Supporting Information

Highly Enantioselective Michael Reaction Employing Cycloheptanone and Cyclooctanone as Nucleophiles

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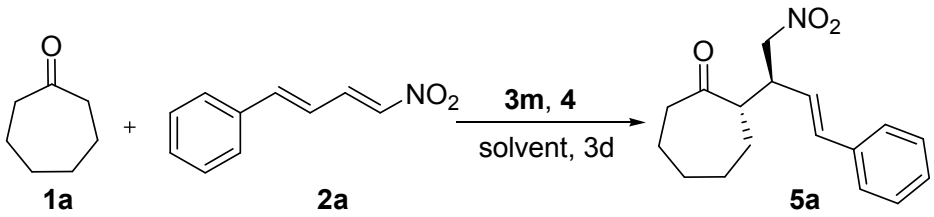
1. Effects of solvents and additives on the Michael reaction

Table **S1**. Effects of solvents and additives on the Michael reaction. [a]

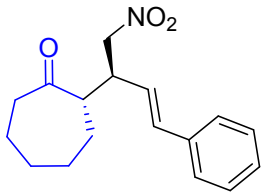


entry	Solvent	**4**	Yield[b] [%]	dr[c] (*anti*:*syn*)	*ee* [%][c] (*anti*/*syn*)
1	PhMe	$PhCO_2H$ **4a**	22	7 : 1	88 / --
2	**xylene**	**$PhCO_2H$ 4a**	**37**	**11 : 1**	**88 / --**
3	*i*-Pr_2O	$PhCO_2H$ **4a**	29	7 : 1	84 / --
4	Et_2O	$PhCO_2H$ **4a**	19	7 : 1	70 / --
5	CH_2Cl_2	$PhCO_2H$ **4a**	28	7 : 1	82 / --
6	$CHCl_3$	$PhCO_2H$ **4a**	30	8 : 1	86 / --
7	1,4-Dioxane	$PhCO_2H$ **4a**	14	12 : 1	85 / --
8	EtOAc	$PhCO_2H$ **4a**	20	10 : 1	87 / --
9	THF	$PhCO_2H$ **4a**	10	11 : 1	85 / --
10	MeOH	$PhCO_2H$ **4a**	trace	n.d.	n.d.
11	EtOH	$PhCO_2H$ **4a**	5<	n.d.	n.d.
12	*i*-PrOH	$PhCO_2H$ **4a**	5	10 : 1	82 / --
13	xylene	CH_3CO_2H **4b**	20	9 : 1	87 / --
14	xylene	CF_3CO_2H **4c**	5<	n.d.	n.d.
15	xylene	$PhCH{=}CHCO_2H$ **4d**	28	9 : 1	86 / --
16	xylene	4- $CH_3C_6H_4CO_2H$ **4e**	29	7 : 1	87 / --
17	xylene	2- $NO_2C_6H_4CO_2H$ **4f**	8	2 : 1	77/85
18	xylene	3- $NO_2C_6H_4CO_2H$ **4g**	13	6 : 1	87 / --

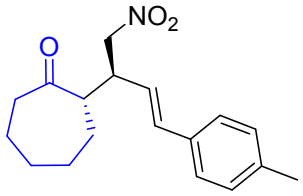
19	xylene	4- $NO_2C_6H_4CO_2H$ **4h**	15	6 : 1	79 / --
20	xylene	2- $CF_3C_6H_4CO_2H$ **4i**	17	4 : 1	76/68
21	xylene	4- $CF_3C_6H_4CO_2H$ **4j**	20	7 : 1	85 / --
22	xylene	4- $FC_6H_4CO_2H$ **4k**	15	8 : 1	87 / --
23	xylene	4- $CH_3C_6H_4SO_3H$ **4l**	11	4 : 1	65/34
24	xylene	2- $C_{10}H_7SO_3H$ **4m**	5<	n.d.	n.d.
25	xylene	2- $OHC_6H_4CO_2H$ **4n**	5<	n.d.	n.d.

[a] Unless otherwise stated, the reaction was conducted by stirring in solvent (0.5 mL) using **1a** (0.5 mmol) and **2a** (0.13 mmol) with 30 mol% catalyst **3** and 30 mol% additive **4** at room temperature. [b] Conversion to the product, as determined by GC. [c] Determined by HPLC analysis on a chiralcel AS-H.

2. Characterization data

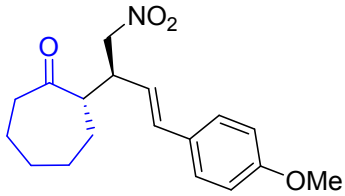


(S)-2-((S,E)-1-nitro-4-phenylbut-3-en-2-yl)cycloheptanone (5a)[1], yield: 26.4 mg, 73%; 89% ee; white solid, Mp: 66−70 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (99:1) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 68.84 min, t^{anti}_{major} = 34.88 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.37−7.26 (m, 5H), 6.54−6.50 (m, 1H), 6.04−5.99 (dd, *J* = 9.5, 15.5 Hz 1H), 4.62−4.51 (m, 2H), 3.31−3.25 (m, 1H), 2.80−2.74 (m, 1H), 2.61−2.46 (m, 2H), 2.00−1.89 (m, 4H), 1.70−1.62 (m, 1H), 1.44−1.26(m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.4, 136.2, 134.8, 128.6 (×2), 128.0, 126.5 (×2), 125.6, 78.1, 52.8, 43.8, 43.7, 29.7, 28.9, 28.7, 23.7 ppm. GC−MS: m/z 240, 197, 129 (100); HRMS: (ESI+) m/z calcd for $C_{17}H_{22}NO_3$ $[M+H]^+$ 288.1600, found 288.1609.

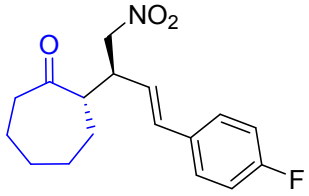


(S)-2-((S,E)-1-nitro-4-p-tolylbut-3-en-2-yl)cycloheptanone (5b), yield: 27.3 mg, 72%; 90% ee; white solid, Mp: 67−70 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/ethyl alcohol (80:20) as the eluent.

Flow: 1.0 mL/min; UV = 256 nm; t^{anti}_{minor} = 18.70 min, t^{anti}_{major} = 11.12 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.28−7.25 (m, 2H), 7.14−7.13 (m, 2H), 6.51−6.47 (m, 1H), 5.98−5.93 (dd, *J* = 9.5, 16Hz, 1H), 4.61−4.50 (m, 2H), 3.30−3.24 (m, 1H), 2.80−2.75 (m, 1H), 2.61−2.48 (m, 2H), 2.35 (S, 3H), 2.01−1.90 (m, 4H), 1.71−1.60 (m, 1H), 1.45−1.25 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.3, 137.9, 134.7, 133.4, 129.3 (×2), 126.4 (×2), 124.5, 78.1, 52.9, 43.8, 43.7, 29.7, 28.9, 28.7, 23.7, 21.2 ppm. GC−MS: m/z 254, 211, 143 (100), 129, 105; HRMS: (ESI+) m/z calcd for $C_{18}H_{24}NO_3$ $[M+H]^+$ 302.1756, found 302.1764.

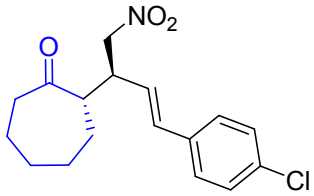


(S)-2-((S,E)-4-(4-methoxyphenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5c), yield: 26.7 mg, 67%; 87% ee; white solid, Mp: 80−87 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (80:20) as the eluent. Flow: 1.0 mL/min; UV = 264 nm; t^{anti}_{minor} = 29.98 min, t^{anti}_{major} = 17.36 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.30−7.28 (m, 2H), 6.87−6.84 (m, 2H), 6.48−6.43 (m, 1H), 5.88−5.83 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.60−4.49 (m, 2H), 3.81 (S, 3H), 3.26−3.23 (m, 1H), 2.78−2.74 (m, 1H), 2.60−2.47 (m, 2H), 2.00−1.89 (m, 4H), 1.68−1.67 (m, 1H), 1.45−1.21 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.4, 159.5, 134.2, 127.7 (×3), 123.2, 114.0 (×2), 78.2, 55.3, 52.9, 43.9, 43.7, 29.7, 28.9, 28.7, 23.7 ppm. GC−MS: m/z 270, 227, 159 (100), 121; HRMS: (ESI+) m/z calcd for $C_{18}H_{24}NO_4$ $[M+H]^+$ 318.1705, found 318.1707.

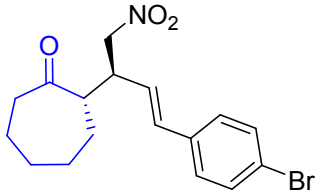


(S)-2-((S,E)-4-(4-fluorophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5d), yield: 30.7mg, 80%; 89% ee; white solid, Mp: 67−70 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (80:20) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 13.15 min, t^{anti}_{major} = 7.95 min; ^{1}H

NMR (500 MHz, $CDCl_3$): δ = 7.33−7.27 (m, 2H), 7.02−6.98 (m, 2H), 6.50−6.44 (m, 1H), 5.95−5.90 (dd, *J* = 10, 16 Hz, 1H), 4.61−4.50 (m, 2H), 3.29−3.23 (m, 1H), 2.80−2.75 (m, 1H), 2.60−2.45 (m, 2H), 1.98−1.89 (m, 4H), 1.70−1.62 (m, 1H), 1.43−1.20 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.2, 163.5(d, $^{1}J_{C\text{-}F}$ = 245.9 Hz), 133.6(d, $^{4}J_{C\text{-}F}$ = 4.8 Hz), 132.4 , 128.1 (×2, $^{3}J_{C\text{-}F}$ = 8 Hz), 125.4, 115.4 (×2, $^{2}J_{C\text{-}F}$ = 21.6 Hz), 78.1, 52.8, 43.8, 43.7, 29.7, 28.9, 28.7, 23.7 ppm. GC−MS: m/z 258, 215 (100), 147, 109; HRMS: (ESI+) m/z calcd for $C_{17}H_{21}FNO_3$ $[M+H]^+$ 306.1505, found 306.1499.

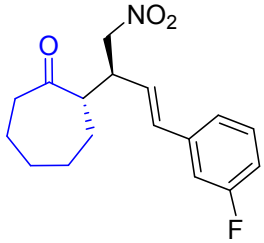


(S)-2-((S,E)-4-(4-chlorophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5e), yield: 30.3 mg, 75%; 90% ee ; white solid, Mp: 66−69 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 21.16 min, t^{anti}_{major} = 10.68 min. ^1H NMR (500 MHz, $CDCl_3$): δ = 7.30−7.26 (m, 4H), 6.49−6.44 (m, 1H), 6.02−5.97 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.62−4.50 (m, 2H), 3.31−3.25 (m, 1H), 2.91−2.76 (m, 1H), 2.61−2.45 (m, 2H), 1.97−1.86 (m, 4H), 1.72−1.60 (m, 1H), 1.48−1.21 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.1, 134.7, 133.7, 133.6, 128.8 (×2), 127.7 (×2), 126.4, 78.0, 52.7, 43.8, 43.7, 29.7, 28.9, 28.7, 23.6 ppm. GC−MS: m/z 274, 231 (100), 129; HRMS: (ESI+) m/z calcd for $C_{17}H_{21}ClNO_3$ $[M+H]^+$ 322.1210, found 322.1208.

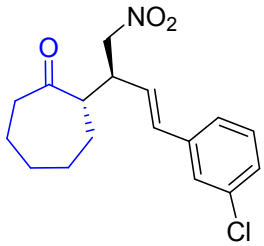


(S)-2-((S,E)-4-(4-bromophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5f), yield: 28.5 mg, 62%; 88% ee; white solid, Mp: 71−73 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 260 nm; t^{anti}_{minor} = 45.28 min, t^{anti}_{major} = 22.44 min. ^1H NMR (500 MHz, $CDCl_3$): δ = 7.44−7.42 (m, 2H), 7.21−7.19 (m, 2H), 6.47−6.41 (m,

1H), 6.03−5.98 (dd, *J* = 10, 16 Hz, 1H), 4.61−4.49 (m, 2H), 3.29−3.23 (m, 1H), 2.79−2.75 (m, 1H), 2.59−2.46 (m, 2H), 1.95−1.90 (m, 4H), 1.67−1.59 (m, 1H), 1.45−1.21 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.1, 135.1, 133.6, 131.7 (×2), 128.0 (×2), 126.5, 121.9, 78.0, 52.7, 43.8, 43.7, 29.7, 28.9, 28.7, 23.6 ppm. GC−MS: m/z 320, 318, 277, 275, 207, 128 (100); HRMS: (ESI+) m/z calcd for $C_{17}H_{21}BrNO_3$ $[M+H]^+$ 366.0705, found 366.0705.

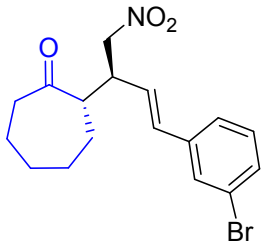


(S)-2-((S,E)-4-(3-fluorophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5g), yield: 29.9 mg, 78%; 86% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (95:5) as the eluent. Flow: 1 mL/min; UV = 248 nm; t^{anti}_{minor} = 14.20 min, t^{anti}_{major} = 10.52 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.31−6.94 (m, 4H), 6.52−6.48 (m, 1H), 6.06−6.01 (dd, *J*= 9.5, 16 Hz , 1H), 4.63−4.51 (m, 2H), 3.32−3.26 (m, 1H), 2.82−2.77 (m, 1H), 2.62−2.48 (m, 2H), 1.98−1.90 (m, 4H), 1.72−1.60 (m, 1H), 1.45−1.27 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.0, 164.0(d, $^1J_{C\text{-}F}$ = 244.4 Hz), 138.5(d, $^3J_{C\text{-}F}$ = 7.9 Hz), 133.7, 130.1(d, $^3J_{C\text{-}F}$ = 8.7 Hz), 127.2, 122.4, 114.9(d, $^2J_{C\text{-}F}$ = 21.3 Hz), 113.0(d, $^2J_{C\text{-}F}$ = 21.6 Hz), 77.9, 52.7, 43.7 (×2), 29.7, 28.9, 28.7, 23.6 ppm. GC−MS: m/z 258, 215, 147 (100), 109; HRMS: (ESI+) m/z calcd for $C_{17}H_{21}FNO_3$ $[M+H]^+$ 306.1505, found 306.1501.

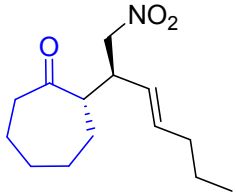


(S)-2-((S,E)-4-(3-chlorophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5h), yield: 30.3 mg, 75%; 91% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1 mL/min; UV = 252 nm; t^{anti}_{minor} = 15.07 min, t^{anti}_{major} = 9.69 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.34−7.19 (m, 4H), 6.48−6.43 (m, 1H), 6.06−6.01 (dd, *J* = 9.5, 16 Hz,

1H), 4.62−4.50 (m, 2H), 3.31−3.24 (m, 1H), 2.81−2.75 (m, 1H), 2.61−2.45 (m, 2H), 1.97−1.89 (m, 4H), 1.68−1.65 (m, 1H), 1.44−1.22 (m, 3H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.0, 138.0, 134.6, 133.5, 129.8, 128.0, 127.3, 126.3, 124.8, 77.9, 52.7, 43.8, 43.7, 29.7, 28.9, 28.7, 23.6ppm. GC−MS: m/z 274, 233, 231 (100), 163, 129; HRMS: (ESI+) m/z calcd for $C_{17}H_{21}ClNO_3$ $[M+H]^+$ 322.1210, found 322.1215.

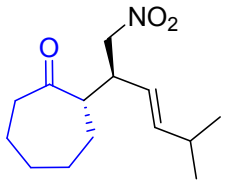


(S)-2-((S,E)-4-(3-bromophenyl)-1-nitrobut-3-en-2-yl)cycloheptanone (5i), yield: 27.5 mg, 60%; 86% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1 mL/min; UV = 252 nm; t^{anti}_{minor} = 13.17 min, t^{anti}_{major} = 9.15 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.48−7.15 (m, 4H), 6.46−6.40 (m, 1H), 6.04−6.00 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.59−4.49 (m, 2H), 3.29−3.26 (m, 1H), 2.79−2.75 (m, 1H), 2.55−2.43 (m, 2H), 1.94−1.87 (m, 4H), 1.68−1.55 (m, 1H), 1.43−1.21 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 213.9, 138.4, 133.2, 130.8, 130.1, 129.2, 127.5, 125.3, 122.7, 77.9, 52.7, 43.7 (×2), 29.6, 28.9, 28.7, 23.6 ppm. GC−MS: m/z 320, 318, 277, 275, 207, 141, 128 (100), 112; HRMS: (ESI+) m/z calcd for $C_{17}H_{21}BrNO_3$ $[M+H]^+$ 366.0705, found 366.0701.

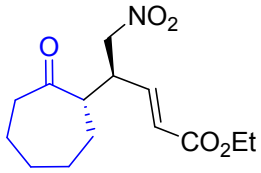


(S)-2-((S,E)-1-nitrohept-3-en-2-yl)cycloheptanone (5j), yield: 26.7 mg, 84%; 80% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (80:20) as the eluent. Flow: 1 mL/min; UV = 215 nm; t^{anti}_{minor} = 9.20 min, t^{anti}_{major} = 6.16 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 5.59−5.53 (m, 1H), 5.22−5.17 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.41−4.39 (d, *J* = 6.5 Hz, 2H), 3.06−2.99 (m, 1H), 2.62−2.57 (m, 1H), 2.60−2.46 (m, 2H), 1.99−1.94 (m, 2H), 1.90−1.83 (m,

4H), 1.65−1.57 (m, 1H), 1.37−1.32 (m, 3H) , 1.29−1.24 (m, 2H), 0.86−0.83 (t, *J* = 7Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.5, 136.3, 125.9, 78.4, 52.8, 43.6, 34.4, 29.4, 28.8, 28.7, 25.6, 23.8, 22.2, 13.4 ppm. GC−MS: m/z 206, 177, 163 (100), 55; HRMS: (ESI+) m/z calcd for $C_{14}H_{24}NO_3$ $[M+H]^+$ 254.1756, found 254.1759.

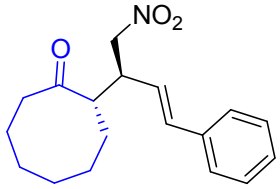


(S)-2-((S,E)-5-methyl-1-nitrohex-3-en-2-yl)cycloheptanone (5k), yield: 24.8 mg, 78%; 83% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (95.5:0.5) as the eluent. Flow: 0.7 mL/min; UV = 220 nm; t^{anti}_{minor} = 42.13 min, t^{anti}_{major} = 32.44 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 5.55−5.50 (m, 1H), 5.17−5.12 (m, 1H), 4.41−4.37 (m, 2H), 3.02−2.96 (m, 1H), 2.61−2.55 (m, 1H), 2.49−2.40 (m, 2H), 2.26−2.20 (m, 1H), 1.91−1.86 (m, 4H), 1.62−1.59 (m, 1H), 1.36−1.23 (m, 3H), 0.94−0.91 (m, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.3, 143.3, 122.7, 78.3, 52.8, 43.5, 43.3, 30.9, 29.2, 28.7, 28.5, 23.8, 22.1 (×2)ppm. GC−MS: m/z 206, 163 (100), 95, 55; HRMS: (ESI+) m/z calcd for $C_{14}H_{24}NO_3$ $[M+H]^+$ 254.1756, found 254.1768.

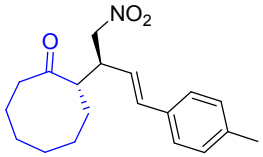


(S,E)-ethyl 5-nitro-4-((S)-2-oxocycloheptyl)pent-2-enoate (5l), yield: 31.3 mg, 88%; 78% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (70:30) as the eluent. Flow: 1 mL/min; UV = 212nm; t^{anti}_{minor} = 17.27 min, t^{anti}_{major} = 12.99 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.75−6.70 (dd, *J* = 9.5, 15.5 Hz, 1H), 5.92−5.89 (d, *J* = 15.5 Hz, 1H), 4.57−4.45 (m, 2H), 4.18−4.14 (dd, *J* = 7, 14 Hz, 2H), 3.34−3.28 (m, 1H), 2.79−2.74 (m, 1H), 2.57−2.40 (m, 2H), 1.91−1.81 (m, 4H), 1.68−1.58 (m, 1H), 1.45−1.38 (m, 1H) , 1.31−1.21 (m, 5H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 213.1, 165.3, 143.5, 125.6, 77.3, 60.6, 51.9, 43.6, 42.3, 29.4, 28.9, 28.6, 23.4, 14.0 ppm. GC−MS: m/z 237, 207,

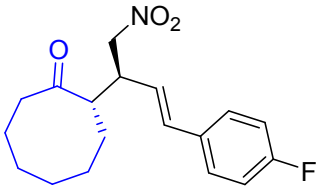
191, 163 (100), 107; HRMS: (ESI+) m/z calcd for $C_{14}H_{22}NO_5$ $[M+H]^+$ 284.1498, found 284.1492.



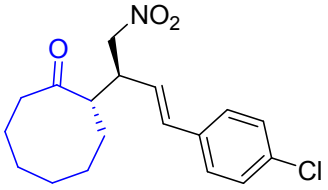
(S)-2-((S,E)-1-nitro-4-phenylbut-3-en-2-yl)cyclooctanone (5m), yield: 17.0 mg, 45%; 92% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (95:5) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 17.00 min, t^{anti}_{major} = 20.41 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.36−7.25 (m, 5H), 6.56−6.52 (d, *J* = 15.5 Hz, 1H), 5.99−5.94 (dd, *J* = 10, 16 Hz, 1H), 4.48−4.43 (m, 2H), 3.26−3.19 (m, 1H), 2.95−2.88 (m, 1H), 2.48−2.39 (m, 2H), 2.09−1.21 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.7, 134.9, 128.6 (×2), 128.6, 128.0, 126.5 (×2), 125.7, 78.2, 50.7, 44.6, 44.2, 33.0, 28.0, 25.0, 24.9, 23.9 ppm. GC−MS: m/z 254, 211, 196, 129 (100), 115; HRMS: (ESI+) m/z calcd for $C_{18}H_{24}NO_3$ $[M+H]^+$ 302.1756, found 302.1767.



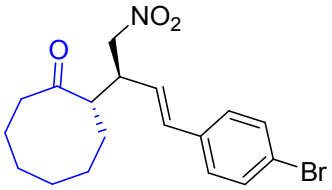
(S)-2-((S,E)-1-nitro-4-p-tolylbut-3-en-2-yl)cyclooctanone (5n), yield: 16.2 mg, 41%; 93% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/*i*-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 256 nm; t^{anti}_{minor} = 17.48 min, t^{anti}_{major} = 13.60 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.28−7.11 (m, 4H), 6.52−6.49 (d, *J* = 15.5 Hz, 1H), 5.93−5.88 (dd, *J* = 10, 16 Hz, 1H), 4.49−4.44 (m, 2H), 3.21−3.15 (m, 1H), 2.95−2.90 (m, 1H), 2.50−2.42 (m, 2H), 2.35 (s, 3H), 2.09−1.20 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.9, 138.0, 134.8, 133.4, 129.3 (×2), 126.4 (×2), 124.6, 78.3, 50.8, 44.6, 44.2, 33.0, 28.0, 25.1, 24.9, 23.9, 21.2 ppm. GC−MS: m/z 268, 211, 143 (100), 129, 105; HRMS: (ESI+) m/z calcd for $C_{19}H_{26}NO_3$ $[M+H]^+$ 316.1913, found 316.1910.



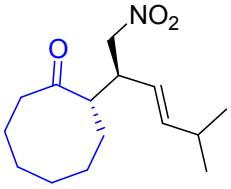
(S)-2-((S,E)-4-(4-fluorophenyl)-1-nitrobut-3-en-2-yl)cyclooctanone (5o), yield: 9.2 mg, 23%; 91% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/*i*-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 18.77 min, t^{anti}_{major} = 12.76 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.33−7.27 (m, 2H), 7.02−6.97 (m, 2H), 6.51−6.48 (d, *J* = 15.5Hz, 1H), 5.89−5.84 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.47−4.45 (m, 2H), 3.24−3.16 (m, 1H), 2.95−2.89 (m, 1H), 2.48−2.38 (m, 2H), 2.08−1.19 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.7, 161.6(d, $^{1}J_{C\text{-}F}$ = 246.4 Hz), 133.7, 128.0 (×2), 128.0 (×2), 115.6, 115.5, 78.2, 50.6, 44.5, 44.2, 33.1, 28.1, 25.0, 24.8, 23.8 ppm. GC−MS: m/z 272, 229, 215 (100), 147, 109; HRMS: (ESI+) m/z calcd for $C_{18}H_{23}FNO_3$ $[M+H]^+$ 320.1662, found 320.1672.



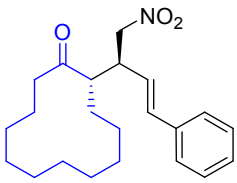
(S)-2-((S,E)-4-(4-chlorophenyl)-1-nitrobut-3-en-2-yl)cyclooctanone (5p), yield: 15.6 mg, 37%; 92% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/*i*-PrOH (80:20) as the eluent. Flow: 1.0 mL/min; UV = 256 nm; t^{anti}_{minor} =17.37 min, t^{anti}_{major} = 9.97 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.31−7.27 (m, 4H), 6.51−6.48 (d, *J* = 15.5 Hz, 1H), 5.97−5.91 (dd, *J* = 10, 16 Hz, 1H), 4.50−4.44 (m, 2H), 3.23−3.16 (m, 1H), 2.96−2.91 (m, 1H), 2.51−2.41 (m, 2H), 2.09−1.16 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.6, 134.6, 133.8, 133.7, 128.8 (×2), 127.7 (×2), 126.4, 78.1, 50.5, 44.5, 44.3, 33.1, 28.1, 25.0, 24.8, 23.8 ppm. GC−MS: m/z : 290, 288, 245, 231 (100), 129; HRMS: (ESI+) m/z calcd for $C_{18}H_{23}ClNO_3$ $[M+H]^+$ 336.1366, found 336.1369.



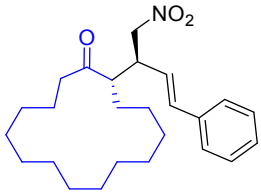
(S)-2-((S,E)-4-(4-bromophenyl)-1-nitrobut-3-en-2-yl)cyclooctanone (5q), yield: 11.0 mg, 23%; 94% ee ; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/*i*-PrOH (80:20) as the eluent. Flow: 1.0 mL/min; UV = 256 nm; t^{anti}_{minor} = 18.80 min, t^{anti}_{major} = 10.31 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.45−7.18 (m, 4H), 6.49−6.46 (d, *J* = 15.5 Hz, 1H), 5.98−5.93 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.47−4.4 6(m, 2H), 3.25−3.16 (m, 1H), 2.95−2.89 (m, 1H), 2.48−2.44 (m, 2H), 2.08−1.17 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.6, 135.1, 133.7, 131.8 (×2), 128.0 (×2), 126.6, 121.9, 78.1, 50.5, 44.5, 44.3, 33.1, 28.1, 25.0, 24.9, 23.8 ppm. GC−MS: m/z: 334, 332, 291, 289, 277, 275, 169, 141, 128 (100); HRMS: (ESI+) m/z calcd for $C_{18}H_{23}BrNO_3$ $[M+H]^+$ 380.0861, found 380.0858.



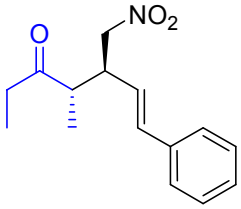
(S)-2-((S,E)-5-methyl-1-nitrohex-3-en-2-yl)cyclooctanone (5r), yield: 27.9 mg, 83%; 99% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/*i*-PrOH (99:1) as the eluent. Flow: 1.0 mL/min; UV = 216 nm; t^{anti}_{major} = 10.76 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 5.59−5.55 (dd, *J* =7, 15.5 Hz, 1H), 5.14−5.09 (m, 1H), 4.38−4.28 (m, 2H), 2.99−2.90 (m, 1H), 2.78−2.70 (m, 1H), 2.42−2.40 (m, 2H), 2.28−2.21 (m, 1H), 1.92−1.36 (m, 10H), 0.96−0.91 (m, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 219.0, 143.6, 123.0, 78.6, 51.0, 44.0, 32.4, 31.1, 28.0, 27.6, 25.2, 24.9, 24.2, 22.3, 22.2 ppm. GC−MS: m/z: 220, 177, 163, 95 (100), 55; HRMS: (ESI+) m/z calcd for $C_{15}H_{26}NO_3$ $[M+H]^+$ 268.1913, found 268.1913.



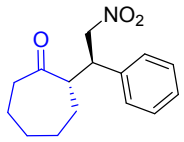
(S)-2-((S,E)-1-nitro-4-phenylbut-3-en-2-yl)cyclododecanone (5s), yield: 9.0mg, 20%; 98% ee; white solid, Mp: 76−80 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/*i*-PrOH (95:5) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 17.06 min, t^{anti}_{major} = 22.03 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.37−7.27 (m, 5H), 6.57−6.54 (d, *J* = 15.5 Hz, 1H), 5.98−5.93 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.49−4.39 (m, 2H), 3.37−3.33 (m, 1H), 2.95−2.89 (m, 1H), 2.81−2.77 (m, 1H), 2.38−2.32 (m, 1H), 2.02−1.77 (m, 4H), 1.33−1.26 (m, 14H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 212.0, 136.3, 134.5, 128.6 (×2), 128.0, 126.6 (×2), 125.3, 78.7, 52.5, 41.3, 38.5, 27.0, 26.2, 26.2, 23.8, 23.2, 22.7, 22.2, 21.6, 20.5 ppm. HRMS: (ESI+) m/z calcd for $C_{22}H_{32}NO_3$ $[M+H]^+$ 358.2382, found 358.2388.



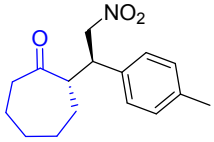
(S)-2-((S,E)-1-nitro-4-phenylbut-3-en-2-yl)cyclopentadecanone (5t), yield: 13.1 mg, 26%; 94% ee; white solid, Mp: 83−87 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/*i*-PrOH (95:5) as the eluent. Flow: 1.0 mL/min; UV = 256 nm; t^{anti}_{minor} = 12.43 min, t^{anti}_{major} = 19.33 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.36−7.26 (m, 5H), 6.55−6.52 (d, *J* = 15.5 Hz, 1H), 5.98−5.93 (dd, *J* = 9.5, 16 Hz, 1H), 4.48−4.47 (d, *J* = 6Hz, 2H), 3.30−3.24 (m, 1H), 2.80−2.76 (m, 1H), 2.69−2.63 (m, 1H), 2.44−2.38 (m, 1H), 1.64–1.52 (m, 4H), 1.36−1.24 (m, 20H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 213.3, 136.2, 134.6, 128.6 (×2), 128.0, 126.5 (×2), 125.5, 78.1, 53.0, 43.2, 43.2, 30.3, 27.4, 27.4, 27.1, 26.6, 26.4, 26.2, 26.2, 26.1, 25.9, 25.6, 22.0 ppm. HRMS: (ESI+) m/z calcd for $C_{25}H_{38}NO_3$ $[M+H]^+$ 400.2852, found 400.2859.



(4S,5S,E)-4-methyl-5-(nitromethyl)-7-phenylhept-6-en-3-one (5u), yield: 22.7mg, 67%; 96% ee; yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/*i*-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 248 nm; t^{anti}_{minor} = 13.89 min, t^{anti}_{major} = 20.40 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.34−7.23 (m, 5H), 6.53−6.51 (d, *J* = 15.5 Hz, 1H), 5.99−5.94 (dd, *J* = 9.5, 15.5 Hz, 1H), 4.54−4.48 (m, 2H), 3.32−3.26 (m, 1H), 2.80−2.74 (m, 1H), 2.63−2.56 (m, 1H), 2.51−2.45 (m, 1H), 1.20−1.16 (m, 3H), 1.09−1.06 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 213.0, 136.2, 134.8, 128.6 (×2), 128.0, 126.5 (×2), 125.1, 78.0, 47.1, 43.8, 35.2, 15.4, 7.6 ppm. GC−MS: m/z: 115, 128 (100), 143, 157, 185, 214, 261; HRMS: (ESI+) m/z calcd for $C_{15}H_{20}NO_3$ $[M+H]^+$ 262.1443, found 262.1450.

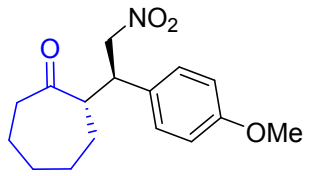


(S)-2-((R)-2-nitro-1-phenylethyl)cycloheptanone (7a), yield: 23.8 mg, 70%; 89% ee; slightly white solid, Mp: 76−78 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/*i*-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 228 nm; t^{anti}_{minor} = 25.21 min, t^{anti}_{major} = 19.29 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.35−7.32 (m, 2H), 7.29−7.26 (m, 1H), 7.18−7.17 (m, 2H), 4.69−4.61 (m, 2H), 3.70−3.66 (m, 1H), 3.03−2.98 (m, 1H), 2.58−2.49 (m, 2H), 1.94−1.84 (m, 2H), 1.79−1.74 (m, 1H), 1.71−1.62 (m, 1H), 1.61−1.57 (m, 1H), 1.29–1.14 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.6, 137.8, 129.0 (×2), 128.1 (×2), 127.9, 78.8, 53.7, 45.6, 43.4, 30.0, 28.6, 28.5, 23.9 ppm. GC−MS: m/z: 91 (100), 117, 129, 155, 171, 214; HRMS: (ESI+) m/z calcd for $C_{15}H_{20}NO_3$ $[M+H]^+$ 262.1438, found 262.1440.

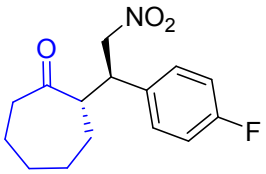


(S)-2-((R)-2-nitro-1-p-tolylethyl)cycloheptanone (7b), yield: 24.6 mg, 69%; 84% ee; slightly white solid, Mp: 65−67 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow:

1.0 mL/min; UV = 220 nm; t^{anti}_{minor} = 9.79 min, t^{anti}_{major} = 11.89 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.13 (d, *J* = 8 Hz, 2H), 7.05 (d, *J* = 8 Hz, 2H), 4.66-4.59 (m, 2H), 3.68-3.62 (m, 1H), 3.00-2.96 (m, 1H), 2.58-2.48 (m, 2H), 2.32 (s, 3H), 1.93-1.84 (m, 2H), 1.78-1.74 (m, 1H), 1.70-1.59 (m, 2H), 1.28-1.13 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.7, 137.6, 134.6, 129.7 (×2), 128.0 (×2), 78.9, 53.8, 45.2, 43.4, 29.9, 28.6, 28.5, 23.9, 21.0 ppm. GC-MS: m/z 105, 118, 185 (100), 228, 275; HRMS: (ESI+) m/z calcd for $C_{16}H_{22}NO_3$ $[M+H]^+$ 276.1594, found 276.1590.

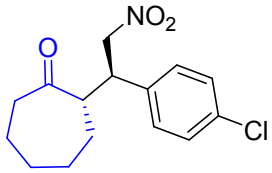


(S)-2-((R)-1-(4-methoxyphenyl)-2-nitroethyl)cycloheptanone (7c), yield: 31.8 mg, 84%; 90% ee; colorless oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 212 nm; t^{anti}_{minor} = 32.86 min, t^{anti}_{major} = 24.24 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.09 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 4.62-4.61 (m, 2H), 2.78 (s, 3H), 3.66-3.61 (m, 1H), 2.98-2.93 (m, 1H), 2.57-2.47 (m, 2H), 1.94-1.84 (m, 2H), 1.78-1.74 (m, 1H), 1.87-1.58 (m, 2H), 1.26-1.21 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.9, 159.1, 129.5, 129.1 (×2), 114.4 (×2), 78.9, 55.2, 53.9, 44.8, 43.3, 29.8, 28.6, 28.4, 22.9 ppm. GC-MS: m/z 91, 121, 134, 201 (100), 244, 291; HRMS: (ESI+) m/z calcd for $C_{16}H_{22}NO_4$ $[M+H]^+$ 292.1543, found 292.1544.

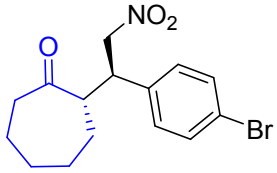


(S)-2-((R)-1-(4-fluorophenyl)-2-nitroethyl)cycloheptanone (7d), yield: 27.6 mg, 76%; 92% ee; slightly white solid, Mp: 48−50 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 212 nm; t^{anti}_{minor} = 37.09 min, t^{anti}_{major} = 21.45 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.17-7.14 (m, 2H), 7.05-7.01 (m, 2H), 4.67-4.60 (m, 2H), 3.72-3.67 (m, 1H), 3.00-2.95 (m, 1H), 2.58-2.48 (m, 2H), 1.94-1.85 (m, 2H),

1.80-1.76 (m, 1H), 1.71-1.63 (m, 1H), 1.60-1.55 (m, 1H), 1.31-1.13 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.3, 162.2 (d, $^{1}J_{C\text{-}F}$ = 245.5 Hz), 133.5 (d, $^{4}J_{C\text{-}F}$ = 3.4 Hz), 129.7 (×2, d, $^{3}J_{C\text{-}F}$ = 8 Hz), 116.5 (×2, d, $^{2}J_{C\text{-}F}$ = 21.6 Hz), 78.7, 53.7, 44.9, 43.4, 29.9, 28.5 (×2), 23.8 ppm. GC-MS: m/z 109, 122, 173, 189 (100), 232; HRMS: (ESI+) m/z calcd for $C_{15}H_{19}FNO_3$ $[M+H]^+$ 280.1343, found 280.1344.

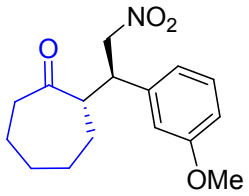


(S)-2-((R)-1-(4-chlorophenyl)-2-nitroethyl)cycloheptanone (7e), yield: 28.7 mg, 79%; 87% ee; slightly white solid, Mp: 58−60 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 224 nm; t^{anti}_{minor} =12.96 min, t^{anti}_{major} = 13.99 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.32-7.27 (m, 2H), 7.13-7.09 (m, 2H), 4.67-4.61 (m, 2H), 3.71-3.66 (m, 1H), 3.00-2.95 (m, 1H), 2.58-2.47 (m, 2H), 1.93-1.85 (m, 2H), 1.79-1.75 (m, 1H), 1.71-1.62 (m, 1H), 1.59-1.54 (m, 1H), 1.32-1.13 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.1, 136.4, 133.8, 129.5 (×2), 129.2 (×2), 78.5, 63.5, 45.0, 43.4, 29.9, 28.6, 28.4, 23.7 ppm. GC-MS: m/z 125, 165, 189, 205 (100), 248; HRMS: (ESI+) m/z calcd for $C_{15}H_{19}ClNO_3$ $[M+H]^+$ 296.1048, found 296.1050.

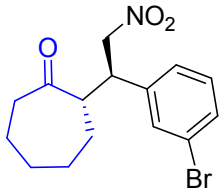


(S)-2-((R)-1-(4-bromophenyl)-2-nitroethyl)cycloheptanone (7f), yield: 34.8 mg, 79%; 83% ee; slightly white solid, Mp: 73−75 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 232 nm; t^{anti}_{minor} = 13.93 min, t^{anti}_{major} = 16.24 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.47-7.42 (m, 2H), 7.07-7.03 (m, 2H), 4.67-4.60 (m, 2H), 3.69-3.65 (m, 1H), 3.00-2.95 (m, 1H), 2.58-2.47 (m, 2H), 1.93-1.85 (m, 2H), 1.78-1.76 (m, 1H), 1.70-1.62 (m, 1H), 1.59-1.55 (m, 1H), 1.35-1.13 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.1, 136.9, 132.2 (×2), 129.8 (×2), 121.9, 78.4, 53.5,

45.0, 43.5, 29.9, 28.6, 28.5, 23.7 ppm. GC-MS: m/z 116, 129, 171, 196, 249 (100), 292; HRMS: (ESI+) m/z calcd for $C_{15}H_{19}BrNO_3$ $[M+H]^+$ 340.0543, found 340.0545.

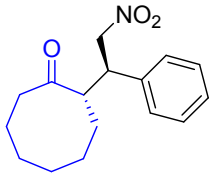


(S)-2-((R)-1-(3-methoxyphenyl)-2-nitroethyl)cycloheptanone (7g), yield: 28.4 mg, 75%; 81% ee; slightly yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 220 nm; t^{anti}_{minor} = 14.00 min, t^{anti}_{major} = 18.41 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.27-7.21 (m, 1H), 6.82-6.80 (m, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 6.71 (s, 1H), 4.64-4.62 (m, 2H), 3.79 (s, 3H), 3.68-3.63 (m, 1H), 3.00-2.96 (m, 1H), 2.57-2.48 (m, 2H), 1.98-1.84 (m, 2H), 1.78-1.74 (m, 1H), 1.70-1.59 (m, 2H) , 1.30-1.14 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.5, 159.9, 139.4, 130.0, 120.2, 114.4, 112.6, 78.7, 55.2, 53.7, 45.6, 43.4, 29.8, 28.6, 28.5, 23.9 ppm. GC-MS: m/z 91, 121, 135, 159, 201 (100), 244, 291; HRMS: (ESI+) m/z calcd for $C_{16}H_{22}NO_4$ $[M+H]^+$ 292.1543, found 292.1544.

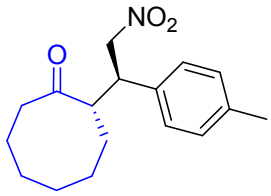


(S)-2-((R)-1-(3-bromophenyl)-2-nitroethyl)cycloheptanone (7h), yield: 22.0 mg, 50%; 86% ee; slightly white solid, Mp: 72−74 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 212 nm; t^{anti}_{minor} = 14.24 min, t^{anti}_{major} = 16.66 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.42 (d, *J* = 8.5Hz, 1H), 7.34 (s, 1H), 7.23-717 (m, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 4.68-4.60 (m, 2H), 3.69-3.64 (m, 1H), 3.00-2.92 (m, 1H), 2.58-2.49 (m, 2H), 1.94-1.87 (m, 2H), 1.79-1.76 (m, 1H), 1.72-1.63 (m, 1H), 1.61-1.56 (m, 1H), 21.32-1.14 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 214.0, 140.3, 131.2, 131.2, 130.6, 126.8, 123.1, 78.3, 53.5, 45.2, 43.4, 30.0, 28.5, 28.4, 23.7

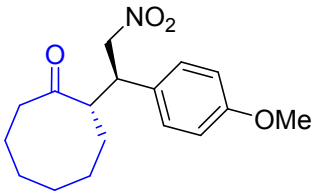
ppm. GC-MS: m/z 116 (100), 129, 169, 196, 251, 292; HRMS: (ESI+) m/z calcd for $C_{15}H_{19}BrNO_3$ $[M+H]^+$ 340.0543, found 340.0545.



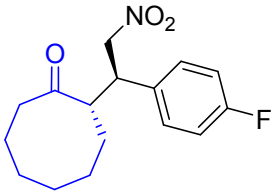
(S)-2-((R)-2-nitro-1-phenylethyl)cyclooctanone (7i), yield: 24.0 mg, 67%; 99% ee; slightly white solid, Mp: 87−88 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 212 nm; t^{anti}_{minor} = 11.55 min, t^{anti}_{major} = 13.64 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.35-7.32 (m, 2H), 7.29-7.26 (m, 1H), 7.18-7.16 (m, 2H), 4.68-4.63 (m, 1H), 4.59-4.56 (m, 1H), 3.67-3.62 (m, 1H), 3.16-3.11 (m, 1H), 2.48-2.36 (m, 2H), 2.10-2.01 (m, 1H), 1.64-1.45 (m, 7H), 1.31-1.18 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.5, 137.9, 129.0 (×2), 127.9 (×3), 78.4, 52.1, 46.5, 44.0, 32.7, 28.0, 25.1, 24.8, 24.1 ppm. GC-MS: m/z 91 (100), 105, 118, 131, 171, 228, 275; HRMS: (ESI+) m/z calcd for $C_{16}H_{22}NO_3$ $[M+H]^+$ 276.1594, found 276.1596.



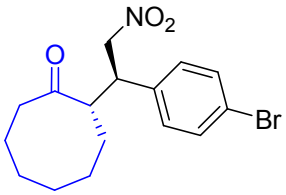
(S)-2-((R)-2-nitro-1-p-tolylethyl)cyclooctanone (7j), yield: 22.6 mg, 60%; 95% ee; slightly white solid, Mp: 80−82 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 220 nm; t^{anti}_{minor} = 9.33 min, t^{anti}_{major} = 10.52 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.13 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 4.64-4.60 (m, 1H), 4.58-4.53 (m, 1H), 3.62-3.57 (m, 1H), 3.13-3.08 (m, 1H), 2.47-2.36 (m, 2H), 2.32 (s, 3H), 2.09-2.00 (m, 1H), 1.88-1.81 (m, 1H), 1.63-1.42 (m, 6H), 1.31-1.18 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 219.0, 137.6, 134.8, 129.7 (×2), 127.8 (×2), 78.6, 52.2, 46.2, 44.0, 32.7, 28.0, 25.1, 24.8, 24.2, 21.0 ppm. GC-MS: m/z 91, 105 (100), 117, 131, 171, 228, 242; HRMS: (ESI+) m/z calcd for $C_{17}H_{24}NO_3$ $[M+H]^+$ 290.1751, found 290.1753.



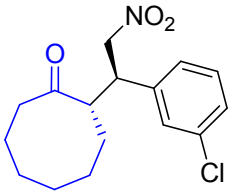
(S)-2-((R)-1-(4-methoxyphenyl)-2-nitroethyl)cyclooctanone (7k), yield: 22.6 mg, 57%; 99% ee; colorless oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 228 nm; t^{anti}_{minor} = 17.08 min, t^{anti}_{major} = 15.09 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.09 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 4.63-4.53 (m, 2H), 3.77 (s, 3H), 3.62-3.57 (m, 1H), 3.10-3.05 (m, 1H), 2.46-2.34 (m, 2H), 2.09-2.00 (m, 1H), 1.86-1.82 (m, 1H), 1.62-1.44 (m, 6H), 1.30-1.17 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 219.0, 159.1, 129.7, 128.9 (×2), 114.4 (×2), 78.6, 55.1, 52.3, 45.8, 44.0, 32.6, 27.9, 25.1, 24.6, 24.1 ppm. GC-MS: m/z 121, 134 (100), 201, 215, 258, 305; HRMS: (ESI+) m/z calcd for $C_{17}H_{24}NO_4$ $[M+H]^+$ 306.1700, found 306.1701.



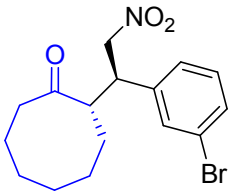
(S)-2-((R)-1-(4-fluorophenyl)-2-nitroethyl)cyclooctanone (7l), yield: 14.9 mg, 39%; 99% ee; slightly yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 212 nm; t^{anti}_{minor} = 27.22 min, t^{anti}_{major} = 20.6 5min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.17-7.14 (m, 2H), 7.04-7.01 (m, 2H), 4.65-4.55 (m, 2H), 3.68-3.63 (m, 1H), 3.12-3.08 (m, 1H), 2.46-2.35 (m, 2H), 2.09-2.00 (m, 1H), 1.90-1.62 (m, 1H), 1.63-1.42 (m, 6H), 1.31-1.17 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.7, 162.2(d, $^1J_{C\text{-}F}$ = 245.6 Hz), 133.7(d, $^4J_{C\text{-}F}$ = 3.3 Hz), 129.5 (×2, d, $^3J_{C\text{-}F}$ = 8 Hz), 116.0(×2, d, $^2J_{C\text{-}F}$ = 21.8 Hz), 78.4, 52.0, 45.8, 44.1, 32.8, 27.9, 24.9, 24.8, 24.0 ppm. GC-MS: m/z 109 (100), 122, 149, 189, 246; HRMS: (ESI+) m/z calcd for $C_{16}H_{21}FNO_3$ $[M+H]^+$ 294.1500, found 294.1501.



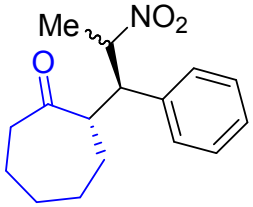
(S)-2-((R)-1-(4-bromophenyl)-2-nitroethyl)cyclooctanone (7m), yield: 24.8 mg, 54%; 99% ee; slightly white solid, Mp: 84−86°C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 228 nm; t^{anti}_{minor} = 29.30 min, t^{anti}_{major} = 24.96 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.46 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.5 Hz, 2H), 4.65-4.55 (m, 2H), 3.65-3.60 (m, 1H), 3.12-3.07 (m, 1H), 2.46-2.36 (m, 2H), 2.09-2.00 (m, 1H), 1.89-1.82 (m, 1H), 1.63-1.42 (m, 6H), 1.31-1.15 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.4, 137.0, 132.2 (×2), 129.6 (×2), 121.9, 78.1, 51.8, 46.0, 44.2, 32.8, 28.0, 24.9, 24.8, 23.9 ppm. GC-MS: m/z 116 (100), 130, 171, 249, 265, 306; HRMS: (ESI+) m/z calcd for $C_{16}H_{21}BrNO_3$ $[M+H]^+$ 354.0699, found 354.0700.



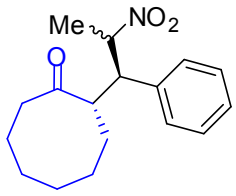
(S)-2-((R)-1-(3-chlorophenyl)-2-nitroethyl)cyclooctanone (7n), yield: 23.3 mg, 58%; >99% ee; slightly white solid, Mp: 80−82 °C. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 1.0 mL/min; UV = 212 nm; t^{anti}_{major} = 13.16 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.23-7.22 (m, 2H), 7.15 (s, 1H), 7.05-7.03 (m, 1H), 4.85-4.81 (m, 1H), 4.68-4.64 (m, 1H), 3.78-3.63 (m, 1H), 3.19-3.10 (m, 1H), 2.12-2.07 (m, 1H), 1.97-1.81 (m, 3H), 1.77-1.29 (m, 8H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.7, 140.0, 134.7, 130.1, 128.2, 128.1, 126.2, 78.0, 51.8, 46.2, 44.5, 31.7, 28.1, 25.4, 25.0, 24.1 ppm. GC-MS: m/z 115, 125 (100), 139, 151, 165, 262, 309; HRMS: (ESI+) m/z calcd for $C_{16}H_{21}ClNO_3$ $[M+H]^+$ 310.1204, found 310.1205.



(S)-2-((R)-1-(3-bromophenyl)-2-nitroethyl)cyclooctanone (7o), yield: 22.9 mg, 50%; 98% ee; slightly yellow oil. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AD-H with hexane/i-PrOH (90:10) as the eluent. Flow: 0.5 mL/min; UV = 216 nm; t^{anti}_{minor} = 21.53 min, t^{anti}_{major} = 19.68 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.42 (d, *J* = 8.5 Hz, 1H), 7.34 (s, 1H), 7.21 (t, *J* = 7.5Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 4.66-4.55 (m, 2H), 3.65-3.61 (m, 1H), 3.12-3.07 (m, 1H), 2.47-2.36 (m, 2H), 2.10-2.02 (m, 1H), 1.94-1.81 (m, 1H), 1.64-1.42 (m, 6H), 1.33-1.15 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 218.4, 140.4, 131.2, 131.0, 130.6, 126.6, 123.1, 78.1, 51.8, 46.1, 44.1, 32.8, 28.0, 24.9, 24.8, 24.0 ppm. GC-MS: m/z 116 (100), 131, 169, 183, 210, 263, 306; HRMS: (ESI+) m/z calcd for $C_{16}H_{21}BrNO_3$ $[M+H]^+$ 354.0699, found 354.0700.

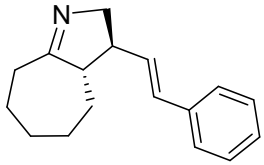


(S)-2-((R)-2-nitro-1-phenylpropyl)cycloheptanone (7p), yield: 12.2 mg, 34%; 93% ee; slightly white solid. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (98:2) as the eluent. Flow: 1 mL/min; UV = 220 nm; t^{anti}_{minor} = 8.32 min, t^{anti}_{major} = 9.57 min. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.31-7.28 (m, 3H), 7.01-6.99 (m, 2H), 4.99-4.93 (m, 1H), 3.40-3.27 (m, 2H), 2.87-2.80 (m, 1H), 2.49-2.40 (m, 1H), 1.97-1.75 (m, 3H), 1.73-1.62 (m, 2H), 1.48-1.42 (m, 1H), 1.28 (d, *J* = 6.4 Hz, 3H), 1.23-1.01 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 215.2, 135.4, 129.0 (×2), 128.5 (×2), 127.9, 82.3, 51.6, 51.0, 44.3, 31.0, 29.3, 27.9, 23.1, 17.2 ppm. GC-MS: m/z 90.9 (100), 116.9 , 185.1, 229.2; HRMS: (ESI+) m/z calcd for $C_{16}H_{22}NO_3$ $[M+H]^+$ 276.1600, found 276.1606.



(S)-2-((R)-2-nitro-1-phenylpropyl)cyclooctanone (7q), yield: 14.28 mg, 38%; 99% ee; slightly white solid. The enantiomeric excess was determined by HPLC on Daicel Chiralpak AS-H with hexane/i-PrOH (98:2) as the eluent. Flow: 1 mL/min; UV = 216 nm; t^{anti}_{major} = 12.04 min. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.34-7.28 (m, 3H), 7.09-7.07 (m, 2H), 4.80-4.74 (m, 1H), 3.71-3.67 (m, 1H), 3.50-3.44 (m, 1H), 3.01-2.95 (m, 1H), 2.40-2.22 (m, 2H), 1.95-1.76 (m, 1H), 1.66-1.47 (m, 3H), 1.22-1.19 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 3H), 1.22-1.19 (m, 2H), 0.88-0.79 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 217.9, 135.4, 128.9 (×2), 128.7 (×2), 127.8, 84.5, 52.3, 51.7, 42.3, 30.5, 27.6, 26.2, 26.0, 25.0, 15.5 ppm. GC-MS: m/z 90.9, 116.9 (100), 185.1, 243; HRMS: (ESI+) m/z calcd for $C_{17}H_{24}NO_3$ $[M+H]^+$ 290.1756, found 290.1760.

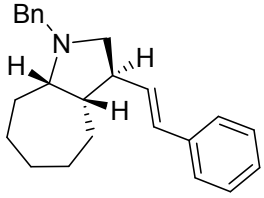
Synthesis of Compound (8a). The mixture of zinc powder (237.0 mg, 3.65 mmol), **5a** (70 mg, 0.24 mmol) and EtOH (3.0 mL) was stirred in a 25 mL round-bottom flask at 35 ℃ for 10 min. Then, 2 mL of 4M aqueous HCl were added. When the reaction was complete (monitored by HPLC-MS), the solvent was removed under reduced pressure and aqueous 3M NaOH (6 mL) was added. After the solution was stirred for 5 min, dichloromethane (20 mL) was added to the mixture. The aqueous layer was extracted with CH_2Cl_2 (3×10 mL), and the combined organic layers were washed with brine and dried over anhydrous Na_2SO_4 and concentrated to obtain crude blackish oil. The crude solid was purified by column chromatography on silica gel (Petroleum ether: EtOAc=7:3) to afford the product **8a**.



(3S,3aS,E)-3-styryl-2,3,3a,4,5,6,7,8-octahydrocyclohepta[b]pyrrole (8a), yield: 55.4 mg, 95%; 85% ee. The enantiomeric excess was determined by HPLC on Daicel

Chiralpak OD-H with hexane/ethyl alcohol (95:5) as the eluent. Flow: 1 mL/min; UV = 252 nm; t_{minor} = 9.80 min, t_{major} = 12.17 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.38−7.21 (m, 5H), 6.43−6.40 (d, *J* = 15.5 Hz, 1H), 6.20−6.16 (dd, *J* = 8, 15.5 Hz, 1H), 2. 70−2.60 (m, 2H), 2.53−2.48 (m, 1H), 1.82−1.28 (m, 11H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 183.0, 137.1, 131.1, 131.0, 128.5 (×2), 127.2, 126.0 (×2), 64.2, 57.2, 50.9, 34.2, 31.5, 29.4, 28.3, 26.2 ppm. GC−MS: m/z: 239, 211, 196, 162 (100), 143, 128, 91; HRMS: (ESI+) m/z calcd for $C_{17}H_{22}N$ $[M+H]^+$ 240.1741, found 240.1752.

Synthesis of Compound (9a). $NaBH_4$ (15 mg, 0.40 mmol) was added to a solution of **8a** (48 mg, 0.20 mmol) in anhydrous ethanol (2 mL) at 0 ℃. After 45 min the reaction was quenched with saturated NH_4Cl solution and concentrated. The residue was diluted with aqueous NaOH solution (1 N, 5 mL) and extracted with CH_2Cl_2 (3×10 mL). The combined organic phases were dried over Na_2SO_4, filtered, and concentrated. The crude material was dissolved in anhydrous ethanol (2 mL), then, benzyl bromide (25 mg, 0.15 mmol) and potassium hydroxide (8.4 mg, 0.15 mmol) were added. After stirring at room temperature for 24 h the reaction mixture was concentrated. The residue was extracted with CH_2Cl_2 (3×10 mL). The combined organic phases were dried over Na_2SO_4, filtered, and concentrated. The crude solid was purified by column chromatography on silica gel (Petroleum ether:ether:$N(Et)_3$ = 50:5:1) to afford the product **9a**.

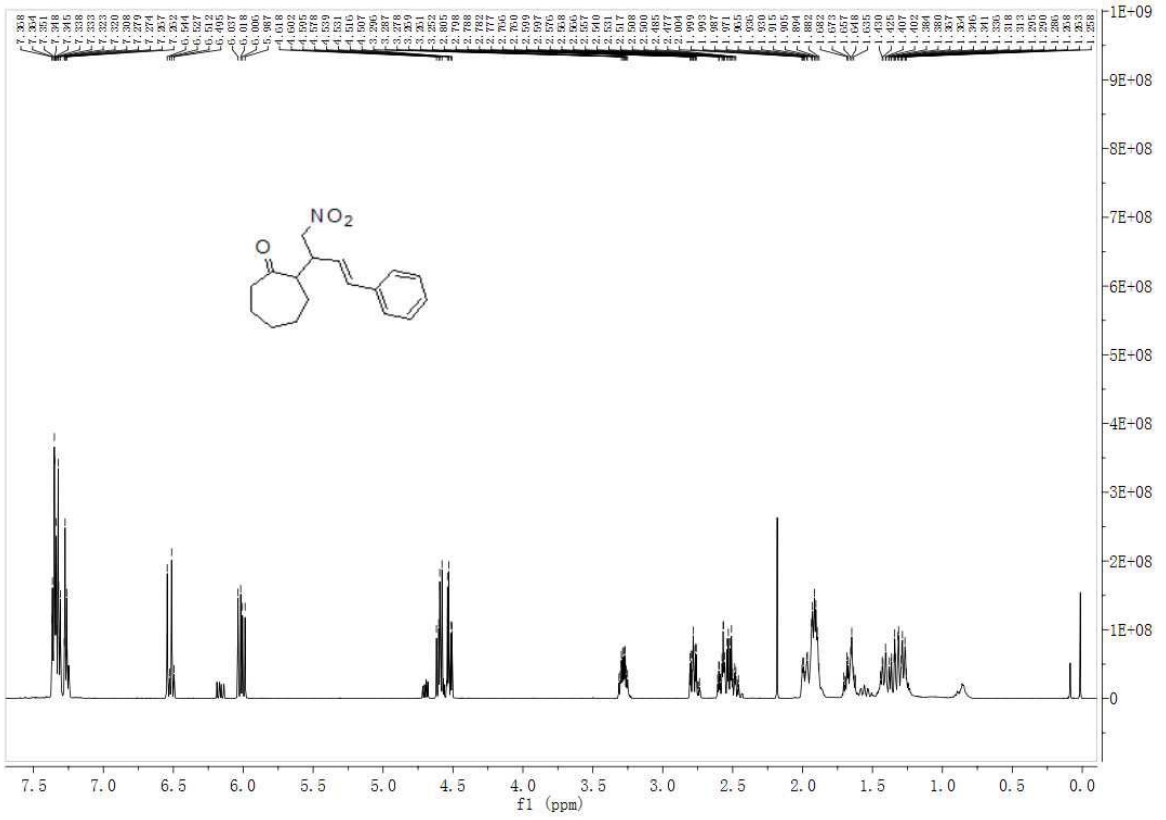


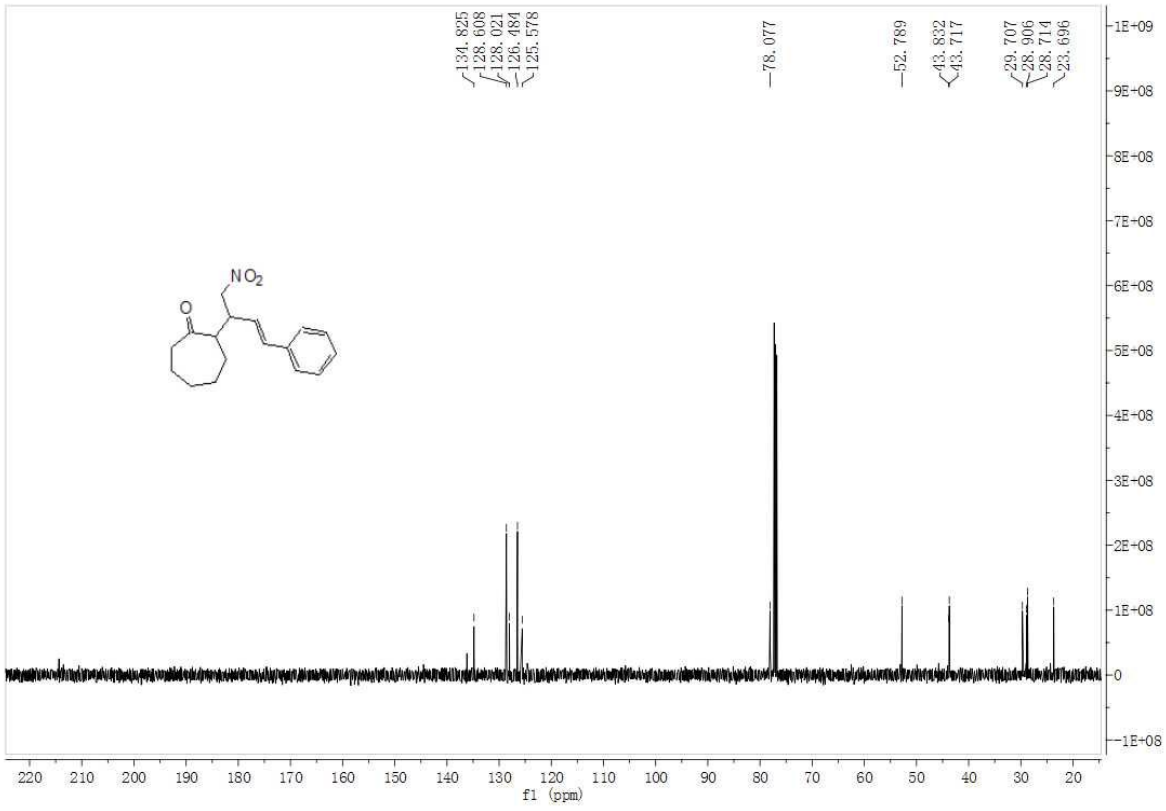
(3S,3aS,8aS,E)-1-benzyl-3-styryl-decahydrocyclohepta[b]pyrrole (9a), yield: 31 mg, 46%; 83% ee. The enantiomeric excess was determined by HPLC on Daicel Chiralpak OD-H with hexane/i-PrOH (99.5:0.5) as the eluent. Flow: 0.7 mL/min; UV = 256 nm; t_{minor} = 20.51 min, t_{major} = 14.01 min. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.34−7.20 (m, 10H), 6.38−6.35 (d, *J* = 15.5 Hz, 1H), 6.09−6.04 (dd, *J* = 8.5, 16 Hz, 1H), 4.04−4.01 (d, *J* = 13 Hz, 1H), 3.30−3.27 (d, *J* = 13 Hz, 1H), 3.00−2.97 (m, 1H), 2.76−2.72 (m,

1H), 2.50−2.43 (m, 1H), 2.18−2.14 (m, 1H), 1.90−1.17(m, 11H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 137.5, 131.8, 130.6, 129.2 (×2), 128.5 (×2), 128.2 (×2), 127.0, 126.9, 126.1, 126.0 (×2), 68.8, 59.7, 58.9, 49.9, 48.7, 31.5, 30.8, 30.0, 29.0, 26.5 ppm. HRMS: (ESI+) m/z calcd for $C_{24}H_{30}N$ $[M+H]^+$ 332.237, found 332.2378.

3. NMR spectra

5a





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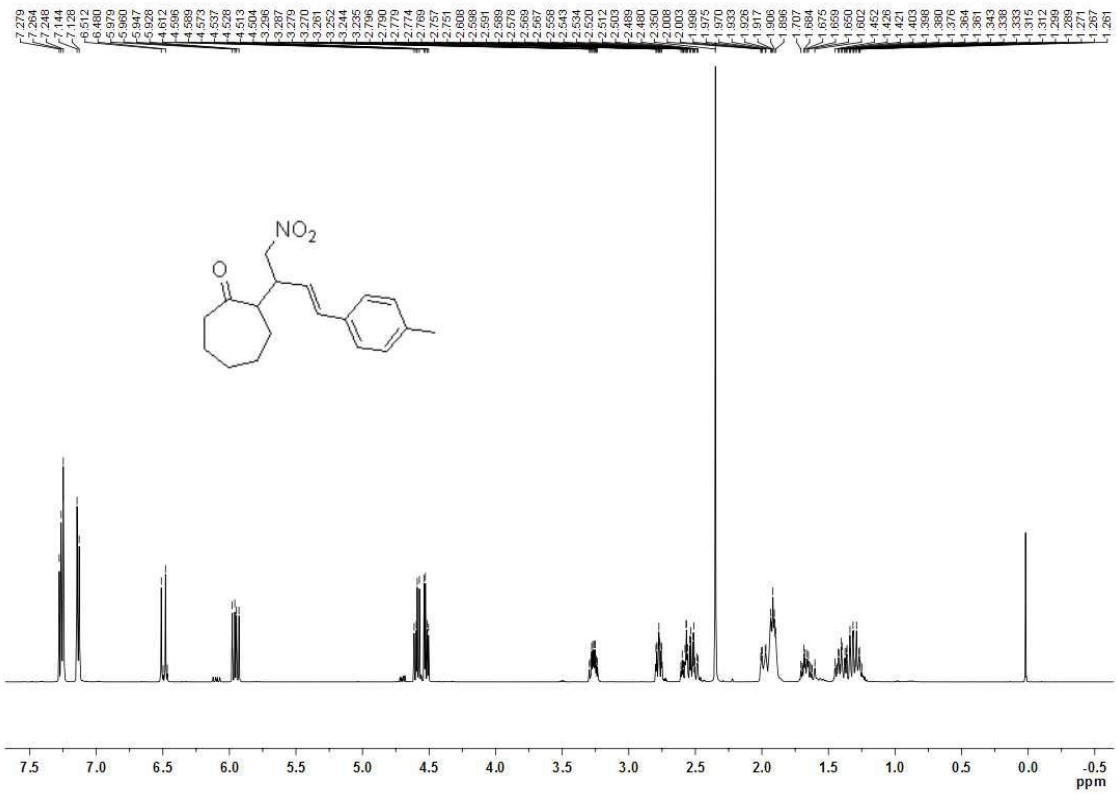
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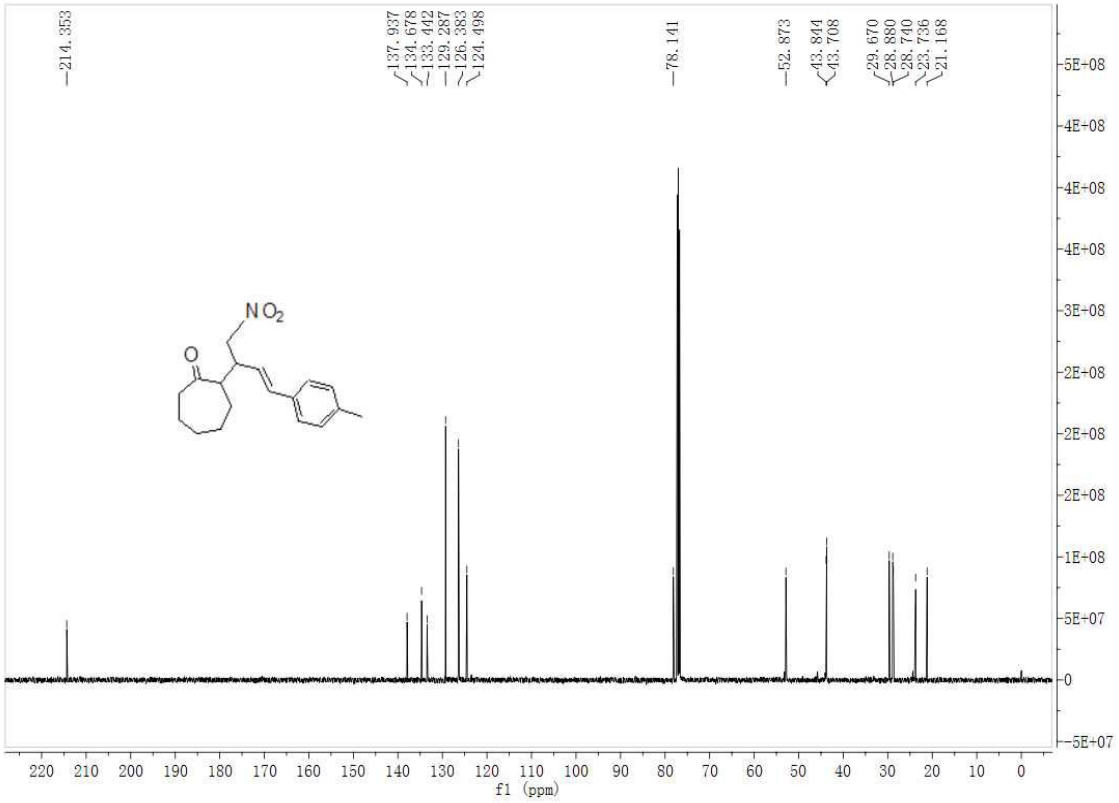
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm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78.141
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28.740
23.736
21.168
NO2
O
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4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
220
210
200
190
180
170
160
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140
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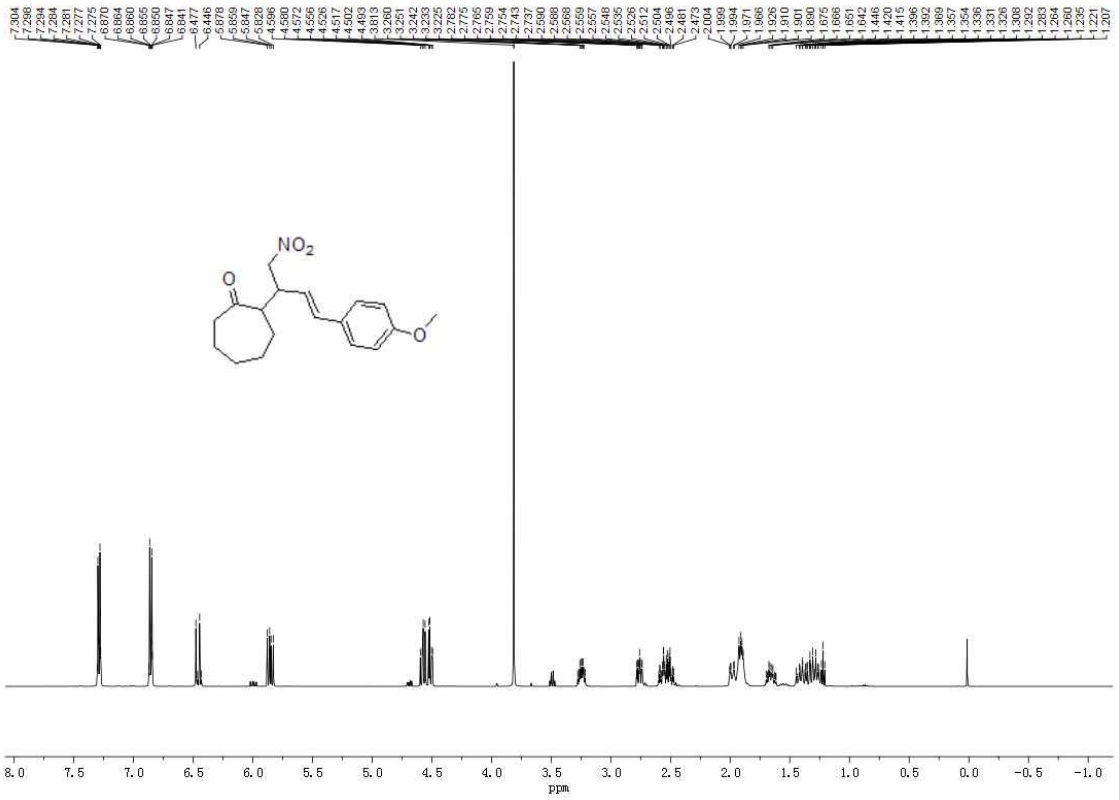
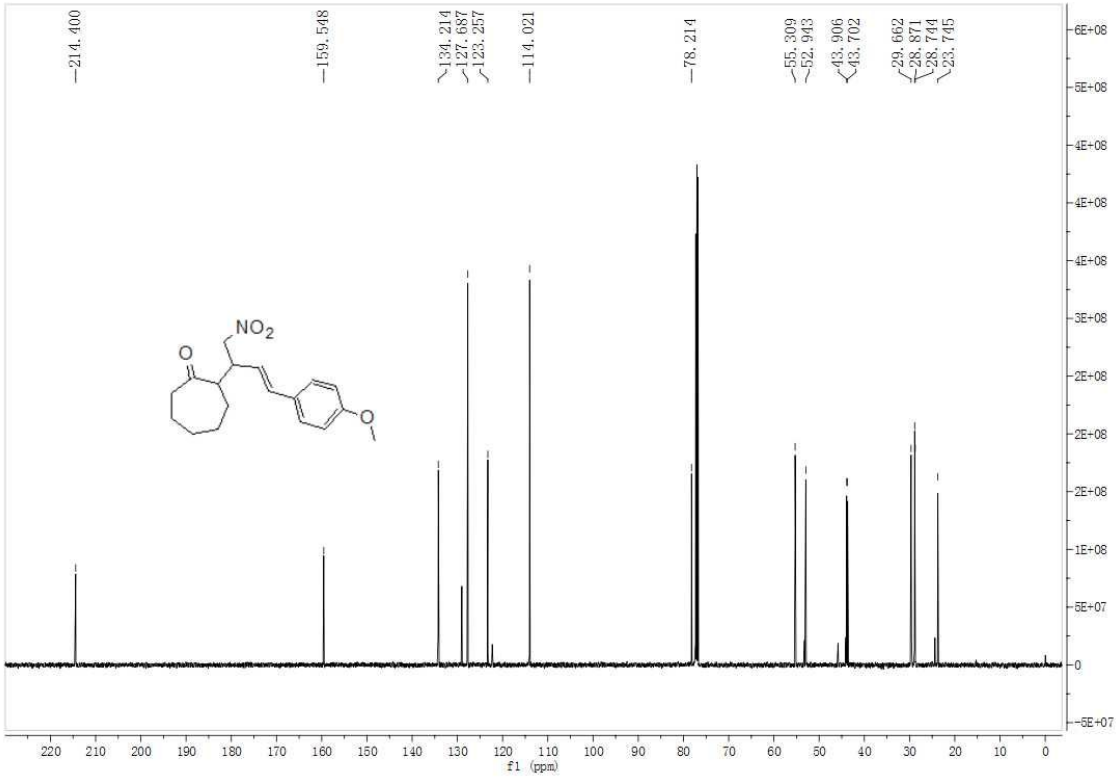
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5c


NO2
O
O
ppm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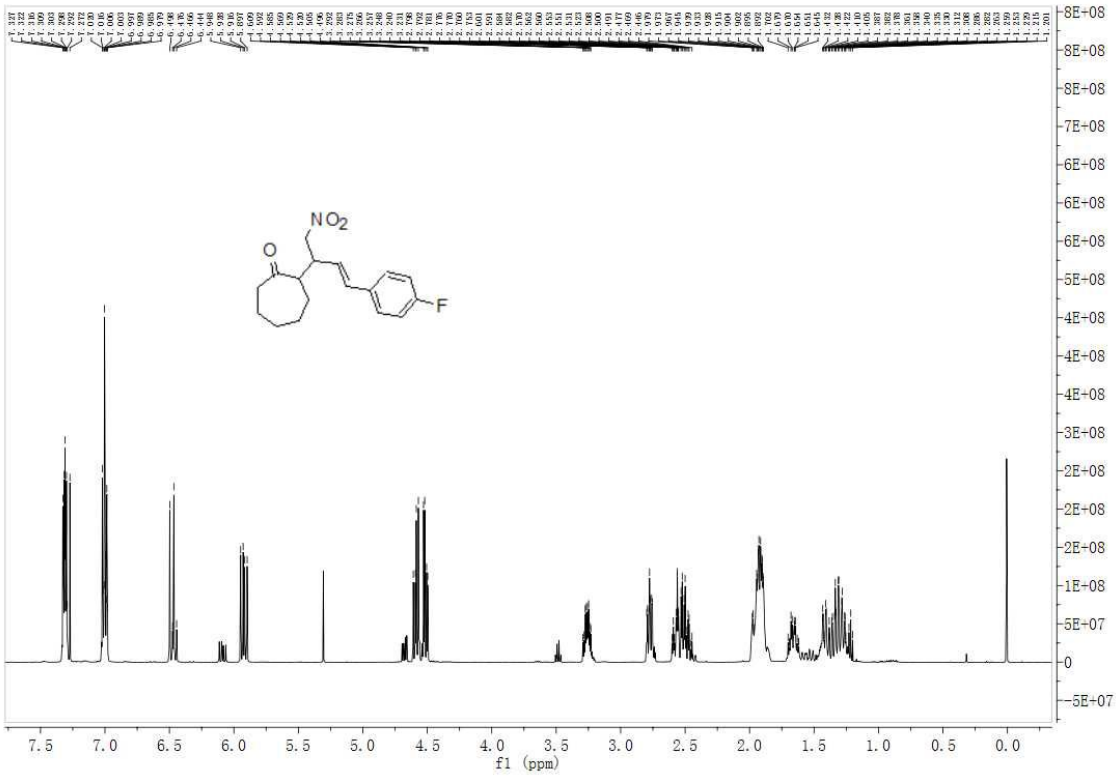
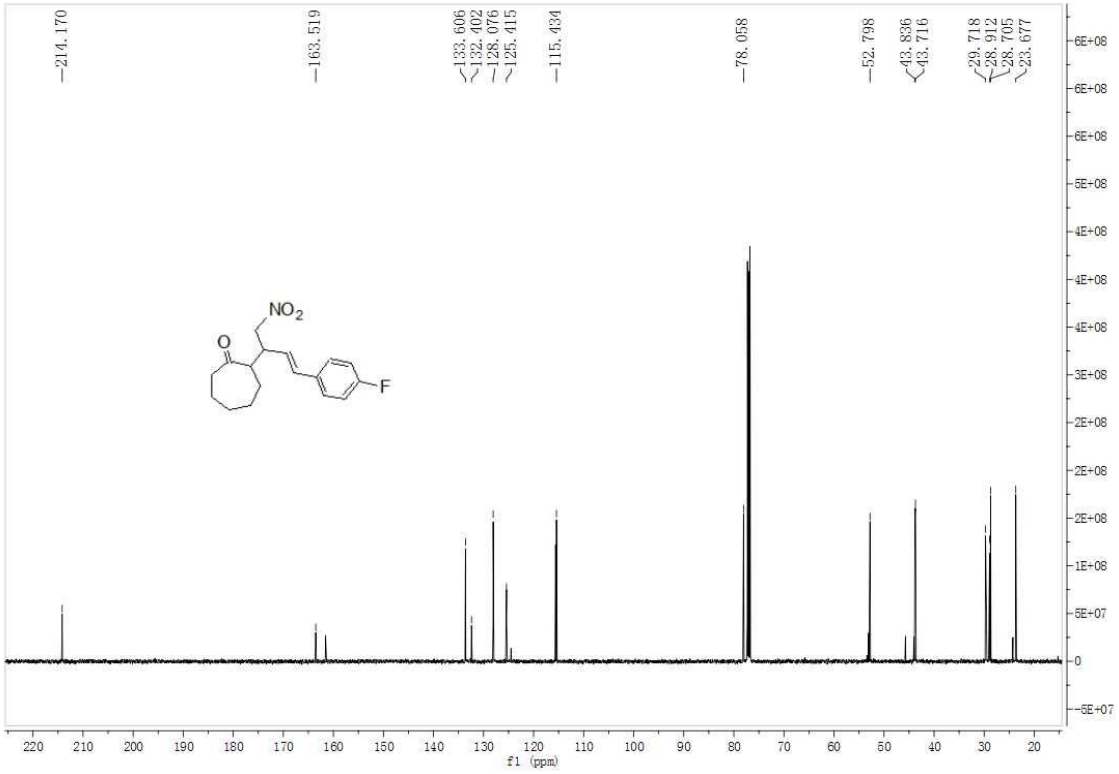
28.744
23.745
NO2
O
O
f1 (ppm)

5d


NO2
O
F
f1 (ppm)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125.415
115.434
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52.798
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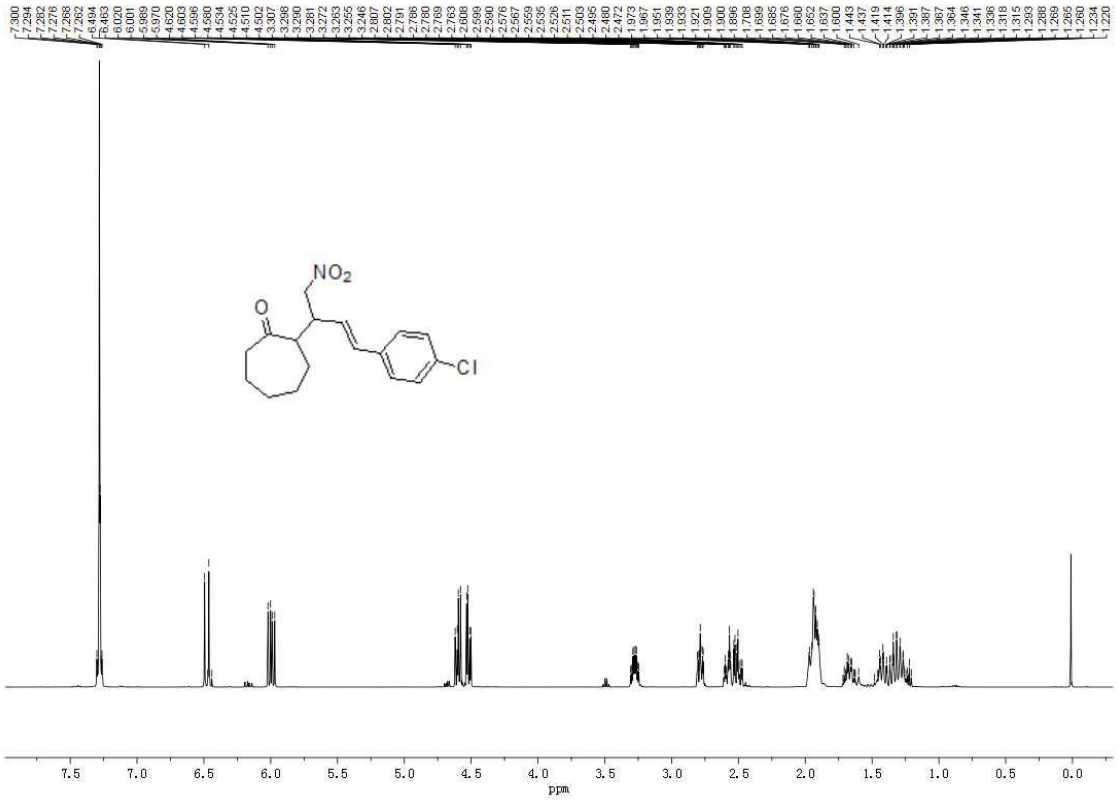
28.912
28.705
23.677
NO2
O
F
f1 (ppm)

5e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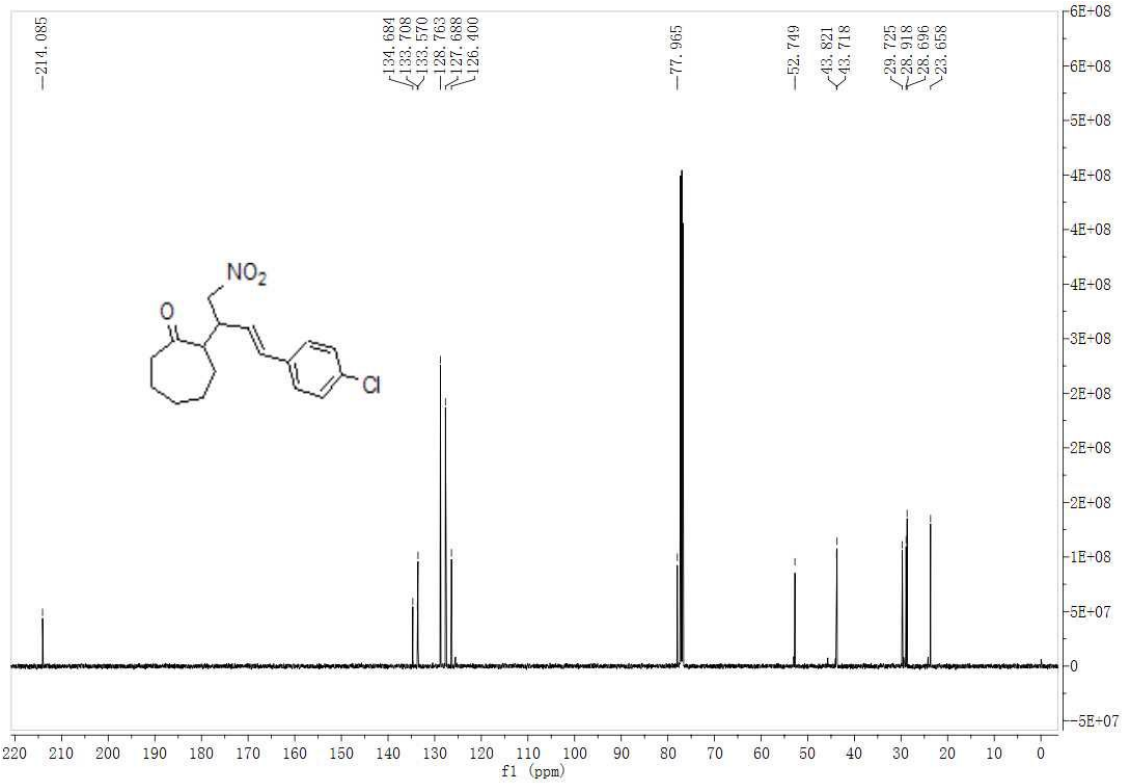
O
Cl
ppm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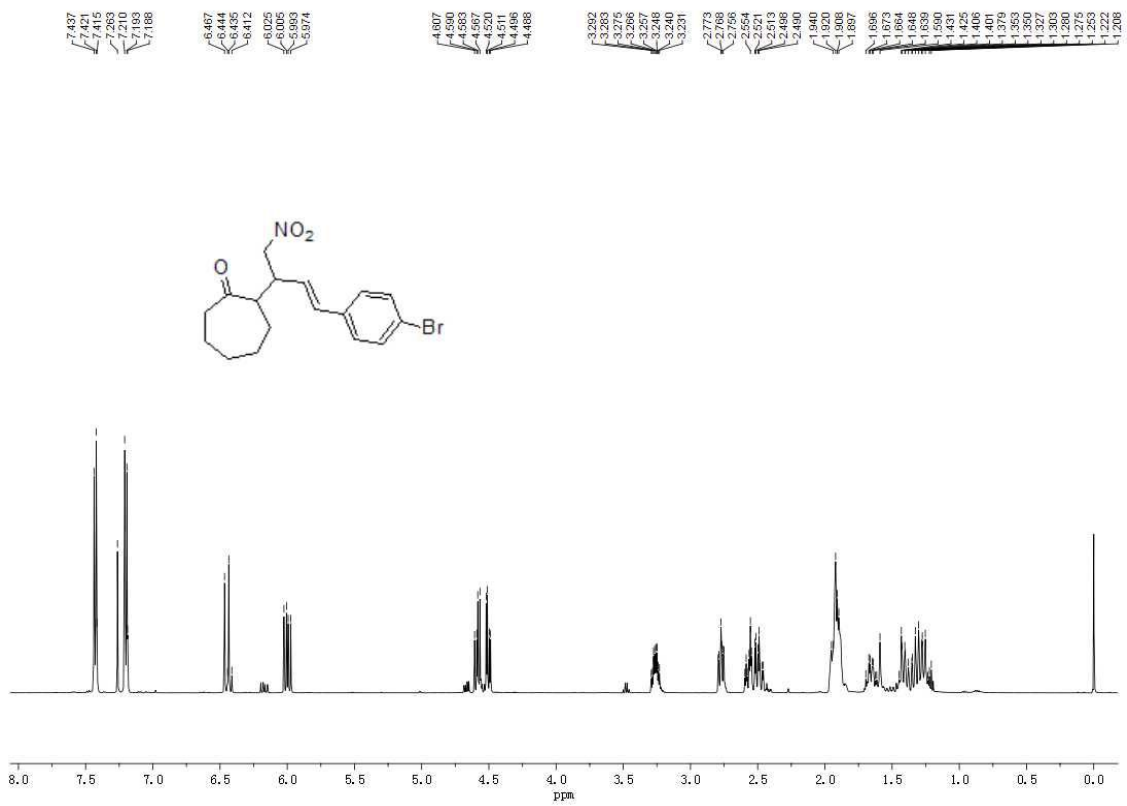
NO2
O
Cl
f1 (ppm)

5f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4.607
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4.583
4.567
4.530
4.511
4.496
4.488
3.292
3.283
3.275
3.266
3.257
3.248
3.240
3.231
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2.768
2.756
2.554
2.521
2.513
2.498
2.490
1.940
1.920
1.908
1.897
1.696
1.673
1.664
1.648
1.639
1.590
1.541
1.425
1.406
1.401
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1.353
1.350
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6.0
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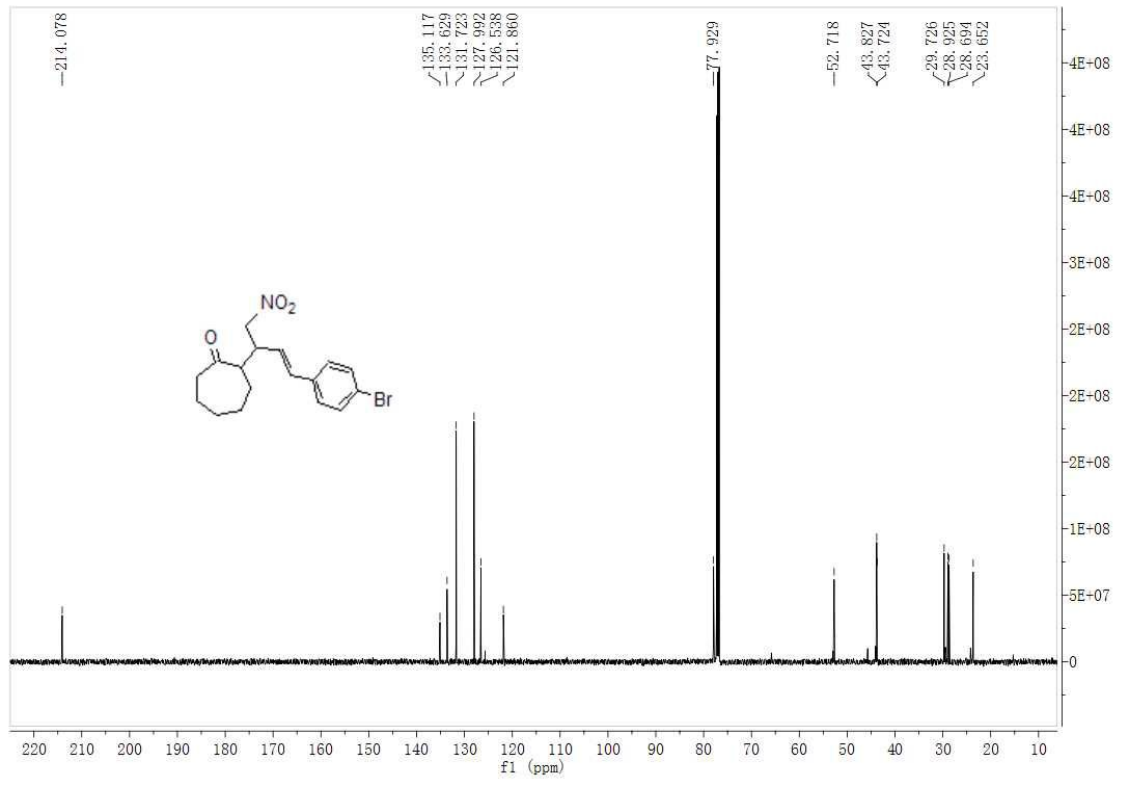
ppm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Br
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4E+08
4E+08
3E+08
2E+08
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2E+08
1E+08
5E+07
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210
200
190
180
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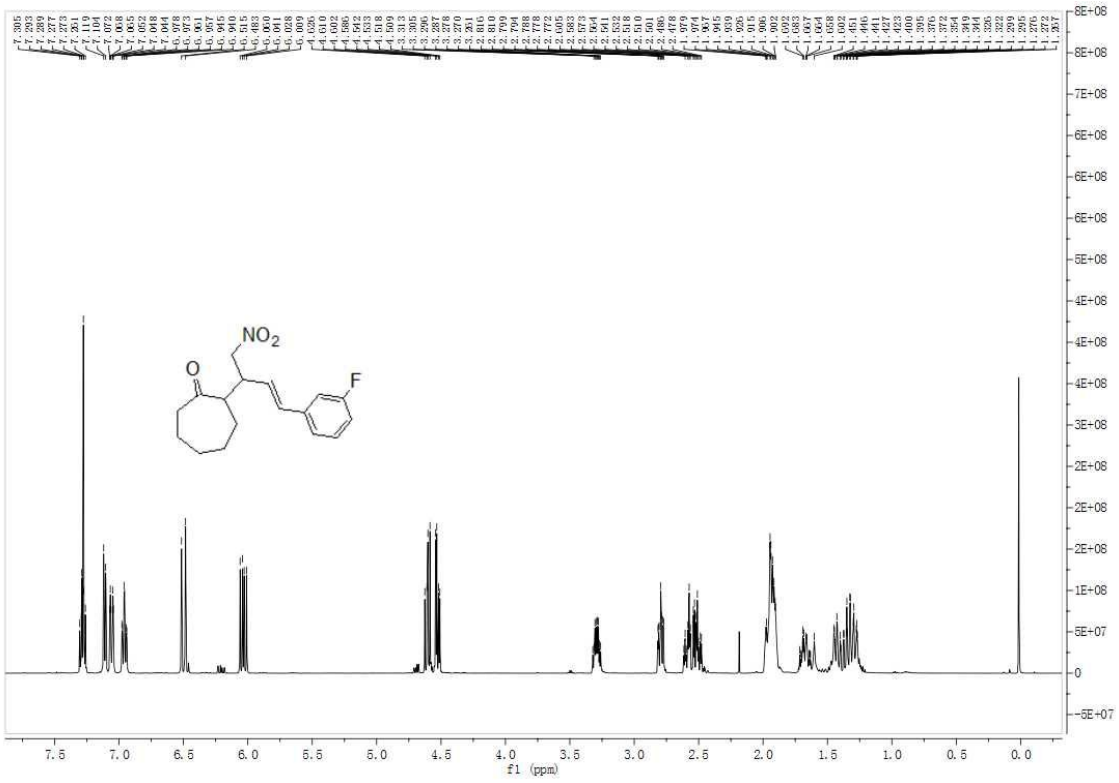
f1 (ppm)

5g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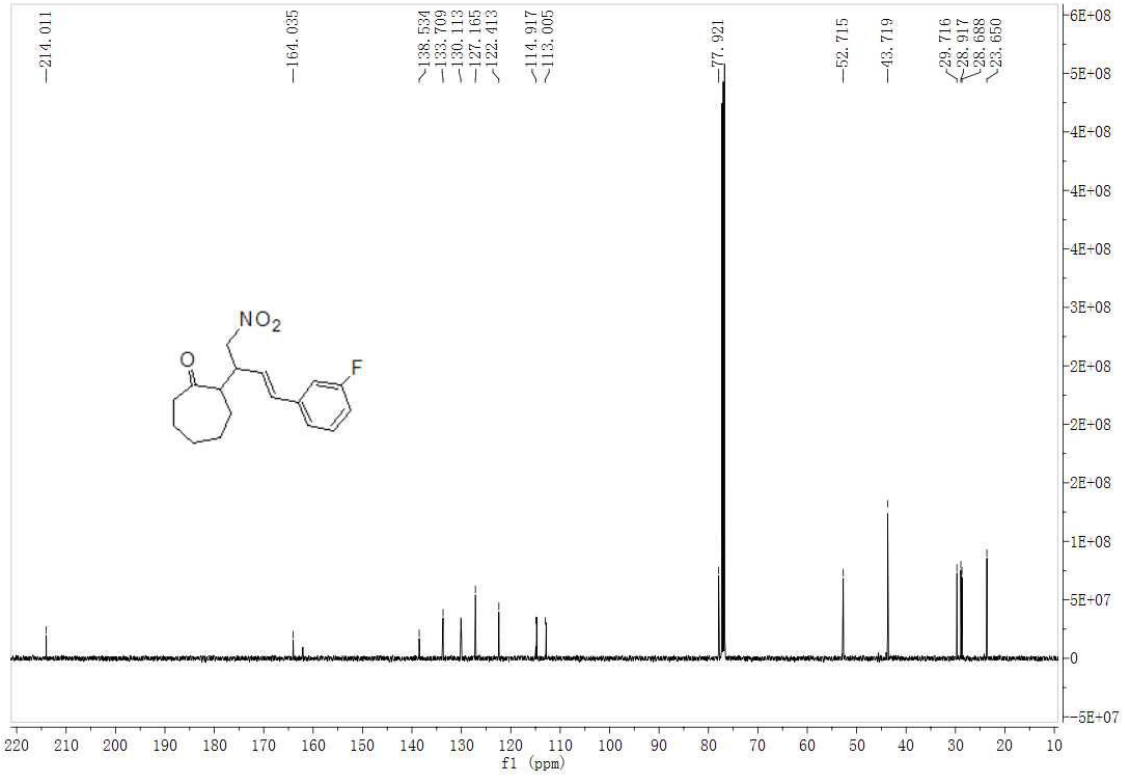
F
f1 (ppm)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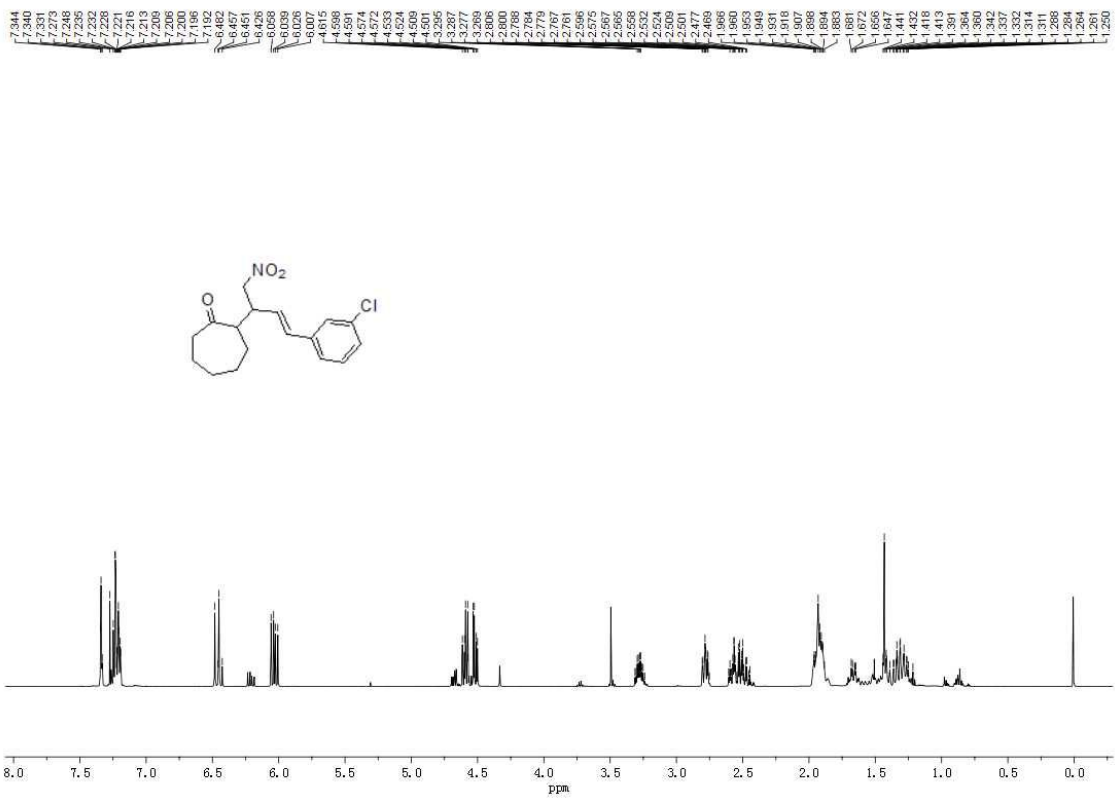
NO2
O
F
f1 (ppm)

5h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1.322
1.314
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1.261
1.250
NO2
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Cl
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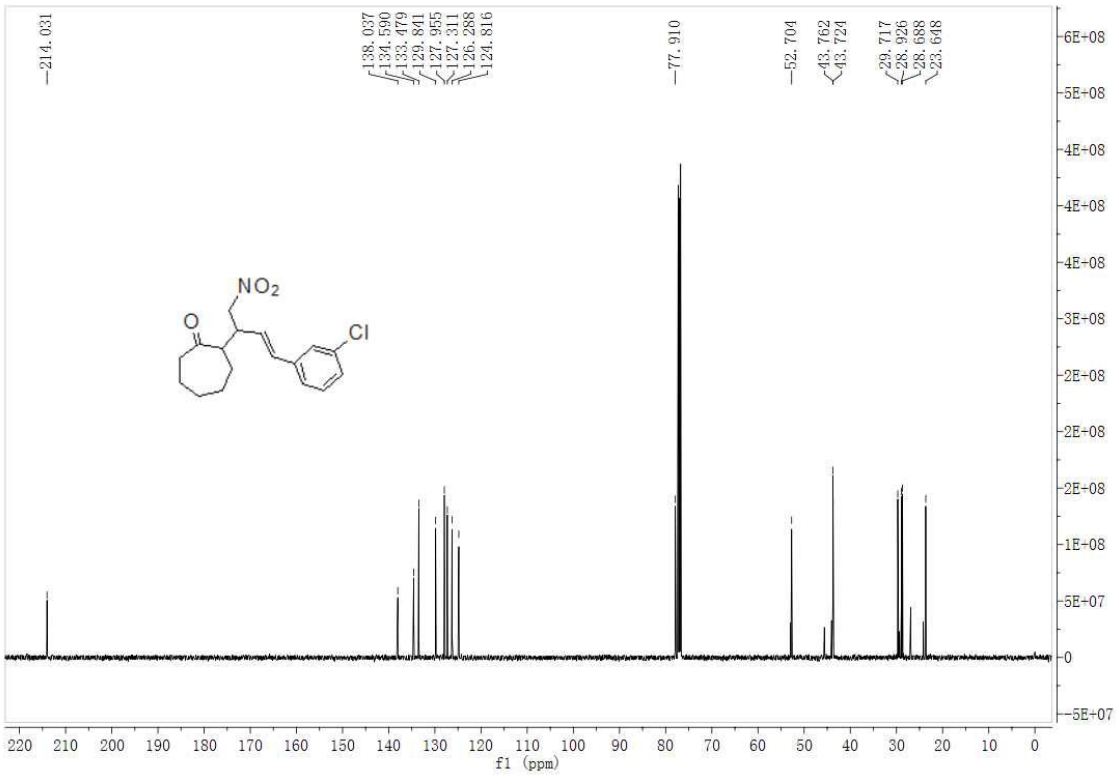
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28.688
23.648
NO2
O
Cl
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5E+08
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4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
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210
200
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180
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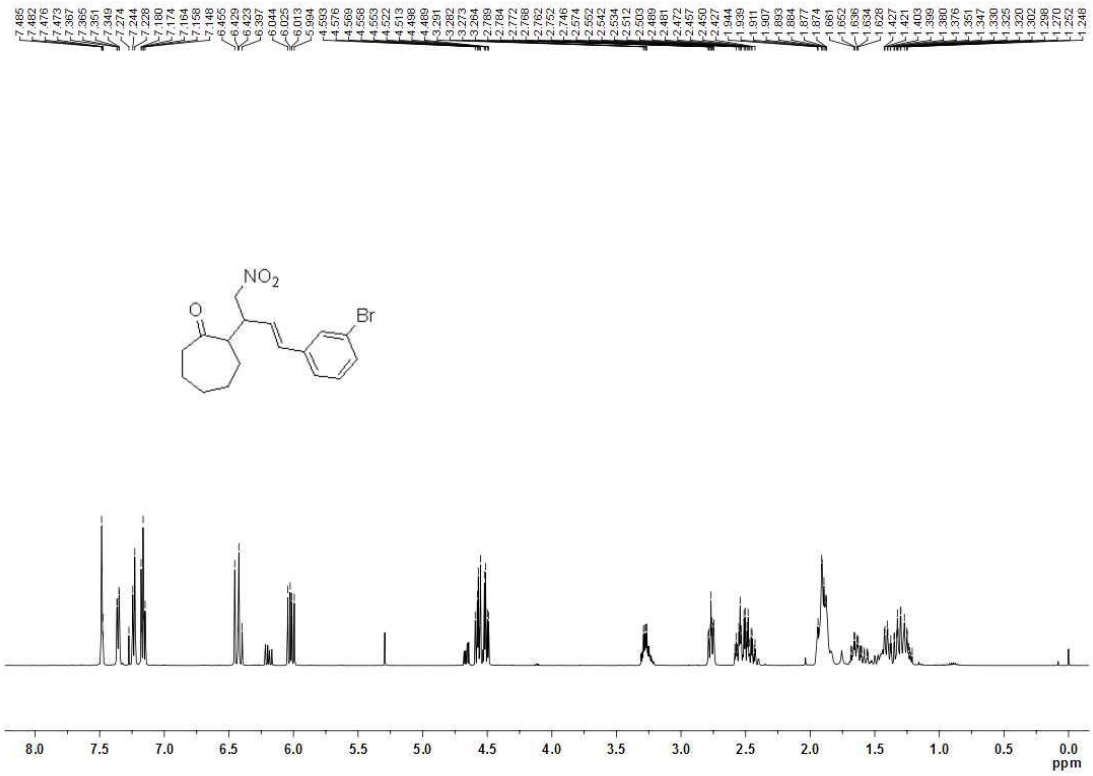
5i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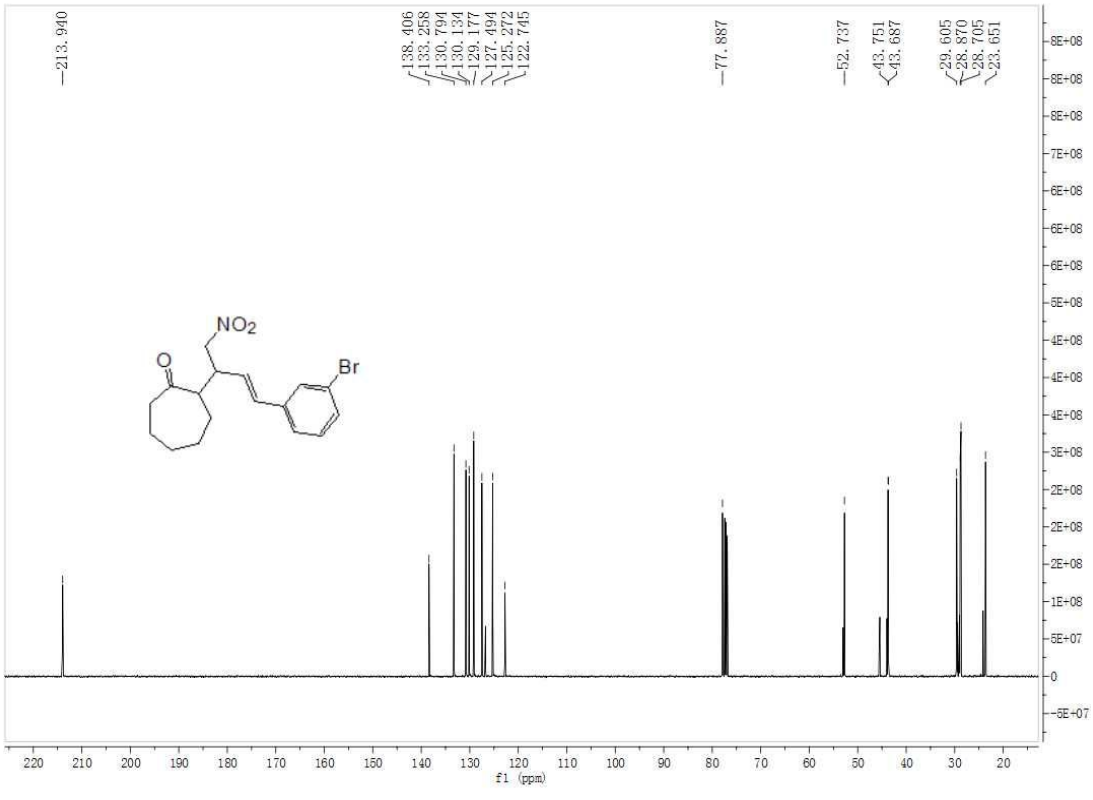
ppm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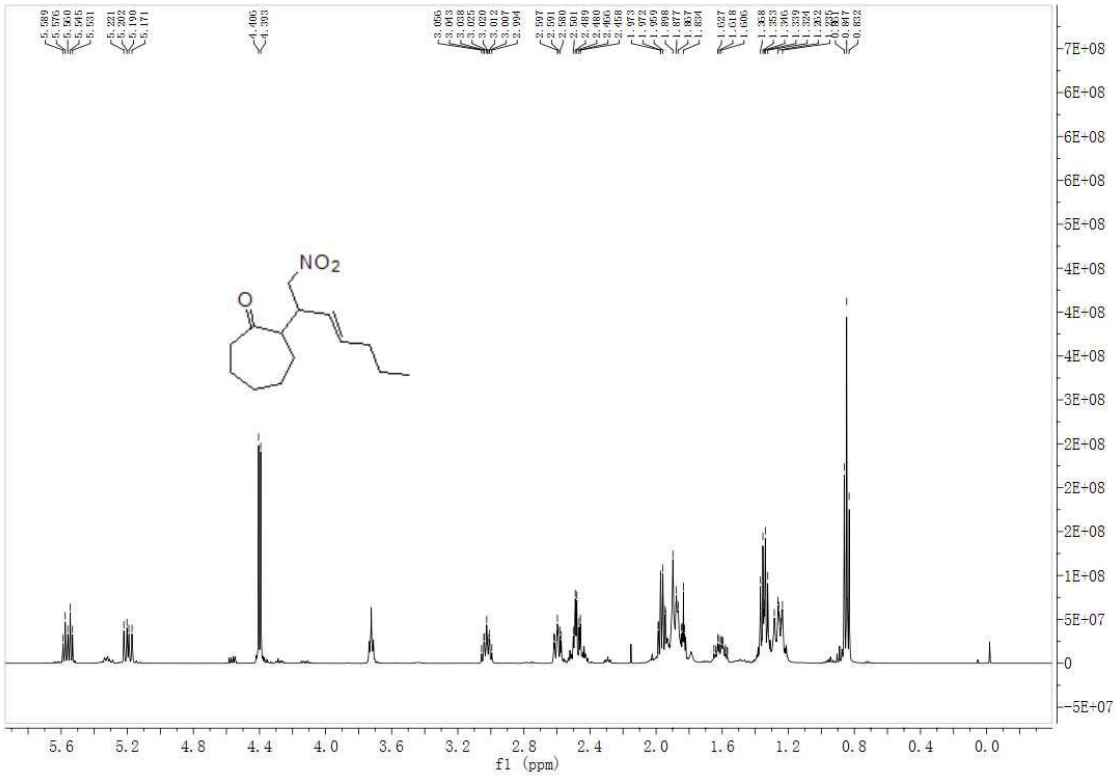
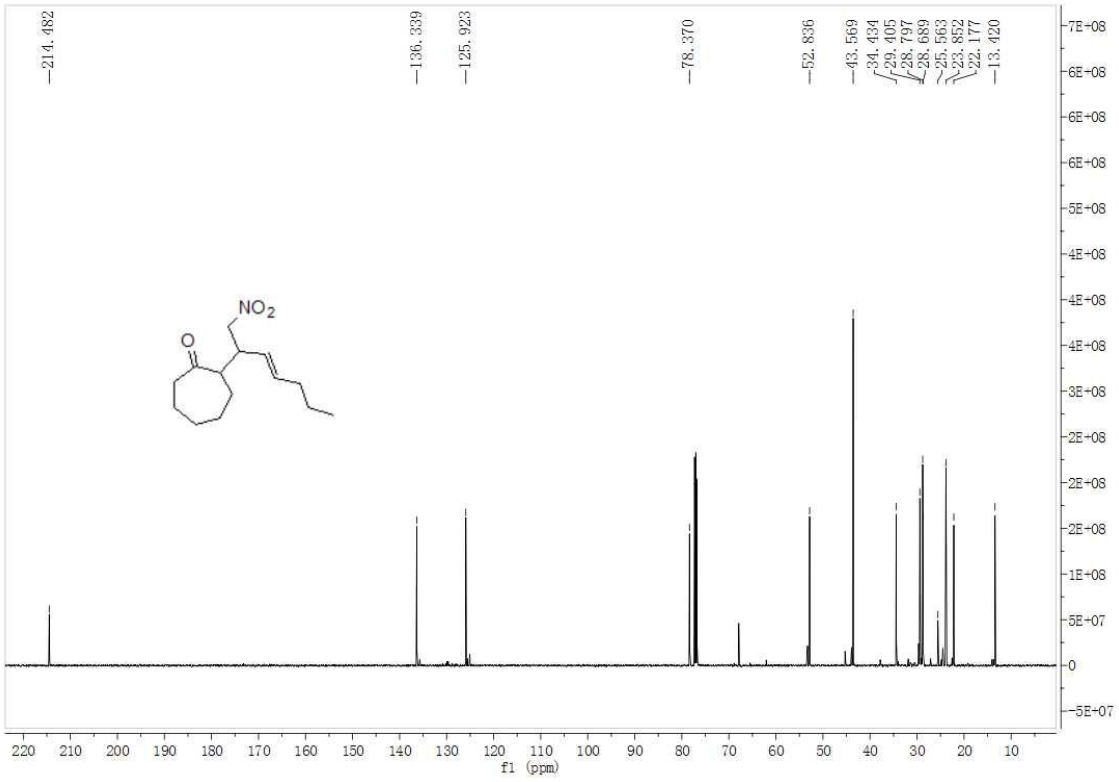
NO2
O
Br
f1 (ppm)

5j


NO2
O
f1 (ppm)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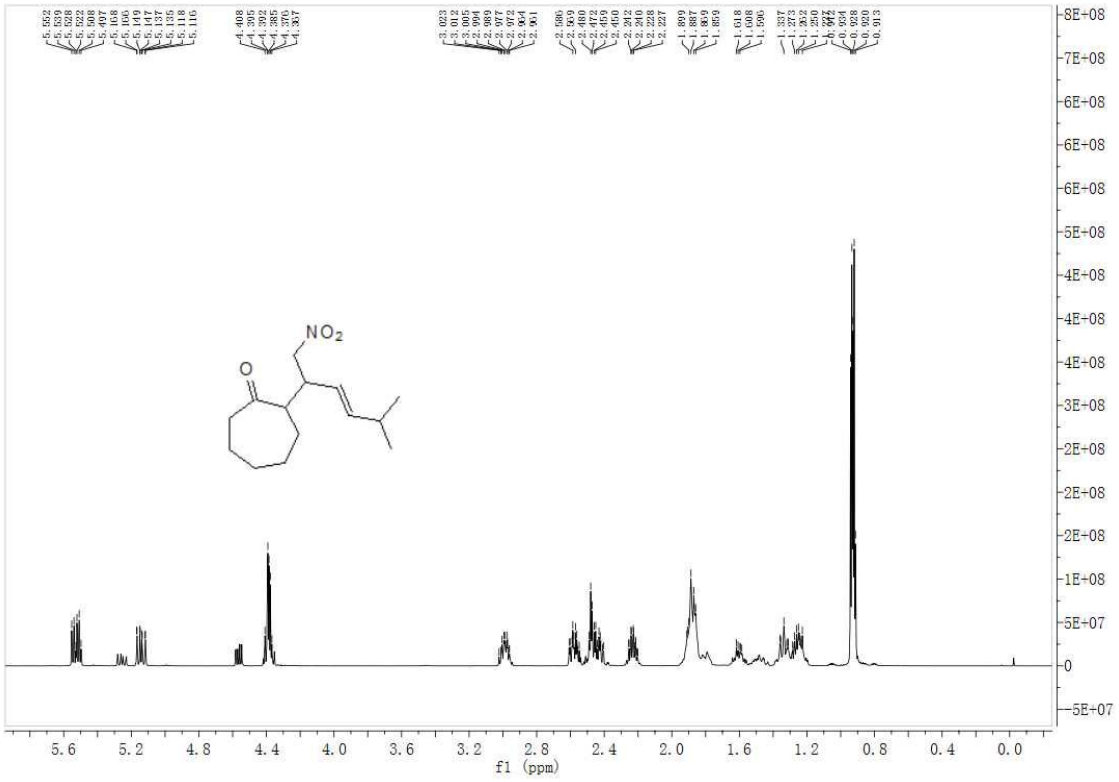
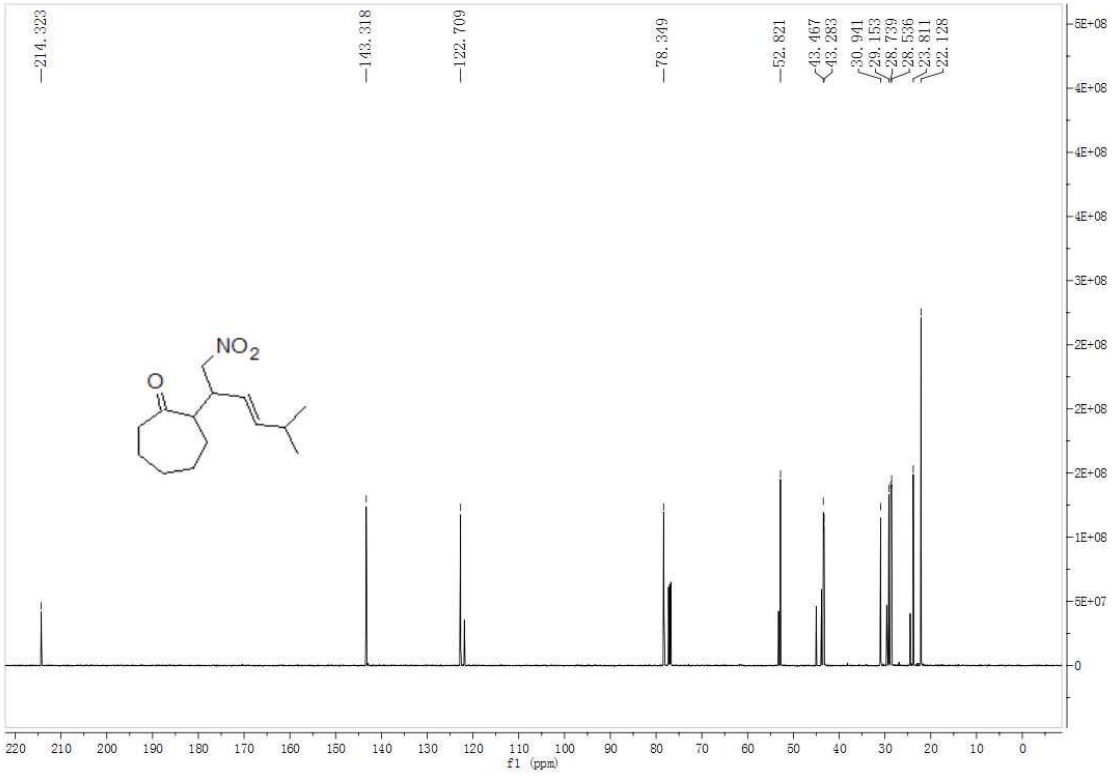
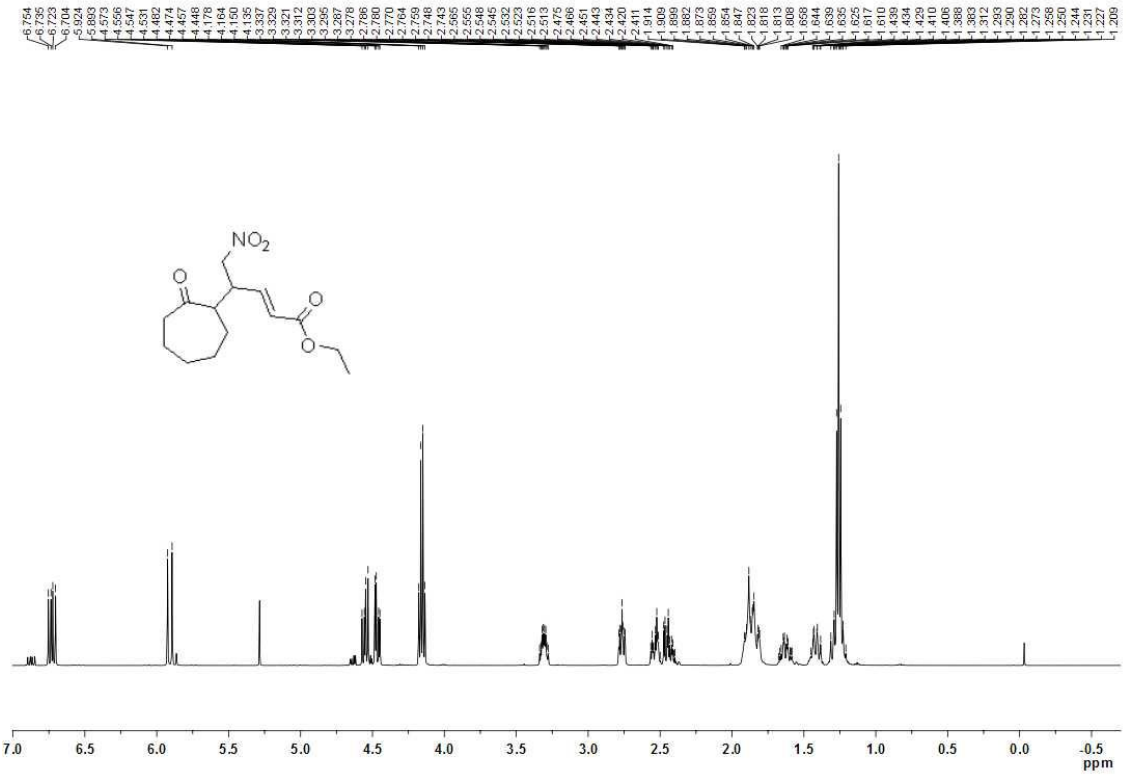
NO2
O
f1 (ppm)

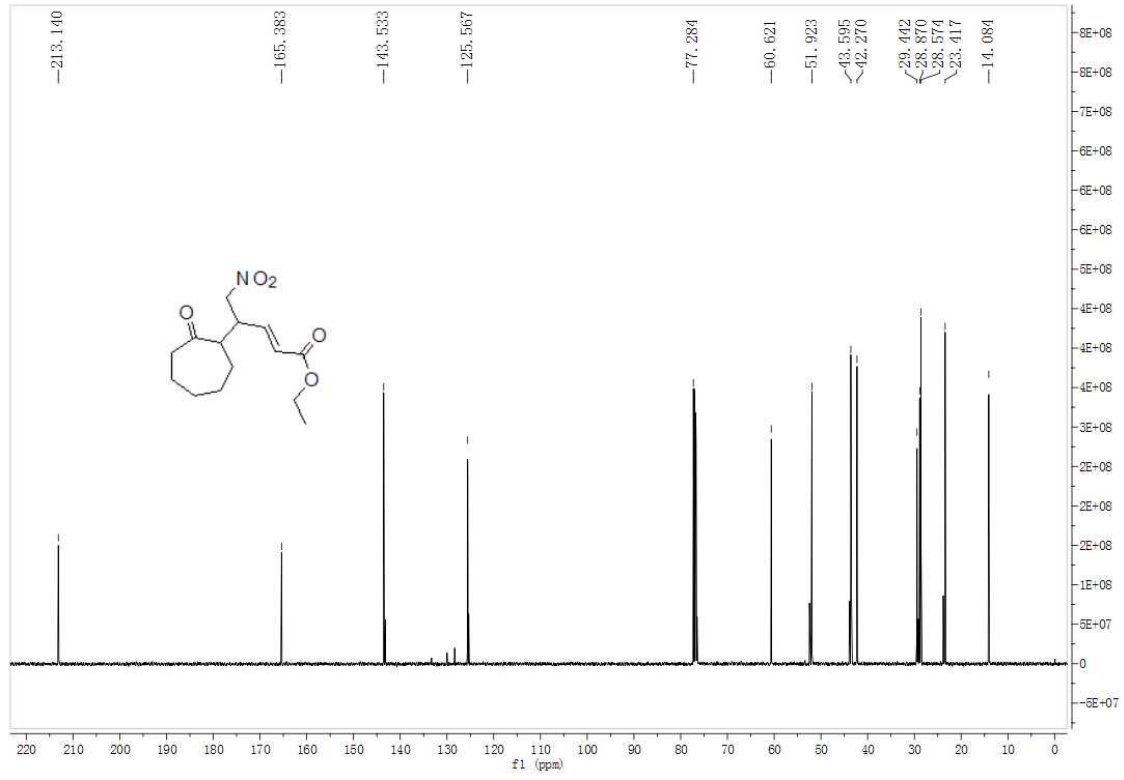
5k


NO2
O
f1 (ppm)

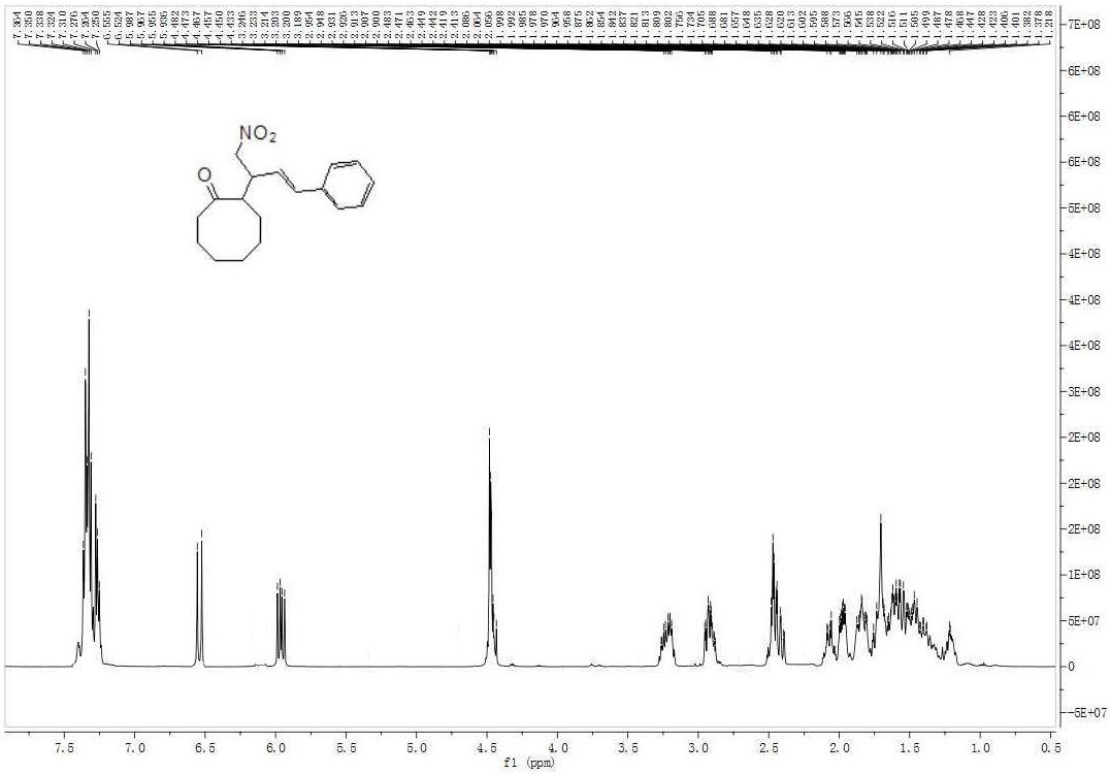

214.323
143.318
122.709
78.349
52.821
43.467
43.283
30.941
29.153
28.739
28.536
23.811
22.128
NO2
O
f1 (ppm)

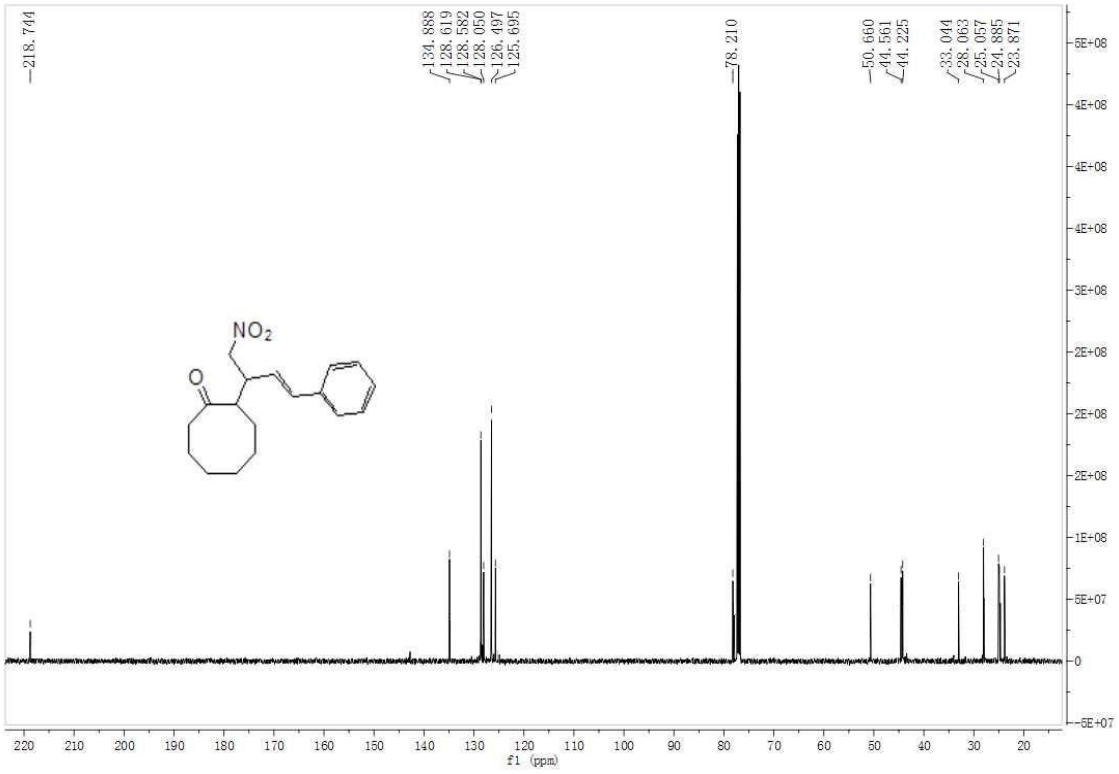
5l


6.754
6.735
6.723
6.704
5.924
5.893
4.573
4.556
4.547
4.531
4.462
4.447
4.437
4.178
4.164
4.150
4.135
3.337
3.329
3.321
3.312
3.303
3.295
3.287
3.278
2.786
2.780
2.770
2.764
2.759
2.748
2.743
2.595
2.565
2.548
2.545
2.532
2.523
2.516
2.513
2.475
2.466
2.451
2.443
2.434
2.420
2.411
1.914
1.909
1.889
1.882
1.873
1.859
1.854
1.847
1.823
1.818
1.813
1.808
1.658
1.644
1.639
1.635
1.625
1.617
1.610
1.439
1.434
1.429
1.410
1.406
1.388
1.383
1.312
1.293
1.290
1.282
1.273
1.258
1.250
1.244
1.231
1.227
1.209
NO2
O
O
O
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

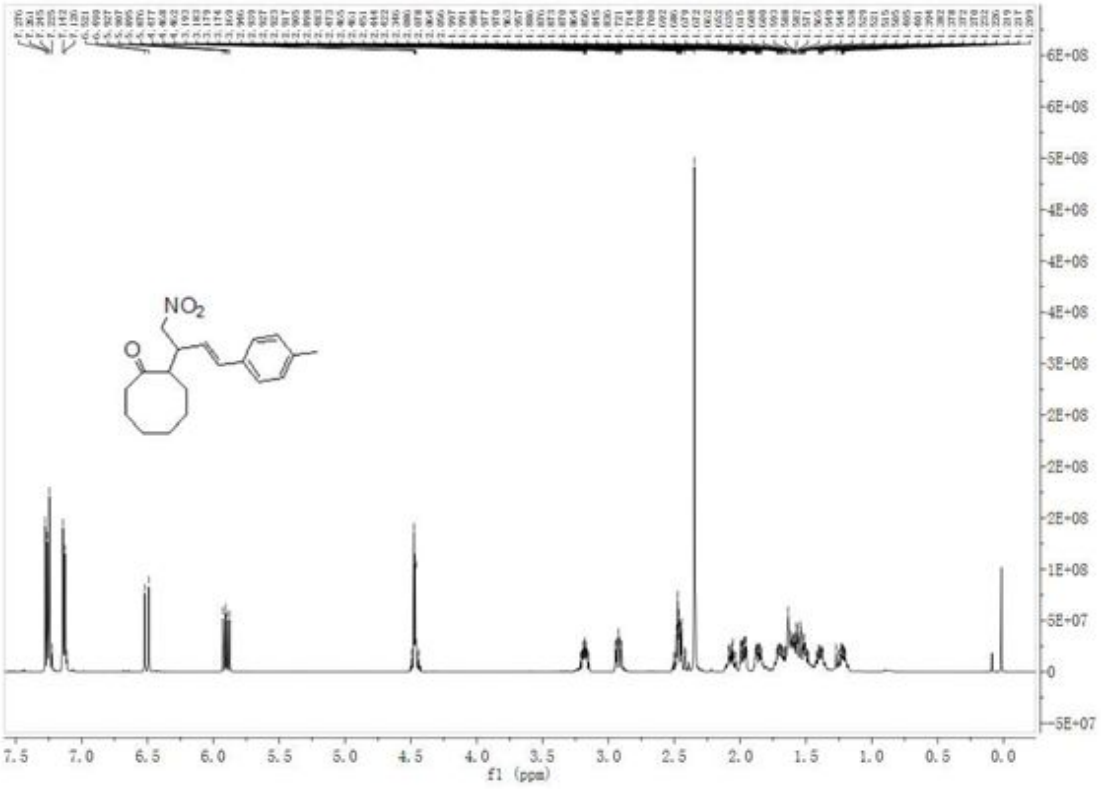

213.140
165.383
143.533
125.567
77.284
60.621
51.923
43.595
42.270
29.442
28.870
28.574
23.417
14.084
NO2
O
O
O
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

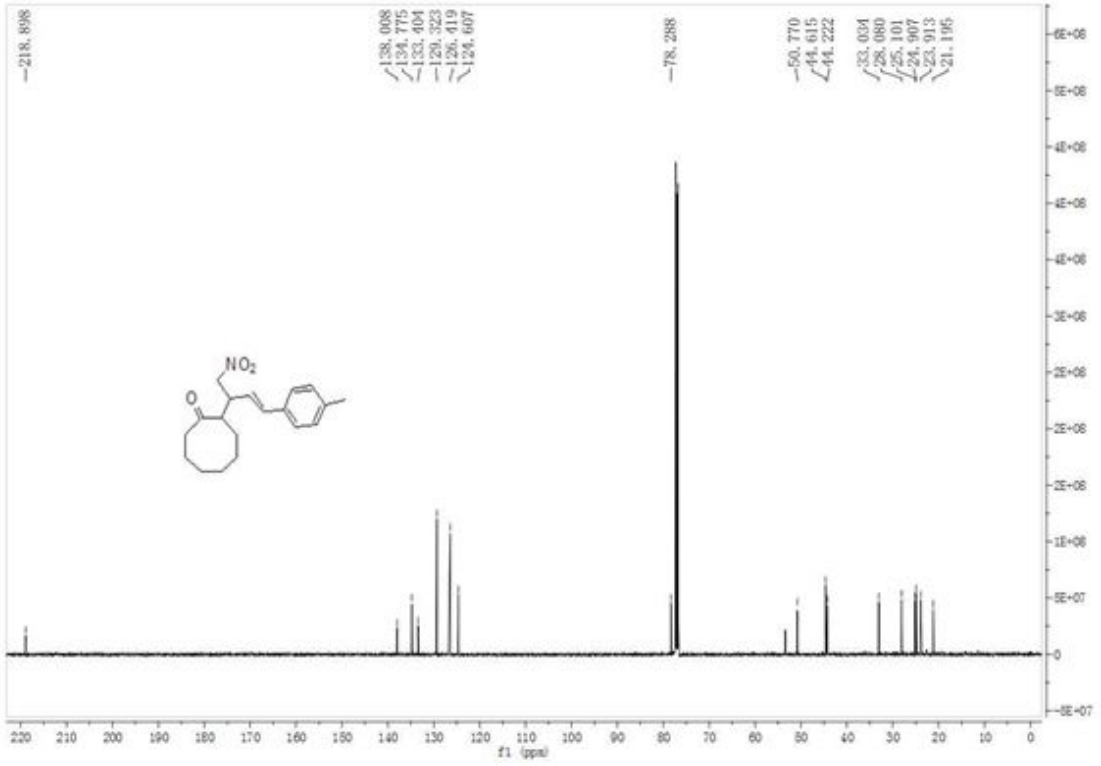
5m


NO2
O
f1 (ppm)

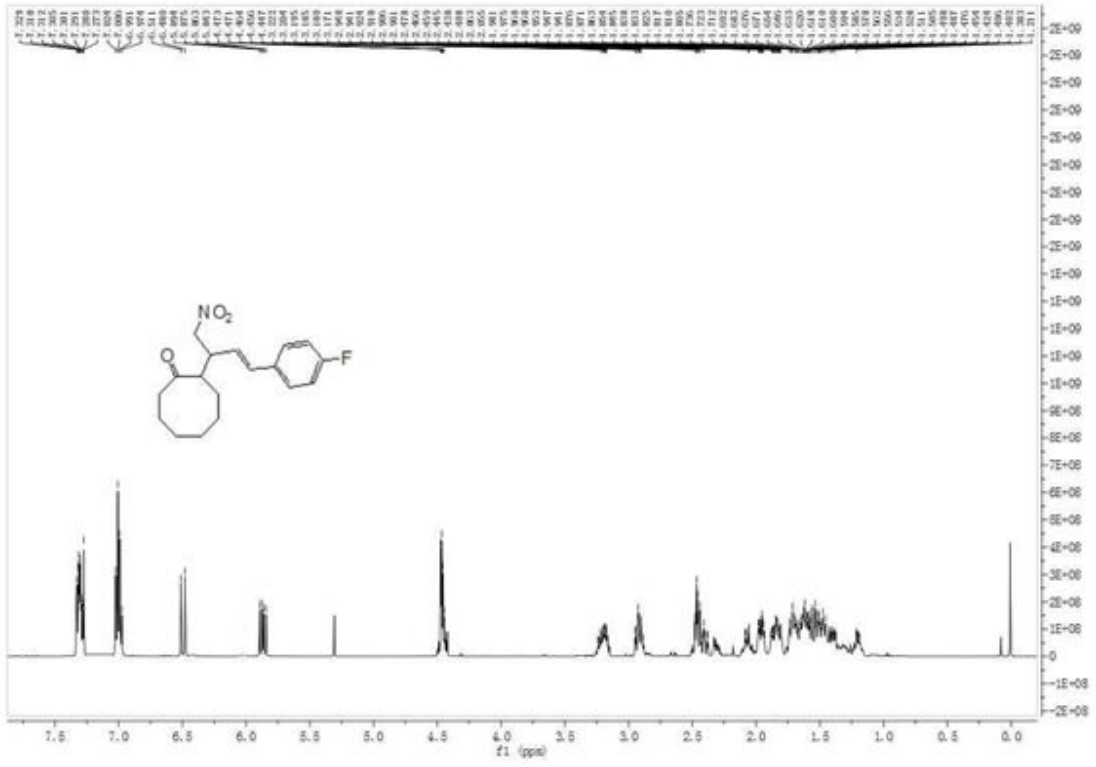

218.744
134.888
128.619
128.582
128.050
126.497
125.695
78.210
50.660
44.561
44.225
33.044
28.063
25.057
24.885
23.871
NO2
O
f1 (ppm)

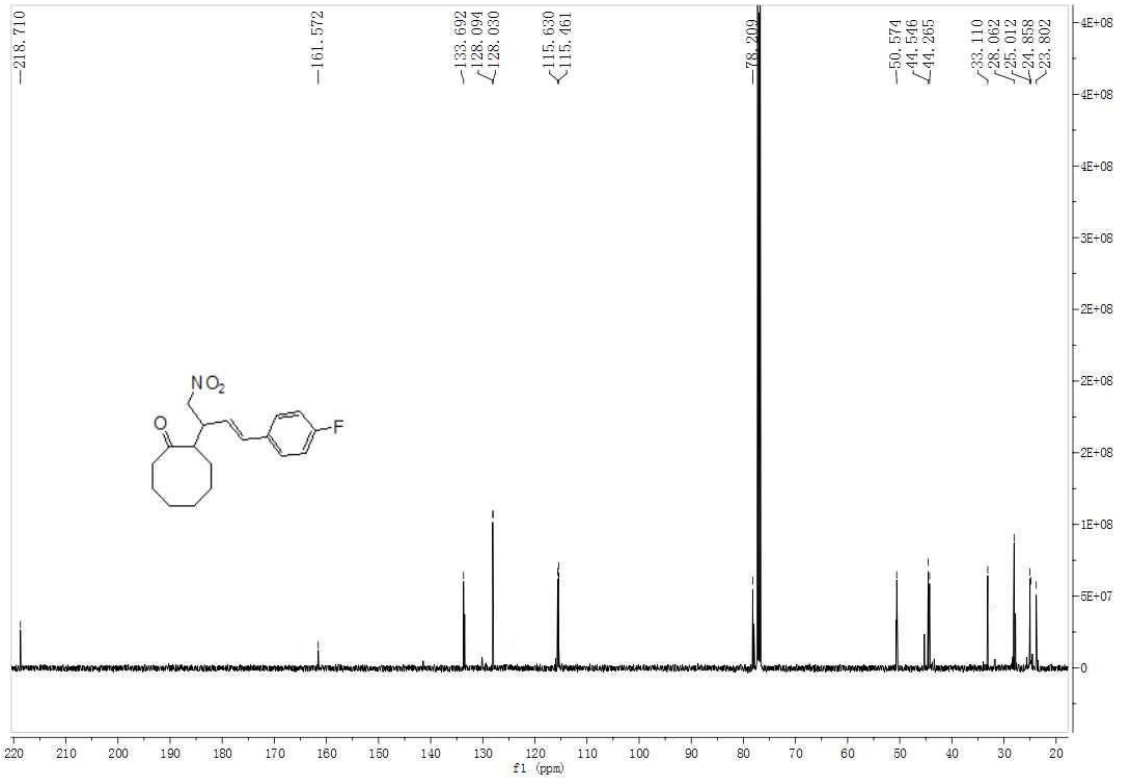
5n


NO2
O
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

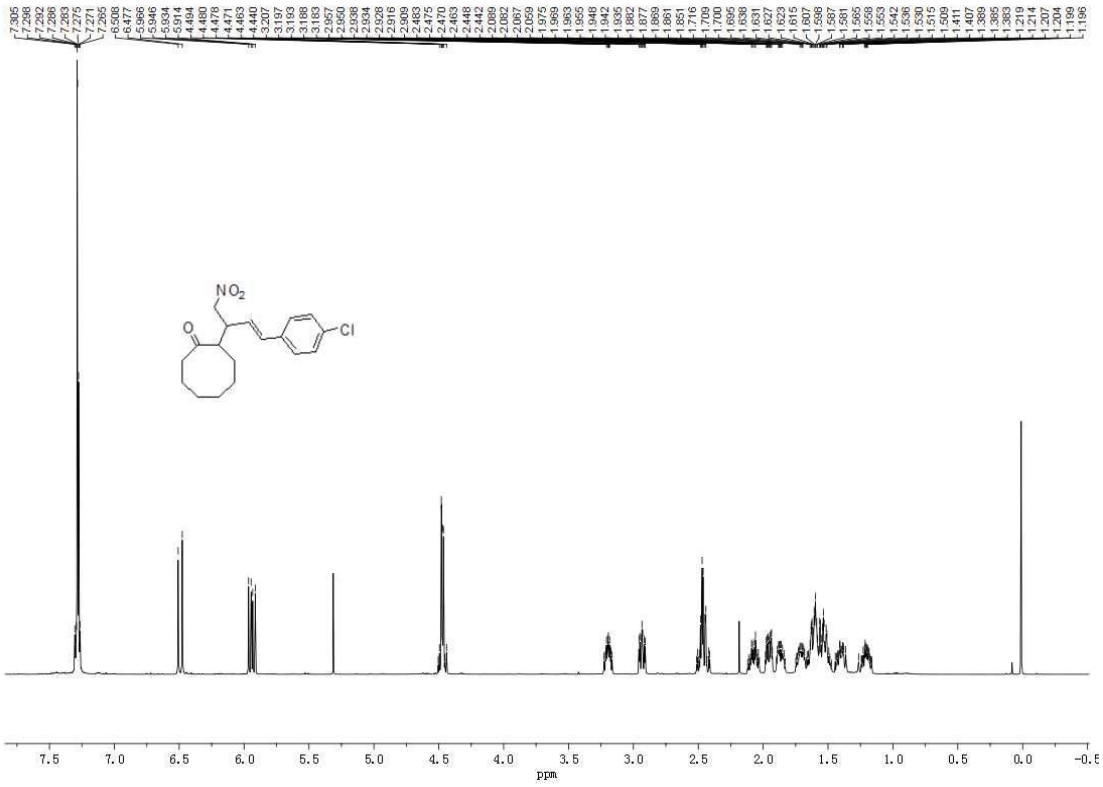

218.898
138.008
134.775
133.404
129.323
126.419
124.607
78.288
50.770
44.615
44.222
33.034
28.080
25.101
24.907
23.913
21.195
NO2
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

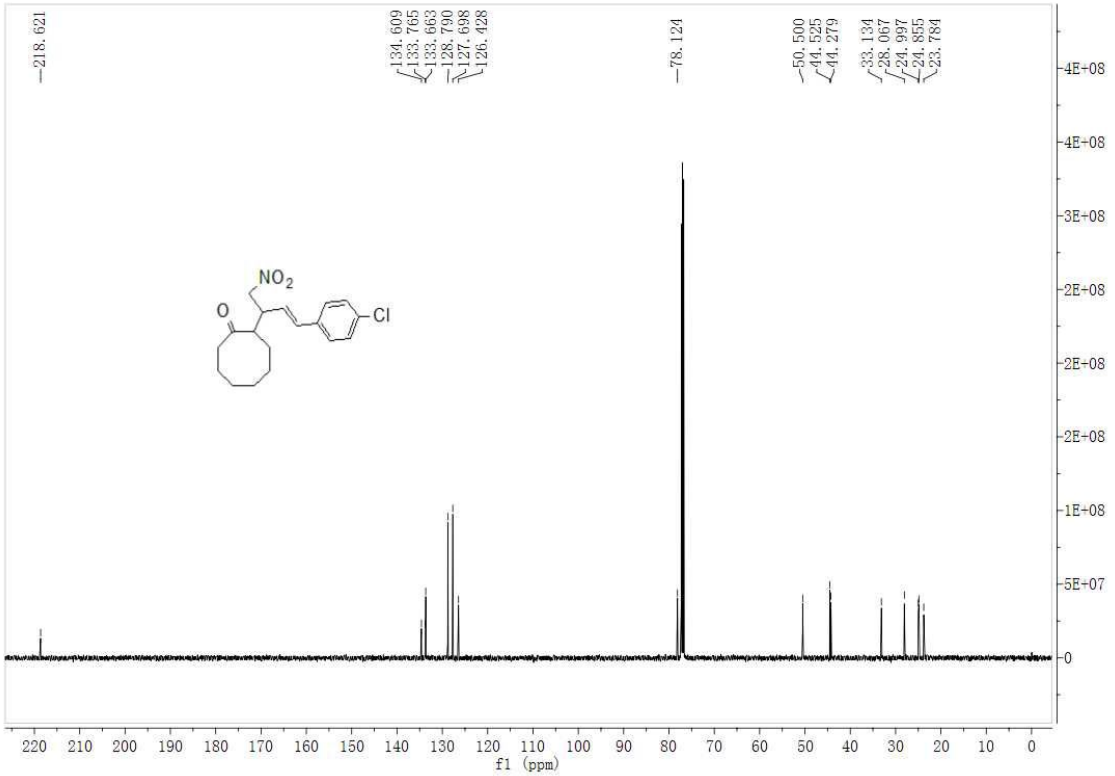
5o


NO2
O
F
f1 (ppm)

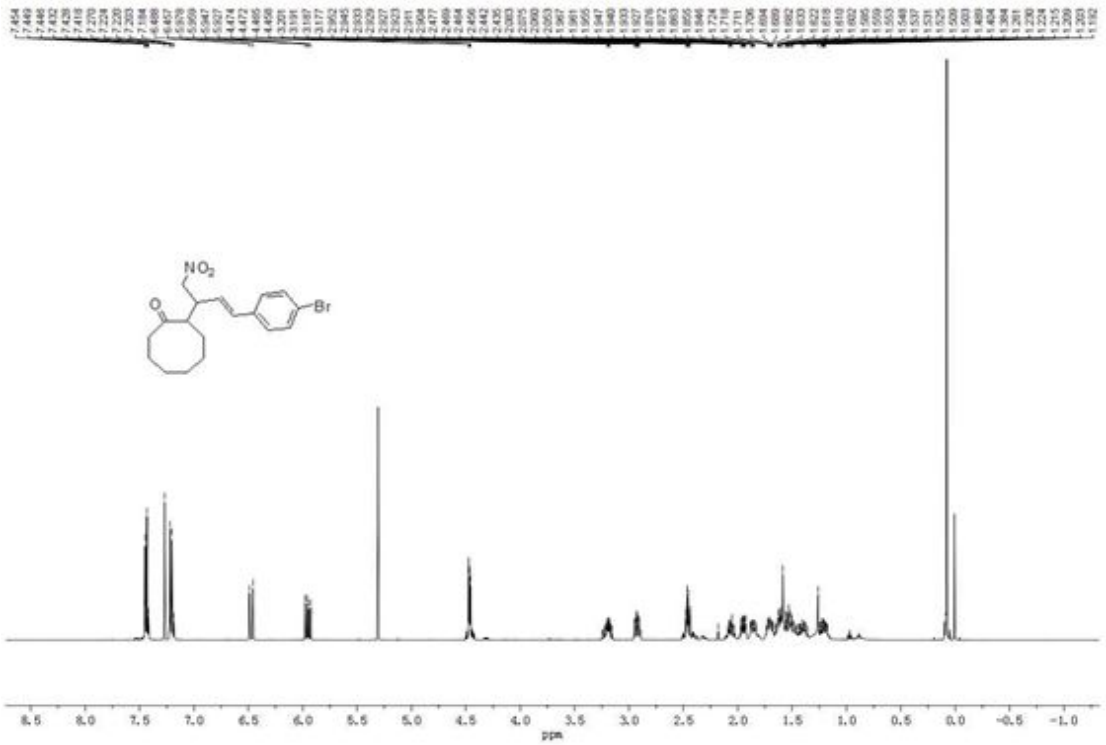

218.710
161.572
133.692
128.094
128.030
115.630
115.461
78.209
50.574
44.546
44.265
33.110
28.062
25.012
24.858
23.802
NO2
O
F
f1 (ppm)

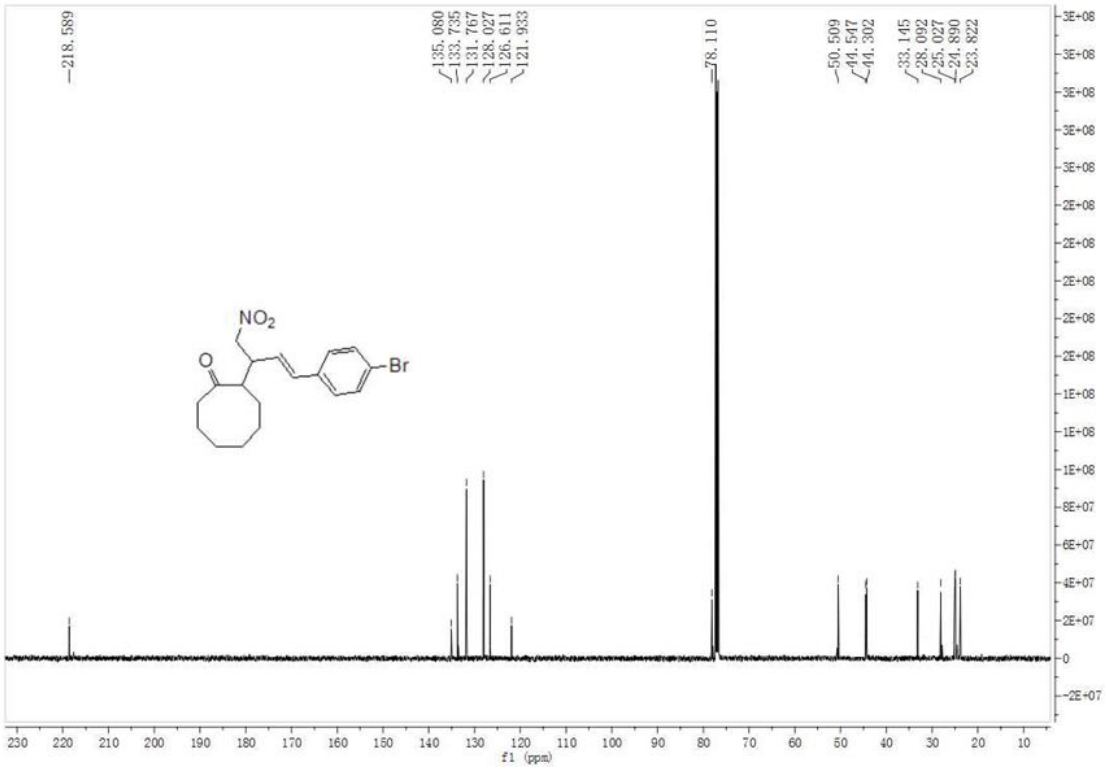
5p


NO2
O
Cl
ppm

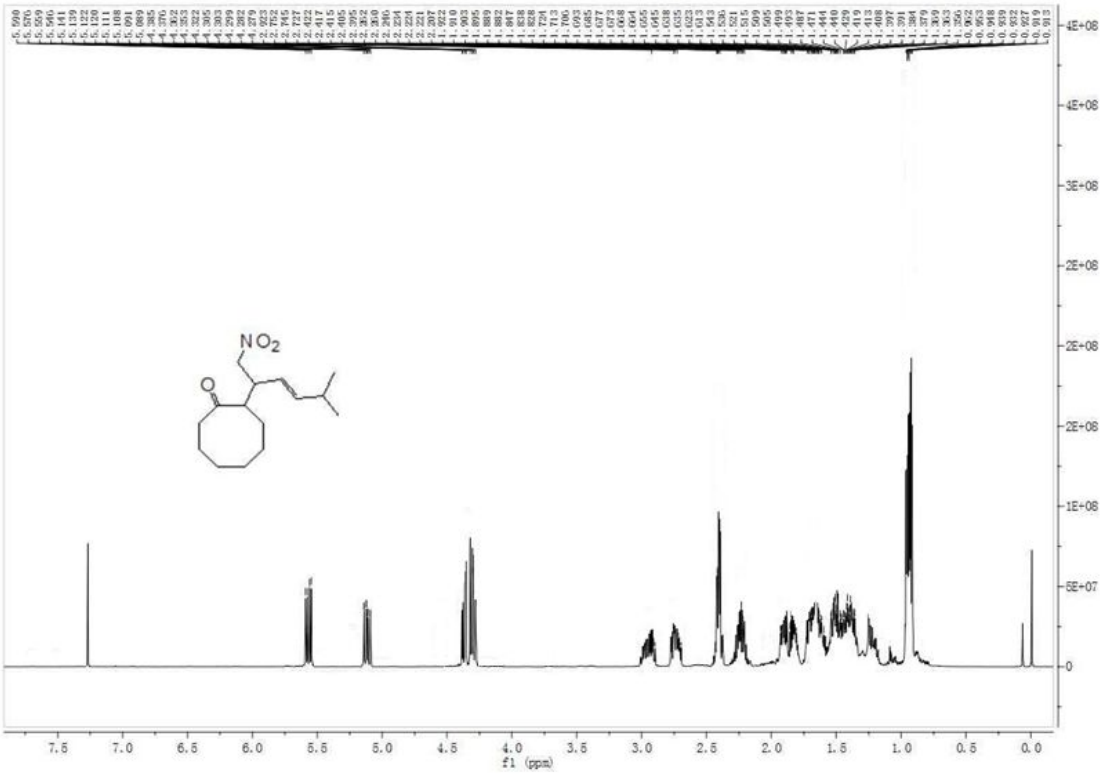

218.621
134.609
133.765
133.663
128.790
127.698
126.428
78.124
50.500
44.525
44.279
33.134
28.067
24.997
24.855
23.784
NO2
O
Cl
f1 (ppm)

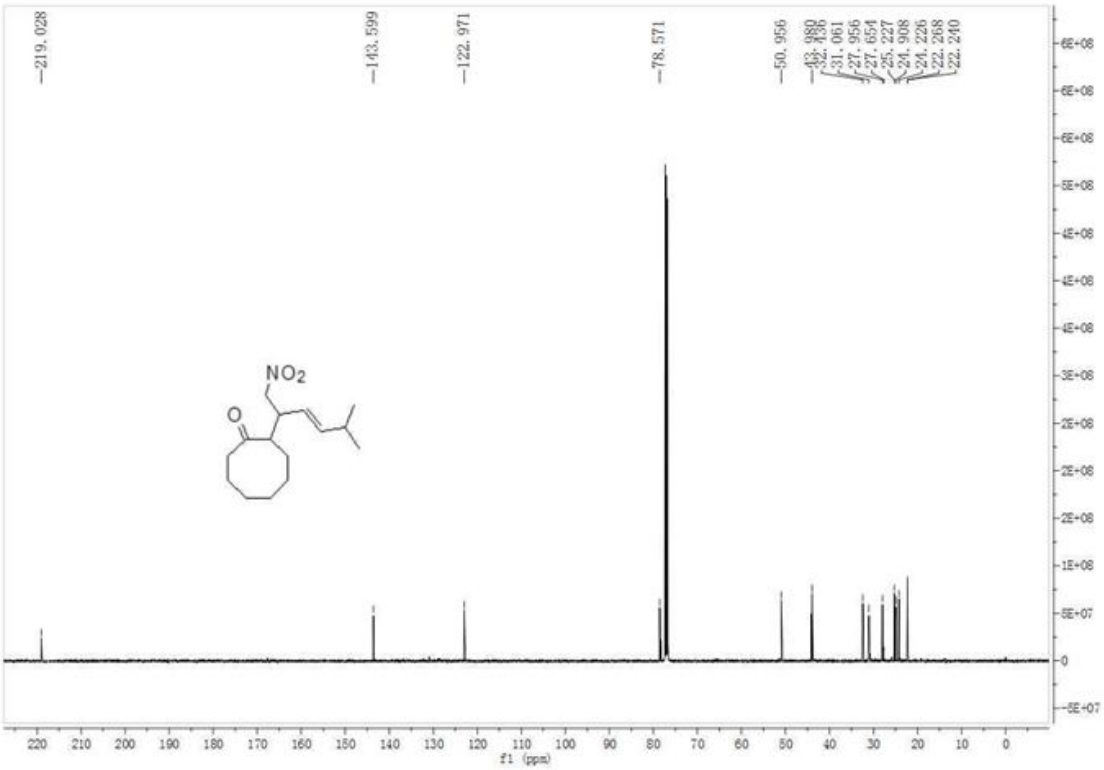
5q


NO2
O
Br
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
ppm

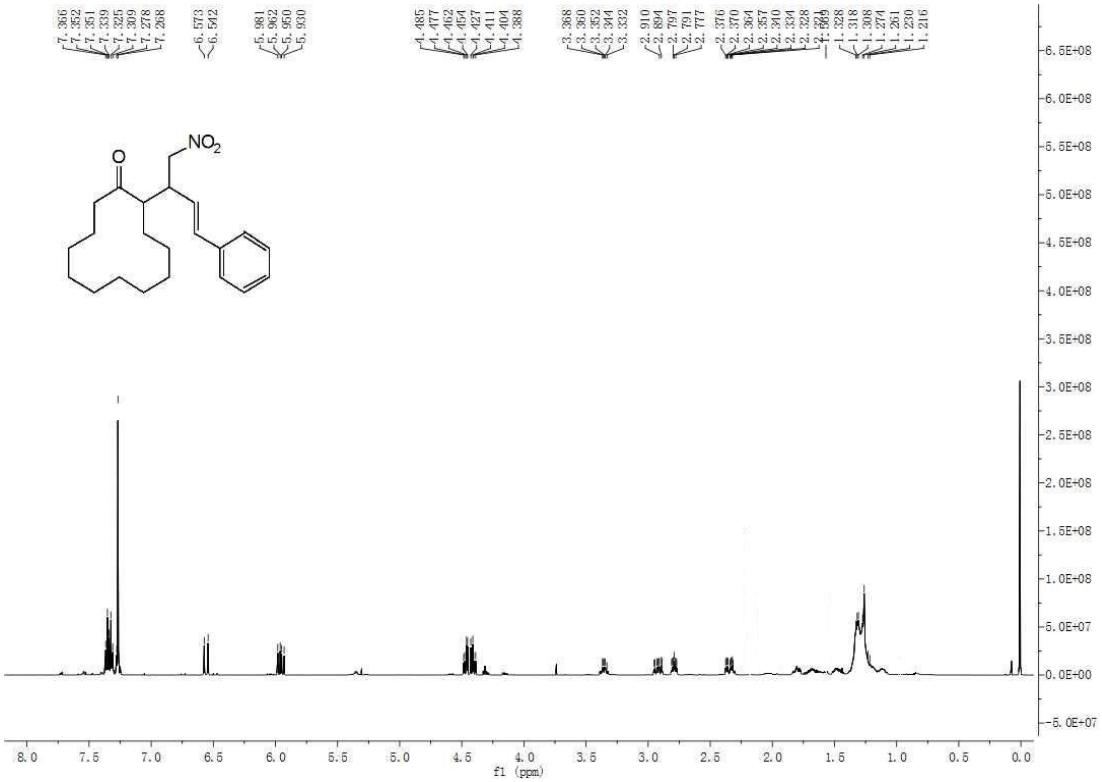

218.589
135.080
133.735
131.767
128.027
126.611
121.933
78.110
50.509
44.547
44.302
33.145
28.092
25.027
24.890
23.822
NO2
O
Br
f1 (ppm)

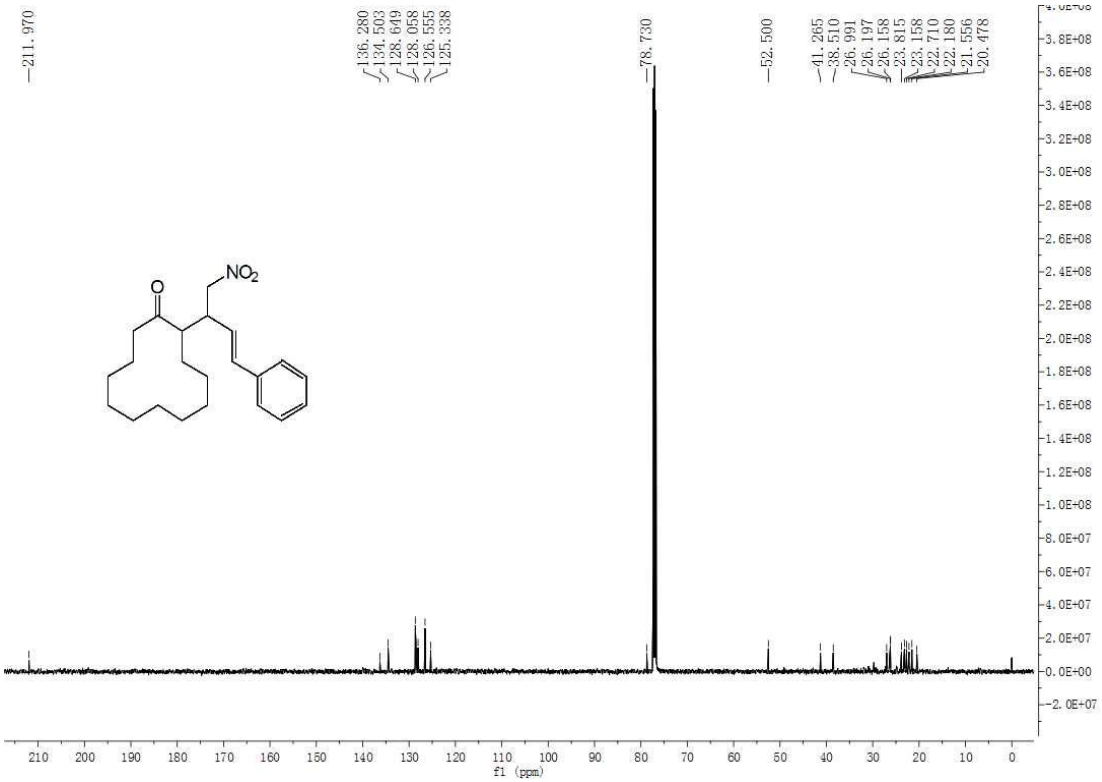
5r


NO2
O
f1 (ppm)

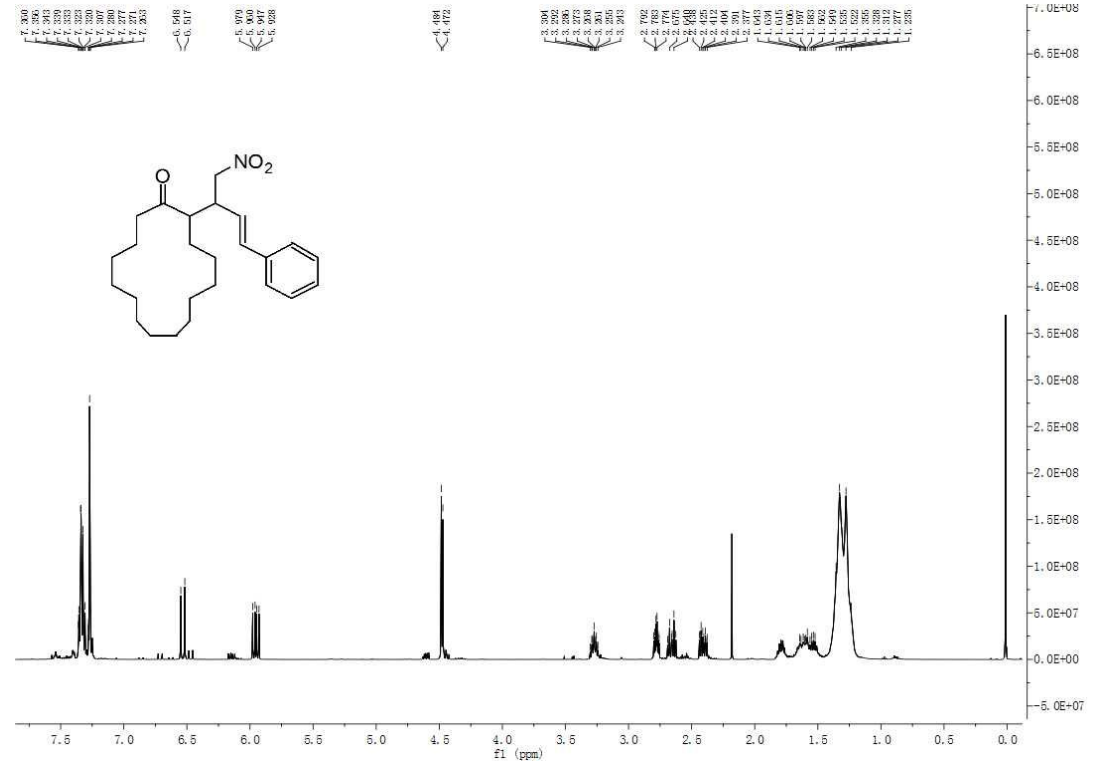

219.028
143.599
122.971
78.571
50.956
43.980
43.436
32.136
31.061
27.956
27.654
25.227
24.908
24.226
22.268
22.240
NO2
O
f1 (ppm)

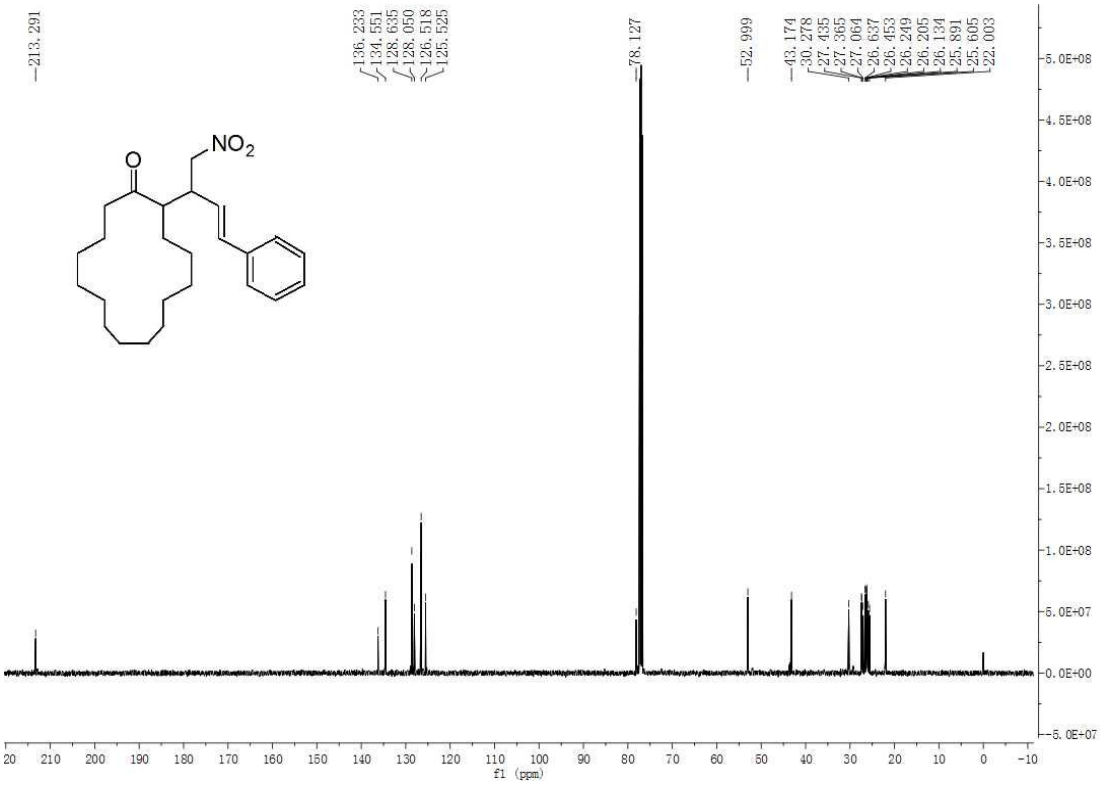
5s


7.366
7.352
7.351
7.339
7.325
7.309
7.278
7.268
6.573
6.542
5.981
5.962
5.950
5.930
4.485
4.477
4.462
4.454
4.427
4.411
4.404
4.388
3.368
3.360
3.352
3.344
3.332
2.910
2.894
2.797
2.791
2.777
2.376
2.370
2.364
2.357
2.340
2.334
2.328
1.328
1.318
1.308
1.274
1.261
1.230
1.215
O
NO2
f1 (ppm)

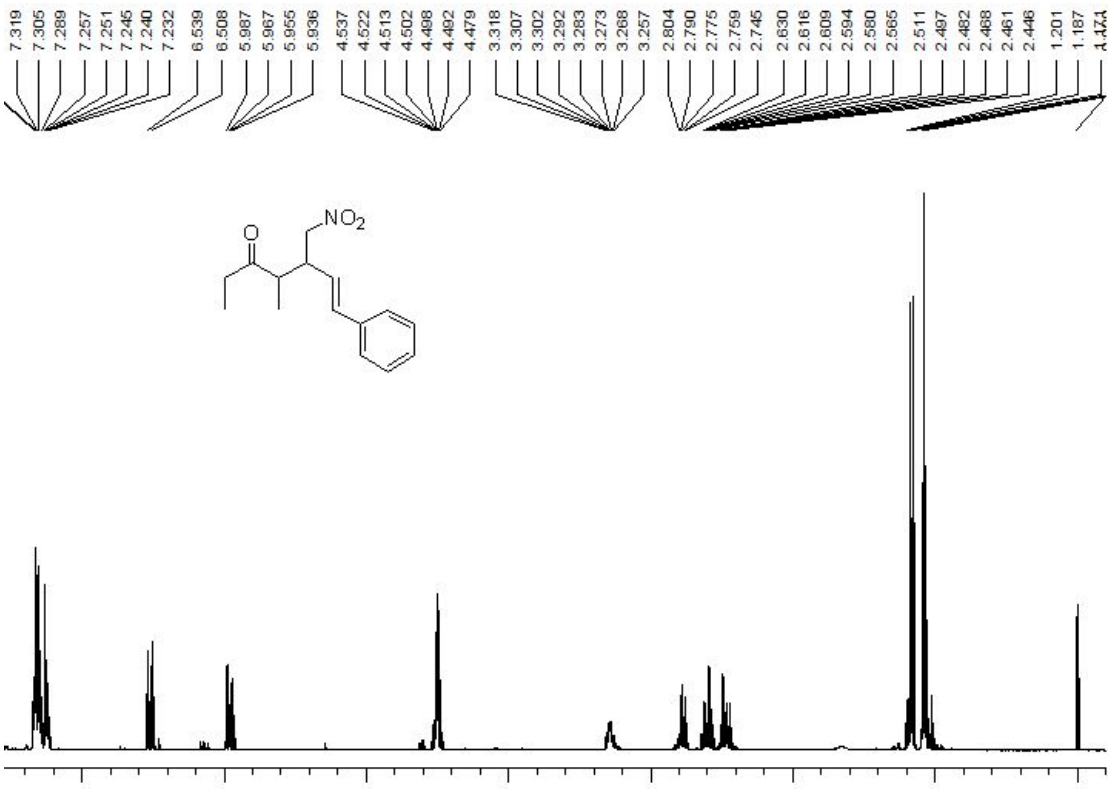

211.970
136.280
134.503
128.649
128.058
126.555
125.338
78.730
52.500
41.265
38.510
26.991
26.197
26.158
23.815
23.158
22.710
22.180
21.556
20.478
O
NO2
f1 (ppm)

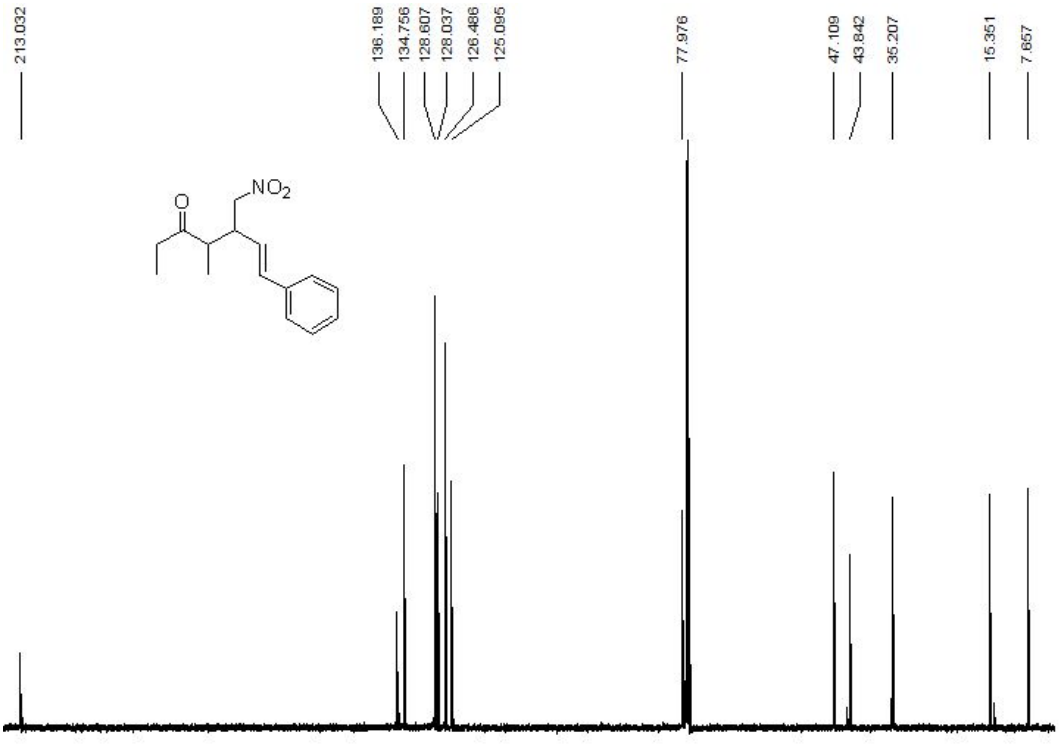
5t


NO2
O
f1 (ppm)

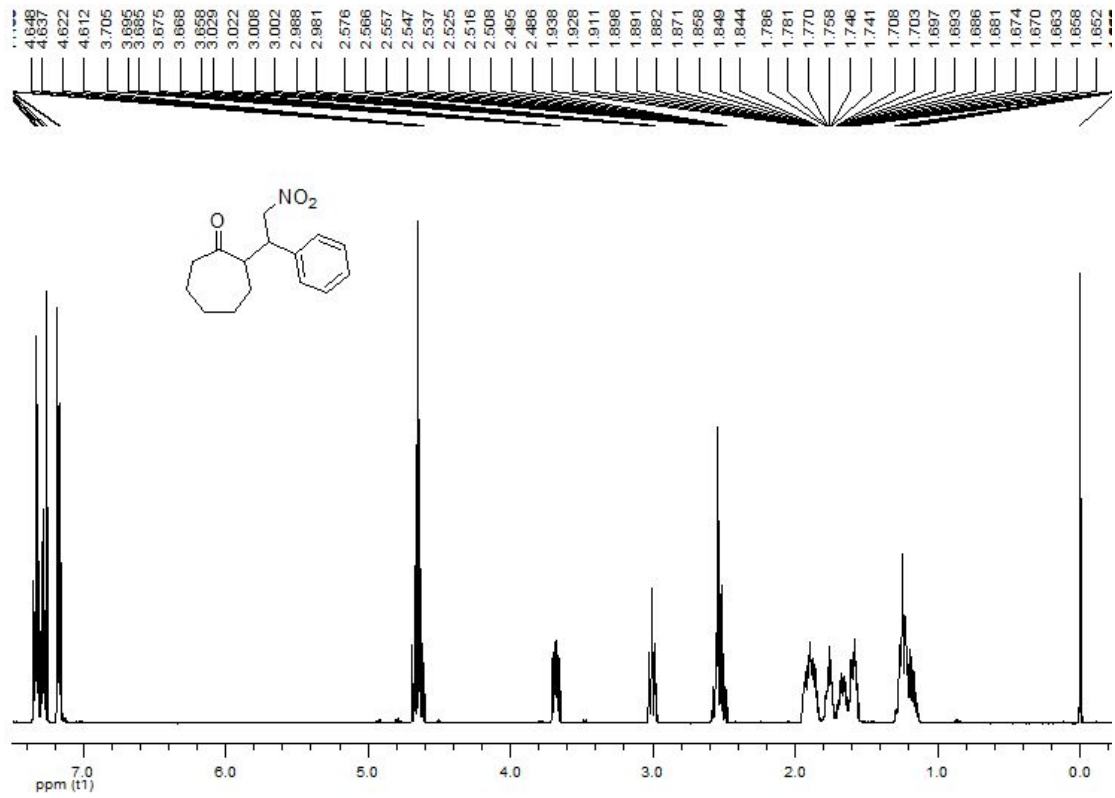

213.291
136.233
134.551
128.635
128.050
126.518
125.525
78.127
52.999
43.174
30.278
27.435
27.365
27.064
26.637
26.453
26.249
26.205
26.134
25.891
25.605
22.003
NO2
O
f1 (ppm)

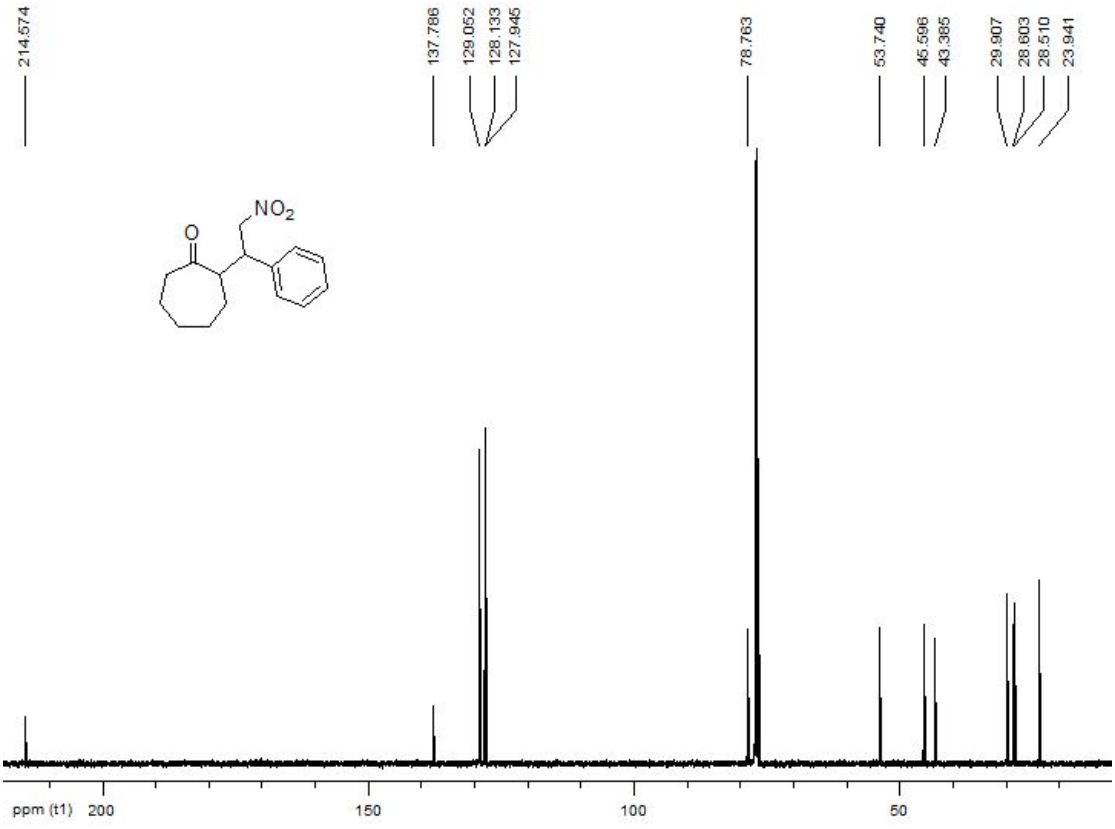
5u


7.319
7.305
7.289
7.257
7.251
7.245
7.240
7.232
6.539
6.508
5.987
5.967
5.955
5.936
4.537
4.522
4.513
4.502
4.498
4.492
4.479
3.318
3.307
3.302
3.292
3.283
3.273
3.268
3.257
2.804
2.790
2.775
2.759
2.745
2.630
2.616
2.609
2.594
2.580
2.565
2.511
2.497
2.482
2.468
2.461
2.446
1.201
1.187
O
NO2

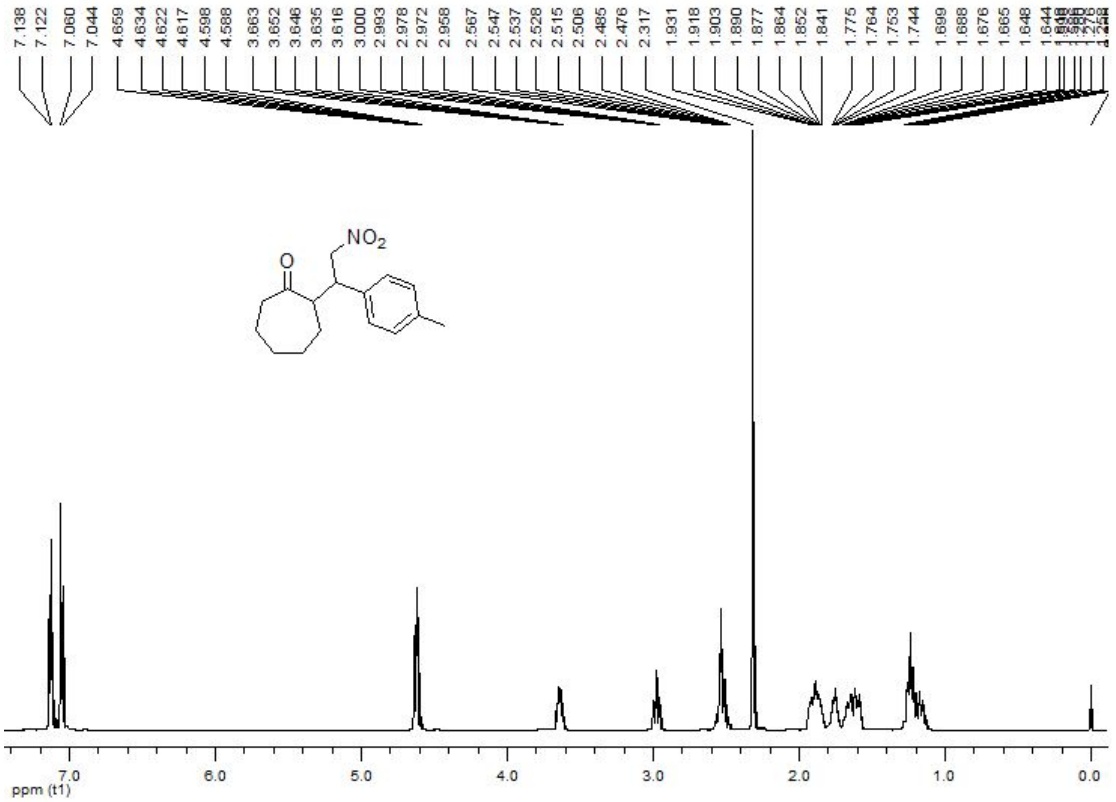

213.032
136.189
134.756
128.607
128.037
126.486
125.095
77.976
47.109
43.842
35.207
15.351
7.657
O
NO2

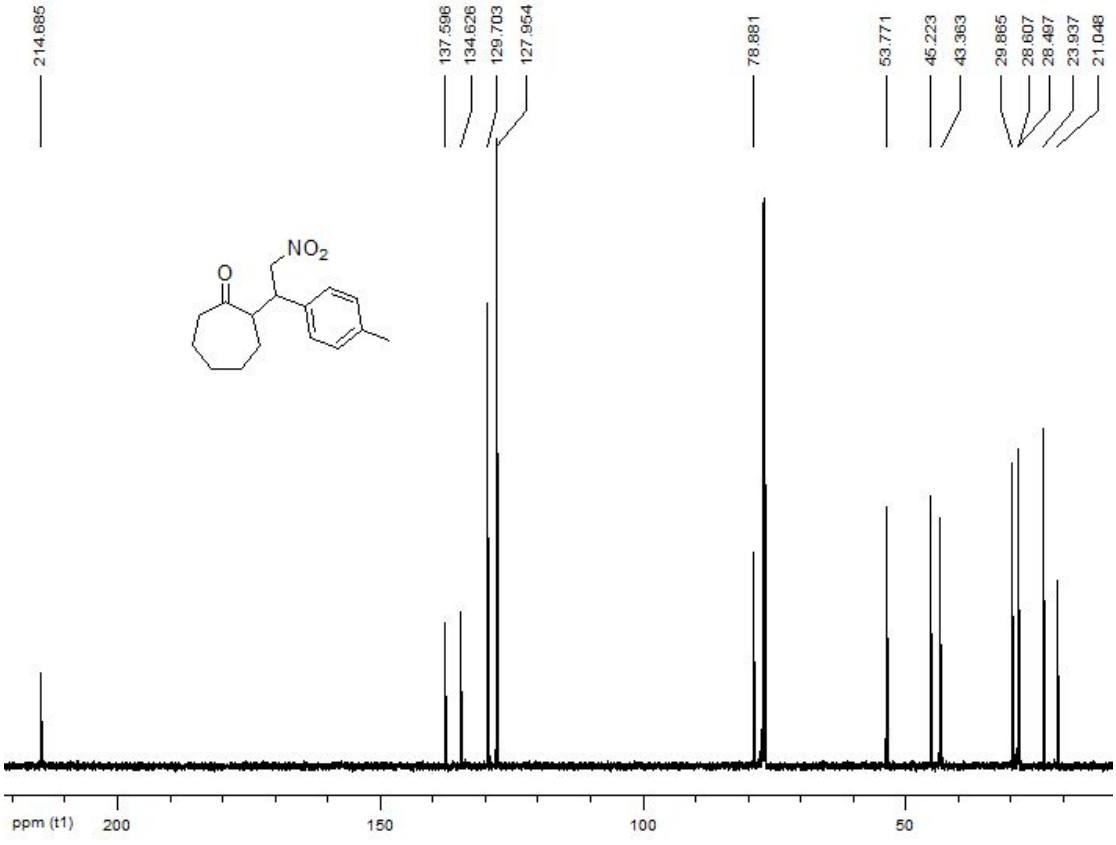
7a


4.648
4.637
4.622
4.612
3.705
3.695
3.685
3.675
3.668
3.658
3.029
3.022
3.008
3.002
2.988
2.981
2.576
2.566
2.557
2.547
2.537
2.525
2.516
2.508
2.495
2.486
1.938
1.928
1.911
1.898
1.891
1.882
1.871
1.858
1.849
1.844
1.786
1.781
1.770
1.758
1.746
1.741
1.708
1.703
1.697
1.693
1.686
1.681
1.674
1.670
1.663
1.658
1.652
NO2
O
7.0
ppm (t1)
6.0
5.0
4.0
3.0
2.0
1.0
0.0

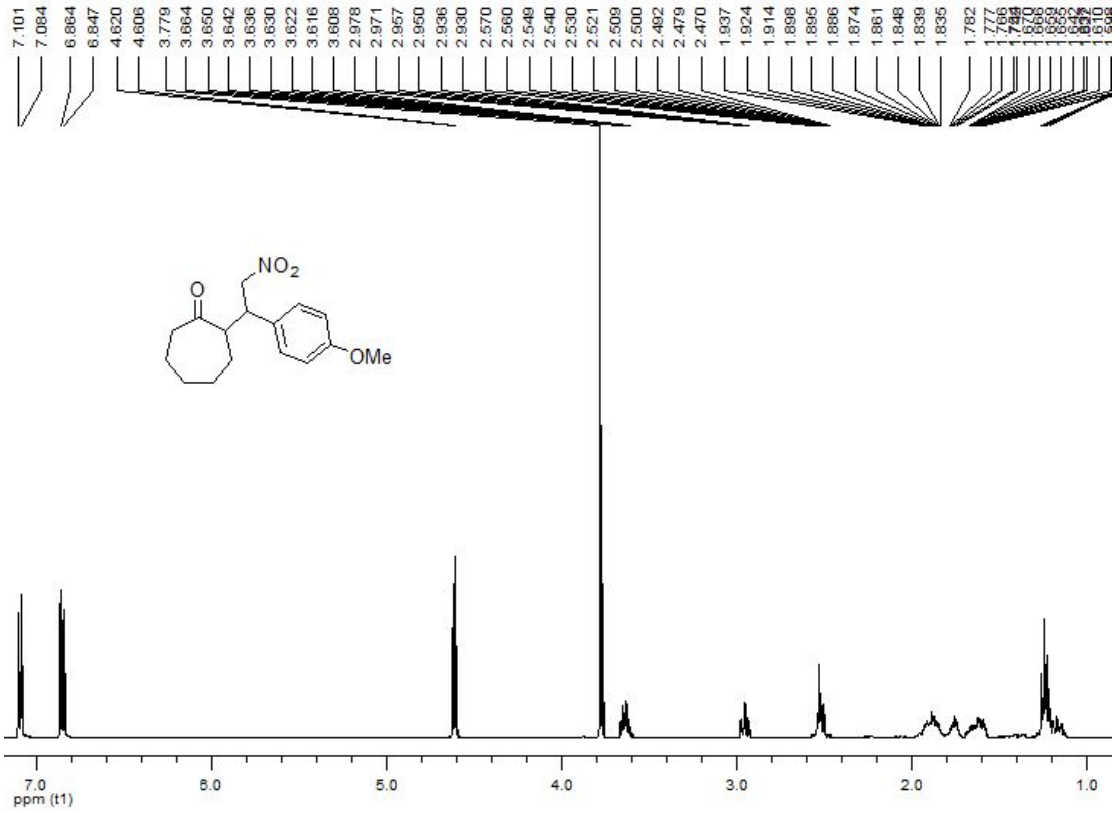

214.574
137.786
129.052
128.133
127.945
78.763
53.740
45.596
43.385
29.907
28.603
28.510
23.941
NO2
O
ppm (t1)
200
150
100
50

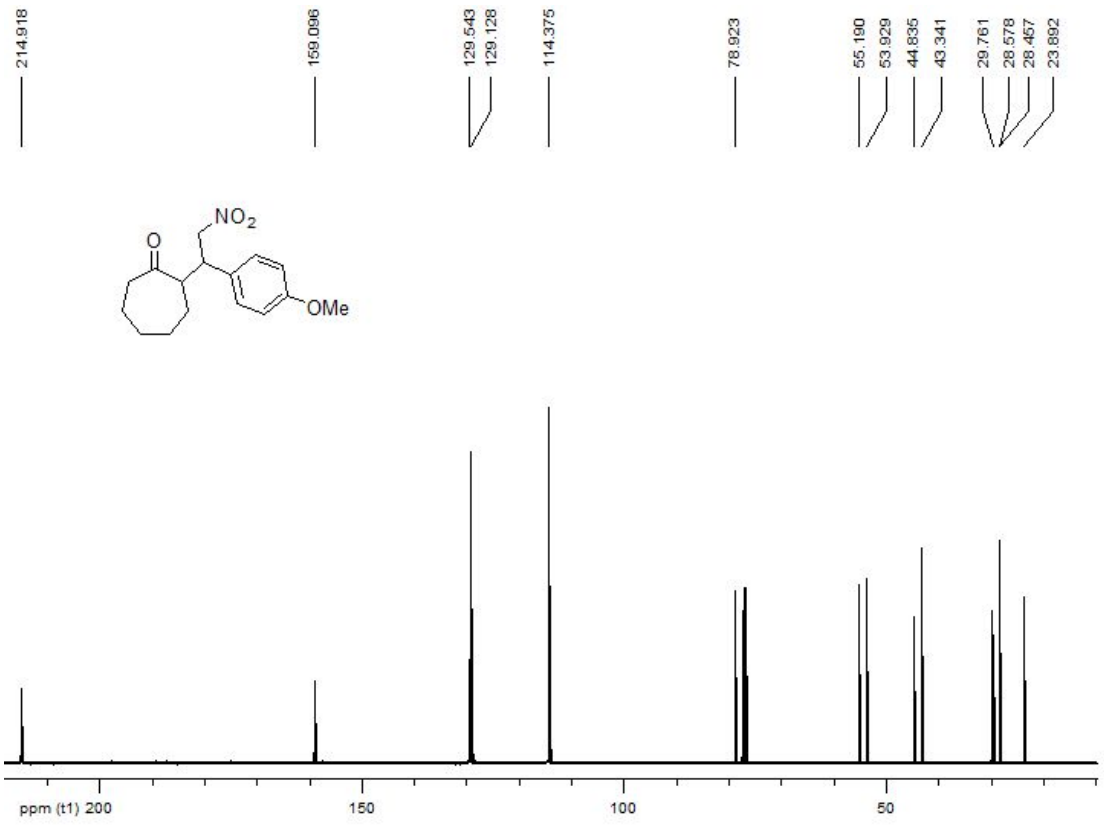
7b


7.138
7.122
7.060
7.044
4.659
4.634
4.622
4.617
4.598
4.588
3.663
3.652
3.646
3.635
3.616
3.000
2.993
2.978
2.972
2.958
2.567
2.547
2.537
2.528
2.515
2.506
2.485
2.476
2.317
1.931
1.918
1.903
1.890
1.877
1.864
1.852
1.841
1.775
1.764
1.753
1.744
1.699
1.688
1.676
1.665
1.648
1.644
NO2
O
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

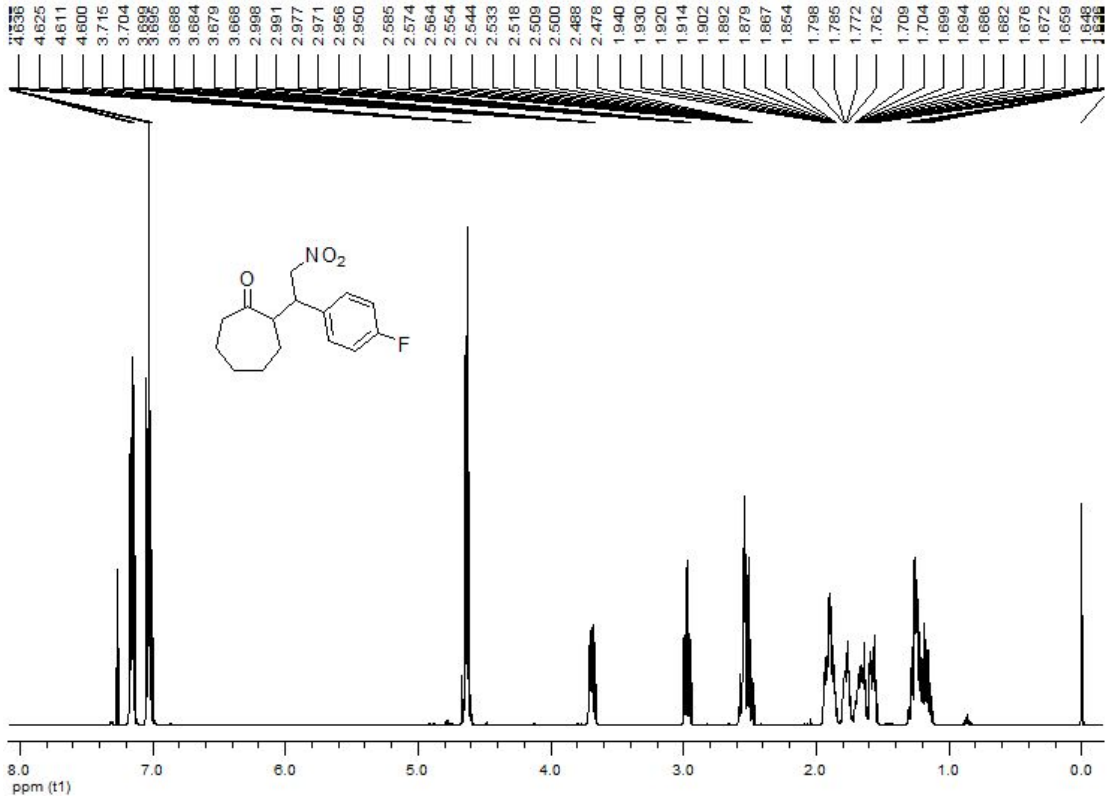

214.685
137.596
134.626
129.703
127.954
78.881
53.771
45.223
43.363
29.865
28.607
28.497
23.937
21.048
NO2
O
ppm (t1)
200
150
100
50

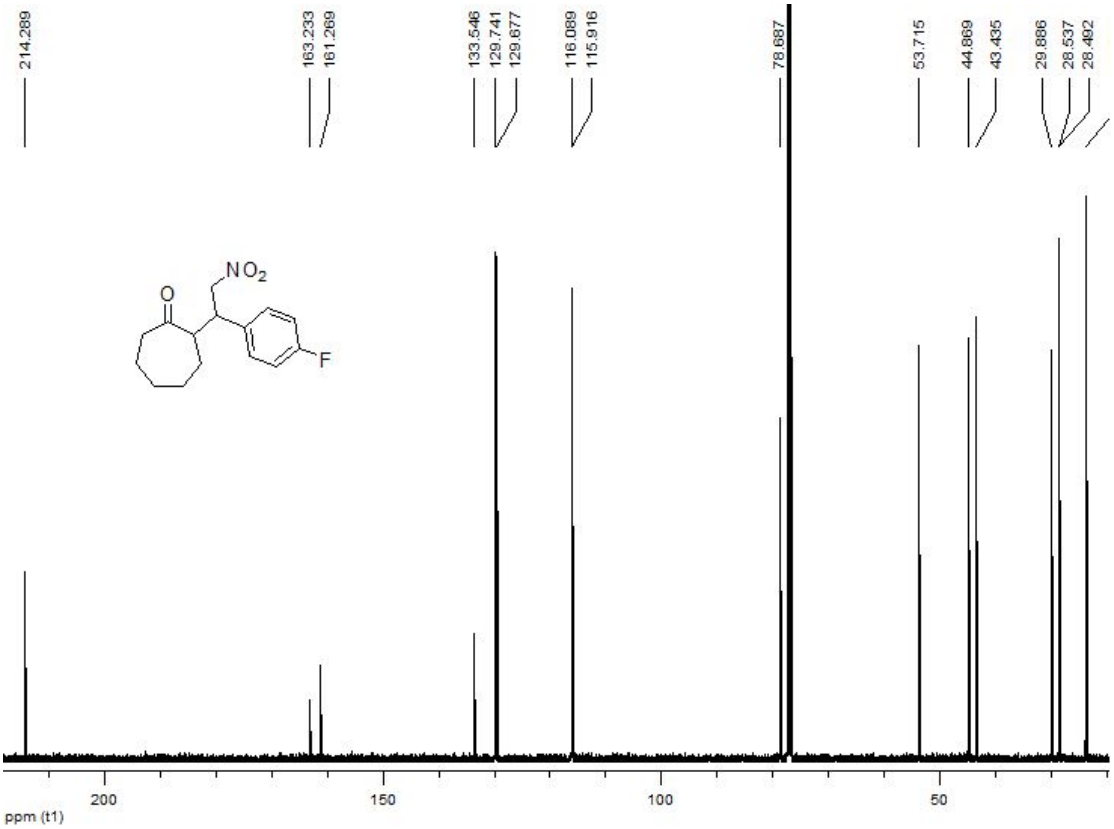
7c


7.101
7.084
6.864
6.847
4.620
4.606
3.779
3.664
3.650
3.642
3.636
3.630
3.622
3.616
3.608
2.978
2.971
2.957
2.950
2.936
2.930
2.570
2.560
2.549
2.540
2.530
2.521
2.509
2.500
2.492
2.479
2.470
1.937
1.924
1.914
1.898
1.895
1.886
1.874
1.861
1.848
1.839
1.835
1.782
1.777
1.766
O
NO2
OMe
7.0
ppm (t1)
6.0
5.0
4.0
3.0
2.0
1.0

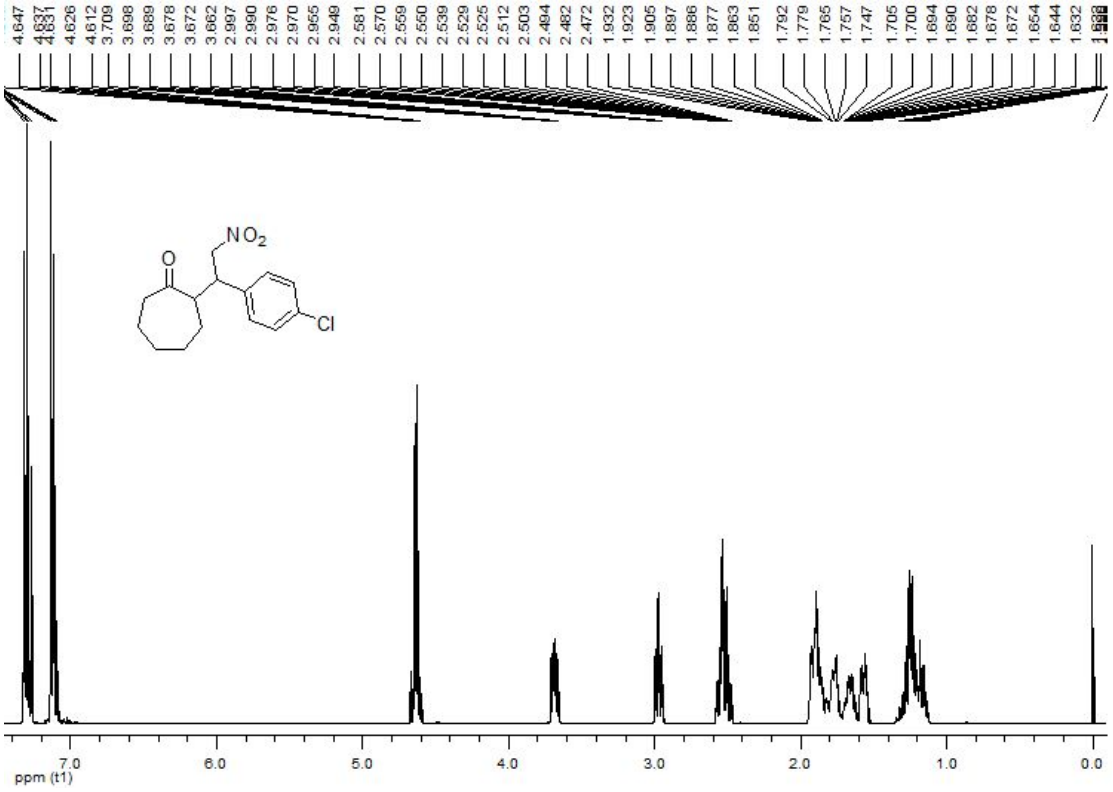

214.918
159.096
129.543
129.128
114.375
78.923
55.190
53.929
44.835
43.341
29.761
28.578
28.457
23.892
O
NO2
OMe
ppm (t1) 200
150
100
50

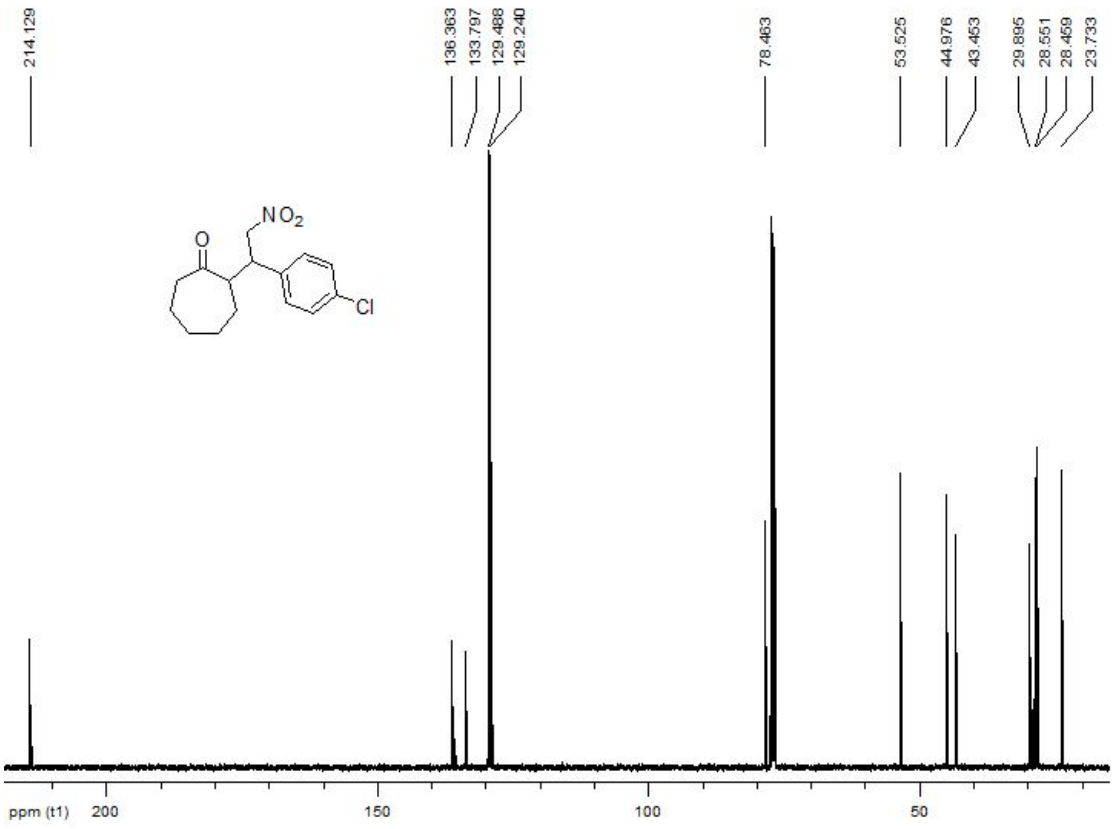
7d


4.636
4.625
4.611
4.600
3.715
3.704
3.688
3.684
3.679
3.668
2.998
2.991
2.977
2.971
2.956
2.950
2.585
2.574
2.564
2.554
2.544
2.533
2.518
2.509
2.500
2.488
2.478
1.940
1.930
1.920
1.914
1.902
1.892
1.879
1.867
1.854
1.798
1.785
1.772
1.762
1.709
1.704
1.699
1.694
1.686
1.682
1.676
1.672
1.659
1.648
NO2
O
F
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

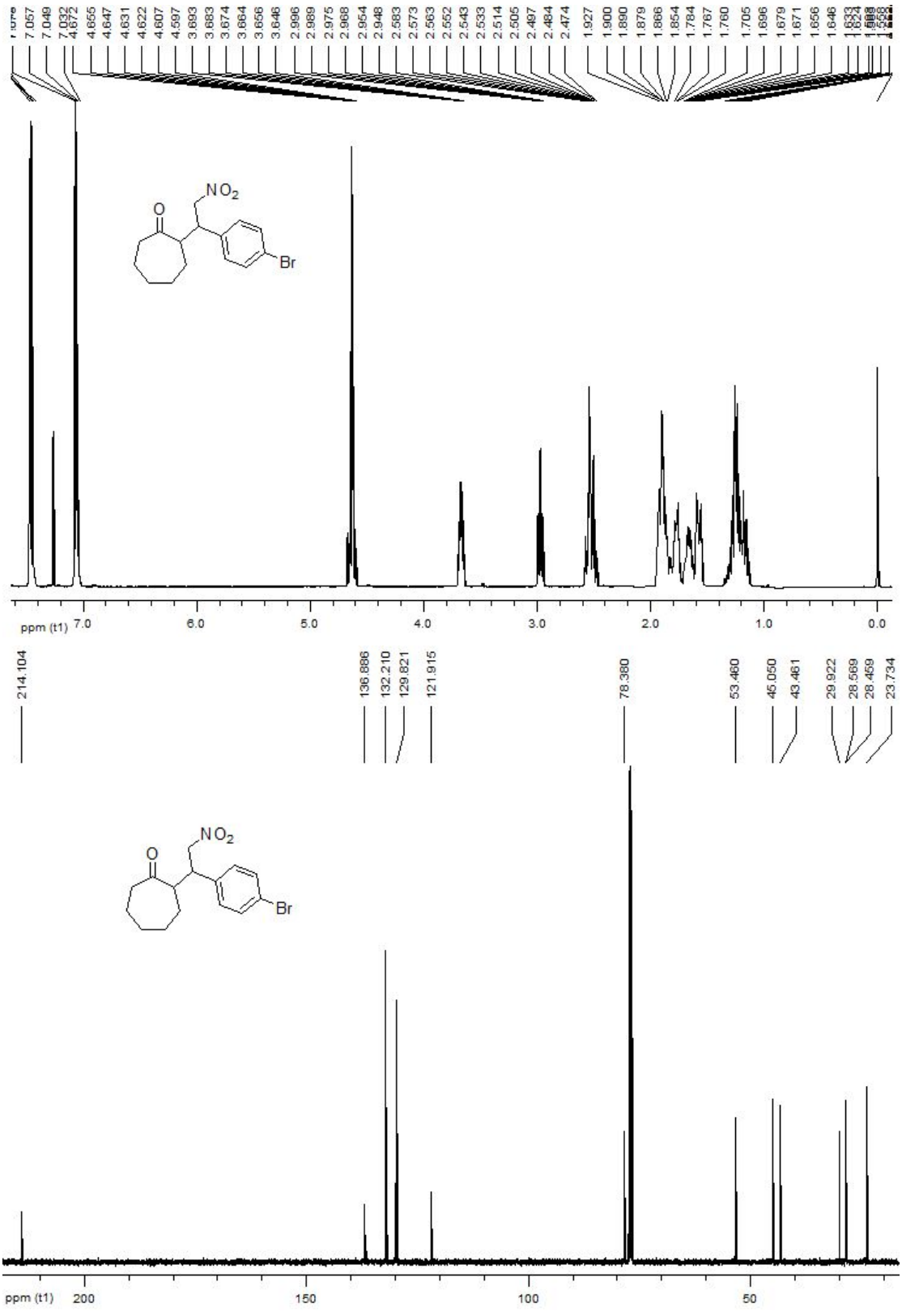

214.289
163.233
161.269
133.546
129.741
129.677
116.089
115.916
78.687
53.715
44.869
43.435
29.886
28.537
28.492
NO2
O
F
200
150
100
50
ppm (t1)

7e

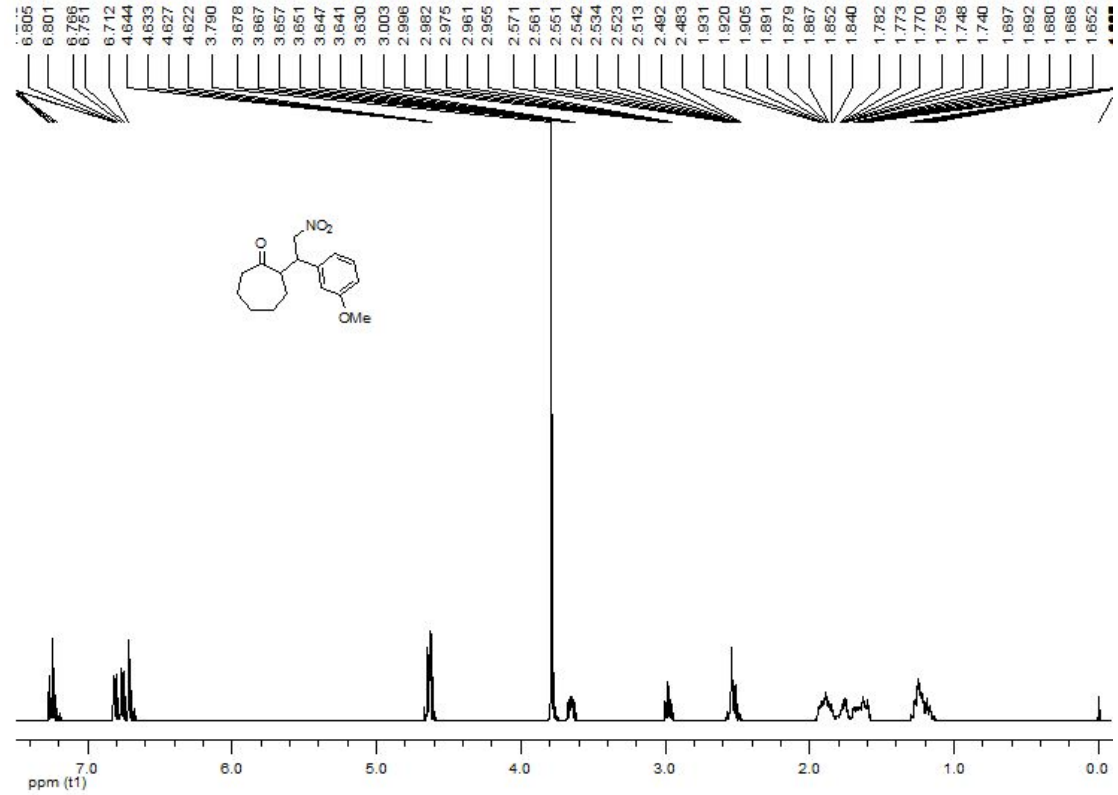

4.647
4.637
4.631
4.626
4.612
3.709
3.698
3.689
3.678
3.672
3.662
2.997
2.990
2.976
2.970
2.955
2.949
2.581
2.570
2.559
2.550
2.539
2.529
2.525
2.512
2.503
2.494
2.482
2.472
1.932
1.923
1.905
1.897
1.886
1.877
1.863
1.851
1.792
1.779
1.765
1.757
1.747
1.705
1.700
1.694
1.690
1.682
1.678
1.672
1.654
1.644
1.632
NO2
O
Cl
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

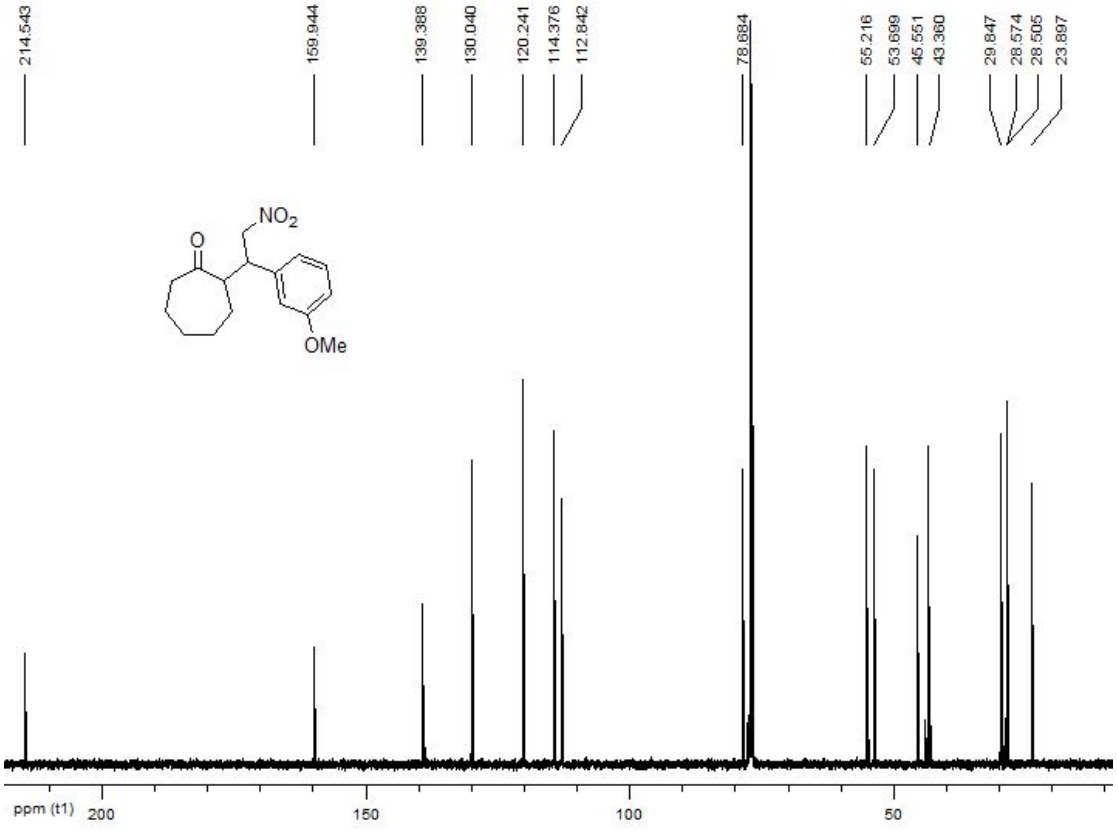

214.129
136.363
133.797
129.488
129.240
78.463
53.525
44.976
43.453
29.895
28.551
28.459
23.733
NO2
O
Cl
ppm (t1)
200
150
100
50

7f

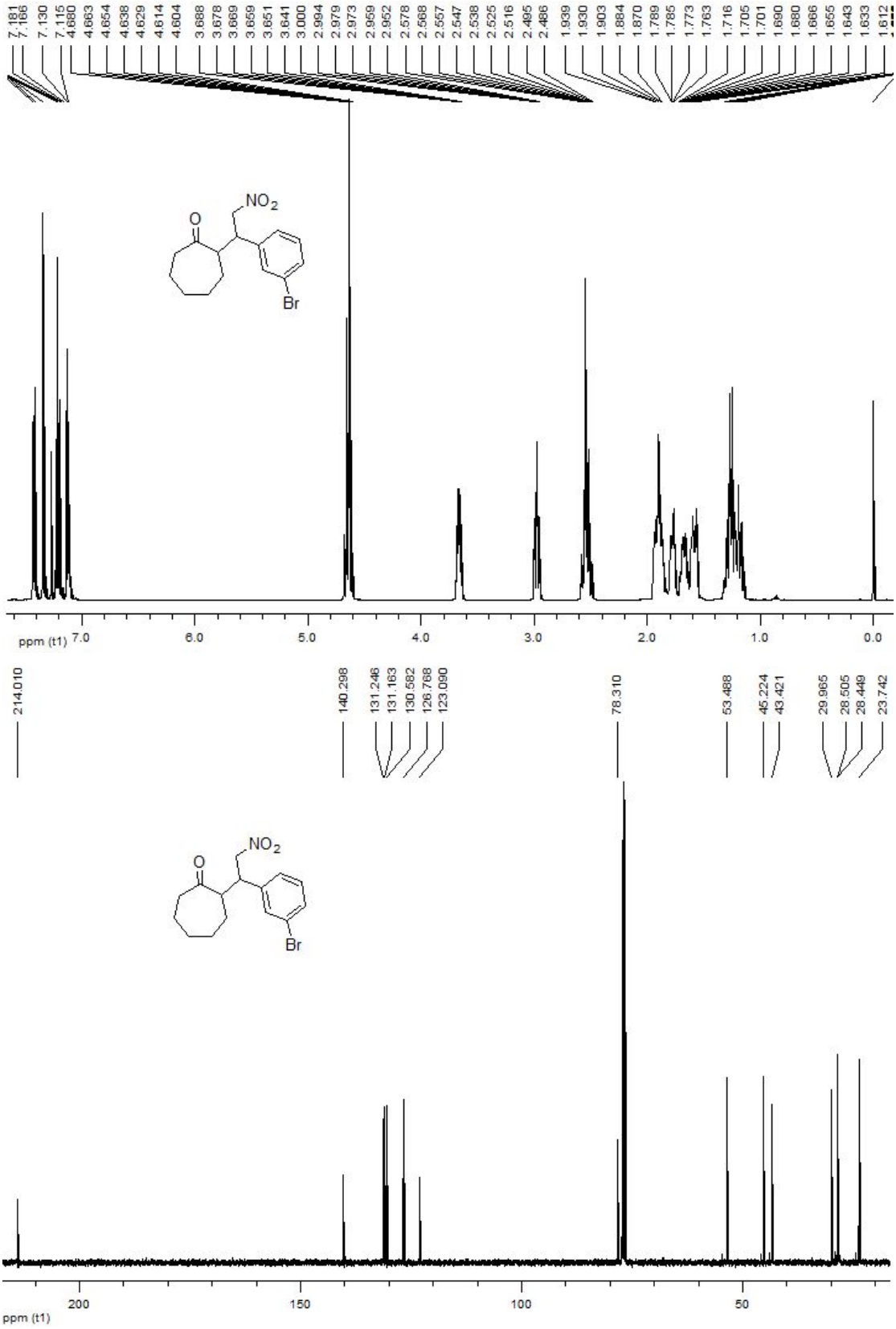

7.057
7.049
7.032
4.672
4.655
4.647
4.631
4.622
4.607
4.597
3.693
3.683
3.674
3.664
3.656
3.646
2.996
2.989
2.975
2.968
2.954
2.948
2.583
2.573
2.563
2.552
2.543
2.533
2.514
2.505
2.497
2.484
2.474
1.927
1.900
1.890
1.879
1.866
1.854
1.784
1.767
1.760
1.705
1.696
1.679
1.671
1.656
1.646
NO2
O
Br
ppm (t1) 7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
214.104
136.886
132.210
129.821
121.915
78.380
53.460
45.050
43.461
29.922
28.569
28.459
23.734
NO2
O
Br
ppm (t1) 200
150
100
50

7g

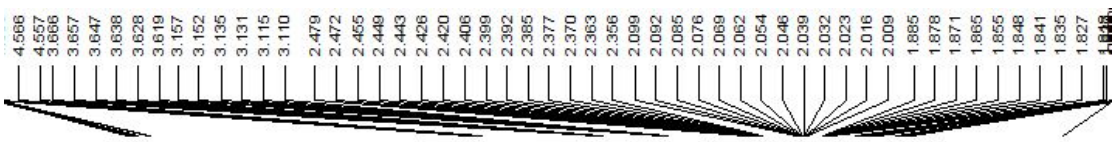

6.805
6.801
6.766
6.751
6.712
4.644
4.633
4.627
4.622
3.790
3.678
3.667
3.657
3.651
3.647
3.641
3.630
3.003
2.996
2.982
2.975
2.961
2.955
2.571
2.561
2.551
2.542
2.534
2.523
2.513
2.492
2.483
1.931
1.920
1.905
1.891
1.879
1.867
1.852
1.840
1.782
1.773
1.770
1.759
1.748
1.740
1.697
1.692
1.680
1.668
1.652
NO2
O
OMe
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

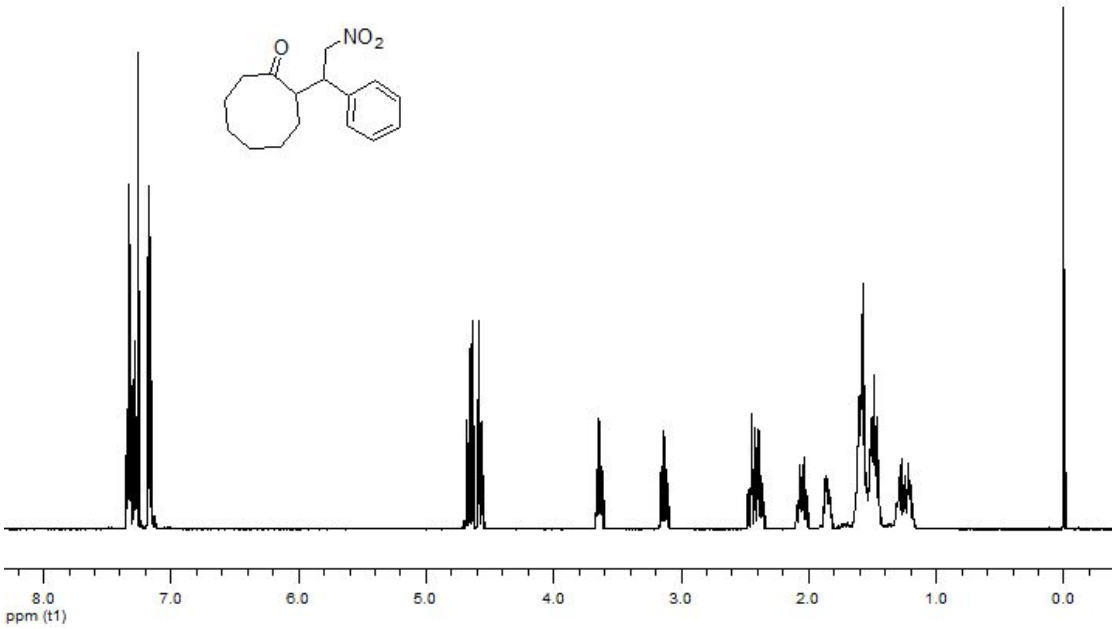

214.543
159.944
139.388
130.040
120.241
114.376
112.842
78.884
55.216
53.699
45.551
43.360
29.847
28.574
28.505
23.897
NO2
O
OMe
ppm (t1)
200
150
100
50

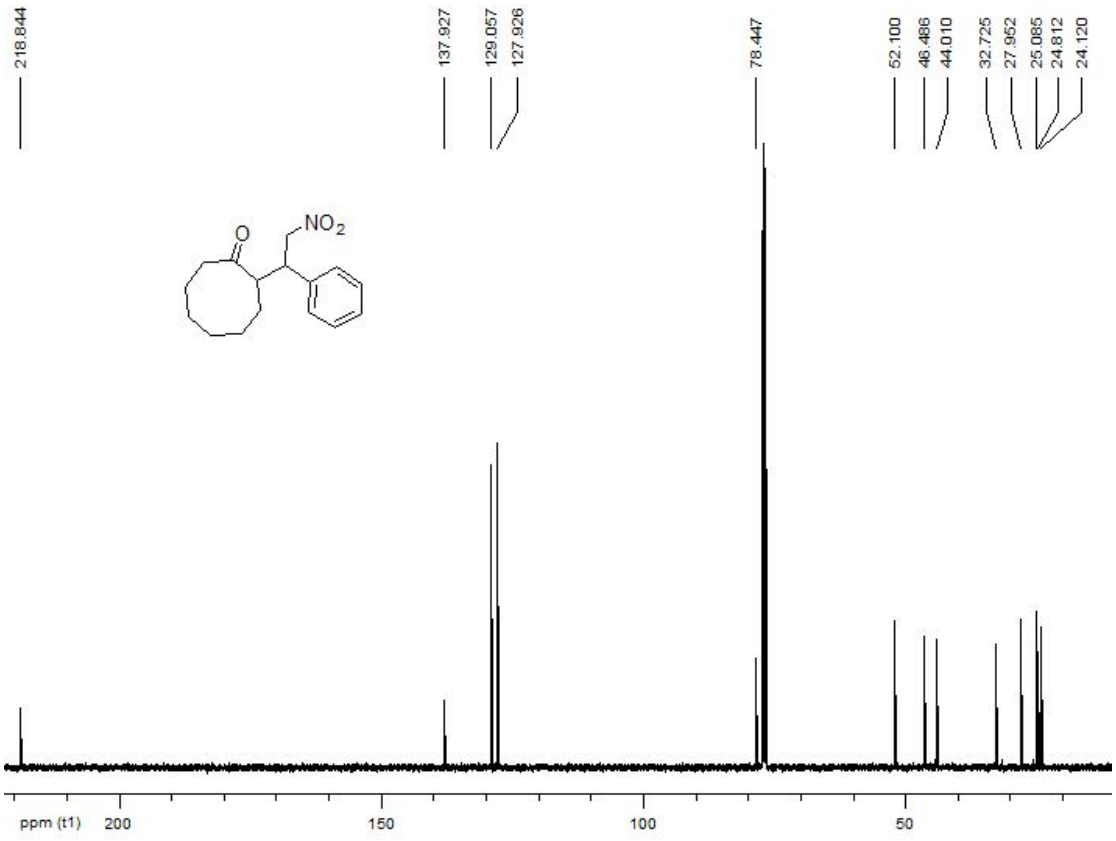
7h


7.181
7.165
7.130
7.115
4.680
4.663
4.654
4.638
4.629
4.614
4.604
3.688
3.678
3.669
3.659
3.651
3.641
3.000
2.994
2.979
2.973
2.959
2.952
2.578
2.568
2.557
2.547
2.538
2.525
2.516
2.495
2.486
1.939
1.930
1.903
1.884
1.870
1.789
1.785
1.773
1.763
1.716
1.705
1.701
1.690
1.680
1.666
1.655
1.643
1.633
1.612
NO2
O
Br
ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
214.010
140.298
131.246
131.163
130.582
126.768
123.090
78.310
53.488
45.224
43.421
29.965
28.505
28.449
23.742
NO2
O
Br
200
150
100
50
ppm (t1)

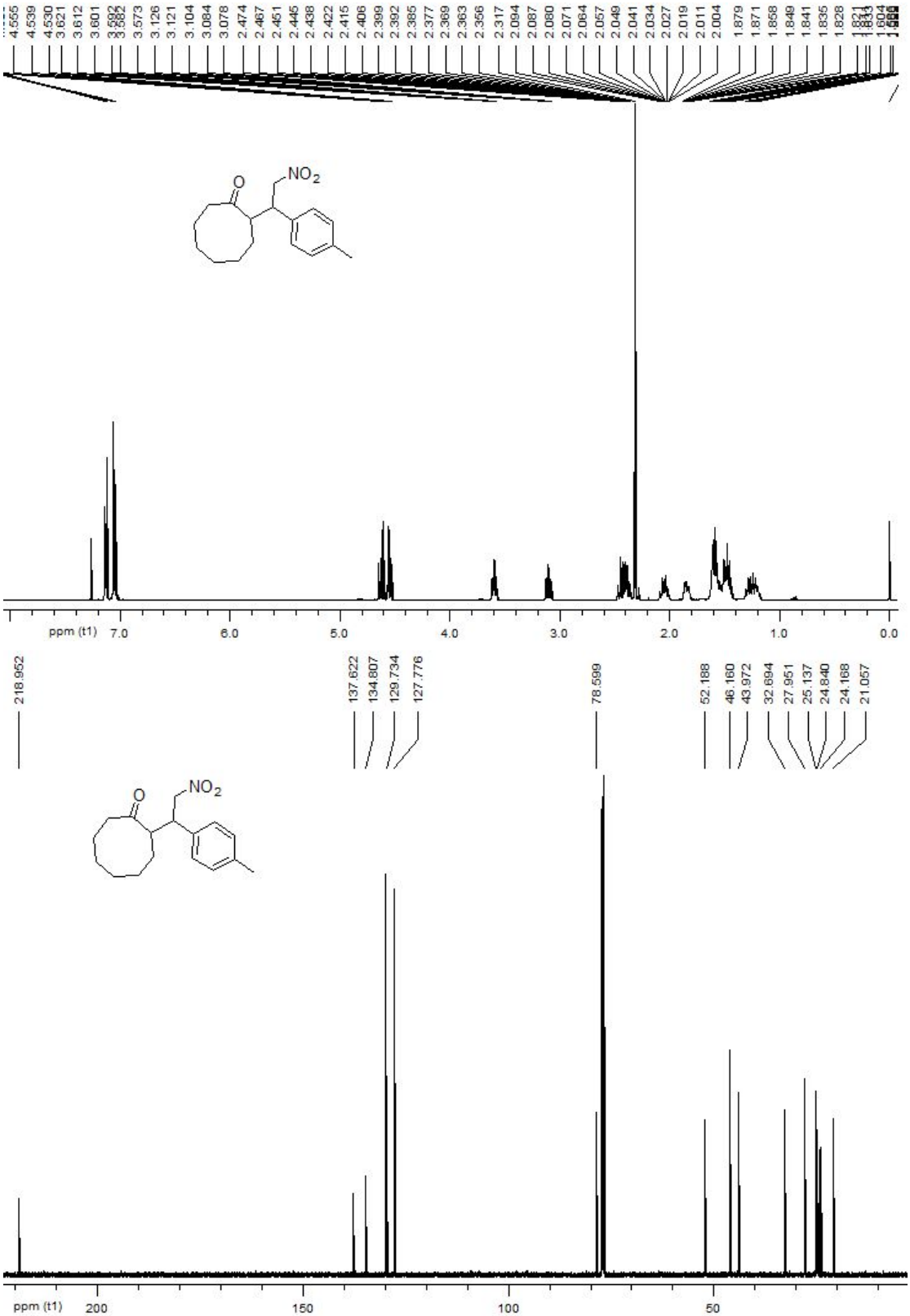
7i


4.566
4.557
3.666
3.657
3.647
3.638
3.628
3.619
3.157
3.152
3.135
3.131
3.115
3.110
2.479
2.472
2.455
2.449
2.443
2.426
2.420
2.406
2.399
2.392
2.385
2.377
2.370
2.363
2.356
2.099
2.092
2.085
2.076
2.069
2.062
2.054
2.046
2.039
2.032
2.023
2.016
2.009
1.885
1.878
1.871
1.865
1.855
1.848
1.841
1.835
1.827

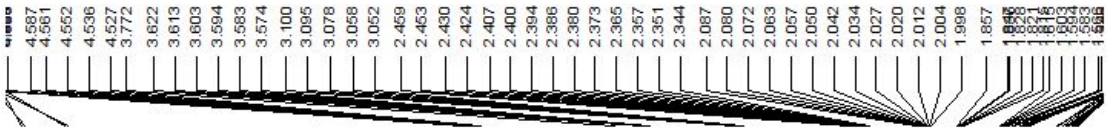

O
NO2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

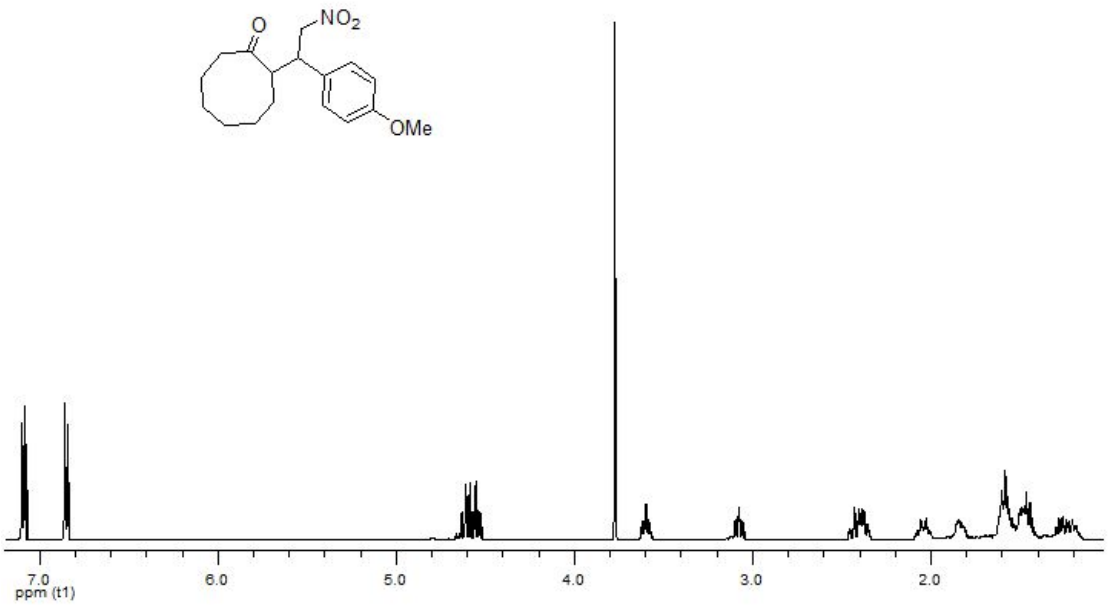

218.844
137.927
129.057
127.926
78.447
52.100
46.486
44.010
32.725
27.952
25.085
24.812
24.120
O
NO2
ppm (t1)
200
150
100
50

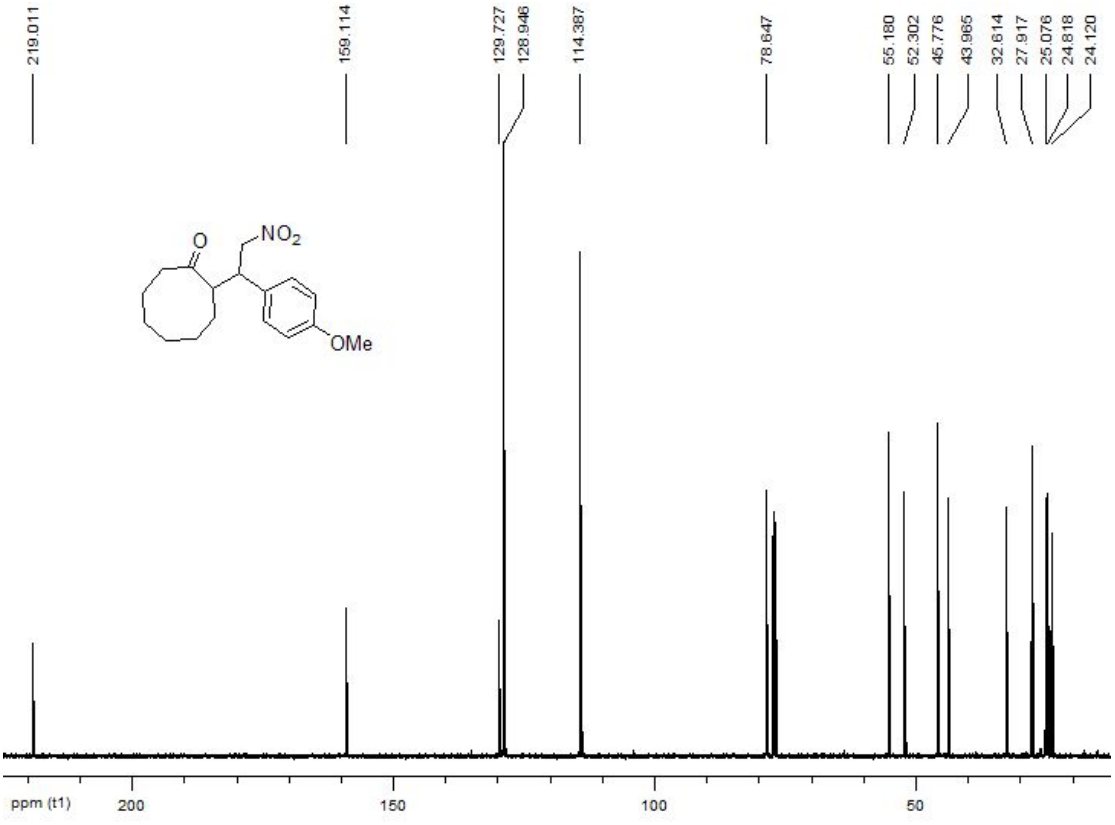
7j


4.555
4.539
4.530
3.621
3.612
3.601
3.592
3.582
3.573
3.126
3.121
3.104
3.084
3.078
2.474
2.467
2.451
2.445
2.438
2.422
2.415
2.406
2.399
2.392
2.385
2.377
2.369
2.363
2.356
2.317
2.094
2.087
2.080
2.071
2.064
2.057
2.049
2.041
2.034
2.027
2.019
2.011
2.004
1.879
1.871
1.858
1.849
1.841
1.835
1.828
O
NO2
ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
218.952
137.622
134.807
129.734
127.776
78.599
52.188
46.160
43.972
32.694
27.951
25.137
24.840
24.168
21.057
O
NO2
ppm (t1)
200
150
100
50

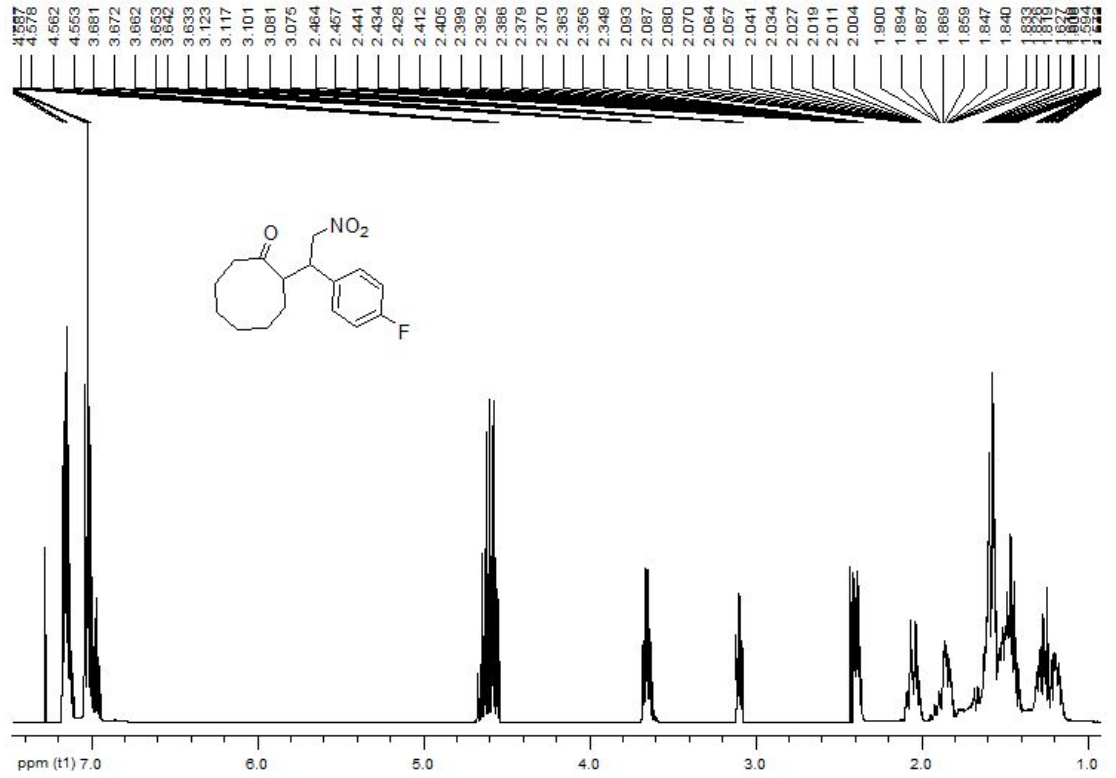
7k

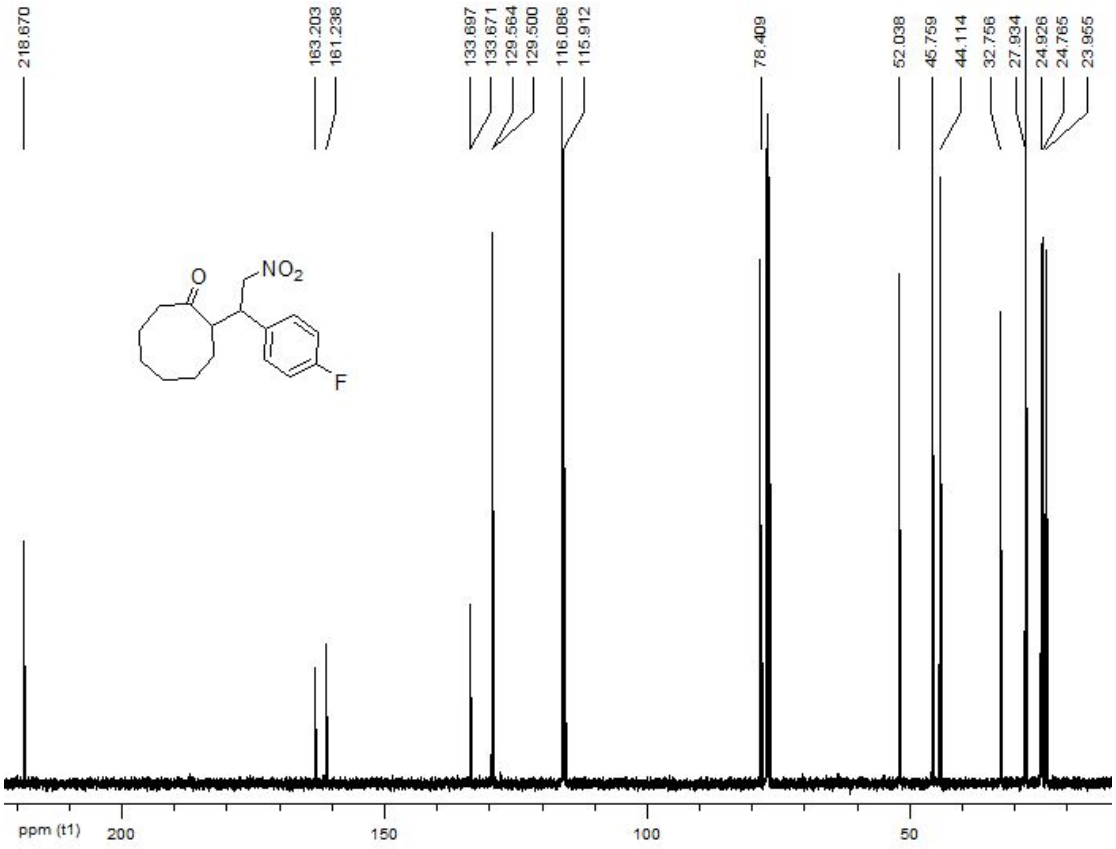

4.587
4.561
4.552
4.536
4.527
3.772
3.622
3.613
3.603
3.594
3.583
3.574
3.100
3.095
3.078
3.058
3.052
2.459
2.453
2.430
2.424
2.407
2.400
2.394
2.386
2.380
2.373
2.365
2.357
2.351
2.344
2.087
2.080
2.072
2.063
2.057
2.050
2.042
2.034
2.027
2.020
2.012
2.004
1.998
1.857


O
NO2
OMe
7.0
ppm (t1)
6.0
5.0
4.0
3.0
2.0

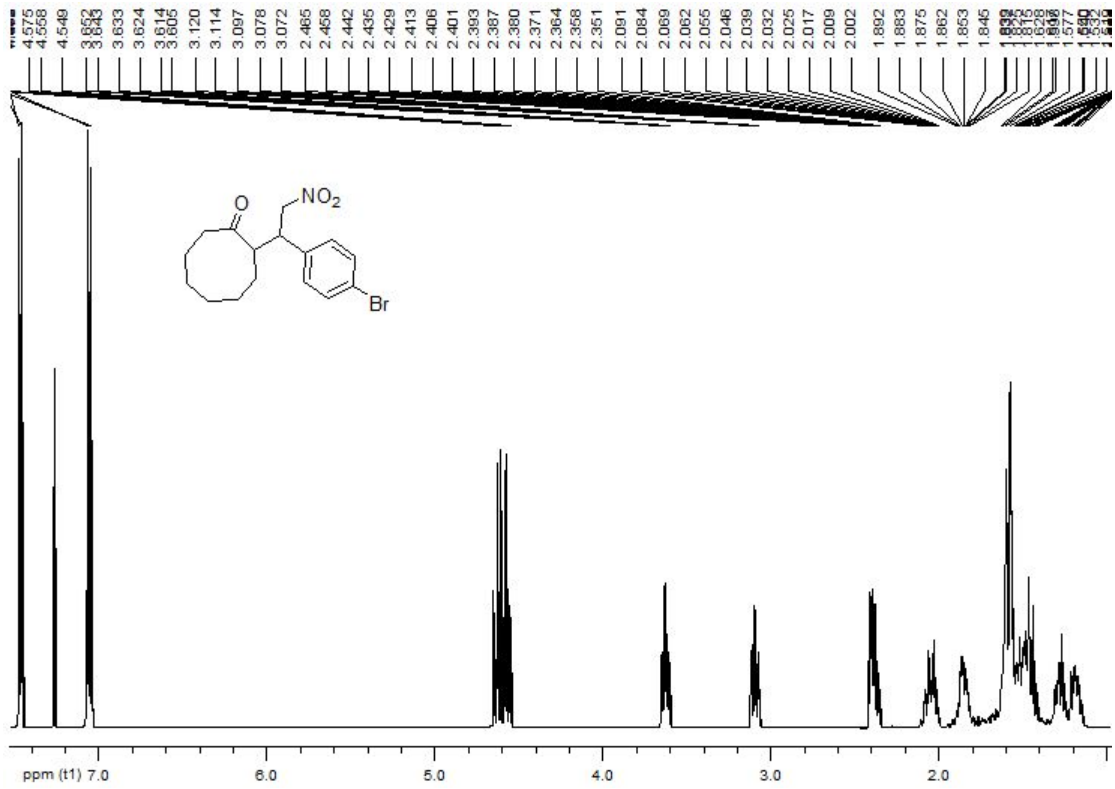

219.011
159.114
129.727
128.946
114.387
78.647
55.180
52.302
45.776
43.965
32.614
27.917
25.076
24.818
24.120
O
NO2
OMe
ppm (t1)
200
150
100
50

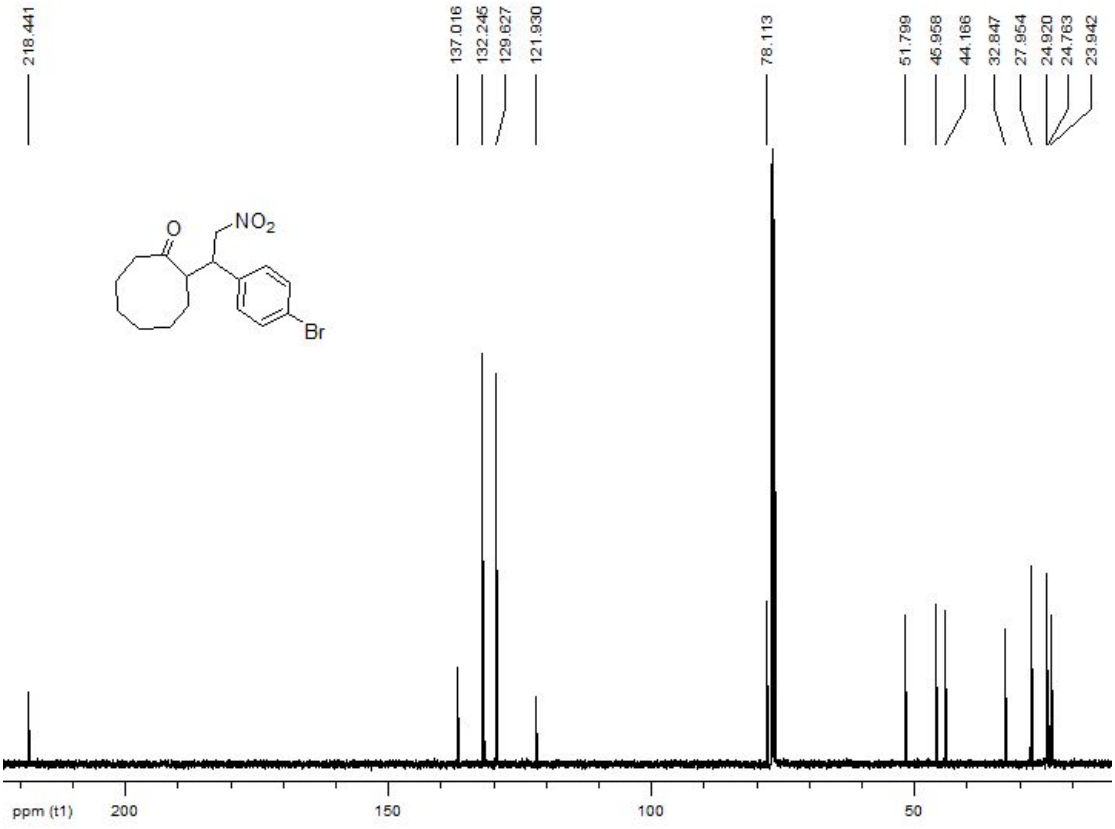
7l


4.587
4.578
4.562
4.553
3.681
3.672
3.662
3.653
3.642
3.633
3.123
3.117
3.101
3.081
3.075
2.464
2.457
2.441
2.434
2.428
2.412
2.405
2.399
2.392
2.386
2.379
2.370
2.363
2.356
2.349
2.093
2.087
2.080
2.070
2.064
2.057
2.041
2.034
2.027
2.019
2.011
2.004
1.900
1.894
1.887
1.869
1.859
1.847
1.840
O
NO2
F
ppm (t1) 7.0
6.0
5.0
4.0
3.0
2.0
1.0

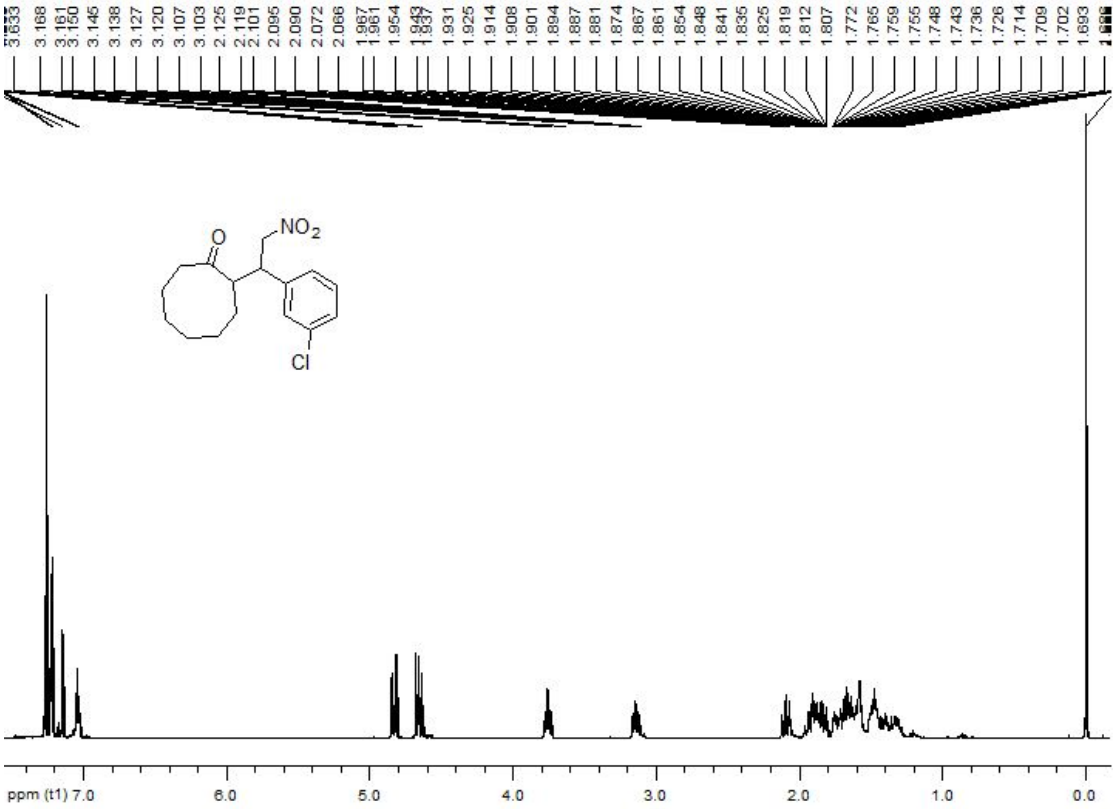

218.670
163.203
161.238
133.697
133.671
129.564
129.500
116.086
115.912
78.409
52.038
45.759
44.114
32.756
27.934
24.926
24.765
23.955
O
NO2
F
ppm (t1)
200
150
100
50

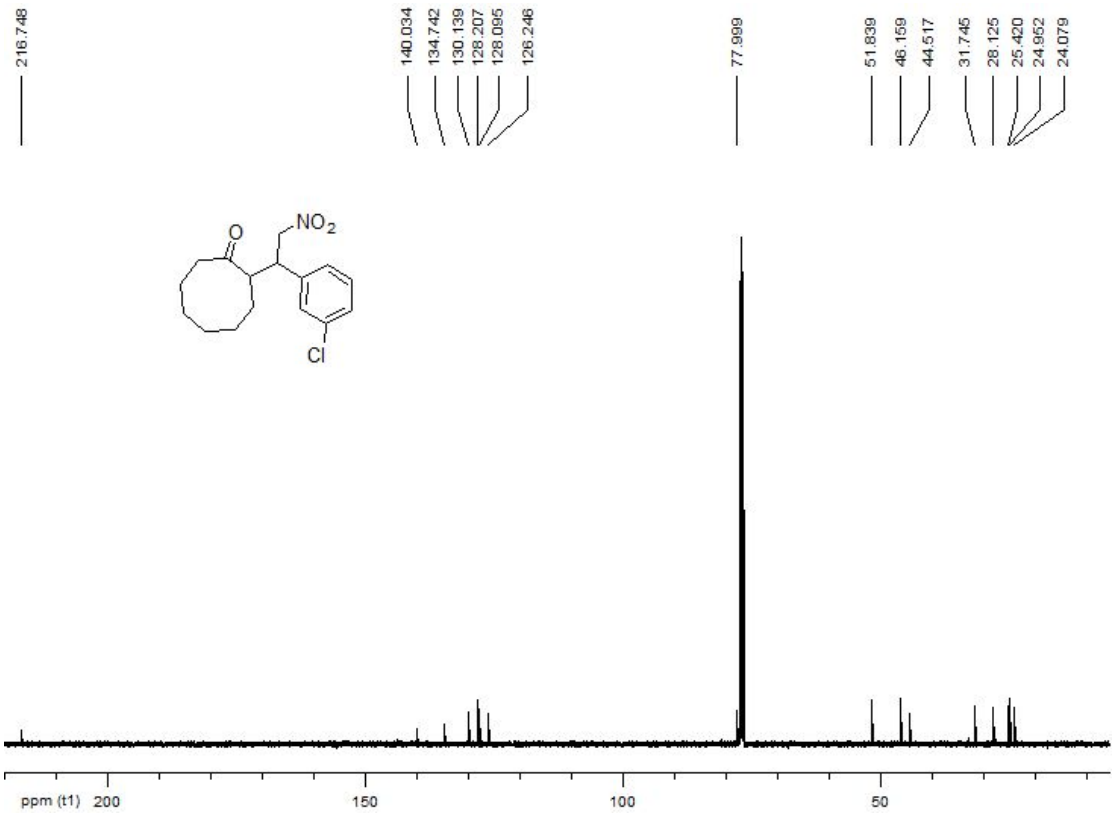
7m


4.575
4.558
4.549
3.852
3.843
3.633
3.624
3.614
3.605
3.120
3.114
3.097
3.078
3.072
2.465
2.458
2.442
2.435
2.429
2.413
2.406
2.401
2.393
2.387
2.380
2.371
2.364
2.358
2.351
2.091
2.084
2.069
2.062
2.055
2.046
2.039
2.032
2.025
2.017
2.009
2.002
1.892
1.883
1.875
1.862
1.853
1.845
O
NO2
Br
ppm (t1) 7.0
6.0
5.0
4.0
3.0
2.0

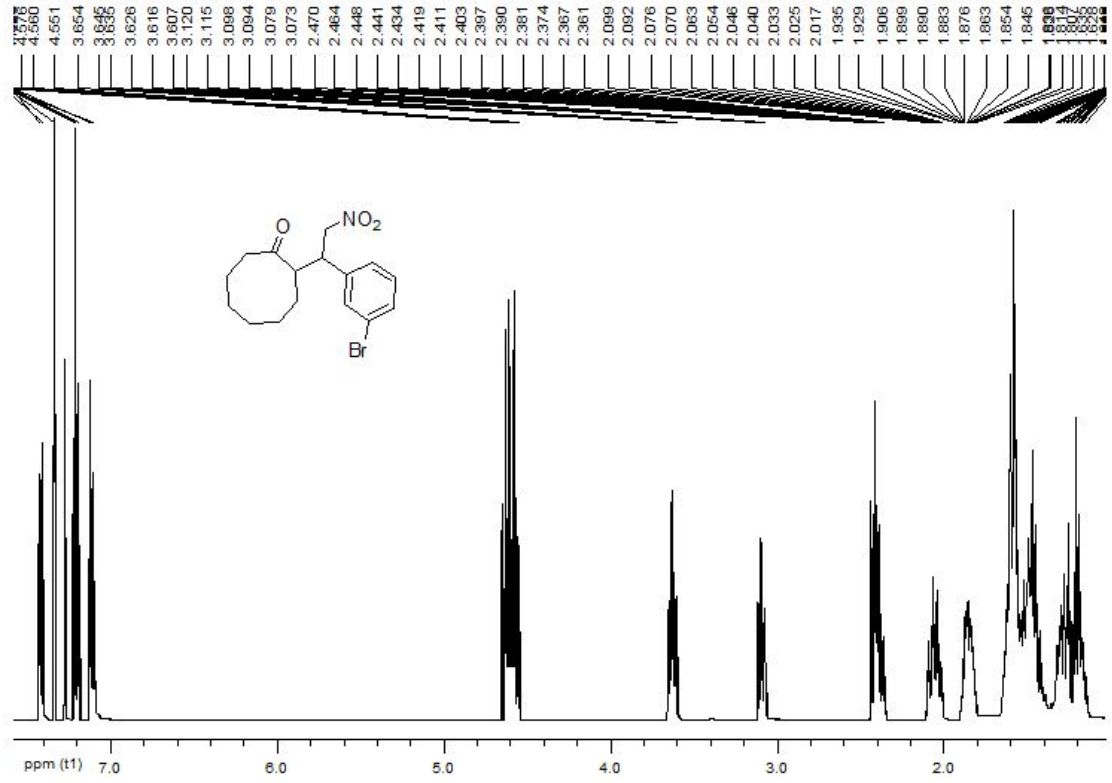

218.441
137.016
132.245
129.627
121.930
78.113
51.799
45.958
44.166
32.847
27.954
24.920
24.763
23.942
O
NO2
Br
ppm (t1)
200
150
100
50

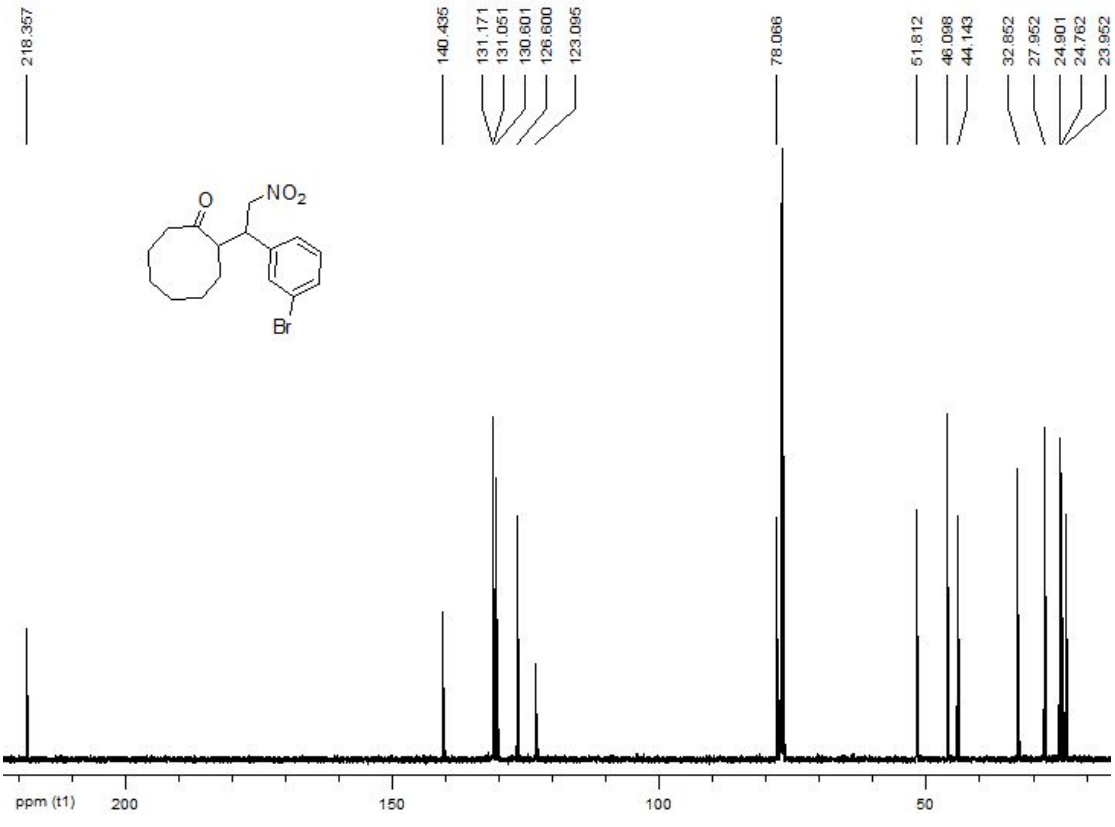
7n


3.168
3.161
3.150
3.146
3.138
3.127
3.120
3.107
3.103
2.125
2.119
2.101
2.095
2.090
2.072
2.066
1.967
1.961
1.954
1.943
1.937
1.931
1.925
1.914
1.908
1.901
1.894
1.887
1.881
1.874
1.867
1.861
1.854
1.848
1.841
1.835
1.825
1.819
1.812
1.807
1.772
1.765
1.759
1.755
1.748
1.743
1.736
1.726
1.714
1.709
1.702
1.693
O
NO2
Cl
ppm (t1) 7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

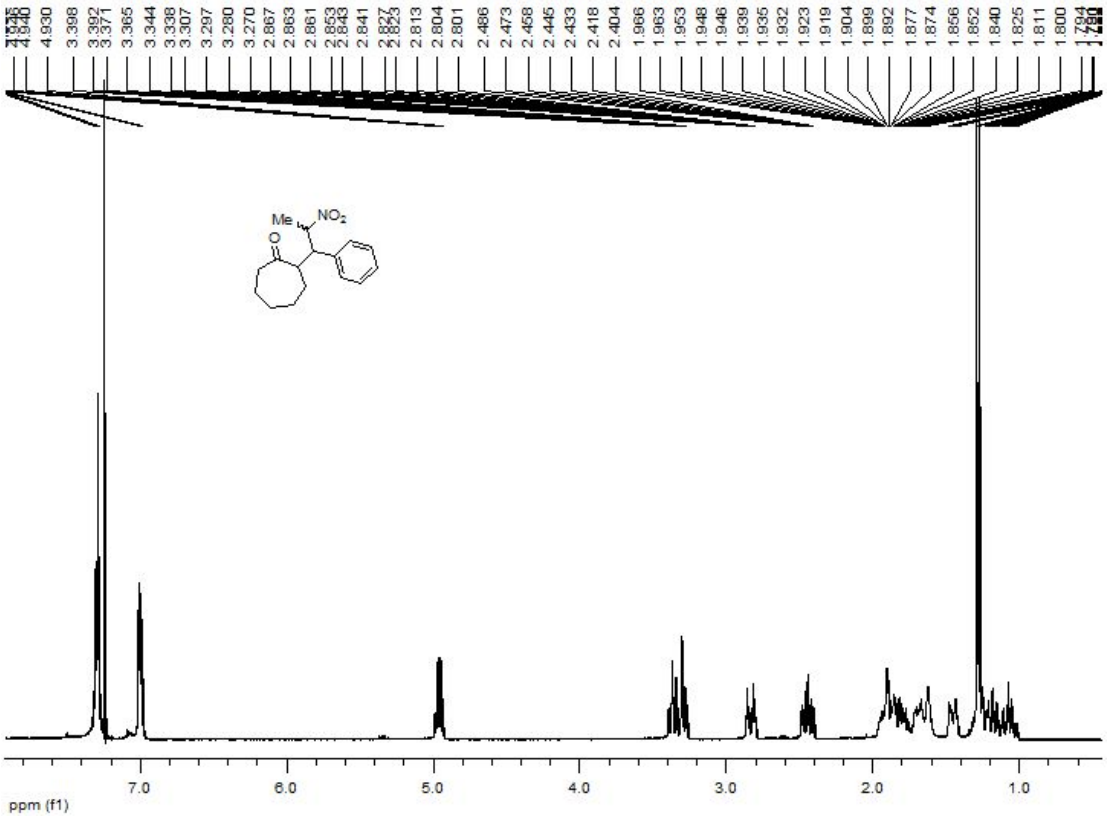

216.748
140.034
134.742
130.139
128.207
128.095
126.246
77.999
51.839
46.159
44.517
31.745
28.125
25.420
24.952
24.079
O
NO2
Cl
ppm (t1) 200
150
100
50

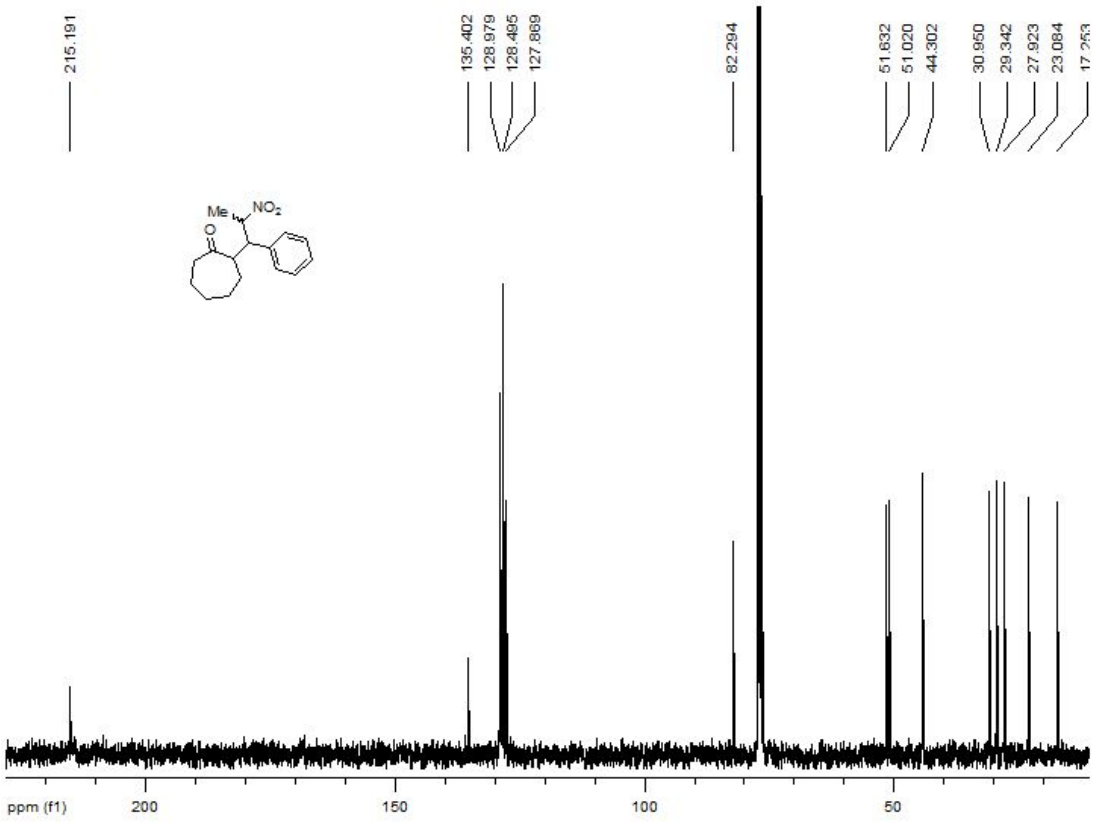
7o


4.560
4.551
3.654
3.626
3.616
3.607
3.120
3.115
3.098
3.094
3.079
3.073
2.470
2.464
2.448
2.441
2.434
2.419
2.411
2.403
2.397
2.390
2.381
2.374
2.367
2.361
2.099
2.092
2.076
2.070
2.063
2.054
2.046
2.040
2.033
2.025
2.017
1.935
1.929
1.906
1.899
1.890
1.883
1.876
1.863
1.854
1.845
O
NO2
Br
ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0

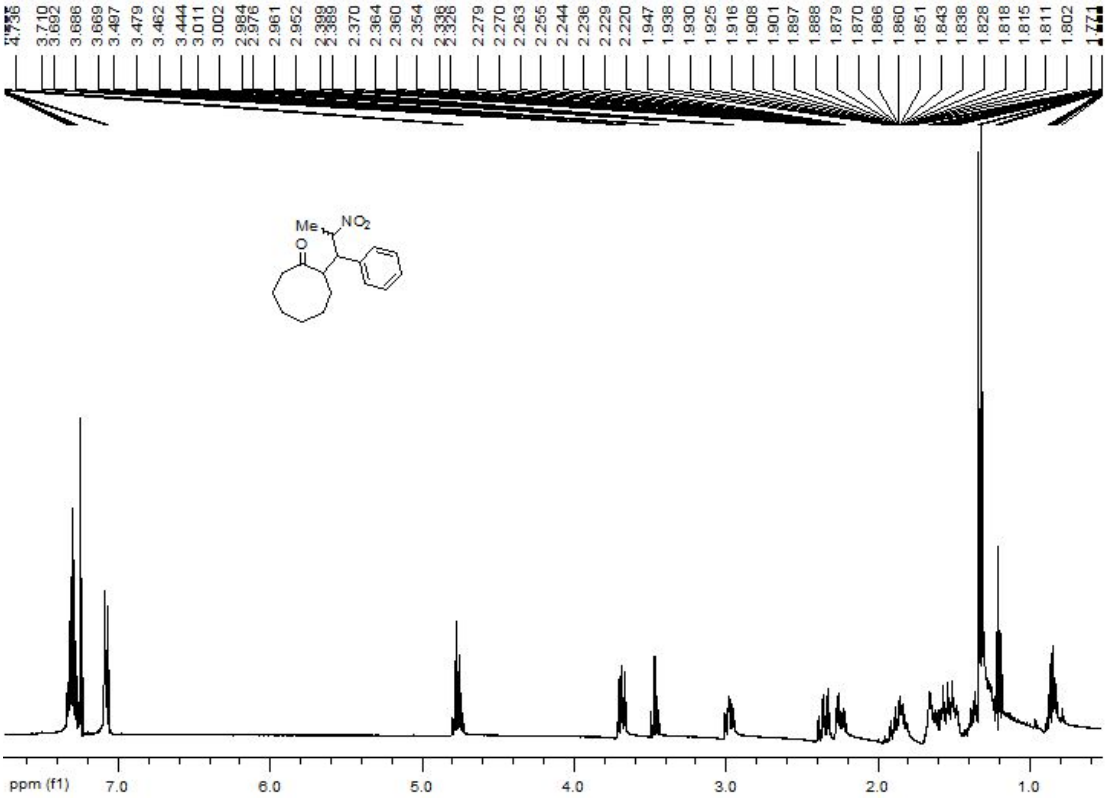

218.357
140.435
131.171
131.051
130.601
126.600
123.095
78.066
51.812
46.098
44.143
32.852
27.952
24.901
24.762
23.952
O
NO2
Br
ppm (t1)
200
150
100
50

7p


4.930
3.398
3.392
3.371
3.365
3.344
3.338
3.307
3.297
3.280
3.270
2.867
2.863
2.861
2.853
2.843
2.841
2.827
2.823
2.813
2.804
2.801
2.486
2.473
2.458
2.445
2.433
2.418
2.404
1.966
1.963
1.953
1.948
1.946
1.939
1.935
1.932
1.923
1.919
1.904
1.899
1.892
1.877
1.874
1.856
1.852
1.840
1.825
1.811
1.800
Me
NO2
O
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)


215.191
135.402
128.979
128.495
127.869
82.294
51.632
51.020
44.302
30.950
29.342
27.923
23.084
Me
NO2
O
ppm (f1)
200
150
100
50

7q


4.735
3.710
3.692
3.686
3.669
3.487
3.479
3.462
3.444
3.011
3.002
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2.976
2.961
2.952
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2.388
2.370
2.364
2.360
2.354
2.338
2.328
2.279
2.270
2.263
2.255
2.244
2.236
2.229
2.220
1.947
1.938
1.930
1.925
1.916
1.908
1.901
1.897
1.888
1.879
1.870
1.866
1.860
1.851
1.843
1.838
1.828
1.818
1.815
1.811
1.802
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NO2
O
ppm (f1)
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6.0
5.0
4.0
3.0
2.0
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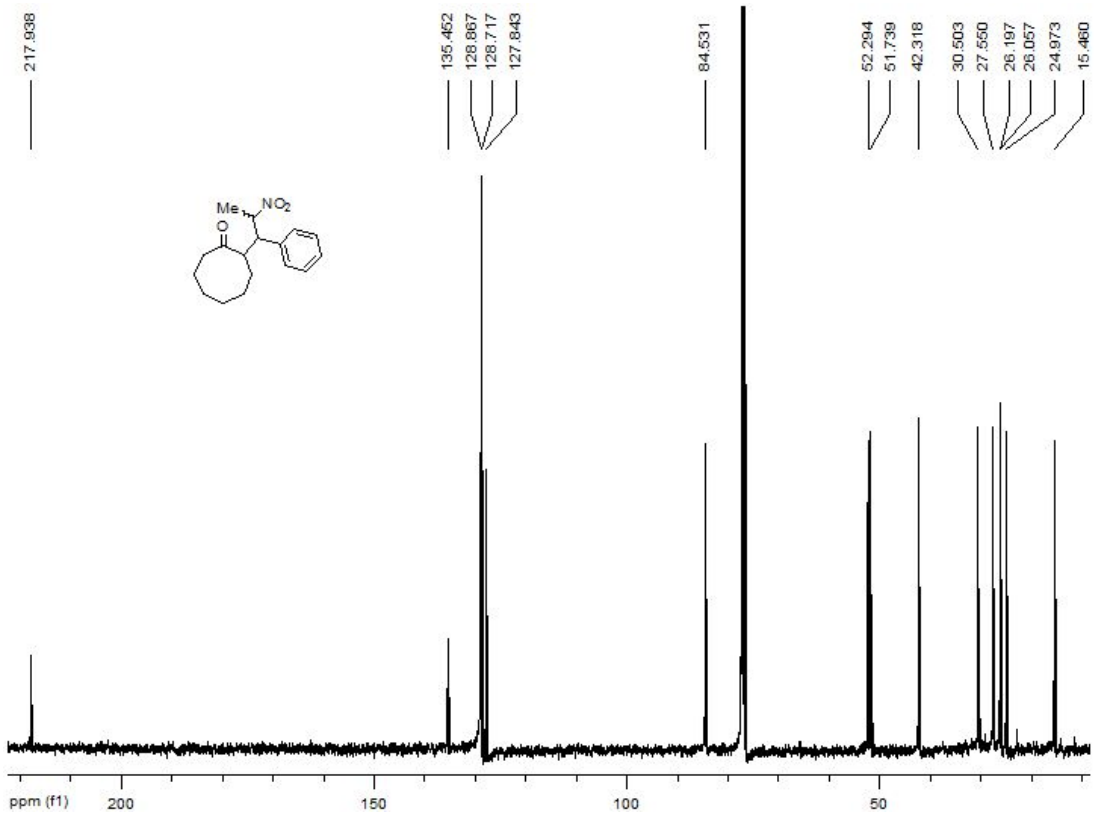
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Me
NO2
O
ppm (f1)
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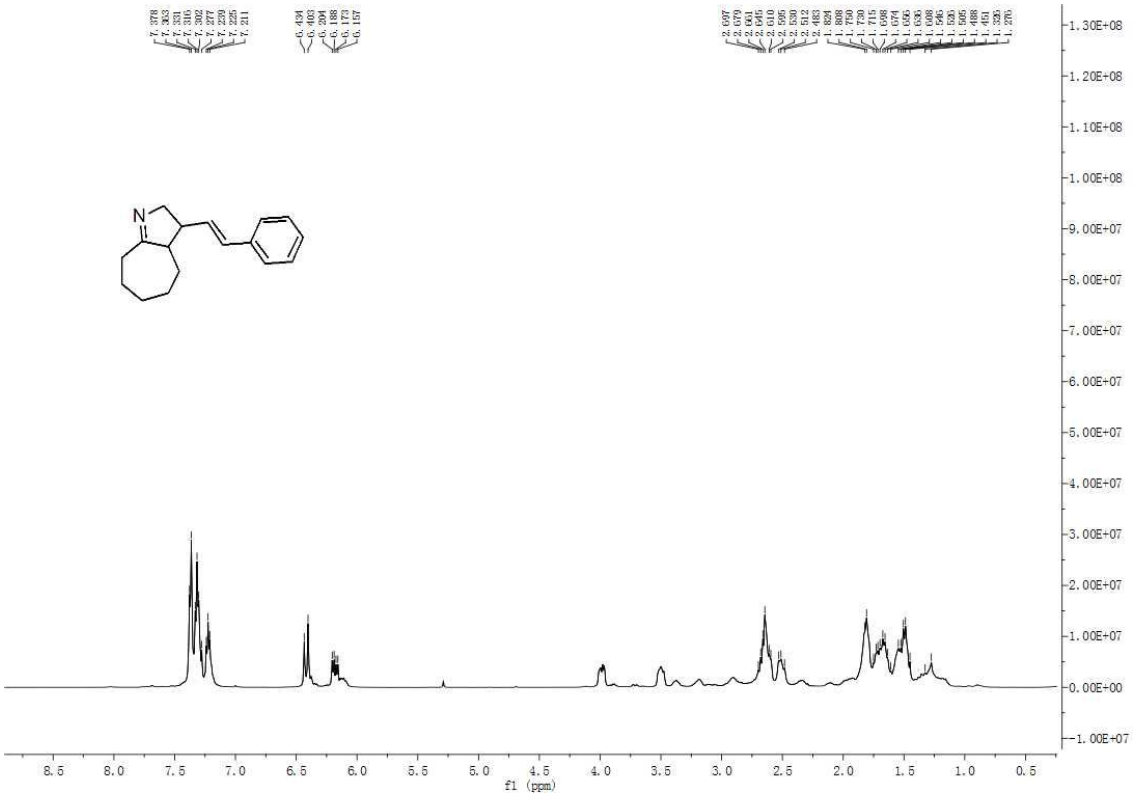
150
100
50

8a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6.173
6.157
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2.079
2.061
2.045
2.010
1.995
1.930
1.912
1.883
1.858
1.808
1.759
1.739
1.715
1.698
1.674
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1.608
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1.535
1.505
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1.461
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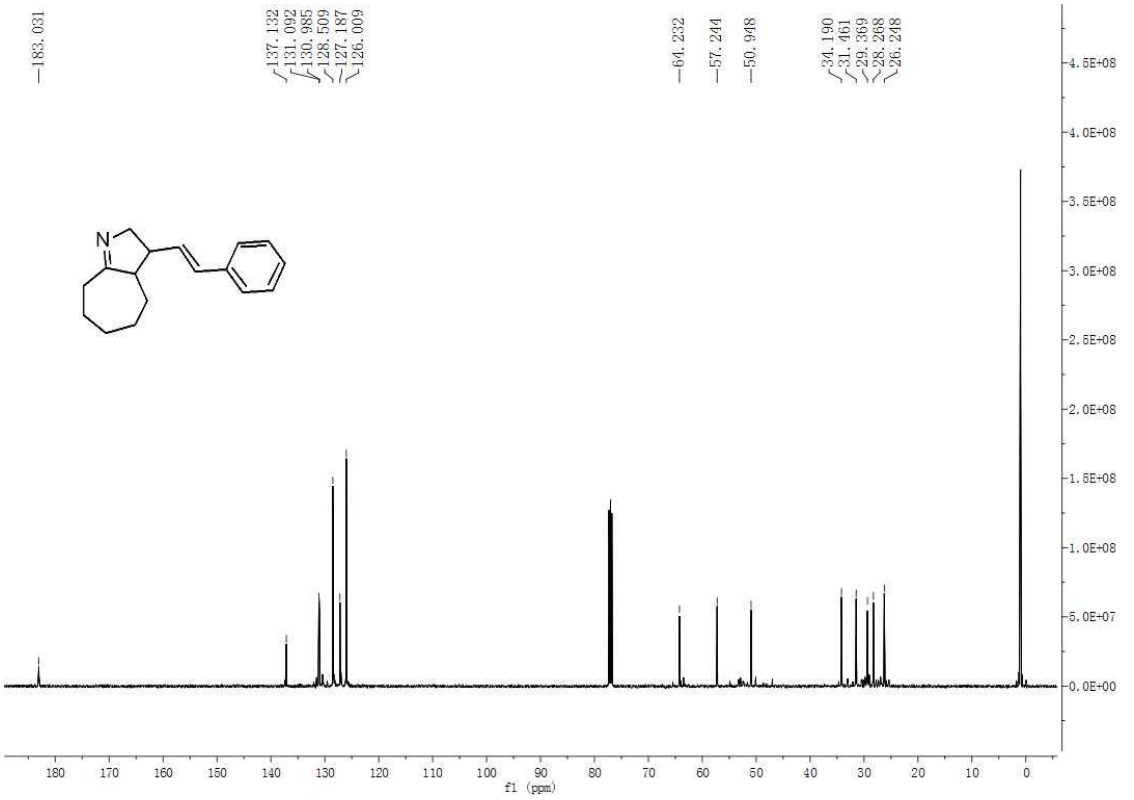
1.295
f1 (ppm)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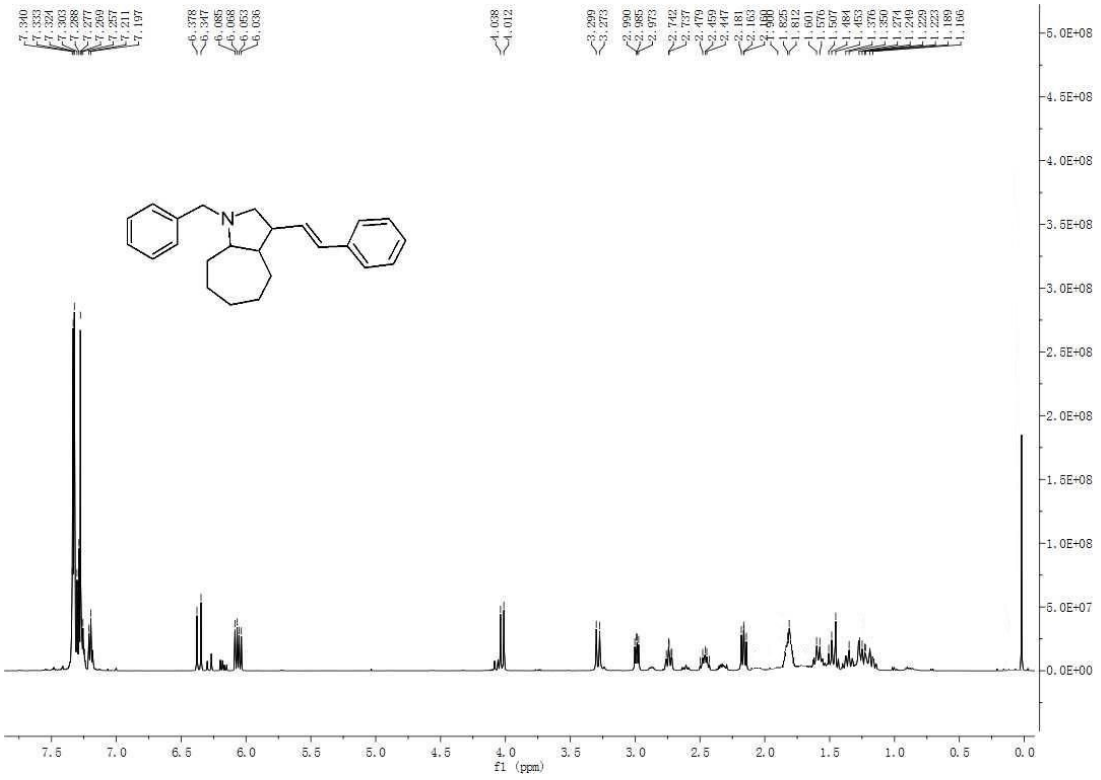
29.369
28.268
26.248
f1 (ppm)

9a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6.068
6.053
6.036
4.038
4.012
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3.273
2.990
2.985
2.973
2.742
2.737
2.479
2.459
2.447
2.181
2.163
1.825
1.812
1.601
1.576
1.507
1.484
1.453
1.376
1.356
1.274
1.249
1.229
1.223
1.189
1.166
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4.5E+08
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3.5E+08
3.0E+08
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7.5
7.0
6.5
6.0
5.5
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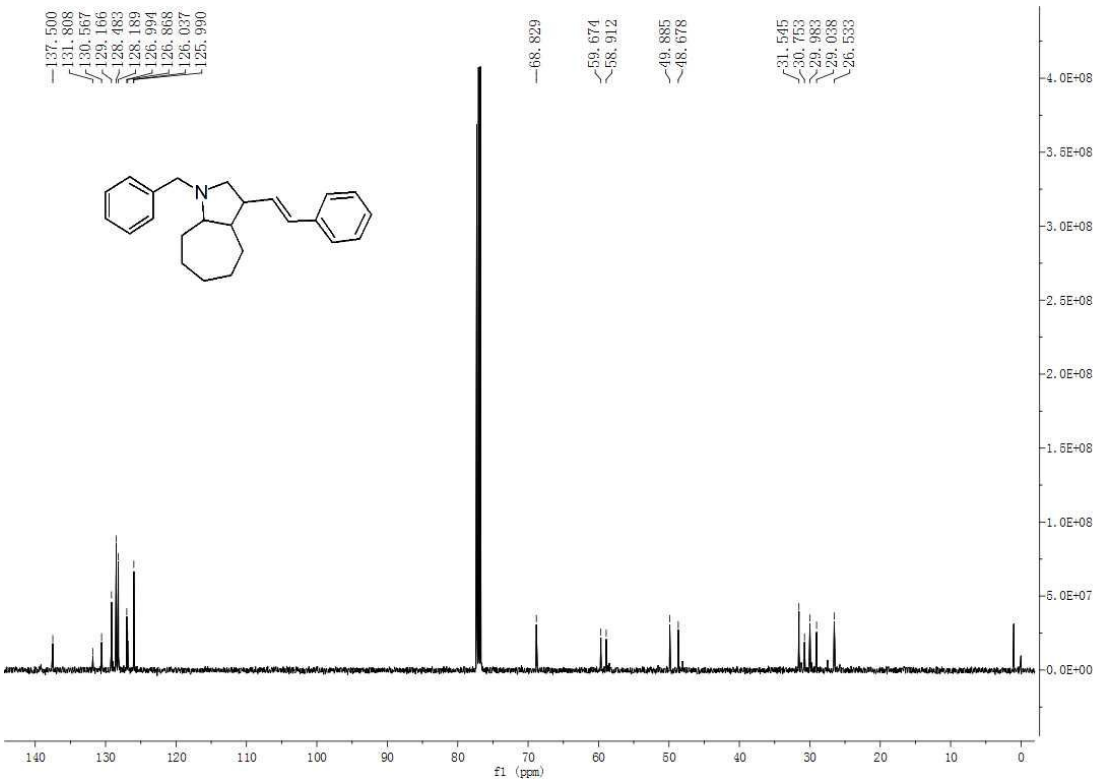
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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49.885
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31.545
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29.983
29.038
26.533
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3.5E+08
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2.5E+08
2.0E+08
1.5E+08
1.0E+08
6.0E+07
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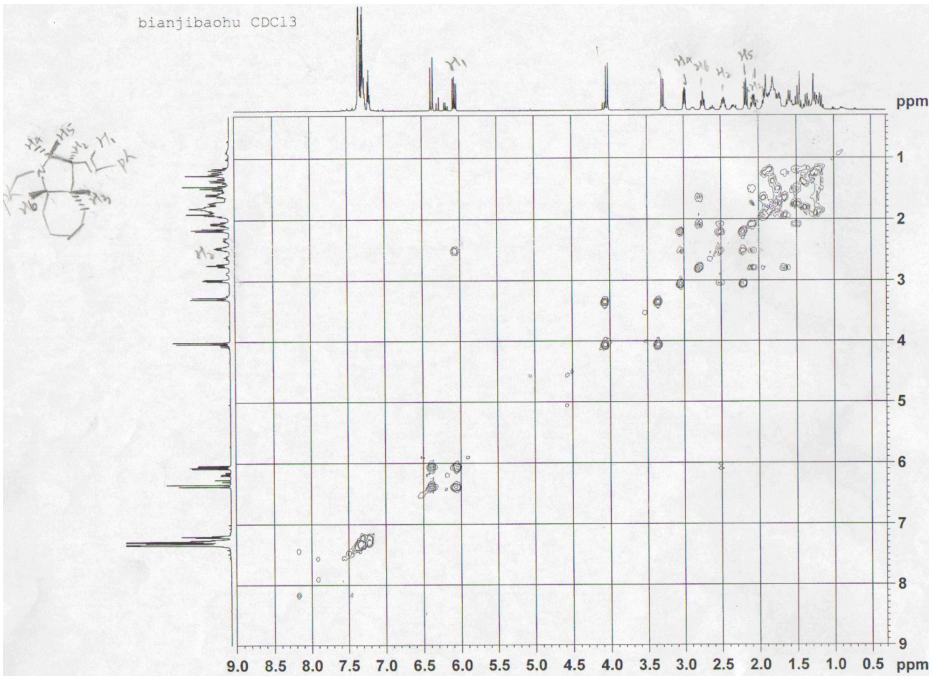
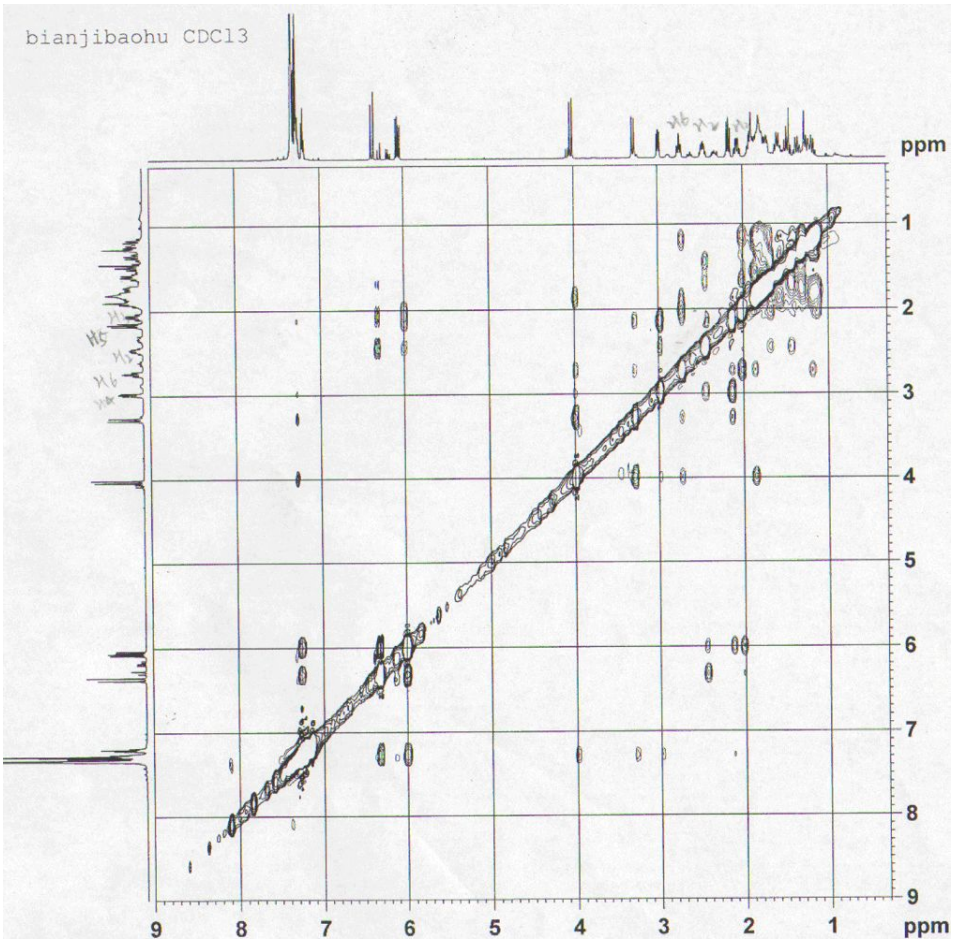
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

H-H COSY spectra of 9a

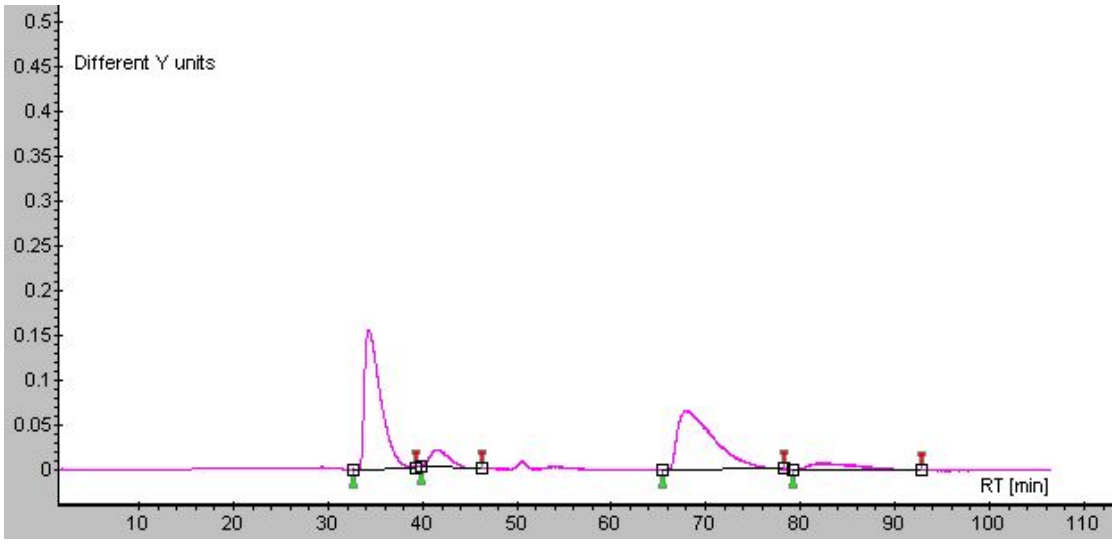


H-H NOESY spectra of 9a

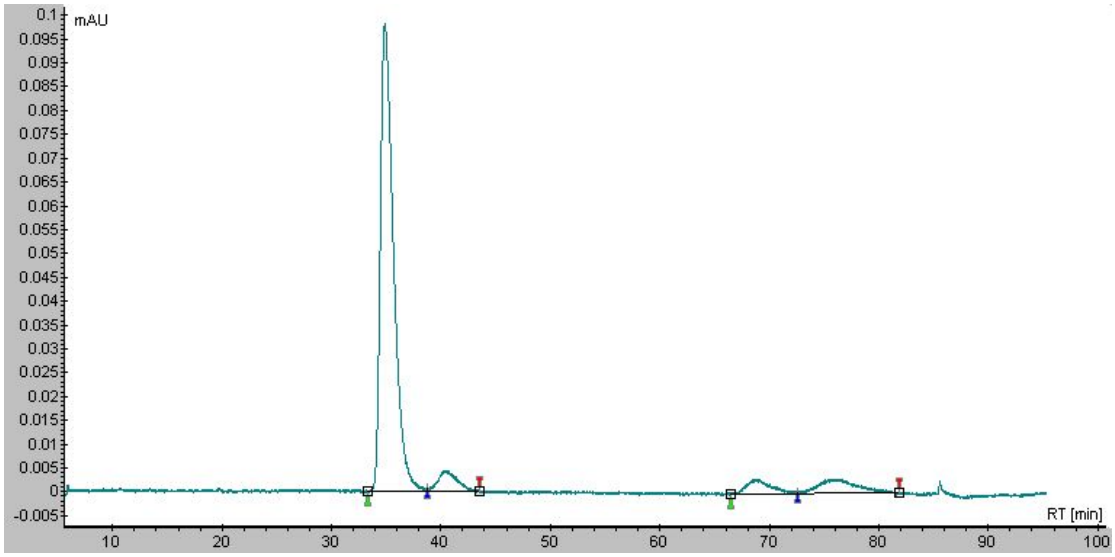


4. HPLC spectra

5a

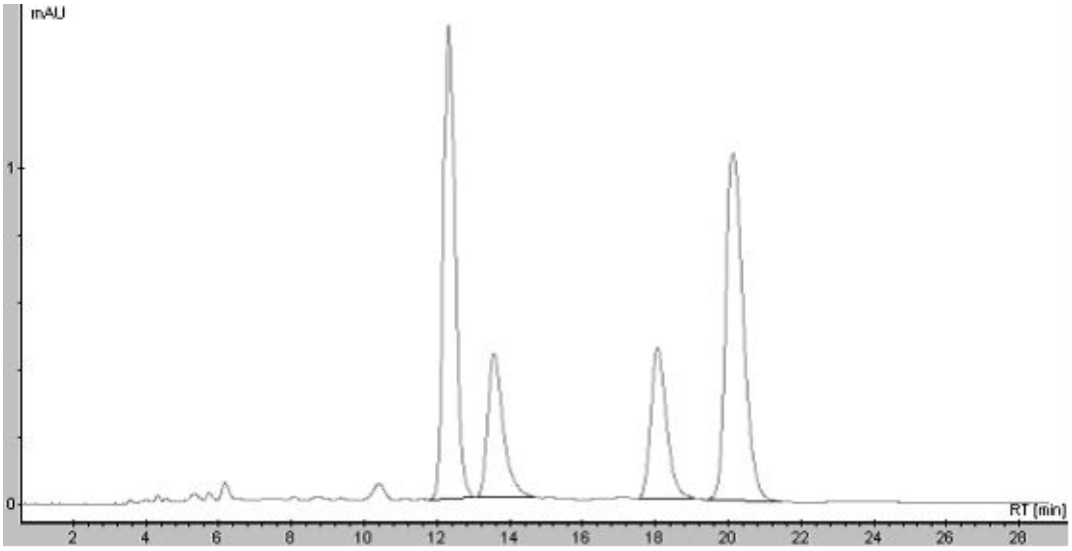


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	32.938	34.521	39.404	44.720
2	40.026	41.781	46.492	6.216
3	65.974	68.509	78.782	43.170
4	79.653	83.002	97.331	5.894

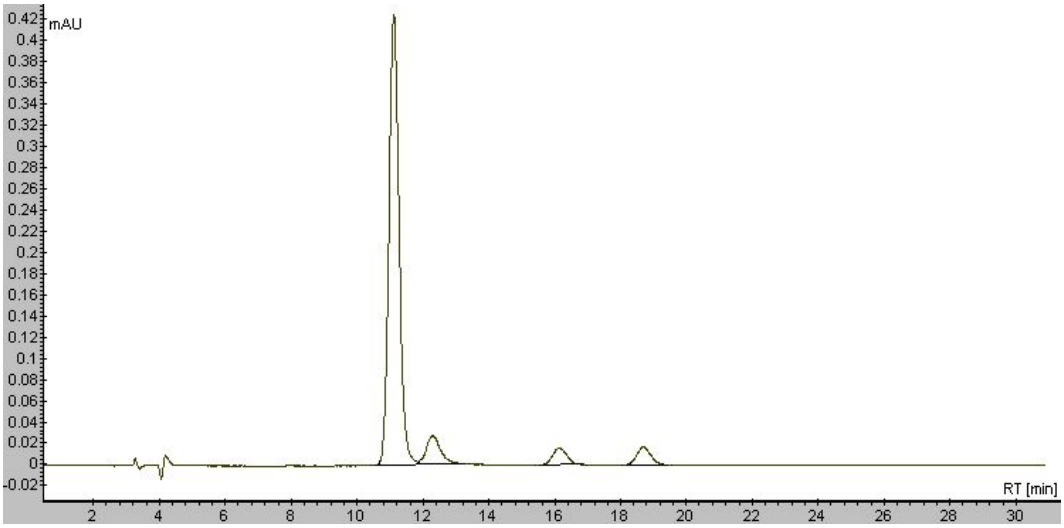


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	33.304	34.881	38.744	82.926
2	38.744	40.479	43.520	5.327
3	66.474	68.842	72.578	4.687
4	72.578	76.333	81.866	7.059

5b

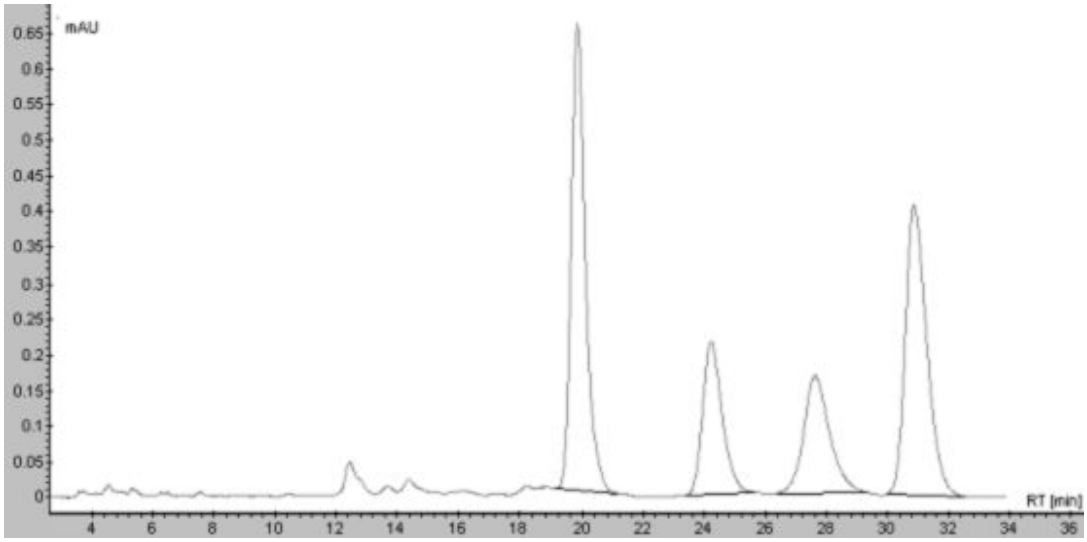


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.769	12.319	13.054	34.453
2	13.094	13.559	14.701	13.635
3	17.553	18.065	19.079	14.311
4	19.401	20.132	21.489	37.602

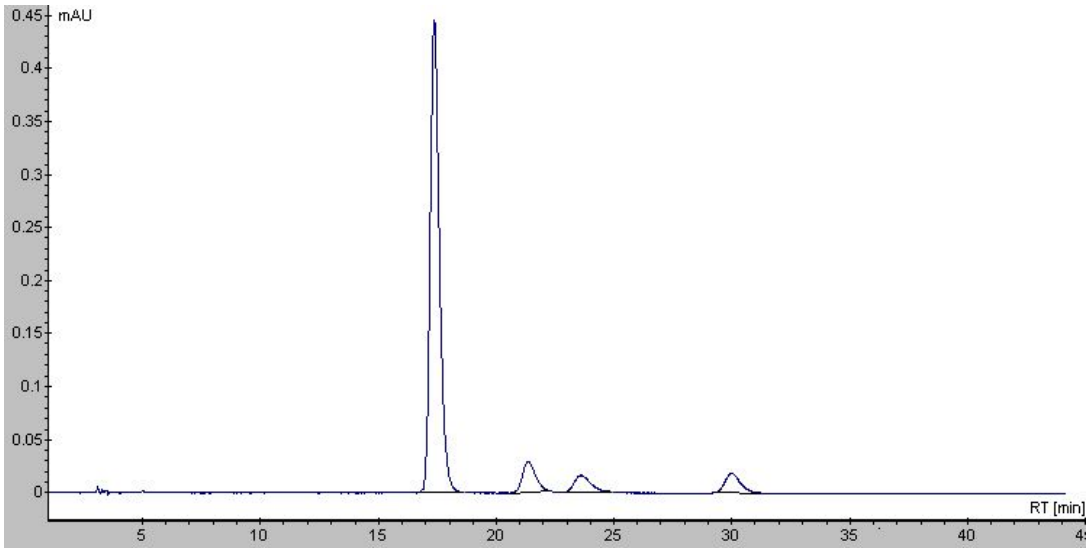


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	10.551	11.119	11.843	83.770
2	11.843	12.292	13.264	7.438
3	15.546	16.145	16.838	4.333
4	18.173	18.705	19.422	4.460

5c

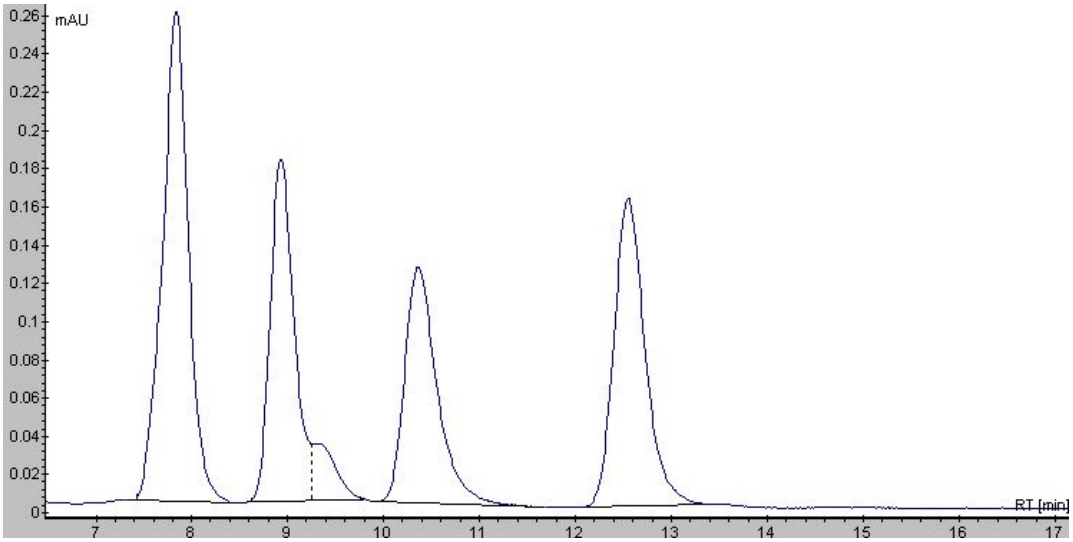


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	19.126	19.839	21.156	34.967
2	23.376	24.212	25.690	16.029
3	26.398	27.625	29.373	16.241
4	29.987	30.864	32.584	32.763

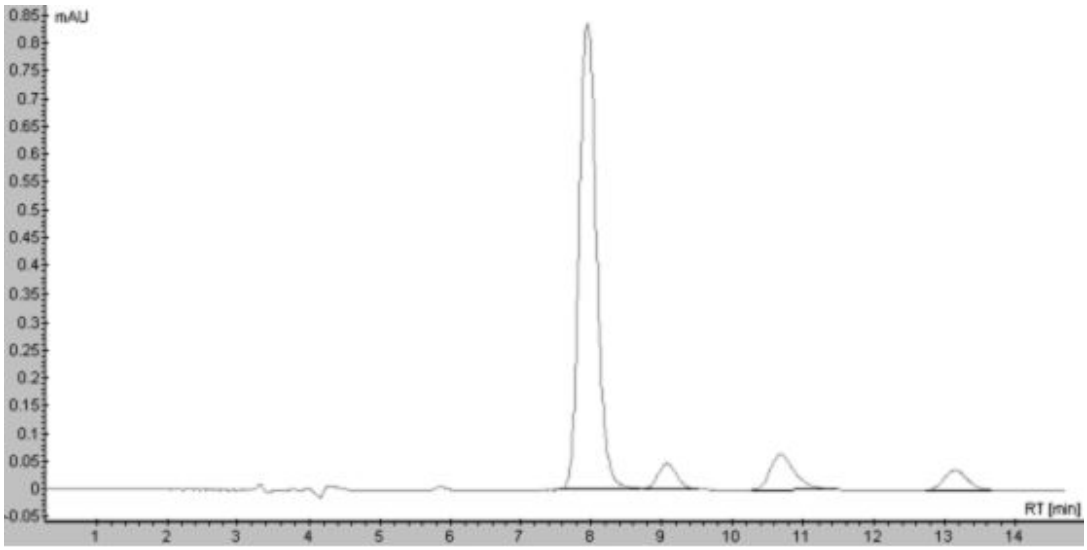


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	16.678	17.359	18.647	81.514
2	20.616	21.345	22.339	7.583
3	22.893	23.585	24.924	5.254
4	29.232	29.984	31.325	5.649

5d

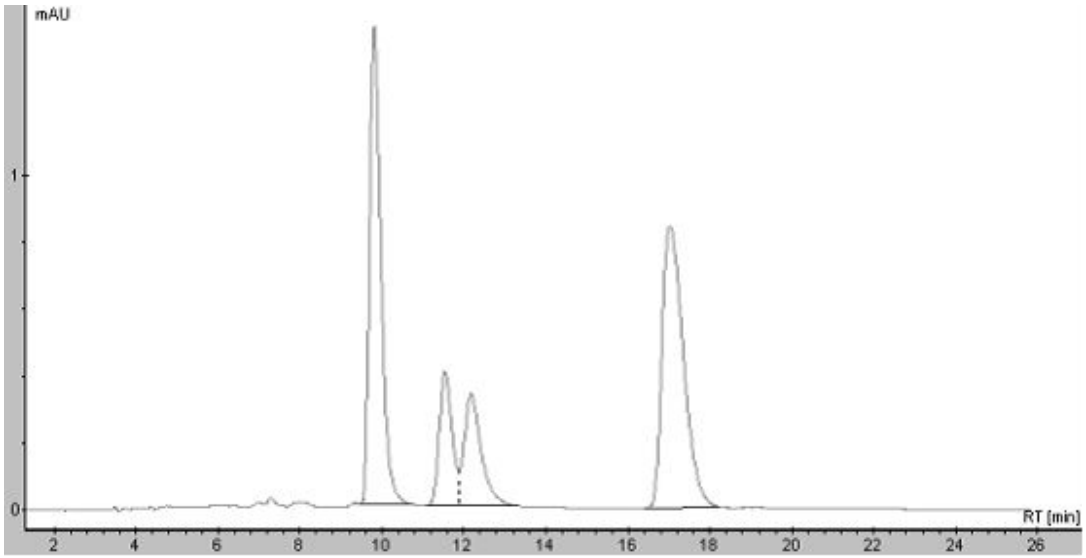


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	7.380	7.839	8.450	33.503
2	8.578	8.933	9.249	21.359
3	9.919	10.359	11.679	20.071
4	12.039	12.546	13.426	25.067

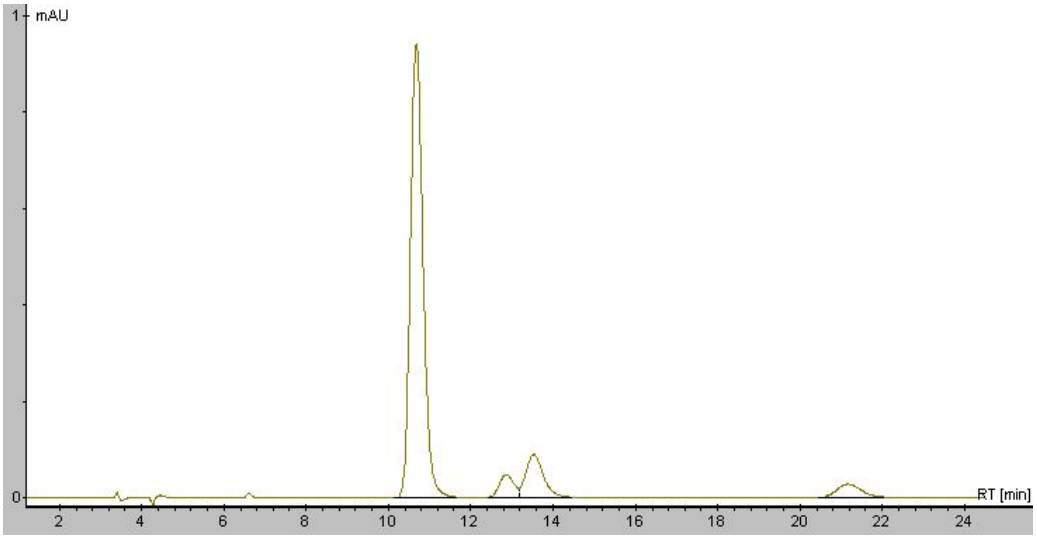


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	7.545	7.947	8.713	81.949
2	8.734	9.080	9.533	4.695
3	10.292	10.693	11.481	8.706
4	12.731	13.147	13.674	4.649

5e

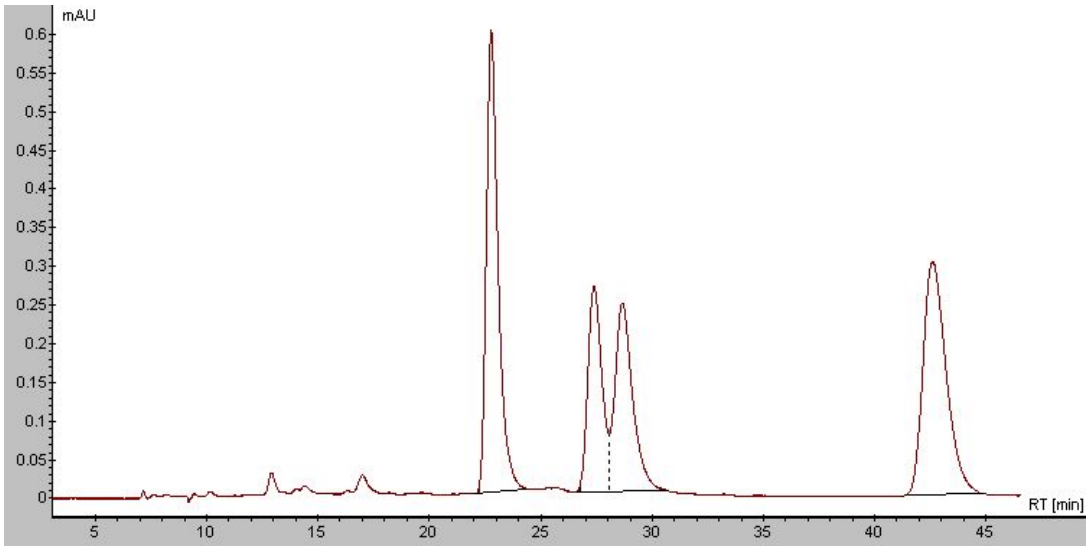


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.465	9.813	10.761	36.294
2	11.085	11.532	11.876	11.305
3	11.876	12.172	13.352	12.735
4	16.411	17.025	18.246	39.666

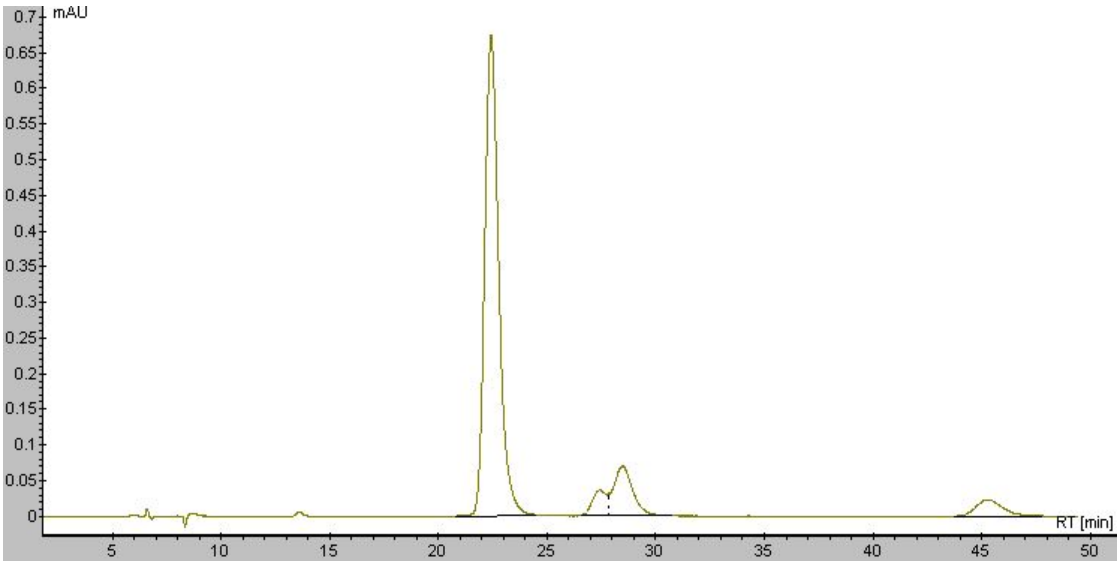


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	10.143	10.679	11.679	80.458
2	12.431	12.866	13.182	4.694
3	13.182	13.532	14.514	10.520
4	20.559	21.158	22.027	4.328

5f

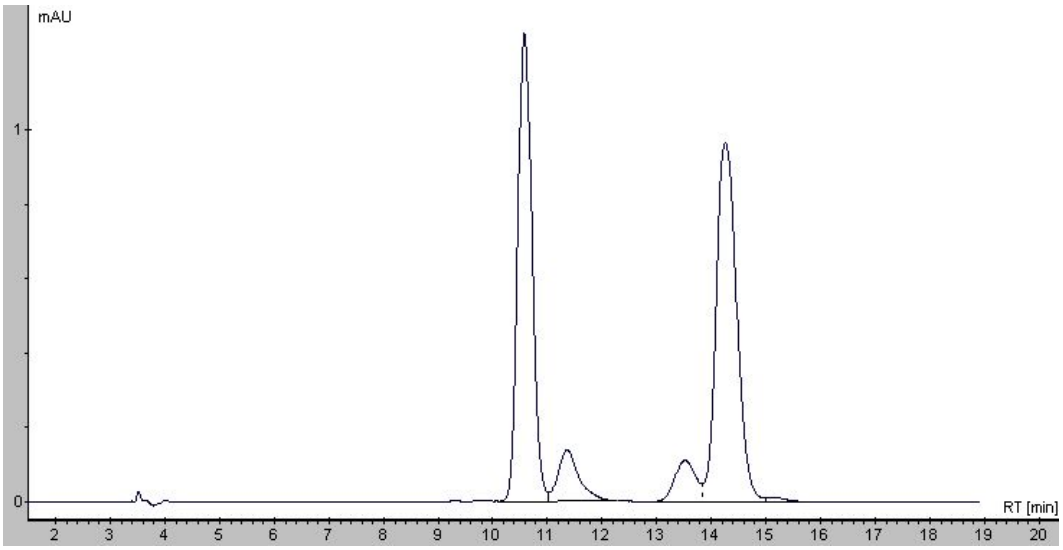


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	22.048	22.722	24.382	31.809
2	26.587	27.398	28.079	16.946
3	28.079	28.665	30.802	19.739
4	41.437	42.610	45.004	31.506

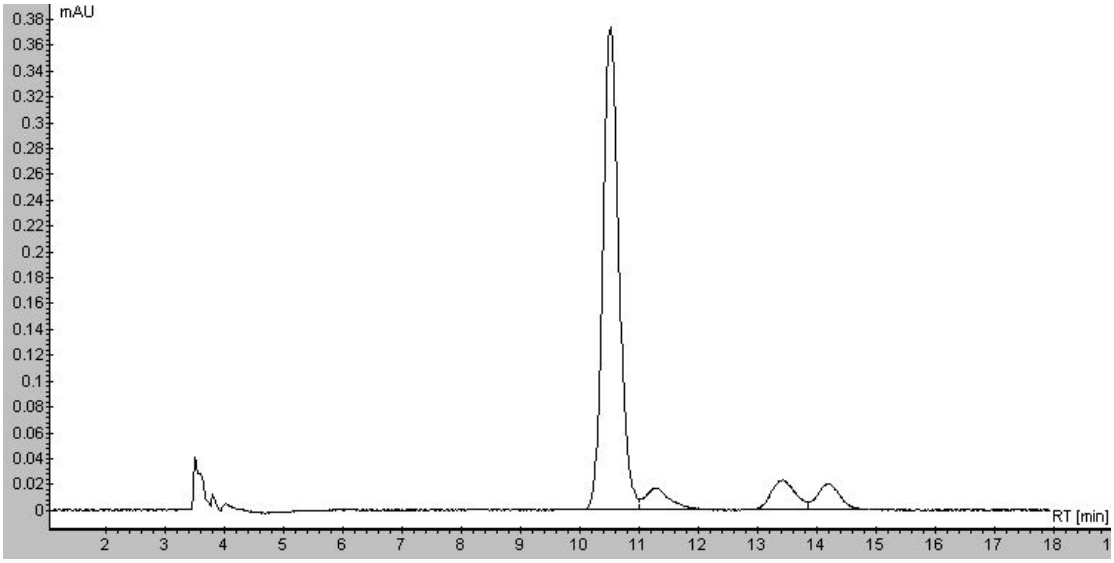


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	20.806	22.438	24.596	79.689
2	26.594	27.438	27.834	4.225
3	27.834	28.465	30.796	10.970
4	43.748	45.277	47.813	5.115

5g

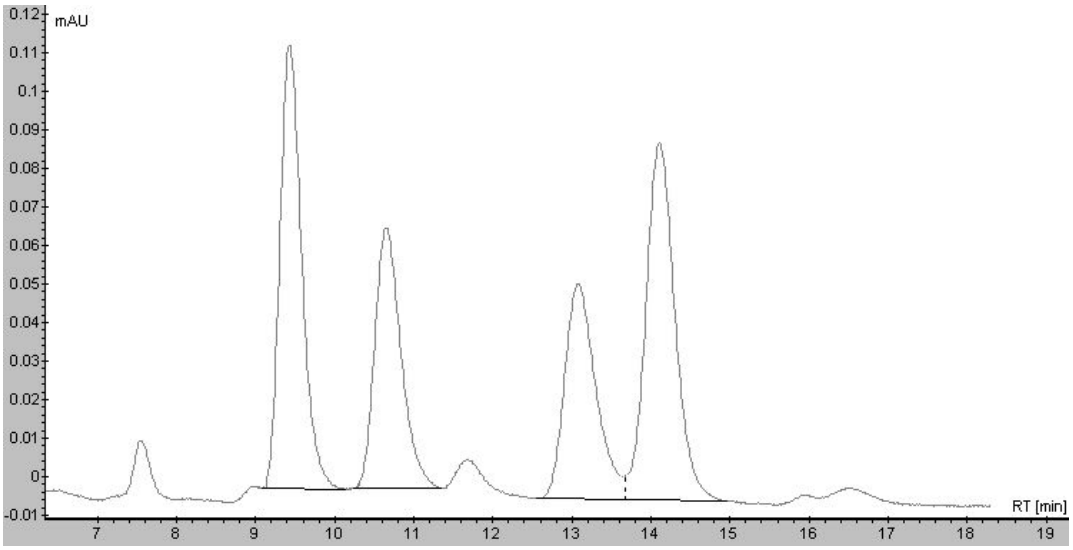


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	10.106	10.573	11.026	42.406
2	11.026	11.359	12.292	6.648
3	12.919	13.519	13.839	5.363
4	13.839	14.252	14.986	45.583

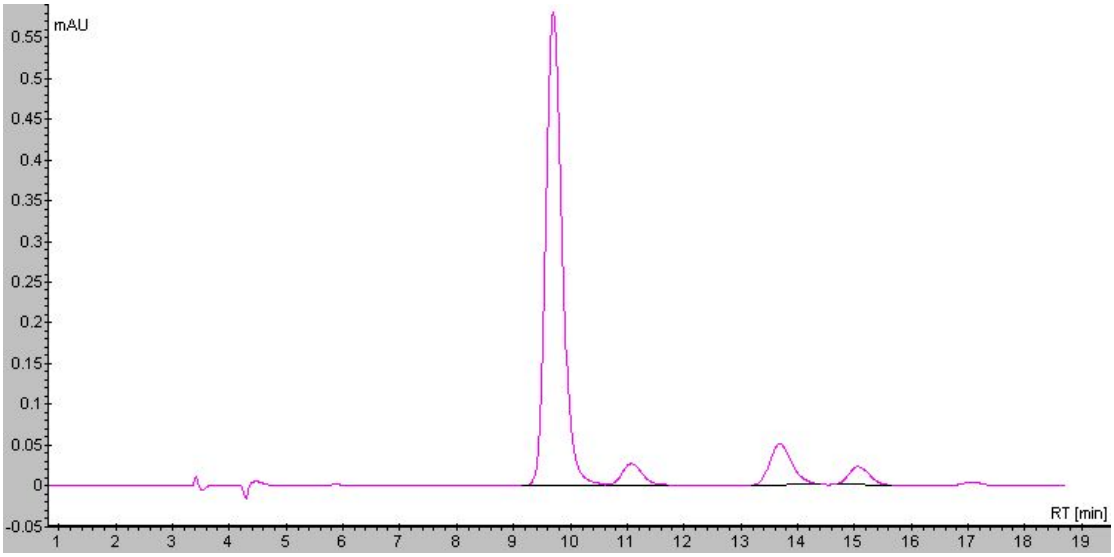


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.986	10.519	11.026	80.997
2	11.026	11.293	12.159	5.402
3	12.839	13.412	13.866	7.592
4	13.866	14.199	14.879	6.009

5h

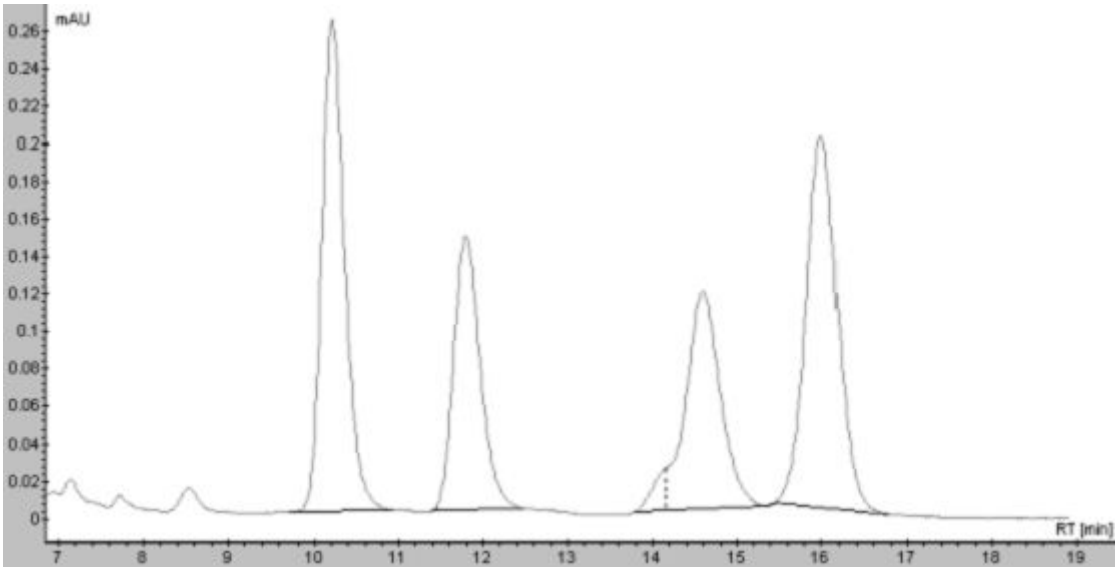


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.084	9.426	10.151	28.789
2	10.241	10.653	11.362	20.341
3	12.555	13.079	13.675	20.030
4	13.675	14.106	14.977	30.840

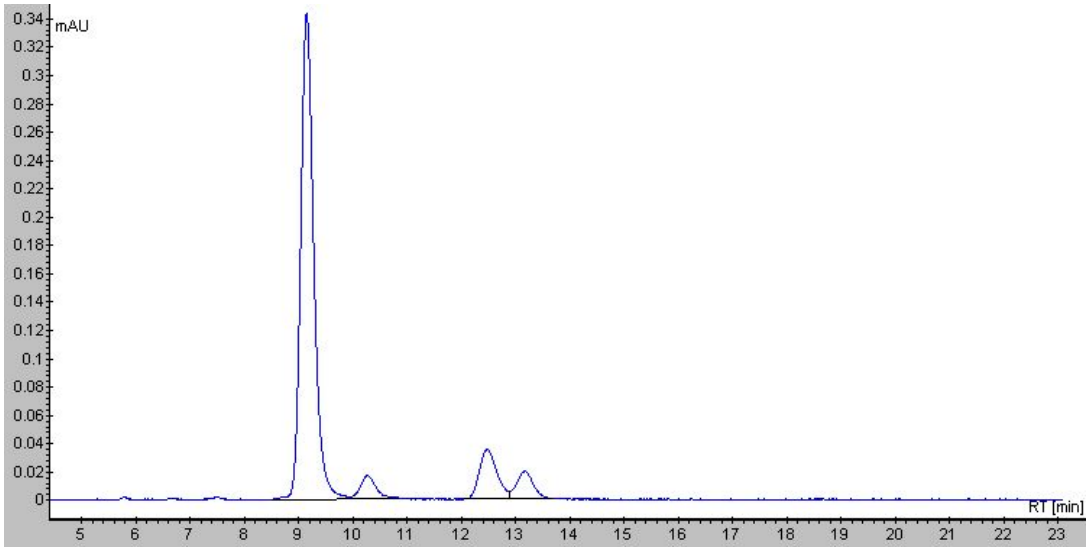


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.153	9.693	10.649	82.365
2	10.649	11.079	11.739	4.446
3	13.188	13.679	14.418	9.487
4	14.699	15.065	15.665	3.702

5i

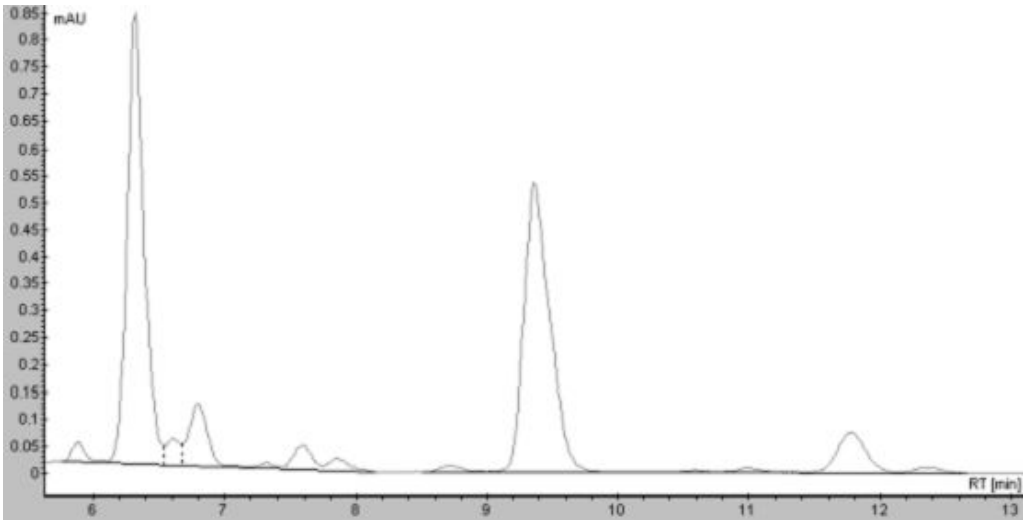


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.709	10.213	10.941	30.002
2	11.399	11.786	12.490	19.438
3	14.162	14.599	15.395	20.082
4	15.447	15.986	16.785	30.478

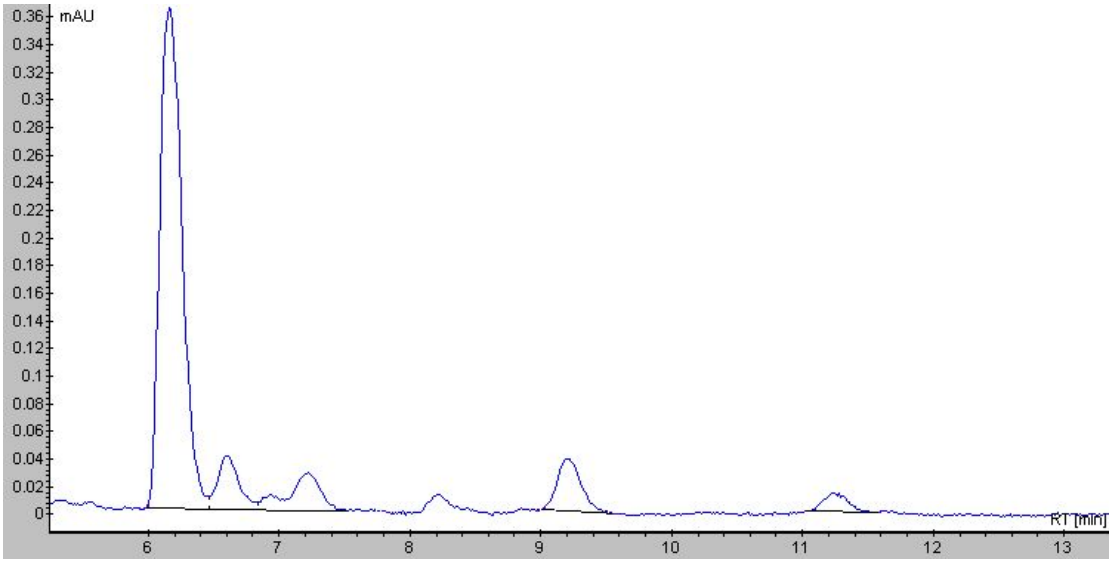


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	8.512	9.146	9.899	78.902
2	9.899	10.266	10.886	4.417
3	12.059	12.479	12.885	10.938
4	12.885	13.172	13.686	5.742

5j

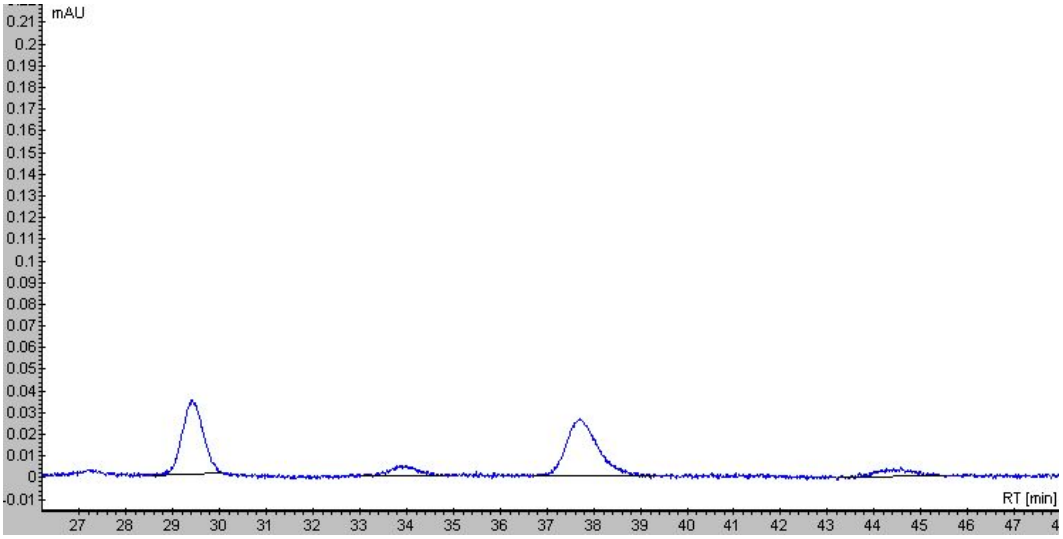


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	6.107	6.320	6.547	43.580
2	6.680	6.800	7.013	6.624
3	8.960	9.360	10.053	42.995
4	11.320	11.773	12.160	6.801

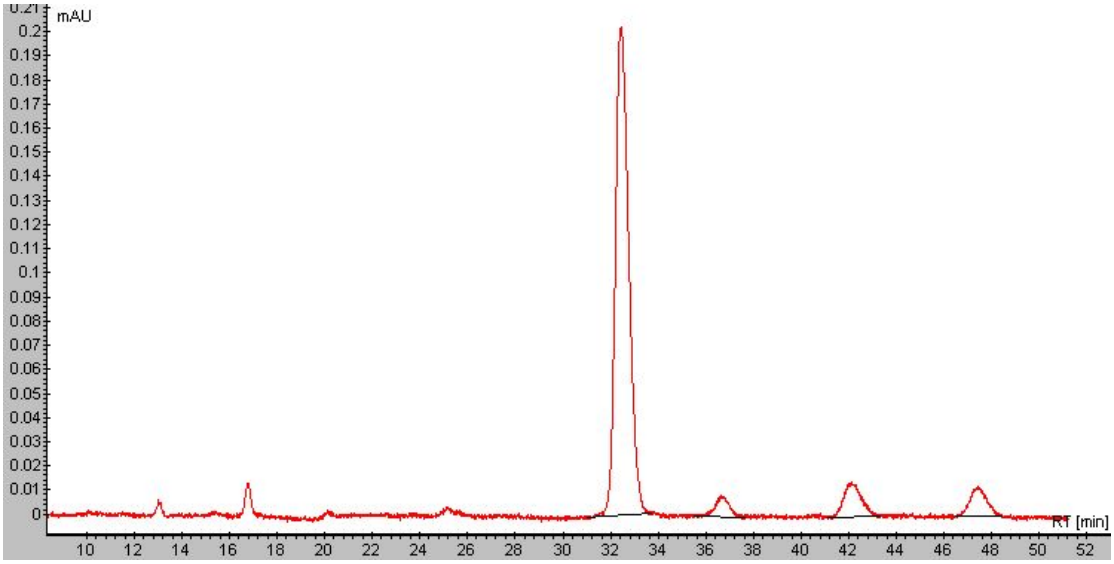


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	5.973	6.160	6.466	79.609
2	6.466	6.600	6.840	8.321
3	9.014	9.199	9.600	8.981
4	11.024	11.239	11.594	3.088

5k

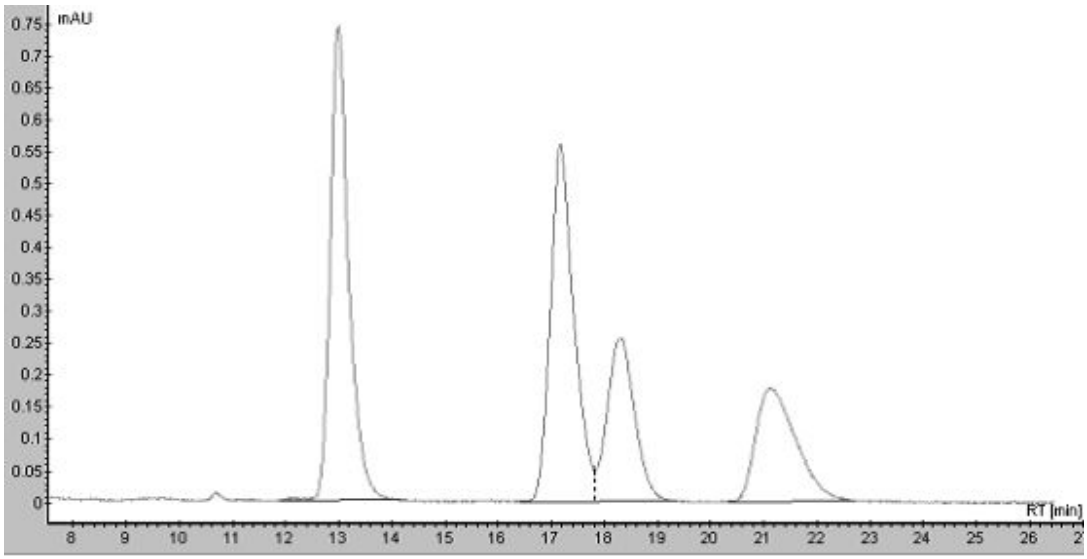


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	28.438	29.425	30.078	40.105
2	33.038	33.958	34.811	6.744
3	36.744	37.691	39.450	46.084
4	43.250	44.423	45.557	7.068

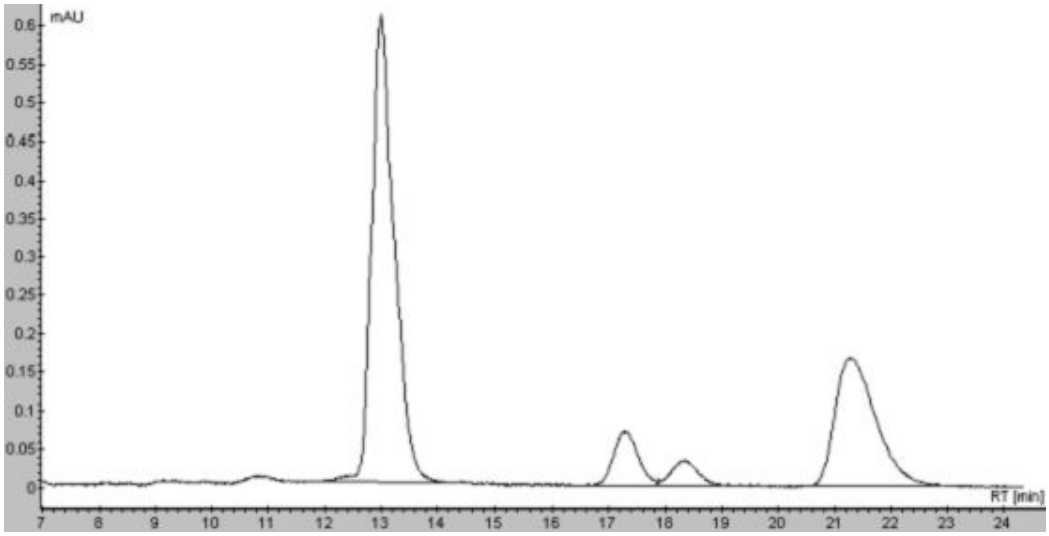


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	30.904	32.438	33.758	82.424
2	35.517	36.704	37.704	3.724
3	41.184	42.130	43.410	7.670
4	46.543	47.463	48.530	6.181

5l

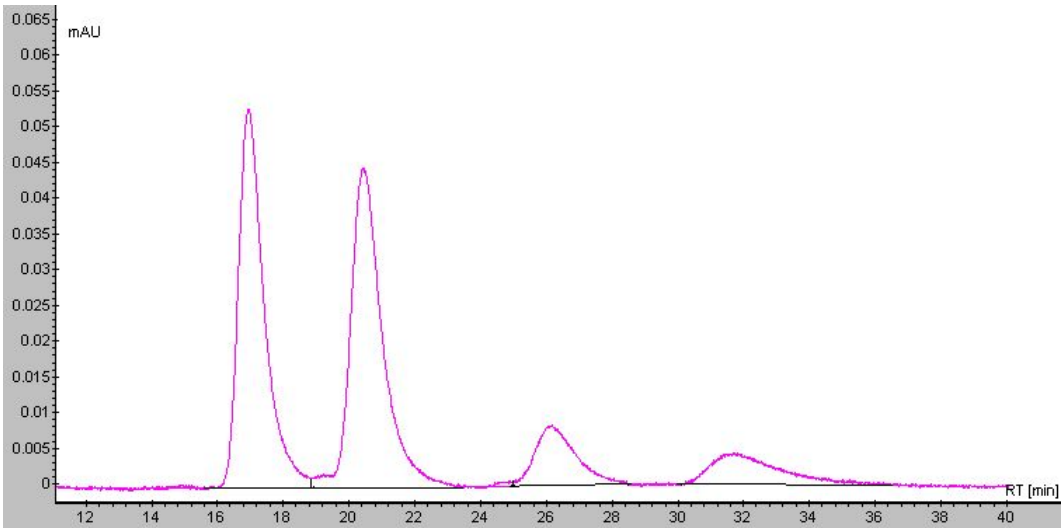


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.319	12.986	14.172	33.471
2	16.439	17.172	17.825	32.098
3	17.825	18.292	19.385	17.118
4	20.345	21.132	22.732	17.313

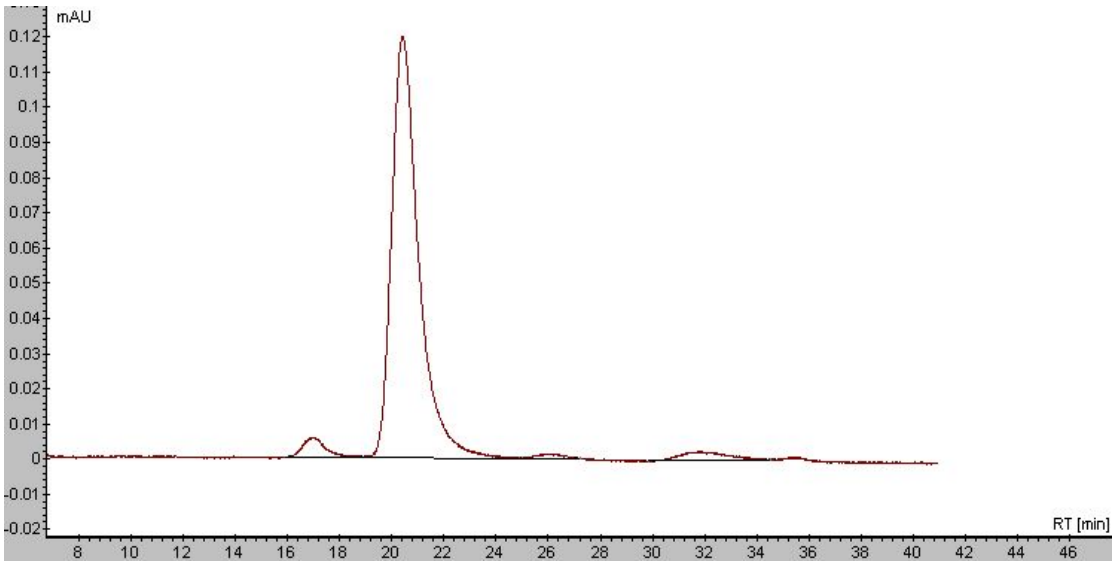


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.782	12.986	14.090	59.506
2	16.705	17.265	17.865	7.537
3	17.865	18.345	19.025	3.594
4	20.479	21.278	22.918	29.364

5m

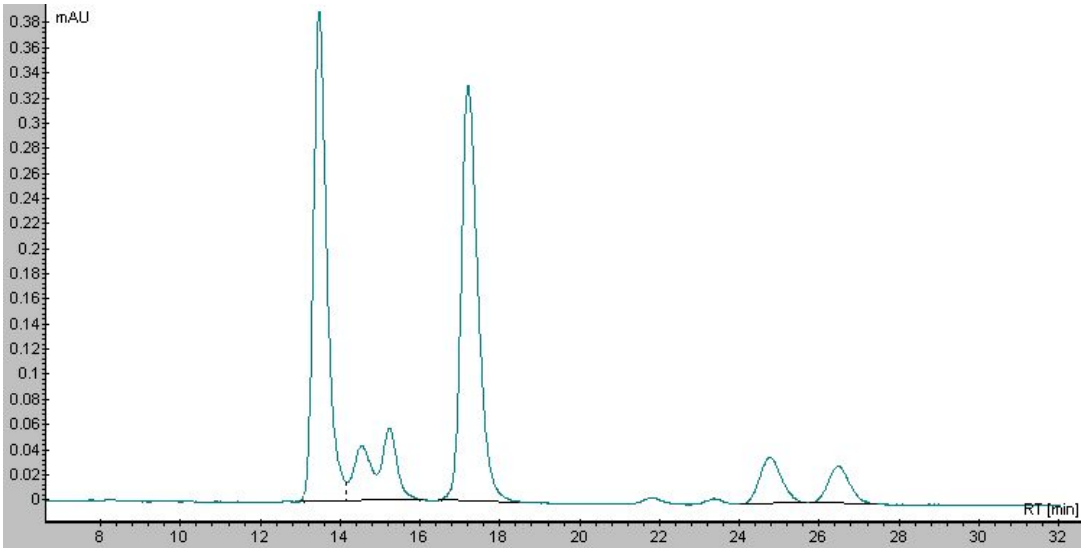


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	15.586	16.945	18.905	40.283
2	19.399	20.452	23.492	40.960
3	24.985	26.118	28.598	10.040
4	29.983	31.638	36.536	8.717

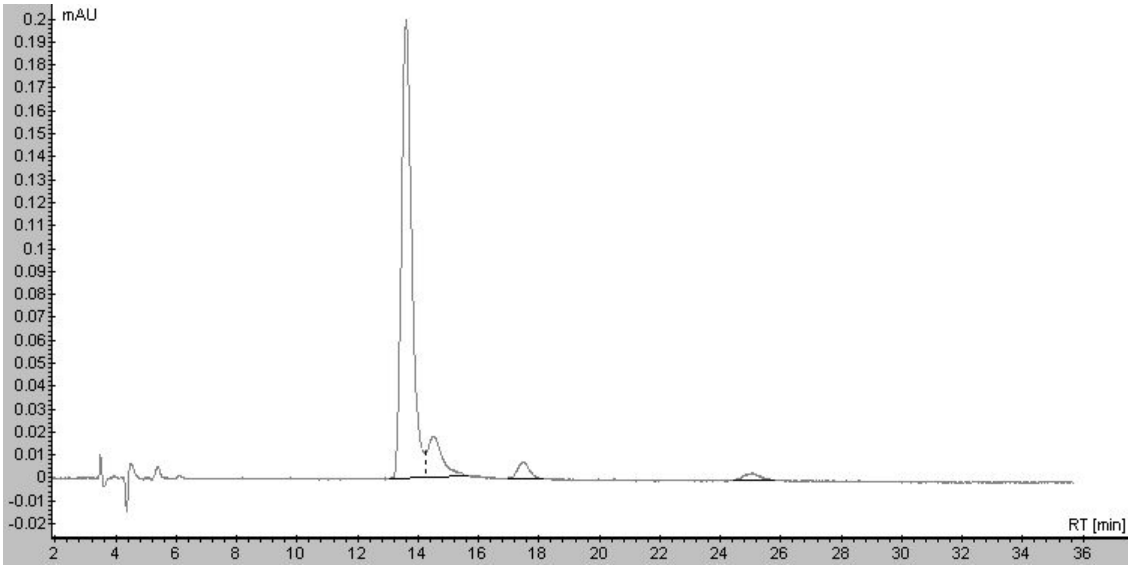


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	15.919	16.999	18.185	3.725
2	18.825	20.412	24.932	92.122
3	24.932	26.051	27.211	0.932
4	29.859	31.731	34.534	3.220

5n

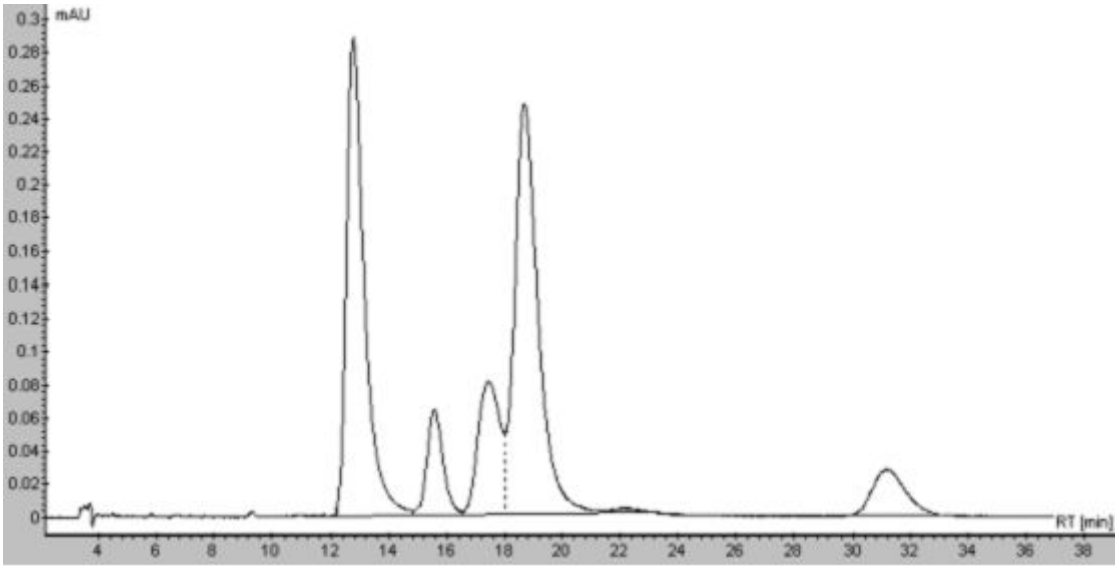


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.991	13.479	14.152	43.042
2	16.428	17.199	18.482	45.187
3	24.018	24.758	25.669	6.559
4	25.759	26.478	27.455	5.212

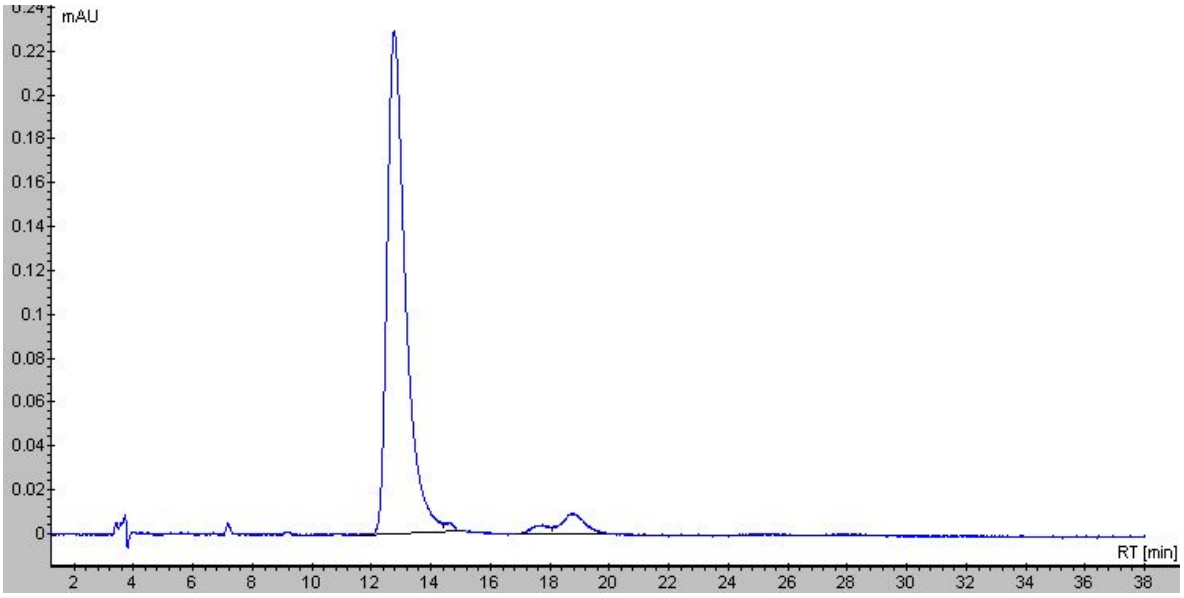


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.065	13.599	14.257	94.251
2	16.989	17.479	18.181	3.656
3	24.440	25.012	25.632	2.093

5o

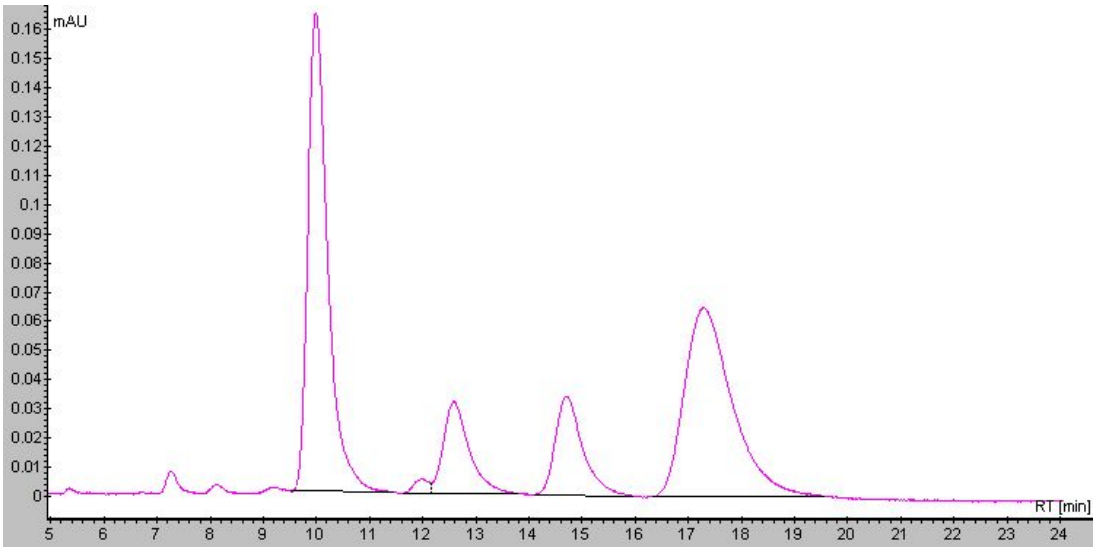


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.999	12.759	14.852	40.026
2	14.852	15.559	16.505	7.896
3	17.999	18.679	21.305	45.084
4	29.811	31.158	33.078	6.994

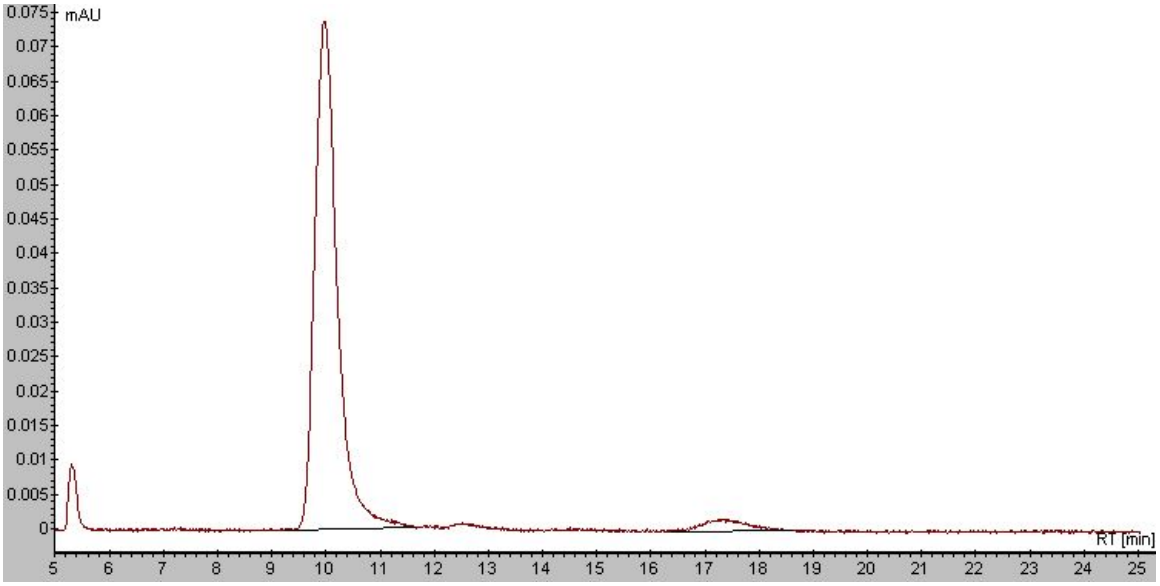


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.559	12.759	14.426	95.265
2	18.092	18.772	19.945	4.735

5p

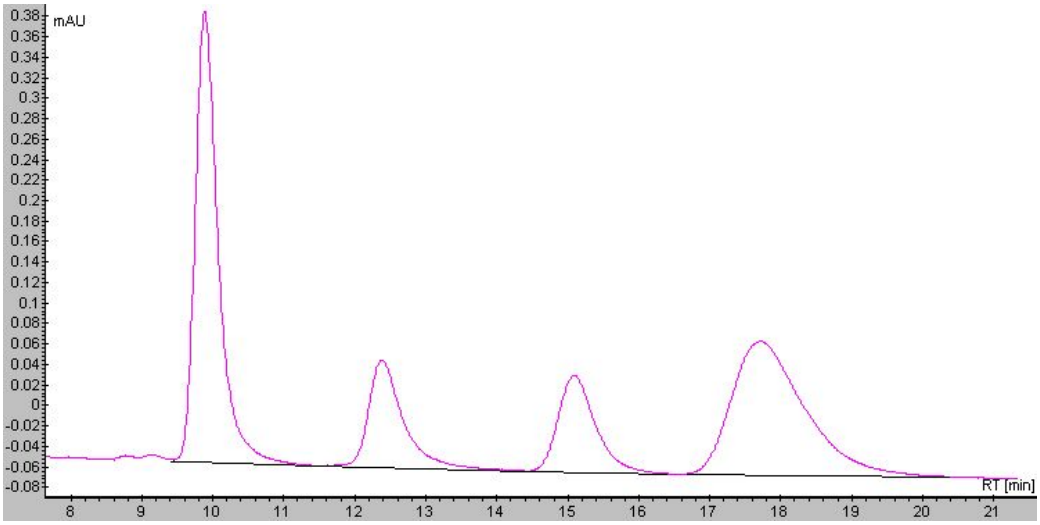


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.515	9.986	11.483	40.363
2	12. 160	12.586	13. 822	9.958
3	14.106	14.706	15.986	11.477
4	16.336	17.292	19.593	38.202

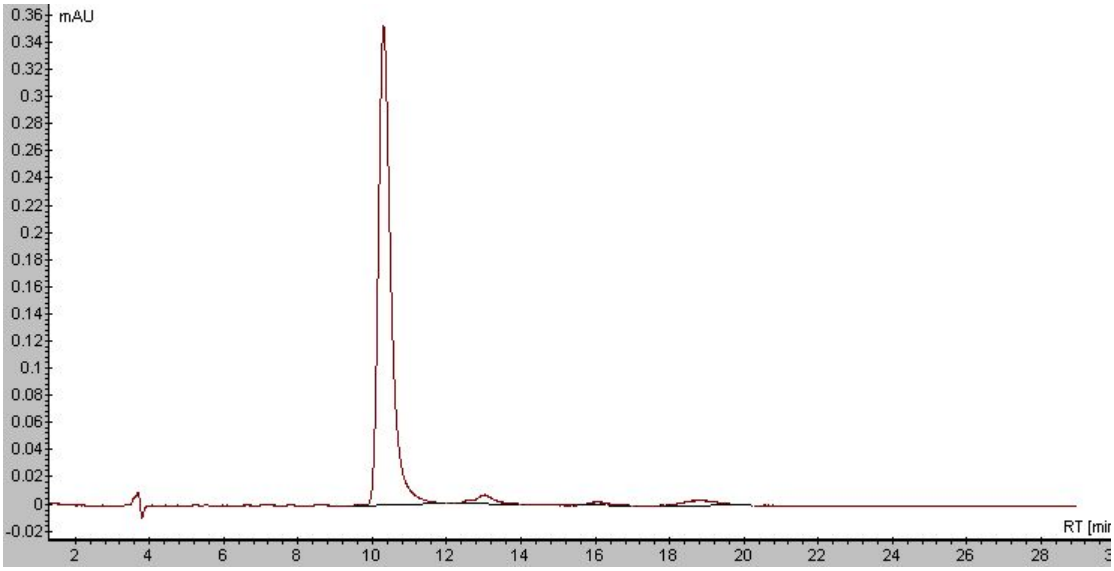


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.257	9.973	11.681	95.835
2	16.385	17.372	18.625	4.165

5q

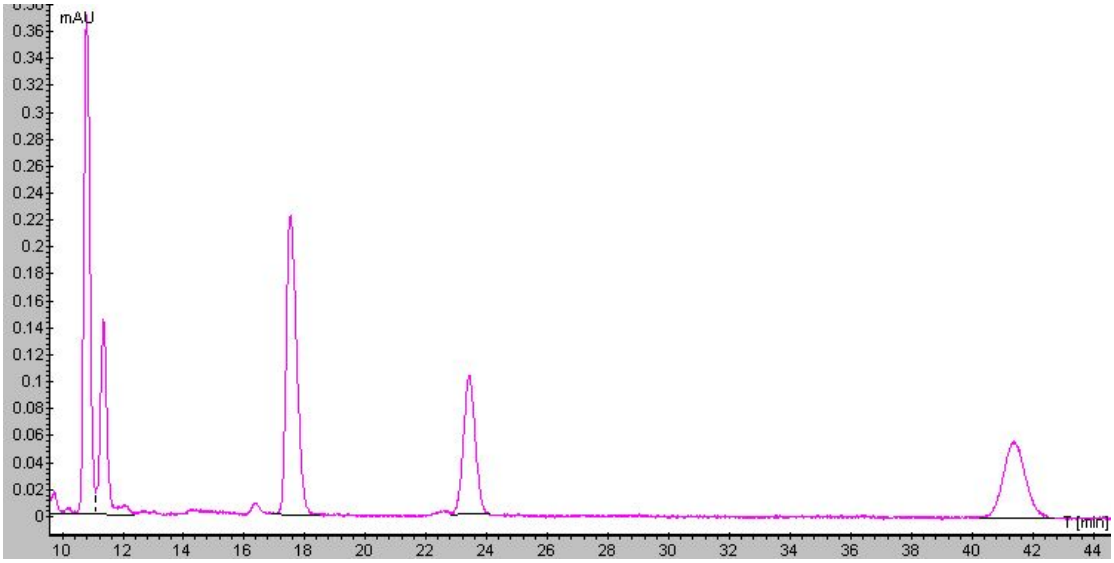


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.453	9.879	11.453	38.172
2	11.453	12.386	14.399	13.470
3	14.399	15.092	16.505	13.050
4	16.532	17.705	20.385	35.308

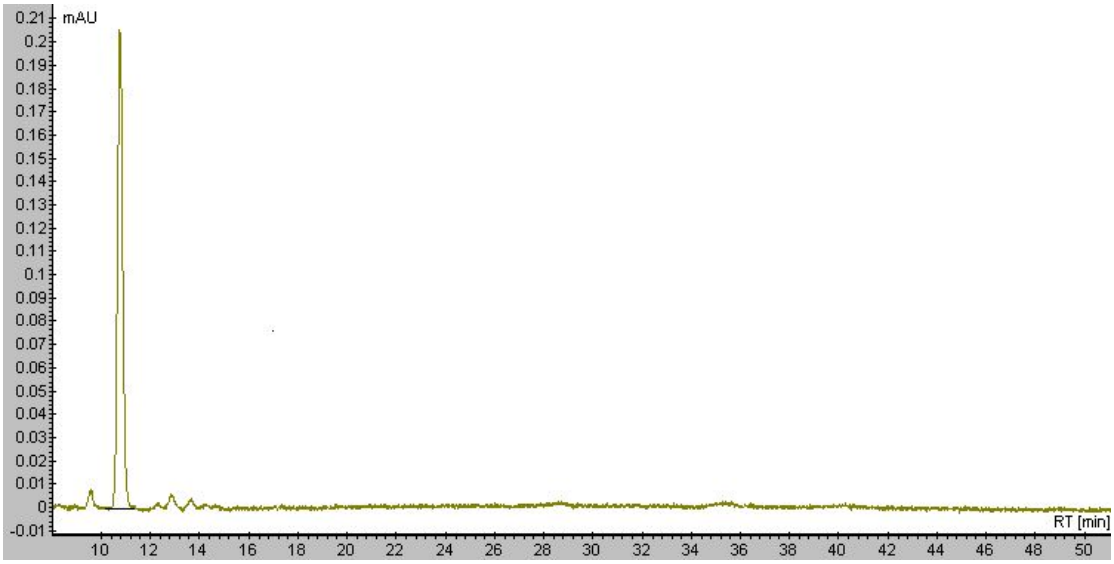


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.494	10.306	11.975	93.510
2	12.275	13.012	13.956	2.781
3	15.516	16.026	16.997	0.974
4	17.857	18.799	20.318	2.735

5r

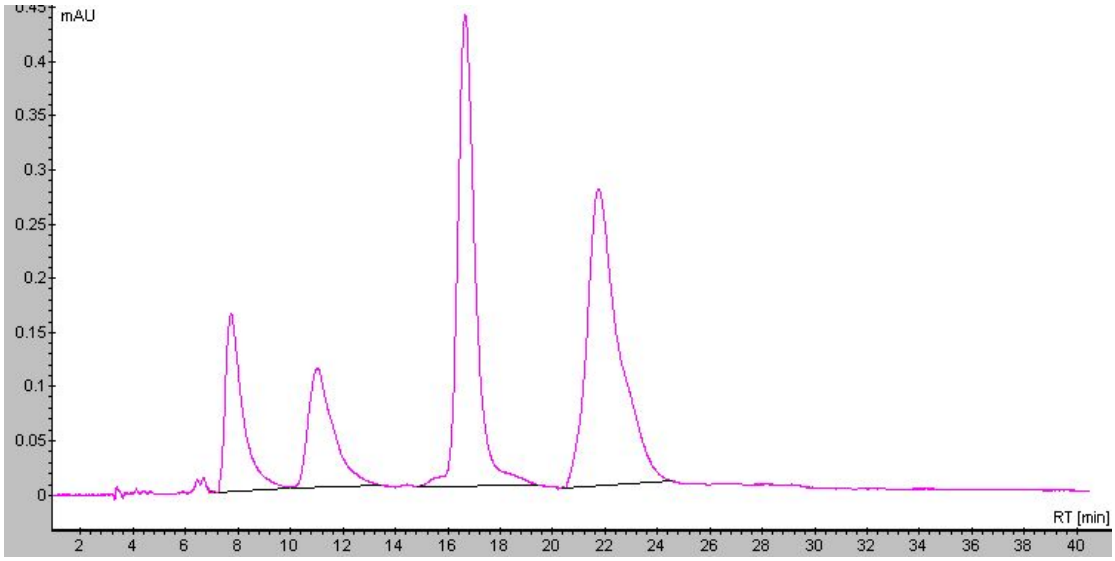


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	10.413	10.799	11.119	31.942
2	17.079	17.519	18.532	32.972
3	22.838	23.412	24.145	17.440
4	40.237	41.370	42.744	17.646

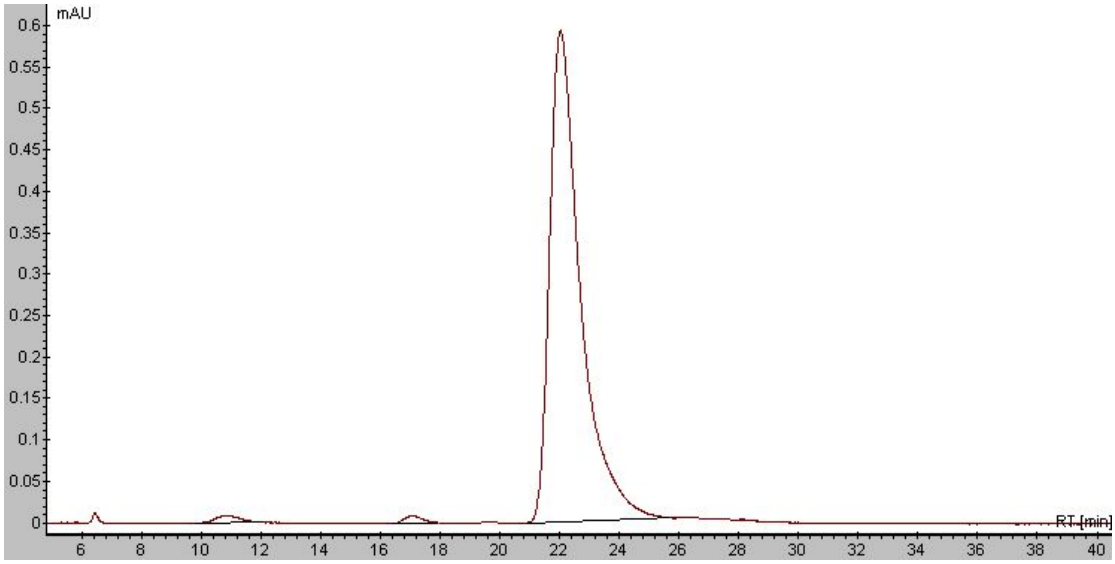


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	10.160	10.759	11.377	100.00

5s

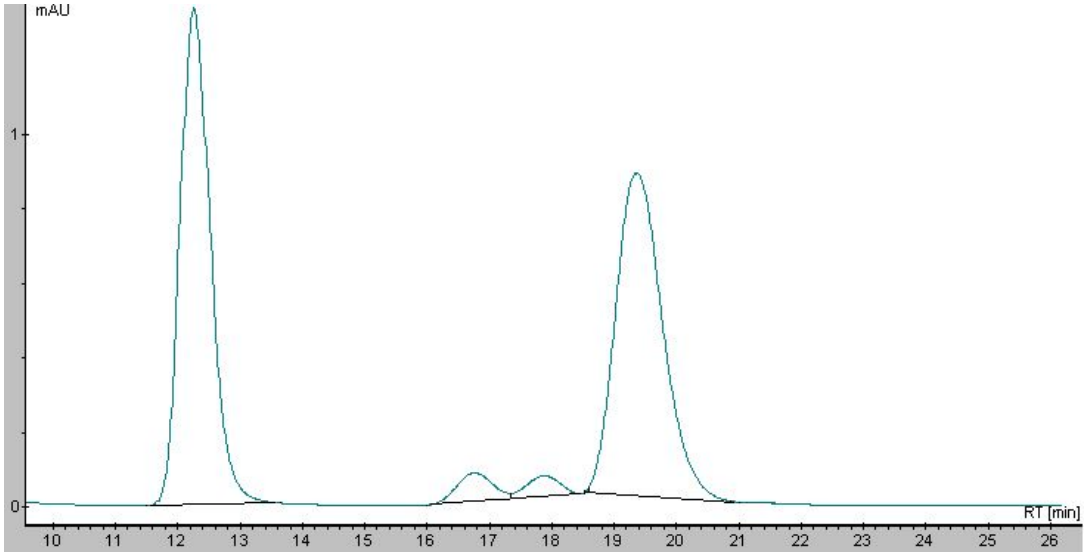


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	7.111	7.733	9.989	12.848
2	10.045	11.026	13.544	12.472
3	14.842	16.665	19.470	35.029
4	20.373	21.758	24.605	39.651

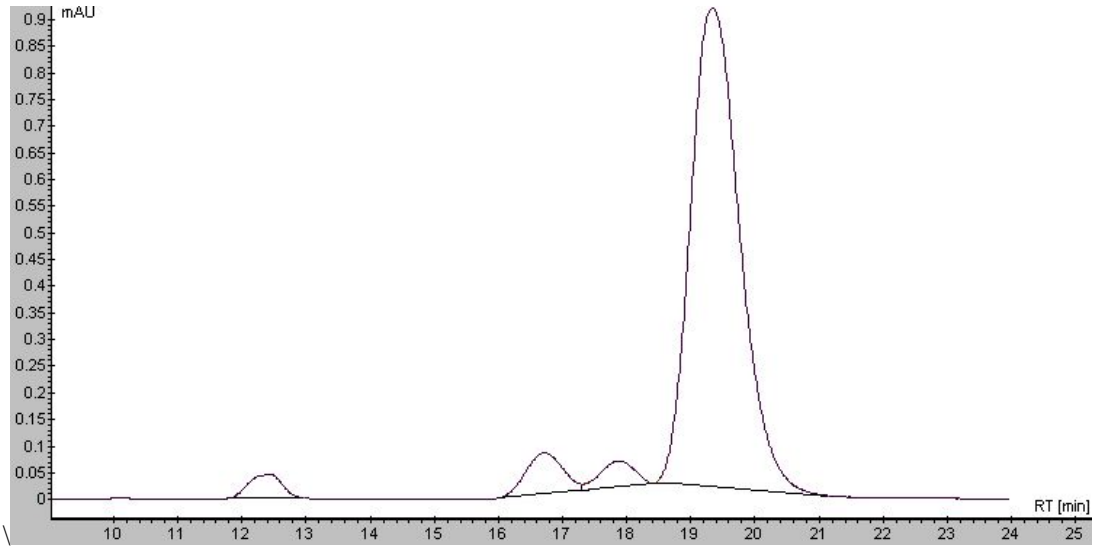


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.800	10.836	12.175	1.189
2	16.421	17.061	17.968	0.866
3	20.919	22.032	25.885	97.945

5t

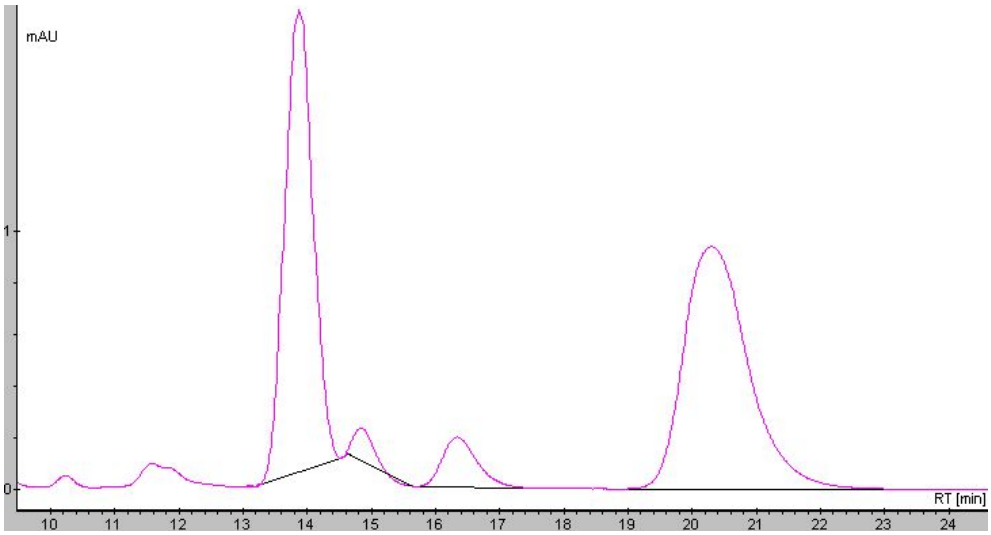


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.563	12.252	13.575	47.236
2	16.061	16.745	17.339	3.202
3	17.339	17.865	18.451	2.215
4	18.522	19.359	20.937	47.347

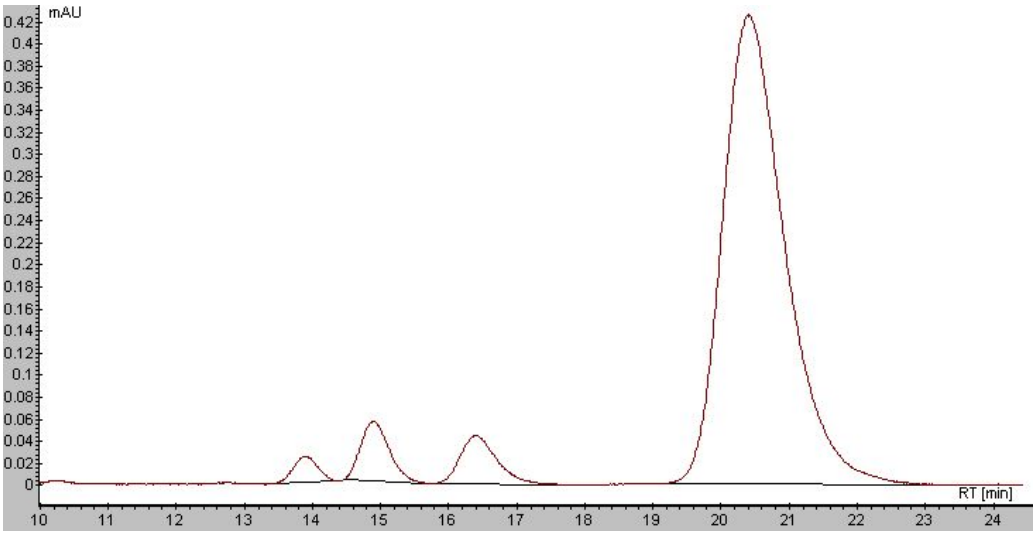


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.789	12.426	12.967	2.953
2	15.981	16.705	17.295	5.649
3	17.295	17.852	18.428	3.324
4	18.473	19.332	21.147	88.073

5u

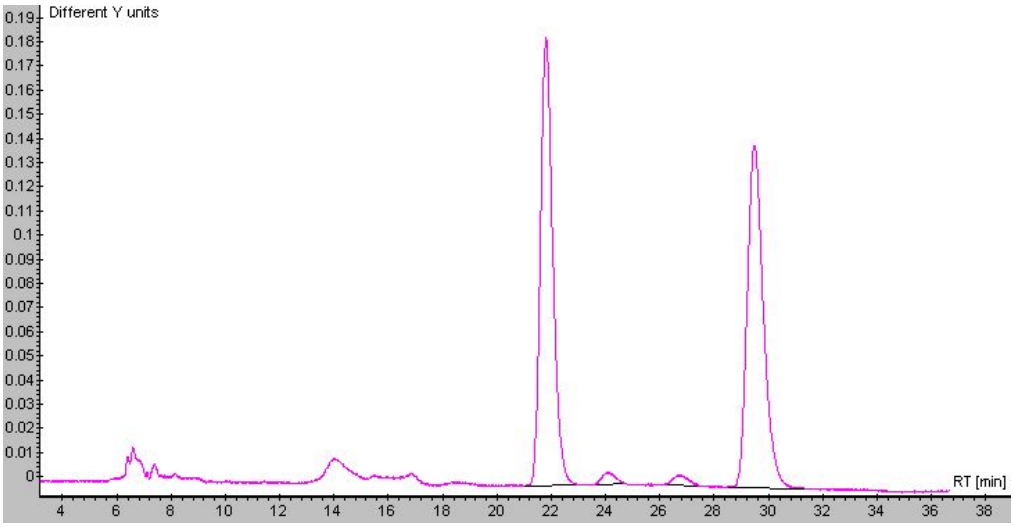


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.171	13.866	14.523	48.590
2	14.607	14.866	15.643	1.450
3	15.748	16.332	17.438	1.466
4	18.981	20.292	23.079	48.953

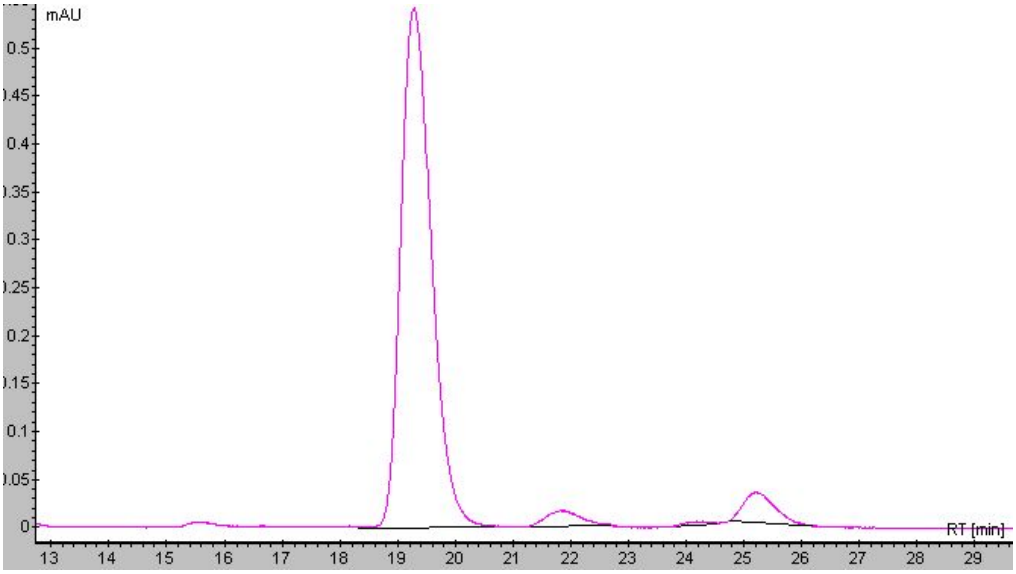


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.450	13.892	14.348	1.864
2	14.476	14.892	15.631	5.041
3	15.802	16.399	17.684	5.232
4	18.988	20.399	23.991	87.862

7a

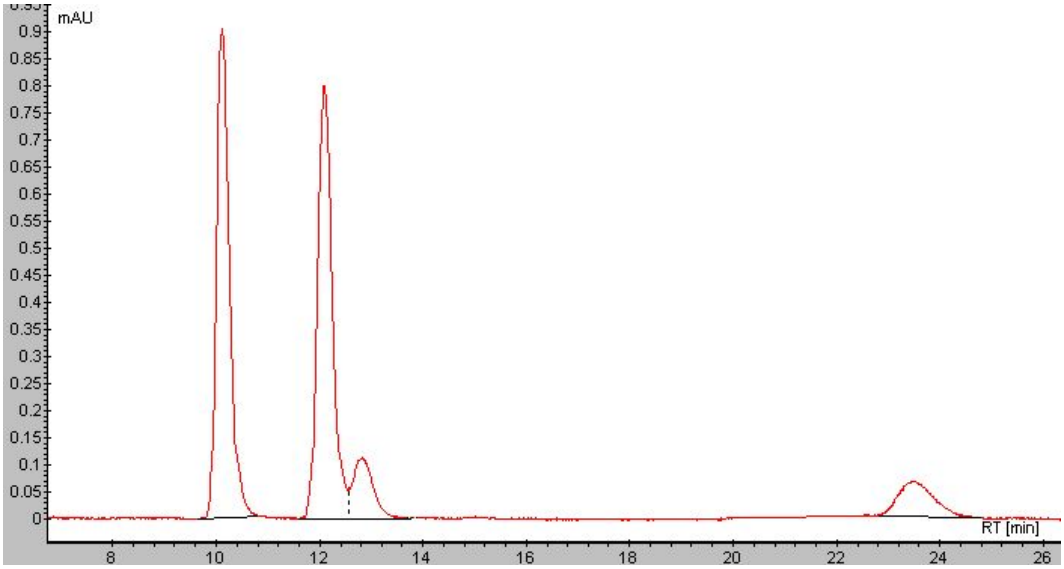


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	21.032	21.812	23.023	48.590
2	23.585	24.092	24.963	1.450
3	26.137	26.731	27.618	1.466
4	28.537	29.478	31.497	48.493

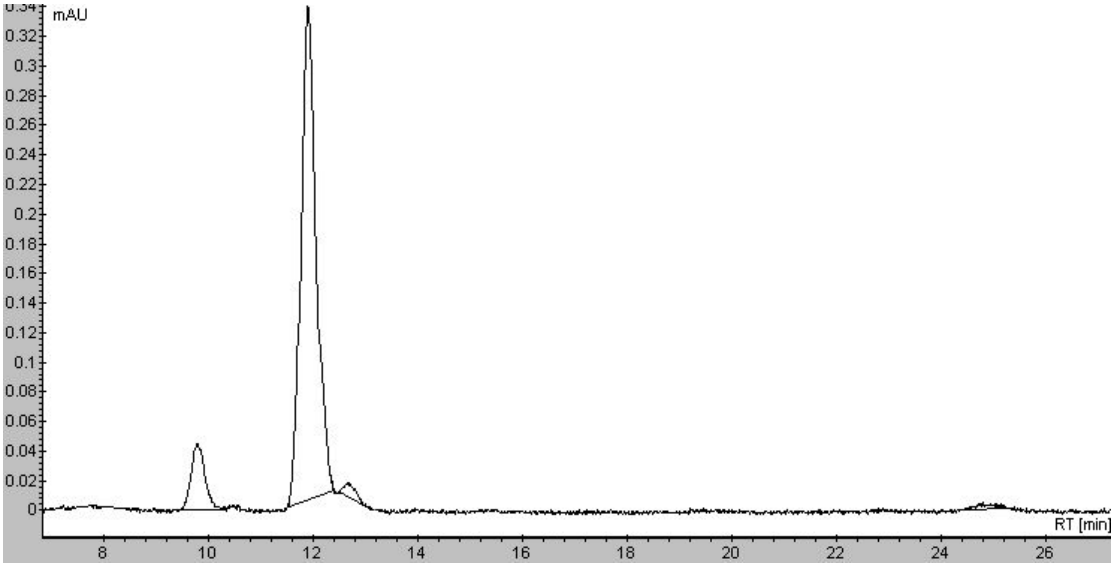


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	18.250	19.292	20.874	91.154
2	21.252	21.838	22.718	3.061
3	23.687	24.172	24.585	0.428
4	24.751	25.212	26.382	5.357

7b

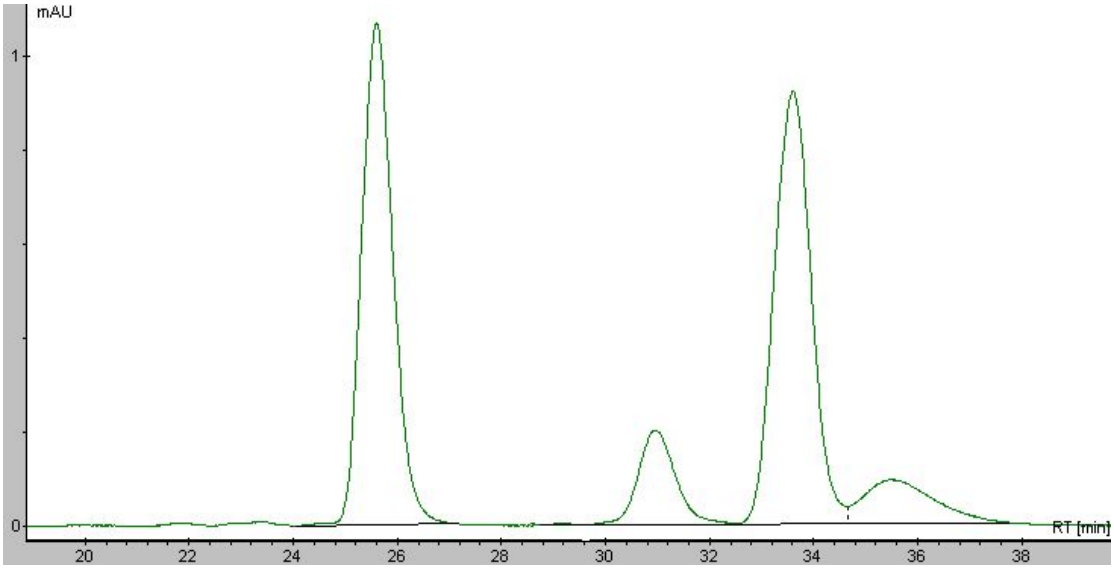


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.653	10.119	10.933	41.896
2	11.599	12.092	12.559	41.832
3	12.599	12.826	13.799	7.974
4	22.705	23.492	24.825	8.299

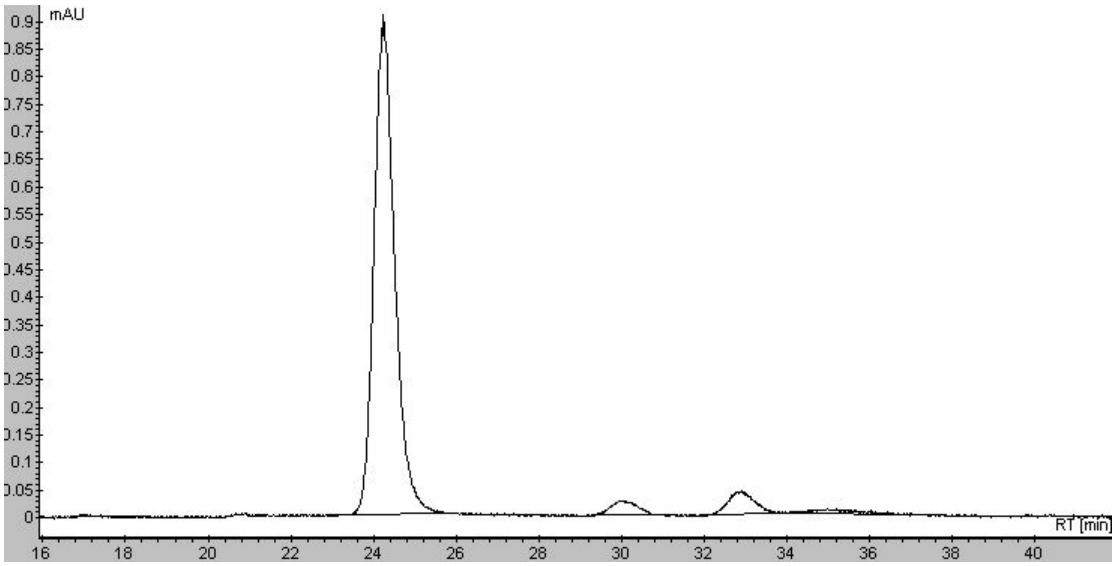


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.575	9.786	10.071	7.765
2	11.463	11.892	12.406	88.986
3	12.486	12.679	13.174	2.076
4	24.460	24.905	25.318	1.173

7c

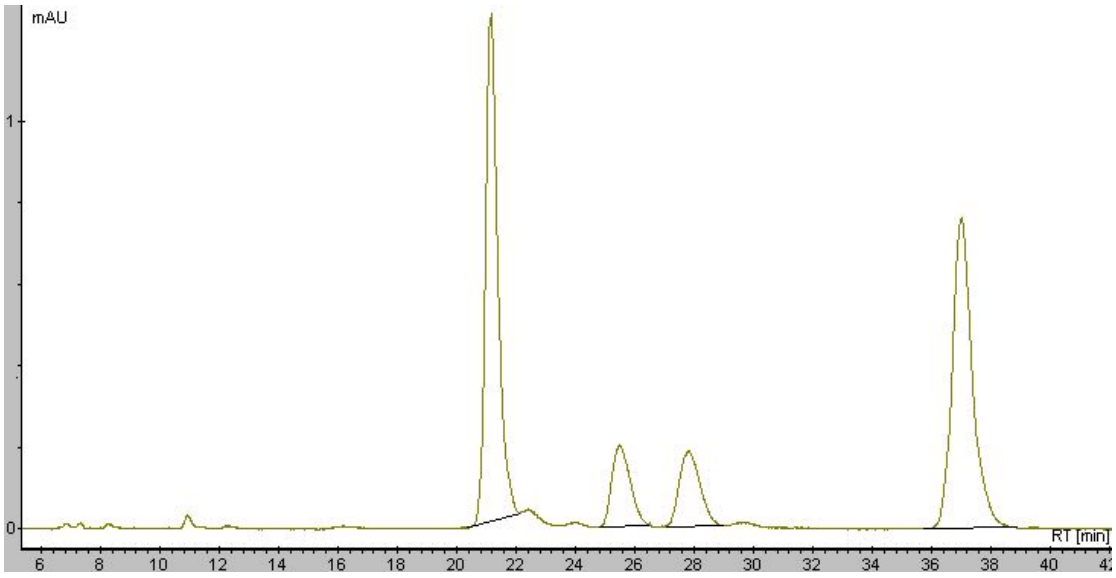


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	24.705	25.611	27.211	40.766
2	29.598	30.971	32.504	9.159
3	32.504	33.611	34.651	41.631
4	34.651	35.504	38.024	8.444

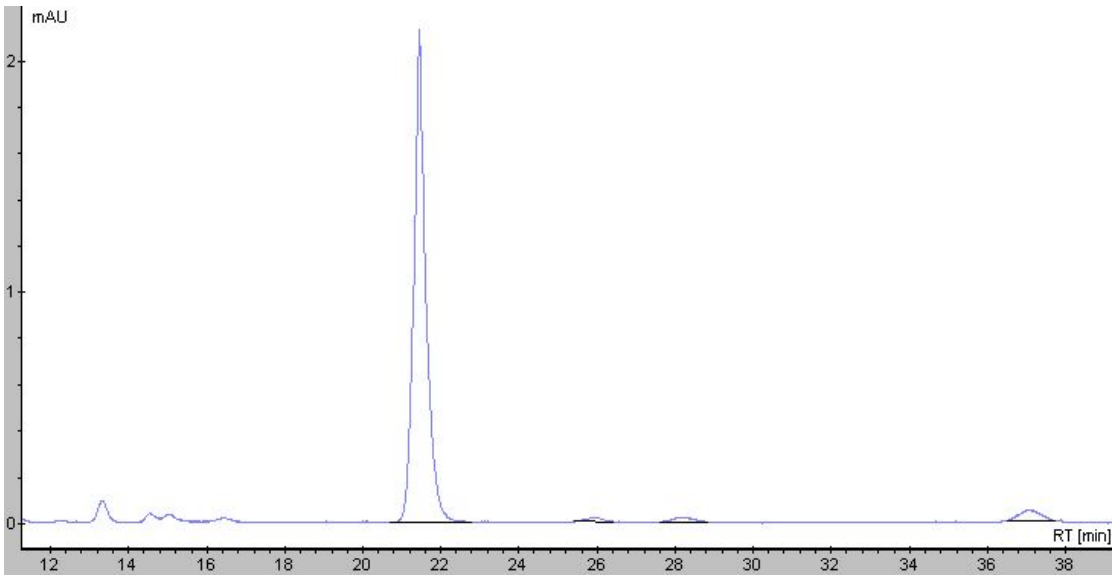


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	23.418	24.238	25.913	90.311
2	29.453	29.998	30.903	3.050
3	32.252	32.864	33.702	4.951
4	34.005	34.997	37.208	1.688

7d

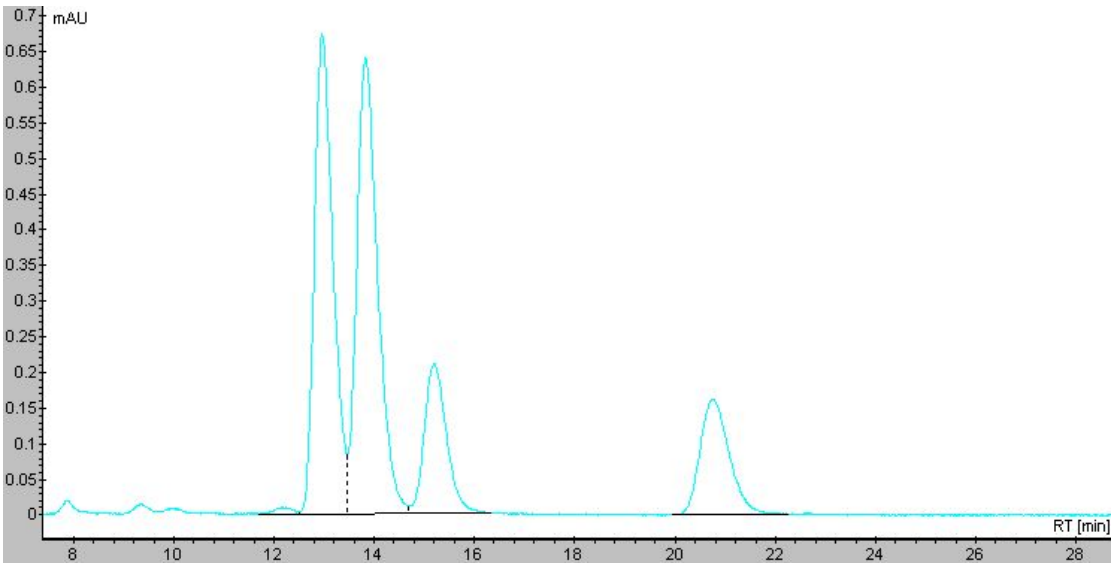


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	20.277	21.158	22.135	40.315
2	24.807	25.478	26.535	9.494
3	27.056	27.811	29.044	9.946
4	35.725	37.011	39.049	40.245

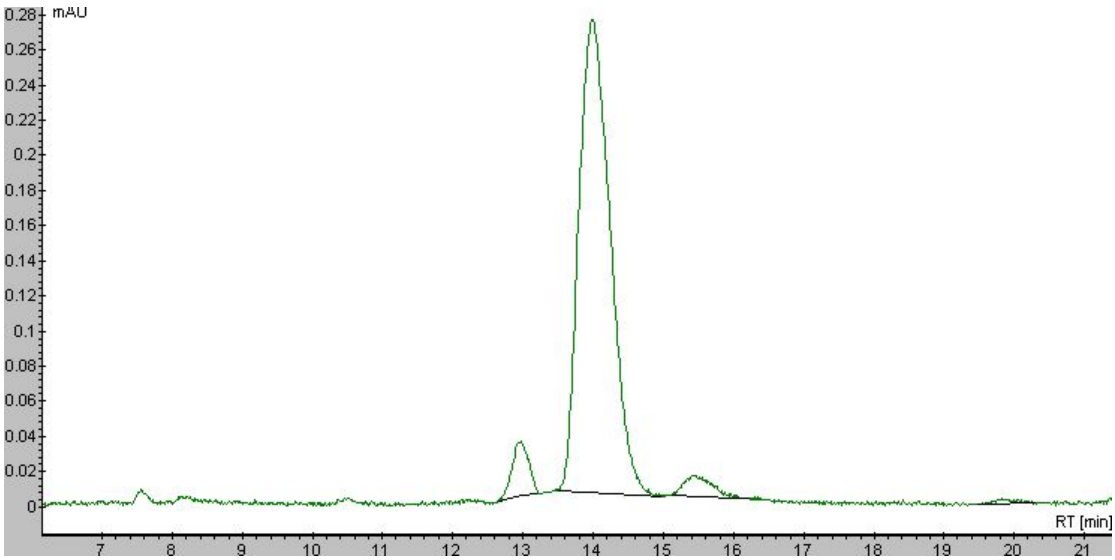


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	20.691	21.452	22.810	93.761
2	25.413	25.918	26.442	0.989
3	27.623	28.171	28.924	1.553
4	36.522	37.091	37.763	3.697

7e

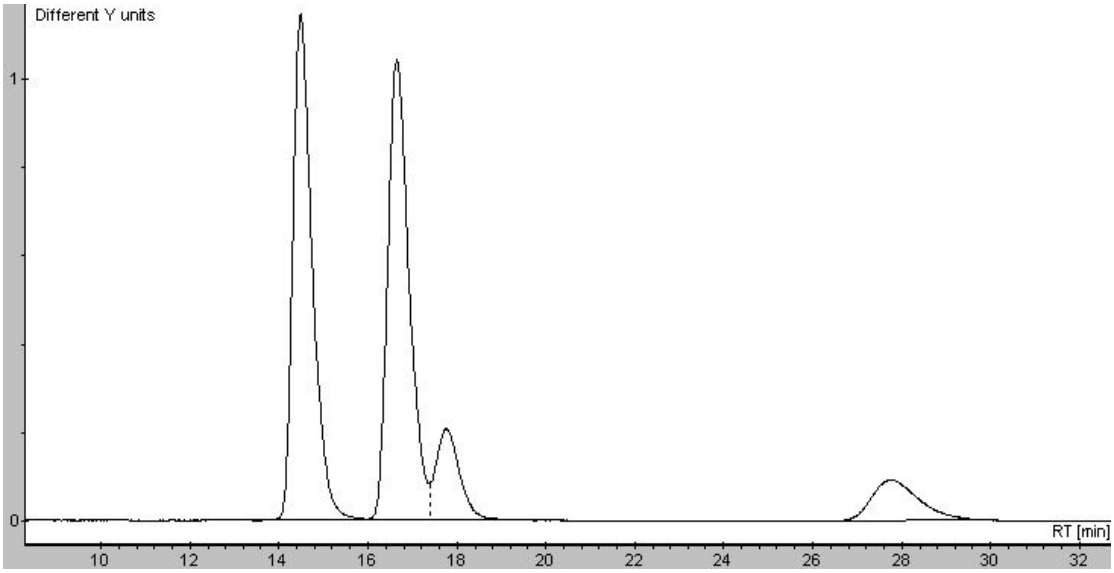


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.492	12.959	13.466	35.587
2	13.466	13.826	14.692	37.924
3	14.692	15.199	16.345	13.143
4	19.945	20.758	22.412	13.346

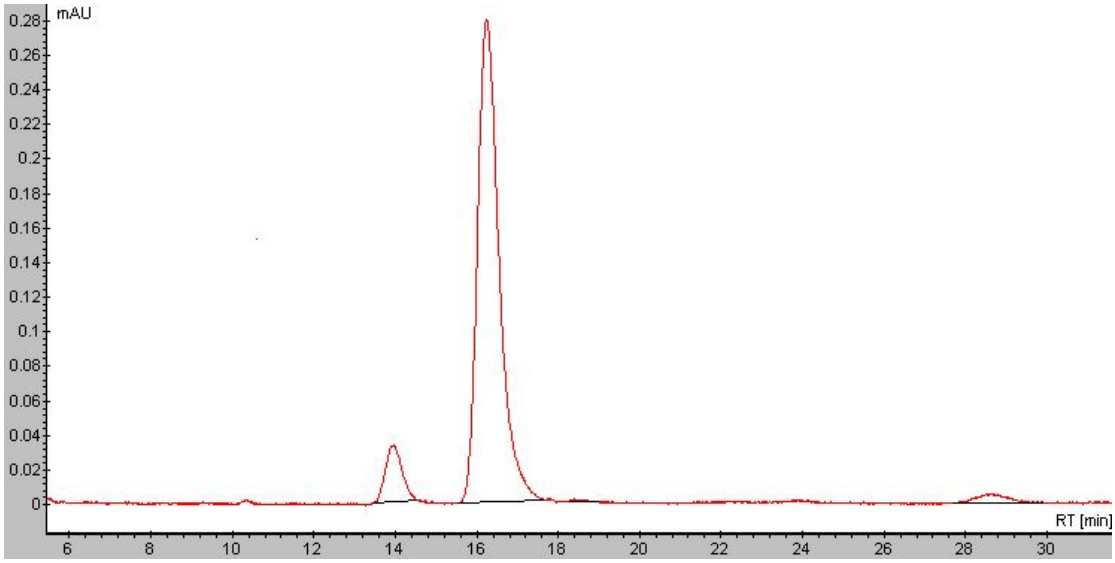


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.633	12.956	13.230	6.250
2	13.498	13.986	15.000	89.762
3	15.113	15.466	16.456	3.465
4	19.459	19.892	20.415	0.523

7f

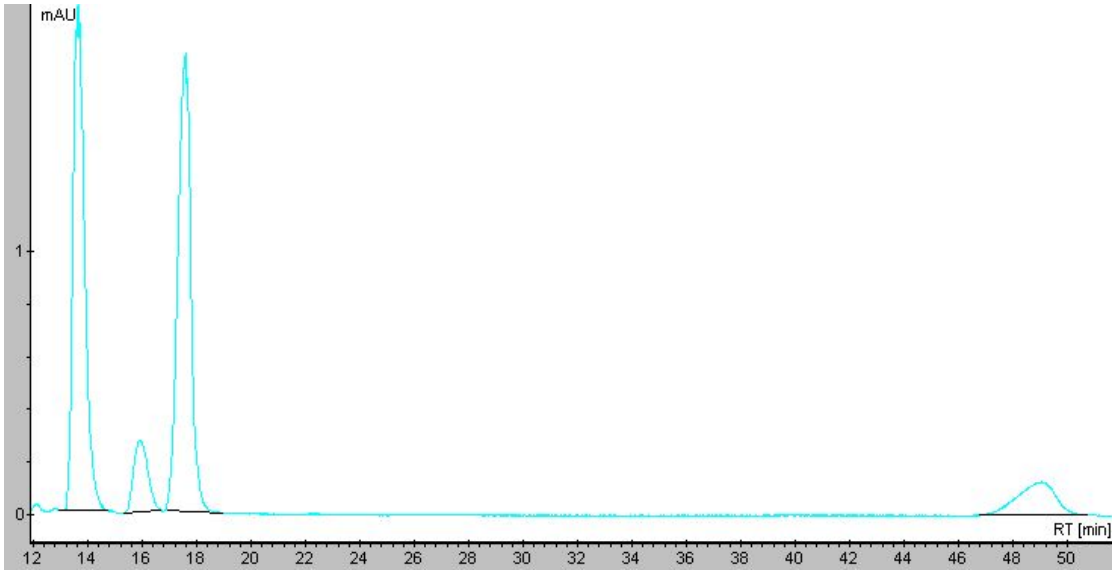


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.746	14.492	15.986	41.619
2	15.986	16.665	17.385	41.486
3	17.385	17.759	18.959	8.946
4	26.585	27.745	29.665	7.950

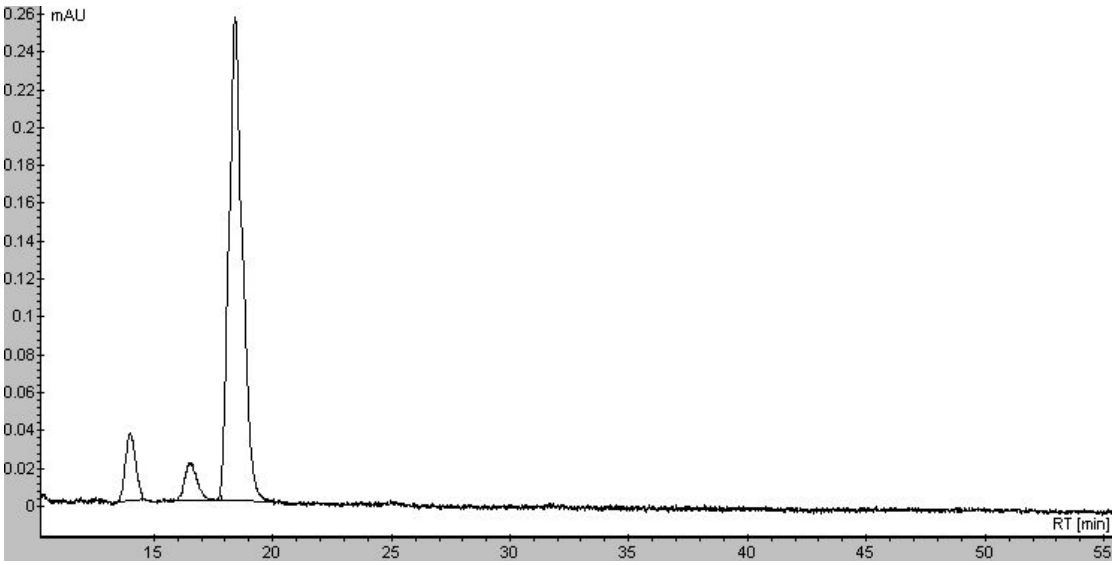


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.455	13.932	14.612	8.114
2	15.557	16.239	17.750	89.332
3	18.268	18.505	19.030	0.177
4	27.591	28.611	30.058	2.377

7g

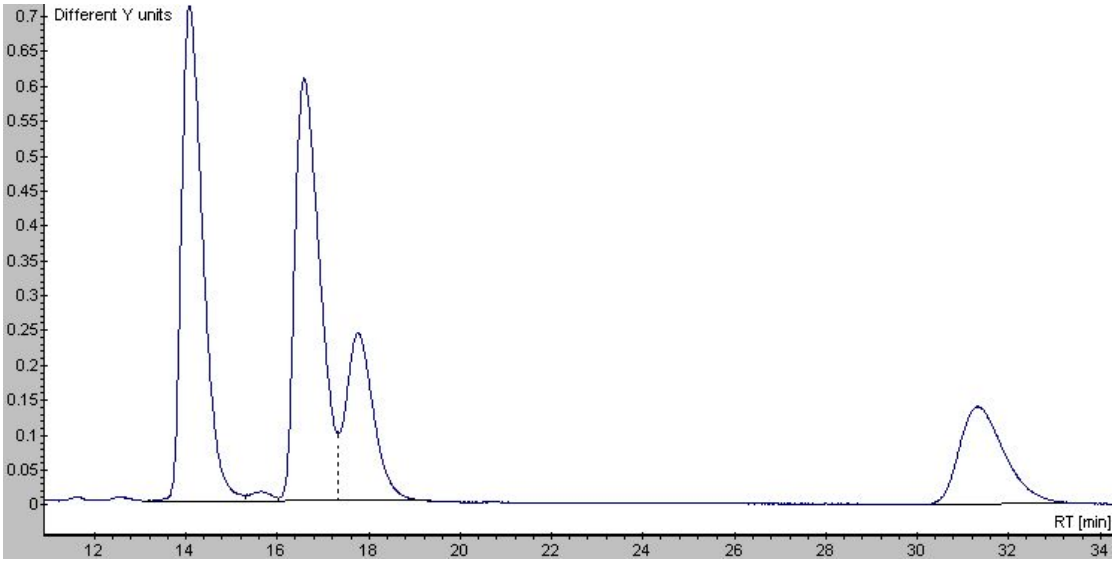


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.034	13.639	14.713	41.646
2	15.324	15.892	16.667	7.209
3	16.820	17.599	18.957	42.193
4	46.706	49.050	50.769	8.952

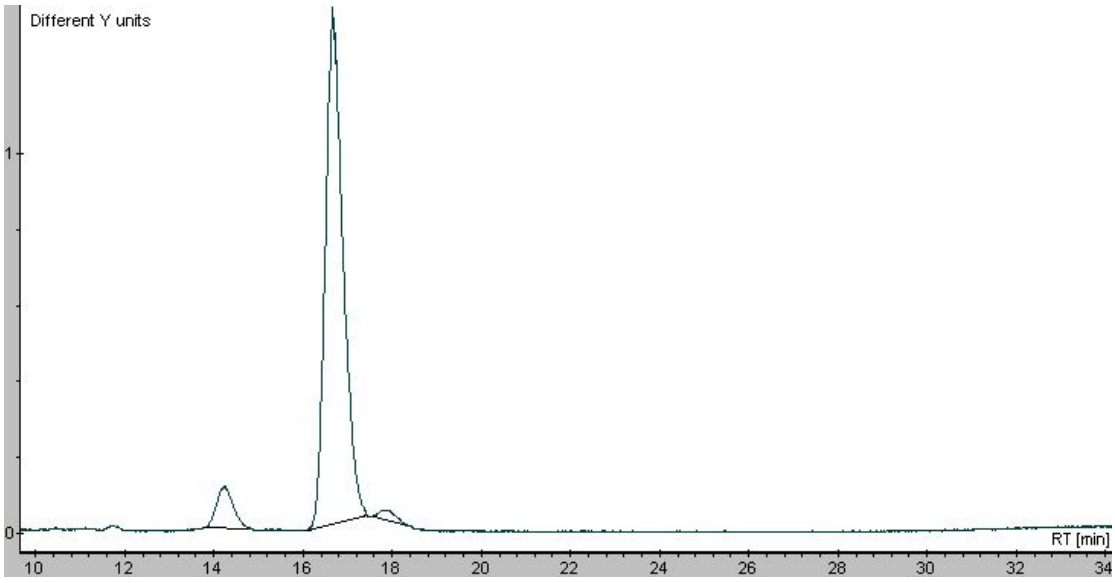


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.478	13.955	14.708	9.234
2	16.156	16.514	17.241	4.356
3	17.675	18.407	20.642	4.951

7h

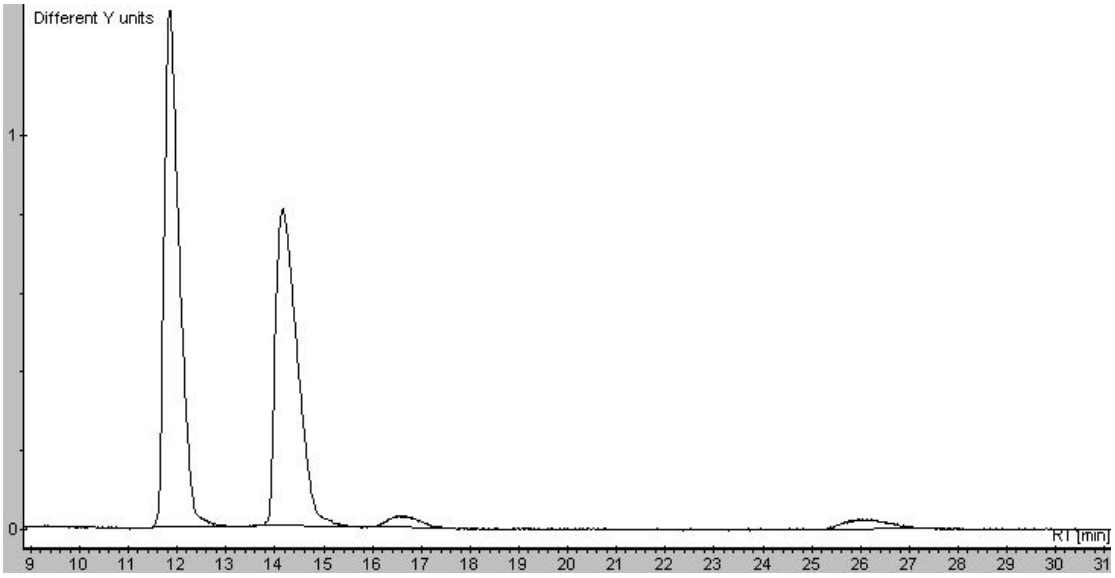


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.079	14.079	15.292	35.190
2	16.026	16.585	17.332	35.029
3	17.332	17.759	19.252	15.344
4	30.198	31.318	33.491	14.437

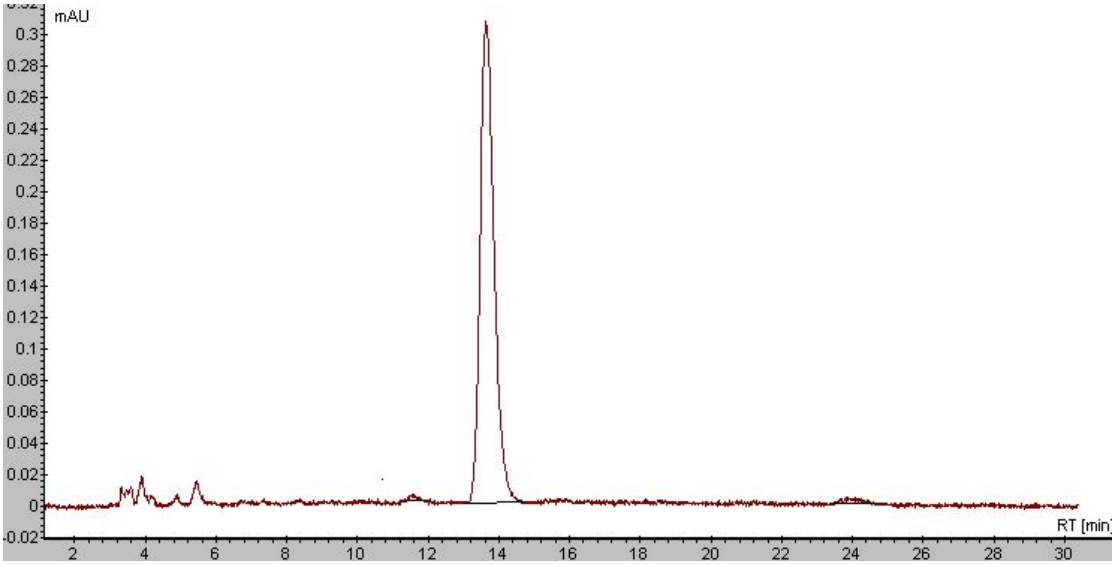


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	13.783	14.239	14.770	6.869
2	16.073	16.665	17.489	91.397
3	17.552	17.905	18.488	1.734

7i

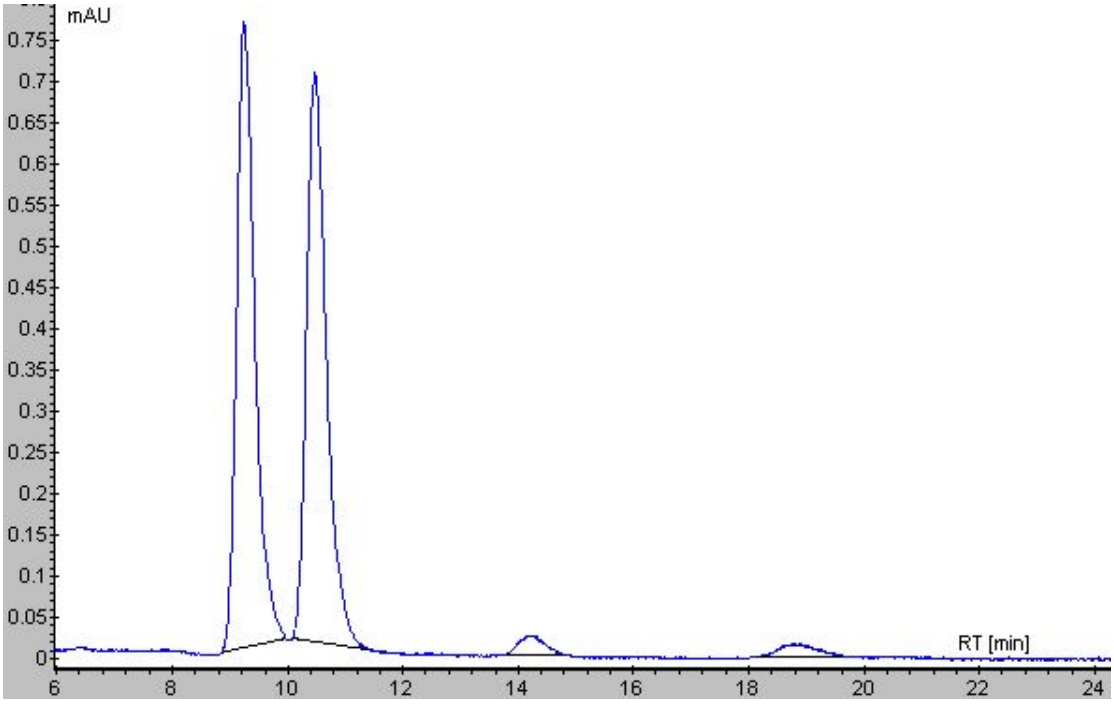


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.509	11.826	12.988	50.807
2	13.710	14.159	15.465	44.374
3	16.015	16.559	17.563	2.274
4	25.200	26.145	27.333	2.545

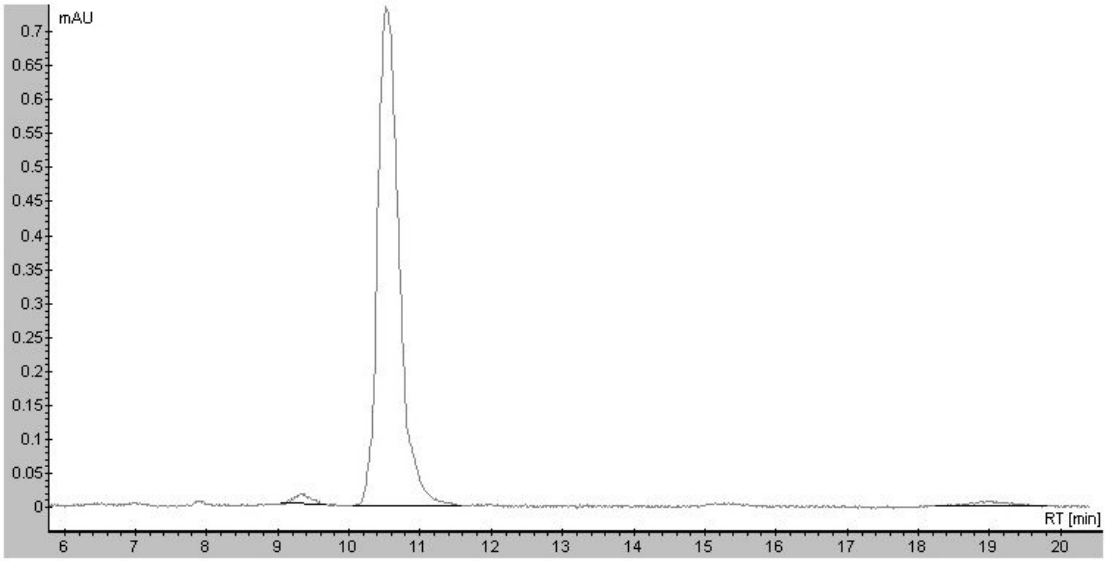


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.324	11.546	11.868	0.676
2	13.014	13.639	14.847	98.172
3	23.498	23.905	24.788	1.152

7j

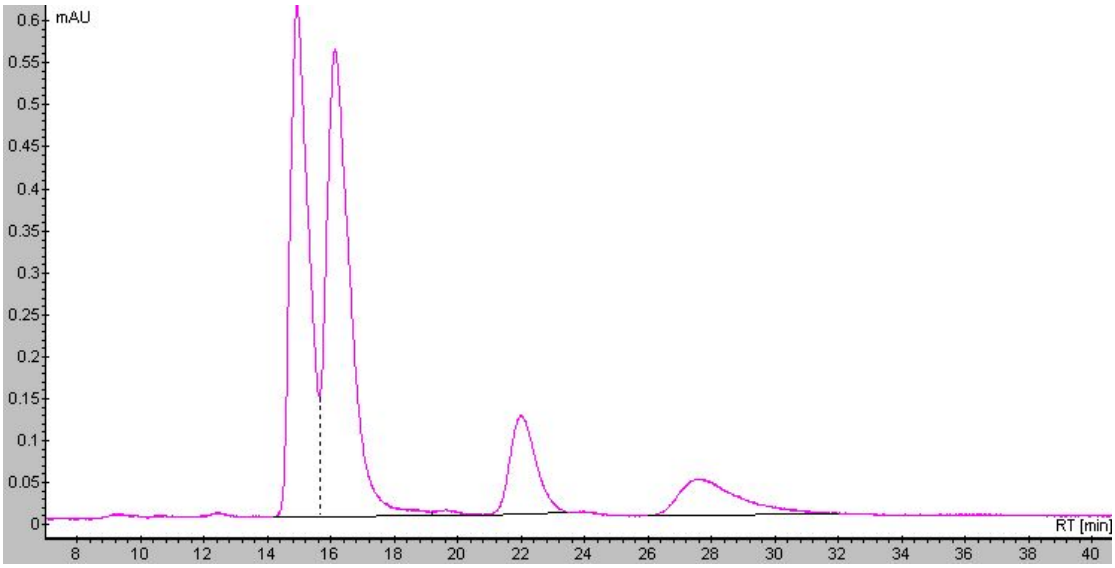


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	8.784	9.225	10.010	48.243
2	10.092	10.479	11.807	47.363
3	13.740	14.199	14.939	2.234
4	18.070	18.812	19.758	2.160

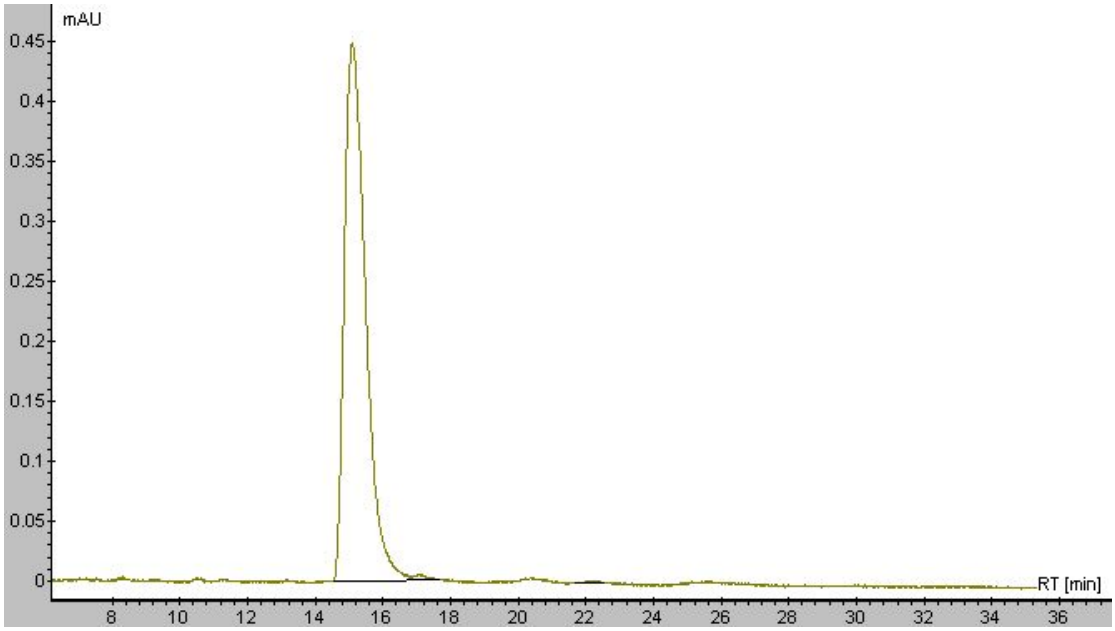


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.036	9.333	9.677	1.379
2	10.055	10.519	11.639	94.949
3	18.259	19.012	19.843	1.673

7k

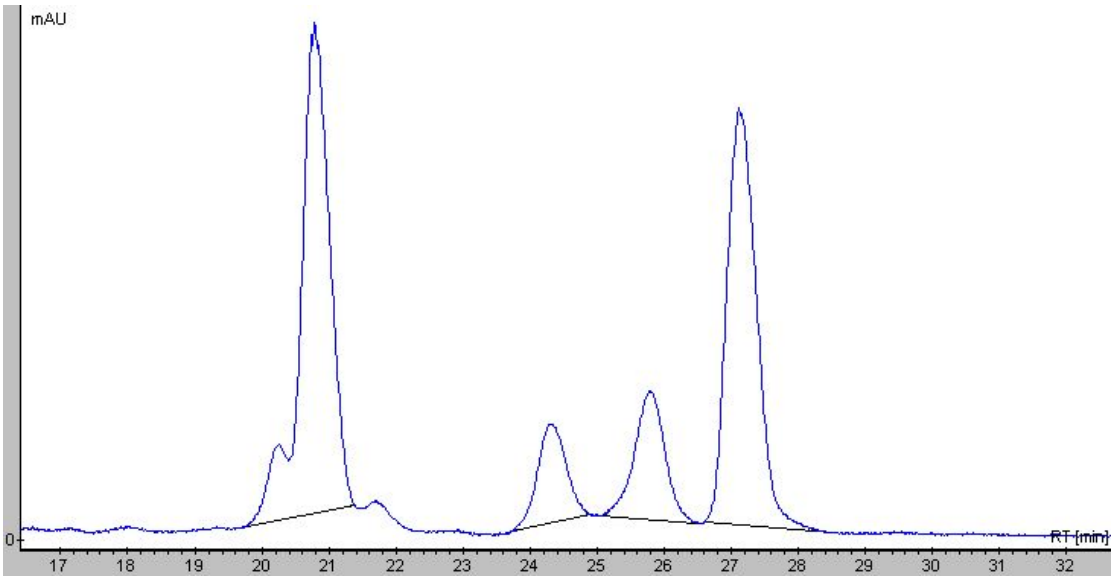


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	14.199	14.932	15.639	37.153
2	15.639	16.132	19.172	43.844
3	20.705	21.998	23.558	9.919
4	25.968	27.585	32.842	9.084

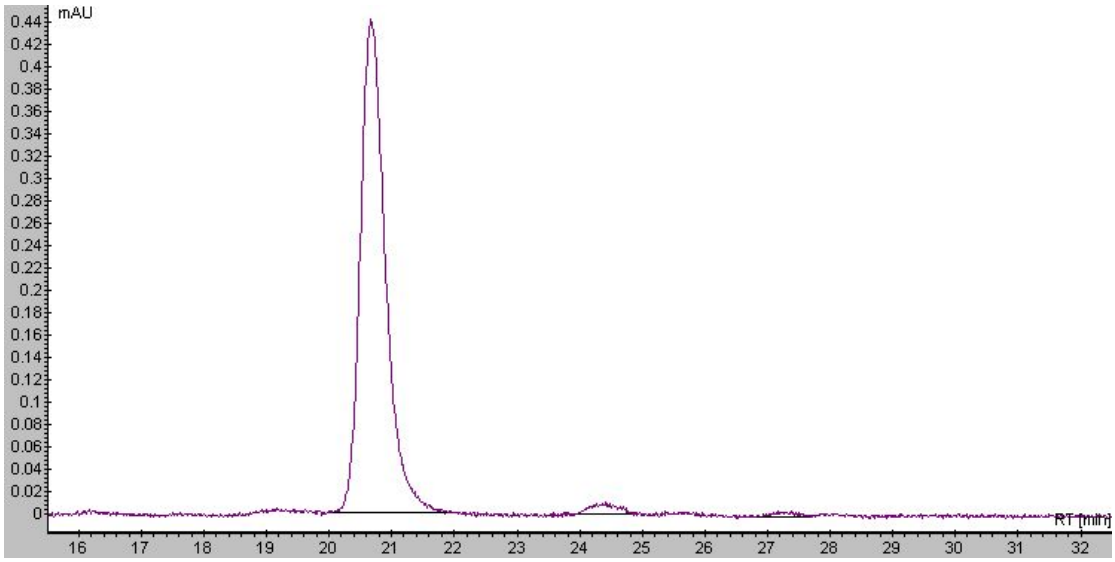


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	14.466	15.092	16.839	99.193
2	16.839	17.079	17.692	0.604
3	21.705	22.145	22.585	0.203

7l

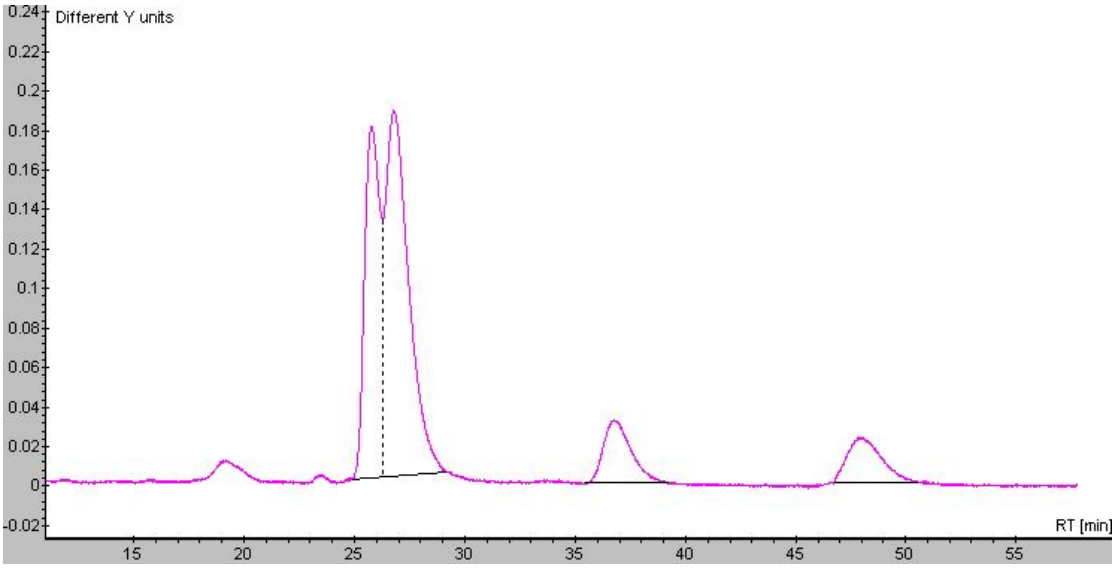


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	19.670	20.772	21.396	42.977
2	23.735	24.318	24.917	8.571
3	25.053	25.798	26.484	11.679
4	26.597	27.118	28.505	36.773

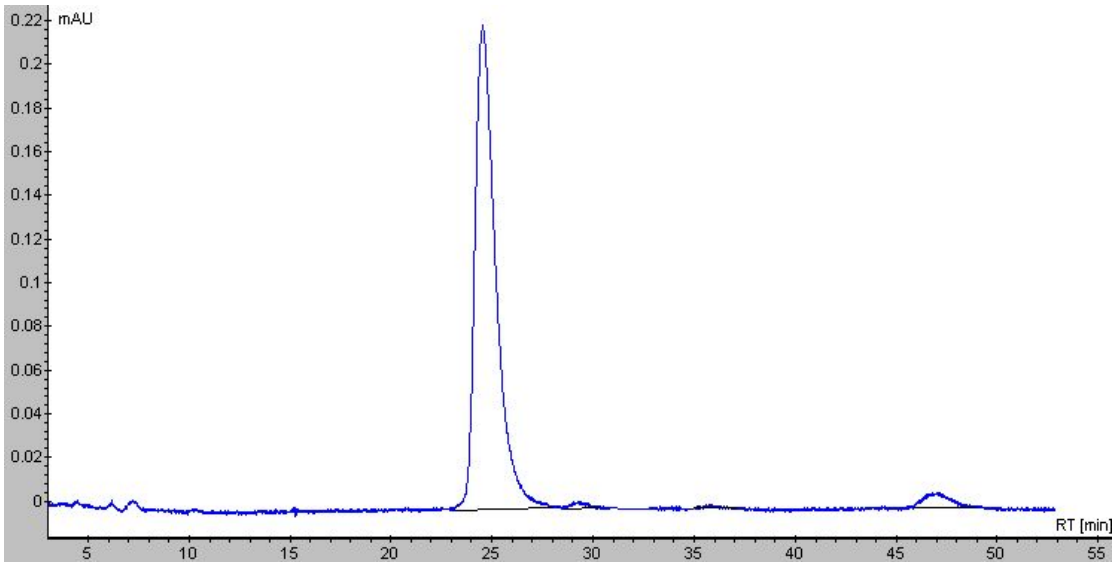


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	20.061	20.652	22.069	96.645
2	23.832	24.372	24.836	2.253
3	26.788	27.225	27.697	1.103

7m

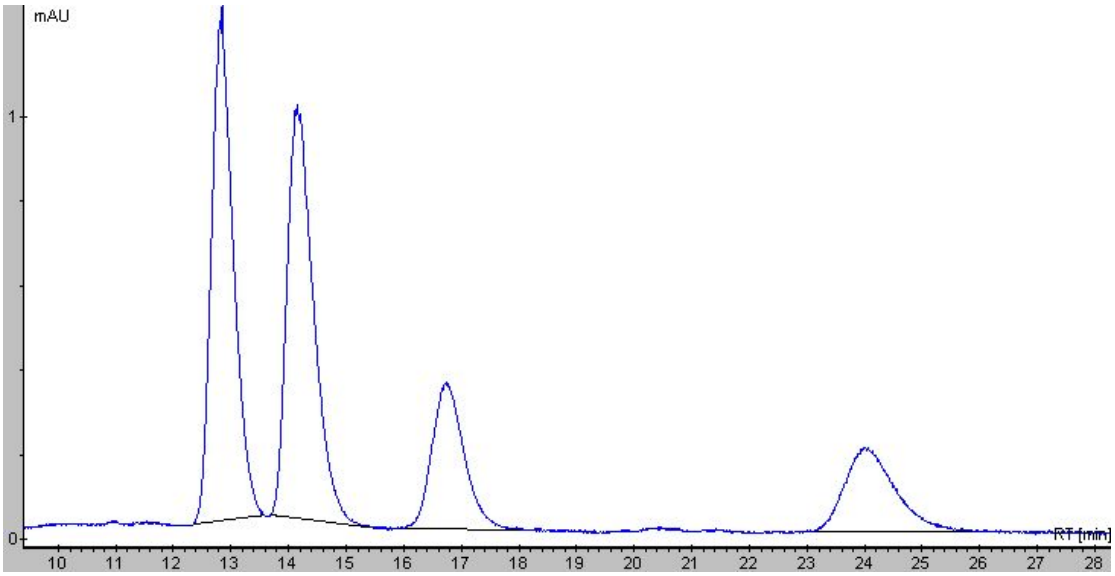


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	24. 785	25. 771	26. 278	31. 050
2	26. 278	26. 785	29. 185	49. 814
3	35. 519	36. 797	39. 563	10. 008
4	46. 495	47. 957	50. 749	9. 128

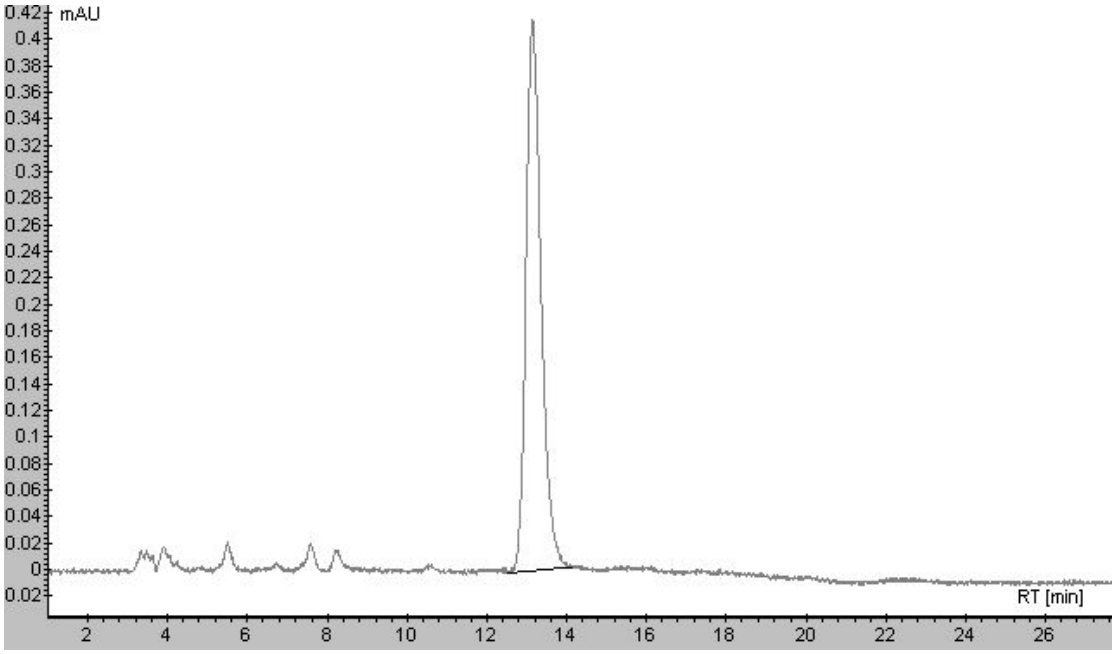


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	23.506	24.959	28.522	96.056
2	28.234	29.305	30.244	0.219
3	35.088	35.985	37.300	0.151
4	45..709	47.051	49.101	3.574

7n

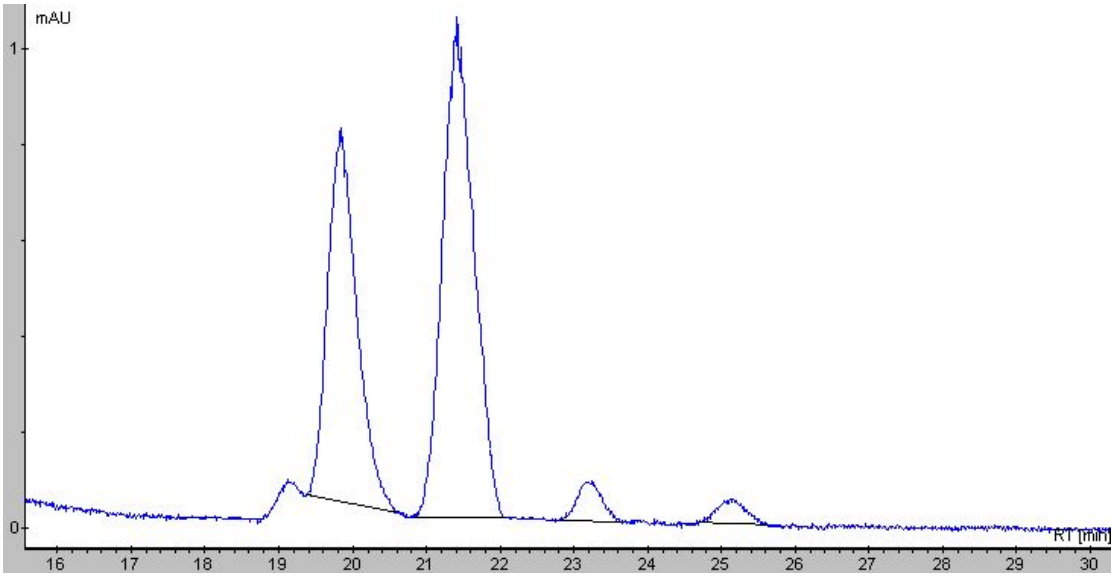


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.168	12.852	13.595	36.100
2	13.697	14.146	15.565	35.572
3	16.041	16.719	18.182	13.945
4	23.075	24.012	26.133	13.383

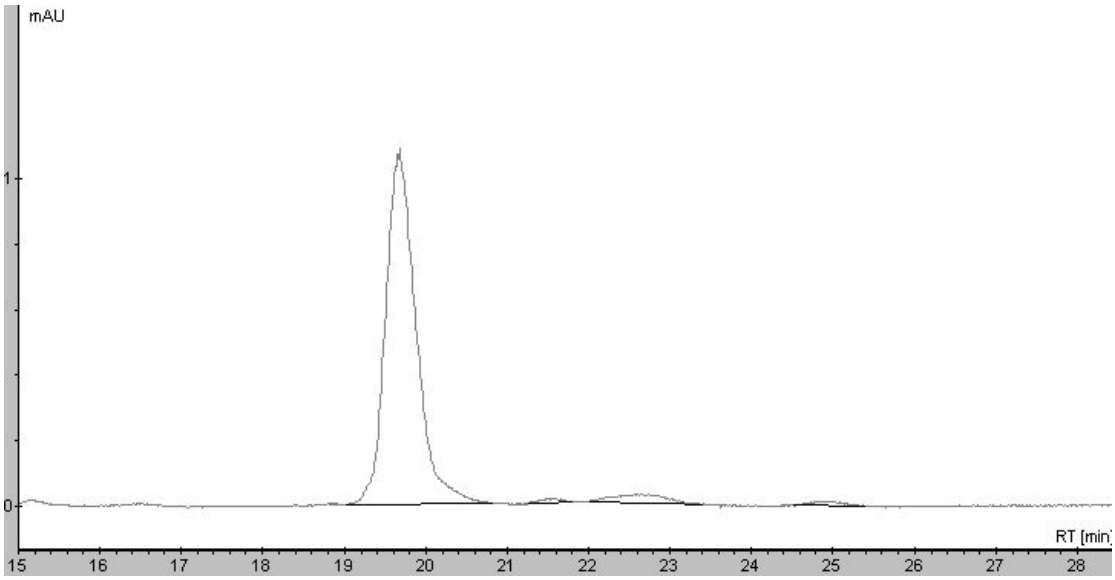


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.521	13.159	14.384	100.000

7o

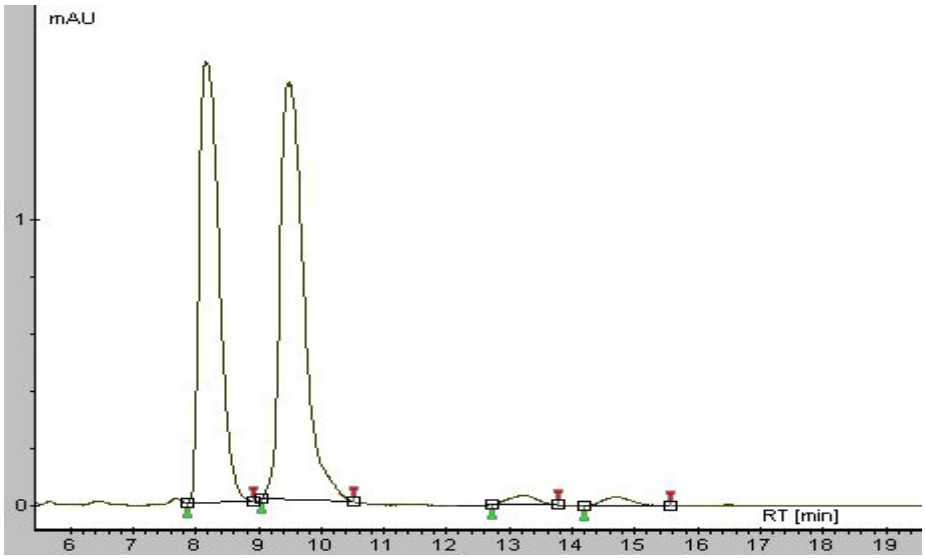


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	19.380	19.852	20.629	45.425
2	20.845	21.412	22.013	47.848
3	22.723	23.187	23.682	3.476
4	24.592	25.145	25.738	3.251

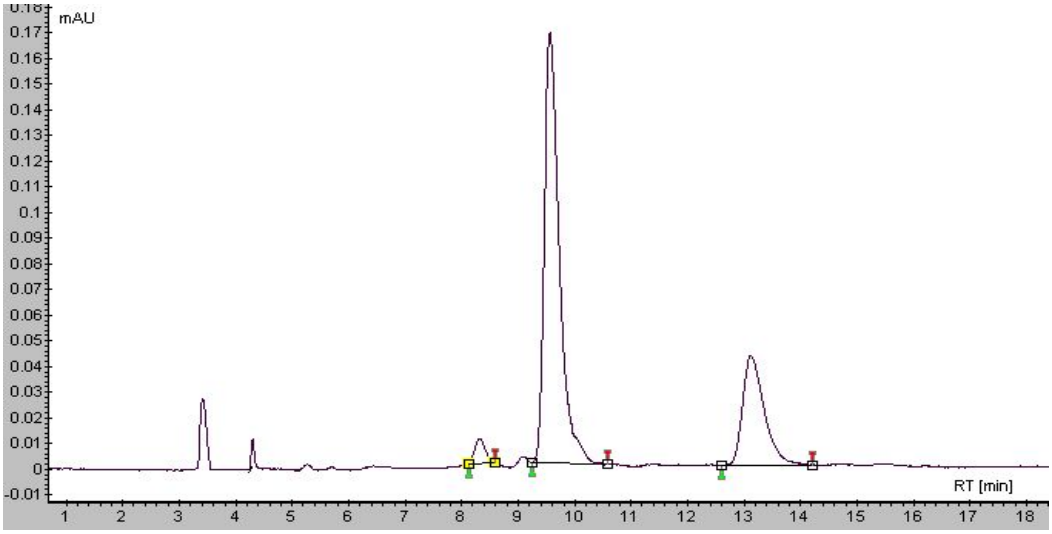


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	18.989	19.679	20.882	93.349
2	21.079	21.532	21.837	0.879
3	21.973	22.652	23.564	4.386
4	24.397	24.918	25.488	1.386

7p

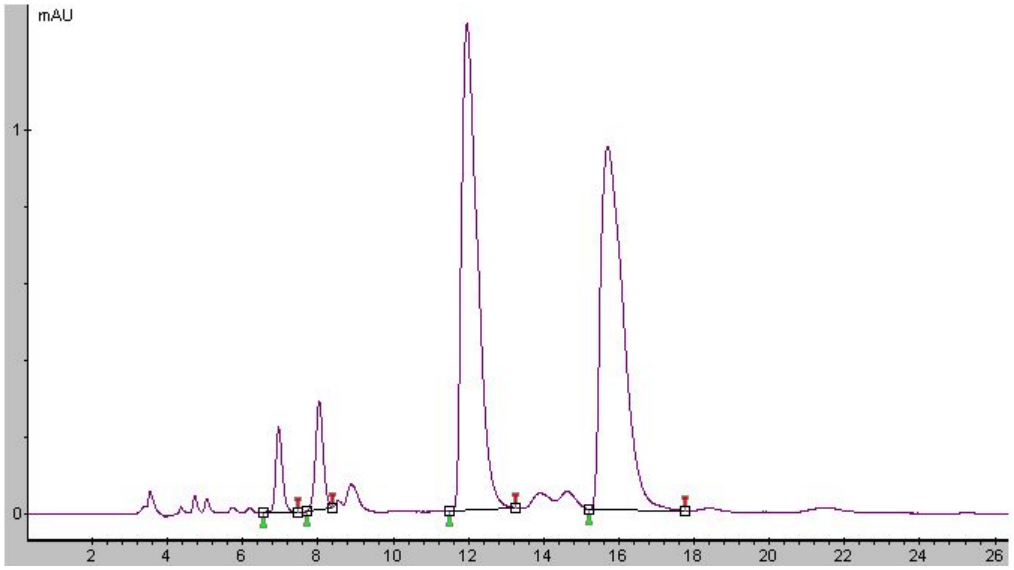


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	7.86	8.159	8.927	47.66
2	9.044	9.493	10.499	49.72
3	12.612	13.226	13.760	1.32
4	14.187	14.706	15.565	1.30

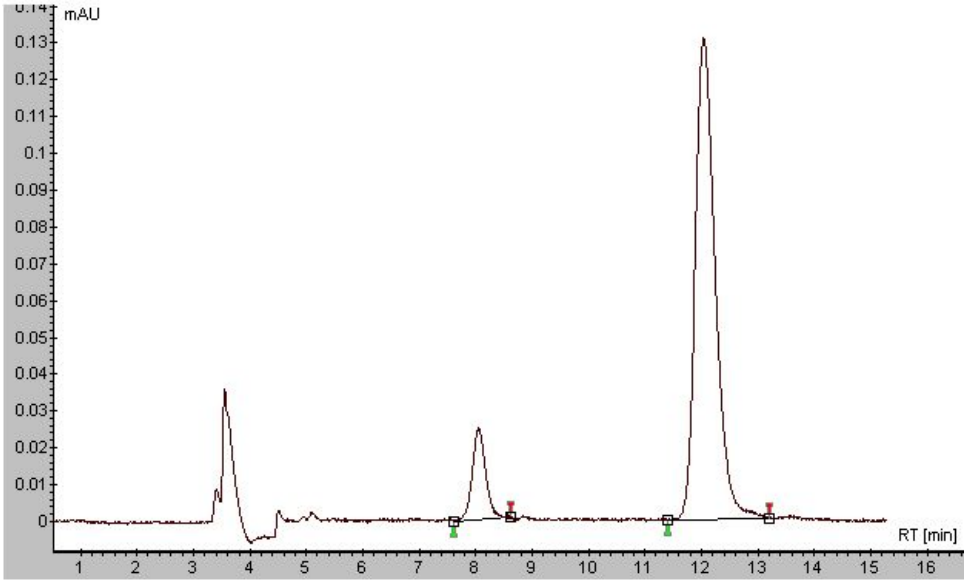


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	8.129	8.319	8.593	2.85
2	9.248	9.573	10.584	72.20
3	12.603	13.119	14.213	24.95
4				

7q

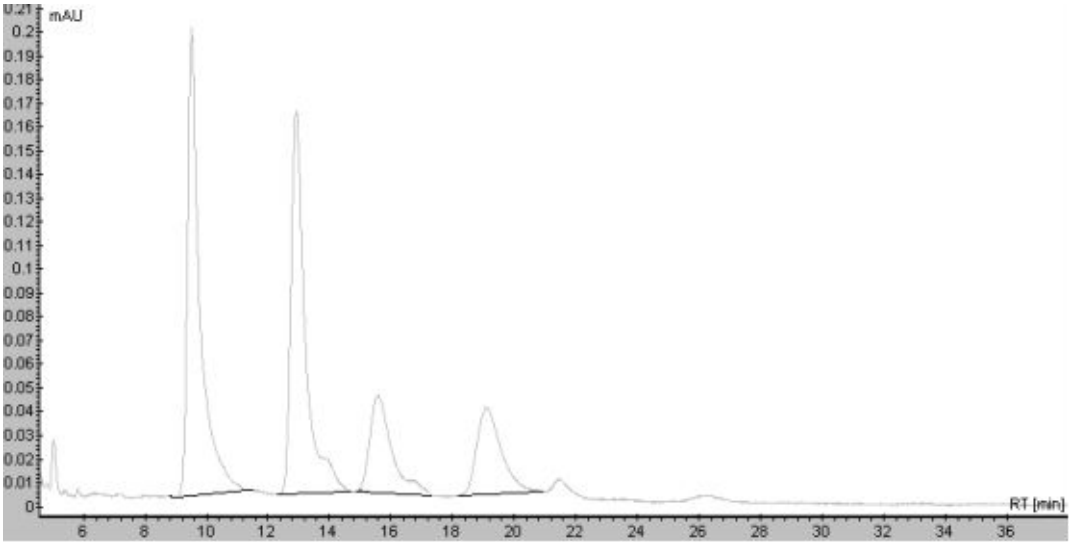


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	6.545	6.959	7.463	3.28
2	7.702	8.039	8.381	4.80
3	11.493	11.959	13.249	44.73
4	15.205	15.706	17.759	47.19

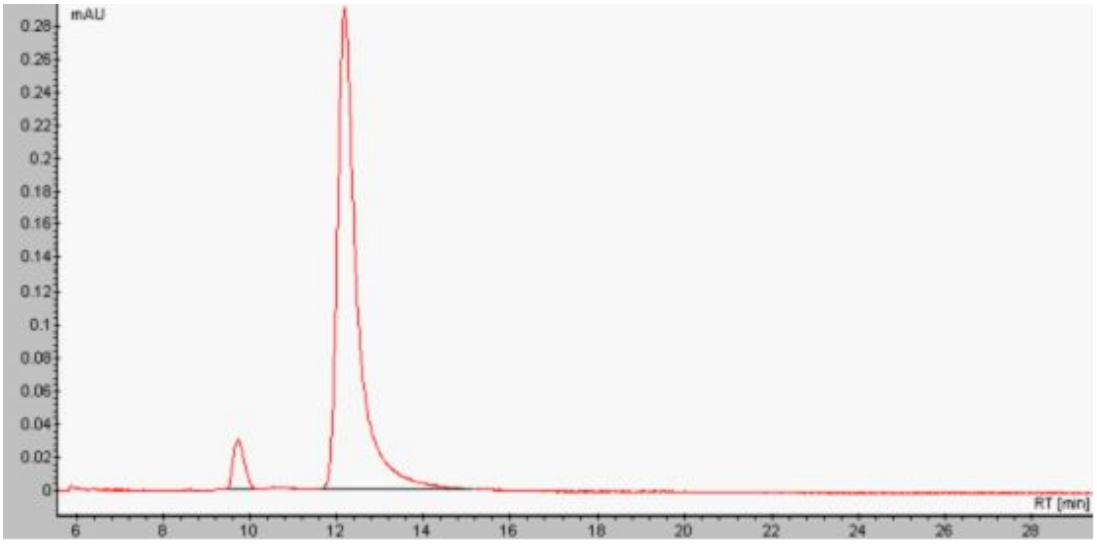


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1				
2	7.611	8.053	8.620	11.57
3	11.403	12.039	13.203	88.43
4				

8a

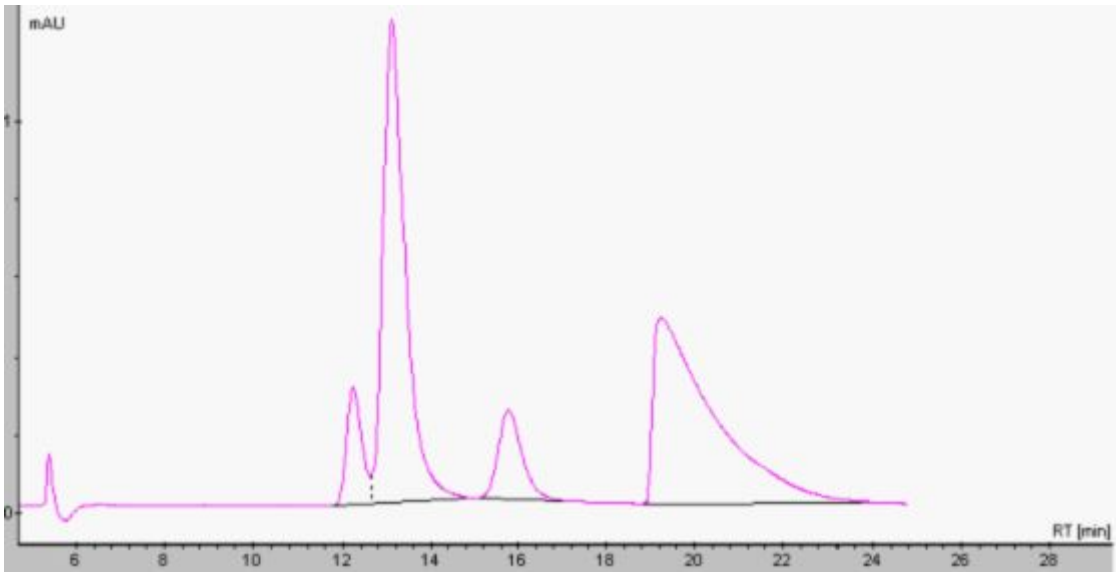


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.006	9.519	11.389	37.555
2	12.318	12.906	14.759	35.232
3	14.875	15.572	17.432	13.641
4	18.187	19.079	20.976	13.571

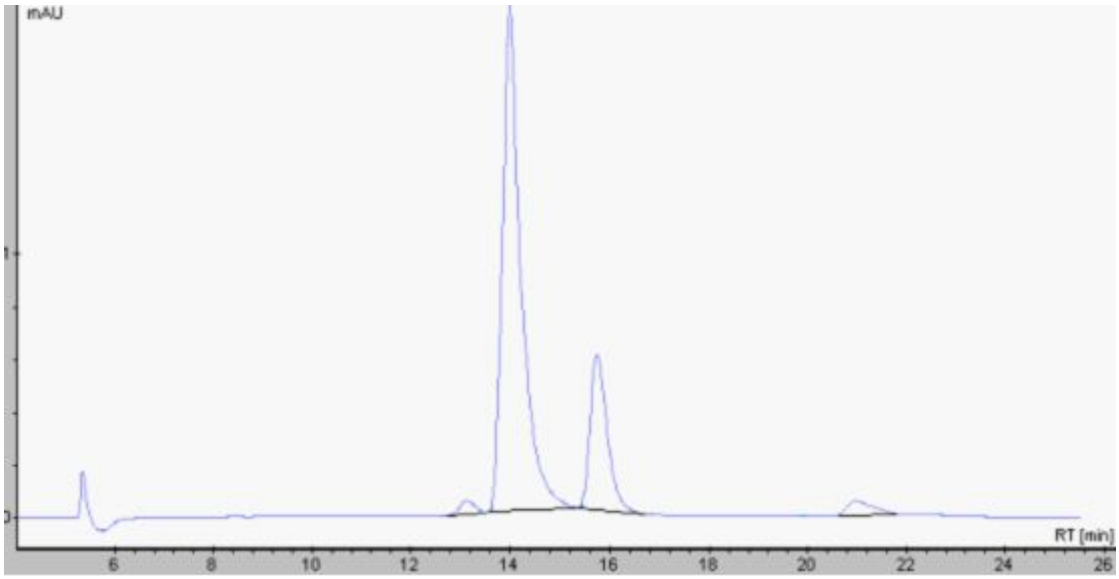


#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	9.406	9.796	10.200	7.419
2	11.622	12.172	15.153	92.581

9a



#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	11.772	12.239	12.670	7.023
2	12.670	13.119	14.948	41.446
3	15.121	15.772	17.088	8.163
4	18.814	19.225	23.855	43.368



#	Start [Min]	Time [Min]	End [Min]	Area% [%]
1	12.742	13.146	13.548	1.528
2	13.579	14.012	15.346	72.087
3	15.377	15.732	16.742	19.648
4	19.997	20.505	22.602	6.736

5. The absolute configuration of the Michael product 5a

The absolute configuration of chiral Michael product **5a** has been assigned by means of TDDFT CD computations. To investigate the unknown chirality of **5a**, four ground-state geometries, known molecules 1-SS (1S, 2S) / 2-SR (1S, 2R) / 3-RS (1R, 2S) / 4-RR (1R, 2R), have been optimized at the Zindo//DFT B3LYP/6-31+G* levels by employing Gaussian 03W Pack. As shown in Figure 6S, in the selected data in the 200-390 nm UV region, the experimental CD spectra (Figure 5S) match well with the calculated data (Figure 1S).

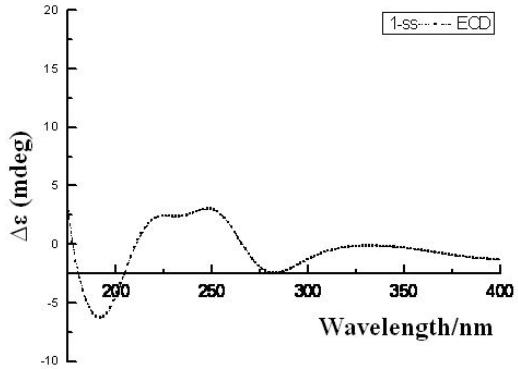


Figure 1S

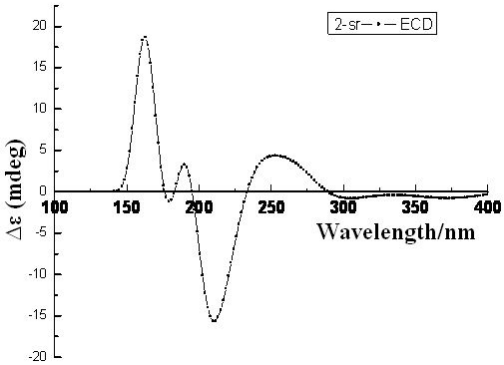


Figure 2S

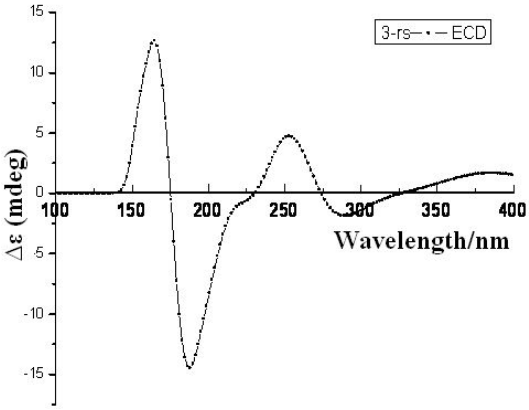


Figure 3S

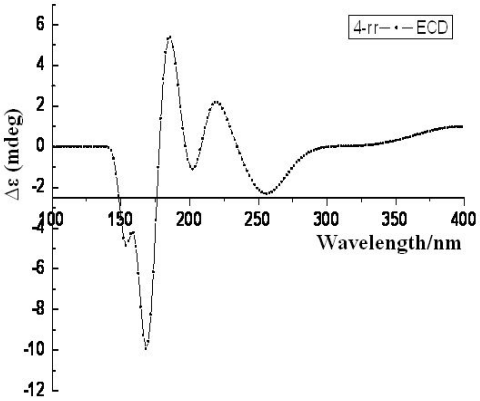


Figure 4S

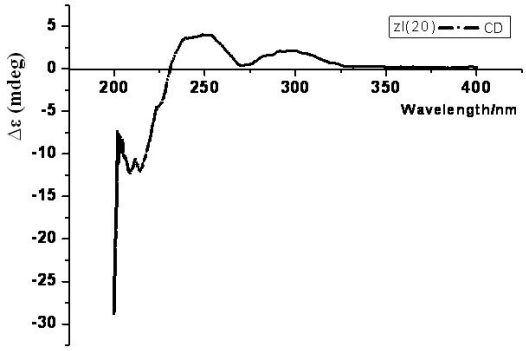


Figure 5S

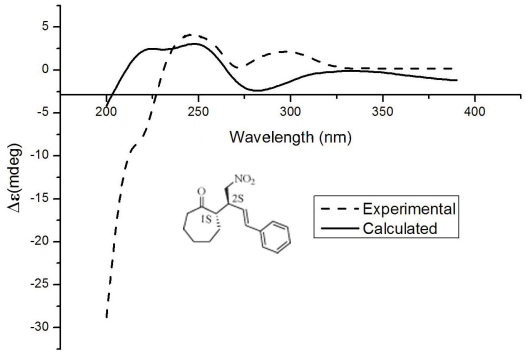


Figure 6S

Wavelength /nm	Δε/1-SS(Calculated) /medg	Δε/zl(20)(Experimental) /medg
200	-28.7644	-4.1191
210	-11.6377	-0.267
220	-7.63086	2.2492
230	-0.548705	2.3887
240	3.56948	2.7024
250	3.96069	3.0323
260	2.62048	1.4632
270	0.360182	-1.2414
280	1.13095	-2.3738
290	1.93125	-2.0678
300	2.11502	-1.2995
310	1.49862	-0.5684
320	0.643492	-0.2489
330	0.22983	-0.119
340	0.236451	-0.1477
350	0.161487	-0.2994
360	0.151642	-0.5426
370	0.184926	-0.7761
380	0.141662	-1.0357
390	0.156171	-1.1962

Experimental CD spectrum data

TITLE zl(20)
DATA TYPE
ORIGINJASCO
OWNER
DATE 13/02/25
TIME 14:22:36
SPECTROMETER/DATA SYSTEM
RESOLUTION
DELTAX -0.5
XUNITS NANOMETERS
YUNITS ARBITRARY UNITS
FIRSTX 400.0000
LASTX 200.0000
NPOINTS 401
FIRSTY 0.16098
MAXY 3.98330
MINY -28.76436
XYDATA

400.0000	0.160983	174.801
399.5000	0.186015	174.765
399.0000	0.190883	174.711
398.5000	0.191542	174.656
398.0000	0.196648	174.579
397.5000	0.215216	174.484
397.0000	0.206371	174.362
396.5000	0.207172	174.211
396.0000	0.207235	174.041
395.5000	0.188146	173.861
395.0000	0.162043	173.664
394.5000	0.151874	173.469
394.0000	0.134778	173.281
393.5000	0.127331	173.114
393.0000	0.106243	172.991
392.5000	0.101474	172.906
392.0000	0.122632	172.868
391.5000	0.146346	172.876
391.0000	0.16229	172.915
390.5000	0.144682	172.983
390.0000	0.156171	173.07
389.5000	0.158121	173.169
389.0000	0.145959	173.271
388.5000	0.144763	173.366
388.0000	0.126835	173.453
387.5000	0.106667	173.535
387.0000	0.108347	173.619
386.5000	0.110095	173.689
386.0000	0.101024	173.758
385.5000	0.072493	173.814
385.0000	0.0820526	173.868
384.5000	0.0917297	173.921
384.0000	0.109032	173.966
383.5000	0.0989761	174.001
383.0000	0.0870125	174.023
382.5000	0.123369	174.034
382.0000	0.149149	174.035
381.5000	0.136638	174.016
381.0000	0.13327	173.99
380.5000	0.128573	173.953
380.0000	0.141662	173.913
379.5000	0.152341	173.862
379.0000	0.132927	173.813
378.5000	0.130643	173.758

378.0000	0.138894	173.709
377.5000	0.14558	173.661
377.0000	0.152209	173.621
376.5000	0.174708	173.586
376.0000	0.170101	173.555
375.5000	0.15892	173.531
375.0000	0.153026	173.521
374.5000	0.174777	173.506
374.0000	0.157671	173.489
373.5000	0.14465	173.47
373.0000	0.143228	173.449
372.5000	0.166852	173.437
372.0000	0.18836	173.418
371.5000	0.172065	173.395
371.0000	0.165159	173.365
370.5000	0.171581	173.347
370.0000	0.184926	173.326
369.5000	0.16972	173.298
369.0000	0.158276	173.264
368.5000	0.143494	173.234
368.0000	0.158421	173.2
367.5000	0.163428	173.175
367.0000	0.160394	173.142
366.5000	0.156448	173.12
366.0000	0.178071	173.103
365.5000	0.19034	173.094
365.0000	0.195311	173.088
364.5000	0.189449	173.09
364.0000	0.189891	173.09
363.5000	0.185782	173.094
363.0000	0.185825	173.101
362.5000	0.149216	173.113
362.0000	0.148774	173.123
361.5000	0.157323	173.132
361.0000	0.150916	173.14
360.5000	0.15805	173.151
360.0000	0.151642	173.171
359.5000	0.162154	173.186
359.0000	0.178808	173.202
358.5000	0.193932	173.216
358.0000	0.186108	173.227
357.5000	0.159354	173.249
357.0000	0.157646	173.276
356.5000	0.178583	173.301

356.0000	0.178978	173.326
355.5000	0.159784	173.361
355.0000	0.150685	173.4
354.5000	0.136272	173.443
354.0000	0.154211	173.475
353.5000	0.131087	173.508
353.0000	0.120078	173.541
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352.0000	0.105558	173.595
351.5000	0.120465	173.63
351.0000	0.136138	173.668
350.5000	0.149608	173.708
350.0000	0.161487	173.748
349.5000	0.174915	173.799
349.0000	0.197005	173.847
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347.5000	0.247948	173.968
347.0000	0.249233	174.006
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346.0000	0.265658	174.069
345.5000	0.270211	174.104
345.0000	0.263303	174.132
344.5000	0.246421	174.169
344.0000	0.265658	174.205
343.5000	0.276304	174.245
343.0000	0.274438	174.285
342.5000	0.241066	174.327
342.0000	0.221308	174.361
341.5000	0.242577	174.399
341.0000	0.235116	174.428
340.5000	0.22006	174.456
340.0000	0.236451	174.474
339.5000	0.226691	174.501
339.0000	0.253697	174.532
338.5000	0.253075	174.569
338.0000	0.221237	174.598
337.5000	0.242591	174.63
337.0000	0.256003	174.669
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336.0000	0.25705	174.743
335.5000	0.257712	174.769
335.0000	0.27038	174.799
334.5000	0.271111	174.836

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328.0000	0.24249	175.394
327.5000	0.271925	175.442
327.0000	0.280924	175.5
326.5000	0.306075	175.558
326.0000	0.330838	175.613
325.5000	0.376003	175.659
325.0000	0.432465	175.703
324.5000	0.464098	175.746
324.0000	0.501227	175.783
323.5000	0.544013	175.809
323.0000	0.570277	175.833
322.5000	0.584206	175.852
322.0000	0.609013	175.866
321.5000	0.633252	175.88
321.0000	0.628011	175.897
320.5000	0.643069	175.923
320.0000	0.643492	175.957
319.5000	0.66396	175.999
319.0000	0.688045	176.055
318.5000	0.72543	176.118
318.0000	0.776959	176.191
317.5000	0.827326	176.259
317.0000	0.843794	176.322
316.5000	0.894479	176.386
316.0000	0.930648	176.444
315.5000	0.97257	176.5
315.0000	1.01624	176.558
314.5000	1.04989	176.608
314.0000	1.08704	176.657
313.5000	1.15725	176.705
313.0000	1.1915	176.752
312.5000	1.24314	176.794

312.0000	1.31129	176.834
311.5000	1.35305	176.879
311.0000	1.42585	176.934
310.5000	1.45795	177.002
310.0000	1.49862	177.081
309.5000	1.56791	177.175
309.0000	1.60212	177.284
308.5000	1.60444	177.401
308.0000	1.64481	177.519
307.5000	1.67715	177.633
307.0000	1.71809	177.748
306.5000	1.74537	177.857
306.0000	1.77282	177.962
305.5000	1.81161	178.067
305.0000	1.82685	178.177
304.5000	1.82248	178.288
304.0000	1.82852	178.404
303.5000	1.84988	178.515
303.0000	1.8821	178.631
302.5000	1.91745	178.746
302.0000	1.95684	178.857
301.5000	2.00632	178.974
301.0000	2.044	179.082
300.5000	2.09772	179.202
300.0000	2.11502	179.322
299.5000	2.11245	179.45
299.0000	2.12157	179.582
298.5000	2.12758	179.718
298.0000	2.13539	179.853
297.5000	2.13673	180.007
297.0000	2.11424	180.171
296.5000	2.09592	180.347
296.0000	2.09086	180.538
295.5000	2.043	180.76
295.0000	2.00742	181.015
294.5000	1.98201	181.305
294.0000	1.96591	181.642
293.5000	1.96689	182.011
293.0000	1.99202	182.416
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292.0000	2.03724	183.231
291.5000	2.0457	183.602
291.0000	2.0251	183.922
290.5000	1.98583	184.179

290.0000 1.93125 184.374
289.5000 1.8409 184.522
289.0000 1.74552 184.646
288.5000 1.6599 184.771
288.0000 1.63018 184.921
287.5000 1.60062 185.116
287.0000 1.586 185.382
286.5000 1.55714 185.735
286.0000 1.56299 186.171
285.5000 1.56802 186.7
285.0000 1.57137 187.315
284.5000 1.54167 188.017
284.0000 1.51458 188.792
283.5000 1.49993 189.614
283.0000 1.46533 190.466
282.5000 1.45105 191.335
282.0000 1.37848 192.204
281.5000 1.32711 193.049
281.0000 1.26743 193.849
280.5000 1.20433 194.598
280.0000 1.13095 195.295
279.5000 1.05713 195.934
279.0000 0.950919 196.504
278.5000 0.912042 197.019
278.0000 0.84565 197.493
277.5000 0.780612 197.946
277.0000 0.673566 198.392
276.5000 0.602904 198.848
276.0000 0.546314 199.348
275.5000 0.516358 199.901
275.0000 0.471913 200.507
274.5000 0.457006 201.181
274.0000 0.439602 201.92
273.5000 0.449249 202.718
273.0000 0.439325 203.568
272.5000 0.445686 204.452
272.0000 0.389413 205.375
271.5000 0.364584 206.336
271.0000 0.351738 207.345
270.5000 0.342418 208.406
270.0000 0.360182 209.527
269.5000 0.422697 210.72
269.0000 0.4598 212
268.5000 0.562109 213.364

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266.5000	1.02321	219.597
266.0000	1.13882	221.291
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265.0000	1.43168	224.706
264.5000	1.52036	226.391
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263.5000	1.73772	229.665
263.0000	1.83276	231.243
262.5000	1.94406	232.781
262.0000	2.03984	234.296
261.5000	2.18269	235.786
261.0000	2.33174	237.256
260.5000	2.45997	238.71
260.0000	2.62048	240.161
259.5000	2.73767	241.611
259.0000	2.87249	243.071
258.5000	2.95074	244.523
258.0000	3.03057	245.982
257.5000	3.14063	247.435
257.0000	3.25011	248.877
256.5000	3.33793	250.286
256.0000	3.50223	251.66
255.5000	3.59165	252.971
255.0000	3.70283	254.212
254.5000	3.81382	255.366
254.0000	3.87777	256.424
253.5000	3.92949	257.387
253.0000	3.95285	258.252
252.5000	3.90502	259.034
252.0000	3.92147	259.746
251.5000	3.94625	260.409
251.0000	3.93724	261.019
250.5000	3.96069	261.593
250.0000	3.96495	262.136
249.5000	3.96882	262.647
249.0000	3.9833	263.119
248.5000	3.96917	263.565
248.0000	3.90276	263.989
247.5000	3.81594	264.404
247.0000	3.79519	264.813
246.5000	3.80711	265.225

246.0000 3.72115 265.647
245.5000 3.71281 266.105
245.0000 3.69818 266.608
244.5000 3.72154 267.193
244.0000 3.7074 267.876
243.5000 3.66429 268.72
243.0000 3.60601 269.764
242.5000 3.61192 271.068
242.0000 3.62489 272.672
241.5000 3.59291 274.635
241.0000 3.5438 277
240.5000 3.54473 279.827
240.0000 3.56948 283.13
239.5000 3.59076 286.936
239.0000 3.5359 291.241
238.5000 3.41318 296.036
238.0000 3.38222 301.297
237.5000 3.15426 306.93
237.0000 2.93474 312.865
236.5000 2.72046 319.019
236.0000 2.52932 325.302
235.5000 2.26261 331.595
235.0000 2.1537 337.822
234.5000 1.87042 343.903
234.0000 1.84306 349.806
233.5000 1.51249 355.507
233.0000 1.18748 361.003
232.5000 0.929455 366.343
232.0000 0.735175 371.568
231.5000 0.482142 376.69
231.0000 0.00285416 381.731
230.5000 -0.548705 386.64
230.0000 -0.908919 391.358
229.5000 -1.31492 395.803
229.0000 -1.68225 399.854
228.5000 -2.3483 403.439
228.0000 -2.95369 406.477
227.5000 -3.20022 408.939
227.0000 -3.63574 410.816
226.5000 -4.00916 412.14
226.0000 -4.13103 412.95
225.5000 -4.26035 413.306
225.0000 -4.40177 413.235
224.5000 -4.5018 412.815

224.0000	-4.52474	412.091
223.5000	-4.54175	411.152
223.0000	-4.99765	410.063
222.5000	-5.56782	408.91
222.0000	-6.19208	407.799
221.5000	-6.44972	406.832
221.0000	-6.90655	406.108
220.5000	-7.63086	405.711
220.0000	-8.11307	405.68
219.5000	-8.58728	406.032
219.0000	-8.82951	406.696
218.5000	-9.27207	407.541
218.0000	-9.71456	408.401
217.5000	-10.1301	409.105
217.0000	-10.5916	409.528
216.5000	-10.8373	409.639
216.0000	-11.1954	409.493
215.5000	-11.6301	409.284
215.0000	-11.9058	409.283
214.5000	-12.0462	409.768
214.0000	-11.8698	411.055
213.5000	-11.5444	413.404
213.0000	-11.4616	416.9
212.5000	-11.0167	421.499
212.0000	-10.6852	427.036
211.5000	-10.7941	433.319
211.0000	-11.081	440.141
210.5000	-11.6377	447.262
210.0000	-11.7642	454.548
209.5000	-12.0296	462.043
209.0000	-12.335	469.932
208.5000	-12.2174	478.448
208.0000	-12.083	487.846
207.5000	-11.5561	498.341
207.0000	-10.9311	510.183
206.5000	-10.804	523.543
206.0000	-10.2973	538.526
205.5000	-10.4763	555.319
205.0000	-9.9113	574.273
204.5000	-8.395	595.853
204.0000	-9.12687	620.882
203.5000	-8.24539	650.162
203.0000	-7.8208	684.535
202.5000	-11.1949	724.243

202.0000 -7.42708 768.039
201.5000 -13.3043 812.968
201.0000 -18.9291 855.91
200.5000 -21.0372 894.384
200.0000 -28.7644 926.658

Extended Information
[Comment]
Sample Name zl(20)
Comment
User
Division
Company JASCO

[Data Information]
Creation Date 2013-2-25 14:22
Data array type Linear data array * 2
Horizontal Wavelength [nm]
Vertical(1) CD[mdeg]
Vertical(2) HT[V]
Start 400 nm
End 200 nm
Data pitch 0.5 nm
Data points 401

[Measurement Information]
Instrument NameJASCO
Model NameJ-815
Serial No. A010961168

Photometric Mode CD, HT
Measure Range 400 - 200 nm
Data pitch 0.5 nm
Sensitivity Standard
D.I.T. 2 sec
Band width 3.00 nm
Start Mode Immediately
Scanning Speed 100 nm/min
Baseline Correction Baseline
Shutter Control Manual
PMT Voltage Auto
Accumulation Times 2

Theoretical ECD spectra data

1-SS ECD Spectrum
X-Axis: Excitation Energy (nm)
Y-Axis: Delta Epsilon

# X	Y	DY/DX
-100.0000000000	0.0000000000	0.0000000000
-98.2000000000	0.0000000000	0.0000000000
-96.4000000000	0.0000000000	0.0000000000
-94.6000000000	0.0000000000	0.0000000000
-92.8000000000	0.0000000000	0.0000000000
-91.0000000000	0.0000000000	0.0000000000
-89.2000000000	0.0000000000	0.0000000000
-87.4000000000	0.0000000000	0.0000000000
-85.6000000000	0.0000000000	0.0000000000
-83.8000000000	0.0000000000	0.0000000000
-82.0000000000	0.0000000000	0.0000000000
-80.2000000000	0.0000000000	0.0000000000
-78.4000000000	0.0000000000	0.0000000000
-76.6000000000	0.0000000000	0.0000000000
-74.8000000000	0.0000000000	0.0000000000
-73.0000000000	0.0000000000	0.0000000000
-71.2000000000	0.0000000000	0.0000000000
-69.4000000000	0.0000000000	0.0000000000
-67.6000000000	0.0000000000	0.0000000000
-65.8000000000	0.0000000000	0.0000000000
-64.0000000000	0.0000000000	0.0000000000
-62.2000000000	0.0000000000	0.0000000000
-60.4000000000	0.0000000000	0.0000000000
-58.6000000000	0.0000000000	0.0000000000
-56.8000000000	0.0000000000	0.0000000000
-55.0000000000	0.0000000000	0.0000000000
-53.2000000000	0.0000000000	0.0000000000
-51.4000000000	0.0000000000	0.0000000000
-49.6000000000	0.0000000000	0.0000000000
-47.8000000000	0.0000000000	0.0000000000
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-42.4000000000	0.0000000000	0.0000000000
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-37.0000000000	0.0000000000	0.0000000000
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-33.4000000000	0.0000000000	0.0000000000
-31.6000000000	0.0000000000	0.0000000000

-29.8000000000	0.0000000000	0.0000000000
-28.0000000000	0.0000000000	0.0000000000
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-22.6000000000	0.0000000000	0.0000000000
-20.8000000000	0.0000000000	0.0000000000
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-11.8000000000	0.0000000000	0.0000000000
-10.0000000000	0.0000000000	0.0000000000
-8.2000000000	0.0000000000	0.0000000000
-6.4000000000	0.0000000000	0.0000000000
-4.6000000000	0.0000000000	0.0000000000
-2.8000000000	0.0000000000	0.0000000000
-1.0000000000	0.0000000000	0.0000000000
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2.6000000000	0.0000000000	0.0000000000
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11.6000000000	0.0000000000	0.0000000000
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15.2000000000	0.0000000000	0.0000000000
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20.6000000000	0.0000000000	0.0000000000
22.4000000000	0.0000000000	0.0000000000
24.2000000000	0.0000000000	0.0000000000
26.0000000000	0.0000000000	0.0000000000
27.8000000000	0.0000000000	0.0000000000
29.6000000000	0.0000000000	0.0000000000
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35.0000000000	0.0000000000	0.0000000000
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38.6000000000	0.0000000000	0.0000000000
40.4000000000	0.0000000000	0.0000000000
42.2000000000	0.0000000000	0.0000000000
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78.2000000000	-0.0000000000	0.0000000000
80.0000000000	-0.0000000000	-0.0000000000
81.8000000000	-0.0000000000	-0.0000000000
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85.4000000000	-0.0000000000	-0.0000000000
87.2000000000	-0.0000000000	-0.0000000000
89.0000000000	-0.0000000000	-0.0000000000
90.8000000000	-0.0000000000	-0.0000000000
92.6000000000	-0.0000000000	-0.0000000000
94.4000000000	-0.0000000000	-0.0000000000
96.2000000000	-0.0000000000	-0.0000000000
98.0000000000	-0.0000000000	-0.0000000000
99.8000000000	-0.0000000000	-0.0000000000
101.6000000000	-0.0000000000	-0.0000000000
103.4000000000	-0.0000000000	-0.0000000000
105.2000000000	-0.0000000000	-0.0000000000
107.0000000000	-0.0000000000	-0.0000000000
108.8000000000	-0.0000000000	-0.0000000000
110.6000000000	-0.0000000000	-0.0000000000
112.4000000000	-0.0000000000	-0.0000000000
114.2000000000	-0.0000000000	-0.0000000000
116.0000000000	-0.0000000000	-0.0000000000
117.8000000000	-0.0000000000	-0.0000000000
119.6000000000	-0.0000000000	-0.0000000000
121.4000000000	-0.0000000000	-0.0000000000
123.2000000000	-0.0000000003	-0.0000000000
125.0000000000	-0.0000000097	-0.0000000000
126.8000000000	-0.0000001987	-0.0000000000

128.6000000000	-0.0000029425	-0.0000000000
130.4000000000	-0.0000323088	-0.0000000002
132.2000000000	-0.0002686925	-0.0000000176
134.0000000000	-0.0017258333	-0.0000007402
135.8000000000	-0.0087161538	-0.0000187169
137.6000000000	-0.0351814651	-0.0002940984
139.4000000000	-0.1151629529	-0.0029569270
141.2000000000	-0.3096096002	-0.0195152454
143.0000000000	-0.6905289800	-0.0863347730
144.8000000000	-1.2854265691	-0.2596324404
146.6000000000	-1.9949737219	-0.5309580967
148.4000000000	-2.5391169660	-0.7113406136
150.2000000000	-2.4961995396	-0.5029565777
152.0000000000	-1.4507537594	0.2129188920
153.8000000000	0.8097623231	1.2303094508
155.6000000000	4.1511220108	2.1864568746
157.4000000000	8.0819519903	2.7416893283
159.2000000000	11.8900194447	2.6212749958
161.0000000000	14.8657557749	1.7392316625
162.8000000000	16.5139815843	0.3883838642
164.6000000000	16.6679719011	-0.8581409391
166.4000000000	15.4760983464	-1.5636059023
168.2000000000	13.2941813790	-1.7114003342
170.0000000000	10.5490779958	-1.5729681883
171.8000000000	7.6296828688	-1.3898112742
173.6000000000	4.8285818122	-1.2196544811
175.4000000000	2.3280407573	-1.0100960738
177.2000000000	0.2122143474	-0.7335702882
179.0000000000	-1.5094937387	-0.4410837073
180.8000000000	-2.8756770332	-0.2226479169
182.6000000000	-3.9463884631	-0.1383039671
184.4000000000	-4.7801411746	-0.1783392394
186.2000000000	-5.4182828339	-0.2716668380
188.0000000000	-5.8793570234	-0.3281558976
189.8000000000	-6.1630570368	-0.2865433581
191.6000000000	-6.2602862664	-0.1418730278
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195.2000000000	-5.8792656477	0.2509132525
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198.8000000000	-4.8235293481	0.4315603179
200.6000000000	-4.1191298766	0.4223436543
202.4000000000	-3.3481742171	0.3862706968
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206.0000000000	-1.7497140007	0.3360729898

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209.6000000000	-0.2669797994	0.3306321468
211.4000000000	0.3778366887	0.3162458322
213.2000000000	0.9390680707	0.2818211198
215.0000000000	1.4079939776	0.2270764045
216.8000000000	1.7808258585	0.1578458997
218.6000000000	2.0590052354	0.0830028555
220.4000000000	2.2492109521	0.0114737672
222.2000000000	2.3629227929	-0.0496785684
224.0000000000	2.4155052435	-0.0959429723
225.8000000000	2.4248786043	-0.1251647954
227.6000000000	2.4099150447	-0.1369438933
229.4000000000	2.3887315069	-0.1319930360
231.2000000000	2.3770562544	-0.1116559551
233.0000000000	2.3868304609	-0.0776632032
234.8000000000	2.4251778315	-0.0321403512
236.6000000000	2.4938380733	0.0221641659
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242.0000000000	2.8208561916	0.1940810763
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245.6000000000	3.0109502633	0.2522564456
247.4000000000	3.0499514220	0.2437504544
249.2000000000	3.0322523610	0.2045287403
251.0000000000	2.9472489890	0.1347293283
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254.6000000000	2.5552015245	-0.0748230354
256.4000000000	2.2503709485	-0.1946152790
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261.8000000000	1.0077079674	-0.4681702304
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265.4000000000	0.0543864763	-0.4952362894
267.2000000000	-0.4100666530	-0.4574644788
269.0000000000	-0.8461439907	-0.3925020714
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274.4000000000	-1.8739699511	-0.1212082157
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278.0000000000	-2.2671820800	0.0413112922
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285.2000000000	-2.3837551826	0.1826591261

287.0000000000	-2.3051063226	0.1830773357
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290.6000000000	-2.0678423135	0.1599444744
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299.6000000000	-1.2994881782	0.0677590571
301.4000000000	-1.1525057869	0.0535026361
303.2000000000	-1.0142696633	0.0415250151
305.0000000000	-0.8861497377	0.0317229877
306.8000000000	-0.7689590059	0.0238871868
308.6000000000	-0.6630517766	0.0177558840
310.4000000000	-0.5684190743	0.0130537483
312.2000000000	-0.4847771268	0.0095173273
314.0000000000	-0.4116463003	0.0069097911
315.8000000000	-0.3484190436	0.0050276353
317.6000000000	-0.2944163568	0.0037018132
319.4000000000	-0.2489330130	0.0027953497
321.2000000000	-0.2112722621	0.0021990168
323.0000000000	-0.1807710667	0.0018262042
324.8000000000	-0.1568170912	0.0016077500
326.6000000000	-0.1388587270	0.0014872059
328.4000000000	-0.1264094162	0.0014168077
330.2000000000	-0.1190474642	0.0013542792
332.0000000000	-0.1164124203	0.0012605102
333.8000000000	-0.1181989826	0.0010980880
335.6000000000	-0.1241492534	0.0008306292
337.4000000000	-0.1340440416	0.0004228268
339.2000000000	-0.1476937895	-0.0001588900
341.0000000000	-0.1649295926	-0.0009452081
342.8000000000	-0.1855946779	-0.0019624365
344.6000000000	-0.2095366252	-0.0032308185
346.4000000000	-0.2366005330	-0.0047628150
348.2000000000	-0.2666232682	-0.0065615203
350.0000000000	-0.2994288791	-0.0086193633
351.8000000000	-0.3348252032	-0.0109172303
353.6000000000	-0.3726016572	-0.0134241145
355.4000000000	-0.4125281632	-0.0160973632
357.2000000000	-0.4543551341	-0.0188835510
359.0000000000	-0.4978144200	-0.0217199647
360.8000000000	-0.5426210972	-0.0245366415
362.6000000000	-0.5884759706	-0.0272588648
364.4000000000	-0.6350686524	-0.0298099892

366.2000000000	-0.6820810755	-0.0321144451
368.0000000000	-0.7291913040	-0.0341007625
369.8000000000	-0.7760775038	-0.0357044528
371.6000000000	-0.8224219489	-0.0368705986
373.4000000000	-0.8679149462	-0.0375560222
375.2000000000	-0.9122585771	-0.0377309302
377.0000000000	-0.9551701653	-0.0373799670
378.8000000000	-0.9963854008	-0.0365026422
380.6000000000	-1.0356610602	-0.0351131348
382.4000000000	-1.0727772838	-0.0332395104
384.2000000000	-1.1075393827	-0.0309224135
386.0000000000	-1.1397791645	-0.0282133238
387.8000000000	-1.1693557806	-0.0251724775
389.6000000000	-1.1961561064	-0.0218665672
391.4000000000	-1.2200946806	-0.0183663341
393.2000000000	-1.2411132339	-0.0147441612
395.0000000000	-1.2591798473	-0.0110717700
396.8000000000	-1.2742877827	-0.0074181043
398.6000000000	-1.2864540343	-0.0038474731
400.4000000000	-1.2957176478	-0.0004180012
402.2000000000	-1.3021378577	0.0028195781
404.0000000000	-1.3057920908	0.0058227771
405.8000000000	-1.3067738810	0.0085578547
407.6000000000	-1.3051907394	0.0109999848
409.4000000000	-1.3011620195	0.0131331195
411.2000000000	-1.2948168117	0.0149495858
413.0000000000	-1.2862919001	0.0164494619
414.8000000000	-1.2757298062	0.0176397785
416.6000000000	-1.2632769429	0.0185335958
418.4000000000	-1.2490818951	0.0191490018
420.2000000000	-1.2332938410	0.0195080762
422.0000000000	-1.2160611213	0.0196358598
423.8000000000	-1.1975299639	0.0195593618
425.6000000000	-1.1778433635	0.0193066334
427.4000000000	-1.1571401165	0.0189059290
429.2000000000	-1.1355540071	0.0183849692
431.0000000000	-1.1132131384	0.0177703168
432.8000000000	-1.0902394009	0.0170868673
434.6000000000	-1.0667480698	0.0163574561
436.4000000000	-1.0428475214	0.0156025758
438.2000000000	-1.0186390568	0.0148401976
440.0000000000	-0.9942168227	0.0140856869
441.8000000000	-0.9696678184	0.0133518008
443.6000000000	-0.9450719776	0.0126487569

445.4000000000	-0.9205023142	0.0119843596
447.2000000000	-0.8960251217	0.0113641722
449.0000000000	-0.8717002177	0.0107917225
450.8000000000	-0.8475812227	0.0102687314
452.6000000000	-0.8237158662	0.0097953538
454.4000000000	-0.8001463121	0.0093704239
456.2000000000	-0.7769094969	0.0089916974
458.0000000000	-0.7540374748	0.0086560833
459.8000000000	-0.7315577633	0.0083598622
461.6000000000	-0.7094936874	0.0080988864
463.4000000000	-0.6878647158	0.0078687590
465.2000000000	-0.6666867884	0.0076649919
467.0000000000	-0.6459726306	0.0074831402
468.8000000000	-0.6257320545	0.0073189145
470.6000000000	-0.6059722438	0.0071682713
472.4000000000	-0.5866980221	0.0070274824
474.2000000000	-0.5679121048	0.0068931857
476.0000000000	-0.5496153328	0.0067624177
477.8000000000	-0.5318068892	0.0066326319
479.6000000000	-0.5144844988	0.0065017024
481.4000000000	-0.4976446110	0.0063679177
483.2000000000	-0.4812825665	0.0062299638
485.0000000000	-0.4653927485	0.0060869009
486.8000000000	-0.4499687201	0.0059381340
488.6000000000	-0.4350033472	0.0057833797
490.4000000000	-0.4204889090	0.0056226304
492.2000000000	-0.4064171969	0.0054561171
494.0000000000	-0.3927796024	0.0052842724
495.8000000000	-0.3795671949	0.0051076934
497.6000000000	-0.3667707905	0.0049271074
499.4000000000	-0.3543810127	0.0047433380
501.2000000000	-0.3423883456	0.0045572752
503.0000000000	-0.3307831802	0.0043698474
504.8000000000	-0.3195558554	0.0041819965
506.6000000000	-0.3086966928	0.0039946565
508.4000000000	-0.2981960278	0.0038087349
510.2000000000	-0.2880442356	0.0036250968
512.0000000000	-0.2782317541	0.0034445527
513.8000000000	-0.2687491037	0.0032678484
515.6000000000	-0.2595869039	0.0030956576
517.4000000000	-0.2507358877	0.0029285767
519.2000000000	-0.2421869140	0.0027671223
521.0000000000	-0.2339309778	0.0026117298
522.8000000000	-0.2259592191	0.0024627536

524.6000000000	-0.2182629302	0.0023204697
526.4000000000	-0.2108335624	0.0021850780
528.2000000000	-0.2036627306	0.0020567065
530.0000000000	-0.1967422178	0.0019354160
531.8000000000	-0.1900639788	0.0018212051
533.6000000000	-0.1836201426	0.0017140160
535.4000000000	-0.1774030149	0.0016137400
537.2000000000	-0.1714050799	0.0015202237
539.0000000000	-0.1656190010	0.0014332744
540.8000000000	-0.1600376218	0.0013526665
542.6000000000	-0.1546539666	0.0012781466
544.4000000000	-0.1494612402	0.0012094389
546.2000000000	-0.1444528276	0.0011462503
548.0000000000	-0.1396222935	0.0010882752
549.8000000000	-0.1349633814	0.0010351995
551.6000000000	-0.1304700122	0.0009867050
553.4000000000	-0.1261362832	0.0009424723
555.2000000000	-0.1219564661	0.0009021847
557.0000000000	-0.1179250054	0.0008655304
558.8000000000	-0.1140365164	0.0008322052
560.6000000000	-0.1102857828	0.0008019144
562.4000000000	-0.1066677543	0.0007743746
564.2000000000	-0.1031775443	0.0007493149
566.0000000000	-0.0998104270	0.0007264784
567.8000000000	-0.0965618345	0.0007056224
569.6000000000	-0.0934273540	0.0006865193
571.4000000000	-0.0904027246	0.0006689572
573.2000000000	-0.0874838341	0.0006527394
575.0000000000	-0.0846667157	0.0006376848
576.8000000000	-0.0819475448	0.0006236277
578.6000000000	-0.0793226353	0.0006104173
580.4000000000	-0.0767884365	0.0005979172
582.2000000000	-0.0743415290	0.0005860050
584.0000000000	-0.0719786217	0.0005745719
585.8000000000	-0.0696965479	0.0005635215
587.6000000000	-0.0674922616	0.0005527695
589.4000000000	-0.0653628342	0.0005422428
591.2000000000	-0.0633054505	0.0005318790
593.0000000000	-0.0613174056	0.0005216250
594.8000000000	-0.0593961007	0.0005114368
596.6000000000	-0.0575390402	0.0005012788
598.4000000000	-0.0557438276	0.0004911224
600.2000000000	-0.0540081624	0.0004809461
602.0000000000	-0.0523298366	0.0004707341

603.8000000000	-0.0507067313	0.0004604760
605.6000000000	-0.0491368136	0.0004501664
607.4000000000	-0.0476181327	0.0004398035
609.2000000000	-0.0461488178	0.0004293895
611.0000000000	-0.0447270740	0.0004189293
612.8000000000	-0.0433511798	0.0004084307
614.6000000000	-0.0420194842	0.0003979032
616.4000000000	-0.0407304035	0.0003873582
618.2000000000	-0.0394824189	0.0003768085
620.0000000000	-0.0382740733	0.0003662677
621.8000000000	-0.0371039695	0.0003557501
623.6000000000	-0.0359707667	0.0003452706
625.4000000000	-0.0348731790	0.0003348440
627.2000000000	-0.0338099721	0.0003244853
629.0000000000	-0.0327799620	0.0003142091
630.8000000000	-0.0317820121	0.0003040298
632.6000000000	-0.0308150312	0.0002939611
634.4000000000	-0.0298779719	0.0002840163
636.2000000000	-0.0289698283	0.0002742078
638.0000000000	-0.0280896339	0.0002645474
639.8000000000	-0.0272364606	0.0002550460
641.6000000000	-0.0264094161	0.0002457135
643.4000000000	-0.0256076430	0.0002365591
645.2000000000	-0.0248303166	0.0002275911
647.0000000000	-0.0240766440	0.0002188168
648.8000000000	-0.0233458622	0.0002102425
650.6000000000	-0.0226372371	0.0002018738
652.4000000000	-0.0219500618	0.0001937153
654.2000000000	-0.0212836558	0.0001857708
656.0000000000	-0.0206373635	0.0001780434
657.8000000000	-0.0200105533	0.0001705352
659.6000000000	-0.0194026163	0.0001632477
661.4000000000	-0.0188129655	0.0001561816
663.2000000000	-0.0182410348	0.0001493371
665.0000000000	-0.0176862777	0.0001427137
666.8000000000	-0.0171481673	0.0001363101
668.6000000000	-0.0166261944	0.0001301249
670.4000000000	-0.0161198676	0.0001241559
672.2000000000	-0.0156287120	0.0001184005
674.0000000000	-0.0151522688	0.0001128559
675.8000000000	-0.0146900945	0.0001075185
677.6000000000	-0.0142417602	0.0001023849
679.4000000000	-0.0138068510	0.0000974510
681.2000000000	-0.0133849658	0.0000927127

683.0000000000	-0.0129757162	0.0000881655
684.8000000000	-0.0125787262	0.0000838049
686.6000000000	-0.0121936319	0.0000796261
688.4000000000	-0.0118200808	0.0000756242
690.2000000000	-0.0114577314	0.0000717943
692.0000000000	-0.0111062528	0.0000681313
693.8000000000	-0.0107653245	0.0000646302
695.6000000000	-0.0104346355	0.0000612857
697.4000000000	-0.0101138846	0.0000580929
699.2000000000	-0.0098027794	0.0000550465
701.0000000000	-0.0095010366	0.0000521415
702.8000000000	-0.0092083813	0.0000493727
704.6000000000	-0.0089245465	0.0000467353
706.4000000000	-0.0086492736	0.0000442243
708.2000000000	-0.0083823112	0.0000418348
710.0000000000	-0.0081234156	0.0000395620
711.8000000000	-0.0078723501	0.0000374013
713.6000000000	-0.0076288848	0.0000353481
715.4000000000	-0.0073927966	0.0000333980
717.2000000000	-0.0071638690	0.0000315465
719.0000000000	-0.0069418914	0.0000297894
720.8000000000	-0.0067266596	0.0000281226
722.6000000000	-0.0065179751	0.0000265422
724.4000000000	-0.0063156452	0.0000250442
726.2000000000	-0.0061194825	0.0000236248
728.0000000000	-0.0059293053	0.0000222805
729.8000000000	-0.0057449369	0.0000210077
731.6000000000	-0.0055662056	0.0000198031
733.4000000000	-0.0053929446	0.0000186633
735.2000000000	-0.0052249919	0.0000175853
737.0000000000	-0.0050621902	0.0000165661
738.8000000000	-0.0049043866	0.0000156028
740.6000000000	-0.0047514325	0.0000146925
742.4000000000	-0.0046031836	0.0000138326
744.2000000000	-0.0044594997	0.0000130205
746.0000000000	-0.0043202446	0.0000122539
747.8000000000	-0.0041852860	0.0000115303
749.6000000000	-0.0040544953	0.0000108476
751.4000000000	-0.0039277476	0.0000102036
753.2000000000	-0.0038049216	0.0000095962
755.0000000000	-0.0036858996	0.0000090236
756.8000000000	-0.0035705670	0.0000084838
758.6000000000	-0.0034588127	0.0000079751
760.4000000000	-0.0033505287	0.0000074958

762.2000000000	-0.0032456101	0.0000070443
764.0000000000	-0.0031439551	0.0000066191
765.8000000000	-0.0030454648	0.0000062188
767.6000000000	-0.0029500431	0.0000058419
769.4000000000	-0.0028575967	0.0000054872
771.2000000000	-0.0027680352	0.0000051533
773.0000000000	-0.0026812705	0.0000048393
774.8000000000	-0.0025972173	0.0000045439
776.6000000000	-0.0025157928	0.0000042660
778.4000000000	-0.0024369164	0.0000040047
780.2000000000	-0.0023605101	0.0000037591
782.0000000000	-0.0022864980	0.0000035281
783.8000000000	-0.0022148067	0.0000033111
785.6000000000	-0.0021453646	0.0000031071
787.4000000000	-0.0020781024	0.0000029154
789.2000000000	-0.0020129530	0.0000027354
791.0000000000	-0.0019498510	0.0000025662
792.8000000000	-0.0018887332	0.0000024073
794.6000000000	-0.0018295380	0.0000022581
796.4000000000	-0.0017722059	0.0000021180
798.2000000000	-0.0017166790	0.0000019865
800.0000000000	-0.0016629013	0.0000018630

2-SR ECD Spectrum
X-Axis: Excitation Energy (nm)
Y-Axis: Delta Epsilon

# X	Y	DY/DX
-100.0000000000	0.0000000000	0.0000000000
-98.2000000000	0.0000000000	0.0000000000
-96.4000000000	0.0000000000	0.0000000000
-94.6000000000	0.0000000000	0.0000000000
-92.8000000000	0.0000000000	0.0000000000
-91.0000000000	0.0000000000	0.0000000000
-89.2000000000	0.0000000000	0.0000000000
-87.4000000000	0.0000000000	0.0000000000
-85.6000000000	0.0000000000	0.0000000000
-83.8000000000	0.0000000000	0.0000000000
-82.0000000000	0.0000000000	0.0000000000
-80.2000000000	0.0000000000	0.0000000000
-78.4000000000	0.0000000000	0.0000000000
-76.6000000000	0.0000000000	0.0000000000
-74.8000000000	0.0000000000	0.0000000000
-73.0000000000	0.0000000000	0.0000000000
-71.2000000000	0.0000000000	0.0000000000

-69.4000000000	0.0000000000	0.0000000000
-67.6000000000	0.0000000000	0.0000000000
-65.8000000000	0.0000000000	0.0000000000
-64.0000000000	0.0000000000	0.0000000000
-62.2000000000	0.0000000000	0.0000000000
-60.4000000000	0.0000000000	0.0000000000
-58.6000000000	0.0000000000	0.0000000000
-56.8000000000	0.0000000000	0.0000000000
-55.0000000000	0.0000000000	0.0000000000
-53.2000000000	0.0000000000	0.0000000000
-51.4000000000	0.0000000000	0.0000000000
-49.6000000000	0.0000000000	0.0000000000
-47.8000000000	0.0000000000	0.0000000000
-46.0000000000	0.0000000000	0.0000000000
-44.2000000000	0.0000000000	0.0000000000
-42.4000000000	0.0000000000	0.0000000000
-40.6000000000	0.0000000000	0.0000000000
-38.8000000000	0.0000000000	0.0000000000
-37.0000000000	0.0000000000	0.0000000000
-35.2000000000	0.0000000000	0.0000000000
-33.4000000000	0.0000000000	0.0000000000
-31.6000000000	0.0000000000	0.0000000000
-29.8000000000	0.0000000000	0.0000000000
-28.0000000000	0.0000000000	0.0000000000
-26.2000000000	0.0000000000	0.0000000000
-24.4000000000	0.0000000000	0.0000000000
-22.6000000000	0.0000000000	0.0000000000
-20.8000000000	0.0000000000	0.0000000000
-19.0000000000	0.0000000000	0.0000000000
-17.2000000000	0.0000000000	0.0000000000
-15.4000000000	0.0000000000	0.0000000000
-13.6000000000	0.0000000000	0.0000000000
-11.8000000000	0.0000000000	0.0000000000
-10.0000000000	0.0000000000	0.0000000000
-8.2000000000	0.0000000000	0.0000000000
-6.4000000000	0.0000000000	0.0000000000
-4.6000000000	0.0000000000	0.0000000000
-2.8000000000	0.0000000000	0.0000000000
-1.0000000000	0.0000000000	0.0000000000
0.8000000000	0.0000000000	0.0000000000
2.6000000000	0.0000000000	0.0000000000
4.4000000000	0.0000000000	0.0000000000
6.2000000000	0.0000000000	0.0000000000
8.0000000000	0.0000000000	0.0000000000

9.8000000000	0.0000000000	0.0000000000
11.6000000000	0.0000000000	0.0000000000
13.4000000000	0.0000000000	0.0000000000
15.2000000000	0.0000000000	0.0000000000
17.0000000000	0.0000000000	0.0000000000
18.8000000000	0.0000000000	0.0000000000
20.6000000000	0.0000000000	0.0000000000
22.4000000000	0.0000000000	0.0000000000
24.2000000000	0.0000000000	0.0000000000
26.0000000000	0.0000000000	0.0000000000
27.8000000000	0.0000000000	0.0000000000
29.6000000000	0.0000000000	0.0000000000
31.4000000000	0.0000000000	0.0000000000
33.2000000000	0.0000000000	0.0000000000
35.0000000000	0.0000000000	0.0000000000
36.8000000000	0.0000000000	0.0000000000
38.6000000000	0.0000000000	0.0000000000
40.4000000000	0.0000000000	0.0000000000
42.2000000000	0.0000000000	0.0000000000
44.0000000000	0.0000000000	0.0000000000
45.8000000000	0.0000000000	0.0000000000
47.6000000000	0.0000000000	0.0000000000
49.4000000000	0.0000000000	0.0000000000
51.2000000000	0.0000000000	0.0000000000
53.0000000000	0.0000000000	0.0000000000
54.8000000000	0.0000000000	0.0000000000
56.6000000000	0.0000000000	0.0000000000
58.4000000000	0.0000000000	0.0000000000
60.2000000000	0.0000000000	0.0000000000
62.0000000000	0.0000000000	0.0000000000
63.8000000000	0.0000000000	0.0000000000
65.6000000000	0.0000000000	0.0000000000
67.4000000000	0.0000000000	0.0000000000
69.2000000000	0.0000000000	0.0000000000
71.0000000000	0.0000000000	0.0000000000
72.8000000000	0.0000000000	0.0000000000
74.6000000000	0.0000000000	0.0000000000
76.4000000000	0.0000000000	0.0000000000
78.2000000000	0.0000000000	0.0000000000
80.0000000000	0.0000000000	0.0000000000
81.8000000000	0.0000000000	0.0000000000
83.6000000000	0.0000000000	0.0000000000
85.4000000000	0.0000000000	0.0000000000
87.2000000000	0.0000000000	0.0000000000

89.0000000000	0.0000000000	0.0000000000
90.8000000000	0.0000000000	0.0000000000
92.6000000000	0.0000000000	0.0000000000
94.4000000000	0.0000000000	0.0000000000
96.2000000000	0.0000000000	0.0000000000
98.0000000000	0.0000000000	0.0000000000
99.8000000000	0.0000000000	0.0000000000
101.6000000000	0.0000000000	0.0000000000
103.4000000000	0.0000000000	0.0000000000
105.2000000000	0.0000000000	0.0000000000
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769.4000000000	-0.1026291014	0.0004088042
771.2000000000	-0.1000270368	0.0003883175
773.0000000000	-0.0974853297	0.0003687899
774.8000000000	-0.0950028940	0.0003501816
776.6000000000	-0.0925786463	0.0003324543
778.4000000000	-0.0902115071	0.0003155710
780.2000000000	-0.0879004017	0.0002994957
782.0000000000	-0.0856442612	0.0002841936
783.8000000000	-0.0834420232	0.0002696312
785.6000000000	-0.0812926329	0.0002557761
787.4000000000	-0.0791950435	0.0002425972
789.2000000000	-0.0771482172	0.0002300642
791.0000000000	-0.0751511254	0.0002181483
792.8000000000	-0.0732027499	0.0002068214
794.6000000000	-0.0713020829	0.0001960569
796.4000000000	-0.0694481278	0.0001858288
798.2000000000	-0.0676398994	0.0001761124
800.0000000000	-0.0658764247	0.0001668839

3-RS ECD Spectrum
X-Axis: Excitation Energy (nm)
Y-Axis: Delta Epsilon

# X	Y	DY/DX
-100.0000000000	0.0000000000	0.0000000000
-98.2000000000	0.0000000000	0.0000000000
-96.4000000000	0.0000000000	0.0000000000
-94.6000000000	0.0000000000	0.0000000000
-92.8000000000	0.0000000000	0.0000000000
-91.0000000000	0.0000000000	0.0000000000
-89.2000000000	0.0000000000	0.0000000000
-87.4000000000	0.0000000000	0.0000000000
-85.6000000000	0.0000000000	0.0000000000
-83.8000000000	0.0000000000	0.0000000000
-82.0000000000	0.0000000000	0.0000000000
-80.2000000000	0.0000000000	0.0000000000
-78.4000000000	0.0000000000	0.0000000000
-76.6000000000	0.0000000000	0.0000000000
-74.8000000000	0.0000000000	0.0000000000
-73.0000000000	0.0000000000	0.0000000000
-71.2000000000	0.0000000000	0.0000000000
-69.4000000000	0.0000000000	0.0000000000
-67.6000000000	0.0000000000	0.0000000000
-65.8000000000	0.0000000000	0.0000000000
-64.0000000000	0.0000000000	0.0000000000
-62.2000000000	0.0000000000	0.0000000000
-60.4000000000	0.0000000000	0.0000000000
-58.6000000000	0.0000000000	0.0000000000
-56.8000000000	0.0000000000	0.0000000000
-55.0000000000	0.0000000000	0.0000000000
-53.2000000000	0.0000000000	0.0000000000
-51.4000000000	0.0000000000	0.0000000000
-49.6000000000	0.0000000000	0.0000000000
-47.8000000000	0.0000000000	0.0000000000
-46.0000000000	0.0000000000	0.0000000000
-44.2000000000	0.0000000000	0.0000000000
-42.4000000000	0.0000000000	0.0000000000
-40.6000000000	0.0000000000	0.0000000000
-38.8000000000	0.0000000000	0.0000000000
-37.0000000000	0.0000000000	0.0000000000
-35.2000000000	0.0000000000	0.0000000000
-33.4000000000	0.0000000000	0.0000000000
-31.6000000000	0.0000000000	0.0000000000

-29.8000000000	0.0000000000	0.0000000000
-28.0000000000	0.0000000000	0.0000000000
-26.2000000000	0.0000000000	0.0000000000
-24.4000000000	0.0000000000	0.0000000000
-22.6000000000	0.0000000000	0.0000000000
-20.8000000000	0.0000000000	0.0000000000
-19.0000000000	0.0000000000	0.0000000000
-17.2000000000	0.0000000000	0.0000000000
-15.4000000000	0.0000000000	0.0000000000
-13.6000000000	0.0000000000	0.0000000000
-11.8000000000	0.0000000000	0.0000000000
-10.0000000000	0.0000000000	0.0000000000
-8.2000000000	0.0000000000	0.0000000000
-6.4000000000	0.0000000000	0.0000000000
-4.6000000000	0.0000000000	0.0000000000
-2.8000000000	0.0000000000	0.0000000000
-1.0000000000	0.0000000000	0.0000000000
0.8000000000	0.0000000000	0.0000000000
2.6000000000	0.0000000000	0.0000000000
4.4000000000	0.0000000000	0.0000000000
6.2000000000	0.0000000000	0.0000000000
8.0000000000	0.0000000000	0.0000000000
9.8000000000	0.0000000000	0.0000000000
11.6000000000	0.0000000000	0.0000000000
13.4000000000	0.0000000000	0.0000000000
15.2000000000	0.0000000000	0.0000000000
17.0000000000	0.0000000000	0.0000000000
18.8000000000	0.0000000000	0.0000000000
20.6000000000	0.0000000000	0.0000000000
22.4000000000	0.0000000000	0.0000000000
24.2000000000	0.0000000000	0.0000000000
26.0000000000	0.0000000000	0.0000000000
27.8000000000	0.0000000000	0.0000000000
29.6000000000	0.0000000000	0.0000000000
31.4000000000	0.0000000000	0.0000000000
33.2000000000	0.0000000000	0.0000000000
35.0000000000	0.0000000000	0.0000000000
36.8000000000	0.0000000000	0.0000000000
38.6000000000	0.0000000000	0.0000000000
40.4000000000	0.0000000000	0.0000000000
42.2000000000	0.0000000000	0.0000000000
44.0000000000	0.0000000000	0.0000000000
45.8000000000	0.0000000000	0.0000000000
47.6000000000	0.0000000000	0.0000000000

49.4000000000	0.0000000000	0.0000000000
51.2000000000	0.0000000000	0.0000000000
53.0000000000	0.0000000000	0.0000000000
54.8000000000	0.0000000000	0.0000000000
56.6000000000	0.0000000000	0.0000000000
58.4000000000	0.0000000000	0.0000000000
60.2000000000	0.0000000000	0.0000000000
62.0000000000	0.0000000000	0.0000000000
63.8000000000	0.0000000000	0.0000000000
65.6000000000	0.0000000000	0.0000000000
67.4000000000	0.0000000000	0.0000000000
69.2000000000	0.0000000000	0.0000000000
71.0000000000	0.0000000000	0.0000000000
72.8000000000	0.0000000000	0.0000000000
74.6000000000	0.0000000000	0.0000000000
76.4000000000	0.0000000000	0.0000000000
78.2000000000	0.0000000000	0.0000000000
80.0000000000	0.0000000000	0.0000000000
81.8000000000	0.0000000000	0.0000000000
83.6000000000	0.0000000000	0.0000000000
85.4000000000	0.0000000000	0.0000000000
87.2000000000	0.0000000000	0.0000000000
89.0000000000	0.0000000000	0.0000000000
90.8000000000	0.0000000000	0.0000000000
92.6000000000	0.0000000000	0.0000000000
94.4000000000	0.0000000000	0.0000000000
96.2000000000	0.0000000000	0.0000000000
98.0000000000	0.0000000000	0.0000000000
99.8000000000	0.0000000000	0.0000000000
101.6000000000	0.0000000000	0.0000000000
103.4000000000	0.0000000000	0.0000000000
105.2000000000	0.0000000000	0.0000000000
107.0000000000	0.0000000000	0.0000000000
108.8000000000	0.0000000000	0.0000000000
110.6000000000	0.0000000000	0.0000000000
112.4000000000	0.0000000000	0.0000000000
114.2000000000	0.0000000000	0.0000000000
116.0000000000	0.0000000000	0.0000000000
117.8000000000	0.0000000000	0.0000000000
119.6000000000	0.0000000000	0.0000000000
121.4000000000	0.0000000000	0.0000000000
123.2000000000	0.0000000000	0.0000000000
125.0000000000	0.0000000002	0.0000000000
126.8000000000	0.0000000062	0.0000000000

128.6000000000	0.0000001257	0.0000000000
130.4000000000	0.0000018722	0.0000000000
132.2000000000	0.0000209458	0.0000000001
134.0000000000	0.0001795020	0.0000000045
135.8000000000	0.0012000213	0.0000002064
137.6000000000	0.0063650302	0.0000058467
139.4000000000	0.0272099804	0.0001051522
141.2000000000	0.0951373944	0.0012341398
143.0000000000	0.2758657564	0.0096827644
144.8000000000	0.6723191235	0.0518248660
146.6000000000	1.3955977917	0.1921623378
148.4000000000	2.5019245668	0.4976479359
150.2000000000	3.9334482261	0.8961224529
152.0000000000	5.5209670488	1.0880059101
153.8000000000	7.0666436665	0.8032191283
155.6000000000	8.4491624165	0.2274207752
157.4000000000	9.6622591231	-0.0681498214
159.2000000000	10.7525750903	0.2268563258
161.0000000000	11.7123069845	0.7743489818
162.8000000000	12.4174292799	0.9704466826
164.6000000000	12.6560871188	0.5654455268
166.4000000000	12.2176032042	-0.1872993305
168.2000000000	10.9775719206	-0.8671220011
170.0000000000	8.9353064832	-1.2533045706
171.8000000000	6.2030389615	-1.4125678284
173.6000000000	2.9724571169	-1.5334257405
175.4000000000	-0.5183240614	-1.7124760904
177.2000000000	-4.0109995625	-1.8712352826
179.0000000000	-7.2519838119	-1.8409673450
180.8000000000	-10.0208507878	-1.5166951240
182.6000000000	-12.1593184773	-0.9467352500
184.4000000000	-13.5918258686	-0.2999654591
186.2000000000	-14.3295710457	0.2417462791
188.0000000000	-14.4561425159	0.5749571676
189.8000000000	-14.0999647940	0.6962251624
191.6000000000	-13.4027717773	0.6654865670
193.4000000000	-12.4930245044	0.5567393336
195.2000000000	-11.4698120007	0.4298498396
197.0000000000	-10.3984488549	0.3266207815
198.8000000000	-9.3154683131	0.2752540551
200.6000000000	-8.2388436825	0.2896632268
202.4000000000	-7.1790692273	0.3633881879
204.2000000000	-6.1477367466	0.4670425153
206.0000000000	-5.1618443232	0.5564172040

207.8000000000	-4.2437037780	0.5895482455
209.6000000000	-3.4175573287	0.5438543162
211.4000000000	-2.7046537557	0.4242689767
213.2000000000	-2.1185548260	0.2591090991
215.0000000000	-1.6619926293	0.0872713792
216.8000000000	-1.3259158240	-0.0561364216
218.6000000000	-1.0906880907	-0.1495603303
220.4000000000	-0.9289093901	-0.1876256677
222.2000000000	-0.8090954999	-0.1777861924
224.0000000000	-0.6994574788	-0.1341534946
225.8000000000	-0.5711946933	-0.0716347556
227.6000000000	-0.4009582500	-0.0022041337
229.4000000000	-0.1723749736	0.0663904343
231.2000000000	0.1233048161	0.1301806790
233.0000000000	0.4872764238	0.1877530662
234.8000000000	0.9137797959	0.2389608144
236.6000000000	1.3910595523	0.2838958749
238.4000000000	1.9025558529	0.3221718972
240.2000000000	2.4282348554	0.3524893079
242.0000000000	2.9459947133	0.3724895657
243.8000000000	3.4330949534	0.3789419907
245.6000000000	3.8675564480	0.3682758446
247.4000000000	4.2294722610	0.3373788157
249.2000000000	4.5021632485	0.2844841889
251.0000000000	4.6731118556	0.2099188240
252.8000000000	4.7346159863	0.1165088537
254.6000000000	4.6841222877	0.0095286829
256.4000000000	4.5242225475	-0.1038041953
258.2000000000	4.2623245760	-0.2151808271
260.0000000000	3.9100358506	-0.3162256790
261.8000000000	3.4823206575	-0.3995054866
263.6000000000	2.9965067610	-0.4593593532
265.4000000000	2.4712243975	-0.4924407732
267.2000000000	1.9253585737	-0.4979249867
269.0000000000	1.3770863673	-0.4773931004
270.8000000000	0.8430560761	-0.4344491092
272.6000000000	0.3377469498	-0.3741537568
274.4000000000	-0.1269708089	-0.3023701202
276.2000000000	-0.5420740294	-0.2251120984
278.0000000000	-0.9014360731	-0.1479719838
279.8000000000	-1.2017129901	-0.0756809197
281.6000000000	-1.4420990278	-0.0118304244
283.4000000000	-1.6239877438	0.0412417738
285.2000000000	-1.7505750235	0.0824192943

287.0000000000	-1.8264375310	0.1116604506
288.8000000000	-1.8571153704	0.1297772444
290.6000000000	-1.8487218154	0.1381804303
292.4000000000	-1.8075966256	0.1386260832
294.2000000000	-1.7400133169	0.1329905320
296.0000000000	-1.6519452288	0.1230904750
297.8000000000	-1.5488906188	0.1105553986
299.6000000000	-1.4357534506	0.0967513941
301.4000000000	-1.3167740375	0.0827497887
303.2000000000	-1.1955021758	0.0693308168
305.0000000000	-1.0748047318	0.0570115458
306.8000000000	-0.9568996399	0.0460879143
308.6000000000	-0.8434087785	0.0366824154
310.4000000000	-0.7354230265	0.0287911025
312.2000000000	-0.6335738275	0.0223257713
314.0000000000	-0.5381066890	0.0171490766
315.8000000000	-0.4489531077	0.0131018378
317.6000000000	-0.3657984006	0.0100228211
319.4000000000	-0.2881437728	0.0077619121
321.2000000000	-0.2153616637	0.0061878765
323.0000000000	-0.1467439732	0.0051919540
324.8000000000	-0.0815431854	0.0046884246
326.6000000000	-0.0190067035	0.0046131067
328.4000000000	0.0415951069	0.0049205406
330.2000000000	0.1009465637	0.0055804205
332.0000000000	0.1596693657	0.0065736797
333.8000000000	0.2183097100	0.0078885132
335.6000000000	0.2773292375	0.0095165372
337.4000000000	0.3370992677	0.0114492317
339.2000000000	0.3978978473	0.0136747821
341.0000000000	0.4599091987	0.0161754138
342.8000000000	0.5232252100	0.0189253018
344.6000000000	0.5878486591	0.0218891232
346.4000000000	0.6536979040	0.0250212989
348.2000000000	0.7206128018	0.0282659499
350.0000000000	0.7883616452	0.0315575629
351.8000000000	0.8566489207	0.0348223235
353.6000000000	0.9251237047	0.0379800466
355.4000000000	0.9933885239	0.0409465958
357.2000000000	1.0610085128	0.0436366597
359.0000000000	1.1275207071	0.0459667324
360.8000000000	1.1924433184	0.0478581350
362.6000000000	1.2552848454	0.0492399159
364.4000000000	1.3155528843	0.0500514779

366.2000000000	1.3727625129	0.0502447994
368.0000000000	1.4264441379	0.0497861453
369.8000000000	1.4761507078	0.0486571968
371.6000000000	1.5214642099	0.0468555608
373.4000000000	1.5620013896	0.0443946611
375.2000000000	1.5974186440	0.0413030425
377.0000000000	1.6274160624	0.0376231483
378.8000000000	1.6517406019	0.0334096576
380.6000000000	1.6701884019	0.0287274812
382.4000000000	1.6826062582	0.0236495272
384.2000000000	1.6888922893	0.0182543462
386.0000000000	1.6889958386	0.0126237639
387.8000000000	1.6829166684	0.0068405987
389.6000000000	1.6707035075	0.0009865453
391.4000000000	1.6524520206	-0.0048597078
393.2000000000	1.6283022720	-0.0106240811
395.0000000000	1.5984357596	-0.0162383971
396.8000000000	1.5630720926	-0.0216413528
398.6000000000	1.5224653895	-0.0267791759
400.4000000000	1.4769004674	-0.0316059844
402.2000000000	1.4266888934	-0.0360838757
404.0000000000	1.3721649616	-0.0401827844
405.8000000000	1.3136816569	-0.0438801477
407.6000000000	1.2516066603	-0.0471604226
409.4000000000	1.1863184447	-0.0500144969
411.2000000000	1.1182025033	-0.0524390335
413.0000000000	1.0476477490	-0.0544357846
414.8000000000	0.9750431152	-0.0560109054
416.6000000000	0.9007743819	-0.0571742934
418.4000000000	0.8252212488	-0.0579389699
420.2000000000	0.7487546676	-0.0583205200
422.0000000000	0.6717344447	-0.0583365945
423.8000000000	0.5945071171	-0.0580064808
425.6000000000	0.5174041041	-0.0573507374
427.4000000000	0.4407401312	-0.0563908910
429.2000000000	0.3648119201	-0.0551491868
431.0000000000	0.2898971361	-0.0536483858
432.8000000000	0.2162535828	-0.0519115993
434.6000000000	0.1441186297	-0.0499621511
436.4000000000	0.0737088597	-0.0478234604
438.2000000000	0.0052199199	-0.0455189366
440.0000000000	-0.0611734399	-0.0430718806
441.8000000000	-0.1253171577	-0.0405053864
443.6000000000	-0.1870774974	-0.0378422419

445.4000000000	-0.2463405489	-0.0351048232
447.2000000000	-0.3030116101	-0.0323149856
449.0000000000	-0.3570144649	-0.0294939485
450.8000000000	-0.4082905740	-0.0266621773
452.6000000000	-0.4567981948	-0.0238392641
454.4000000000	-0.5025114422	-0.0210438094
456.2000000000	-0.5454193072	-0.0182933075
458.0000000000	-0.5855246434	-0.0156040402
459.8000000000	-0.6228431340	-0.0129909794
461.6000000000	-0.6574022511	-0.0104677026
463.4000000000	-0.6892402150	-0.0080463243
465.2000000000	-0.7184049637	-0.0057374428
467.0000000000	-0.7449531408	-0.0035501062
468.8000000000	-0.7689491064	-0.0014917969
470.6000000000	-0.7904639794	0.0004315649
472.4000000000	-0.8095747148	0.0022155983
474.2000000000	-0.8263632205	0.0038574215
476.0000000000	-0.8409155170	0.0053555941
477.8000000000	-0.8533209427	0.0067100444
479.6000000000	-0.8636714064	0.0079219831
481.4000000000	-0.8720606892	0.0089938056
483.2000000000	-0.8785837952	0.0099289850
485.0000000000	-0.8833363526	0.0107319584
486.8000000000	-0.8864140643	0.0114080080
488.6000000000	-0.8879122071	0.0119631402
490.4000000000	-0.8879251792	0.0124039638
492.2000000000	-0.8865460942	0.0127375699
494.0000000000	-0.8838664202	0.0129714152
495.8000000000	-0.8799756620	0.0131132099
497.6000000000	-0.8749610854	0.0131708116
499.4000000000	-0.8689074793	0.0131521267
501.2000000000	-0.8618969567	0.0130650199
503.0000000000	-0.8540087885	0.0129172319
504.8000000000	-0.8453192715	0.0127163070
506.6000000000	-0.8359016250	0.0124695292
508.4000000000	-0.8258259167	0.0121838684
510.2000000000	-0.8151590125	0.0118659355
512.0000000000	-0.8039645506	0.0115219463
513.8000000000	-0.7923029367	0.0111576942
515.6000000000	-0.7802313568	0.0107785314
517.4000000000	-0.7678038089	0.0103893564
519.2000000000	-0.7550711476	0.0099946095
521.0000000000	-0.7420811431	0.0095982740
522.8000000000	-0.7288785510	0.0092038831

524.6000000000	-0.7155051918	0.0088145310
526.4000000000	-0.7020000386	0.0084328892
528.2000000000	-0.6883993116	0.0080612247
530.0000000000	-0.6747365776	0.0077014227
531.8000000000	-0.6610428541	0.0073550098
533.6000000000	-0.6473467167	0.0070231800
535.4000000000	-0.6336744074	0.0067068209
537.2000000000	-0.6200499455	0.0064065412
539.0000000000	-0.6064952382	0.0061226976
540.8000000000	-0.5930301903	0.0058554220
542.6000000000	-0.5796728139	0.0056046481
544.4000000000	-0.5664393357	0.0053701366
546.2000000000	-0.5533443028	0.0051515002
548.0000000000	-0.5404006856	0.0049482266
549.8000000000	-0.5276199781	0.0047597005
551.6000000000	-0.5150122948	0.0045852238
553.4000000000	-0.5025864648	0.0044240349
555.2000000000	-0.4903501217	0.0042753252
557.0000000000	-0.4783097906	0.0041382552
558.8000000000	-0.4664709701	0.0040119682
560.6000000000	-0.4548382118	0.0038956027
562.4000000000	-0.4434151952	0.0037883032
564.2000000000	-0.4322047988	0.0036892299
566.0000000000	-0.4212091675	0.0035975659
567.8000000000	-0.4104297761	0.0035125245
569.6000000000	-0.3998674891	0.0034333546
571.4000000000	-0.3895226172	0.0033593445
573.2000000000	-0.3793949694	0.0032898257
575.0000000000	-0.3694839027	0.0032241748
576.8000000000	-0.3597883679	0.0031618152
578.6000000000	-0.3503069522	0.0031022180
580.4000000000	-0.3410379192	0.0030449015
582.2000000000	-0.3319792452	0.0029894313
584.0000000000	-0.3231286539	0.0029354189
585.8000000000	-0.3144836471	0.0028825208
587.6000000000	-0.3060415342	0.0028304359
589.4000000000	-0.2977994580	0.0027789043
591.2000000000	-0.2897544199	0.0027277048
593.0000000000	-0.2819033012	0.0026766523
594.8000000000	-0.2742428842	0.0026255956
596.6000000000	-0.2667698699	0.0025744146
598.4000000000	-0.2594808951	0.0025230178
600.2000000000	-0.2523725476	0.0024713398
602.0000000000	-0.2454413795	0.0024193386

603.8000000000	-0.2386839197	0.0023669931
605.6000000000	-0.2320966847	0.0023143010
607.4000000000	-0.2256761888	0.0022612760
609.2000000000	-0.2194189522	0.0022079460
611.0000000000	-0.2133215094	0.0021543508
612.8000000000	-0.2073804156	0.0021005402
614.6000000000	-0.2015922527	0.0020465723
616.4000000000	-0.1959536348	0.0019925117
618.2000000000	-0.1904612125	0.0019384279
620.0000000000	-0.1851116768	0.0018843941
621.8000000000	-0.1799017626	0.0018304857
623.6000000000	-0.1748282513	0.0017767793
625.4000000000	-0.1698879735	0.0017233517
627.2000000000	-0.1650778103	0.0016702789
629.0000000000	-0.1603946954	0.0016176353
630.8000000000	-0.1558356164	0.0015654932
632.6000000000	-0.1513976150	0.0015139221
634.4000000000	-0.1470777883	0.0014629882
636.2000000000	-0.1428732892	0.0014127541
638.0000000000	-0.1387813262	0.0013632785
639.8000000000	-0.1347991637	0.0013146158
641.6000000000	-0.1309241218	0.0012668161
643.4000000000	-0.1271535760	0.0012199249
645.2000000000	-0.1234849570	0.0011739835
647.0000000000	-0.1199157498	0.0011290282
648.8000000000	-0.1164434935	0.0010850913
650.6000000000	-0.1130657805	0.0010422002
652.4000000000	-0.1097802558	0.0010003783
654.2000000000	-0.1065846163	0.0009596447
656.0000000000	-0.1034766096	0.0009200144
657.8000000000	-0.1004540338	0.0008814986
659.6000000000	-0.0975147362	0.0008441047
661.4000000000	-0.0946566125	0.0008078367
663.2000000000	-0.0918776061	0.0007726952
665.0000000000	-0.0891757068	0.0007386779
666.8000000000	-0.0865489504	0.0007057794
668.6000000000	-0.0839954173	0.0006739917
670.4000000000	-0.0815132320	0.0006433044
672.2000000000	-0.0791005619	0.0006137049
674.0000000000	-0.0767556169	0.0005851784
675.8000000000	-0.0744766478	0.0005577083
677.6000000000	-0.0722619462	0.0005312765
679.4000000000	-0.0701098430	0.0005058633
681.2000000000	-0.0680187082	0.0004814477

683.0000000000	-0.0659869494	0.0004580077
684.8000000000	-0.0640130116	0.0004355202
686.6000000000	-0.0620953763	0.0004139615
688.4000000000	-0.0602325603	0.0003933071
690.2000000000	-0.0584231155	0.0003735320
692.0000000000	-0.0566656278	0.0003546108
693.8000000000	-0.0549587166	0.0003365179
695.6000000000	-0.0533010340	0.0003192274
697.4000000000	-0.0516912641	0.0003027136
699.2000000000	-0.0501281224	0.0002869505
701.0000000000	-0.0486103550	0.0002719125
702.8000000000	-0.0471367383	0.0002575738
704.6000000000	-0.0457060778	0.0002439093
706.4000000000	-0.0443172080	0.0002308940
708.2000000000	-0.0429689917	0.0002185032
710.0000000000	-0.0416603191	0.0002067127
711.8000000000	-0.0403901076	0.0001954987
713.6000000000	-0.0391573010	0.0001848381
715.4000000000	-0.0379608690	0.0001747080
717.2000000000	-0.0367998069	0.0001650863
719.0000000000	-0.0356731346	0.0001559514
720.8000000000	-0.0345798964	0.0001472823
722.6000000000	-0.0335191605	0.0001390585
724.4000000000	-0.0324900183	0.0001312603
726.2000000000	-0.0314915841	0.0001238684
728.0000000000	-0.0305229946	0.0001168644
729.8000000000	-0.0295834081	0.0001102302
731.6000000000	-0.0286720046	0.0001039487
733.4000000000	-0.0277879848	0.0000980031
735.2000000000	-0.0269305701	0.0000923772
737.0000000000	-0.0260990018	0.0000870558
738.8000000000	-0.0252925408	0.0000820239
740.6000000000	-0.0245104673	0.0000772672
742.4000000000	-0.0237520801	0.0000727721
744.2000000000	-0.0230166964	0.0000685253
746.0000000000	-0.0223036515	0.0000645144
747.8000000000	-0.0216122980	0.0000607273
749.6000000000	-0.0209420057	0.0000571525
751.4000000000	-0.0202921614	0.0000537789
753.2000000000	-0.0196621679	0.0000505961
755.0000000000	-0.0190514443	0.0000475940
756.8000000000	-0.0184594252	0.0000447630
758.6000000000	-0.0178855605	0.0000420940
760.4000000000	-0.0173293151	0.0000395783

762.2000000000	-0.0167901685	0.0000372077
764.0000000000	-0.0162676141	0.0000349743
765.8000000000	-0.0157611597	0.0000328705
767.6000000000	-0.0152703263	0.0000308892
769.4000000000	-0.0147946483	0.0000290237
771.2000000000	-0.0143336730	0.0000272676
773.0000000000	-0.0138869603	0.0000256147
774.8000000000	-0.0134540824	0.0000240593
776.6000000000	-0.0130346235	0.0000225959
778.4000000000	-0.0126281795	0.0000212192
780.2000000000	-0.0122343577	0.0000199243
782.0000000000	-0.0118527767	0.0000187067
783.8000000000	-0.0114830658	0.0000175617
785.6000000000	-0.0111248647	0.0000164854
787.4000000000	-0.0107778239	0.0000154736
789.2000000000	-0.0104416034	0.0000145227
791.0000000000	-0.0101158734	0.0000136292
792.8000000000	-0.0098003134	0.0000127896
794.6000000000	-0.0094946123	0.0000120008
796.4000000000	-0.0091984680	0.0000112599
798.2000000000	-0.0089115873	0.0000105640
800.0000000000	-0.0086336854	0.0000099105

4-RR ECD Spectrum
X-Axis: Excitation Energy (nm)
Y-Axis: Delta Epsilon

# X	Y	DY/DX
-100.0000000000	0.0000000000	0.0000000000
-98.2000000000	0.0000000000	0.0000000000
-96.4000000000	0.0000000000	0.0000000000
-94.6000000000	0.0000000000	0.0000000000
-92.8000000000	0.0000000000	0.0000000000
-91.0000000000	0.0000000000	0.0000000000
-89.2000000000	0.0000000000	0.0000000000
-87.4000000000	0.0000000000	0.0000000000
-85.6000000000	0.0000000000	0.0000000000
-83.8000000000	0.0000000000	0.0000000000
-82.0000000000	0.0000000000	0.0000000000
-80.2000000000	0.0000000000	0.0000000000
-78.4000000000	0.0000000000	0.0000000000
-76.6000000000	0.0000000000	0.0000000000
-74.8000000000	0.0000000000	0.0000000000
-73.0000000000	0.0000000000	0.0000000000
-71.2000000000	0.0000000000	0.0000000000

-69.4000000000	0.0000000000	0.0000000000
-67.6000000000	0.0000000000	0.0000000000
-65.8000000000	0.0000000000	0.0000000000
-64.0000000000	0.0000000000	0.0000000000
-62.2000000000	0.0000000000	0.0000000000
-60.4000000000	0.0000000000	0.0000000000
-58.6000000000	0.0000000000	0.0000000000
-56.8000000000	0.0000000000	0.0000000000
-55.0000000000	0.0000000000	0.0000000000
-53.2000000000	0.0000000000	0.0000000000
-51.4000000000	0.0000000000	0.0000000000
-49.6000000000	0.0000000000	0.0000000000
-47.8000000000	0.0000000000	0.0000000000
-46.0000000000	0.0000000000	0.0000000000
-44.2000000000	0.0000000000	0.0000000000
-42.4000000000	0.0000000000	0.0000000000
-40.6000000000	0.0000000000	0.0000000000
-38.8000000000	0.0000000000	0.0000000000
-37.0000000000	0.0000000000	0.0000000000
-35.2000000000	0.0000000000	0.0000000000
-33.4000000000	0.0000000000	0.0000000000
-31.6000000000	0.0000000000	0.0000000000
-29.8000000000	0.0000000000	0.0000000000
-28.0000000000	0.0000000000	0.0000000000
-26.2000000000	0.0000000000	0.0000000000
-24.4000000000	0.0000000000	0.0000000000
-22.6000000000	0.0000000000	0.0000000000
-20.8000000000	0.0000000000	0.0000000000
-19.0000000000	0.0000000000	0.0000000000
-17.2000000000	0.0000000000	0.0000000000
-15.4000000000	0.0000000000	0.0000000000
-13.6000000000	0.0000000000	0.0000000000
-11.8000000000	0.0000000000	0.0000000000
-10.0000000000	0.0000000000	0.0000000000
-8.2000000000	0.0000000000	0.0000000000
-6.4000000000	0.0000000000	0.0000000000
-4.6000000000	0.0000000000	0.0000000000
-2.8000000000	0.0000000000	0.0000000000
-1.0000000000	0.0000000000	0.0000000000
0.8000000000	0.0000000000	0.0000000000
2.6000000000	0.0000000000	0.0000000000
4.4000000000	0.0000000000	0.0000000000
6.2000000000	0.0000000000	0.0000000000
8.0000000000	0.0000000000	0.0000000000

9.8000000000	0.0000000000	0.0000000000
11.6000000000	0.0000000000	0.0000000000
13.4000000000	0.0000000000	0.0000000000
15.2000000000	0.0000000000	0.0000000000
17.0000000000	0.0000000000	0.0000000000
18.8000000000	0.0000000000	0.0000000000
20.6000000000	0.0000000000	0.0000000000
22.4000000000	0.0000000000	0.0000000000
24.2000000000	0.0000000000	0.0000000000
26.0000000000	0.0000000000	0.0000000000
27.8000000000	0.0000000000	0.0000000000
29.6000000000	0.0000000000	0.0000000000
31.4000000000	0.0000000000	0.0000000000
33.2000000000	0.0000000000	0.0000000000
35.0000000000	0.0000000000	0.0000000000
36.8000000000	0.0000000000	0.0000000000
38.6000000000	0.0000000000	0.0000000000
40.4000000000	0.0000000000	0.0000000000
42.2000000000	0.0000000000	0.0000000000
44.0000000000	0.0000000000	0.0000000000
45.8000000000	0.0000000000	0.0000000000
47.6000000000	0.0000000000	0.0000000000
49.4000000000	0.0000000000	0.0000000000
51.2000000000	0.0000000000	0.0000000000
53.0000000000	0.0000000000	0.0000000000
54.8000000000	0.0000000000	0.0000000000
56.6000000000	0.0000000000	0.0000000000
58.4000000000	0.0000000000	0.0000000000
60.2000000000	0.0000000000	0.0000000000
62.0000000000	0.0000000000	0.0000000000
63.8000000000	0.0000000000	0.0000000000
65.6000000000	0.0000000000	0.0000000000
67.4000000000	0.0000000000	0.0000000000
69.2000000000	0.0000000000	0.0000000000
71.0000000000	0.0000000000	0.0000000000
72.8000000000	0.0000000000	0.0000000000
74.6000000000	0.0000000000	0.0000000000
76.4000000000	0.0000000000	0.0000000000
78.2000000000	0.0000000000	0.0000000000
80.0000000000	0.0000000000	0.0000000000
81.8000000000	0.0000000000	0.0000000000
83.6000000000	0.0000000000	0.0000000000
85.4000000000	0.0000000000	0.0000000000
87.2000000000	0.0000000000	0.0000000000

89.0000000000	0.0000000000	0.0000000000
90.8000000000	0.0000000000	0.0000000000
92.6000000000	0.0000000000	0.0000000000
94.4000000000	0.0000000000	0.0000000000
96.2000000000	0.0000000000	0.0000000000
98.0000000000	0.0000000000	0.0000000000
99.8000000000	0.0000000000	0.0000000000
101.6000000000	0.0000000000	0.0000000000
103.4000000000	0.0000000000	0.0000000000
105.2000000000	0.0000000000	0.0000000000
107.0000000000	0.0000000000	0.0000000000
108.8000000000	0.0000000000	0.0000000000
110.6000000000	0.0000000000	0.0000000000
112.4000000000	0.0000000000	0.0000000000
114.2000000000	0.0000000000	0.0000000000
116.0000000000	0.0000000000	0.0000000000
117.8000000000	0.0000000000	0.0000000000
119.6000000000	0.0000000000	0.0000000000
121.4000000000	0.0000000000	0.0000000000
123.2000000000	0.0000000002	0.0000000000
125.0000000000	0.0000000044	0.0000000000
126.8000000000	0.0000000838	0.0000000000
128.6000000000	0.0000011352	0.0000000000
130.4000000000	0.0000110805	0.0000000001
132.2000000000	0.0000783727	0.0000000101
134.0000000000	0.0003971569	0.0000003948
135.8000000000	0.0013631347	0.0000092776
137.6000000000	0.0024132908	0.0001331409
139.4000000000	-0.0040434583	0.0011736825
141.2000000000	-0.0484963243	0.0061850398
143.0000000000	-0.2061092107	0.0168428884
144.8000000000	-0.5982539381	0.0007382761
146.6000000000	-1.3357712229	-0.1652347209
148.4000000000	-2.4055846685	-0.6200254269
150.2000000000	-3.5852603452	-1.1804351388
152.0000000000	-4.5026123139	-1.1894166081
153.8000000000	-4.8578025913	-0.1889351190
155.6000000000	-4.6603692980	1.2227493035
157.4000000000	-4.2791668429	1.7663670138
159.2000000000	-4.2389112743	0.8451934336
161.0000000000	-4.9006409915	-0.8470209986
162.8000000000	-6.2460263694	-2.0867153823
164.6000000000	-7.8898506085	-2.1805404119
166.4000000000	-9.2777486591	-1.3055314458

168.2000000000	-9.9268613464	-0.1188516649
170.0000000000	-9.5840325294	0.8139844623
171.8000000000	-8.2595847189	1.3144503775
173.6000000000	-6.1685781014	1.5103538866
175.4000000000	-3.6369834777	1.5771640852
177.2000000000	-1.0156304843	1.5615331081
179.0000000000	1.3814738737	1.3960383953
180.8000000000	3.3150927872	1.0250270608
182.6000000000	4.6399749712	0.4957084647
184.4000000000	5.3083994979	-0.0567950035
186.2000000000	5.3597538461	-0.4926501966
188.0000000000	4.8992096648	-0.7392470114
189.8000000000	4.0708689225	-0.8071575620
191.6000000000	3.0315775003	-0.7588482228
193.4000000000	1.9301134505	-0.6634292139
195.2000000000	0.8935997806	-0.5640564257
197.0000000000	0.0203690960	-0.4678004379
198.8000000000	-0.6227842380	-0.3554839067
200.6000000000	-1.0008728879	-0.2028003989
202.4000000000	-1.1094429816	-0.0015832643
204.2000000000	-0.9717361016	0.2288489534
206.0000000000	-0.6338741015	0.4452748985
207.8000000000	-0.1579265324	0.5967317350
209.6000000000	0.3866187388	0.6449951247
211.4000000000	0.9318242304	0.5796867124
213.2000000000	1.4192647207	0.4216898386
215.0000000000	1.8057104641	0.2144775967
216.8000000000	2.0658032064	0.0082455604
218.6000000000	2.1916916177	-0.1559656627
220.4000000000	2.1902096975	-0.2562190973
222.2000000000	2.0785616453	-0.2913258295
224.0000000000	1.8795671915	-0.2756038620
225.8000000000	1.6173646583	-0.2304390177
227.6000000000	1.3141628974	-0.1764640774
229.4000000000	0.9882868689	-0.1287175890
231.2000000000	0.6534621039	-0.0952336266
233.0000000000	0.3190800227	-0.0781158463
234.8000000000	-0.0089090319	-0.0756584256
236.6000000000	-0.3268305883	-0.0843395677
238.4000000000	-0.6321432623	-0.1001142866
240.2000000000	-0.9225204183	-0.1189878407
242.0000000000	-1.1952605434	-0.1371589665
243.8000000000	-1.4470456457	-0.1510682488
245.6000000000	-1.6740042125	-0.1575648527

247.4000000000	-1.8719972295	-0.1542317320
249.2000000000	-2.0370303875	-0.1397736899
251.0000000000	-2.1656983451	-0.1143158367
252.8000000000	-2.2555822266	-0.0794817349
254.6000000000	-2.3055439850	-0.0381938117
256.4000000000	-2.3158860959	0.0057734315
258.2000000000	-2.2883685265	0.0483869356
260.0000000000	-2.2260944320	0.0859624466
261.8000000000	-2.1332900804	0.1156615602
263.6000000000	-2.0150126115	0.1357943813
265.4000000000	-1.8768217452	0.1458982635
267.2000000000	-1.7244494058	0.1466147293
269.0000000000	-1.5634957116	0.1394229074
270.8000000000	-1.3991722769	0.1263033701
272.6000000000	-1.2361055909	0.1094025306
274.4000000000	-1.0782054495	0.0907506501
276.2000000000	-0.9285967779	0.0720634564
278.0000000000	-0.7896081491	0.0546350181
279.8000000000	-0.6628070131	0.0393122604
281.6000000000	-0.5490700310	0.0265312303
283.4000000000	-0.4486766971	0.0163916566
285.2000000000	-0.3614153080	0.0087479503
287.0000000000	-0.2866919300	0.0032994870
288.8000000000	-0.2236349924	-0.0003311278
290.6000000000	-0.1711902155	-0.0025375195
292.4000000000	-0.1282025412	-0.0036879887
294.2000000000	-0.0934834499	-0.0041011774
296.0000000000	-0.0658634215	-0.0040355721
297.8000000000	-0.0442303266	-0.0036889375
299.6000000000	-0.0275552228	-0.0032040019
301.4000000000	-0.0149074226	-0.0026773655
303.2000000000	-0.0054608568	-0.0021693997
305.0000000000	0.0015062716	-0.0017136776
306.8000000000	0.0066166942	-0.0013251202
308.6000000000	0.0104025269	-0.0010065235
310.4000000000	0.0133156003	-0.0007534537
312.2000000000	0.0157385826	-0.0005576794
314.0000000000	0.0179960573	-0.0004093985
315.8000000000	0.0203649498	-0.0002985325
317.6000000000	0.0230838898	-0.0002153388
319.4000000000	0.0263612608	-0.0001505560
321.2000000000	0.0303818147	-0.0000952486
323.0000000000	0.0353118304	-0.0000404844
324.8000000000	0.0413028673	0.0000230593

326.6000000000	0.0484942197	0.0001054834
328.4000000000	0.0570142123	0.0002179911
330.2000000000	0.0669805000	0.0003731001
332.0000000000	0.0784995496	0.0005847055
333.8000000000	0.0916654816	0.0008679643
335.6000000000	0.1065584536	0.0012389827
337.4000000000	0.1232427555	0.0017142982
339.2000000000	0.1417647805	0.0023101664
341.0000000000	0.1621510193	0.0030416742
342.8000000000	0.1844062109	0.0039217197
344.6000000000	0.2085117644	0.0049599161
346.4000000000	0.2344245466	0.0061614863
348.2000000000	0.2620761105	0.0075262269
350.0000000000	0.2913724166	0.0090476221
351.8000000000	0.3221940803	0.0107121857
353.6000000000	0.3543971559	0.0124990987
355.4000000000	0.3878144490	0.0143801957
357.2000000000	0.4222573318	0.0163203330
359.0000000000	0.4575180187	0.0182781440
360.8000000000	0.4933722469	0.0202071665
362.6000000000	0.5295822950	0.0220572973
364.4000000000	0.5659002663	0.0237765087
366.2000000000	0.6020715557	0.0253127430
368.0000000000	0.6378384189	0.0266158879
369.8000000000	0.6729435623	0.0276397317
371.6000000000	0.7071336743	0.0283437957
373.4000000000	0.7401628245	0.0286949514
375.2000000000	0.7717956637	0.0286687418
377.0000000000	0.8018103657	0.0282503466
378.8000000000	0.8300012626	0.0274351498
380.6000000000	0.8561811338	0.0262288936
382.4000000000	0.8801831198	0.0246474236
384.2000000000	0.9018622442	0.0227160515
386.0000000000	0.9210965335	0.0204685805
387.8000000000	0.9377877385	0.0179460527
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5. Reference

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