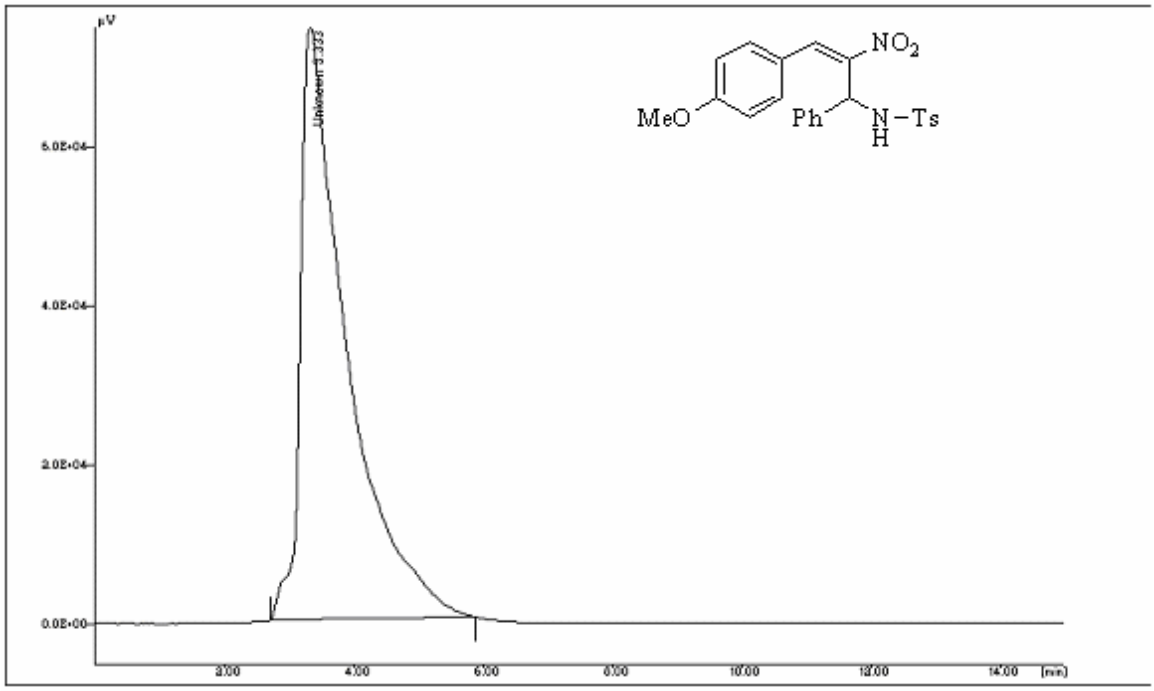
File name: NR-179

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 15.77 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3h**	5.367	13003129.500	100.000

Total Area of Peak = 13003129.500 [µV.Sec]
Injection Volume = 20.00 µl



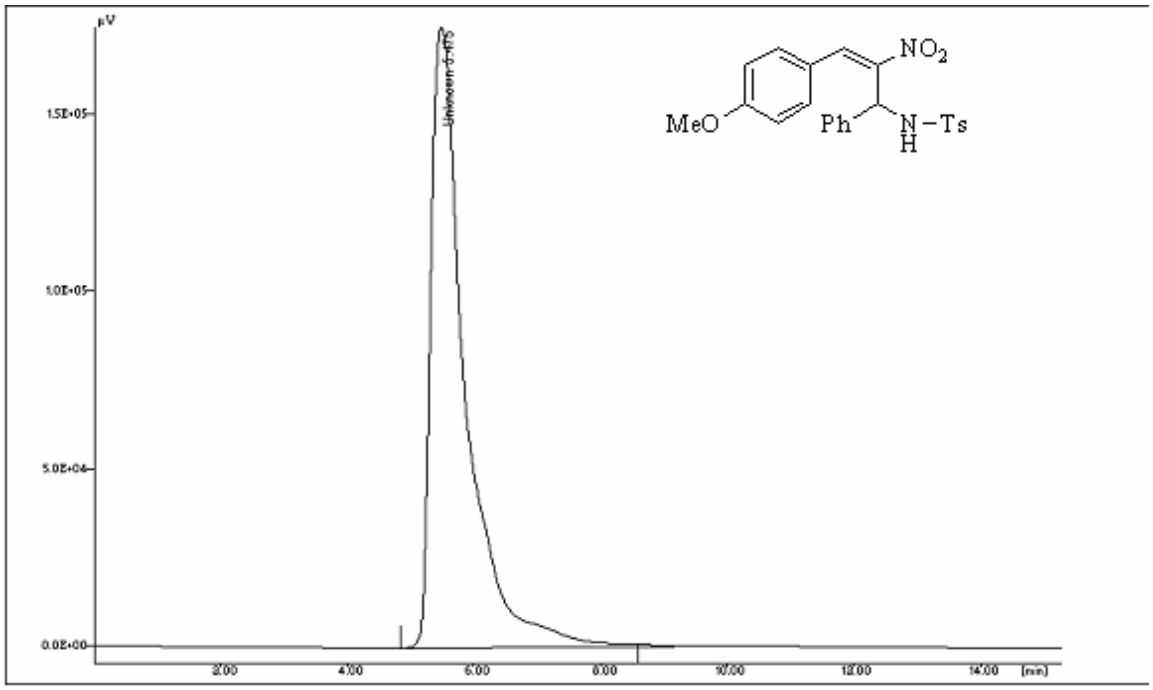
File name: NR-165

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3i**	3.333	3603709.250	100.000

Total Area of Peak = 3603709.250 [µV.Sec]
Injection Volume = 20.00 µl



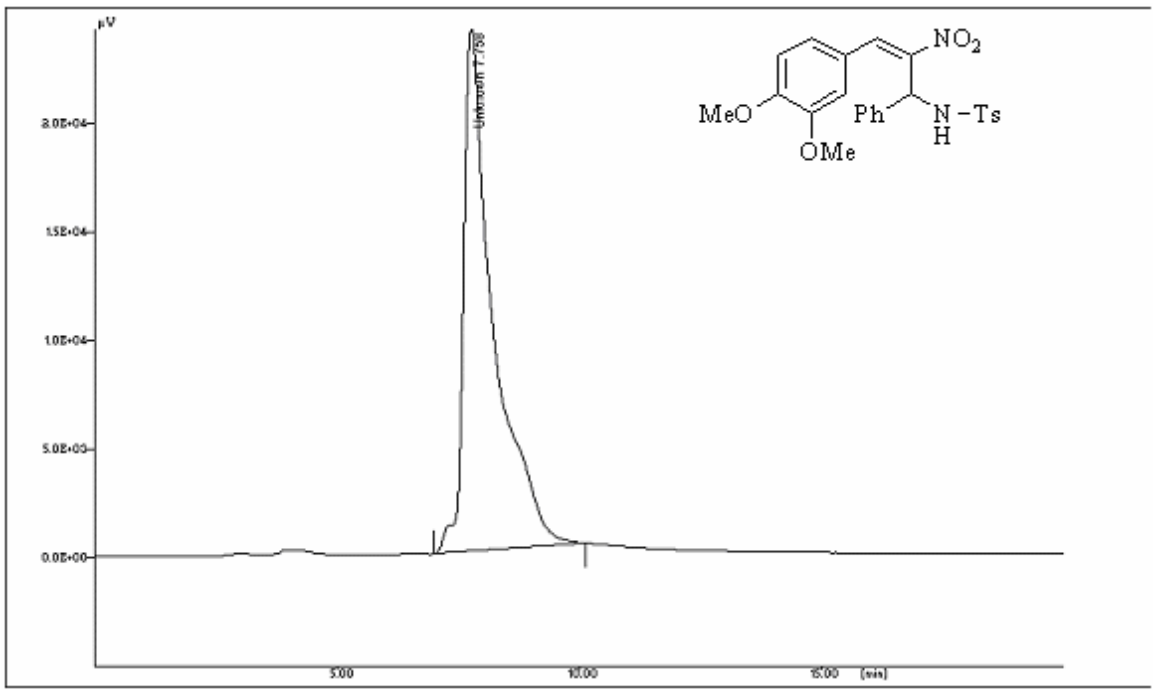
File name: NR-165

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: μV
Acquisition Time: 15.30 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3i**	5.475	6415787.786	100.000

Total Area of Peak = 6415787.786 [μV.Sec]
Injection Volume = 20.00 μl



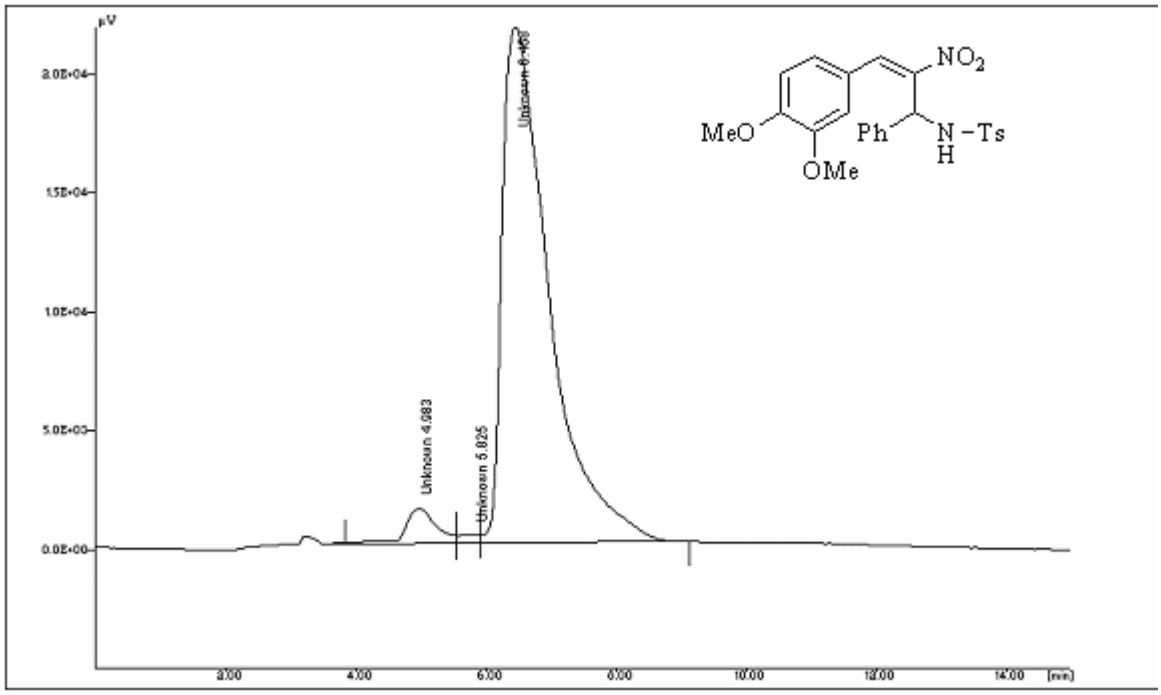
File name: NR-175

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: µV
Acquisition Time: 19.99 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3j**	7.758	996629.324	100.000

Total Area of Peak = 996629.324 [µV.Sec]
Injection Volume = 20.00 µl



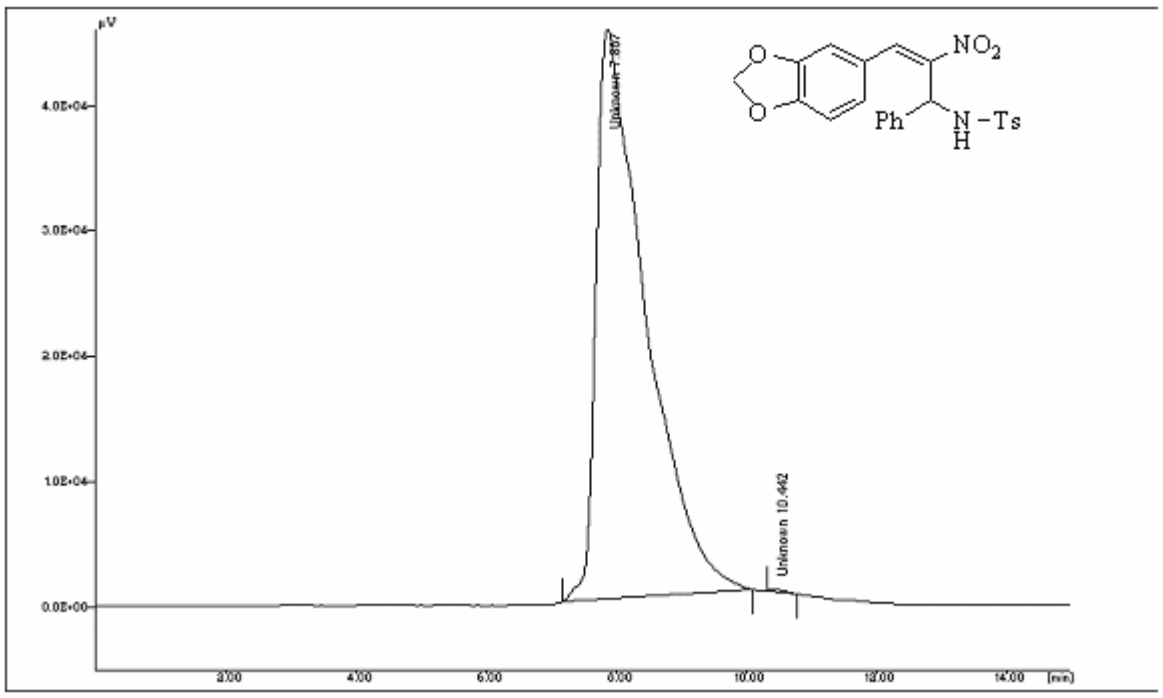
File name: NR-175

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 15.00 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1		4.983	46195.472	4.148
2		5.825	7312.233	0.657
3	**3j**	6.458	1060304.247	95.196

Total Area of Peak = 1113811.952 [µV.Sec]
Injection Volume = 20.00 µl



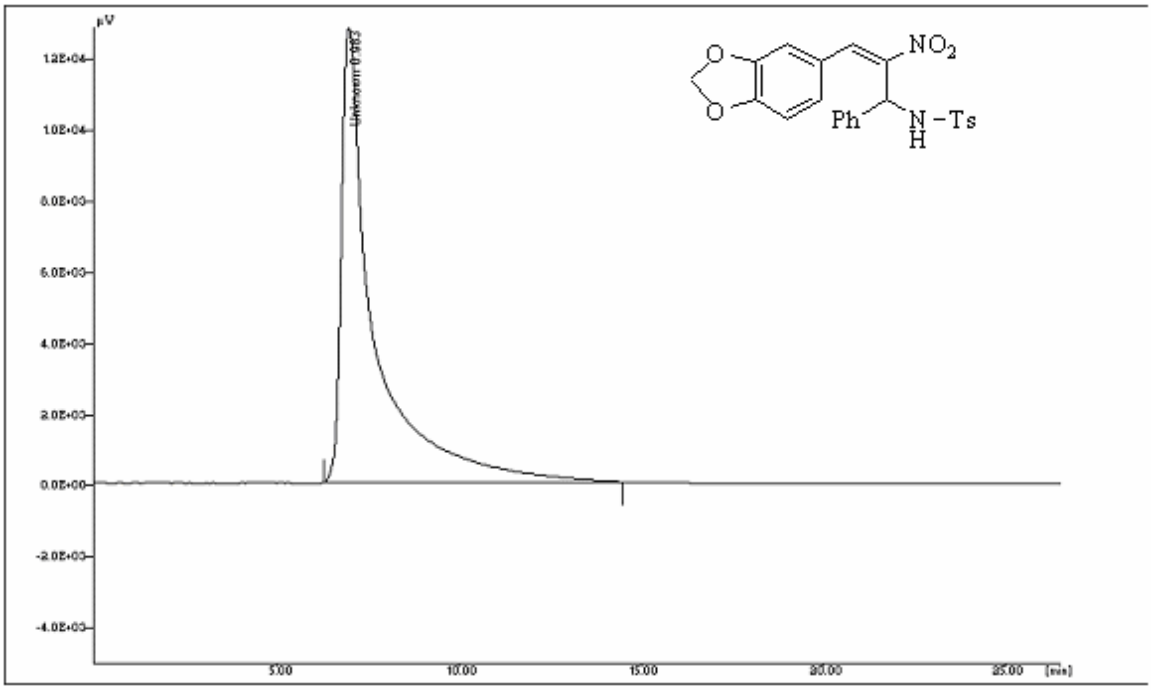
File name: NR-177

Info:
Sample: Aza-MBH
Gradient: 90:10 MeCN/H2O
Wavelength: 355 nm
Flow rate: 1 ml/min

Vial # = 1 Rack # = 1
X Units: [min] Y Units: μV
Acquisition Time: 10.15 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [μV.Sec]	% Area
1	**3k**	7.867	2346177.750	99.913
2		10.442	2043.500	0.087

Total Area of Peak = 2348221.250 [μV.Sec]
Injection Volume = 20.00 μl



File name: NR-177

Info:
Sample: Aza-MBH
Gradient: 40:60 MeOH/H2O
Wavelength: 355 nm
Flow rate: 0.5 ml/min

X Units: [min] Y Units: µV
Acquisition Time: 26.53 [min]
Control Method:
Code of system chromatographic: JASCO HPLC

#	Name	RT	Area [µV.Sec]	% Area
1	**3k**	6.983	777680.000	100.000

Total Area of Peak = 777680.000 [µV.Sec]
Injection Volume = 20.00 µl