Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Regioselective and Diastereodivergent Organocatalytic Asymmetric Vinylogous Michael Addition

A: General Remarks and Starting Materials

A1：General Remarks

^{1}H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker AV-400/500 spectrometer (400/500 MHz and 100/125 MHz). Chemical shifts (δ) for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to residual solvent peak. Chemical shifts (δ) for carbon are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent. Data are reported as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, dd = doublet of doublets, t = triplet, dt = doublet of triplets, q = quartet, quint = quintet, m = multiplet), coupling constants (*J*) in Hertz (Hz), integration; "app" is used to denote the apparent splitting of a signal.

High resolution mass spectrometry (HRMS) was carried out using MicroMass GCT CA 055 instrument and recorded on a MicroMass LCTTM spectrometer.

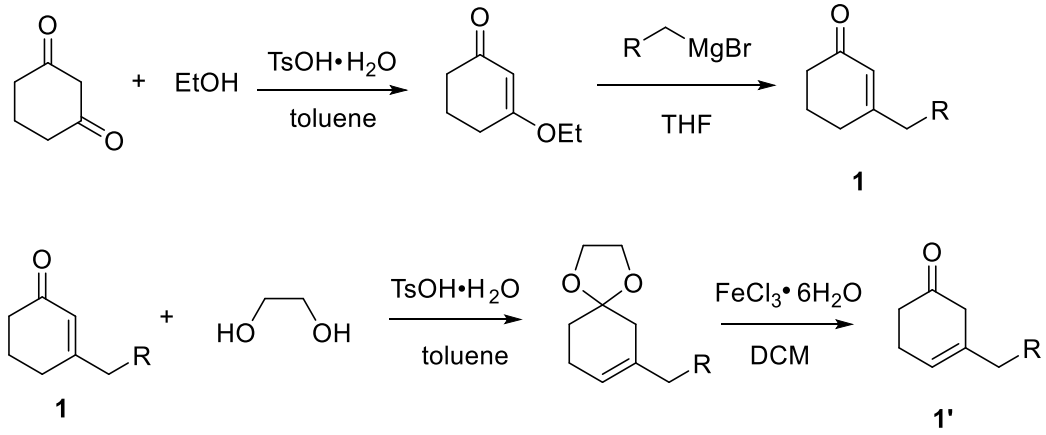
Optical rotations were measured on an Autopol III automatic polarimeter (Rudolph Research analytical). $[\alpha]_D^T$ values are reported in 10^{-1} deg cm^2 g^{-1}; concentrations (*c*) are quoted in g/100 mL; D refers to the D-line of sodium (589 nm); temperatures (T) are given in degrees Celsius (°C).

Melting points were measured on a XT3A apparatus.

Enantiomeric excesses were determined by HPLC analysis on an Agilent HPLC 1200 or 1220 Series instrument, using the chiral stationary phase column (25 cm x 4.6 mm internal diameter, Daicel Chiralpak IA, IB, AD-H, AS-H as noted) specified in the individual experiment.

A2：Starting Materials.

All solvents and inorganic reagents were from commercial sources (Adamas-beta, TCI, or Energy Chemical) and used without purification unless otherwise noted. Nitroalkenes were synthesized following the literature produre.[1] The aminocatalysts **3a** and **3b** were prepared according our previous papers.[2] The different β-alkyl-cyclohex-2-enones **1**[3] and β-substituted-cyclohex-3-enones **1′**[4] were achieved as showed in Scheme S1.



Scheme S1. Synthesis of starting materials **1** and **1′**

p-Toluenesulfonic acid (400 mg, 2.1 mmol) was added to a stirred solution of 1,3-cyclohexanedione (12.6 g, 112 mmol) in EtOH (50 mL) and PhMe (180 mL) at rt. The reaction mixture was heated at

reflux overnight. The reaction mixture was allowed too cool to rt before concentration to give orange oil under reduced pressure. The crude material was dissolved in EtOAc (100 mL) and neutralized using 1 M NaOH. The organic layer was washed by brine, dried by $MgSO_4$ and concentrated to afford intermediate 3-ethoxy-cyclohexenones which was used without futher purification.

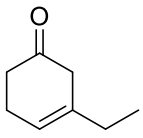
3-ethoxy-cyclohex-2-enones (20 mmol, 1.0 equiv) in anhydrous THF (15 mL) was added dropwise to a solution of a Grignard regent (30 mmol 1.5 equiv) under argon at 0 °C. Once the addition was completed, the solution was stirred at 45 °C for about 2 h. The reaction was slowly quenched with diluted aqueous acid (1 M HCl) at 0 °C. The layers were separated and the aqueous layer extracted with EtOAc (3×50 mL). The combined organic layers were washed with saturated $NaHCO_3$ and brine, dried with Na_2SO_4, then filtered and evaporated under reduced pressure. The crude product was purified by flash colume chromatography (PE/EA = 10 :1) to give the product β-alkyl-cyclohex-2-enones **1**.

A mixture of β-alkyl-2-cyclohex-2-enones **1** (36.00 mmol), toluenesulfonic acid (100 mg) and ethylene glycol (7 mL) in 100 mL of toluene is refluxed overnight and water formed is removed by Dean-Stark trap. The residue after concentration is chromatographed on silica gel (PE/EA = 95:5) to give the 7-alkyl-1,4-dioxaspiro[4.5]dec-7-enes.

To a solution of 7-alkyl-1,4-dioxaspiro[4.5]dec-7-enes (17 mmol) in CH_2Cl_2 (25 mL) at rt was added $FeCl_3 \cdot 6H_2O$ (1.66 g, 3.5 equiv). The resulting yellow to amber colored suspension was stirred for about 15 min and TLC was conducted to make sure the reactant was consumed. Then saturated aqueous $NaHCO_3$ was added to quench the reaction. The aqueous layer was extracted three times with CH_2Cl_2 and the combined organics were washed with brine, dry over $MgSO_4$, and concentrated under reduced pressure. The resulting oil was chromatographed on silica gel (PE/EA = 95:5) to give differernt β-alkyl-cyclohex-3-enones **1′**.

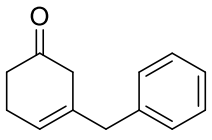
A3：For some selected Starting Materials NMR data.

1′a: β-ethyl-cyclohex-3-enone



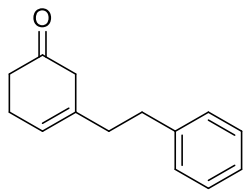
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.04 (t, J = 7.6 Hz, 3H), 2.00-2.06 (q, J_1 = 7.2 Hz, J_2 = 14.8 Hz, 2H), 2.45 (s, 4H), 2.81 (s, 2H), 5.61 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.9, 29.4, 38.5, 42.9, 119.2, 137.7, 211.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_8H_{12}O$) requires m/z 124.0888, found m/z 124.0891.

1′f: β-benzyl-cyclohex-3-enone



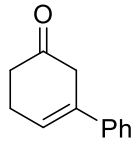
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.42 (s, 4H), 2.71 (s, 2H), 3.31 (s, 2H), 5.68 (s, 1H), 7.14-7.16 (m, 2H), 7.20-7.21 (m, 1H), 7.26-7.30 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.0, 38.4, 42.6, 43.4, 122.4, 126.4, 128.5, 128.9, 135.6, 138.7, 210.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{13}H_{14}O$) requires m/z 186.1045, found m/z 186.1044.

1′g: β-phenethyl-cyclohex-3-enone



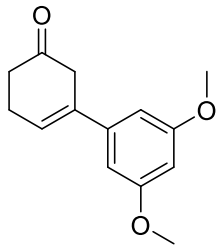
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.29-2.33 (m, 2H), 2.42 (s, 4H), 2.71-2.75 (m, 2H), 2.83 (s, 2H), 5.62 (s, 1H), 7.15-7.20 (m, 3H), 7.26-7.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.9, 34.0, 38.4, 38.4, 43.1, 121.2, 126.0, 128.3, 128.4, 135.5, 141.6, 210.6. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{16}O$) requires m/z 200.1201, found m/z 200.1202.

1′q: 4,5-dihydro-[1,1'-biphenyl]-3(2*H*)-one



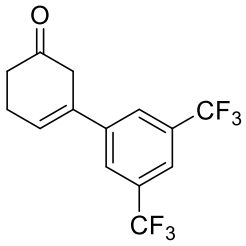
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.53-2.57 (m, 2H), 2.62-2.68 (m, 2H), 3.27-3.28 (m, 2H), 6.31-6.34 (m, 1H), 7.25-7.29 (m, 1H), 7.32-7.38 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.3, 38.0, 42.0, 123.6, 125.1, 127.6, 128.6, 134.9, 139.7, 210.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{12}H_{12}O$) requires m/z 172.0888, found m/z 172.0890.

1′r: 3',5'-dimethoxy-4,5-dihydro-[1,1'-biphenyl]-3(2*H*)-one



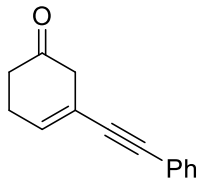
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.54-2.57 (m, 2H), 2.63-2.66 (m, 2H), 3.25 (s, 2H), 3.80 (s, 6H), 6.32-6.34 (m, 1H), 6.40-6.41 (m, 1H), 6.51-6.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.2, 38.0, 42.1, 55.4, 99.4, 103.6, 124.0, 134.9, 142.0, 160.8, 209.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{16}O_3$) requires m/z 232.1099, found m/z 232.1101.

1′s: 3',5'-bis(trifluoromethyl)-4,5-dihydro-[1,1'-biphenyl]-3(2*H*)-one



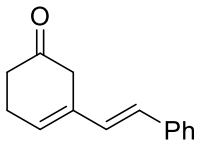
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.59-2.62 (m, 2H), 2.71-2.74 (m, 2H), 3.30 (s, 2H), 6.51-6.53 (m, 1H), 7.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.3, 37.3, 41.5, 121.1, 121.2, 121.2, 121.9, 124.6, 125.2, 127.5, 131.4, 131.8, 132.1, 132.4, 132.9, 141.7, 208.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{10}F_6O$) requires m/z 308.0636, found m/z 308.0637.

1′u: 3-(phenylethynyl)cyclohex-3-en-1-one



^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.50-2.53 (m, 2H), 2,58-2.63 (m, 2H), 3.09-3.09 (m, 2H), 6.37-6.39 (m, 1H), 7.31-7.33 (m, 3H), 7.42-7.45 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.4, 37.7, 43.2, 88.4, 88.5, 119.0, 122.9, 128.4, 131.5, 133.5, 208.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{12}O$) requires m/z 196.0888, found m/z 196.0891.

1′v: (*E*)-3-styrylcyclohex-3-en-1-one



^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.53-2.57 (m, 2H), 2.63-2.64 (m, 2H), 3.14 (s, 2H), 6.08 (s, 1H), 6.37-6.41 (d, *J* = 16.0 Hz, 1H), 6.83-6.87 (d, *J* = 16.0 Hz, 1H), 7.21-7.26 (m, 1H), 7.30-7.34 (m, 2H), 7.40-7.42 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.5, 38.5, 39.6, 126.4, 126.8, 127.6, 128.5, 128.7, 129.8, 134.1, 137.1, 209.7. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{14}O$) requires m/z 198.1045, found m/z 198.1046.

[1] J. M. Lopchuk, R. P. Hughes, G. W. Gribble. *Org. Lett.* **2013**, *15*, 5218-5221.

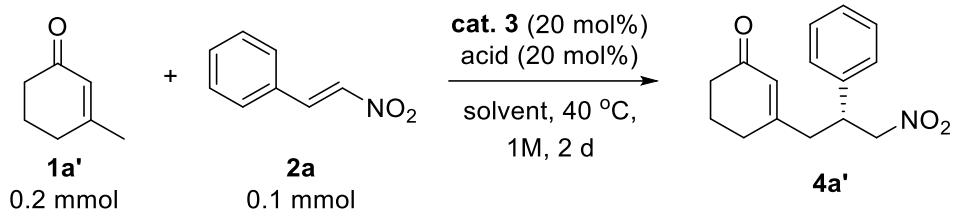
[2] a) H. Huang, F. Yu, Z. Jin, W. Li, W. Wu, X. Liang, J. Ye. *Chem. Commun.* **2010**, *46*, 5957-5959; b) P. Li, Y. Wang, X. Liang, J. Ye. *Chem. Commun.* **2008**, 3302-3304.

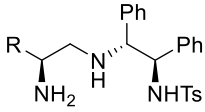
[3] a) B. K. Bharat, R. M. James, Z. Murray. *Synthesis* **1991**, *2*, 176; b) X. Yin, Y. Zheng, X. Feng, K. Jiang, X.-Z. Wei, N. Gao, Y.-C. Chen. *Angew. Chem. Int. Ed.* **2014**, *53*, 6245-6248.

[4] a) J. H. Babler, N. C. Malek, M. J. Coghlan. *J. Org. Chem.* **1978**, *43*, 1821-1823; b) D. Becker, Z. Harel, M. Nagler, A. Gillon. *J. Org. Chem.* **1982**, *47*, 3297-3306; c) S. E. Sen, S. L. Roach, J. K. Boggs, G. J. Ewing, J. Magrath. *J. Org. Chem.* **1997**, *62*, 6684-6686.

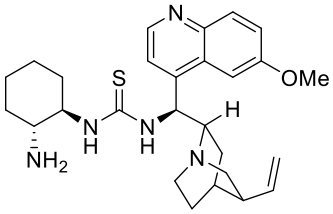
B: Optimization Tables

Table S1. The effect of the primary amine on γ-AVMA reaction of β-methyl-cyclohex-2-enone[a]

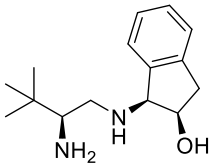




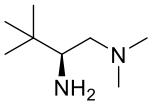
3a: R = *t*-Bu
3c: R = Bn
3d: R = Ph
3e: R = *i*-Bu
3f: R = *i*-Pr



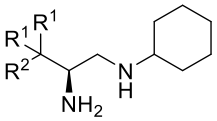
3b



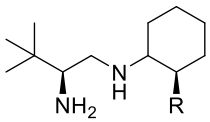
3g



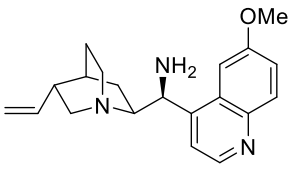
3h



3i: $R^1 = R^2$ = Me
3j: R^1 = Et, R^2 = OMe
3k: R^1 = Ph, R^2 = OMe



3l: R = NHTs
3m: R= OH

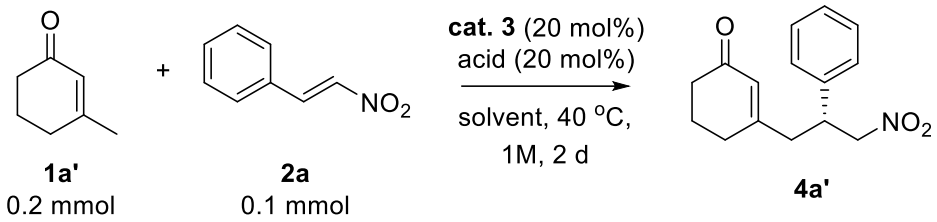


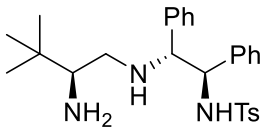
3n

entry	catalyst	conv. (%)[b]	ee (%)[c]
1[d]	**3a**	90	87
2	**3b**	74	90
3[d]	**3c**	24	47
4[d]	**3d**	15	-14
5[d]	**3e**	66	71
6[d]	**3f**	50	81
7	**3g**	79	32
8	**3h**	36	35
9	**3i**	88	40
10	**3j**	80	60
11	**3k**	20	37
12	**3l**	84	43
13	**3m**	68	15
14	**3n**	57	81

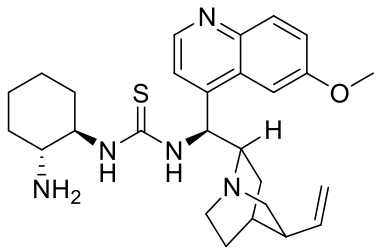
[a] All reactions were performed with **2a** (0.1 mmol), **1a'** (0.2 mmol), **cat. 3** (20 mol%) and 2-F-$C_6H_4CO_2H$ (30 mol%) in 100 μL of toluene. [b] Determined by GC analysis. [c] Determined by chiral HPLC analysis. [d] 2-F-$C_6H_4CO_2H$ (40 mmol%) was added.

Table S2. The effect of the concentration and acid additives on γ-regioselective AVMA reaction[a]





3a

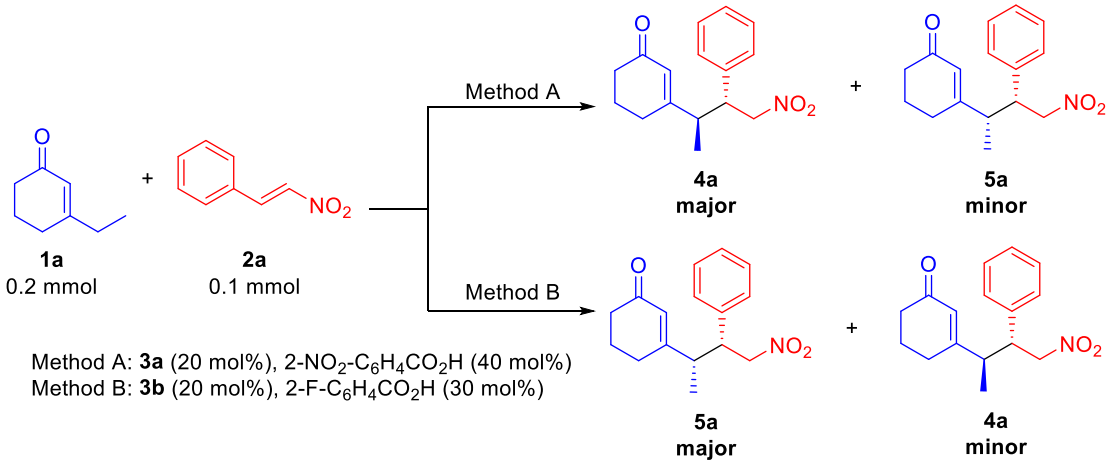


3b

entry	catalyst	acid	conv. (%)[b]	ee (%)[c]
1	**3a**	2-F-$C_6H_4CO_2H$	74	90
2[d]	**3a**	2-F-$C_6H_4CO_2H$	60	94
3	**3a**	2-F-$C_6H_4CO_2H$	84	76
4[e]	**3a**	2-F-$C_6H_4CO_2H$	90	87
5[d, e]	**3a**	2-F-$C_6H_4CO_2H$	84	89
6[d, e]	**3a**	$C_6H_5CO_2H$	74	45
7[d, e]	**3a**	AcOH	78	-16
8[d, e]	**3a**	2-MeO-$C_6H_4CO_2H$	75	40
9[d, e]	**3a**	3-Br-2-F-$C_6H_3CO_2H$	83	90
10[d, e]	**3b**	2-NO_2-$C_6H_4CO_2H$	67	95
11[d, e]	**3b**	3,5-$(NO_2)_2$-$C_6H_3CO_2H$	36	93
12[d, e]	**3b**	4-NO_2-$C_6H_4CO_2H$	61	85

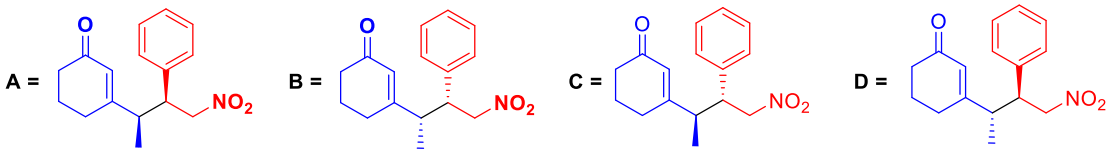
[a] All reactions were performed with **2a** (0.1 mmol), **1a'** (0.2 mmol), **cat. 3** (20 mol%) and acid (30 mol%) in 100 μL of toluene. [b] Determined by GC analysis. [c] Determined by chiral HPLC analysis. [d] Reaction in 500 μL of toluene. [e] acid (40 mol%) was added.

Table S3. Study of γ-regioselective AVMA reaction catalyzed by 3a and 3b[a]



entry	Method	conv. (%)[b]	ee (%)[c]	d.r. (*anti* : *syn*)[d]
1	A	96	55 (**4a**)/56 (**5a**)	88 (**4a**):12 (**5a**)
2	B	77	94 (**4a**)/93 (**5a**)	13 (**4a**):87 (**5a**)

[a] All reactions were performed with **2a** (0.1 mmol), **1a** (0.2 mmol), **cat. 3** (20 mol%) in toluene (0.2 M) for 3 days. [b] Determined by GC analysis. [c] Determined by chiral HPLC analysis. [d] was determined by ^{1}H NMR analysis of the crude reactions.



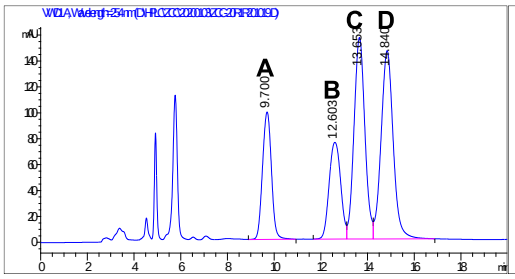


Figure S1

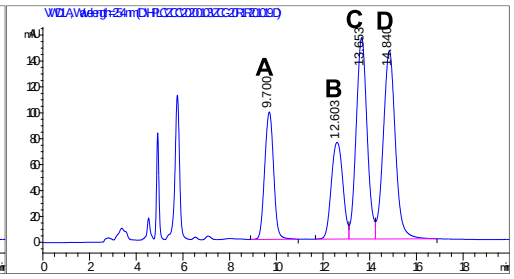


Figure S2

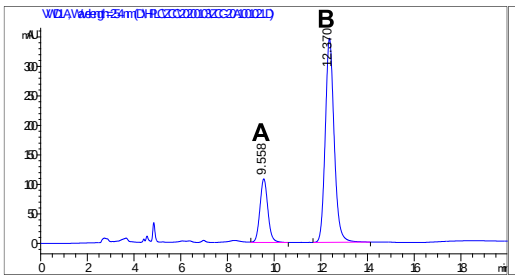


Figure S3.

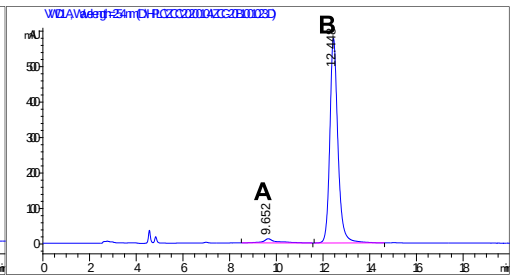


Figure S4

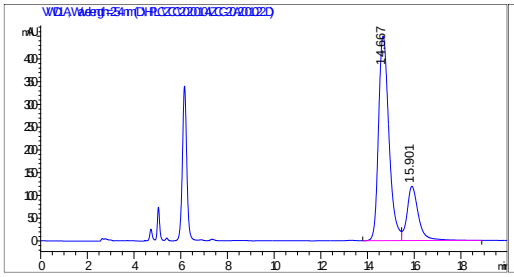


Figure S5

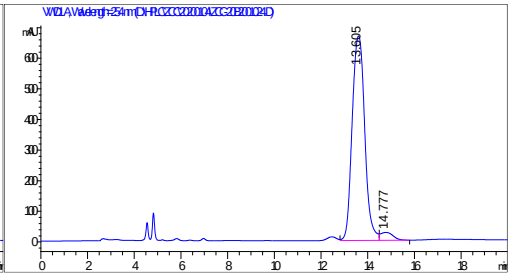


Figure S6

Notes:

(1) Figure S1 and Figure S2: Chiral HPLC analysis for racemic stereoiosmers of the reaction in Table S1.

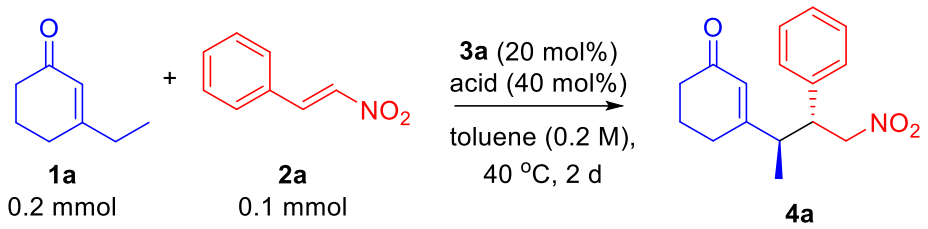
(2) Figure S3: Chiral HPLC analysis for minor diastereoisomer (**5a**) of Method A in Table S1.

(3) Figure S5: Chiral HPLC analysis for major diastereoisomer (**4a**) of Method A in Table S1.

(4) Figure S4: Chiral HPLC analysis for major diastereoisomer (**5a**) of Method B in Table S1.

(5) Figure S6: Chiral HPLC analysis for minor diastereoisomer (**4a**) of Method B in Table S1.

Table S4. The effect of the acids on γ-regioselective *anti*-AVMA reaction[a]

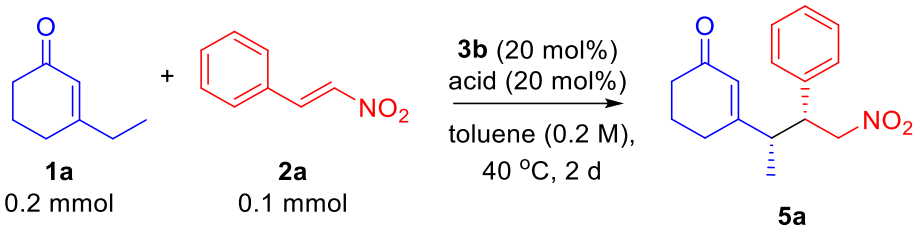


1a 0.2 mmol **2a** 0.1 mmol **4a**

entry	acid	conv. (%)[b]	ee (%)[c]	d.r. [d]
1	2-F-$C_6H_4CO_2H$	91	76	80:20
2	2-OH-$C_6H_4CO_2H$	64	75	83:17
3	2-NO_2-$C_6H_4CO_2H$	96	88	88:12
4	3-NO_2-$C_6H_4CO_2H$	71	75	84:16
5	4-NO_2-$C_6H_4CO_2H$	81	71	81:19
6	2-MeO-$C_6H_4CO_2H$	85	38	66:34
7	3,5-$(NO_2)_2$-$C_6H_3CO_2H$	88	81	77:23
8	2-F-4-NO_2-$C_6H_3CO_2H$	89	85	88:12
9	2-NO_2-4-F-$C_6H_3CO_2H$	77	89	90:10
10[e]	2-NO_2-4-F-$C_6H_3CO_2H$	76	90	92:8
11[e, f]	2-NO_2-4-F-$C_6H_3CO_2H$	69	91	94:6
12[e, g]	2-NO_2-4-F-$C_6H_3CO_2H$	68	92	94:6

[a] All reactions were performed with **2a** (0.1 mmol), **1a** (0.2 mmol), **cat. 3a** (20 mol%), and acid (40 mol%) in toluene. [b] Determined by GC analysis. [c] Determined by chiral HPLC analysis. [d] Determined by GC analysis. [e] The reaction was reacted at 30 °C. [f] Acid (50 mol%) was added. [g] Acid (60 mol%) was added.

Table S5. The effect of the acids on γ-regioselective *syn*-AVMA reaction[a]



1a 0.2 mmol

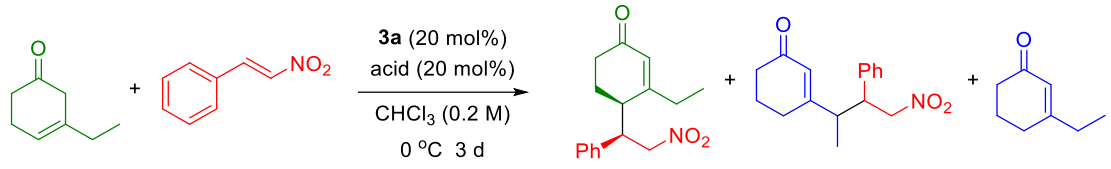
2a 0.1 mmol

5a

entry	acid	conv. (%)[b]	ee (%)[c]	d.r. [d]
1	$C_6H_5CO_2H$	70	94	37:63
2	2-MeO-$C_6H_4CO_2H$	74	93	37:63
3	2-OH-$C_6H_4CO_2H$	48	97	26:74
4	2-F-$C_6H_4CO_2H$	58	96	44:56
5	2-NO_2-$C_6H_4CO_2H$	50	97	21:79
6	3-NO_2-$C_6H_4CO_2H$	75	98	28:72
7	4-NO_2-$C_6H_4CO_2H$	54	97	38:62
8	3,5-$(NO_2)_2$-$C_6H_3CO_2H$	29	97	39:61
9	2-NO_2-4-F-$C_6H_3CO_2H$	43	97	25:75
10	2-F-4-NO_2-$C_6H_3CO_2H$	43	96	58:42
11[f]	2-NO_2-$C_6H_4CO_2H$	60	98	15:85
12[g]	2-NO_2-$C_6H_4CO_2H$	42	98	12:88
13[e, f]	2-NO_2-$C_6H_4CO_2H$	48	99	12:88
14[e, h]	2-NO_2-$C_6H_4CO_2H$	35	99	10:90

[a] All reactions were performed with **2a** (0.1 mmol), **1a** (0.2 mmol), **cat. 3b** (20 mol%), and acid (20 mol%) in toluene. [b] Determined by GC analysis. [c] Determined by chiral HPLC analysis. [d] Determined by GC analysis. [e] The reaction was reacted at 30 °C. [f] Acid (40 mol%) was added. [g] Acid (60 mol%) was added. [h] Acid (50 mol%) was added.

Table S6. Research on γ′-regioselective *syn*-AVMA reaction[a]

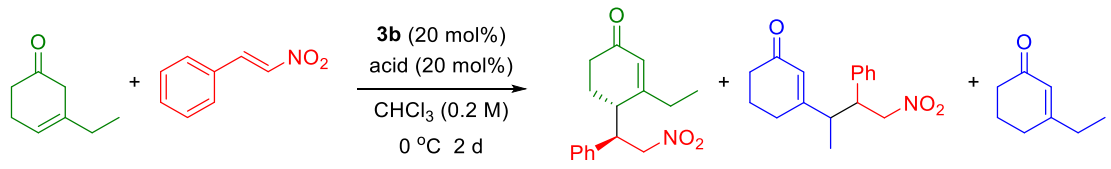


1'a 0.1 mmol | **2a** 0.2 mmol | **6a** | **4a+5a** | **1a**

entry	acid	conv.[b] (**6a**)	conv.[b] (**4a+5a**)	conv.[b] (**1a**)	d.r.[c]	ee (%)[d]
1	$C_6H_5CO_2H$	86.0	0	14.0	>19:1	96
2	4-Me-$C_6H_4CO_2H$	86.3	0	13.7	>19:1	98
3	4-NO_2-$C_6H_4CO_2H$	90.0	0	trace	>19:1	99
4	4-OH-$C_6H_4CO_2H$	83.4	0	16.7	>19:1	94
5[e]	4-NO_2-$C_6H_4CO_2H$	75%	0	trace	>19:1	97
6[f]	4-NO_2-$C_6H_4CO_2H$	<5	0	trace	N. D.	N. D.
7[g]	4-NO_2-$C_6H_4CO_2H$	<5	0	trace	N. D.	N. D.
8[h]	4-NO_2-$C_6H_4CO_2H$	<5	0	trace	N. D.	N. D.

[a] Reactions performed using 1.0 equiv of **1′a** (0.1 mmol, 0.2 M), 2.0 equiv of **2a**, 0.2 equiv of **cat. 3a**, and 0.2 equiv of acid in TCM at 0 °C. [b] Determined by GC analysis. [c] The dr values were determined by HPLC analysis of the crude reaction mixture. [d] The ee values were determined by chiral HPLC analysis. [e] Toluene (0.2 M) was used as solvent. [f] EtOAc (0.2 M) was used as solvent. [g] MeOH (0.2 M) was used as solvent. [h] CH_3CN (0.2 M) was used as solvent. N. D. = not detected.

Table S7. Research on γ′-regioselective *anti*-AVMA reaction[a]

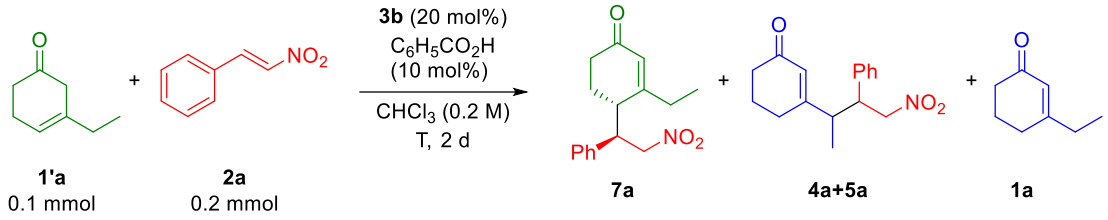


1'a 0.1 mmol | **2a** 0.2 mmol | **7a** | **4a+5a** | **1a**

entry	acid	conv.[b] (**7a**)	conv.[b] (**4a+5a**)	conv.[b] (**1a**)	dr[c]	ee (%)[d]
1	$C_6H_5CO_2H$	0	35	55	N. D.	N. D.

[a] Reactions performed using 1.0 equiv of **1′a** (0.1 mmol, 0.2 M), 2.0 equiv of **2a**, 0.2 equiv of **cat. 3b**, and 0.2 equiv of benzoic acid in solvent at 0 °C. [b] Determined by GC analysis. N. D. = not detected.

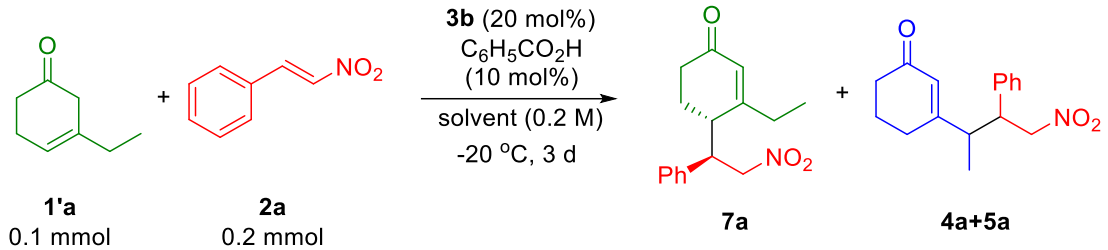
Table S8. The effect of temperature on γ′-regioselective *anti*-AVMA reaction[a]



entry	T (°C)	conv.[b] (**7a**)	conv.[b] (**4a+5a**)	conv.[b] (**1a**)	dr[c]
1	0	23	20	25	1:6
2	-20	20	15	trace	1:7

[a] Reactions performed using 1.0 equiv of **1′a** (0.1 mmol, 0.2 M), 2.0 equiv of **2a**, 0.2 equiv of **cat. 3b**, and 0.1 equiv of benzoic acid in solvent TCM. [b] Determined by GC analysis. [c] The dr values were determined by HPLC analysis of the crude reaction mixture.

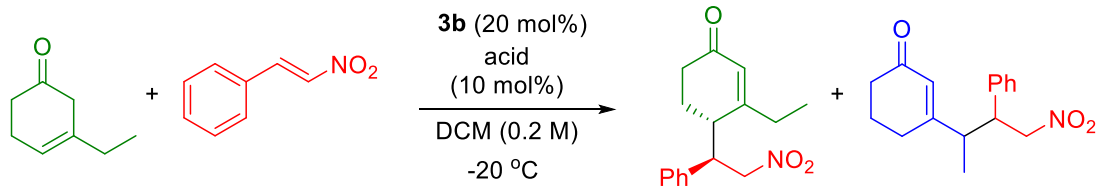
Table S9. The effect of the solvent on γ′-regioselective *anti*-AVMA reaction[a]



entry	solvent	conv.[b]	dr [c]
1	Toluene	0	N. D.
2	TCM	35	1:7
3	DCM	40	1:10
4	THF	0	N. D.
5	DCM/MeOH (1:1)	0	N. D.

[a] Reactions performed using 1.0 equiv of **1′a** (0.1 mmol, 0.2 M), 2.0 equiv of **2a**, 0.2 equiv of **cat. 3b**, and 0.1 equiv of benzoic acid in solvent at -20 °C. [b] Determined by GC analysis. [c] The dr values were determined by HPLC analysis of the crude reaction mixture. N. D. = not detected.

Table S10. The effect of the acids on γ′-regioselective *anti*-AVMA reaction[a]



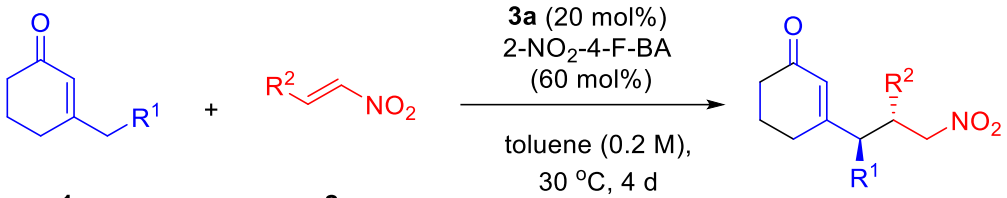
1'a 0.2 mmol | **2a** 0.1 mmol | **7a** | **4a+5a**

Entry	acid	Time (h)	conv. (**7a**, **4a**+**5a**)(%)[b]	dr[c]	ee (%)[d]
1	$C_6H_5CO_2H$	36	46, 36	1:8	97
2	4-MeO-$C_6H_4CO_2H$	36	27, 40	1:5	N. D.
3	4-NO_2-$C_6H_4CO_2H$	36	52, 42	1:8	N. D.
4	TsOH	36	50, 42	1:5	N. D.
5	3,5-$(NO_2)_2$-$C_6H_3CO_2H$	36	39, 48	1:6	N. D.
6	CF_3COOH	36	24, 66	1:4	N. D.
7	*t*Bu-COOH	36	58, 34	1:6	N. D.
8	$(Ph)_3COOH$	36	48, 35	1:5	N. D.
9	N-Boc-D-Phg	36	50, 41	1:7	N. D.
10	Ph_3CCOOH	36	67, 31	1:7	N. D.
11	Ph_3CCOOH (3 Å MS)	36	18, 12	1:9	N. D.
12[e]	2,6-(*t*Bu)$_2$-4-Me-C_6H_2OH	72	55, 5	1:19	98
13[f]	2,6-(*t*Bu)$_2$-4-Me-C_6H_2OH	72	64, 7	1:19	98
14[g]	2,6-(*t*Bu)$_2$-4-Me-C_6H_2OH	72	26, 55	1:19	N. D
15	none	72	37, 7	1:19	N. D

[a] Reactions performed using 1.0 equiv of **2a** (0.1 mmol, 0.2 M), 2.0 equiv of **1′a**, 0.2 equiv of **cat. 3b**, and 0.1 equiv of acid in DCM at -20 °C. [b] Determined by GC analysis. [c] The dr values were determined by HPLC analysis of the crude reaction mixture. [d] The ee values were determined by chiral HPLC analysis. [e] c = 0.1 M. [f] c = 0.1 M, additive (20 mol%) was added. [g] c = 0.1 M, T = 0 °C. N. D. = not detected.

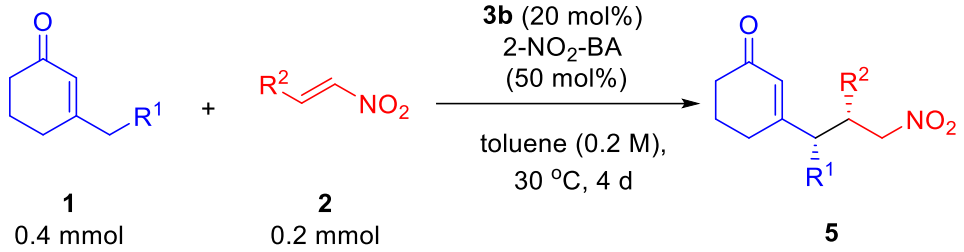
C: General procedure for γ- and γ′-regioselective AVMA Reaction

C1: General procedure for γ-*anti*-AVMA reaction



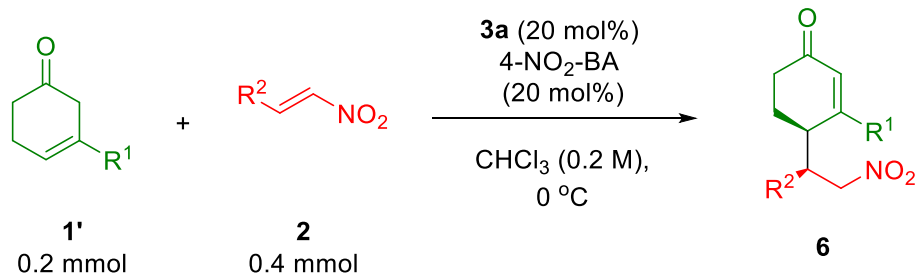
β-Alkyl-cyclohex-2-enones **1** (0.4 mmol, 2.0 equiv) and nitroalkenes **2** (0.2 mmol, 1.0 equiv) were added to a solution of catalyst **3a** (0.04 mmol, 0.2 equiv) and 4-fluoro-2-nitro-benzoic acid (0.12 mmol, 0.6 equiv) in toluene (1 mL, 0.2 M). The reaction mixture was stirred at 30 °C for several days. The toluene was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **4**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **4** that used for chiral HPLC analysis.

C2: General procedure for γ-regioselective *syn*-AVMA reaction



β-Alkyl-cyclohex-2-enones **1** (0.4 mmol, 2.0 equiv) and nitroalkenes **2** (0.2 mmol, 1.0 equiv) were added to a solution of catalyst **3b** (0.04 mmol, 0.2 equiv) and 2-nitro-benzoic acid (0.1 mmol, 0.5 equiv) in toluene (1 mL, 0.2 M). The reaction mixture was stirred at 30 °C for several days. The toluene was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **5**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **5** that used for chiral HPLC analysis.

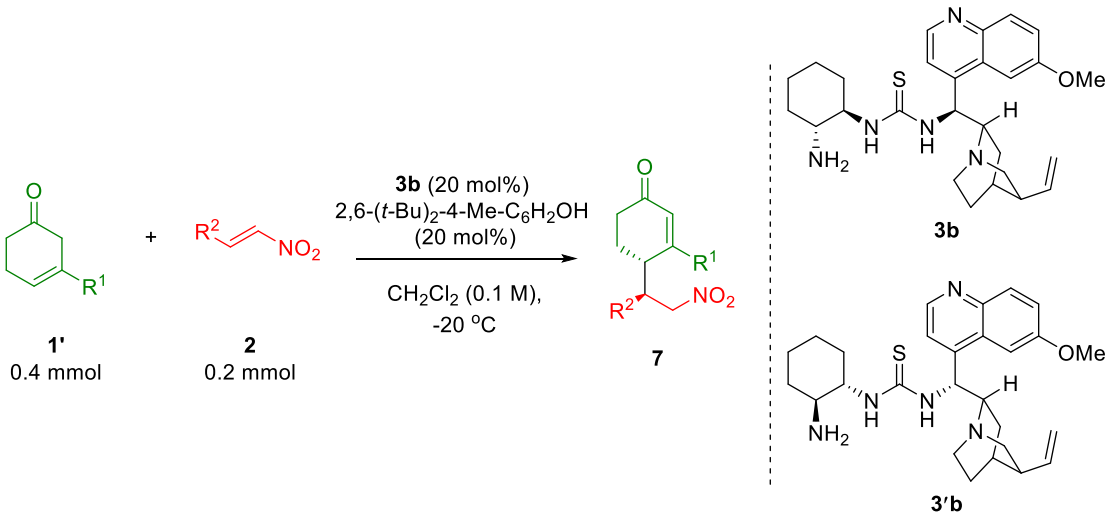
C3: General procedure for γ′-regioselective *syn*-AVMA reaction



β-Substituted-cyclohex-3-enones **1′** (0.2 mmol, 1.0 equiv) and nitroalkenes **2** (0.4 mmol, 2.0 equiv) were added to a solution of catalyst **3a** (0.04 mmol, 0.2 equiv) and 4-nitro-benzoic acid (0.04 mmol,

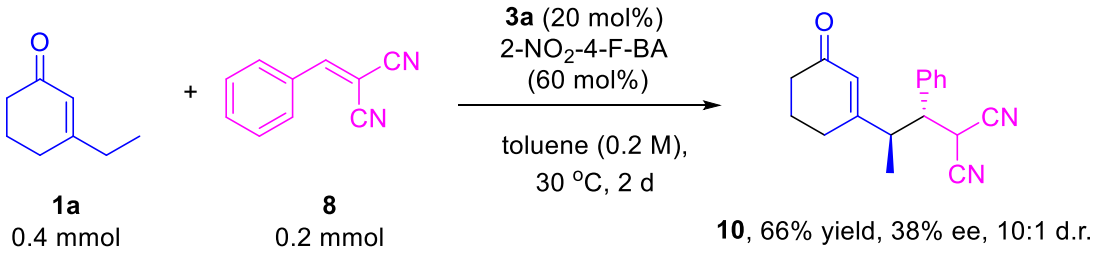
0.2 equiv) in chloroform (1 mL, 0.2 M). The reaction mixture was stirred at 0 °C for several days. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **6**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **6** that used for chiral HPLC analysis.

C4: General procedure for γ′-regioselective *anti*-AVMA reaction

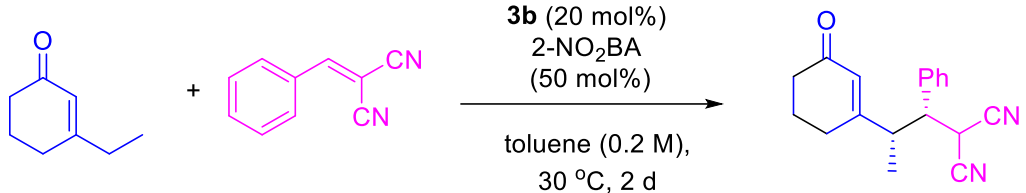


β-Substituted -cyclohex-3-enones **1′** (0.4 mmol, 2.0 equiv) and nitroalkenes **2** (0.2 mmol, 1.0 equiv) were added to a solution of catalyst **3b** (0.04 mmol, 0.2 equiv) and 2,6-(*t*-Bu)$_2$-4-Me-C$_6$H$_2$OH (0.04 mmol, 0.2 equiv) in CH$_2$Cl$_2$ (2 mL, 0.1 M). The reaction mixture was stirred at -20 °C for several days The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **7**. For chiral HPLC analysis, the reactions were also conducted under the cat. **3′b** for synthesis of the enantiomers of **7b-7p**, **7r-7s**, and **7u**. Others were procured under the racemic cat. **3i**.

C5: Procedure for γ-AVMA between β-ethyl-cyclohex-2-enone and benzylidenemalononitrile



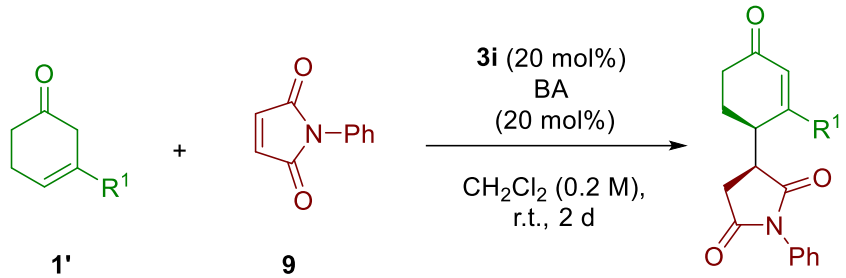
β-Ethyl-cyclohex-2-enones **1a** (0.4 mmol, 2.0 equiv) and benzylidenemalononitrile **8** (0.2 mmol, 1.0 equiv) were added to a solution toluene of catalyst **3a** (0.04 mmol, 0.2 equiv) and 4-fluoro-2-nitro-benzoic acid (0.12 mmol, 0.6 equiv) in toluene (1 mL, 0.2 M). The reaction mixture was stirred at 30 °C for 2 days. The toluene was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **10**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **10** that used for chiral HPLC analysis



1a 0.4 mmol + **8** 0.2 mmol → **11**, 57% yield, 40% ee, 1:3 d.r.

β-Ethyl -cyclohex-2-enones **1a** (0.4 mmol, 2.0 equiv) and benzylidenemalononitrile **8** (0.2 mmol, 1.0 equiv) were added to a solution of catalyst **3b** (0.04 mmol, 0.2 equiv) and 2-nitro-benzoic acid (0.1 mmol, 0.5 equiv) in toluene (1 mL, 0.2 M). The reaction mixture was stirred at 30 °C for 2 days. The toluene was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 8:1-5:1) to obtain product **11**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **11** that used for chiral HPLC analysis

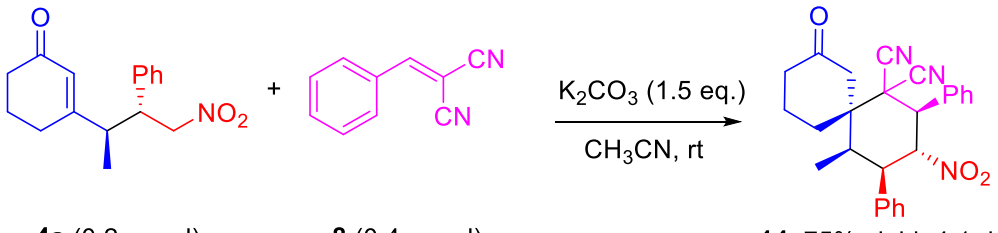
C6: Procedure for γ′-*syn*-AVMA between β-styryl-cyclohex-3-enone and *N*-phenyl-maleimide



1' 0.2 mmol + **9** 0.4 mmol → **12**

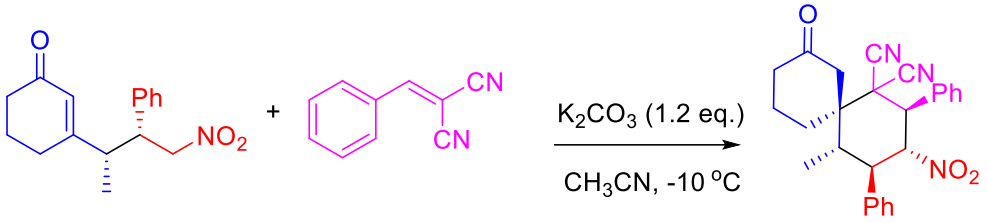
β-Substituted-cyclohex-3-enones **1′** (0.2 mmol, 1.0 equiv) and *N*-phenyl-maleimide **9** (0.4 mmol, 2.0 equiv) were added to a solution of catalyst **3i** (0.04 mmol, 0.2 equiv) and benzoic acid (0.04 mmol, 0.2 equiv) in CH_2Cl_2 (1 mL, 0.2 M). The reaction mixture was stirred at room temperture for 1 days. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 3:1-1:1) to obtain product **12**. The reactions were also catalyzed by racemic **3i** (Table S1) for synthesis of racemic products **12** that used for chiral HPLC analysis

C7: Derivation of the adducts



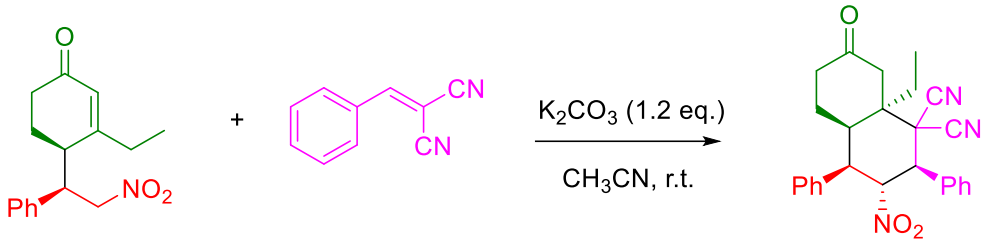
4a (0.2 mmol) + **8** (0.4 mmol) → **14**, 75% yield, 4:1 d.r.

γ-*Anti*-adduct **4a** (0.2 mmol, 1.0 equiv), **8** (0.4 mmol, 2.0 equiv) and potassium carbonate (0.3 mmol, 1.5 equiv) were added to CH_3CN (2 mL, 0.1 M). The reaction mixture was stirred at r.t. for 12 h. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 6:1-4:1) to obtain product **14**.



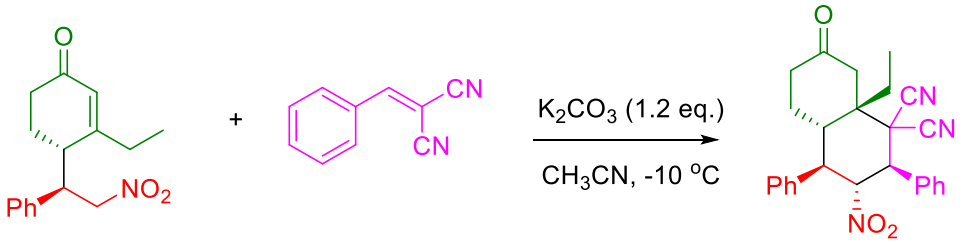
5a (0.2 mmol) **8** (0.24 mmol) **15**, 70% yield, 3:1 d.r.

γ-*Syn*-adduct **5a** (0.2 mmol, 1.0 equiv), **8** (0.24 mmol, 1.2 equiv) and potassium carbonate (0.24 mmol, 1.2 equiv) were added to CH_3CN (2 mL, 0.1 M). The reaction mixture was stirred at -10 °C. for 12 h. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 6:1-4:1) to obtain product **15**.



6a (0.2 mmol) **8** (0.24 mmol) **16**, 72% yield, 3:1 d.r.

γ′-*Syn*-adduct **6a** (0.2 mmol, 1.0 equiv), **8** (0.24 mmol, 1.2 equiv) and potassium carbonate (0.24 mmol mmol, 1.2 equiv) were added to CH_3CN (2 mL, 0.1 M). The reaction mixture was stirred at r.t. for 12 h. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 6:1-4:1) to obtain product **16**.

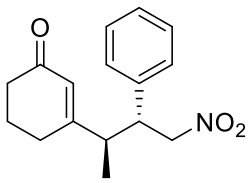


7a (0.2 mmol) **8** (0.24 mmol) **17**, 85% yield, 2:1 d.r.

γ′-*Anti*-adduct **7a** (0.2 mmol, 1.0 equiv), **8** (0.24 mmol, 1.2 equiv) and potassium carbonate (0.24 mmol mmol, 1.2 equiv) were added to CH_3CN (2 mL, 0.1 M). The reaction mixture was stirred at -10 °C. for 12 h. The solvent was removed under vacuum and the residue was purified by silica gel chromatography (PE/EA= 6:1-4:1) to obtain product **17**.

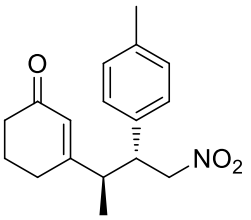
D: Products of γ- and γ′-regioselective AVMA and [4+2] cycloadducts.

4a: 3-((2*R*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one



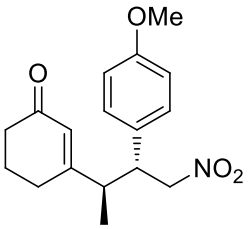
The product was obtained in 77% yield, pale yellow solid. Mp 94-96 °C; $[\alpha]_D^{25}$ 14.6 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.25 (d, *J* = 6.8 Hz, 3H), 1.61-1.71 (m, 1H), 1.75-1.84 (m, 1H), 2.08-2.12 (m, 2H), 2.17-2.22 (m, 2H), 2.66-2.74 (m, 1H), 3.54-3.62 (m, 1H), 4.62-4.68 (m, 1H), 4.73-4.78 (m, 1H), 5.74 (s, 1H), 7.10-7.12 (m, 2H), 7.21-7.25 (m, 1H), 7.26-7.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.9, 22.5, 27.2, 37.4, 45.2, 48.0, 78.5, 127.4, 127.8, 128.0, 128.9, 137.8, 166.5, 199.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{19}NO_3$) requires m/z 273.1365, found m/z 273.1366. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 19.90 min (major), 24.98 min (minor), ee = 92%.

4b: 3-((2*R*,3*R*)-4-nitro-3-(*p*-tolyl)butan-2-yl)cyclohex-2-en-1-one



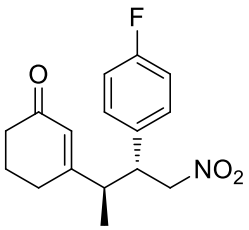
The product was obtained in 79% yield, yellow oil. $[\alpha]_D^{25}$ 12.6 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.24 (d, *J* = 6.8 Hz, 3H), 1.65-1.73 (m, 1H), 1.77-1.86 (m, 1H), 2.10-2.13 (m, 2H), 2.19-2.22 (m, 2H), 2.28 (s, 3H), 2.65-2.72 (m, 1H), 3.51-3.57 (m, 1H), 4.59-4.65 (m, 1H), 4.71-4.75 (m, 1H), 5.74 (s, 1H), 6.99 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.9, 21.1, 22.5, 27.2, 37.4, 45.2, 47.6, 78.7, 127.4, 127.6, 129.6, 134.6, 137.6, 166.9, 199.7. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1524. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 16.29 min (major), 18.59 min (minor), ee = 92%.

4c: 3-((2*R*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



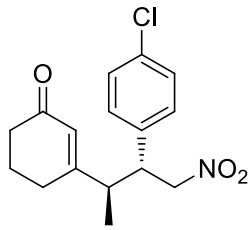
The product was obtained in 73% yield, yellow solid. Mp 98-101°C; $[\alpha]_D^{25}$ 36.4 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 7.2 Hz, 3H), 2.00-2.11 (m, 2H), 2.37-2.45 (m, 4H), 2.53-2.61 (m, 1H), 3.41-3.47 (m, 1H), 3.79 (s, 3H), 4.47-4.54 (m, 2H), 5.97 (s, 1H), 6.86-6.88 (m, 2H), 7.08-7.11 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.3, 22.8, 26.1, 37.6, 45.5, 46.8, 55.3, 79.7, 114.4, 127.5, 129.0, 159.3, 166.4, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_4$) requires m/z 303.1471, found m/z 303.1473. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 24.37 min (major), 27.07 min (minor), ee = 93%.

4d: 3-((2*R*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



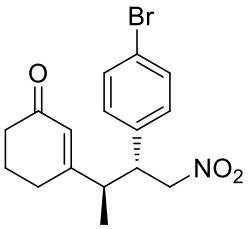
The product was obtained in 72% yield, yellow oil. $[\alpha]_D^{25}$ 13.8 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.26 (d, *J* = 6.8 Hz, 3H), 1.63-1.71 (m, 1H), 1.78-1.87 (m, 1H), 2.09-2.11 (m, 2H), 2.20-2.23 (m, 2H), 2.63-2.71 (m, 1H), 3.54-3.60 (m, 1H), 4.58-4.63 (m, 1H), 4.73-4.78 (m, 1H), 5.73 (s, 1H), 6.97-7.01 (m, 2H), 7.08-7.12 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.0, 22.5, 27.2, 37.3, 45.2, 47.3, 78.6, 115.8, 116.0, 127.5, 129.4, 129.4, 133.5, 133.6, 166.5, 199.7. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}FNO_3$) requires m/z 291.1271, found m/z 291.1269. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 22.55 min (major), 28.53 min (minor), ee = 93%.

4e: 3-((2*R*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



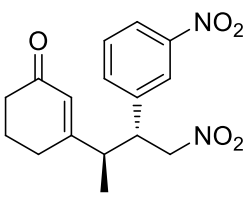
The product was obtained in 69% yield, yellow solid. Mp 64-66°C; $[\alpha]_D^{25}$ 12.1 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.26 (d, *J* = 6.8 Hz, 3H), 1.64-1.71 (m, 1H), 1.79-1.88 (m, 1H), 2.10-2.11 (m, 2H), 2.21-2.24 (m, 2H), 2.64-2.71 (m, 1H) , 3.54-3.60 (m, 1H), 4.58-4.63 (m, 1H), 4.73-4.77 (m, 1H), 5.74 (s, 1H) , 7.07 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.9, 22.5, 27.2, 37.3, 45.0, 47.3, 78.4, 127.5, 129.1, 133.9, 136.4, 166.0, 199.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}ClNO_3$) requires m/z 307.0975, found m/z 307.0973. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 24.56 min (major), 31.53 min (minor), ee = 94%.

4f: 3-((2*R*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



The product was obtained in 65% yield, yellow oil. $[\alpha]_D^{25}$ 11.0 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.26 (d, *J* = 6.8 Hz, 3H), 1.68-1.75 (m, 1H), 1.79-1.89 (m, 1H), 2.11-2.12 (m, 2H), 2.21-2.25 (m, 2H), 2.64-2.71 (m, 1H), 3.53-3.59 (m ,1H), 4.57-4.63 (m, 1H), 4.72-4.77 (m, 1H), 5.74 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.9, 22.5, 27.2, 37.3, 45.0, 47.4, 78.3, 122.0, 127.5, 129.5, 132.1, 136.9, 166.4, 199.7. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}BrNO_3$) requires m/z 351.0470, found m/z 351.0469. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 16.26 min (major), 16.38 min (minor), ee = 93%.

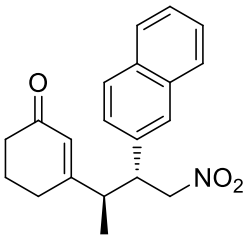
4g: 3-((2*R*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one



The product was obtained in 58% yield, yellow oil. $[\alpha]_D^{25}$ 4.0 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.30 (d, *J* = 6.8 Hz, 3H), 1.67-1.76 (m, 1H), 1.84-1.90 (m, 1H), 2.17-2.24 (m, 4H), 2.72-2.80 (m, 1H), 3.71-3.77 (m, 1H), 5.73 (s, 1H), 7.48-7.52 (m, 2H), 8.05 (s, 1H), 8.10-8.15 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.8, 22.5, 27.2, 37.3, 45.0, 47.4, 77.9, 122.5, 123.2,

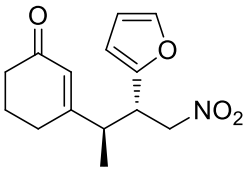
127.8, 130.1, 134.0, 140.2, 148.4, 165.0, 199.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}N_2O_5$) requires m/z 318.1216, found m/z 318.1217. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 34.80 min (major), 73.83 min (minor), ee = 91%.

4h: 3-((2*R*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



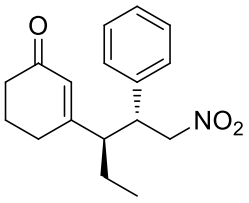
The product was obtained in 84% yield, yellow solid. Mp 94-95°C; $[\alpha]_D^{25}$ 32.5 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.28 (d, *J* = 6.8 Hz, 3H), 1.55-1.66 (m, 1H), 1.70-1.80 (m, 1H), 2.11-2.15 (m ,4H), 2.77-2.85 (m, 1H), 3.73-3.79 (m, 1H), 4.72-4.83 (m, 2H), 5.78 (s, 1H), 7.23-7.25 (m, 1H), 7.43-7.49 (m, 2H), 7.56 (s, 1H), 7.42-7.79 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.8, 22.5, 27.3, 37.3, 45.1, 48.0, 78.4, 124.9, 126.4, 126.6, 127.2, 127.4, 127.7, 127.8, 128.9, 132.8, 133.2, 135.2, 166.4, 199.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{21}NO_3$) requires m/z 323.1521, found m/z 323.1524. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 20.96 min (major), 24.24 min (minor), ee = 93%.

4i: 3-((2*R*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



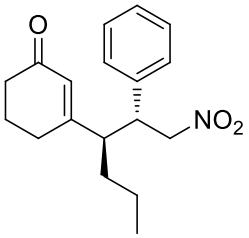
The product was obtained in 80% yield, yellow solid. Mp 58-59°C; $[\alpha]_D^{25}$ 19.5 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (d, *J* = 6.8 Hz, 3H), 1.84-1.96 (m, 2H), 2.13-2.21 (m, 2H), 2.29-2.33 (m, 2H), 2.76-2.83 (m, 1H), 3.74-3.79 (m, 1H), 4.60-4.73 (m, 2H), 5,80 (s, 1H), 6.13 (d, *J* = 3.2 Hz, 1H), 6.26-6.28 (m, 1H), 7.32-7.33 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.0, 22.7, 27.1, 37.5, 41.5, 43.4, 76.0, 108.2, 110.5, 127.1, 142.5, 150.8, 165.7, 199.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{17}NO_4$) requires m/z 263.1158, found m/z 263.1159. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 18.57 min (major), 28.77 min (minor), ee = 91%.

4j: 3-((2*R*,3*R*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one



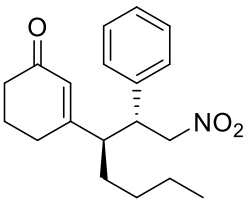
The product was obtained in 72% yield, yellow solid. Mp 72-74°C; $[\alpha]_D^{25}$ 31.1 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.88 (t, *J* = 7.2 Hz, 3H), 1.52-1.64 (m, 2 H), 1.69-1.79 (m, 2H), 1.98-2.01 (m, 2H), 2.16-2.19 (m, 2H), 2.43-2.50 (m, 1H), 3.54-3.60 (m, 1H), 4.60-4.66 (m, 1H), 4.79-4.83 (m, 1H), 5.72 (s, 1H), 7.08-7.10 (m, 2H), 7.20-7.24 (m, 1H), 7.25-7.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.1, 22.4, 23.7, 27.2, 37.4, 47.5, 52.8, 79.2, 128.0, 128.0, 128.8, 129.3, 137.7, 164.7, 199.4. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1523. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 0.5 mL/min, λ = 254 nm, 29.08 min (major), 34.08 min (minor), ee = 93%.

4k: 3-((2*R*,3*R*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one



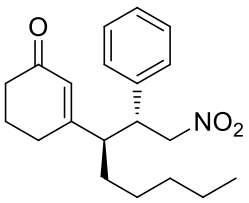
The product was obtained in 65% yield, yellow oil. $[\alpha]_D^{25}$ 53.8 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.91-0.94 (m, 3H), 1.13-1.24 (m, 1H), 1.28-1.37 (m, 1H), 1.54-1.65 (m, 4H), 1.69-1.78 (m, 1H), 1.99-2.01 (m, 2H), 2.15-2.18 (m, 1H), 2.52-2.59 (m, 1H), 3.53-3.59 (m, 1H), 4.60-4.66 (m, 1H), 4.79-4.84 (m, 1H), 5.70 (s, 1H), 7.08-7.10 (m, 2H), 7.20-7.25 (m, 2H), 7.27-7.29 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.0, 20.8, 22.4, 27.1, 32.9, 37.5, 47.6, 50.9, 79.2, 128.0, 128.8, 129.2, 137.7, 164.7, 199.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{23}NO_3$) requires m/z 301.1678, found m/z 301.1675. The enantiomeric ratio was determined by Daicel Chiralpak AS (25 cm), *n*-Hexane / EtOH = 7/3, 0.55 mL/min, λ = 254 nm, 24.18 min (major), 28.57 min (minor), ee = 92%.

4l: 3-((2*R*,3*R*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one



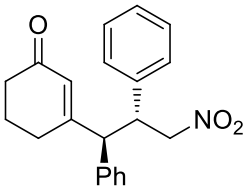
The product was obtained in 63% yield, yellow oil. $[\alpha]_D^{25}$ 128.2 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.87-0.91 (m, 3H), 1.12-1.40 (m, 4H), 1.60-1.79 (m, 4H), 1.98-2.01 (m, 2H), 2.15-2.19 (m, 2H), 2,50-2.56 (m, 1H), 3.53-3.59 (m, 1H), 4.60-4.66 (m, 1H), 4.79-4.83 (m, 1H), 5.70 (s, 1H), 7.08-7.10 (m, 2H), 7.20-7.25 (m, 2H), 7.27-7.29 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 22.4, 22.6, 27.1, 29.8, 29.8, 30.5, 37.5, 47.6, 51.2, 79.2, 128.0, 128.8, 129.2, 137.7, 164.8, 199.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{19}H_{25}NO_3$) requires m/z 315.1834, found m/z 315.1832. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 19/1, 1.0 mL/min, λ = 254 nm, 15.03 min (major), 16.39 min (minor), ee = 94%.

4m: 3-((2*R*,3*R*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one



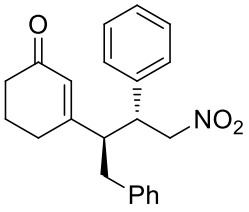
The product was obtained in 67% yield, yellow oil. $[\alpha]_D^{25}$ 29.7 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ 0.86-0.89 (m, 3H), 1.16-1.30 (m, 6H), 1.54-1.64 (m, 3H), 1.70-1.78 (m, 1H), 1.98-2.01 (m, 2H), 2.15-2.18 (m, 2H), 2.50-2.56 (m, 1H), 3.52-3.58 (m, 1H), 4.60-4.66 (m, 1H), 4,79-4.83 (m, 1H), 5.70 (s, 1H), 7.07-7.10 (m, 2H), 7.20-7.29 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.0, 22.4, 22.5, 27.1, 27.3, 30.7, 31.7, 37.5, 47.6, 51.2, 79.2, 128.0, 128.8, 129.2, 137.7, 164.8, 199.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{27}NO_3$) requires m/z 329.1991, found m/z 329.1994. The enantiomeric ratio was determined by Daicel Chiralpak AD (25 cm), *n*-Hexane / EtOH = 19/1, 0.8 mL/min, λ = 254 nm, 22.43 min (major), 25.26 min (minor), ee = 93%.

4n: 3-((1*R*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one



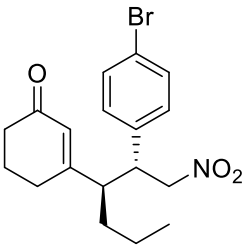
The product was obtained in 69% yield, yellow oil. $[\alpha]_D^{25}$ 12.5 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.49-1.59 (m, 1H), 1.68-1.76 (m, 1H), 2.00-2.12 (m, 3H), 2.18-2.45 (m,1H), 3.79 (d, *J* = 12.0 Hz, 1H), 4.15-4.22 (m, 1H), 4.38-4.49 (m, 2H), 5.93 (s, 1H), 7.25-7.27 (m, 3H), 7.30-7.44 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 22.4, 27.8, 37.1, 46.0, 56.5, 79.8, 127.6, 127.9, 128.0, 128.2, 128.4, 129.1, 129.6, 137.2, 137.8, 163.5, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1521. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane / EtOH = 7/3, 0.9 mL/min, λ = 220 nm, 10.05 min (minor), 15.31 min (major), ee = 99%.

4o: 3-((2*R*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one



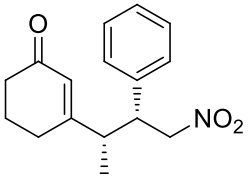
The product was obtained in 58% yield, yellow solid. Mp 101-103°C; $[\alpha]_D^{25}$ 45.2 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.42-1.56 (m, 2H), 1.65-1.72 (m, 1H), 1.84-1.92 (m, 1H), 2.01-2.04 (m, 2H), 2.75-2.81 (m, 1H), 2.88-2.94 (m, 1H), 3.09-3.13 (m, 1H), 3.66-3.73 (m, 1H), 4.69-4.74 (m, 1H), 4.86-4.90 (m, 1H), 5.67 (s, 1H), 7.10-7.13 (m ,4H), 7.18-7.25 (m, 3H), 7.26-7.31 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 22.1, 28.8, 37.2, 37.8, 47.6, 52.4, 79.0, 126.8, 128.1, 128.7, 128.8, 129.2, 137.4, 138.0, 164.3, 198.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.1682. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 19/1, 1.0 mL/min, λ = 254 nm, 19.80 min (major), 22.48 min (minor), ee = 99%.

4p: 3-((2*R*,3*R*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one



The product was obtained in 78% yield, yellow solid. Mp 99-101°C; $[\alpha]_D^{25}$ 40.5 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.90-0.94 (t, *J* = 7.2 Hz, 3H), 1.13-1.31 (m, 2H), 1.54-1.65 (m, 3H), 1.74-1.80 (m, 1H), 2.00-2.03 (m, 2H), 2.18-2.21 (m, 2H), 2.49-2.56 (m, 1H), 3.50-3.56 (m, 1H), 4.55-4.61 (m, 1H), 4.78-4.82 (m, 1H), 5.72 (s, 1H), 6.98 (d, *J* = 8 Hz, 2H), 7.42 (m, *J* = 8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.9, 19.7, 21.4, 26.1, 31.9, 36.4, 46.0, 49.6, 77.9, 120.9, 128.2, 128.6, 131.0, 135.8, 163.1, 198.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{22}BrNO_3$) requires m/z 379.0783, found m/z 379.0784. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 0.95 mL/min, λ = 220 nm, 12.43 min (major), 13.32 min (minor), ee = 95%.

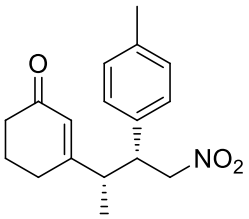
5a: 3-((2*S*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one



The product was obtained in 68% yield, pale yellow solid. Mp 138-140 °C; $[\alpha]_D^{25}$ 38.3 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 2.00-2.12 (m, 2H), 2.33-2.49 (m, 4H), 2.58-2.65 (m, 1H), 3.46-3.53 (m, 1H), 4.49-4.59 (m, 2H), 5.98 (s, 1H), 7.18 (m, 2H), 7.28-7.37 (m, 3H). ^{13}C NMR (100

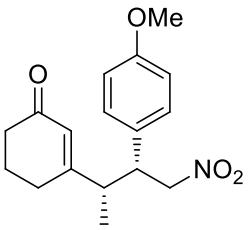
MHz, $CDCl_3$): δ (ppm) 17.4, 22.8, 26.1, 37.6, 45.4, 47.4, 79.5, 127.5, 128.0, 128.2, 129.1, 137.3, 166.2, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{19}NO_3$) requires m/z 273.1365, found m/z 273.1367. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 15.80 min (minor), 23.33 min (major), ee = 99%.

5b: 3-((2*S*,3*R*)-4-nitro-3-(*p*-tolyl)butan-2-yl)cyclohex-2-en-1-one



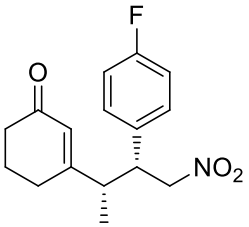
The product was obtained in 76% yield, pale yellow solid. Mp 145-147 °C; $[\alpha]_D^{25}$ 45.1 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 1.99-2.11 (m, 2H), 2.33 (s, 3H), 2.38-2.45 (m, 4H), 2.55-2.63 (m, 1H), 3.42-3.49 (m, 1H), 4.47-4.56 (m, 2H), 5.97 (s, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.3, 21.1, 22.8, 26.1, 37.6, 45.4, 47.1, 79.6, 127.5, 127.8, 129.7, 134.1, 137.9, 166.4, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1522. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 14.67 min (minor), 24.36 min (major), ee = 98%.

5c: 3-((2*S*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



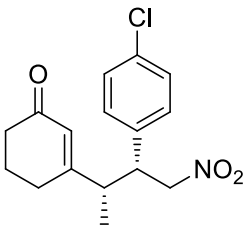
The product was obtained in 63% yield, pale yellow solid. Mp 136-138 °C; $[\alpha]_D^{25}$ 53.3 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 1.98-2.13 (m, 2H), 2.37-2.46 (m, 4H), 2.53-2.61 (m, 1H), 3.41-3.48 (m, 1H), 3.79 (s, 3H), 4.47-4.54 (m, 2H), 5.97 (s, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.3, 22.8, 26.1, 37.6, 45.5, 46.8, 55.3, 79.7, 114.4, 127.5, 129.0, 159.3, 166.4, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_4$) requires m/z 303.1471, found m/z 303.1473. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 25.22 min (major), 40.32 min (minor), ee = 99%.

5d: 3-((2*S*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



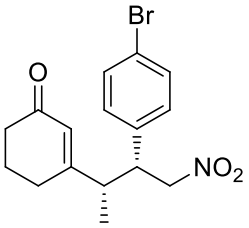
The product was obtained in 83% yield, pale yellow solid. Mp 111-113 °C; $[\alpha]_D^{25}$ 37.8 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 2.00-2.12 (m, 2H), 2.37-2.46 (m, 4H), 2.54-2.62 (m, 1H), 3.46-3.52 (m, 1H), 4.48-4.55 (m, 2H), 5.97 (s, 1H), 7.03-7.07 (m, 2H), 7.15-7.19 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.4, 22.8, 26.4, 37.6, 45.4, 46.8, 79.5, 116.0, 116.2, 127.6, 129.5, 129.6, 133.0, 133.0, 165.8, 199.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}FNO_3$) requires m/z 291.1271, found m/z 291.1269. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 19.29 min (minor), 26.30 min (major), ee = 99%.

5e: 3-((2*S*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



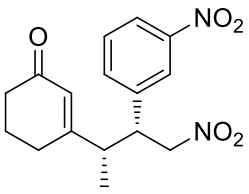
The product was obtained in 73% yield, pale yellow solid. Mp 111-113 °C; $[\alpha]^{25}_{D}$ 48.7 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 1.99-2.14 (m, 2H), 2.33-2.50 (m, 4H), 2.54-2.62 (m, 1H), 3.45-3.51 (m, 1H), 4.48-4.55 (m, 2H), 5.97 (s, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.4, 22.8, 26.0, 37.6, 45.2, 46.9, 79.3, 127.6, 129.3, 129.3, 134.1, 135.8, 165.6, 199.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}ClNO_3$) requires m/z 307.0975, found m/z 307.0973. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 20.48 min (major), 28.09 min (minor), ee = 97%.

5f: 3-((2*S*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



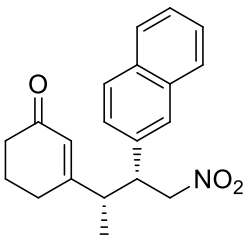
The product was obtained in 66% yield, pale yellow solid. Mp 126-128 °C; $[\alpha]_{D}^{25}$ 74.3 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.92 (d, *J* = 6.8 Hz, 3H), 1.99-2.14 (m, 2H), 2.32-2.50 (m, 4H), 2.54-2.61 (m, 1H), 3.44-3.50 (m, 1H), 4.48-4.55 (m, 2H), 5.97 (s, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.4, 22.8, 26.0, 37.6, 45.2, 46.9, 79.2, 122.2, 127.6, 129.6, 136.3, 165.6, 199.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}BrNO_3$) requires m/z 351.0470, found m/z 351.0471. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 22.00 min (minor), 30.13 min (major), ee = 99%.

5g: 3-((2*S*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one



The product was obtained in 55% yield, pale yellow solid. Mp 137-140 °C; $[\alpha]_{D}^{25}$ 40.0 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.94 (d, *J* = 6.8 Hz, 3H), 2.02-2.16 (m, 2H), 2.36-2.52 (m, 4H), 2.63-2.71 (m, 1H), 3.62-3.69 (m, 1H), 4.55-4.64 (m, 2H), 6.01 (s, 1H), 7.55-7.60 (m, 2H), 8.11 (s, 1H), 8.19-8.22 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.5, 22.8, 26.1, 37.6, 45.0, 47.1, 78.9, 122.8, 123.4, 127.8, 130.2, 134.3, 139.7, 148.7, 164.7, 198.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}N_2O_5$) requires m/z 318.1216, found m/z 318.1218. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 42.37 min (minor), 47.95 min (major), ee = 98%.

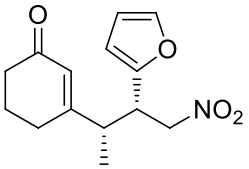
5h: 3-((2*S*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



The product was obtained in 82% yield, pale yellow solid. Mp 171-172 °C; $[\alpha]_{D}^{25}$ 53.2 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.93 (d, *J* = 7.2 Hz, 3H), 2.01-2.15 (m, 2H), 2.39-2.51 (m, 4H), 2.69-2.77 (m, 1H), 3.63-3.70 (m, 1H), 4.56-4.69 (m, 2H), 6.04 (s, 1H), 7.30-7.32 (m, 1H), 7.49-7.51 (m, 2H), 7.65 (s, 1H), 7.80-7.87 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.6, 22.9, 26.0, 37.6, 45.3, 47.6, 79.5, 124.7, 126.4, 126.6, 127.7, 127.7, 127.8, 129.1, 133.0,

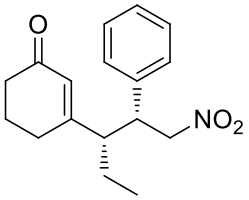
133.4, 134.6, 166.1, 199.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{21}NO_3$) requires m/z 323.1521, found m/z 323.1522. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 18.38 min (minor), 29.92 min (major), ee = 98%.

5i: 3-((2*S*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



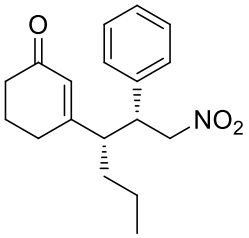
The product was obtained in 61% yield, pale yellow oil. $[\alpha]_D^{25}$ 31.5 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01 (d, *J* = 6.8 Hz, 3H), 1.96-2.11 (m, 2H), 2.25-2.43 (m, 4H), 2.66-2.74 (m, 1H), 3.67-3.73 (m, 1H), 4.46-4.50 (m, 1H), 4.60-4.66 (m, 1H), 5.92 (s, 1H), 6.20 (d, *J* = 3.2 Hz, 1H), 6.30-6.32 (m, 1H), 7.38 (d, *J* = 1.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.5, 22.8, 26.5, 37.6, 41.1, 43.3, 77.0, 109.2, 110.4, 127.4, 142.7, 150.1, 165.6, 199.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{17}NO_4$) requires m/z 263.1158, found m/z 263.1159. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 21.10 min (major), 22.81 min (minor), ee = 97%.

5j: 3-((2*R*,3*S*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one



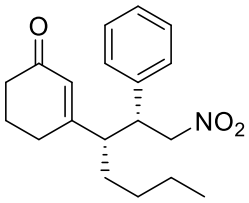
The product was obtained in 78% yield, pale yellow solid. Mp 192-194 °C; $[\alpha]_D^{25}$ 99.1 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.69 (t, *J* = 7.2 Hz, 3H), 1.21-1.35 (m, 2H), 2.04-2.10 (m, 2H), 2.34-2.40 (m, 3H), 2.44-2.47 (m, 2H), 3.46-3.52 (m, 1H), 4.44-4.56 (m, 2H), 6.01 (s, 1H), 7.18-7.20 (m, 2H), 7.28-7.37 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.8, 22.8, 23.7, 25.7, 37.8, 47.0, 53.1, 79.7, 127.9, 128.2, 129.1, 129.7, 137.6, 164.2, 198.9. HRMS (ESI): exact mass calculated for $[M+H]^+$ ($C_{17}H_{21}NO_3$+H) requires m/z 288.1600, found m/z 288.1601. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 12.33 min (minor), 15.92 min (major), ee = 95%.

5k: 3-((2*R*,3*S*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one



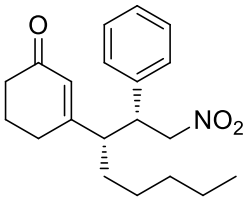
The product was obtained in 78% yield, pale yellow solid. Mp 128-130 °C; $[\alpha]_D^{25}$ 53.9 (*c* 1.00, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): 0.66 (t, J = 8 Hz, 3H), 0.89-0.96 (m, 1H), 1.00-1.13(m, 2H), 1.23-1.30 (m, 1H), 1.95-2.02 (m, 2H), 2.27-2.28 (m, 2H), 2.36-2.45 (m, 3H), 3.37-3.44 (m, 1H), 4.36-4.48 (m, 2H), 5,93 (s, 1H), 7.10-7.12 (m, 2H), 7.21-7.30 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.7, 19.4, 21.7, 24.7, 31.7, 36.7, 46.1, 50.1, 78.8, 126.9, 127.1, 128.1, 128.4, 136.6, 163.5, 197.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{23}NO_3$) requires m/z 301.1678, found m/z 301.1679. The enantiomeric ratio was determined by Daicel Chiralpak AS (25 cm), *n*-Hexane / EtOH = 7/3, 0.55 mL/min, λ = 220 nm, 14.87 min (minor), 23.16 min (major), ee = 99%.

5l: 3-((2*R*,3*S*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one



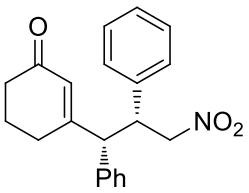
The product was obtained in 57% yield, white solid. Mp 108-110 °C; $[\alpha]^{25}_{D}$ 99.7 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.74 (t, *J* = 7.2 Hz, 3H), 0.95-1.20 (m, 5H), 1.30-1.34 (m, 1H), 2.04-2.10 (m, 2H), 2.35-2.36 (m, 2H), 2.43-2.50 (m, 3H), 3.44-3.51 (m, 1H), 4.43-4.54 (m, 2H), 6.00 (s, 1H), 7.17-7.19 (m, 2H), 7.28-7.37 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.7, 19.4, 21.7, 24.7, 31.7, 36.7, 46.1, 50.1, 78.8, 126.9, 127.1, 128.1, 136.6, 163.5, 197.9.HRMS (EI): exact mass calculated for $[M]^+$ ($C_{19}H_{25}NO_3$) requires m/z 315.1834, found m/z 315.1833. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 19/1, 1.0 mL/min, λ = 254 nm, 9.94 min (major), 12.59 min (minor), ee = 99%.

5m: 3-((2*R*,3*S*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one



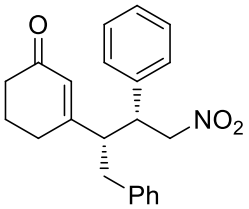
The product was obtained in 58% yield, white solid. Mp 95-97 °C; $[\alpha]_D^{25}$ 67.3 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.78 (t, *J* = 7.2 Hz, 3H), 1.18-0.95 (m, 7H), 1.33-1.28 (m, 1H), 2.10-2.03 (m, 2H), 2.37-2.34(m, 2H), 2.50-2.44 (m, 3H), 3.47 (td, J_1 = 4.8 Hz, J_2 = 10.8 Hz, 1H), 4.55-4.43 (m, 2H), 6.00 (m, 1H), 7.19-7.17 (m, 2H), 7.38-7.28 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 22.4, 22.8, 25.7, 26.9, 29.7, 30.5, 31.4, 37.8, 47.1, 51.3, 79.8, 127.9, 128.2, 129.1, 129.5, 137.6, 164.6, 199.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{27}NO_3$) requires m/z 329.1991, found m/z 329.1994. The enantiomeric ratio was determined by Daicel Chiralpak AD (25 cm), *n*-Hexane / EtOH = 19/1, 0.8 mL/min, λ = 254 nm, 20.21 min (major), 22.48 min (minor), ee = 98%.

5n: 3-((1*S*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one



The product was obtained in 34% yield, yellow oil. $[\alpha]_D^{25}$ 8.5 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.17-7.03 (m, 10H), 6.33 (s, 1H), 4.75-4.61 (m, 2H), 4.20-4.14 (m, 1H), 3.79-3.76 (m, 1H), 2.44-2.24 (m, 4H), 2.03-1.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 22.4, 27.8, 37.1, 46.0, 56.6, 79.8, 127.6, 127.9, 128.0, 128.4, 129.1, 129.6, 137.2, 137.9, 163.4, 199.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1522. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / IPA = 9/1, 1.0 mL/min, λ = 254 nm, 11.49 min (major), 14.64 min (minor), ee = 92%.

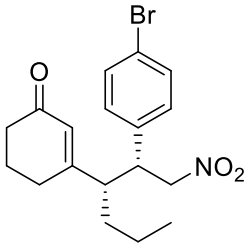
5o: 3-((2*S*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one



The product was obtained in 56% yield, pale yellow solid. Mp 108-110 °C; $[\alpha]_D^{25}$ 57.0 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.84-1.95 (m, 2H), 2.05-2.15 (m, 1H), 2.27-2.39 (m, 3H), 2.45 (dd, *J* = 13.8, 11.5 Hz, 1H), 2.63 (dd, *J* = 13.8, 3.7 Hz, 1H), 2.79 (td, *J* = 11.5, 3.7 Hz, 1H), 3.62 (td, *J* = 10.6, 4.9 Hz, 1H), 4.54 (qd, *J* = 12.5, 7.5 Hz, 2H), 5.83 (s, 1H), 6.85-6.94 (m, 2H), 7.10-7.21 (m, 3H), 7.28-7.37 (m, 3H), 7.41 (t, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 22.4, 27.4,

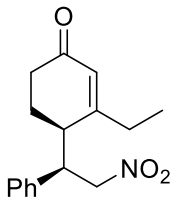
37.5, 38.0, 47.3, 53.3, 79.5, 126.6, 128.0, 128.1, 128.5, 128.5, 128.7, 128.9, 129.4, 129.4, 137.4, 138.3, 163.7, 198.7. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.1680. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane / EtOH = 19/1, 1.0 mL/min, λ = 220 nm, 19.65 min (minor), 20.64 min (major), ee = 98%.

5p: 3-((2*R*,3*S*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one



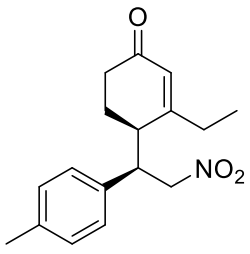
The product was obtained in 46% yield, pale yellow solid. Mp 56-59 °C; $[\alpha]_D^{25}$ 24.9 (*c* 1.00, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.75 (t, *J* = 7.2 Hz, 3H), 0.94-1.20 (m, 3H), 1.22-1.34 (m, 1H), 2.02-2.11 (m, 2H), 2.32-2.37 (m, 2H), 2.40-2.48 (m, 3H), 3.39-3.51 (m, 1H), 4.41-4.52 (m, 2H), 5.99 (s, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.7, 20.4, 22.7, 25.6, 32.7, 37.7, 46.6, 50.9, 79.5, 122.1, 129.6, 129.6, 132.3, 136.7, 164.0, 198.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{22}BrNO_3$) requires m/z 379.0783, found m/z 379.0784. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 19/1, 1.0 mL/min, λ = 220 nm, 14.60 min (minor), 18.44 min (major), ee = 99%.

6a: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



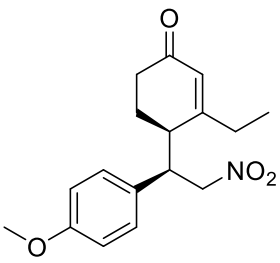
The product was obtained in 68% yield, pale yellow oil. $[\alpha]_D^{25}$ -138 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01 (t, *J* = 7.2 Hz, 3H), 1.84-1.97 (m, 3H), 1.99-2.08 (m, 1H), 2.31-2.38 (m, 1H), 2.45- 2.53 (m, 1H), 2.67-2.71 (m, 1H), 3.94-3.99 (m, 1H), 4.59-4.63 (m, 1H), 4.88-4.94 (m, 1H), 5.96 (s, 1H), 7.22 (d, *J* = 7.2 Hz, 2H), 7.29-7.32 (m, 1H), 7.35-7.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.6, 24.6, 29.3, 34.3, 43.1, 45.3, 76.6, 126.8, 127.8, 128.2, 129.1, 137.5, 167.4, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{19}NO_3$) requires m/z 273.1365, found m/z 273.1366. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 4/1, 1.0 mL/min, λ = 220 nm, 10.76 min (major), 13.02 min (minor), ee = 99%.

6b: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(*p*-tolyl)ethyl)cyclohex-2-en-1-one



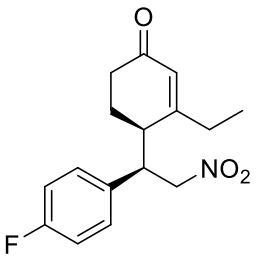
The product was obtained in 70% yield, colorless oil. $[\alpha]_D^{25}$ -141 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.02 (t, *J* = 7.2 Hz, 3H), 1.82-1.90 (m, 1H), 1.93-2.07 (m, 3H), 2.29-2.38 (m, 4H), 2.44-2.51 (m, 1H), 2.64-2.69 (m, 1H), 3.90-3.96 (m, 1H), 4.56-4.60 (m, 1H), 4.85-4.91 (m, 1H), 5.95 (s, 1H), 7.10 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 10.6, 20.0, 23.6, 28.3, 33.3, 42.0, 44.0, 125.7, 126.6, 128.7, 133.3, 136.9, 166.5, 197.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1519. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 14.94 min (minor), 22.26 min (major), ee = 98%.

6c: (*R*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one



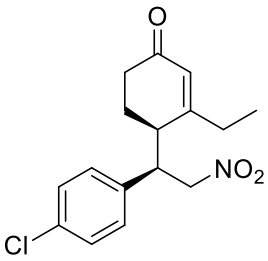
The product was obtained in 66% yield, colorless oil. $[\alpha]_D^{25}$ -165 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01 (t, *J* = 7.2 Hz, 3H), 1.84-1.96 (m, 3H), 2.00-2.09 (m, 1H), 2.31-2.38 (m, 1H), 2.45-2.53 (m, 1H), 2.62-2.66 (m, 1H), 3.34 (s, 3H), 3.86-3.92 (m, 1H), 4.58-4.62 (m, 1H), 4.81-4.87 (m, 1H), 5.94 (s, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 7.13 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 10.6, 23.7, 28.4, 33.1, 42.0, 43.8, 54.3, 113.4, 125.7, 127.8, 128.2, 158.3, 166.7, 197.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_4$) requires m/z 303.1471, found m/z 303.1473. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 16.98 min (minor), 25.70 (major), ee = 95%.

6d: (*R*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one



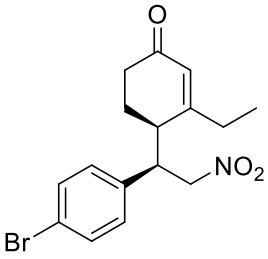
The product was obtained in 74% yield, pale yellow oil. $[\alpha]_D^{25}$ -167 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.94 (t, *J* = 7.2 Hz, 3H), 1.78-1.88 (m, 3H), 1.93-2.02 (m, 1H), 2.25-2.32 (m, 1H), 2.38-2.47 (m, 1H), 2.55-2.60 (m, 1H), 3.84-3.90 (m, 1H), 4.53-4.57 (m, 1H), 4.75-4.81 (m, 1H), 5.88 (s, 1H), 6.97-7.01 (m, 2H), 7.12-7.15 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 10.6, 23.6, 28.4, 33.1, 42.0, 43.8, 115.0, 115.2, 125.9, 128.3, 128.4, 166.1, 197.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}FNO_3$) requires m/z 291.1271, found m/z 291.1273. The enantiomeric ratio was determined by Daicel Chiralpak IA, *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 18.95 min (major), 21.35 (minor), ee = 99%.

6e: (*R*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



The product was obtained in 76% yield, pale yellow oil. $[\alpha]_D^{25}$ -148 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.03 (t, *J* = 7.6 Hz, 3H), 1.82-2.08 (m, 4H), 2.31-2.39 (m ,1H), 2.44-2.52 (m, 1H), 2.63-2.68 (m, 1H), 3.91-3.97 (m, 1H), 4.58-4.62 (m, 1H), 4.82-4.88 (m, 1H), 5.96 (s, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.6, 24.6, 29.4, 34.2, 42.9, 44.9, 76.4, 127.0, 129.1, 129.4, 134.2, 136.0, 166.8, 198.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}ClNO_3$) requires m/z 307.0975, found m/z 307.0973. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 15.75 min (minor), 27.64 (major), ee = 99%.

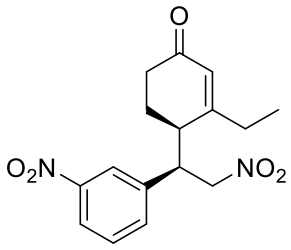
6f: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



The product was obtained in 80% yield, pale yellow oil. $[\alpha]_D^{25}$ -98 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.03 (t, *J* = 7.2 Hz, 3H), 1.82-1.89 (m, 1H), 1.93-2.07 (m, 3H), 2.31-2.38 (m, 1H), 2.44-2.52 (m, 1H), 2.63-2.68 (m, 1H), 3.90-3.96 (m, 1H), 4.58-4.62 (m, 1H), 4.82-4.88 (m, 1H), 5.96 (s, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.7, 24.5, 29.4, 34.2, 42.9, 44.9, 76.3, 122.2, 127.0, 129.4, 132.3, 136.6, 166.7, 198.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}BrNO_3$) requires m/z

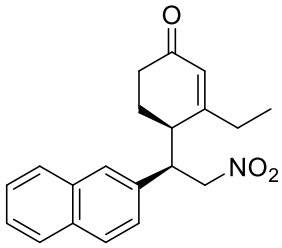
351.0470, found m/z 351.0470. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 19.71 min (minor), 36.38 (major), ee = 98%.

6g: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(3-nitrophenyl)ethyl)cyclohex-2-en-1-one



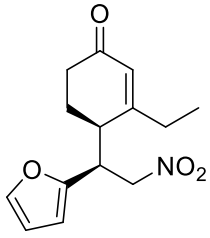
The product was obtained in 79% yield, pale yellow oil. $[\alpha]_D^{25}$ -102 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.06 (t, *J* = 7.2 Hz, 3H), 1.85-1.94 (m, 1H), 1.97-2.07 (m, 3H), 2.34-2.41 (m, 1H), 2.46-2.55 (m, 1H), 2.73-2.77 (m, 1H), 4.10-4.16 (m, 1H), 4.65-4.69 (m, 1H), 4.95-5.01 (m, 1H), 6.01 (s, 1H), 7.57-7.60 (m, 2H), 8.18 (s, 1H), 8.21-8.22 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 10.6, 23.3, 28.2, 33.3, 41.9, 44.0, 74.8, 121.6, 122.3, 126.5, 129.2, 133.0, 138.9, 147.6, 164.6, 196.8. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}N_2O_5$) requires m/z 318.1216, found m/z 318.1219. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 7/3, 0.8 mL/min, λ = 220 nm, 13.57 min (minor), 20.74 (major), ee = 94%.

6h: (*R*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



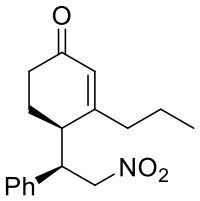
The product was obtained in 80% yield, colorless oil. $[\alpha]_D^{25}$ -144 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.99 (t, *J* = 7.2 Hz, 3H), 1.87-2.06 (m, 4H), 2.30-2.37 (m, 1H), 4.65-4.68 (m, 1H), 4.99-5.06 (m, 1H), 5.98 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.49-7.51 (m, 2H), 7.67 (s, 1H), 7.80-7.86 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 10.6, 23.5, 28.3, 33.3, 41.9, 44.3, 75.4, 124.2, 125.5, 125.7, 125.8, 125.9, 126.7, 126.8, 128.0, 131.8, 132.2, 133.8, 166.3, 197.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{21}NO_3$) requires m/z 323.1521, found m/z 323.1526. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 7/3, 0.8 mL/min, λ = 220 nm, 13.36 (minor), 24.64 min (major), ee = 99%.

6i: (*R*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



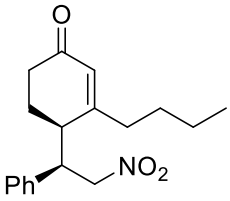
The product was obtained in 82% yield, pale yellow oil. $[\alpha]_D^{25}$ -142 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01 (t, *J* = 7.2 Hz, 3H), 1.78-1.83 (m, 1H), 2.02-2.13 (m, 3H), 2.33-2.40 (m, 1H), 2.91-2.93 (m, 1H), 4.09-4.13 (m, 1H), 4.49-4.52 (m, 1H), 4.80-4.86 (m, 1H), 5.99 (s, 1H), 6.20 (s, 1H), 6.34 (s, 1H), 7.40 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.6, 24.7, 28.5, 34.6, 39.1, 40.7, 75.4, 108.1, 110.7, 127.2, 142.5, 151.0, 166.2, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{17}NO_4$) requires m/z 263.1158, found m/z 263.1160. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 7/3, 0.8 mL/min, λ = 220 nm, 8.66 min (minor), 13.91 min (major), ee = 96%.

6j: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one



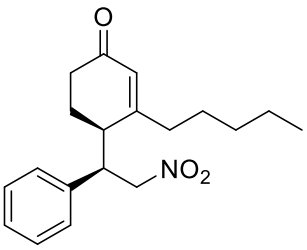
The product was obtained in 83% yield, pale yellow solid. $[\alpha]_D^{25}$ -141 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.77 (t, *J* = 6.4 Hz, 3H), 1.25-1.34 (m, 1H), 1.40-1.52 (m, 1H), 1.70-1.86 (m, 3H), 1.91-1.99 (m, 1H), 2.23-2.30 (m, 1H), 2.37-2.46 (m, 1H), 2.58-2.63 (m, 1H), 3.85-3.91 (m, 1H), 4.53-4.57 (m, 1H), 4.81-4.87 (m, 1H), 5.87 (s, 1H), 7.15-7.16 (m, 2H), 7.21-7.25 (m, 1H), 7.27-7.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.7, 19.5, 23.5, 33.2, 37.3, 41.7, 44.4, 75.6, 126.8, 126.8, 127.1, 128.1, 136.5, 165.0, 197.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1523. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 11.44 min (minor), 16.49 min (major), ee = 99%.

6k: (*R*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



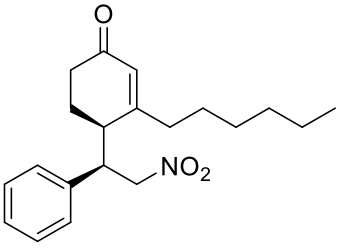
The product was obtained in 74% yield, pale yellow oil. $[\alpha]_D^{25}$ -145 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.79 (t, *J* = 7.2 Hz, 3H), 1.13-1.23 (m, 3H), 1.34-1.44 (m, 1H), 1.75-1.84 (m, 3H), 1.91-2.00 (m, 1H), 2.23-2.30 (m, 1H), 2.38-2.46 (m, 1H), 2.59-2.63 (m, 1H), 3.85-3.90 (m, 1H), 4.53-4.57 (m, 1H), 4.80-4.86 (m, 1H), 5.87 (s, 1H), 7.14-7.16 (m, 2H), 7.22-7.25 (m, 1H), 7.27-7.31 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.8, 22.3, 24.6, 29.4, 34.2, 36.1, 42.7, 45.4, 76.7, 127.7, 127.8, 128.2, 129.1, 137.5, 166.4, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{23}NO_3$) requires m/z 301.1678, found m/z 301.1680. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 10.81 min (minor), 16.71 min (major), ee = 98%.

6l: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one



The product was obtained in 75% yield, pale yellow oil. $[\alpha]_D^{25}$ -150 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.86 (t, *J* = 7.2 Hz, 3H), 1.16-1.37 (m, 5H), 1.41-1.51 (m, 1H), 1.85-1.92 (m, 3H), 1.98-2.07 (m, 1H), 2.30-2.38 (m, 1H), 2.45-2.53 (m, 1H), 2.66-2.71 (m, 1H), 3.92-3.98 (m, 1H), 4.60-4.64 (m, 1H), 4.87-4.93 (m, 1H), 5.94 (s, 1H), 7.23 (d, *J* = 7.2 Hz, 2H), 7.29-7.32 (m, 1H), 7.34-7.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.7, 21.3, 23.6, 28.4, 33.2, 35.1, 41.7, 44.4, 75.7, 126.7, 126.8, 127.2, 128.1, 136.5, 165.4, 197.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{19}H_{25}NO_3$) requires m/z 315.1834, found m/z 315.1839. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 10.68 min (minor), 16.66 min (major), ee = 98%.

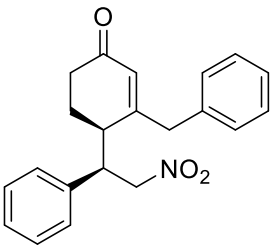
6m: (*R*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



The product was obtained in 75% yield, pale yellow oil. $[\alpha]_D^{25}$ -148 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.87 (t, *J* = 7.2 Hz, 3H), 1.21-1.35 (m, 7H), 1.42-1.47 (m, 1H), 1.80-1.91 (m, 3H), 1.98-2.07 (m, 1H), 2.30-2.38 (m, 1H), 2.45-2.53 (m, 1H), 2.66-2.70 (m, 1H), 3.92-3.97 (m, 1H), 4.60-4.64 (m, 1H), 4.87-4.93 (m, 1H), 5.94 (s, 1H), 7.22 (d, *J* = 7.2 Hz, 2H), 7.29-7.32 (m, 1H), 7.34-7.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.0, 22.5, 24.6, 27.3, 28.8, 31.4, 34.2, 36.4, 42.7, 45.4, 76.7, 127.7, 127.8, 128.2,

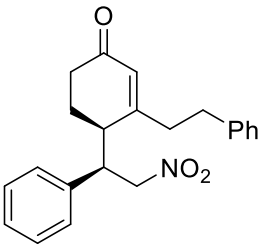
129.1, 137.5, 166.5, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{27}NO_3$) requires m/z 329.1991, found m/z 329.1990. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 10.63 min (minor), 18.92 min (major), ee = 99%.

6n: (*R*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



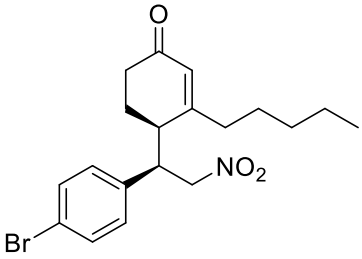
The product was obtained in 79% yield, pale yellow oil. $[\alpha]_D^{25}$ -142 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.83-1.99 (m, 2H), 2.33-2.41 (m, 1H), 2.50-2.58 (m, 2H), 2.90 (d, *J* = 15.6 Hz, 1H), 3.20 (d, *J* = 15.6 Hz, 1H), 3.94-4.00 (m, 1H), 4.65-4.69 (m, 1H), 4.84-4.90 (m, 1H), 5.91 (s, 1H), 7.00 (d, *J* = 7.2 Hz, 2H), 7.12 (d, *J* = 7.2 Hz, 2H), 7.27-7.40 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.9, 33.9, 41.7, 43.2, 45.2, 77.0, 127.2, 127.9, 128.3, 128.9, 129.1, 129.2, 129.4, 136.4, 137.6, 165.0, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1525. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 15.07 min (minor), 25.50 min (major), ee = 98%.

6o: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one



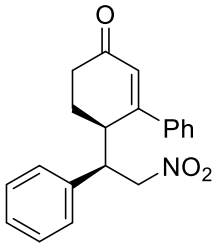
The product was obtained in 77% yield, pale yellow oil. $[\alpha]_D^{25}$ -146 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.82-1.89 (m, 1H), 1.94-2.02 (m, 1H), 2.09-2.12 (m, 2H), 2.30-2.38 (m, 1H), 2.46-2.54 (m, 2H), 2.55-2.65 (m, 1H), 3.88-3.93 (m, 1H), 4.60-4.64 (m, 1H), 4.83-4.89 (m, 1H), 5.96 (s, 1H), 7.03 (d, *J* = 7.2 Hz, 2H), 7.18-7.21 (m, 3H), 7.25-7.28 (m, 2H), 7.32-7.38 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.7, 32.8, 32.8, 37.1, 41.9, 44.5, 75.9, 125.4, 126.8, 127.0, 127.2, 127.2, 127.6, 128.1, 136.4, 139.1, 164.6, 197.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.1681. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.8 mL/min, λ = 220 nm, 16.36 min (minor), 29.11 min (major), ee = 99%.

6p: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-pentylcyclohex-2-en-1-one



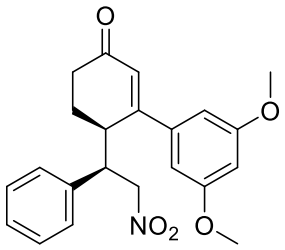
The product was obtained in 79% yield, pale yellow soild, Mp 96-99 °C. $[\alpha]_D^{25}$ -144 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.87 (t, *J* = 7.2 Hz, 3H), 1.19-1.51 (m, 6H), 1.81-1.92 (m, 3H), 1.97-2.06 (m, 1H), 2.30-2.38 (m, 1H), 2.44-2.52 (m, 1H), 2.63-2.67 (m, 1H), 3.89-3.94 (m, 1H), 4.58-4.63 (m, 1H), 4.82-4.88 (m, 1H), 5.95 (s, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.7, 32.8, 32.8, 37.1, 41.8, 44.5, 75.9, 125.4, 126.8, 127.0, 127.2, 127.6, 128.1, 136.4, 139.1, 164.6, 197.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{19}H_{24}BrNO_3$) requires m/z 393.0904, found m/z 393.0910. The enantiomeric ratio was determined by Daicel Chiralpak IB, *n*-Hexane / EtOH = 4/1, 0.9 mL/min, λ = 220 nm, 11.432 min (minor), 21.310 min (major), ee = 98%.

6q: (*R*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



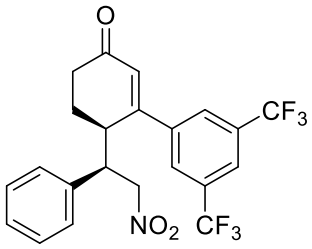
The product was obtained in 80% yield, white solid, Mp 126-127 °C. $[\alpha]_D^{25}$ -116 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.08-2.16 (m, 1H), 2.26-2.43 (m, 3H), 3.46-3.49 (m, 1H), 3.90-3.96 (m, 1H), 4.47-4.51 (m, 1H), 4.63-4.69 (m, 1H), 6.22 (s, 1H), 7.06-7.08 (m, 2H), 7.16-7.21 (m, 3H), 7.28-7.31 (m, 2H), 7.35-7.38 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.3, 33.7, 40.7, 46.7, 126.3, 128.0, 128.8, 129.1, 129.3, 129.8, 136.8, 139.1, 161.2, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{19}NO_3$) requires m/z 321.1365, found m/z 321.1368. The enantiomeric ratio was determined by Daicel Chiralpak AD-H (25 cm), *n*-Hexane/iPrOH = 7/3, 0.7 mL/min, λ = 254 nm, 8.35 min (major), 9.14 min (minor), ee = 95%.

6r: (*R*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



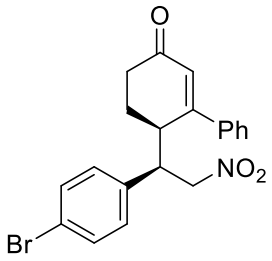
The product was obtained in 74% yield, yellow oil. $[\alpha]_D^{25}$ -123 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.08-2.15 (m, 1H), 2.23-2.37 (m, 3H), 3.39-3.41 (m, 1H), 3.80 (s, 6H), 3.92-3.97 (m, 1H), 4.50-4.55 (m, 1H), 4.63-4.69 (m, 1H), 6.21 (s, 1H), 6.39-6.40 (m, 2H), 6.45-6.46 (m, 1H), 7.07-7.10 (m, 2H), 7.19-7.21 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.4, 33.7, 40.8, 46.8, 55.5, 101.3, 104.7, 128.1, 128.2, 128.8, 129.2, 136.9, 141.3, 161.1, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_5$) requires m/z 381.1576, found m/z 381.1572. The enantiomeric ratio was determined by Daicel Chiralpak AD-H (25 cm), *n*-Hexane/iPrOH = 7/3, 0.7 mL/min, λ = 254 nm, 9.53 min (major), 10.34 min (minor), ee = 93%.

6s: (*R*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



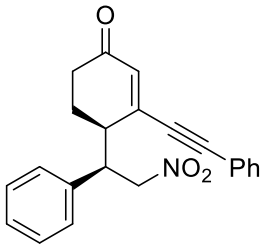
The product was obtained in 67% yield, pale yellow oil. $[\alpha]_D^{25}$ -127 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.28-2.32 (M, 1H), 2.41-2.50 (m, 1H), 2.59-2.64 (m, 1H), 2.74-2.83 (m, 1H), 3.38-3.40 (m, 1H), 3.74-3.80 (m, 1H), 4.76-4.88 (m, 2H), 6.12 (s, 1H), 6.86-6.87 (m, 2H), 6.93-6.94 (m, 3H), 7.32 (s, 2H), 7.63 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.7, 32.3, 41.3, 46.2, 78.4, 121.5, 122.2, 122.2, 124.2, 126.2, 128.2, 128.5, 128.7, 129.7, 131.4, 136.1, 142.0, 160.0, 197.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{17}F_6NO_3$) requires m/z 457.1113, found m/z 457.1116. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane/*i*PrOH = 7/3, 0.9 mL/min, λ = 254 nm, 8.34 min (minor), 10.01 min (major), ee = 90%.

6t: (*R*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



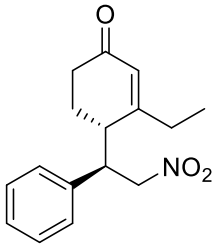
The product was obtained in 60% yield, white solid, Mp 110-111 °C; $[\alpha]_D^{25}$ -143 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.09-2.15 (m, 1H), 2.28-2.39 (m, 1H), 2.41-2.46 (m, 2H), 3.39-3.43 (m, 1H), 3.83-3.89 (m, 1H), 4.53-4.58 (m, 1H), 4.62-4.68 (m, 1H), 6.19 (s, 1H), 6.89-6.91 (m, 2H), 7.18-7.20 (m, 2H), 7.24-7.26 (m, 2H), 7.31-7.40 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.3, 33.5, 40.7, 46.1, 122.1, 126.2, 129.0, 129.1, 129.7, 129.8, 131.8,135.8, 139.0, 161.3, 197.9. HRMS(EI) exact mass calculated for $M^+(C_{20}H_{18}BrNO_3)$ requires m/z 399.0470, found m/z 399.0473. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / *i*PrOH = 4/1, 1.0 mL/min, λ = 254 nm, 22.12 min (minor), 48.63 min (major), ee =92%.

6u: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one



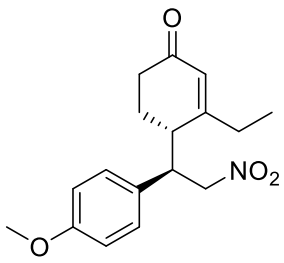
The product was obtained in 74% yield, pale yellow oil. $[\alpha]_D^{25}$ -143 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.69-1.79 (m, 1H), 2.02-2.09 (m, 1H), 2.18-2.26 (m, 1H), 2.33-2.40 (m, 1H), 2.92-2.97 (m, 1H), 4.55-4.60 (m, 1H), 4.80-4.84 (m, 1H), 4.95-5.01 (m, 1H), 6.42-6.43 (d, *J* = 2.0 Hz, 1H), 7.30-7.33 (m, 5H), 7.36-7.43 (m, 5H), 7.57-7.59 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.4, 36.3, 43.3, 45.9, 75.0, 86.5, 102.9, 121.3, 128.0, 128.2, 128.7, 129.1, 130.1, 132.3, 134.7, 137.1, 143.0, 197.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{19}NO_3$) requires m/z 345.1365, found m/z 345.1363. The enantiomeric ratio was determined by Daicel Chiralpak AS-H (25 cm), *n*-Hexane / *i*PrOH = 4/1, 0.9 mL/min, λ = 254 nm, 26.10 min (minor), 29.63 min (major), ee >99%.

7a: (*S*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



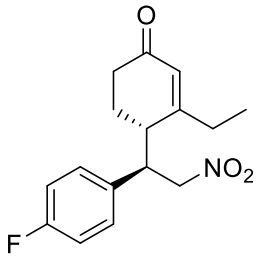
The product was obtained in 66% yield, colorless oil. $[\alpha]_D^{25}$ 43 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (t, *J* = 7.6 Hz, 3H), 1.77-1.82 (m, 1H), 1.93-2.05 (m, 2H), 2.10-2.19 (m, 1H), 2.29-2.38 (m, 1H), 2.42-2.51 (m, 1H), 2.56-2.58 (m, 1H), 3.78-3.84 (m, 1H), 4.70-4.75 (m, 1H), 4.78-4.84 (m, 1H), 5.98 (s, 1H), 7.16-7.18 (m, 2H), 7.30-7.36 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.7, 30.4, 32.6, 40.8, 45.8, 78.9, 126.9, 127.5, 128.4, 129.2, 137.0, 166.4, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{19}NO_3$) requires m/z 273.1365, found m/z 273.1363. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 11.26 min (minor), 16.83 min (major), ee = 98%.

7c: (*S*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one



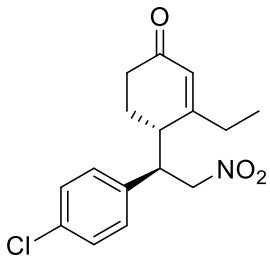
The product was obtained in 66% yield, colorless oil. $[\alpha]_D^{25}$ 34 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (t, *J* = 7.6 Hz, 3H), 1.78-1.86 (m, 1H), 1.93-1.99 (m, 1H), 2.02-2.06 (m, 1H), 2.10-2.18 (m, 1H), 2.93-2.37 (m, 1H), 2.40-2.48 (m, 1H), 2.48-2.54 (m, 1H), 3.75-3.81 (m, 4H)， 4.67-4.79 (m, 2H), 5.97 (s, 1H), 6.86 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.7, 30.4, 32.6, 40.9, 45.1, 55.3, 79.1, 114.5, 126.9, 128.6, 128.7, 159.4, 166.6, 198.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_4$) requires m/z 303.1471, found m/z 303.1469. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 19.83 min (minor), 34.59 min (major), ee = 99%.

7d: (*S*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one



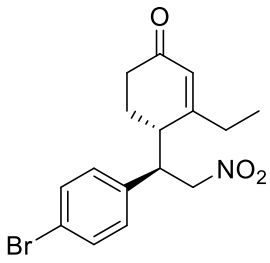
The product was obtained in 57% yield, pale yellow oil. $[\alpha]_D^{25}$ 22 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (t, *J* = 7.2 Hz, 3H), 1.74-1.79 (m, 1H), 1.98-2.04 (m, 1H), 2.07-2.12 (m, 1H), 2.17-2.23 (m, 1H), 2.29-2.35 (m, 1H), 2.39-2.45 (m, 1H), 2.53-2.56 (m, 1H), 3.76-3.82 (m, 1H), 4.66-4.71 (m, 1H), 4.74-4.79 (m, 1H), 5.99 (s, 1H), 7.03-7.08 (m, 2H), 7.15-7.18 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.8, 30.6, 32.5, 41.0, 45.3, 79.0, 116.2, 116.4, 127.0, 129.1, 129.2, 166.2, 198.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}FNO_3$) requires m/z 291.1271, found m/z 291.1271. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 13.42 min (minor), 22.98 min (major), ee = 96%.

7e: (*S*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



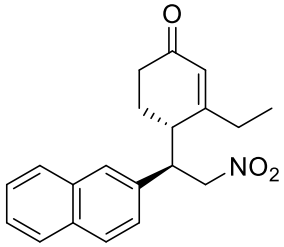
The product was obtained in 52% yield, pale yellow oil. $[\alpha]_D^{25}$ 18 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (t, *J* = 7.6 Hz, 3H), 1.73-1.79 (m, 1H), 1.94-2.03 (m, 1H), 2.10-2.14 (m, 1H), 2.17-2.24 (m, 1H), 2.29-2.37 (m, 1H), 2.39-2.47 (m, 1H), 2.53-2.57 (m, 1H), 3.75-3.81 (m, 1H), 4.65-4.70 (m, 1H), 4.73-4.78 (m, 1H), 5.99 (s, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.9, 30.6, 32.5, 40.9, 45.5, 78.9, 127.0, 128.9, 129.4, 130.8, 135.6, 166.2, 198.1. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}ClNO_3$) requires m/z 307.0975, found m/z 307.0979. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane / EtOH = 4/1, 1.0 mL/min, λ = 254 nm, 11.80 min (minor), 12.45 min (major), ee = 97%.

7f: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



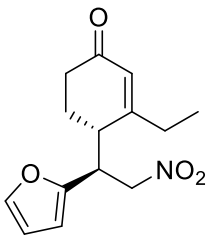
The product was obtained in 70% yield, pale yellow oil. $[\alpha]_D^{25}$ 21 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.20 (t, *J* = 7.6 Hz, 3H), 1.73-1.78 (m, 1H), 1.94-2.03 (m, 1H), 2.06-2.15 (m, 1H), 2.18-2.24 (m, 1H), 2.27-2.36 (m, 1H), 2.39-2.47 (m,1H), 2.53-2.57 (m, 1H), 3.74-3.80 (m, 1H), 4.65-4.70 (m, 1H), 4.73-4.78 (m, 1H), 5.99 (s, 1H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 24.9, 30.6, 32.5, 40.8, 45.6, 78.8, 122.4, 127.0, 129.2, 132.4, 136.1, 166.1, 198.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{16}H_{18}BrNO_3$) requires m/z 351.0470, found m/z 351.0474. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 16.40 min (minor), 33.03min (major), ee = 94%.

7h: (*S*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



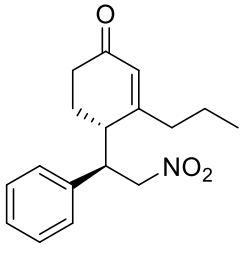
The product was obtained in 63% yield, colorless oil. $[\alpha]_D^{25}$ 22 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.22 (t, *J* = 7.2 Hz, 3H), 1.77-1.83 (m, 1H), 1.93-2.02 (m, 1H), 2.17-2.21 (m, 2H), 2.32-2.42 (m, 1H), 2.45-2.54 (m, 1H), 2.66-2.70 (m, 1H), 3.93-3.99 (m, 1H), 4.75-4.79 (m, 1H), 4.87-4.92 (m, 1H), 6.00 (s, 1H), 7.29-7.32 (m, 1H), 7.48-7.53 (m, 2H), 7.64 (s, 1H), 7.78-7.85 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 12.0, 25.2, 30.8, 32.6, 41.0, 46.3, 79.1, 124.6, 126.6, 126.8, 126.9, 127.1, 127.8, 129.2, 132.9, 133.3, 134.6, 166.7, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{21}NO_3$) requires m/z 323.1521, found m/z 323.1524. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 15.25 min (minor), 19.78 min (major), ee = 98%.

7i: (*S*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



The product was obtained in 52% yield, pale yellow oil. $[\alpha]_D^{25}$ 40 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.17 (t, *J* = 7.2 Hz, 3H), 1.71-1.79 (m, 1H), 1.89-1.97 (m, 1H), 2.02-2.11 (m, 1H), 2.14-2.21 (m, 1H), 2.30-2.50 (m, 2H), 4.09-4.14 (m, 1H), 4.74-4.80 (m, 1H), 4.86-4.92 (m, 1H), 5.98 (s, 1H), 6.08 (d, *J* = 3.2 Hz, 2H), 6.30-6.31 (m, 1H), 7.35 (d, *J* = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 11.8, 23.3, 28.7, 33.4, 38.4, 39.6, 76.1, 108.7, 110.9, 127.2, 142.4, 149.2, 165.0, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{14}H_{17}NO_3$) requires m/z 263.1158, found m/z 263.1162. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane/EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 11.69 min (minor), 15.08 min (major), ee = 93%.

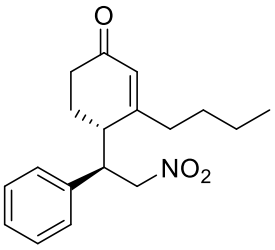
7j: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one



The product was obtained in 63% yield, pale yellow oil. $[\alpha]_D^{25}$ 37 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.01 (t, *J* = 7.2 Hz, 3H), 1.50-1.60 (m, 1H), 1.64-1.71 (m, 1H), 1.76-1.80 (m, 1H), 1.93-2.06 (m, 2H), 2.10-2.18 (m, 1H), 2.26-2.41 (m, 2H), 2.55-2.58 (m, 1H), 3.77-3.83 (m, 1H), 4.71-4.76 (m, 1H), 4.79-4.84 (m, 1H), 5.97 (s, 1H), 7.17 (m, 2H), 7.30-7.36 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 21.3, 24.7, 32.5, 39.6, 40.7, 45.9, 79.0, 127.5, 127.9,

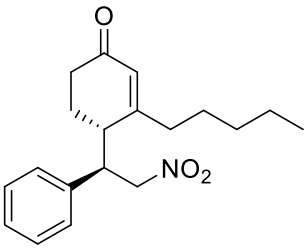
128.3, 129.2, 137.0, 165.0, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{17}H_{21}NO_3$) requires m/z 287.1521, found m/z 287.1520. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 10.72 min (minor), 18.97 min (major), ee = 97%.

7k: (*S*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



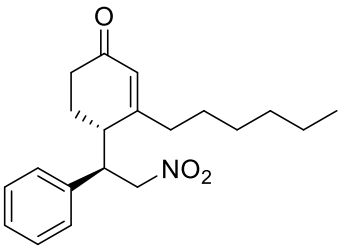
The product was obtained in 66% yield, colorless oil. $[\alpha]_D^{25}$ 36 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.97 (t, *J* = 7.6 Hz, 3H), 1.37-1.45 (m, 2H), 1.48-1.54 (m, 1H), 1.58-1.65 (m, 1H), 1.77-1.80 (m, 1H), 1.91-2.06 (m, 2H), 2.09-2.17 (m, 1H), 2.26-2.33 (m, 1H), 2.36-2.44 (m, 1H), 2.56-2.59 (m, 1H), 3.77-3.83 (m, 1H), 4.71-4.76 (m, 1H), 4.78-4.84 (m, 1H), 5.97 (s, 1H), 7.12-7.19 (m, 2H), 7.30-7.36 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 22.5, 24.7, 30.2, 32.5, 37.3, 40.7, 45.9, 79.0, 127.5, 127.8, 128.3, 129.2, 137.0, 165.3, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{23}NO_3$) requires m/z 301.1678, found m/z 301.1680. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 10.71 min (minor), 13.08 min (major), ee = 94%.

7l: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one



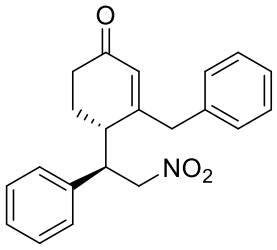
The product was obtained in 55% yield, pale yellow oil. $[\alpha]_D^{25}$ 24 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.97 (t, *J* = 7.2 Hz, 3H), 1.39-1.43 (m, 2H), 1.46-1.51 (m, 1H), 1.56-1.65 (m, 3H), 1.76-1.81 (m, 1H), 1.92-2.01 (m, 2H), 2.12-2.28 (m, 1H), 2.26-2.33 (m, 1H), 2.36-2.44 (m, 1H), 2.55-2.59 (m ,1H), 3.78-3.83 (m, 1H), 4.71-4.76 (m, 1H), 4.78-4.83 (m, 1H), 5.97 (s, 1H), 7.16-7.18 (m, 2H), 7.31-7.36 (m, 3H).^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 22.5, 24.7, 30.2, 32.5, 37.3, 40.7, 45.9, 79.0, 127.5, 127.9, 128.4, 129.2, 137.0, 175.7, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{19}H_{25}NO_3$) requires m/z 315.1834, found m/z 315.1830. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 9.60 min (minor), 11.53 min (major), ee = 96%.

7m: (*S*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



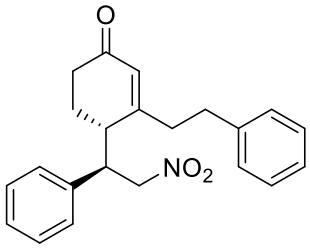
The product was obtained in 64% yield, pale yellow oil. $[\alpha]_D^{25}$ 36 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.91(t, *J* = 6.8 Hz, 3H), 1.32-1.42 (m, 6H), 1.46-1.53 (m, 1H), 1.60-1.65 (m, 1H), 1.76-1.83 (m, 1H), 1.91-2.06 (m, 2H), 2.12-2.17 (m, 1H), 2.25-2.33 (m, 1H), 2.36-2.43 (m, 1H), 2.55-2.58 (m, 1H), 3.77-3.83 (m, 1H), 4.70-4.75 (m, 1H), 4.78-4.84 (m, 1H), 5.96 (s, 1H), 7.16-7.18 (m, 2H), 7.30-7.36 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.0, 22.5, 24.7, 28.0, 29.0, 31.6, 32.5, 37.6, 40.7, 45.9, 79.0, 127.5, 127.8, 128.3, 129.2, 137.0, 165.4, 198.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{27}NO_3$) requires m/z 329.1991, found m/z 329.1996. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 8.85 min (minor), 11.77 min (major), ee = 99%.

7n: (*S*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



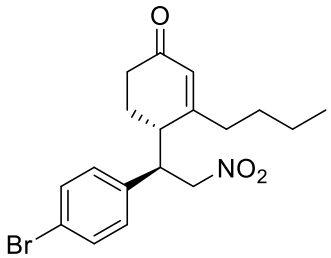
The product was obtained in 58% yield, pale yellow oil. $[\alpha]_D^{25}$ 60 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.77-1.90 (m, 3H), 2.04-2.14 (m, 1H), 2.55-2.56 (m, 1H), 3.60 (d, *J* = 15.2 Hz, 1H), 3.78 (d, *J* = 15.2 Hz, 1H), 3.89-3.95 (m, 1H), 4.77-4.82 (m, 1H), 4.84-4.89 (m, 1H), 5.96 (s, 1H), 7.14-7.16 (m, 2H), 7.20-7.22 (m, 2H), 7.28-7.38 (m, 6H).^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.6, 32.5, 39.4, 43.8, 45.4, 78.8, 127.4, 128.4, 129.1, 129.2, 129.5, 136.4, 136.7, 163.0, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{21}H_{21}NO_3$) requires m/z 335.1521, found m/z 335.1527. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 4/1, 0.8 mL/min, λ = 254 nm, 12.09 min (major), 13.16 min (minor), ee = 97%.

7o: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one



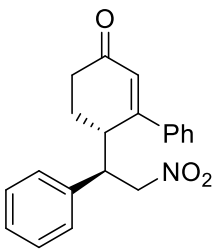
The product was obtained in 68% yield, pale yellow oil. $[\alpha]_D^{25}$ 27 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.72-1.79 (m, 1H), 1.85-1.95 (m, 2H), 2.01-2.11 (m, 1H), 2.43-2.46 (m, 1H), 2.59-2.67 (m, 1H), 2.70-2.77 (m, 1H), 2.84-2.96 (m, 2H), 3.76-3.81 (m, 1H), 4.65-4.70 (m, 1H), 4.73-4.78 (m, 1H), 6.02 (s, 1H), 7.07-7.11 (m, 2H), 7.22-7.24 (m, 3H), 7.28-7.35 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.4, 32.4, 34.5, 39.1, 40.8, 45.6, 78.7, 126.6, 127.5, 128.4, 128.4, 128.8, 129.2, 136.8, 140.1, 163.9, 198.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_3$) requires m/z 349.1678, found m/z 349.16740. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 254 nm, 13.73 min (minor), 14.52 min (major), ee = 99%

7p: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-butylcyclohex-2-en-1-one



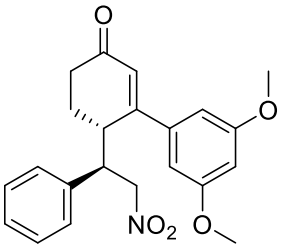
The product was obtained in 56% yield, pale yellow soild. $[\alpha]_D^{25}$ 30 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.96 (t, *J* = 7.2 Hz, 3H), 1.35-1.46 (m, 2H), 1.47-1.65 (m, 2H), 1.71-1.77 (m, 1H), 1.92-2.19 (m, 3H), 2.21-2.30 (m, 1H), 2.34-2.42 (m, 1H), 2.53-2.57 (m, 1H), 3.72-3.78 (m, 1H), 4.66-4.78 (m, 2H), 5.97 (s, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H).^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 13.9, 22.5, 24.9, 30.2, 32.4, 37.5, 40.7, 45.7, 78.8, 122.4, 127.9, 129.2, 132.4, 136.2, 165.1, 198.0. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{22}BrNO_3$) requires m/z 379.0783, found m/z 379.0786. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 0.8 mL/min, λ = 254 nm, 18.18 min (minor), 29.87 min (major), ee = 99%.

7q: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



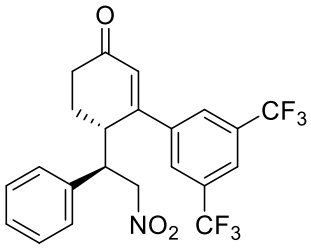
The product was obtained in 69% yield, yellow oil. $[\alpha]_D^{25}$ 107 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.85-1.91 (m, 1H), 2.11-2.21 (m, 1H), 2.29-2.35 (m, 1H), 2.37-2.47 (m, 1H), 3.34-3.38 (m, 1H), 3.74-3.80 (m, 1H), 4.27-4.37 (m, 2H), 6.35 (s, 1H), 7.17-7.19 (m, 2H), 7.30-7.38 (m, 3H), 7.51-7.53 (m, 3H), 7.54-7.58 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.1, 32.3, 38.9, 46.8, 79.4, 126.3, 127.5, 128.2, 128.4, 129.2, 129.7, 130.7, 137.5, 139.2, 160.7, 198.6. HRMS(EI) exact mass calculated for $M^+(C_{20}H_{19}NO_3)$ requires m/z 321.1365, found m/z 321.1368. The enantiomeric ratio was determined by Daicel Chiralpak AD-H (25 cm), *n*-Hexane / EtOH = 7/3, 0.7 mL/min, λ = 254 nm, 11.51 min (minor), 14.95 min (major), ee = 97%.

7r: (*S*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



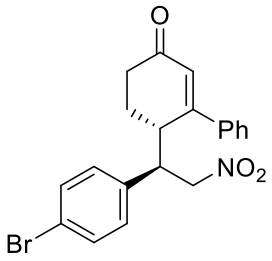
The product was obtained in 72% yield, pale yellow oil. $[\alpha]_D^{25}$ 72 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.82-1.87 (m, 1H), 2.09-2.18 (m, 1H), 2.28-2.45 (m, 2H), 3.25-3.29 (m, 1H), 3.73-3.77 (m, 1H), 3.87 (s, 6H), 4.38-4.40 (m, 2H), 6.34 (s, 1H), 6.57-6.58 (m, 1H), 6.66-6.66 (m, 2H), 7.18-7.19 (m, 2H), 7.30-7.37 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 24.0, 31.3, 38.0, 45.8, 54.6, 78.4, 100.9, 103.5, 126.5, 127.1, 127.3, 128.2, 136.5, 140.2, 159.6, 160.6, 197.6. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{23}NO_5$) requires m/z 381.1576, found m/z 381.1579. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane/*i*PrOH = 7/3, 0.9 mL/min, λ = 254 nm, 6.50 min (major), 10.08 min (minor), ee = 99%.

7s: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



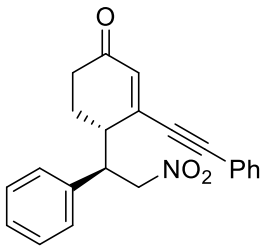
The product was obtained in 49% yield, pale yellow oil. $[\alpha]_D^{25}$ 45 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.04-2.10 (m, 1H), 2.18-2.34 (m, 3H), 3.37-3.40 (m, 1H), 3.73-3.79 (m, 1H), 4.42-4.47 (m, 1H), 4.53-4.58 (m, 1H), 6.34 (s, 1H), 7.03-7.05 (m, 2H), 7.32-7.36 (m, 3H), 7.96 (s, 2H), 8.02 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.1, 31.7, 37.4, 44.8, 77.3, 120.5, 122.8, 123.2, 125.6, 126.5, 127.7, 128.3, 129.9, 131.6, 131.9, 132.2, 135.1, 140.1, 196.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{17}F_6NO_3$) requires m/z 457.1113, found m/z 457.1110. The enantiomeric ratio was determined by Daicel Chiralpak IB (25 cm), *n*-Hexane/*i*PrOH = 7/3, 0.9 mL/min, λ = 254 nm, 10.11 min (major), 11.07 min (minor), ee = 91%.

7t: (*S*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



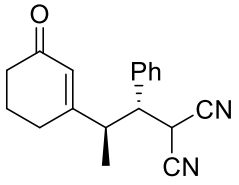
The product was obtained in 68% yield, pale yellow oil. $[\alpha]_D^{25}$ 133 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.82-1.88 (m, 1H), 2.13-2.22 (m, 1H), 2.32-2.49 (m, 2H), 3.30-3.35 (m, 1H), 3.72-3.78 (m, 1H), 4.21-4.33 (m, 2H), 6.35 (s, 1H), 7.06-7.09 (m, 2H), 7.47-7.56 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 25.2, 32.3, 38.8, 46.4, 79.2, 122.4, 126.2, 128.3, 129.2, 129.7, 130.8, 132.4, 136.6, 139.1, 160.3, 198.2. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{20}H_{18}BrNO_3$) requires m/z 399.0470, found m/z 399.0468. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / *i*-PrOH = 4/1, 1.0 mL/min, λ = 254 nm, 13.4 min (major), 16.07 min (minor), ee = 97%.

7u: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one



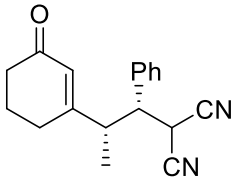
The product was obtained in 55% yield, pale yellow oil. $[\alpha]_D^{25}$ 47 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.68-1.76 (m, 1H), 2.03-2.12 (m, 1H), 2.26-2.41 (m, 2H), 2.85-2.89 (m, 1H), 4.08-4.14 (m, 1H), 4.86-4.92 (m, 1H), 5.10-5.14 (m, 1H), 6.37 (s, 1H), 7.28-7.36 (m, 5H), 7.42-7.45 (m, 3H), 7.56-7.58 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 23.6, 32.4, 40.5, 45.3, 77.9, 87.3, 101.4, 120.4, 126.8, 127.3, 127.7, 128.2, 129.0, 131.0, 133.0, 135.8, 142.3, 196.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{22}H_{19}NO_3$) requires m/z 345.1365, found m/z 345.1367. The enantiomeric ratio was determined by Daicel Chiralpak AS-H (25 cm), *n*-Hexane / *i*-PrOH = 4/1, 0.9 mL/min, λ = 254 nm, 19.80 min (minor), 20.67 min (major), ee = 99%.

10: 2-((1*S*,2*R*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile



The product was obtained in 66% yield, white solid. $[\alpha]_D^{25}$ 20 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.37-1.39 (d, *J* = 6.8 Hz, 3H), 1.62-1.78 (m, 2H), 2.02-2.05 (m, 2H), 2.15-2.18 (m, 2H), 3.06-3.11 (m, 1H), 3.20-3.24 (m, 1H), 4.26-4.28 (d, *J* = 4.8 Hz, 1H), 5.80 (s, 1H), 7.28-7.32 (m, 2H), 7.35-7.40 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.0, 21.4, 26.3, 26.7, 36.2, 42.7, 48.9, 110.4, 110.6, 126.8, 127.1, 128.2, 128.3, 134.5, 164.2, 198.3. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{12}N_2O$) requires m/z 278.1419, found m/z 278.1417. The enantiomeric ratio was determined by Daicel Chiralpak AY-H (25 cm), *n*-Hexane / *i*-PrOH = 7/3, 0.7 mL/min, λ = 254 nm, 20.38 min (minor), 29.24 min (major), ee = 38%.

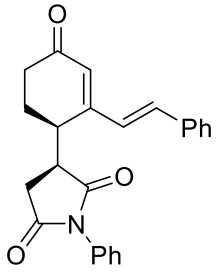
11: 2-((1*S*,2*S*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile



The product was obtained in 57% yield, white solid. $[\alpha]_D^{25}$ 47 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 0.98 (d, *J* = 6.8 Hz, 3H), 2.04-2.16 (m, 2H), 2.35-2.54 (m, 4H), 3.02-3.10 (m, 1H), 3.19-3.22 (m, 1H), 4.06-4.07 (m, 1H), 6.15 (s, 1H), 7.39-7.41 (m, 2H), 7.43-7.48 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 16.9, 21.6, 25.7, 27.4, 36.5, 42.7, 48.1, 110.3, 110.7, 126.9, 127.3, 128.4, 128.5, 133.8, 163.6, 197.9. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{18}H_{12}N_2O$) requires m/z 278.1419, found m/z 278.1416. The enantiomeric ratio was determined by Daicel Chiralpak AY-H (25 cm), *n*-Hexane / *i*-PrOH = 7/3, 0.7 mL/min, λ = 254 nm, 13.72 min (minor), 20.86 min (major), ee =

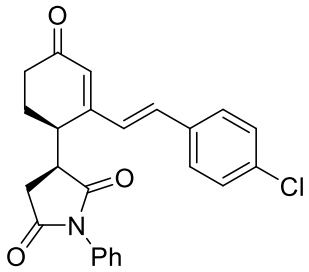
40%.

12a: (*S*)-3-((*R*)-4-oxo-2-((*E*)-styryl)cyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione



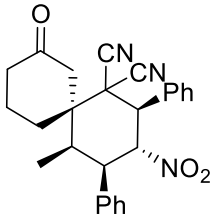
The product was obtained in 68% yield, white solid. Mp 170-171°C. ^{1}H NMR (400MHz, $CDCl_3$): δ 2.20-2.25(m, 1H), 2.33-2.50 (m, 2H), 2.54-2.59 (m, 1H), 2.69-2.75 (m, 1H), 2.96-3.03 (m, 1H), 3.28-3.33 (m, 1H), 3.83-3.85 (m, 1H), 6.32 (s, 1H), 6.74-6.78 (d, J = 16 Hz, 1H), 7.03-7.07 (m, 3H), 7.31-7.38 (m, 5H), 7.44-7.46 (m, 2H). ^{13}C NMR(100MHz, $CDCl_3$): δ 29.7, 32.1, 34.2, 35.1, 43.7, 126.5, 127.0, 127.6, 128.7, 128.9, 129.0, 129.0, 129.7, 131.4, 135.2, 137.3, 156.1, 174.6, 178.2, 198.3; HRMS(EI) exact mass calculated for M^+($C_{24}H_{21}NO_3$) requires m/z 371.1521, found m/z 371.1524; The enantiomeric excess was determined by Daicel Chiralpak AS-H, *n*-Hexane / EtOH = 4:1, 0.7 mL/min, λ = 254 nm, 38.06 min (minor), 43.63 min (major), ee = 99%.

12b: (*S*)-3-((*R*)-2-((*E*)-4-chlorostyryl)-4-oxocyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione



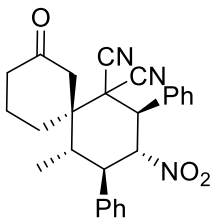
The product was obtained in 50% yield, white solid. Mp 183-184°C. ^{1}H NMR(400MHz, $CDCl_3$): δ 2.21-2.27(m, 1H), 2.38-2.48(m, 2H), 2.54-2.58(m, 1H), δ 2.65-2.71 (m, 1H), 2.94-3.01 (m, 1H), 3.26-3.31(m, 1H), 3.80-3.82 (m, 1H), 6.32 (s, 1H), 6.72-6.76 (d, J = 16.4 Hz, 1H), 6.89-6.91(m, 2H), 7.00-7.05 (d, J = 16.4 Hz, 1H), δ 7.24-7.7.34 (m, 7H); ^{13}C NMR(100MHz, $CDCl_3$): δ 29.7, 32.1, 34.2, 35.0, 43.7, 126.3, 127.7, 128.7, 128.8, 129.0, 129.2, 129.3, 131.4, 133.8, 135.5, 135.8, 155.7, 174.6, 178.2, 198.1. HRMS(EI) exact mass calculated for M^+ ($C_{24}H_{20}ClNO_3$) requires m/z 405.1132, found m/z 405.1133; The enantiomeric excess was determined by Daicel Chiralpak AS-H, *n*-Hexane / EtOH = 7:3, 0.7 mL/min, λ = 254 nm, 27.61 min (minor), 36.87 min (major), ee = 98%.

14: (2*R*,3*R*,4*R*,5*R*,6*S*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile



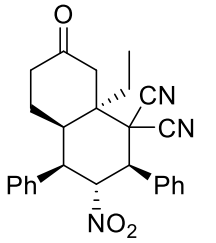
The product was obtained in 75% yield, white soild. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.11 (d, J = 7.6 Hz, 3H), 1.66-1.83 (m, 1H), 2.02-2.26 (m, 3H), 2.44-2.60 (m, 3H), 2.96 (d, J = 13.6 Hz, 1H), 3.38-3.44 (m, 1H), 3.88 (dd, J_1 = 4.0 Hz, J_2 = 12.0 Hz, 1H), 4.07 (d, J = 12.0 Hz, 1H), 5.82 (t, J = 12.0 Hz, 1H), 7.20-7.25 (m, 2H), 7.26-7.37 (m, 3H), 7.43-7.48 (m, 3H), 7.57 (s, 2H). ^{13}C NMR (100 MHz, d6-DMSO): δ (ppm) 9.54, 19.8, 31.9, 39.0, 46.1, 47.7, 47.8, 48.1, 49.0, 79.6, 84.2, 113.9, 128.1, 128.8, 128.9, 130.2, 132.4, 137.4, 208.4. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{26}H_{25}N_3O_3$) requires m/z 427.1896, found m/z 427.1898. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 11.38 min (minor), 13.87 min (major), ee = 84%.

15: (2*R*,3*R*,4*R*,5*S*,6*R*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile



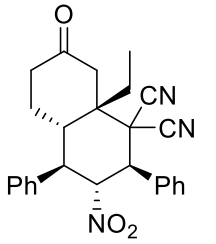
The product was obtained in 70% yield, white soild; ^{1}H NMR (400 MHz, d6-DMSO) δ (ppm) 0.64 (d, *J* = 6.8 Hz, 3H), 2.00-2.16 (m, 2H), 2.22-2.42 (m, 4H), 2.46-2.47 (m, 1H), 2.68-2.83 (m, 2H), 3.29-3.32 (m, 1H), 4.39 (d, *J* = 12 Hz, 1H), 5.60-5.66 (t, *J* = 11.6 Hz, 1H), 7.10-7.11 (m, 1H), 7.26-7.33 (m, 2H), 7.45-7.47 (m, 4H), 7.64-7.65 (m, 1H), 7.77-7.78 (m, 2H). ^{13}C NMR (100 MHz, d6-DMSO): δ (ppm) 13.8, 20.55, 24.8, 38.5, 42.8, 46.4, 46.7, 49.2, 49.3, 52.8, 55.4, 90.6, 113.2, 113.9, 126.3, 128.6, 129.0, 129.2, 129.8, 130.3, 131.0, 132.4, 137.2, 209.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{26}H_{25}N_3O_3$) requires m/z 427.1896, found m/z 427.1892. The enantiomeric ratio was determined by Daicel Chiralpak IA (25 cm), *n*-Hexane / EtOH = 9/1, 1.0 mL/min, λ = 220 nm, 13.50 min (minor), 15.73 min (major), ee = 83%.

16: (2*R*,3*R*,4*R*,4a*R*,8a*R*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile



The product was obtained in 72% yield, white soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.20-1.23 (t, *J* = 6.8 Hz, 3H), 1.80-1.90 (m, 2H), 2.04-2.13 (m, 1H), 2.39-2.48 (m, 3H), 2.53-2.57 (m, 2H), 2.63-2.67 (m, 1H), 3.79-3.83 (m, 1H), 4.04-4.06 (d, *J* = 12 Hz, 1H), 5.75-5.81 (t, *J* = 12 Hz, 3H), 7.20-7.21 (m, 2H), 7.26-7.34 (m, 3H), 7.37-7.39 (m, 3H), 7.49 (m, 2H).^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 8.1, 22.2, 28.6, 39.3, 40.3, 45.9, 46.3, 46.7, 48.6, 49.9, 84.0, 112.2, 113.9, 128.1, 128.6, 129.2, 129.3, 130.4, 130.6, 135.2, 205.5. HRMS (EI): exact mass calculated for $[M]^+$ ($C_{26}H_{25}N_3O_3$) requires m/z 427.1896, found m/z 427.1894. The enantiomeric ratio was determined by Daicel Chiralpak AD (25 cm), *n*-Hexane / EtOH = 7/3, 0.55 mL/min, λ = 220 nm, 15.23 min (minor), 16.89 min (major), ee = 88%.

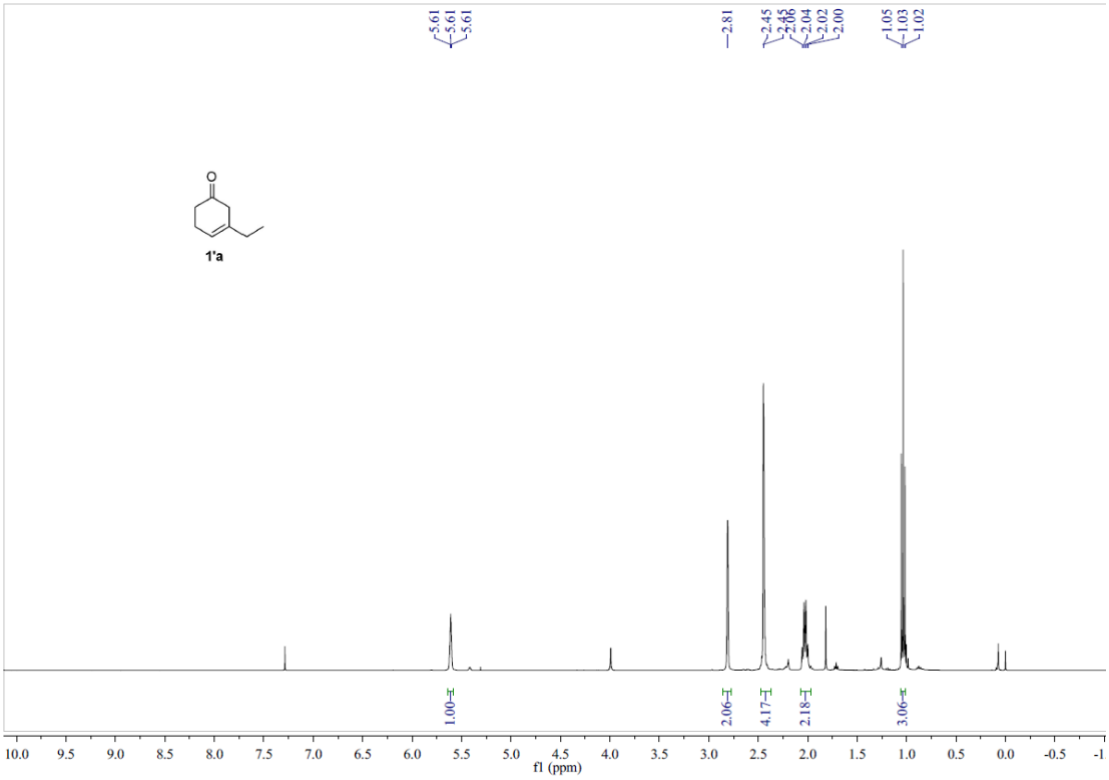
17: (2*R*,3*R*,4*R*,4a*S*,8a*S*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile

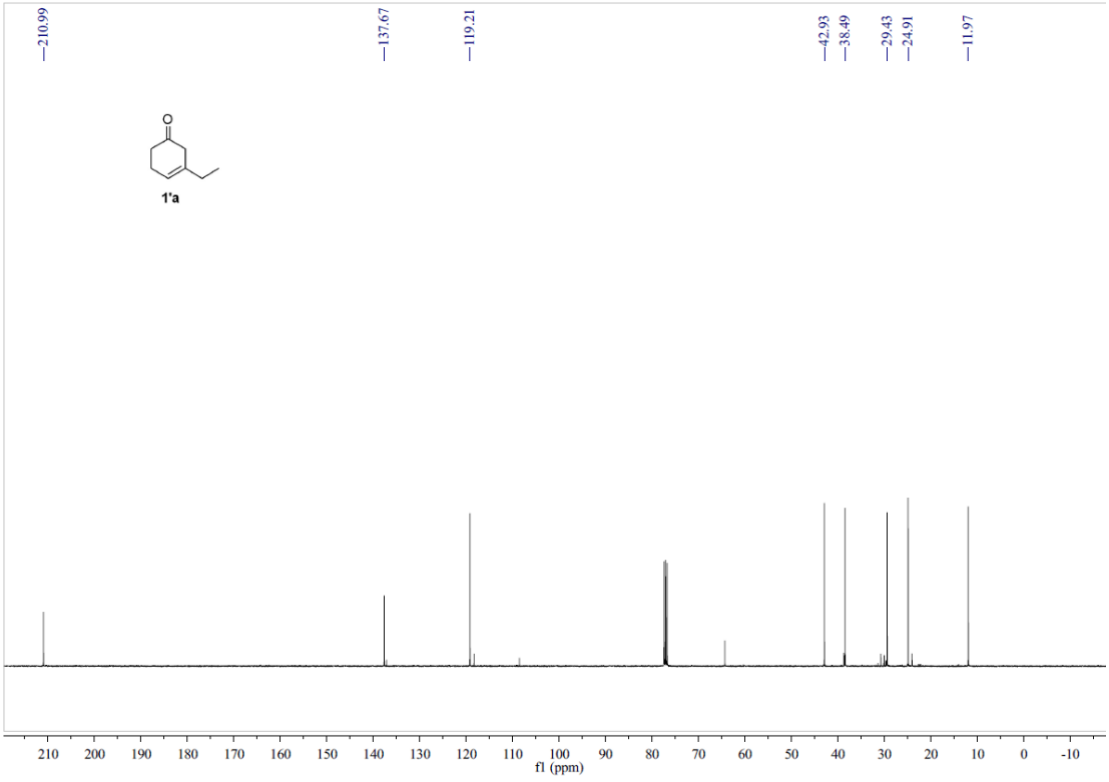


The product was obtained in 80% yield, white soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.22-1.26 (t, *J* = 7.6 Hz, 3H), 1.58-1.62 (m, 1H), 1.85-2.04 (m, 3H), 2.29-2.51 (m, 3H), 2.90-2.93 (m, 1H), 3.00-3.04 (m, 1H), 3.66-3.72 (t, *J* = 11.6 Hz, 1H), 3.94 (d, *J* = 12 Hz, 1H), 5.44-5.50 (t, *J* = 11.6 Hz, 1H), 7.07-7.09 (m, 1H), 7.32-7.38 (m, 2H), 7.40-7.44 (m, 3H), 7.51-7.54 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 7.7, 12.1, 21.6, 28.7, 31.0, 34.1, 39.6, 40.9, 46.0, 46.2, 47.4, 48.1, 89.8, 111.0, 111.4, 128.2, 128.3, 129.2, 129.5, 134.6, 204.4 HRMS (EI): exact mass calculated for $[M]^+$ ($C_{26}H_{25}N_3O_3$) requires m/z 427.1896, found m/z 427.1897. The enantiomeric ratio was determined by Daicel Chiralpak AD (25 cm), *n*-Hexane / EtOH = 7/3, 0.55 mL/min, λ = 220 nm, 13.50 min (minor), 15.25 min (major), ee = 84%.

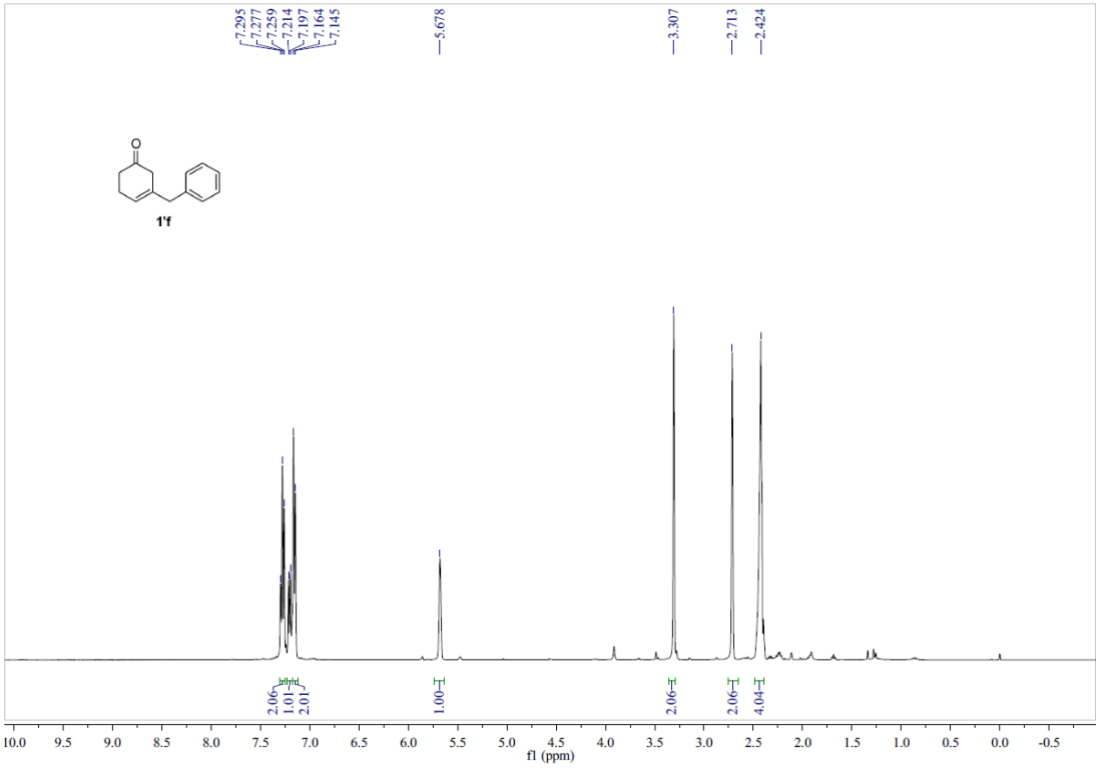
E: NMR spectra of substrates and products

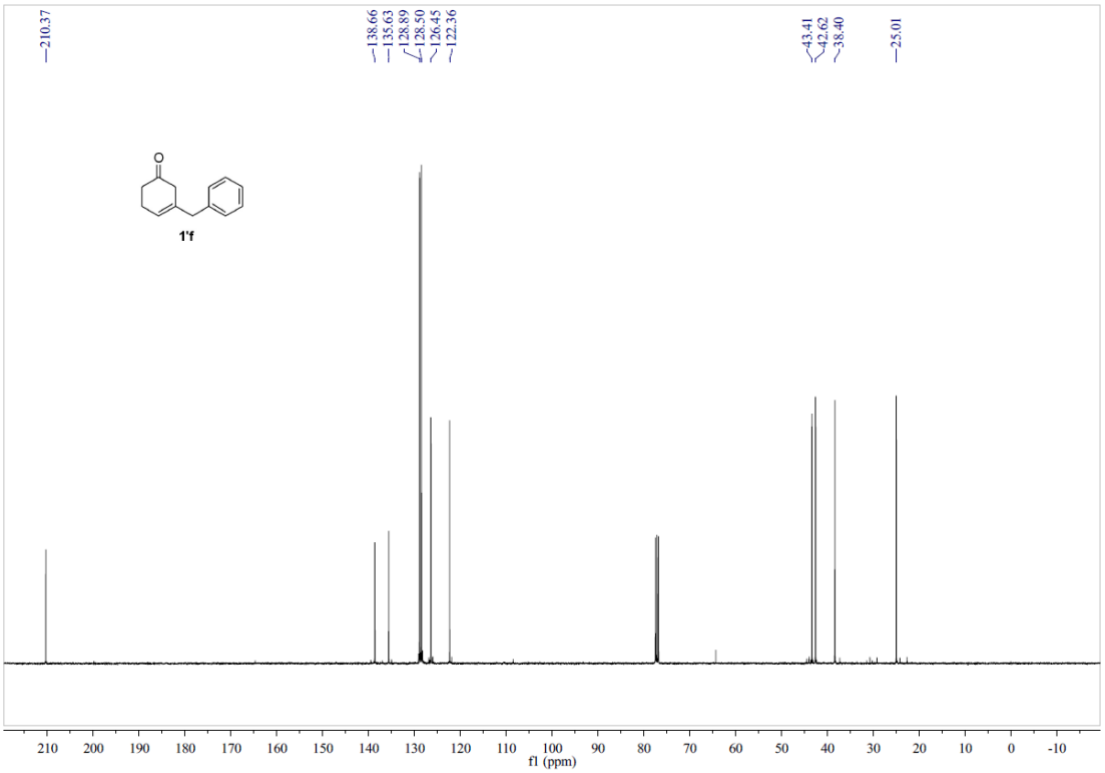
1′a: 3-ethylcyclohex-3-en-1-one



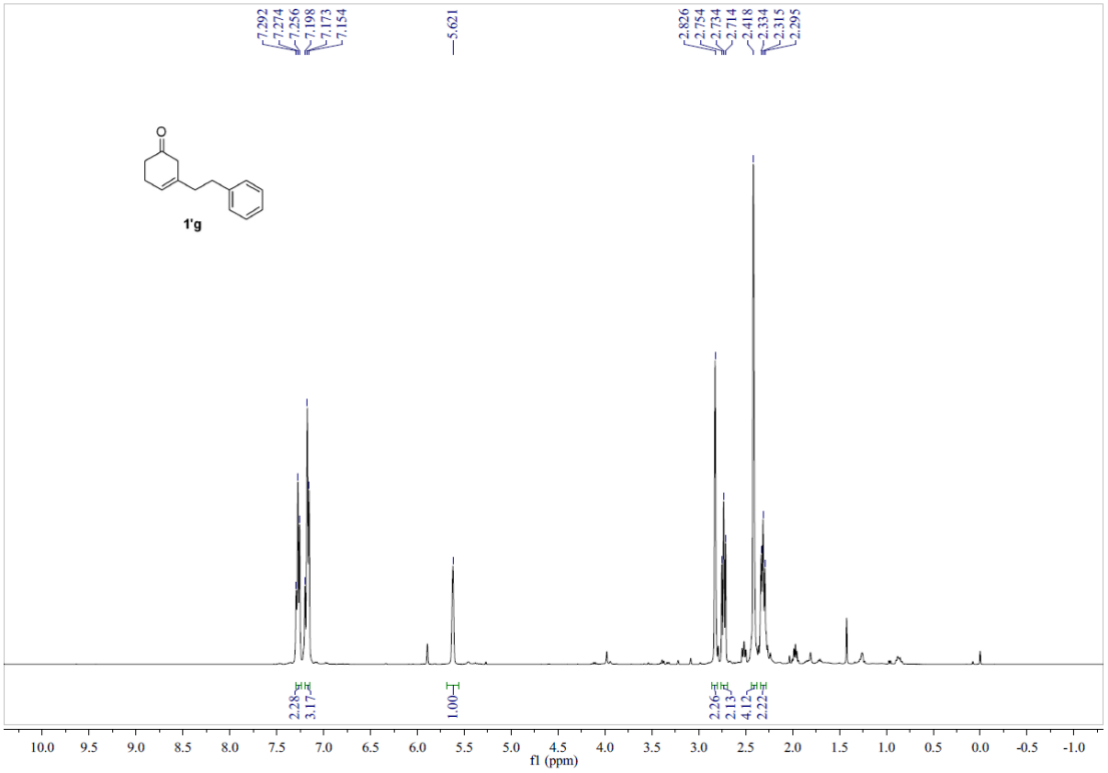


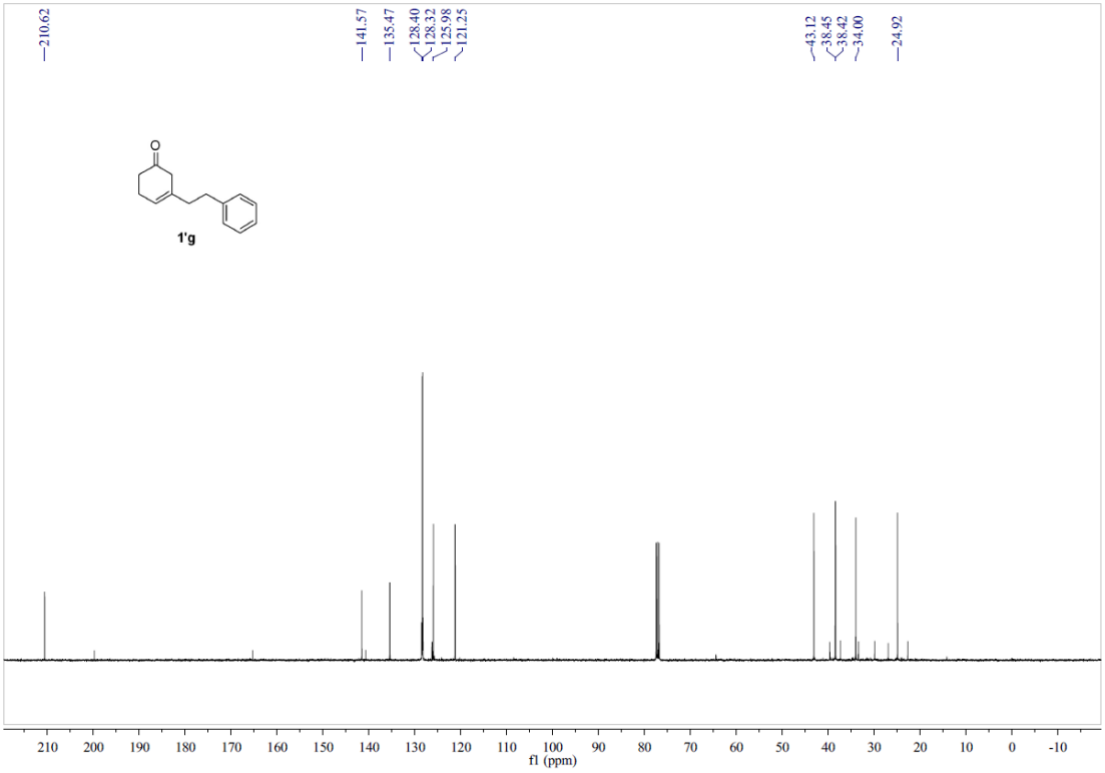
1′f: 3-benzylcyclohex-3-en-1-one



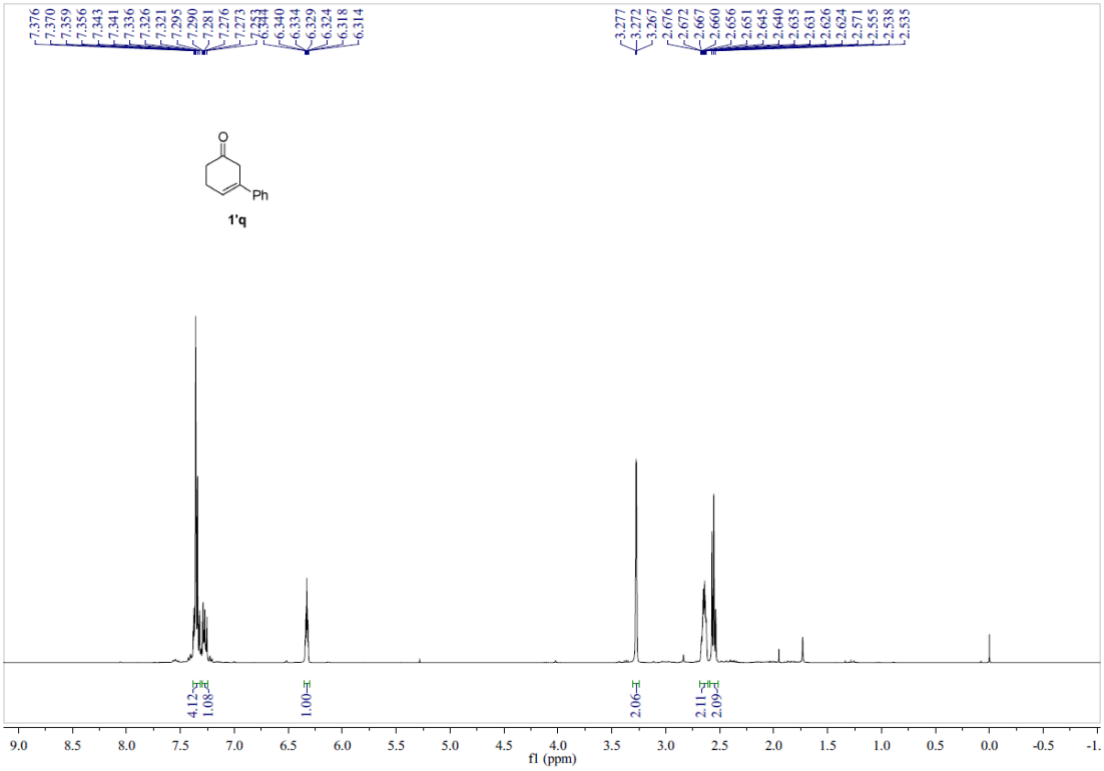


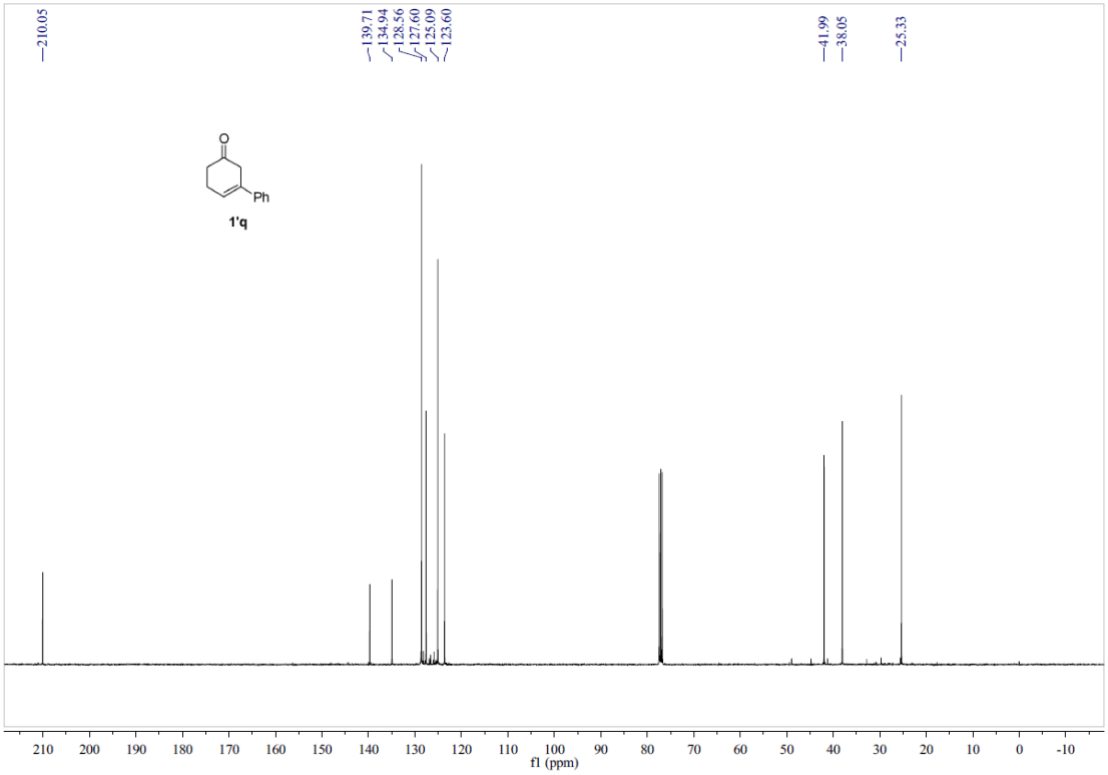
1′g: 3-phenethylcyclohex-3-en-1-one



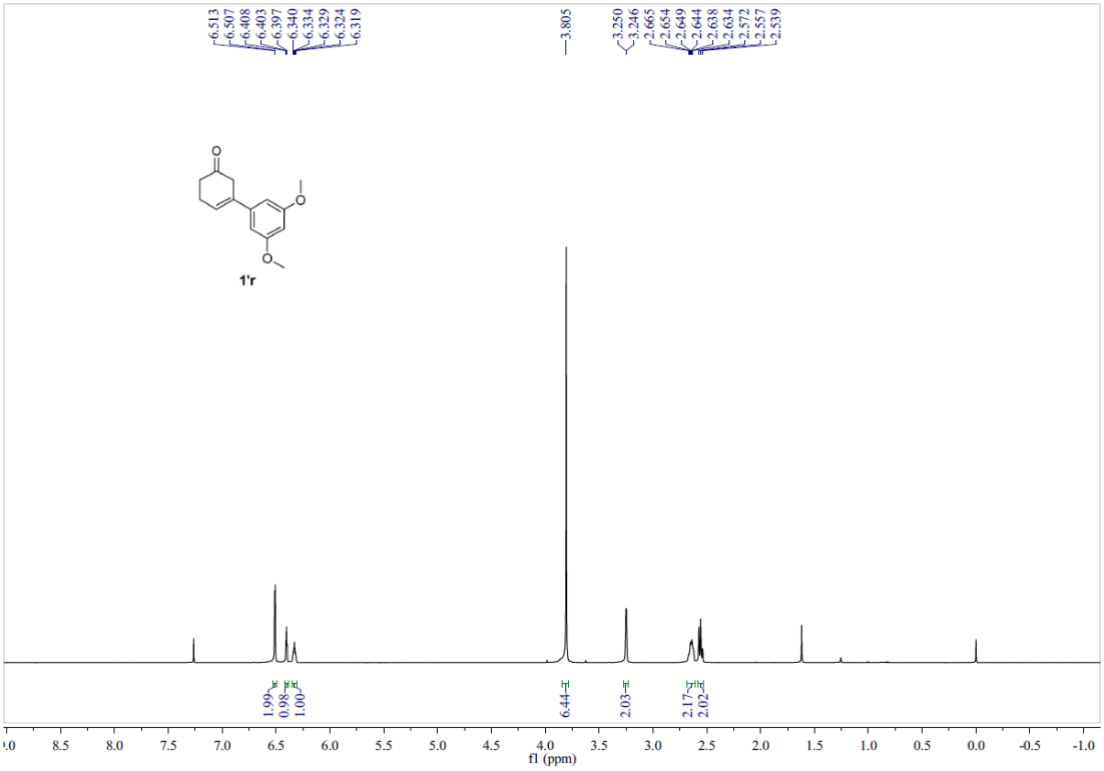


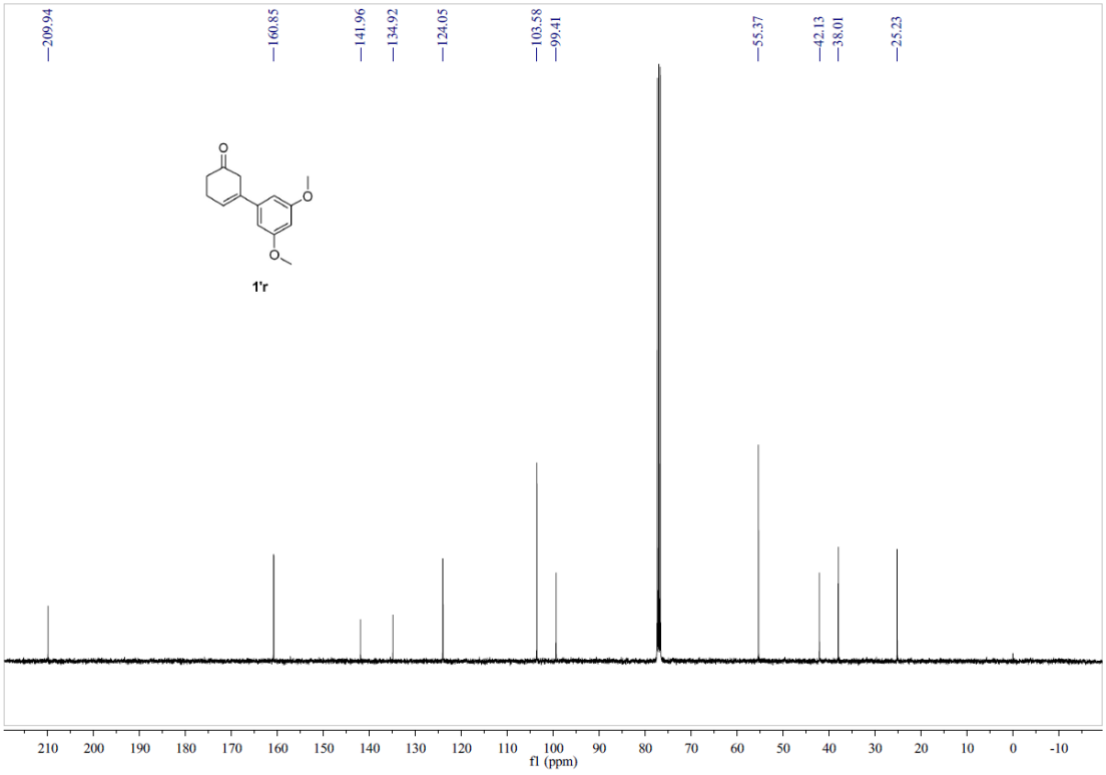
1′q:4,5-dihydro-[1,1'-biphenyl]-3(2H)-one



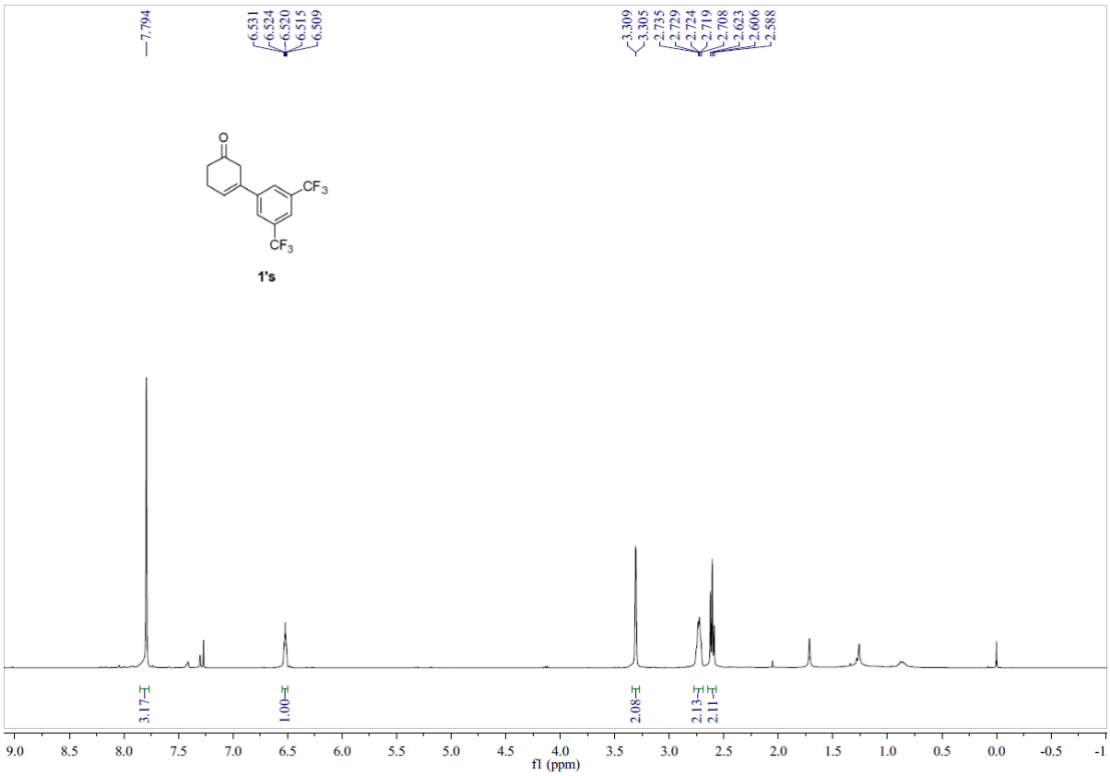


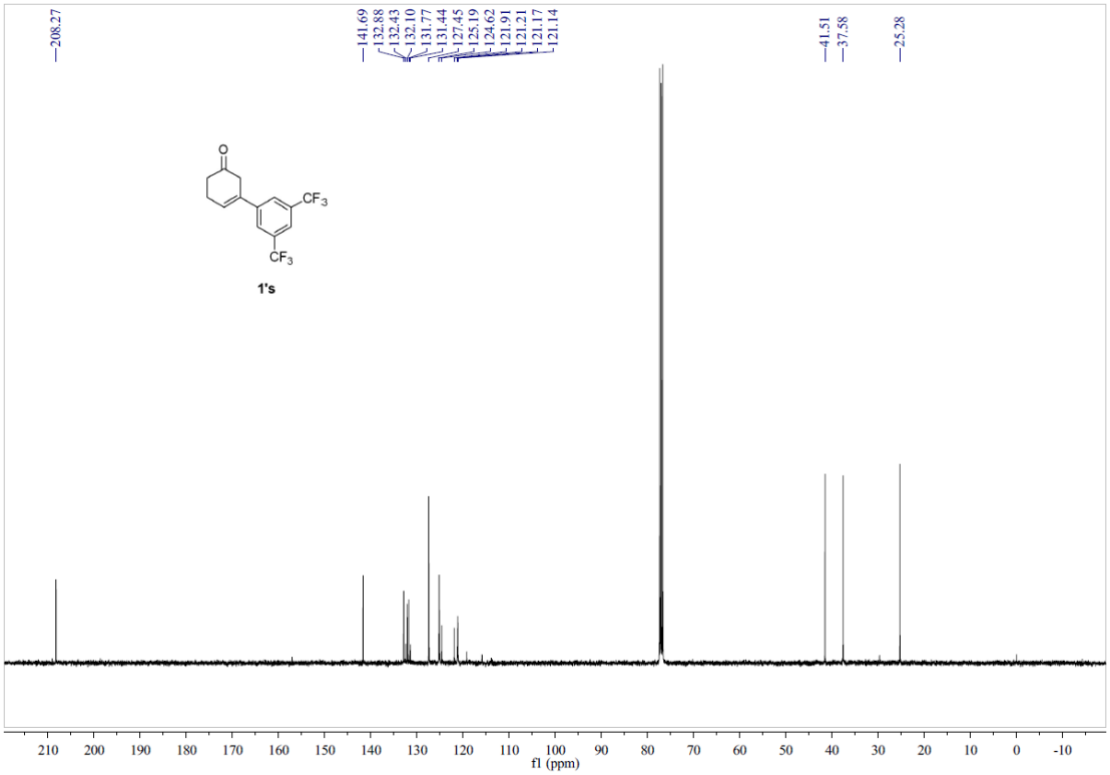
1′r: 3',5'-dimethoxy-4,5-dihydro-[1,1'-biphenyl]-3(2*H*)-one



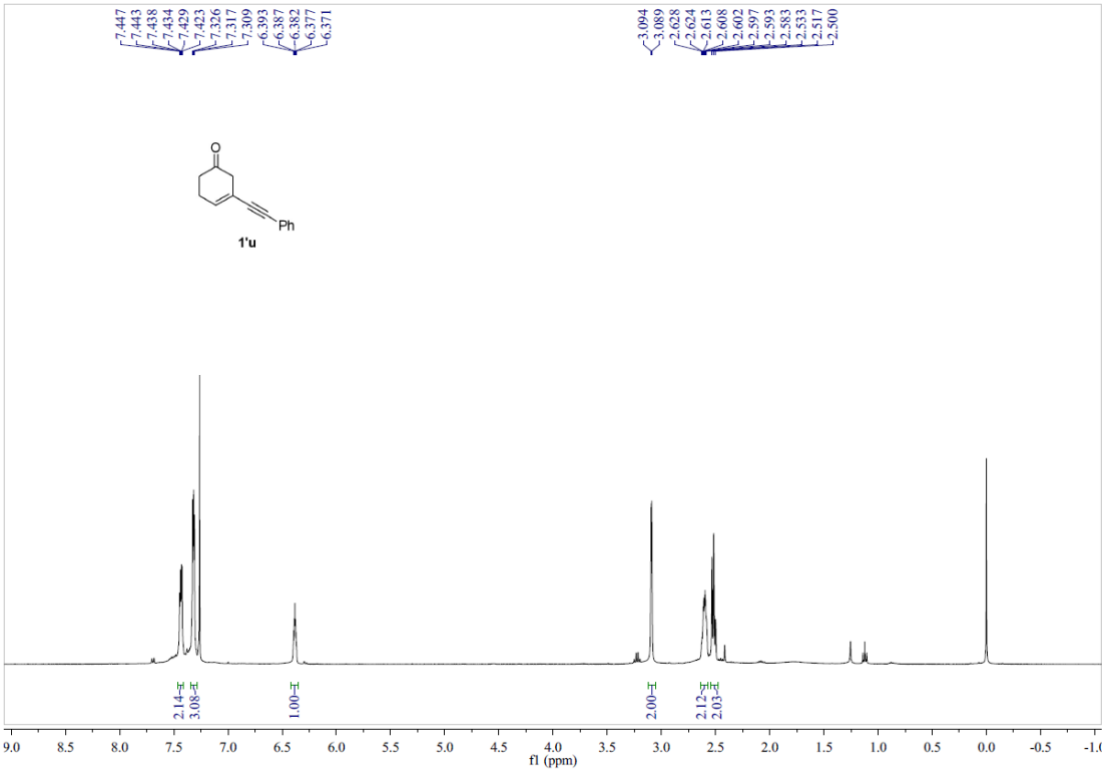


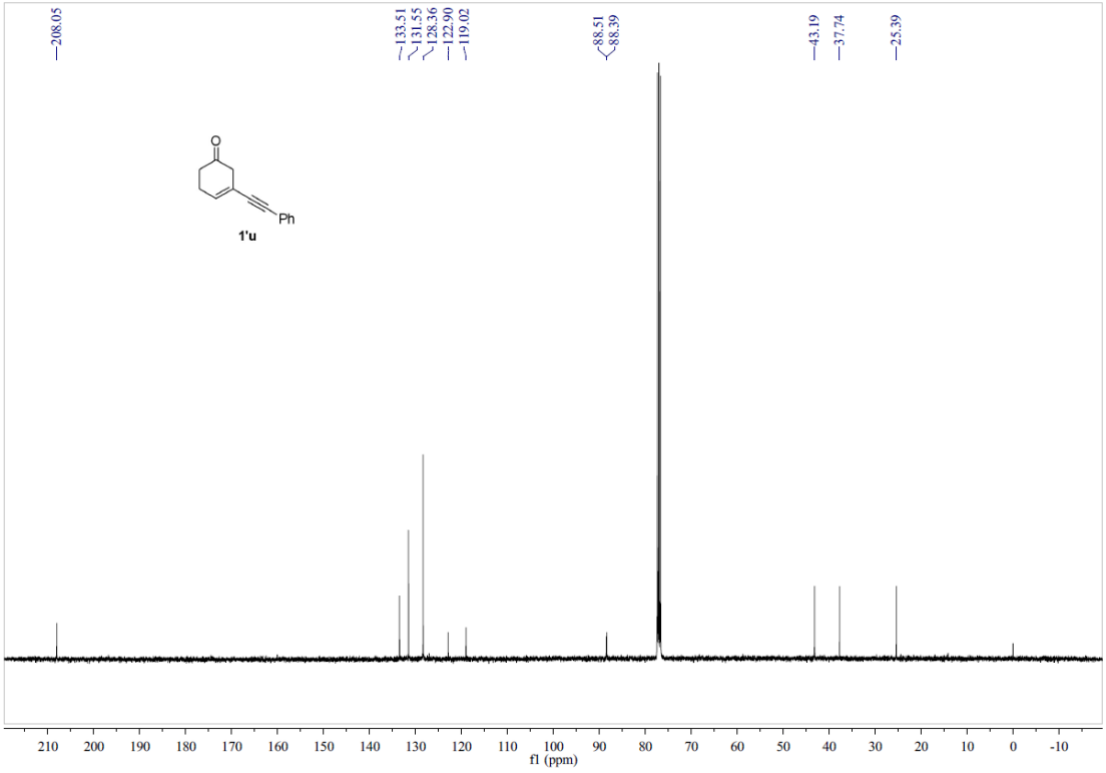
1′s: 3',5'-bis(trifluoromethyl)-4,5-dihydro-[1,1'-biphenyl]-3(2*H*)-one



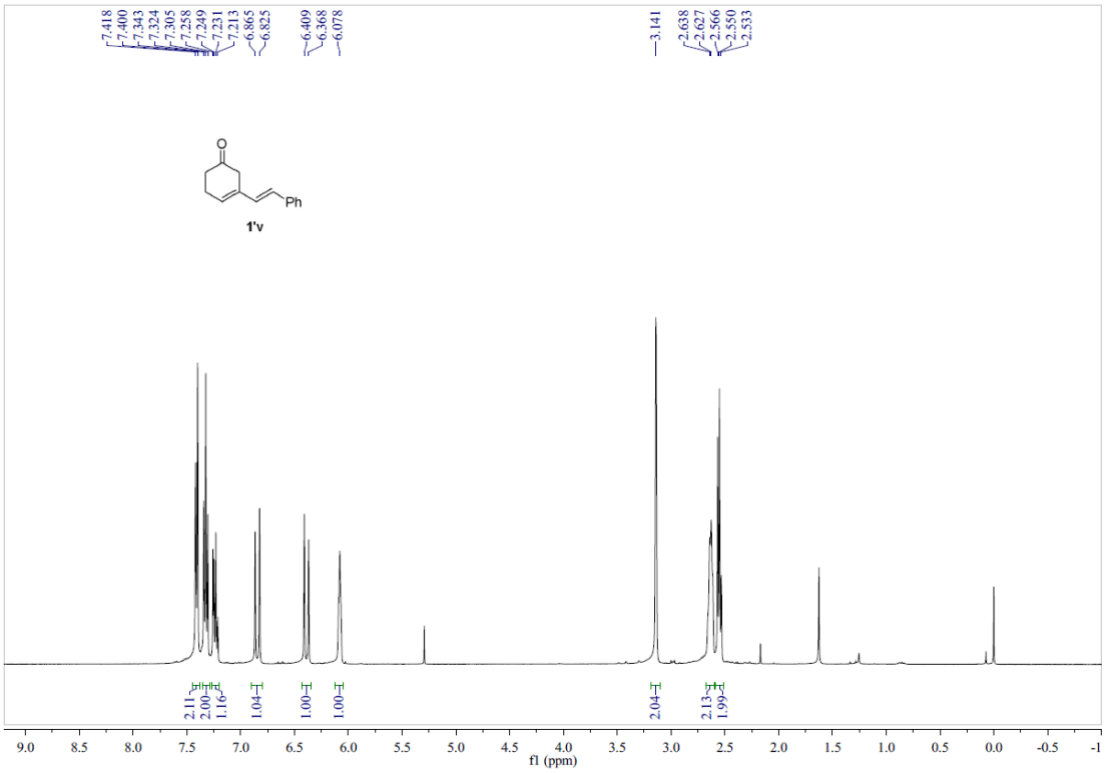


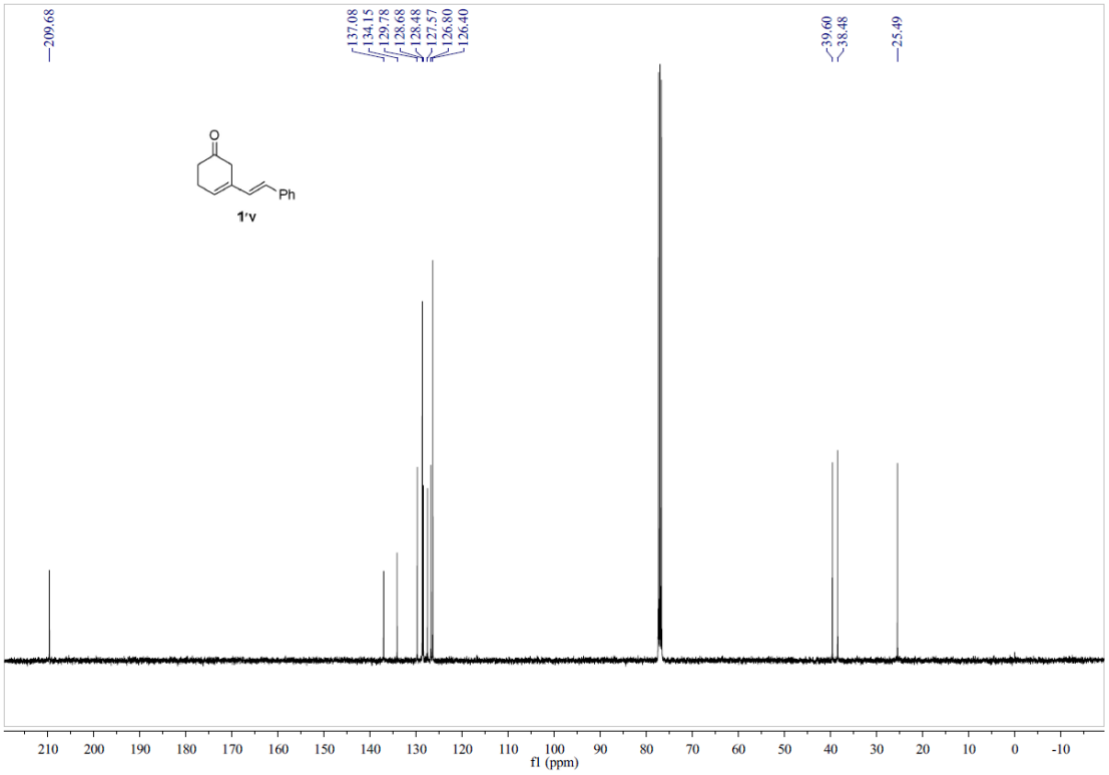
1′u: 3-(phenylethynyl)cyclohex-3-en-1-one



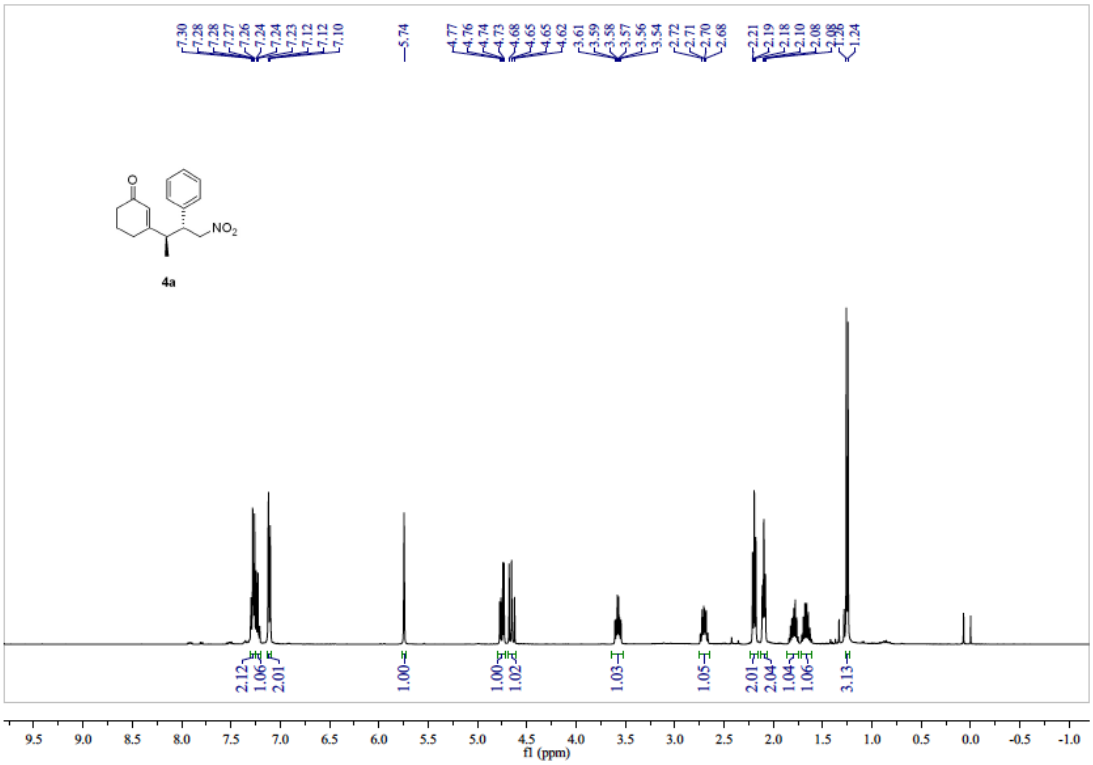


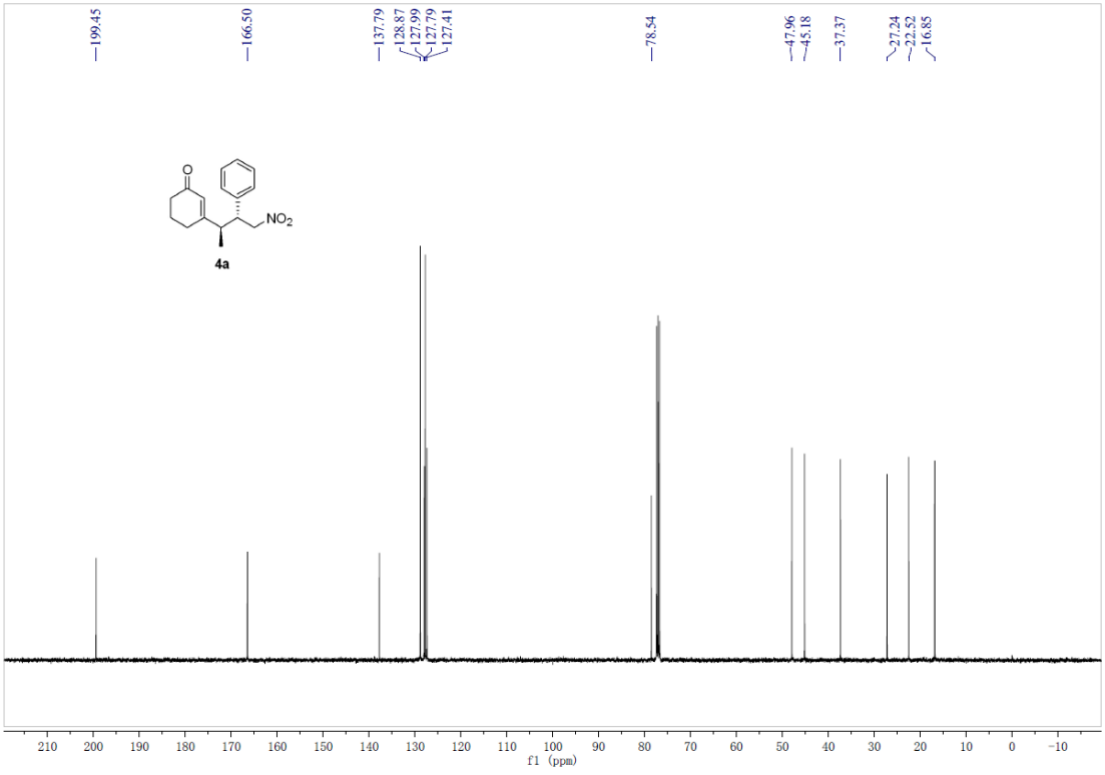
1′v: (*E*)-3-styrylcyclohex-3-en-1-one



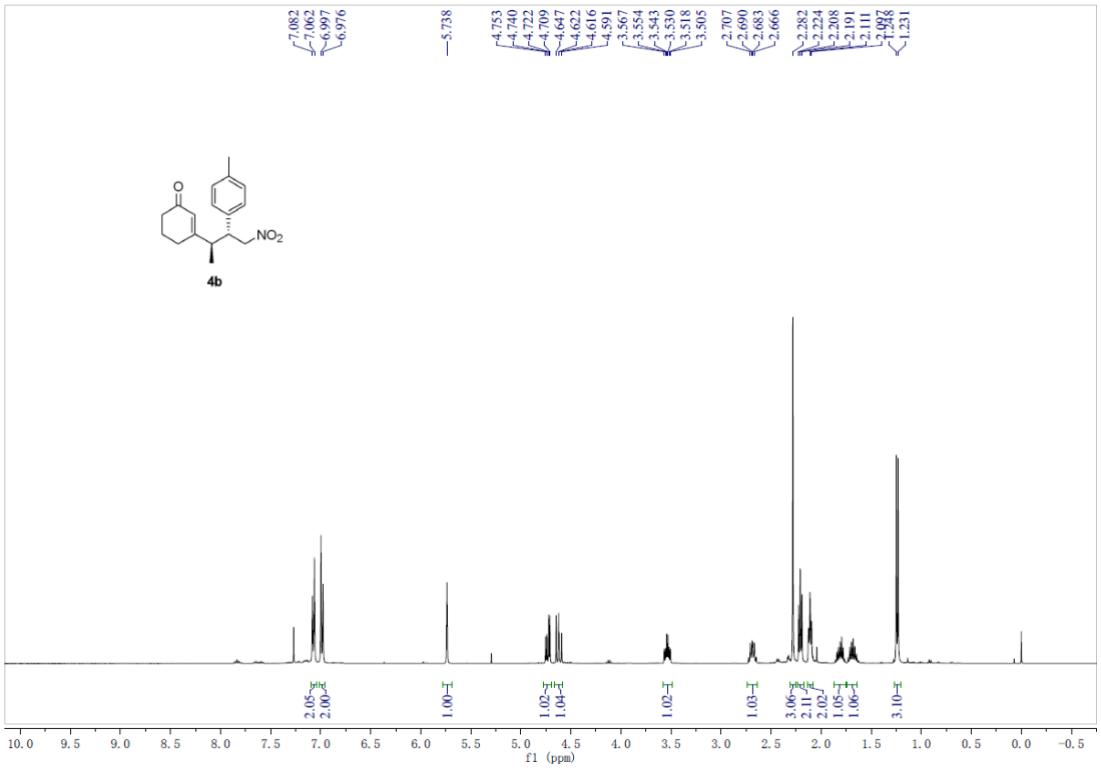


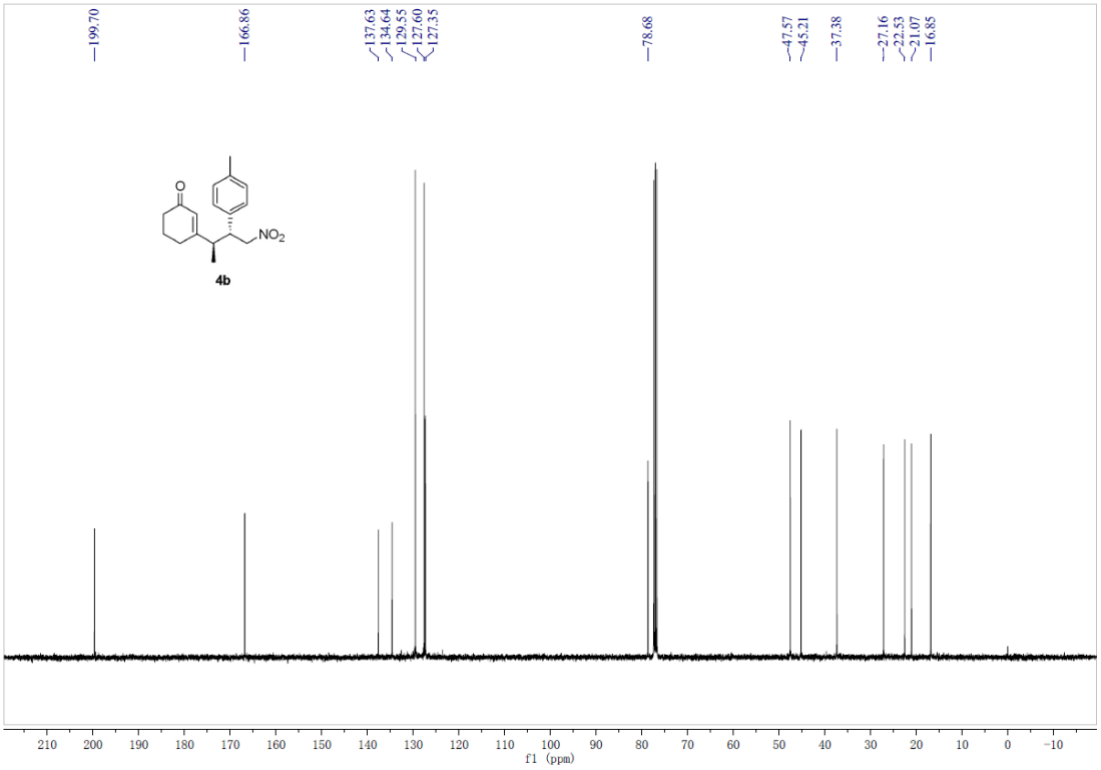
4a: 3-((2*R*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one



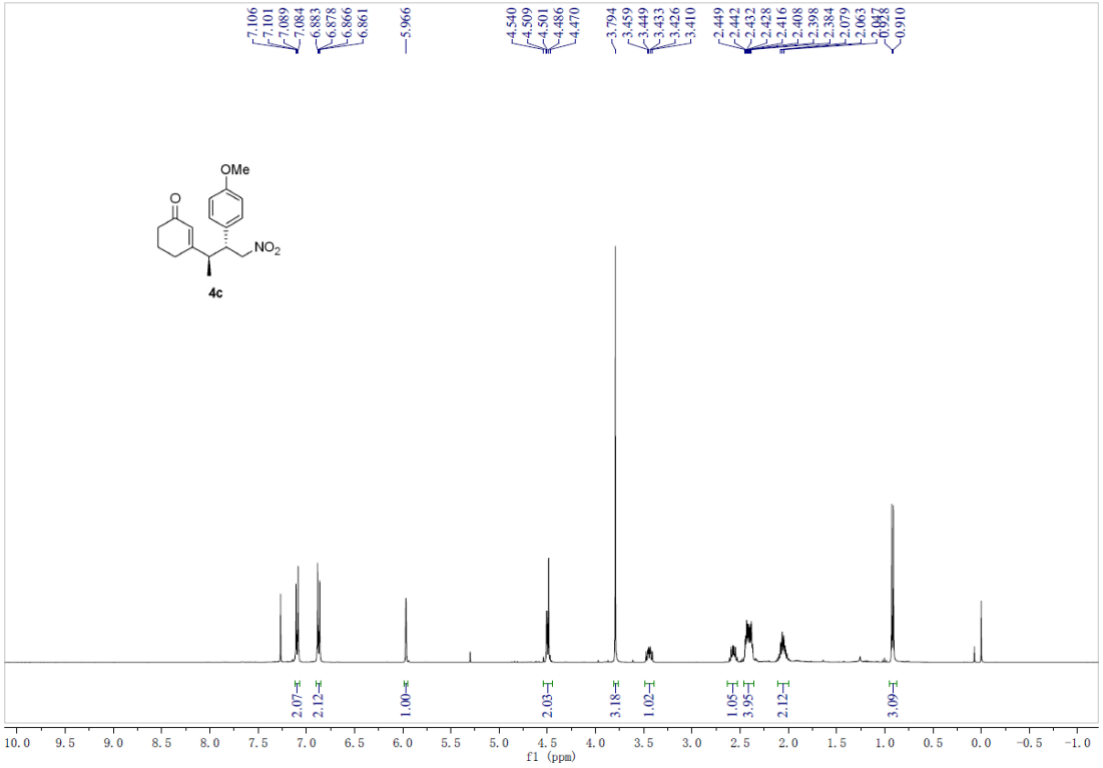


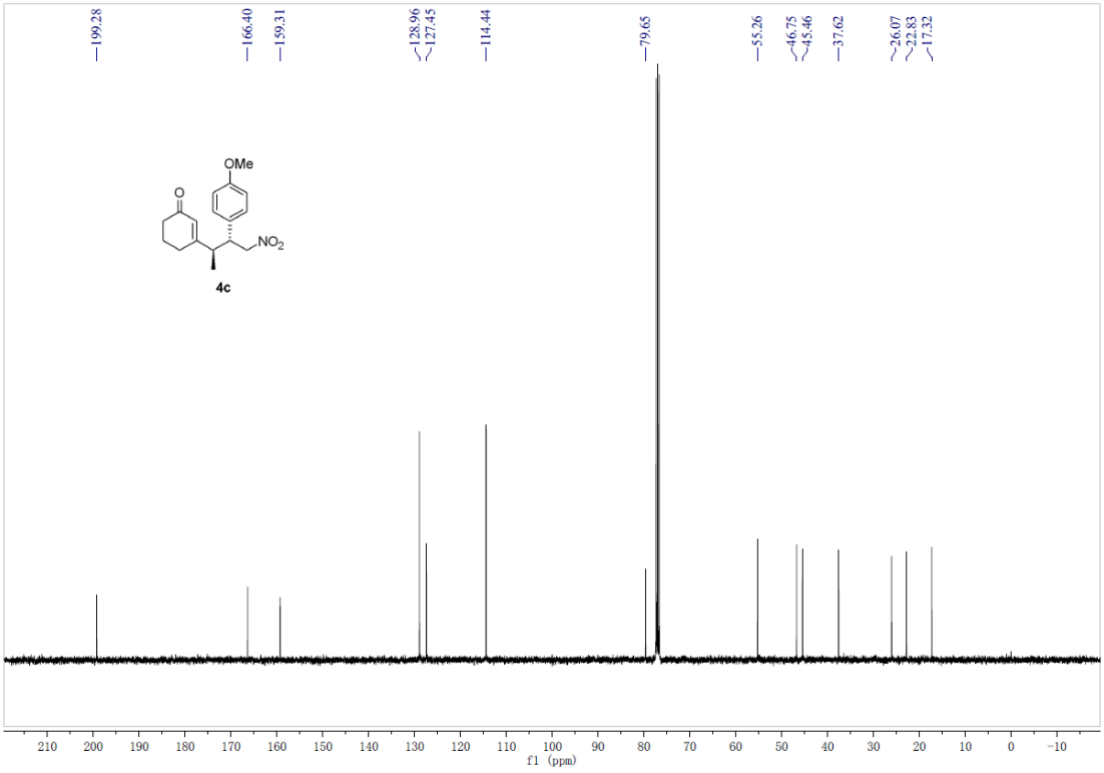
4b: 3-((2*R*,3*R*)-4-nitro-3-(*p*-tolyl)butan-2-yl)cyclohex-2-en-1-one



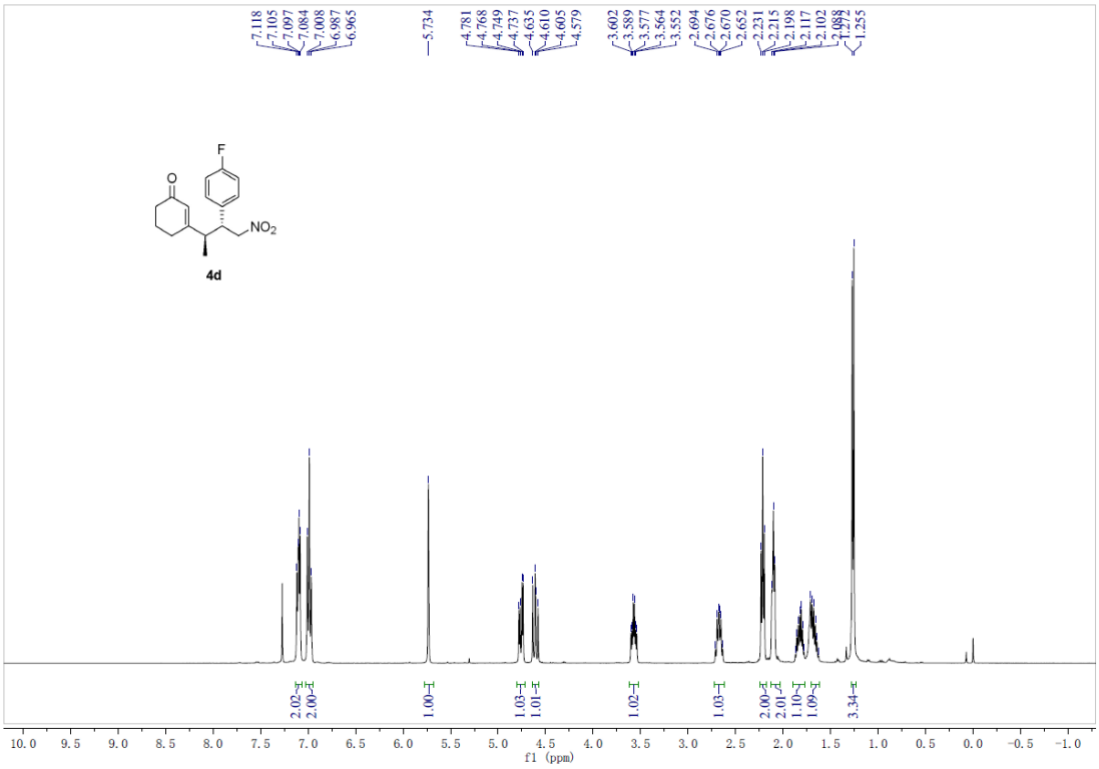


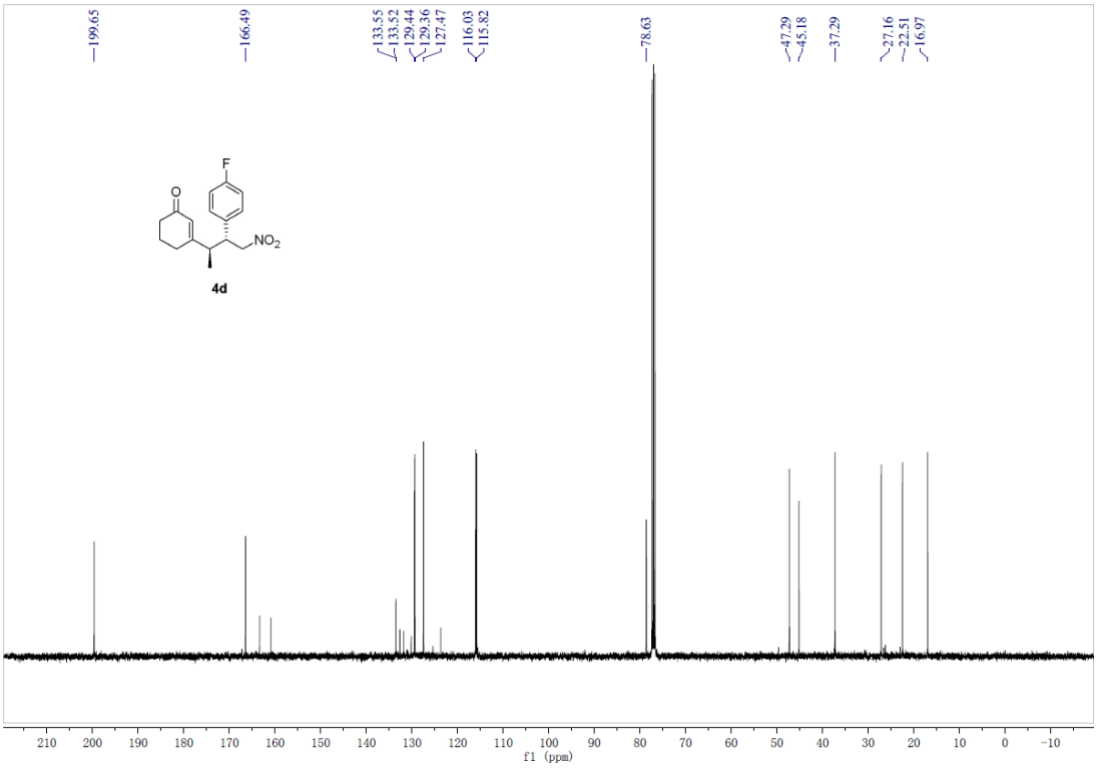
4c: 3-((2*R*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



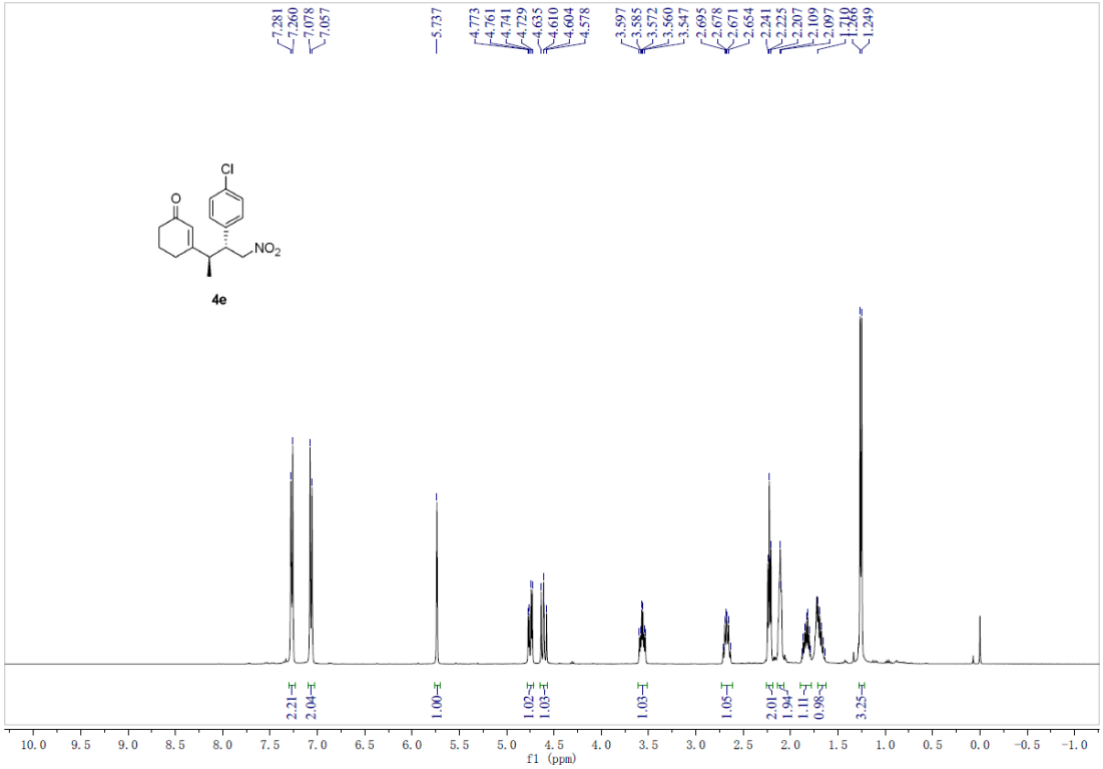


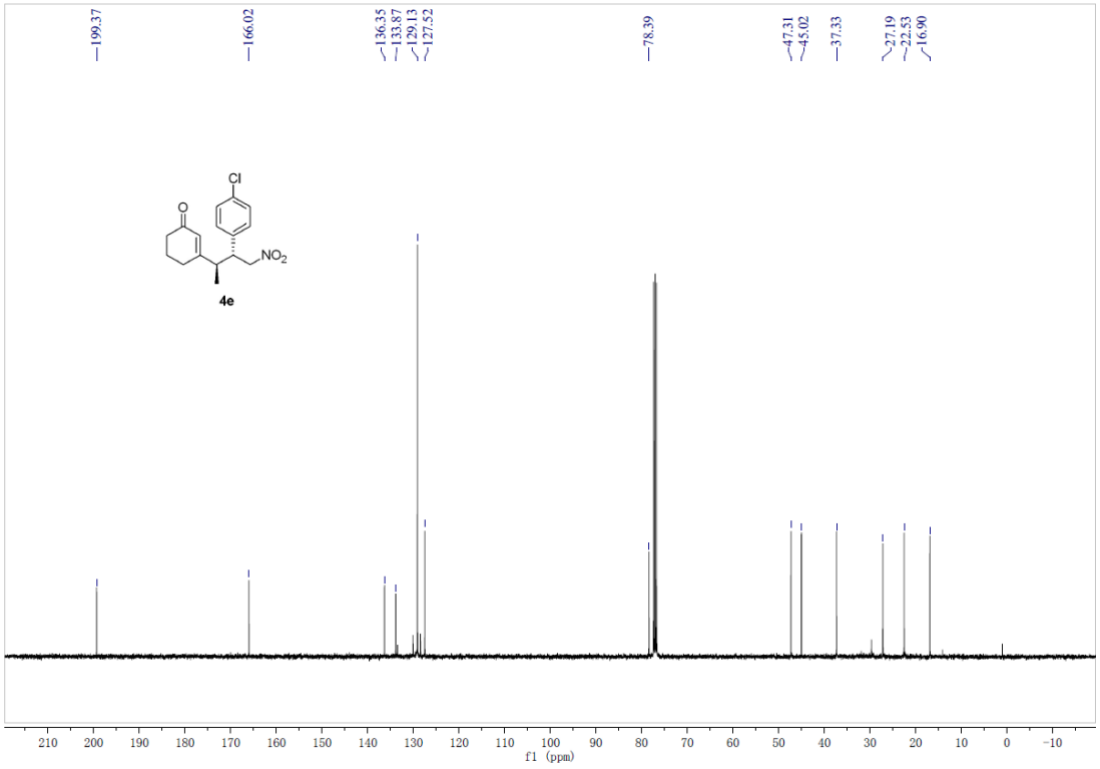
4d: 3-((2*R*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



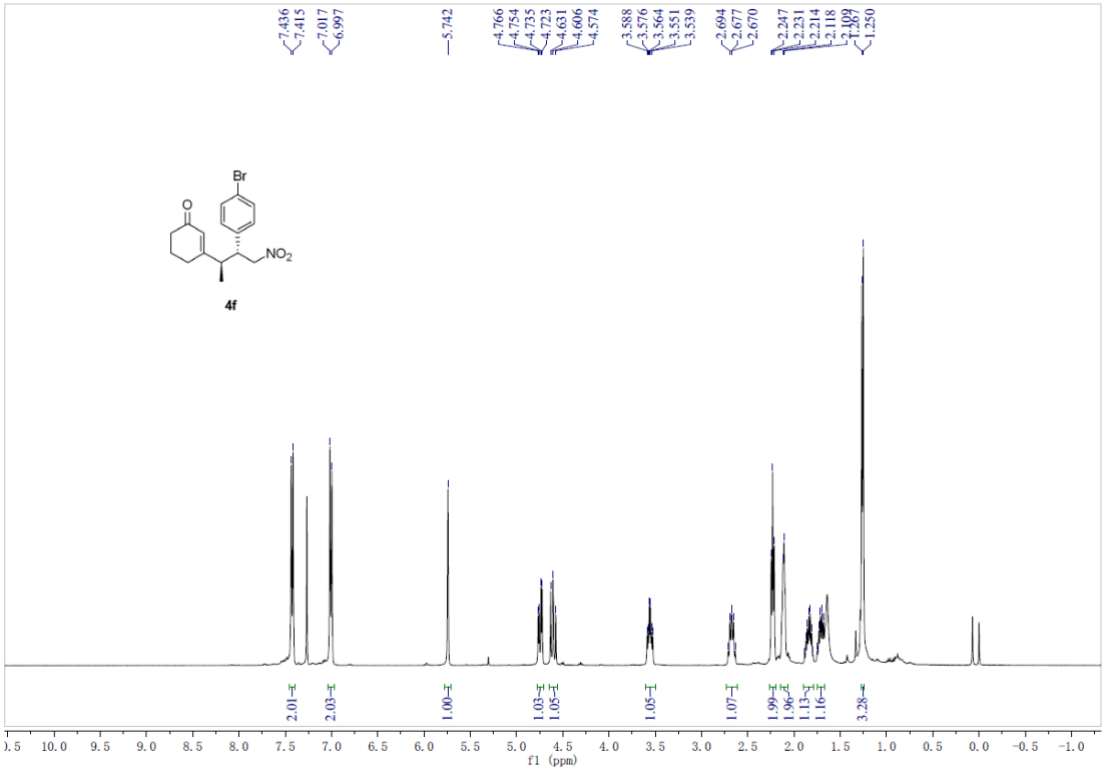


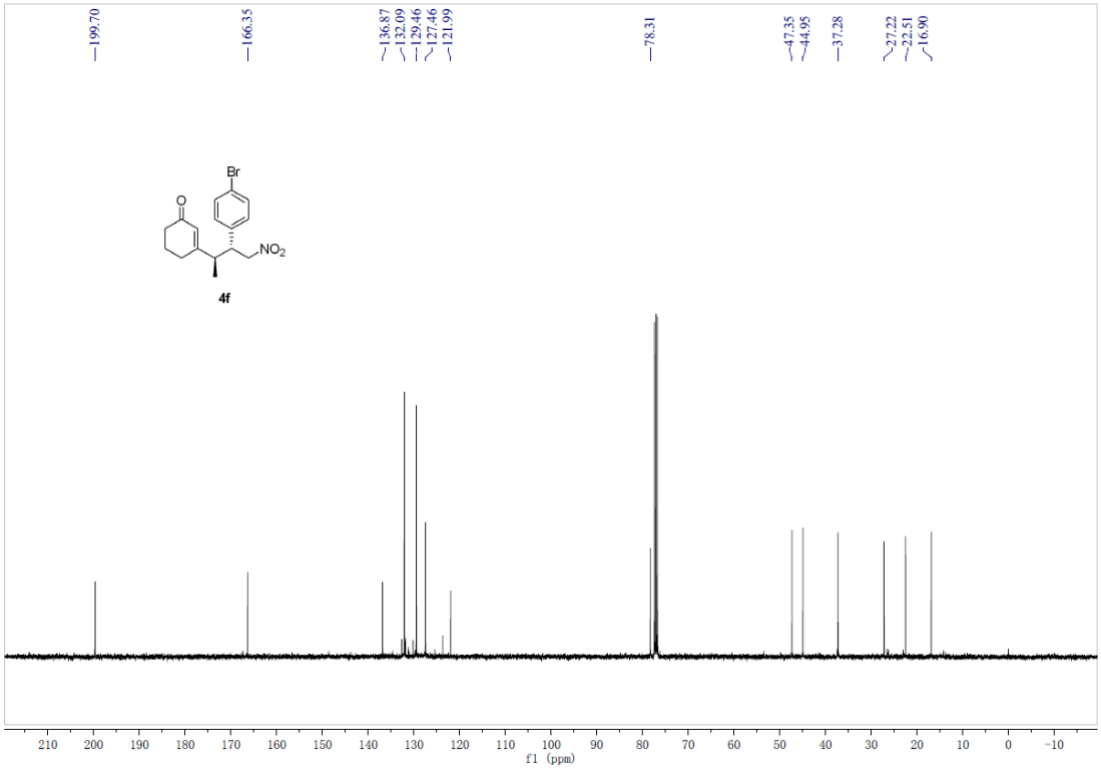
4e: 3-((2*R*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



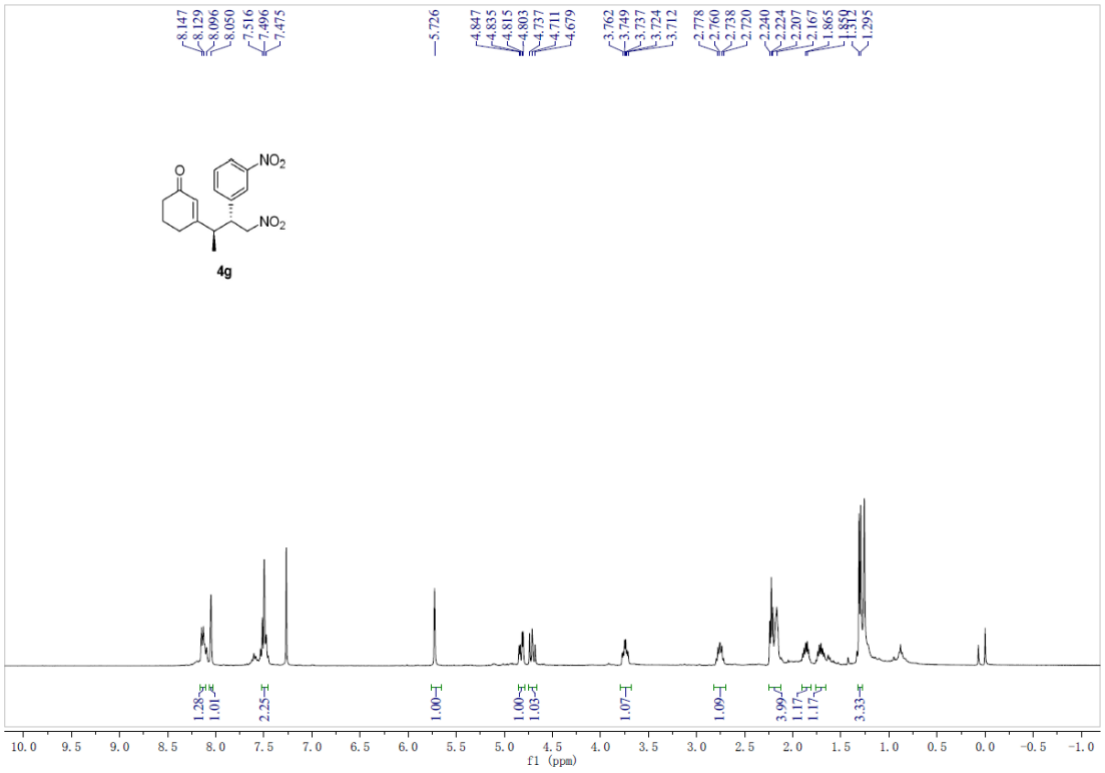


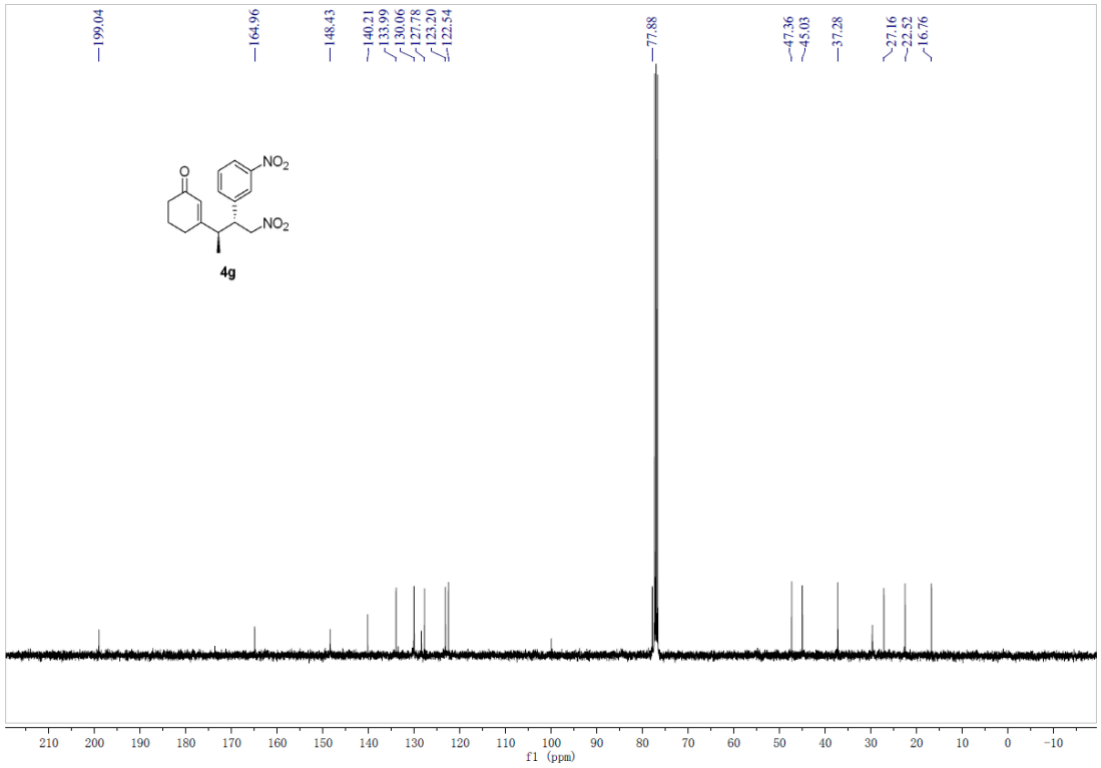
4f: 3-((2*R*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



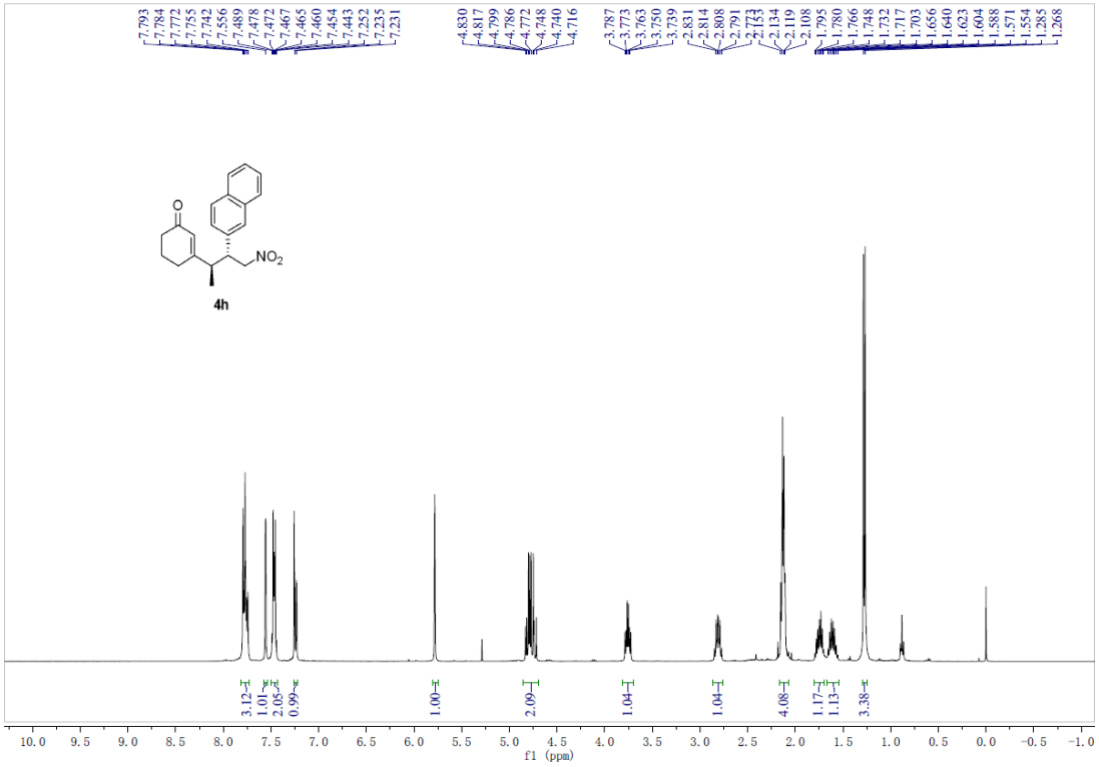


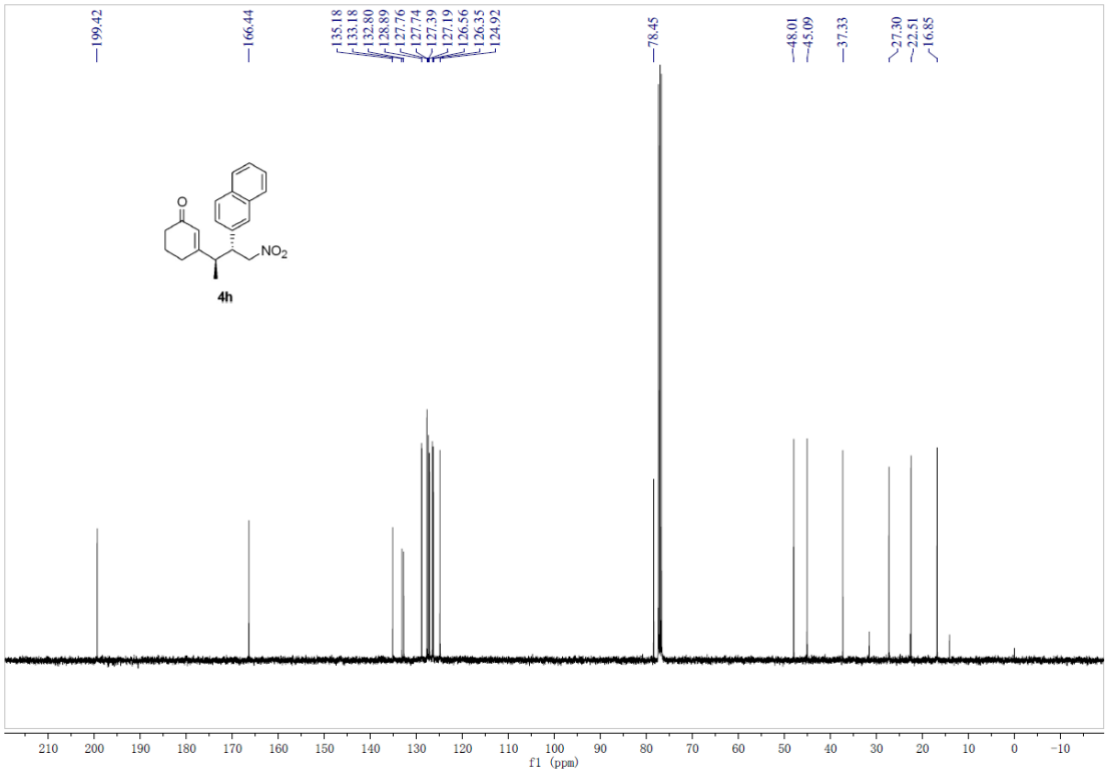
4g: 3-((2*R*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one



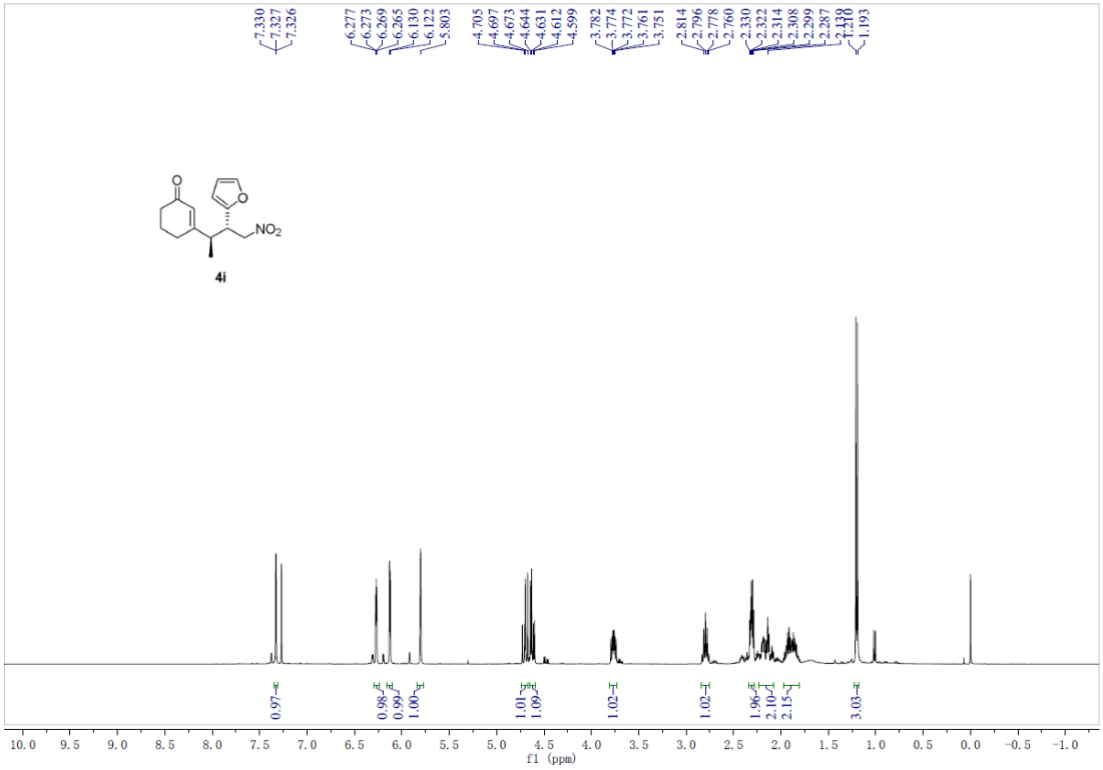


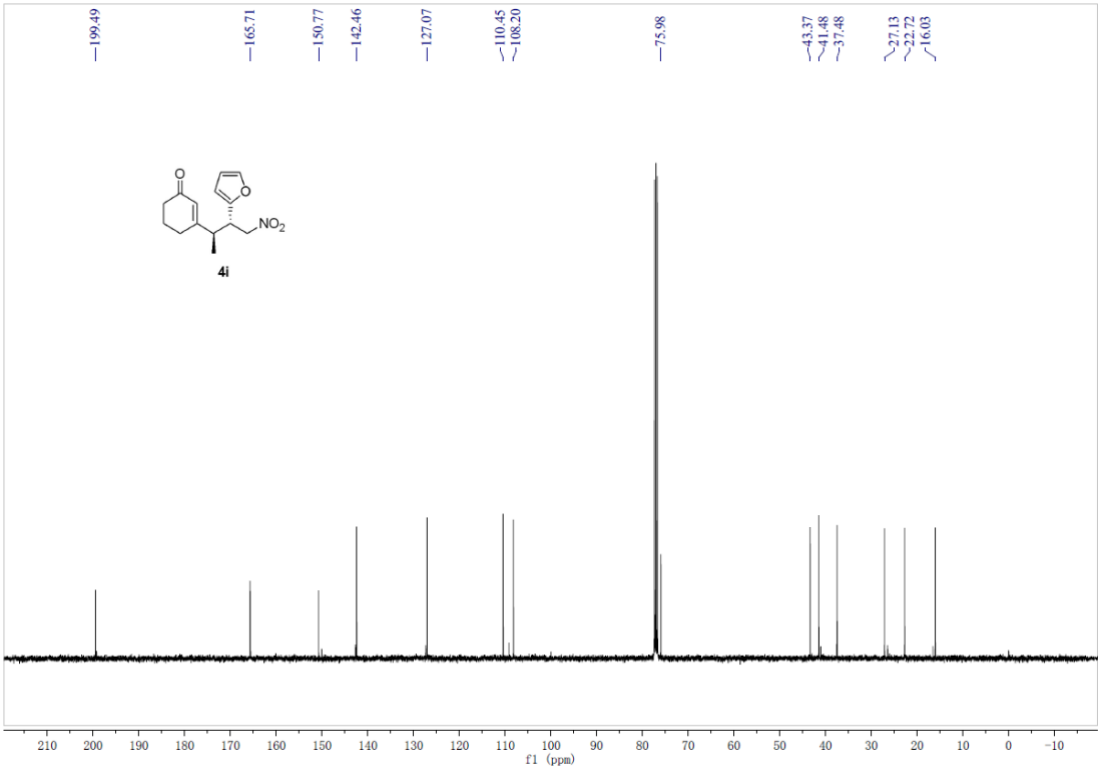
4h: 3-((2*R*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



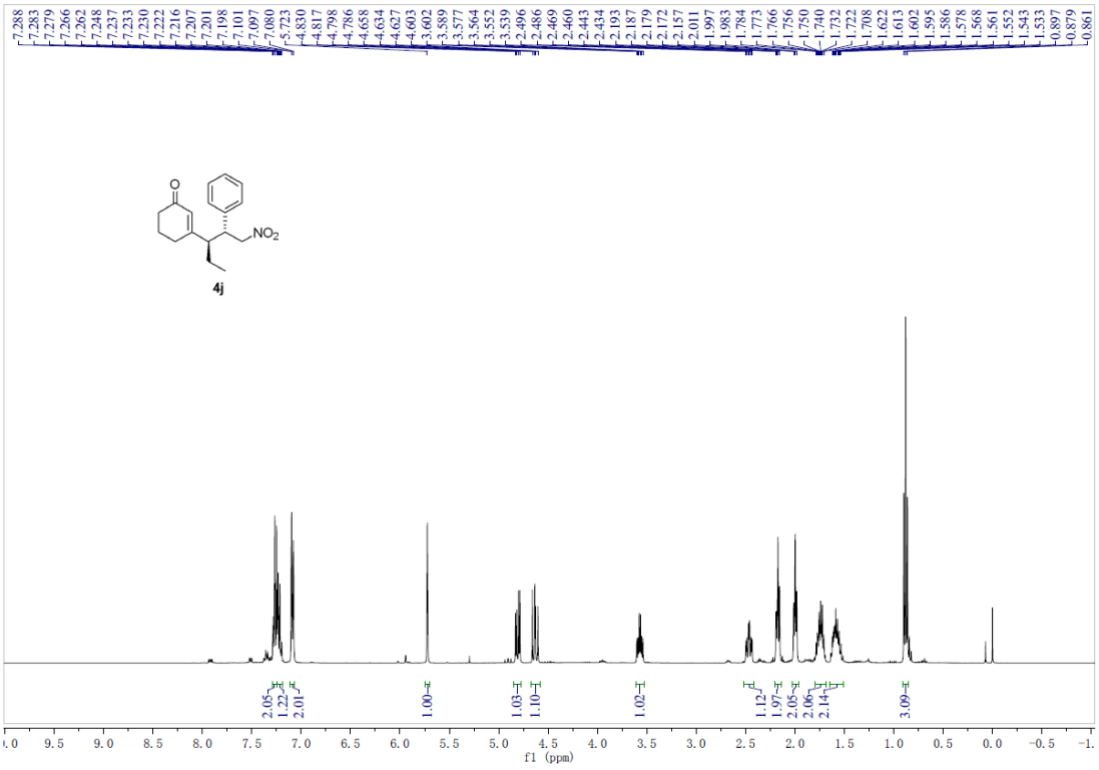


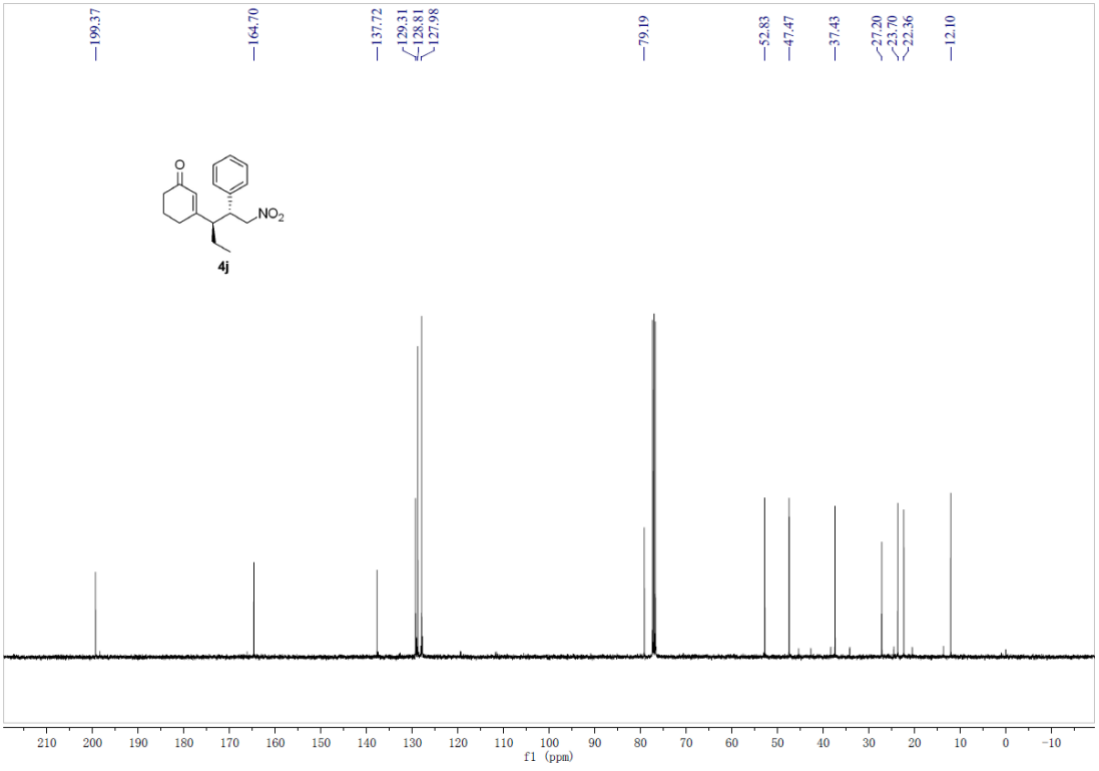
4i: 3-((2*R*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



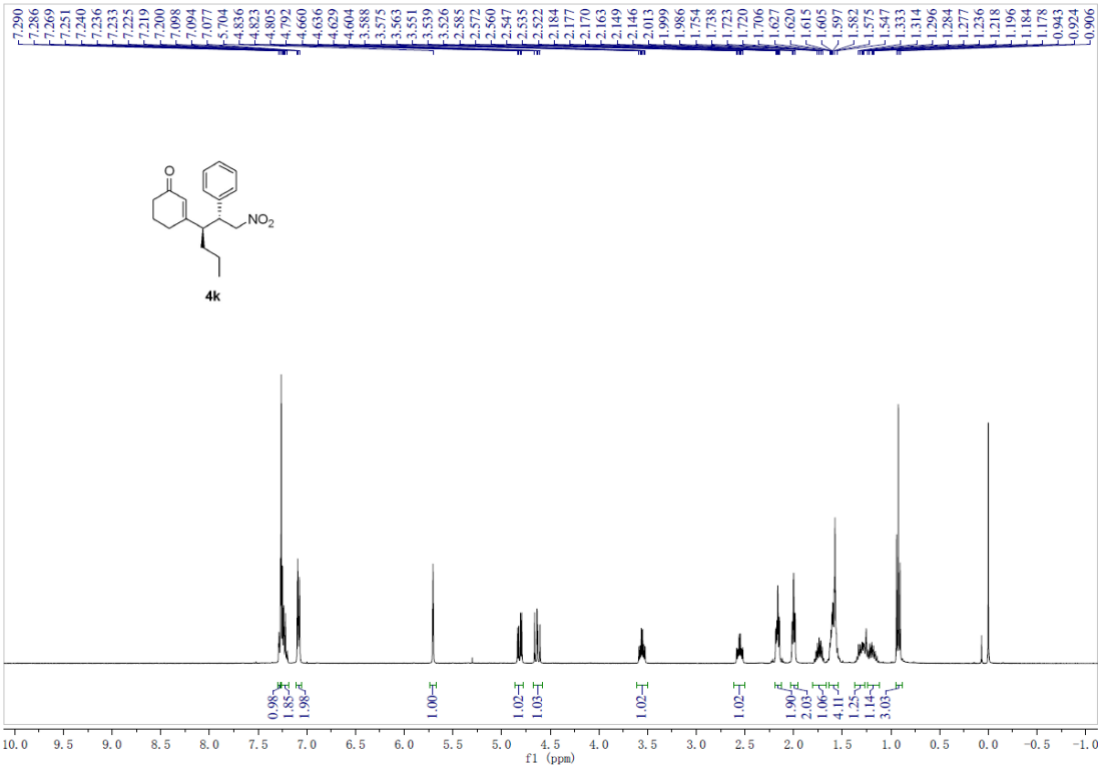


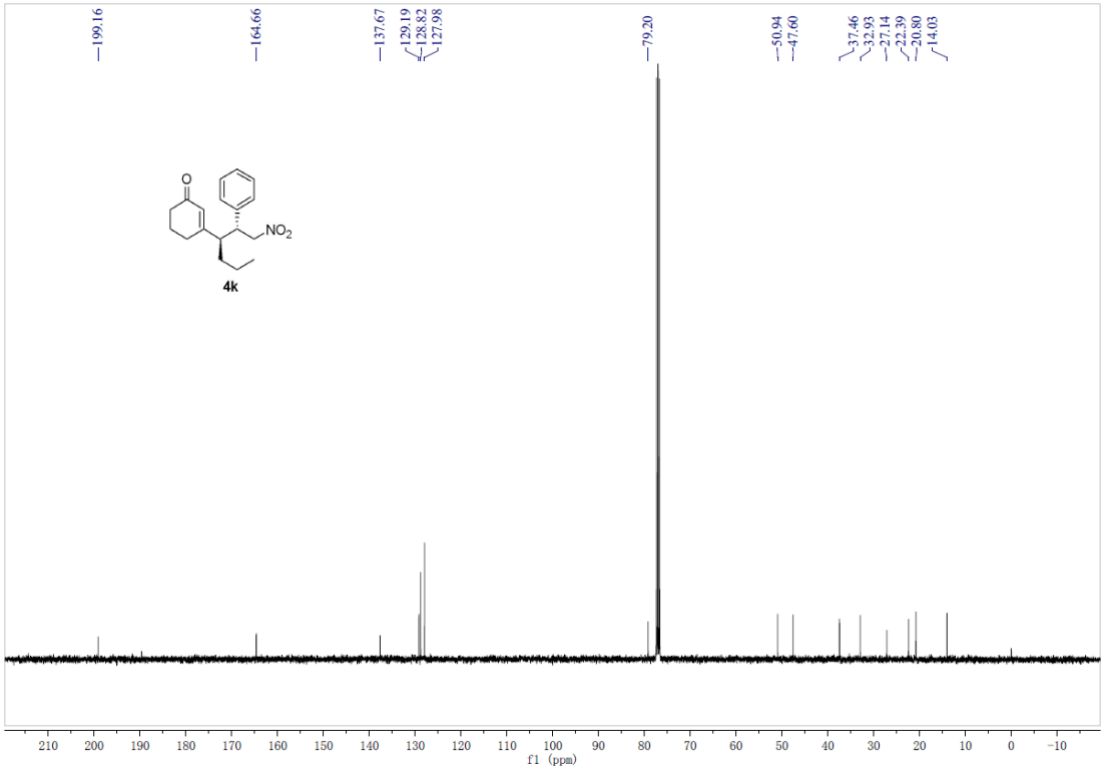
4j:3-((2*R*,3*R*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one



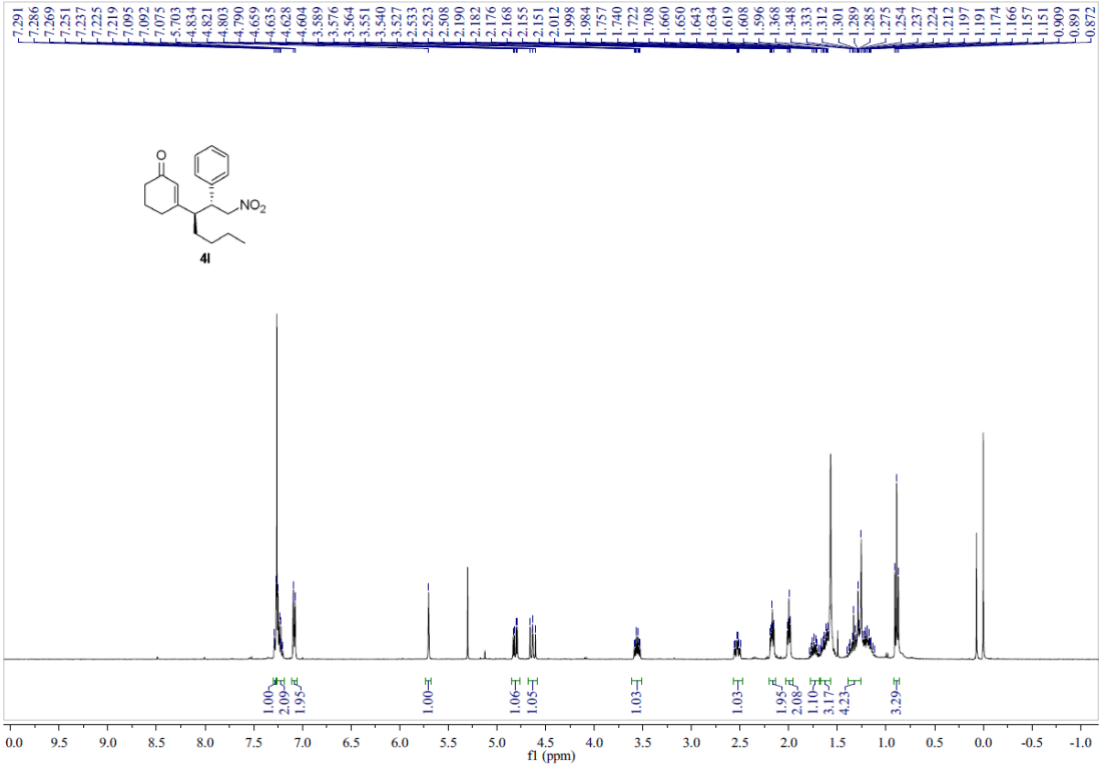


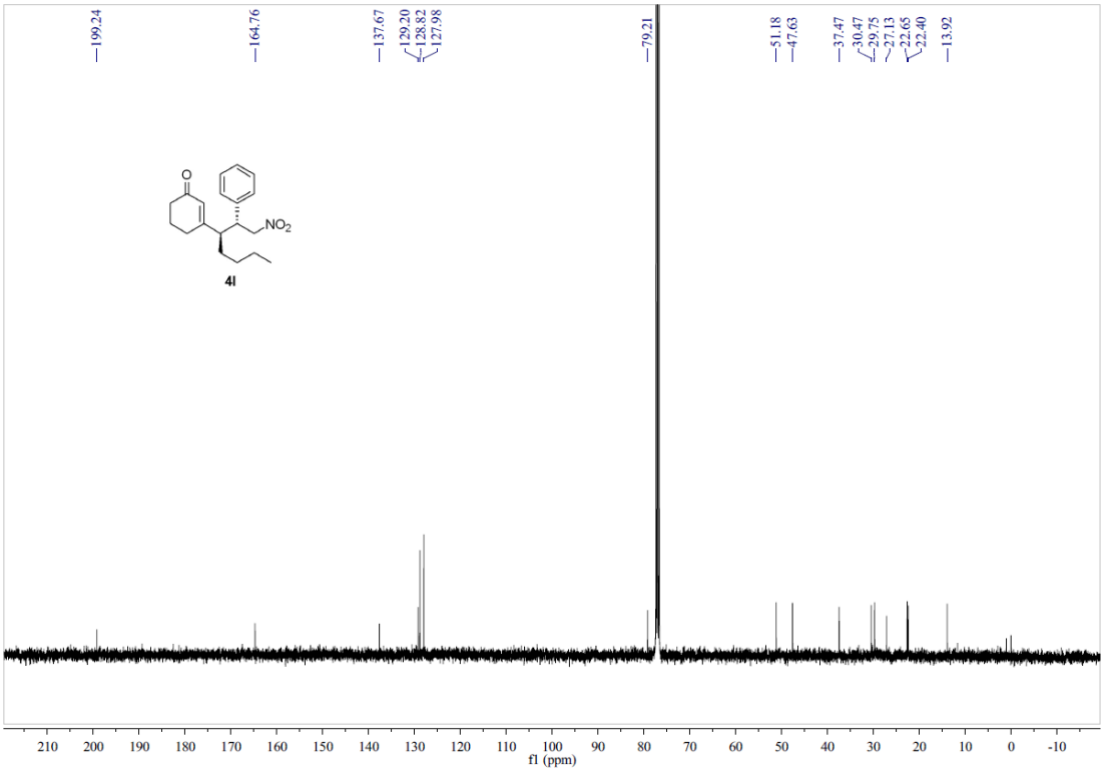
4k: 3-((2*R*,3*R*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one



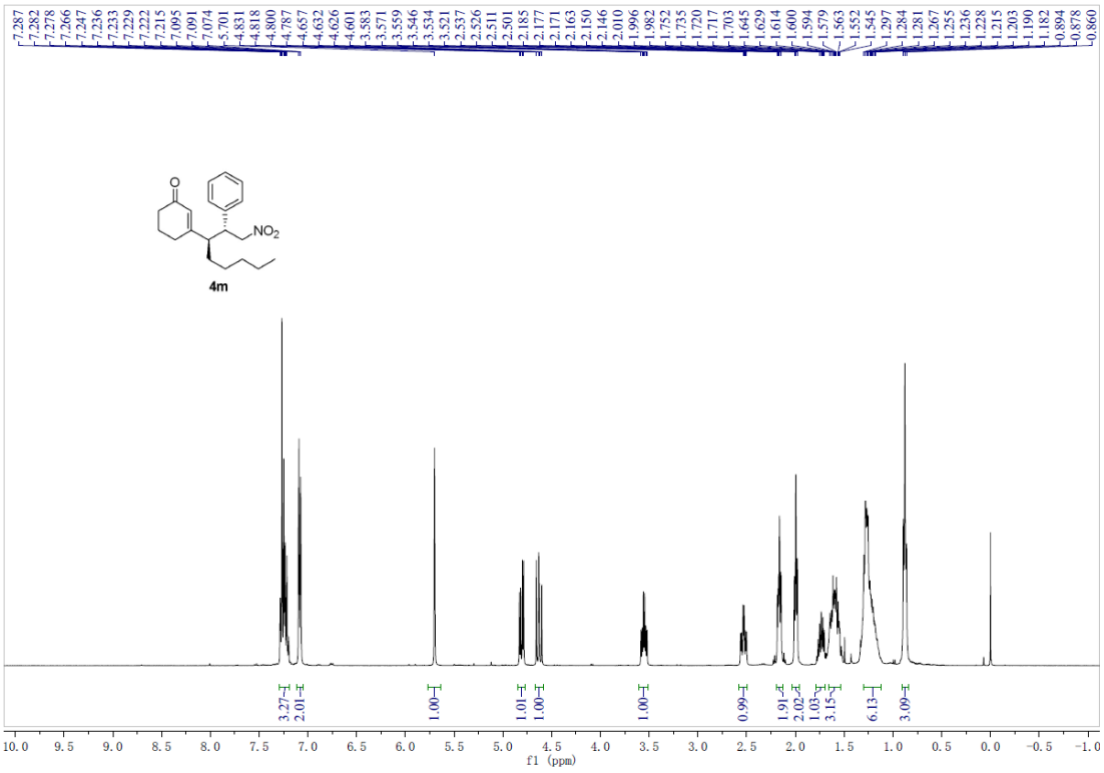


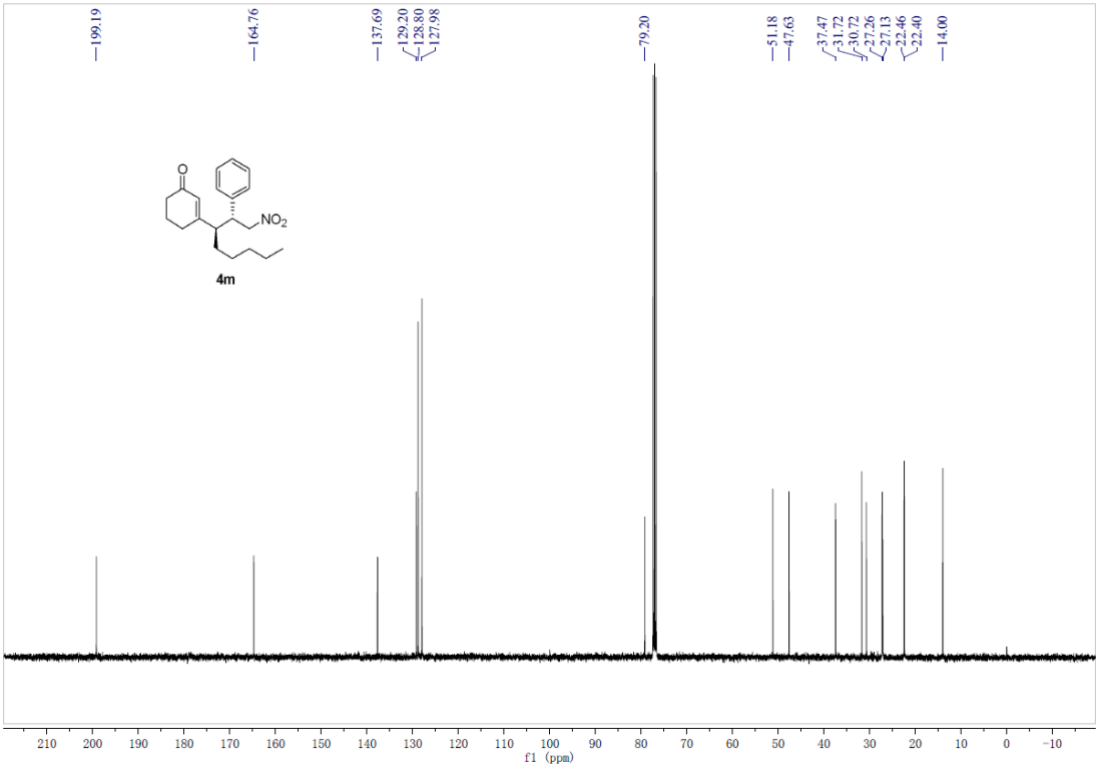
4l: 3-((2*R*,3*R*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one



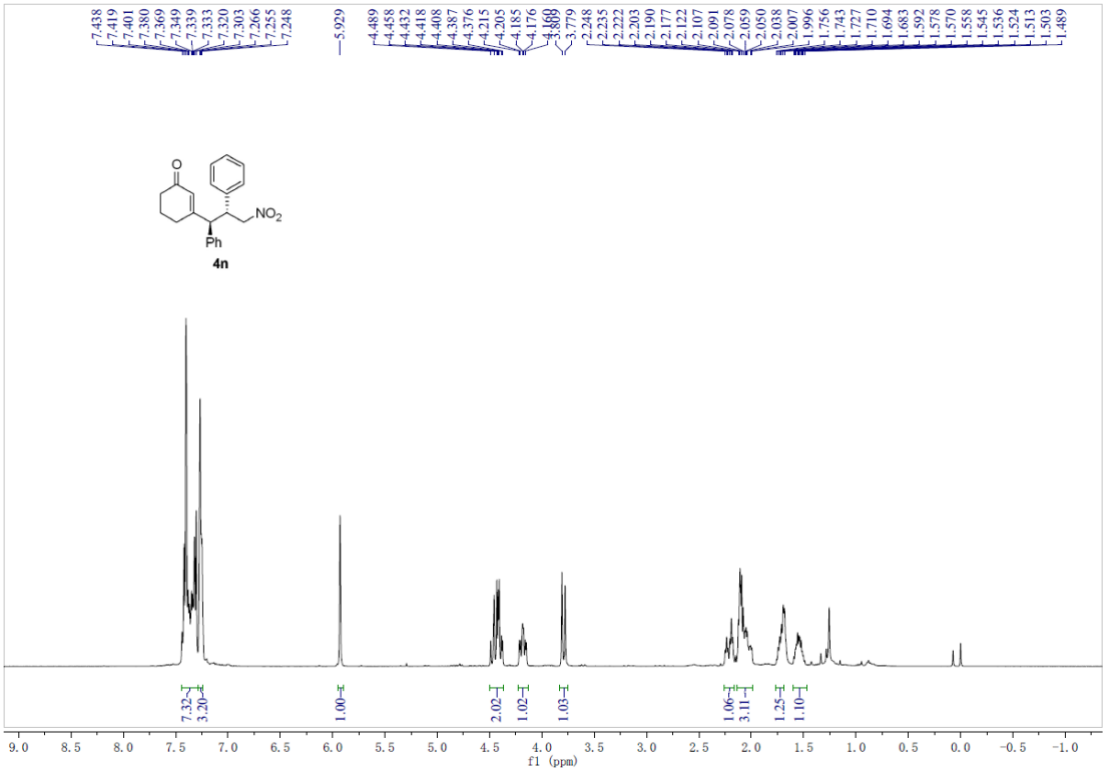


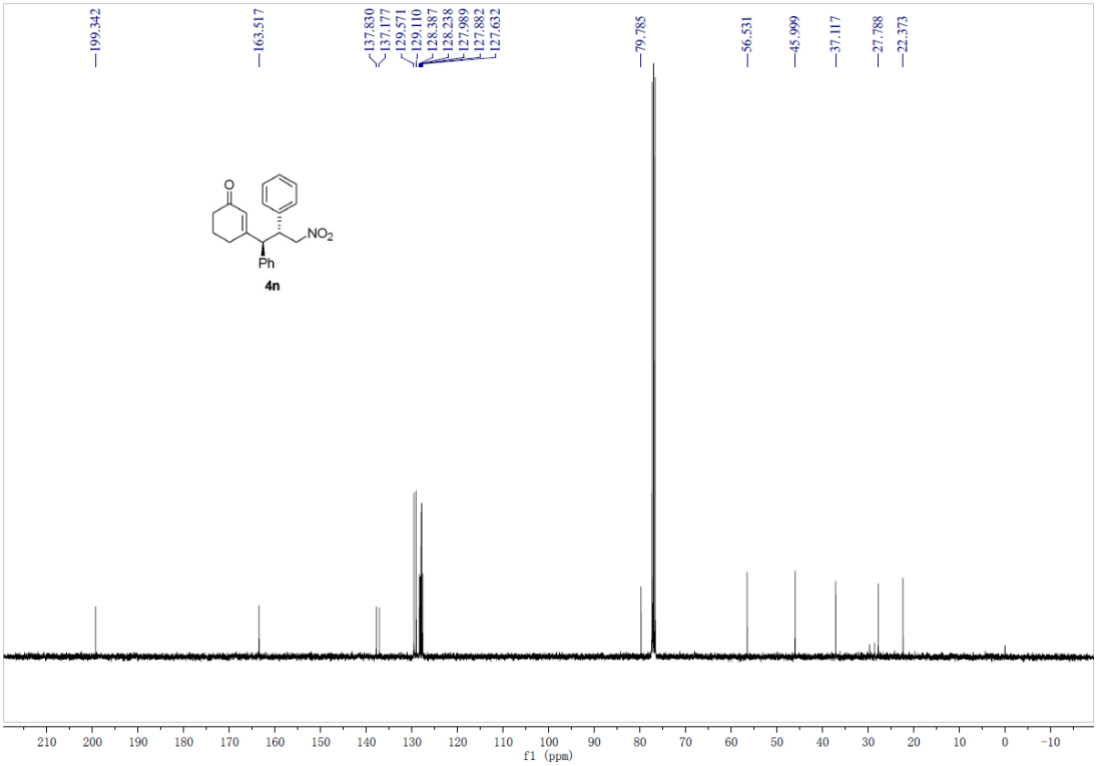
4m: 3-((2*R*,3*R*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one



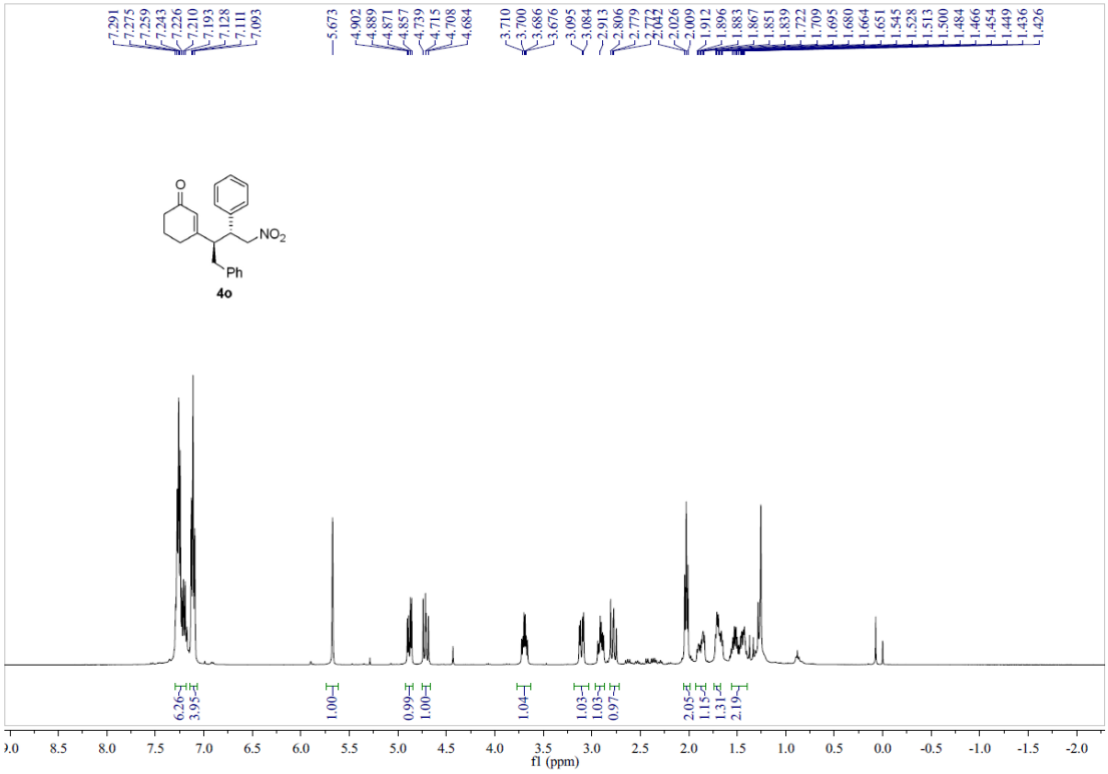


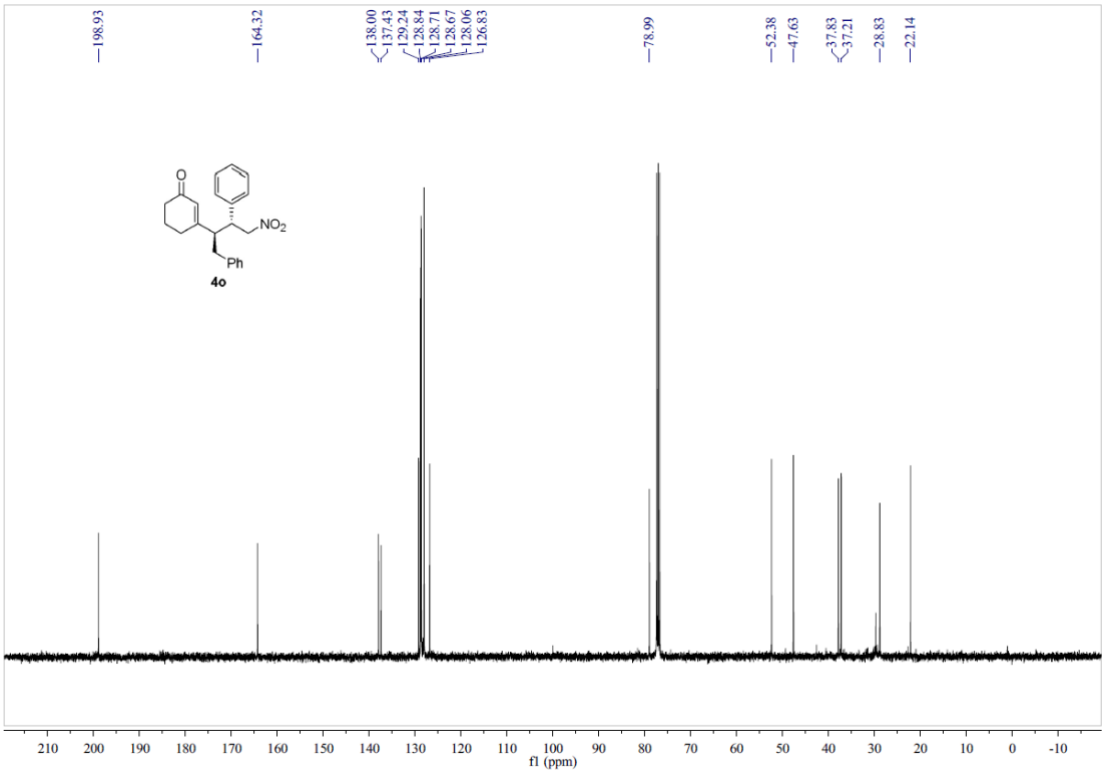
4n: 3-((1*R*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one



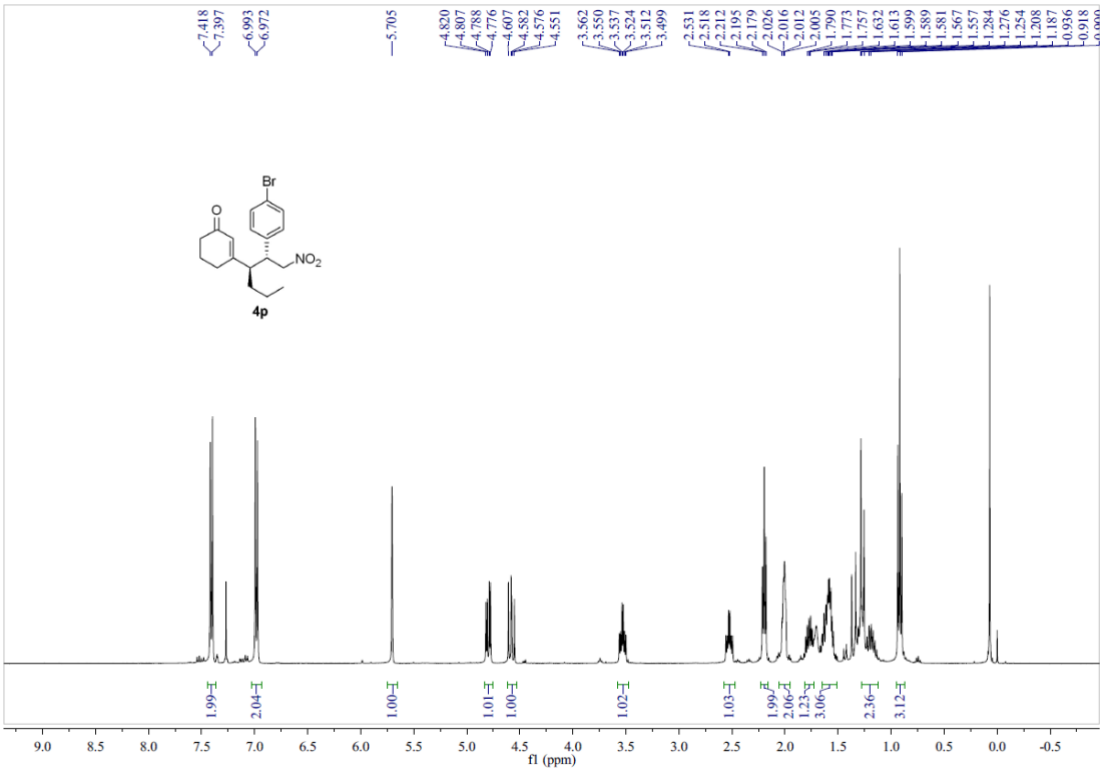


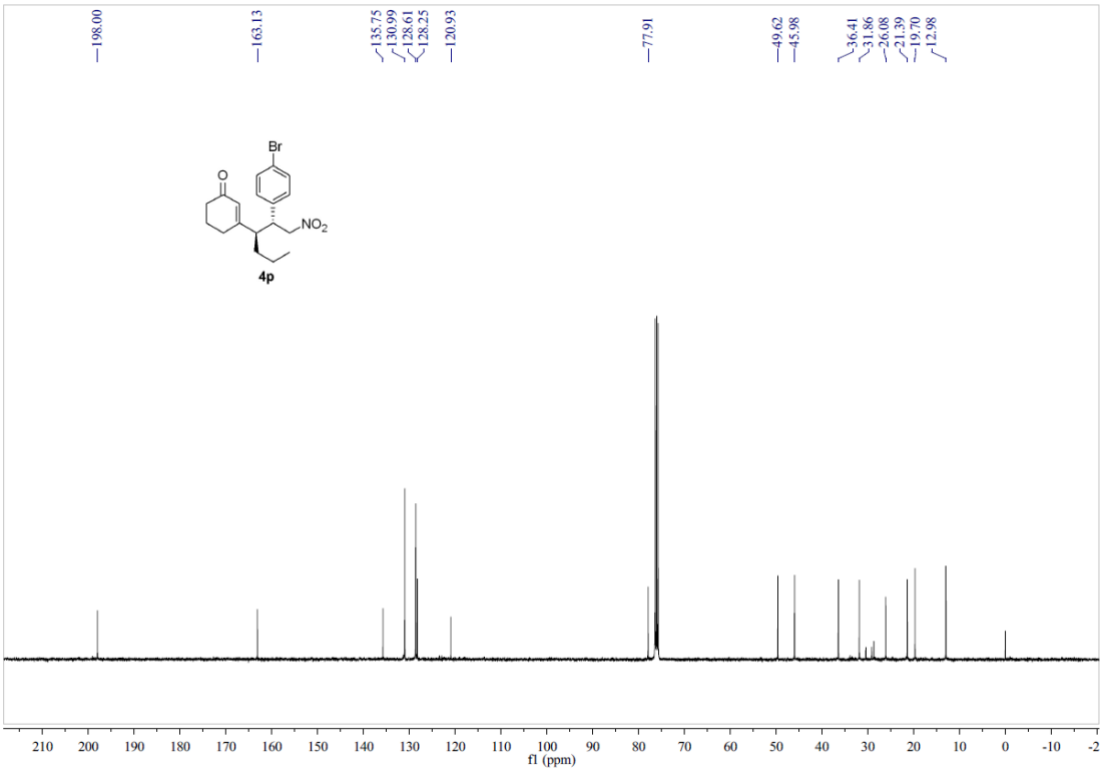
4o: 3-((2*R*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one



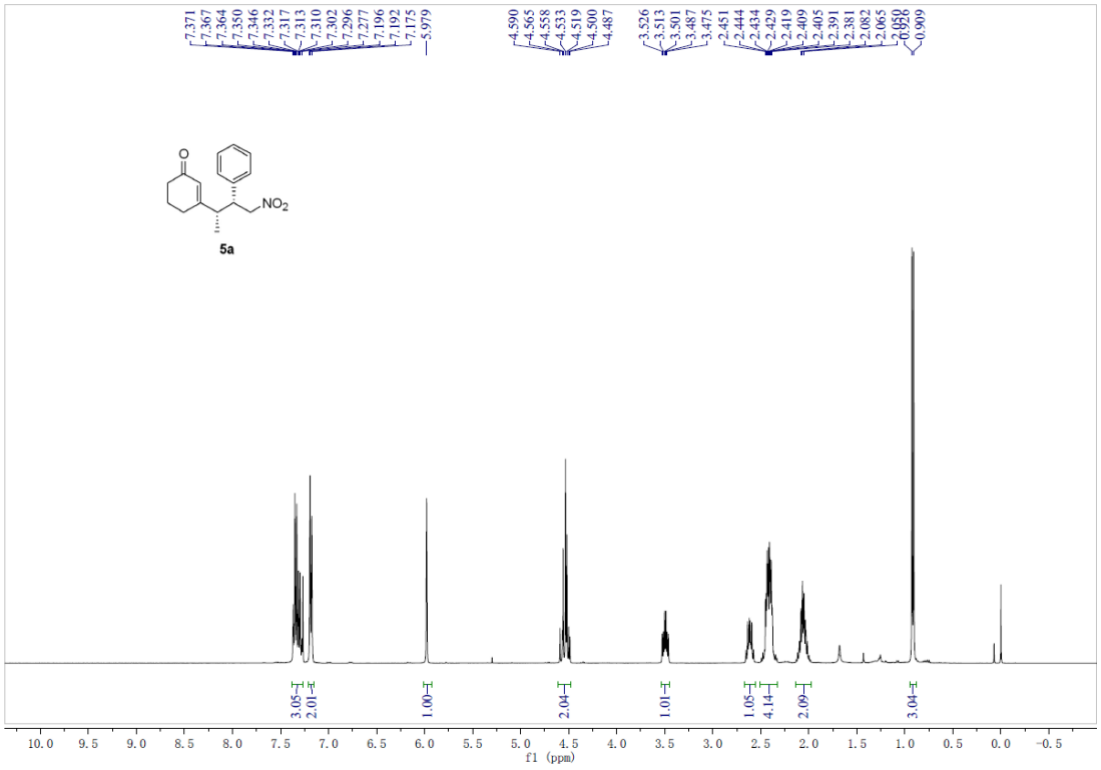


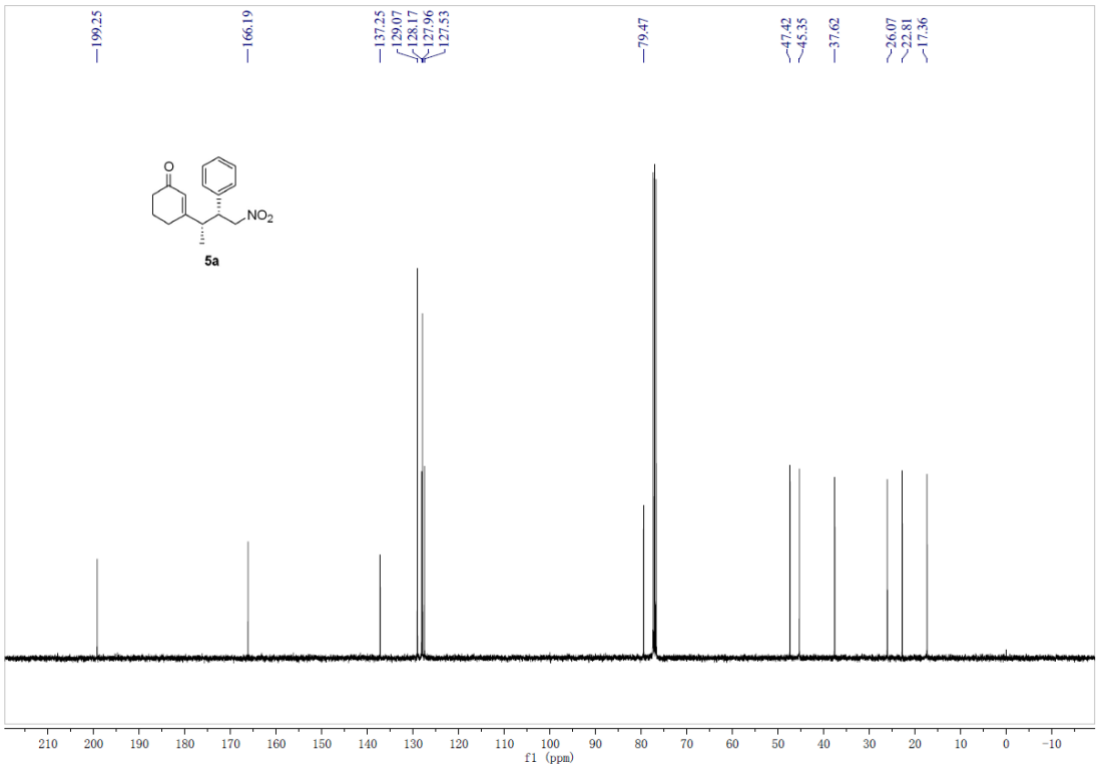
4p: 3-((2*R*,3*R*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one



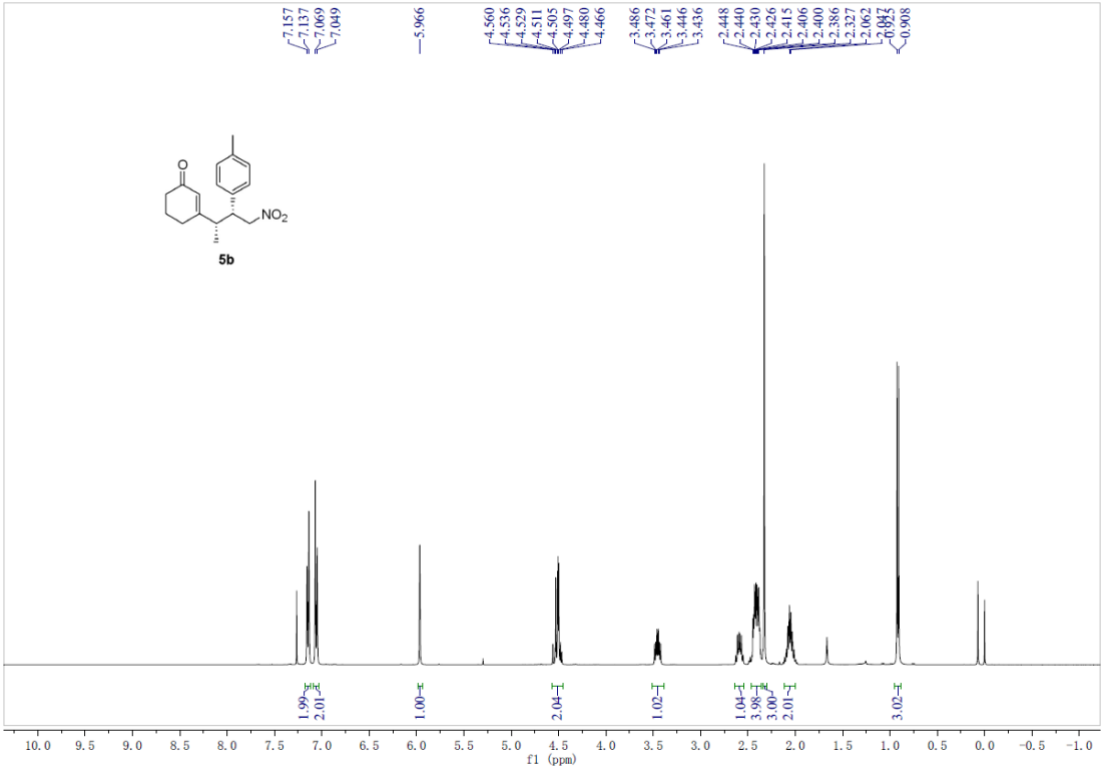


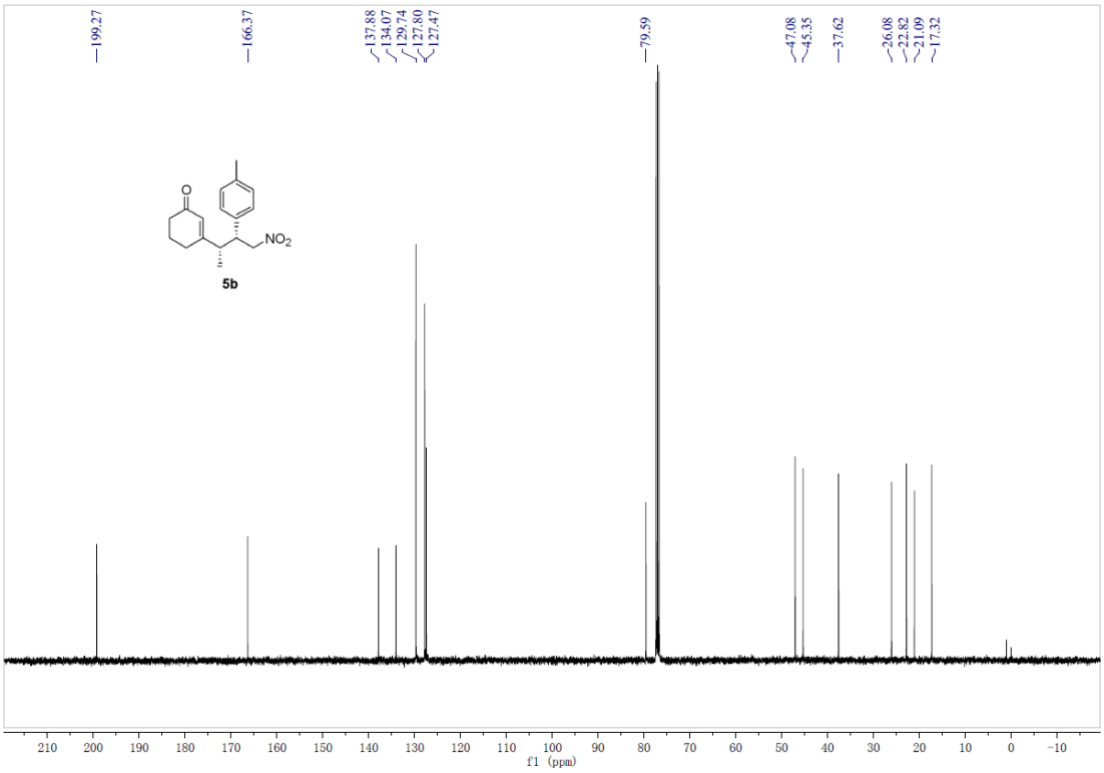
5a: 3-((2*S*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one



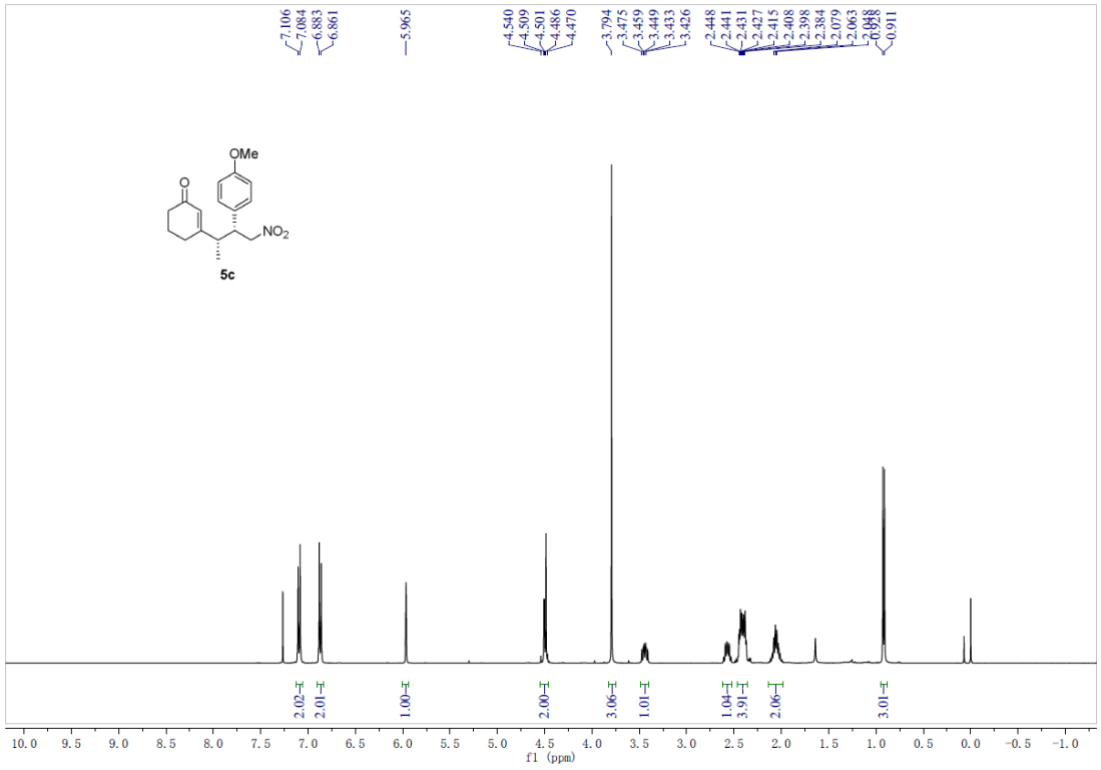


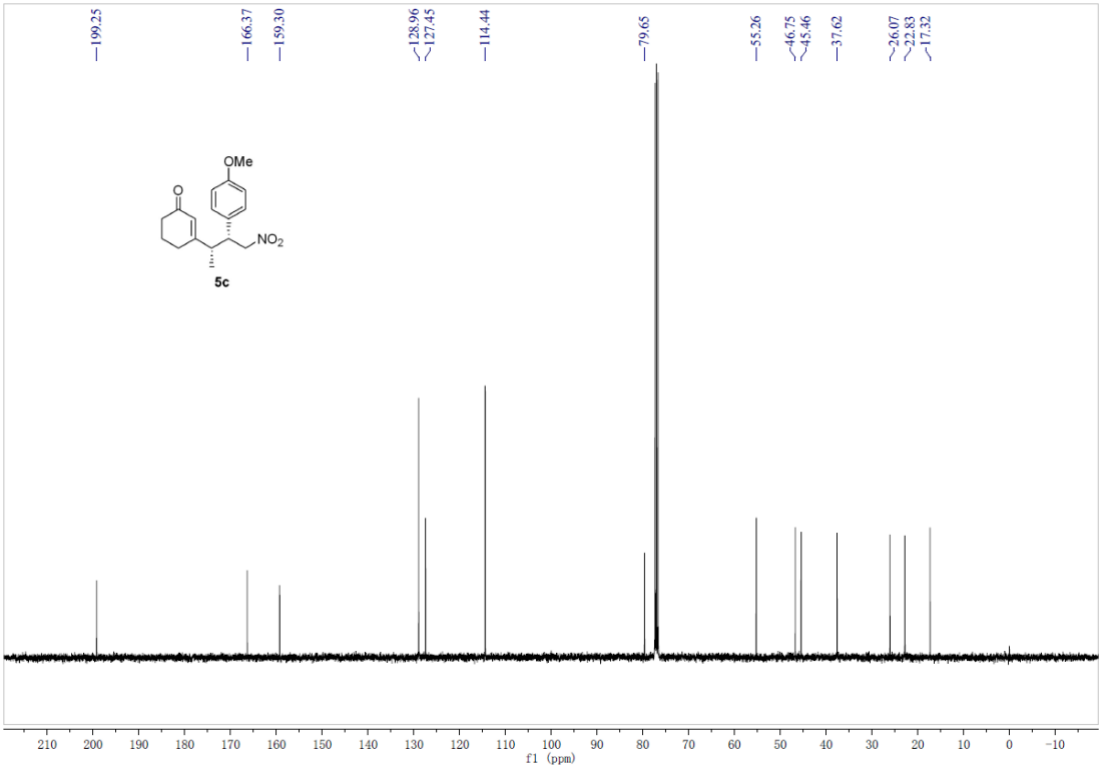
5b: 3-((2*S*,3*R*)-4-nitro-3-(*p*-tolyl)butan-2-yl)cyclohex-2-en-1-one



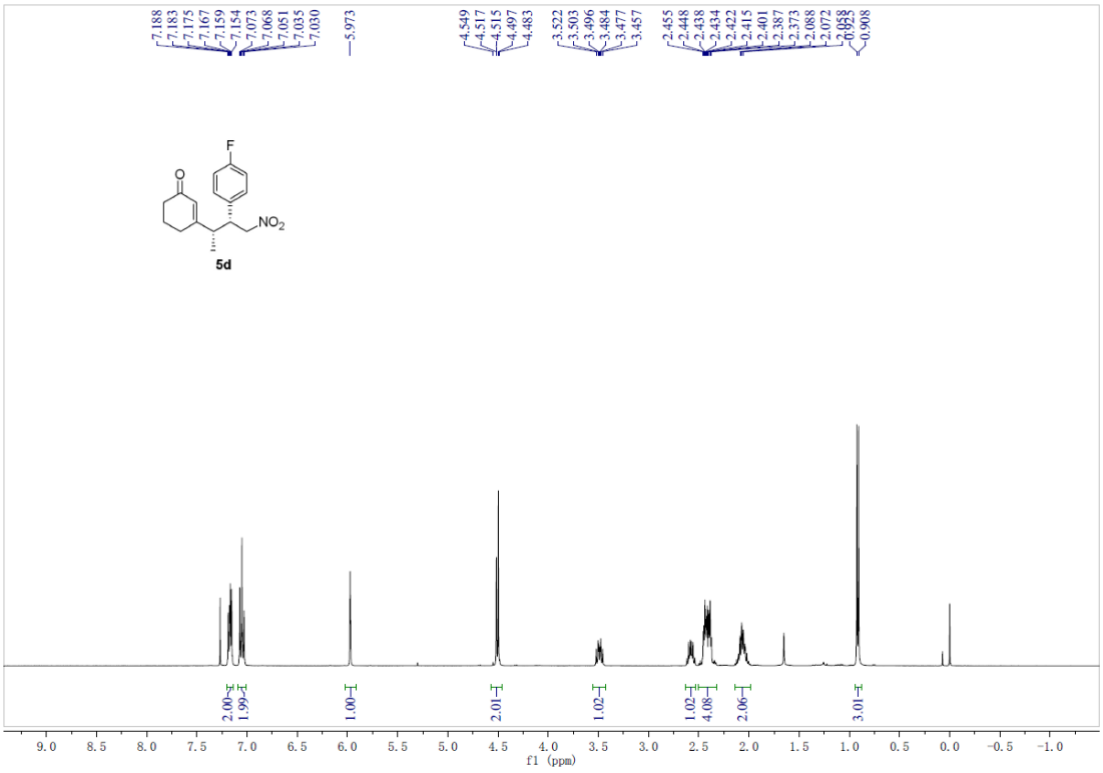


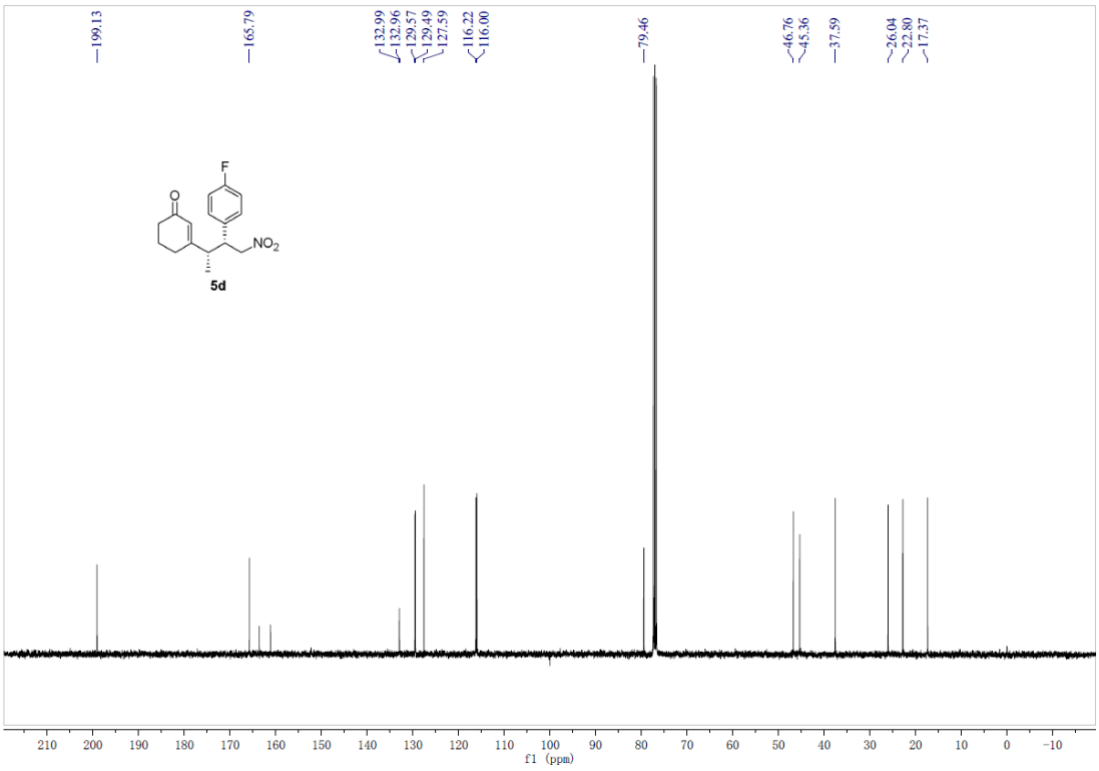
5c: 3-((2*S*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



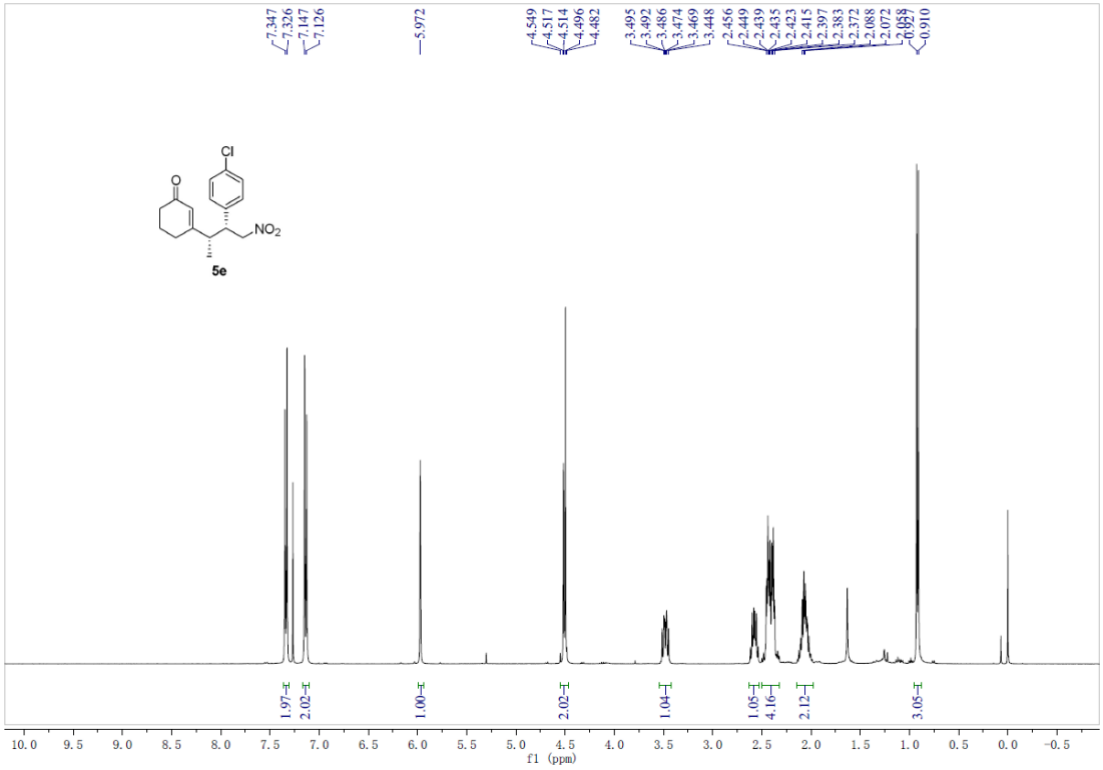


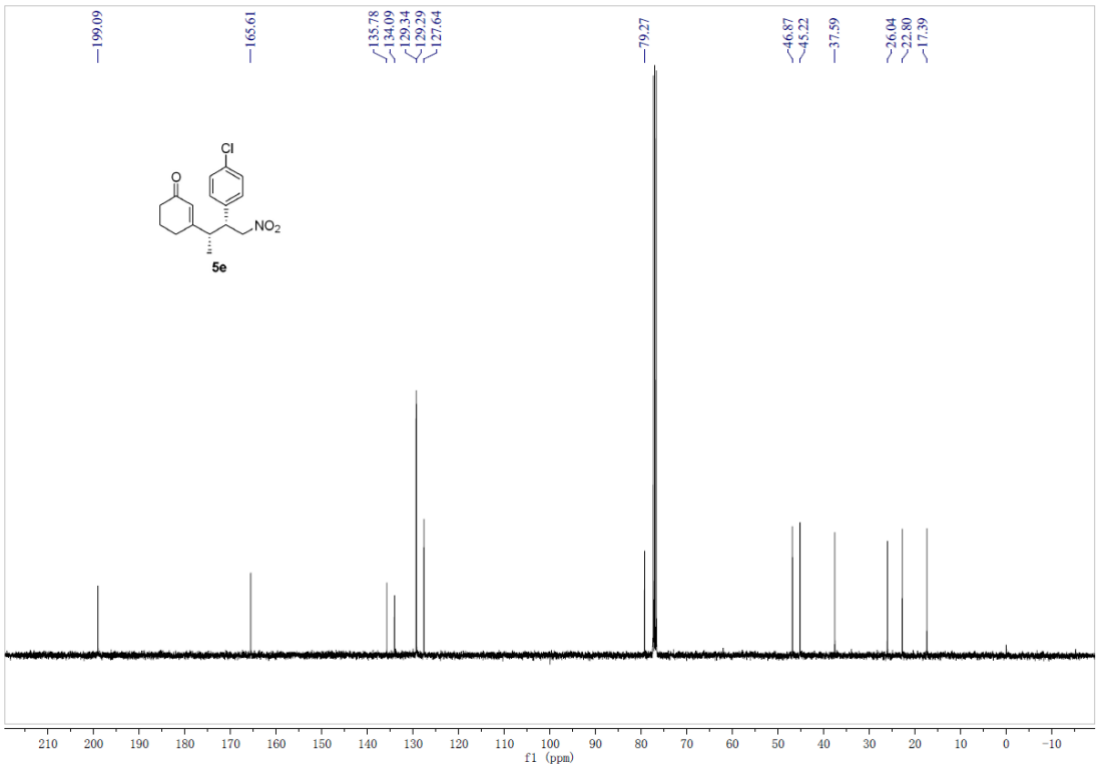
5d: 3-((2*S*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



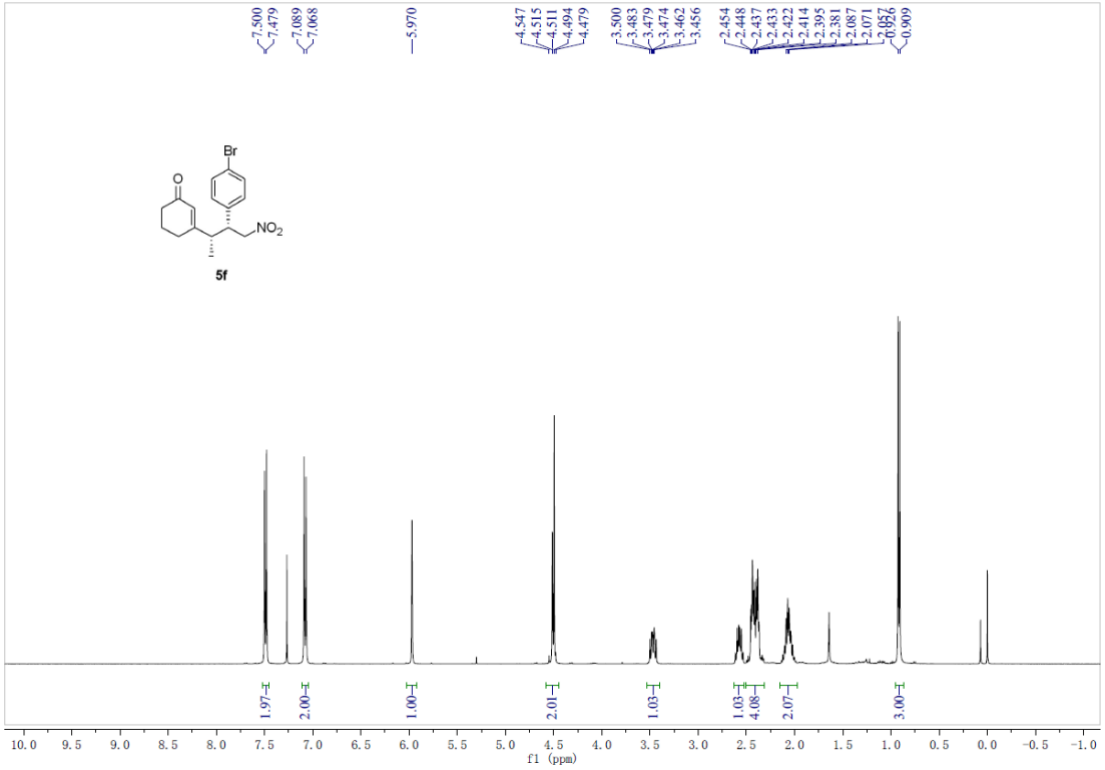


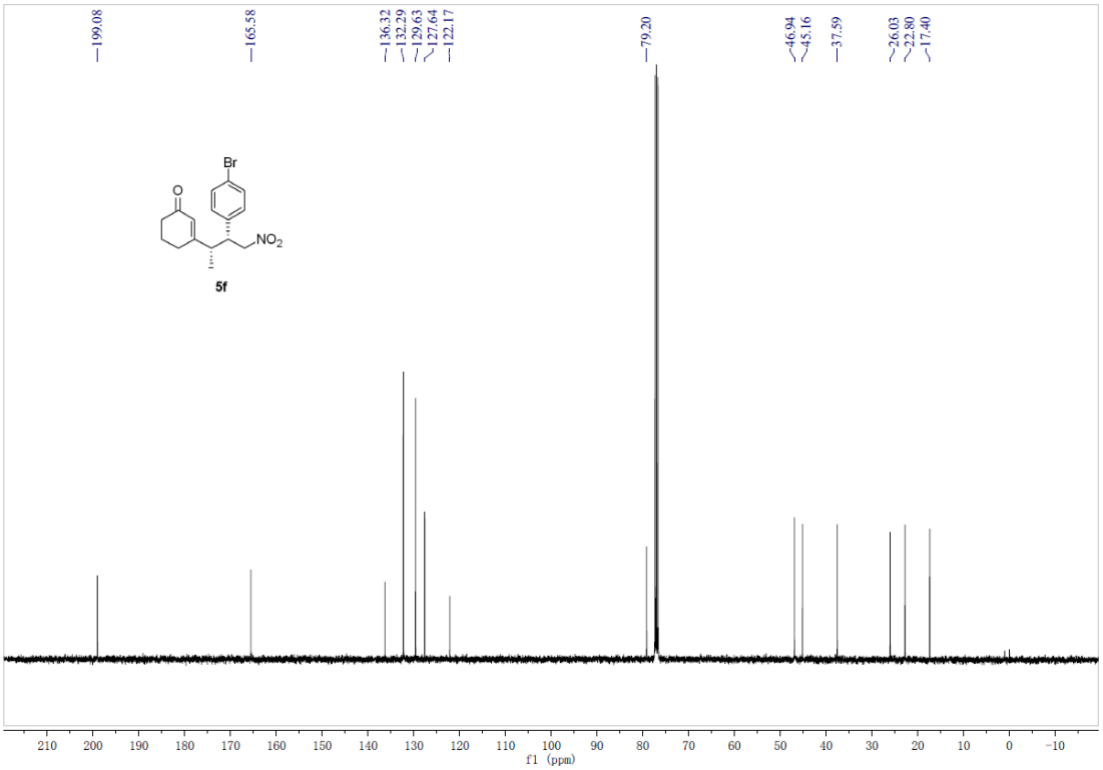
5e: 3-((2*S*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



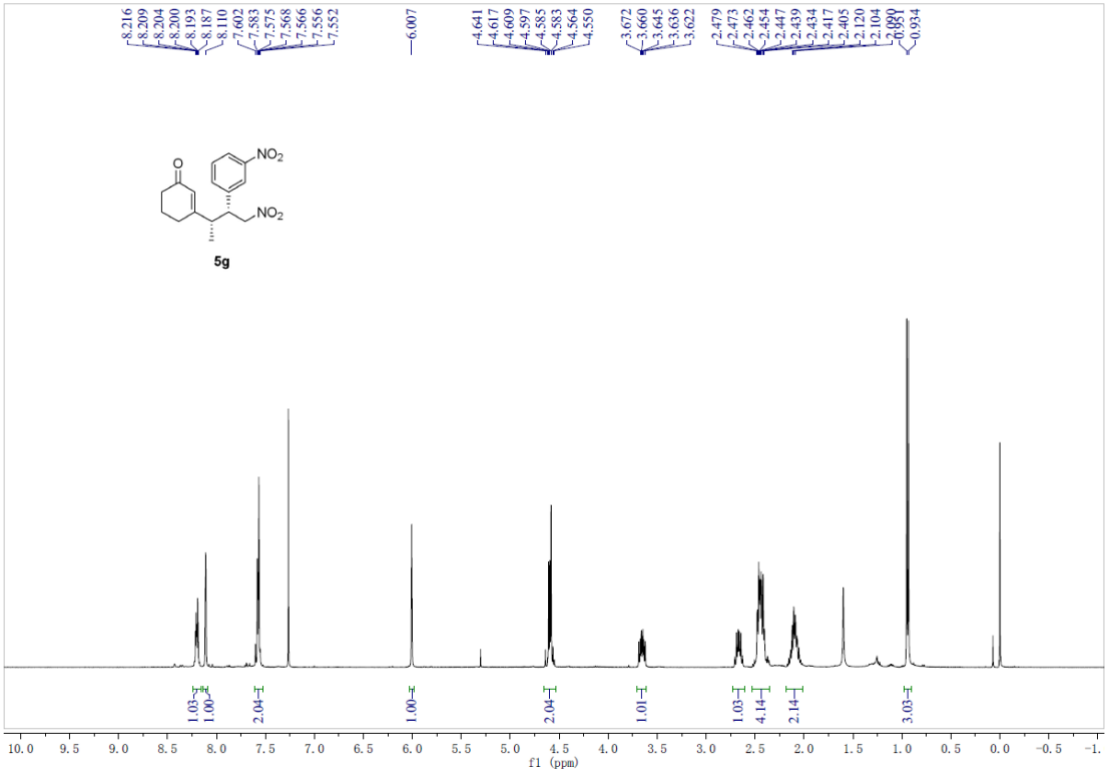


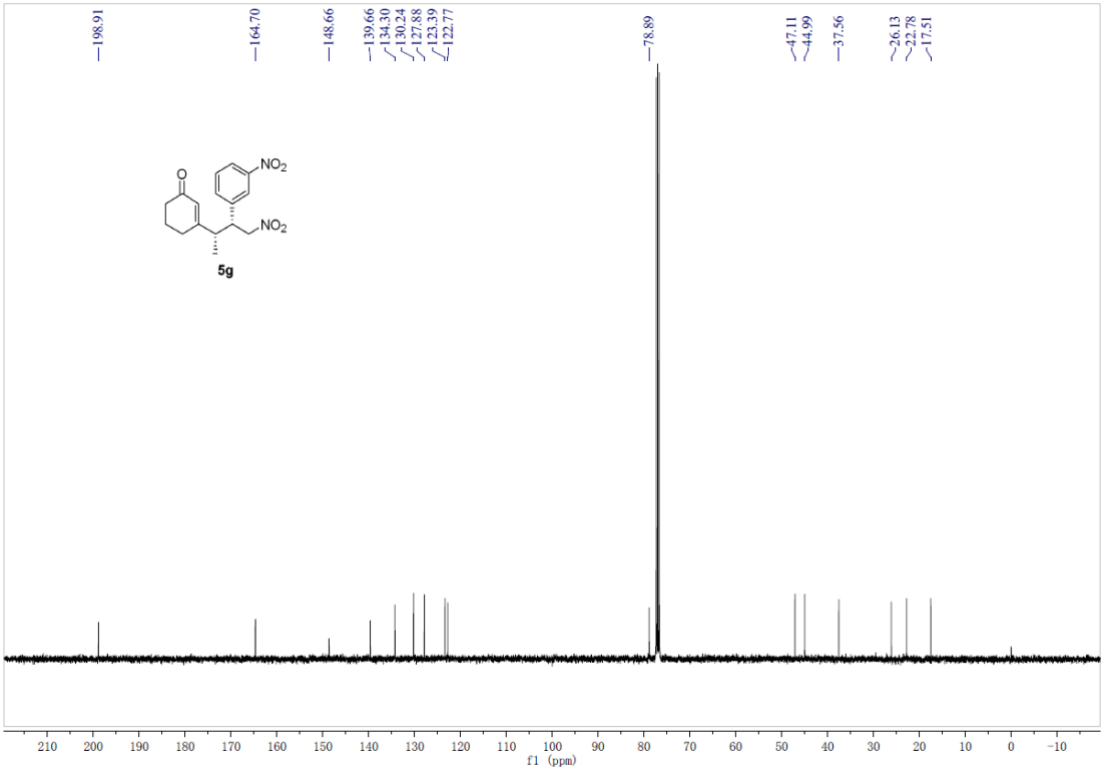
5f: 3-((2*S*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



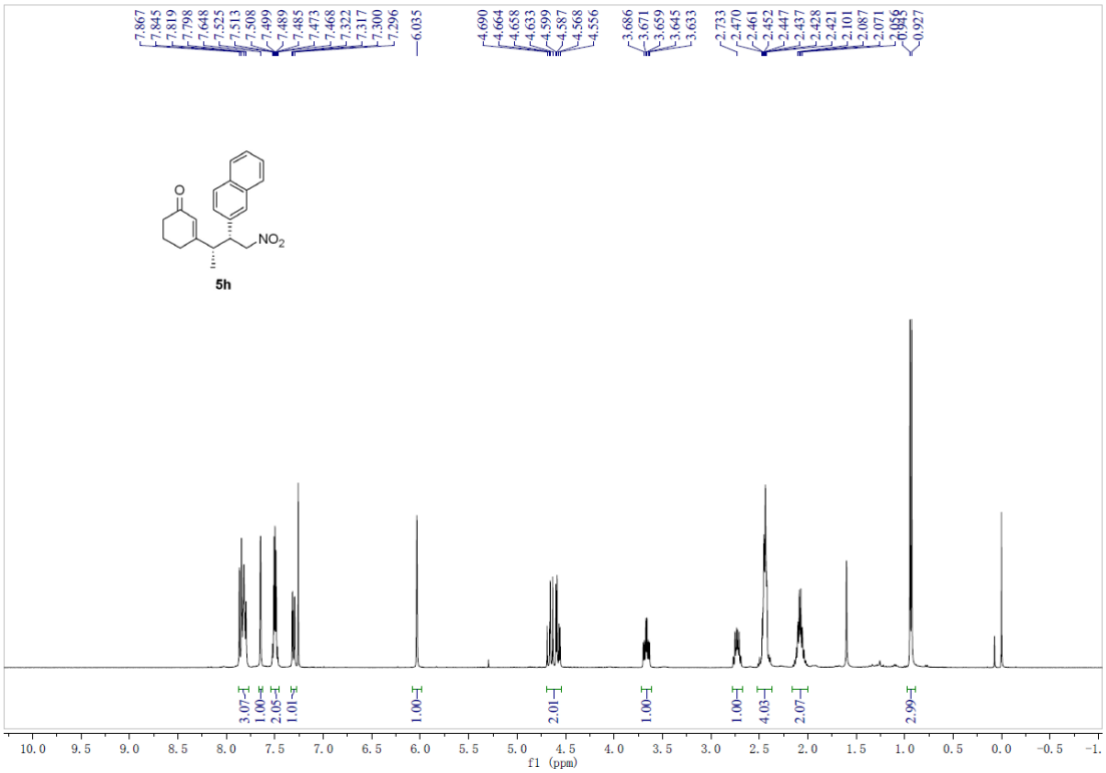


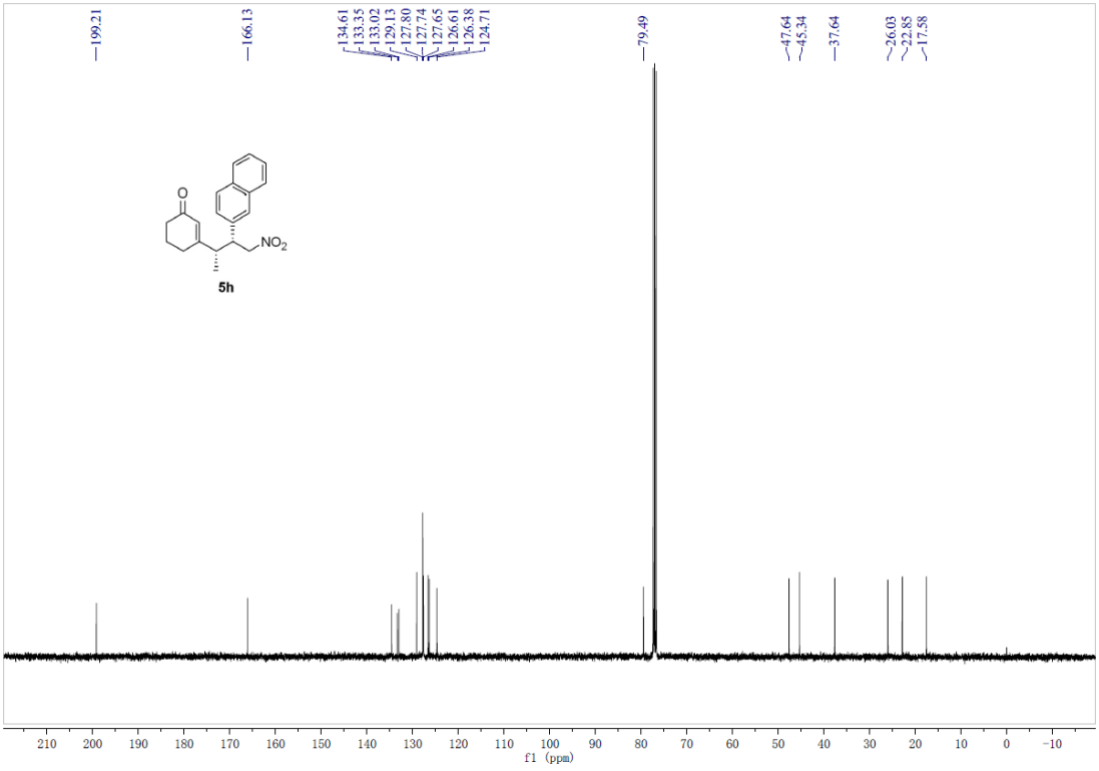
5g: 3-((2*S*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one



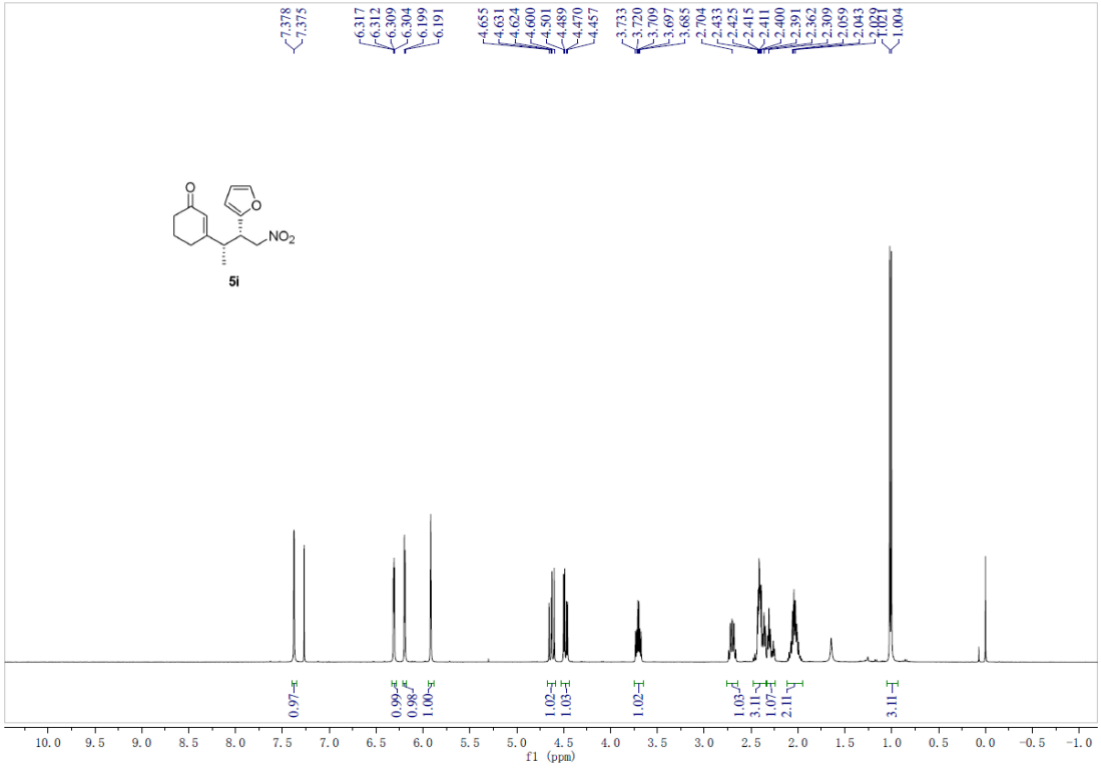


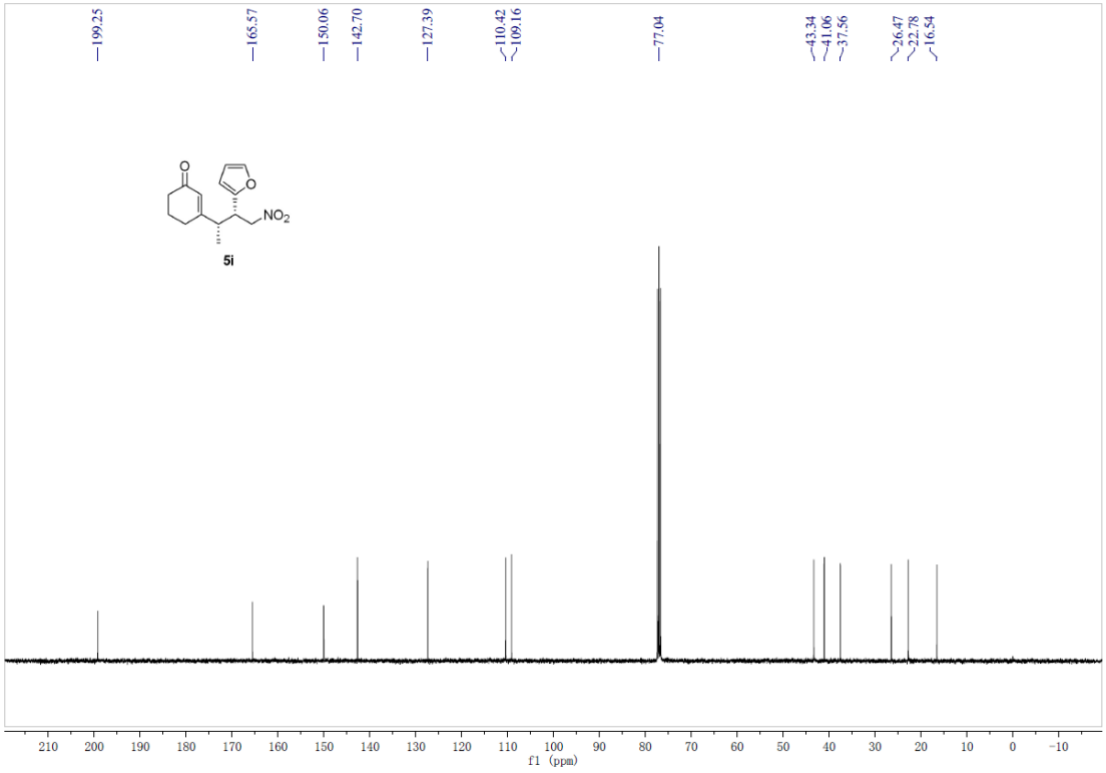
5h: 3-((2*S*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



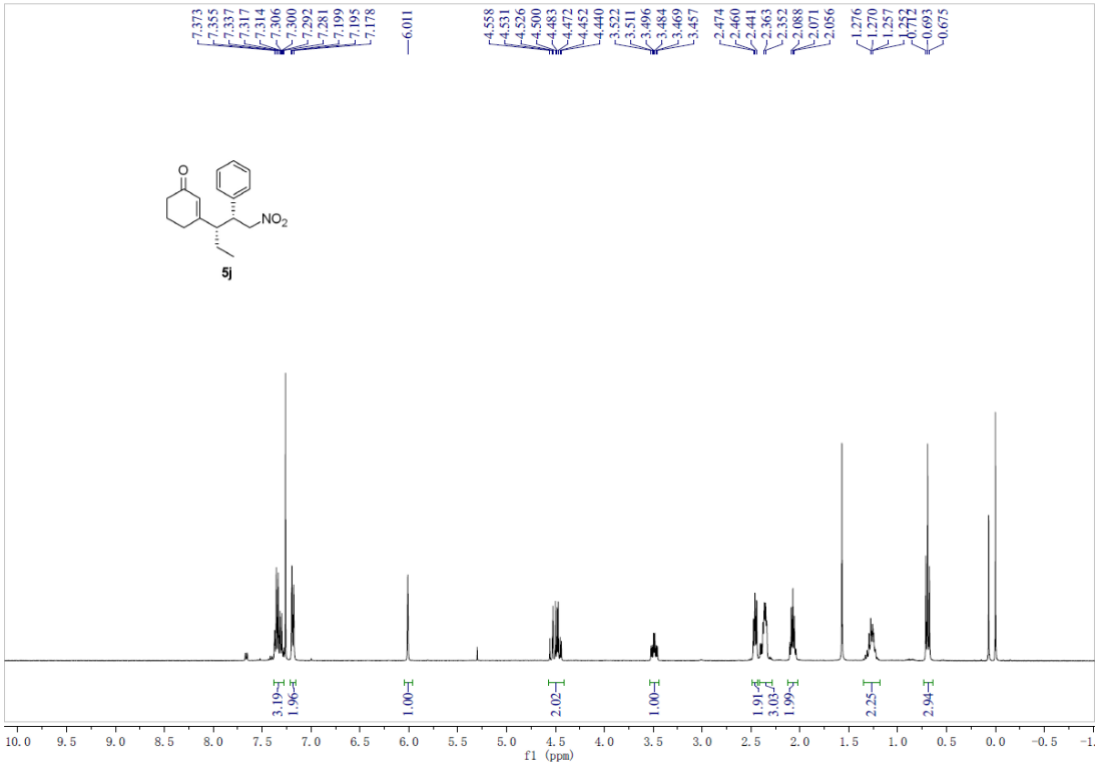


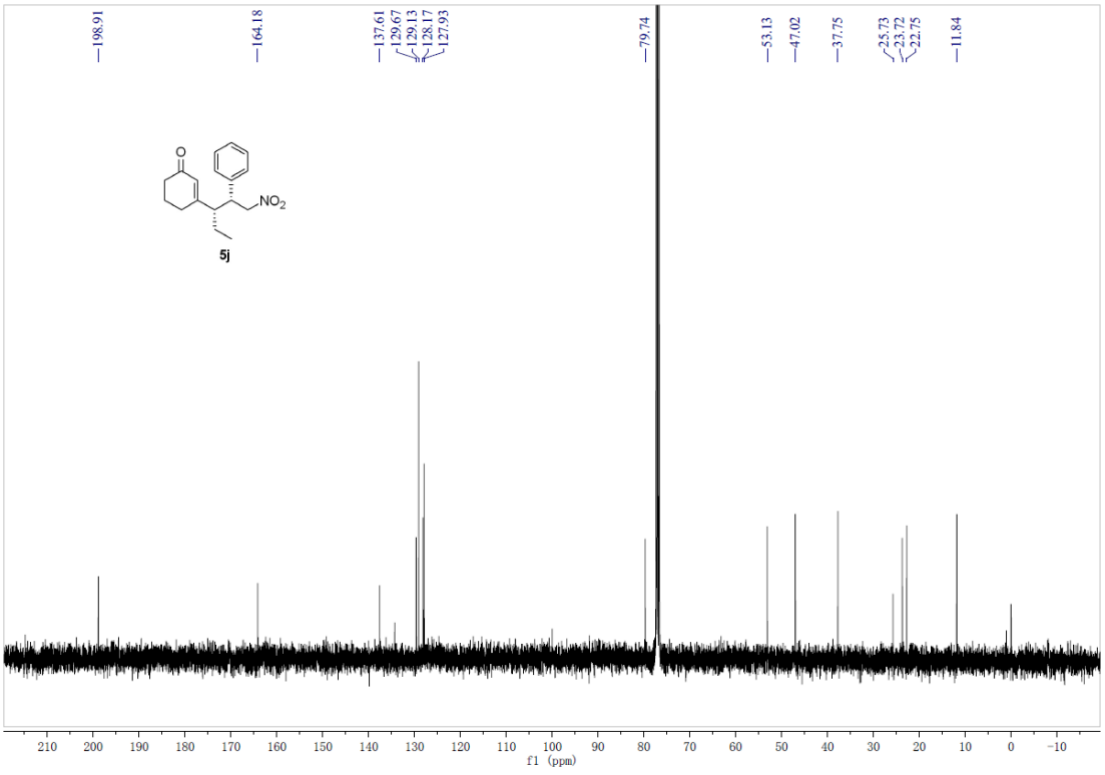
5i: 3-((2*S*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one



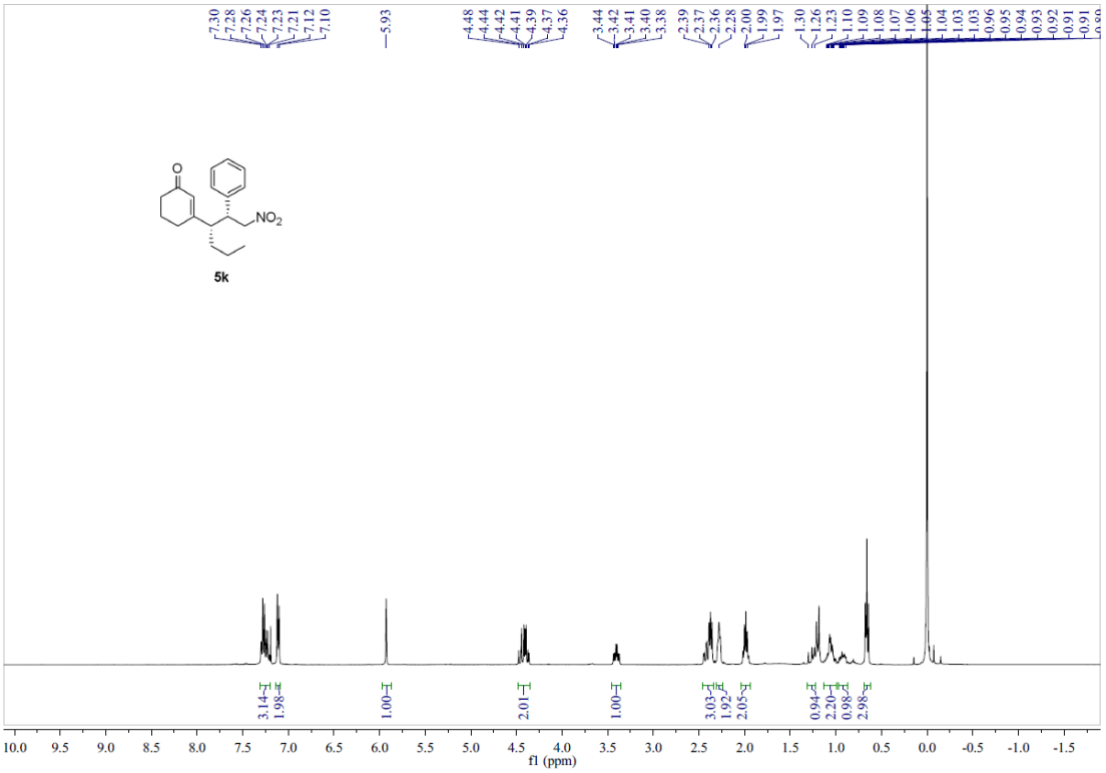


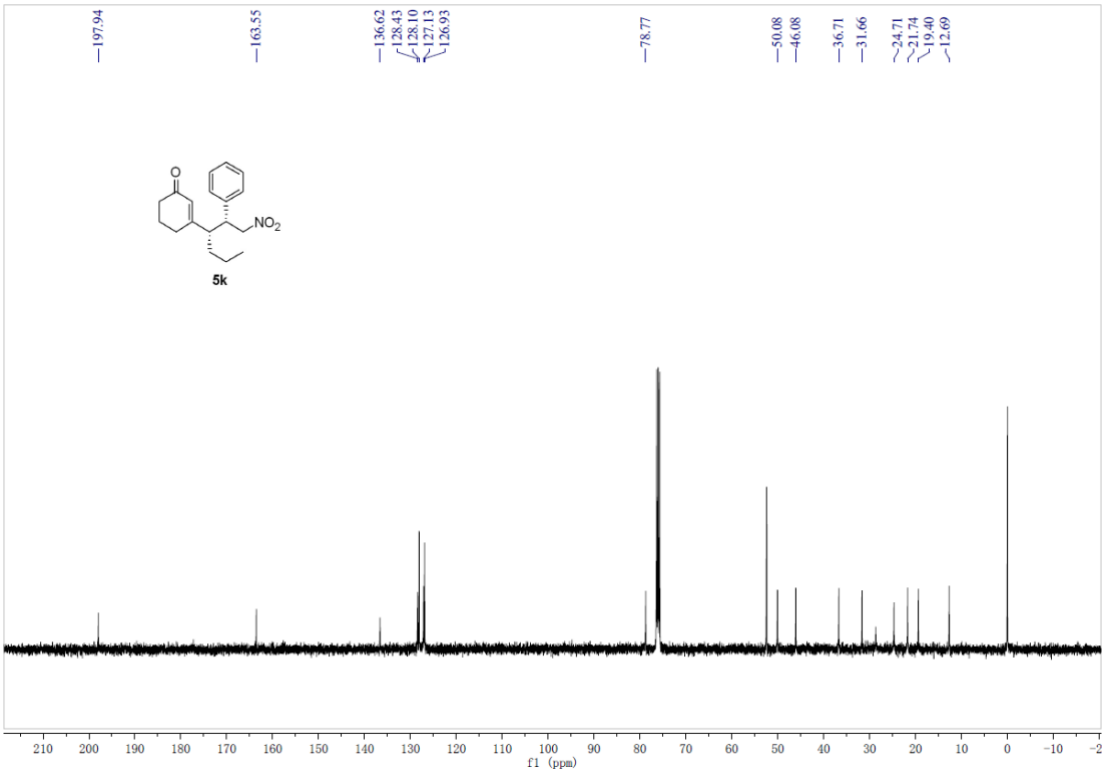
5j: 3-((2*R*,3*S*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one



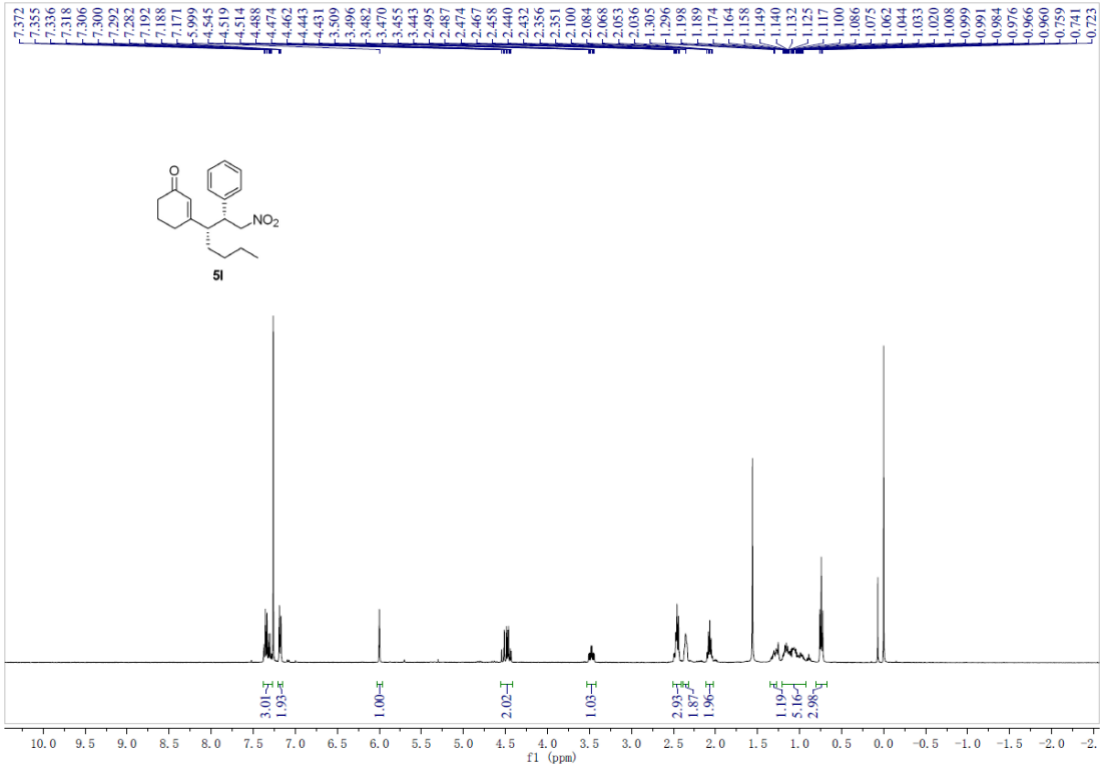


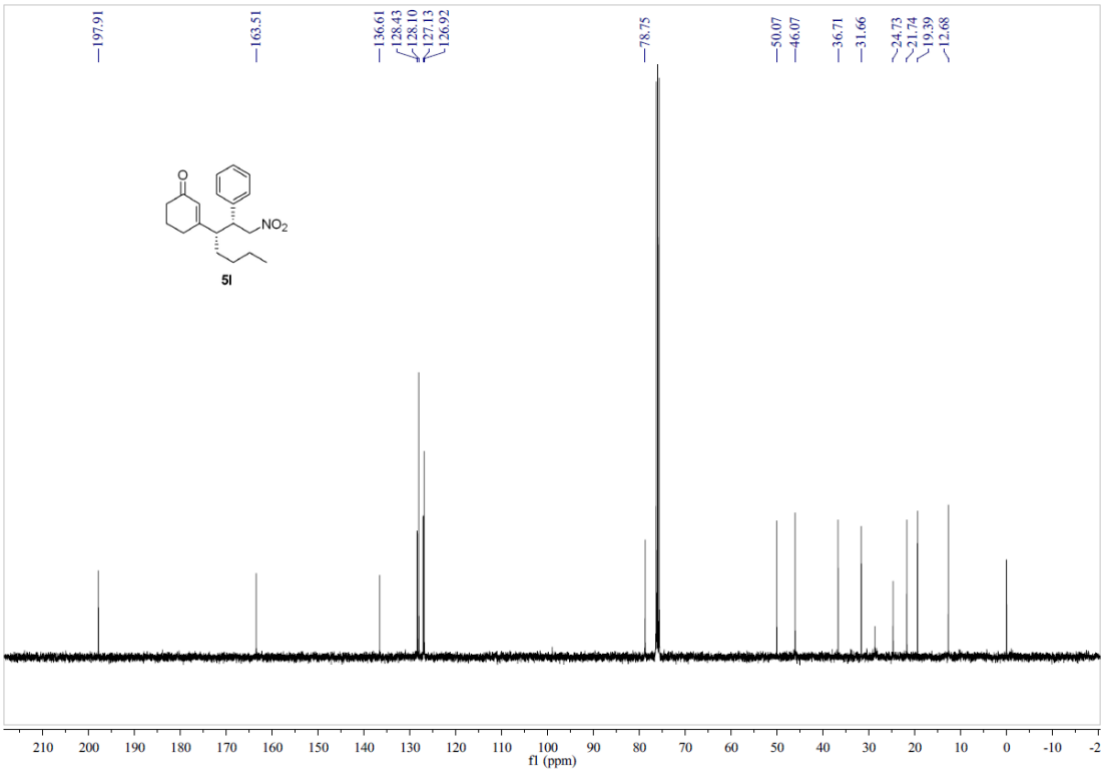
5k: 3-((2*R*,3*S*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one



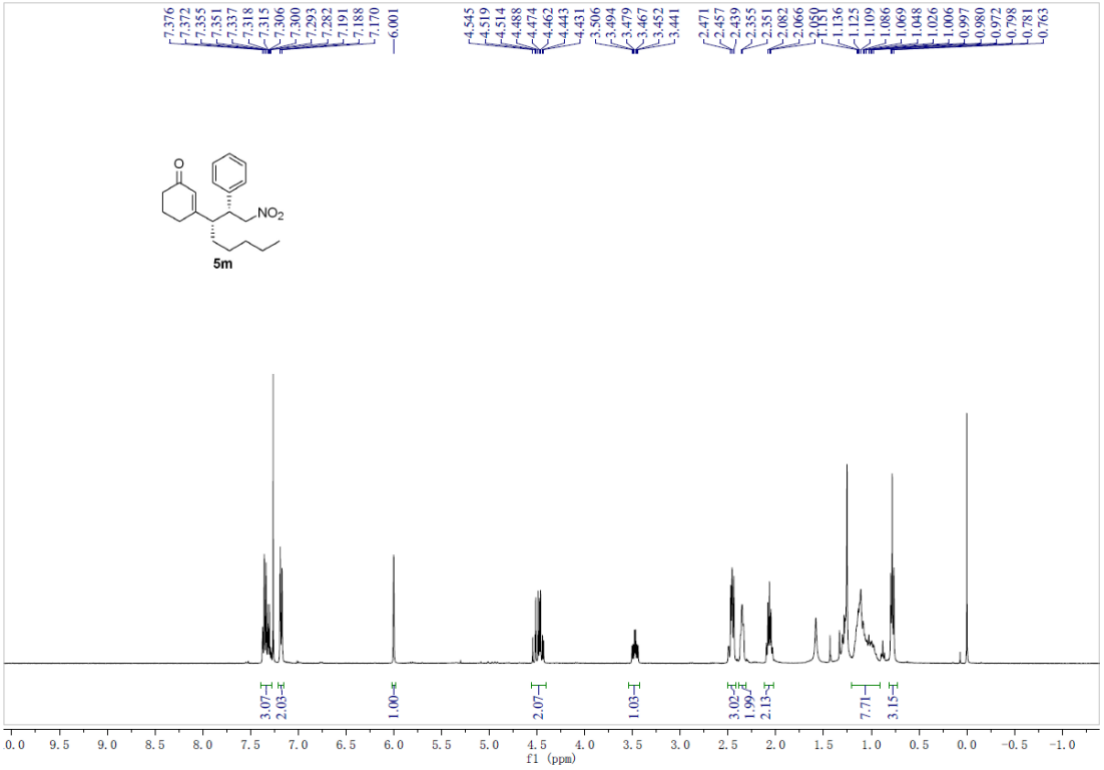


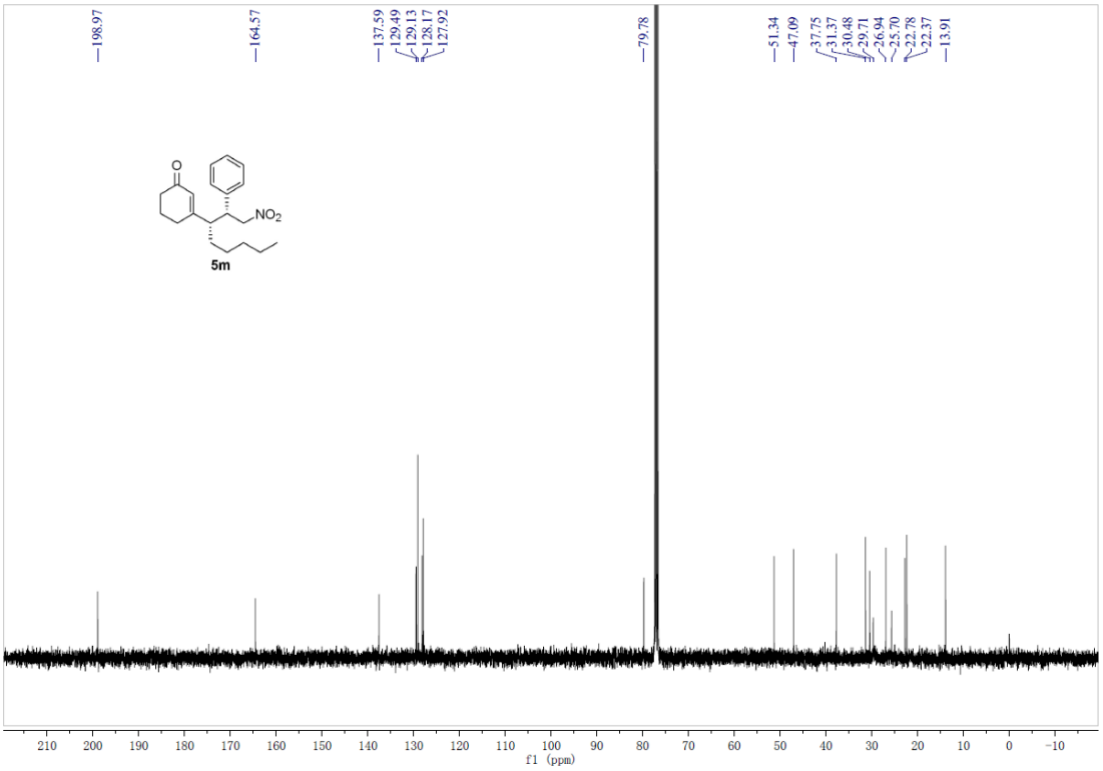
5l: 3-((2*R*,3*S*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one



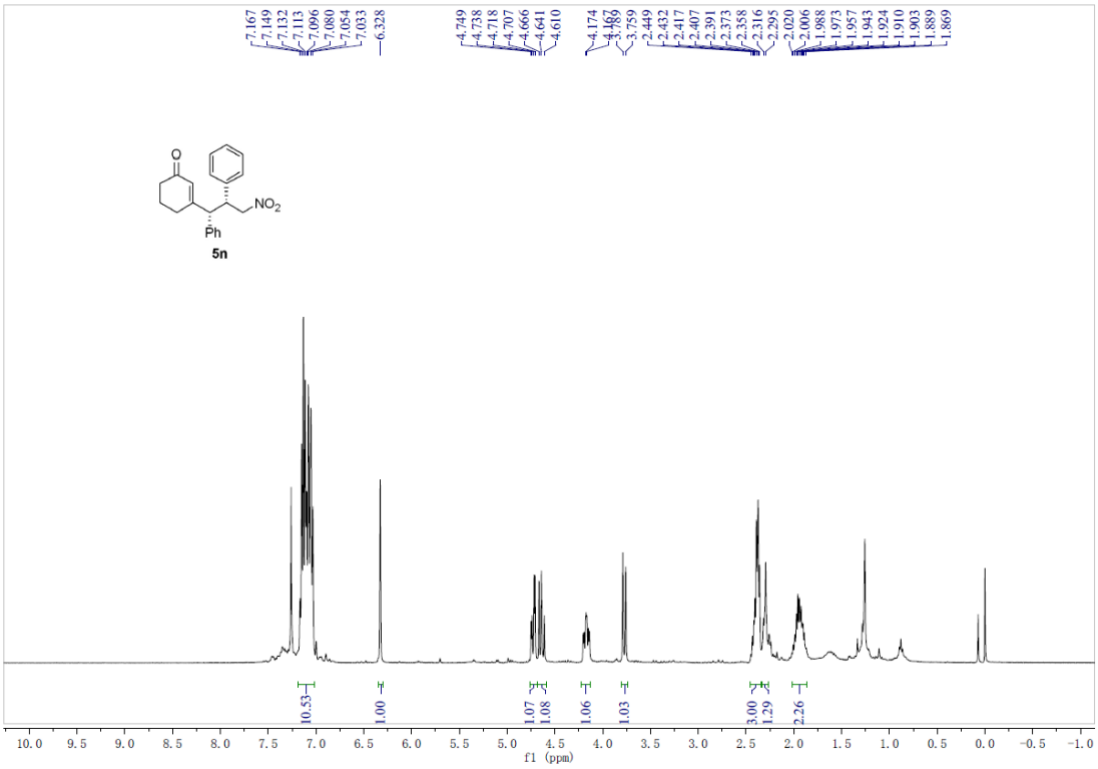


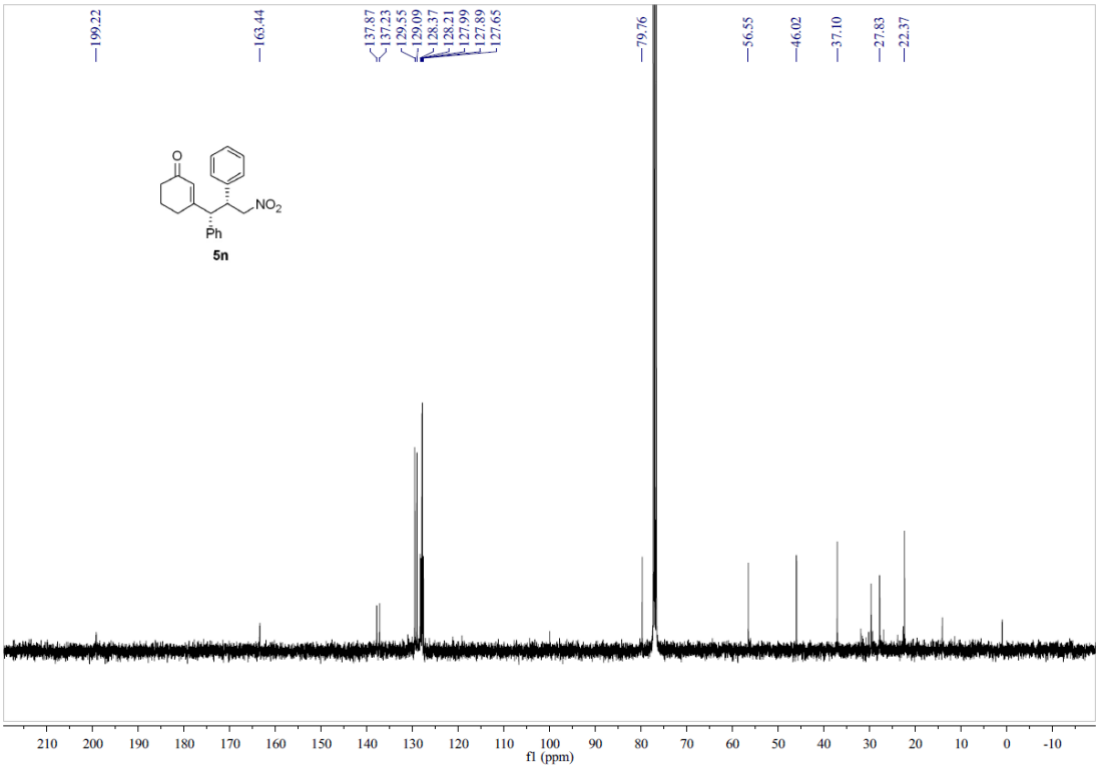
5m: 3-((2*R*,3*S*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one



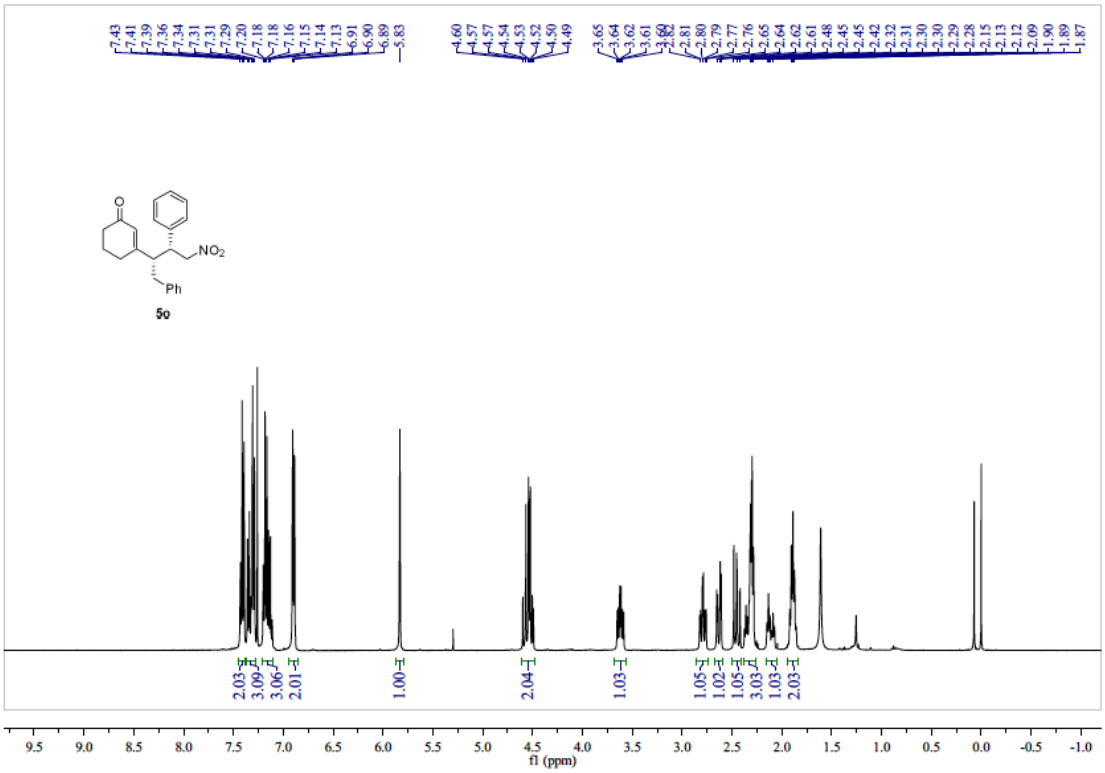


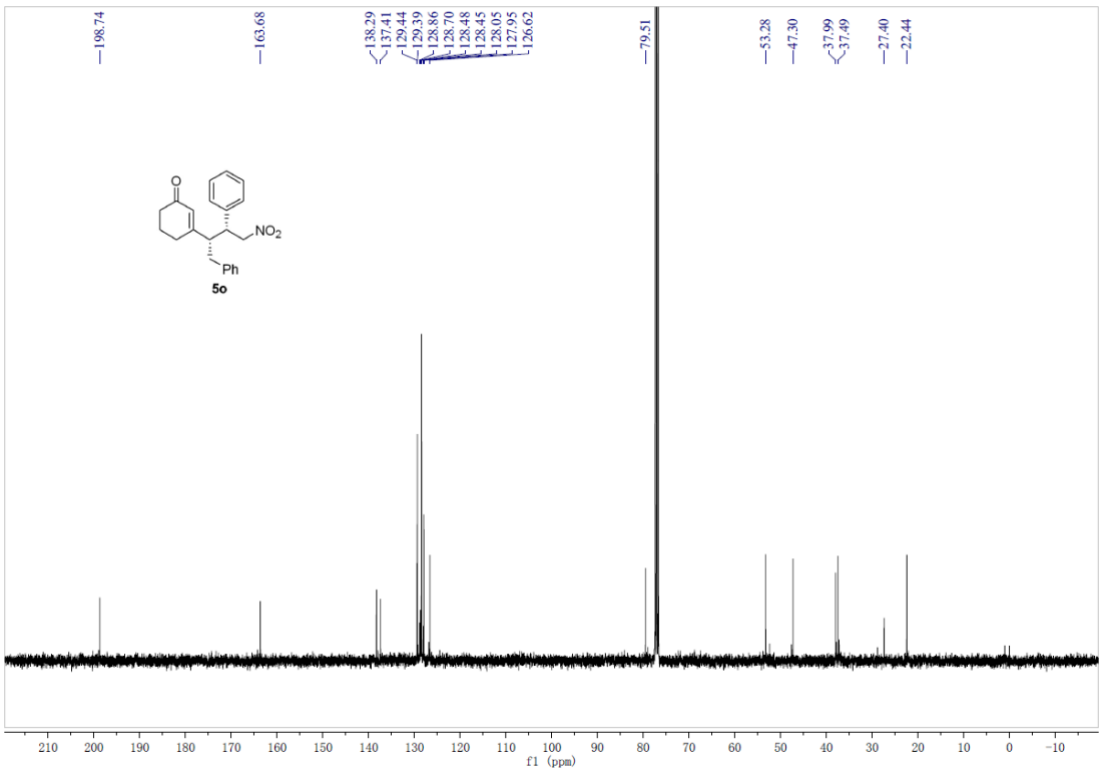
5n: 3-((1*S*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one



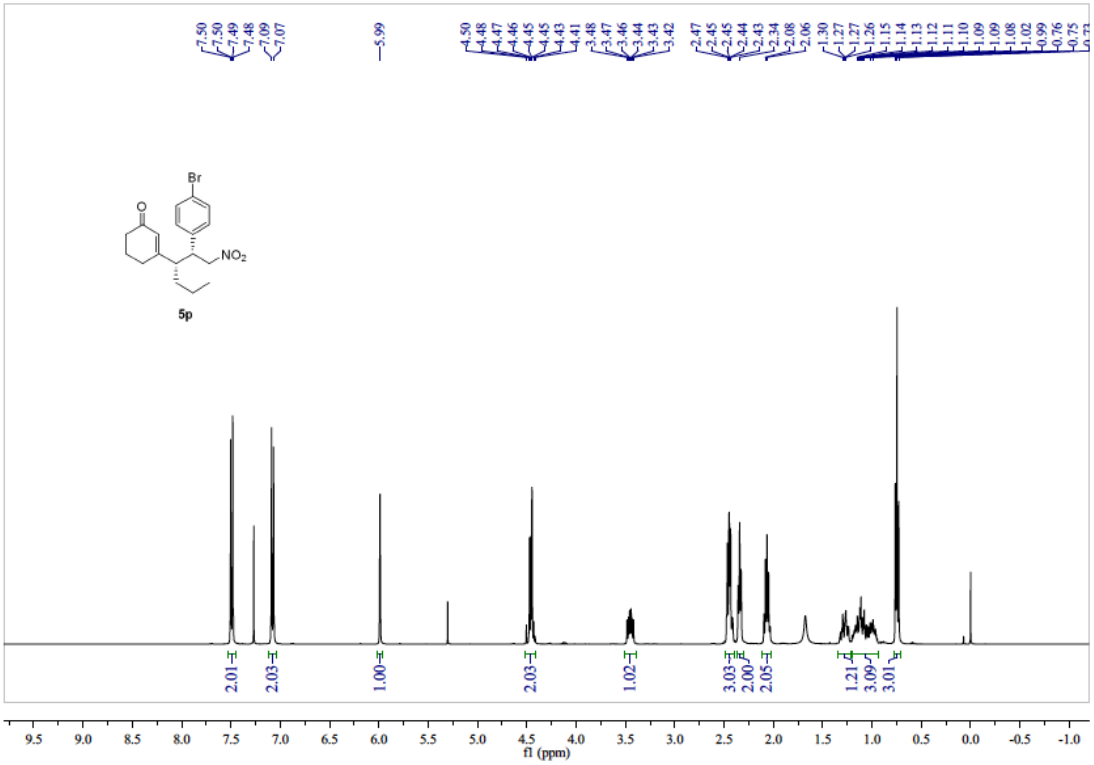


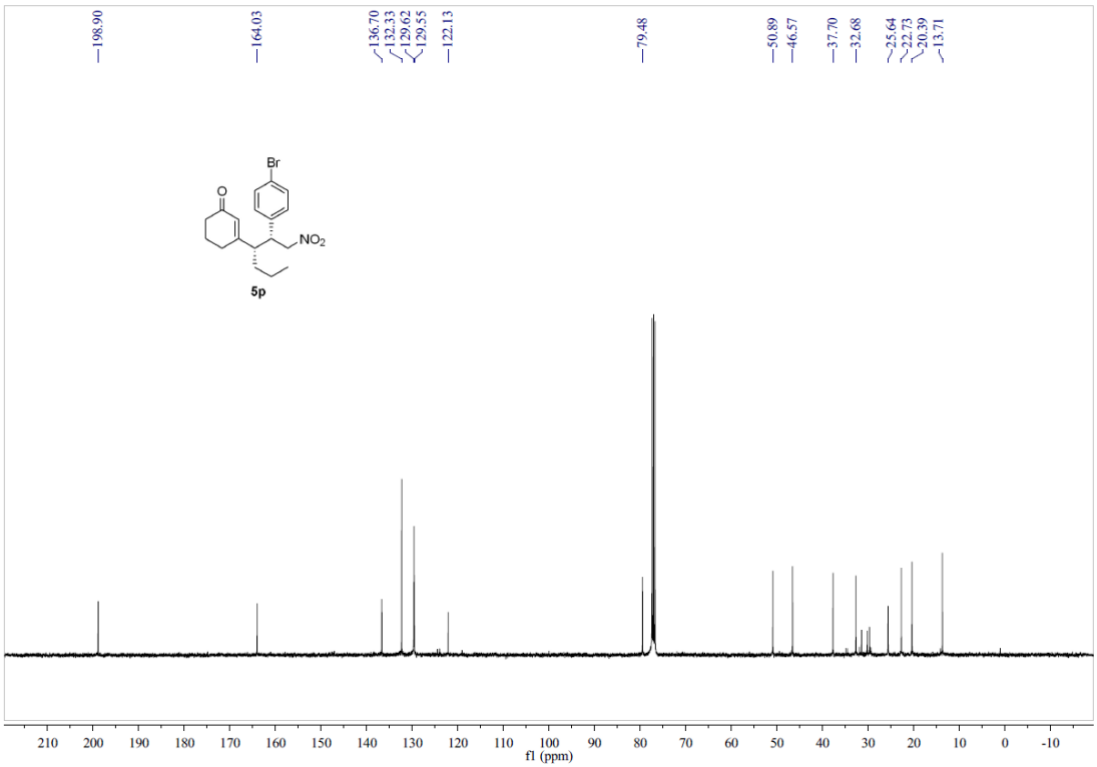
5o: 3-((2*S*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one



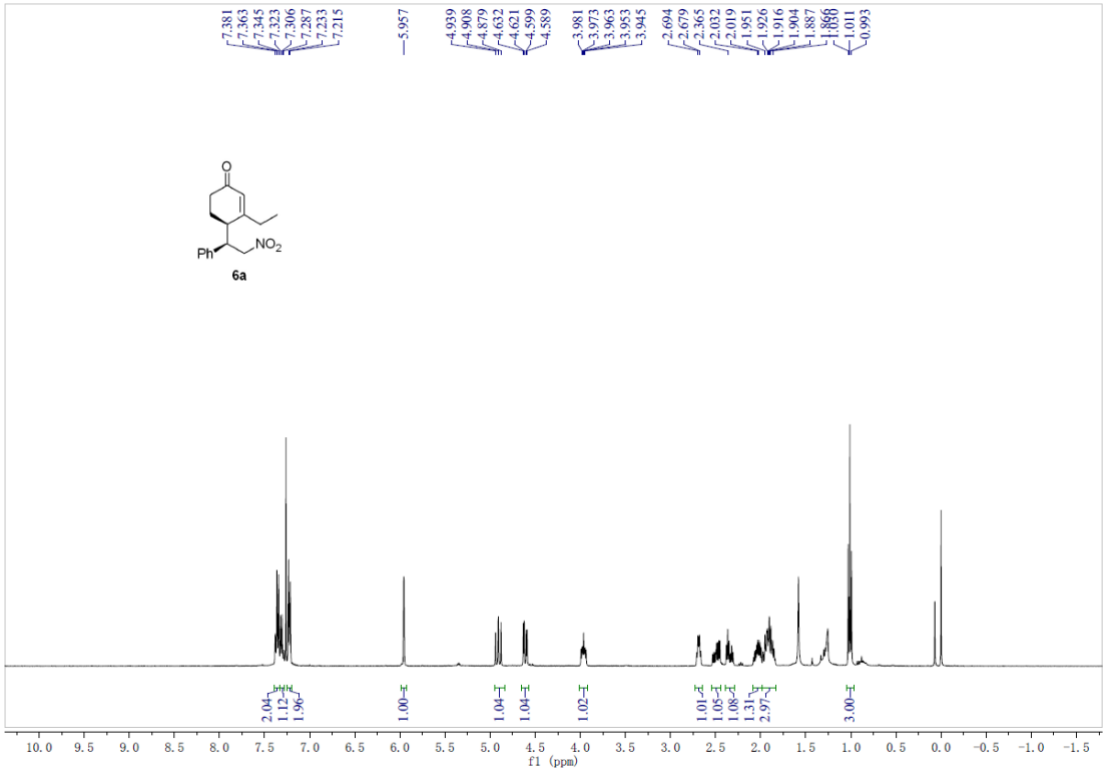


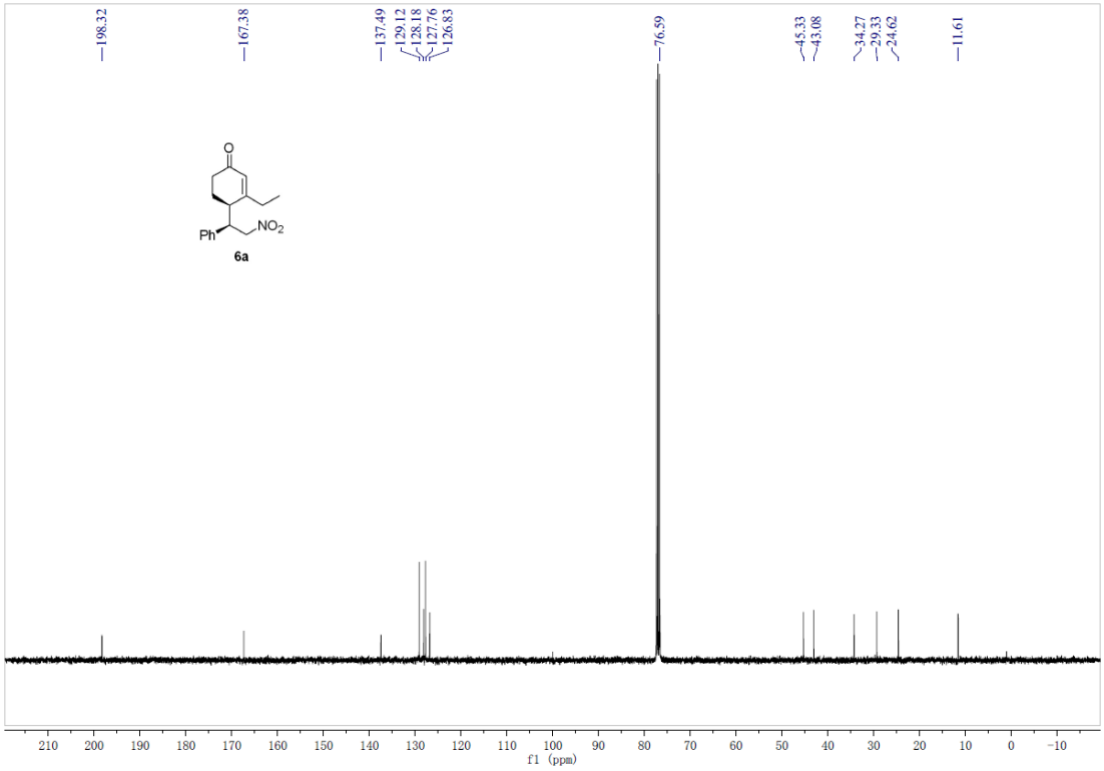
5p: 3-((2*R*,3*S*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one



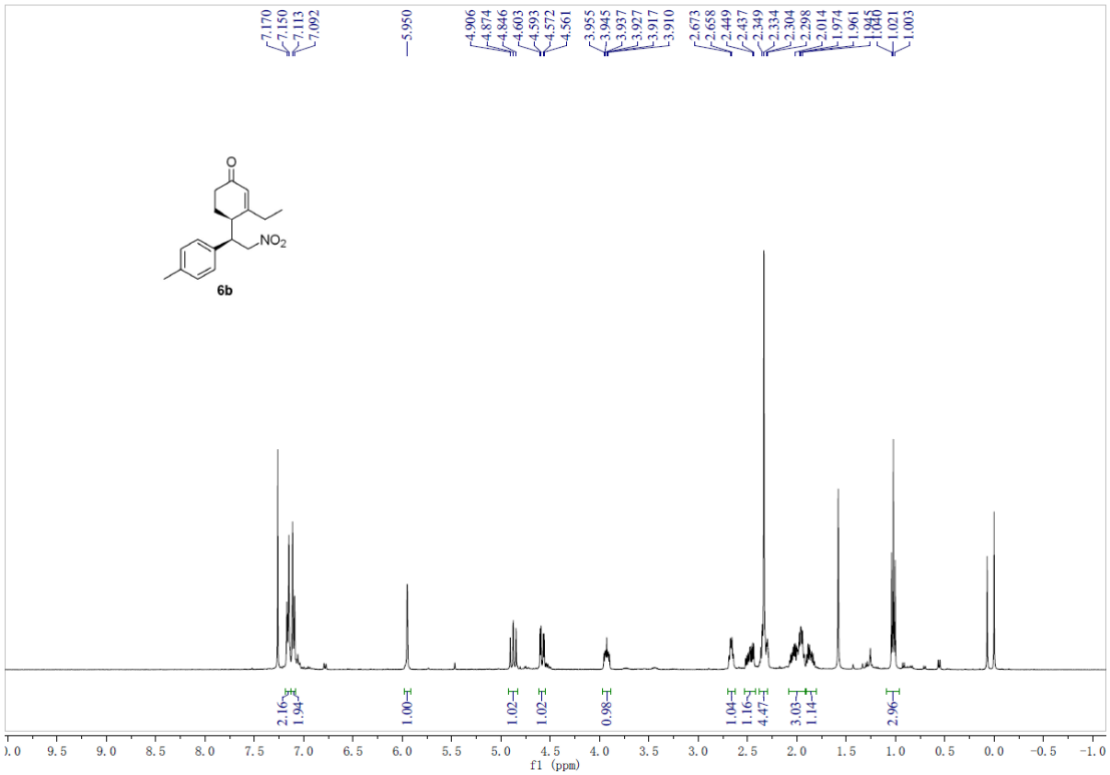


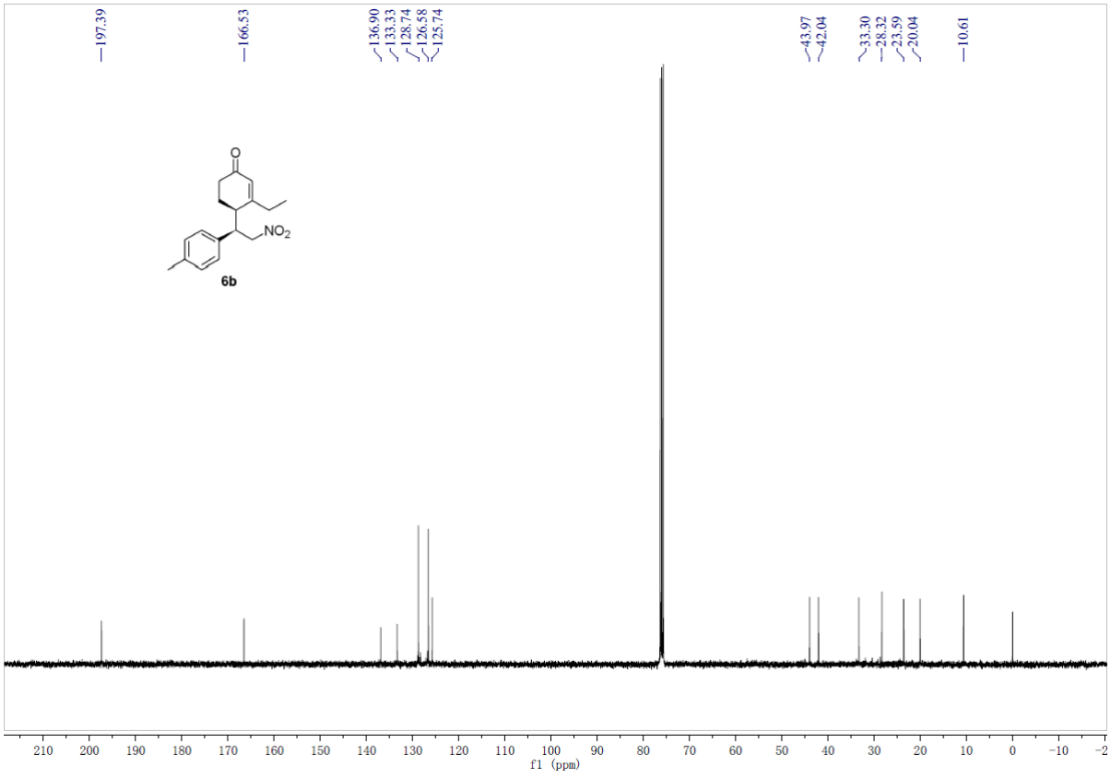
6a: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



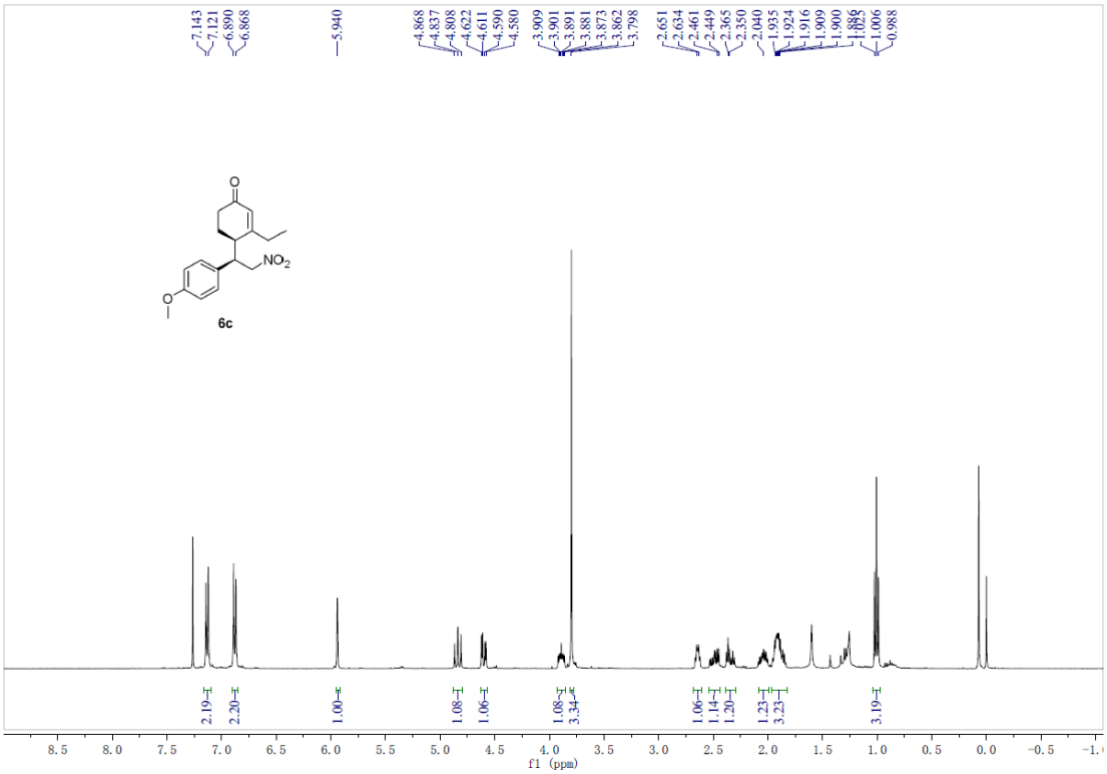


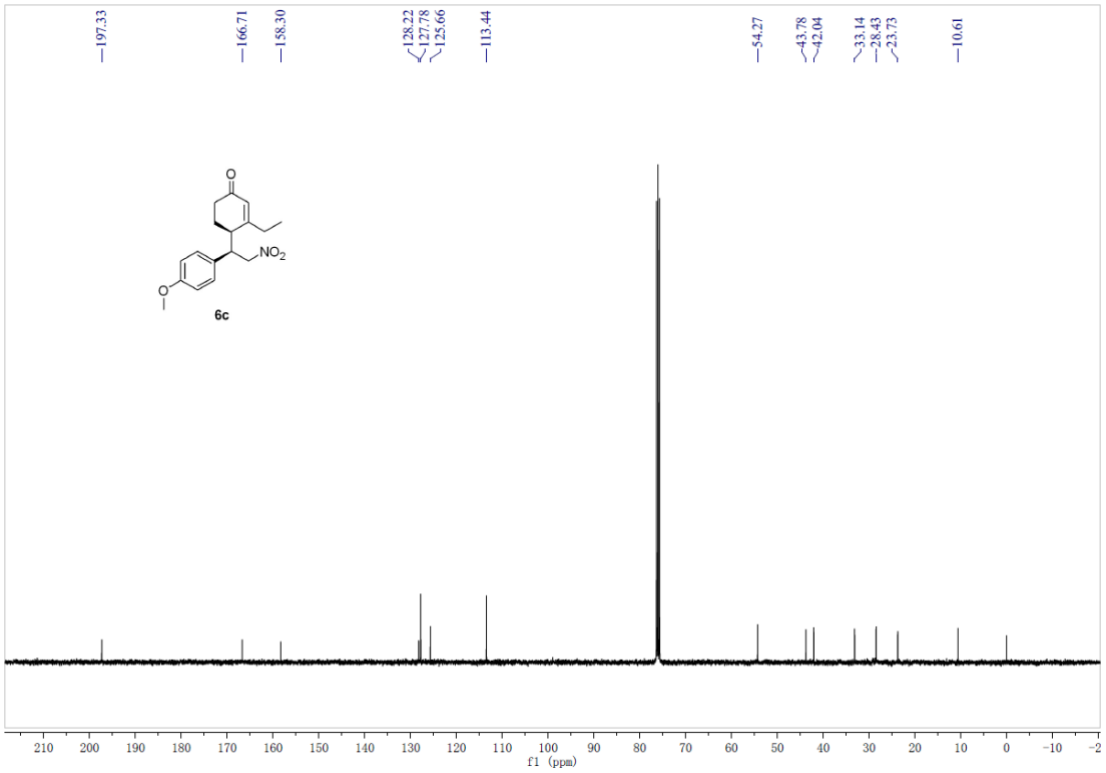
6b: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(p-tolyl)ethyl)cyclohex-2-en-1-one



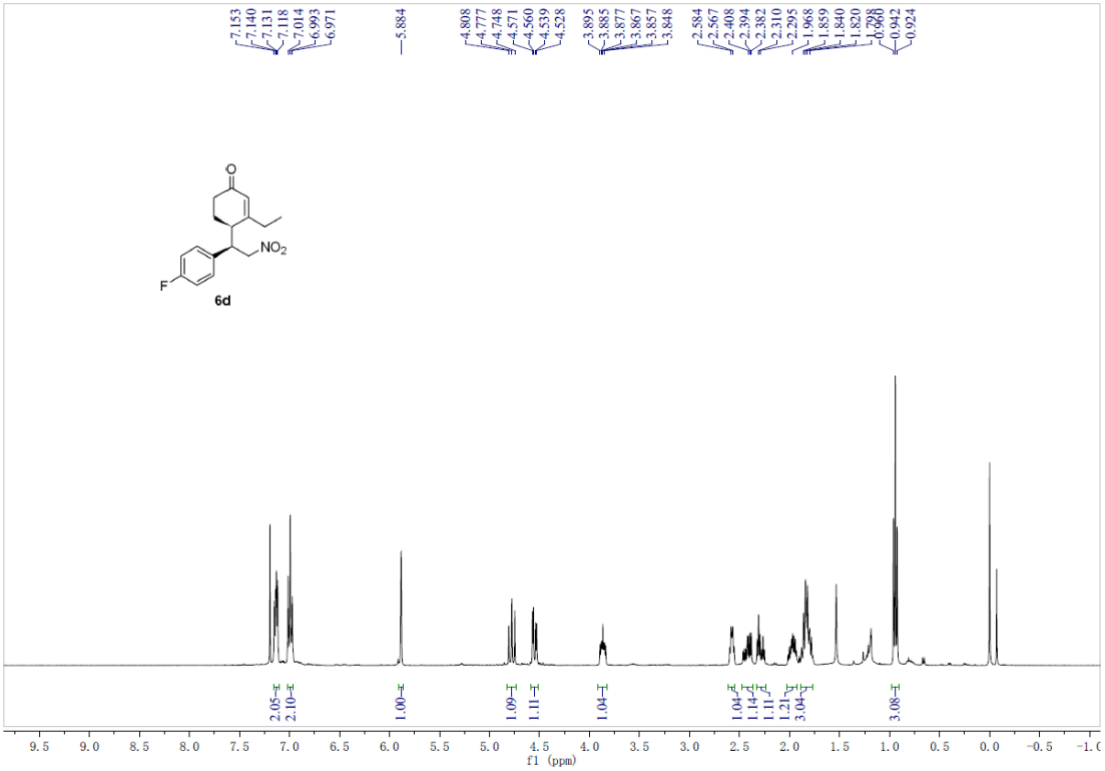


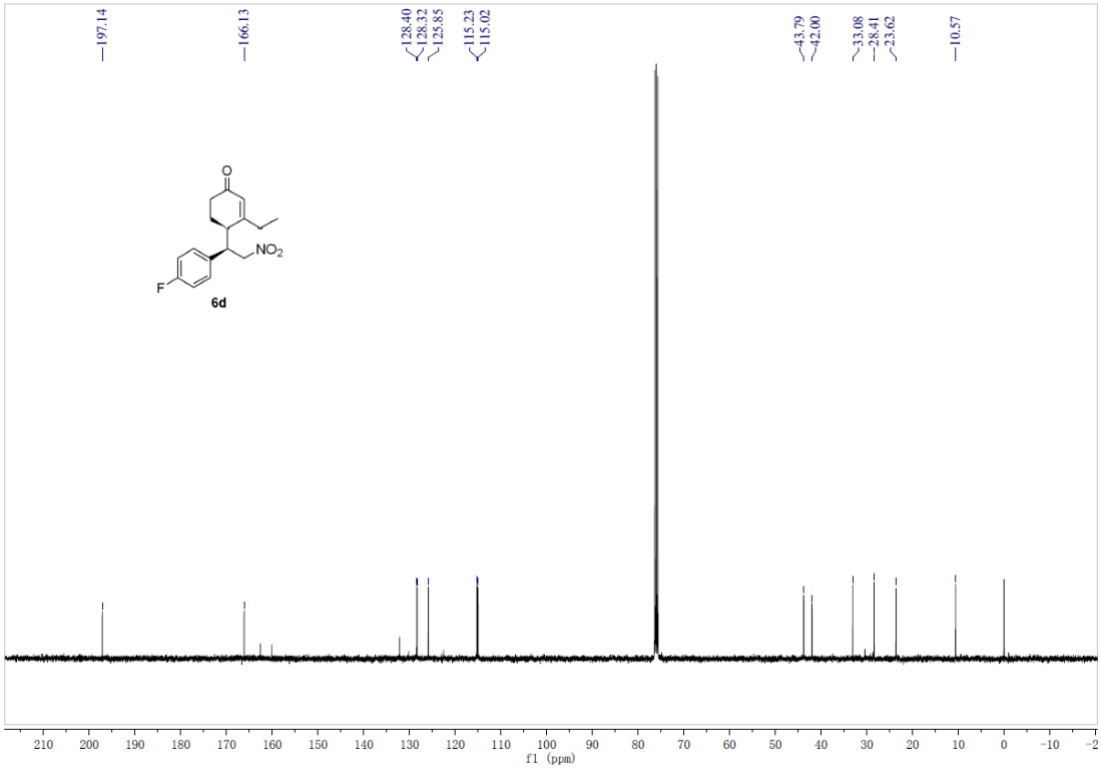
6c: (*R*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one



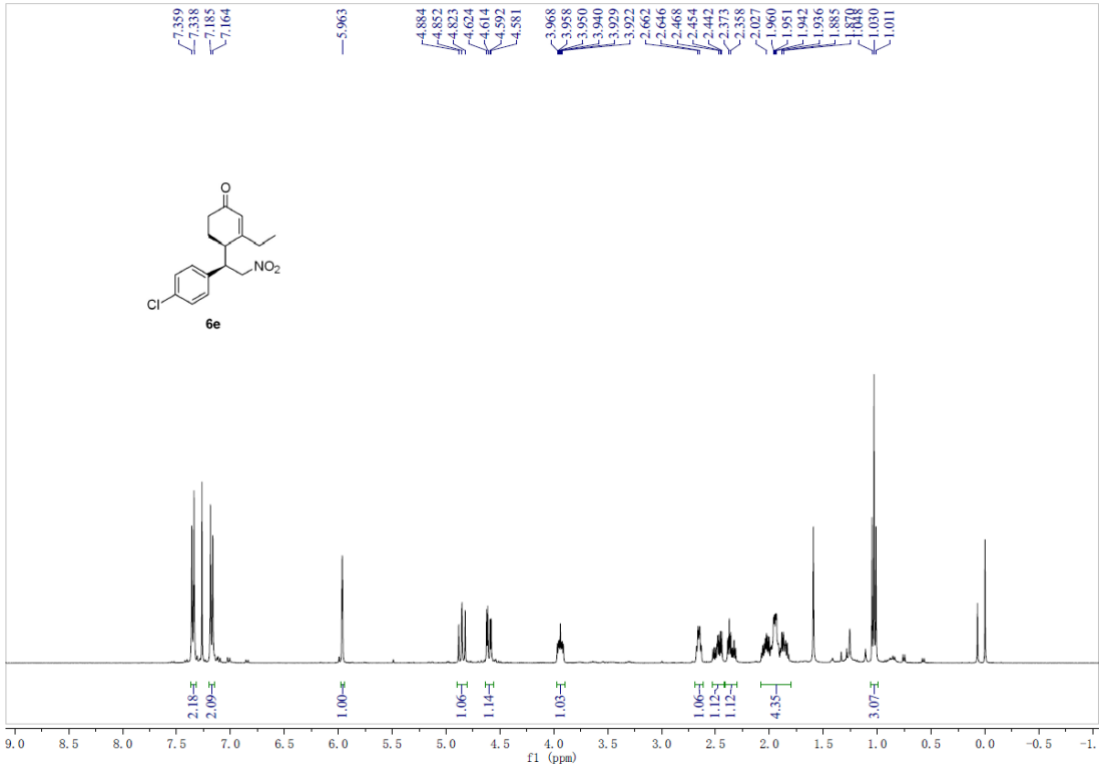


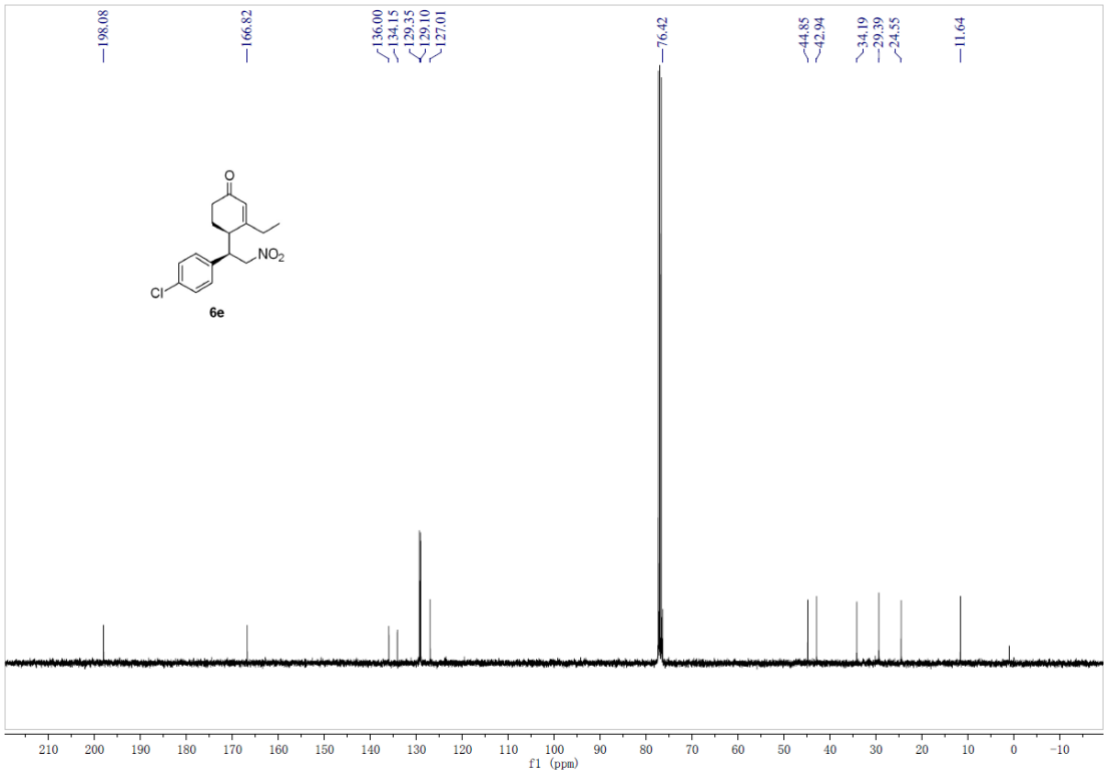
6d: (*R*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one



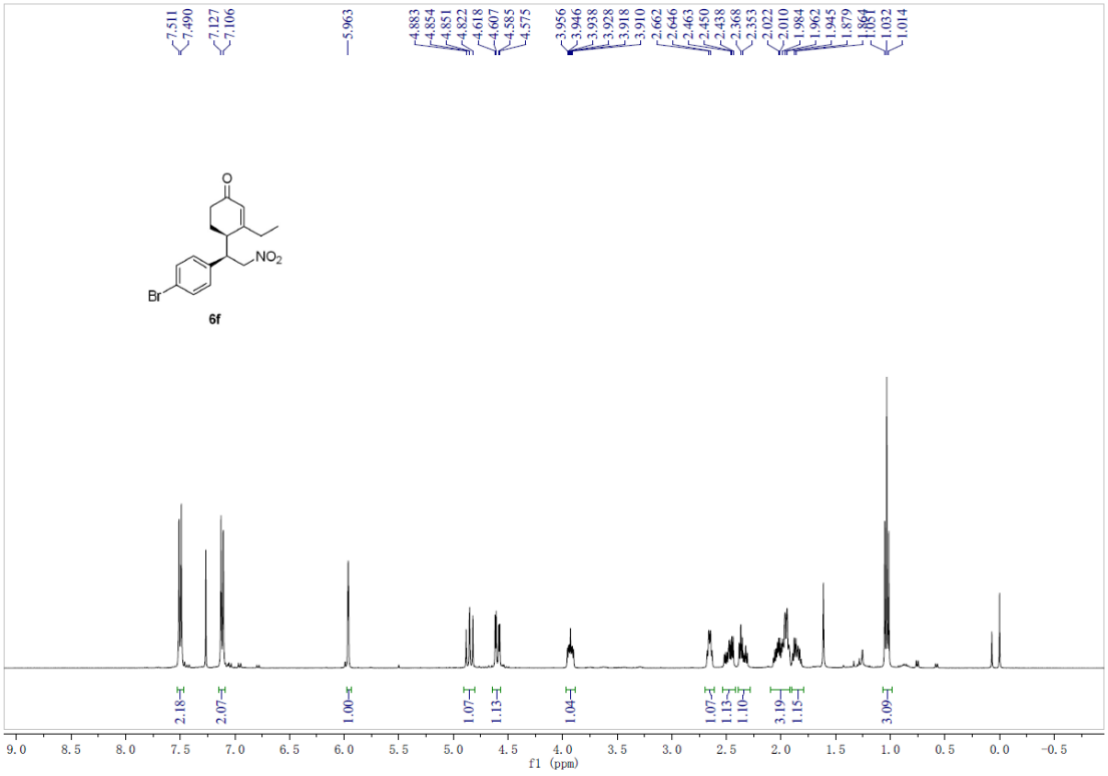


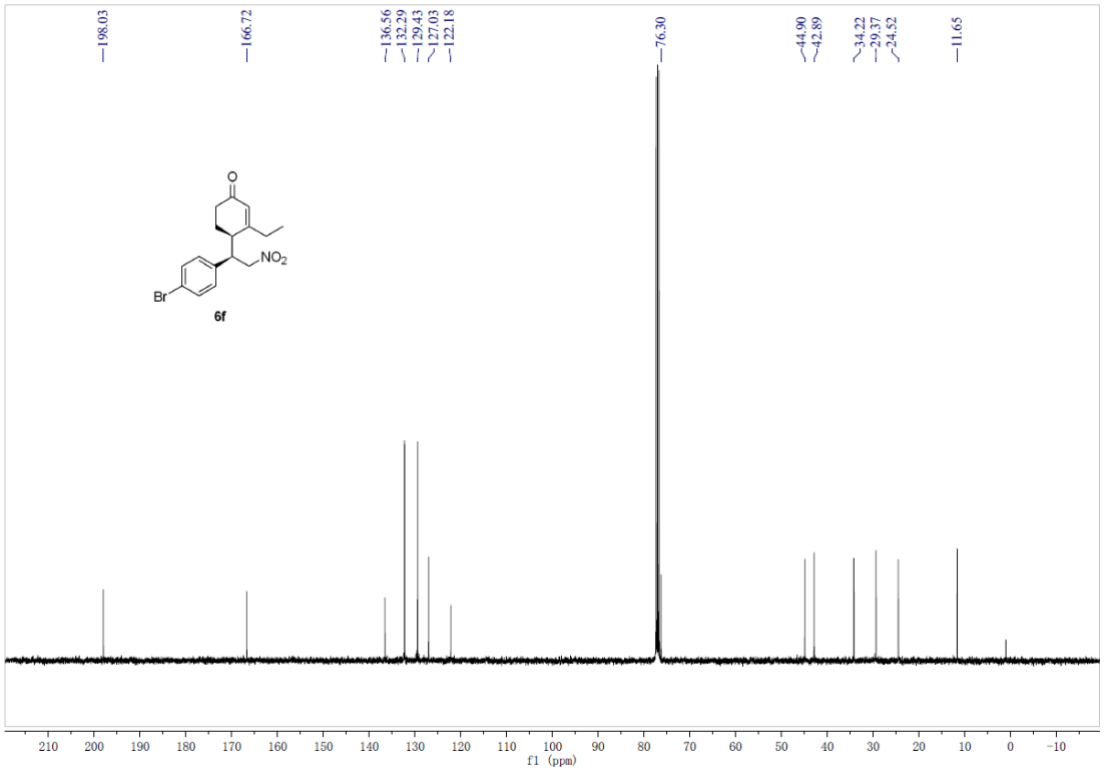
6e: (*R*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



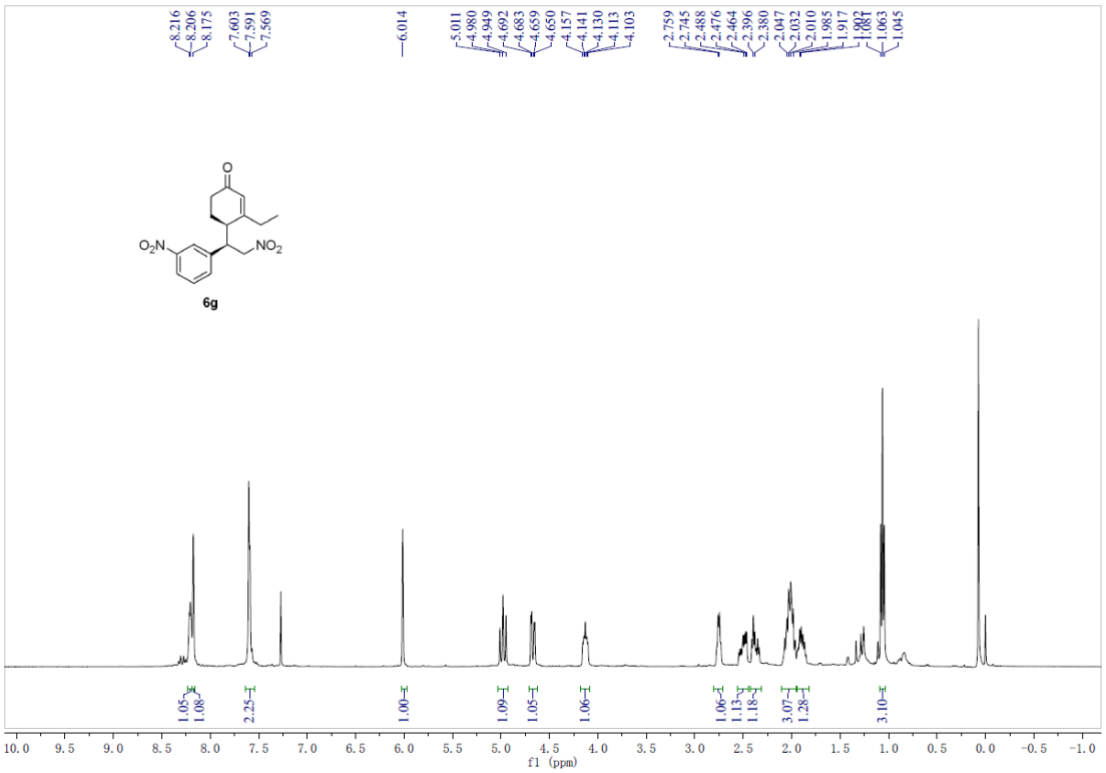


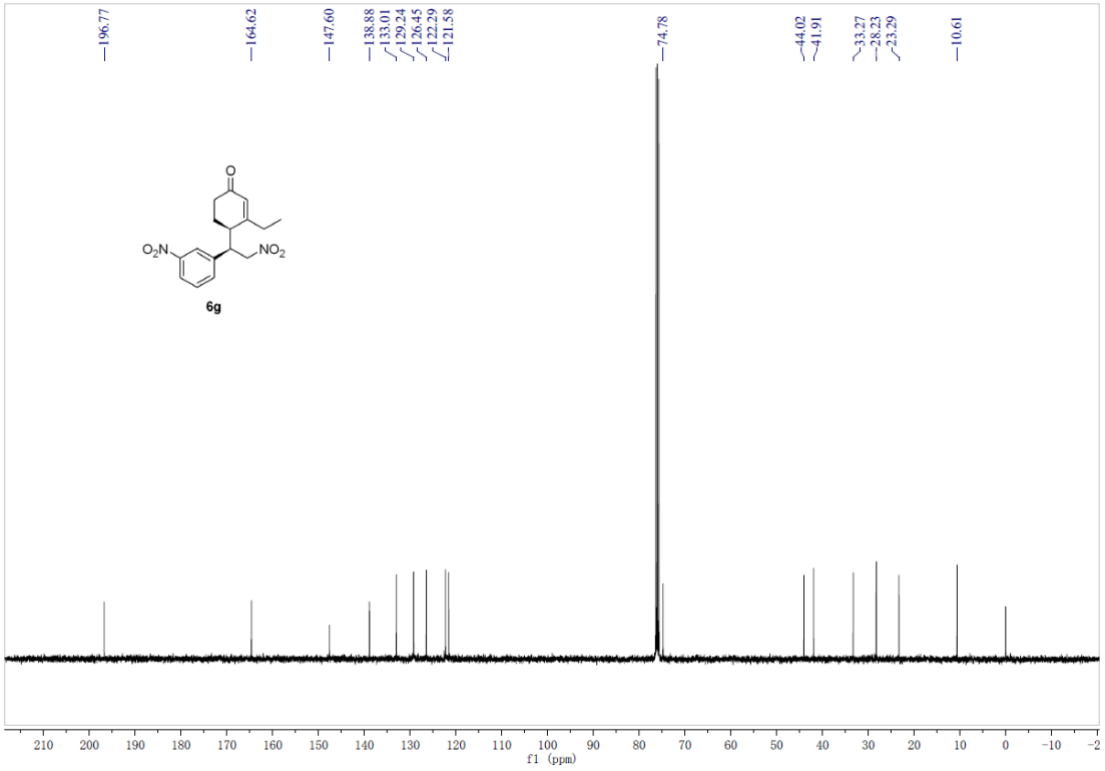
6f: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



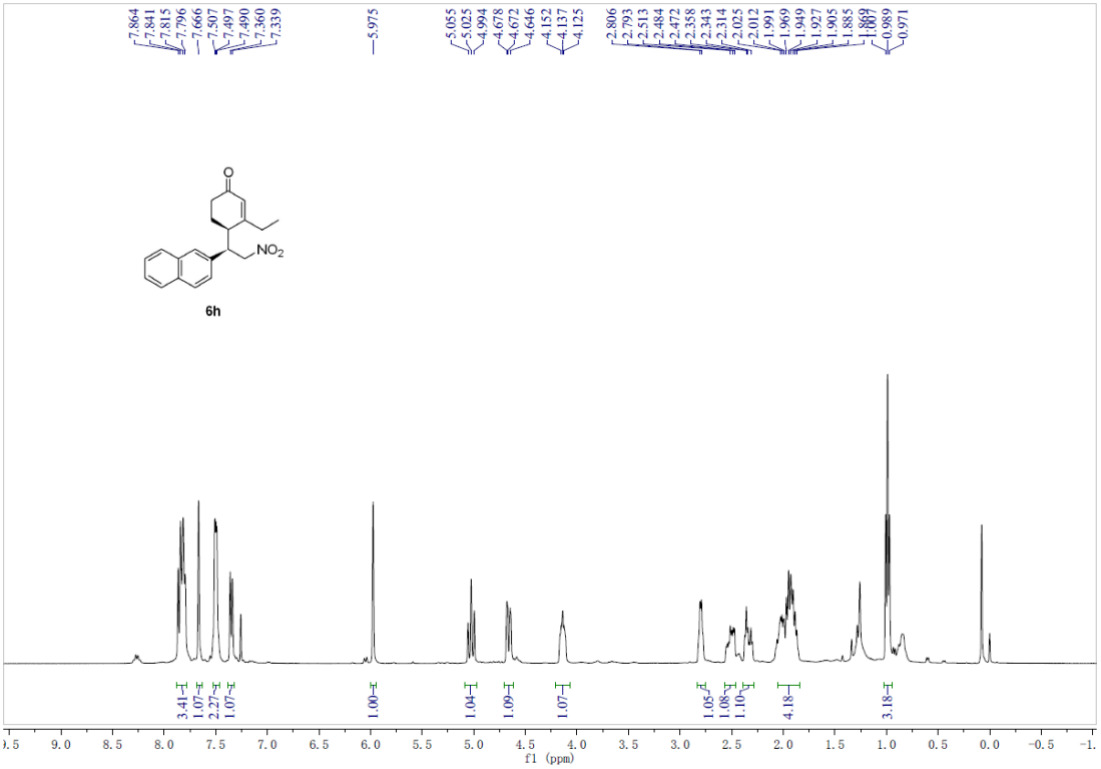


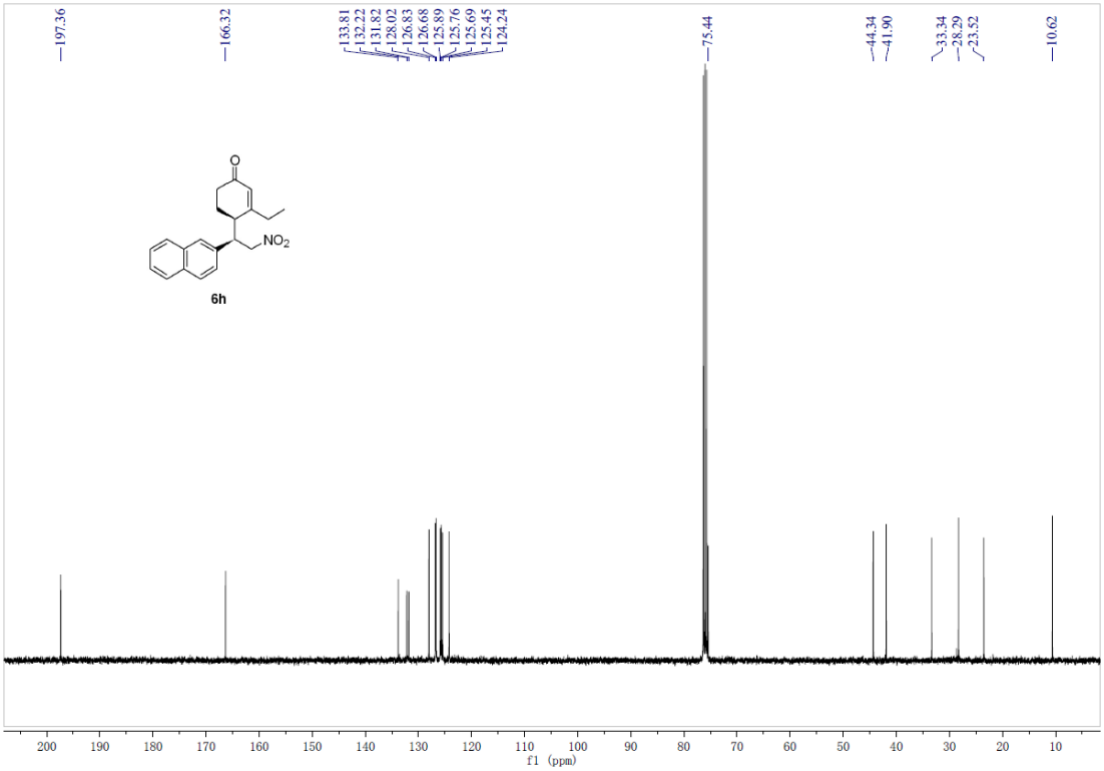
6g: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(3-nitrophenyl)ethyl)cyclohex-2-en-1-one



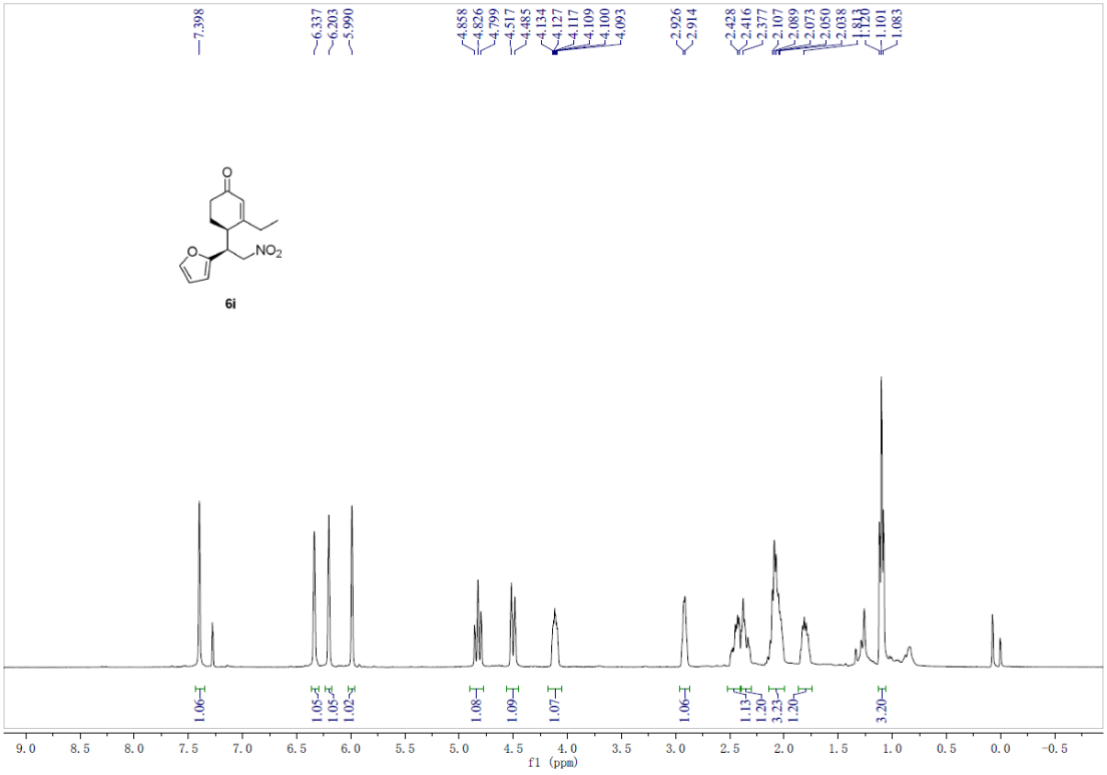


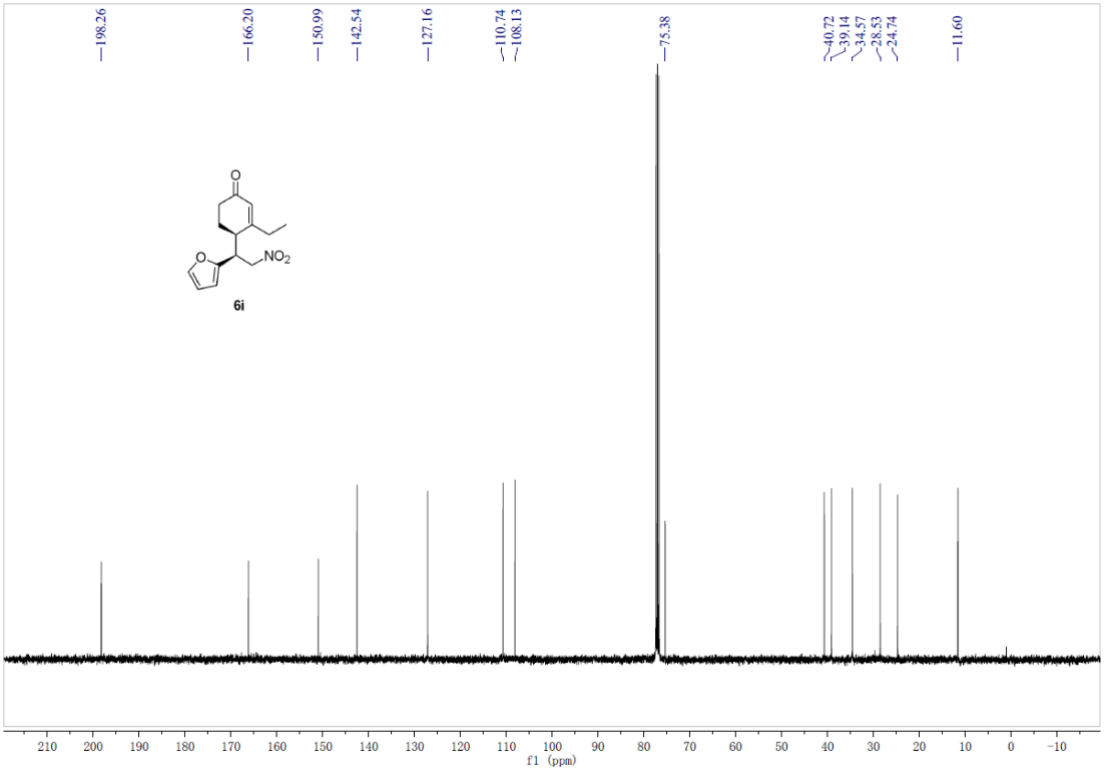
6h: (*R*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



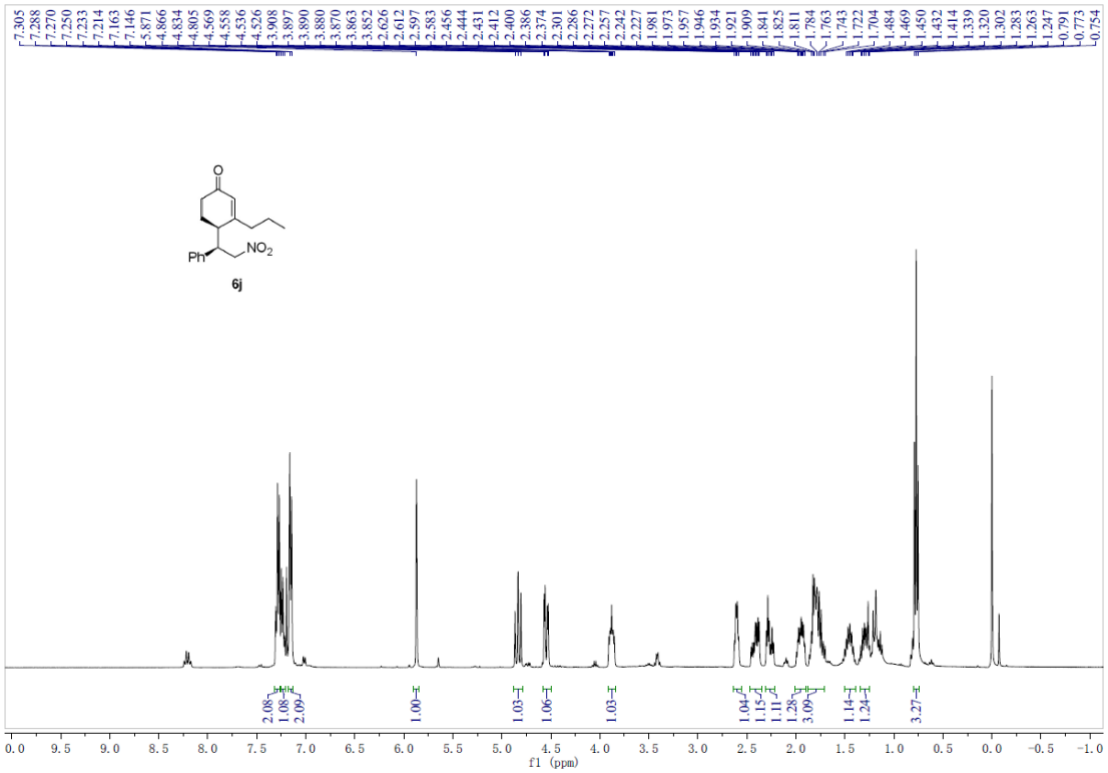


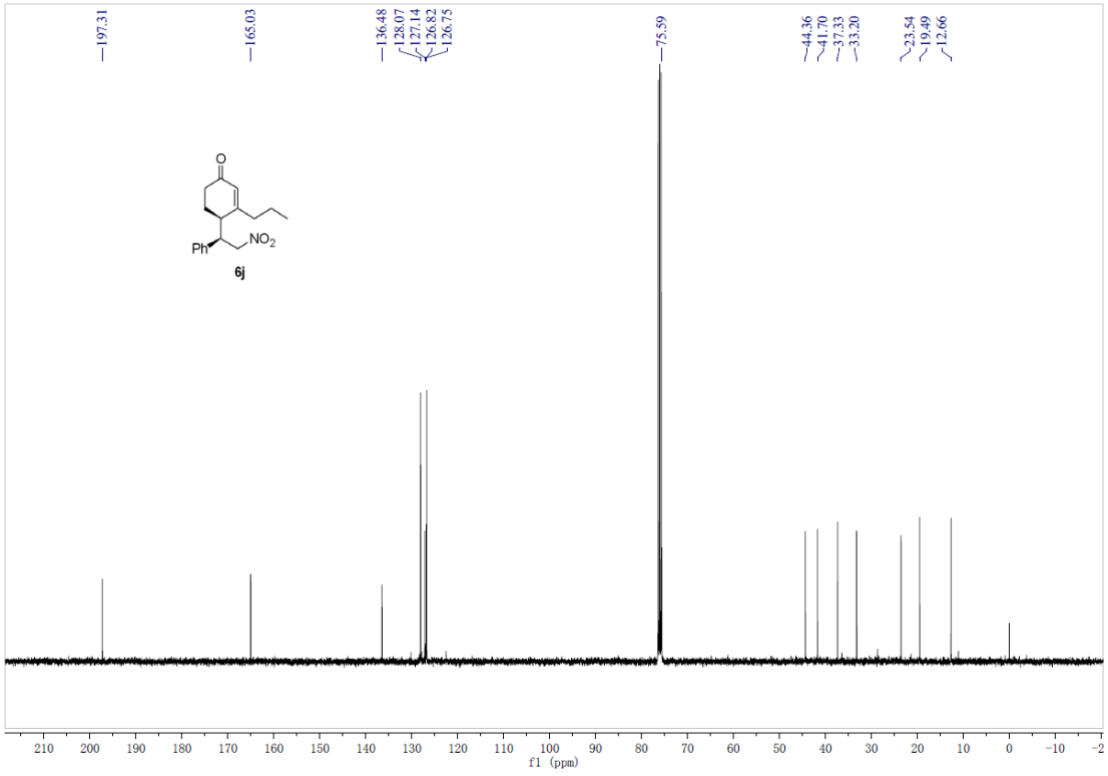
6i: (*R*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



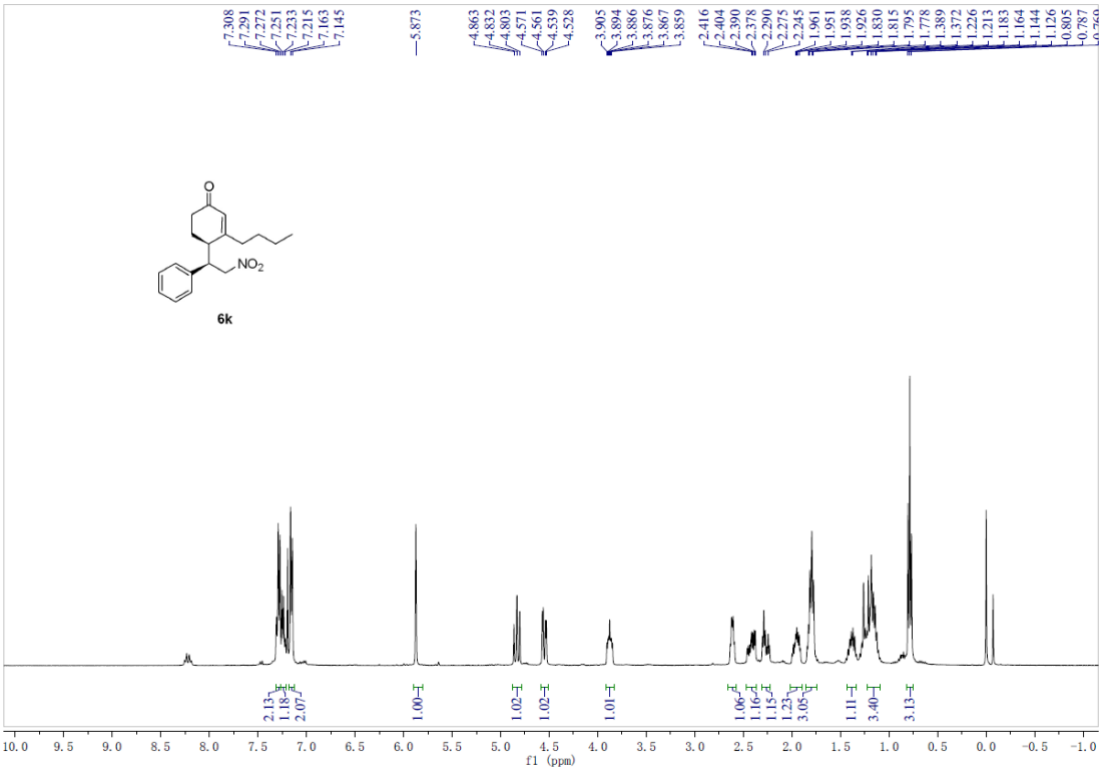


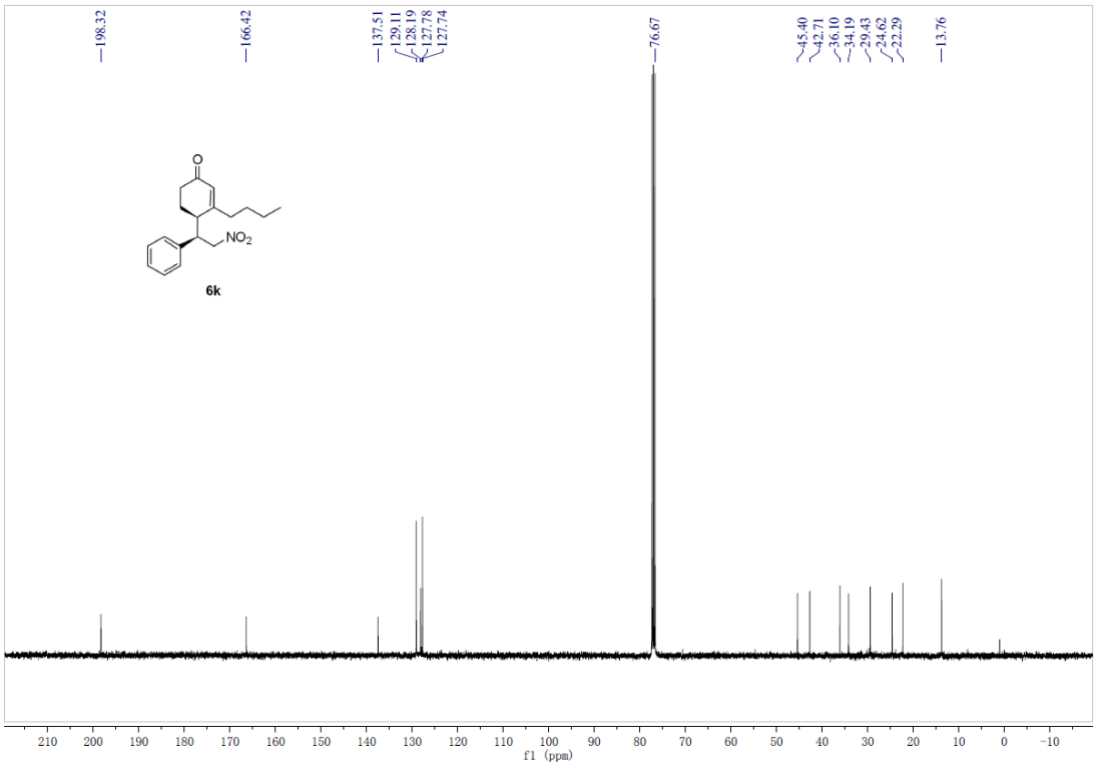
6j: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one



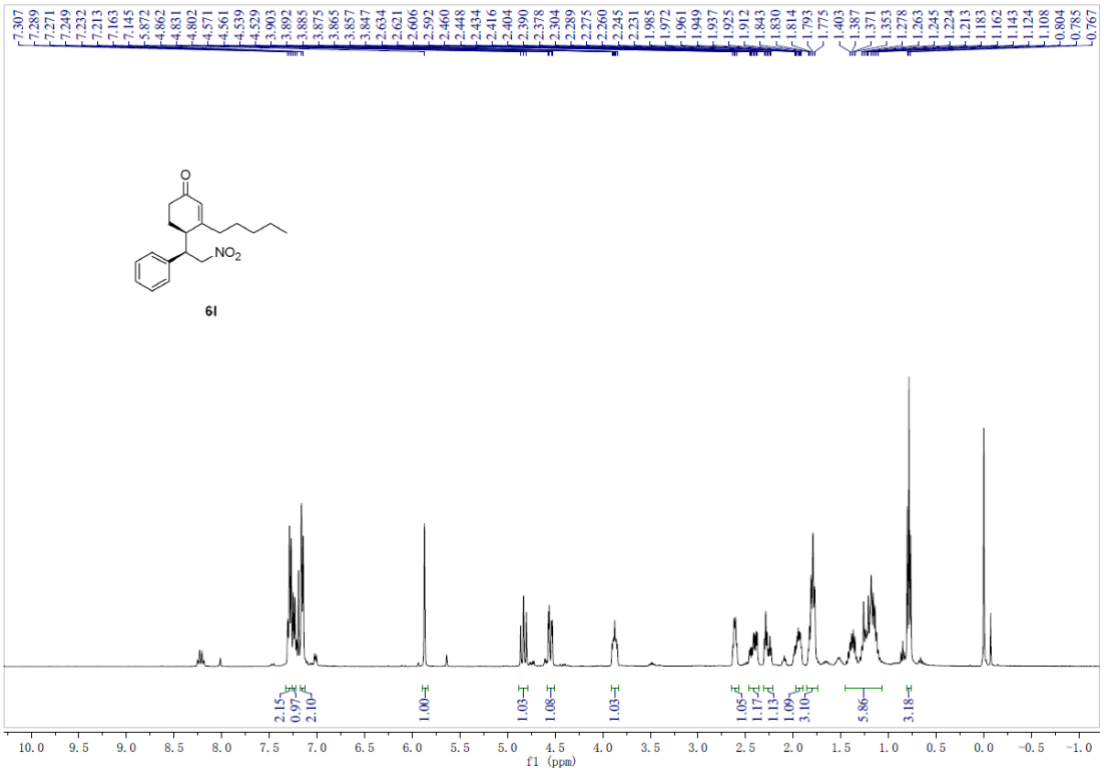


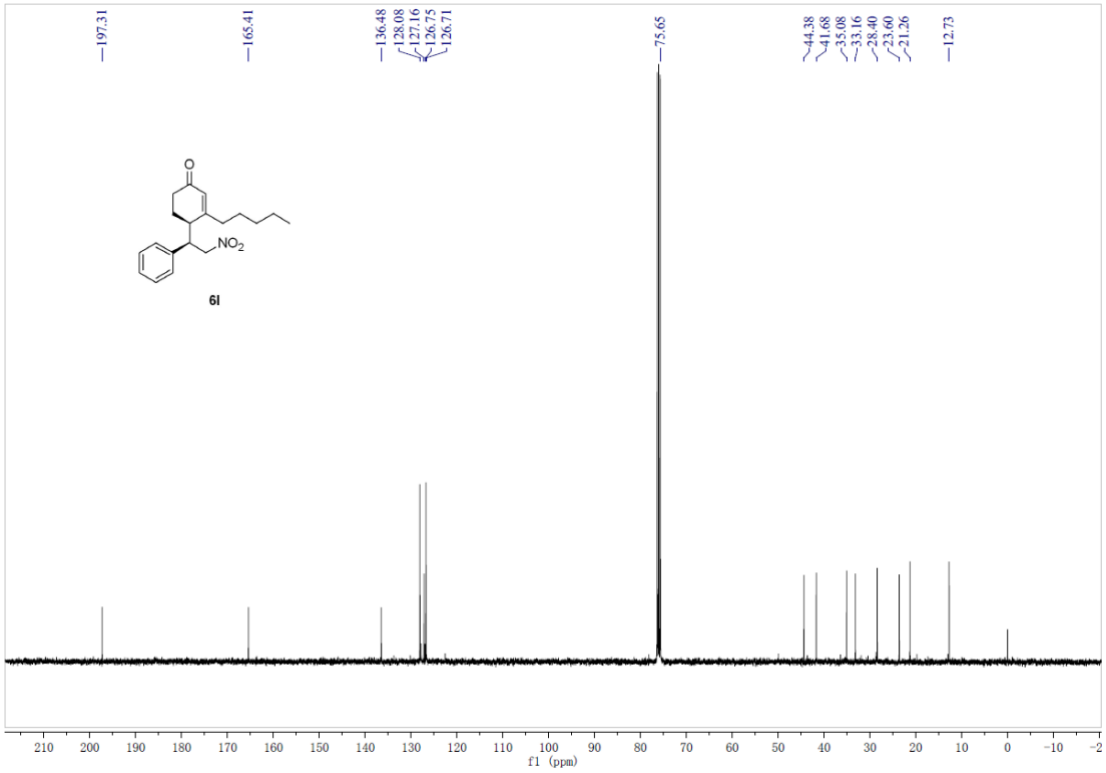
6k: (*R*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



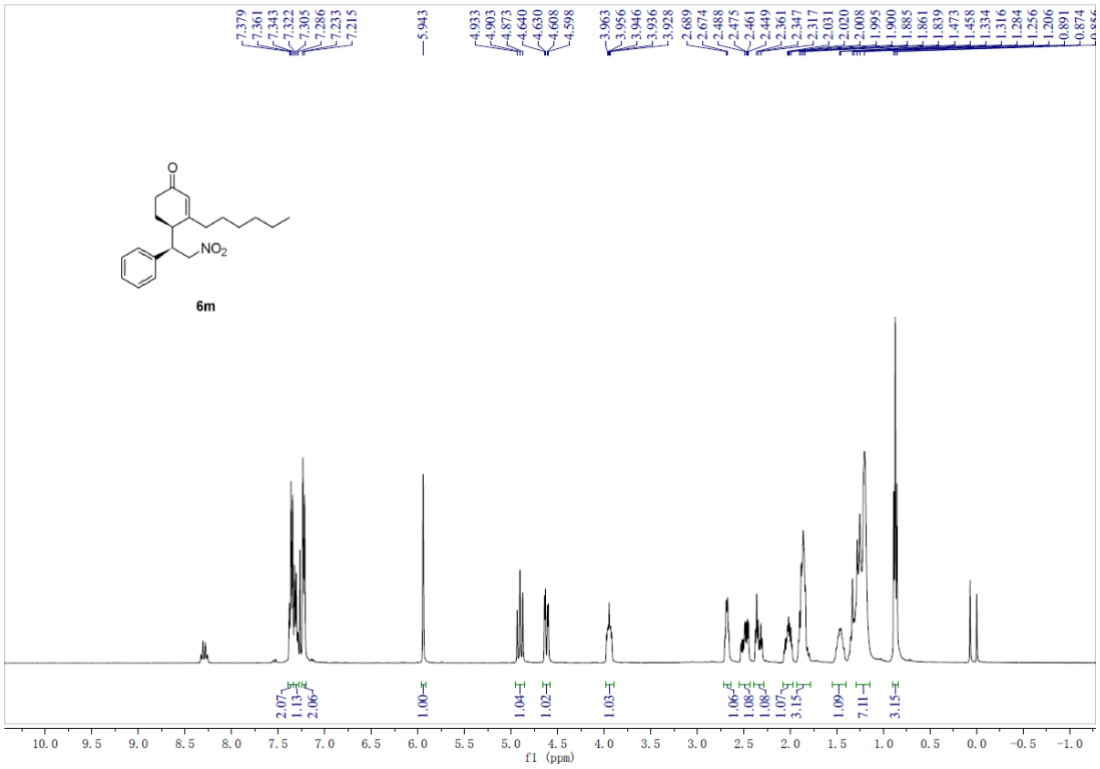


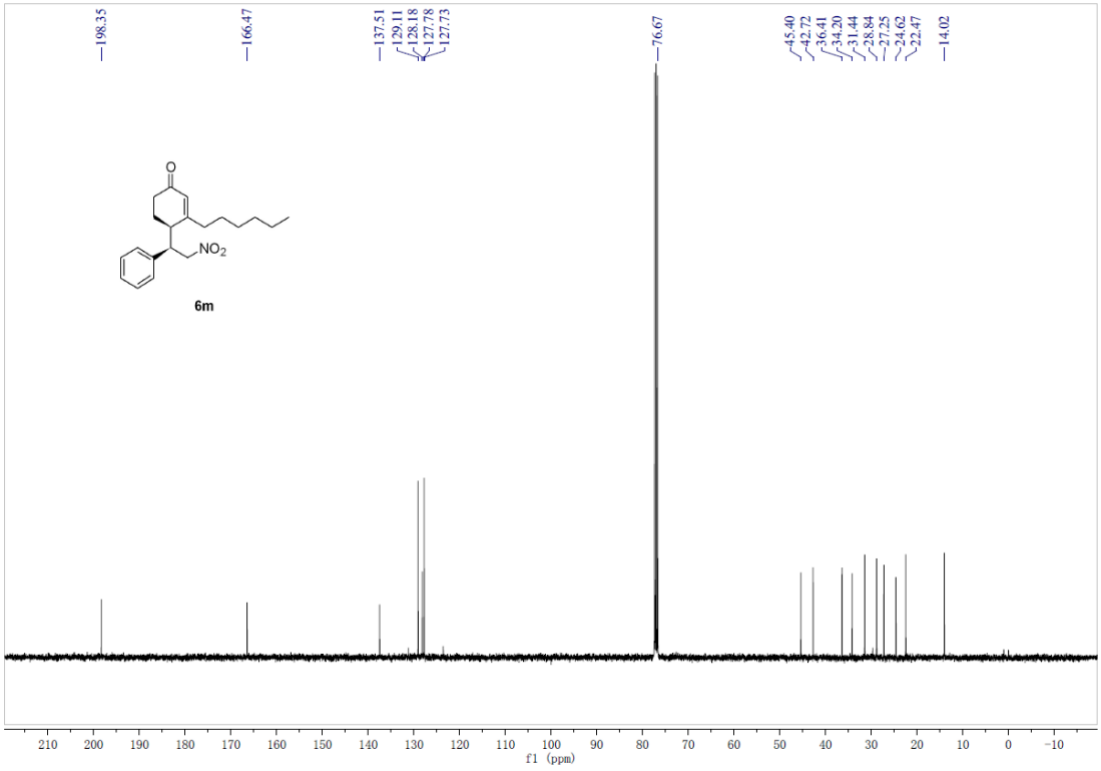
6l: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one



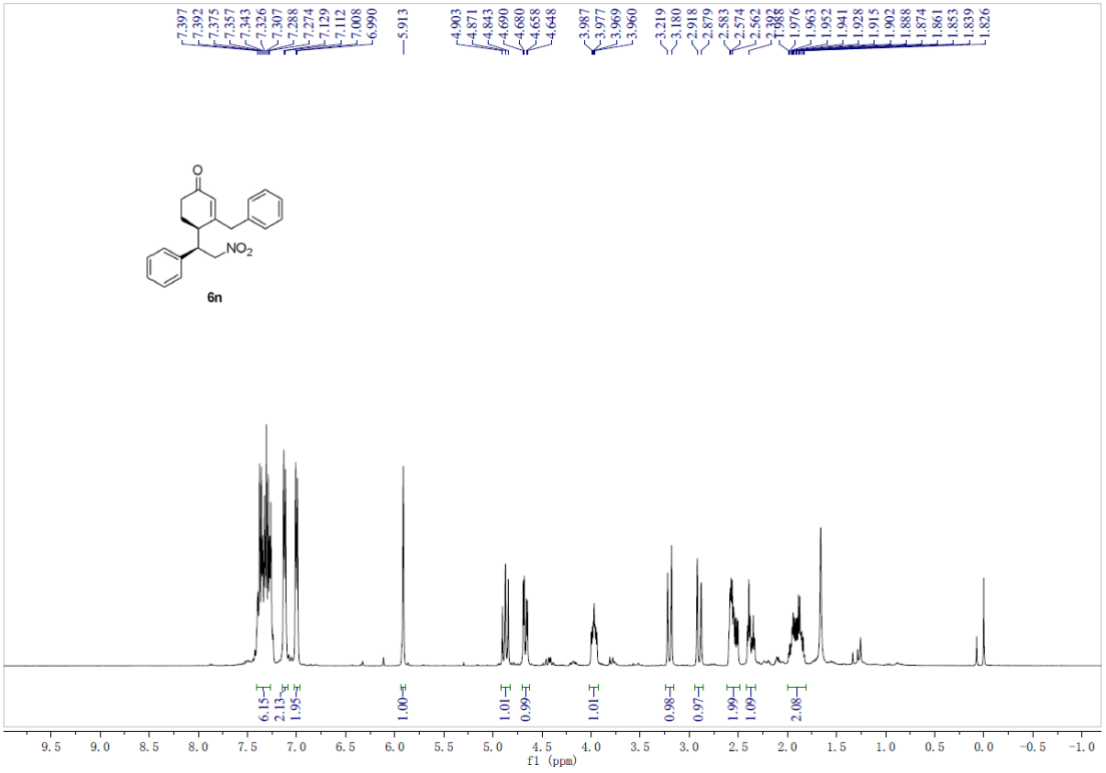


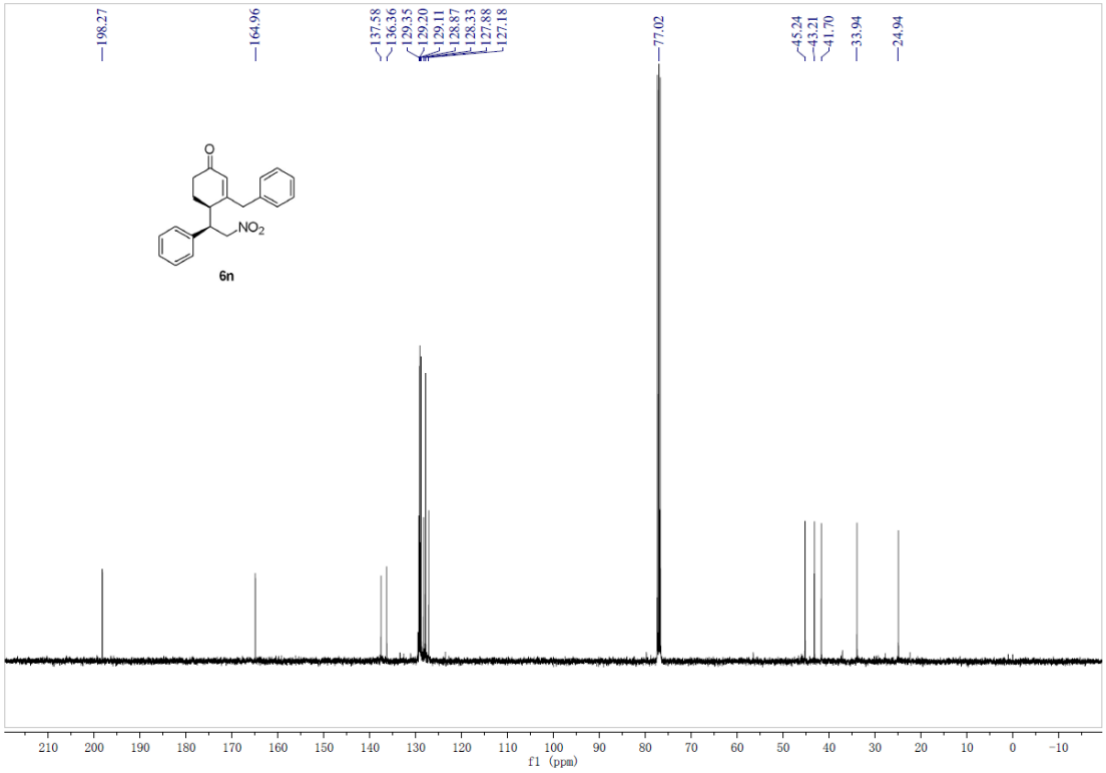
6m: (*R*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



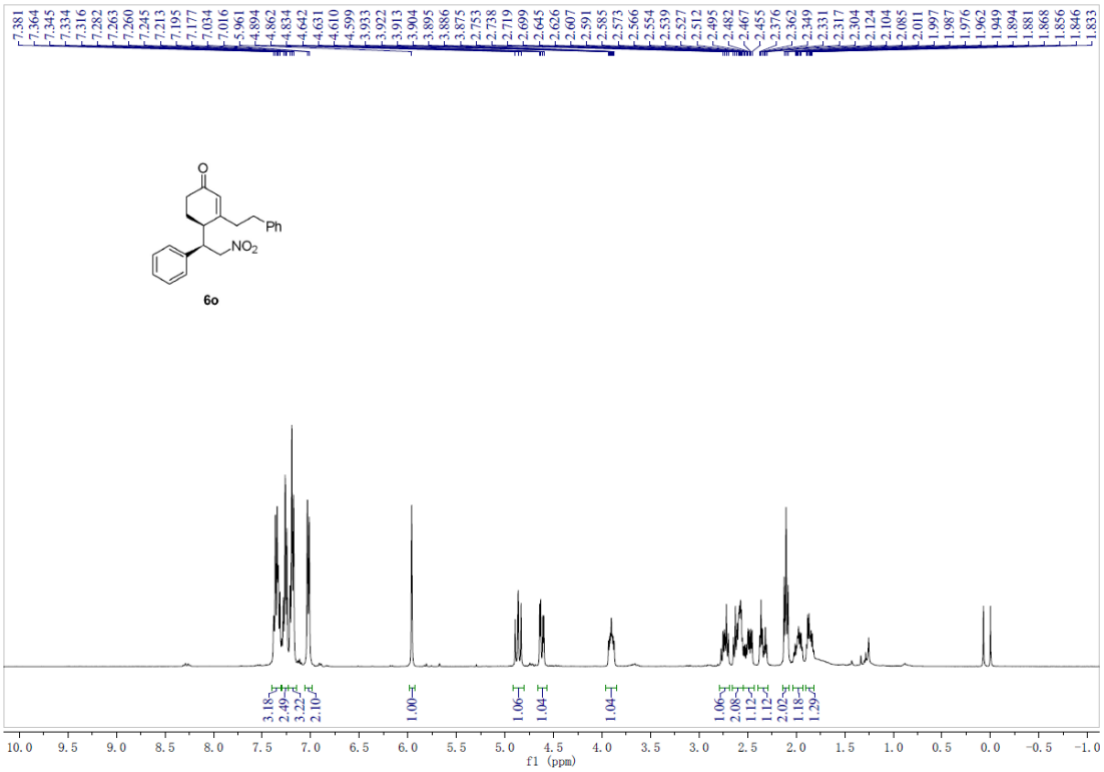


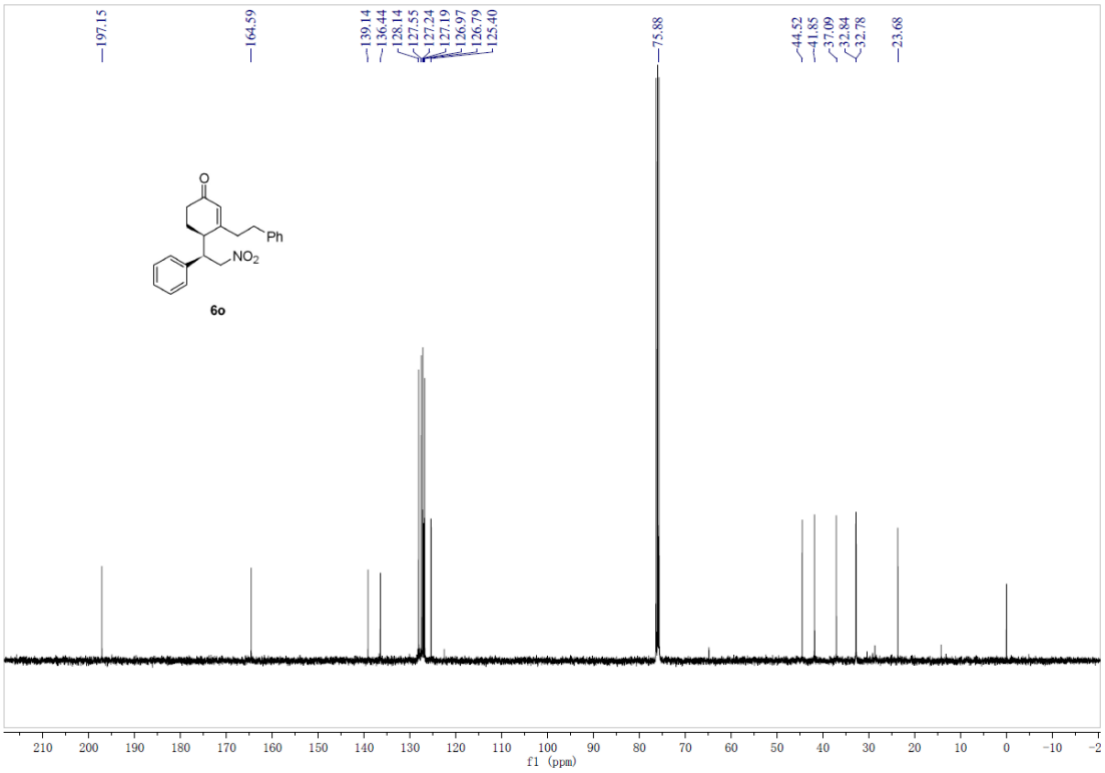
6n: (*R*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



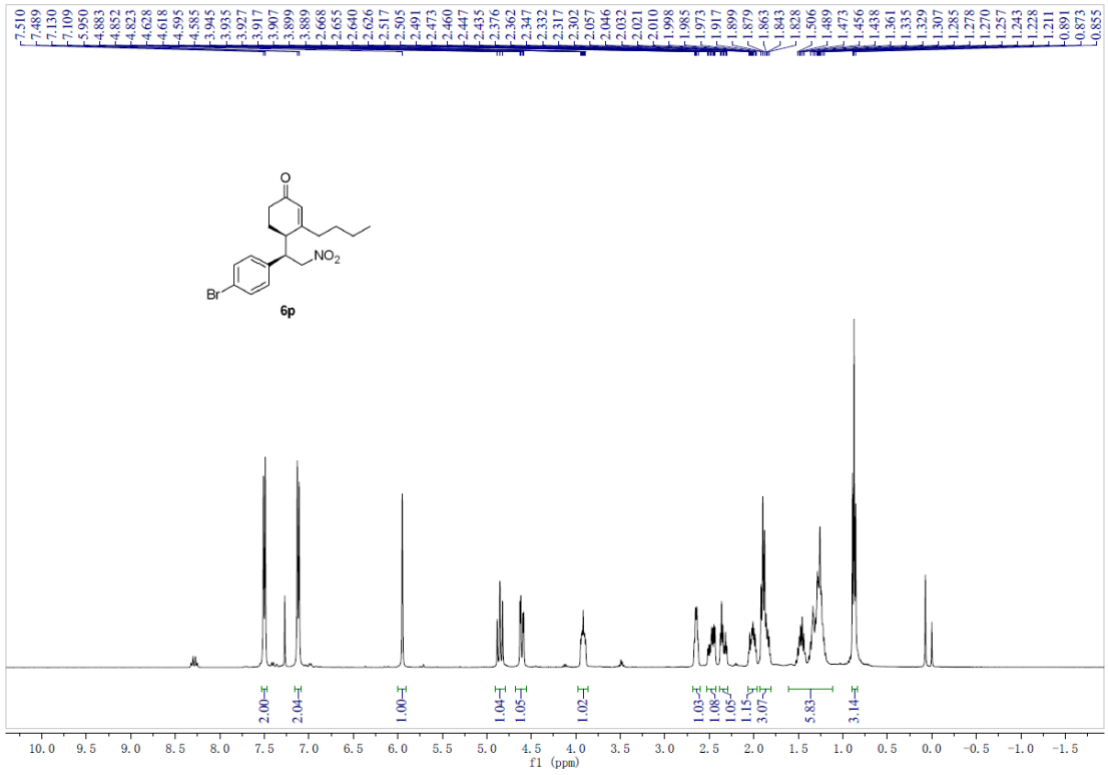


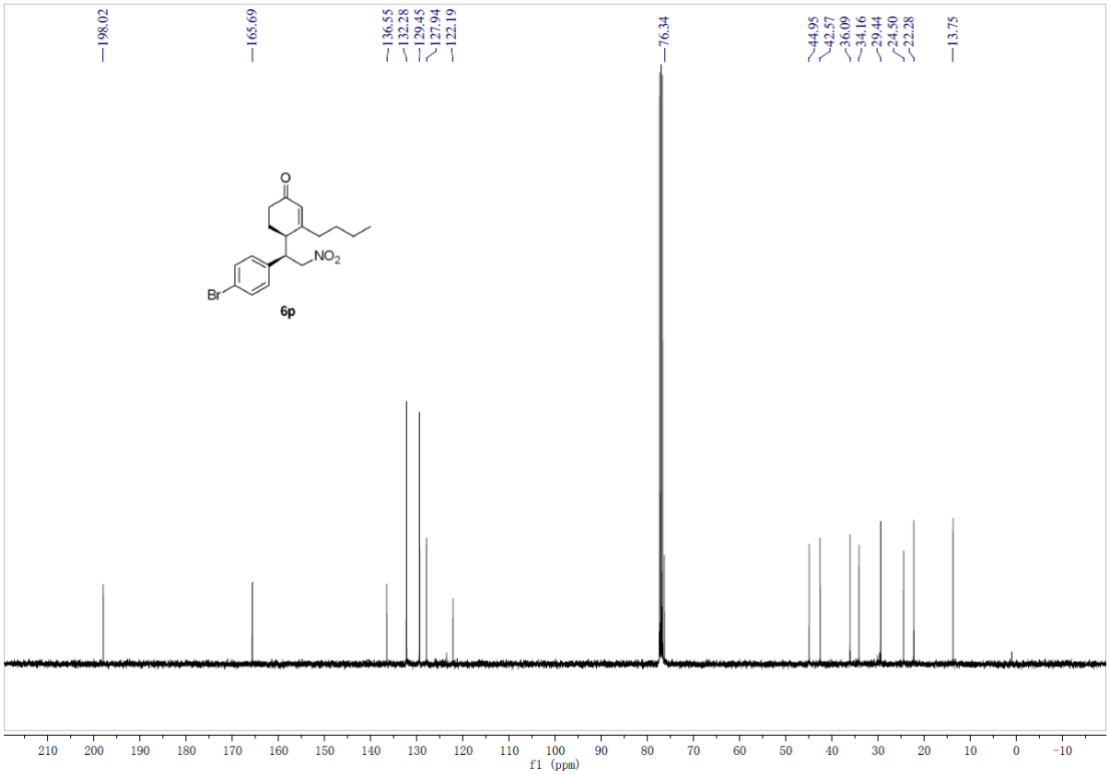
6o: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one



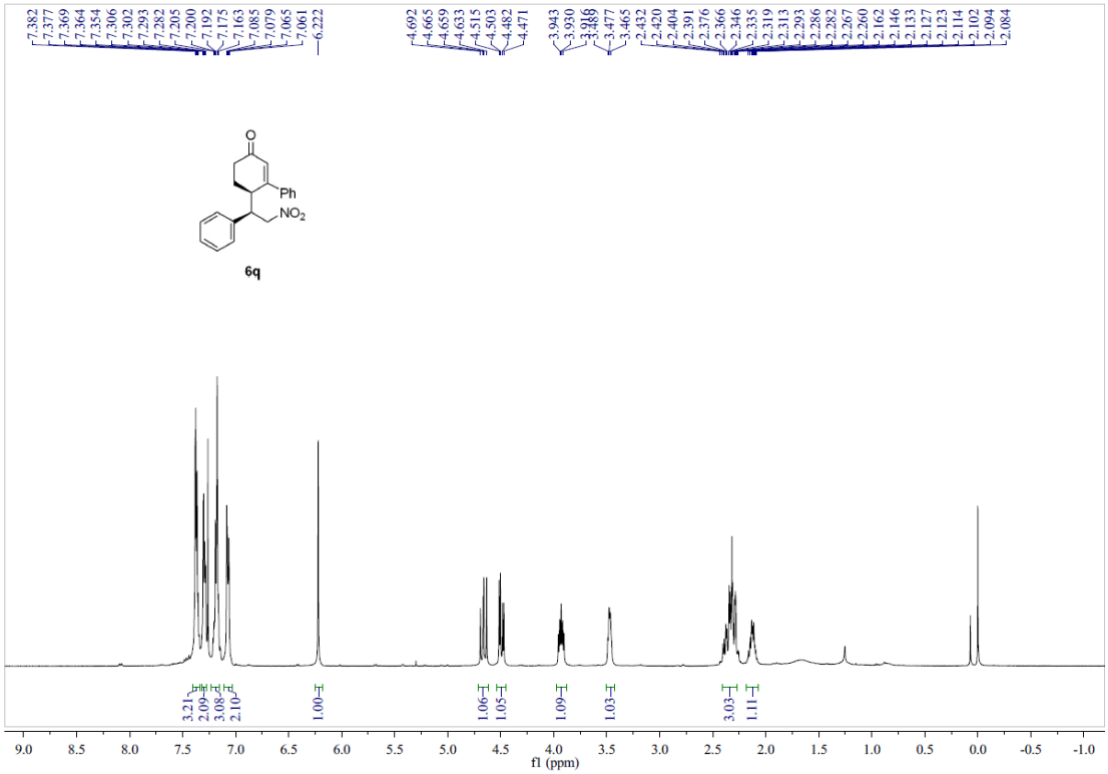


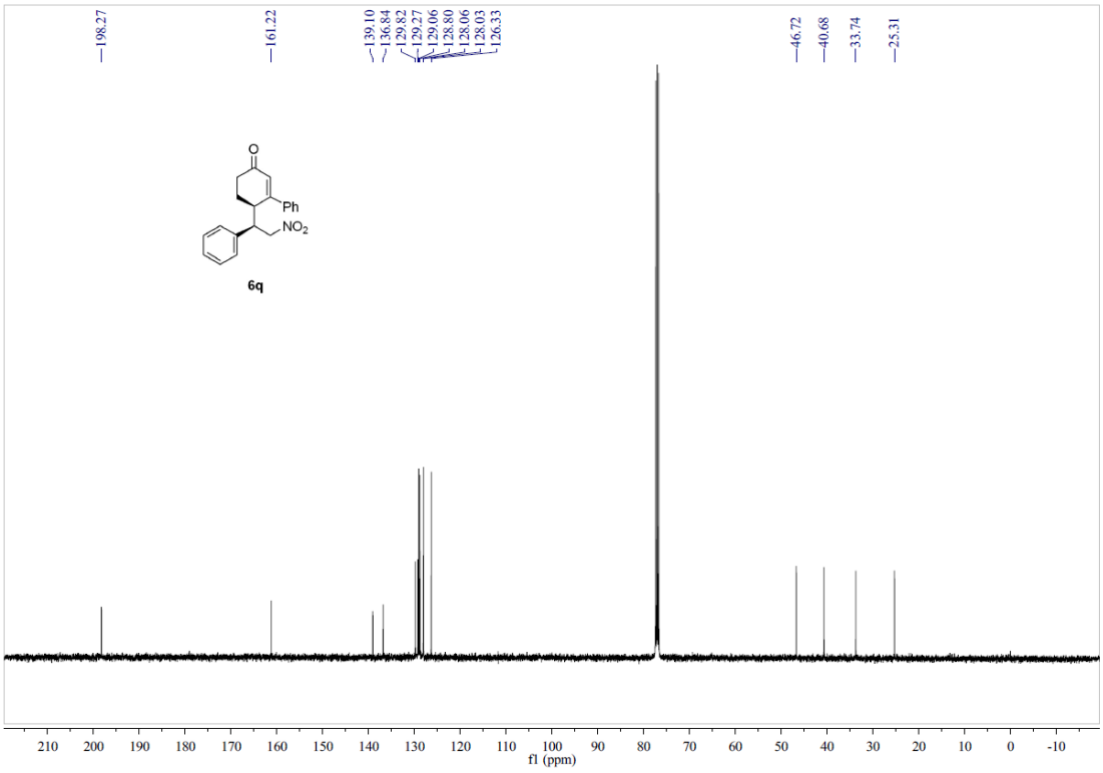
6p: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-pentylcyclohex-2-en-1-one



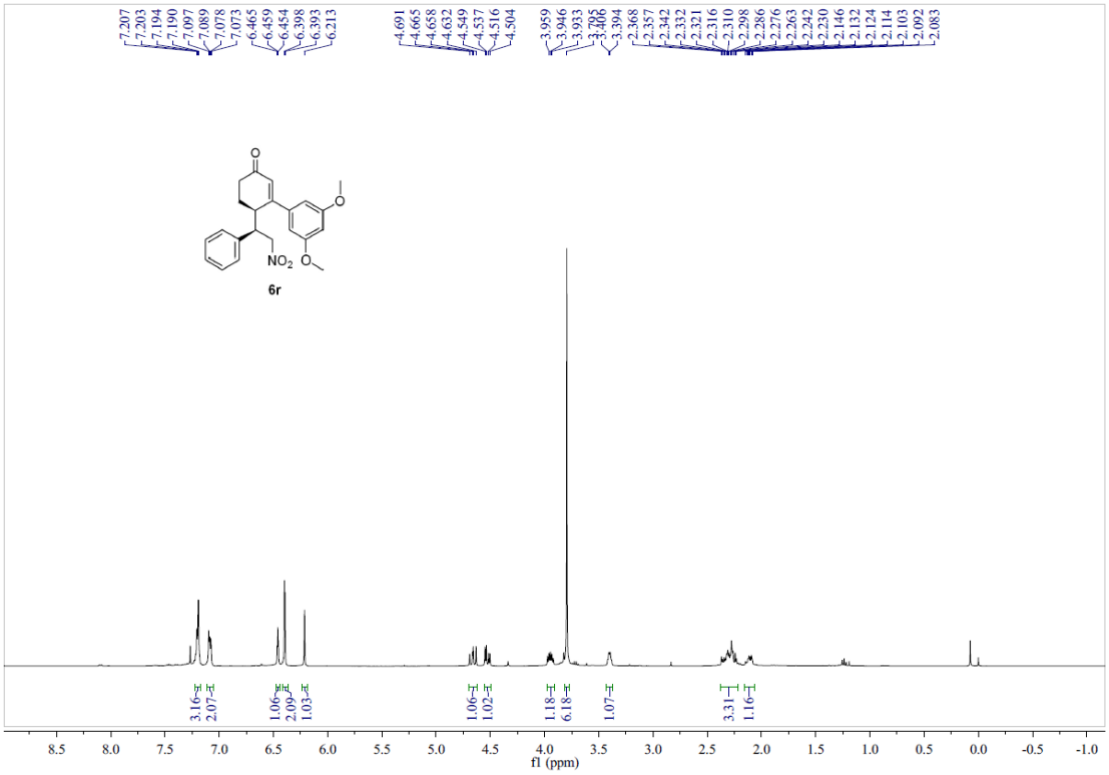


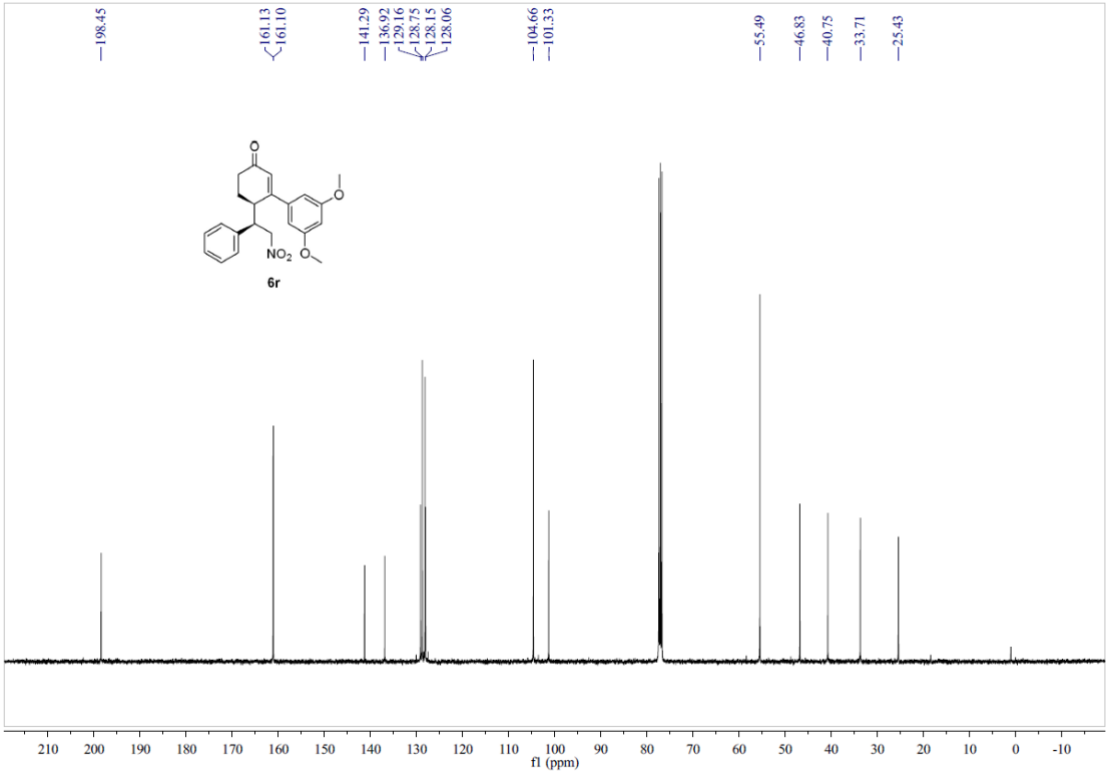
6q: (*R*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



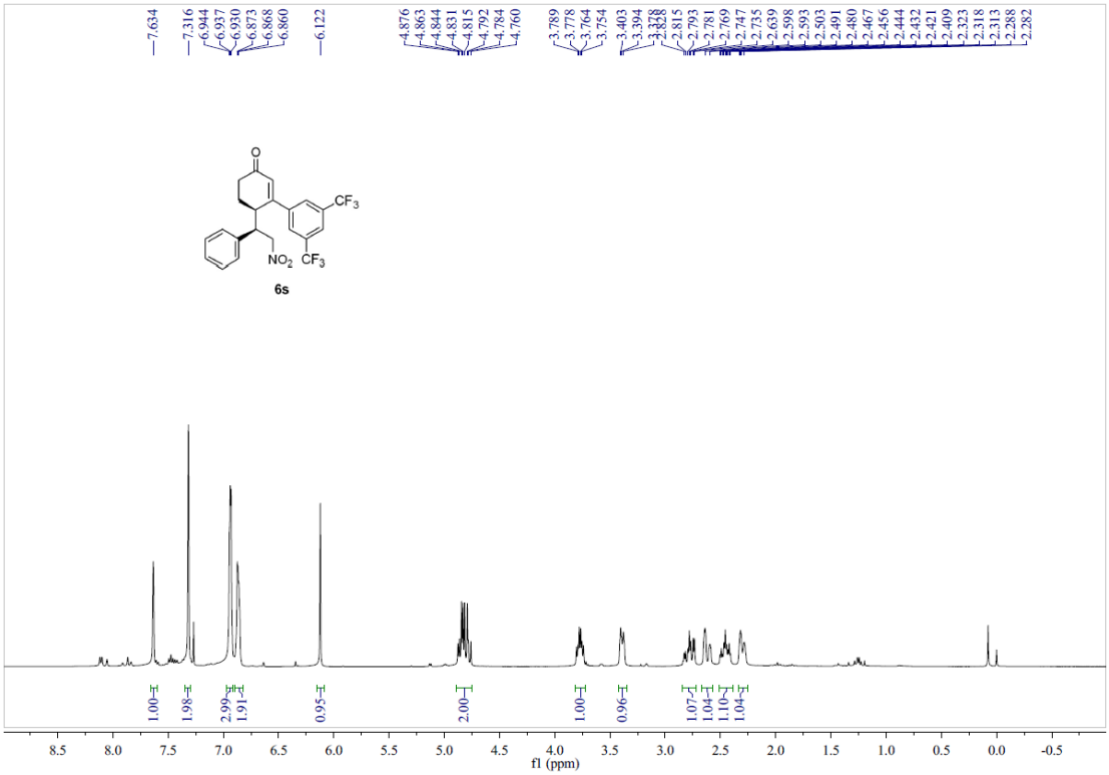


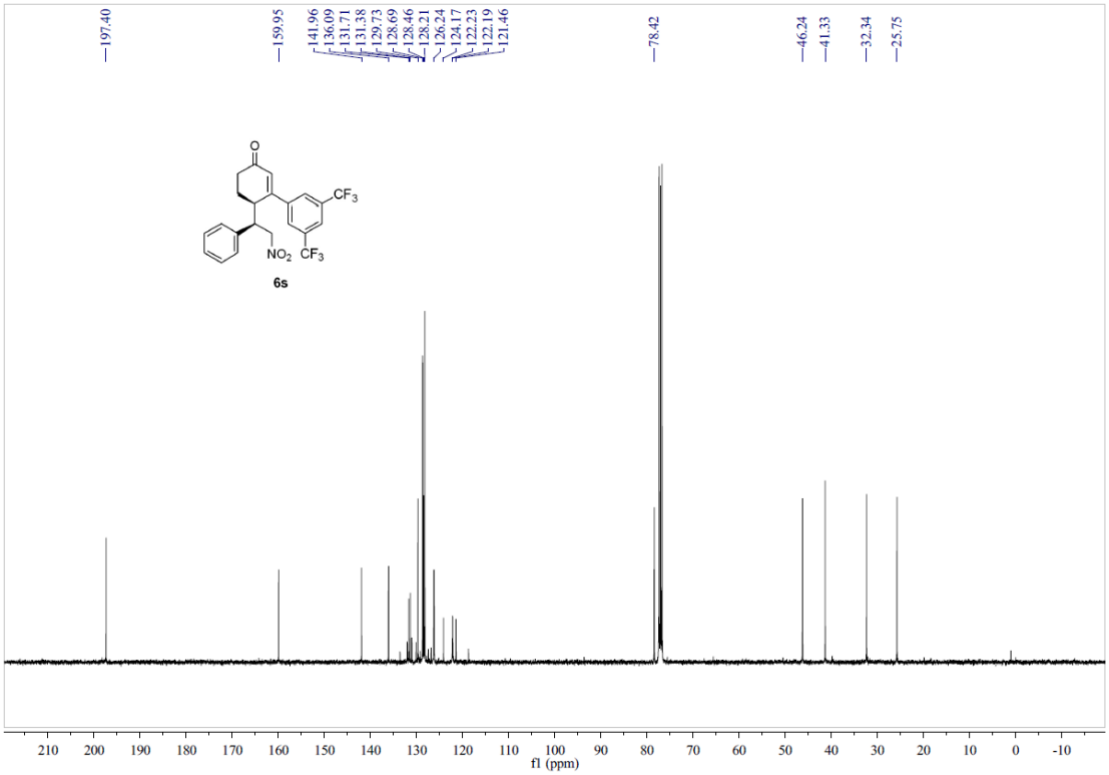
6r: (*R*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



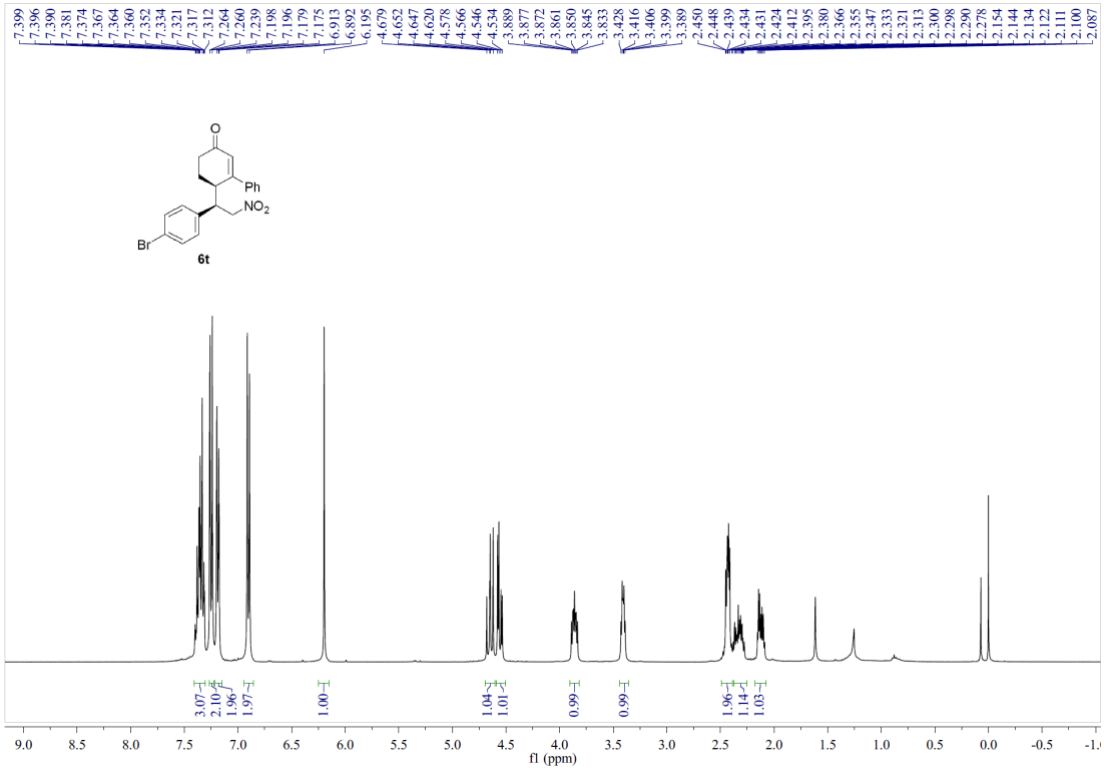


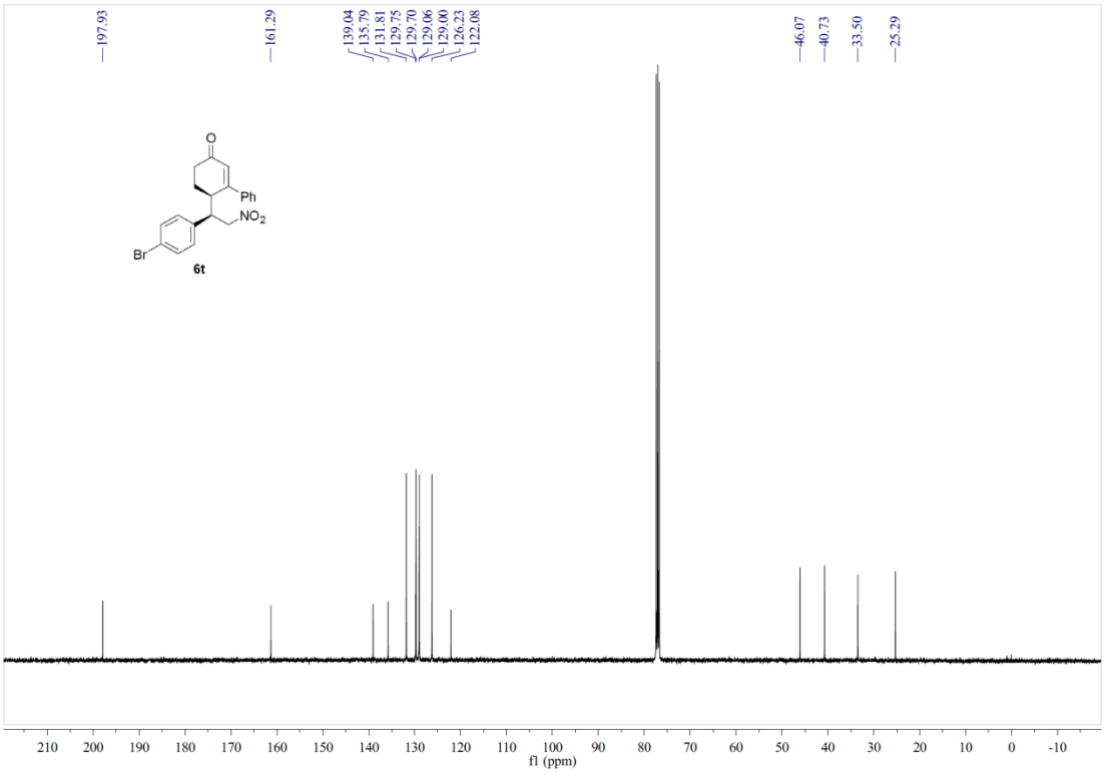
6s: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



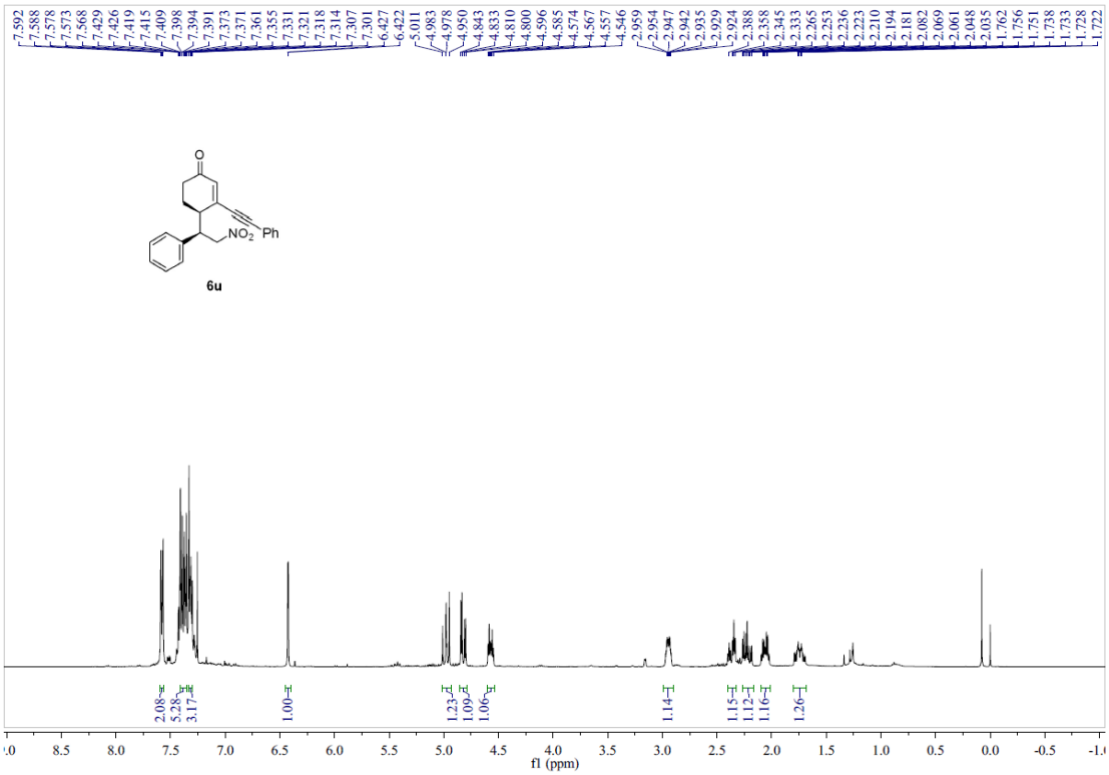


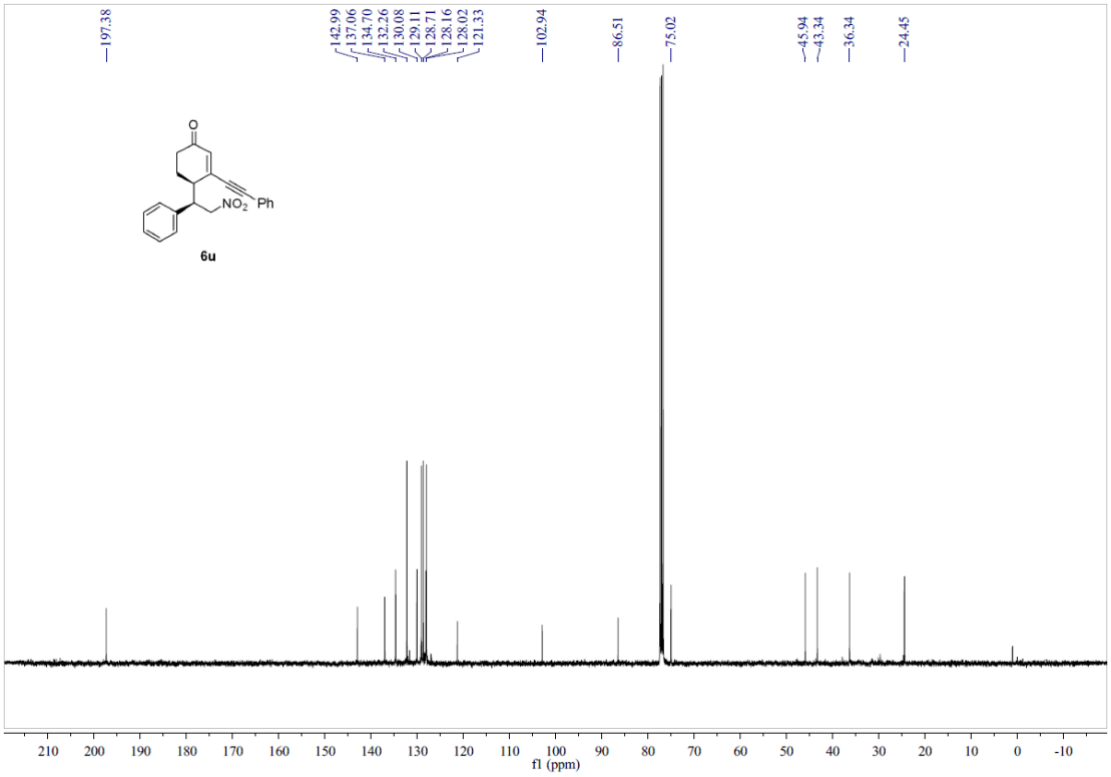
6t: (*R*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



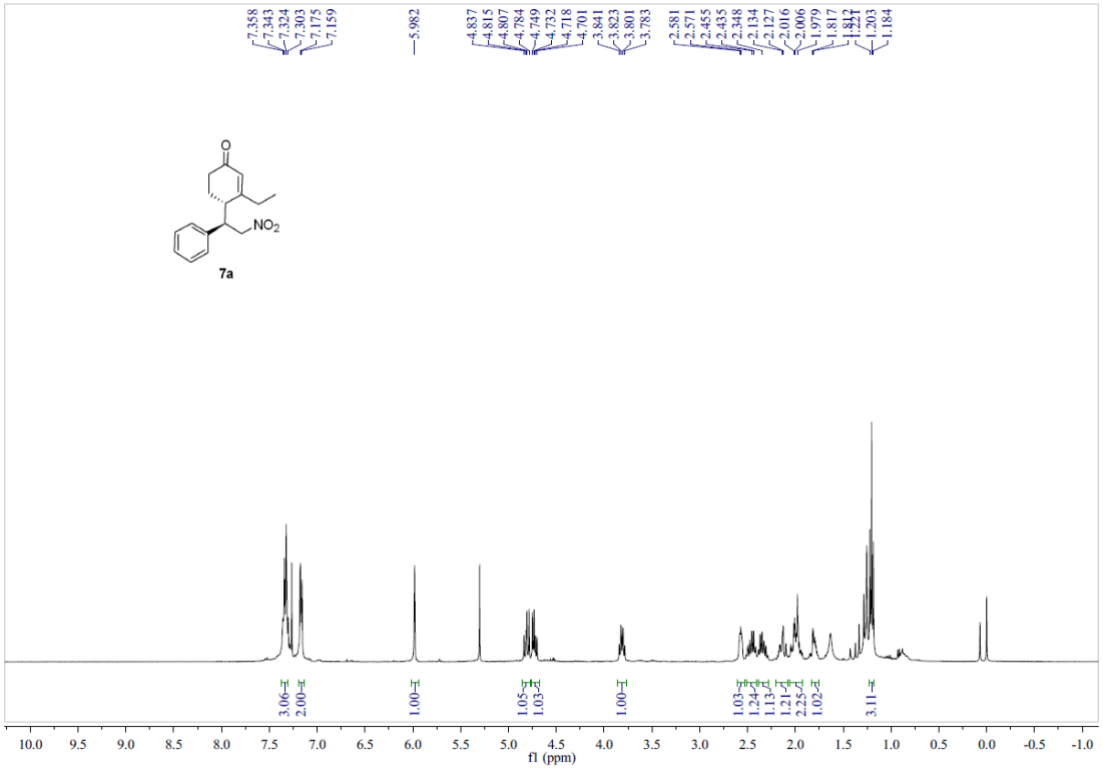


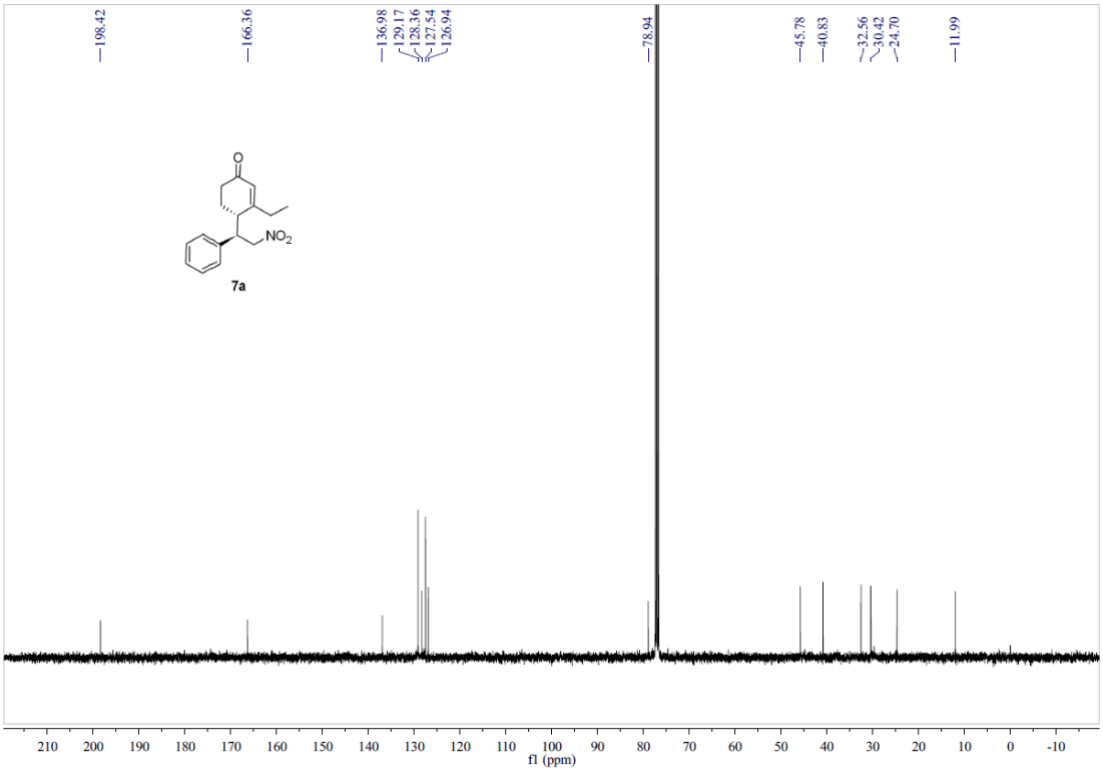
6u: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one



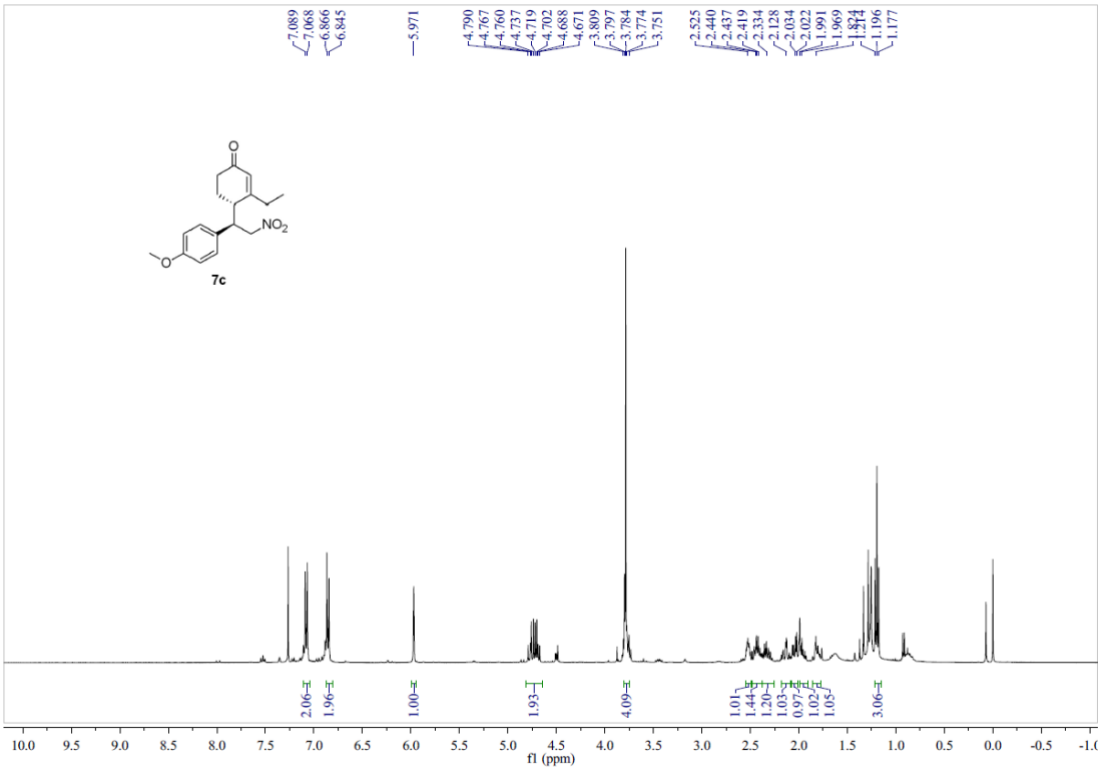


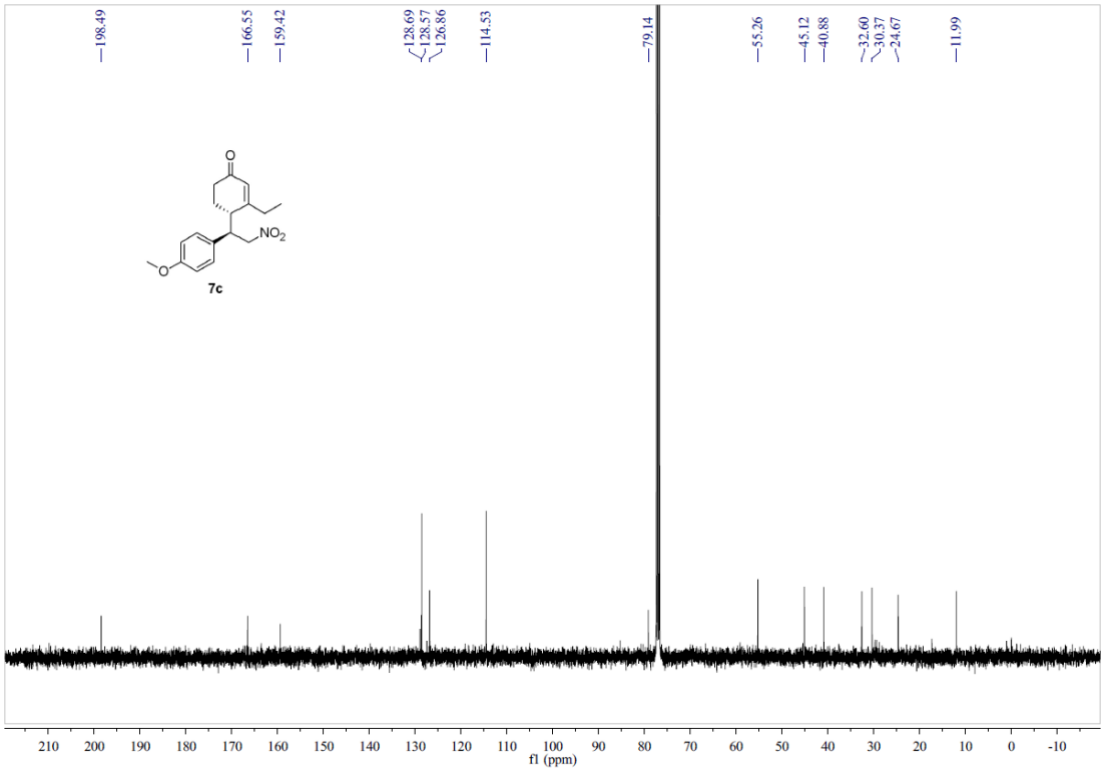
7a: (*S*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



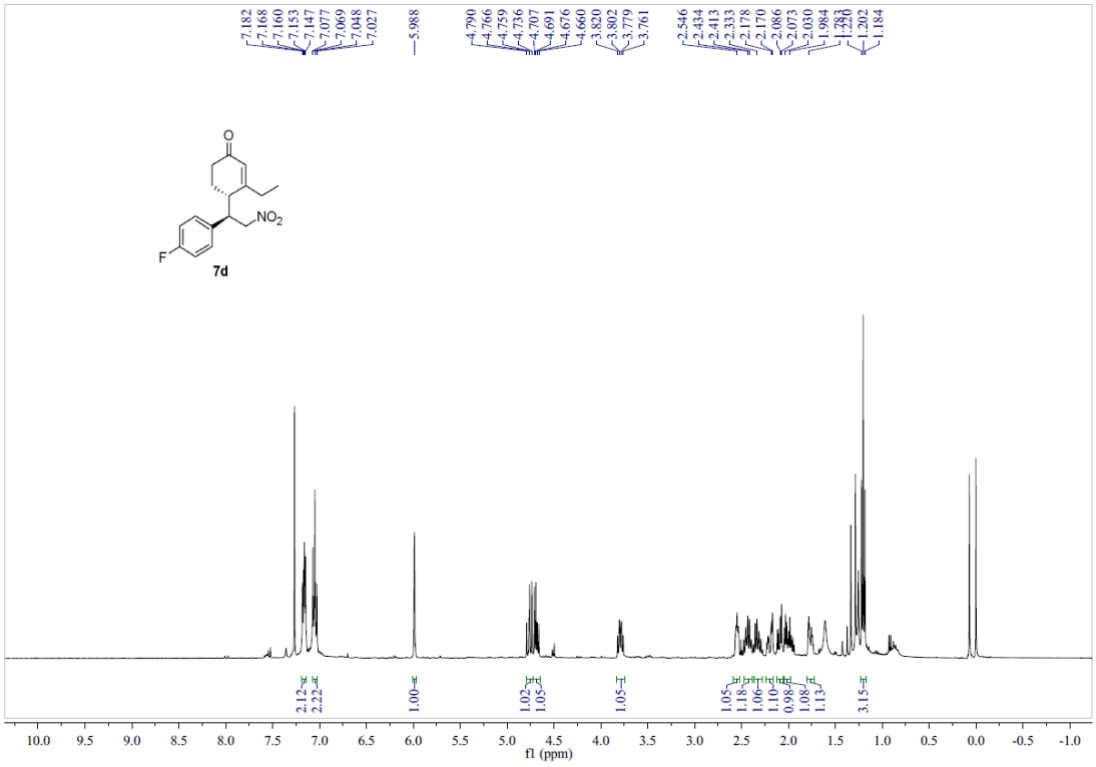


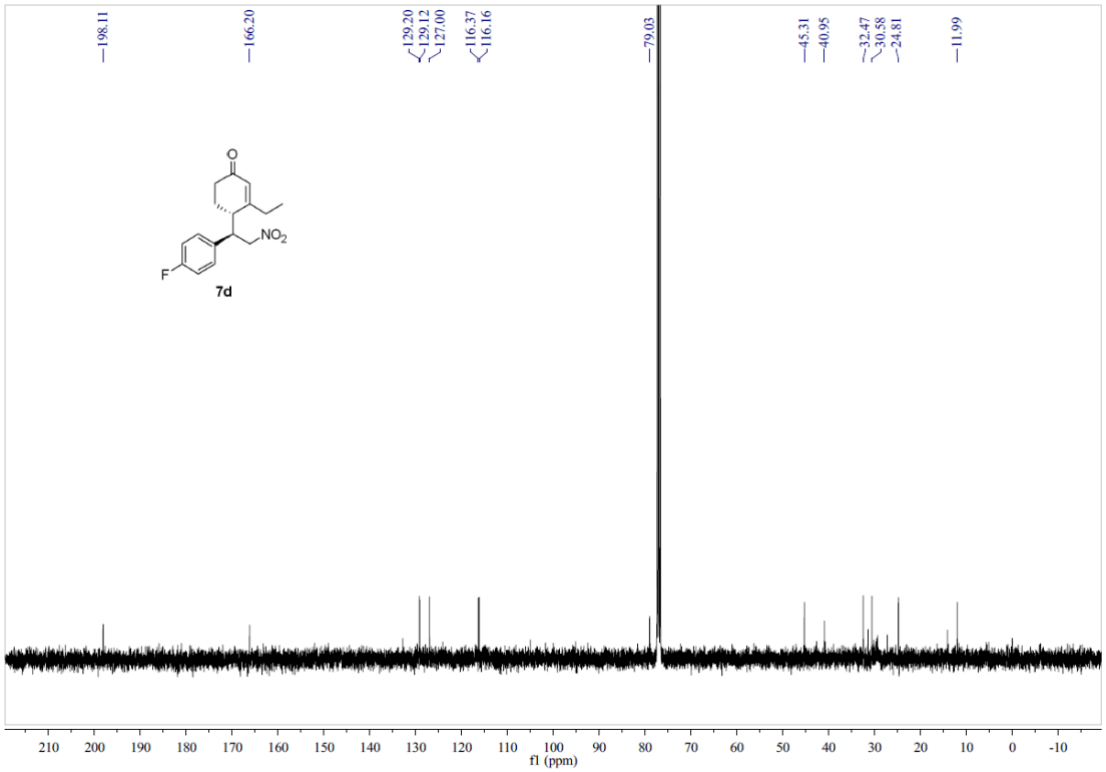
7c: (*S*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one



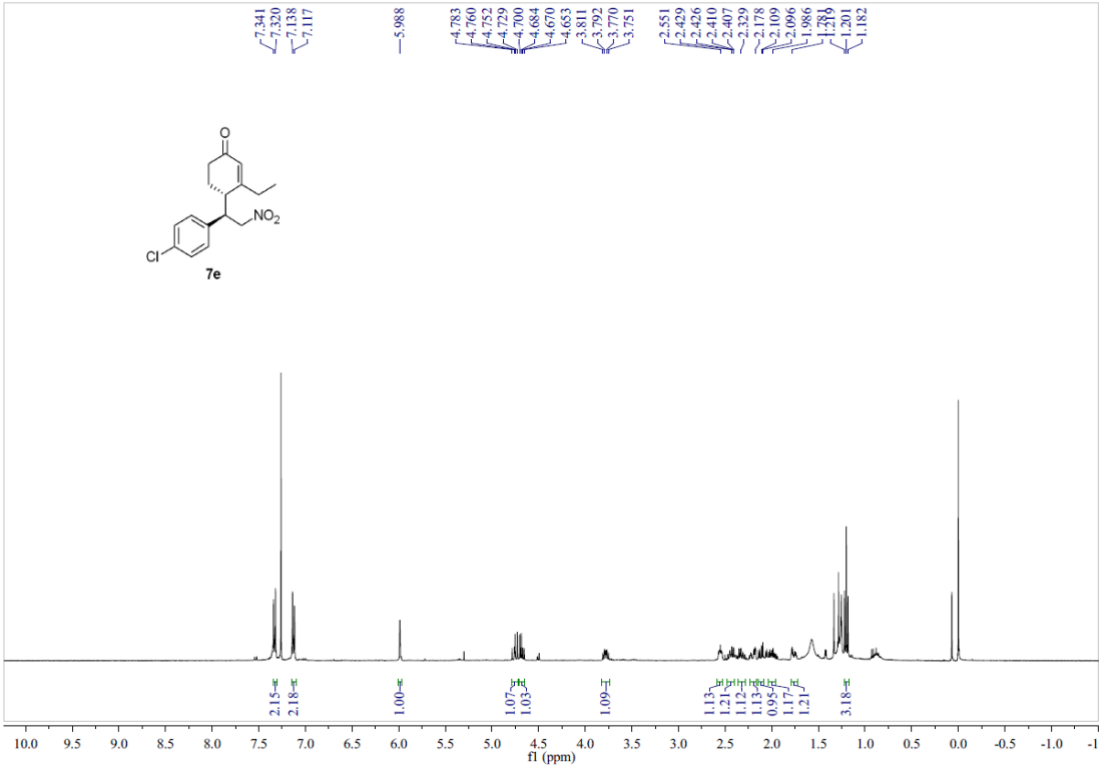


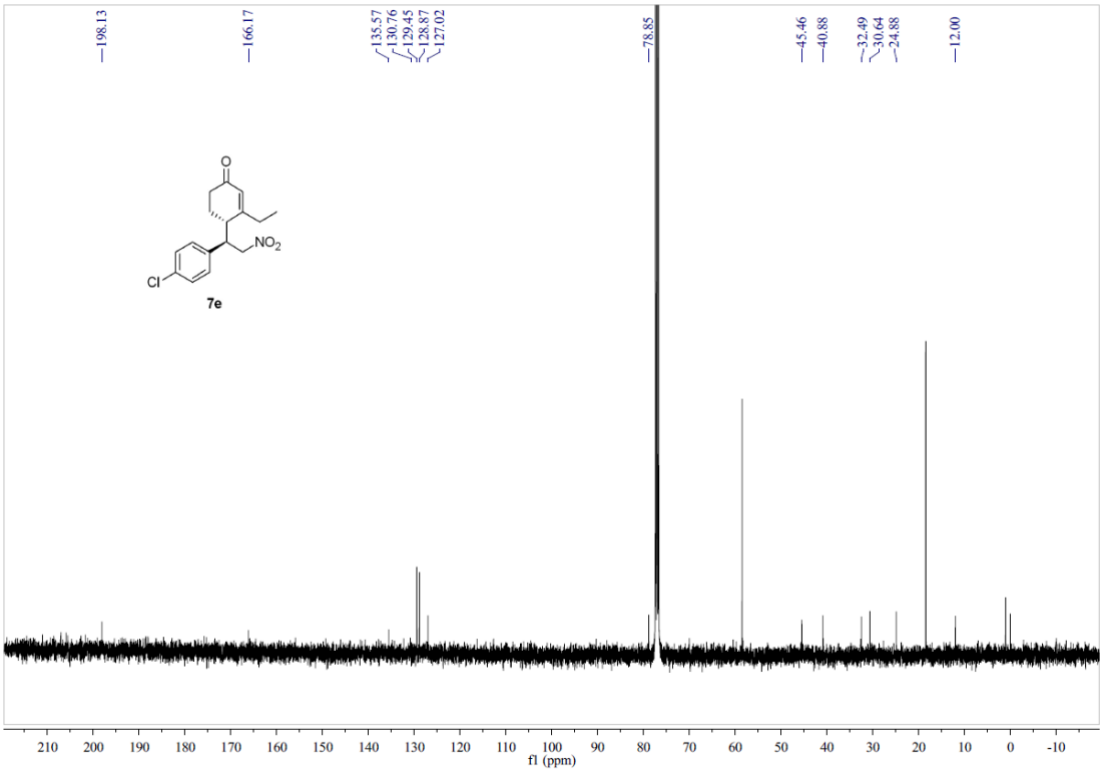
7d: (*S*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one



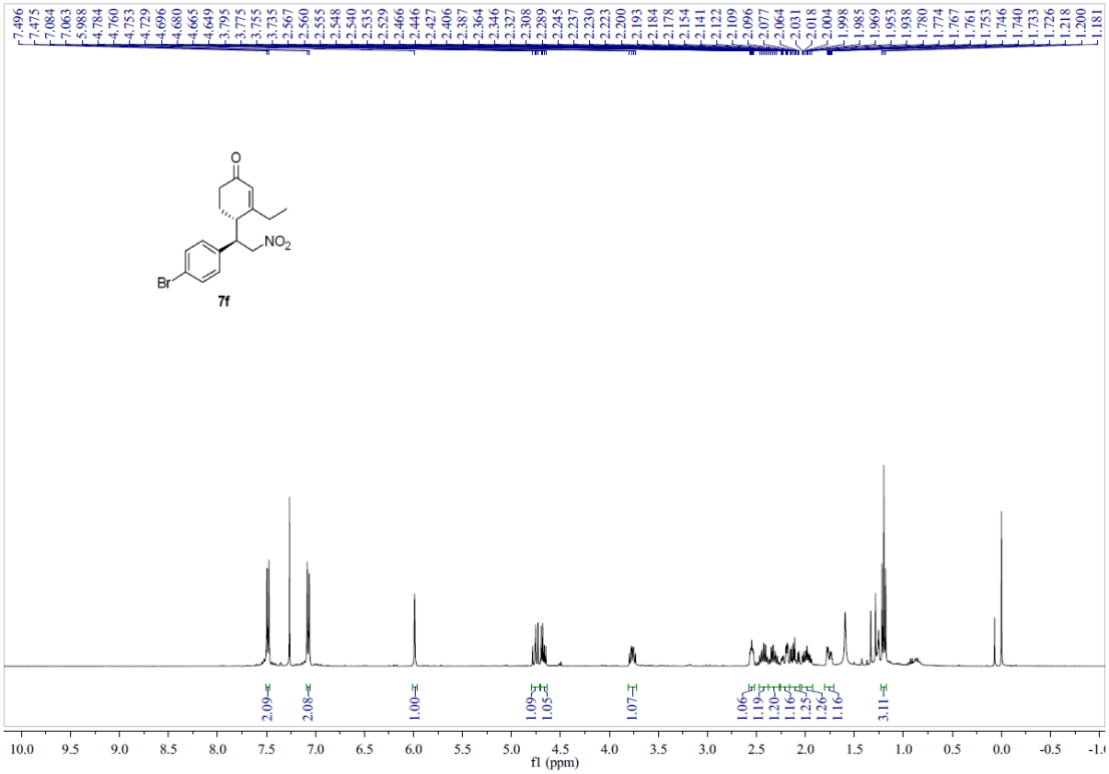


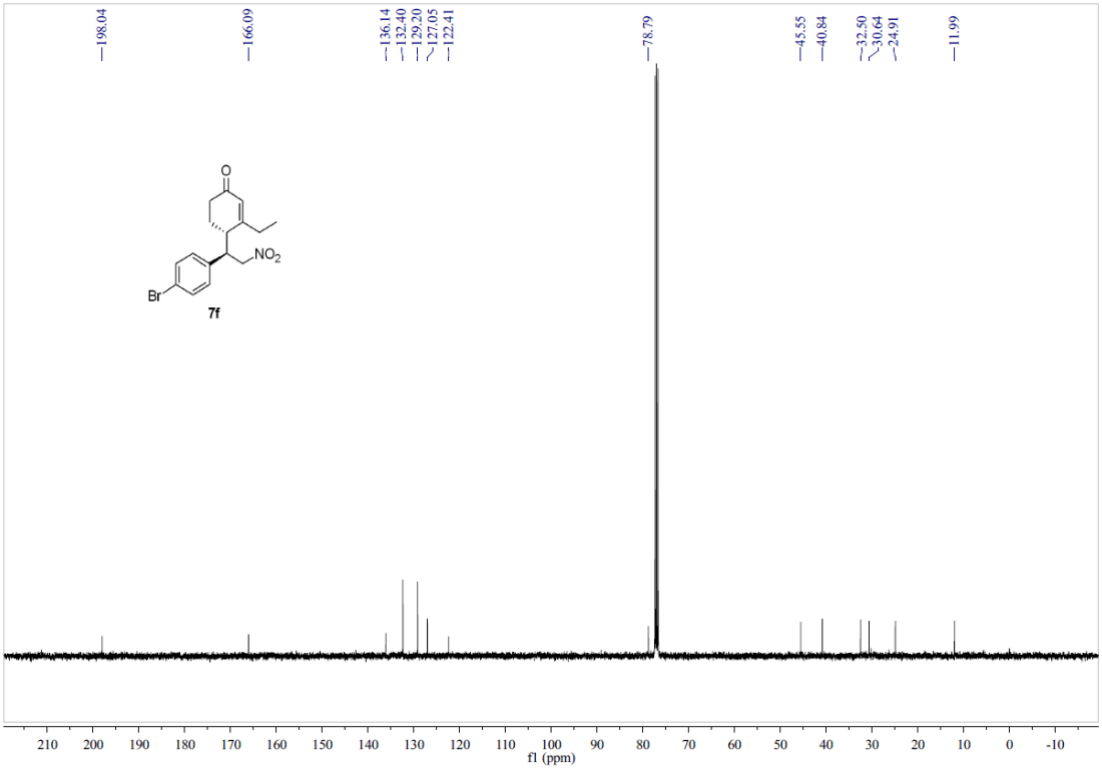
7e: (*S*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



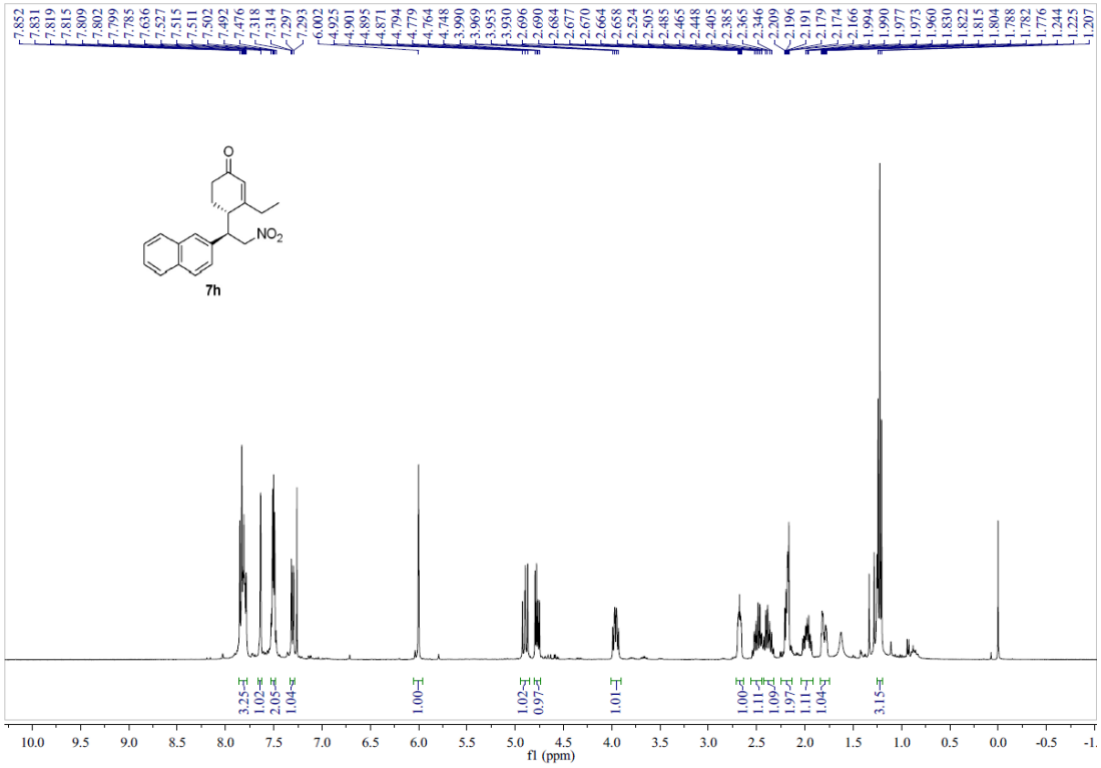


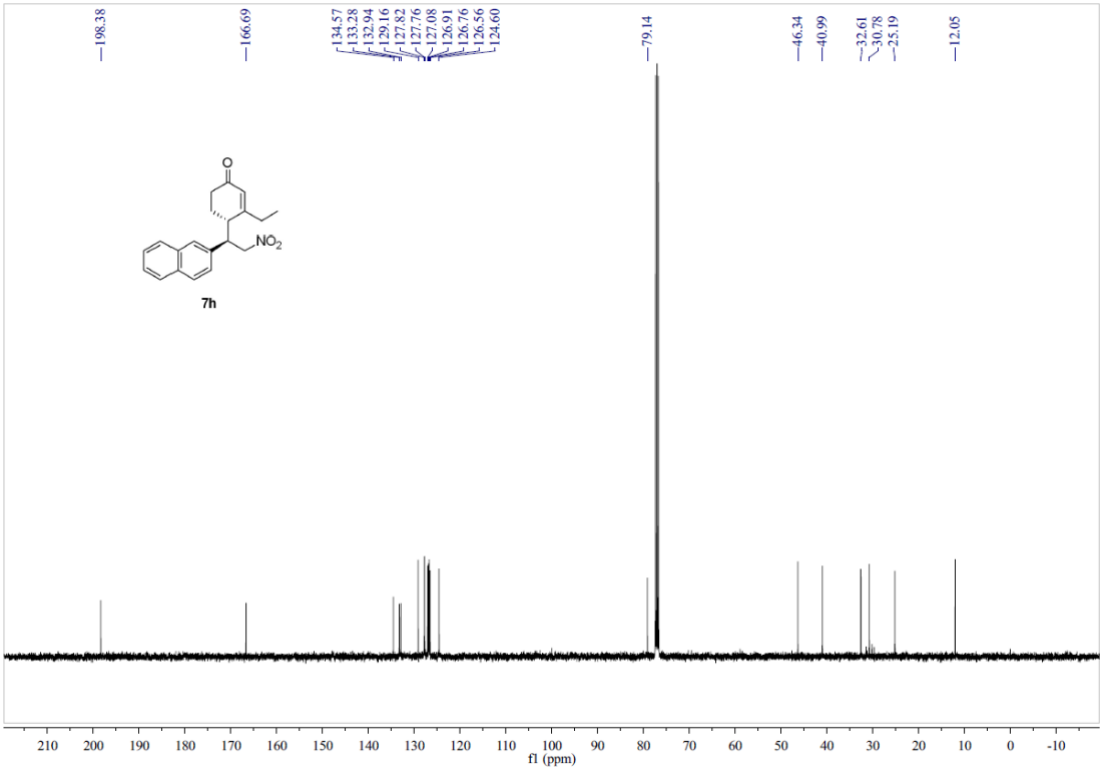
7f: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one



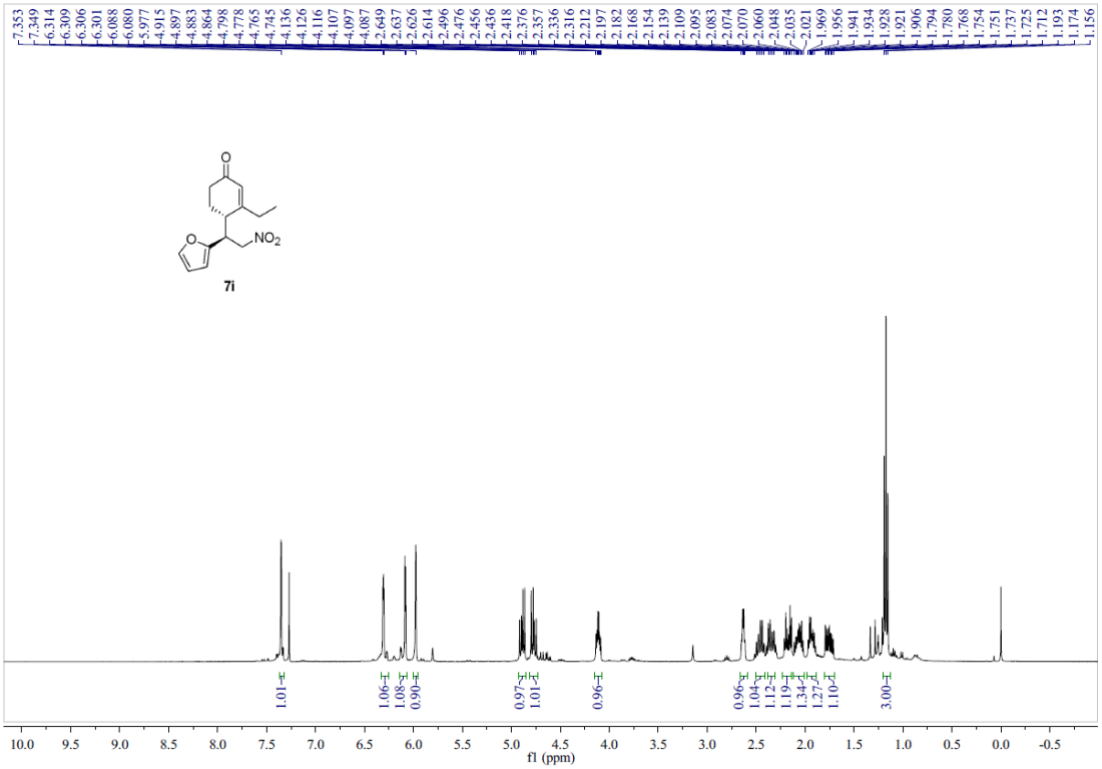


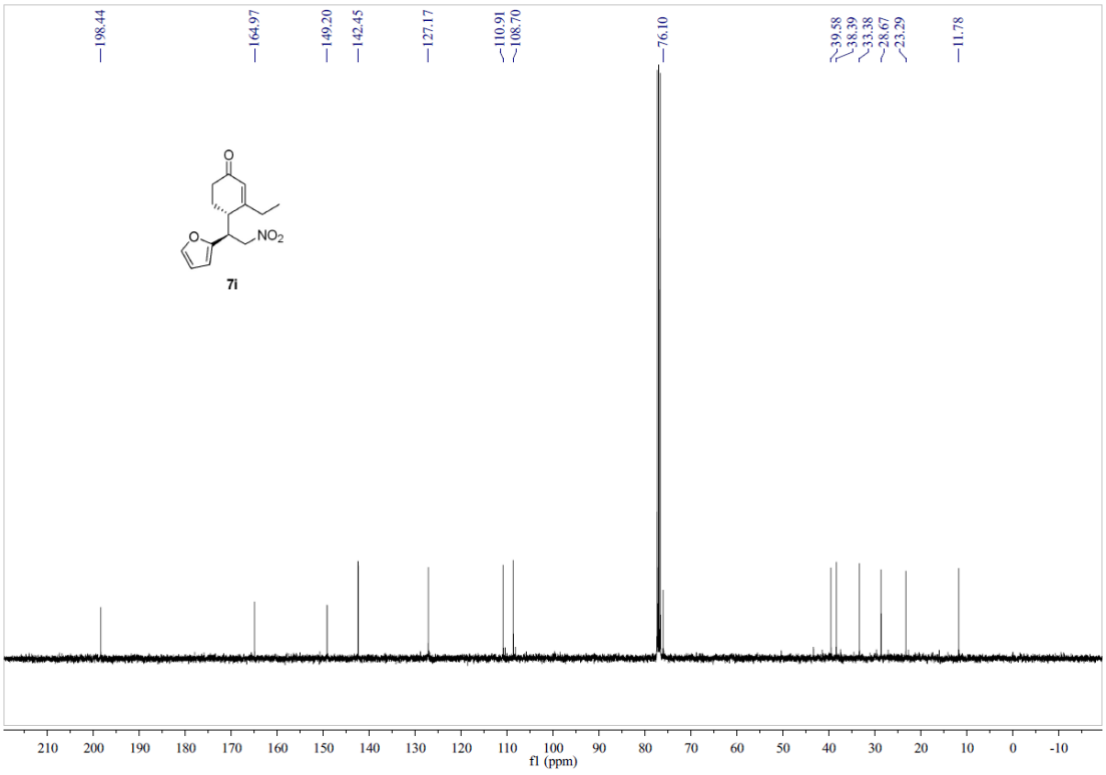
7h: (*S*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



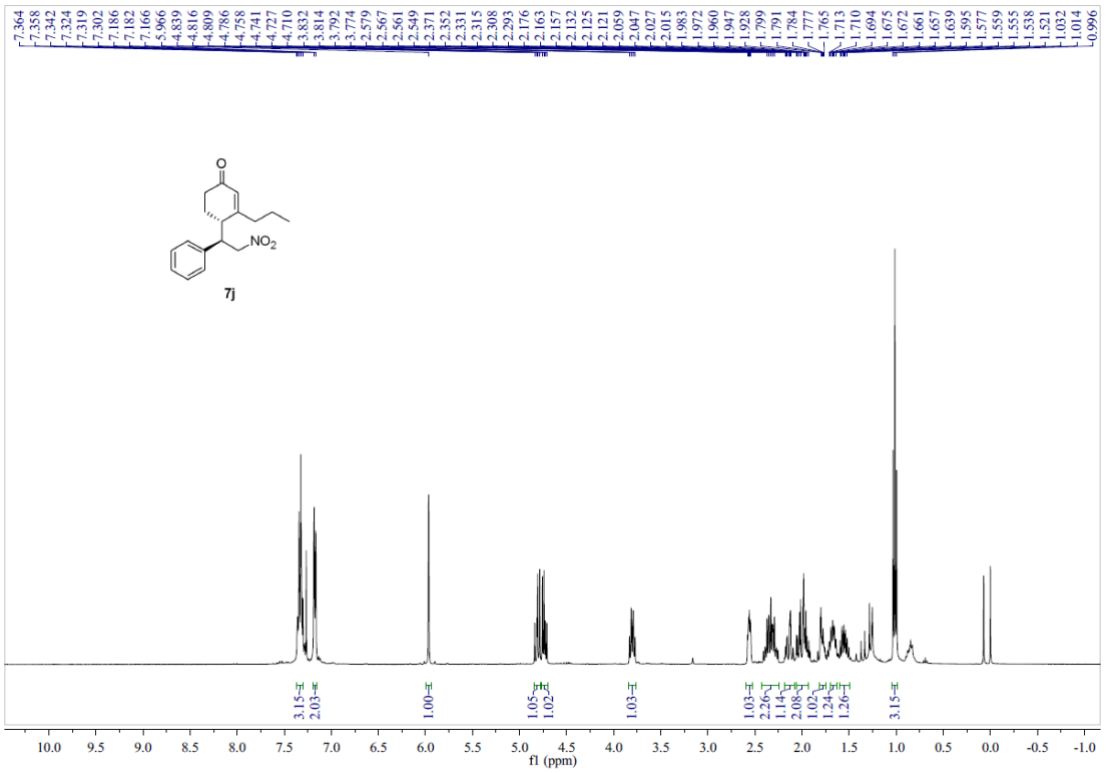


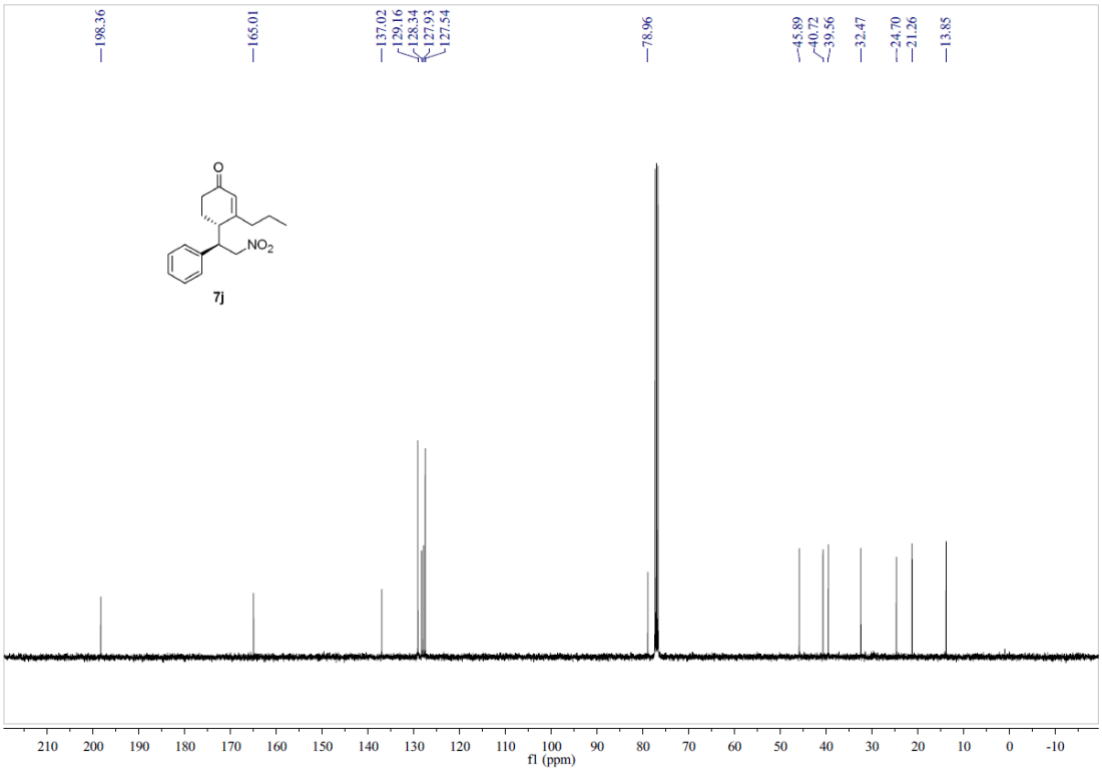
7i: (*S*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one



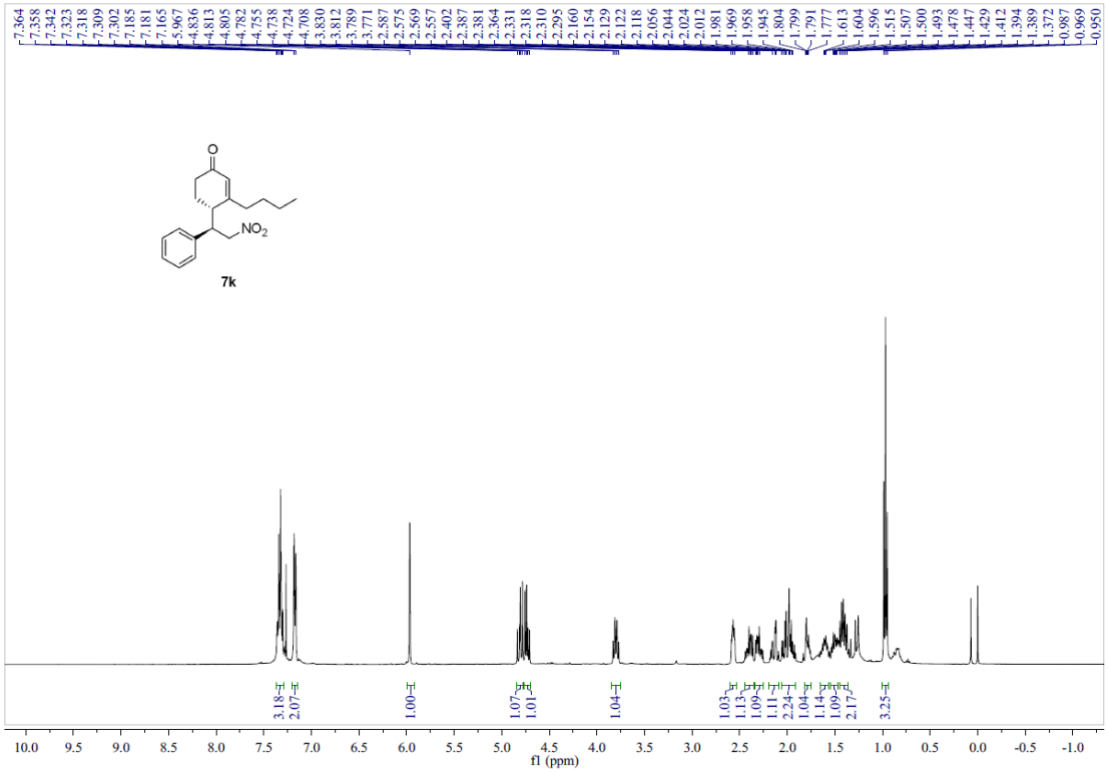


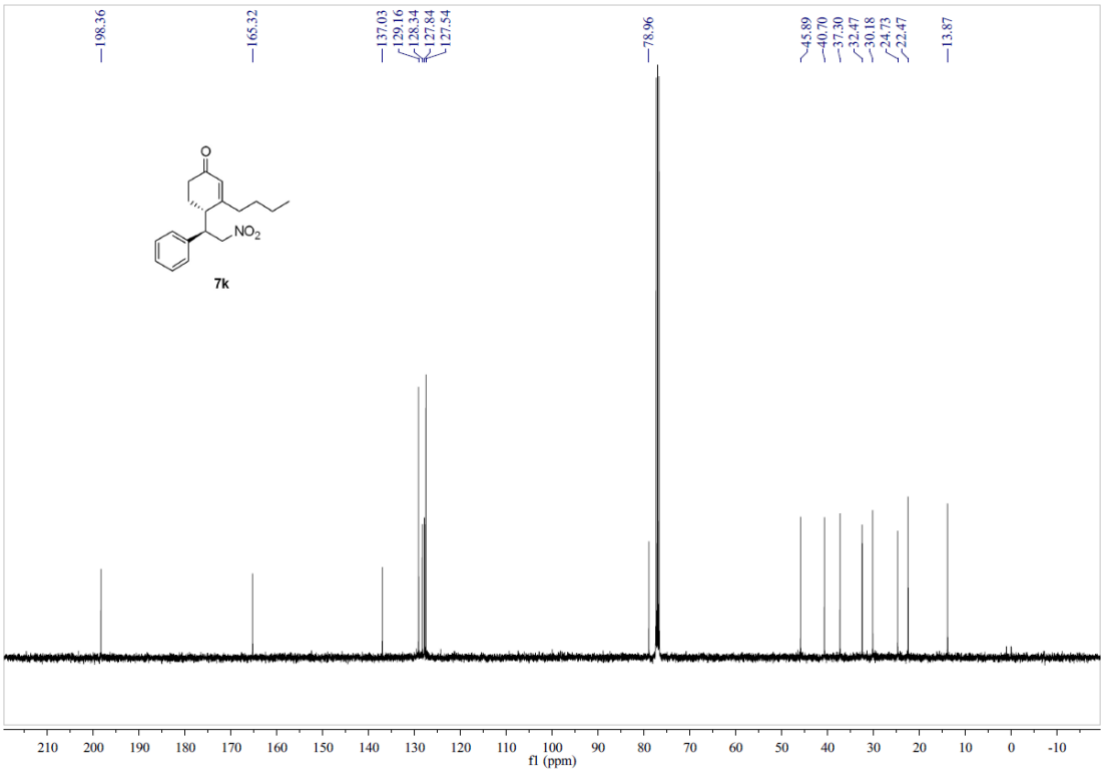
7j: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one



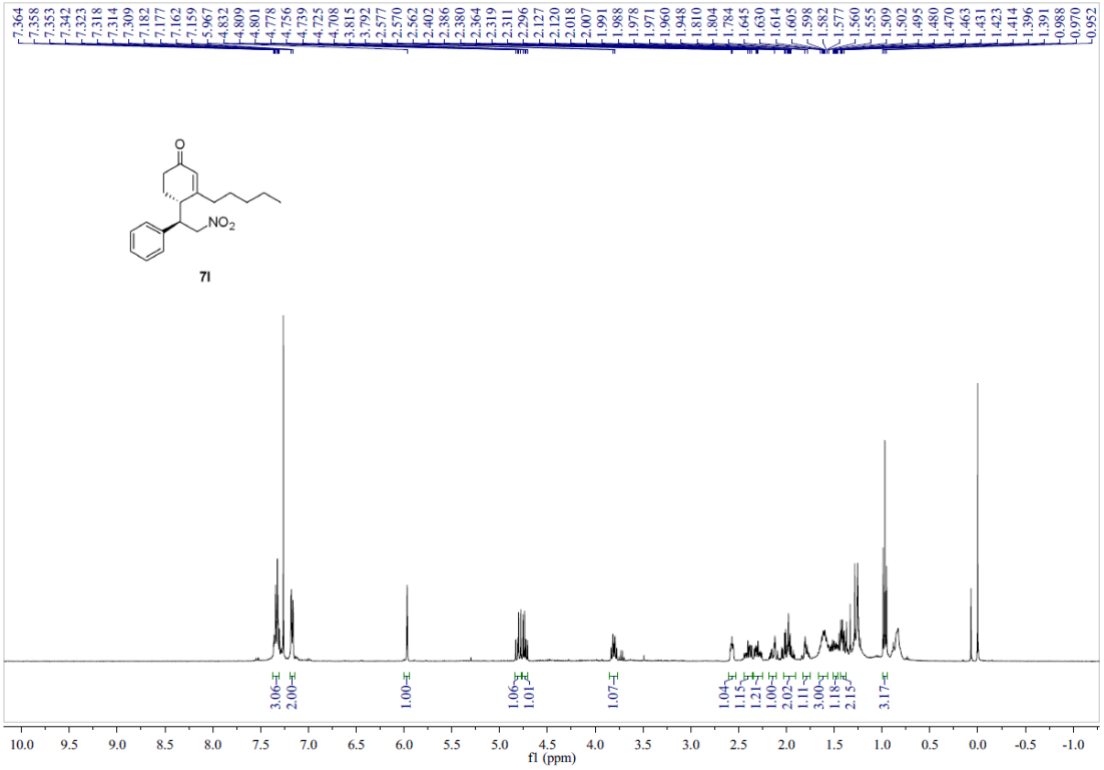


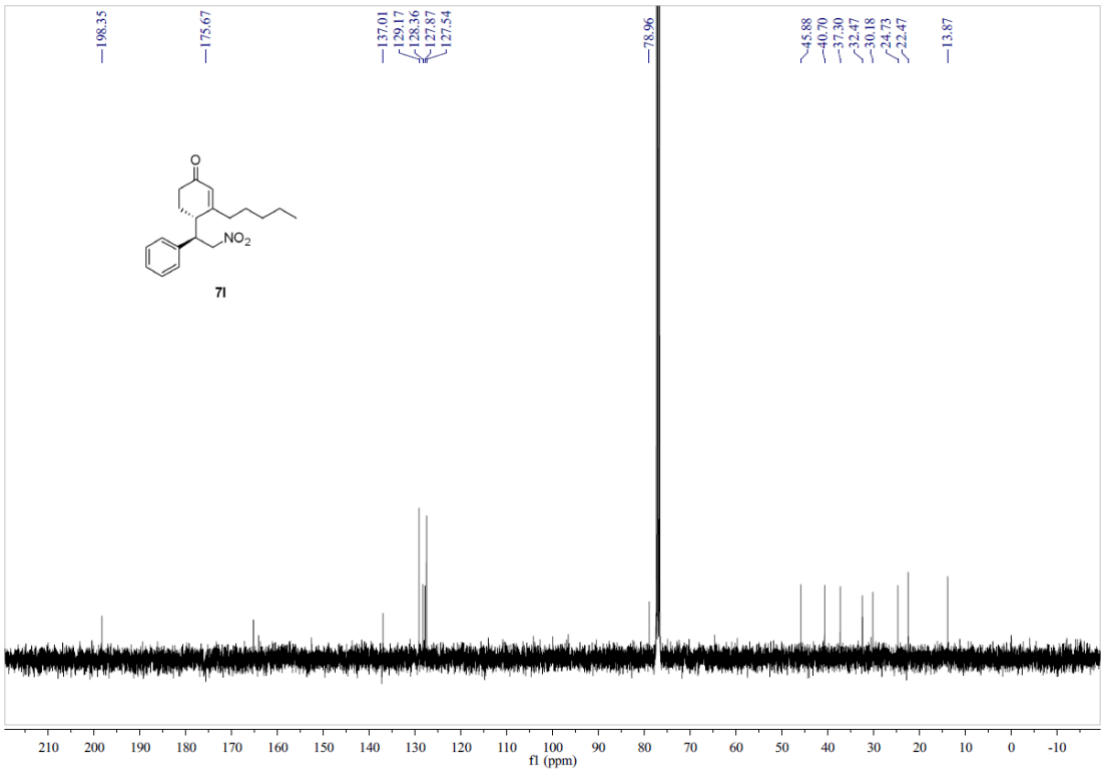
7k: (*S*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



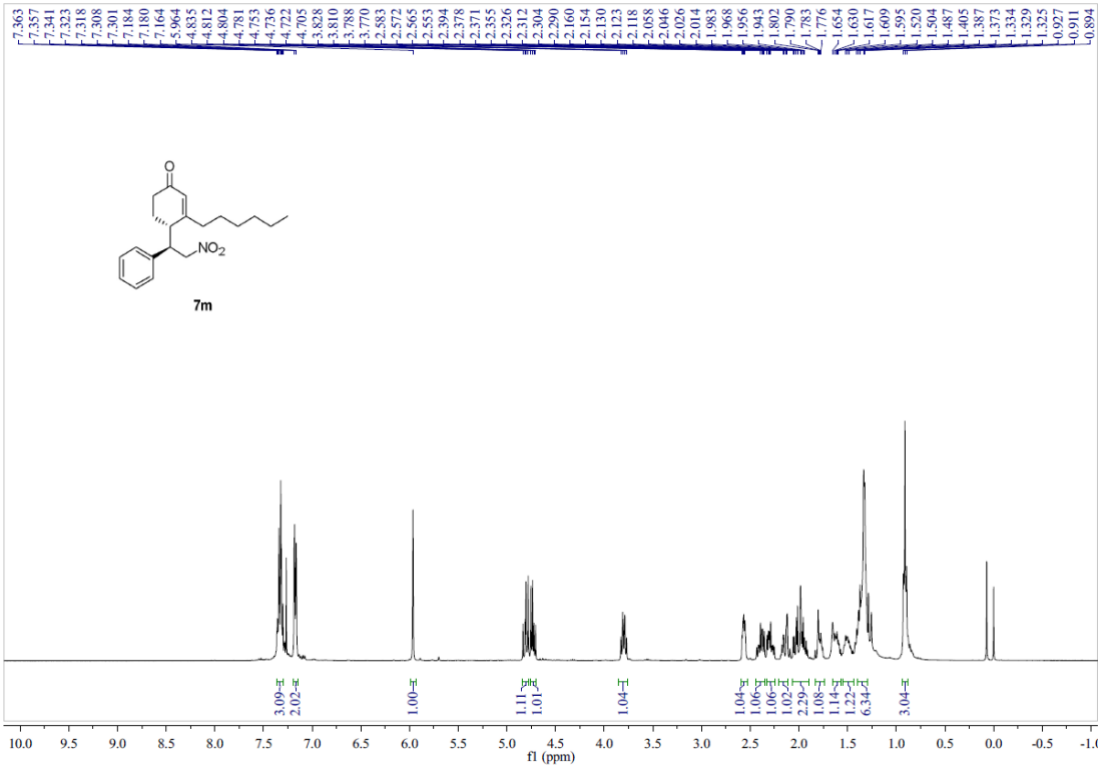


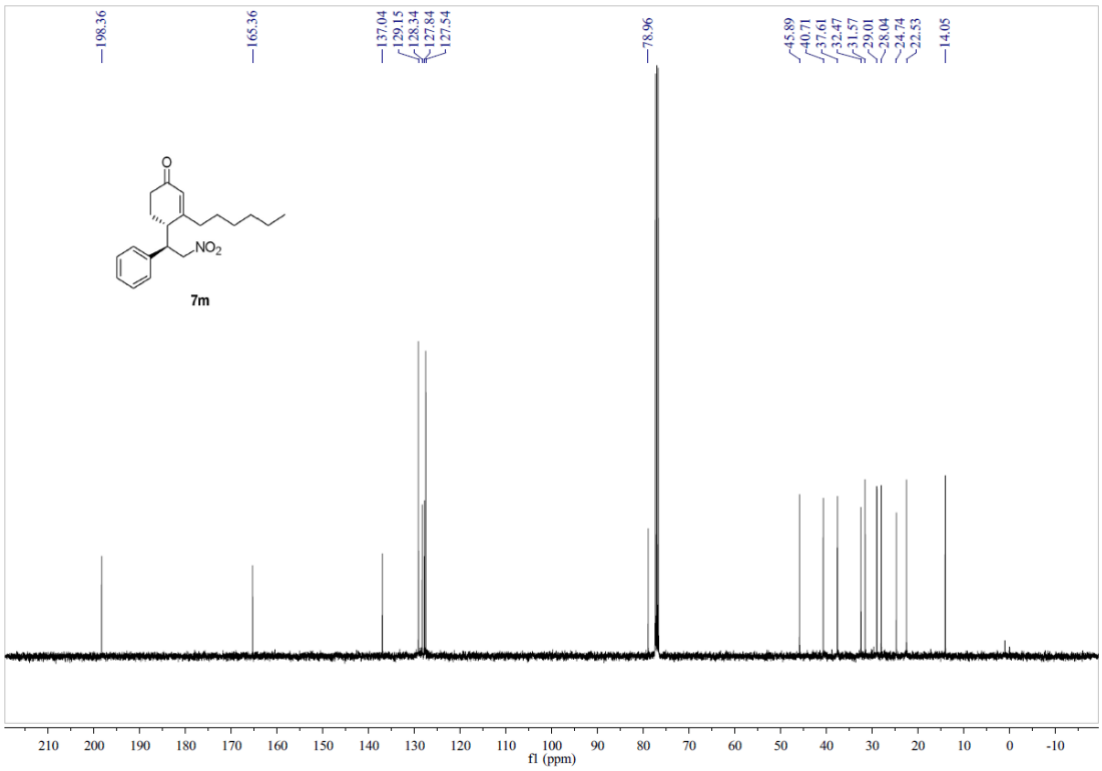
7l: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one



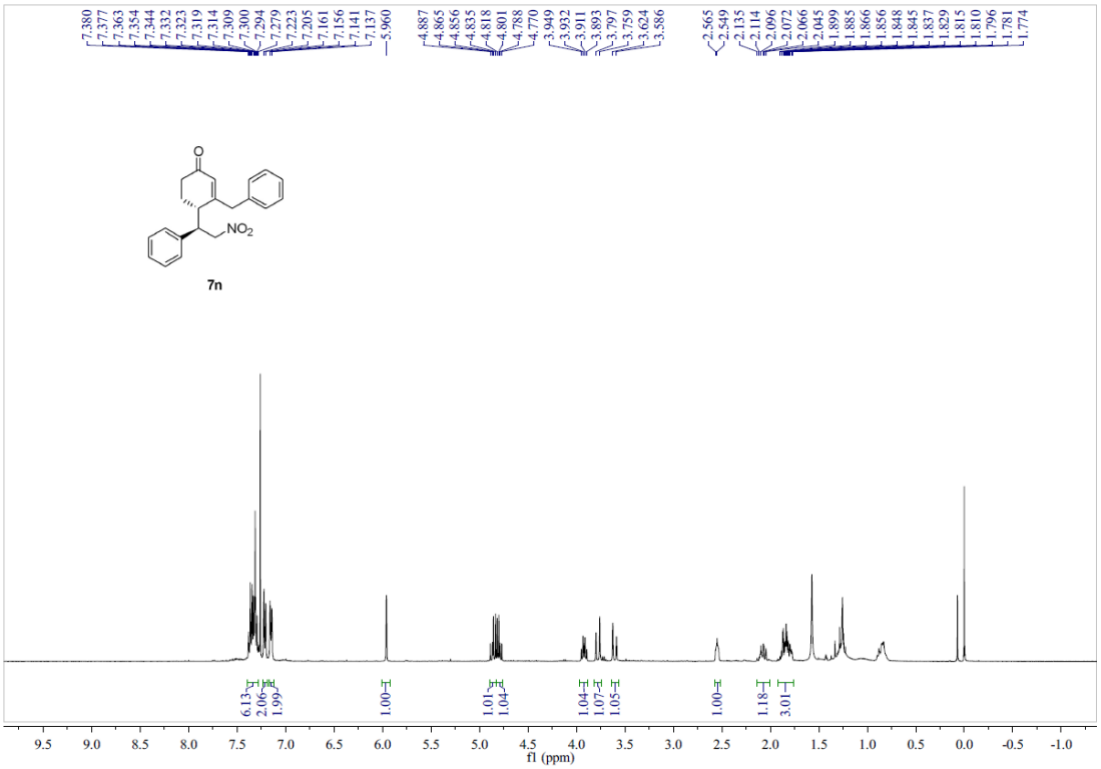


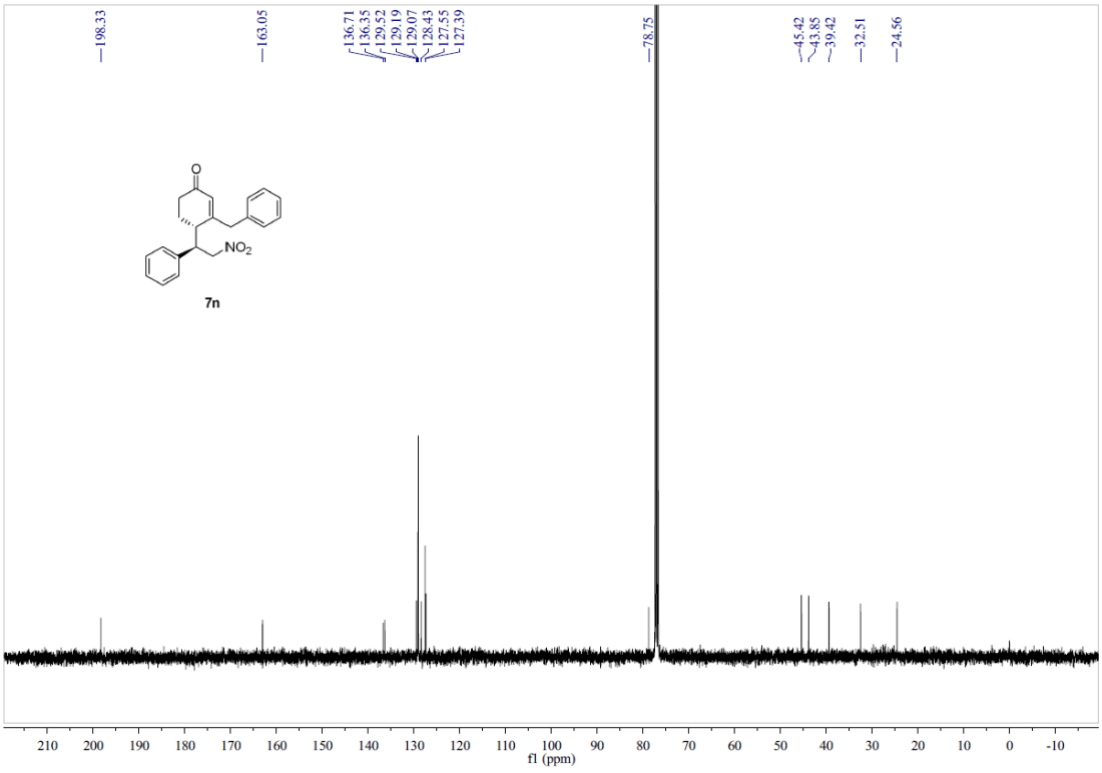
7m: (*S*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



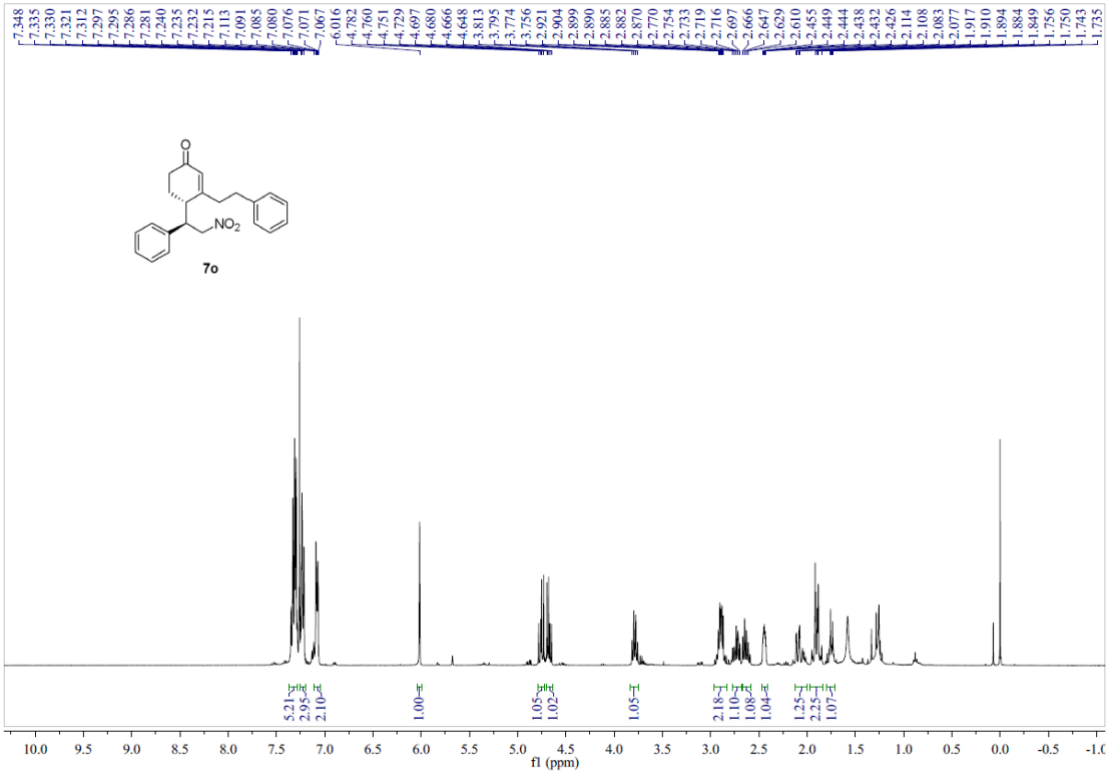


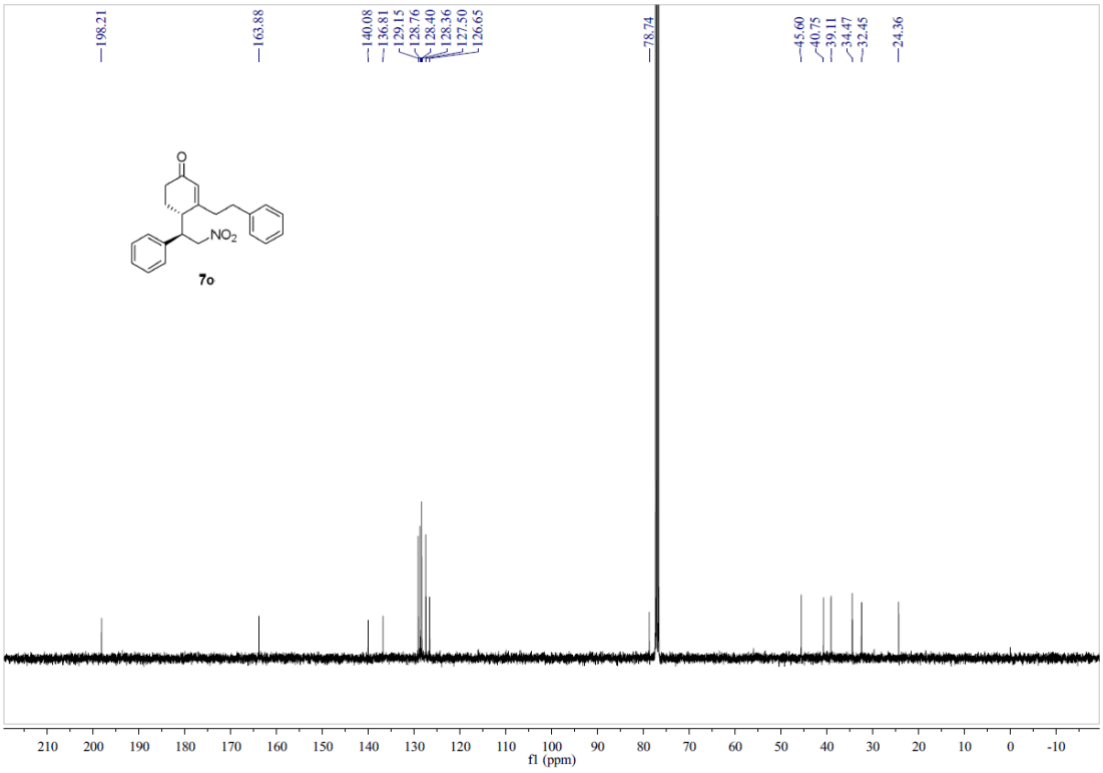
7n: (*S*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one



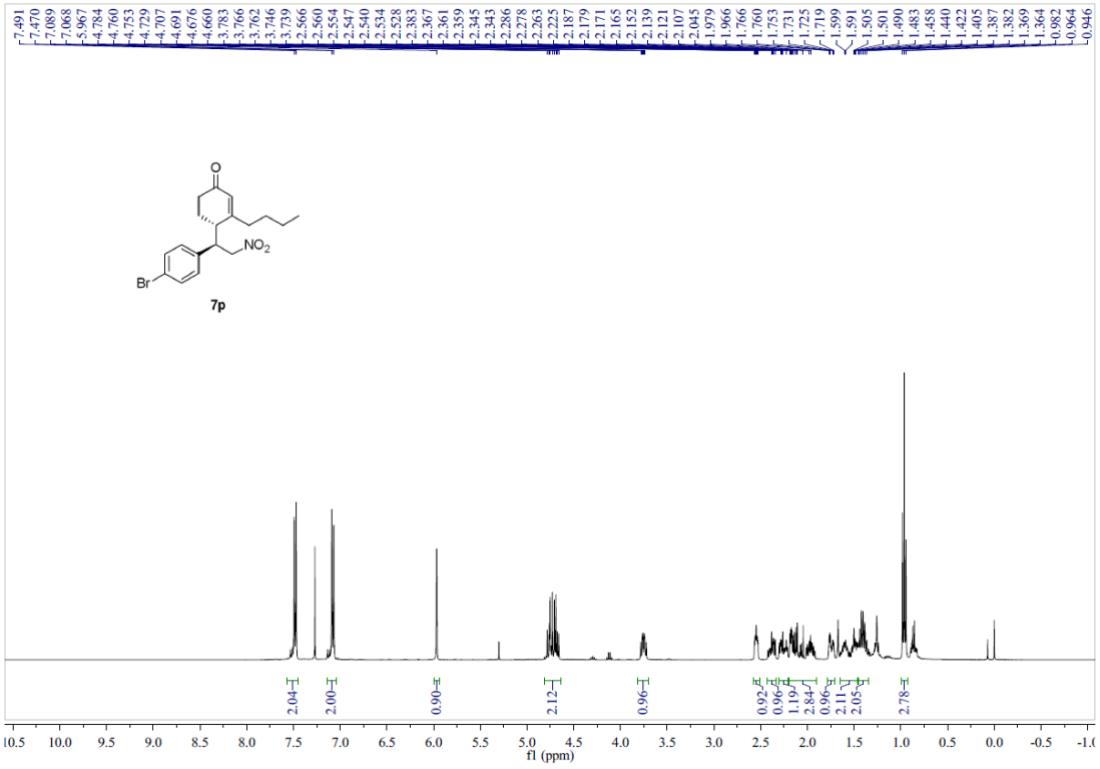


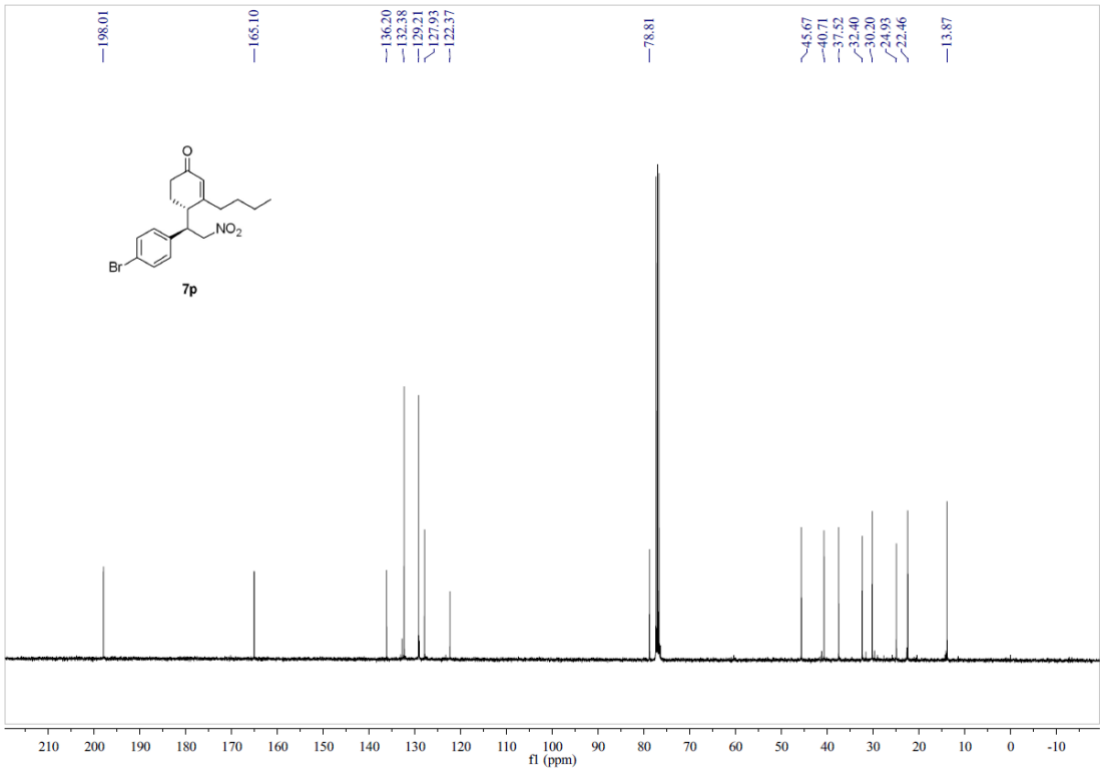
7o: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one



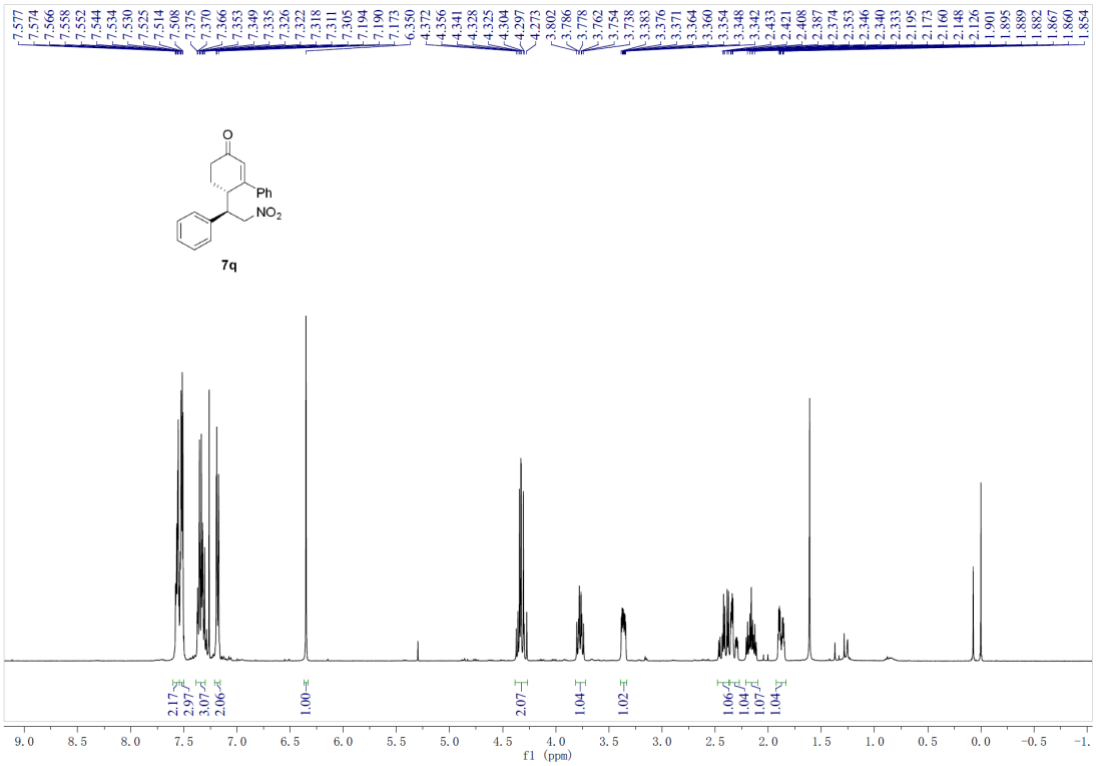


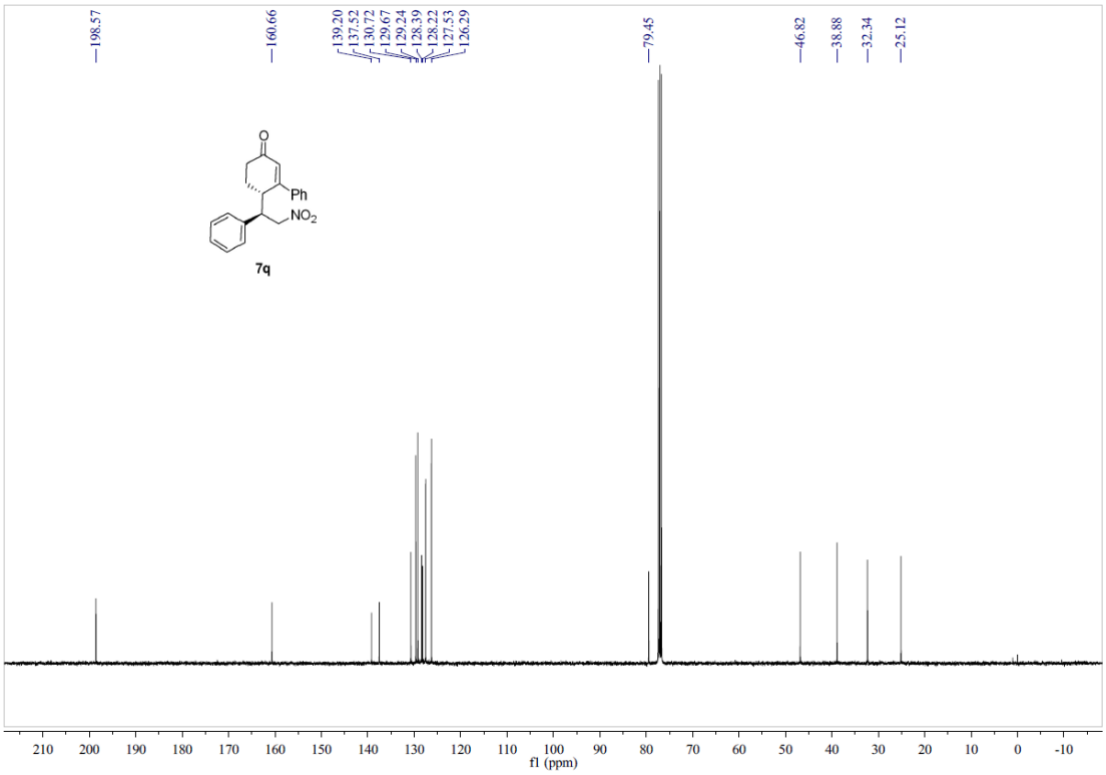
7p: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-butylcyclohex-2-en-1-one



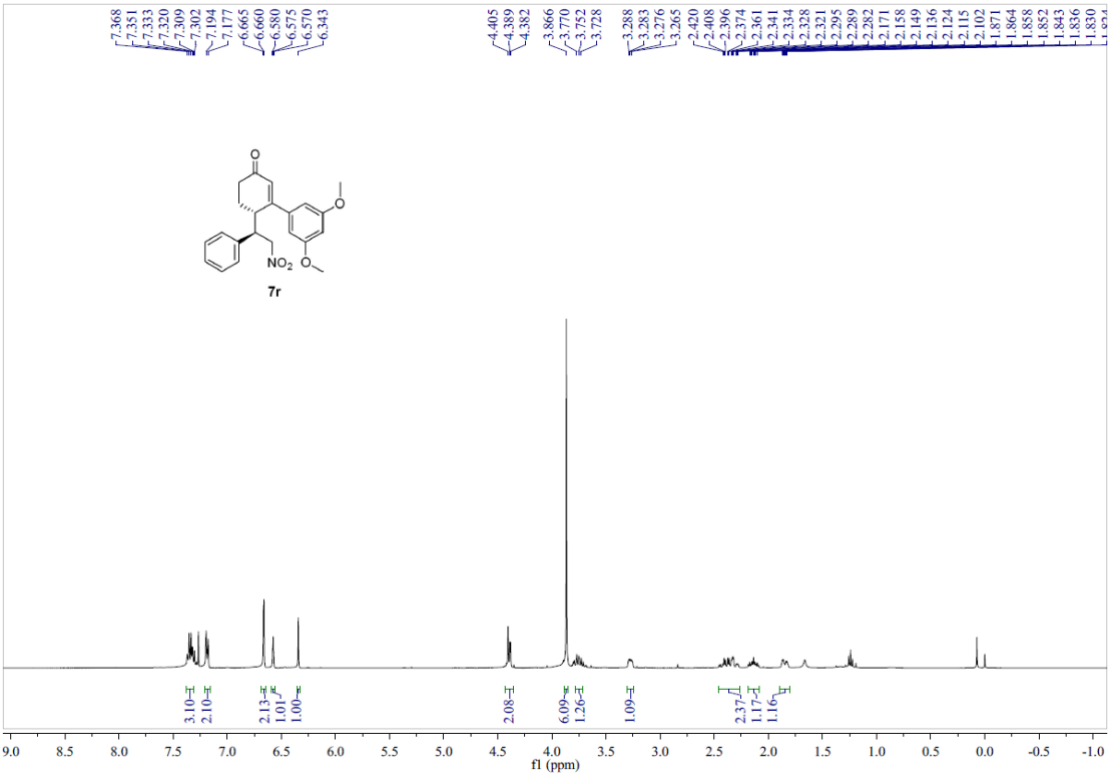


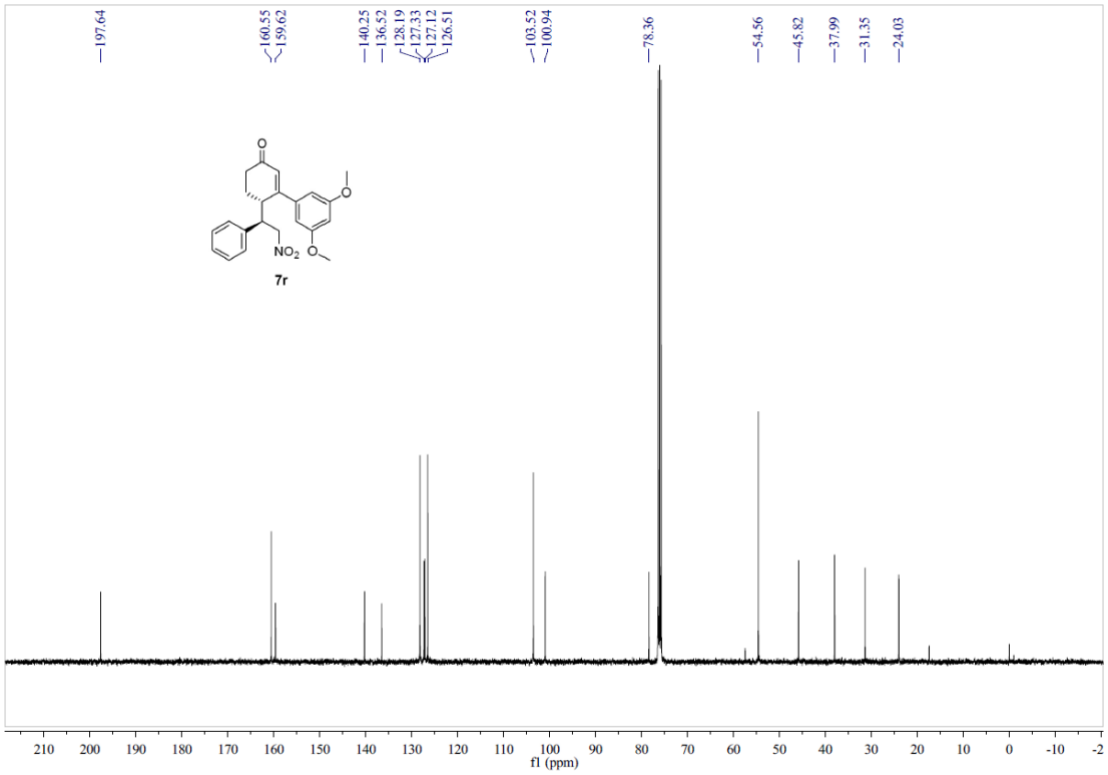
7q: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



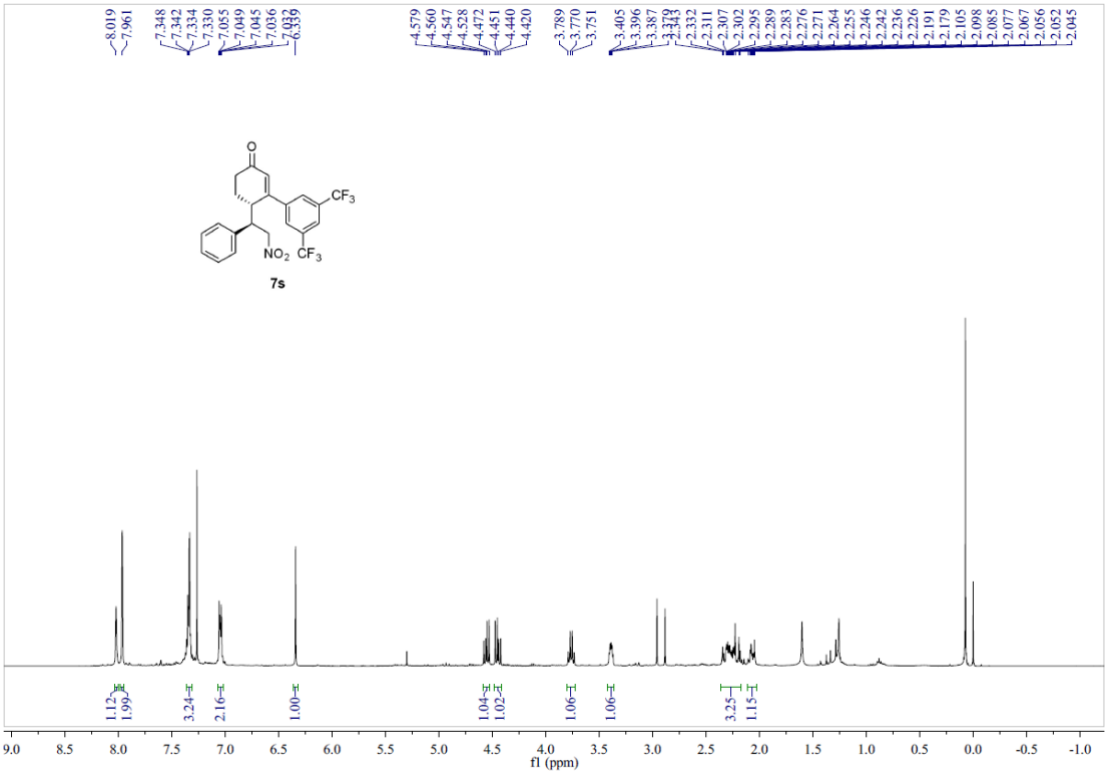


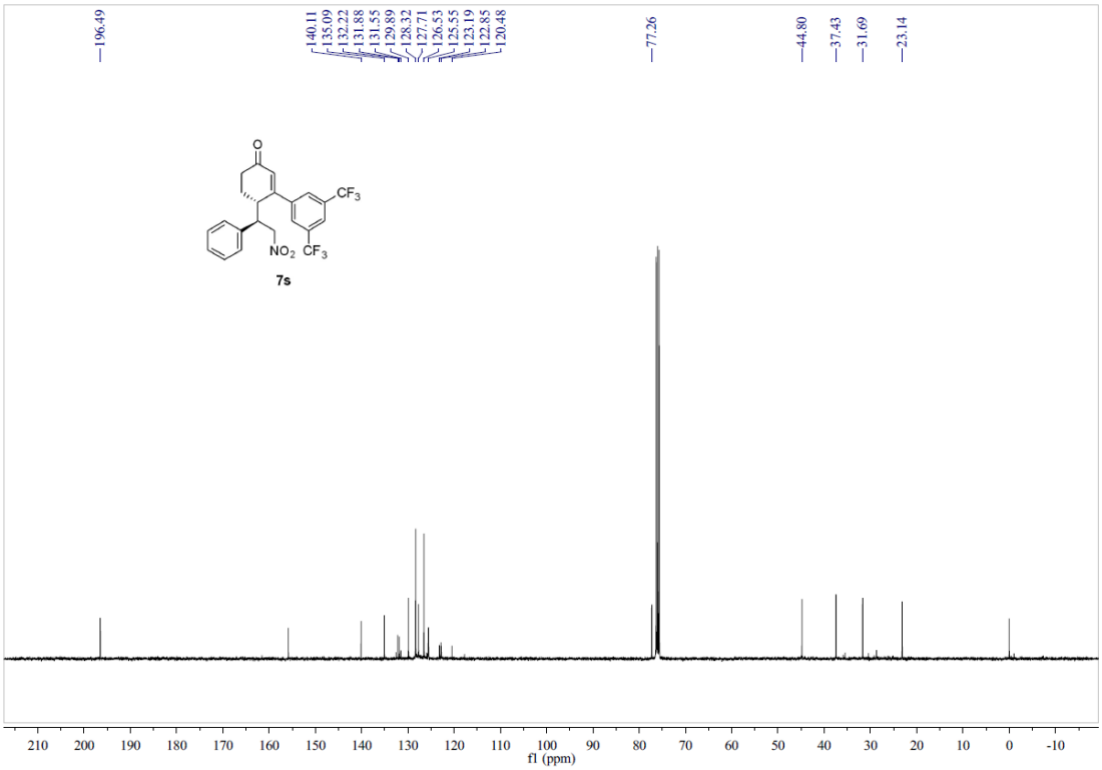
7r: (*S*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



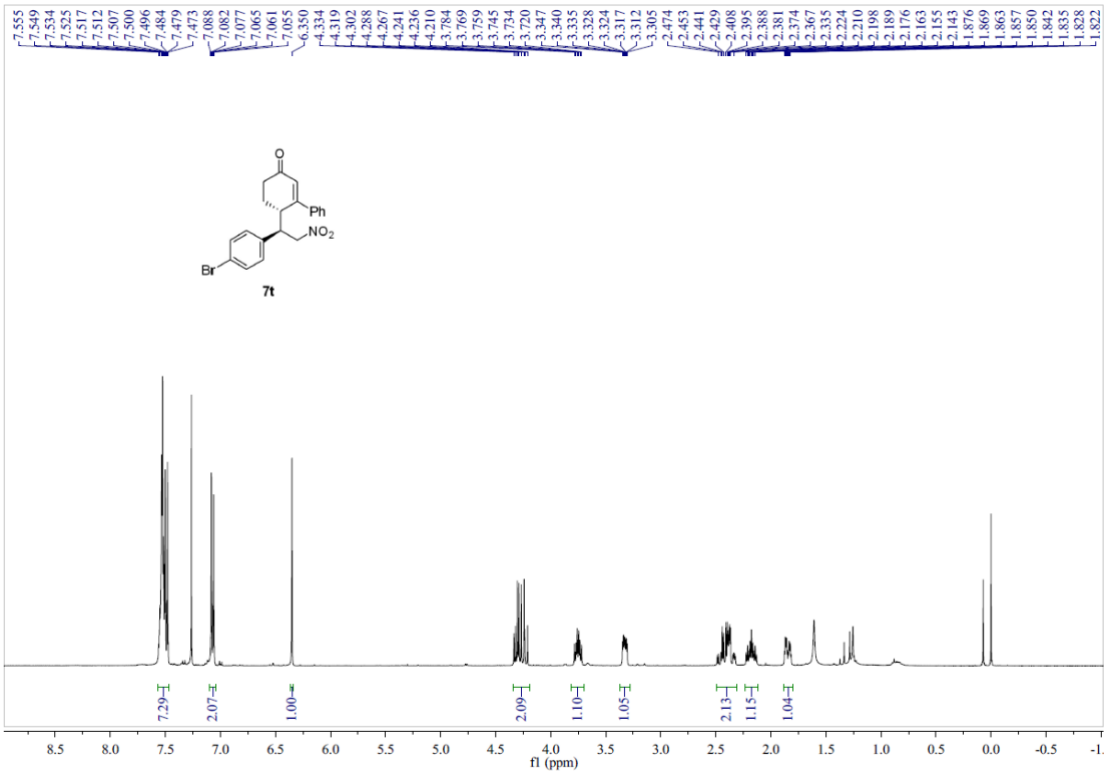


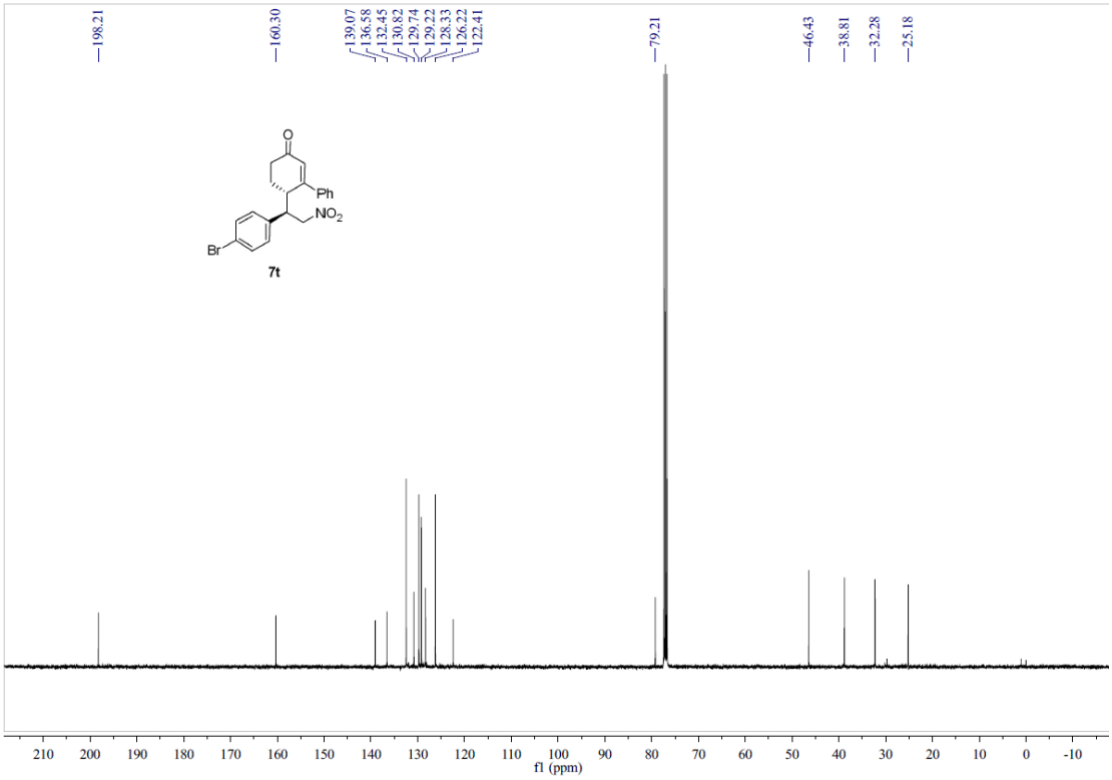
7s: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



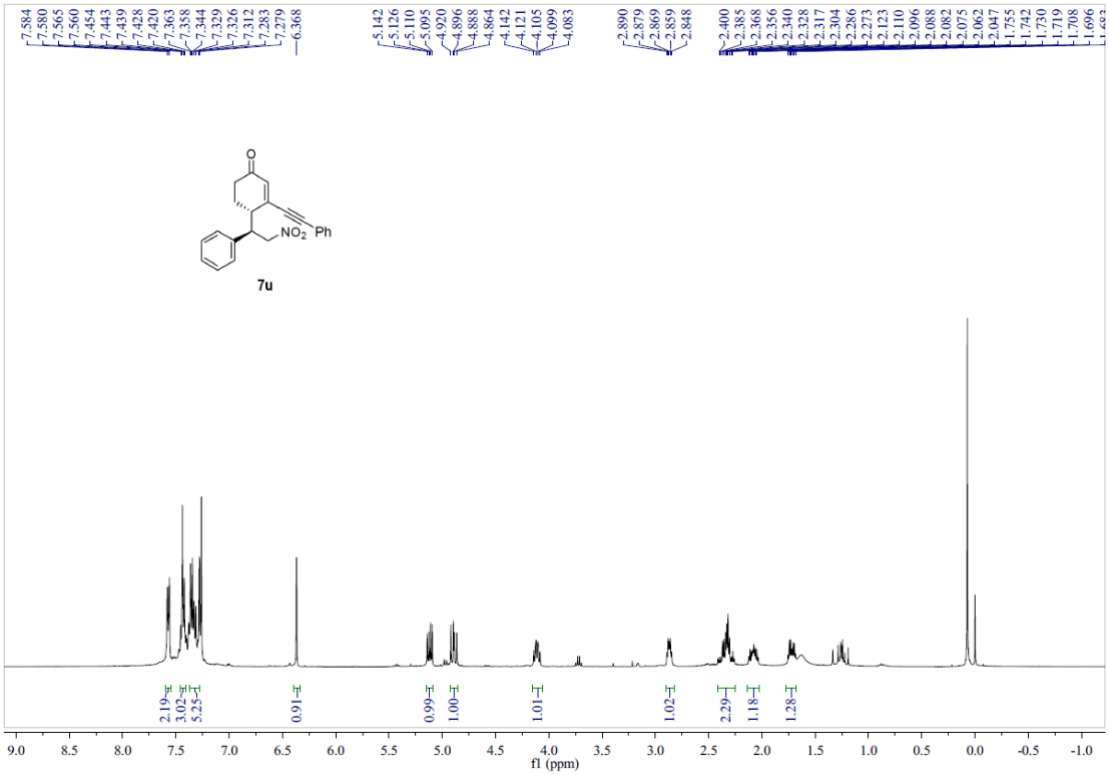


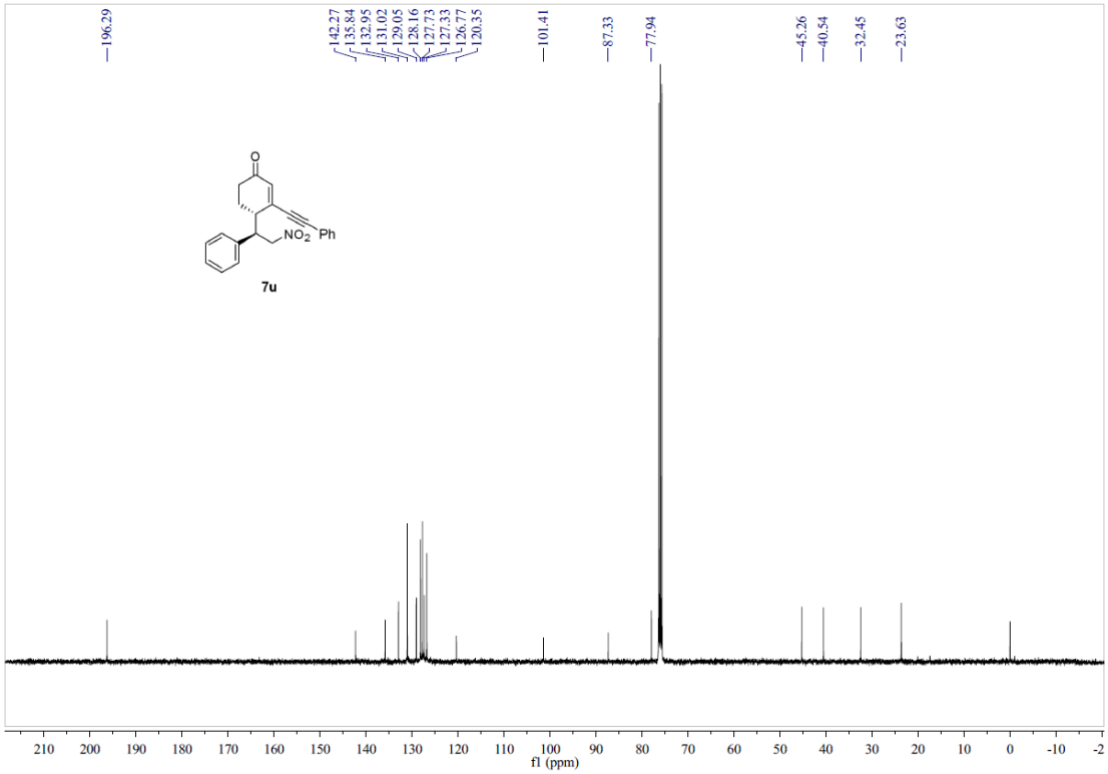
7t: (*S*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one



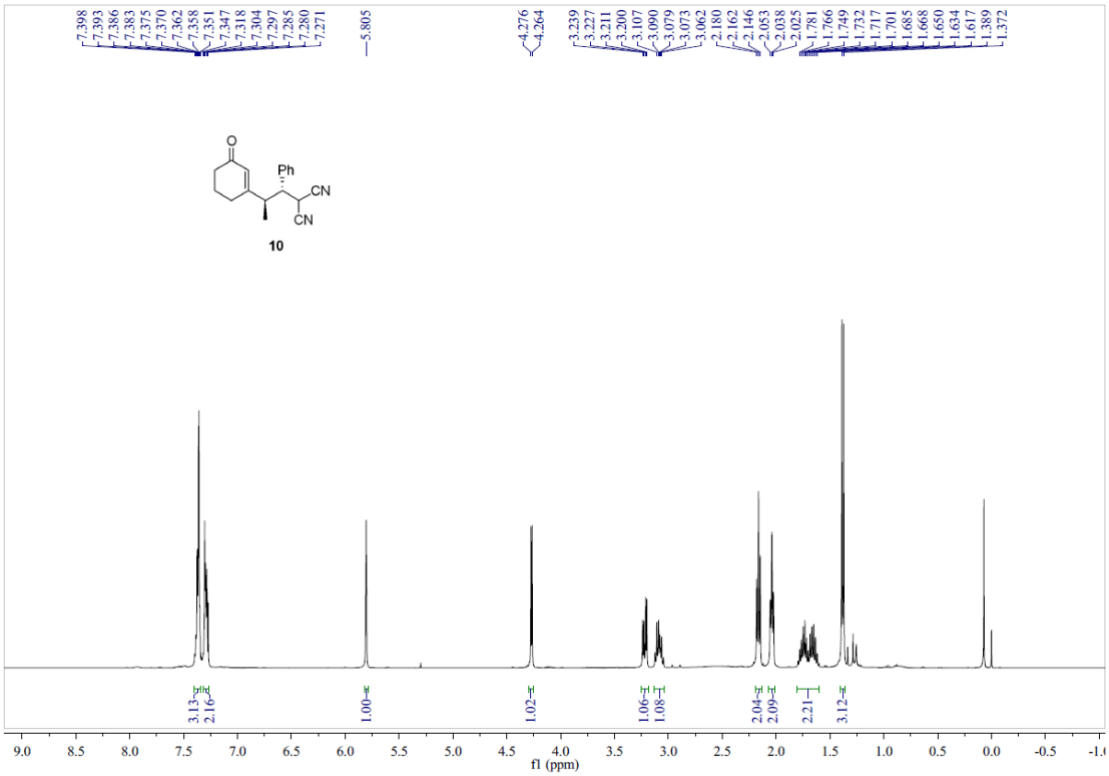


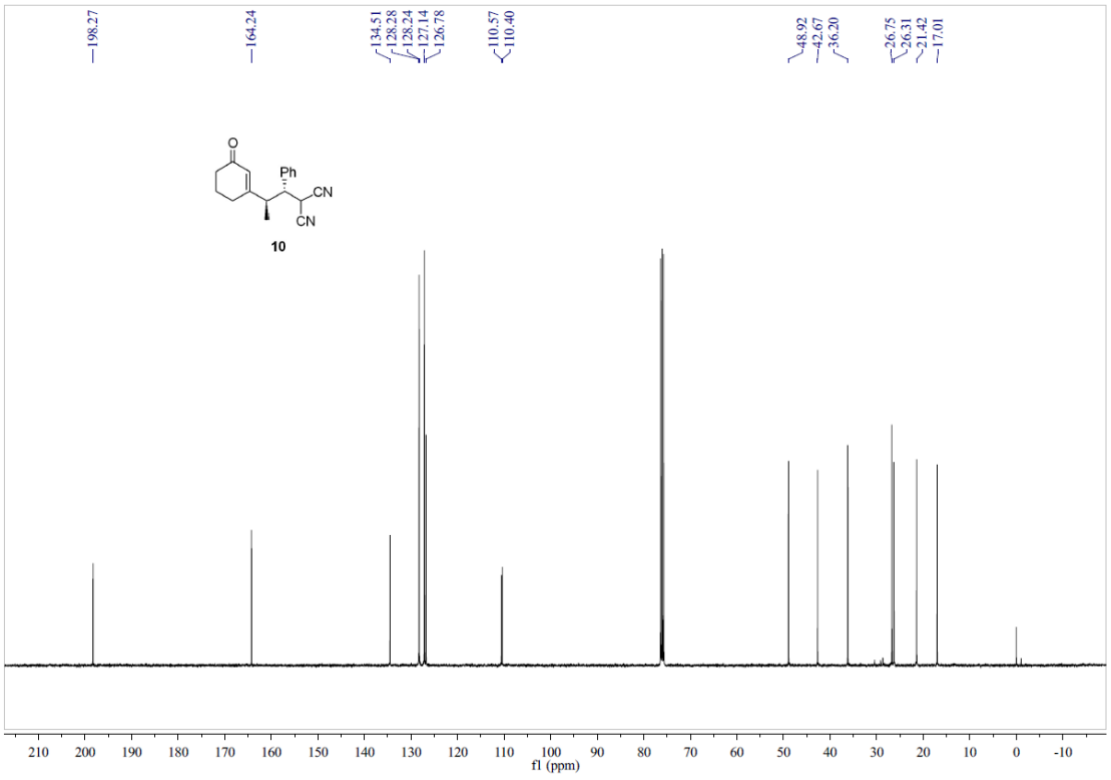
7u: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one



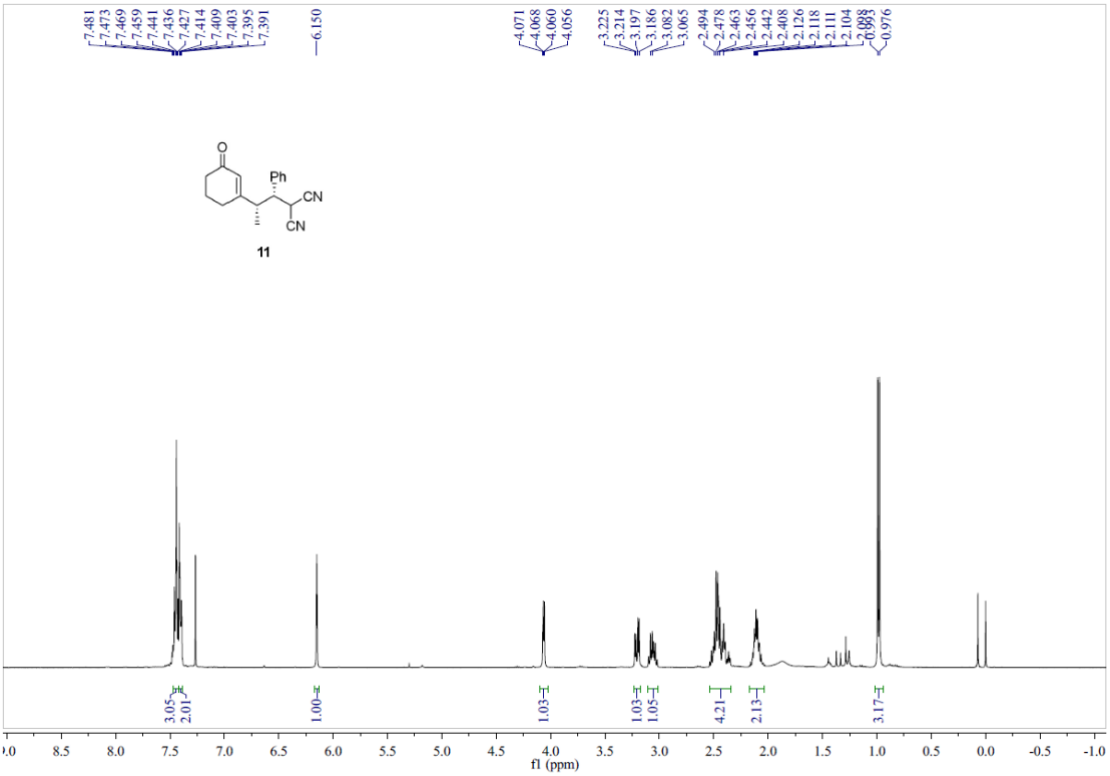


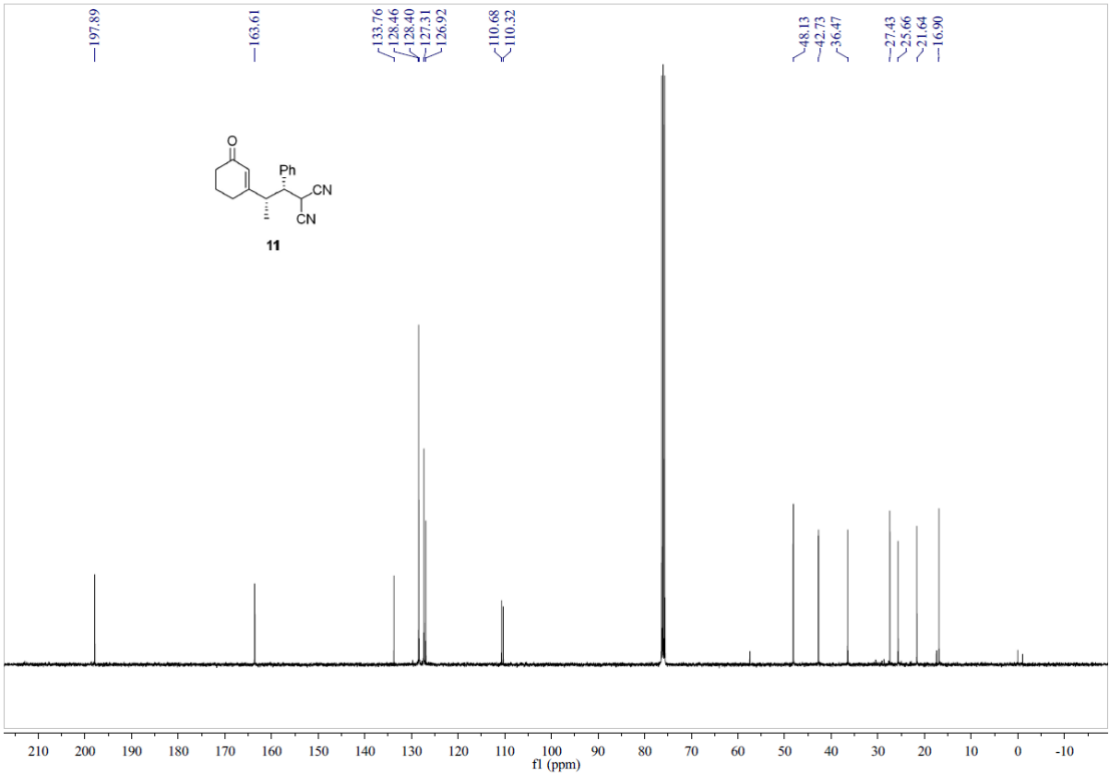
10: 2-((1*S*,2*R*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile



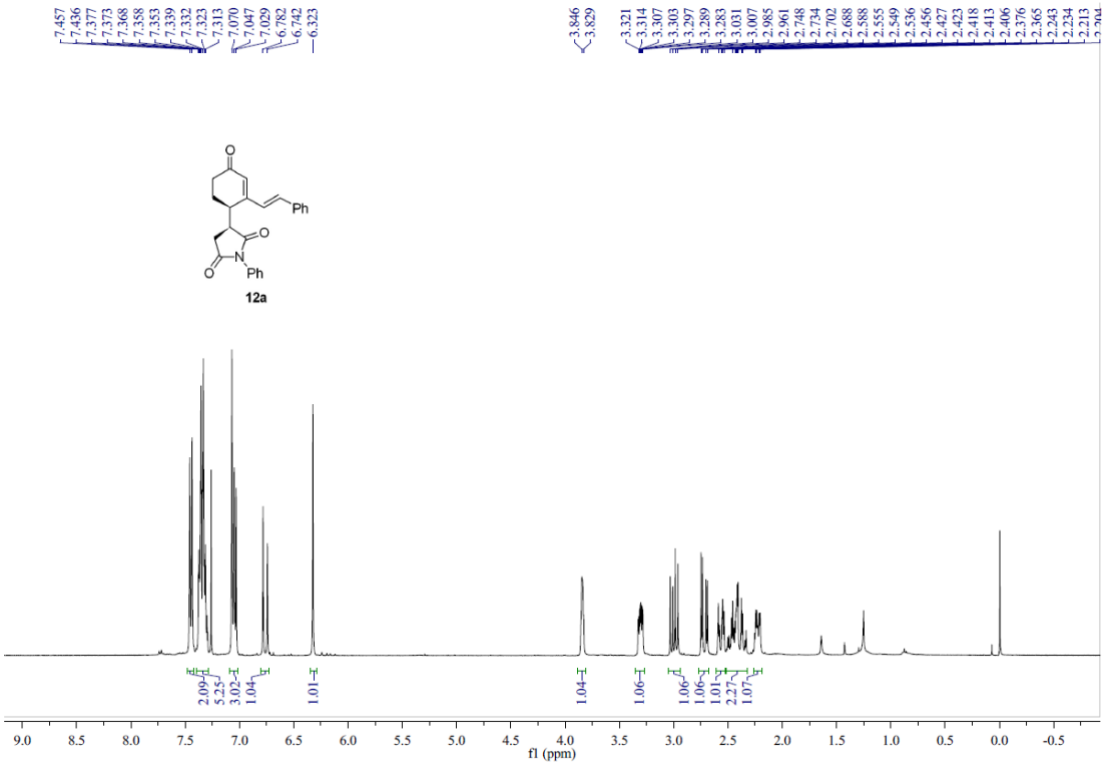


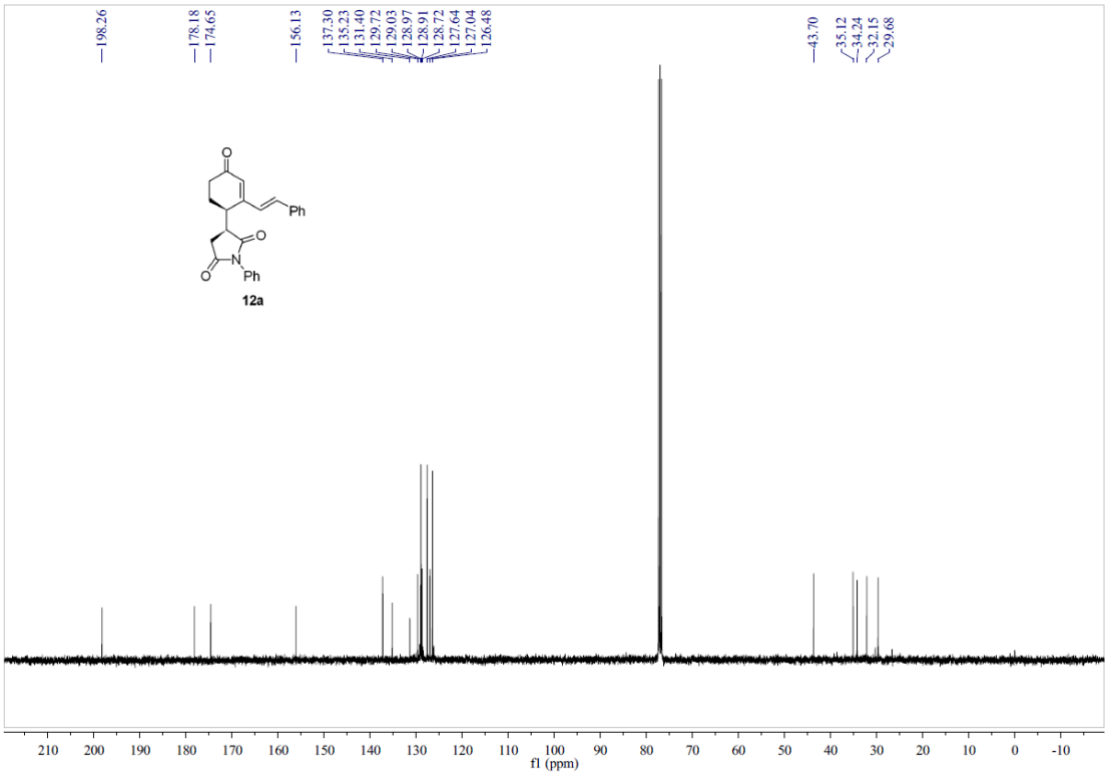
11: 2-((1*S*,2*S*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile



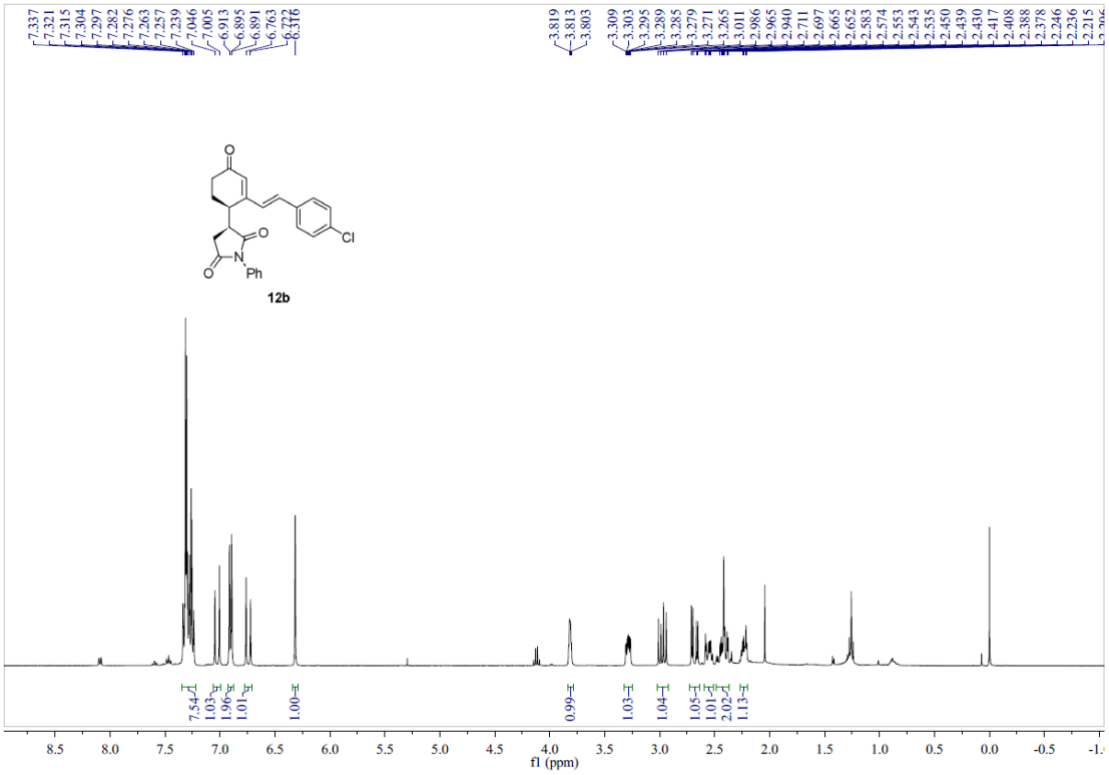


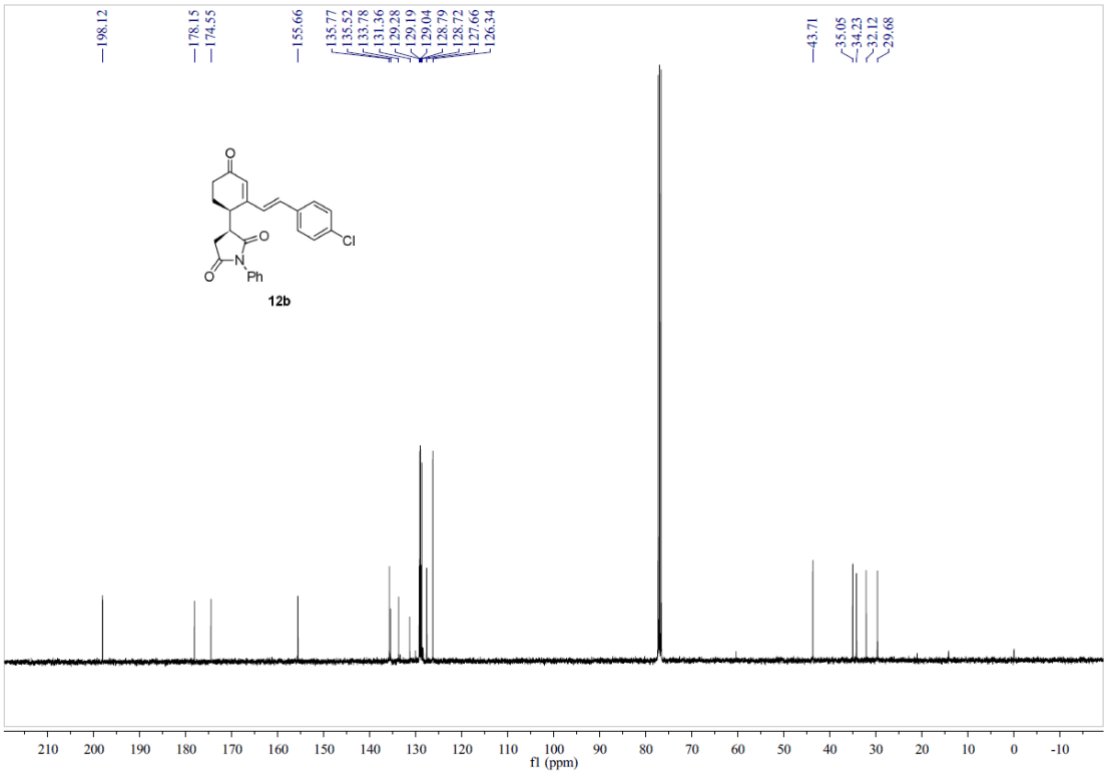
12a: (*S*)-3-((*R*)-4-oxo-2-((*E*)-styryl)cyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione



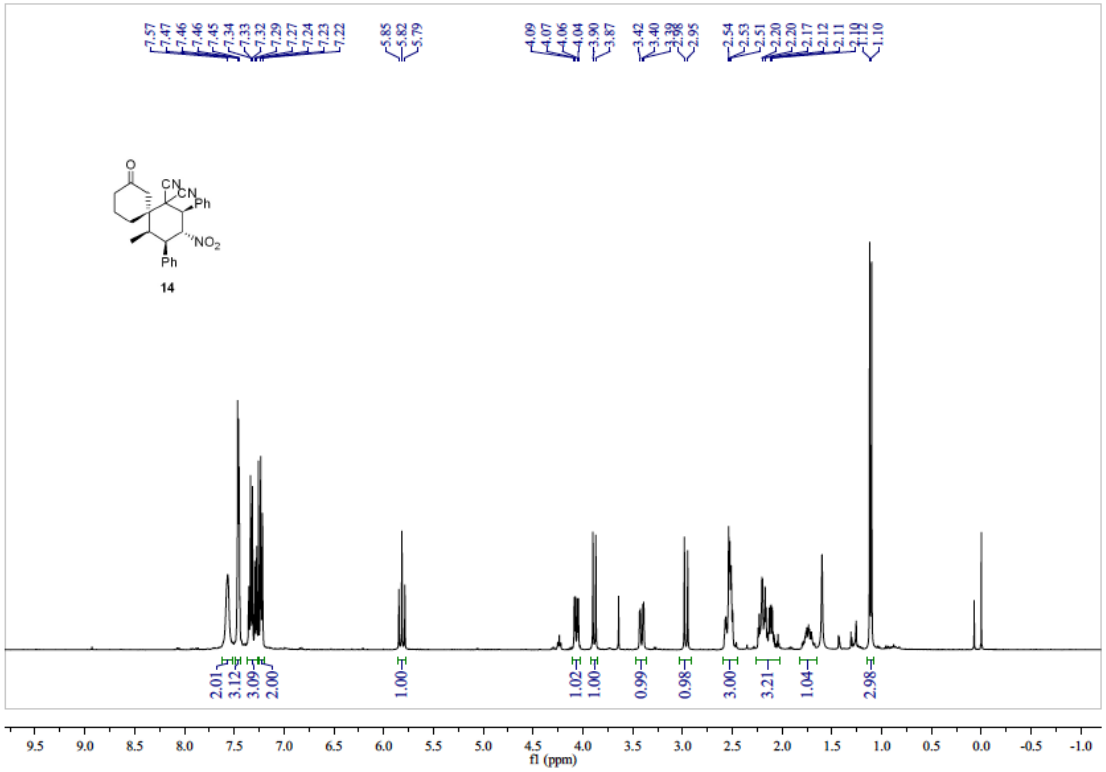


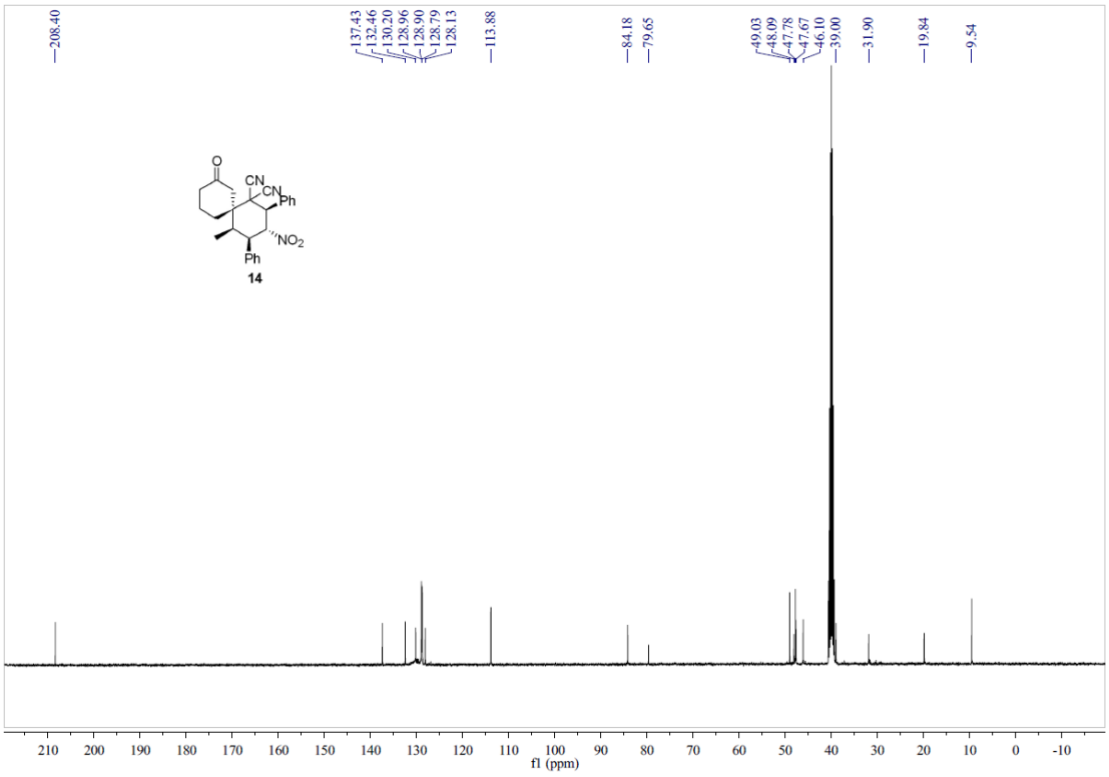
12b: (*S*)-3-((*R*)-2-((*E*)-4-chlorostyryl)-4-oxocyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione



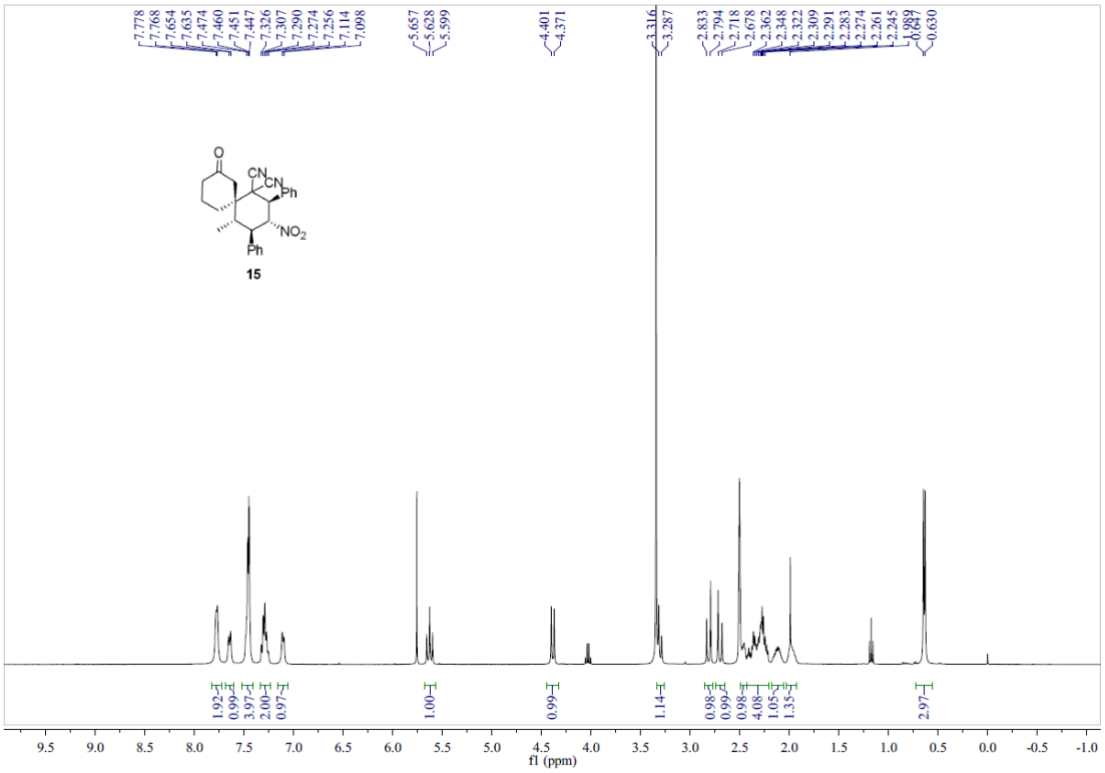


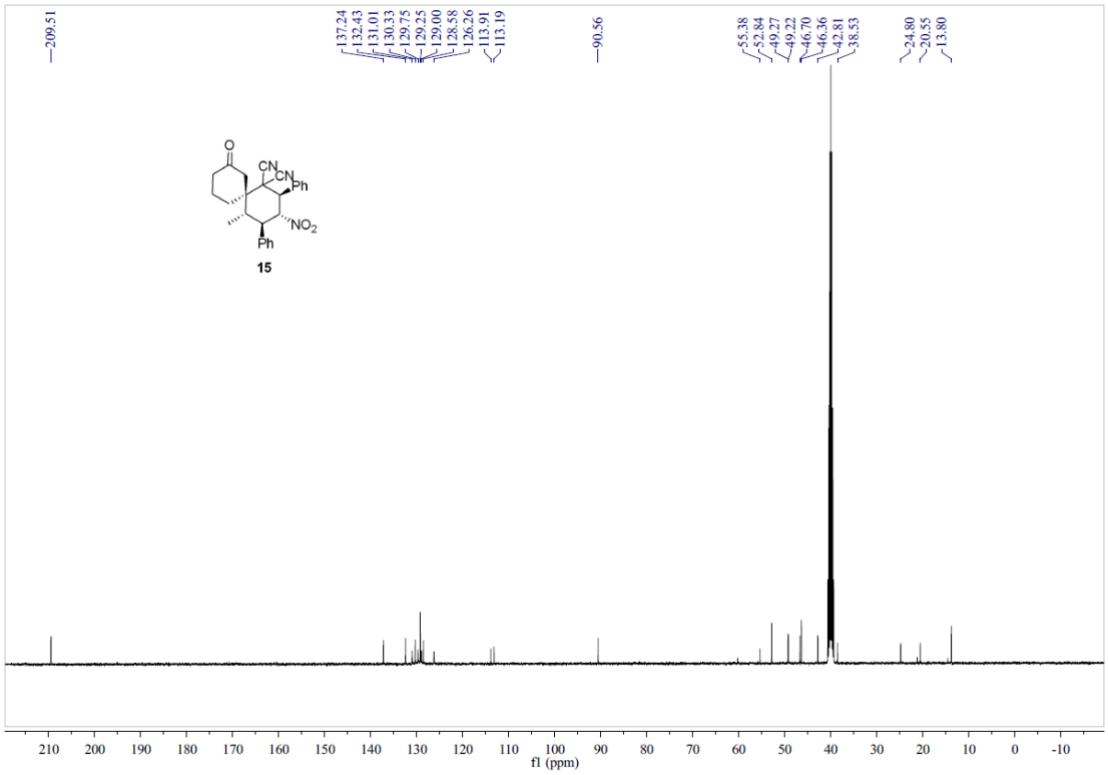
14: (2*R*,3*R*,4*R*,5*R*,6*S*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile



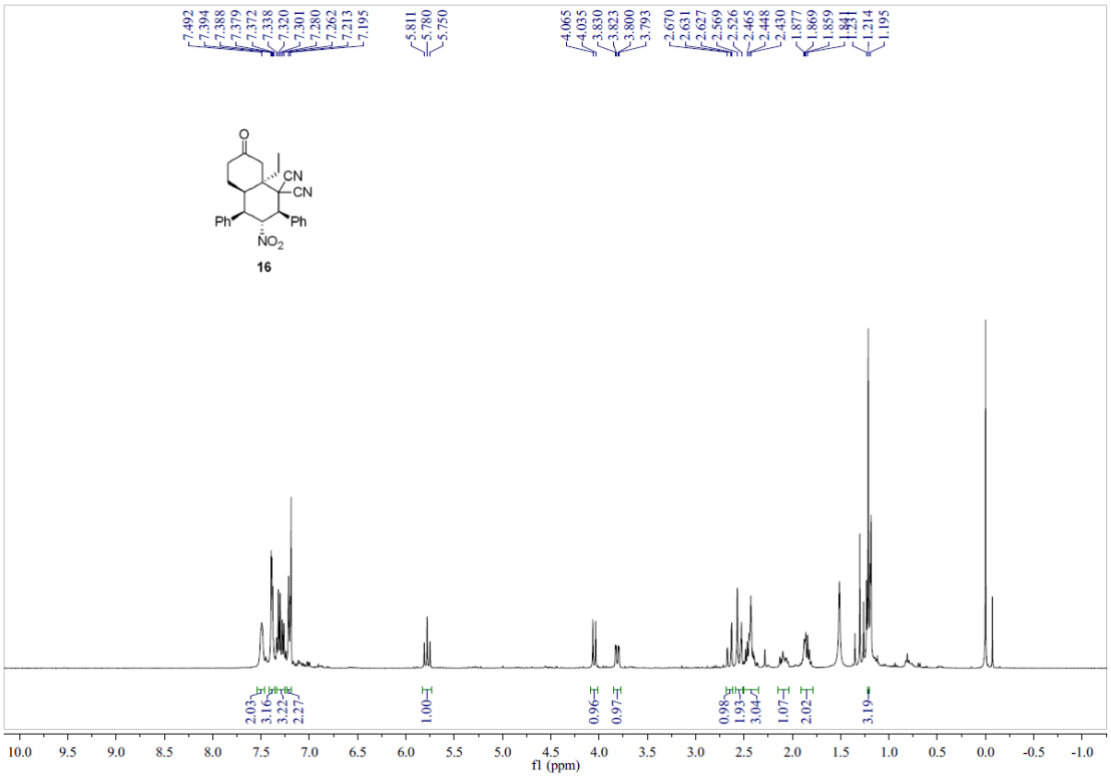


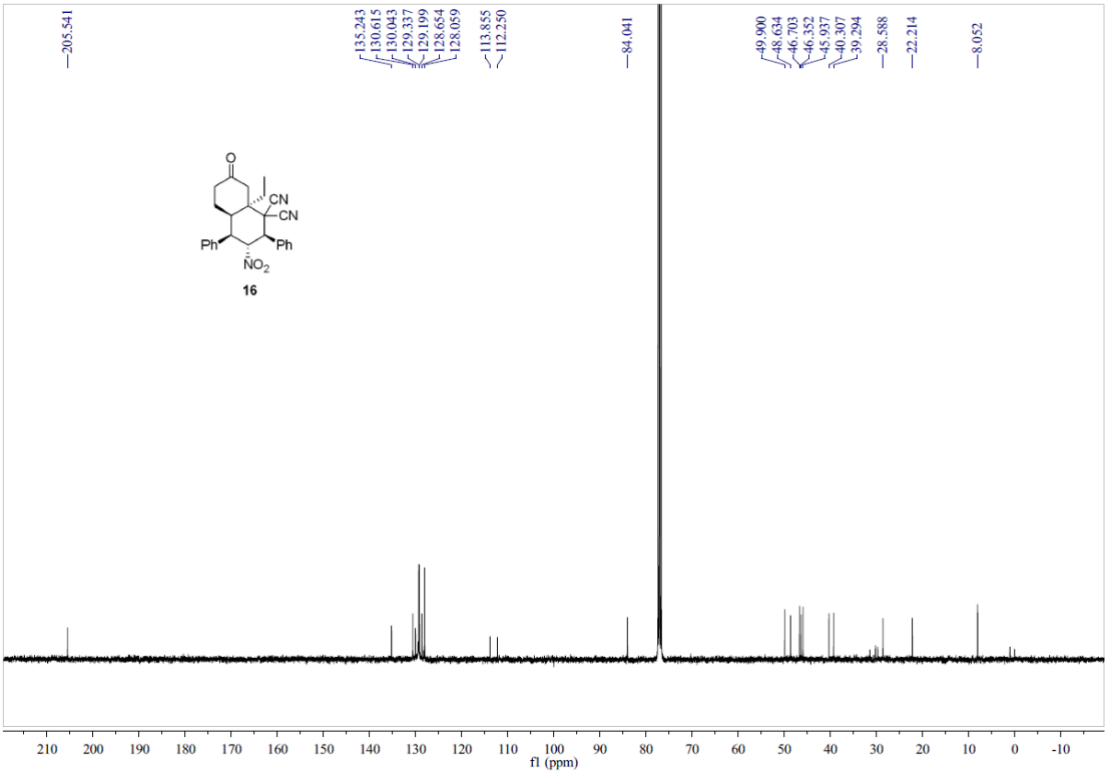
15: (2*R*,3*R*,4*R*,5*S*,6*R*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile



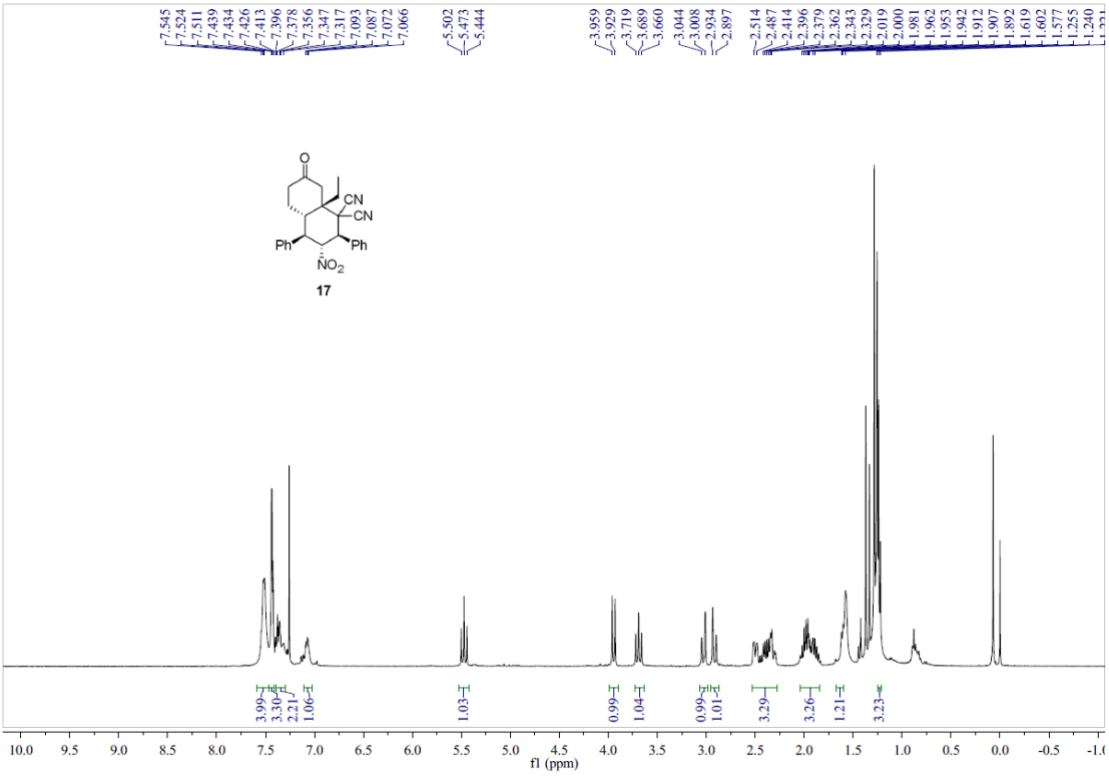


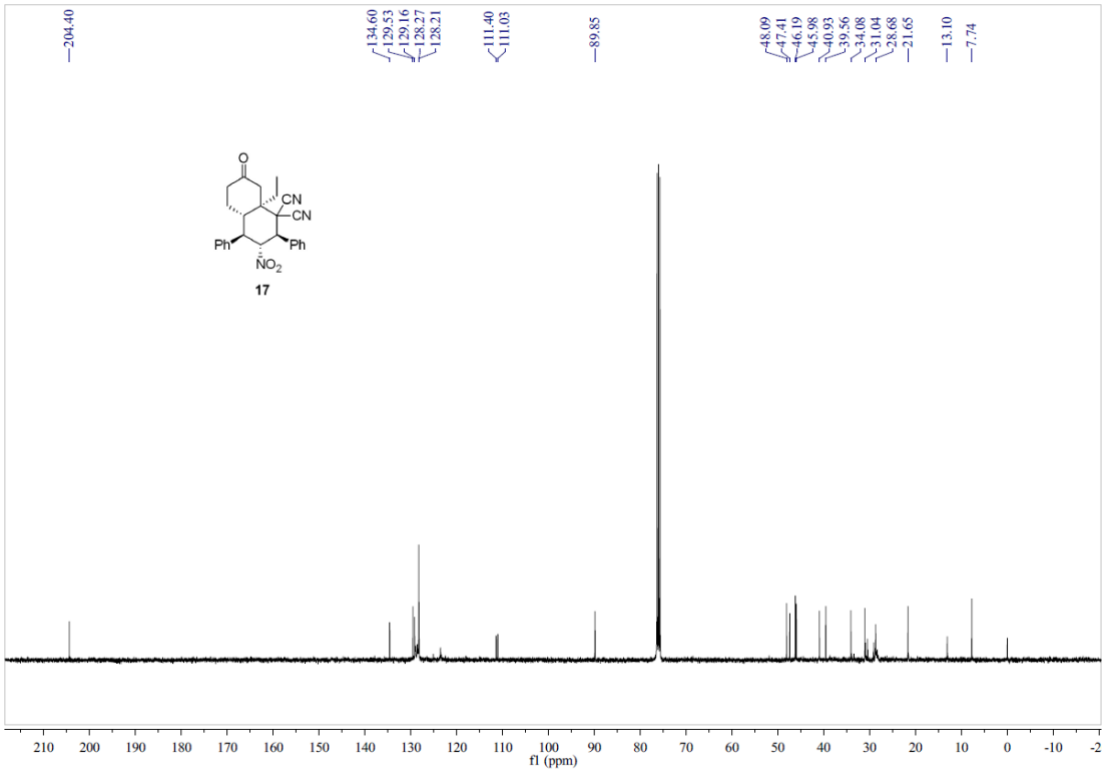
16: (2*R*,3*R*,4*R*,4a*R*,8a*R*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile





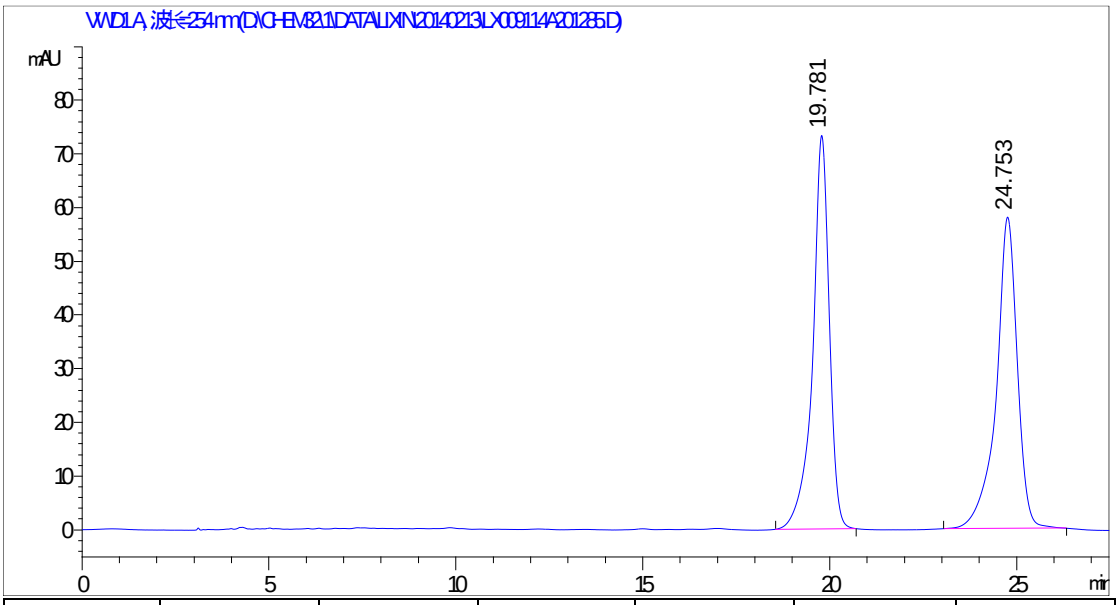
17: (2*R*,3*R*,4*R*,4a*S*,8a*S*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile



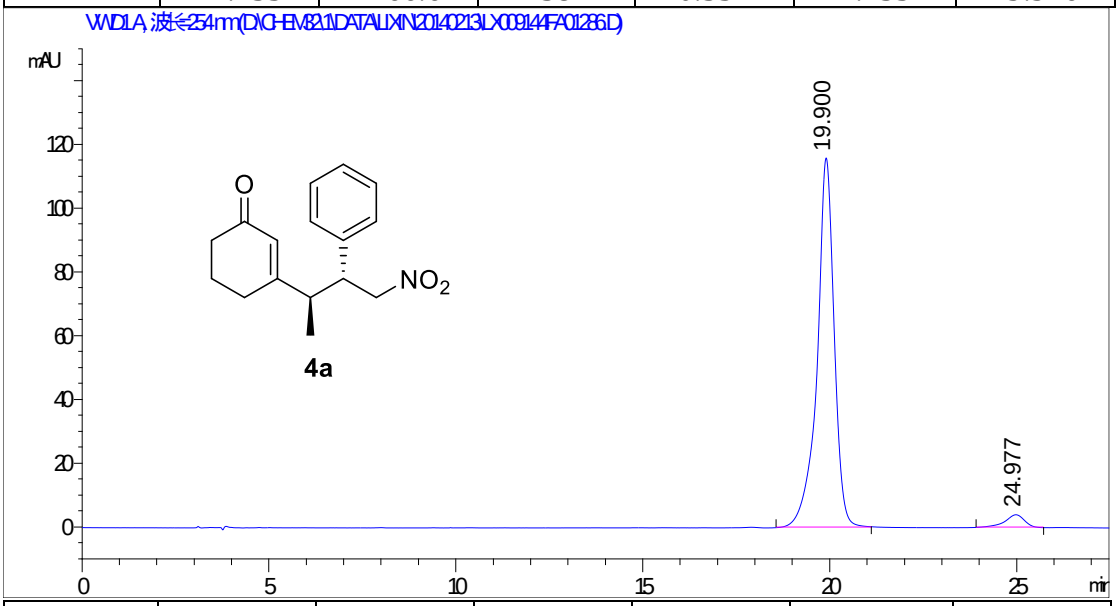


F: HPLC Charts of Products.

4a: 3-((2*R*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one

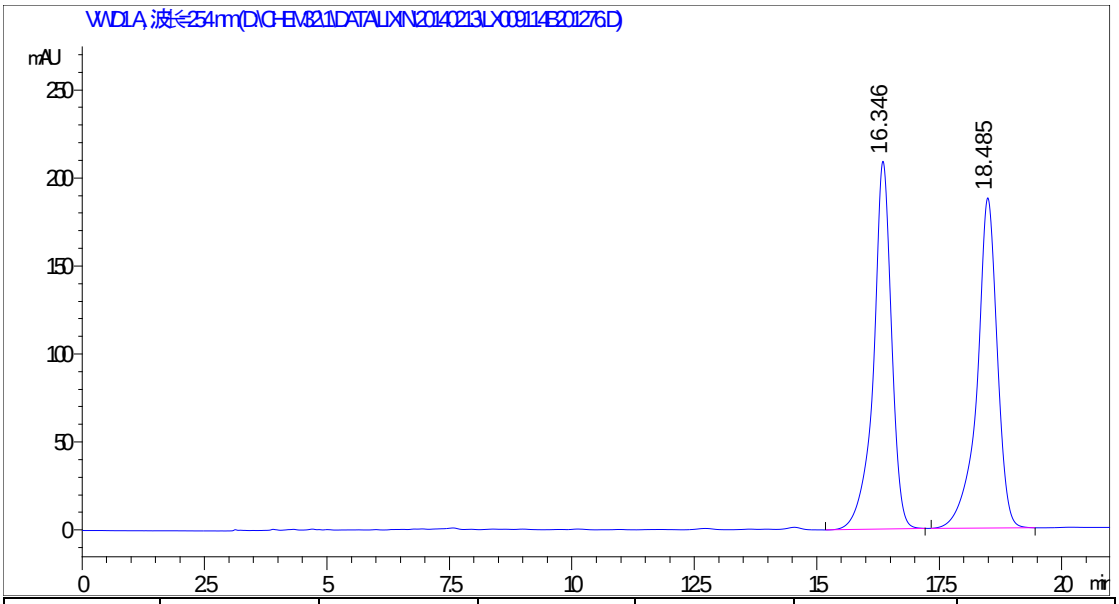


#	Time	Area	Height	Width	Symmetry	Area %
1	19.781	2268.8	73.3	0.4556	1.195	50.024
2	24.753	2266.6	58	0.531	1.153	49.976

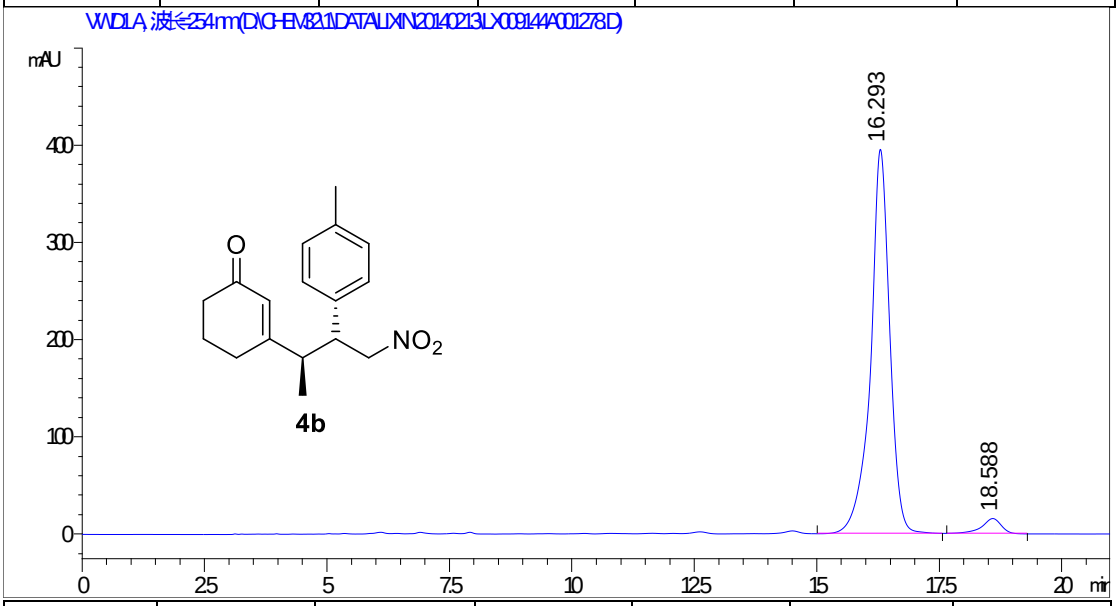


#	Time	Area	Height	Width	Symmetry	Area %
1	19.9	3674.4	115.9	0.5268	1.117	96.132
2	24.977	147.8	4	0.605	1.395	3.868

4b: 3-((2*R*,3*R*)-4-nitro-3-(p-tolyl)butan-2-yl)cyclohex-2-en-1-one

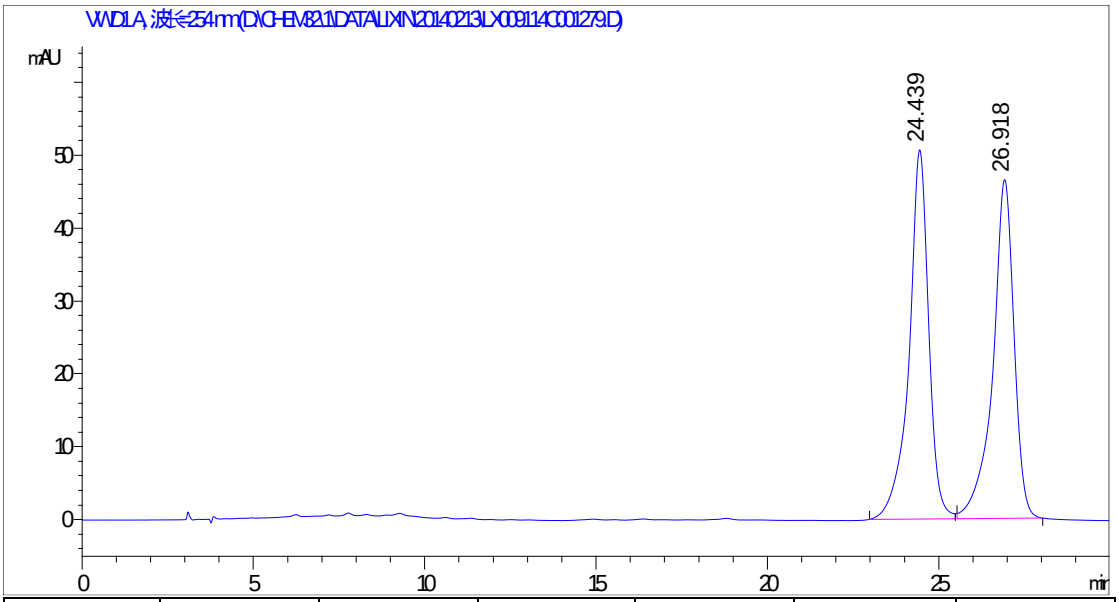


#	Time	Area	Height	Width	Symmetry	Area %
1	16.346	5363.5	209.1	0.3779	1.109	49.976
2	18.485	5368.5	187.7	0.4225	1.141	50.024

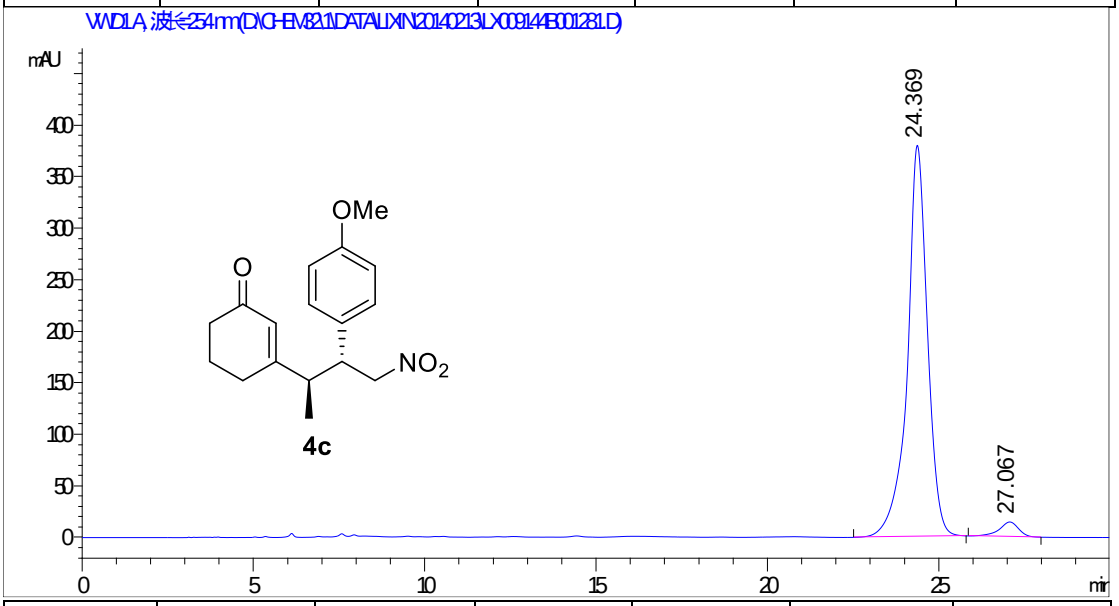


#	Time	Area	Height	Width	Symmetry	Area %
1	16.293	10735.8	395.2	0.4527	1.050	96.127
2	18.588	432.6	15.6	0.4592	1.318	3.873

4c: 3-((2*R*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

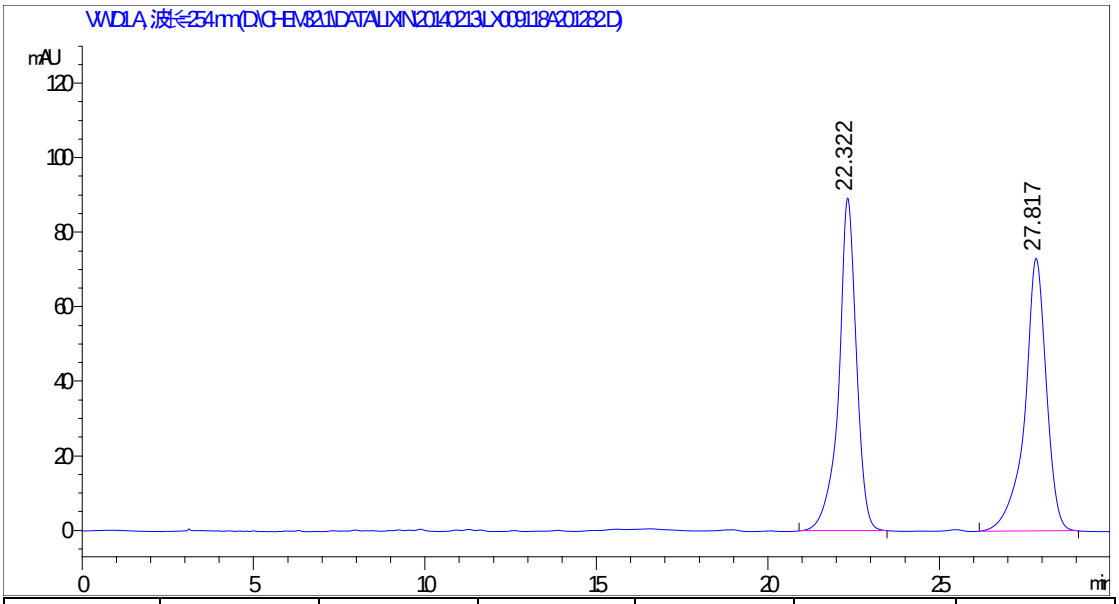


#	Time	Area	Height	Width	Symmetry	Area %
1	24.439	2024.5	50.7	0.5851	1.173	50.242
2	26.918	2005	46.5	0.6351	1.266	49.758

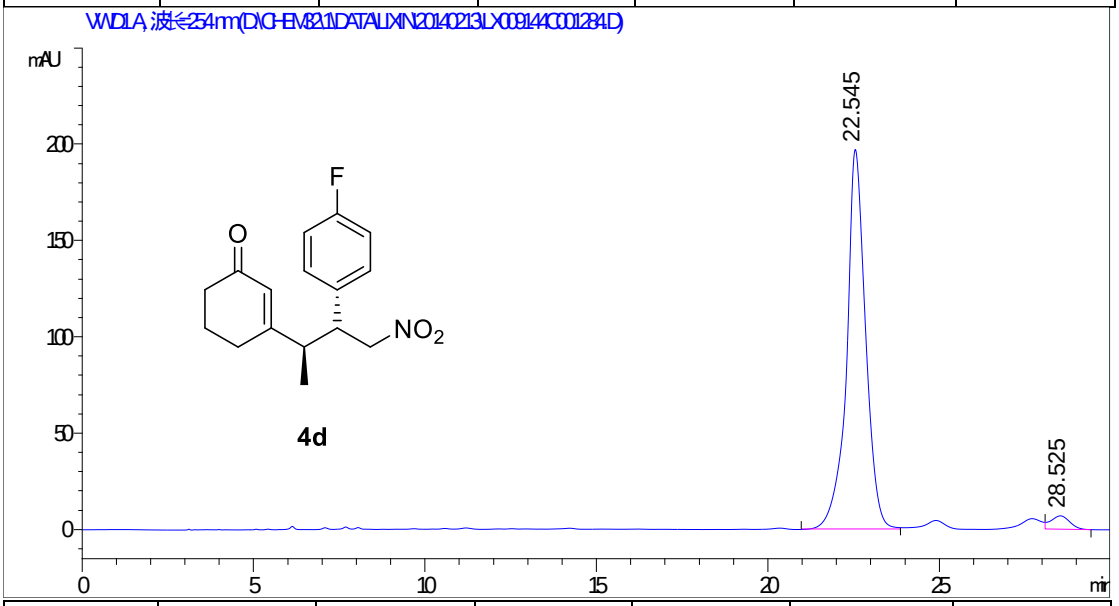


#	Time	Area	Height	Width	Symmetry	Area %
1	24.369	15453.9	379.6	0.6541	0.992	96.503
2	27.067	560	14.2	0.5492	1.221	3.497

4d: 3-((2*R*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

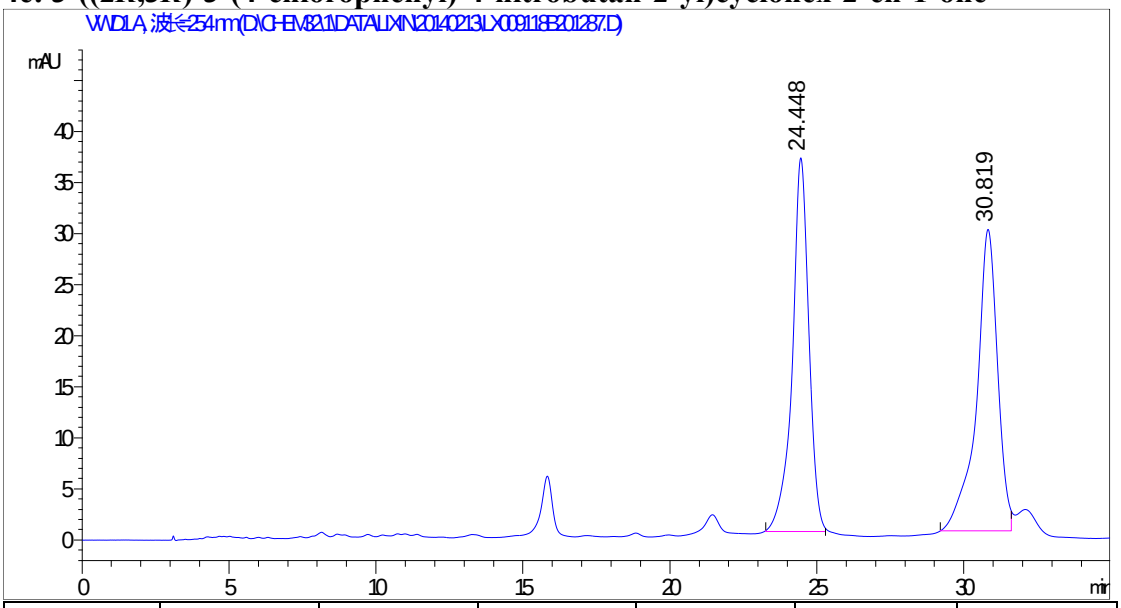


#	Time	Area	Height	Width	Symmetry	Area %
1	22.322	3202.1	89.4	0.5273	1.035	49.971
2	27.817	3205.8	73.2	0.6447	1.118	50.029

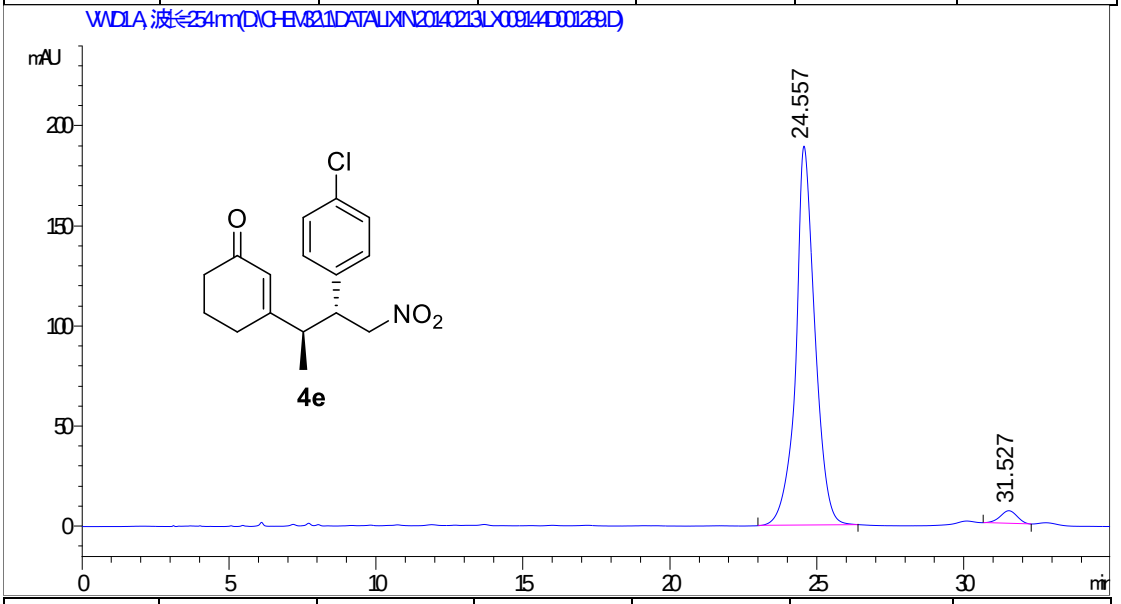


#	Time	Area	Height	Width	Symmetry	Area %
1	22.545	7601.3	197.2	0.6421	0.864	96.455
2	28.525	279.4	7.1	0.592	0.981	3.545

4e: 3-((2*R*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

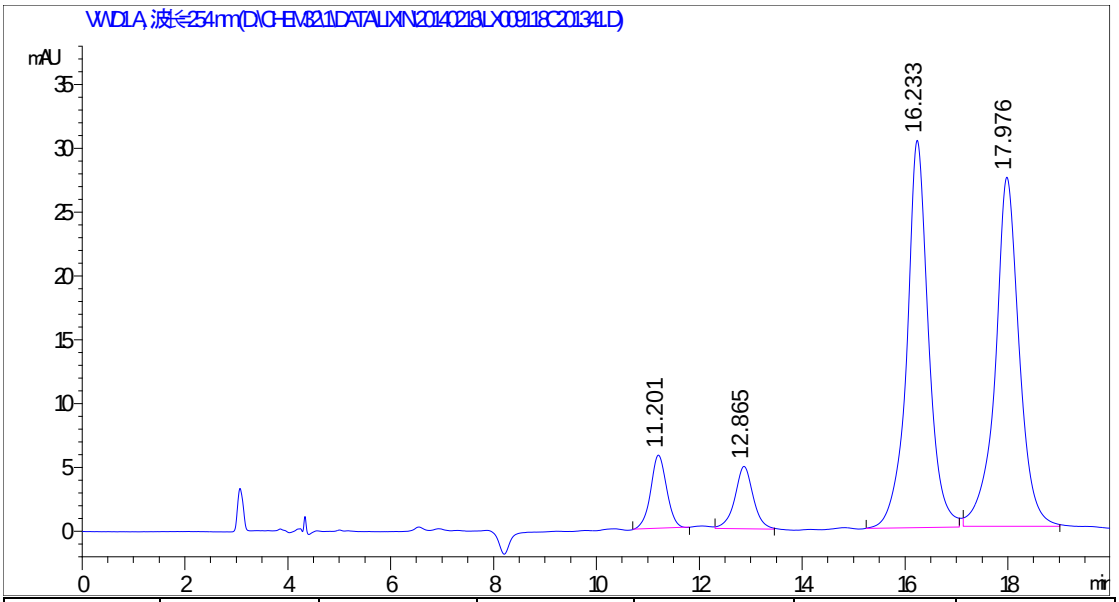


#	Time	Area	Height	Width	Symmetry	Area %
1	24.448	1430.9	36.6	0.6319	1.045	49.184
2	30.819	1478.4	29.6	0.7818	1.287	50.816

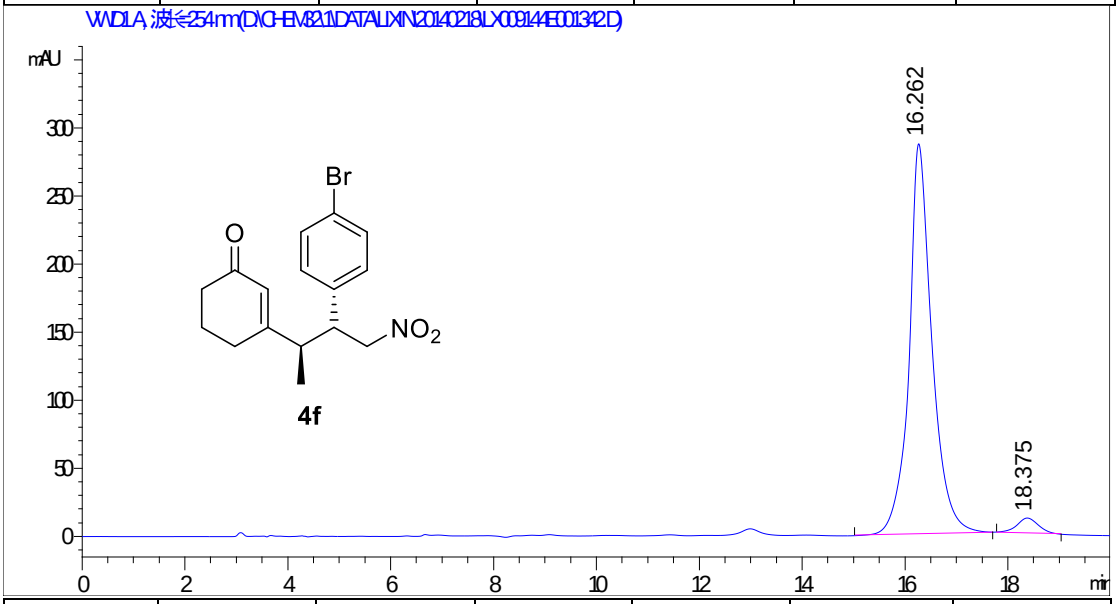


#	Time	Area	Height	Width	Symmetry	Area %
1	24.557	8556	189.4	0.658	0.754	97.043
2	31.527	260.7	6.4	0.6703	1.029	2.957

4f: 3-((2*R*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

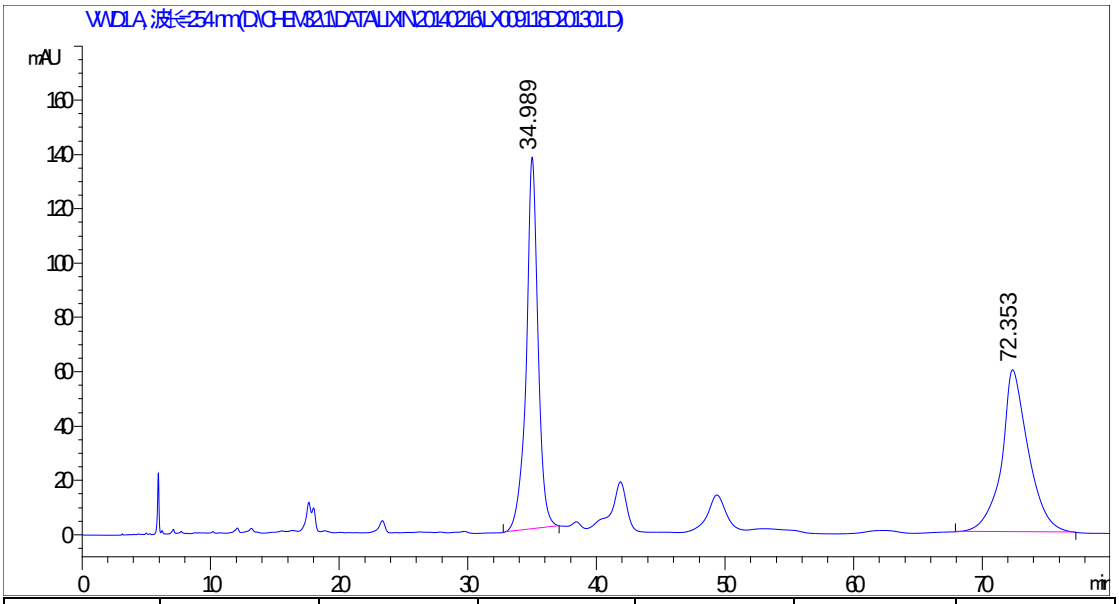


#	Time	Area	Height	Width	Symmetry	Area %
1	11.201	125.3	5.8	0.3338	0.929	6.191
2	12.865	122.8	4.9	0.4162	0.97	6.066
3	16.233	888.3	30.4	0.4273	0.908	43.887
4	17.976	887.7	27.4	0.5403	0.925	43.856

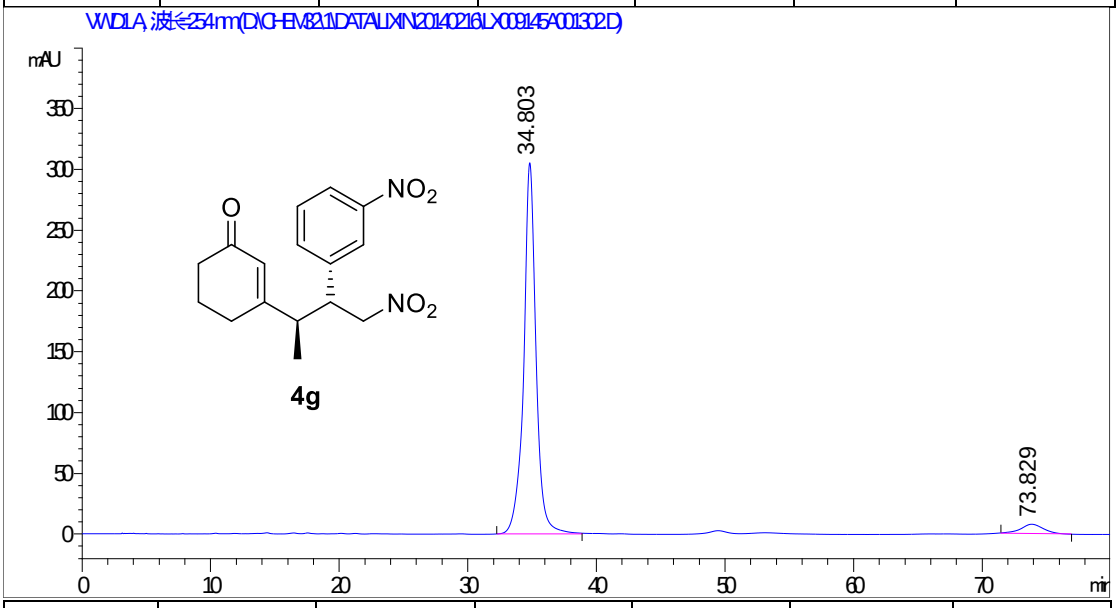


#	Time	Area	Height	Width	Symmetry	Area %
1	16.262	8850.9	286.6	0.5147	0.727	96.477
2	18.375	323.2	11.1	0.4852	0.898	3.523

4g: 3-((2*R*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one

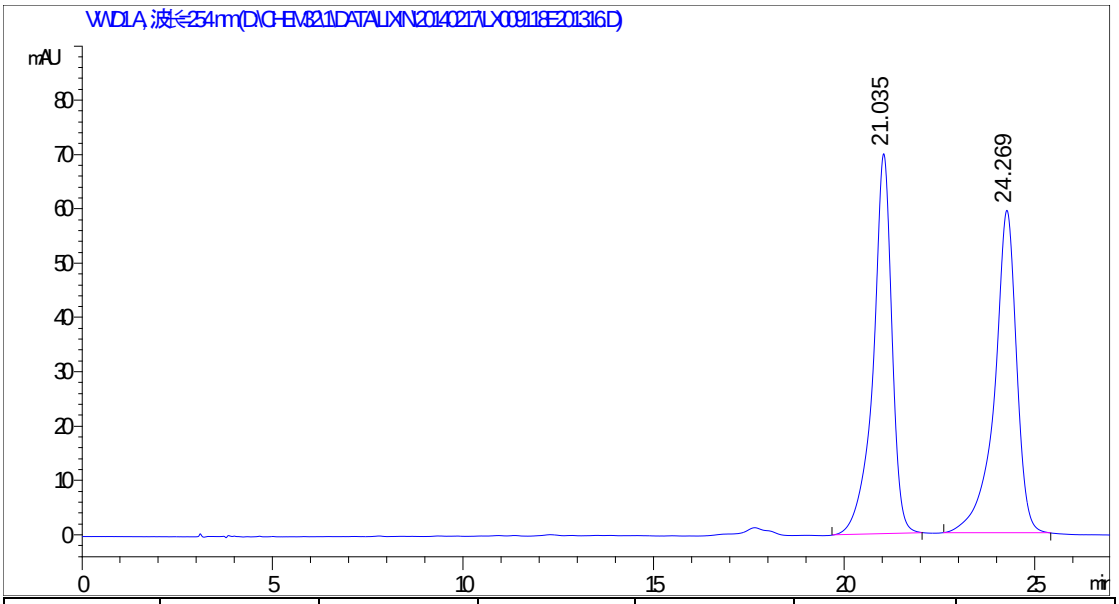


#	Time	Area	Height	Width	Symmetry	Area %
1	34.989	8709.7	137	0.9278	0.991	50.209
2	72.353	8637.1	59.8	2.4085	0.707	49.791

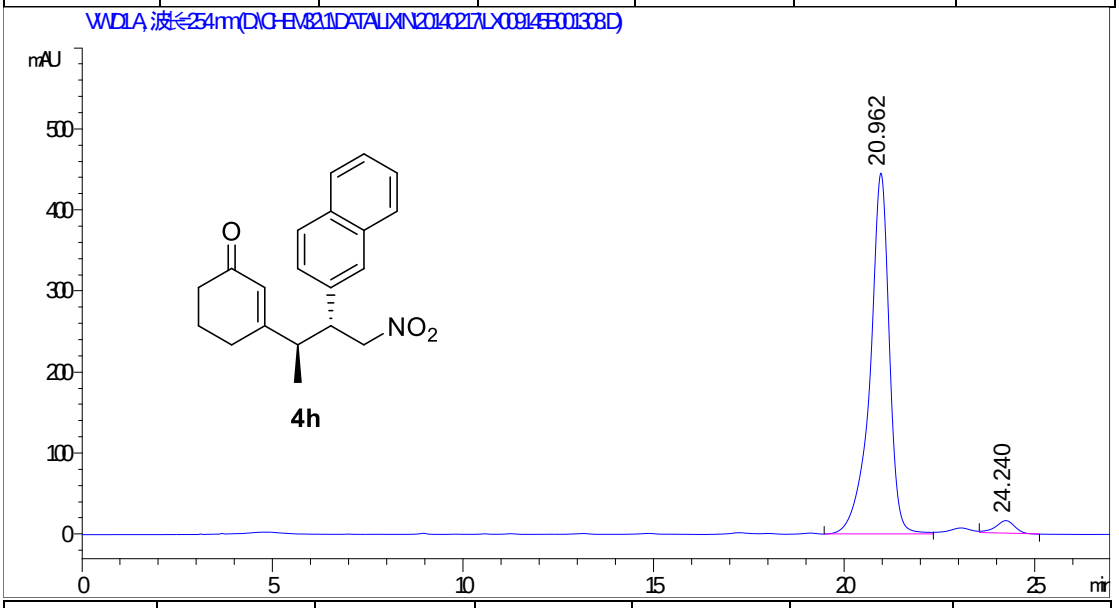


#	Time	Area	Height	Width	Symmetry	Area %
1	34.803	20467.1	305.7	1.116	0.934	95.324
2	73.829	1003.9	7.9	1.5127	0.917	4.676

4h: 3-((2*R*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

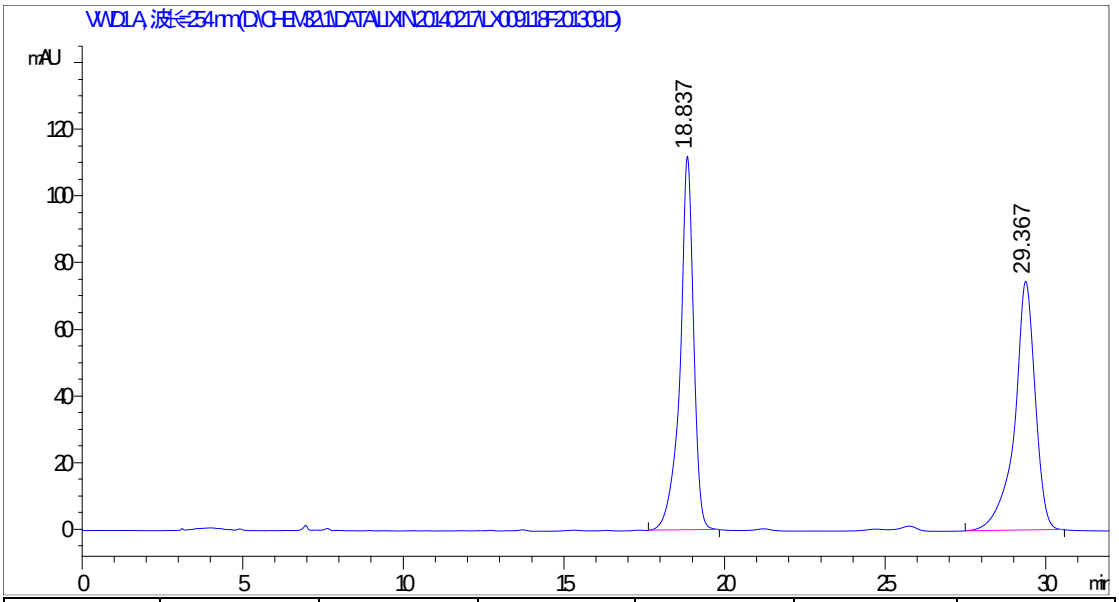


#	Time	Area	Height	Width	Symmetry	Area %
1	21.035	2390.9	70	0.5018	1.278	49.826
2	24.269	2407.6	59.4	0.5935	1.292	50.174

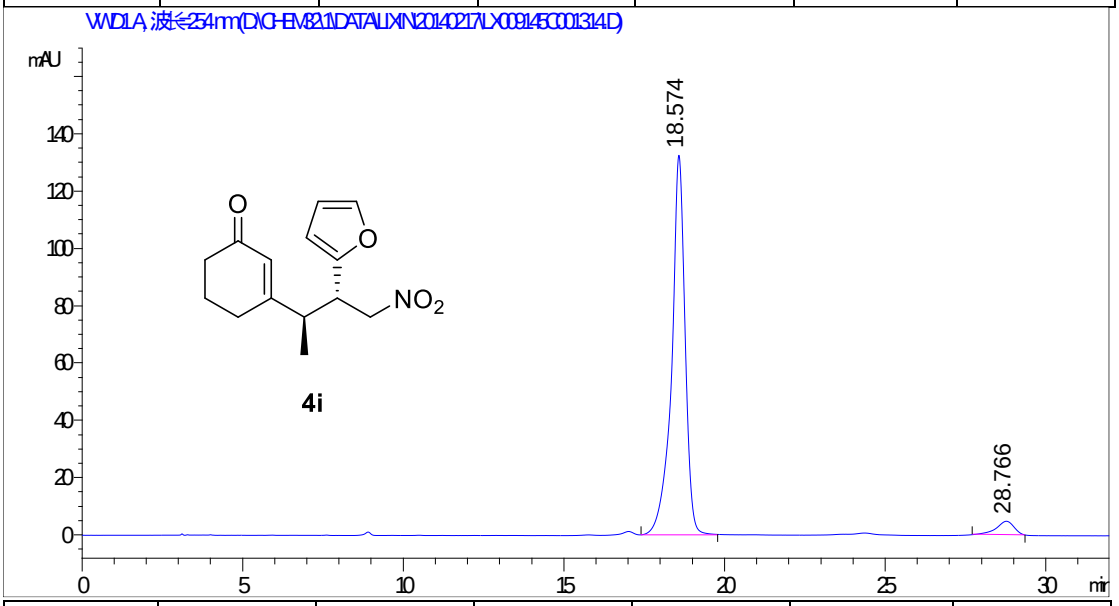


#	Time	Area	Height	Width	Symmetry	Area %
1	20.962	15616.1	445.3	0.5844	1.243	96.424
2	24.24	579.1	16	0.5437	1.202	3.576

4i: 3-((2*R*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

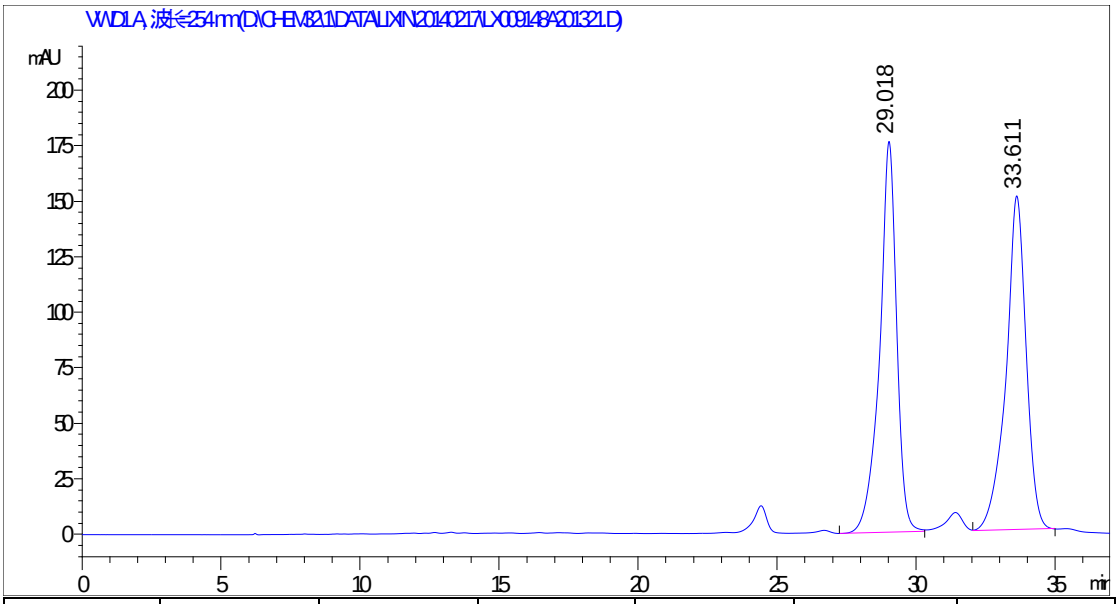


#	Time	Area	Height	Width	Symmetry	Area %
1	18.837	3292.5	112.1	0.4299	1.185	49.625
2	29.367	3342.3	74.7	0.6544	1.185	50.375

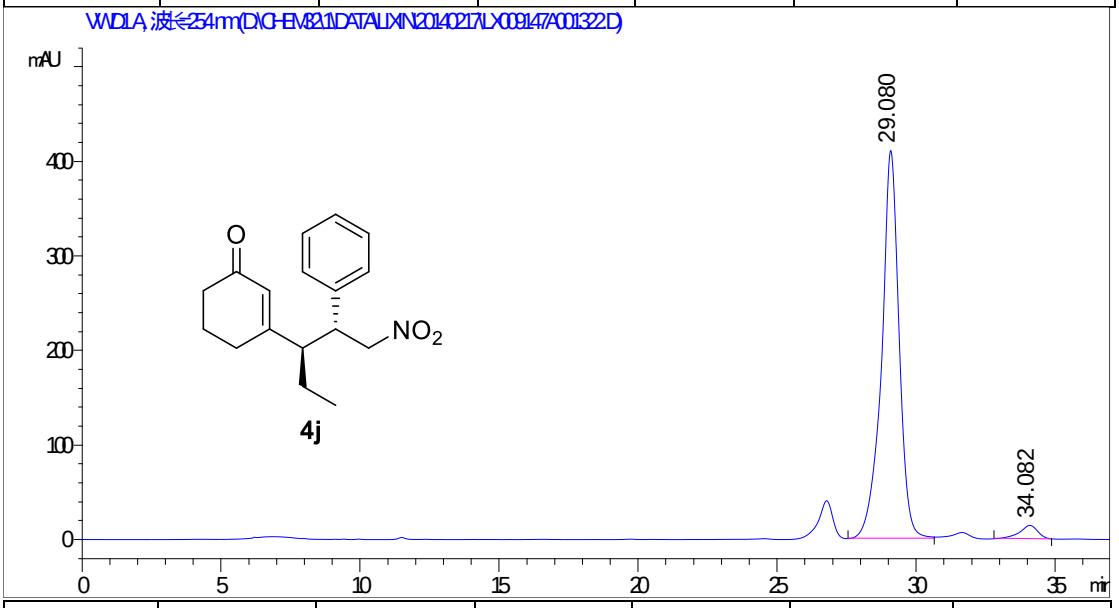


#	Time	Area	Height	Width	Symmetry	Area %
1	18.574	3863.4	132.5	0.4836	1.182	95.390
2	28.766	186.7	4.8	0.5941	1.466	4.610

4j:3-((2*R*,3*R*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one

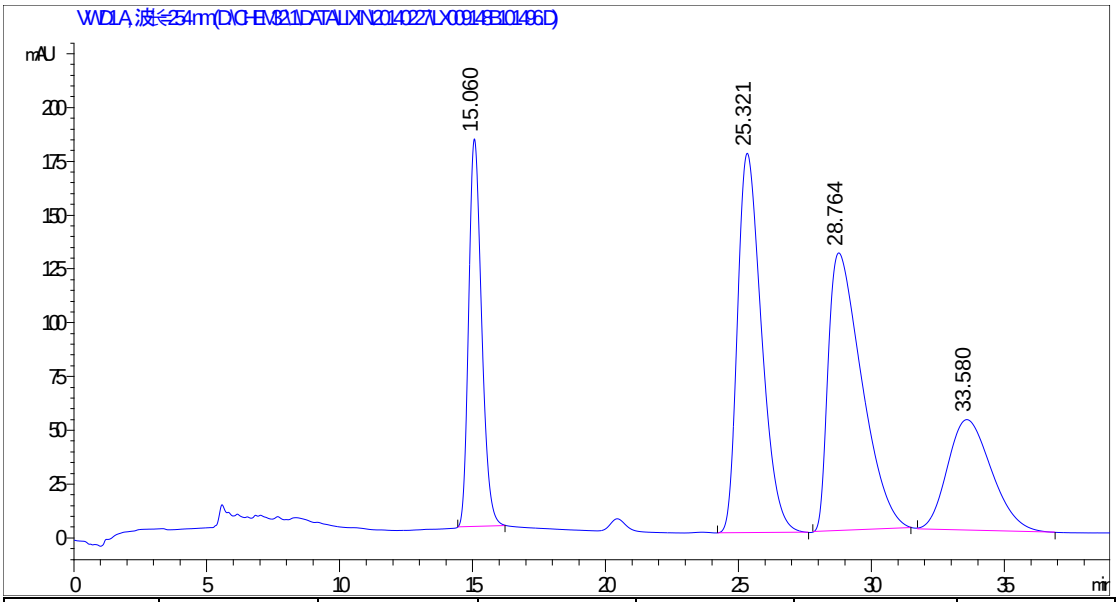


#	Time	Area	Height	Width	Symmetry	Area %
1	29.018	7499.1	176.2	0.6204	1.220	49.713
2	33.611	7585.5	150.4	0.7382	1.135	50.287

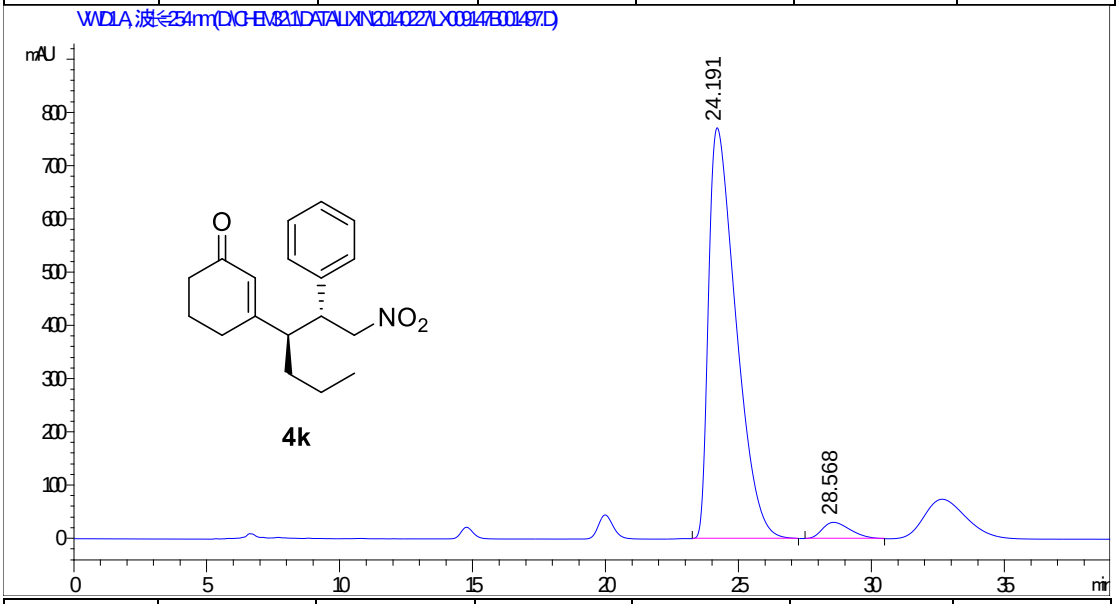


#	Time	Area	Height	Width	Symmetry	Area %
1	29.08	17942.7	410.2	0.7289	1.070	96.468
2	34.082	656.9	14.2	0.7699	1.322	3.532

4k: 3-((2*R*,3*R*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one

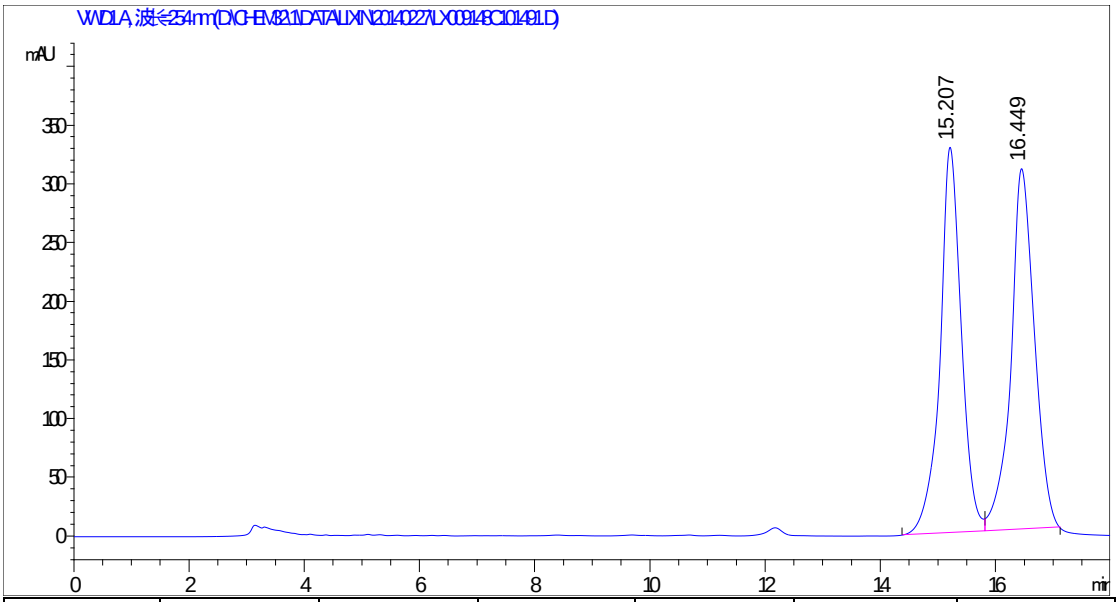


#	Time	Area	Height	Width	Symmetry	Area %
1	15.06	6093.1	180.1	0.5639	0.761	17.705
2	25.321	11086.5	176.4	0.9678	0.638	32.214
3	28.764	11312	129	1.4613	0.443	32.870
4	33.58	5923.2	51.4	1.9195	0.758	17.211

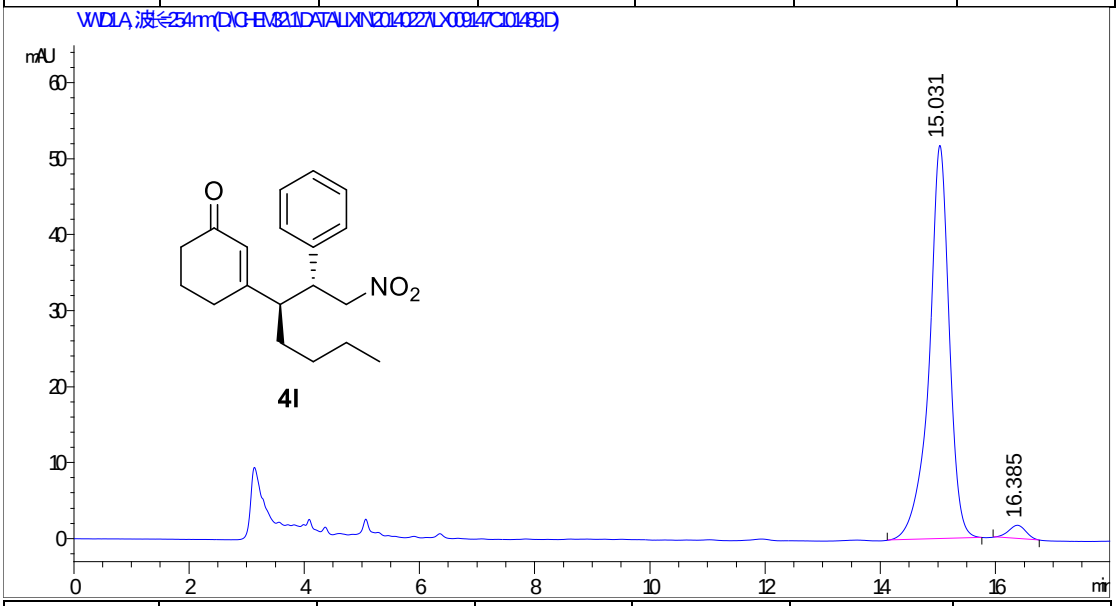


#	Time	Area	Height	Width	Symmetry	Area %
1	24.191	55202.1	771.4	1.1926	0.445	96.110
2	28.568	2234.5	30.5	1.222	0.649	3.890

4l: 3-((2*R*,3*R*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one

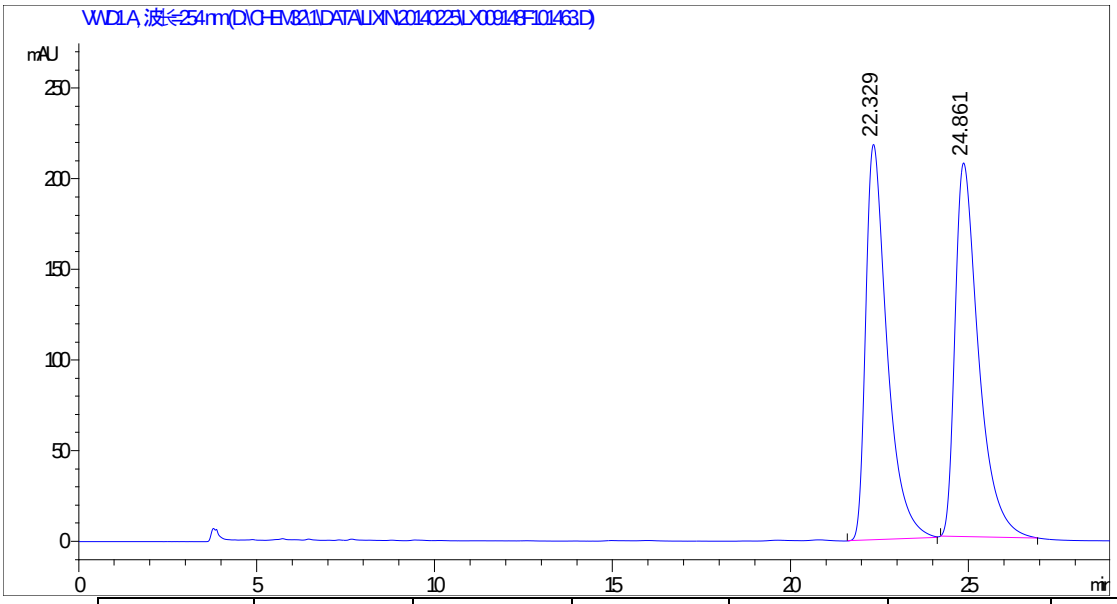


#	Time	Area	Height	Width	Symmetry	Area %
1	15.207	8431.9	328.3	0.4281	0.897	49.131
2	16.449	8730.4	307.2	0.4736	0.821	50.869

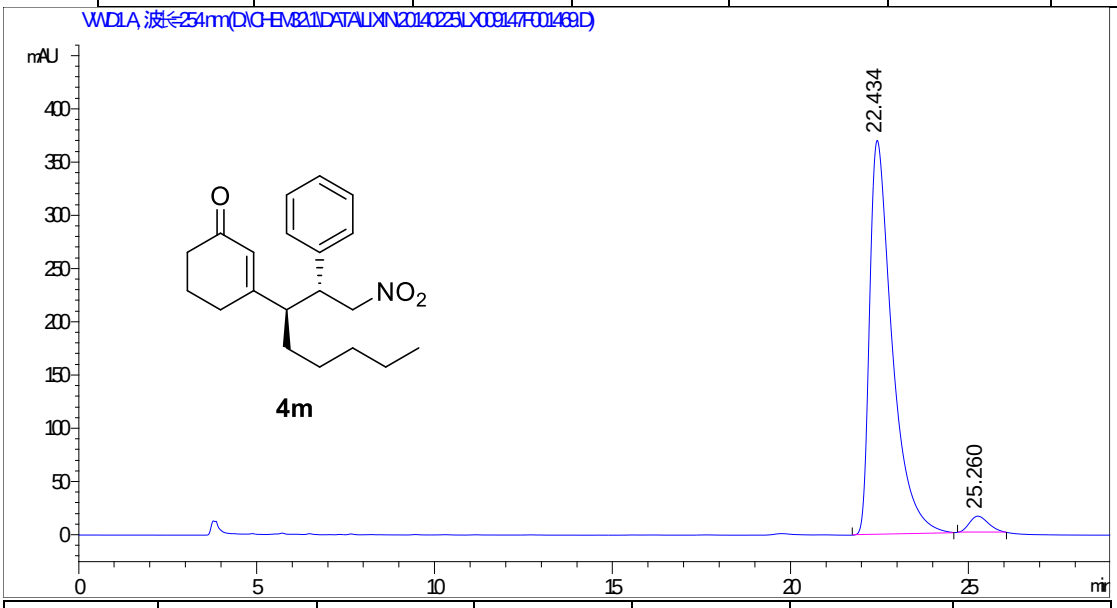


#	Time	Area	Height	Width	Symmetry	Area %
1	15.031	1257.4	51.8	0.3573	1.142	97.057
2	16.385	38.1	1.8	0.3566	1.042	2.943

4m: 3-((2*R*,3*R*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one

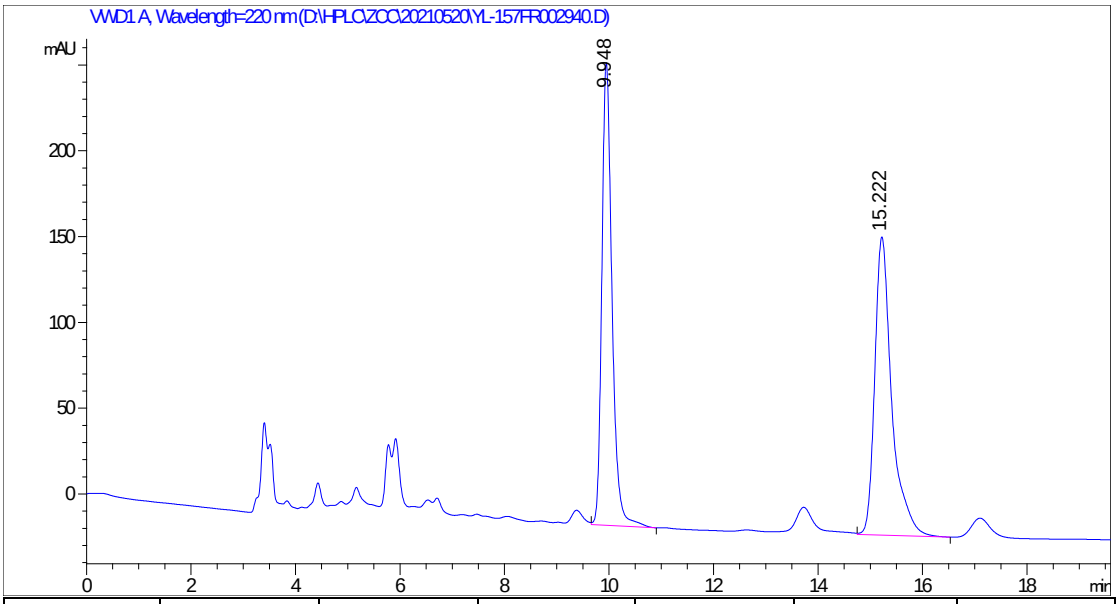


#	Time	Area	Height	Width	Symmetry	Area %
1	22.329	9121.1	218.3	0.6964	0.548	49.053
2	24.861	9473.3	206.3	0.7655	0.547	50.947

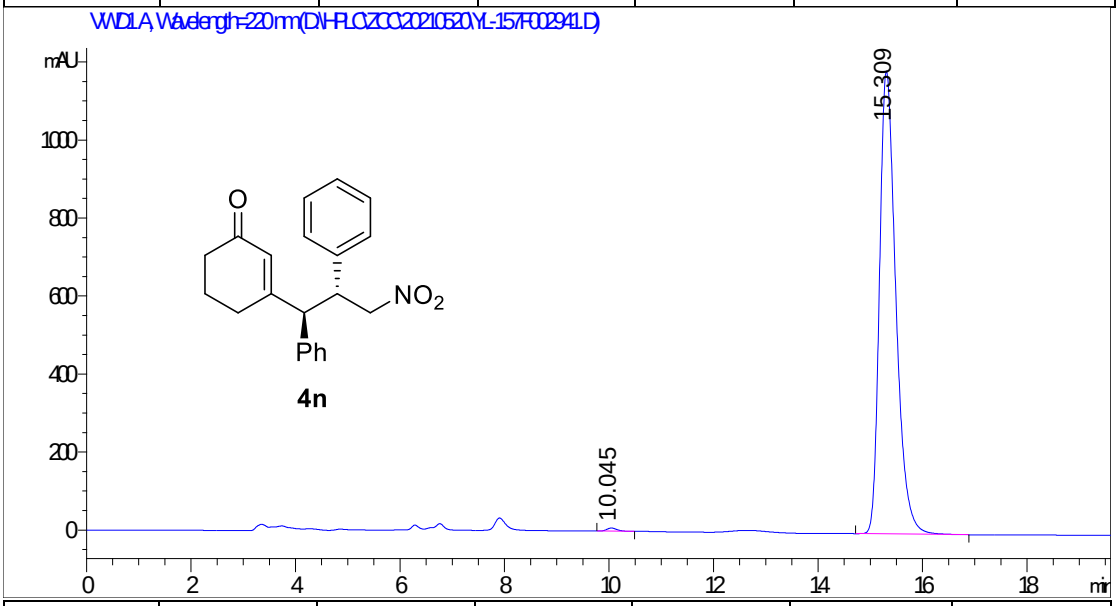


#	Time	Area	Height	Width	Symmetry	Area %
1	22.434	16257	370.1	0.7321	0.488	96.495
2	25.26	590.5	15.5	0.6367	0.766	3.505

4n: 3-((1*R*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one

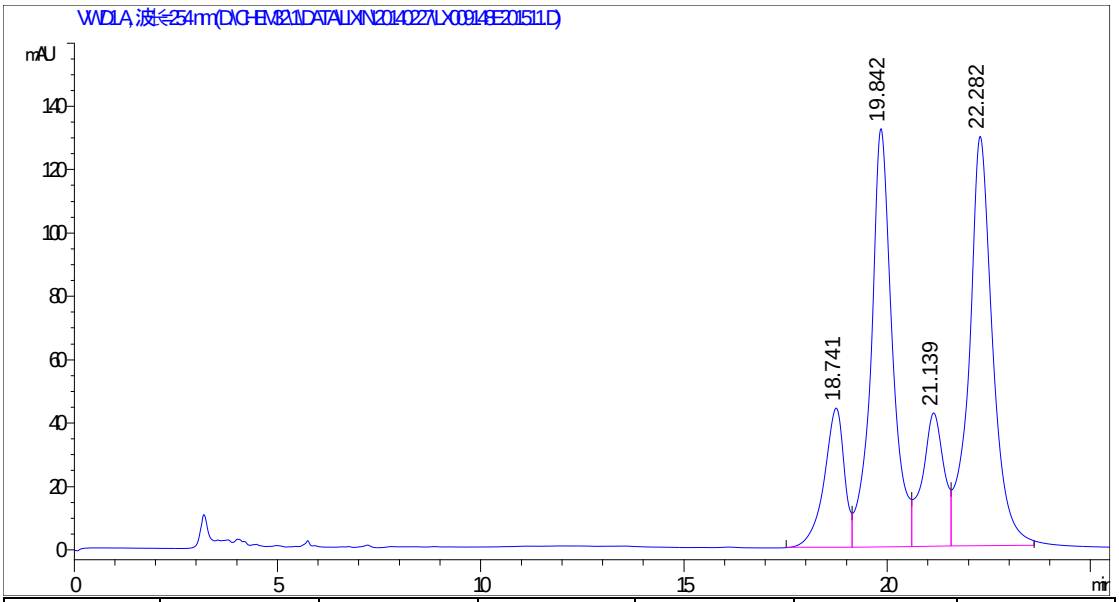


#	Time	Area	Height	Width	Symmetry	Area %
1	9.948	3642.7	269.6	0.2058	0.719	48.203
2	15.222	3914.3	173.7	0.3372	0.656	51.797

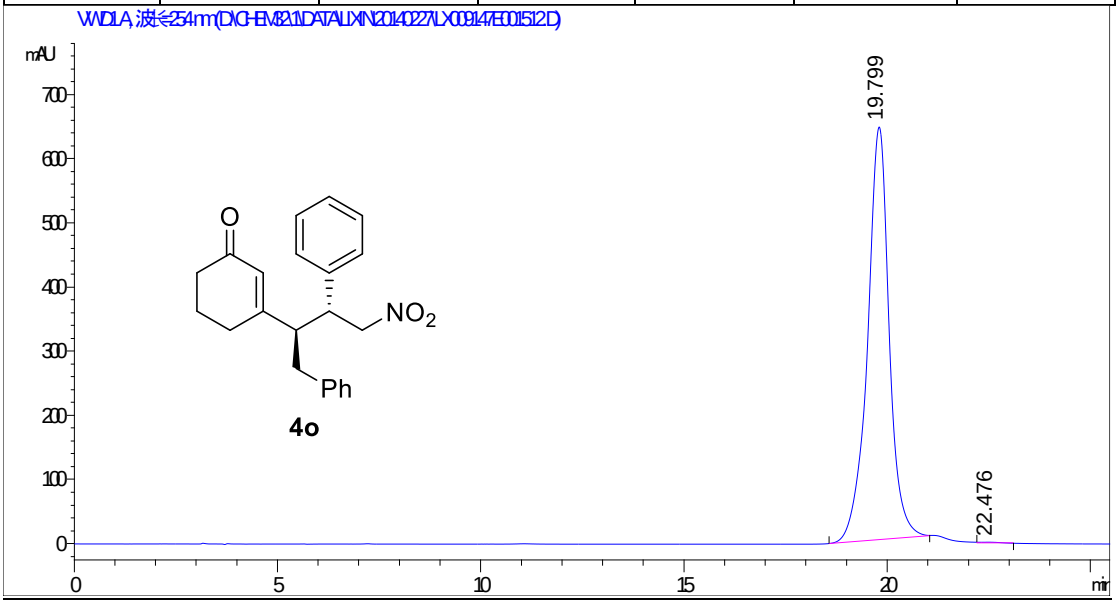


#	Time	Area	Height	Width	Symmetry	Area %
1	10.045	112.8	8.2	0.2112	0.786	0.436
2	15.309	25762.8	1186.8	0.3334	0.676	99.564

4o: 3-((2*R*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one

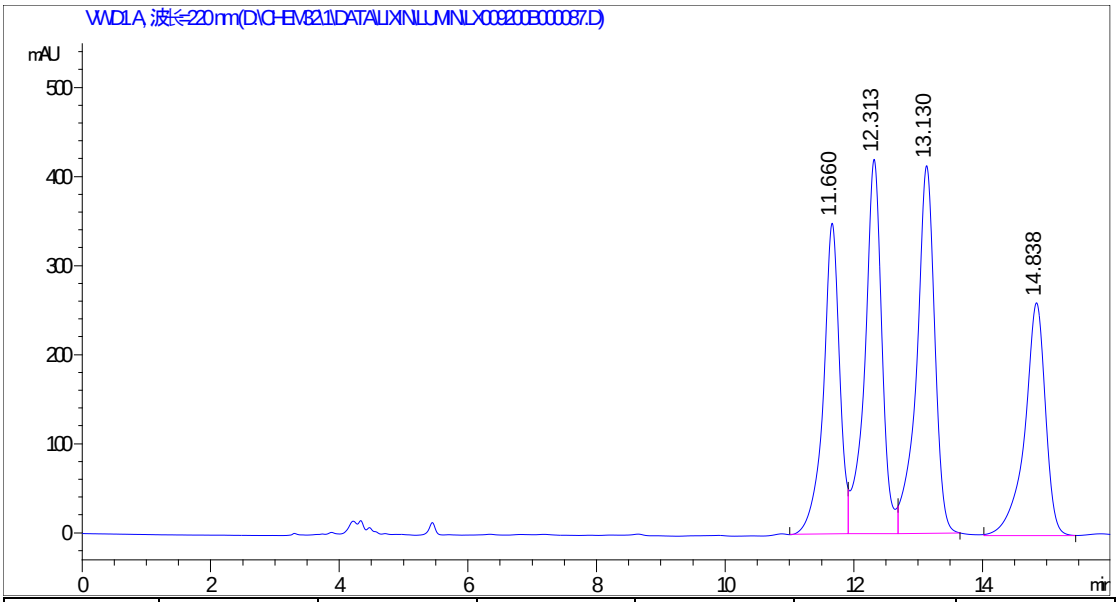


#	Time	Area	Height	Width	Symmetry	Area %
1	18.741	1519.6	44	0.5169	1.475	11.593
2	19.842	4792.3	132	0.5225	0.857	36.560
3	21.139	1571.7	42.2	0.5381	1.093	11.991
4	22.282	5224.2	129.3	0.6733	0.862	39.856

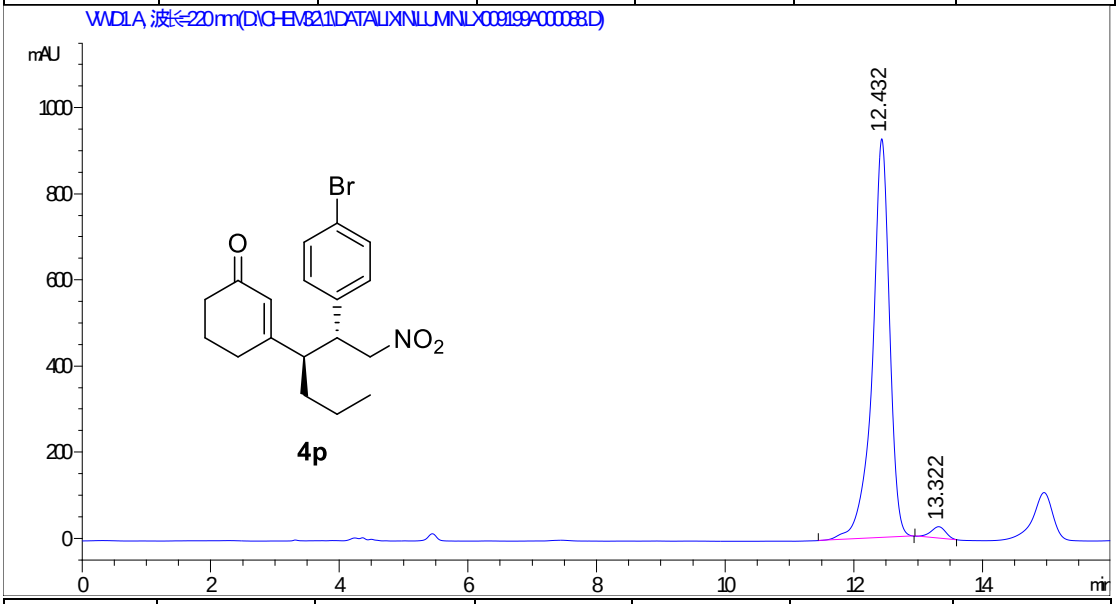


#	Time	Area	Height	Width	Symmetry	Area %
1	19.799	23746.6	643.3	0.6152	1.128	99.752
2	22.476	58.9	1.6	0.6104	0.730	0.248

4p: 3-((2*R*,3*R*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one

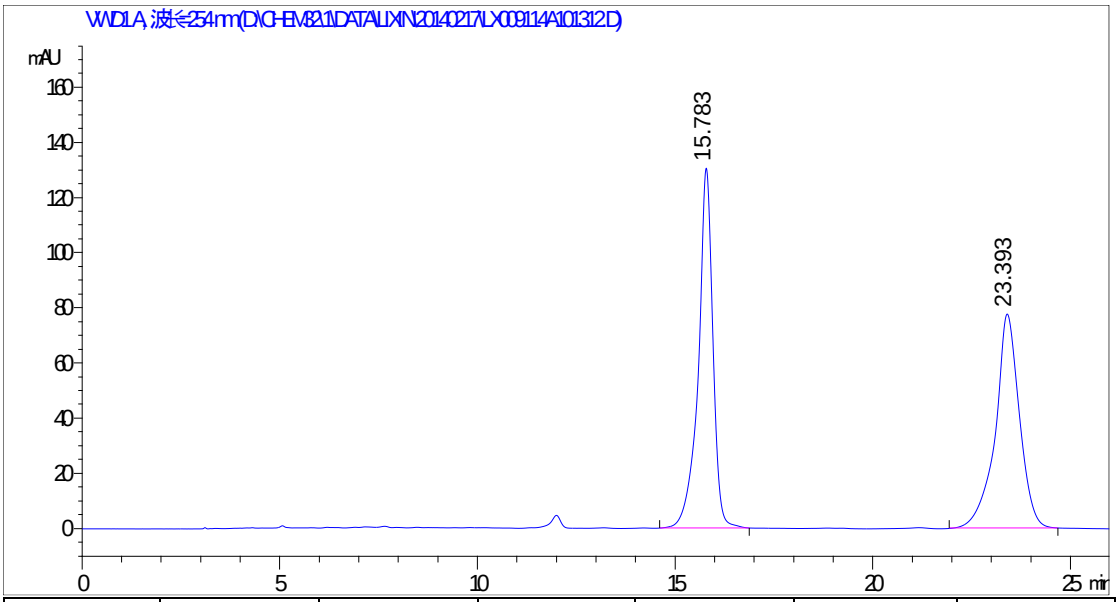


#	Time	Area	Height	Width	Symmetry	Area %
1	11.66	6112.5	349.4	0.2916	1.172	21.941
2	12.313	7784.8	420.7	0.3084	1.238	27.943
3	13.13	8065.5	413	0.3255	1.137	28.951
4	14.838	5896.5	262	0.3751	1.309	21.165

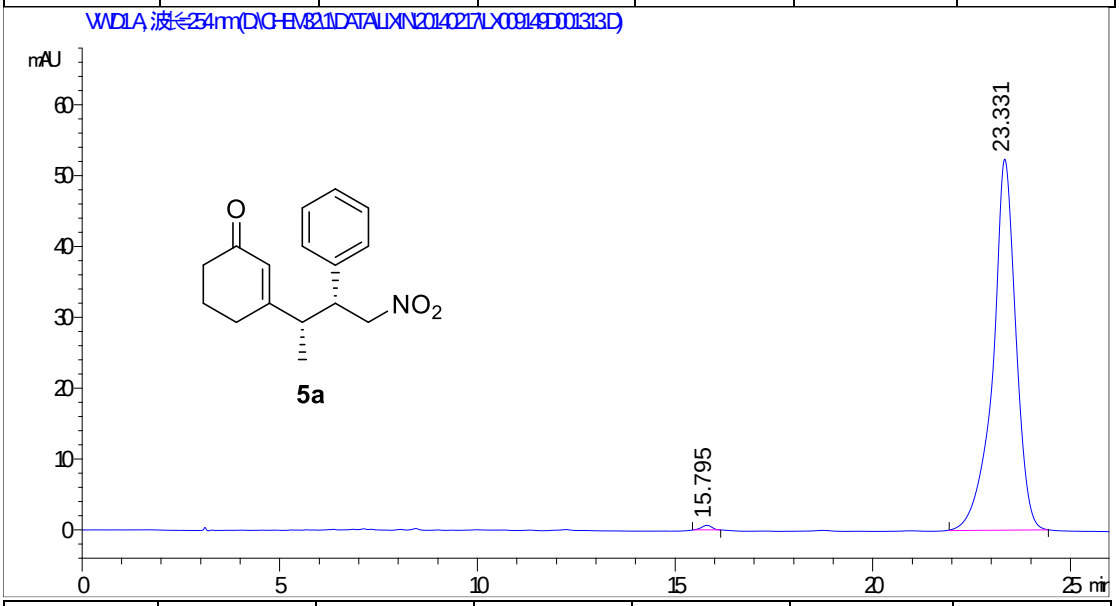


#	Time	Area	Height	Width	Symmetry	Area %
1	12.432	17171.1	927.2	0.3087	1.195	97.516
2	13.322	437.3	27	0.2703	1.041	2.484

5a: 3-((2*S*,3*R*)-4-nitro-3-phenylbutan-2-yl)cyclohex-2-en-1-one

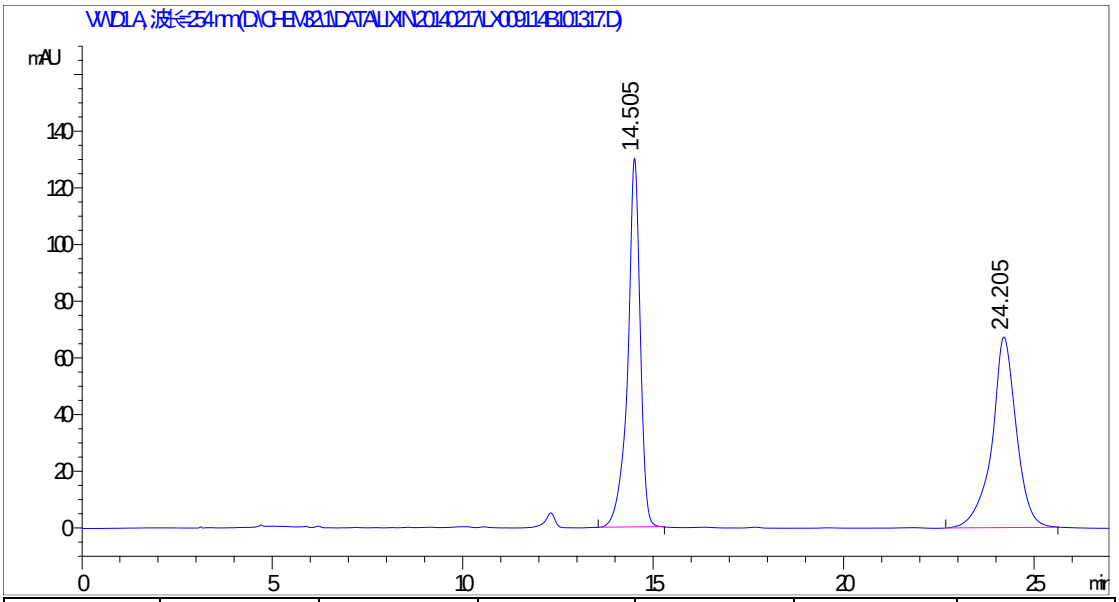


#	Time	Area	Height	Width	Symmetry	Area %
1	15.783	3351.4	130.6	0.3738	1.192	50.369
2	23.393	3302.3	77.7	0.6151	0.994	49.631

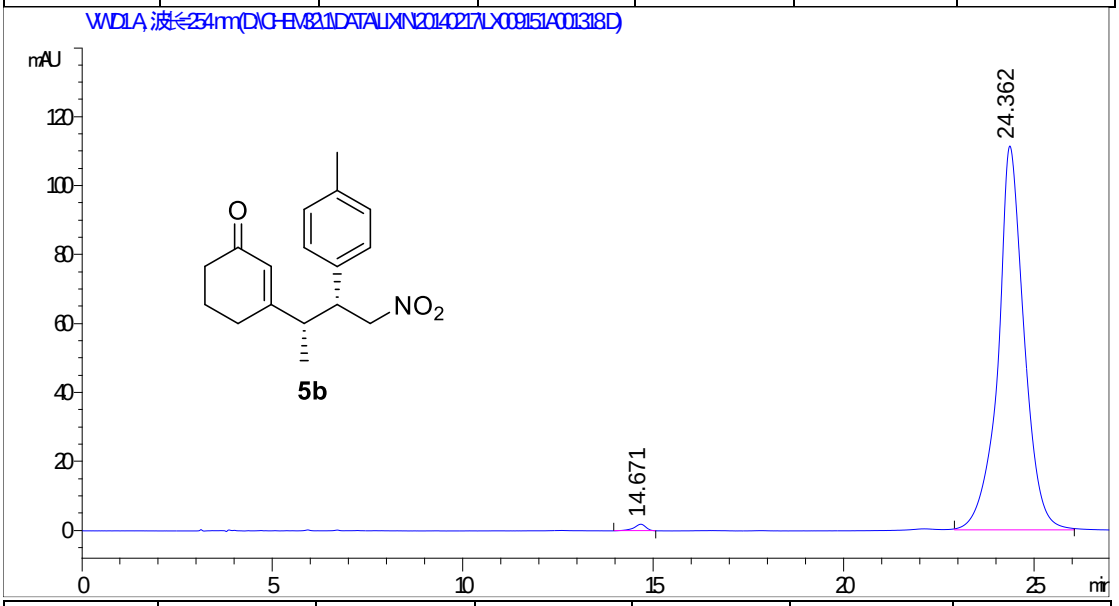


#	Time	Area	Height	Width	Symmetry	Area %
1	15.795	12.3	6.6E-1	0.3118	1.035	0.577
2	23.331	2117.5	52.4	0.585	1.083	99.423

5b: 3-((2*S*,3*R*)-4-nitro-3-(p-tolyl)butan-2-yl)cyclohex-2-en-1-one

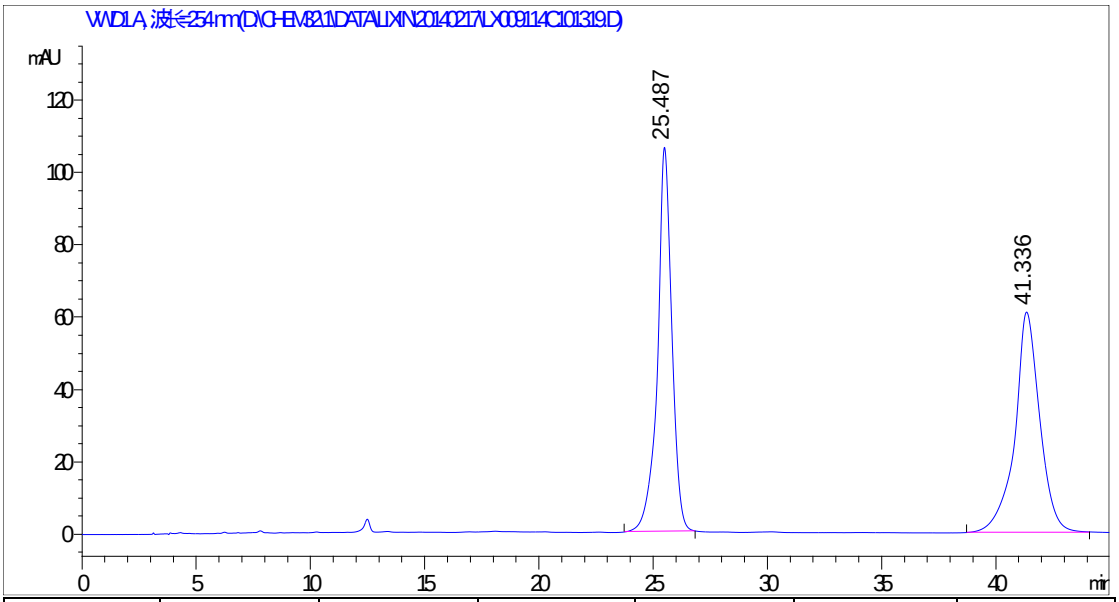


#	Time	Area	Height	Width	Symmetry	Area %
1	14.505	2964.3	130.2	0.3341	1.186	49.708
2	24.205	2999.2	67.3	0.6467	0.969	50.292

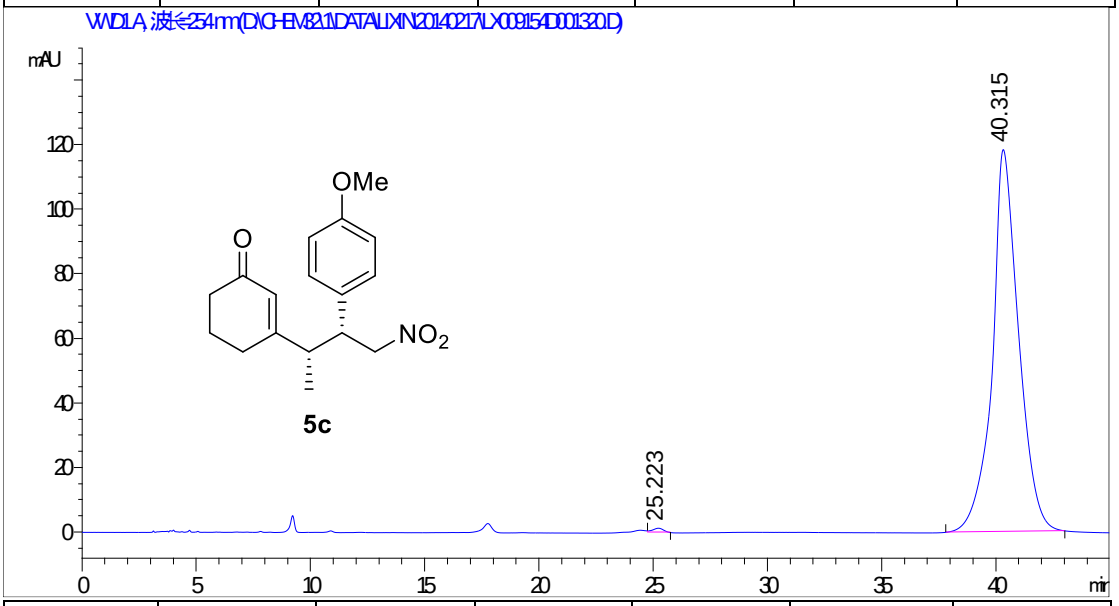


#	Time	Area	Height	Width	Symmetry	Area %
1	14.671	42.6	1.9	0.371	1.378	0.794
2	24.362	5325.2	111.5	0.7958	0.828	99.206

5c: 3-((2*S*,3*R*)-3-(4-methoxyphenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

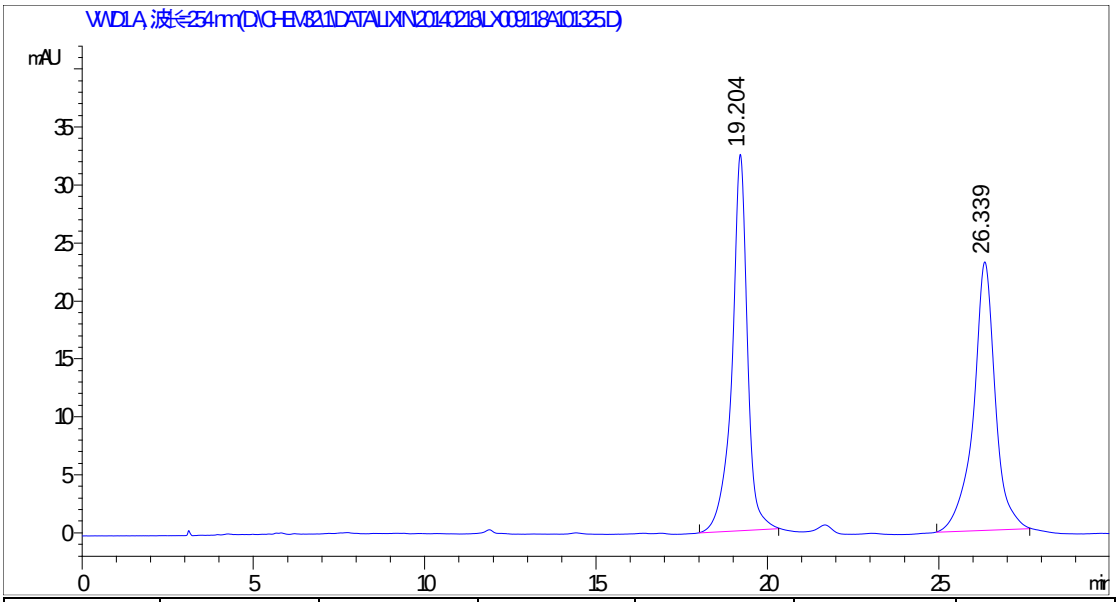


#	Time	Area	Height	Width	Symmetry	Area %
1	25.487	4637.1	106.2	0.636	0.966	50.052
2	41.336	4627.5	60.9	1.2656	0.889	49.948

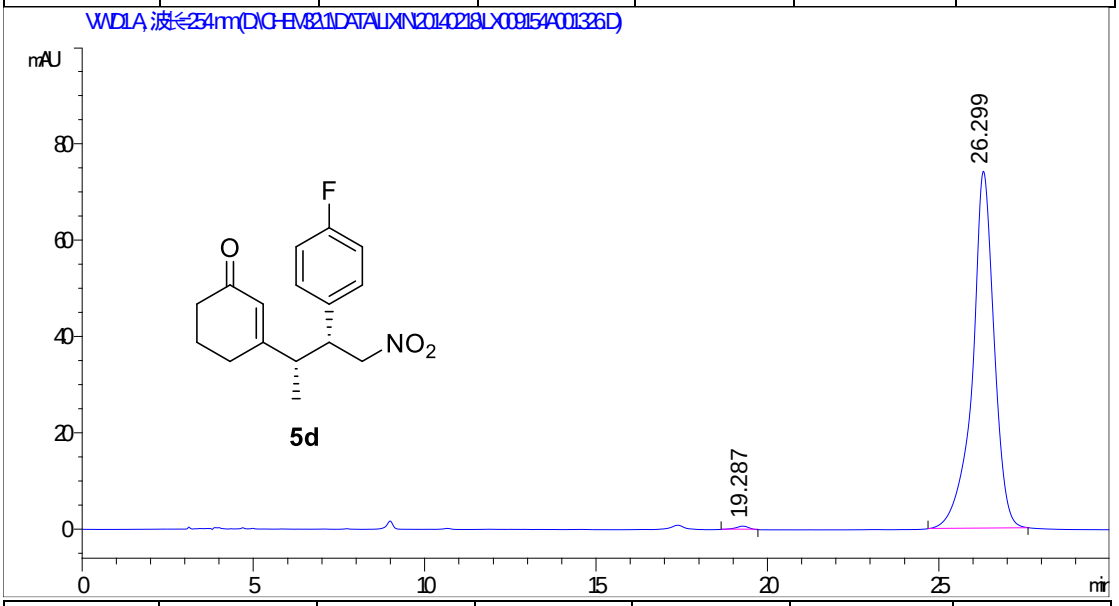


#	Time	Area	Height	Width	Symmetry	Area %
1	25.223	46.3	1.3	0.5724	1.168	0.485
2	40.315	9487.5	118.4	1.1372	0.733	99.515

5d: 3-((2*S*,3*R*)-3-(4-fluorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

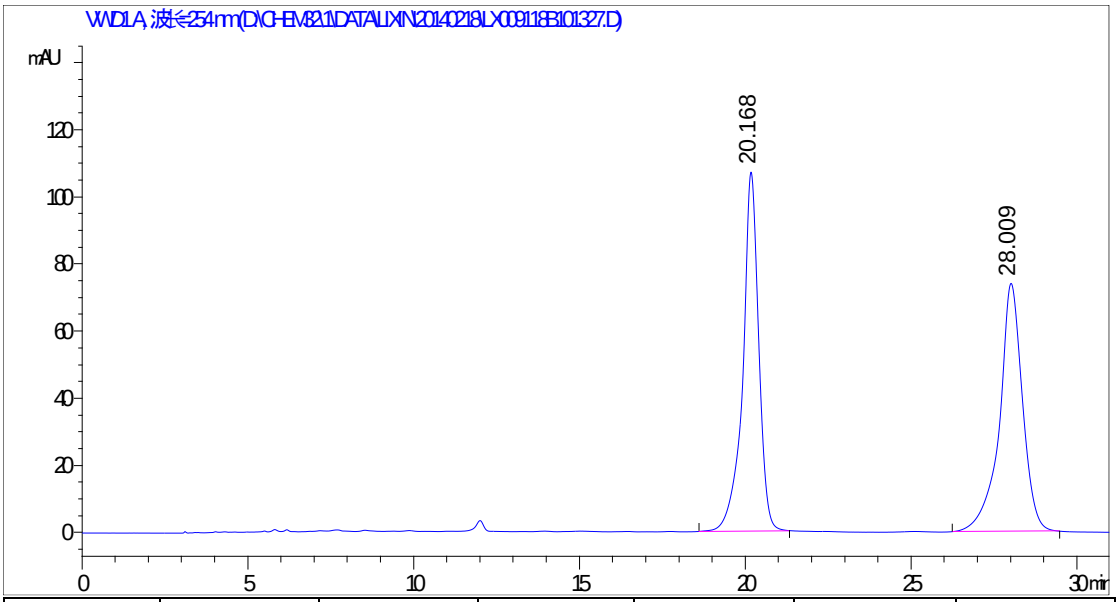


#	Time	Area	Height	Width	Symmetry	Area %
1	19.204	1016.4	32.5	0.4552	1.140	49.742
2	26.339	1026.9	23.2	0.6376	1.066	50.258

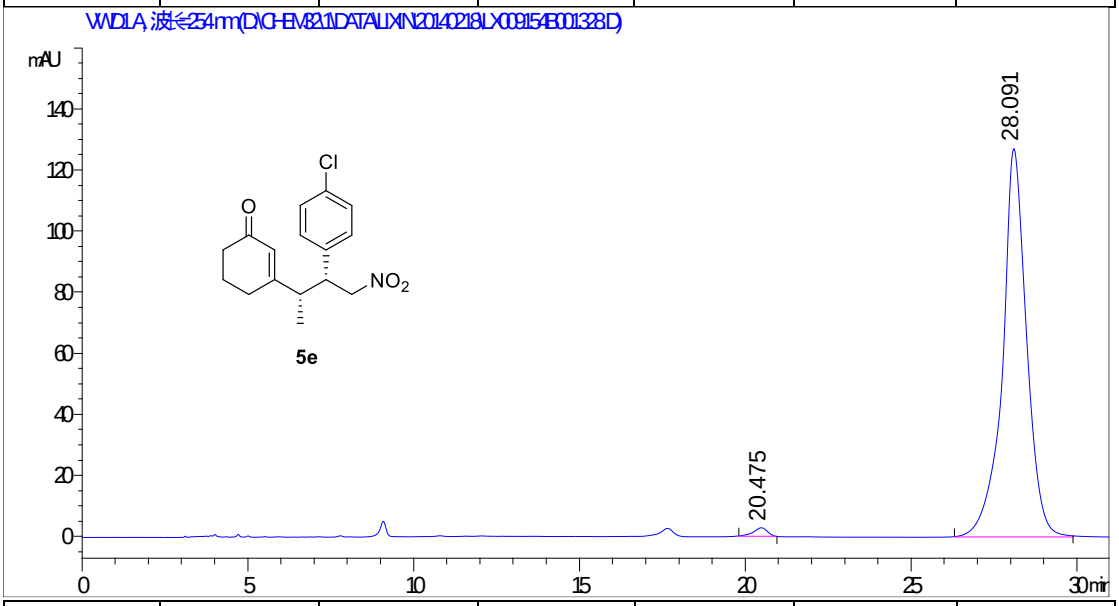


#	Time	Area	Height	Width	Symmetry	Area %
1	19.287	18.7	7E-1	0.4428	1.256	0.568
2	26.299	3268.8	74.2	0.6418	1.040	99.432

5e: 3-((2*S*,3*R*)-3-(4-chlorophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

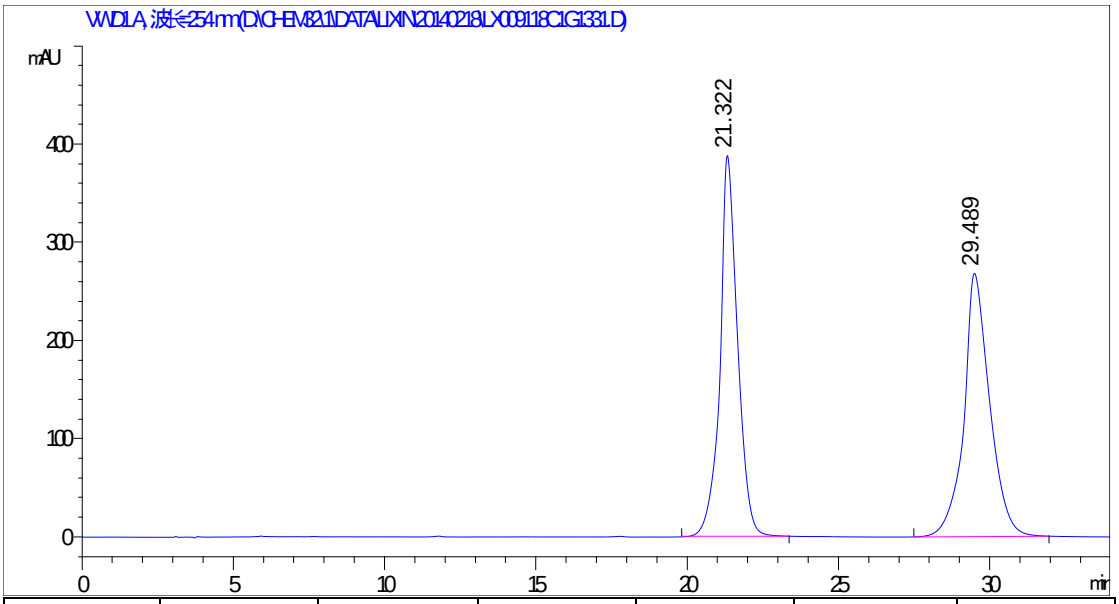


#	Time	Area	Height	Width	Symmetry	Area %
1	20.168	3568.9	107	0.4881	1.087	49.905
2	28.009	3582.5	74	0.7048	1.037	50.095

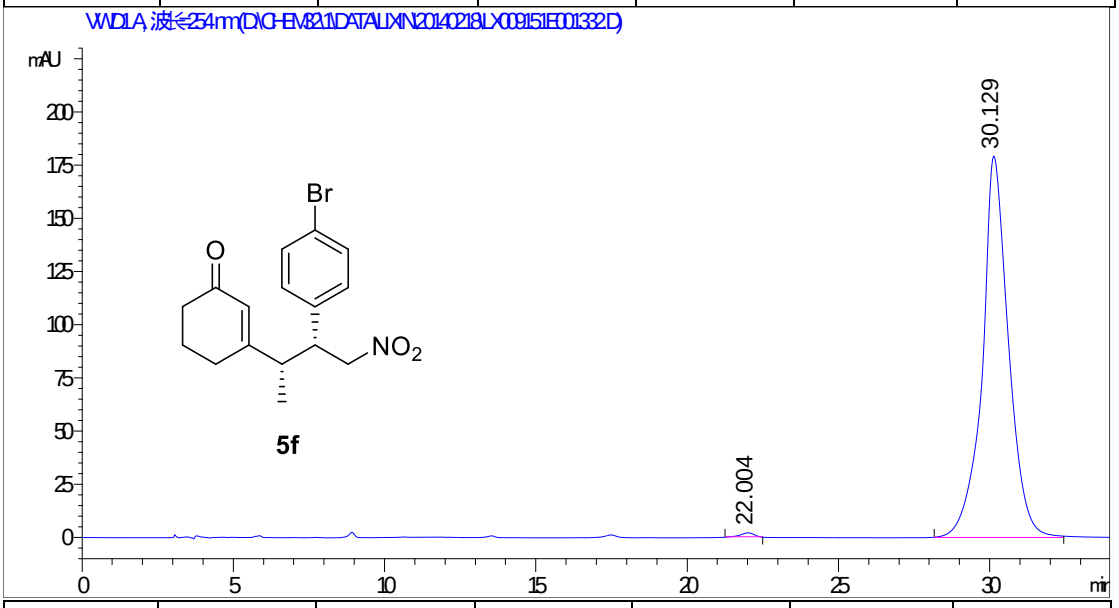


#	Time	Area	Height	Width	Symmetry	Area %
1	20.475	92.1	2.9	0.5244	1.323	1.413
2	28.091	6429.9	127.2	0.8428	0.890	98.587

5f: 3-((2*S*,3*R*)-3-(4-bromophenyl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

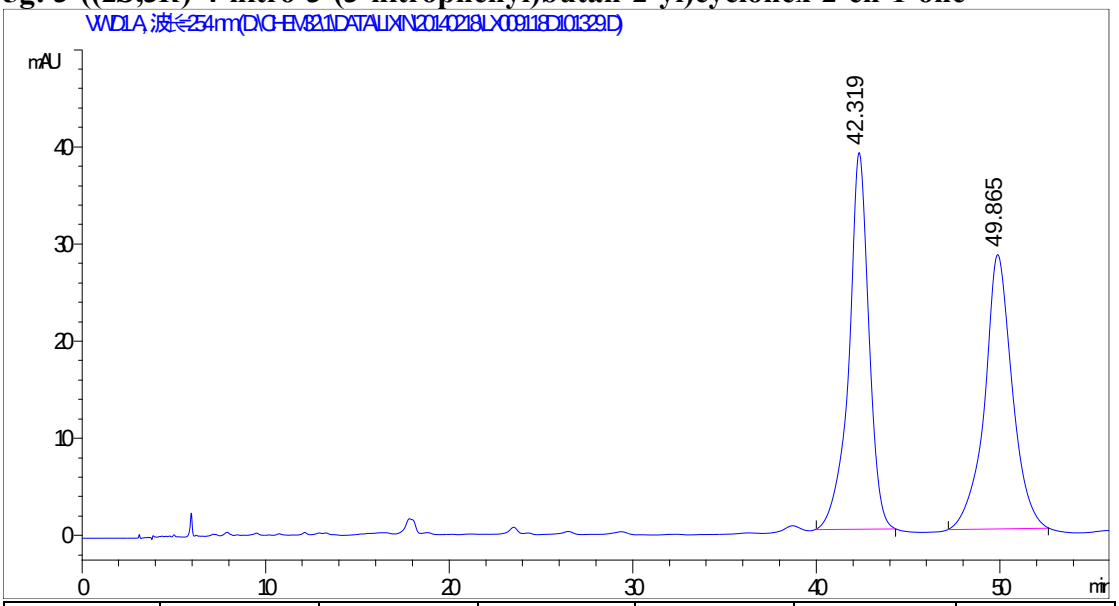


#	Time	Area	Height	Width	Symmetry	Area %
1	21.322	15679.6	388	0.585	0.736	49.721
2	29.489	15855.5	268.1	0.8503	0.707	50.279

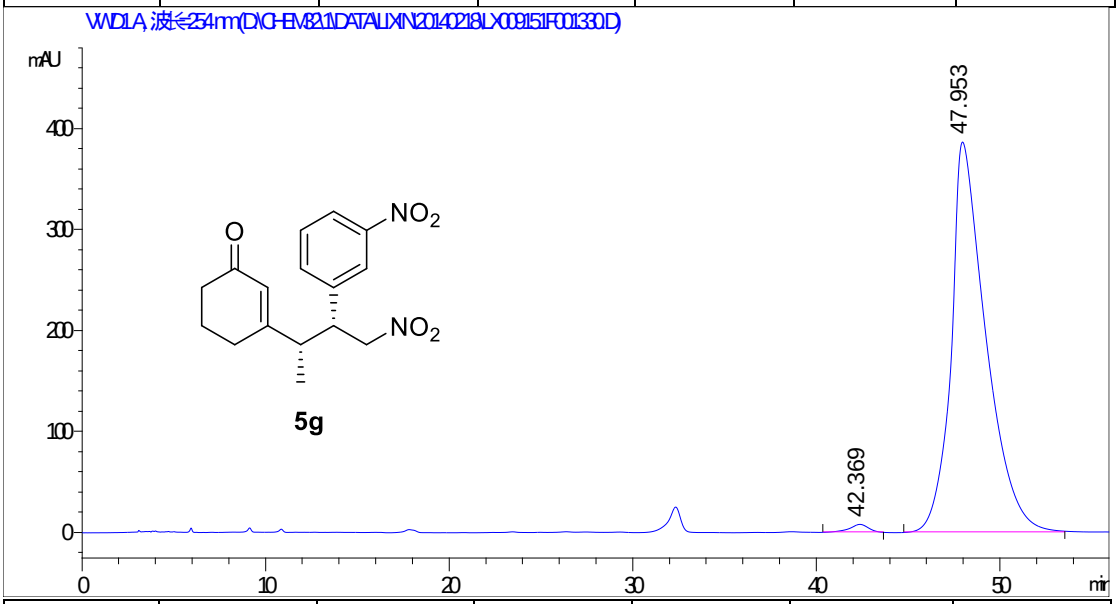


#	Time	Area	Height	Width	Symmetry	Area %
1	22.004	66.1	2	0.5422	1.252	0.606
2	30.129	10830.7	179.3	1.0067	0.790	99.394

5g: 3-((2*S*,3*R*)-4-nitro-3-(3-nitrophenyl)butan-2-yl)cyclohex-2-en-1-one

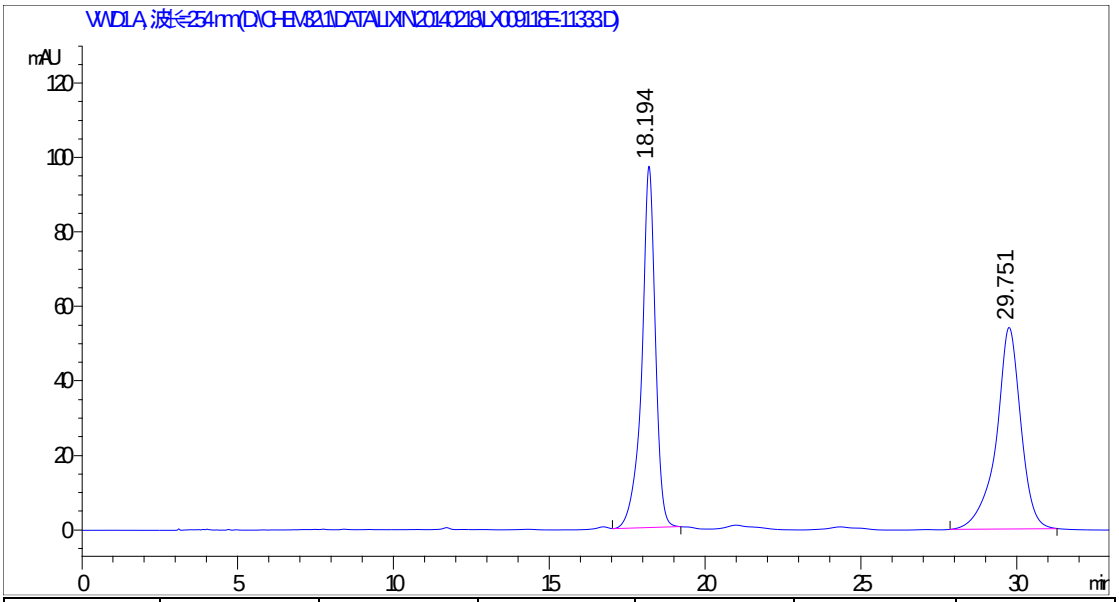


#	Time	Area	Height	Width	Symmetry	Area %
1	42.319	2943.8	38.8	1.0978	1.055	49.787
2	49.865	2968.9	28.3	1.4637	0.896	50.213

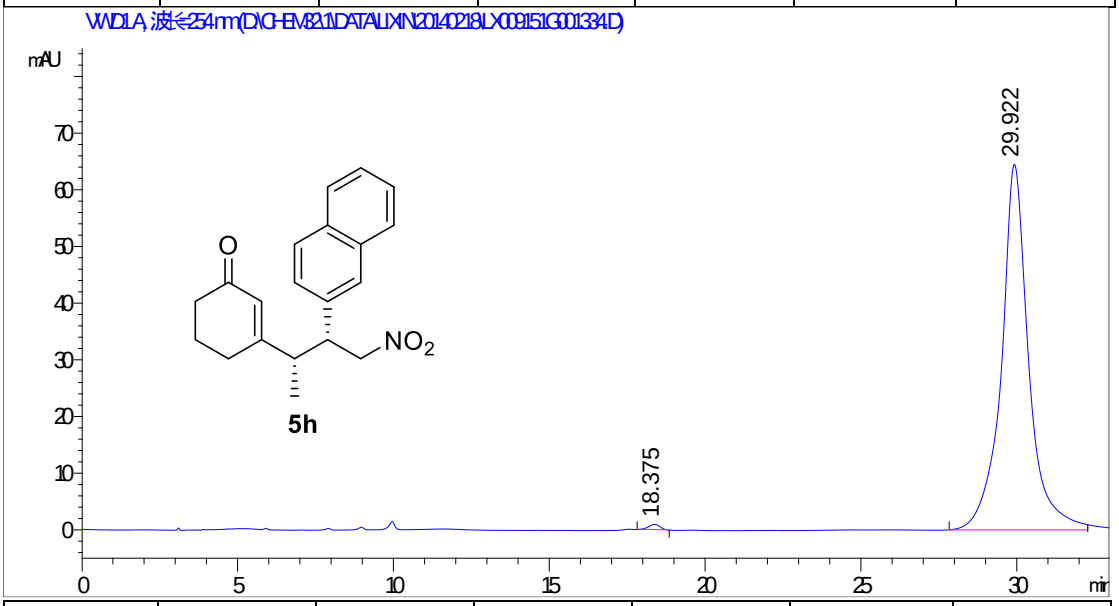


#	Time	Area	Height	Width	Symmetry	Area %
1	42.369	574.3	7.9	1.214	1.267	1.115
2	47.953	50914	386.5	2.1955	0.493	98.885

5h: 3-((2*S*,3*R*)-3-(naphthalen-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

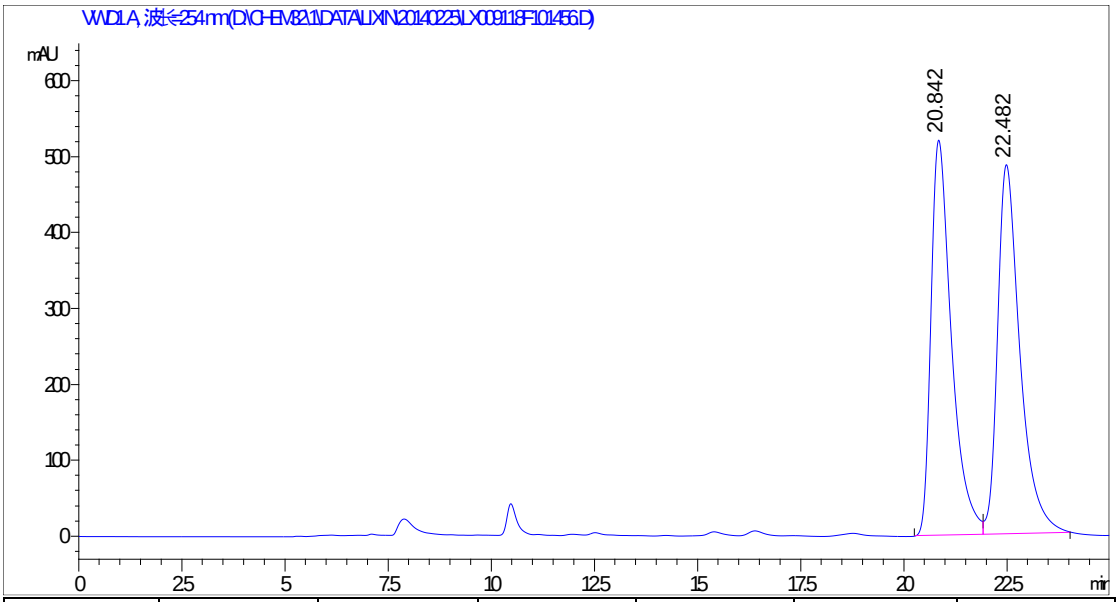


#	Time	Area	Height	Width	Symmetry	Area %
1	18.194	2946.3	97.1	0.4472	1.126	49.725
2	29.751	2978.9	54.2	0.8058	1.097	50.275

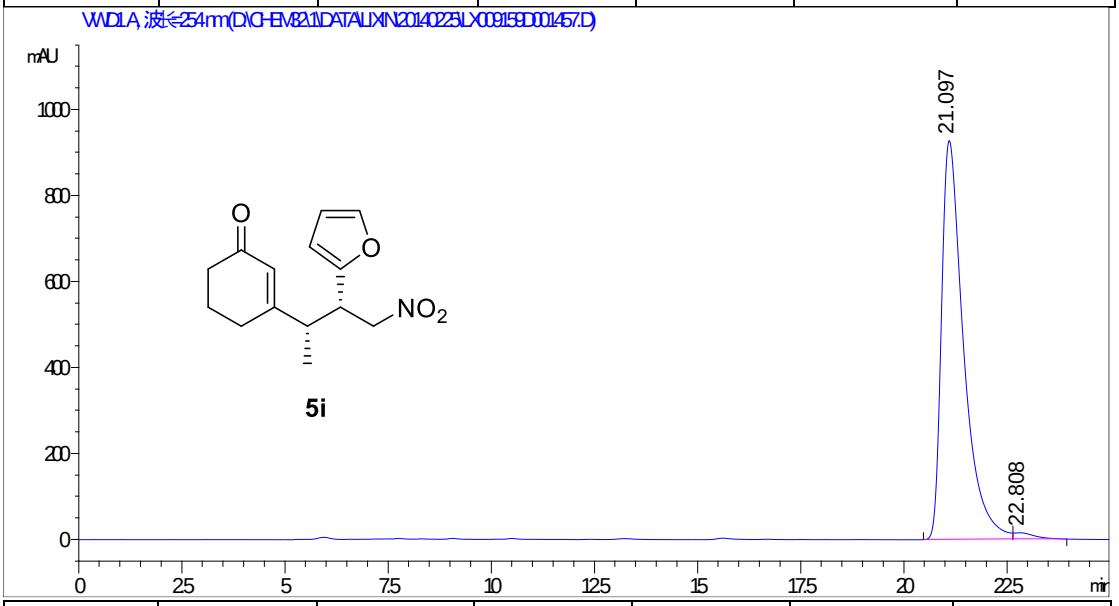


#	Time	Area	Height	Width	Symmetry	Area %
1	18.375	25.7	9.8E-1	0.4387	1.095	0.648
2	29.922	3938.1	64.5	1.0173	0.890	99.352

5i: 3-((2*S*,3*S*)-3-(furan-2-yl)-4-nitrobutan-2-yl)cyclohex-2-en-1-one

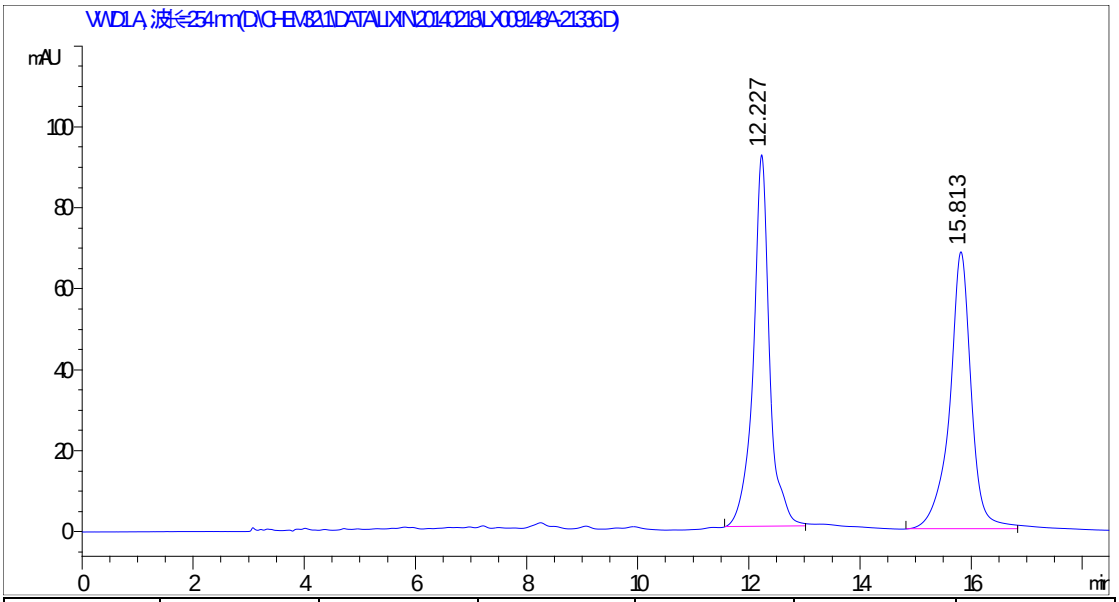


#	Time	Area	Height	Width	Symmetry	Area %
1	20.842	18010.8	520.9	0.5763	0.580	49.514
2	22.482	18364.5	486.6	0.629	0.622	50.486

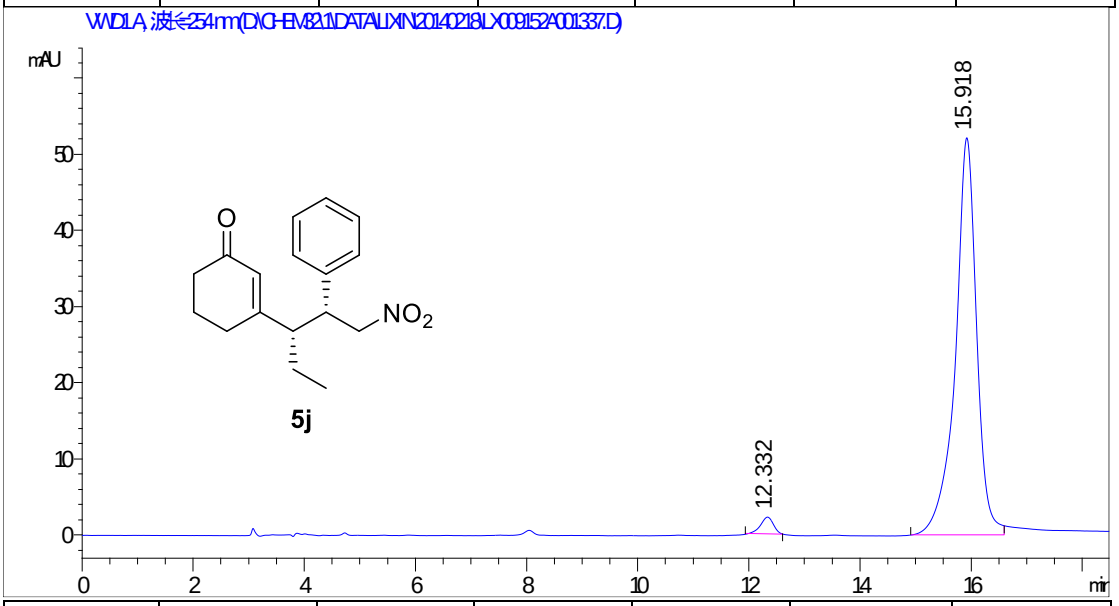


#	Time	Area	Height	Width	Symmetry	Area %
1	21.097	34554	927.8	0.6207	0.514	98.493
2	22.808	528.8	15.1	0.583	0.363	1.507

5j: 3-((2*R*,3*S*)-1-nitro-2-phenylpentan-3-yl)cyclohex-2-en-1-one

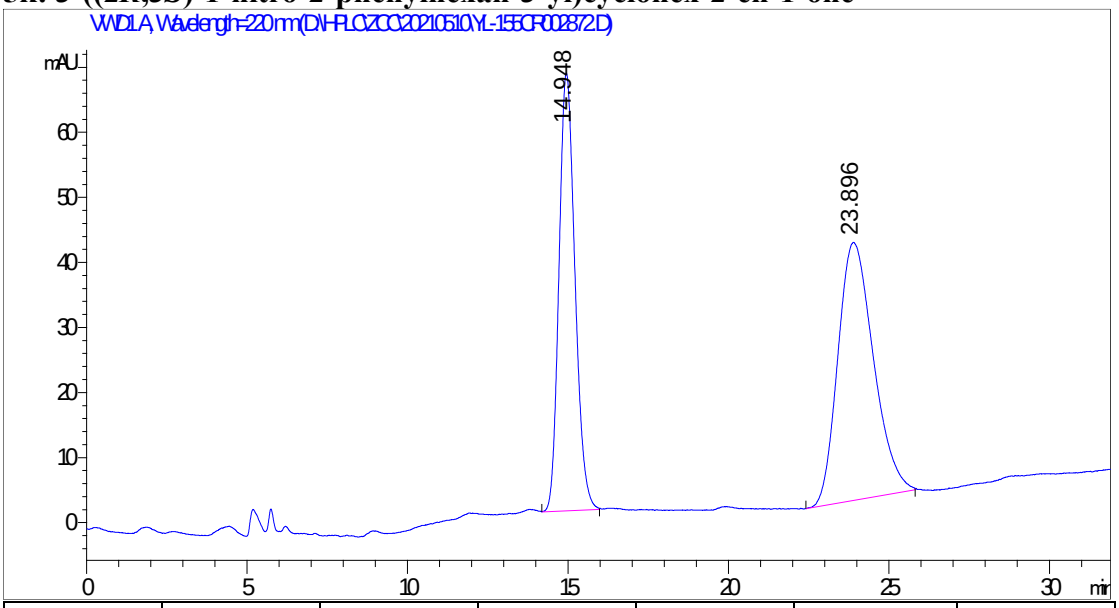


#	Time	Area	Height	Width	Symmetry	Area %
1	12.227	1869.3	91.9	0.3392	1.023	50.203
2	15.813	1854.2	68.5	0.4511	1.058	49.797

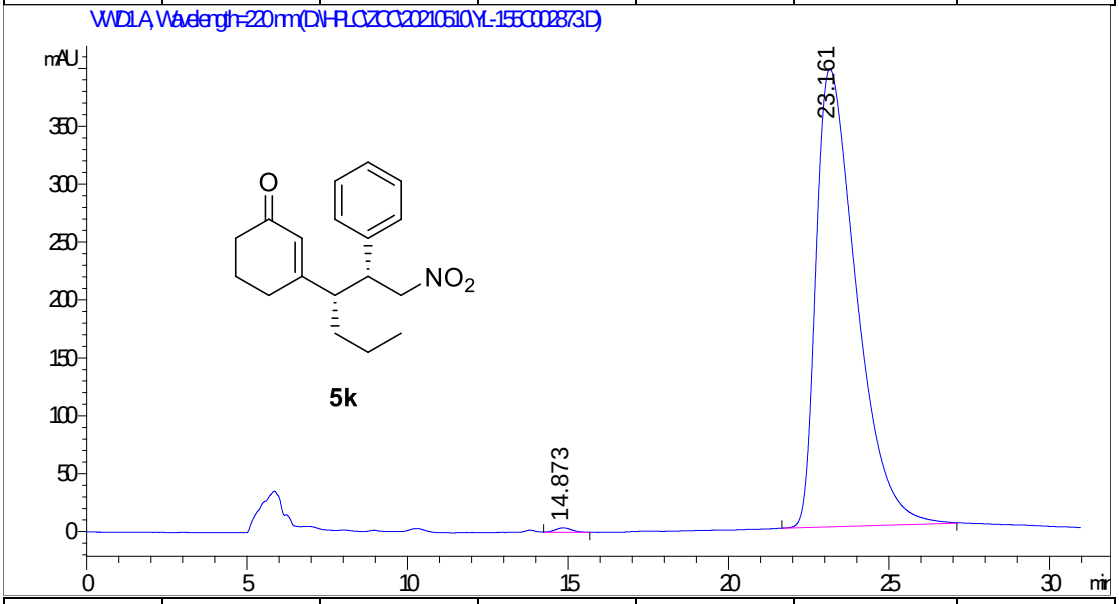


#	Time	Area	Height	Width	Symmetry	Area %
1	12.332	37.2	2.3	0.2755	1.183	2.605
2	15.918	1392	52.2	0.4441	1.131	97.395

5k: 3-((2*R*,3*S*)-1-nitro-2-phenylhexan-3-yl)cyclohex-2-en-1-one

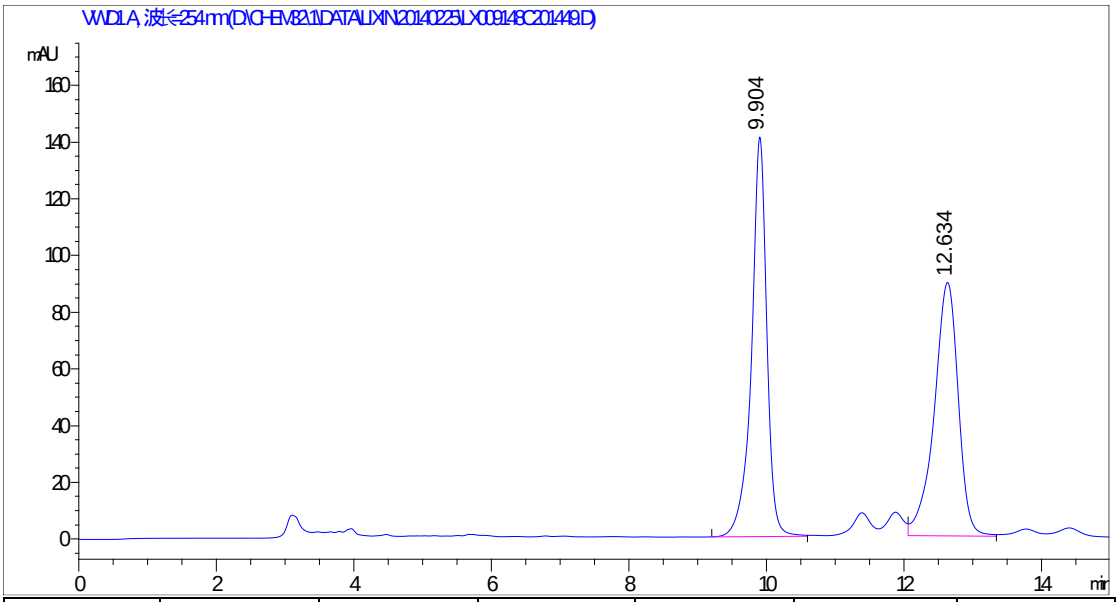


#	Time	Area	Height	Width	Symmetry	Area %
1	14.948	2327.6	67.3	0.5318	0.805	43.245
2	23.896	3054.7	39.7	0.9258	0.769	56.755

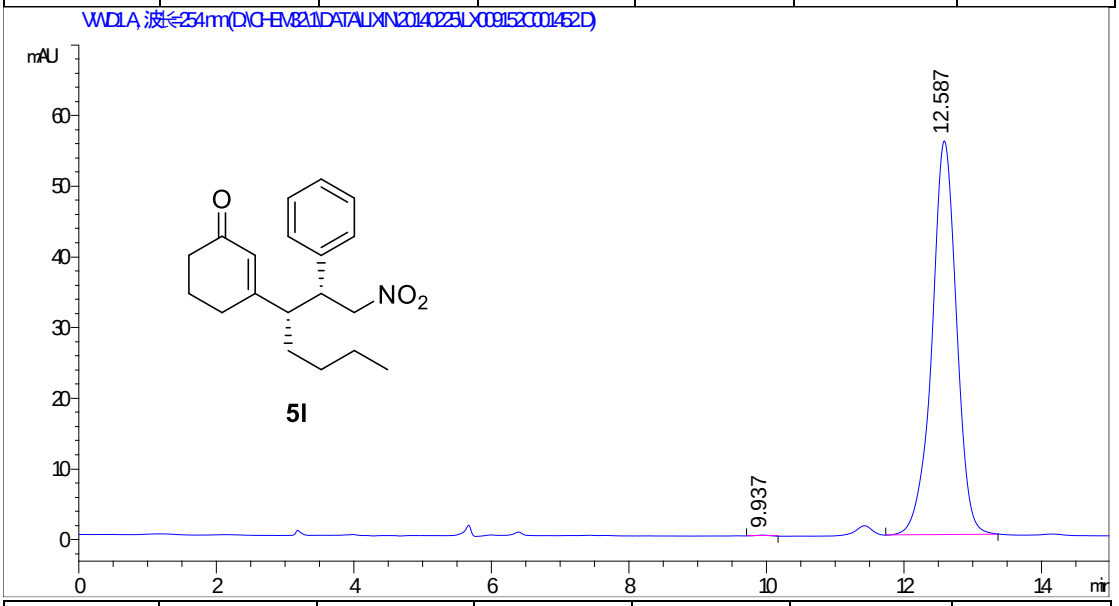


#	Time	Area	Height	Width	Symmetry	Area %
1	14.873	144.4	3.9	0.4457	1.054	0.416
2	23.161	34533.3	395.4	1.287	0.489	99.584

5l: 3-((2*R*,3*S*)-1-nitro-2-phenylheptan-3-yl)cyclohex-2-en-1-one

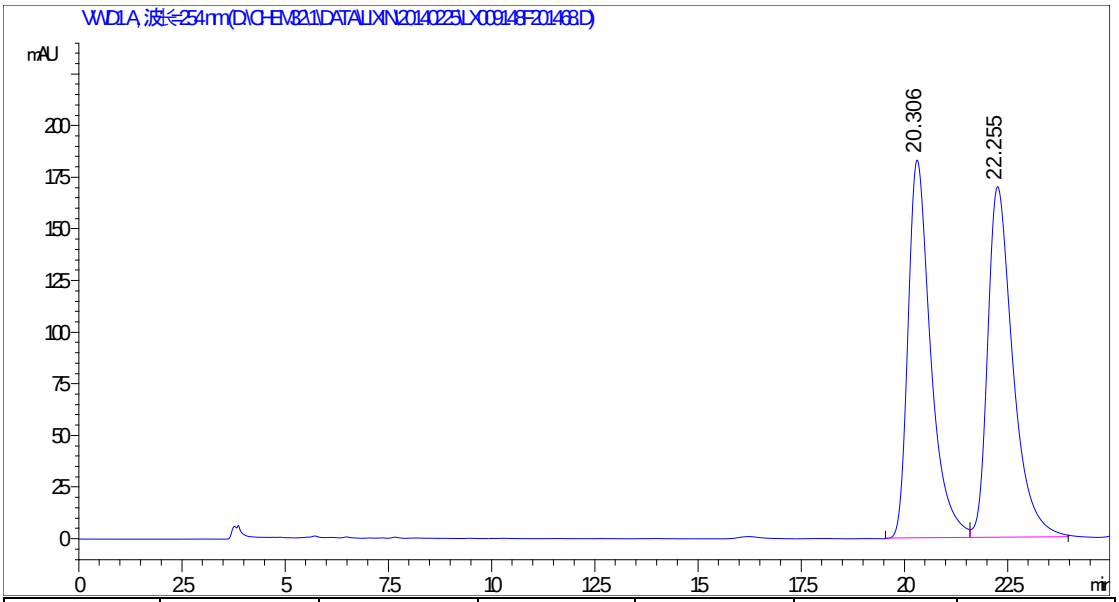


#	Time	Area	Height	Width	Symmetry	Area %
1	9.904	2188.1	141.1	0.2585	1.149	50.098
2	12.634	2179.5	89.5	0.37	1.220	49.902

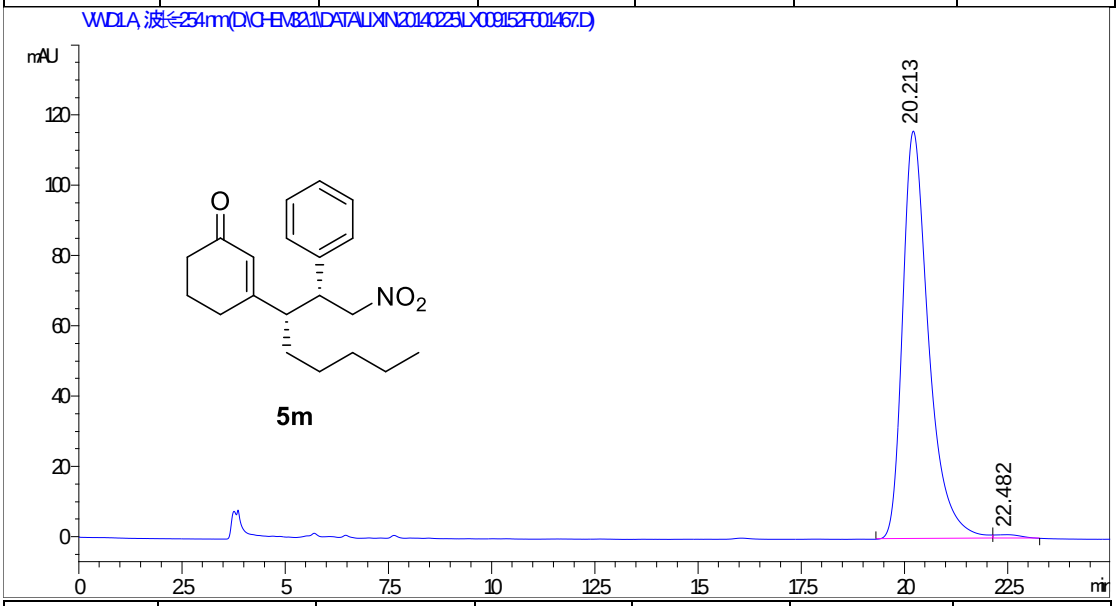


#	Time	Area	Height	Width	Symmetry	Area %
1	9.937	2.1	1.5E-1	0.2355	0.986	0.147
2	12.587	1389	55.7	0.381	1.007	99.853

5m: 3-((2*R*,3*S*)-1-nitro-2-phenyloctan-3-yl)cyclohex-2-en-1-one

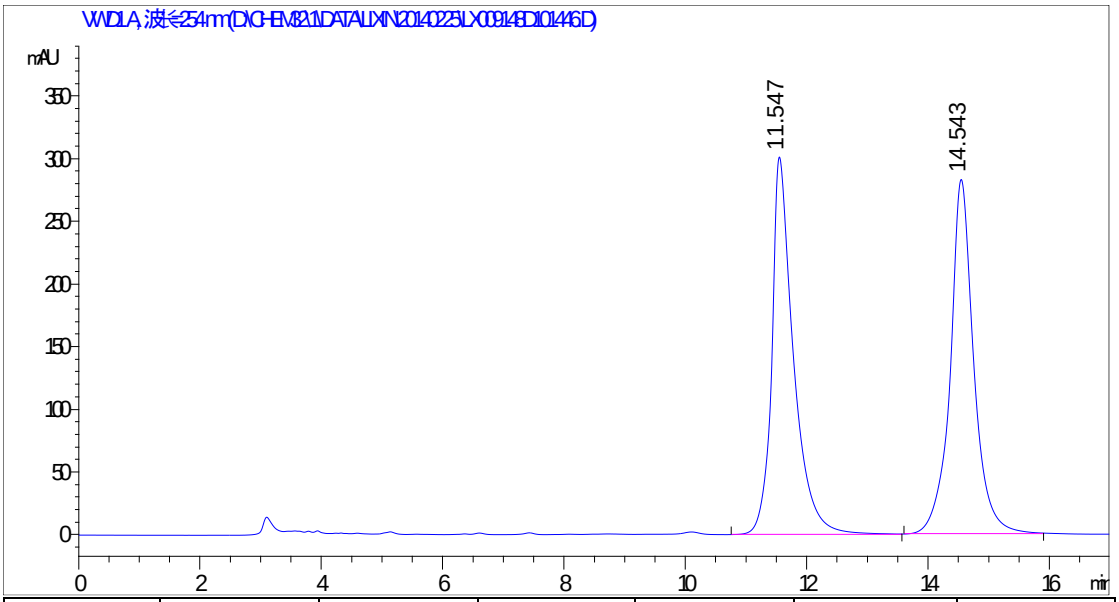


#	Time	Area	Height	Width	Symmetry	Area %
1	20.306	7004	183.1	0.5743	0.620	49.122
2	22.255	7254.5	170	0.7112	0.624	50.878

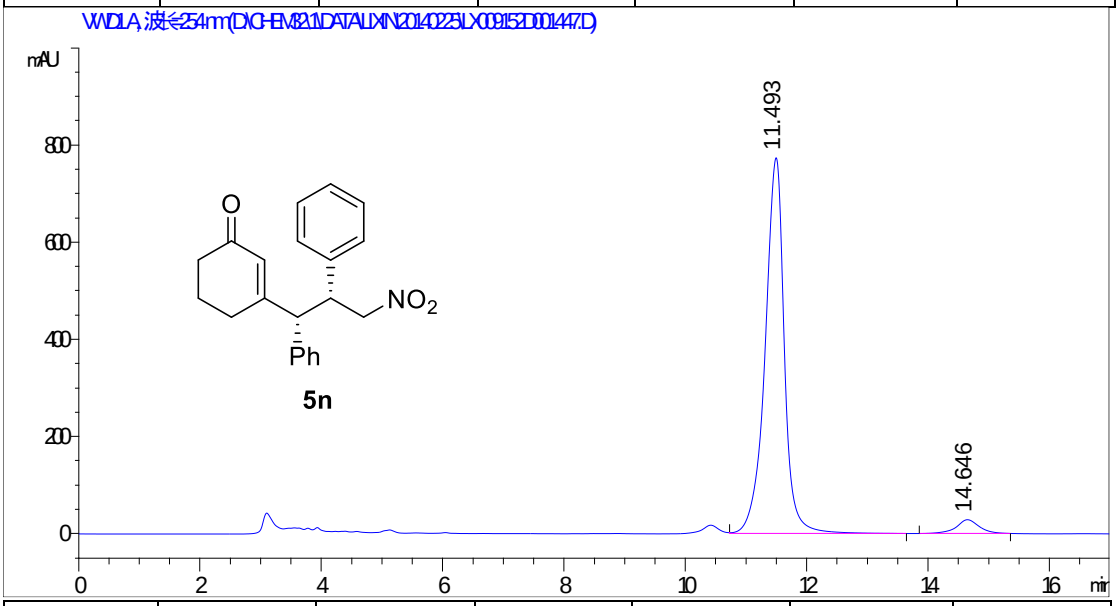


#	Time	Area	Height	Width	Symmetry	Area %
1	20.213	5107.2	116.1	0.7332	0.654	99.053
2	22.482	48.8	1.1	0.7372	0.809	0.947

5n: 3-((1*S*,2*R*)-3-nitro-1,2-diphenylpropyl)cyclohex-2-en-1-one

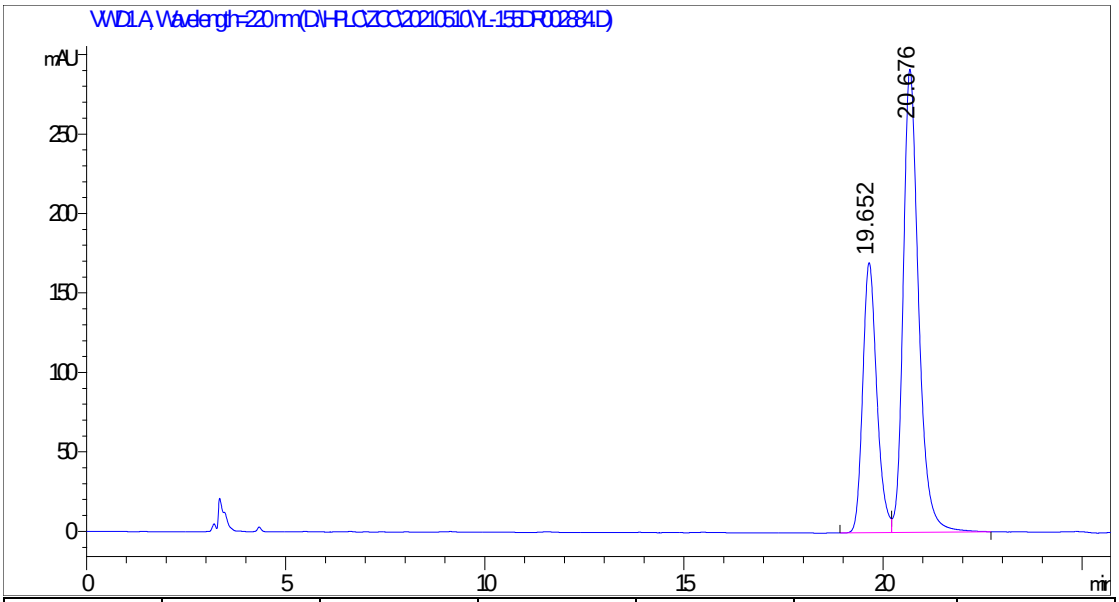


#	Time	Area	Height	Width	Symmetry	Area %
1	11.547	7493.5	301.2	0.4146	0.534	49.567
2	14.543	7624.6	282.8	0.4494	0.855	50.433

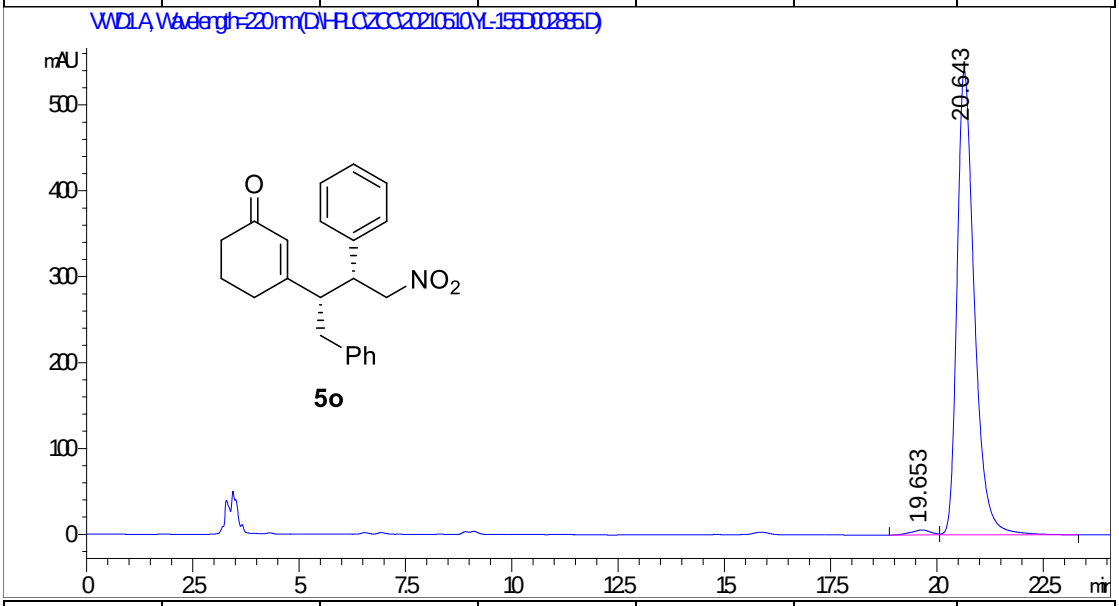


#	Time	Area	Height	Width	Symmetry	Area %
1	11.493	17058.3	773.8	0.3343	1.253	95.812
2	14.646	745.6	28.4	0.4382	0.943	4.188

5o: 3-((2*S*,3*R*)-4-nitro-1,3-diphenylbutan-2-yl)cyclohex-2-en-1-one

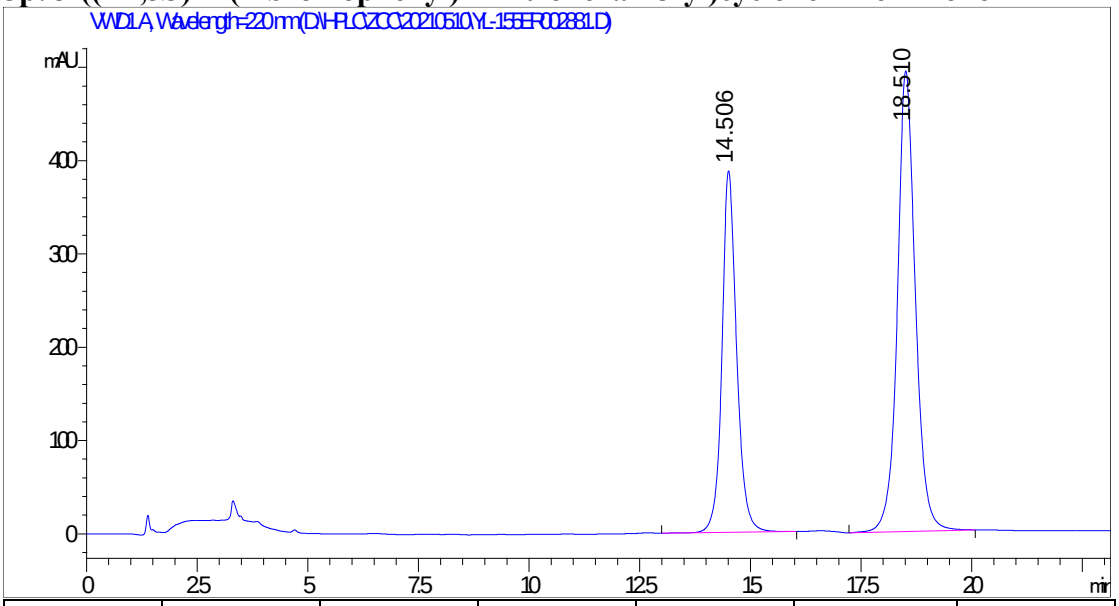


#	Time	Area	Height	Width	Symmetry	Area %
1	19.652	4173.3	170	0.3754	0.789	34.762
2	20.676	7832	291.5	0.4083	0.718	65.238

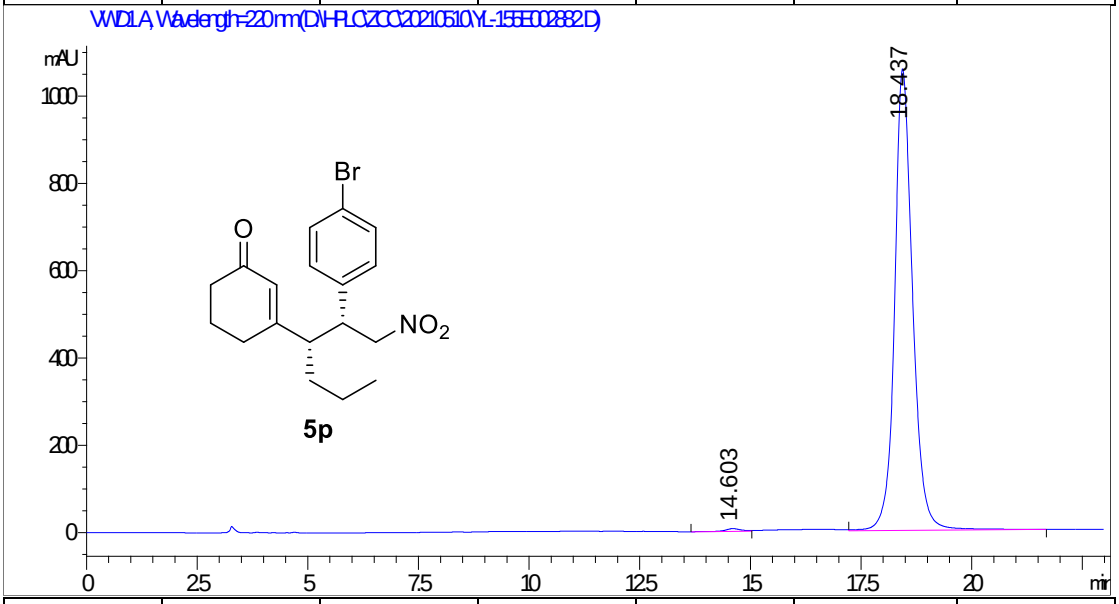


#	Time	Area	Height	Width	Symmetry	Area %
1	19.653	189.1	5.9	0.4636	1.282	1.218
2	20.643	15336.8	540.2	0.4318	0.656	98.782

5p: 3-((2*R*,3*S*)-2-(4-bromophenyl)-1-nitrohexan-3-yl)cyclohex-2-en-1-one

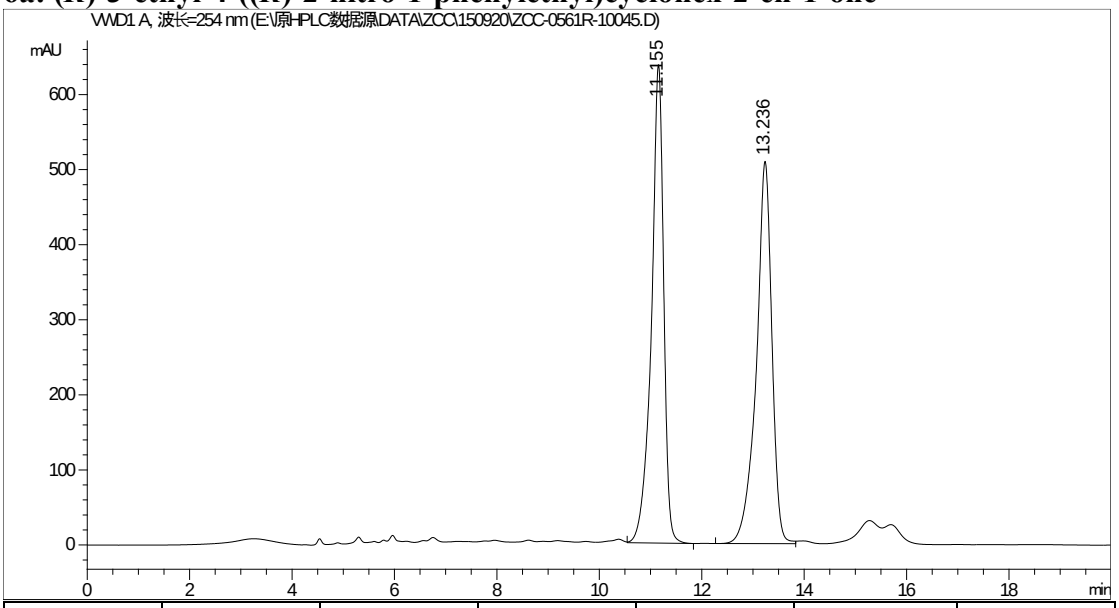


#	Time	Area	Height	Width	Symmetry	Area %
1	14.506	8934.1	387.7	0.3447	0.783	39.039
2	18.51	13951.3	493.6	0.4245	0.844	60.961

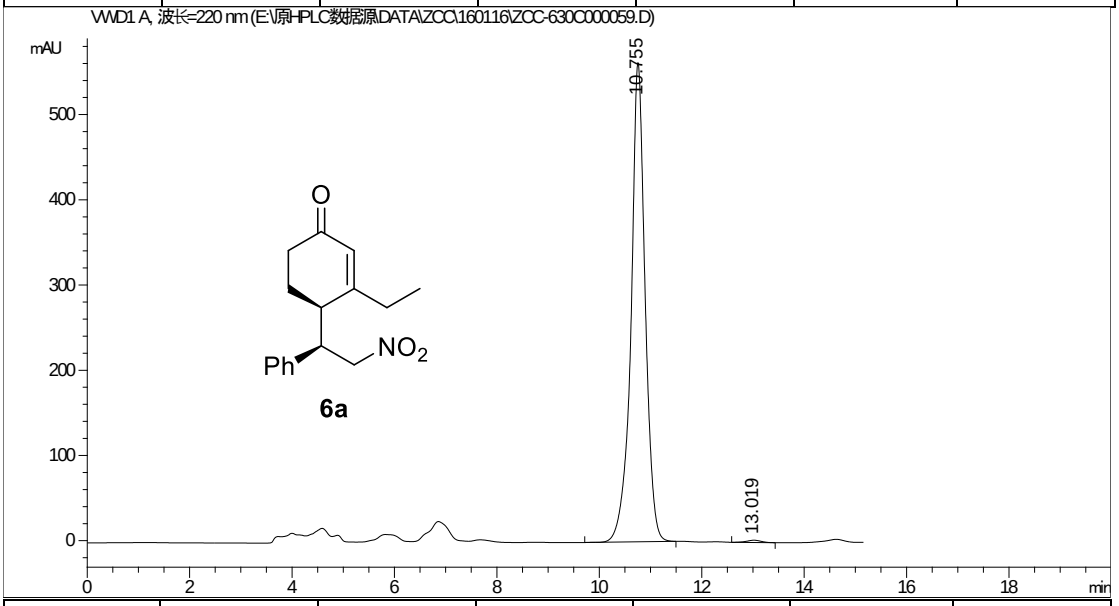


#	Time	Area	Height	Width	Symmetry	Area %
1	14.603	172.9	6.6	0.3769	0.811	0.575
2	18.437	29876.3	1057.1	0.4245	0.754	99.425

6a: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

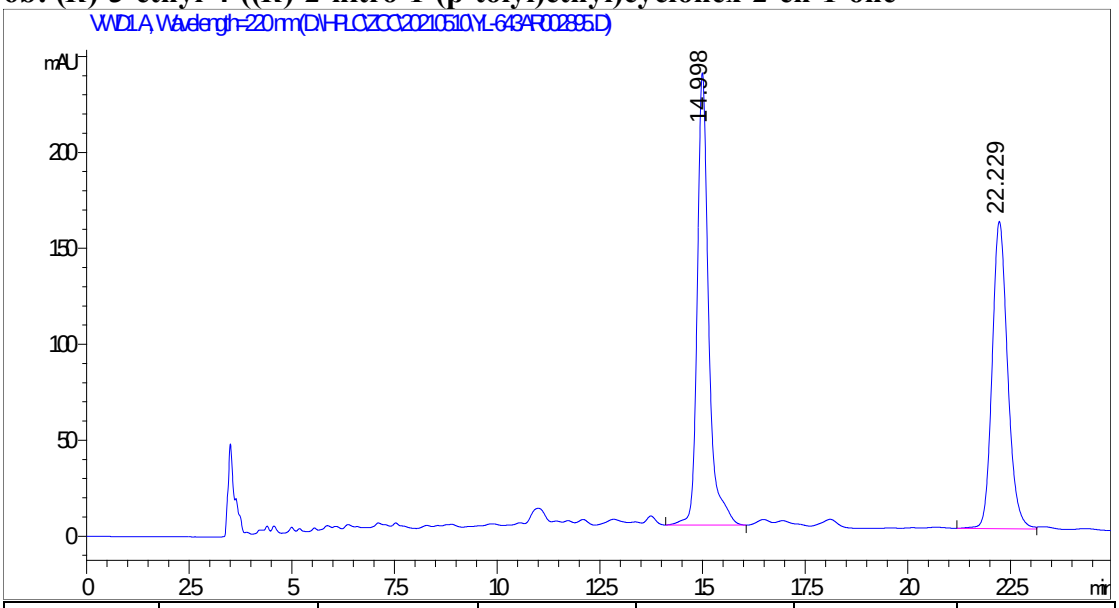


#	Time	Area	Height	Width	Symmetry	Area %
1	11.155	10546.4	637.3	0.2426	1.329	49.540
2	13.236	10742.2	509.3	0.3087	1.267	50.460

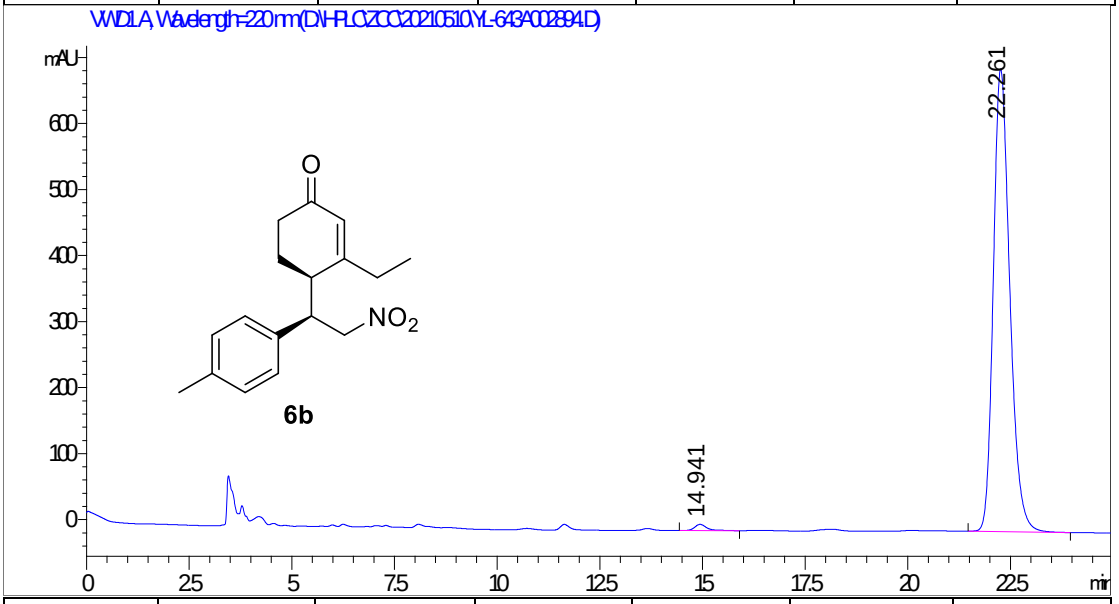


#	Time	Area	Height	Width	Symmetry	Area %
1	10.755	10766.5	562.2	0.2802	0.967	99.519
2	13.019	52	2.7	0.2877	0.997	0.481

6b: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(p-tolyl)ethyl)cyclohex-2-en-1-one

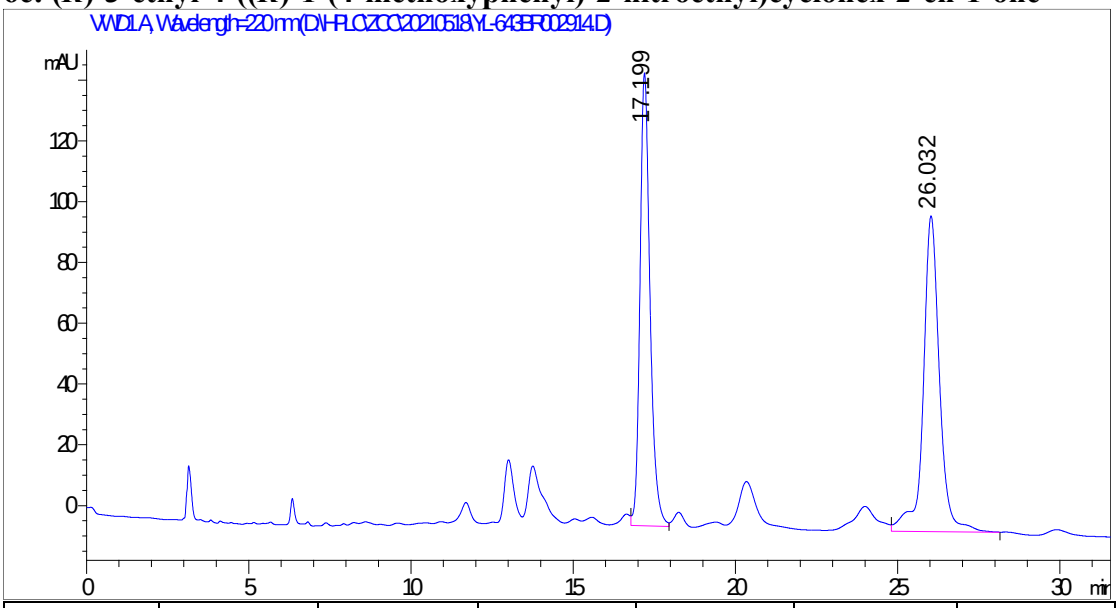


#	Time	Area	Height	Width	Symmetry	Area %
1	14.998	4537.9	235.6	0.2888	0.763	51.928
2	22.229	4200.9	160.2	0.4021	0.822	48.072

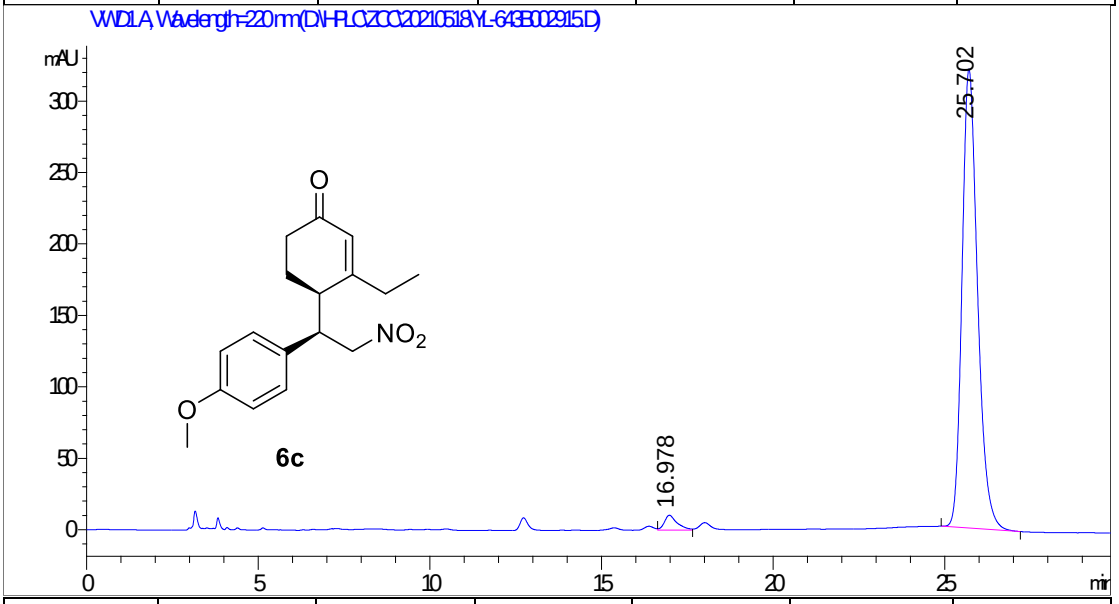


#	Time	Area	Height	Width	Symmetry	Area %
1	14.941	191.6	9.3	0.3048	0.721	0.972
2	22.261	19524.6	700.7	0.4286	0.749	99.028

6c: (*R*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one

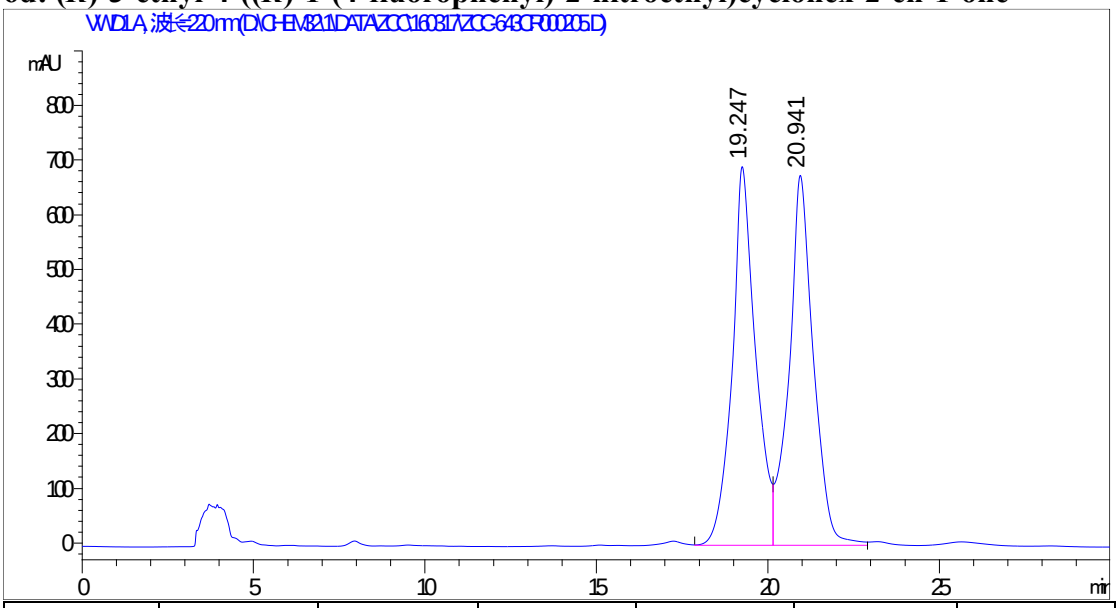


#	Time	Area	Height	Width	Symmetry	Area %
1	17.199	3204.2	149.1	0.3252	0.759	47.013
2	26.032	3611.5	103.9	0.5207	0.906	52.987

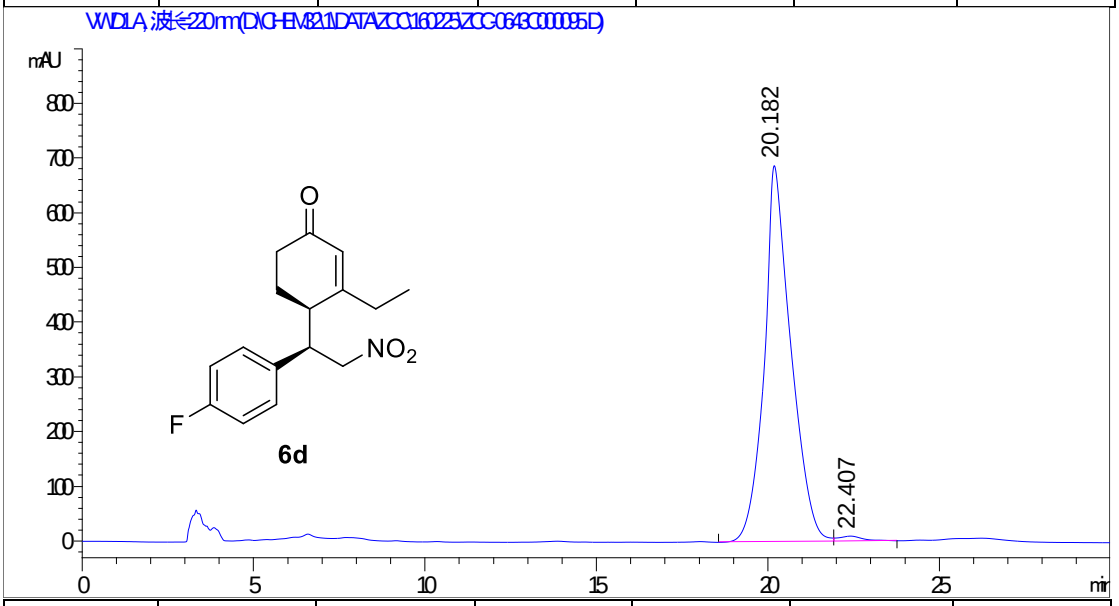


#	Time	Area	Height	Width	Symmetry	Area %
1	16.978	268	10.4	0.3737	0.613	2.583
2	25.702	10108.4	321.4	0.4835	0.752	97.417

6d: (*R*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one

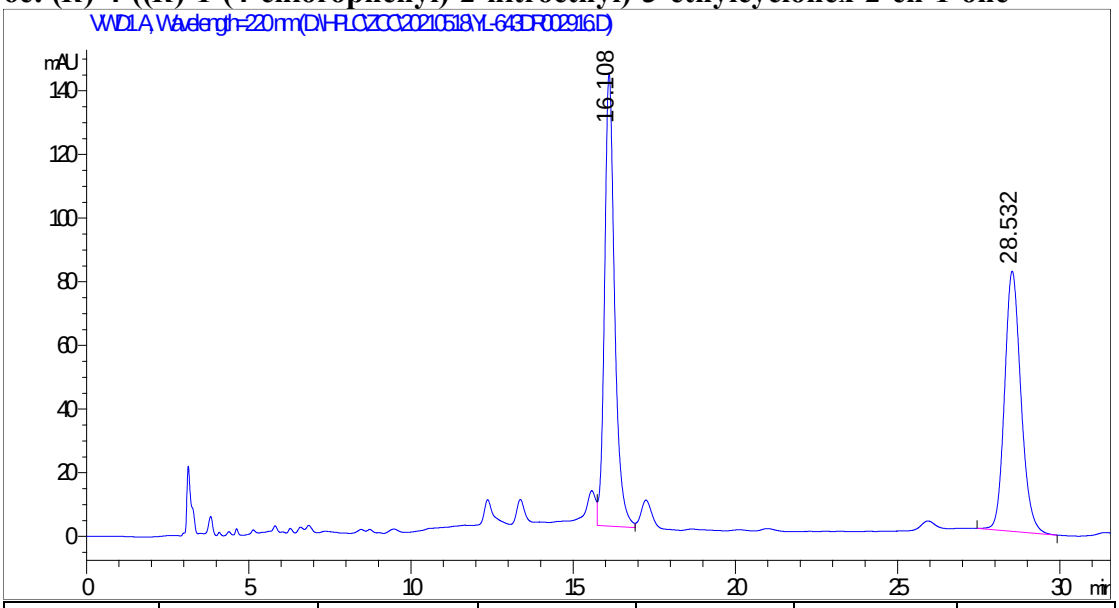


#	Time	Area	Height	Width	Symmetry	Area %
1	19.247	32895.6	692.6	0.6546	0.750	49.628
2	20.941	33388.5	676.6	0.6893	0.829	50.372

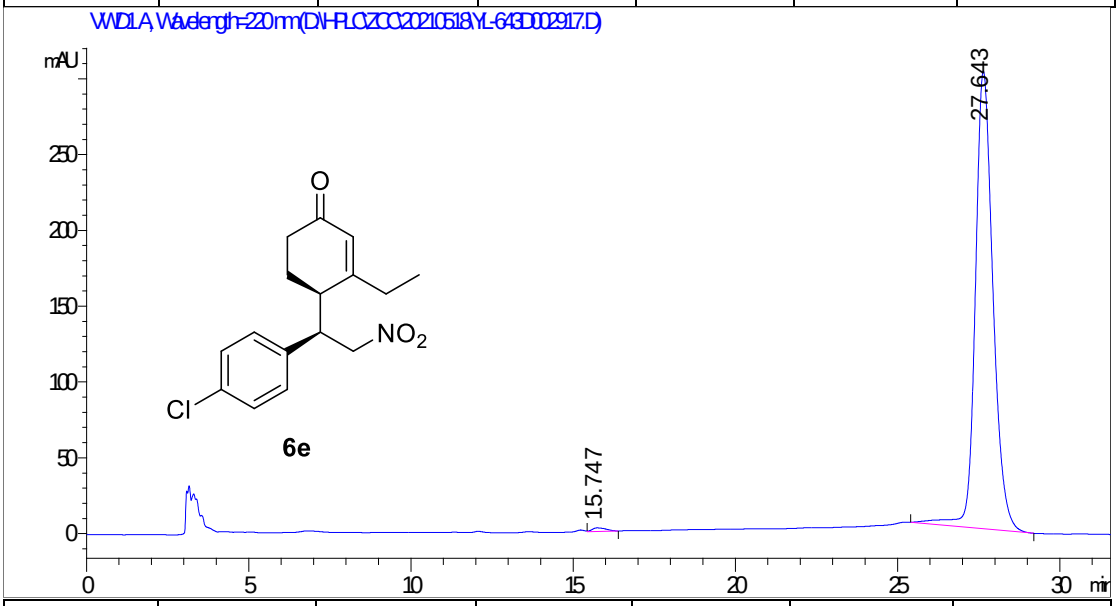


#	Time	Area	Height	Width	Symmetry	Area %
1	20.182	37295.4	687.5	0.7421	0.616	98.776
2	22.407	462.3	9.3	0.6774	0.857	1.224

6e: (*R*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one

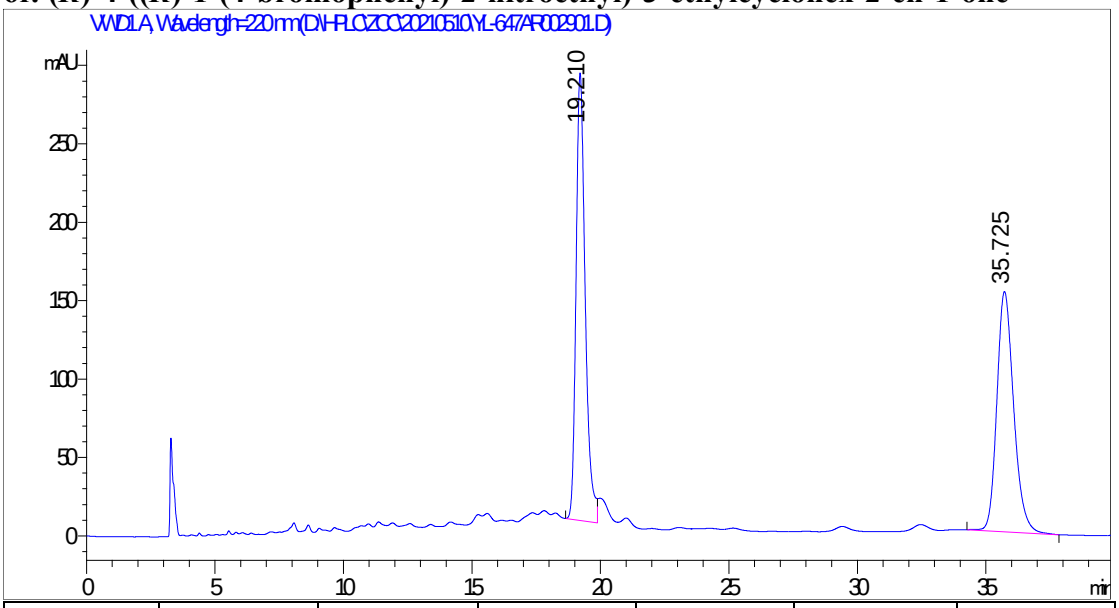


#	Time	Area	Height	Width	Symmetry	Area %
1	16.108	3073.8	142.3	0.3248	0.754	51.755
2	28.532	2865.4	81.8	0.5371	0.825	48.245

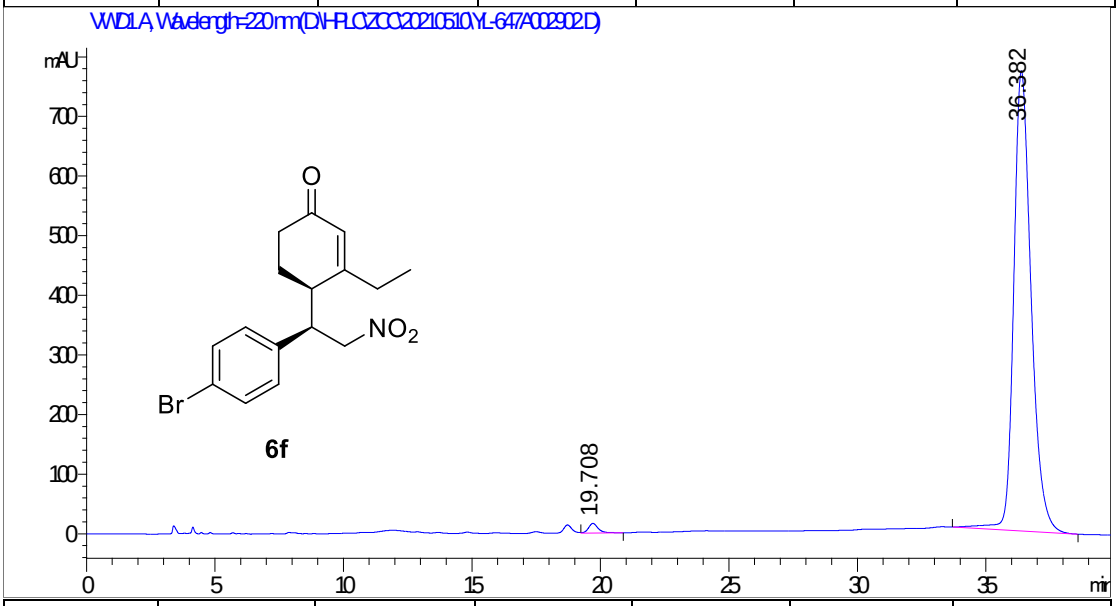


#	Time	Area	Height	Width	Symmetry	Area %
1	15.747	73.2	2.4	0.4082	0.594	0.635
2	27.643	11459.2	302	0.5768	0.809	99.365

6f: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one

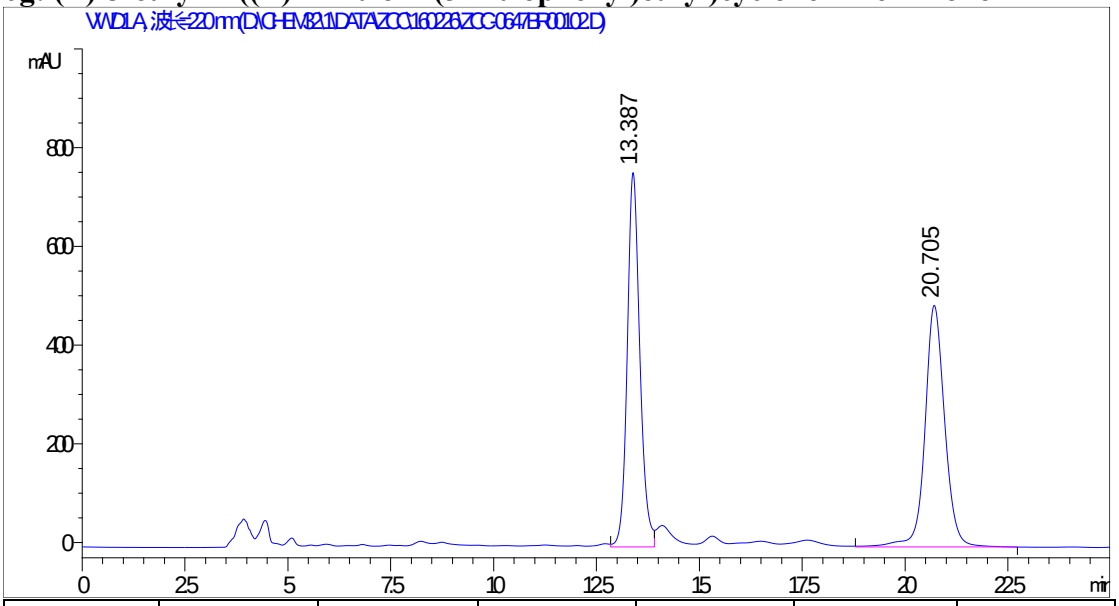


#	Time	Area	Height	Width	Symmetry	Area %
1	19.21	7070.1	285.3	0.3751	0.73	50.360
2	35.725	6969	153.2	0.6985	0.782	49.640

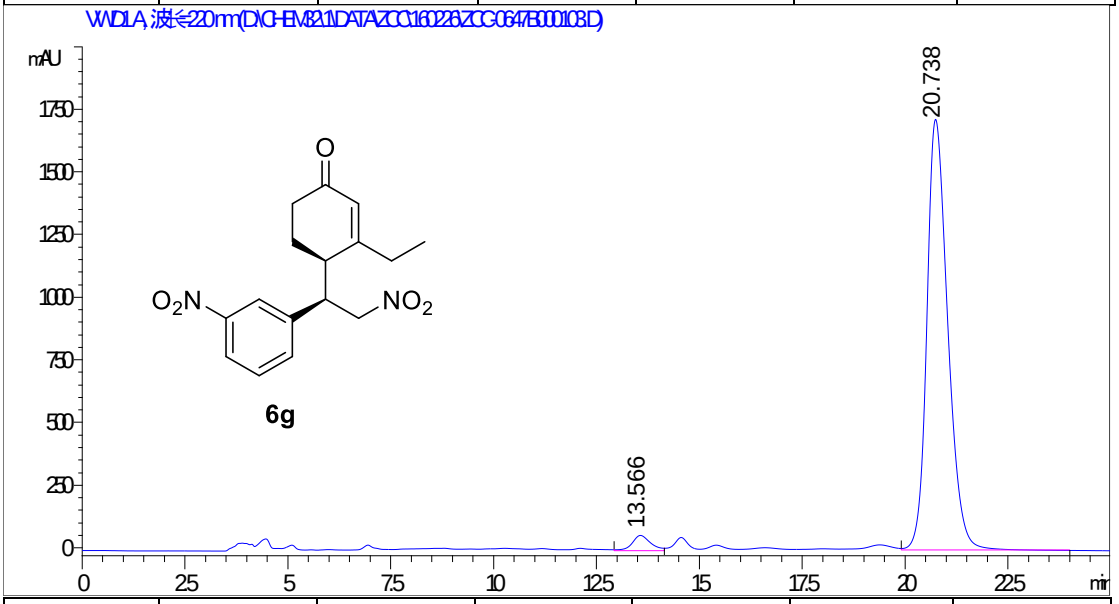


#	Time	Area	Height	Width	Symmetry	Area %
1	19.708	420	16.1	0.3936	0.788	1.144
2	36.382	36298.6	771.6	0.7179	0.75	98.856

6g: (*R*)-3-ethyl-4-((*R*)-2-nitro-1-(3-nitrophenyl)ethyl)cyclohex-2-en-1-one

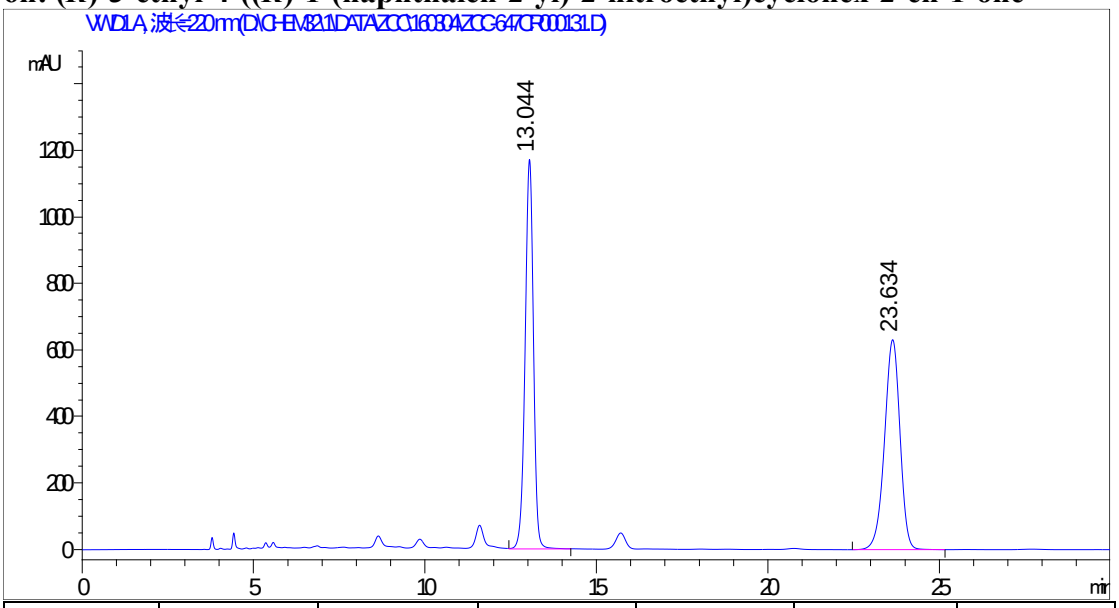


#	Time	Area	Height	Width	Symmetry	Area %
1	13.387	16202.6	758.5	0.322	0.820	49.630
2	20.705	16443.9	489.3	0.5056	0.886	50.370

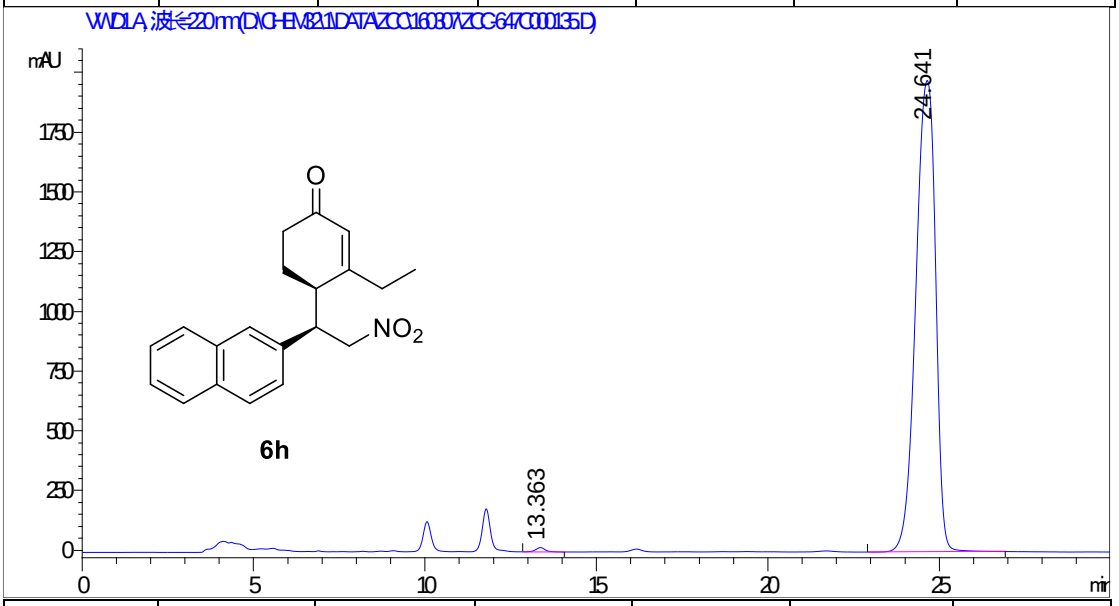


#	Time	Area	Height	Width	Symmetry	Area %
1	13.566	1929	61.2	0.4667	0.805	3.063
2	20.738	61044	1720	0.5393	0.678	96.937

6h: (*R*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one

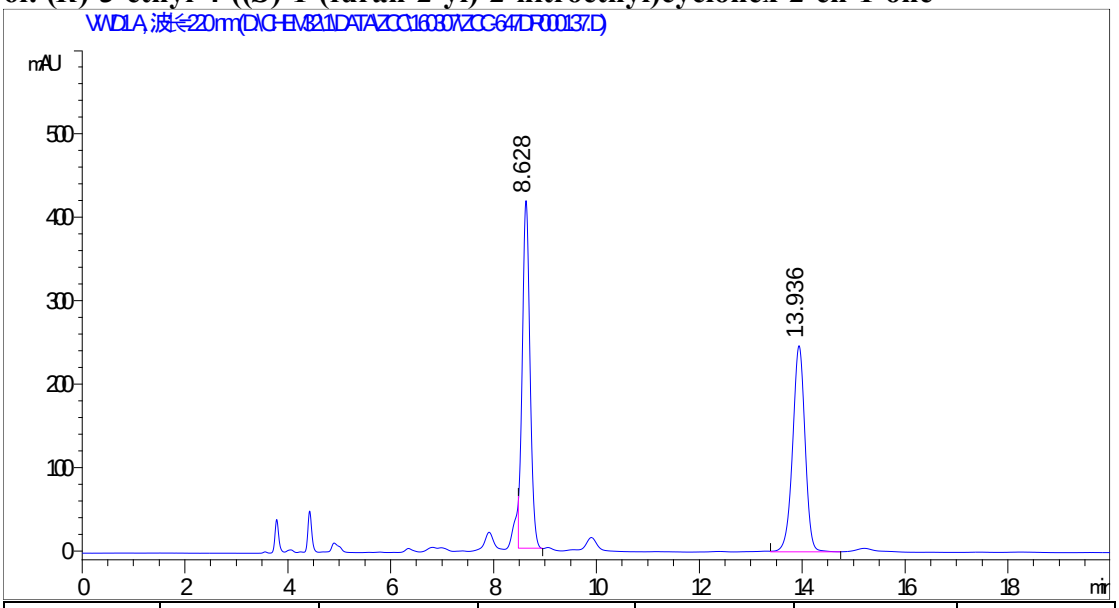


#	Time	Area	Height	Width	Symmetry	Area %
1	13.044	19741.4	1171.3	0.2607	1.072	49.932
2	23.634	19794.8	631.3	0.4881	1.092	50.068

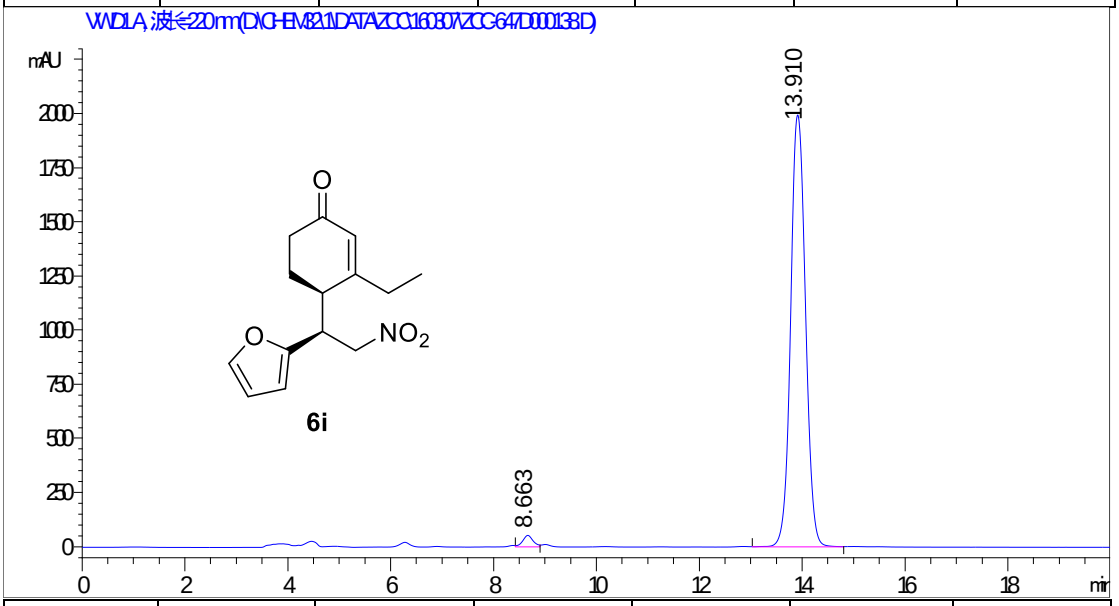


#	Time	Area	Height	Width	Symmetry	Area %
1	13.363	381.6	18.6	0.306	1.020	0.481
2	24.641	79009.4	1973.1	0.6404	1.301	99.519

6i: (*R*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one

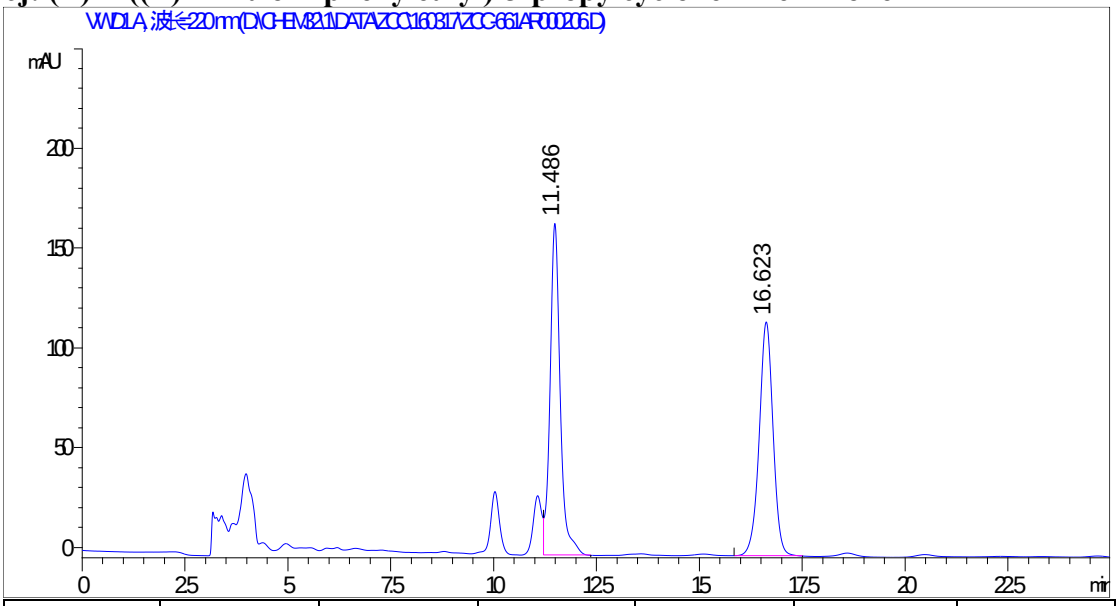


#	Time	Area	Height	Width	Symmetry	Area %
1	8.628	4311	417.1	0.1722	0.901	50.874
2	13.936	4162.9	247.5	0.2588	1.033	49.126

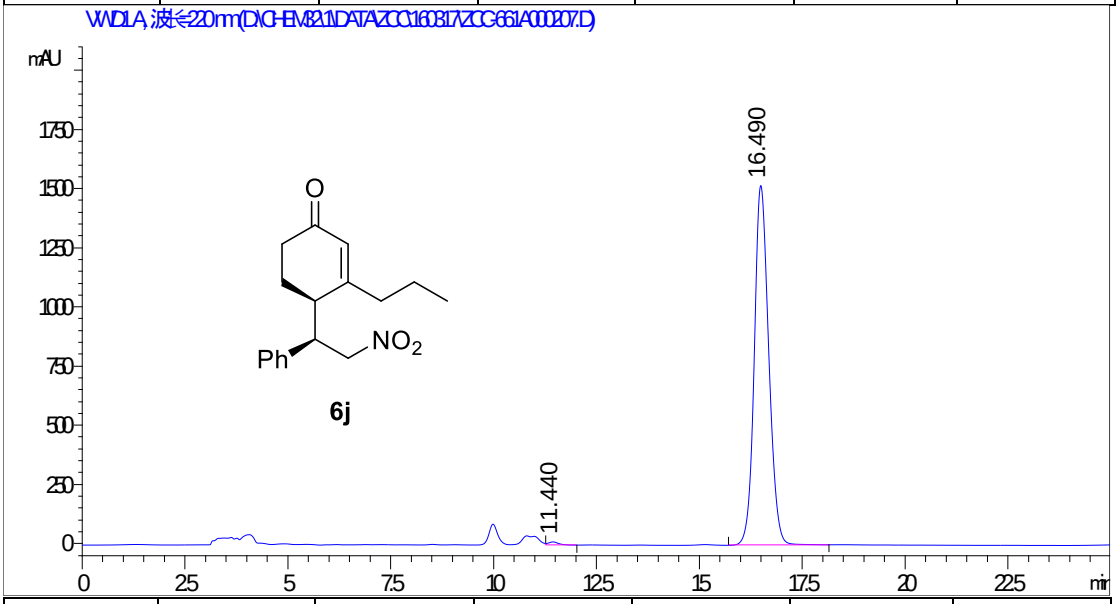


#	Time	Area	Height	Width	Symmetry	Area %
1	8.663	777.9	53.9	0.2135	0.923	1.901
2	13.91	40153.5	1995.9	0.3133	0.875	98.099

6j: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one

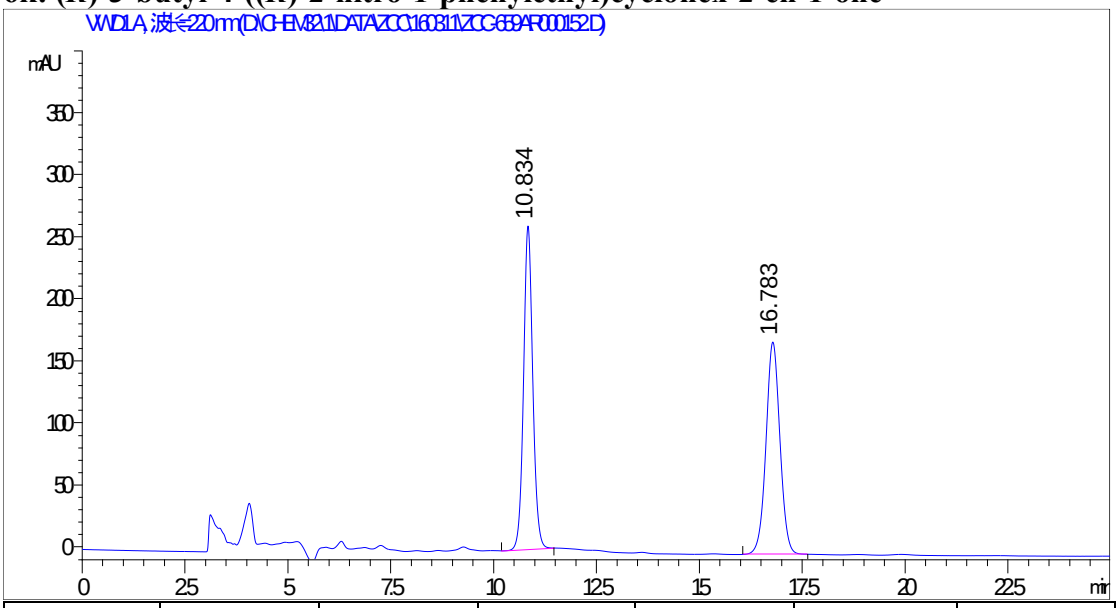


#	Time	Area	Height	Width	Symmetry	Area %
1	11.486	2856	166.3	0.2572	0.829	50.976
2	16.623	2746.6	117.3	0.3561	1.007	49.024

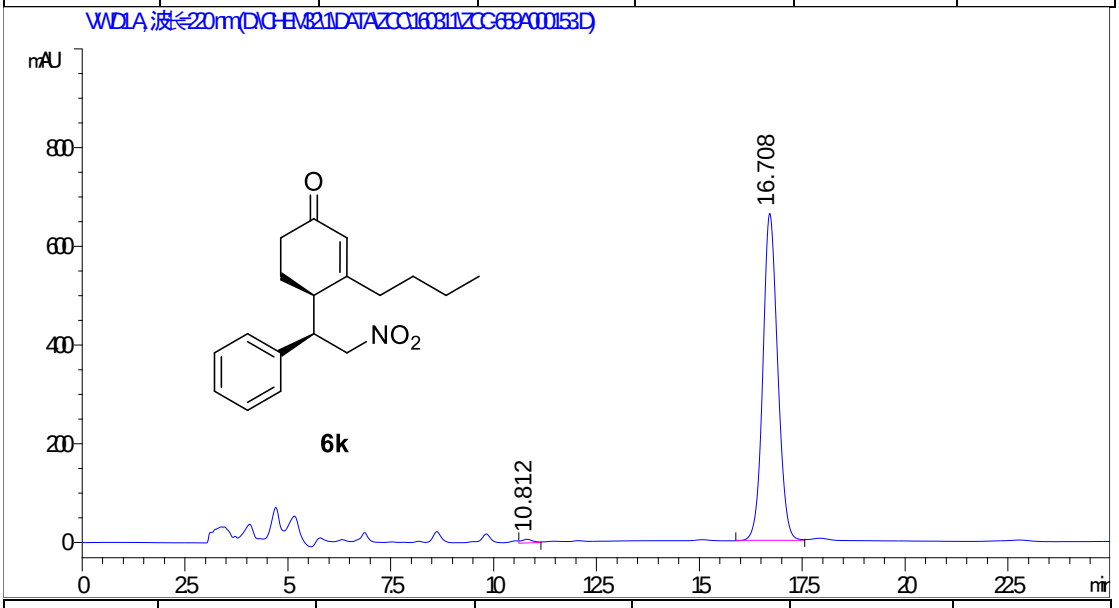


#	Time	Area	Height	Width	Symmetry	Area %
1	11.44	271.2	14.2	0.2758	0.668	0.723
2	16.49	37255.8	1520.1	0.3733	0.781	99.277

6k: (*R*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

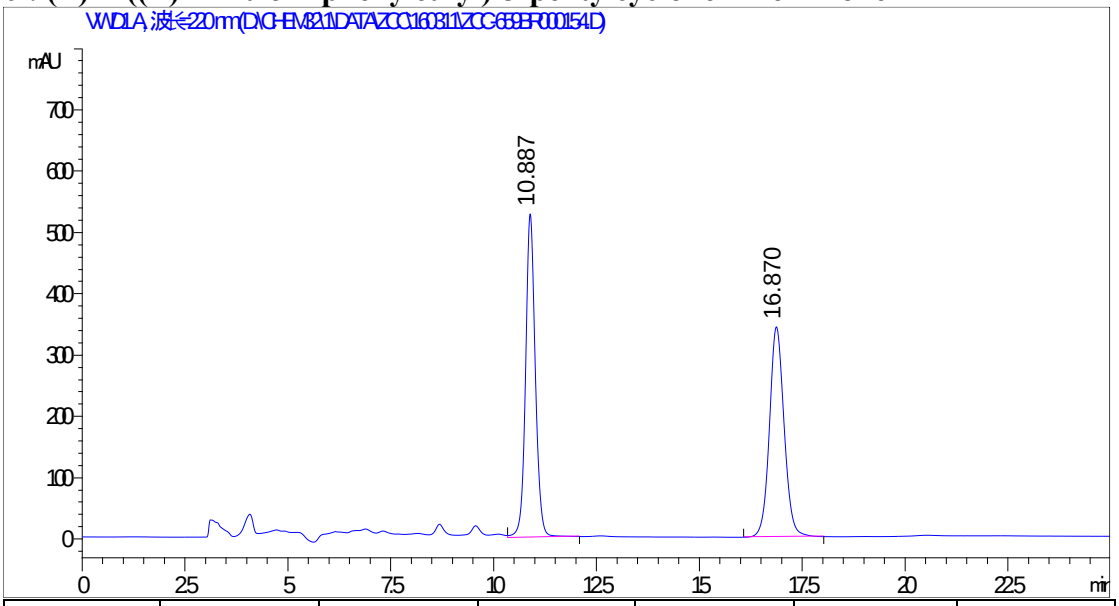


#	Time	Area	Height	Width	Symmetry	Area %
1	10.834	4077.8	260.8	0.2377	0.908	50.274
2	16.783	4033.4	171.1	0.3624	0.942	49.726

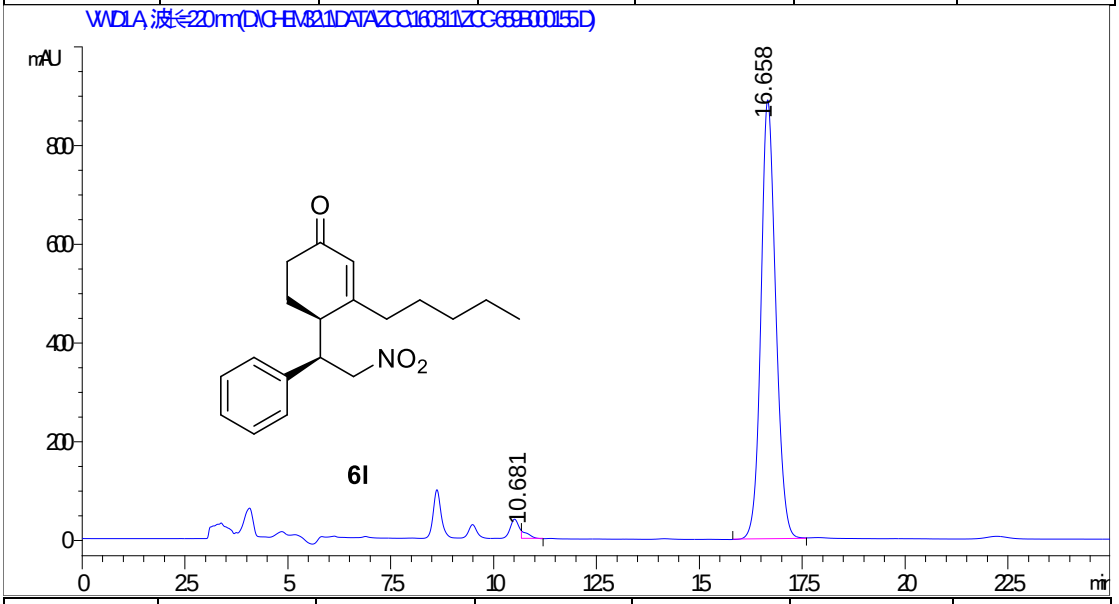


#	Time	Area	Height	Width	Symmetry	Area %
1	10.812	158.7	7.9	0.287	0.795	0.947
2	16.708	16602.6	662.5	0.3826	0.840	99.053

6l: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one

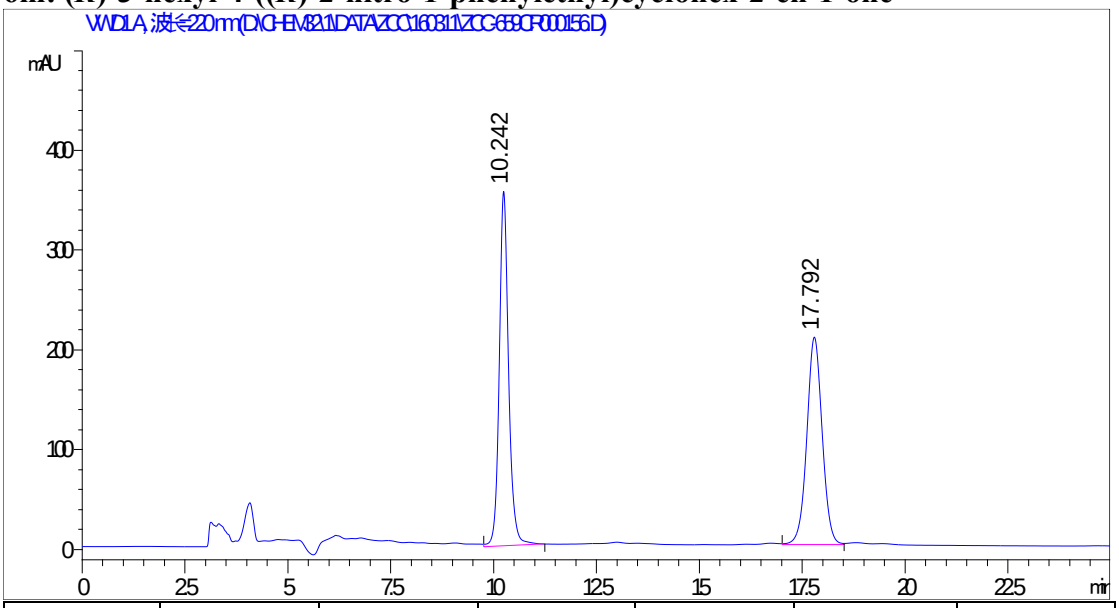


#	Time	Area	Height	Width	Symmetry	Area %
1	10.887	8715.1	528	0.2493	0.874	50.621
2	16.87	8501.2	342.7	0.3796	0.867	49.379

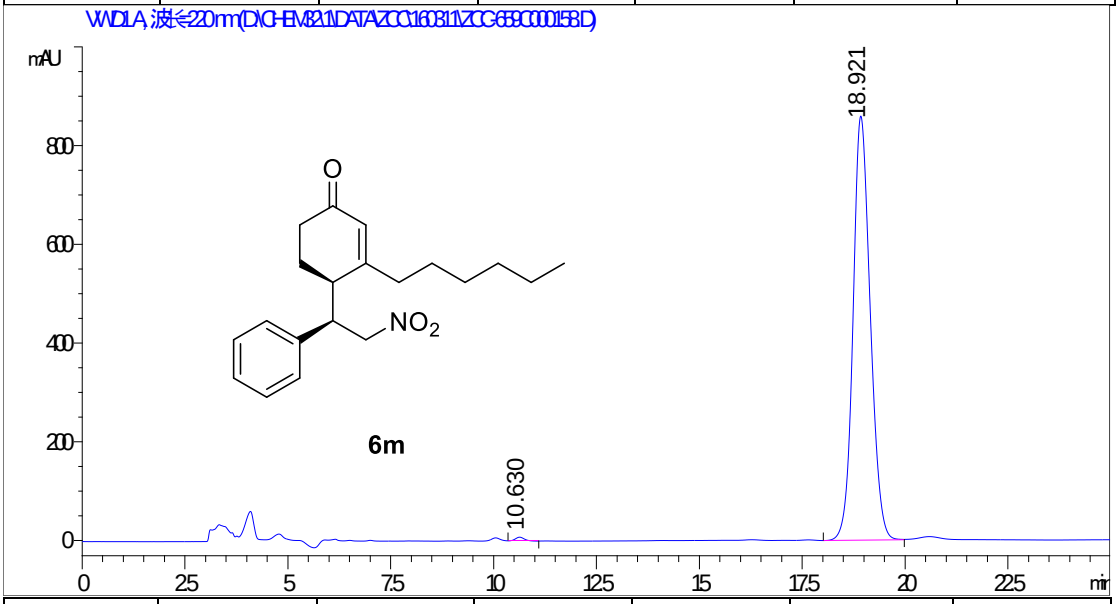


#	Time	Area	Height	Width	Symmetry	Area %
1	10.681	183.3	15.5	0.1973	0.589	0.814
2	16.658	22339.3	889.4	0.3818	0.803	99.186

6m: (*R*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

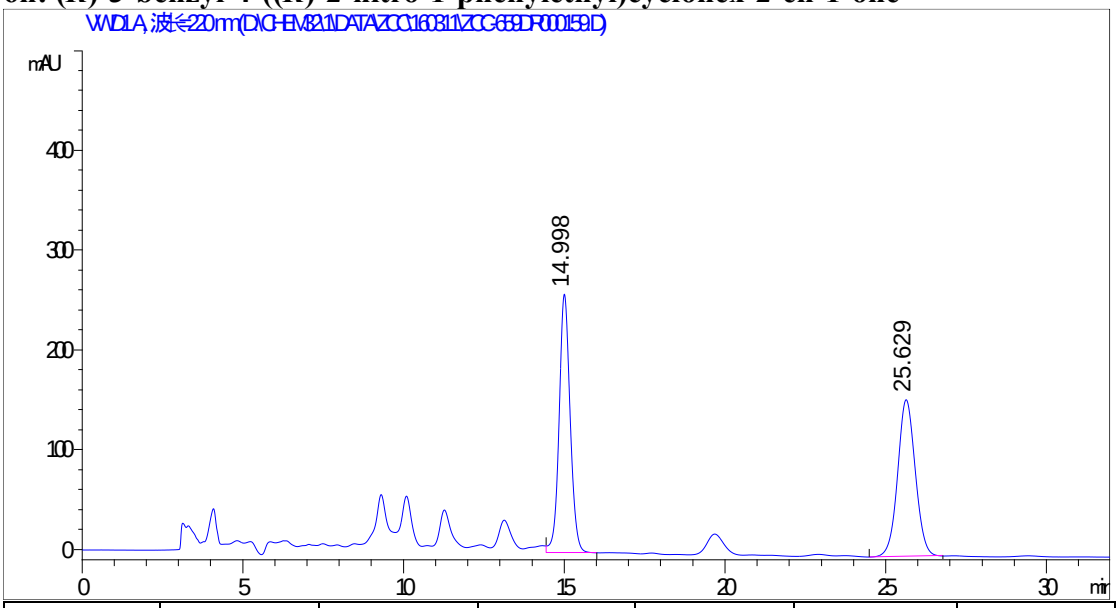


#	Time	Area	Height	Width	Symmetry	Area %
1	10.242	5612.1	355.5	0.2366	0.836	50.833
2	17.792	5428.1	208.3	0.3986	0.940	49.167

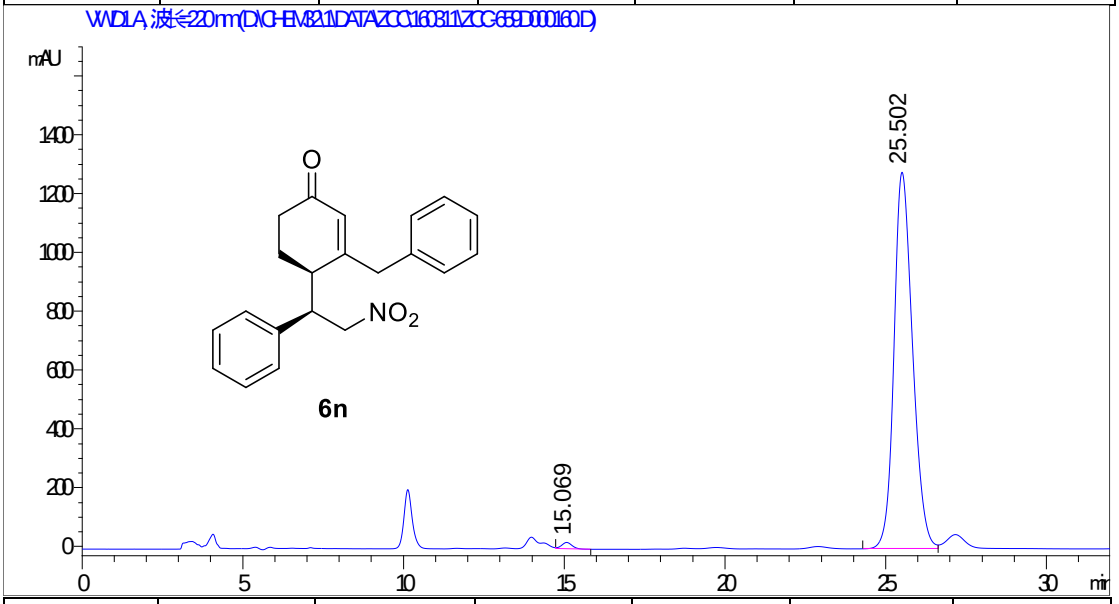


#	Time	Area	Height	Width	Symmetry	Area %
1	10.63	129.5	8	0.2447	0.874	0.516
2	18.921	24969	858.9	0.444	0.791	99.484

6n: (*R*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

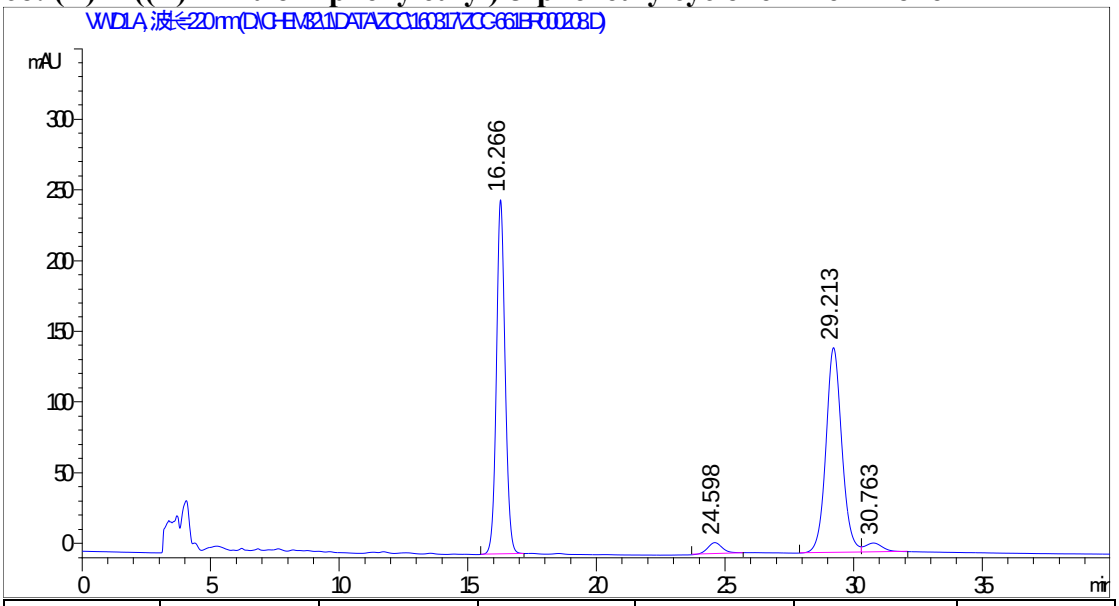


#	Time	Area	Height	Width	Symmetry	Area %
1	14.998	6201.1	259.4	0.3633	0.886	50.836
2	25.629	5997.1	157.1	0.5865	0.908	49.164

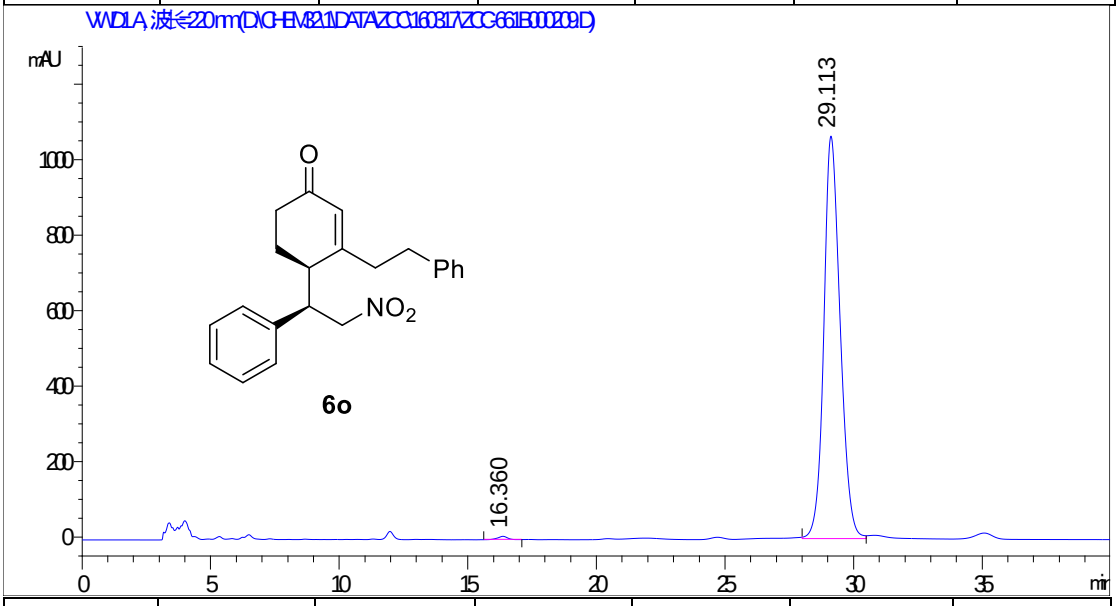


#	Time	Area	Height	Width	Symmetry	Area %
1	15.069	538.2	22.8	0.3565	0.928	1.037
2	25.502	51372.1	1279.9	0.6124	0.739	98.963

6o: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one

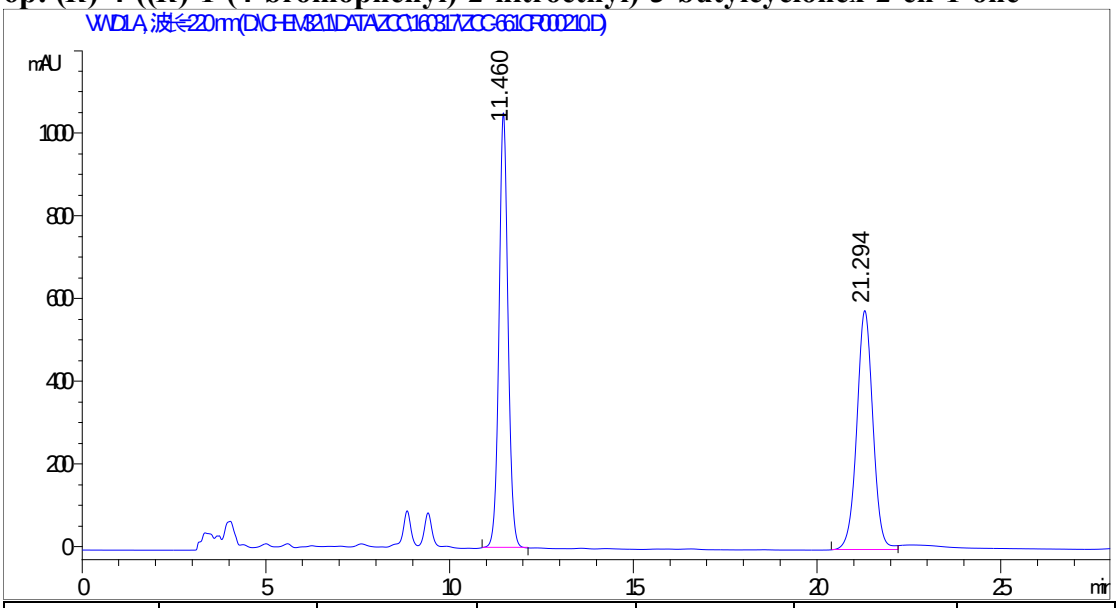


#	Time	Area	Height	Width	Symmetry	Area %
1	16.266	5878.1	250.6	0.3595	0.872	46.066
2	24.598	322.8	8	0.6086	0.925	2.530
3	29.213	6247	145	0.6554	0.880	48.958
4	30.763	312.1	6.5	0.6625	0.823	2.446

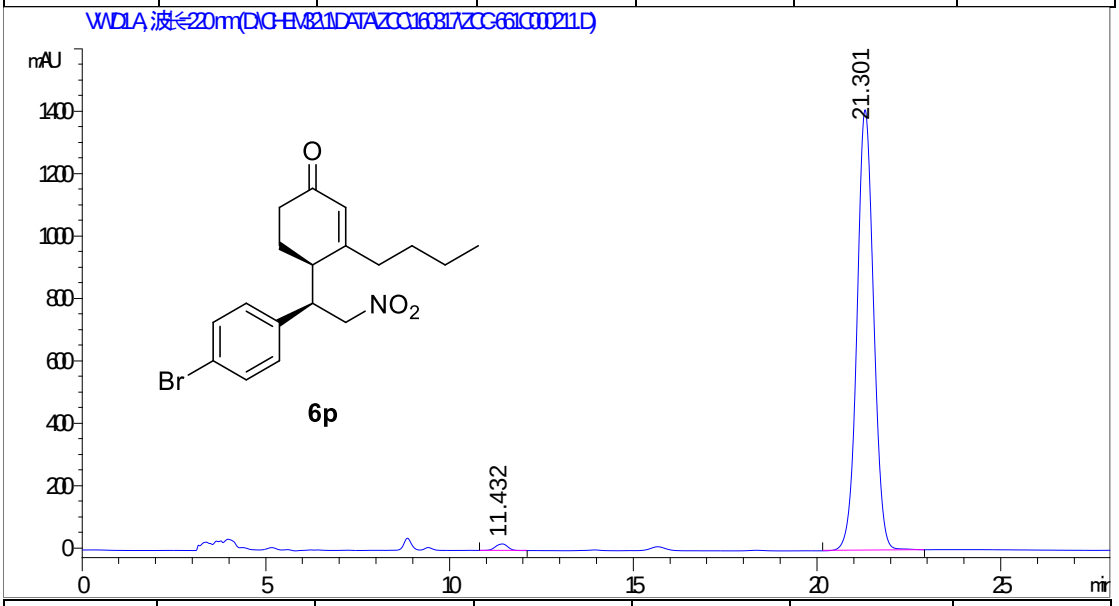


#	Time	Area	Height	Width	Symmetry	Area %
1	16.36	256.9	9.1	0.4161	1.142	0.539
2	29.113	47412.1	1069.3	0.739	0.763	99.461

6p: (*R*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-butylcyclohex-2-en-1-one

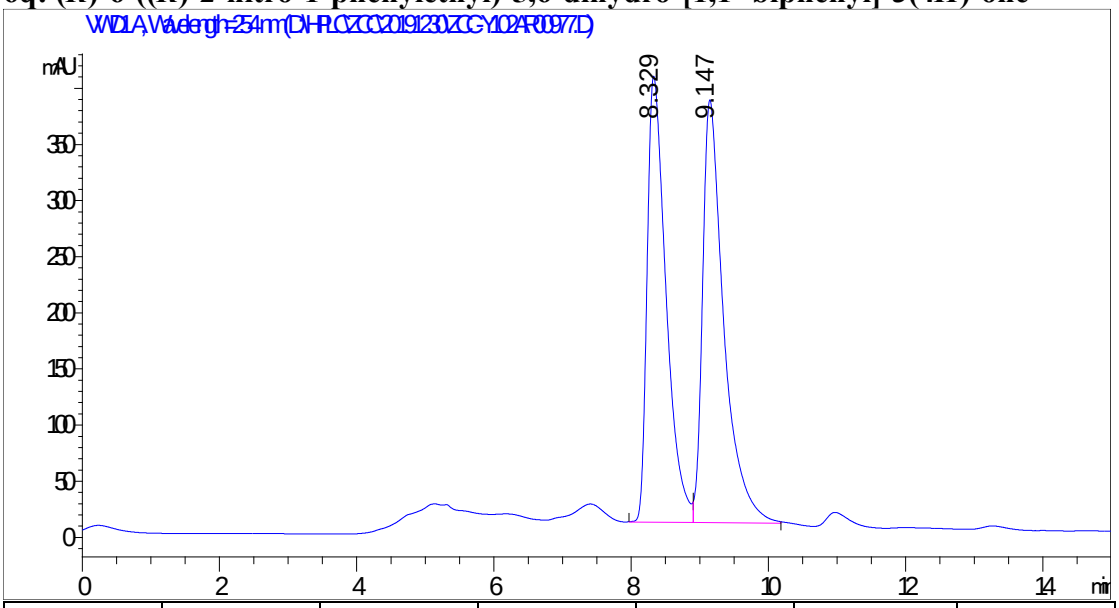


#	Time	Area	Height	Width	Symmetry	Area %
1	11.46	17919.5	1052.2	0.2838	0.923	50.349
2	21.294	17671.3	578.8	0.5089	0.948	49.651

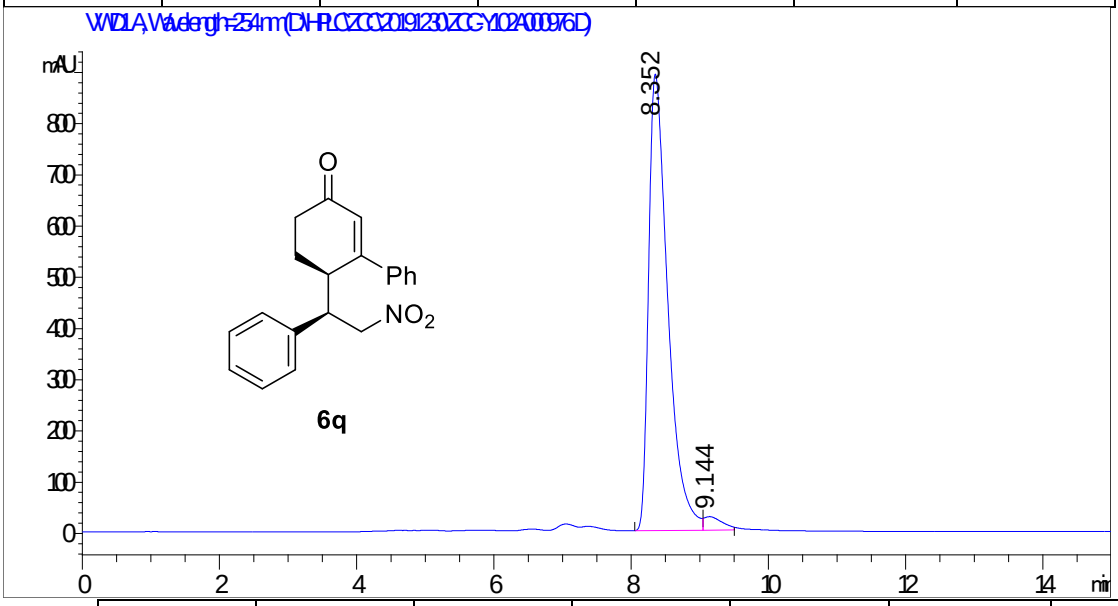


#	Time	Area	Height	Width	Symmetry	Area %
1	11.432	493.6	21	0.3764	1.225	1.101
2	21.301	44323.6	1411.9	0.4842	0.906	98.899

6q: (*R*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

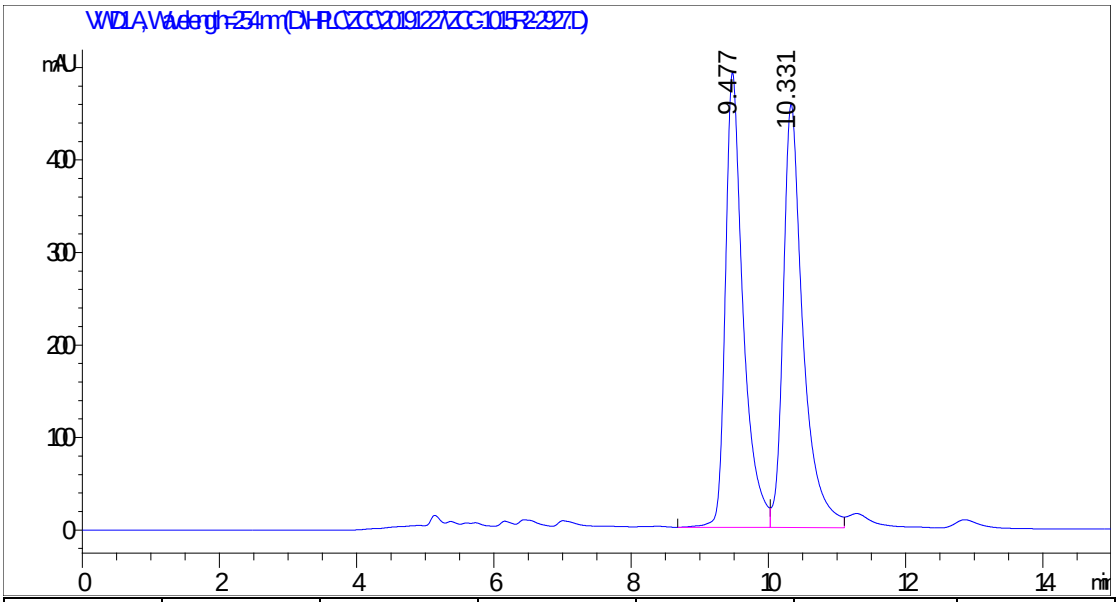


#	Time	Area	Height	Width	Symmetry	Area %
1	8.329	7624	397.4	0.3197	0	48.483
2	9.147	8101.1	376.6	0.3585	0.496	51.517

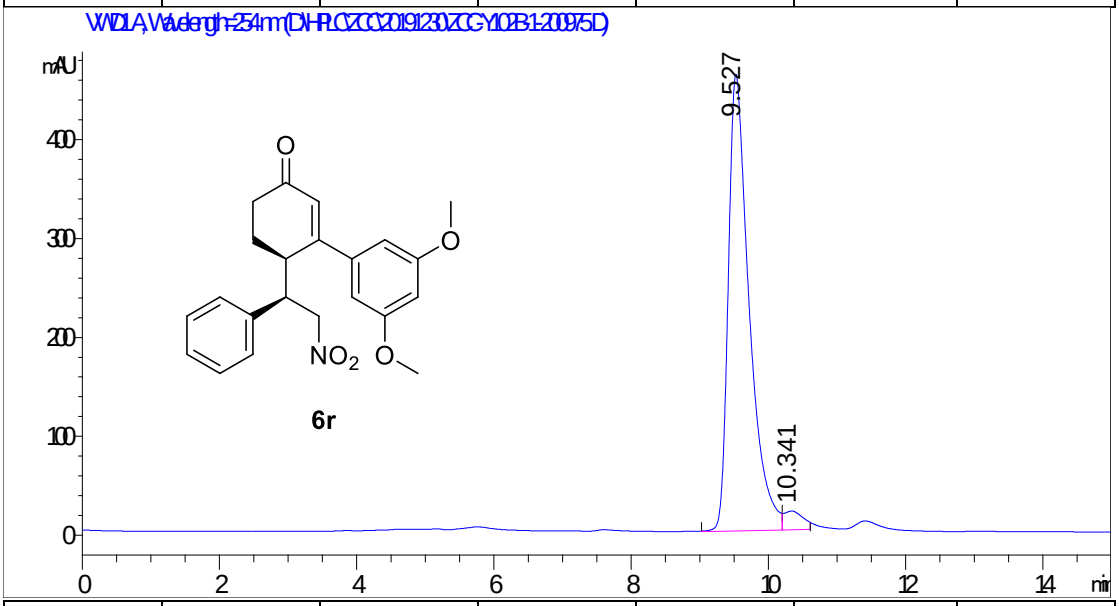


#	Time	Area	Height	Width	Symmetry	Area %
1	8.352	17335.2	891.1	0.3242	0	97.278
2	9.144	485.1	26.3	0.3069	0.423	2.722

6r: (*R*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

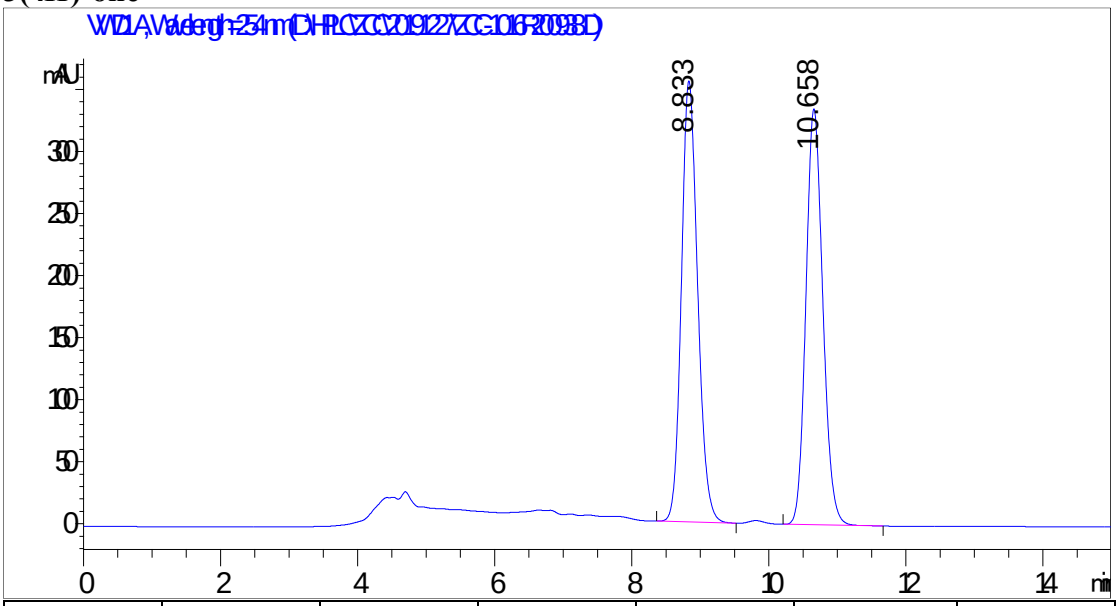


#	Time	Area	Height	Width	Symmetry	Area %
1	9.477	8845.1	491.9	0.2637	0.62	49.022
2	10.331	9198	458.1	0.294	0.611	50.978

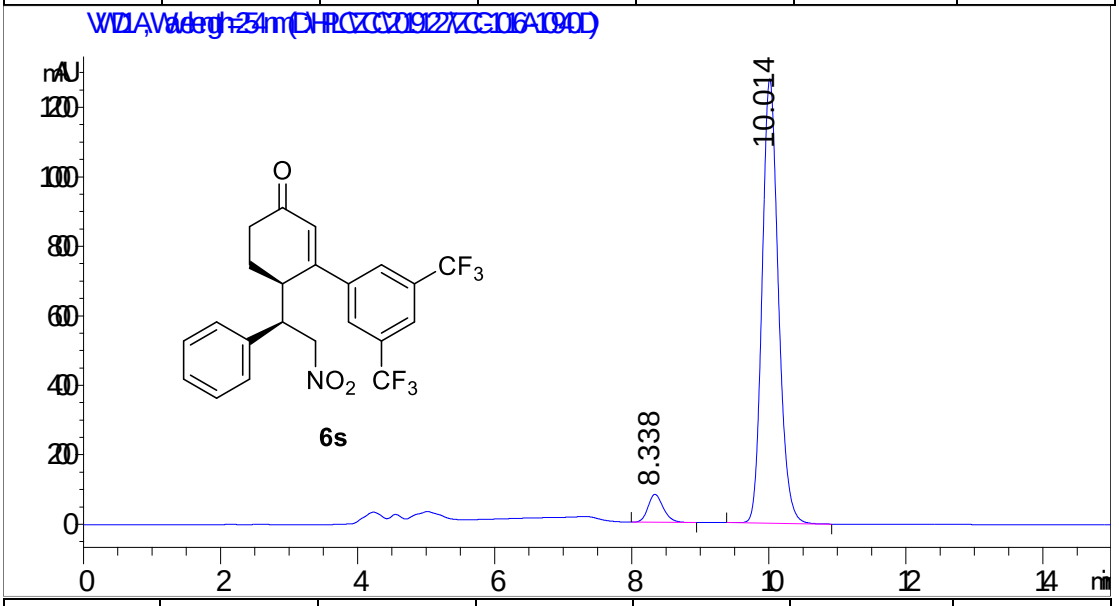


#	Time	Area	Height	Width	Symmetry	Area %
1	9.527	9757.3	461.6	0.3332	0	96.417
2	10.341	362.6	18.9	0.3202	0.674	3.583

6s: (*R*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

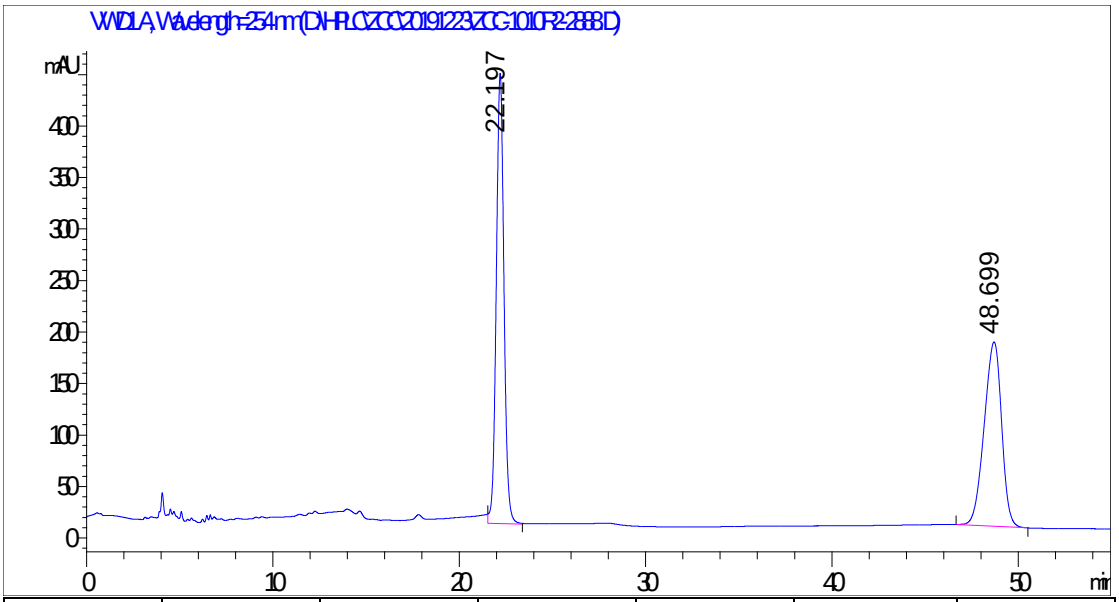


#	Time	Area	Height	Width	Symmetry	Area %
1	8.833	5842.8	355.5	0.253	0.81	50.430
2	10.658	5743.1	335.2	0.2669	0.846	49.570

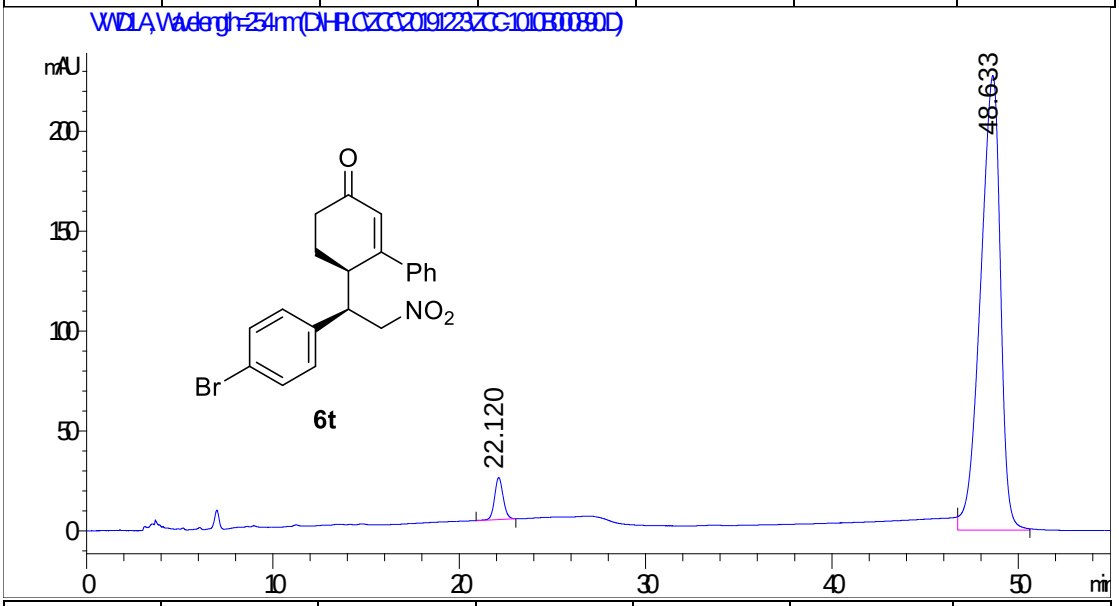


#	Time	Area	Height	Width	Symmetry	Area %
1	8.338	1244.8	80.7	0.2353	0.781	5.587
2	10.014	21035.1	1279.5	0.253	0.833	94.413

6t: (*R*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

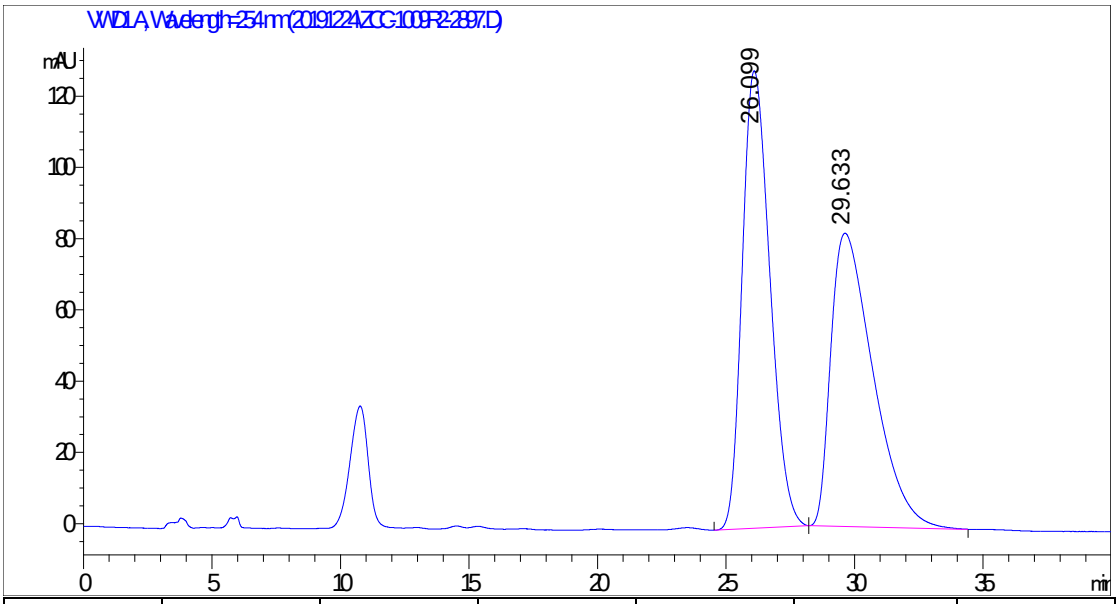


#	Time	Area	Height	Width	Symmetry	Area %
1	22.197	12497.5	436.9	0.4767	0.98	51.799
2	48.699	11629.3	179	1.01	1.266	48.201

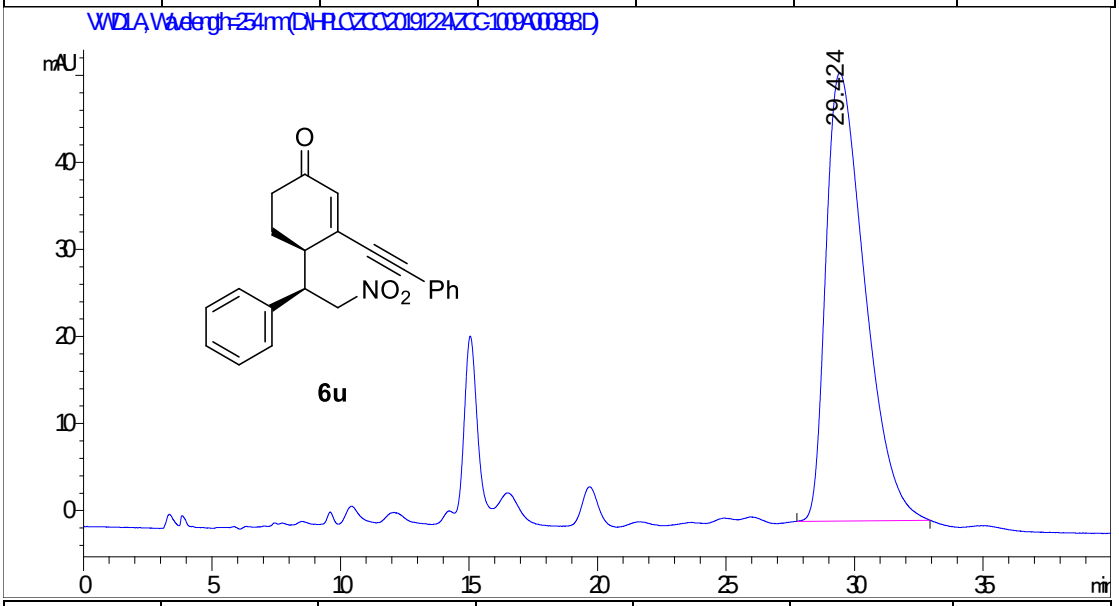


#	Time	Area	Height	Width	Symmetry	Area %
1	22.12	675.1	21.1	0.495	0.899	3.846
2	48.633	16881	227.6	1.2364	1.539	96.154

6u: (*R*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one

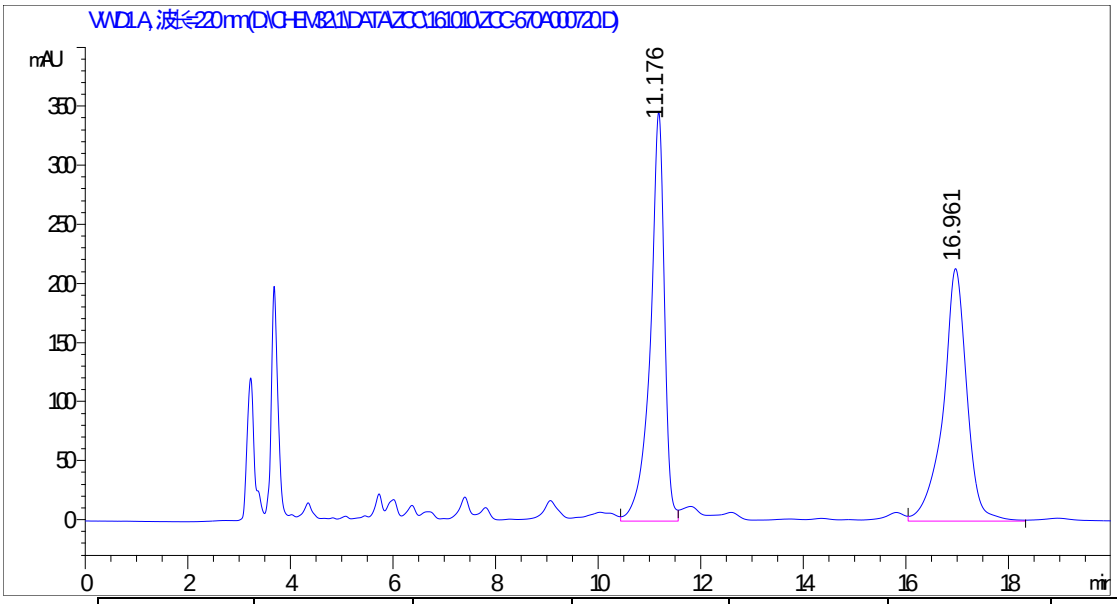


#	Time	Area	Height	Width	Symmetry	Area %
1	26.099	9622.9	128.4	1.1598	0.728	50.597
2	29.633	9395.7	82.4	1.5993	0.476	49.403

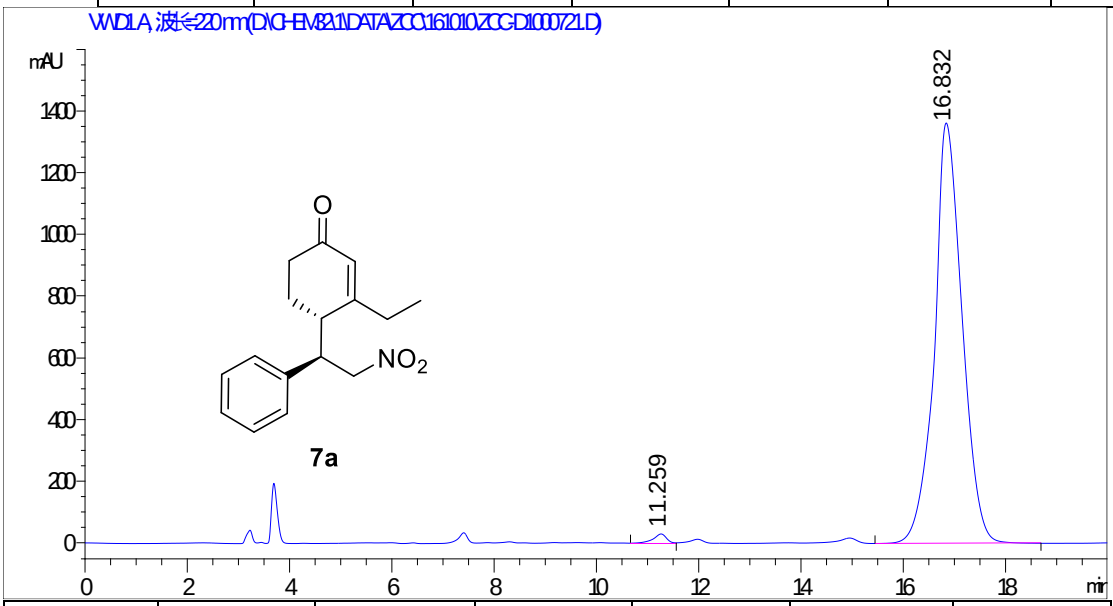


#	Time	Area	Height	Width	Symmetry	Area %
1	29.424	5420.5	51.5	1.4304	0.51	100.000

7a: (*S*)-3-ethyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

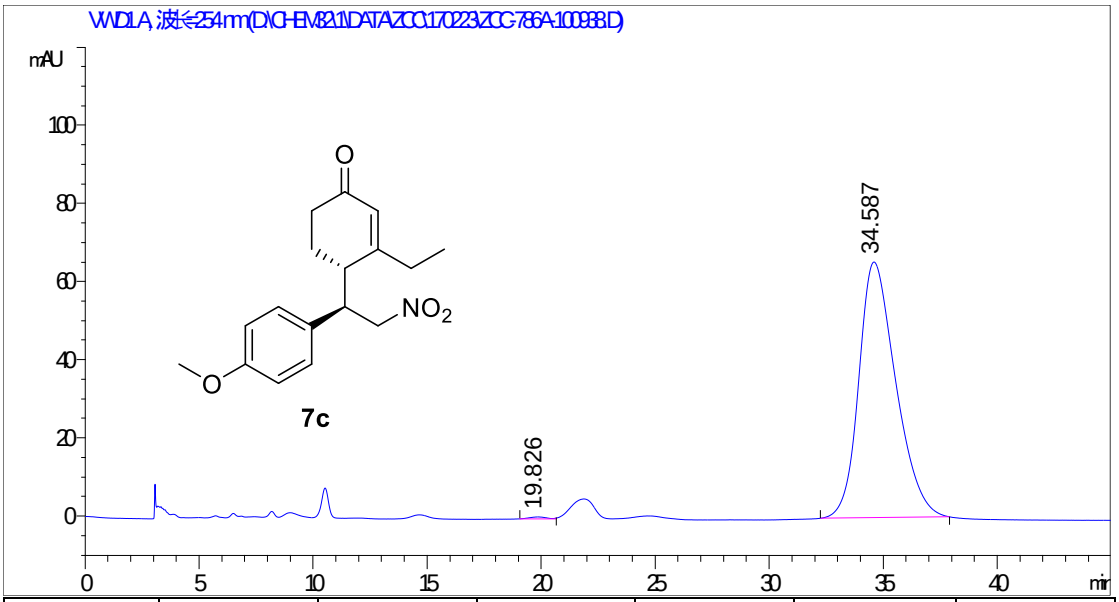


#	Time	Area	Height	Width	Symmetry	Area %
1	11.176	6651.8	346.8	0.2791	1.456	48.974
2	16.961	6930.7	214.3	0.472	1.074	51.026

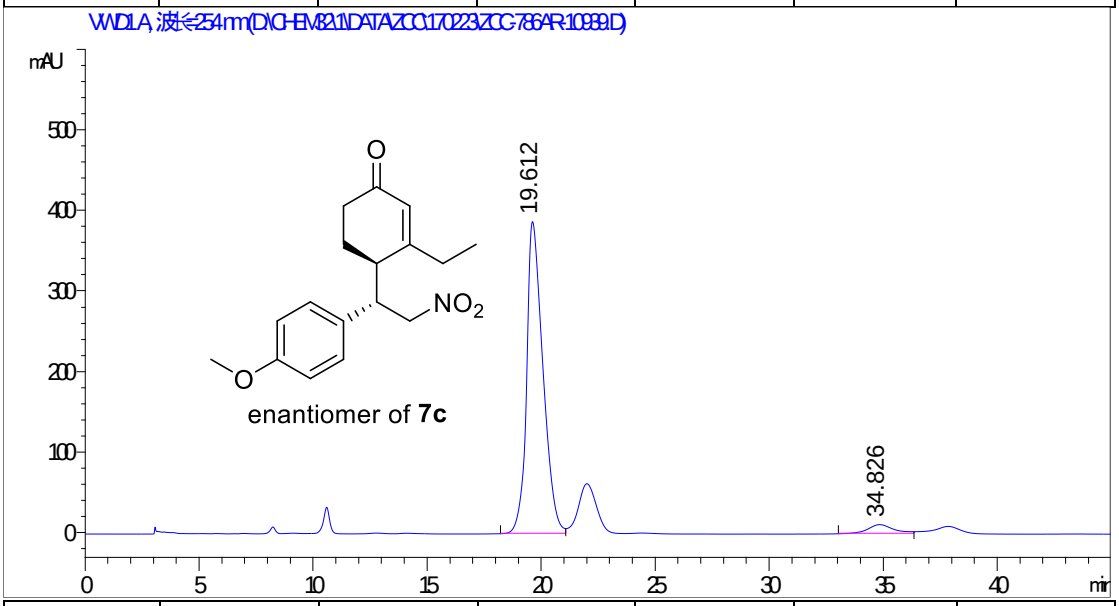


#	Time	Area	Height	Width	Symmetry	Area %
1	11.259	597.8	31	0.2786	1.514	1.150
2	16.832	51367.3	1361.8	0.5624	0.752	98.850

7c: (*S*)-3-ethyl-4-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)cyclohex-2-en-1-one

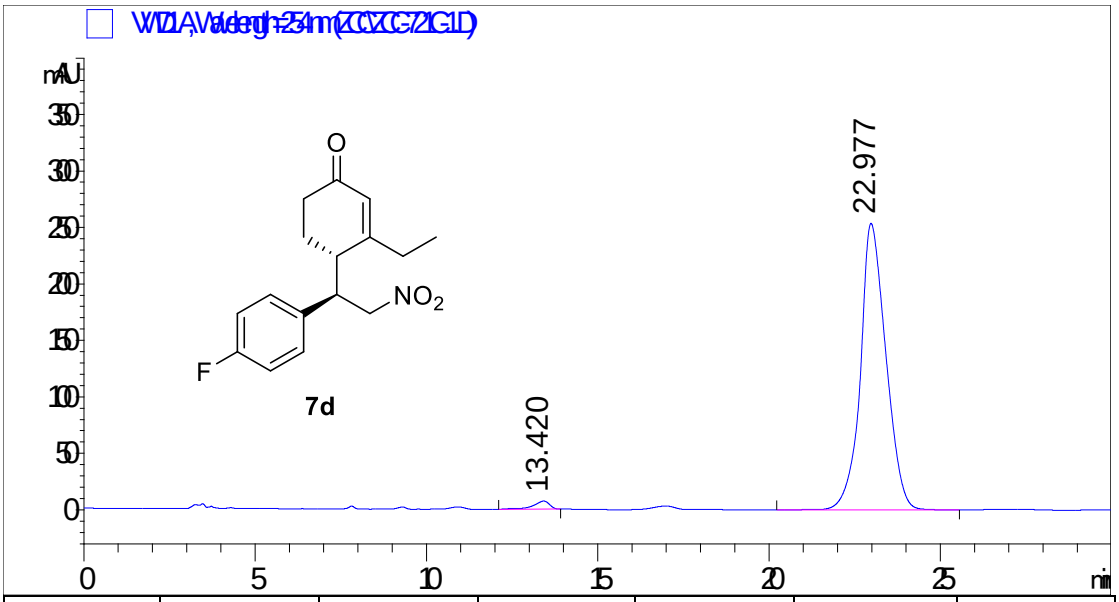


#	Time	Area	Height	Width	Symmetry	Area %
1	19.826	39.3	6.4E-1	1.0276	0.804	0.529
2	34.587	7393.5	65.5	1.6634	0.676	99.471

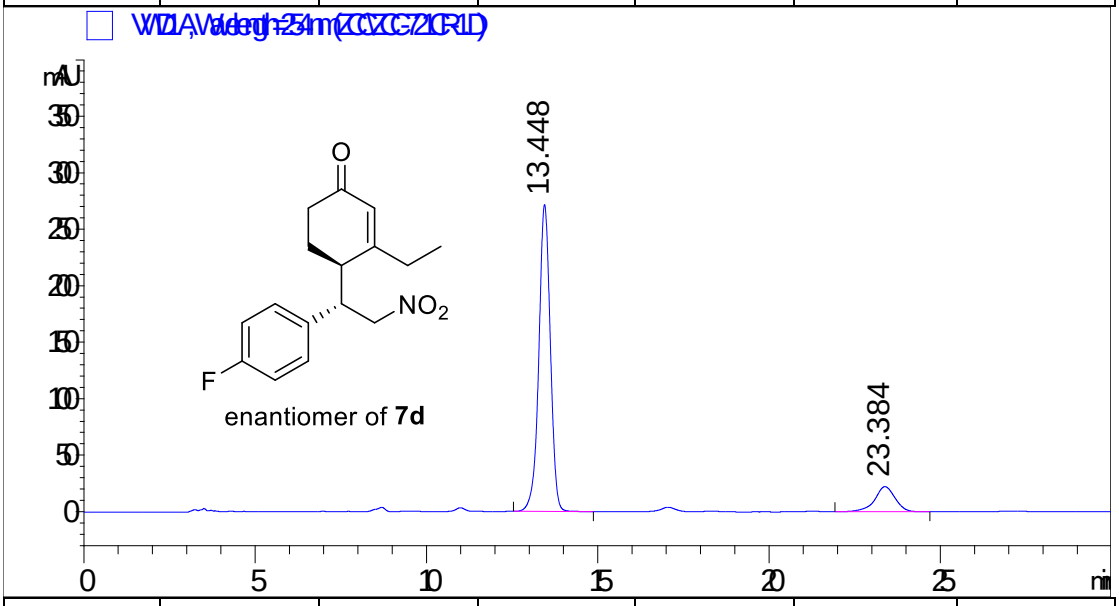


#	Time	Area	Height	Width	Symmetry	Area %
1	19.612	19236.8	387	0.743	0.560	95.232
2	34.826	963.2	11.6	1.0752	0.795	4.768

7d: (*S*)-3-ethyl-4-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)cyclohex-2-en-1-one

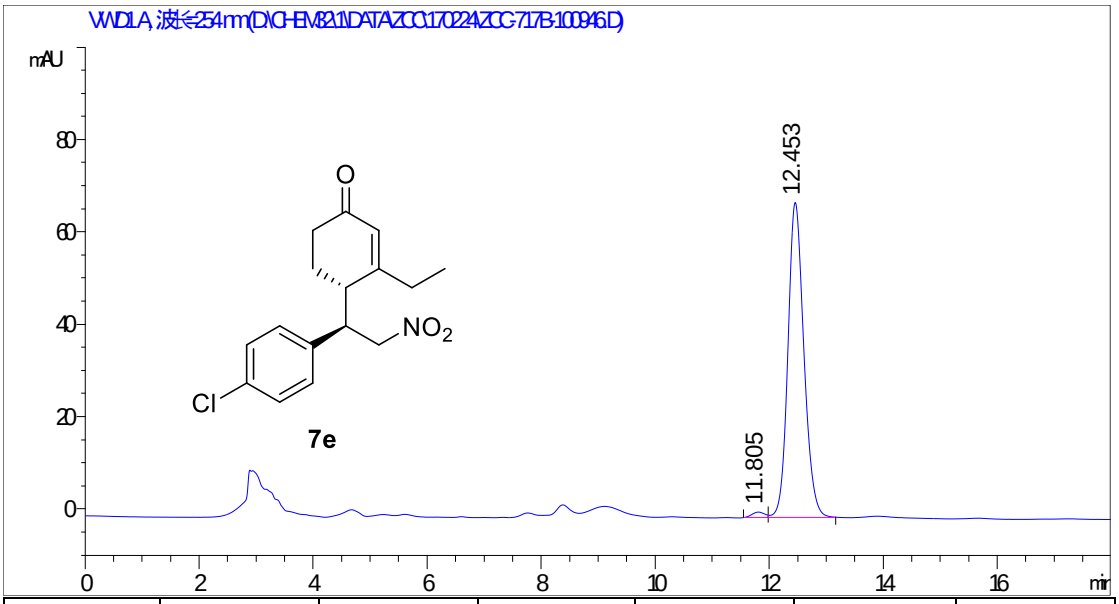


#	Time	Area	Height	Width	Symmetry	Area %
1	13.42	237.6	7.2	0.4806	1.820	1.773
2	22.977	13165.9	253.8	0.7783	0.721	98.227

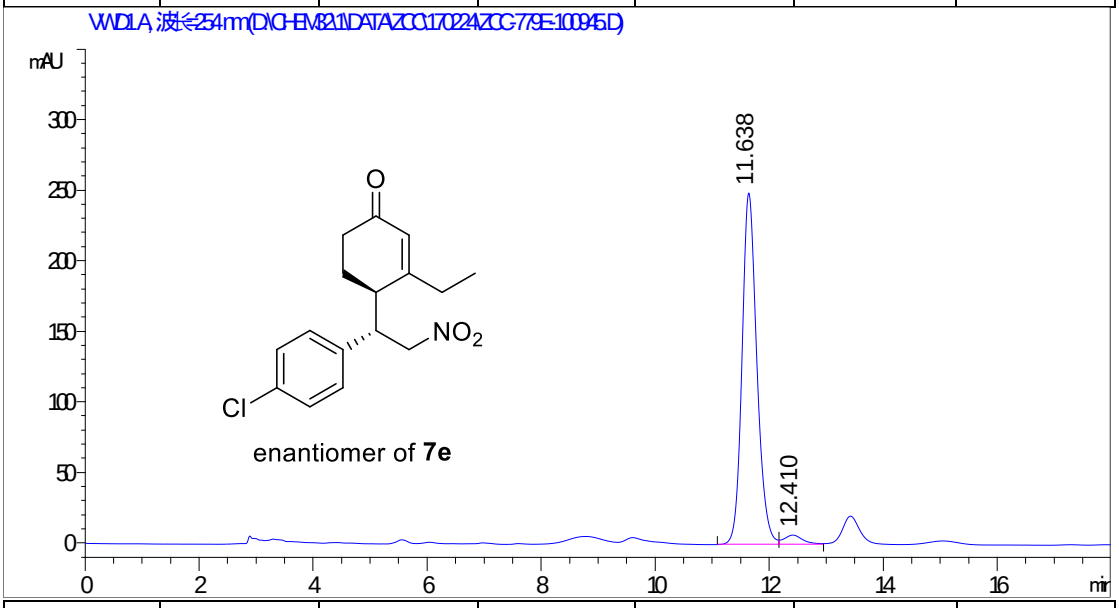


#	Time	Area	Height	Width	Symmetry	Area %
1	13.448	6352.3	271.7	0.3597	0.979	87.199
2	23.384	932.5	22.3	0.6299	1.021	12.801

7e: (*S*)-4-((*R*)-1-(4-chlorophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one

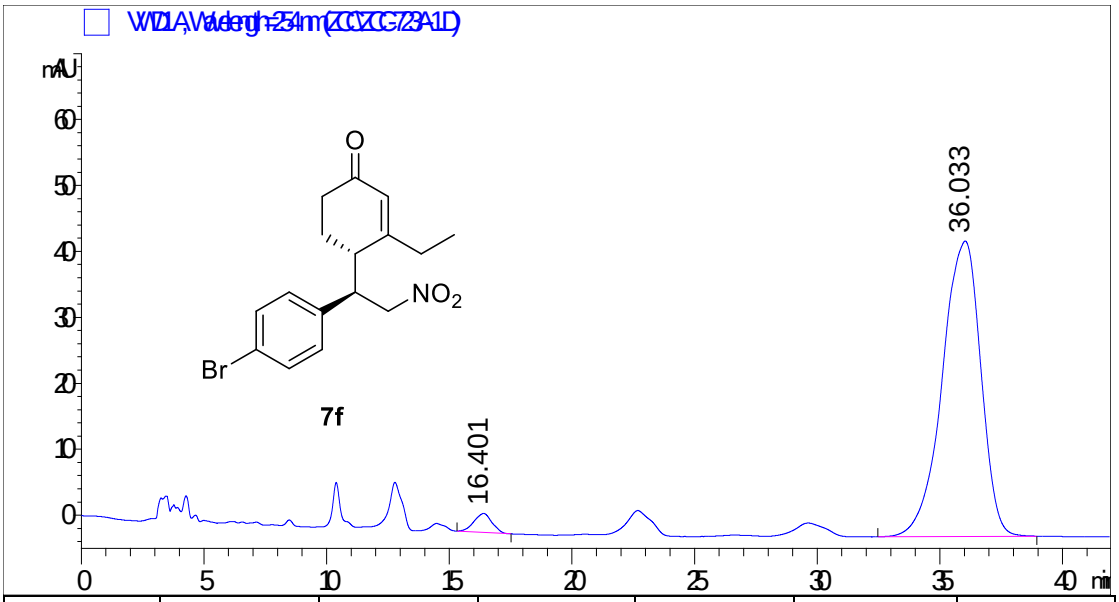


#	Time	Area	Height	Width	Symmetry	Area %
1	11.805	19.3	1.2	0.2643	0.923	1.431
2	12.453	1328.1	68.2	0.2969	0.806	98.569

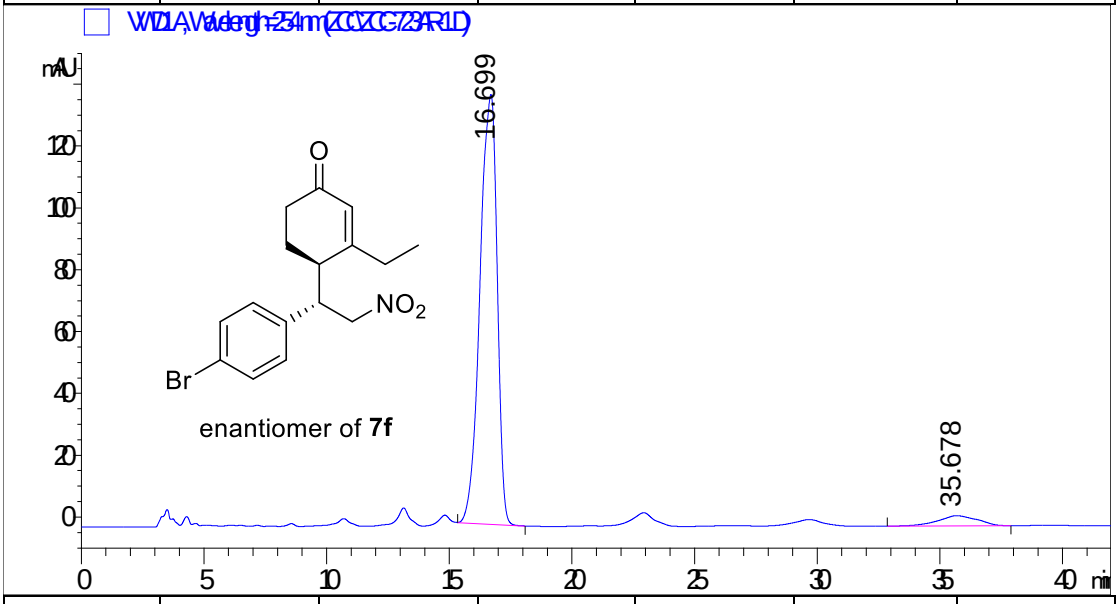


#	Time	Area	Height	Width	Symmetry	Area %
1	11.638	4508.3	249.2	0.2737	0.798	96.584
2	12.41	159.5	6.7	0.3461	0.762	3.416

7f: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-ethylcyclohex-2-en-1-one

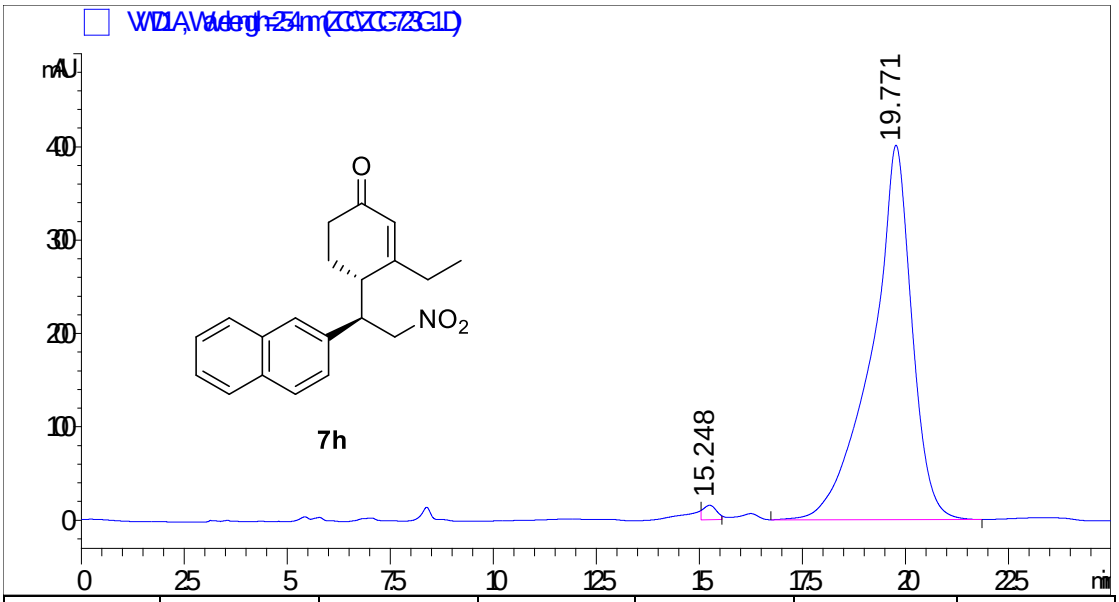


#	Time	Area	Height	Width	Symmetry	Area %
1	16.401	146.2	2.9	0.6981	1.111	2.897
2	36.033	4900.2	44.8	1.5549	1.391	97.103

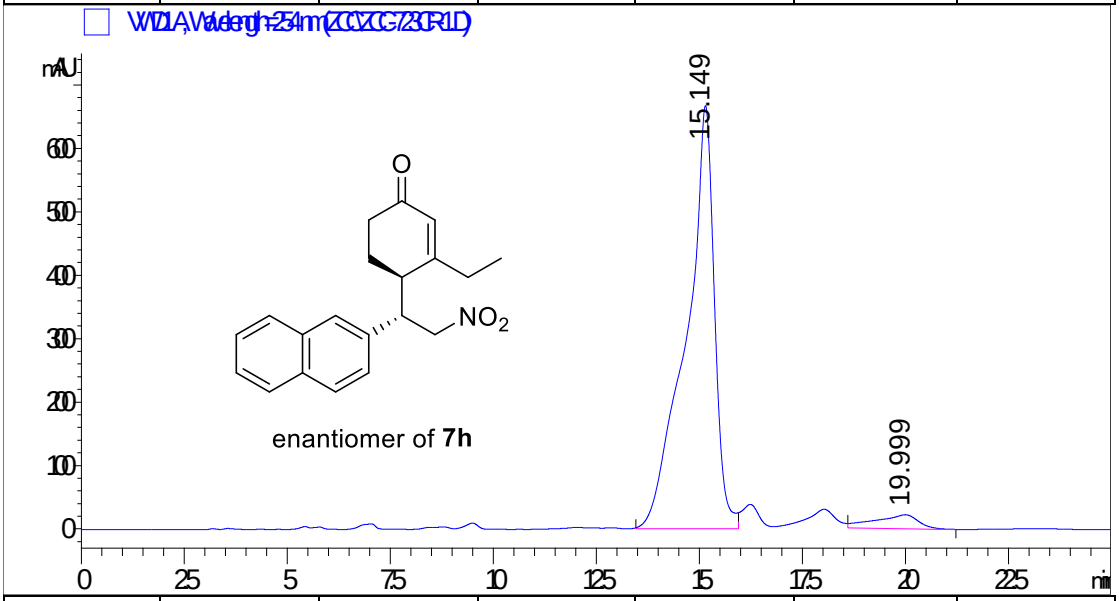


#	Time	Area	Height	Width	Symmetry	Area %
1	16.699	6754.1	139	0.7748	1.625	94.855
2	35.678	366.3	3.3	1.3698	0.895	5.145

7h: (*S*)-3-ethyl-4-((*R*)-1-(naphthalen-2-yl)-2-nitroethyl)cyclohex-2-en-1-one

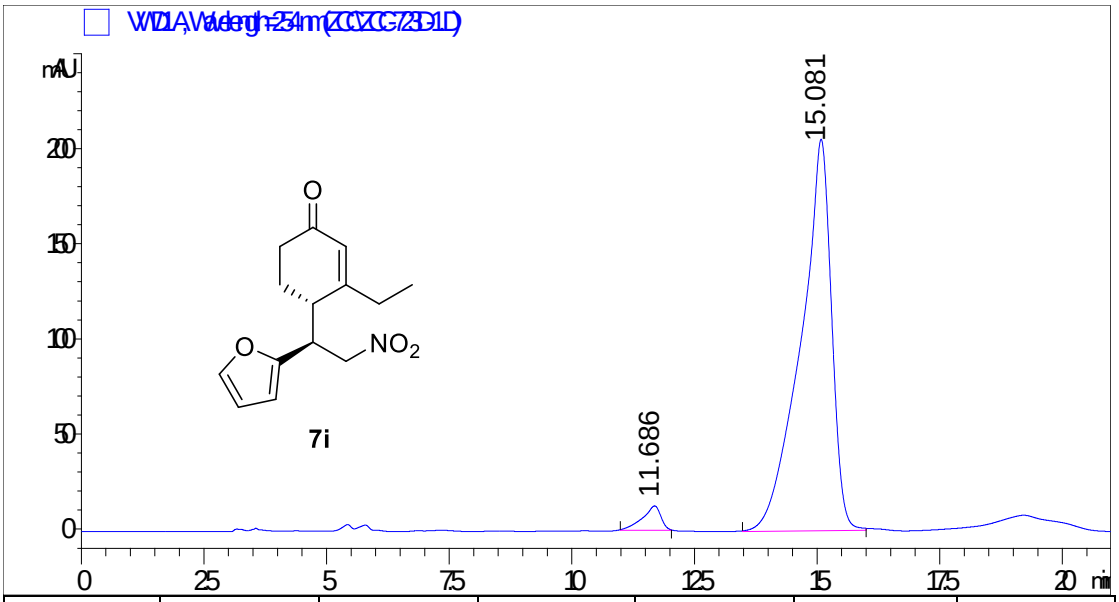


#	Time	Area	Height	Width	Symmetry	Area %
1	15.248	346.4	15.6	0.3706	0.902	1.256
2	19.771	27233.3	401.2	0.933	1.527	98.744

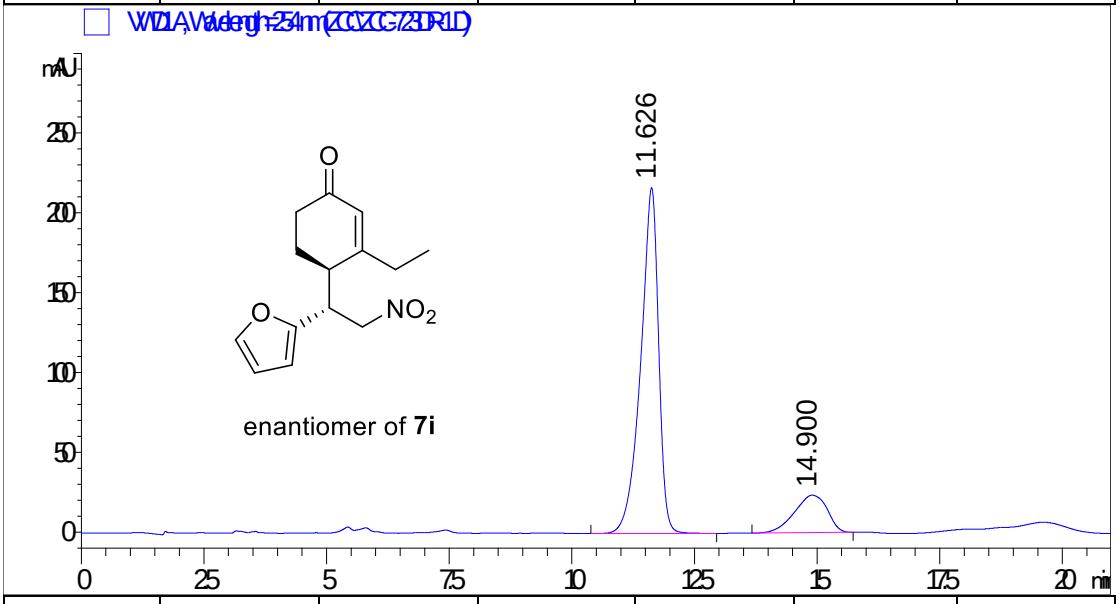


#	Time	Area	Height	Width	Symmetry	Area %
1	15.149	31889.6	667.5	0.7962	2.019	95.216
2	19.999	1602.2	22	0.9778	2.264	4.784

7i: (*S*)-3-ethyl-4-((*S*)-1-(furan-2-yl)-2-nitroethyl)cyclohex-2-en-1-one

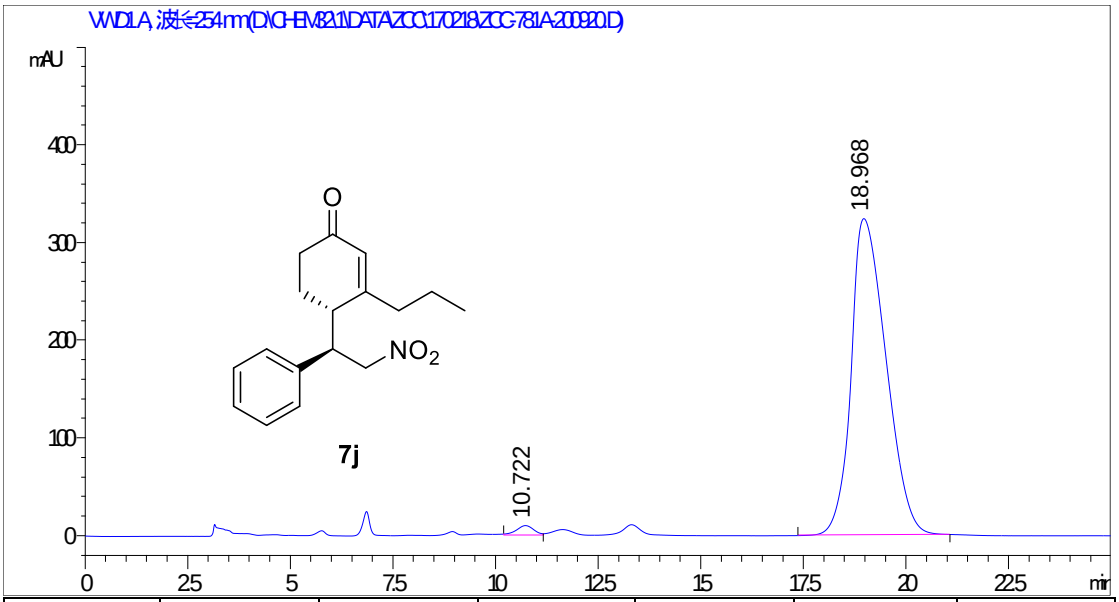


#	Time	Area	Height	Width	Symmetry	Area %
1	11.686	342.5	12.9	0.4411	1.881	3.675
2	15.081	8976	205.9	0.7176	1.765	96.325

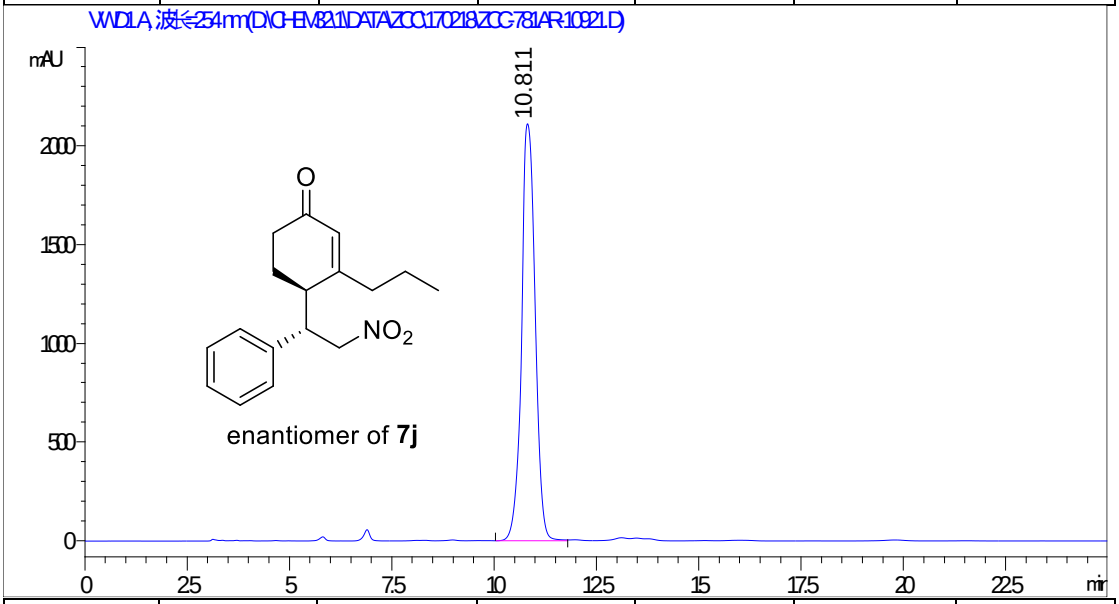


#	Time	Area	Height	Width	Symmetry	Area %
1	11.626	5507.7	216.7	0.3695	1.516	83.409
2	14.9	1095.6	23.5	0.7241	1.21	16.591

7j: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-propylcyclohex-2-en-1-one

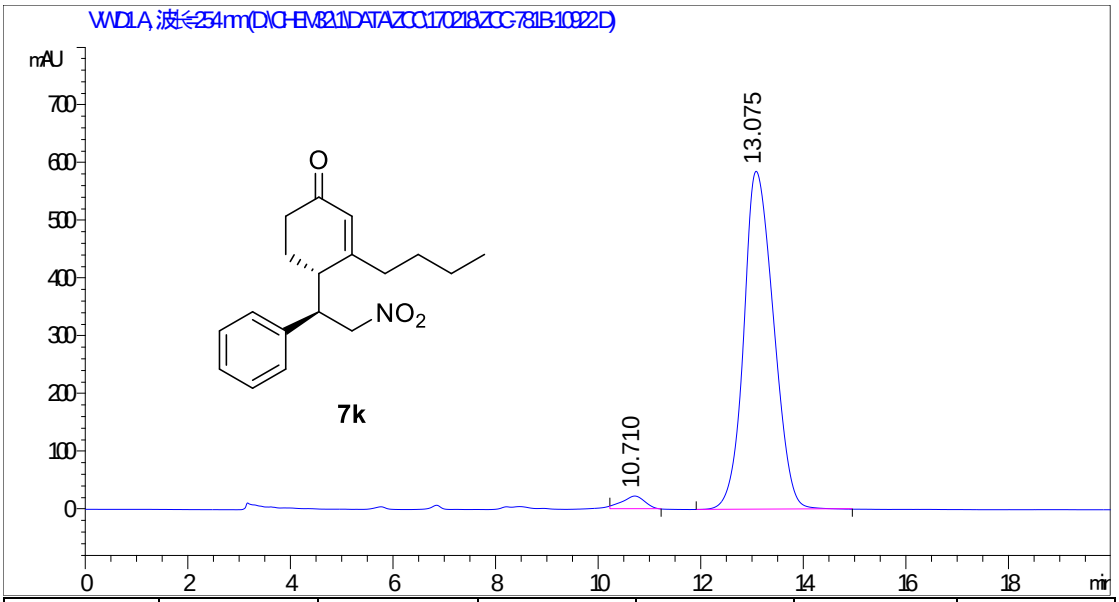


#	Time	Area	Height	Width	Symmetry	Area %
1	10.722	320.3	10.2	0.5212	1.079	1.639
2	18.968	19219.3	324	0.9192	0.571	98.361

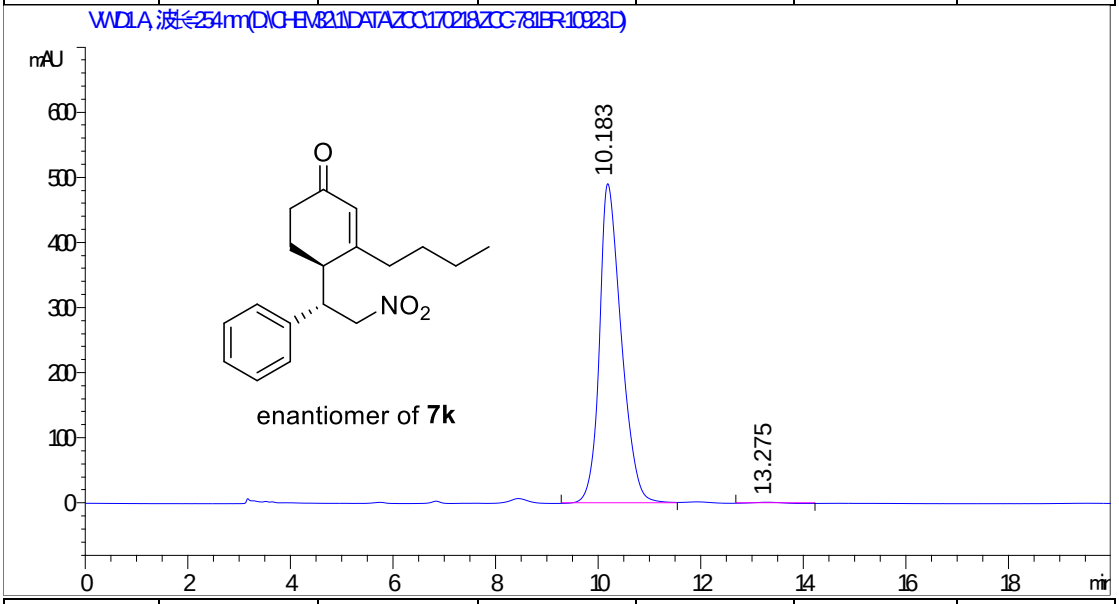


#	Time	Area	Height	Width	Symmetry	Area %
1	10.811	48965.8	2112.6	0.3563	0.779	100.000

7k: (*S*)-3-butyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

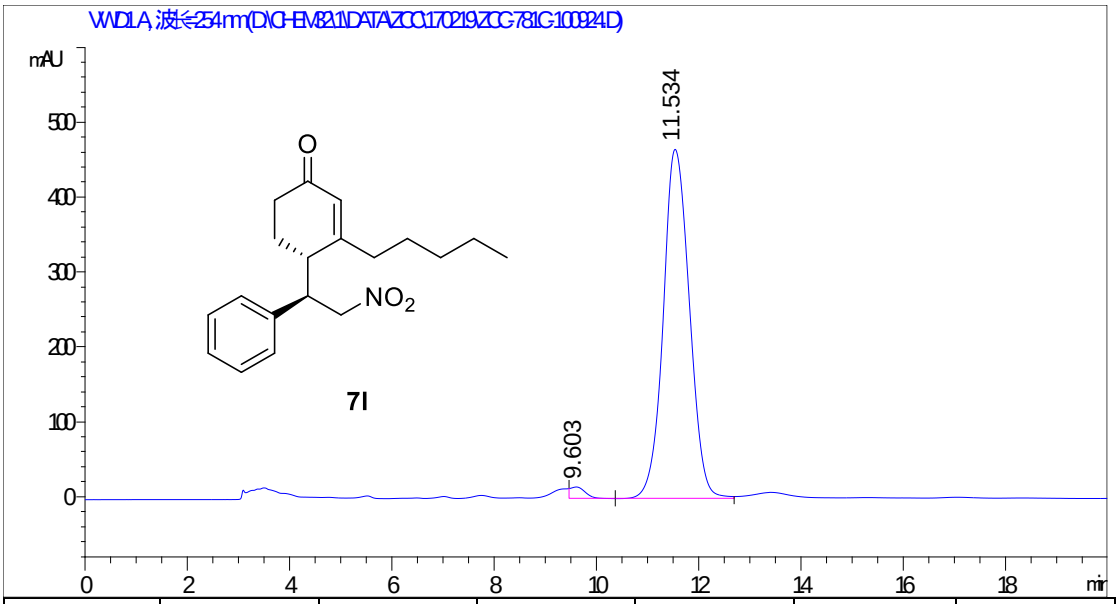


#	Time	Area	Height	Width	Symmetry	Area %
1	10.71	709.7	22.6	0.5233	1.269	2.913
2	13.075	23654.5	585.6	0.6285	0.706	97.087

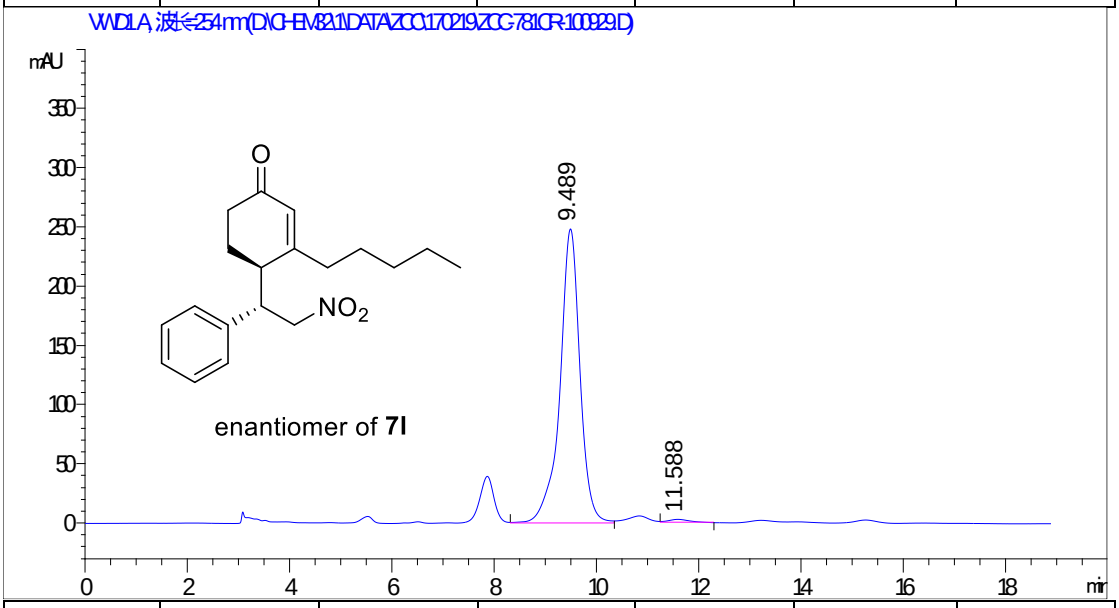


#	Time	Area	Height	Width	Symmetry	Area %
1	10.183	14594.5	490.8	0.4444	0.601	99.538
2	13.275	67.7	1.8	0.476	1.025	0.462

7l: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-pentylcyclohex-2-en-1-one

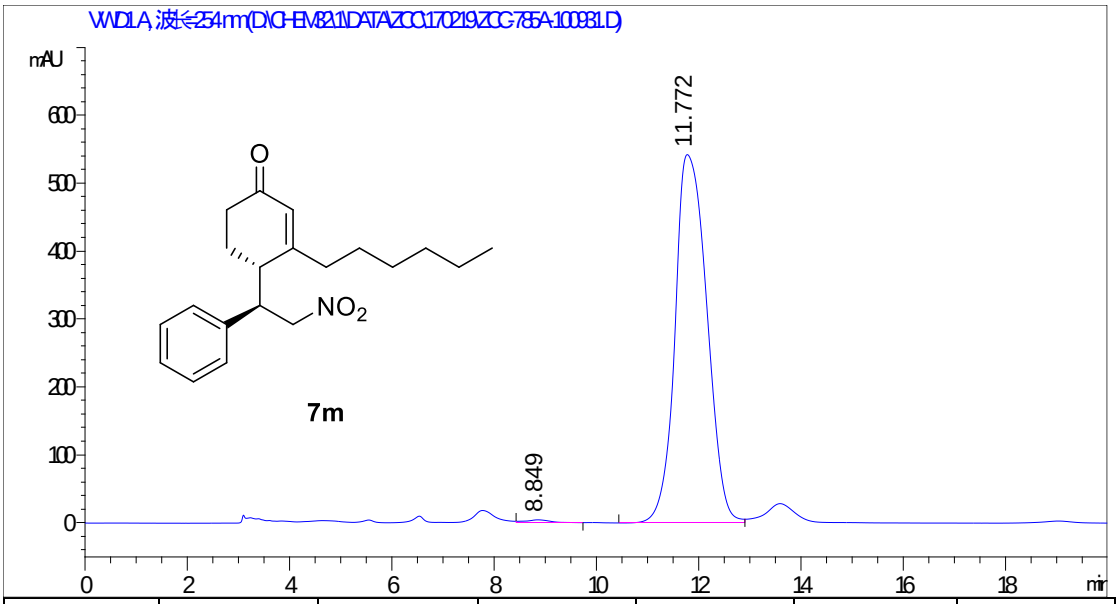


#	Time	Area	Height	Width	Symmetry	Area %
1	9.603	335.6	16	0.349	0.578	1.982
2	11.534	16598	466.3	0.5918	0.8231	98.018

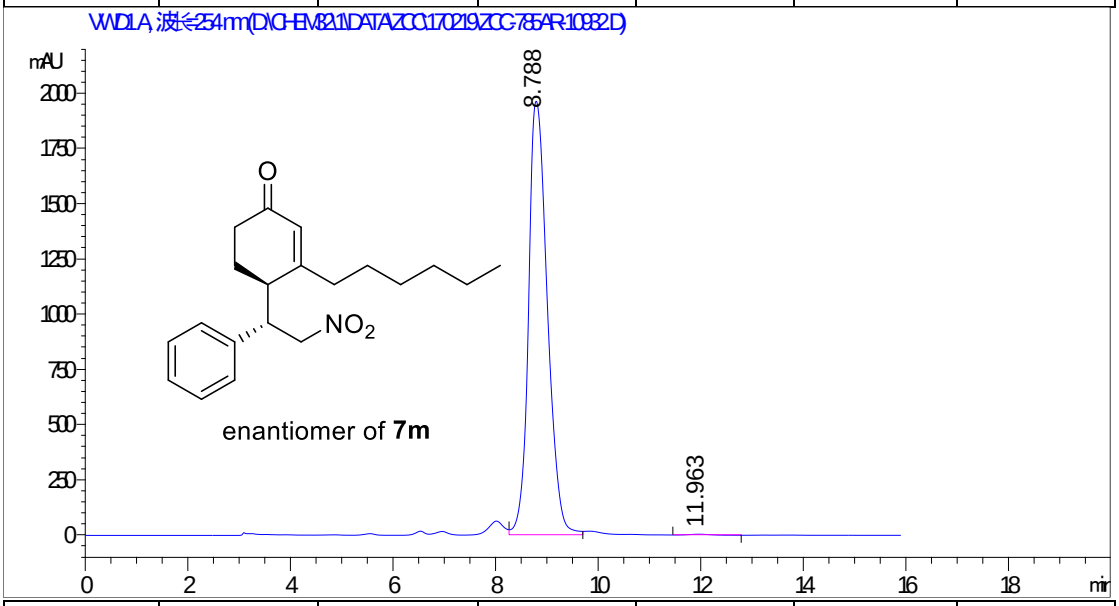


#	Time	Area	Height	Width	Symmetry	Area %
1	9.489	6775.1	248.3	0.4072	1.105	98.660
2	11.588	92.1	2.9	0.4527	0.774	1.340

7m: (*S*)-3-hexyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

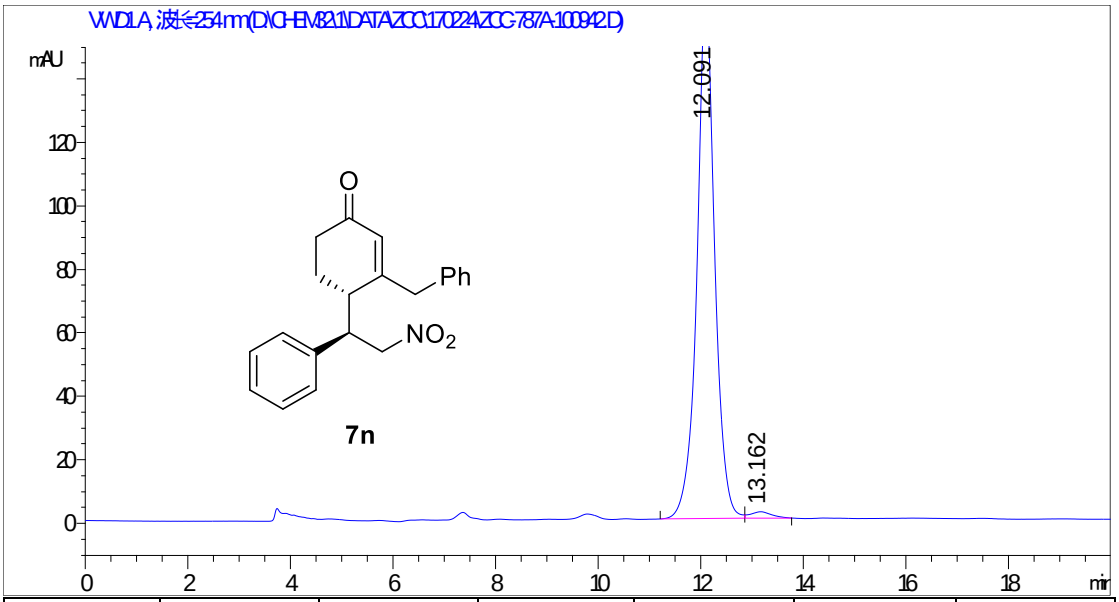


#	Time	Area	Height	Width	Symmetry	Area %
1	8.849	148.3	4.2	0.5004	0.912	0.628
2	11.772	23444.8	542.2	0.6836	0.641	99.372

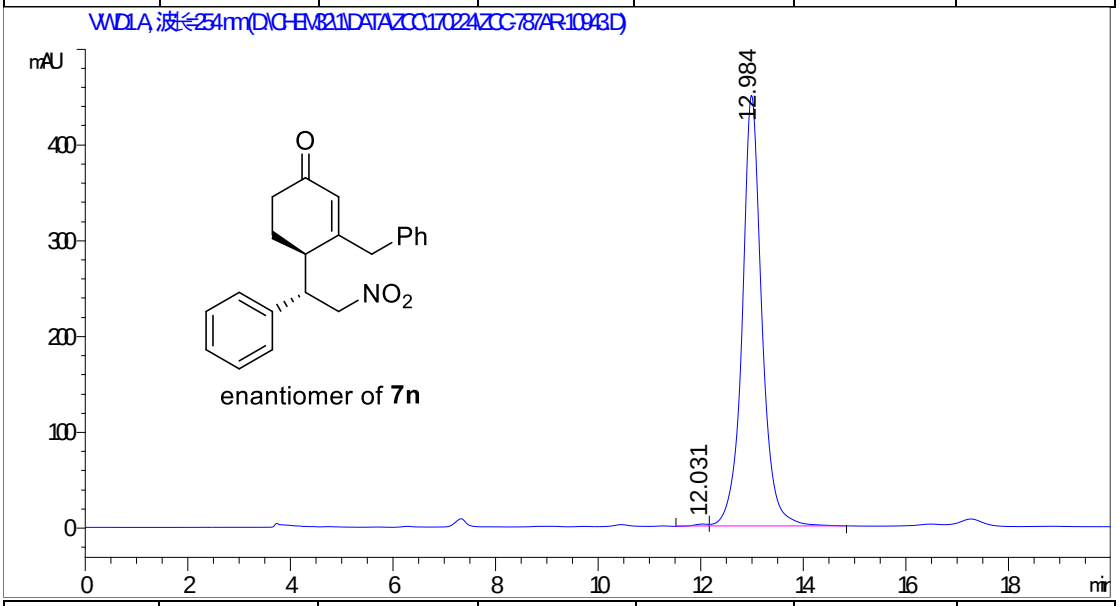


#	Time	Area	Height	Width	Symmetry	Area %
1	8.788	50287.7	1964.9	0.3903	0.663	99.709
2	11.963	146.6	4.6	0.462	1.115	0.291

7n: (*S*)-3-benzyl-4-((*R*)-2-nitro-1-phenylethyl)cyclohex-2-en-1-one

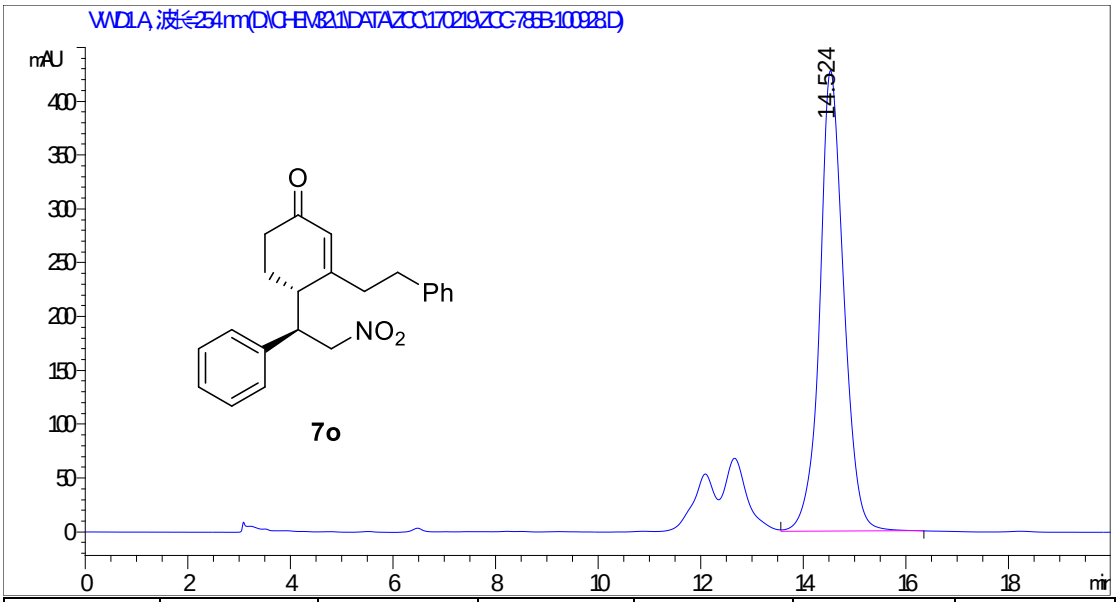


#	Time	Area	Height	Width	Symmetry	Area %
1	12.091	3963.2	166	0.3528	0.941	98.429
2	13.162	63.3	2.1	0.4172	0.844	1.571

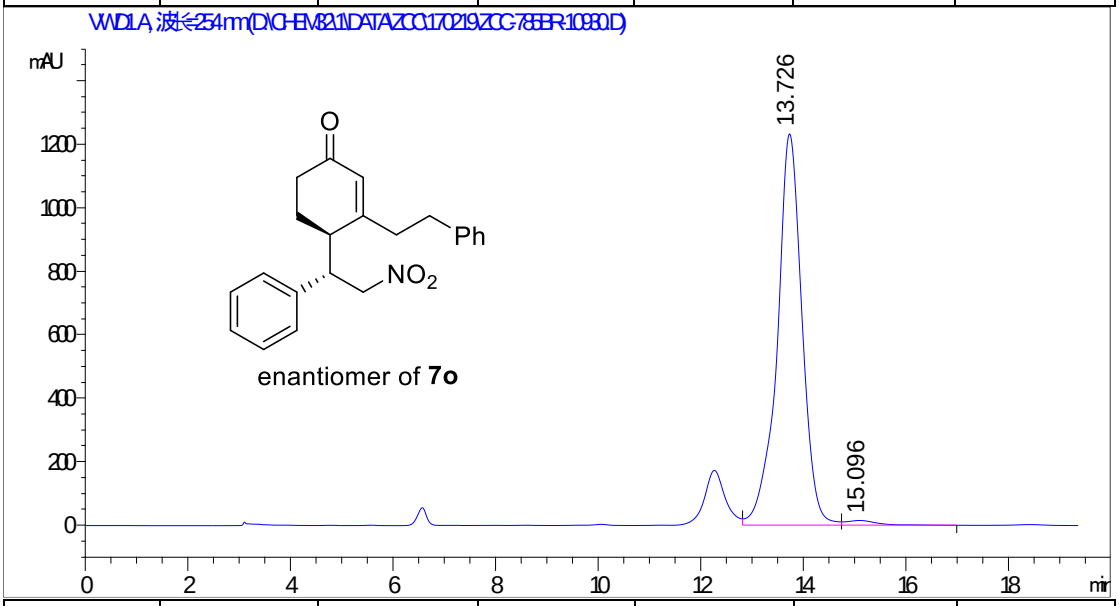


#	Time	Area	Height	Width	Symmetry	Area %
1	12.031	48.7	2.5	0.284	1.781	0.406
2	12.984	11955.4	449.5	0.3918	0.867	99.594

7o: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-phenethylcyclohex-2-en-1-one

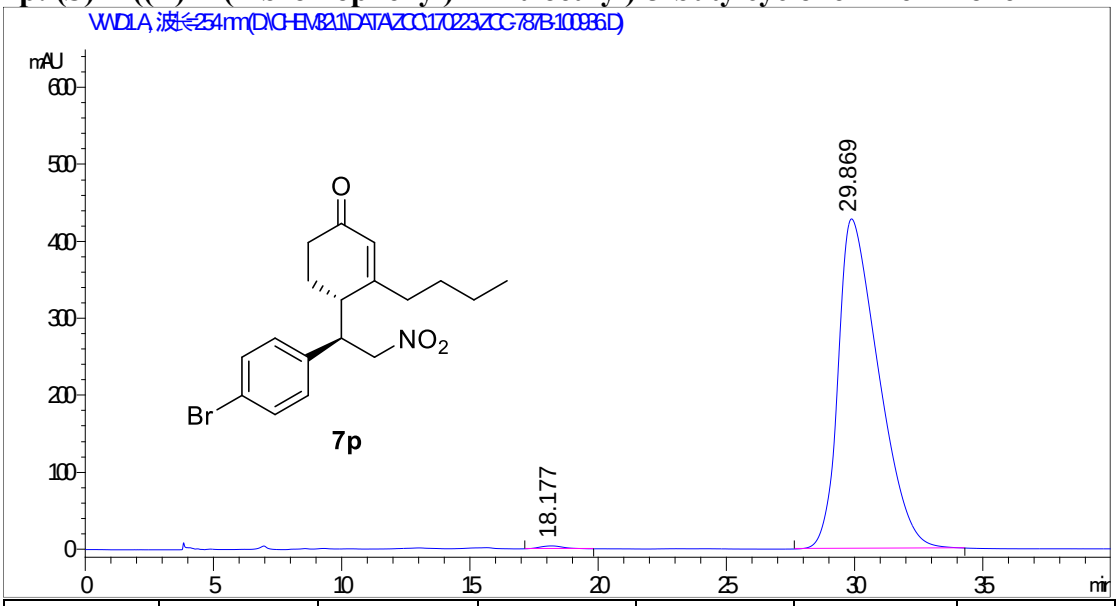


#	Time	Area	Height	Width	Symmetry	Area %
1	14.524	13930.6	428	0.4874	0.801	100.000

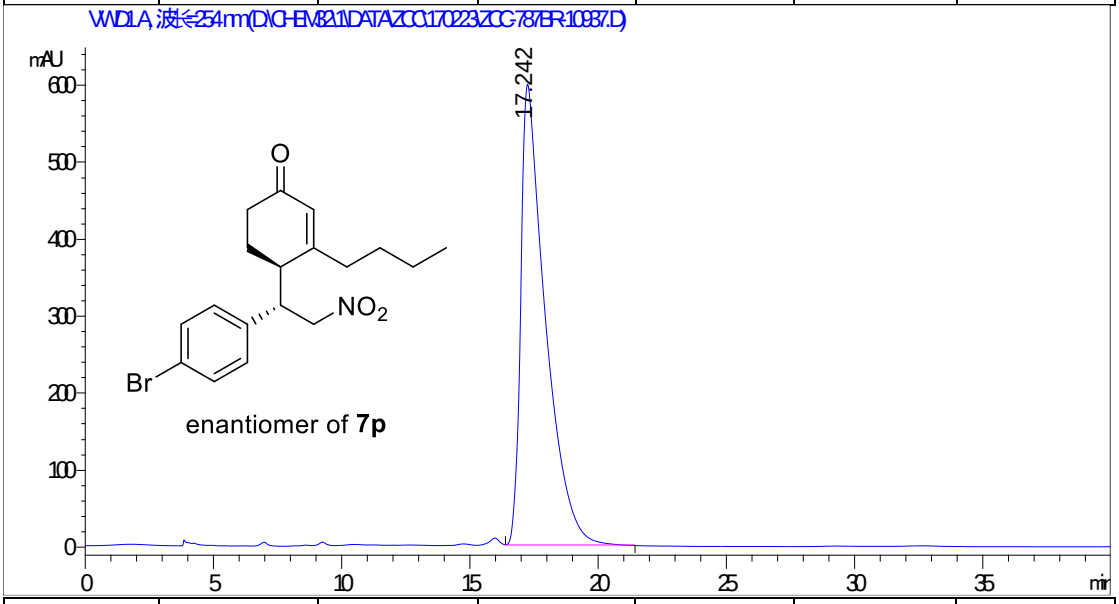


#	Time	Area	Height	Width	Symmetry	Area %
1	13.726	41541.2	1233	0.5023	1.002	98.419
2	15.096	667.3	15.4	0.6011	0.667	1.581

7p: (*S*)-4-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-3-butylcyclohex-2-en-1-one

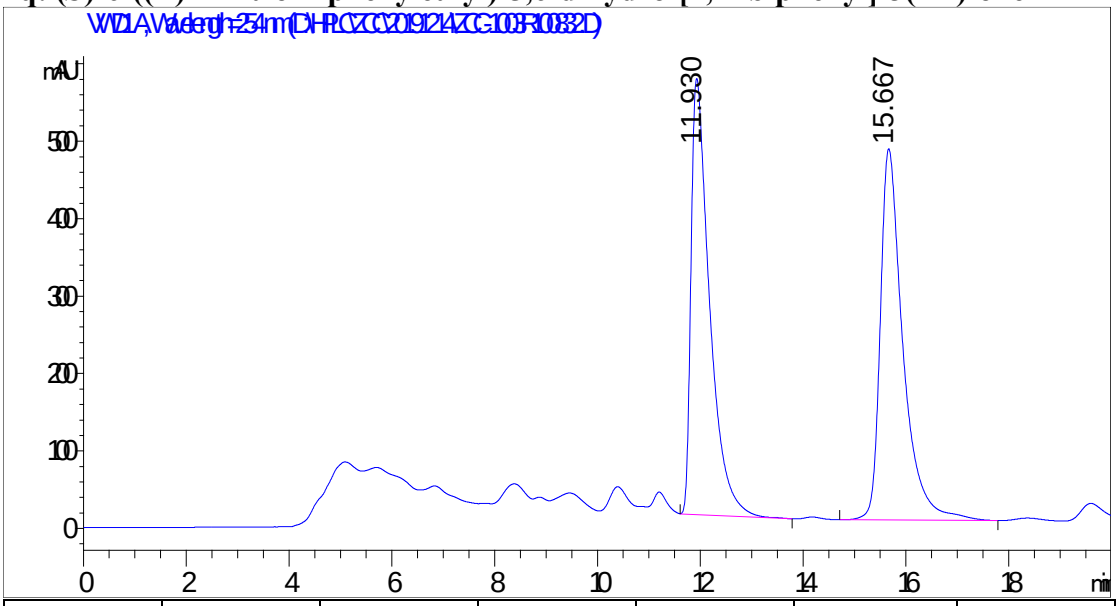


#	Time	Area	Height	Width	Symmetry	Area %
1	18.177	244.7	3.8	0.7676	0.942	0.520
2	29.869	46837.3	428.5	1.6	0.486	99.480

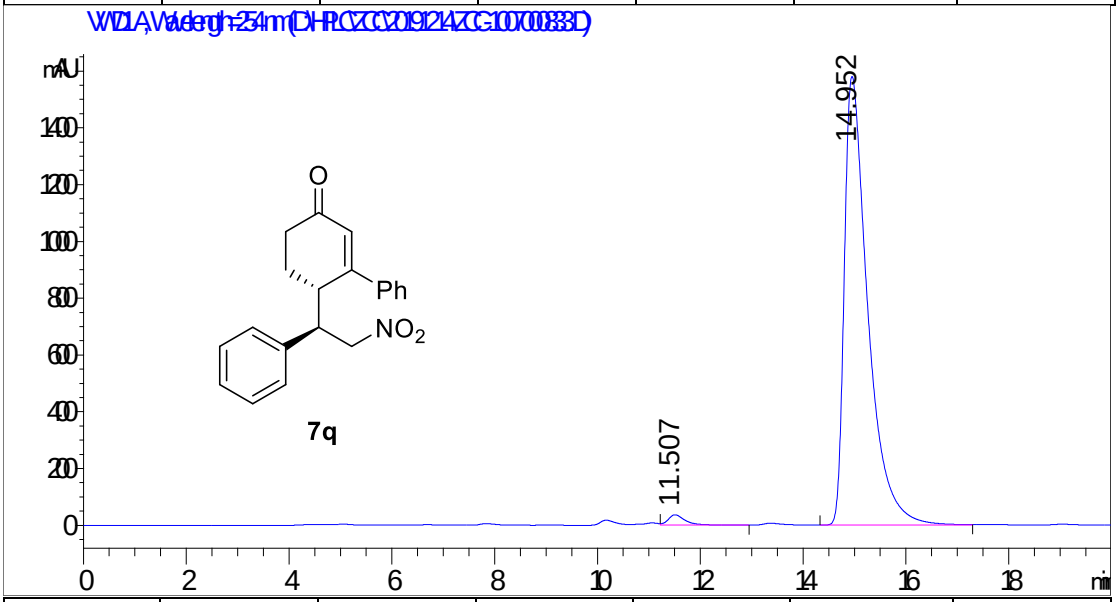


#	Time	Area	Height	Width	Symmetry	Area %
1	17.242	40067.7	599.2	0.9359	0.356	100.000

7q: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

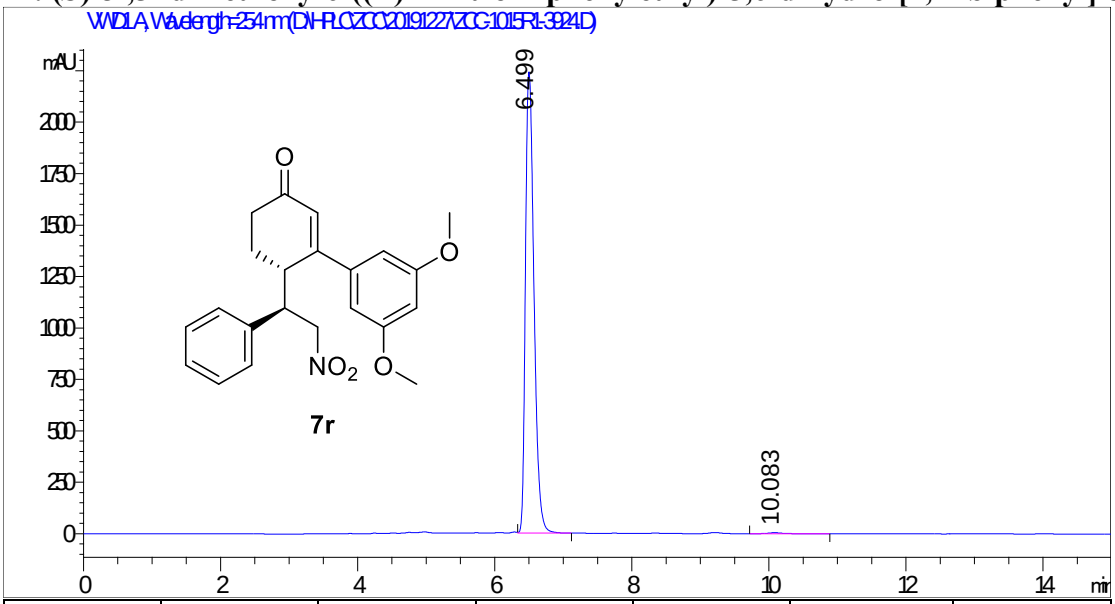


#	Time	Area	Height	Width	Symmetry	Area %
1	11.93	14121.5	563.2	0.3698	0.4	48.979
2	15.667	14710.3	479.5	0.4527	0.549	51.021

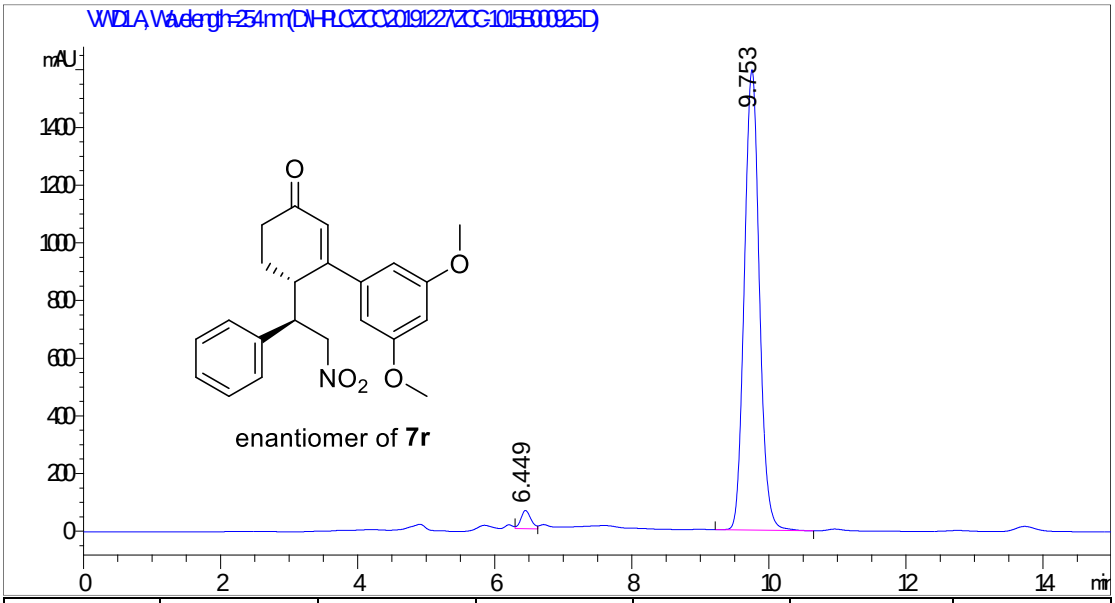


#	Time	Area	Height	Width	Symmetry	Area %
1	11.507	855.8	36.9	0.3437	0.618	1.677
2	14.952	50162.1	1580.4	0.4738	0.443	98.323

7r: (*S*)-3',5'-dimethoxy-6-((*R*)-2-nitro-1-phenylethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

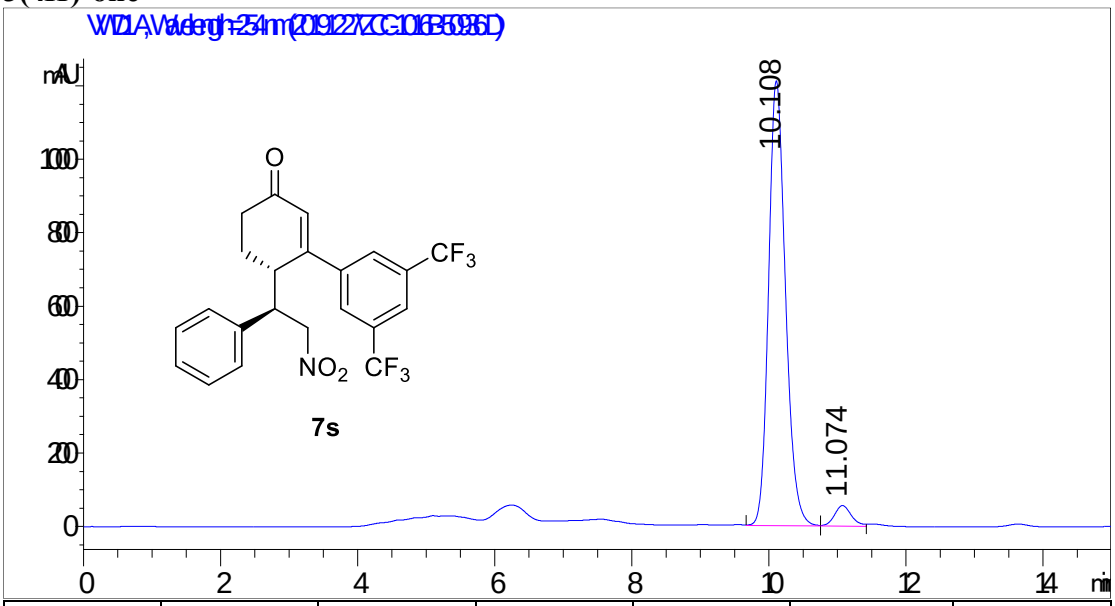


#	Time	Area	Height	Width	Symmetry	Area %
1	6.499	19385.3	2241.8	0.1344	0.648	99.543
2	10.083	89	5.2	0.247	0.675	0.457

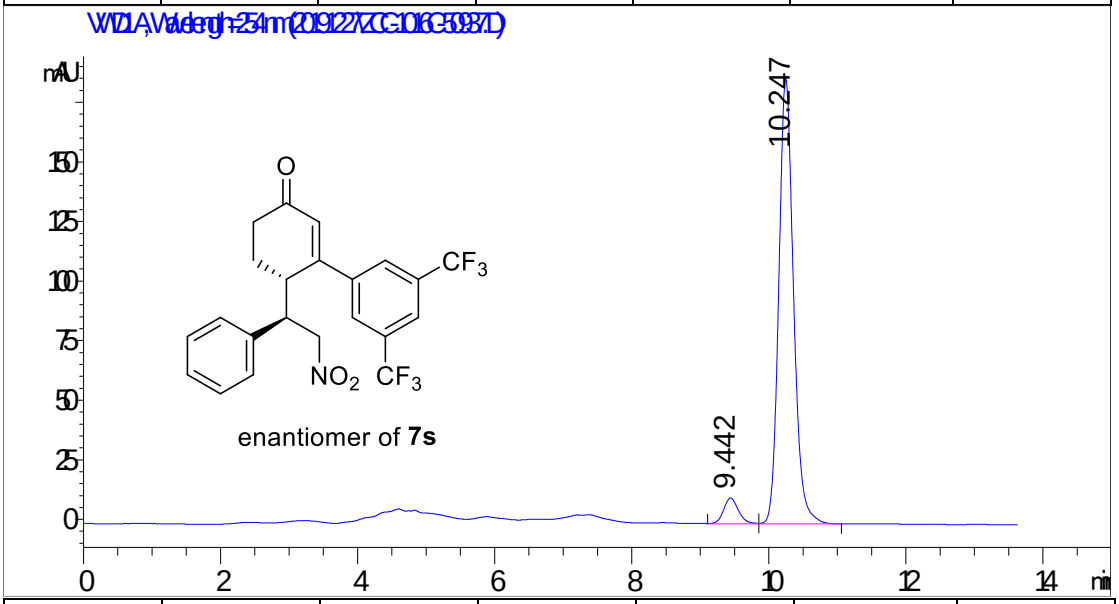


#	Time	Area	Height	Width	Symmetry	Area %
1	6.449	641.5	63.2	0.1548	0.826	2.572
2	9.753	24299.5	1595.8	0.236	0.956	97.428

7s: (*S*)-6-((*R*)-2-nitro-1-phenylethyl)-3',5'-bis(trifluoromethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

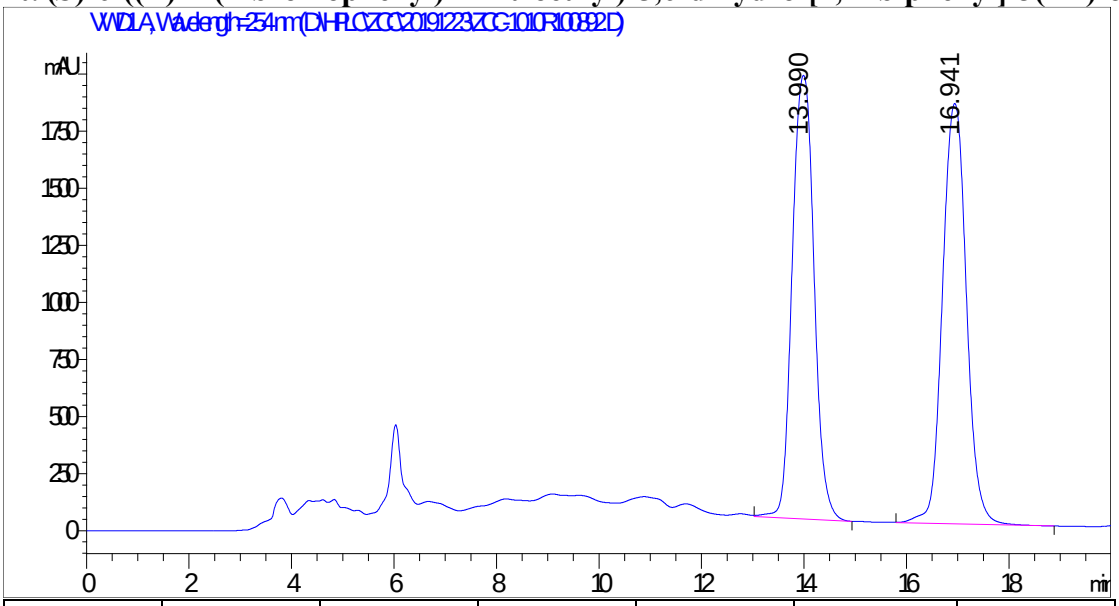


#	Time	Area	Height	Width	Symmetry	Area %
1	10.108	20792.1	1212	0.2643	0.793	95.507
2	11.074	978.1	56.3	0.2654	0.856	4.493

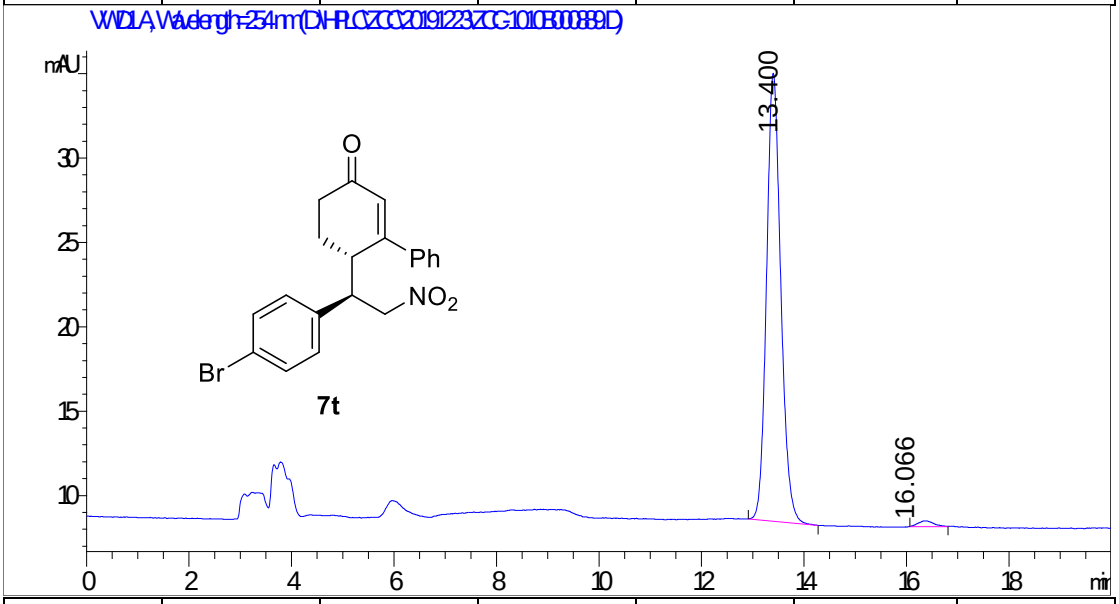


#	Time	Area	Height	Width	Symmetry	Area %
1	9.442	160.6	10.8	0.2295	0.841	5.445
2	10.247	2790	186.8	0.2297	0.833	94.555

7t: (*S*)-6-((*R*)-1-(4-bromophenyl)-2-nitroethyl)-5,6-dihydro-[1,1'-biphenyl]-3(4*H*)-one

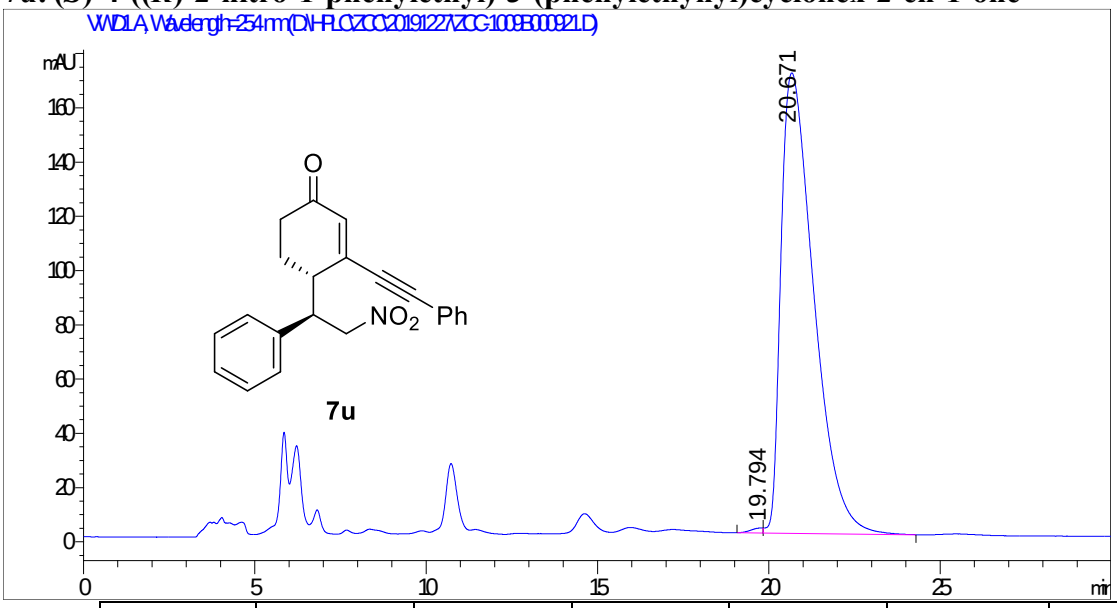


#	Time	Area	Height	Width	Symmetry	Area %
1	13.99	57537.4	1943.4	0.4722	1.01	49.074
2	16.941	59709.3	1841.9	0.5138	0.997	50.926

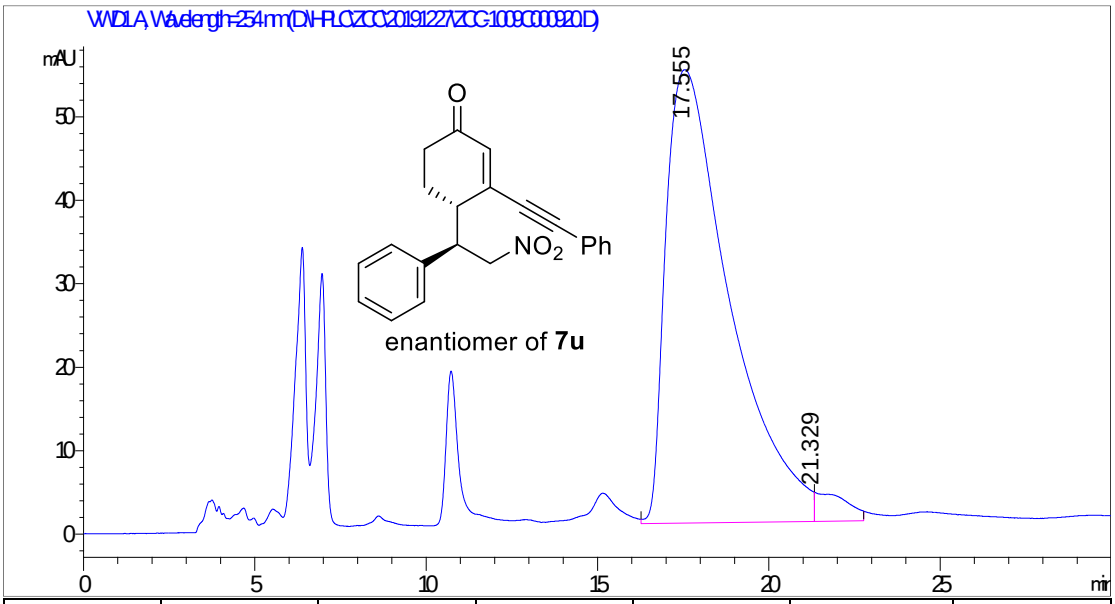


#	Time	Area	Height	Width	Symmetry	Area %
1	13.4	513.6	26.5	0.2957	0.837	98.623
2	16.066	7.2	4.7E-3	0.3495	1.063	1.377

7u: (*S*)-4-((*R*)-2-nitro-1-phenylethyl)-3-(phenylethynyl)cyclohex-2-en-1-one

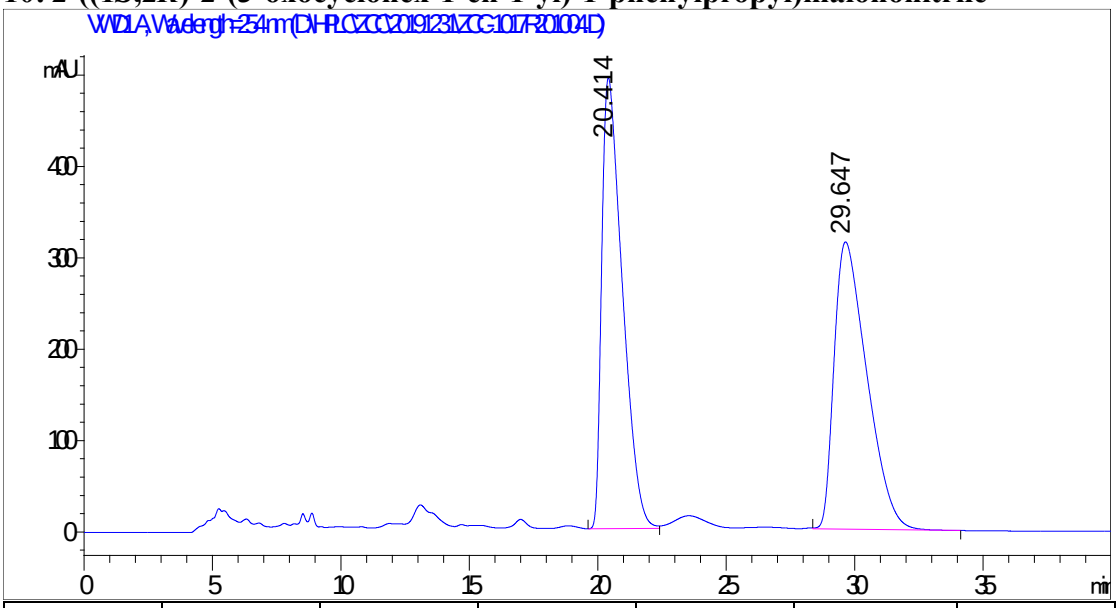


#	Time	Area	Height	Width	Symmetry	Area %
1	19.794	44.4	1.9	0.2812	8.949	0.391
2	20.671	11305.4	169.8	1.0028	0.455	99.609

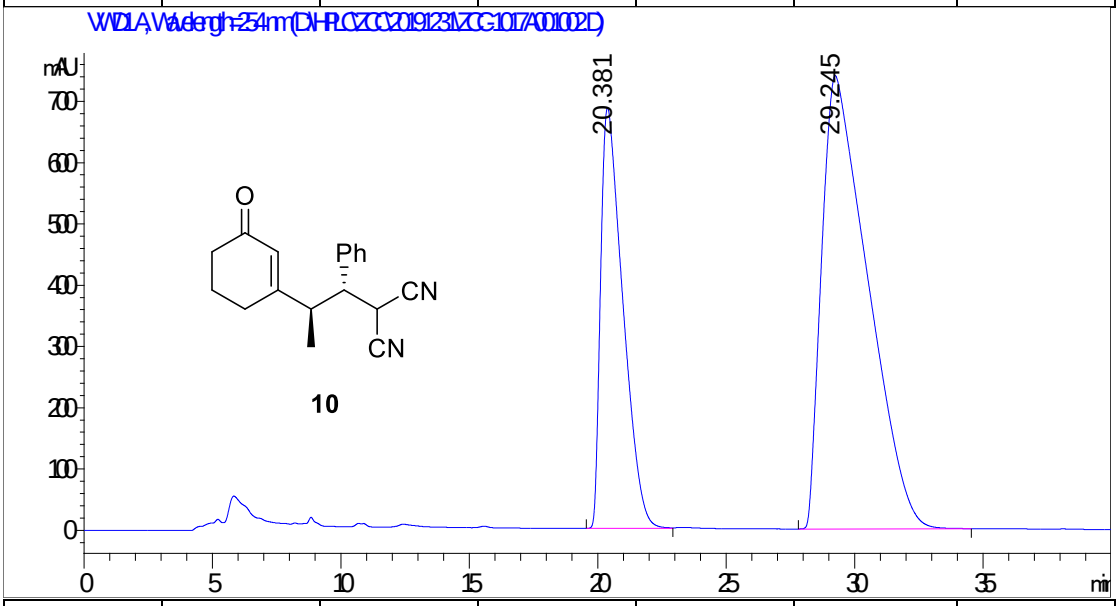


#	Time	Area	Height	Width	Symmetry	Area %
1	17.555	7043.1	54.3	2.1601	0.413	96.951
2	21.329	221.5	3.5	1.058	0	3.049

10: 2-((1*S*,2*R*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile

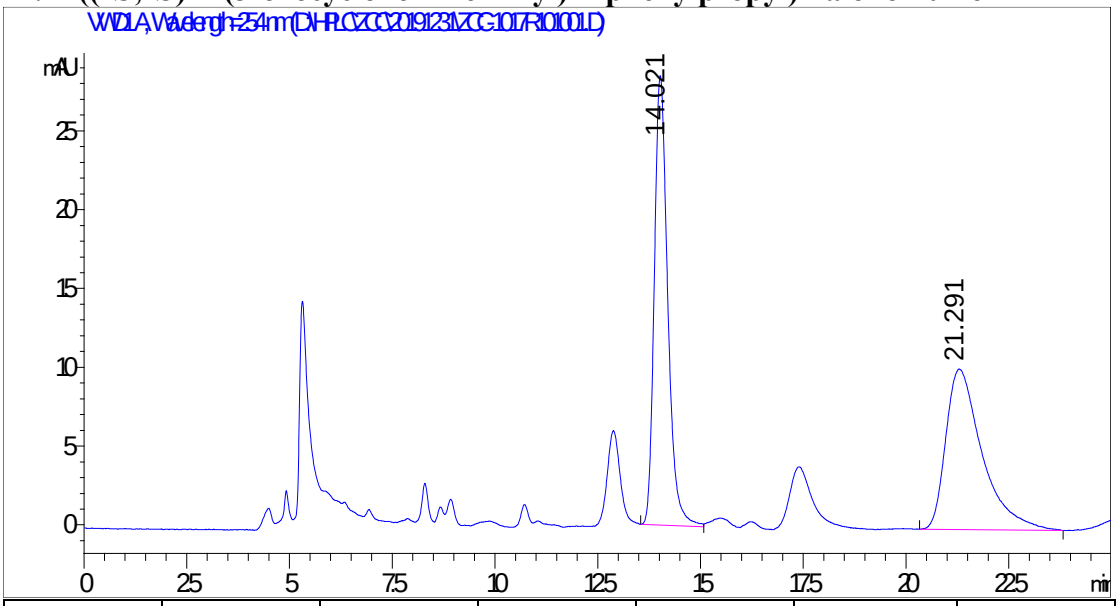


#	Time	Area	Height	Width	Symmetry	Area %
1	20.414	27558.1	493.7	0.8335	0.442	49.719
2	29.647	27869.6	314.5	1.2889	0.502	50.281

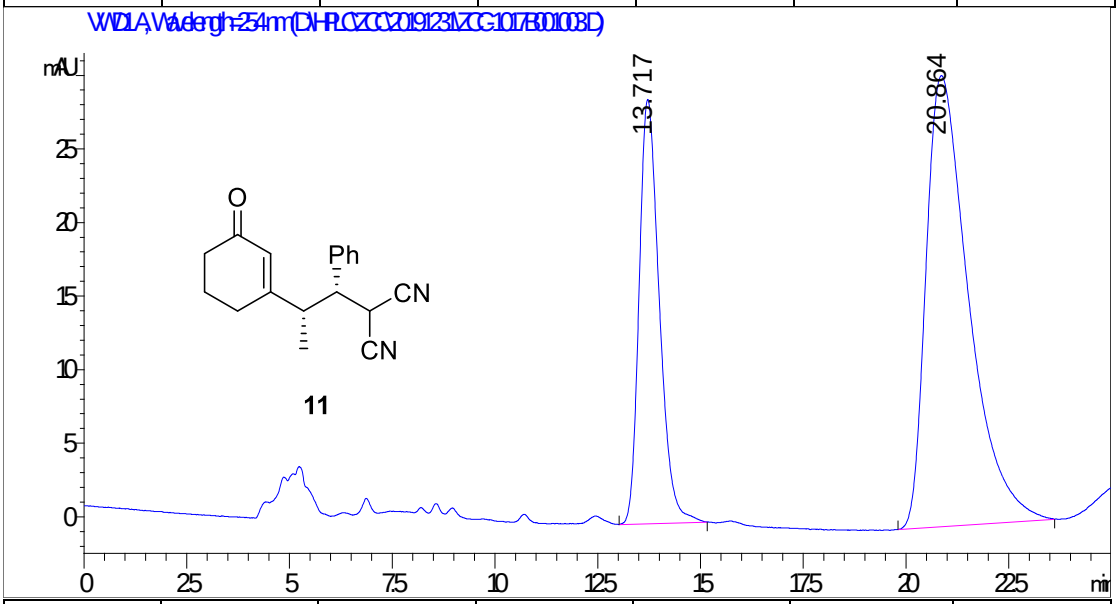


#	Time	Area	Height	Width	Symmetry	Area %
1	20.381	41314.7	686.9	0.9058	0.418	30.971
2	29.245	92081.2	739.9	1.7319	0.395	69.029

11: 2-((1*S*,2*S*)-2-(3-oxocyclohex-1-en-1-yl)-1-phenylpropyl)malononitrile

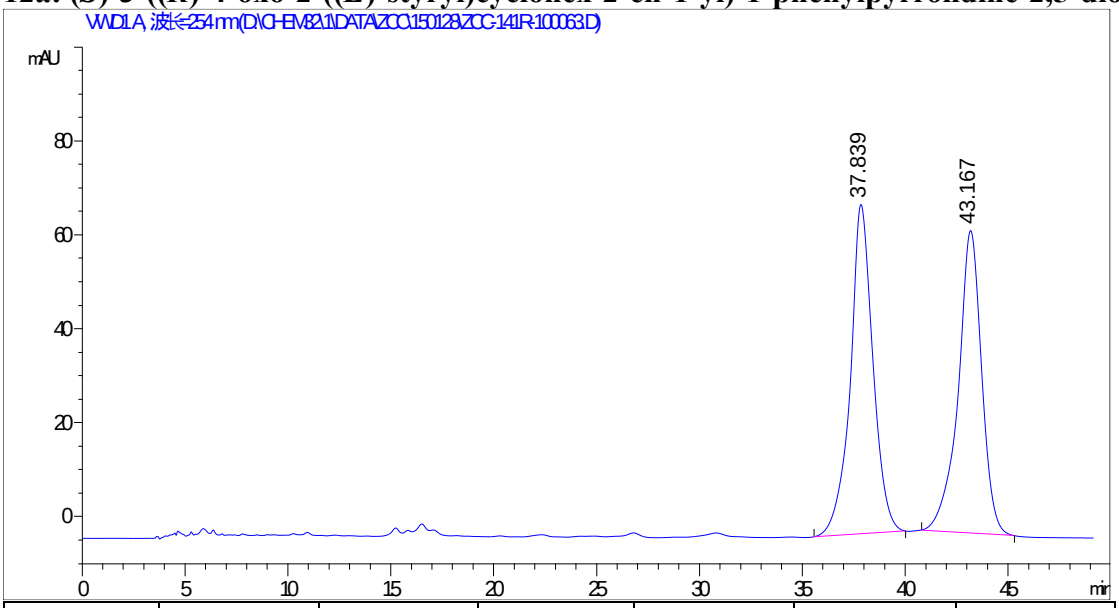


#	Time	Area	Height	Width	Symmetry	Area %
1	14.021	647	28.5	0.3463	0.735	50.889
2	21.291	624.4	10.2	0.8292	0.541	49.111

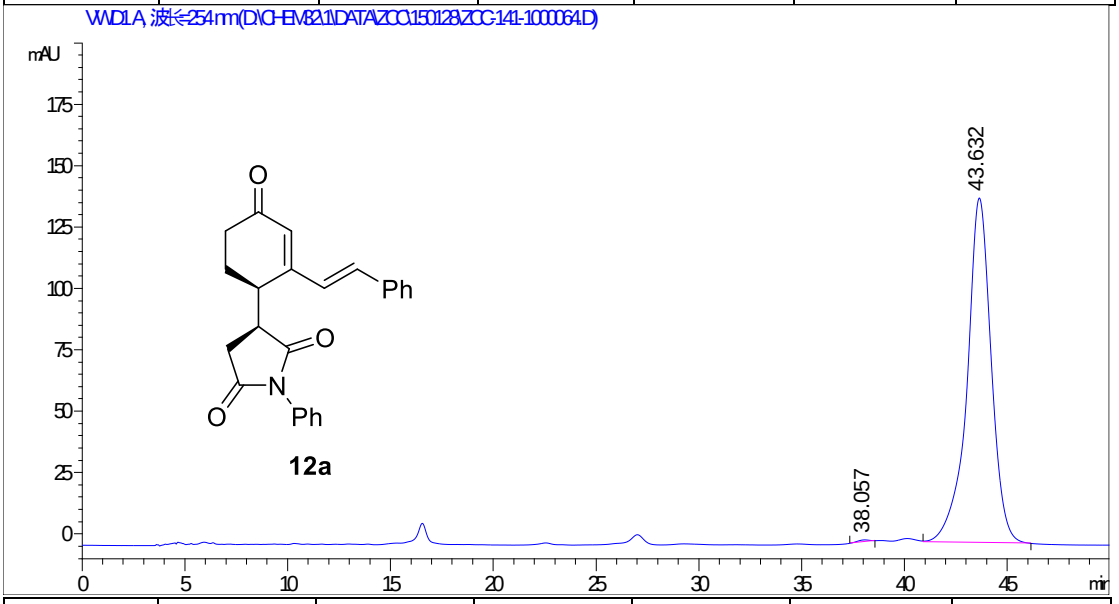


#	Time	Area	Height	Width	Symmetry	Area %
1	13.717	983.6	28.8	0.5204	0.695	30.162
2	20.864	2277.5	30.8	1.1791	0	69.838

12a: (*S*)-3-((*R*)-4-oxo-2-((*E*)-styryl)cyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione

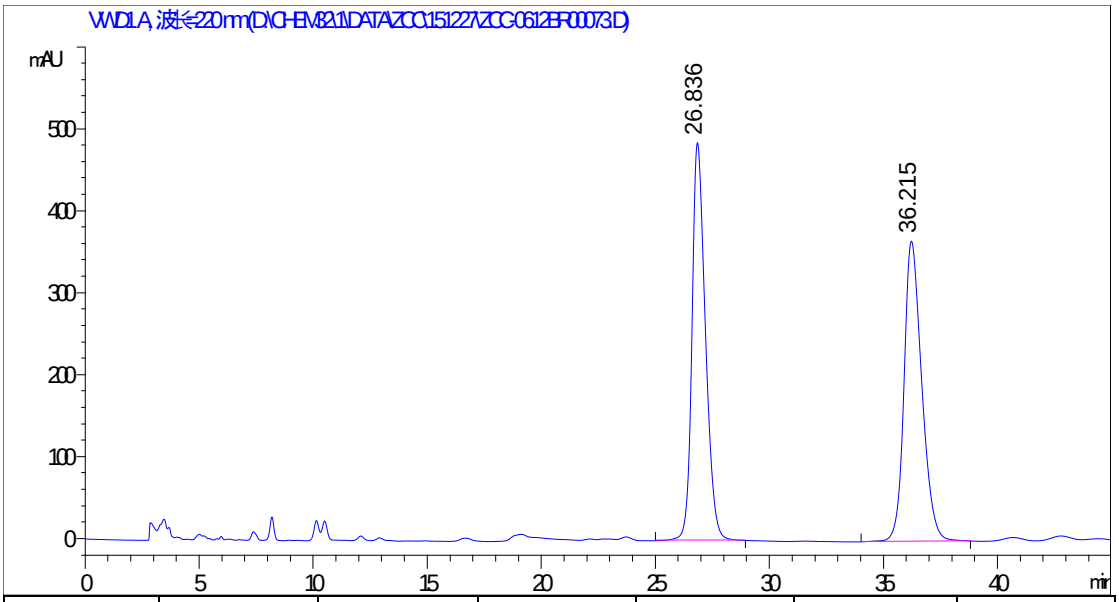


#	Time	Area	Height	Width	Symmetry	Area %
1	37.839	5377.4	70.2	1.0991	0.897	51.227
2	43.167	5119.8	64.5	1.1709	1.123	48.773

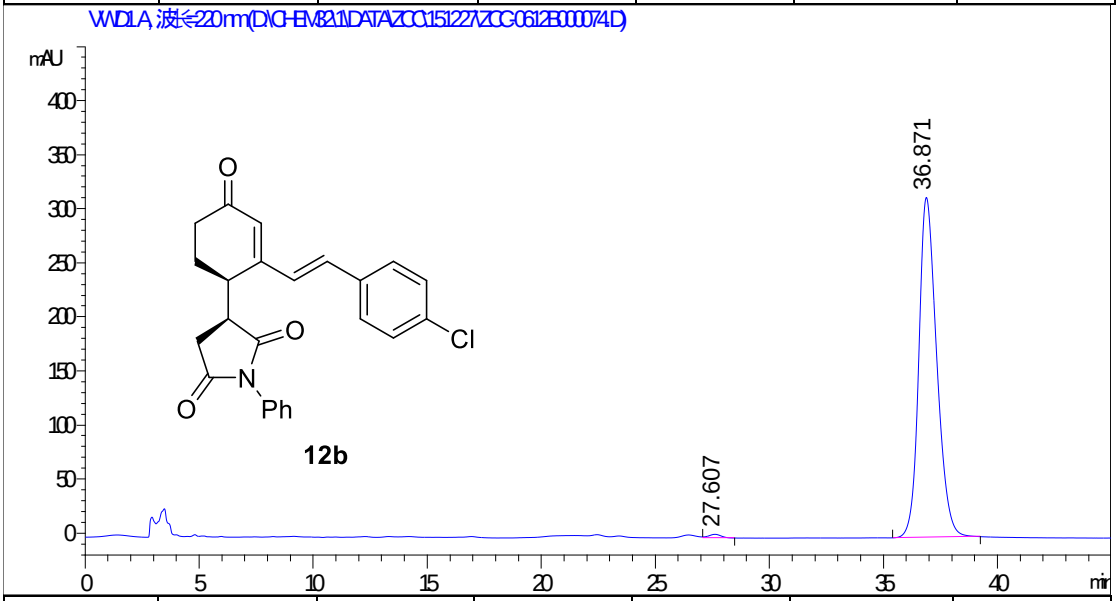


#	Time	Area	Height	Width	Symmetry	Area %
1	38.057	39.3	8.8E-1	0.7473	1.645	0.342
2	43.632	11473	140.4	1.2085	1.039	99.658

12b: (*S*)-3-((*R*)-2-((*E*)-4-chlorostyryl)-4-oxocyclohex-2-en-1-yl)-1-phenylpyrrolidine-2,5-dione

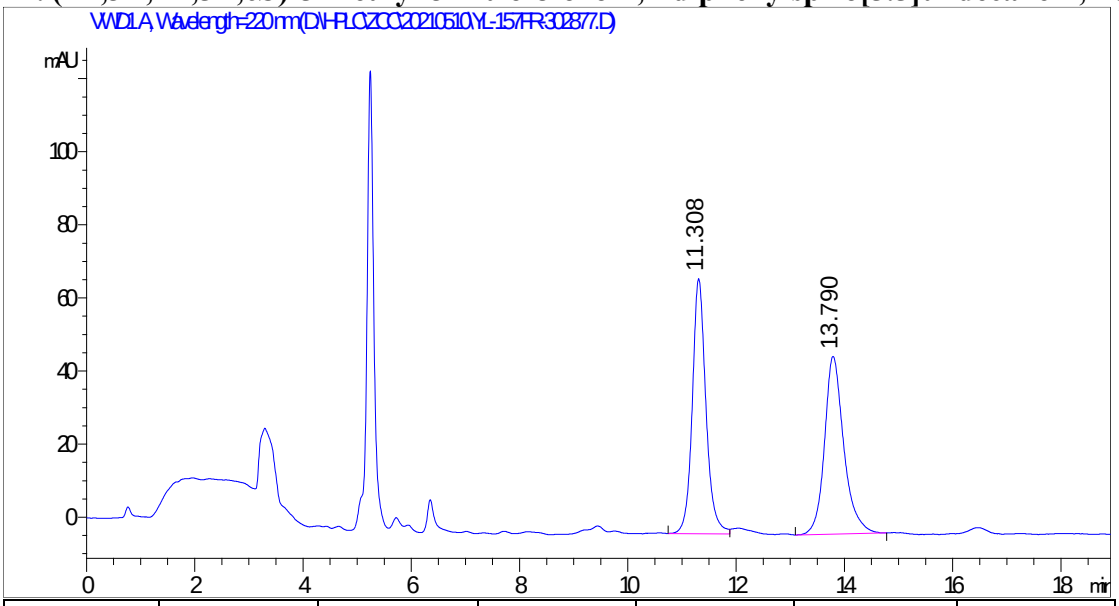


#	Time	Area	Height	Width	Symmetry	Area %
1	26.836	19961.9	485.6	0.6238	0.666	50.141
2	36.215	19849.7	366.5	0.8212	0.688	49.859

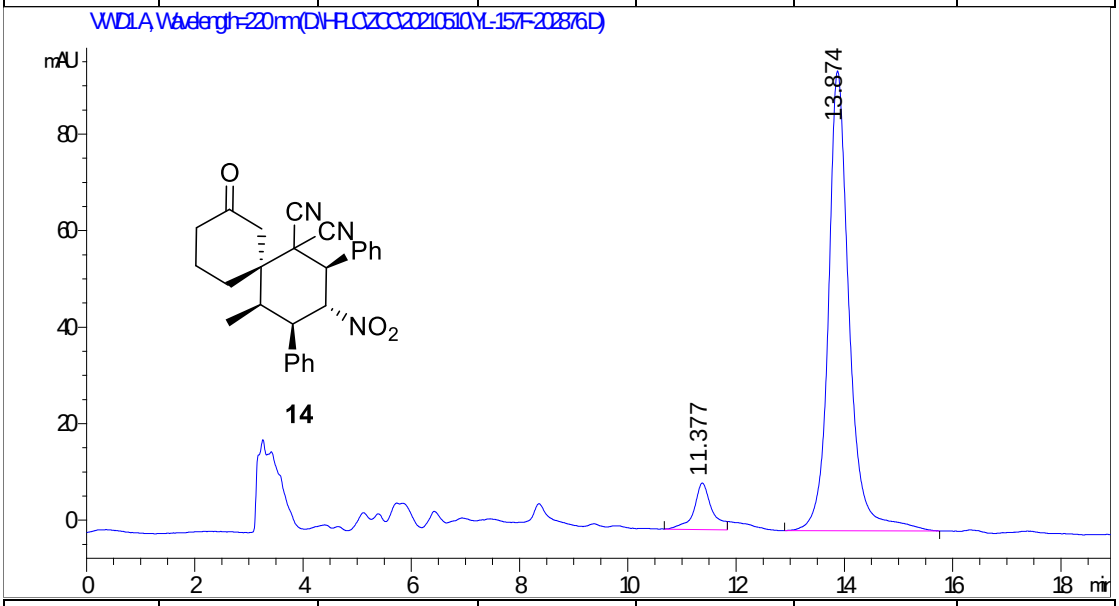


#	Time	Area	Height	Width	Symmetry	Area %
1	27.607	131.5	3.4	0.5592	1.048	0.760
2	36.871	17165	314.5	0.8319	0.702	99.240

14: (2*R*,3*R*,4*R*,5*R*,6*S*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile

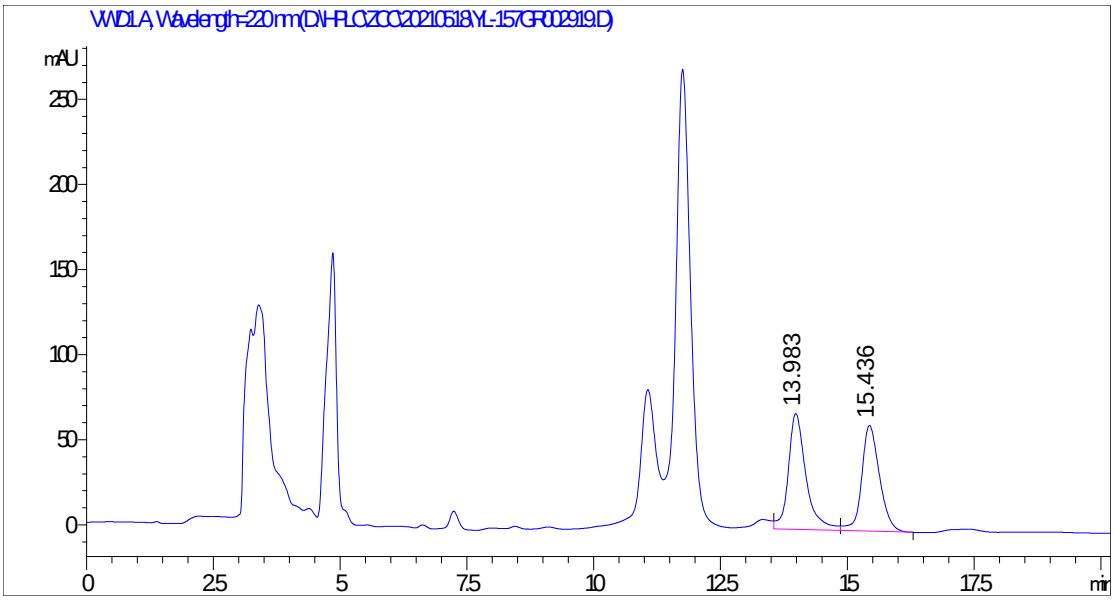


#	Time	Area	Height	Width	Symmetry	Area %
1	11.308	1224	69.8	0.2658	0.83	50.388
2	13.79	1205.2	48.6	0.3721	0.755	49.612

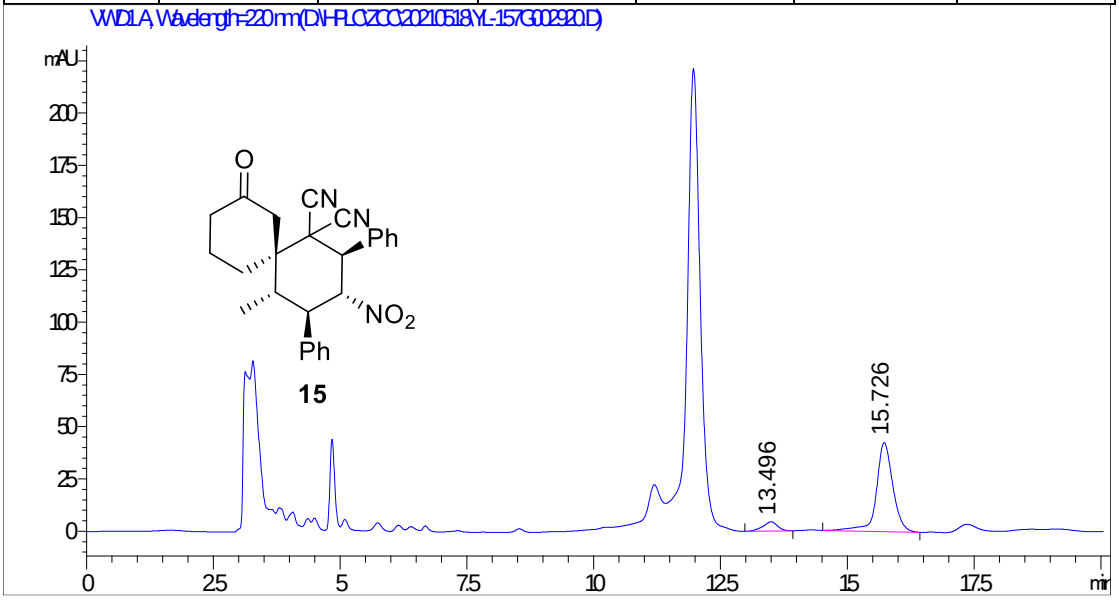


#	Time	Area	Height	Width	Symmetry	Area %
1	11.377	221	9.6	0.3299	0.89	7.974
2	13.874	2550	95.3	0.3967	0.736	92.026

15: (2*R*,3*R*,4*R*,5*S*,6*R*)-5-methyl-3-nitro-8-oxo-2,4-diphenylspiro[5.5]undecane-1,1-dicarbonitrile

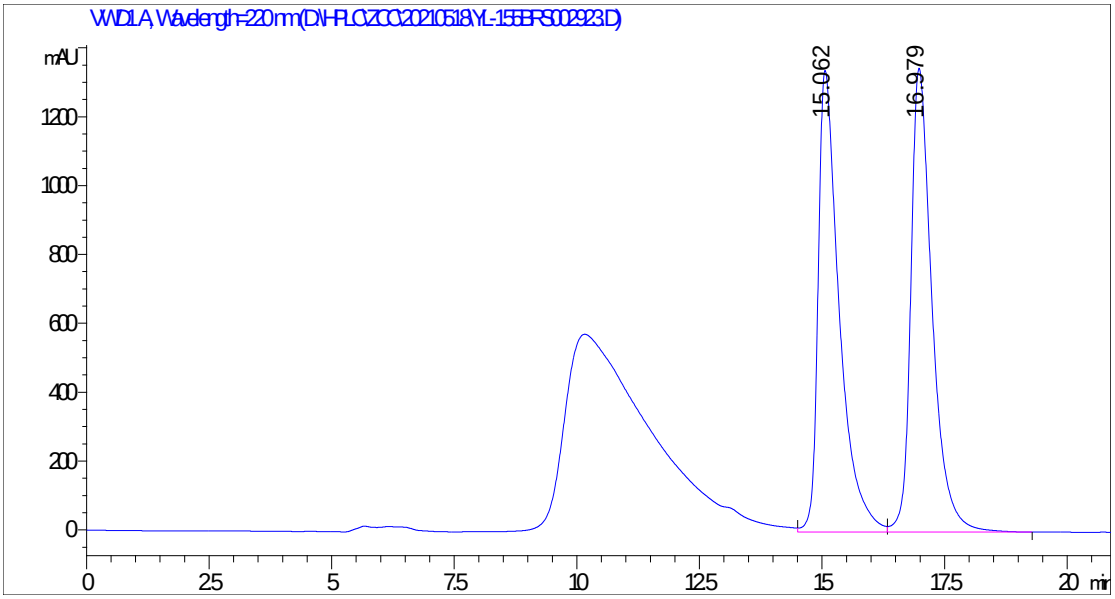


#	Time	Area	Height	Width	Symmetry	Area %
1	13.983	1655.7	68.1	0.3622	0.685	52.061
2	15.436	1524.7	62.2	0.3721	0.761	47.939

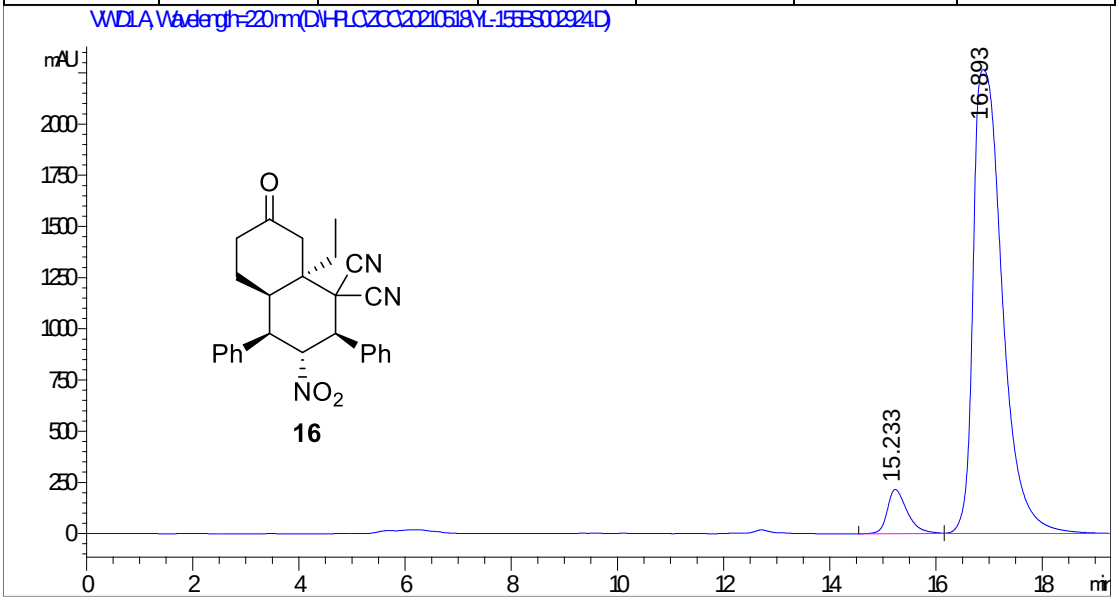


#	Time	Area	Height	Width	Symmetry	Area %
1	13.496	89.1	4.4	0.2931	1.254	8.490
2	15.726	960	42.5	0.3377	0.907	91.510

16:(2*R*,3*R*,4*R*,4a*R*,8a*R*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile

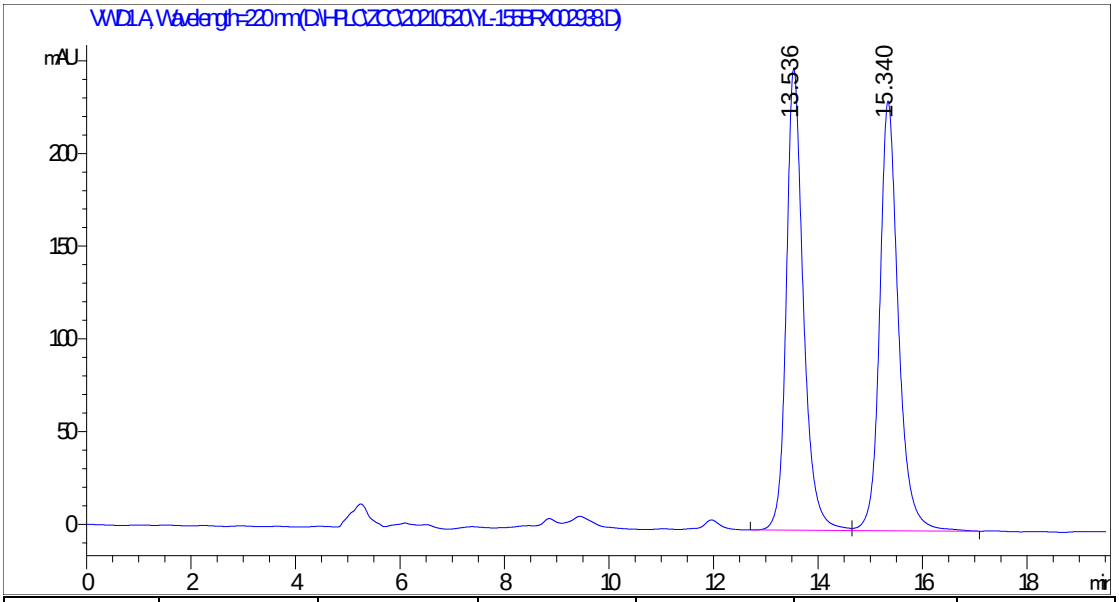


#	Time	Area	Height	Width	Symmetry	Area %
1	15.062	40246.7	1340.2	0.4437	0.456	49.703
2	16.979	40728.1	1346.9	0.4548	0.594	50.297

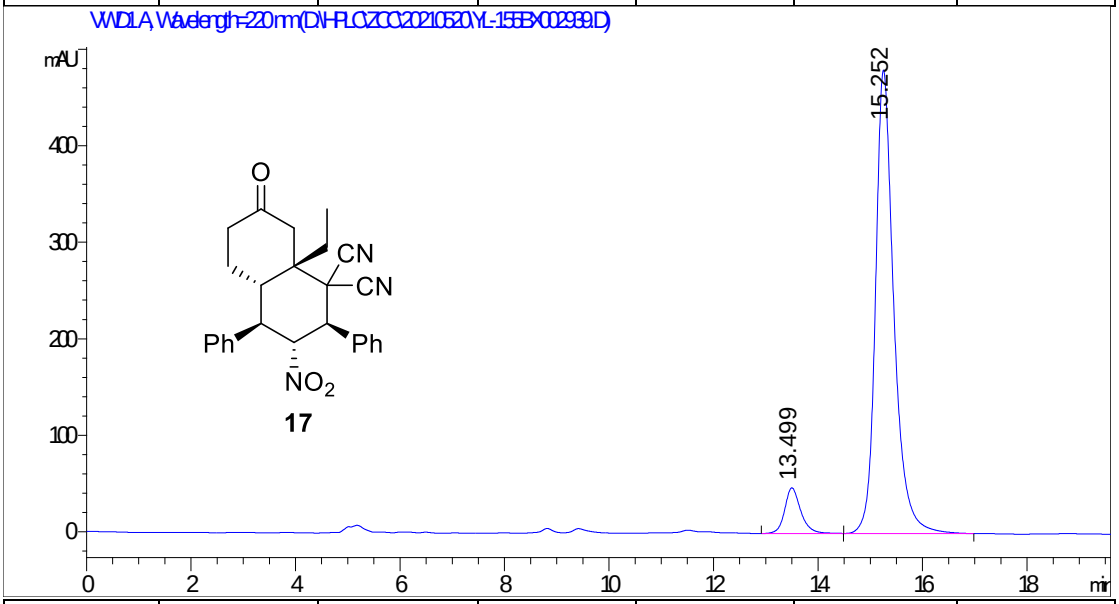


#	Time	Area	Height	Width	Symmetry	Area %
1	15.233	5641.9	216.6	0.3928	0.625	6.126
2	16.893	86461.2	2265.4	0.5881	0.506	93.874

17: (2*R*,3*R*,4*R*,4a*S*,8a*S*)-8a-ethyl-3-nitro-7-oxo-2,4-diphenyloctahydronaphthalene-1,1(2*H*)-dicarbonitrile



#	Time	Area	Height	Width	Symmetry	Area %
1	13.536	5655.4	249.2	0.3406	0.732	49.529
2	15.34	5762.9	231.7	0.3733	0.765	50.471

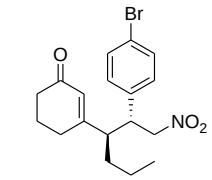


#	Time	Area	Height	Width	Symmetry	Area %
1	13.499	1012.9	47.3	0.3225	0.768	7.952
2	15.252	11725.5	480.4	0.3635	0.712	92.048

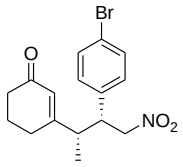
G: Determination of Absolute Configuration

The absolute configuration of compound **4p** (CCDC 1957050), **5f** (CCDC 1957048), **6p** (CCDC 1957049), **7p** (CCDC 1957051), **12b** (CDCC 1978462), **14** (CDCC 1978463) and **16** (CDCC 1978464) were unambiguously assigned by single crystal X-ray analysis.

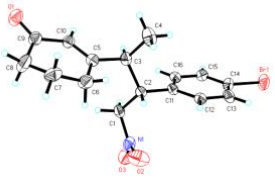
CCDC 1957050



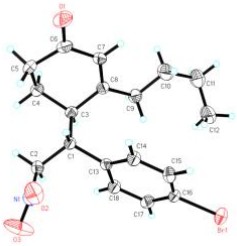
4p



5f



CCDC 1957048



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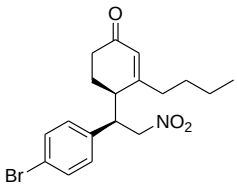
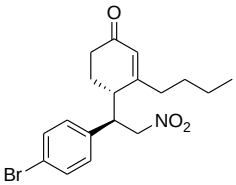
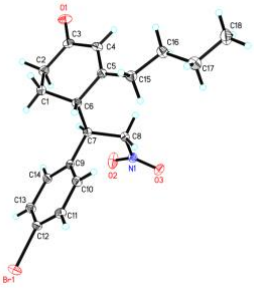


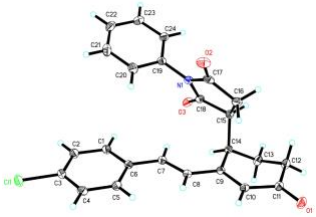
6p



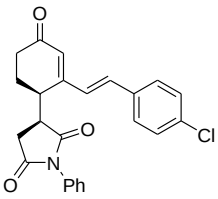
7p



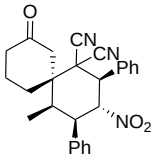
CCDC 1957051



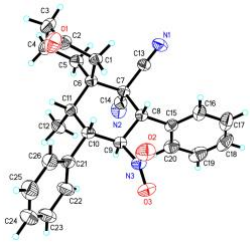
CCDC 1978462



12b



14



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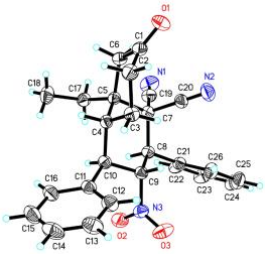

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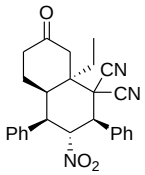


16

Crystal data and structure refinement for **4p** (CCDC 1957050)

Identification code	**4p**	
Empirical formula	$C_{18}H_{22}BrNO_3$	
Formula weight	380.27	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.9889(10) Å	a= 90°.
	b = 10.1859(11) Å	b= 90°.
	c = 20.073(2) Å	g = 90°.
Volume	1837.9(3) $Å^3$	
Z	4	
Density (calculated)	1.374 Mg/m^3	
Absorption coefficient	2.250 mm^{-1}	
F(000)	784	
Crystal size	0.211 x 0.175 x 0.123 mm^3	
Theta range for data collection	2.029 to 25.999°.	
Index ranges	-11<=h<=9, -12<=k<=11, -24<=l<=20	
Reflections collected	11129	
Independent reflections	3617 [R(int) = 0.0387]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3617 / 36 / 242	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.0934	
R indices (all data)	R1 = 0.0626, wR2 = 0.1018	
Absolute structure parameter	0.005(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.407 and -0.223 e.$Å^{-3}$	

Crystal data and structure refinement for **5f** (CCDC 1957048)

Identification code	**5f**
Empirical formula	$C_{16}H_{18}BrNO_3$
Formula weight	352.22
Temperature	293(2) K

Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.4827(10) Å	a= 90°.
	b = 10.4094(12) Å	b= 90°.
	c = 17.8022(19) Å	g = 90°.
Volume	1571.9(3) $Å^3$	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	2.624 mm^{-1}	
F(000)	720	
Crystal size	0.211 x 0.175 x 0.123 mm^3	
Theta range for data collection	2.266 to 25.997°.	
Index ranges	-9<=h<=10, -12<=k<=12, -21<=l<=16	
Reflections collected	9482	
Independent reflections	3090 [R(int) = 0.0523]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5346	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3090 / 1 / 192	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0811	
R indices (all data)	R1 = 0.0488, wR2 = 0.0863	
Absolute structure parameter	0.016(9)	
Extinction coefficient	0.0097(14)	
Largest diff. peak and hole	0.238 and -0.292 $e.Å^{-3}$	

Crystal data and structure refinement for **6p** (CCDC 1957049)

Identification code	**6p**	
Empirical formula	$C_{18}H_{22}BrNO_3$	
Formula weight	380.27	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.5022(3) Å	α = 90°.
	b = 7.3534(2) Å	β = 101.5450(10)°.

	c = 11.4093(3) Å γ = 90°.
Volume	863.28(4) Å^3
Z	2
Density (calculated)	1.463 Mg/m^3
Absorption coefficient	2.395 mm^{-1}
F(000)	392
Crystal size	0.180 x 0.150 x 0.120 mm^3
Theta range for data collection	2.947 to 25.992°.
Index ranges	-12<=h<=12, -8<=k<=9, -14<=l<=14
Reflections collected	14120
Independent reflections	3291 [R(int) = 0.0364]
Completeness to theta = 25.242°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.4350
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3291 / 1 / 210
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0232, wR2 = 0.0563
R indices (all data)	R1 = 0.0244, wR2 = 0.0568
Absolute structure parameter	0.032(5)
Largest diff. peak and hole	0.387 and -0.391 e.Å^{-3}

Crystal data and structure refinement for **7p** (CCDC 1957051)

Identification code	**7p**
Empirical formula	$C_{18}H_{22}BrNO_3$
Formula weight	380.27
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 5.5537(11) Å α = 90°.
	b = 10.753(2) Å β = 90°.
	c = 29.963(5) Å γ = 90°.
Volume	1789.3(6) Å^3
Z	4
Density (calculated)	1.412 Mg/m^3
Absorption coefficient	2.311 mm^{-1}

F(000)	784
Crystal size	0.200 x 0.160 x 0.120 mm^3
Theta range for data collection	1.359 to 25.494°.
Index ranges	-6<=h<=6, -13<=k<=12, -36<=l<=31
Reflections collected	10277
Independent reflections	3326 [R(int) = 0.0498]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5127
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3326 / 40 / 228
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0927
R indices (all data)	R1 = 0.0594, wR2 = 0.1000
Absolute structure parameter	0.020(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.421 and -0.297 e.$Å^{-3}$

Crystal data and structure refinement for **12b** (CCDC 1978462)

Identification code	**12b**	
Empirical formula	$C_{24}H_{20}ClNO_3$	
Formula weight	405.86	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.9525(7) Å	a= 90°.
	b = 13.3638(9) Å	b= 90°.
	c = 13.3808(9) Å	γ = 90°.
Volume	1958.5(2) $Å^3$	
Z	4	
Density (calculated)	1.376 Mg/m^3	
Absorption coefficient	0.221 mm^{-1}	
F(000)	848	
Crystal size	0.35 x 0.3 x 0.22 mm^3	
Theta range for data collection	2.154 to 30.543°.	
Index ranges	-15<=h<=15, -17<=k<=19, -19<=l<=18	
Reflections collected	19828	

Independent reflections	5979 [R(int) = 0.0274]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6990
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5979 / 0 / 262
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0836
R indices (all data)	R1 = 0.0430, wR2 = 0.0876
Absolute structure parameter	0.012(18)
Extinction coefficient	n/a
Largest diff. peak and hole	0.228 and -0.236 e.$Å^{-3}$

Crystal data and structure refinement for **14** (CCDC 1978463)

Identification code	**14**	
Empirical formula	C_{26} H_{25} N_3 O_3	
Formula weight	427.49	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.56750(10) Å	a= 90°.
	b = 28.7020(6) Å	b= 99.5090(10)°.
	c = 12.4932(3) Å	γ = 90°.
Volume	2322.61(8) $Å^3$	
Z	4	
Density (calculated)	1.223 Mg/m^3	
Absorption coefficient	0.652 mm^{-1}	
F(000)	904	
Crystal size	0.200 x 0.140 x 0.100 mm^3	
Theta range for data collection	3.904 to 67.466°.	
Index ranges	-7<=h<=7, -34<=k<=34, -14<=l<=14	
Reflections collected	31317	
Independent reflections	4115 [R(int) = 0.0595]	
Completeness to theta = 67.679°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6132	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4115 / 1 / 291
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1129
R indices (all data)	R1 = 0.0543, wR2 = 0.1208
Extinction coefficient	0.0066(10)
Largest diff. peak and hole	0.171 and -0.136 e.Å^{-3}

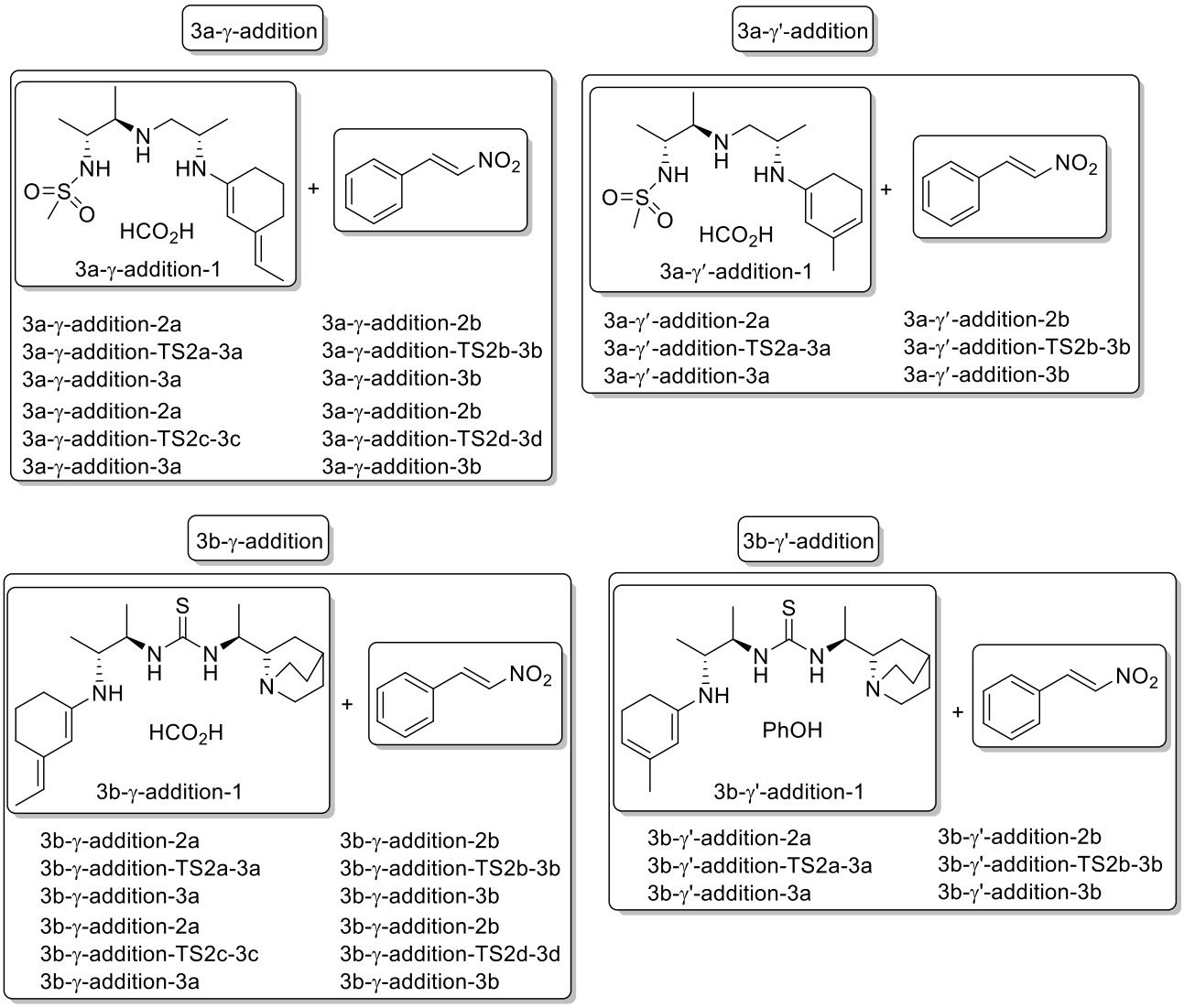
Crystal data and structure refinement for **16** (CCDC 1978464)

Identification code	**16**	
Empirical formula	C_{28} H_{28} N_4 O_3	
Formula weight	468.54	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Hexagonal	
Space group	P 63	
Unit cell dimensions	a = 24.6130(6) Å	a= 90°.
	b = 24.6130(6) Å	b= 90°.
	c = 8.0200(2) Å	γ = 120°.
Volume	4207.6(2) Å^3	
Z	6	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.590 mm^{-1}	
F(000)	1488	
Crystal size	0.200 x 0.160 x 0.120 mm^3	
Theta range for data collection	5.491 to 66.976°.	
Index ranges	-29<=h<=27, -28<=k<=28, -8<=l<=9	
Reflections collected	69597	
Independent reflections	4925 [R(int) = 0.0583]	
Completeness to theta = 67.679°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.5333	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4925 / 1 / 319	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0939	
R indices (all data)	R1 = 0.0388, wR2 = 0.0956	
Absolute structure parameter	0.04(8)	
Extinction coefficient	0.0045(5)	
Largest diff. peak and hole	0.129 and -0.135 e.Å^{-3}	

H. DFT Calculations details

To make the calculation more efficiently, the reaction models were simplified and named as followings:

Simplified reaction models



All the structure were optimized with the Gaussian 09 program using the M06-2X functional together with the 6-31+G(d) basis set, the –D3 dispersion correction, and the SMD continuum solvent model with parameters for toluene, followed by frequency calculations at the same level of theory. Gas-phase single point energy calculations at these optimized structures were performed using M06-2X-D3 and the larger 6-311+G(2d,p) basis set. Combining the gas-phase 6-31+G(d) and 6-311+G(2d,p) electronic energies, the SMD-corrected 6-31+G(d) energy, and the free-energy correction yields the solution-phase free energies that were used to compare the various reaction pathways. That is, the relative free energy was calculated using the following equation:

$$\Delta G_A = \Delta E^{elec} + \Delta E^{thermal} - T\Delta S \ + \Delta G^{solv}$$

where ΔG is the free energy change relative to the separated reactants for species A; ΔE^{elec} is the total electronic energy change in vacuum; $\Delta E^{thermal}$ is the total internal thermal energy change including the

contributions due to translation, rotational, and vibrational motions; ΔS is the total solute entropy change; and ΔG^{solv} is the solvation free energy change in a specific solvent. Unless we specify otherwise, the Gibbs freen energy should be taken as referring to combination of the single-point electronic energies at M06-2X-D3/6-311+G(2d,p) level of theory and the SMD solvation free energies and the vibrational free-energy corrections at M06-2X-D3/6-31+G(d) level.

Gaussian 09, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

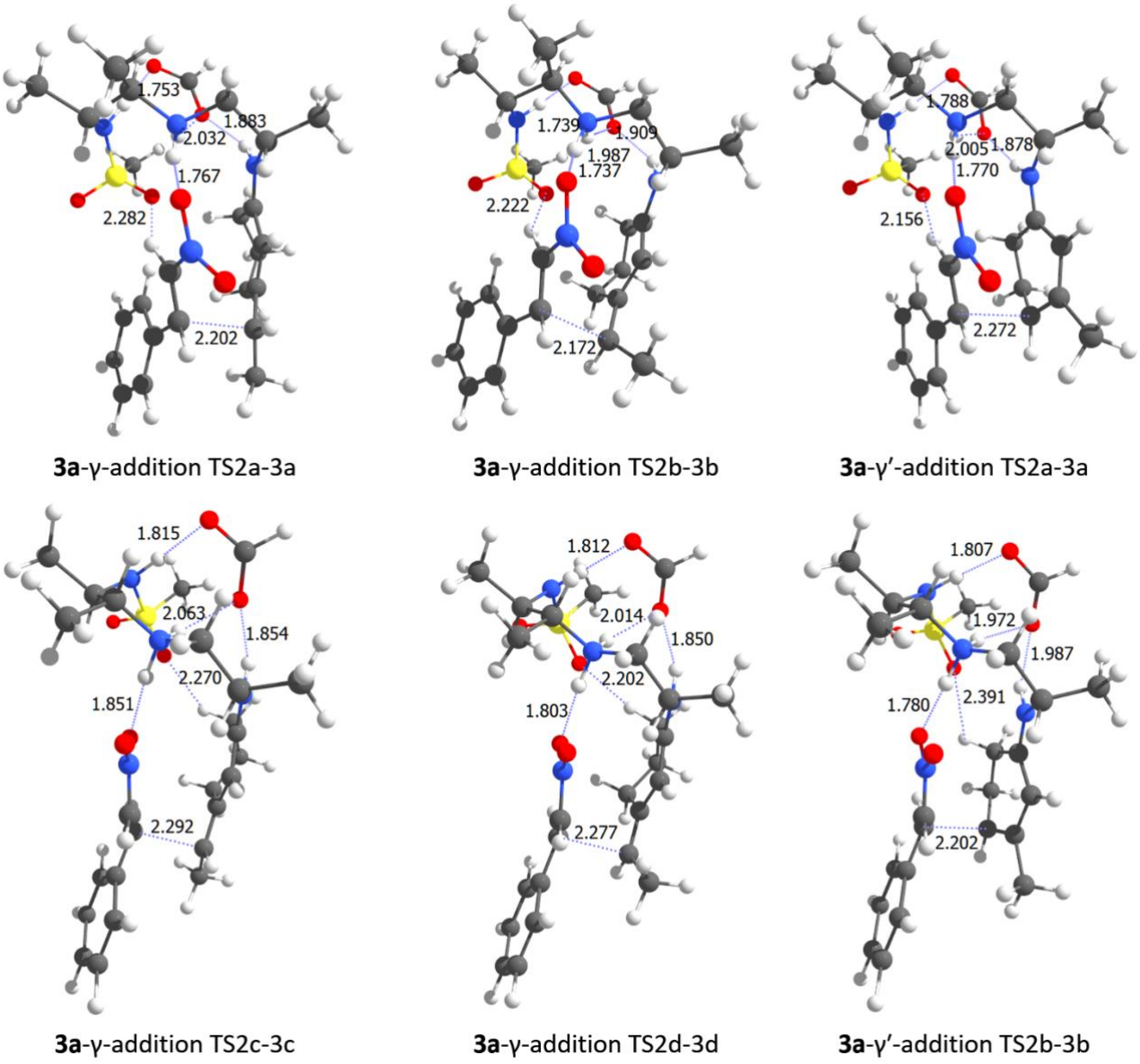
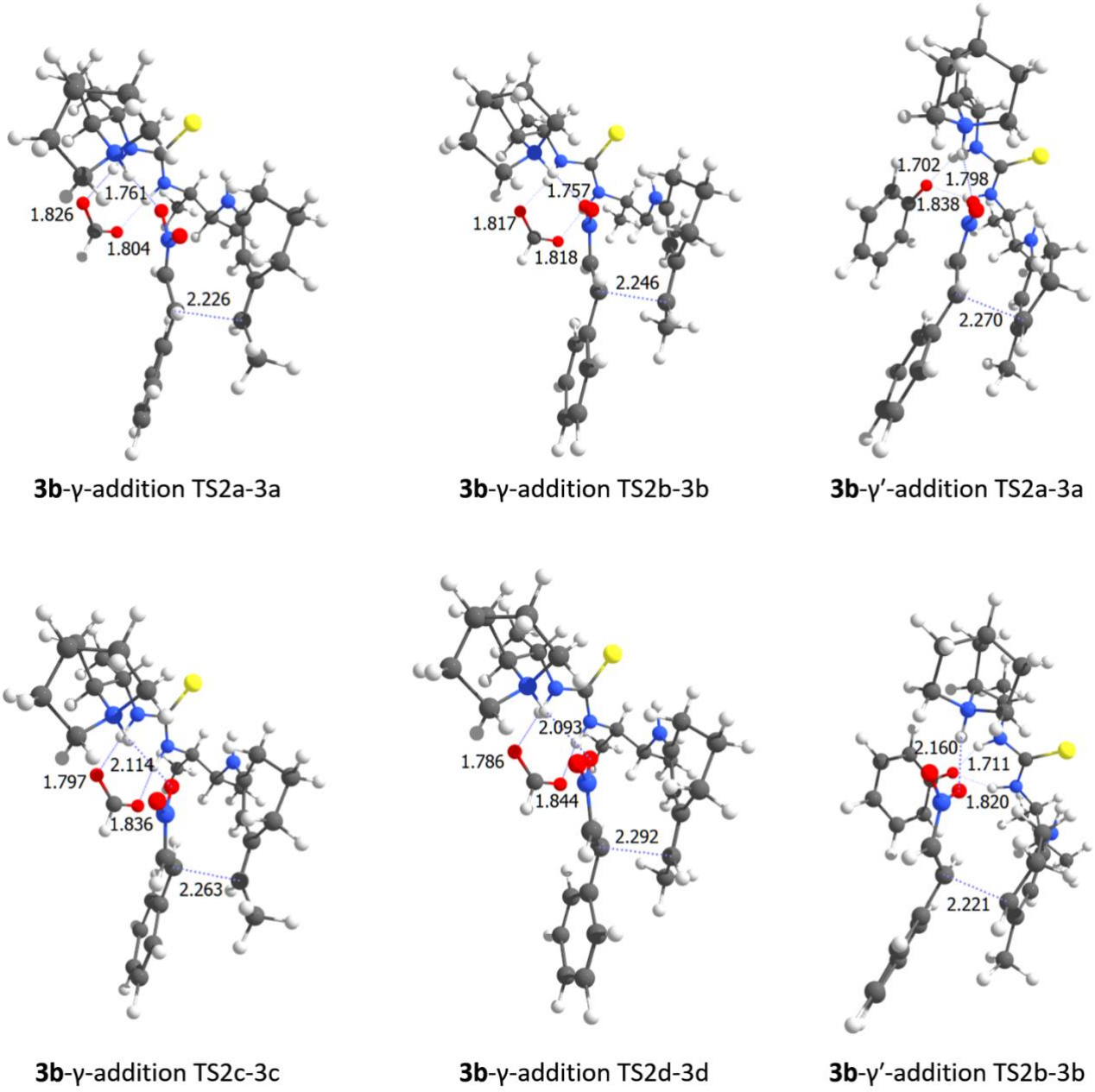


Figure S7. Optimized geometries of the transition states for 3a-γ/γ′-addition. The bond lengths are in angstrom.



3b-γ-addition TS2a-3a | **3b**-γ-addition TS2b-3b | **3b**-γ′-addition TS2a-3a

3b-γ-addition TS2c-3c | **3b**-γ-addition TS2d-3d | **3b**-γ′-addition TS2b-3b

Figure S8. Optimized geometries of the transition states for 3b-γ/γ′-addition. The bond lengths are in angstrom.

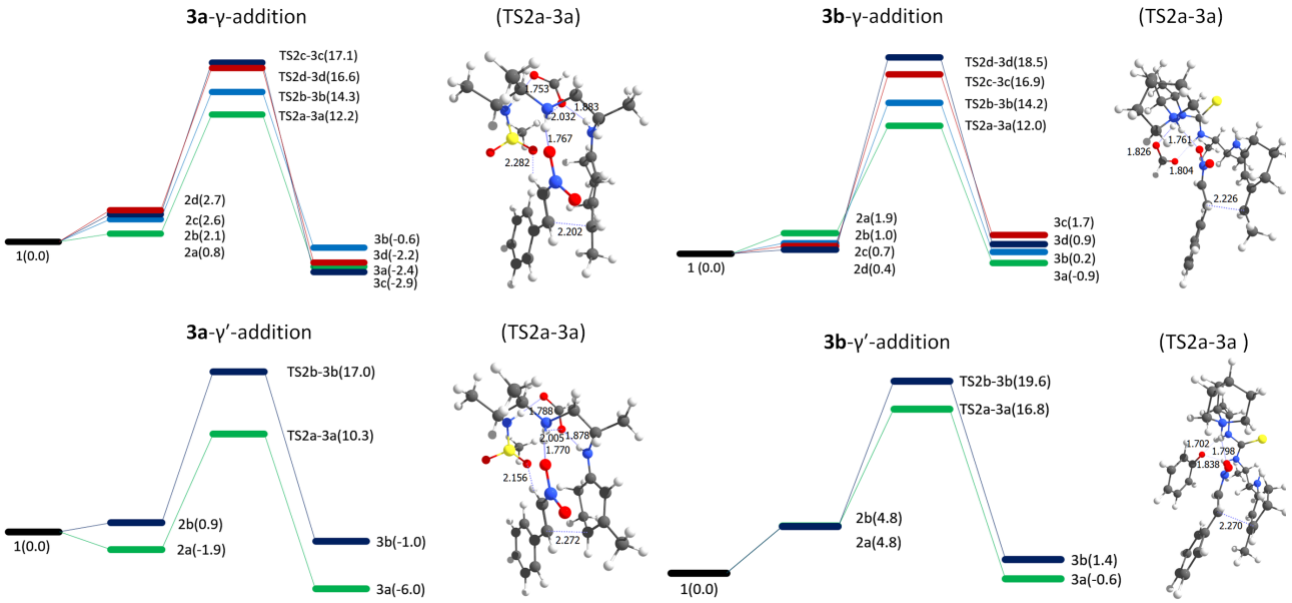


Figure S9. Gibbs free energy profiles for the four additions. All the energies are in kcal/mol, and ralative to the catalyst-die namine-additive plus a free nitrostyrene.

nitroethylene

Geometry with 18 atoms:

N	2.98034	0.03463	0.00865
C	1.59180	0.45278	0.03396
C	0.61748	-0.45904	-0.03419
O	3.25326	-1.15338	-0.07624
O	3.81232	0.92942	0.07648
C	-0.81989	-0.18032	-0.02090
C	-1.34413	1.12198	-0.05606
C	-1.70405	-1.26702	0.02789
C	-2.71778	1.32550	-0.03539
C	-3.08097	-1.06160	0.05051
C	-3.58979	0.23492	0.02008
H	1.49543	1.52670	0.11604
H	0.91421	-1.50442	-0.09647
H	-0.67790	1.97844	-0.10810
H	-1.30461	-2.27805	0.05067
H	-3.11270	2.33669	-0.06577
H	-3.75410	-1.91280	0.09018
H	-4.66333	0.39954	0.03557

3a-γ-addition-1

Geometry with 58 atoms:

C	-0.76543	2.47725	0.09176
N	-1.10877	1.36532	0.94540
C	-2.18547	0.53827	0.72362
C	0.75342	2.63805	0.01997
N	1.39934	1.34259	-0.33873
C	2.81483	1.39983	-0.83385
C	3.26700	-0.02558	-1.23980
N	2.81584	-1.04574	-0.29710
C	-2.14617	-0.73538	1.52974
C	-3.18966	0.79590	-0.15274
C	-4.26077	-0.15863	-0.45008
S	1.52369	-1.98520	-0.67743
O	0.32839	-1.16308	-0.95547
O	1.89377	-2.92434	-1.73544
C	1.28410	-2.84541	0.85608
C	-5.26221	0.17670	-1.28846
C	-3.51672	-1.39897	1.60232
C	-4.12911	-1.51771	0.20519
C	4.78878	-0.11323	-1.34224
C	2.94647	2.37736	-1.99467
C	-6.40749	-0.67911	-1.74473
H	-1.11683	2.23083	-0.92252
H	-0.44973	1.08895	1.66858
H	1.17321	2.94275	0.98476
H	0.99609	3.39137	-0.72971
H	0.80878	0.80740	-0.99430
H	3.41116	1.72778	0.02711
H	2.82446	-0.25443	-2.21963
H	3.00818	-0.89584	0.72060
H	-3.22095	1.74417	-0.68594
H	-5.23854	1.18286	-1.71216
H	-7.37212	-0.22411	-1.48380
H	-6.39970	-0.78927	-2.83717
H	-6.38579	-1.68450	-1.31697
H	3.91376	2.25034	-2.48475
H	2.16614	2.19399	-2.74344
H	2.88806	3.41904	-1.67140
H	5.23965	0.05121	-0.35723
H	5.06382	-1.11533	-1.67979
H	5.20476	0.61445	-2.04391
H	-1.41735	-1.40701	1.05370
H	-1.76524	-0.51598	2.53583
H	-3.42918	-2.38942	2.06261
H	-4.17973	-0.79952	2.23915
H	-3.47380	-2.14828	-0.41470
H	-5.09802	-2.02084	0.26403
C	-1.40557	3.79505	0.53185
H	-1.03525	4.08392	1.52182
H	-1.18800	4.60318	-0.17614
H	-2.49074	3.67831	0.59984
H	1.39621	0.77082	0.55342
O	1.32929	0.46356	2.20156
C	2.29921	-0.01254	2.86398
O	3.30000	-0.59208	2.39728
H	2.23564	0.09663	3.96482
H	2.20172	-3.38103	1.10614
H	1.01805	-2.12060	1.62888
H	0.46452	-3.54761	0.68308

3a-γ-addition-2a

Geometry with 76 atoms:

C	1.35141	-2.92894	-0.10496
N	0.83686	-2.14161	-1.20334
C	-0.48344	-1.83126	-1.39068
C	2.65909	-2.32355	0.41277
N	2.48608	-0.85934	0.63707
C	3.58547	-0.15025	1.37769
C	3.25232	1.35760	1.41811
N	3.08715	1.89599	0.06245

C	-0.73391	-0.89464	-2.54805
C	-1.51386	-2.29372	-0.62753
C	-2.89589	-1.86469	-0.81261
S	1.57254	2.26244	-0.44716
O	0.66677	1.09929	-0.32417
O	1.10196	3.47274	0.22881
C	1.85828	2.57722	-2.16880
C	-3.86842	-2.29121	0.02282
C	-2.15844	-1.03354	-3.07465
C	-3.16768	-0.88591	-1.93649
C	4.33199	2.16636	2.13399
C	3.76055	-0.73538	2.77204
C	-5.32279	-1.91511	-0.03918
H	0.62724	-2.86573	0.71405
H	1.51100	-1.75740	-1.86176
H	3.47448	-2.43638	-0.30878
H	2.92891	-2.80686	1.35164
H	1.58507	-0.69691	1.11454
H	4.49028	-0.29640	0.77364
H	2.30195	1.48373	1.95760
H	3.72404	1.50382	-0.67377
H	-1.33369	-3.01291	0.16961
H	-3.58362	-2.98397	0.81675
H	-5.91551	-2.66141	-0.58784
H	-5.75128	-1.86014	0.96887
H	-5.48604	-0.94551	-0.51998
N	-0.92030	-1.14217	2.45969
C	-1.44610	-0.02460	1.73609
C	-2.76822	0.20127	1.72383
O	-1.65994	-1.93001	3.02252
O	0.31567	-1.25499	2.48106
C	-3.40480	1.29772	0.99836
C	-2.67081	2.20427	0.21302
C	-4.79790	1.43335	1.07334
C	-3.32454	3.21490	-0.48000
C	-5.45097	2.44409	0.37253
C	-4.71505	3.33575	-0.40594
H	-0.67744	0.53289	1.21666
H	-3.41389	-0.46478	2.29196
H	-1.58996	2.11374	0.13500
H	-5.36824	0.73560	1.68202
H	-2.74767	3.91212	-1.08099
H	-6.53137	2.53594	0.43599
H	-5.22132	4.12701	-0.95158
H	4.57739	-0.22558	3.28606
H	2.84644	-0.61376	3.36468
H	4.02109	-1.79537	2.74573
H	5.31062	1.99398	1.67091
H	4.09147	3.22773	2.03751
H	4.39243	1.92293	3.19762
H	-0.54368	0.13034	-2.20069
H	-0.00441	-1.10095	-3.34163
H	-2.34795	-0.27915	-3.84620
H	-2.27786	-2.01855	-3.54368
H	-3.10481	0.13956	-1.53915
H	-4.18525	-1.01447	-2.31866
C	1.55772	-4.39694	-0.47567
H	2.29234	-4.48717	-1.28371
H	1.90544	-4.98094	0.38404
H	0.61284	-4.82435	-0.82410
H	2.40447	-0.44313	-0.31520
O	3.03485	-0.54473	-2.07076
C	4.18421	-0.12082	-2.37845
O	4.80535	0.80644	-1.81316
H	4.68265	-0.61543	-3.23760
H	2.62408	3.34914	-2.26512
H	2.15900	1.63964	-2.64218
H	0.90526	2.92830	-2.57271

3a-γ-addition-TS2a-3a

Geometry with 76 atoms:

C	1.55407	-2.90245	-0.02404
N	1.02335	-2.19721	-1.18461
C	-0.25977	-1.89417	-1.41188
C	2.73601	-2.12901	0.56443
N	2.35647	-0.71003	0.79805
C	3.36068	0.12419	1.54486
C	2.92354	1.60168	1.46958
N	2.86885	2.05435	0.07080
C	-0.52639	-1.07715	-2.64934
C	-1.31597	-2.25734	-0.58346
C	-2.63391	-1.80798	-0.81679
S	1.38806	2.29694	-0.59837
O	0.55751	1.07420	-0.52719
O	0.77929	3.48978	-0.01046
C	1.82472	2.58373	-2.29326
C	-3.56697	-1.89672	0.21504
C	-1.92381	-1.35808	-3.19344
C	-2.97626	-1.11881	-2.11349
C	3.87013	2.51838	2.24054
C	3.48349	-0.36724	2.98069
C	-5.03730	-1.65184	0.01760

H	0.77749	-2.93423	0.74358
H	1.71906	-1.80096	-1.82309
H	3.59904	-2.12954	-0.10827
H	3.01177	-2.58673	1.51487
H	1.45142	-0.70053	1.32209
H	4.30792	0.00955	1.00264
H	1.91695	1.68737	1.90389
H	3.56932	1.61342	-0.56864
H	-1.14103	-2.84182	0.31520
H	-3.29770	-2.56649	1.03209
H	-5.50964	-2.50233	-0.49354
H	-5.54442	-1.53794	0.98180
H	-5.24101	-0.75251	-0.57252
N	-0.95048	-1.27858	2.36955
C	-1.51009	-0.27334	1.63828
C	-2.89646	-0.21213	1.46375
O	-1.64523	-2.18775	2.85595
O	0.31263	-1.28209	2.54103
C	-3.48509	0.98070	0.82873
C	-2.76672	1.75246	-0.09965
C	-4.78678	1.37798	1.16702
C	-3.33936	2.88567	-0.66908
C	-5.35991	2.50988	0.59305
C	-4.63812	3.26699	-0.32920
H	-0.79861	0.39885	1.17935
H	-3.50410	-0.69658	2.22461
H	-1.75026	1.47365	-0.37013
H	-5.34770	0.79924	1.89719
H	-2.76353	3.47906	-1.37426
H	-6.36778	2.80432	0.87201
H	-5.08095	4.15385	-0.77367
H	4.27972	0.17788	3.49119
H	2.54440	-0.21666	3.52470
H	3.74397	-1.42691	3.03109
H	4.89990	2.38950	1.88671
H	3.57452	3.55479	2.06133
H	3.83572	2.33062	3.31663
H	-0.42410	-0.02059	-2.36484
H	0.24455	-1.28580	-3.39945
H	-2.12279	-0.72100	-4.06103
H	-1.97768	-2.39981	-3.53389
H	-3.07283	-0.03891	-1.91789
H	-3.96136	-1.45371	-2.45851
C	1.97709	-4.32167	-0.39184
H	2.74489	-4.30229	-1.17348
H	2.37796	-4.84742	0.48105
H	1.11566	-4.88165	-0.76688
H	2.19194	-0.29292	-0.13749
O	3.01352	-0.44304	-1.99014
C	4.22468	-0.10890	-2.12695
O	4.81003	0.80517	-1.50710
H	4.81905	-0.67902	-2.87171
H	2.53170	3.41404	-2.33956
H	2.24668	1.65847	-2.69362
H	0.89446	2.84224	-2.80590

3a-γ-addition-3a

Geometry with 76 atoms:

C	2.00942	-2.73182	0.39262
N	1.60000	-2.29320	-0.94870
C	0.39028	-2.11098	-1.40642
C	2.87286	-1.64041	1.02487
N	2.11084	-0.37666	1.13443
C	2.86649	0.75757	1.75923
C	2.15587	2.07687	1.40468
N	2.24257	2.31624	-0.04687
C	0.25945	-1.53299	-2.78810
C	-0.77360	-2.37035	-0.61392
C	-1.96757	-1.80867	-0.93609
S	0.88064	2.17286	-0.94309
O	0.29049	0.81860	-0.82422
O	-0.04134	3.26353	-0.62333
C	1.53564	2.36581	-2.58032
C	-3.06181	-1.90718	0.09667
C	-1.17691	-1.60499	-3.29675
C	-2.15033	-1.08450	-2.23884
C	2.75770	3.27477	2.13297
C	2.97700	0.53738	3.26329
C	-4.46544	-2.04176	-0.49151
H	1.11960	-2.86433	1.01415
H	2.36658	-1.91416	-1.52889
H	3.78034	-1.45975	0.43879
H	3.14954	-1.96772	2.02895
H	1.21395	-0.59903	1.77971
H	3.86269	0.77036	1.29657
H	1.09610	1.98581	1.68463
H	3.09983	1.94070	-0.51796
H	-0.68701	-2.89240	0.33503
H	-2.84007	-2.80769	0.67702
H	-4.51633	-2.89978	-1.17149
H	-5.18906	-2.21423	0.31261
H	-4.78515	-1.14874	-1.03632

N	-0.89180	-1.37273	2.31476
C	-1.62062	-0.46711	1.72201
C	-2.99222	-0.74945	1.18138
O	-1.24994	-2.58892	2.44199
O	0.29692	-1.03130	2.79938
C	-3.63996	0.54208	0.71398
C	-2.92262	1.49484	-0.01803
C	-4.98443	0.79944	1.00374
C	-3.53467	2.66806	-0.45714
C	-5.60284	1.96714	0.55959
C	-4.87940	2.90535	-0.17613
H	-1.19418	0.52604	1.70014
H	-3.60347	-1.15558	2.00176
H	-1.86949	1.33280	-0.23570
H	-5.55213	0.07911	1.58956
H	-2.94691	3.39920	-1.00576
H	-6.64752	2.14851	0.79797
H	-5.35666	3.82109	-0.51444
H	3.66760	1.26524	3.69495
H	1.99953	0.63644	3.74653
H	3.36840	-0.45649	3.49638
H	3.83409	3.34189	1.93488
H	2.28400	4.18693	1.76215
H	2.59685	3.21401	3.21254
H	0.59277	-0.49071	-2.70954
H	0.95703	-2.04699	-3.45846
H	-1.26777	-1.02084	-4.21718
H	-1.43281	-2.64320	-3.54107
H	-1.97701	-0.01256	-2.06129
H	-3.18415	-1.18000	-2.58331
C	2.77892	-4.04283	0.28504
H	3.66967	-3.92064	-0.34169
H	3.09425	-4.37585	1.27811
H	2.14628	-4.81873	-0.15460
H	1.78816	-0.10174	0.19253
O	3.20936	-0.33492	-1.82042
C	4.33823	0.22682	-1.74643
O	4.58109	1.32611	-1.20354
H	5.19486	-0.30620	-2.21164
H	2.05124	3.32609	-2.63883
H	2.20969	1.52743	-2.77799
H	0.67597	2.35127	-3.25574

3a-γ-addition-2b

Geometry with 76 atoms:

C	1.33214	2.92829	0.22389
N	0.86345	2.15123	1.35001
C	-0.43951	1.77946	1.55378
C	2.61882	2.32414	-0.34454
N	2.42953	0.86732	-0.60266
C	3.51122	0.16899	-1.38043
C	3.13675	-1.32415	-1.50774
N	2.96570	-1.93836	-0.18505
C	-0.60995	0.79856	2.68983
C	-1.50022	2.22978	0.82245
C	-2.85414	1.71946	1.01358
S	1.44377	-2.27728	0.32233
O	0.58194	-1.07700	0.28714
O	0.91764	-3.42173	-0.42572
C	1.73916	-2.71331	2.01539
C	-3.94539	2.17866	0.36269
C	-2.05482	0.72852	3.17348
C	-2.98442	0.55740	1.97385
C	4.19123	-2.11831	-2.27618
C	3.71436	0.82910	-2.73676
C	-4.01103	3.28810	-0.64739
H	0.57552	2.85832	-0.56508
H	1.56732	1.73325	1.95503
H	3.45667	2.41383	0.35479
H	2.86388	2.82927	-1.27858
H	1.51929	0.72293	-1.06712
H	4.41700	0.25234	-0.76599
H	2.18109	-1.39418	-2.04812
H	3.61992	-1.60850	0.56615
H	-1.34598	2.99718	0.06920
H	-4.89859	1.70095	0.59630
H	-3.03748	3.74203	-0.84613
H	-4.40280	2.93085	-1.60952
H	-4.68799	4.08360	-0.30911
N	-1.02424	1.23687	-2.33081
C	-1.53423	0.05409	-1.70080
C	-2.85549	-0.15835	-1.63542
O	-1.77600	2.08393	-2.77757
O	0.21042	1.33855	-2.39139
C	-3.45783	-1.32459	-0.99201
C	-2.69024	-2.41158	-0.53975
C	-4.84475	-1.33598	-0.78976
C	-3.30329	-3.47476	0.11138
C	-5.45503	-2.39965	-0.13089
C	-4.68450	-3.46941	0.32263
H	-0.75135	-0.55536	-1.26911
H	-3.52605	0.58089	-2.06801

H	-1.61402	-2.43222	-0.69324
H	-5.43910	-0.49495	-1.13948
H	-2.70098	-4.31230	0.45173
H	-6.52934	-2.39356	0.02844
H	-5.15923	-4.30154	0.83483
H	4.49887	0.30630	-3.28668
H	2.79349	0.79983	-3.33095
H	4.03810	1.86774	-2.64424
H	5.17811	-1.99043	-1.81621
H	3.92811	-3.17768	-2.23123
H	4.24586	-1.82183	-3.32655
H	-0.27772	-0.18377	2.32779
H	0.06402	1.08269	3.50820
H	-2.17253	-0.10530	3.87451
H	-2.31302	1.64956	3.71191
H	-2.69975	-0.36944	1.45070
H	-4.02778	0.44255	2.28813
C	1.54896	4.39976	0.57415
H	2.31492	4.49948	1.35130
H	1.85906	4.97816	-0.30341
H	0.61756	4.82628	0.95791
H	2.36475	0.42374	0.34006
O	3.01879	0.41044	2.05859
C	4.14812	-0.07846	2.34485
O	4.72698	-1.00717	1.73949
H	4.66737	0.35613	3.22374
H	2.47541	-3.51846	2.05086
H	2.08389	-1.82016	2.54169
H	0.77847	-3.05176	2.41186

3a-γ-addition-TS2b-3b

Geometry with 76 atoms:

C	1.61850	2.89324	0.05643
N	1.21904	2.23272	1.29263
C	-0.01974	1.86037	1.63015
C	2.73521	2.09249	-0.61819
N	2.31255	0.68048	-0.81818
C	3.24476	-0.18541	-1.62167
C	2.68880	-1.62497	-1.60868
N	2.65626	-2.14818	-0.23431
C	-0.09097	0.98364	2.85605
C	-1.16791	2.23268	0.93109
C	-2.40145	1.59662	1.16854
S	1.19725	-2.32747	0.49234
O	0.44922	-1.05212	0.52972
O	0.47265	-3.44085	-0.12136
C	1.69387	-2.73704	2.14495
C	-3.52249	1.81642	0.36434
C	-1.51796	0.80415	3.36014
C	-2.43287	0.48157	2.18074
C	3.51532	-2.57590	-2.47091
C	3.39695	0.36532	-3.03256
C	-3.76984	3.09263	-0.40182
H	0.76229	2.89193	-0.62368
H	1.97997	1.83301	1.84946
H	3.64897	2.08157	-0.01503
H	2.94043	2.54226	-1.58954
H	1.37862	0.69120	-1.29115
H	4.20398	-0.17262	-1.08805
H	1.66073	-1.59903	-1.99895
H	3.41637	-1.80778	0.40097
H	-1.10109	2.97092	0.13872
H	-4.42776	1.30511	0.68926
H	-2.87514	3.48005	-0.89022
H	-4.52099	2.93863	-1.18466
H	-4.16203	3.86295	0.27550
N	-1.00911	1.36514	-2.20559
C	-1.60162	0.38572	-1.46570
C	-2.97768	0.41295	-1.20121
O	-1.64336	2.34239	-2.63819
O	0.23508	1.25447	-2.47037
C	-3.65874	-0.82190	-0.74877
C	-2.95747	-1.94430	-0.28341
C	-5.05943	-0.88513	-0.80735
C	-3.64249	-3.08938	0.11779
C	-5.74278	-2.02812	-0.40709
C	-5.03446	-3.13644	0.06105
H	-0.91326	-0.35068	-1.07890
H	-3.56491	1.05871	-1.85042
H	-1.87145	-1.94077	-0.23962
H	-5.61325	-0.02214	-1.17352
H	-3.07869	-3.95092	0.46532
H	-6.82730	-2.05760	-0.46548
H	-5.56519	-4.03270	0.36987
H	4.10370	-0.24972	-3.59275
H	2.43495	0.36728	-3.55733
H	3.79699	1.38155	-3.03462
H	4.56836	-2.55396	-2.16629
H	3.13842	-3.59111	-2.32662
H	3.44496	-2.33020	-3.53347
H	0.33625	0.01492	2.56798
H	0.56161	1.40784	3.62828

H	-1.54902	-0.00141	4.10058
H	-1.86427	1.72003	3.85477
H	-2.06927	-0.43704	1.69114
H	-3.46071	0.28879	2.50387
C	2.07018	4.32711	0.31525
H	2.92786	4.34454	0.99696
H	2.35511	4.82008	-0.61978
H	1.25616	4.89680	0.77250
H	2.20057	0.26382	0.12548
O	3.12358	0.30427	1.88518
C	4.27476	-0.20250	2.00576
O	4.71612	-1.18912	1.37723
H	4.95310	0.27158	2.74561
H	2.32825	-3.62458	2.11445
H	2.21822	-1.87616	2.56690
H	0.77223	-2.94179	2.69598

3a-γ-addition-3b

Geometry with 76 atoms:

C	1.90522	2.71326	-0.49793
N	1.60937	2.29732	0.88000
C	0.44338	2.08948	1.43121
C	2.80238	1.65362	-1.13872
N	2.10426	0.35034	-1.16868
C	2.86400	-0.77691	-1.79652
C	2.15094	-2.09439	-1.43470
N	2.23721	-2.32700	0.01717
C	0.44546	1.51152	2.82003
C	-0.78667	2.31508	0.73098
C	-1.92295	1.70433	1.15121
S	0.88229	-2.17332	0.92244
O	0.29289	-0.81989	0.80534
O	-0.04453	-3.26466	0.61897
C	1.55810	-2.35902	2.55277
C	-3.14538	1.72203	0.27317
C	-0.94536	1.51142	3.44292
C	-1.97378	0.96439	2.45578
C	2.74668	-3.29890	-2.15711
C	2.96322	-0.56263	-3.30190
C	-3.50738	3.14214	-0.18592
H	0.97199	2.75791	-1.06741
H	2.42363	1.94433	1.40799
H	3.74662	1.54463	-0.59329
H	3.00859	1.96485	-2.16432
H	1.16224	0.51014	-1.77115
H	3.86346	-0.78743	-1.34043
H	1.09117	-1.99919	-1.71361
H	3.10329	-1.96891	0.48454
H	-0.78541	2.83173	-0.22517
H	-3.98319	1.35246	0.87454
H	-2.77254	3.53213	-0.89217
H	-4.48068	3.12048	-0.68883
H	-3.58745	3.81849	0.67234
N	-0.95814	1.25120	-2.17700
C	-1.68033	0.39413	-1.51125
C	-3.03919	0.72020	-0.96326
O	-1.26850	2.48057	-2.31043
O	0.17461	0.84310	-2.74009
C	-3.76210	-0.57042	-0.61461
C	-3.12014	-1.59953	0.08492
C	-5.11252	-0.72338	-0.94211
C	-3.81373	-2.75483	0.44253
C	-5.80931	-1.87664	-0.58278
C	-5.16112	-2.89690	0.11235
H	-1.28162	-0.60979	-1.47851
H	-3.59769	1.22514	-1.76444
H	-2.06562	-1.51236	0.34084
H	-5.62166	0.06723	-1.49025
H	-3.29161	-3.54817	0.97065
H	-6.85677	-1.98034	-0.85334
H	-5.70017	-3.79953	0.38636
H	3.62343	-1.31434	-3.74015
H	1.97685	-0.63220	-3.77298
H	3.38828	0.41492	-3.54334
H	3.82416	-3.36695	-1.96498
H	2.27336	-4.20715	-1.77629
H	2.57920	-3.24694	-3.23606
H	0.82815	0.48884	2.71610
H	1.16683	2.06255	3.43344
H	-0.93606	0.91329	4.35881
H	-1.22752	2.53384	3.72234
H	-1.78008	-0.09914	2.24507
H	-2.98666	1.02232	2.86859
C	2.58261	4.07803	-0.49101
H	3.51478	4.04964	0.08444
H	2.81266	4.38635	-1.51506
H	1.92054	4.82625	-0.04654
H	1.84881	0.09274	-0.20257
O	3.26311	0.34616	1.69242
C	4.37979	-0.24316	1.64636
O	4.59760	-1.37425	1.16204
H	5.24808	0.29535	2.08254

H	2.05359	-3.32936	2.61826
H	2.25620	-1.53531	2.72743
H	0.71090	-2.31407	3.24262

3a-γ-addition-2c

Geometry with 76 atoms:

C	-0.95548	1.39808	2.23140
N	-0.82166	1.96026	0.90865
C	0.36977	2.13801	0.25658
C	-2.25210	0.58927	2.32484
N	-2.40506	-0.28388	1.12418
C	-3.36194	-1.43325	1.26748
C	-3.60802	-2.06803	-0.11752
N	-4.02060	-1.06358	-1.10929
C	0.20973	2.60003	-1.17193
C	1.59658	1.90080	0.79607
C	2.84132	2.00720	0.03236
S	-2.88880	-0.66467	-2.25125
O	-1.65023	-0.16528	-1.63445
O	-2.73629	-1.80871	-3.15183
C	-3.70851	0.67101	-3.08073
C	4.03927	1.83433	0.62951
C	1.49726	3.20890	-1.71526
C	2.68013	2.27708	-1.44894
C	-4.67535	-3.15824	-0.05383
C	-2.81350	-2.45884	2.25184
H	-0.12703	0.69463	2.37621
H	-1.67009	2.28810	0.45077
H	-3.13395	1.23690	2.35362
H	-2.23346	-0.02492	3.22516
H	-1.47928	-0.63240	0.81817
H	-4.29807	-0.99108	1.62806
H	-2.66377	-2.51649	-0.45802
H	-4.54495	-0.26091	-0.70793
H	1.68928	1.62007	1.84453
H	-3.56945	-3.22129	2.45039
H	-1.92268	-2.94924	1.84310
H	-2.54531	-2.01611	3.21338
H	-5.61177	-2.75172	0.34562
H	-4.86511	-3.52050	-1.06711
H	-4.36399	-4.00663	0.56145
H	-0.09978	1.73352	-1.77218
H	-0.61406	3.32363	-1.22449
H	1.39750	3.39698	-2.78999
H	1.68289	4.17542	-1.22927
H	2.49161	1.32329	-1.96817
H	3.59501	2.69735	-1.87465
C	-0.90780	2.44766	3.34207
H	-1.73259	3.15965	3.22542
H	-0.98015	1.98453	4.33301
H	0.03231	3.00458	3.28837
H	-2.72311	0.35585	0.36267
H	-4.67828	0.32106	-3.43836
H	-3.79825	1.50138	-2.37577
H	-3.06551	0.94674	-3.92037
N	0.97544	-1.51797	1.48049
C	2.39658	-1.63877	1.30734
C	2.94348	-1.36778	0.11463
O	0.25469	-1.33451	0.50282
O	0.54287	-1.60689	2.62521
C	4.36503	-1.44917	-0.21055
C	5.34843	-1.76906	0.73954
C	4.75333	-1.19631	-1.53354
C	6.68398	-1.84491	0.36631
C	6.09263	-1.27168	-1.90611
C	7.05926	-1.59891	-0.95766
H	2.89594	-1.92044	2.22371
H	2.27116	-1.06953	-0.68860
H	5.07336	-1.95268	1.77455
H	3.99539	-0.94219	-2.27078
H	7.43797	-2.09117	1.10822
H	6.37936	-1.07293	-2.93453
H	8.10536	-1.65716	-1.24443
O	-3.49308	1.99738	-0.13435
C	-4.71109	1.98159	0.20114
O	-5.42856	0.96201	0.30189
H	-5.18143	2.96289	0.42080
C	5.40118	1.89347	0.00119
H	5.36744	2.02956	-1.08287
H	5.99560	2.71595	0.42245
H	5.96252	0.96997	0.19681
H	4.03289	1.61944	1.70109

3a-γ-addition-TS2c-3c

Geometry with 76 atoms:

C	0.90554	-0.99999	2.43484
N	0.92553	-1.79949	1.21931
C	-0.14096	-2.14657	0.49061
C	1.94439	0.13043	2.36704
N	2.06467	0.71246	1.00097
C	2.87870	1.97981	0.94748
C	3.30707	2.24074	-0.50660

N	4.11620	1.11662	-1.01282
C	0.18476	-2.75558	-0.84693
C	-1.46087	-1.92195	0.86717
C	-2.52185	-2.04001	-0.06129
S	3.41073	0.21155	-2.20428
O	2.15423	-0.39891	-1.74069
O	3.31375	1.03989	-3.40607
C	4.62535	-1.06043	-2.42601
C	-3.79882	-1.58006	0.24832
C	-1.00617	-3.49084	-1.44131
C	-2.22731	-2.57577	-1.44357
C	4.11043	3.53084	-0.64329
C	2.08963	3.14612	1.52559
H	-0.07689	-0.53042	2.50129
H	1.85445	-2.07465	0.88400
H	2.94343	-0.21880	2.64072
H	1.63667	0.91780	3.05595
H	1.12079	0.87859	0.58632
H	3.77483	1.77414	1.54541
H	2.39811	2.32430	-1.11953
H	4.57383	0.54965	-0.26973
H	-1.69669	-1.56023	1.86397
H	2.75495	4.00201	1.66094
H	1.27123	3.43481	0.85727
H	1.65388	2.90916	2.49803
H	4.97960	3.51491	0.02496
H	4.47133	3.61062	-1.67156
H	3.50530	4.41357	-0.41954
H	0.49539	-1.92987	-1.50173
H	1.05738	-3.41138	-0.74270
H	-0.77379	-3.81389	-2.46082
H	-1.22599	-4.38981	-0.85194
H	-2.04409	-1.72612	-2.12158
H	-3.10100	-3.10640	-1.83406
C	1.15652	-1.85725	3.67276
H	2.12045	-2.37144	3.58766
H	1.16936	-1.23999	4.57774
H	0.37034	-2.61065	3.77827
H	2.51238	-0.01629	0.41106
H	5.58970	-0.59379	-2.63336
H	4.64462	-1.67105	-1.52071
H	4.29212	-1.65326	-3.28167
N	-1.24819	1.23248	0.92570
C	-2.61287	1.09510	0.97025
C	-3.35075	0.63770	-0.11584
O	-0.58858	0.98389	-0.11531
O	-0.65945	1.66105	1.94675
C	-4.76957	1.00638	-0.26894
C	-5.61165	1.22282	0.83265
C	-5.30021	1.13996	-1.55862
C	-6.94652	1.56172	0.64529
C	-6.63701	1.48547	-1.74616
C	-7.46507	1.69418	-0.64544
H	-3.03512	1.42436	1.90871
H	-2.79884	0.47241	-1.03810
H	-5.22646	1.10897	1.84286
H	-4.65550	0.97237	-2.41862
H	-7.58757	1.72206	1.50770
H	-7.03133	1.58895	-2.75305
H	-8.50875	1.95864	-0.78932
O	3.65516	-1.72112	0.62003
C	4.73204	-1.41303	1.20094
O	5.28500	-0.29064	1.17304
H	5.23275	-2.21260	1.78748
C	-5.00731	-1.93352	-0.57992
H	-4.89182	-1.65667	-1.63409
H	-5.20285	-3.01470	-0.54518
H	-5.90201	-1.42841	-0.20592
H	-3.98901	-1.33728	1.29310

3a-γ-addition-3c

Geometry with 76 atoms:

C	-1.00034	1.50365	2.36499
N	-1.23819	2.17526	1.08227
C	-0.35015	2.45341	0.17255
C	-1.90549	0.26956	2.46210
N	-1.85732	-0.54589	1.22411
C	-2.51148	-1.89283	1.33397
C	-2.70452	-2.45496	-0.08629
N	-3.56107	-1.55518	-0.88280
C	-0.86197	2.92406	-1.16153
C	1.06759	2.28440	0.38397
C	1.80835	1.81067	-0.64653
S	-2.83030	-0.76589	-2.13384
O	-1.72875	0.09420	-1.66509
O	-2.47536	-1.74715	-3.15868
C	-4.15988	0.26587	-2.69864
C	3.24200	1.39813	-0.43257
C	0.18202	2.75355	-2.27236
C	1.14366	1.59655	-1.97907
C	-3.32789	-3.84739	-0.07542
C	-1.67608	-2.82730	2.19863

H	0.03127	1.14809	2.37758
H	-2.23709	2.26739	0.81508
H	-2.95028	0.54807	2.63843
H	-1.54139	-0.33283	3.29431
H	-0.82960	-0.67264	0.88485
H	-3.49947	-1.72038	1.78085
H	-1.71531	-2.51018	-0.56255
H	-4.20343	-0.95435	-0.32722
H	1.48679	2.36886	1.38256
H	-2.24278	-3.73913	2.40180
H	-0.73841	-3.08494	1.69643
H	-1.41525	-2.37760	3.15842
H	-4.26982	-3.84218	0.48601
H	-3.54402	-4.14365	-1.10483
H	-2.65539	-4.58883	0.36409
H	-1.77067	2.35626	-1.38211
H	-1.14590	3.97825	-1.04868
H	-0.33288	2.57584	-3.22053
H	0.76508	3.67503	-2.38264
H	0.59051	0.64791	-1.93142
H	1.88148	1.51251	-2.77988
C	-1.26332	2.45650	3.52374
H	-2.29015	2.83765	3.48836
H	-1.11728	1.93832	4.47642
H	-0.57609	3.30677	3.48554
H	-2.33345	-0.00290	0.48377
H	-5.01654	-0.36461	-2.94227
H	-4.38981	0.98812	-1.91129
H	-3.79063	0.77421	-3.59325
N	1.39167	-0.73897	1.35069
C	2.65865	-0.44733	1.22130
C	3.29332	-0.14151	-0.10262
O	0.60816	-0.78094	0.30352
O	0.85463	-0.97428	2.49613
C	4.72735	-0.64093	-0.11126
C	5.66192	-0.14992	0.80895
C	5.14541	-1.59190	-1.04408
C	6.97988	-0.59868	0.79641
C	6.46512	-2.04612	-1.05973
C	7.38661	-1.55029	-0.13995
H	3.22437	-0.45625	2.14406
H	2.73565	-0.66505	-0.88885
H	5.35696	0.59486	1.54244
H	4.42916	-1.98382	-1.76300
H	7.69092	-0.20624	1.51838
H	6.77131	-2.78865	-1.79174
H	8.41425	-1.90238	-0.15035
O	-3.74026	1.58196	0.26854
C	-4.81866	1.18219	0.79977
O	-5.24626	0.01108	0.79291
H	-5.43506	1.94915	1.31467
C	4.13539	1.75989	-1.62484
H	3.99996	1.06392	-2.45982
H	3.92320	2.77374	-1.98359
H	5.18867	1.71944	-1.33510
H	3.60810	1.92516	0.45893

3a-γ-addition-2d

Geometry with 76 atoms:

C	0.84128	1.94681	-1.67880
N	0.74597	2.10768	-0.24622
C	-0.42479	2.06601	0.45645
C	2.13182	1.20977	-2.04208
N	2.32731	0.02518	-1.15487
C	3.28342	-1.01263	-1.67061
C	3.64573	-1.99488	-0.53706
N	4.09836	-1.29058	0.67263
C	-0.23302	2.09675	1.95467
C	-1.66387	1.97335	-0.10819
C	-2.87479	1.80765	0.68731
S	3.02785	-1.26417	1.93907
O	1.74923	-0.64529	1.55639
O	2.94434	-2.62137	2.48070
C	3.87730	-0.19854	3.07526
C	-4.11137	1.81557	0.14675
C	-1.52294	2.44062	2.69509
C	-2.67053	1.57927	2.16779
C	4.73997	-2.96599	-0.97438
C	2.67289	-1.74556	-2.85875
H	0.00794	1.30862	-1.99416
H	1.60878	2.28637	0.26580
H	3.01484	1.84345	-1.91364
H	2.08103	0.88204	-3.08080
H	1.41469	-0.41200	-0.93414
H	4.18294	-0.45773	-1.96051
H	2.74413	-2.56855	-0.28033
H	4.56752	-0.38572	0.47640
H	-1.77293	2.02114	-1.18931
H	3.42592	-2.38222	-3.32804
H	1.83666	-2.37655	-2.53670
H	2.30496	-1.06299	-3.62788
H	5.63219	-2.41384	-1.29203

H	5.01182	-3.59466	-0.12322
H	4.41319	-3.61480	-1.79171
H	0.14275	1.11118	2.26203
H	0.55845	2.81790	2.19652
H	-1.38571	2.28515	3.77081
H	-1.76715	3.50000	2.54415
H	-2.41118	0.52185	2.33997
H	-3.60144	1.77572	2.71125
C	0.76101	3.27233	-2.43692
H	1.59790	3.92050	-2.15381
H	0.78897	3.11447	-3.52121
H	-0.17001	3.78949	-2.18652
H	2.67017	0.41564	-0.25045
H	4.86818	-0.61282	3.26870
H	3.92044	0.80118	2.63562
H	3.27702	-0.19285	3.98846
N	-1.09084	-1.05203	-1.73032
C	-2.50768	-1.21801	-1.55632
C	-3.01979	-1.31021	-0.32158
O	-0.34082	-1.14392	-0.76216
O	-0.69277	-0.81592	-2.86662
C	-4.43733	-1.45058	-0.00021
C	-5.44765	-1.36879	-0.97173
C	-4.79500	-1.63868	1.34213
C	-6.78272	-1.46562	-0.60150
C	-6.13265	-1.74044	1.71092
C	-7.12862	-1.64959	0.73978
H	-3.03471	-1.22074	-2.50002
H	-2.32260	-1.27543	0.51428
H	-5.19436	-1.20917	-2.01645
H	-4.01450	-1.69758	2.09695
H	-7.55858	-1.39045	-1.35782
H	-6.39678	-1.88434	2.75437
H	-8.17449	-1.72012	1.02476
O	3.44703	1.88928	0.67685
C	4.62237	2.02564	0.23350
O	5.32839	1.11552	-0.25429
H	5.06192	3.04371	0.28643
C	-4.39676	1.98486	-1.32053
H	-4.02934	2.94572	-1.70504
H	-3.91439	1.20039	-1.92505
H	-5.47132	1.94014	-1.52069
H	-4.96495	1.66185	0.80660

3a-γ-addition-TS2d-3d

Geometry with 76 atoms:

C	0.91348	1.99444	-1.78892
N	0.96920	2.26918	-0.35969
C	-0.07924	2.26237	0.46979
C	1.97109	0.95668	-2.18643
N	2.05184	-0.16685	-1.21175
C	2.82901	-1.35864	-1.70982
C	3.18083	-2.26613	-0.51868
N	3.98108	-1.53017	0.47649
C	0.27429	2.26557	1.93528
C	-1.40425	2.20506	0.04553
C	-2.42699	1.79650	0.92967
S	3.22450	-1.24717	1.92048
O	1.98162	-0.48250	1.72798
O	3.08760	-2.52365	2.62195
C	4.42211	-0.22527	2.73898
C	-3.72308	1.54363	0.49372
C	-0.94766	2.44319	2.82770
C	-2.04951	1.49426	2.35992
C	3.95271	-3.50815	-0.95661
C	2.03554	-2.10888	-2.77095
H	-0.06235	1.55126	-1.99734
H	1.90716	2.36007	0.04554
H	2.97176	1.39475	-2.24372
H	1.70072	0.55556	-3.16395
H	1.09438	-0.46573	-0.91319
H	3.75698	-0.94783	-2.12556
H	2.24022	-2.58384	-0.04664
H	4.48810	-0.70544	0.09506
H	-1.64554	2.35579	-1.00193
H	2.68517	-2.83832	-3.25979
H	1.18507	-2.63448	-2.32387
H	1.64483	-1.44526	-3.54441
H	4.85456	-3.22421	-1.51168
H	4.25920	-4.06129	-0.06558
H	3.34263	-4.16726	-1.58019
H	0.76255	1.30410	2.14358
H	1.02547	3.04492	2.11460
H	-0.67752	2.23373	3.86726
H	-1.30985	3.47758	2.78072
H	-1.67061	0.46167	2.42174
H	-2.93441	1.55634	3.00168
C	1.09319	3.26417	-2.61562
H	2.05319	3.73885	-2.38331
H	1.06654	3.03865	-3.68718
H	0.29381	3.97667	-2.39161
H	2.50816	0.22018	-0.36138

H	5.37614	-0.75445	2.76171
H	4.48465	0.72415	2.20280
H	4.04339	-0.07045	3.75253
N	-1.29584	-0.68283	-1.38055
C	-2.66784	-0.62411	-1.29406
C	-3.31900	-0.62649	-0.06628
O	-0.58144	-0.82937	-0.35667
O	-0.76175	-0.62716	-2.51085
C	-4.73357	-1.02904	0.06067
C	-5.62258	-1.03754	-1.02385
C	-5.20383	-1.43995	1.31713
C	-6.94285	-1.44526	-0.85256
C	-6.52096	-1.85273	1.48681
C	-7.39722	-1.85522	0.40078
H	-3.14504	-0.57934	-2.26154
H	-2.69743	-0.82576	0.80219
H	-5.28827	-0.72588	-2.00942
H	-4.52144	-1.43564	2.16494
H	-7.61787	-1.44659	-1.70376
H	-6.86382	-2.17584	2.46560
H	-8.42630	-2.17817	0.52958
O	3.64212	1.75839	0.27374
C	4.74940	1.70256	-0.33168
O	5.28855	0.66612	-0.77768
H	5.28943	2.66212	-0.47714
C	-4.26320	2.06532	-0.80704
H	-4.29085	3.16317	-0.81070
H	-3.65056	1.75654	-1.66412
H	-5.28417	1.70894	-0.97387
H	-4.45690	1.31730	1.26445

3a-γ-addition-3d

Geometry with 76 atoms:

C	1.03659	2.32974	-1.51449
N	1.25596	2.40561	-0.06501
C	0.34855	2.31379	0.86305
C	1.93962	1.24054	-2.10527
N	1.86555	-0.01527	-1.32146
C	2.51878	-1.20228	-1.96575
C	2.66804	-2.30475	-0.90198
N	3.50344	-1.82650	0.21621
C	0.82662	2.18673	2.28360
C	-1.06383	2.28245	0.56773
C	-1.83564	1.43982	1.29457
S	2.74347	-1.60826	1.66378
O	1.66234	-0.61034	1.56849
O	2.35449	-2.91761	2.18698
C	4.06547	-0.92189	2.63004
C	-3.26001	1.13482	0.92029
C	-0.24920	1.59370	3.20427
C	-1.21375	0.68356	2.43672
C	3.28609	-3.57784	-1.47153
C	1.70527	-1.67986	-3.16134
H	0.00378	2.02041	-1.68599
H	2.24958	2.35916	0.23262
H	2.98788	1.55759	-2.13450
H	1.58799	1.04483	-3.11832
H	0.82754	-0.25867	-1.08325
H	3.52001	-0.87501	-2.27605
H	1.66523	-2.53614	-0.51554
H	4.17017	-1.06452	-0.02568
H	-1.44170	2.78254	-0.31852
H	2.27509	-2.43104	-3.71357
H	0.75378	-2.11141	-2.83529
H	1.47117	-0.86703	-3.85134
H	4.24894	-3.35798	-1.94812
H	3.46118	-4.28129	-0.65386
H	2.62771	-4.05479	-2.20257
H	1.72601	1.56427	2.27251
H	1.11905	3.18967	2.61989
H	0.23915	1.02818	4.00261
H	-0.82341	2.39885	3.67577
H	-0.66780	-0.17702	2.02428
H	-1.99118	0.30031	3.10547
C	1.31825	3.67683	-2.16783
H	2.34495	4.00033	-1.96282
H	1.18595	3.60301	-3.25161
H	0.63136	4.43855	-1.78749
H	2.32449	0.16509	-0.41259
H	4.91150	-1.61085	2.61079
H	4.31800	0.05456	2.20951
H	3.67666	-0.81723	3.64628
N	-1.39143	-0.11915	-1.55684
C	-2.66446	0.07552	-1.32533
C	-3.26548	-0.16940	0.02387
O	-0.60420	-0.56367	-0.61047
O	-0.85333	0.12798	-2.69796
C	-4.67342	-0.73811	-0.03671
C	-5.60801	-0.35355	-1.00423
C	-5.07255	-1.65553	0.94183
C	-6.90275	-0.87179	-0.99315
C	-6.36469	-2.17666	0.95698

C	-7.28653	-1.78491	-0.01297
H	-3.22122	0.43064	-2.18112
H	-2.63180	-0.90336	0.53395
H	-5.33260	0.35750	-1.77866
H	-4.35486	-1.97162	1.69708
H	-7.61143	-0.56026	-1.75585
H	-6.64864	-2.89359	1.72273
H	-8.29420	-2.19089	-0.00720
O	3.74413	1.51011	0.46353
C	4.83411	1.33922	-0.15878
O	5.25670	0.25627	-0.60933
H	5.46727	2.23862	-0.31149
C	-3.99321	2.30047	0.26057
H	-3.90992	3.20562	0.87132
H	-3.59618	2.52277	-0.73569
H	-5.05636	2.06669	0.15136
H	-3.78766	0.86721	1.84533

3a-γ′-addition-1

Geometry with 55 atoms:

C	-1.21075	2.19733	0.01859
N	-1.55868	0.97240	0.69911
C	-2.66339	0.22418	0.39446
C	0.29251	2.44032	0.13140
N	1.06442	1.23605	-0.29714
C	2.47215	1.50022	-0.74948
C	3.23587	0.17453	-1.00807
N	2.89655	-0.89851	-0.07052
C	-2.73069	-1.11961	1.08408
C	-3.60827	0.54349	-0.52919
C	-4.68397	-0.40292	-0.84894
S	1.78576	-2.02055	-0.57072
O	0.53577	-1.37884	-1.01804
O	2.42988	-2.89660	-1.54677
C	1.47876	-2.88885	0.94465
C	-5.46927	-0.14073	-2.10579
C	-4.17320	-1.59454	1.25331
C	-4.94935	-1.43684	-0.02991
C	4.74176	0.41540	-0.91723
C	2.45877	2.35834	-2.00984
H	-1.44667	2.06021	-1.04881
H	-0.96540	0.65733	1.46377
H	0.58760	2.64514	1.16657
H	0.57015	3.29347	-0.48753
H	0.55428	0.69987	-1.01444
H	2.94832	2.01949	0.08967
H	2.98374	-0.17653	-2.01771
H	2.82868	-0.58083	0.91022
H	-3.56476	1.47443	-1.08944
H	3.46063	2.40171	-2.44318
H	1.79007	1.92126	-2.76158
H	2.14856	3.38815	-1.81927
H	5.01179	0.66395	0.11485
H	5.27172	-0.49612	-1.20353
H	5.07004	1.22936	-1.57030
H	-2.16683	-1.82999	0.46004
H	-2.22255	-1.07185	2.05430
H	-4.18132	-2.63482	1.59466
H	-4.65543	-0.99885	2.04648
H	-5.75921	-2.12793	-0.25406
C	-1.97008	3.41812	0.54246
H	-1.70967	3.60383	1.59036
H	-1.73566	4.31420	-0.04334
H	-3.04788	3.24278	0.48868
H	1.05923	0.59733	0.54510
O	0.74623	0.07820	2.16150
C	1.76943	0.41147	2.83486
O	2.91340	0.58260	2.36948
H	1.61956	0.55397	3.92357
H	2.42436	-3.28419	1.31990
H	1.01272	-2.19439	1.64900
H	0.79540	-3.70352	0.69204
H	-4.81537	-0.14709	-2.98672
H	-6.25208	-0.89088	-2.25284
H	-5.94602	0.84731	-2.06666

3a-γ′-addition-2a

Geometry with 73 atoms:

C	1.06758	-2.90376	-0.54415
N	0.31702	-1.86235	-1.21250
C	-1.05129	-1.78681	-1.20055
C	2.45740	-2.37229	-0.18144
N	2.34699	-0.98686	0.36641
C	3.50289	-0.51562	1.20240
C	3.38615	1.00590	1.41958
N	3.27355	1.72371	0.13852
C	-1.61025	-0.55097	-1.87002
C	-1.88363	-2.63663	-0.54058
C	-3.31872	-2.35130	-0.44374
S	1.79858	2.38504	-0.19305
O	0.73629	1.35928	-0.20067
O	1.57467	3.50512	0.72141

C	2.04162	2.96799	-1.84873
C	-4.10443	-3.14949	0.56247
C	-3.07565	-0.70764	-2.28175
C	-3.88637	-1.41506	-1.22599
C	4.58367	1.55560	2.18976
C	3.52709	-1.25867	2.53296
H	0.54644	-3.11972	0.39733
H	0.81738	-1.29635	-1.89674
H	3.11118	-2.31038	-1.05602
H	2.92114	-3.02488	0.55880
H	1.46850	-0.89980	0.90438
H	4.39936	-0.72599	0.60762
H	2.47260	1.19517	2.00214
H	3.72146	1.23514	-0.66640
H	-1.50213	-3.50498	-0.00808
N	-1.05309	-1.18436	2.25506
C	-1.50366	-0.00599	1.56680
C	-2.81340	0.26612	1.49445
O	-1.83726	-1.90248	2.84722
O	0.16412	-1.40947	2.21940
C	-3.38589	1.42083	0.80291
C	-2.58895	2.41679	0.21415
C	-4.78139	1.52105	0.71390
C	-3.18323	3.48091	-0.45323
C	-5.37361	2.58614	0.04184
C	-4.57471	3.56726	-0.54377
H	-0.68702	0.54634	1.11668
H	-3.50966	-0.42174	1.97061
H	-1.50452	2.35777	0.27310
H	-5.39858	0.74787	1.16630
H	-2.55932	4.24807	-0.90296
H	-6.45569	2.65026	-0.02557
H	-5.03460	4.40047	-1.06762
H	4.47392	-1.07397	3.04489
H	2.70954	-0.92296	3.18052
H	3.43636	-2.34035	2.40839
H	5.51537	1.31984	1.66257
H	4.49182	2.64242	2.25381
H	4.63713	1.15301	3.20485
H	-1.49600	0.28001	-1.16050
H	-0.99587	-0.28929	-2.73993
H	-3.49787	0.27969	-2.50218
H	-3.12775	-1.28555	-3.21906
H	-4.95362	-1.21159	-1.15740
C	1.18908	-4.18804	-1.36310
H	1.71586	-3.98801	-2.30286
H	1.73466	-4.96258	-0.81201
H	0.19427	-4.57351	-1.60481
H	2.22547	-0.37608	-0.47121
O	2.38841	-0.20725	-2.35404
C	3.62147	-0.20129	-2.62349
O	4.53523	0.18397	-1.85837
H	3.91814	-0.56799	-3.62806
H	2.91411	3.62314	-1.86559
H	2.15807	2.09770	-2.49862
H	1.13648	3.52262	-2.10885
H	-3.68953	-3.02895	1.57069
H	-5.15723	-2.84924	0.57819
H	-4.06074	-4.22067	0.32625

3a-γ′-addition-TS2a-3a

Geometry with 73 atoms:

C	1.25279	-2.92763	-0.56308
N	0.45915	-1.95787	-1.30380
C	-0.88078	-1.85416	-1.24327
C	2.54553	-2.27166	-0.06712
N	2.27320	-0.91866	0.49761
C	3.36088	-0.37674	1.38380
C	3.16565	1.14038	1.55186
N	3.16706	1.81185	0.23858
C	-1.44373	-0.62973	-1.92865
C	-1.69688	-2.76199	-0.58603
C	-3.06047	-2.47157	-0.32794
S	1.72686	2.46636	-0.23094
O	0.67621	1.43307	-0.32897
O	1.42010	3.59047	0.65207
C	2.11565	3.03933	-1.86262
C	-3.88552	-3.43465	0.48134
C	-2.97621	-0.58308	-1.94675
C	-3.60606	-1.27505	-0.76489
C	4.25081	1.75910	2.42798
C	3.33805	-1.10126	2.72380
H	0.67258	-3.20820	0.32141
H	0.97210	-1.30361	-1.90175
H	3.27609	-2.13960	-0.86924
H	2.98704	-2.89975	0.70785
H	1.37324	-0.94087	1.02919
H	4.29916	-0.55736	0.84546
H	2.18874	1.30553	2.02874
H	3.66120	1.28698	-0.51466
H	-1.27290	-3.65969	-0.14669
N	-1.16136	-1.31641	1.94791

C	-1.59529	-0.22473	1.22798
C	-2.95334	-0.02985	1.02041
O	-1.96538	-2.12472	2.42651
O	0.08594	-1.46578	2.12420
C	-3.48305	1.25881	0.53287
C	-2.65990	2.25054	-0.02185
C	-4.85991	1.50490	0.63086
C	-3.20627	3.45224	-0.46391
C	-5.40504	2.70569	0.18639
C	-4.57832	3.68430	-0.36618
H	-0.79791	0.40820	0.86530
H	-3.62580	-0.61622	1.64004
H	-1.58678	2.09439	-0.10245
H	-5.50607	0.74360	1.06361
H	-2.55248	4.21303	-0.88159
H	-6.47385	2.87932	0.27470
H	-4.99930	4.62370	-0.71314
H	4.23773	-0.86021	3.29382
H	2.45947	-0.80860	3.30888
H	3.31480	-2.18734	2.60267
H	5.24343	1.54625	2.01427
H	4.11231	2.84279	2.44532
H	4.20489	1.38905	3.45571
H	-1.01948	0.24611	-1.42667
H	-1.05548	-0.59954	-2.95426
H	-3.31356	0.45669	-2.01914
H	-3.34171	-1.09074	-2.85155
H	-4.67143	-1.10944	-0.60965
C	1.57432	-4.16665	-1.39420
H	2.13564	-3.88611	-2.29231
H	2.17071	-4.88215	-0.81741
H	0.65019	-4.66107	-1.70796
H	2.12366	-0.29213	-0.31857
O	2.41606	-0.17023	-2.29859
C	3.66419	-0.16502	-2.48512
O	4.52506	0.22083	-1.66173
H	4.02812	-0.53386	-3.46685
H	2.98750	3.69317	-1.80664
H	2.28702	2.16643	-2.49623
H	1.23775	3.59444	-2.20317
H	-3.26299	-4.08648	1.09804
H	-4.57507	-2.89740	1.14147
H	-4.49113	-4.06164	-0.18565

3a-γ′-addition-3a

Geometry with 73 atoms:

C	1.31597	-2.94501	-0.38635
N	0.54677	-2.02983	-1.23844
C	-0.75970	-1.92626	-1.25895
C	2.53482	-2.20390	0.17291
N	2.16237	-0.85568	0.67156
C	3.19868	-0.21592	1.55027
C	2.95189	1.30107	1.58234
N	3.06638	1.86002	0.21910
C	-1.33835	-0.75634	-2.01123
C	-1.61305	-2.89292	-0.63485
C	-2.88334	-2.55985	-0.28227
S	1.67890	2.47423	-0.42746
O	0.64616	1.42772	-0.57131
O	1.28150	3.64698	0.34834
C	2.23094	2.95195	-2.04308
C	-3.79992	-3.52010	0.39598
C	-2.86250	-0.69694	-1.90847
C	-3.38018	-1.17073	-0.54527
C	3.93202	2.02138	2.50219
C	3.14323	-0.83424	2.94203
H	0.67398	-3.21048	0.45892
H	1.10685	-1.36348	-1.79747
H	3.31839	-2.07842	-0.57898
H	2.93580	-2.78899	1.00269
H	1.22746	-0.92878	1.23568
H	4.16828	-0.40418	1.07139
H	1.92993	1.47131	1.95106
H	3.59987	1.26658	-0.45201
H	-1.21090	-3.86210	-0.35598
N	-1.13675	-1.22810	1.84640
C	-1.56173	-0.26148	1.06081
C	-3.00370	-0.21991	0.67347
O	-1.90325	-2.15161	2.25024
O	0.12208	-1.26718	2.22555
C	-3.51127	1.18126	0.38268
C	-2.69463	2.18829	-0.14303
C	-4.86303	1.46791	0.60456
C	-3.21847	3.44797	-0.43383
C	-5.38992	2.72395	0.31122
C	-4.56665	3.72114	-0.21098
H	-0.83203	0.49355	0.80484
H	-3.57205	-0.62090	1.52269
H	-1.63784	2.00644	-0.32301
H	-5.50912	0.69765	1.02274
H	-2.56225	4.21885	-0.82910
H	-6.44074	2.92626	0.50040

H	-4.97132	4.70468	-0.43317
H	4.01846	-0.53077	3.52082
H	2.23582	-0.52391	3.46995
H	3.14526	-1.92686	2.89913
H	4.96579	1.79032	2.21943
H	3.78195	3.09920	2.40372
H	3.77830	1.74537	3.54907
H	-0.86626	0.15142	-1.61950
H	-1.02233	-0.83919	-3.05914
H	-3.20322	0.32280	-2.11028
H	-3.30744	-1.34293	-2.67409
H	-4.47689	-1.18722	-0.57578
C	1.74788	-4.18598	-1.15858
H	2.34465	-3.90345	-2.03254
H	2.35016	-4.84160	-0.52158
H	0.87482	-4.74757	-1.50368
H	1.99043	-0.25905	-0.15568
O	2.45925	-0.33969	-2.28202
C	3.71828	-0.31580	-2.37065
O	4.50609	0.14894	-1.51762
H	4.16390	-0.74356	-3.29350
H	3.07393	3.63638	-1.93628
H	2.49632	2.04879	-2.59643
H	1.38323	3.45347	-2.51680
H	-3.29179	-4.44620	0.67423
H	-4.20763	-3.05834	1.30188
H	-4.64400	-3.75654	-0.26550

3a-γ′-addition-2b

Geometry with 73 atoms:

C	-0.95048	2.48418	0.98463
N	-0.58371	1.86683	-0.27388
C	0.69755	1.78449	-0.74672
C	-2.09768	1.69767	1.66870
N	-2.24019	0.32876	1.09912
C	-3.11785	-0.60672	1.87708
C	-3.44679	-1.83491	1.00482
N	-3.99627	-1.43484	-0.30186
C	0.83925	0.95094	-1.99904
C	1.81650	2.25165	-0.12479
C	3.14599	1.93885	-0.65705
S	-2.98833	-1.66781	-1.59978
O	-1.73592	-0.91024	-1.46229
O	-2.84779	-3.11128	-1.79554
C	-3.95741	-0.95776	-2.90551
C	4.32227	2.20918	0.23990
C	2.08769	1.31502	-2.79963
C	3.29027	1.44581	-1.90267
C	-4.44267	-2.76257	1.69596
C	-2.43733	-1.01526	3.17695
H	-0.07508	2.39926	1.63335
H	-1.33629	1.74523	-0.94908
H	-3.06572	2.18400	1.51930
H	-1.90417	1.62081	2.73896
H	-1.31275	-0.10015	0.93371
H	-4.04229	-0.04939	2.06847
H	-2.51301	-2.38743	0.82843
H	-4.47712	-0.51390	-0.29248
H	1.75870	2.81544	0.80352
H	-3.14234	-1.55962	3.80918
H	-1.57703	-1.66403	2.97659
H	-2.08625	-0.15378	3.74915
H	-5.36301	-2.21936	1.94030
H	-4.69663	-3.57730	1.01359
H	-4.03177	-3.19570	2.61219
H	0.87403	-0.10058	-1.67256
H	-0.06308	1.03941	-2.61383
H	2.25409	0.56793	-3.58300
H	1.91645	2.27518	-3.31421
H	4.28080	1.21925	-2.29363
C	-1.33475	3.95474	0.83477
H	-2.18741	4.04749	0.15265
H	-1.61021	4.39166	1.80222
H	-0.49562	4.52477	0.42382
H	-2.63431	0.48443	0.14555
H	-4.93862	-1.43505	-2.91598
H	-4.01892	0.11905	-2.73322
H	-3.41667	-1.16692	-3.83203
N	1.08307	-0.44807	1.59449
C	2.51526	-0.55474	1.55231
C	3.10851	-1.11152	0.48734
O	0.39953	-1.00603	0.74069
O	0.59292	0.20187	2.51548
C	4.54970	-1.26260	0.29701
C	5.48336	-1.00968	1.31414
C	5.01033	-1.66409	-0.96555
C	6.84424	-1.14140	1.06507
C	6.37278	-1.79197	-1.21491
C	7.29212	-1.52772	-0.20017
H	2.98004	-0.10259	2.41765
H	2.46568	-1.46476	-0.31679
H	5.14818	-0.71747	2.30559

H	4.28831	-1.85806	-1.75550
H	7.55948	-0.94554	1.85848
H	6.71672	-2.09741	-2.19861
H	8.35678	-1.62780	-0.39144
O	-3.34305	1.69544	-1.10153
C	-4.51409	1.90983	-0.68487
O	-5.18908	1.13767	0.03481
H	-4.98562	2.86900	-0.98614
H	4.20783	1.70294	1.20762
H	5.26119	1.87608	-0.21372
H	4.40519	3.28288	0.45383

3a-γ′-addition-TS2b-3b

Geometry with 73 atoms:

C	-1.02548	2.66489	0.48844
N	-0.63381	1.86762	-0.67224
C	0.61698	1.66327	-1.08220
C	-2.06134	1.91459	1.36678
N	-2.12760	0.46162	1.06221
C	-2.95275	-0.36099	2.00847
C	-3.22723	-1.72051	1.33892
N	-3.90256	-1.52860	0.04097
C	0.78939	0.49970	-2.02325
C	1.71756	2.37551	-0.59370
C	3.02758	1.94363	-0.85279
S	-3.01407	-1.91619	-1.30300
O	-1.80517	-1.08472	-1.42168
O	-2.79877	-3.36302	-1.29631
C	-4.14781	-1.46290	-2.59116
C	4.15239	2.63372	-0.14215
C	2.21276	0.32584	-2.55314
C	3.26184	0.76680	-1.56408
C	-4.08272	-2.62684	2.21848
C	-2.23565	-0.51825	3.34186
H	-0.12466	2.77174	1.09518
H	-1.39014	1.42183	-1.19795
H	-3.07076	2.30445	1.21253
H	-1.78469	2.03827	2.41391
H	-1.17077	0.04042	0.99129
H	-3.90170	0.17644	2.12485
H	-2.25910	-2.20955	1.15936
H	-4.41491	-0.62651	-0.04454
H	1.56923	3.23195	0.05714
H	-2.91265	-0.96660	4.07270
H	-1.35193	-1.15598	3.23405
H	-1.90401	0.44155	3.74423
H	-5.01947	-2.12551	2.48919
H	-4.32767	-3.53238	1.65822
H	-3.55674	-2.91700	3.13227
H	0.47840	-0.37764	-1.44034
H	0.06687	0.58334	-2.84292
H	2.36531	-0.71781	-2.85086
H	2.34659	0.92888	-3.46324
H	4.29282	0.53389	-1.81795
C	-1.55780	4.03461	0.08153
H	-2.42595	3.91639	-0.57496
H	-1.85751	4.60758	0.96613
H	-0.78789	4.60055	-0.45219
H	-2.54365	0.39969	0.11385
H	-5.09043	-1.98934	-2.43417
H	-4.27008	-0.37768	-2.57117
H	-3.68089	-1.77531	-3.52870
N	1.13694	-0.01034	1.44615
C	2.48763	0.01679	1.27083
C	3.11073	-0.58458	0.16737
O	0.40145	-0.75471	0.73526
O	0.60717	0.68826	2.34923
C	4.53494	-0.98591	0.22115
C	5.44681	-0.44316	1.13736
C	4.99448	-1.95472	-0.68365
C	6.77802	-0.85301	1.14007
C	6.32276	-2.36808	-0.67810
C	7.22270	-1.81492	0.23353
H	2.99065	0.62799	2.00666
H	2.47179	-1.23998	-0.42092
H	5.12177	0.29785	1.86209
H	4.29459	-2.38722	-1.39585
H	7.46970	-0.42336	1.85934
H	6.65599	-3.12454	-1.38309
H	8.26039	-2.13565	0.24165
O	-3.37345	1.50224	-1.29436
C	-4.53982	1.71100	-0.86635
O	-5.14598	1.02584	-0.00913
H	-5.07974	2.58458	-1.29031
H	4.06518	2.46045	0.94079
H	5.12937	2.27360	-0.47331
H	4.10319	3.71766	-0.29412

3a-γ′-addition-3b

Geometry with 73 atoms:

C	-1.57734	2.94554	0.16329
N	-0.98879	2.23806	-0.98265

C	0.29282	2.04870	-1.15734
C	-2.64905	2.06445	0.82295
N	-2.21769	0.64580	0.89105
C	-2.92960	-0.19473	1.90925
C	-2.67132	-1.66946	1.56177
N	-3.24137	-1.96768	0.23012
C	0.71868	0.97257	-2.11273
C	1.27646	2.84534	-0.46448
C	2.56608	2.44544	-0.39787
S	-2.15534	-2.48213	-0.91013
O	-1.13232	-1.46401	-1.18281
O	-1.66709	-3.80043	-0.50551
C	-3.21075	-2.62553	-2.33128
C	3.60304	3.27073	0.29343
C	2.23050	0.92301	-2.33328
C	3.01219	1.15022	-1.03374
C	-3.26475	-2.62933	2.58697
C	-2.43186	0.16921	3.30082
H	-0.77668	3.07732	0.89498
H	-1.65542	1.69115	-1.55239
H	-3.59737	2.09653	0.28111
H	-2.81261	2.43911	1.83472
H	-1.14759	0.56429	1.04840
H	-4.00128	0.01658	1.79767
H	-1.58121	-1.81221	1.52464
H	-3.89189	-1.24732	-0.13962
H	0.96746	3.76034	0.03160
H	-3.00235	-0.37481	4.05684
H	-1.36603	-0.06416	3.40590
H	-2.55909	1.23556	3.50802
H	-4.33517	-2.43506	2.72342
H	-3.14622	-3.65114	2.21822
H	-2.76030	-2.55116	3.55400
H	0.35360	0.03823	-1.66945
H	0.17974	1.09918	-3.05945
H	2.49859	-0.05010	-2.75978
H	2.52940	1.68846	-3.05953
H	4.07255	1.26273	-1.28850
C	-2.16008	4.28960	-0.25143
H	-2.92480	4.15267	-1.02346
H	-2.62011	4.78661	0.60869
H	-1.37832	4.94223	-0.65100
H	-2.37682	0.25335	-0.05610
H	-4.06085	-3.26148	-2.08028
H	-3.52059	-1.62235	-2.63117
H	-2.60285	-3.08347	-3.11563
N	1.27379	0.55684	1.71309
C	2.52914	0.37630	1.38133
C	2.88387	-0.05637	-0.01861
O	0.36103	0.32190	0.80643
O	0.89017	0.96128	2.85998
C	4.13351	-0.91652	-0.01630
C	5.38438	-0.38096	0.31320
C	4.04977	-2.27731	-0.32174
C	6.52226	-1.18377	0.33648
C	5.18769	-3.08501	-0.30451
C	6.42689	-2.54078	0.02451
H	3.25676	0.54750	2.16390
H	2.05142	-0.67787	-0.36570
H	5.47117	0.67759	0.55619
H	3.08183	-2.70864	-0.56854
H	7.48414	-0.75093	0.59841
H	5.10214	-4.14073	-0.54719
H	7.31392	-3.16776	0.03921
O	-3.15768	0.77408	-1.89480
C	-4.40041	0.69930	-1.68822
O	-4.95309	0.10691	-0.73470
H	-5.06067	1.20443	-2.42456
H	4.16793	2.66091	1.00672
H	4.32231	3.64444	-0.44780
H	3.16814	4.12119	0.82461

3b-γ-addition-1

Geometry with 70 atoms:

C	3.06671	0.52752	-0.65243
C	3.17791	-0.71036	0.25891
N	2.11355	1.47994	-0.10954
C	3.79393	-1.93099	-0.46525
C	2.72841	-3.02881	-0.61115
C	2.34513	-3.54292	0.78385
C	1.99152	-2.33316	1.66890
N	1.83091	-1.12571	0.79461
C	0.84375	-1.41618	-0.29156
C	1.47725	-2.42563	-1.26870
H	2.13489	1.62078	0.90322
C	1.05432	2.00207	-0.78788
S	0.91663	1.87062	-2.48815
N	0.15669	2.60012	-0.00047
H	0.32715	2.55798	1.02066
C	-1.12344	3.18392	-0.38182
C	-2.23419	2.13582	-0.16450
N	-2.06977	1.07773	-1.14671

C	-2.41288	-0.23051	-0.95970
H	0.75496	-3.21311	-1.50749
H	3.17264	-4.10056	1.23239
H	-2.07465	1.70995	0.83796
H	-1.07606	3.44240	-1.44578
H	0.57319	-0.47345	-0.77160
H	-0.04958	-1.80636	0.20506
H	2.77094	-2.08747	2.39289
H	1.05015	-2.45670	2.20863
H	3.11962	-3.84605	-1.22304
H	4.65773	-2.31311	0.08898
H	4.15026	-1.62882	-1.45605
H	3.74659	-0.43979	1.15548
H	2.68117	0.21968	-1.62923
C	-2.12026	-1.11557	-2.15327
C	-2.98889	-0.72731	0.17375
H	-2.34888	-0.55572	-3.06829
H	-1.04147	-1.32957	-2.19247
C	-3.27863	-2.14608	0.35272
C	-3.92496	-2.62916	1.43379
C	-2.77935	-3.07221	-0.73531
C	-4.42936	-1.78594	2.57542
H	1.49155	-4.22508	0.70825
C	-2.91229	-2.42055	-2.11051
H	-3.31893	-4.02469	-0.69620
H	-3.97042	-2.21175	-2.31128
H	-3.24353	-0.05286	0.98648
H	-2.55727	-3.09696	-2.89618
H	-1.49141	1.29063	-1.95466
H	-4.92649	-2.40393	3.32853
H	-5.15440	-1.03292	2.23958
H	-4.09642	-3.70342	1.49207
H	-3.61743	-1.24504	3.08046
H	-1.71513	-3.30040	-0.56058
C	-3.64577	2.72127	-0.24185
H	-4.37980	1.90901	-0.23728
H	-3.86033	3.37876	0.60631
H	-3.77488	3.28870	-1.17153
C	-1.33423	4.44757	0.44714
H	-2.22758	4.98778	0.12367
H	-1.43813	4.20563	1.51162
H	-0.47220	5.11115	0.33217
C	4.44394	1.16341	-0.83119
H	4.37248	1.98865	-1.54484
H	4.80505	1.56031	0.12423
H	5.17739	0.44232	-1.20738
H	1.74274	-1.92847	-2.20905
H	1.51735	-0.34841	1.42584
O	1.86484	0.60223	2.78790
C	1.29068	1.58838	3.33583
O	0.65355	2.49539	2.76615
H	1.38039	1.64808	4.44020

3b-γ-addition-2a

Geometry with 88 atoms:

C	2.83699	-1.44093	-0.51082
C	1.75758	-0.66636	-0.67293
N	0.58865	-0.87457	0.13682
O	-0.33229	-0.08143	-0.01832
O	0.53435	-1.82161	0.91852
H	2.78561	-2.22915	0.23730
H	1.62274	0.15706	-1.36133
C	-4.15017	0.15374	-0.96966
C	-3.96138	-1.37027	-0.90624
N	-2.87965	0.80422	-1.22617
C	-5.17244	-2.10714	-0.28721
C	-4.75873	-2.72947	1.05476
C	-3.70360	-3.81571	0.79924
C	-2.58064	-3.21662	-0.06842
N	-2.74169	-1.72738	-0.10011
C	-2.80080	-1.19135	1.29660
C	-4.13326	-1.63298	1.92955
H	-2.31887	0.47357	-2.02612
C	-2.42371	1.92275	-0.61780
S	-3.21532	2.64153	0.72120
N	-1.28227	2.39438	-1.14195
H	-0.85225	1.80690	-1.86374
C	-0.52926	3.56842	-0.72572
C	0.69826	3.15762	0.10766
N	0.25357	2.51246	1.32976
C	1.00506	1.58982	2.00135
H	-3.95444	-2.00618	2.94258
H	-4.15018	-4.67395	0.28798
H	1.26730	2.42098	-0.48665
H	-1.19003	4.17506	-0.09808
H	-2.68277	-0.10689	1.24903
H	-1.92842	-1.60412	1.80812
H	-2.60946	-3.54966	-1.10736
H	-1.58032	-3.41112	0.32383
H	-5.63382	-3.15892	1.55037
H	-5.54109	-2.88090	-0.96905
H	-5.99129	-1.39782	-0.12548

H	-3.72980	-1.73855	-1.91184
H	-4.50999	0.51858	-0.00310
C	0.27081	0.84972	3.09149
C	2.30706	1.29758	1.71945
H	-0.47482	1.51608	3.54262
H	-0.28212	0.01872	2.62580
C	3.04884	0.23968	2.39067
C	4.29447	-0.09911	1.99359
C	2.33826	-0.52043	3.49295
H	-3.30181	-4.17440	1.75288
C	1.23480	0.31205	4.14621
H	3.05998	-0.84900	4.24922
H	1.68279	1.15552	4.68667
H	2.83085	1.83177	0.92939
H	0.69010	-0.29315	4.87939
H	-0.75210	2.47529	1.48226
H	1.89174	-1.42981	3.06365
C	5.11579	-1.21681	2.57950
H	5.94541	-1.47671	1.91421
H	5.55728	-0.94617	3.54962
H	4.52367	-2.12665	2.74218
H	4.74992	0.47482	1.18580
C	4.08643	-1.31583	-1.26268
C	5.11244	-2.23668	-1.00843
C	4.30251	-0.30517	-2.21353
C	6.32508	-2.15584	-1.68748
H	4.95231	-3.01748	-0.26836
C	5.51354	-0.22465	-2.88973
H	3.52434	0.42297	-2.42547
C	6.52839	-1.14871	-2.62955
H	7.11032	-2.87729	-1.48104
H	5.66848	0.56115	-3.62325
H	7.47373	-1.08149	-3.16038
C	-5.16568	0.50767	-2.05691
H	-4.77652	0.22823	-3.04275
H	-6.12255	-0.00222	-1.90425
H	-5.34720	1.58609	-2.05038
H	-4.81691	-0.78002	2.01112
C	-0.14291	4.35522	-1.97651
H	0.32212	5.31085	-1.72158
H	0.55831	3.78321	-2.59775
H	-1.03716	4.55853	-2.57233
C	1.60099	4.35183	0.43062
H	2.15320	4.69408	-0.45031
H	1.00204	5.18497	0.81791
H	2.32689	4.07673	1.20117
H	-1.92405	-1.35060	-0.62047
O	-1.06458	-1.75572	-2.23592
C	-0.48370	-0.92557	-2.97735
O	-0.74989	0.29631	-3.10577
H	0.35659	-1.31619	-3.59388

3b-γ-addition-TS2a-3a

Geometry with 88 atoms:

C	3.00230	-1.20157	0.00453
C	1.84342	-0.55637	-0.42245
N	0.67954	-0.70715	0.28417
O	-0.34614	-0.07382	-0.08685
O	0.62397	-1.47953	1.27037
H	2.86786	-2.03476	0.68997
H	1.74631	0.09569	-1.28041
C	-4.18297	-0.01605	-0.69144
C	-3.82020	-1.50580	-0.68996
N	-3.03138	0.73865	-1.14523
C	-4.89277	-2.40693	-0.04761
C	-4.19654	-3.50367	0.77290
C	-3.09416	-4.13890	-0.08908
C	-1.98438	-3.09401	-0.31648
N	-2.52713	-1.74377	0.04501
C	-2.70040	-1.64982	1.52935
C	-3.54390	-2.84967	2.00033
H	-2.48353	0.29163	-1.90332
C	-2.57141	1.89244	-0.62188
S	-3.31477	2.65632	0.72940
N	-1.48460	2.37277	-1.23853
H	-1.02775	1.75644	-1.93858
C	-0.75506	3.58486	-0.91260
C	0.49496	3.24289	-0.08191
N	0.06539	2.62309	1.17009
C	0.81820	1.82706	1.92045
H	-2.91414	-3.57896	2.52166
H	-3.51146	-4.46997	-1.04636
H	1.06440	2.48750	-0.64432
H	-1.41282	4.22268	-0.31242
H	-3.17041	-0.68644	1.74088
H	-1.69254	-1.63769	1.94869
H	-1.65231	-3.02038	-1.35398
H	-1.11454	-3.25145	0.32698
H	-4.92110	-4.26039	1.08591
H	-5.52149	-2.84276	-0.83011
H	-5.54505	-1.81269	0.60578
H	-3.60447	-1.81331	-1.71906

H	-4.42082	0.31277	0.32494
C	0.14186	1.13396	3.06786
C	2.15050	1.52845	1.62569
H	-0.65334	1.77126	3.47024
H	-0.33345	0.23521	2.64552
C	2.83896	0.49177	2.28056
C	3.96069	-0.06089	1.65829
C	2.27924	-0.10725	3.55180
H	-2.67558	-5.01933	0.40808
C	1.15191	0.74074	4.14326
H	3.08908	-0.21504	4.28466
H	1.57204	1.65088	4.58933
H	2.62755	1.99069	0.76671
H	0.64827	0.19036	4.94430
H	-0.93383	2.67607	1.38645
H	1.91393	-1.11887	3.33321
C	4.82411	-1.09267	2.33038
H	5.54741	-1.51510	1.62632
H	5.39727	-0.65733	3.16100
H	4.22951	-1.91726	2.74257
H	4.44856	0.56436	0.91205
C	4.16503	-1.27941	-0.90374
C	4.99654	-2.40694	-0.87574
C	4.46256	-0.24898	-1.80889
C	6.08932	-2.50882	-1.73478
H	4.77439	-3.21429	-0.18127
C	5.55213	-0.35053	-2.66659
H	3.83916	0.64162	-1.83911
C	6.37060	-1.48161	-2.63341
H	6.71835	-3.39413	-1.70398
H	5.76438	0.45536	-3.36354
H	7.22107	-1.55918	-3.30470
C	-5.39411	0.22715	-1.59188
H	-5.16584	-0.06391	-2.62364
H	-6.27048	-0.33537	-1.25221
H	-5.64515	1.29150	-1.58124
H	-4.30772	-2.51031	2.70665
C	-0.39087	4.29611	-2.21393
H	0.06042	5.27345	-2.02393
H	0.30881	3.69311	-2.80512
H	-1.29561	4.44630	-2.80954
C	1.36433	4.46955	0.19911
H	1.88532	4.79848	-0.70448
H	0.74714	5.29675	0.56963
H	2.11763	4.24562	0.96002
H	-1.81632	-1.03201	-0.23290
O	-1.52713	-1.04393	-2.70074
C	-0.43060	-0.53247	-3.05598
O	-0.12881	0.68201	-3.07485
H	0.35354	-1.24665	-3.39656

3b-γ-addition-3a

Geometry with 88 atoms:

C	3.28615	-0.62344	0.30761
C	2.01765	-0.38726	-0.44905
N	0.86442	-0.48444	0.16705
O	-0.23655	-0.10835	-0.41242
O	0.78862	-0.91624	1.37722
H	3.09698	-1.40013	1.05774
H	1.97623	-0.03266	-1.47094
C	-4.09056	-0.72063	-0.31906
C	-3.36983	-2.07180	-0.30938
N	-3.22334	0.23441	-0.98066
C	-4.14165	-3.19929	0.40236
C	-3.13277	-4.10995	1.12038
C	-1.97573	-4.42413	0.15901
C	-1.17834	-3.12821	-0.08415
N	-2.01844	-1.96266	0.34451
C	-2.13323	-1.94057	1.83656
C	-2.56938	-3.33652	2.32111
H	-2.72274	-0.14477	-1.81079
C	-2.94163	1.48303	-0.58034
S	-3.63405	2.18571	0.83679
N	-2.07623	2.12595	-1.37587
H	-1.63598	1.57322	-2.14070
C	-1.56474	3.47272	-1.21919
C	-0.20620	3.43225	-0.49579
N	-0.43369	2.89195	0.85523
C	0.45018	2.31288	1.61548
H	-1.71830	-3.87699	2.75113
H	-2.36782	-4.81846	-0.78497
H	0.42582	2.71299	-1.03193
H	-2.27509	4.04410	-0.61031
H	-2.85812	-1.16332	2.09085
H	-1.15320	-1.63799	2.20645
H	-0.93591	-2.95532	-1.13589
H	-0.26195	-3.07226	0.50935
H	-3.61889	-5.03230	1.45059
H	-4.72591	-3.75947	-0.33443
H	-4.84786	-2.78105	1.13244
H	-3.14882	-2.34523	-1.34634
H	-4.26299	-0.37227	0.70400

C	0.00163	1.71960	2.91646
C	1.80336	2.10404	1.18250
H	-0.83239	2.29768	3.32644
H	-0.36525	0.71456	2.66216
C	2.62339	1.26116	1.86459
C	3.78251	0.65951	1.11708
C	2.33277	0.83827	3.27496
H	-1.31825	-5.18801	0.58590
C	1.17273	1.62014	3.89118
H	3.23950	0.97171	3.87822
H	1.51182	2.63008	4.15461
H	2.08950	2.42984	0.18792
H	0.84343	1.13800	4.81606
H	-1.41802	2.86524	1.16572
H	2.11712	-0.23852	3.25638
C	4.97913	0.30267	1.99664
H	5.82507	-0.01211	1.37919
H	5.30212	1.16213	2.59430
H	4.73956	-0.52021	2.68037
H	4.09655	1.38942	0.35900
C	4.39488	-1.09268	-0.61446
C	5.06450	-2.29337	-0.36589
C	4.78052	-0.32984	-1.72316
C	6.09423	-2.72579	-1.20175
H	4.77440	-2.89564	0.49248
C	5.80661	-0.75821	-2.56215
H	4.27046	0.60745	-1.93958
C	6.46882	-1.95858	-2.30299
H	6.60198	-3.66341	-0.99218
H	6.08700	-0.15606	-3.42201
H	7.26866	-2.29368	-2.95730
C	-5.42997	-0.83560	-1.04684
H	-5.27499	-1.17398	-2.07793
H	-6.10529	-1.53541	-0.54354
H	-5.91226	0.14566	-1.07536
H	-3.32594	-3.23565	3.10579
C	-1.43994	4.10823	-2.60188
H	-1.17151	5.16574	-2.53349
H	-0.68569	3.58666	-3.20253
H	-2.39866	4.02961	-3.12142
C	0.46937	4.79819	-0.39652
H	0.81221	5.13141	-1.37926
H	-0.22875	5.54295	0.00321
H	1.33909	4.75707	0.26667
H	-1.47363	-1.10017	0.02588
O	-1.77637	-1.25356	-2.83782
C	-0.83266	-0.55608	-3.29489
O	-0.80290	0.68961	-3.42557
H	0.06924	-1.11442	-3.63438

3b-γ-addition-2b

Geometry with 88 atoms:

C	2.74820	-1.71569	-0.18865
C	1.74366	-0.88699	-0.49606
N	0.51981	-0.93367	0.26006
O	-0.31514	-0.07378	0.01226
O	0.34291	-1.81908	1.09452
H	2.59939	-2.39732	0.64624
H	1.71555	-0.11815	-1.25705
C	-4.16812	0.09257	-0.95331
C	-3.99845	-1.42026	-0.74448
N	-2.88937	0.69632	-1.27373
C	-5.22383	-2.07929	-0.06853
C	-4.82745	-2.58177	1.32728
C	-3.78673	-3.70007	1.17988
C	-2.64636	-3.19509	0.27575
N	-2.78807	-1.71278	0.10259
C	-2.85572	-1.04464	1.44105
C	-4.19514	-1.41765	2.10362
H	-2.33930	0.28337	-2.04195
C	-2.42066	1.86782	-0.78641
S	-3.19224	2.72526	0.47983
N	-1.28159	2.27515	-1.36703
H	-0.86115	1.61410	-2.02808
C	-0.52559	3.48727	-1.08898
C	0.71985	3.16369	-0.24479
N	0.30253	2.65241	1.04901
C	1.07257	1.80742	1.79592
H	-4.02346	-1.70035	3.14678
H	-4.24092	-4.59330	0.74008
H	1.27355	2.36515	-0.77017
H	-1.17640	4.15133	-0.51087
H	-2.73431	0.03004	1.28999
H	-1.98958	-1.40840	1.99749
H	-2.66693	-3.62293	-0.72830
H	-1.65336	-3.36340	0.69654
H	-5.71193	-2.95204	1.85319
H	-5.60198	-2.90612	-0.67909
H	-6.03152	-1.34511	0.02378
H	-3.76447	-1.88491	-1.70887
H	-4.52174	0.55325	-0.02576
C	0.36228	1.18166	2.97149

C	2.37681	1.51234	1.51787
H	-0.34608	1.90677	3.39086
H	-0.23515	0.33544	2.59675
C	3.15210	0.54646	2.28223
C	4.43671	0.24136	1.99677
C	2.41539	-0.18458	3.38674
C	5.26036	0.84099	0.88994
H	-3.39958	-3.98070	2.16534
C	1.34710	0.69652	4.03328
H	3.12879	-0.55091	4.13338
H	1.82151	1.56172	4.51363
H	2.86783	2.00488	0.68489
H	0.81308	0.14078	4.81195
H	-0.70016	2.62797	1.22315
H	6.04925	0.14949	0.57311
H	5.75204	1.77312	1.20257
H	4.93435	-0.49694	2.62682
H	4.66084	1.07368	0.00224
H	1.91679	-1.06680	2.95757
C	1.62736	4.38600	-0.07445
H	2.36862	4.20409	0.70854
H	2.16174	4.62513	-0.99924
H	1.03388	5.25827	0.22491
C	-0.16849	4.14653	-2.41926
H	0.29557	5.12418	-2.26804
H	0.52454	3.51927	-2.99449
H	-1.07576	4.28514	-3.01407
C	-5.18127	0.35417	-2.06891
H	-5.34459	1.43097	-2.16852
H	-4.80002	-0.02777	-3.02284
H	-6.14592	-0.12208	-1.86554
H	-4.87129	-0.55492	2.10623
C	4.04315	-1.77098	-0.86578
C	5.05795	-2.55146	-0.29442
C	4.31308	-1.06390	-2.04765
C	6.31922	-2.61431	-0.87845
H	4.85231	-3.09840	0.62294
C	5.57258	-1.12888	-2.63188
H	3.53411	-0.46877	-2.51713
C	6.57960	-1.90084	-2.04803
H	7.09817	-3.21772	-0.42136
H	5.77106	-0.57918	-3.54736
H	7.56282	-1.94924	-2.50740
H	-1.96259	-1.39662	-0.44703
O	-1.09095	-1.96054	-1.99547
C	-0.50922	-1.22451	-2.83026
O	-0.77181	-0.02626	-3.10153
H	0.32928	-1.68844	-3.39700

3b-γ-addition-TS2b-3b

Geometry with 88 atoms:

C	2.99138	-1.17966	0.29589
C	1.84475	-0.62754	-0.27659
N	0.66311	-0.64343	0.41847
O	-0.33892	-0.05431	-0.06876
O	0.55300	-1.26754	1.50230
H	2.83042	-1.75474	1.20342
H	1.76866	-0.12245	-1.23020
C	-4.18063	-0.21977	-0.60976
C	-3.74050	-1.68098	-0.48231
N	-3.06817	0.54202	-1.14166
C	-4.77537	-2.59970	0.19119
C	-4.03318	-3.62423	1.06392
C	-2.87079	-4.21811	0.25157
C	-1.81813	-3.11645	0.02380
N	-2.45905	-1.78938	0.30425
C	-2.69373	-1.63995	1.77657
C	-3.45229	-2.88395	2.27822
H	-2.50886	0.05613	-1.86787
C	-2.65249	1.75408	-0.72597
S	-3.40339	2.59859	0.57151
N	-1.59793	2.22543	-1.40260
H	-1.12135	1.57453	-2.05619
C	-0.95017	3.51086	-1.22467
C	0.34286	3.34463	-0.40838
N	-0.00459	2.81594	0.91179
C	0.82217	2.14246	1.70045
H	-2.77856	-3.54519	2.83446
H	-3.23960	-4.60143	-0.70608
H	0.95384	2.58402	-0.91666
H	-1.63763	4.15929	-0.67073
H	-3.25306	-0.71288	1.92160
H	-1.70802	-1.52103	2.22901
H	-1.45081	-3.06578	-1.00364
H	-0.96827	-3.19224	0.70692
H	-4.71631	-4.41357	1.38897
H	-5.37496	-3.09709	-0.57739
H	-5.46097	-2.00979	0.81389
H	-3.47403	-2.05001	-1.47863
H	-4.42798	0.18924	0.37465
C	0.24805	1.54790	2.95451
C	2.15671	1.89422	1.35811

H	-0.53049	2.20820	3.35262
H	-0.23649	0.60350	2.66255
C	2.94319	0.96815	2.05825
C	4.07180	0.41999	1.44317
C	2.46359	0.42778	3.38895
C	4.79944	1.13455	0.33140
H	-2.41579	-5.05693	0.78700
C	1.34332	1.28081	3.98643
H	3.31199	0.38051	4.08161
H	1.75460	2.23801	4.33056
H	2.54491	2.30927	0.43605
H	0.91382	0.77948	4.85965
H	-0.99482	2.84855	1.17047
H	5.68421	0.57189	0.02187
H	5.13098	2.12981	0.65593
H	4.67520	-0.25672	2.04877
H	4.17373	1.27260	-0.56017
H	2.10945	-0.59989	3.24319
C	1.12100	4.65403	-0.27281
H	1.91622	4.55644	0.47206
H	1.58094	4.93817	-1.22349
H	0.45343	5.46210	0.04945
C	-0.67400	4.10924	-2.60274
H	-0.29802	5.13305	-2.52750
H	0.05847	3.50414	-3.15045
H	-1.60085	4.12705	-3.18262
C	-5.40570	-0.11596	-1.51878
H	-5.69479	0.93415	-1.61745
H	-5.17409	-0.50612	-2.51668
H	-6.25916	-0.66951	-1.11268
H	-4.25083	-2.57817	2.96111
C	4.13876	-1.60538	-0.52794
C	5.13659	-2.40030	0.05580
C	4.27585	-1.24273	-1.87571
C	6.24371	-2.81293	-0.67828
H	5.03866	-2.69133	1.09993
C	5.38520	-1.65344	-2.61033
H	3.51200	-0.64190	-2.36196
C	6.37488	-2.43560	-2.01565
H	7.00485	-3.42941	-0.20795
H	5.47366	-1.36265	-3.65337
H	7.23946	-2.75331	-2.59145
H	-1.78737	-1.04509	0.00807
O	-1.50959	-1.27787	-2.59065
C	-0.42521	-0.76757	-2.98107
O	-0.15623	0.44806	-3.10645
H	0.38190	-1.48776	-3.25138

3b-γ-addition-3b

Geometry with 88 atoms:

C	3.31048	-0.53105	0.34060
C	2.04558	-0.37317	-0.43991
N	0.89204	-0.48226	0.17911
O	-0.21236	-0.13933	-0.41113
O	0.81157	-0.89587	1.39542
H	3.08100	-1.18278	1.18930
H	1.97777	0.00251	-1.45181
C	-4.05679	-0.87963	-0.25995
C	-3.28156	-2.19975	-0.27422
N	-3.23662	0.11895	-0.91641
C	-4.00439	-3.36826	0.42177
C	-2.95725	-4.24983	1.12069
C	-1.79213	-4.50096	0.14970
C	-1.04793	-3.17018	-0.07247
N	-1.93335	-2.04664	0.37793
C	-2.04572	-2.05296	1.87053
C	-2.41894	-3.47462	2.33195
H	-2.74076	-0.22464	-1.76475
C	-3.00907	1.37541	-0.50748
S	-3.70052	2.02799	0.93324
N	-2.19476	2.06952	-1.31420
H	-1.74141	1.54908	-2.09382
C	-1.76979	3.44616	-1.16207
C	-0.39015	3.48735	-0.48190
N	-0.53703	2.92142	0.87067
C	0.40493	2.37848	1.58646
H	-1.54299	-3.98619	2.74697
H	-2.17208	-4.89335	-0.80006
H	0.26576	2.81588	-1.04882
H	-2.49768	3.96496	-0.52761
H	-2.80474	-1.31394	2.13819
H	-1.08054	-1.71202	2.24521
H	-0.81490	-2.97031	-1.12149
H	-0.13261	-3.08803	0.51963
H	-3.40445	-5.19632	1.43721
H	-4.57006	-3.93872	-0.32159
H	-4.72269	-2.98966	1.16175
H	-3.05362	-2.44717	-1.31629
H	-4.23587	-0.55142	0.76855
C	0.05243	1.76975	2.90863
C	1.74097	2.22507	1.07924
H	-0.79431	2.30018	3.35489

H	-0.26255	0.74160	2.67703
C	2.63923	1.44210	1.73015
C	3.79818	0.85701	0.97125
C	2.44200	1.02508	3.15826
C	4.37229	1.78305	-0.10305
H	-1.10285	-5.24519	0.56046
C	1.27373	1.74937	3.82692
H	3.37555	1.21287	3.70473
H	1.56741	2.77972	4.06423
H	1.94775	2.55057	0.06689
H	1.01704	1.25971	4.77056
H	-1.50462	2.85185	1.22369
H	5.33290	1.39828	-0.45594
H	4.53383	2.79184	0.29144
H	4.59216	0.60315	1.68526
H	3.71183	1.85718	-0.97443
H	2.28105	-0.06134	3.16352
C	0.20676	4.88946	-0.39024
H	1.10825	4.88866	0.23057
H	0.48251	5.25511	-1.38263
H	-0.51356	5.58682	0.05309
C	-1.72934	4.09935	-2.54133
H	-1.52211	5.17026	-2.46871
H	-0.96525	3.63044	-3.17231
H	-2.69839	3.96827	-3.03019
C	-5.39600	-1.04059	-0.98001
H	-5.92278	-0.08207	-0.98463
H	-5.23429	-1.35044	-2.01900
H	-6.03423	-1.78096	-0.48639
H	-3.17365	-3.41953	3.12301
C	4.46256	-1.15494	-0.42612
C	5.50143	-1.75445	0.29650
C	4.55653	-1.12577	-1.82058
C	6.60541	-2.30469	-0.34979
H	5.43756	-1.79650	1.38275
C	5.66070	-1.67613	-2.47274
H	3.76497	-0.67642	-2.41312
C	6.68990	-2.26504	-1.74169
H	7.39599	-2.77141	0.23179
H	5.71182	-1.64463	-3.55773
H	7.54719	-2.69647	-2.25079
H	-1.42729	-1.16035	0.06717
O	-1.77050	-1.26992	-2.82997
C	-0.85353	-0.53129	-3.27558
O	-0.86831	0.71659	-3.38738
H	0.06814	-1.05149	-3.62386

3b-γ-addition-2c

Geometry with 88 atoms:

C	1.98045	-0.15587	-1.30840
C	1.74705	-1.41484	-1.69036
N	0.52208	-2.06023	-1.29842
O	0.29732	-3.16857	-1.77341
O	-0.23754	-1.49892	-0.51541
H	1.19902	0.35559	-0.74845
H	2.37113	-2.05136	-2.30274
C	-3.47146	1.75356	-0.11193
C	-3.78273	0.67256	-1.15906
N	-2.03438	1.92266	-0.00636
C	-5.24973	0.18640	-1.11858
C	-5.29090	-1.27117	-0.63660
C	-4.59823	-2.16476	-1.67626
C	-3.21482	-1.56778	-1.99464
N	-2.89219	-0.52694	-0.96513
C	-3.02512	-1.11411	0.40566
C	-4.51772	-1.36552	0.68739
H	-1.51338	2.10537	-0.87975
C	-1.33625	2.11234	1.13546
S	-2.03946	1.96498	2.68709
N	-0.03738	2.40563	0.92968
H	0.25069	2.47166	-0.05069
C	0.98255	2.68685	1.93499
C	1.85698	1.43907	2.15894
N	1.01835	0.38714	2.70429
C	1.13894	-0.93584	2.37628
H	-4.64360	-2.35479	1.13742
H	-5.19496	-2.22469	-2.59140
H	2.22080	1.11398	1.17120
H	0.45947	2.92105	2.86880
H	-2.56581	-0.42257	1.11625
H	-2.43909	-2.03457	0.39214
H	-3.17164	-1.06313	-2.96154
H	-2.40606	-2.30160	-1.95521
H	-6.32817	-1.58654	-0.49412
H	-5.71120	0.27535	-2.10773
H	-5.82753	0.81421	-0.43197
H	-3.50520	1.05157	-2.14888
H	-3.83929	1.43463	0.86797
C	-0.02750	-1.78732	2.81646
C	2.19260	-1.48111	1.70785
H	-0.40353	-1.41198	3.77643
H	-0.83720	-1.65994	2.08528

C	2.18978	-2.86089	1.24019
C	3.15900	-3.33282	0.42616
C	1.00803	-3.72910	1.62023
C	3.17612	-4.71059	-0.18038
H	-4.49607	-3.18186	-1.28330
C	0.35700	-3.25904	2.91962
H	1.32428	-4.77446	1.70863
H	1.06214	-3.39103	3.75016
H	3.04541	-0.86536	1.42684
H	-0.52831	-3.86449	3.14387
H	0.10474	0.67731	3.04433
H	3.96367	-4.79447	-0.93559
H	2.22363	-4.95146	-0.67146
H	3.98276	-2.66418	0.17264
H	3.36135	-5.49593	0.56585
H	0.26161	-3.69657	0.81017
C	1.79204	3.90067	1.48801
H	2.46372	4.23712	2.28203
H	2.40059	3.66742	0.60528
H	1.11877	4.72537	1.23694
C	3.06276	1.70466	3.06073
H	3.80682	2.33839	2.56738
H	2.74628	2.18729	3.99349
H	3.54271	0.75544	3.31857
C	-4.13913	3.07331	-0.49907
H	-3.72093	3.44852	-1.44022
H	-5.22186	2.96501	-0.61971
H	-3.95473	3.81692	0.28144
H	-4.90176	-0.62925	1.40262
C	3.20991	0.58247	-1.61764
C	3.16080	1.98193	-1.70089
C	4.43367	-0.07314	-1.81974
C	4.31139	2.70952	-1.99208
H	2.20291	2.48427	-1.57991
C	5.58259	0.65812	-2.10408
H	4.48822	-1.15534	-1.73006
C	5.52395	2.05005	-2.19234
H	4.25937	3.79221	-2.06657
H	6.52759	0.14292	-2.25025
H	6.42281	2.61801	-2.41503
H	-1.92025	-0.21582	-1.16726
O	-1.01684	0.40825	-2.68108
C	-0.22724	1.37222	-2.80841
O	-0.09511	2.34987	-2.02166
H	0.42488	1.37020	-3.70831

3b-γ-addition-TS2c-3c

Geometry with 88 atoms:

C	2.75535	-1.05797	-0.07240
C	2.18802	-2.19662	0.48712
N	0.88084	-2.17967	0.91847
O	0.40339	-3.21038	1.44357
O	0.17516	-1.15351	0.76394
H	2.07778	-0.23095	-0.27786
H	2.66956	-3.15600	0.60805
C	-3.92506	0.11634	-0.70949
C	-3.67062	-1.38034	-0.89822
N	-2.70139	0.84137	-1.00164
C	-4.87380	-2.24805	-0.47445
C	-4.36069	-3.53030	0.19521
C	-3.26696	-4.13747	-0.69458
C	-2.04282	-3.20589	-0.66482
N	-2.47078	-1.86719	-0.12374
C	-2.76311	-1.98370	1.34263
C	-3.74139	-3.15492	1.54990
H	-2.05869	0.39974	-1.68386
C	-2.44055	2.10631	-0.60791
S	-3.41033	2.91891	0.54915
N	-1.35628	2.64705	-1.18877
H	-0.72196	1.99640	-1.68748
C	-0.77510	3.94599	-0.88542
C	0.44700	3.74095	0.02565
N	0.00216	3.03226	1.21989
C	0.70414	2.07546	1.84326
H	-3.21414	-4.01735	1.97249
H	-3.64059	-4.25667	-1.71759
H	1.13374	3.07521	-0.51423
H	-1.53110	4.53010	-0.35101
H	-3.17368	-1.02411	1.66516
H	-1.80145	-2.13804	1.83220
H	-1.60882	-3.00933	-1.64606
H	-1.26155	-3.56135	0.01011
H	-5.18098	-4.23962	0.33399
H	-5.48165	-2.48092	-1.35396
H	-5.50877	-1.69092	0.22652
H	-3.40318	-1.56115	-1.94578
H	-4.20601	0.32248	0.32895
C	-0.04066	1.26522	2.86784
C	2.02308	1.77738	1.54824
H	-0.83077	1.87423	3.32203
H	-0.52577	0.43699	2.32876
C	2.66803	0.64441	2.10402

C	3.82499	0.12928	1.53005
C	2.04513	-0.07874	3.27004
C	4.66309	-0.91747	2.20783
H	-2.97925	-5.12872	-0.33146
C	0.91101	0.70909	3.92227
H	2.82238	-0.30273	4.01090
H	1.33376	1.54113	4.49925
H	2.55343	2.33235	0.77935
H	0.36446	0.07012	4.62325
H	-0.98680	3.11596	1.45400
H	5.50411	-1.21372	1.57499
H	4.07663	-1.81639	2.44243
H	4.31672	0.74916	0.78227
H	5.08245	-0.54884	3.15412
H	1.68426	-1.05851	2.91846
C	-0.40662	4.64883	-2.18823
H	-0.05996	5.66930	-2.00205
H	0.38428	4.10297	-2.71682
H	-1.28394	4.69796	-2.83918
C	1.16191	5.03906	0.39433
H	1.65958	5.48223	-0.47329
H	0.45102	5.76749	0.80219
H	1.92257	4.84365	1.15698
C	-5.06919	0.55671	-1.62640
H	-4.82269	0.34127	-2.67251
H	-6.00770	0.05318	-1.37282
H	-5.22217	1.63354	-1.51775
H	-4.51982	-2.86320	2.26154
C	3.92346	-1.15633	-0.96887
C	4.07077	-0.18268	-1.96829
C	4.86148	-2.19526	-0.88774
C	5.13662	-0.24419	-2.86206
H	3.32142	0.60356	-2.05053
C	5.93041	-2.24954	-1.77697
H	4.76062	-2.96368	-0.12554
C	6.07256	-1.27421	-2.76542
H	5.23372	0.50983	-3.63808
H	6.65319	-3.05718	-1.70115
H	6.90575	-1.32177	-3.46094
H	-1.67042	-1.22738	-0.26383
O	-0.91504	-0.84342	-2.29706
C	0.26204	-0.38723	-2.27044
O	0.60684	0.80616	-2.12237
H	1.07578	-1.13513	-2.40471

3b-γ-addition-3c

Geometry with 88 atoms:

C	2.81509	-0.64488	0.28980
C	2.18527	-1.74443	1.08299
N	0.90100	-1.75057	1.35342
O	0.37744	-2.67256	2.08301
O	0.12232	-0.79859	0.92290
H	2.03882	-0.20723	-0.34597
H	2.73152	-2.57639	1.50575
C	-3.57473	-0.28922	-0.84308
C	-3.24773	-1.78341	-0.81359
N	-2.34475	0.44425	-1.09391
C	-4.47232	-2.65929	-0.47635
C	-4.01206	-3.86608	0.35444
C	-2.77522	-4.47748	-0.31937
C	-1.60543	-3.48528	-0.18560
N	-2.16294	-2.13280	0.17029
C	-2.67689	-2.14892	1.57874
C	-3.60864	-3.36193	1.74797
H	-1.62797	-0.07282	-1.64581
C	-2.17692	1.76001	-0.89103
S	-3.36515	2.73920	-0.12926
N	-0.99213	2.24830	-1.31646
H	-0.32290	1.57372	-1.73747
C	-0.69724	3.65785	-1.45770
C	-0.09263	4.30884	-0.17059
N	-0.47848	3.56564	1.02488
C	0.18381	2.59660	1.59627
H	-3.10003	-4.15869	2.30204
H	-2.98880	-4.68972	-1.37312
H	0.99809	4.27712	-0.23055
H	-1.63914	4.17667	-1.66592
H	-3.19102	-1.19768	1.73963
H	-1.78963	-2.18772	2.21297
H	-1.04337	-3.34270	-1.11072
H	-0.91494	-3.73754	0.62199
H	-4.81530	-4.60445	0.43020
H	-4.95370	-2.98106	-1.40510
H	-5.21062	-2.07637	0.09087
H	-2.82917	-2.05812	-1.78767
H	-3.98113	0.03354	0.12238
C	-0.46159	1.85576	2.72287
C	1.47670	2.16118	1.15432
H	-1.31946	2.41133	3.11394
H	-0.81336	0.90340	2.29390
C	2.15653	1.20518	1.84076
C	3.34485	0.55310	1.18258

C	1.73047	0.74387	3.20406
C	4.44377	0.13531	2.15737
H	-2.50711	-5.42510	0.15812
C	0.58533	1.56283	3.79577
H	2.60084	0.77210	3.87011
H	0.96965	2.50781	4.20013
H	1.85109	2.48691	0.18903
H	0.12308	1.01658	4.62259
H	-1.45839	3.68005	1.29693
H	5.33162	-0.18689	1.60673
H	4.12403	-0.69199	2.80125
H	3.76024	1.27763	0.47000
H	4.73922	0.97286	2.79926
H	1.44914	-0.31634	3.13187
C	0.27081	3.84451	-2.62236
H	0.55467	4.89719	-2.72336
H	1.18085	3.25320	-2.46773
H	-0.18929	3.51760	-3.55898
C	-0.55114	5.75399	-0.02397
H	-0.31712	6.31371	-0.93464
H	-1.63587	5.79543	0.12774
H	-0.05462	6.24351	0.81888
C	-4.61262	-0.02804	-1.93884
H	-4.23613	-0.38362	-2.90502
H	-5.56082	-0.53039	-1.72233
H	-4.80581	1.04475	-2.01128
H	-4.49305	-3.07239	2.32438
C	3.93197	-1.13510	-0.61614
C	4.05479	-0.57746	-1.89493
C	4.85991	-2.10463	-0.21981
C	5.08058	-0.97462	-2.75203
H	3.31395	0.15071	-2.22453
C	5.88654	-2.50356	-1.07492
H	4.78758	-2.55895	0.76529
C	6.00184	-1.93852	-2.34430
H	5.15229	-0.53763	-3.74462
H	6.59516	-3.25976	-0.74738
H	6.79903	-2.25279	-3.01244
H	-1.35313	-1.46350	0.15663
O	-0.59620	-1.32377	-2.28095
C	0.55648	-0.82415	-2.35396
O	0.85098	0.39570	-2.36899
H	1.40071	-1.54532	-2.42124

3b-γ-addition-2d

Geometry with 88 atoms:

C	2.01172	-0.90726	-1.02900
C	1.35352	-1.97225	-0.55710
N	0.07647	-1.76755	0.06678
O	-0.52074	-2.77223	0.45185
O	-0.36129	-0.63306	0.20444
H	1.50097	0.05136	-0.95761
H	1.65372	-3.01077	-0.56363
C	-3.92814	1.09250	-0.73094
C	-4.23479	-0.38145	-1.02689
N	-2.50371	1.33603	-0.86411
C	-5.65511	-0.80858	-0.58707
C	-5.55092	-1.79351	0.58734
C	-4.87887	-3.08420	0.09850
C	-3.58248	-2.70999	-0.64302
N	-3.24723	-1.28186	-0.33400
C	-3.22513	-1.06421	1.14829
C	-4.66878	-1.16188	1.67488
H	-2.03744	1.01839	-1.72655
C	-1.78098	2.17837	-0.09001
S	-2.38036	2.83816	1.37011
N	-0.54269	2.41923	-0.55375
H	-0.27941	1.90991	-1.40343
C	0.41940	3.37929	-0.02935
C	1.56785	2.65398	0.68976
N	1.02350	1.87809	1.78833
C	1.58867	0.70763	2.21840
H	-4.68683	-1.76960	2.58459
H	-5.54318	-3.63734	-0.57255
H	2.02421	1.95861	-0.03540
H	-0.10975	3.99943	0.70154
H	-2.75972	-0.09477	1.33785
H	-2.57124	-1.83952	1.55158
H	-3.67600	-2.77306	-1.72904
H	-2.72105	-3.30554	-0.33889
H	-6.54775	-2.00709	0.98292
H	-6.19490	-1.26690	-1.42264
H	-6.22383	0.07393	-0.27588
H	-4.06466	-0.56937	-2.09313
H	-4.20219	1.32432	0.30254
C	0.73674	-0.06890	3.19611
C	2.82278	0.27033	1.83501
H	0.26360	0.63984	3.88760
H	-0.07798	-0.55360	2.63912
C	3.35819	-1.02465	2.23678
C	4.61441	-1.42572	1.94798
C	2.40198	-1.92553	2.98811

C	5.65002	-0.60316	1.22702
H	-4.65836	-3.73526	0.95142
C	1.54746	-1.11213	3.96101
H	2.95530	-2.71376	3.51016
H	2.20138	-0.61156	4.68632
H	3.43729	0.89157	1.18965
H	0.87401	-1.76766	4.52413
H	0.02928	1.99393	1.97199
H	6.44624	-1.24011	0.82864
H	6.12366	0.12765	1.89793
H	4.92615	-2.41123	2.29438
H	5.23030	-0.04124	0.38333
H	1.72843	-2.42517	2.27326
C	0.91285	4.25188	-1.18107
H	1.55813	5.05750	-0.82171
H	1.47684	3.65702	-1.91125
H	0.05916	4.70128	-1.69641
C	2.64328	3.62272	1.18852
H	3.24449	4.02209	0.36537
H	2.18068	4.45880	1.72691
H	3.31612	3.10984	1.88197
C	-4.72022	1.99483	-1.67838
H	-4.40771	1.82361	-2.71496
H	-5.79833	1.81835	-1.60699
H	-4.52848	3.04208	-1.42813
H	-5.04800	-0.16770	1.93787
C	3.33850	-0.91679	-1.63789
C	3.77244	0.24432	-2.29324
C	4.19898	-2.02355	-1.56408
C	5.03562	0.29928	-2.87459
H	3.10460	1.10097	-2.35249
C	5.45972	-1.96691	-2.14457
H	3.89391	-2.91626	-1.02534
C	5.88111	-0.80670	-2.79924
H	5.35991	1.20265	-3.38267
H	6.12390	-2.82366	-2.07619
H	6.87080	-0.76468	-3.24539
H	-2.31947	-1.08942	-0.76524
O	-1.43343	-1.35286	-2.36738
C	-0.60569	-0.60149	-2.93924
O	-0.52470	0.64967	-2.84543
H	0.13111	-1.09581	-3.60996

3b-γ-addition-TS3d-3d

Geometry with 88 atoms:

C	2.85557	-1.09184	0.03625
C	2.22106	-2.12600	0.71222
N	0.88310	-2.06244	1.02859
O	0.36569	-3.02586	1.63877
O	0.19567	-1.06803	0.69699
H	2.22520	-0.29742	-0.36466
H	2.68723	-3.05667	1.00338
C	-3.96844	-0.02378	-0.70325
C	-3.67270	-1.51839	-0.83772
N	-2.76380	0.72115	-1.02061
C	-4.85287	-2.40288	-0.38671
C	-4.30787	-3.64359	0.33389
C	-3.19259	-4.25403	-0.52620
C	-1.99593	-3.28717	-0.52931
N	-2.46326	-1.94140	-0.04202
C	-2.76008	-2.00707	1.42664
C	-3.70721	-3.19695	1.67550
H	-2.11752	0.27659	-1.69855
C	-2.53377	2.00360	-0.66883
S	-3.51808	2.82823	0.46795
N	-1.46497	2.55205	-1.26977
H	-0.81572	1.90448	-1.75333
C	-0.94091	3.88868	-1.03796
C	0.29094	3.79132	-0.12233
N	-0.11356	3.11490	1.10625
C	0.63132	2.20752	1.75165
H	-3.15881	-4.02632	2.13554
H	-3.55695	-4.42538	-1.54522
H	1.01134	3.13736	-0.63166
H	-1.72171	4.46644	-0.53337
H	-3.20036	-1.04791	1.70844
H	-1.79798	-2.11631	1.92762
H	-1.56481	-3.11571	-1.51652
H	-1.20711	-3.59365	0.16047
H	-5.10883	-4.36963	0.49693
H	-5.44963	-2.68540	-1.25921
H	-5.50664	-1.83808	0.29042
H	-3.39545	-1.72854	-1.87698
H	-4.25654	0.21292	0.32647
C	-0.06836	1.38764	2.79877
C	1.96230	1.96668	1.45265
H	-0.87560	1.97270	3.25434
H	-0.52952	0.53294	2.27854
C	2.65738	0.86539	2.01033
C	3.84785	0.40828	1.45694
C	2.06308	0.12059	3.17989
C	4.66299	1.24881	0.50852

H	-2.87849	-5.22124	-0.12229
C	0.92063	0.88419	3.84653
H	2.85568	-0.09348	3.90593
H	1.32632	1.74004	4.40044
H	2.45087	2.54973	0.68082
H	0.40851	0.23982	4.56828
H	-1.10528	3.15915	1.34108
H	5.56921	0.72374	0.19493
H	4.96930	2.18854	0.98874
H	4.38170	-0.36580	2.00666
H	4.10620	1.51512	-0.39884
H	1.70745	-0.86070	2.83351
C	-0.60931	4.53510	-2.37960
H	-0.30452	5.57770	-2.25224
H	0.19959	3.99430	-2.88563
H	-1.49204	4.51399	-3.02486
C	0.93571	5.14244	0.17836
H	1.39630	5.57147	-0.71654
H	0.18937	5.84814	0.56210
H	1.71475	5.02524	0.93846
C	-5.12200	0.35224	-1.63694
H	-4.86720	0.10708	-2.67451
H	-6.04698	-0.16789	-1.36729
H	-5.30513	1.42762	-1.56719
H	-4.49788	-2.89855	2.37064
C	4.10055	-1.38370	-0.70280
C	4.28083	-0.81093	-1.96831
C	5.09678	-2.22484	-0.18745
C	5.43146	-1.08038	-2.70749
H	3.51005	-0.15576	-2.36986
C	6.24799	-2.48520	-0.92223
H	4.98028	-2.65774	0.80362
C	6.41870	-1.91426	-2.18613
H	5.55677	-0.63361	-3.68974
H	7.01677	-3.13201	-0.50869
H	7.31900	-2.11979	-2.75822
H	-1.68060	-1.28461	-0.20413
O	-0.96850	-0.95752	-2.28758
C	0.20299	-0.48696	-2.24947
O	0.53263	0.71573	-2.16639
H	1.02551	-1.23578	-2.30887

3b-γ-addition-3d

Geometry with 88 atoms:

C	2.80821	-0.77625	0.35694
C	2.04663	-1.81709	1.11753
N	0.75465	-1.74347	1.32612
O	0.15142	-2.60826	2.06679
O	0.04523	-0.77128	0.82508
H	2.12881	-0.29074	-0.35223
H	2.53138	-2.66193	1.58960
C	-3.58353	-0.12874	-0.91708
C	-3.36447	-1.64013	-0.83021
N	-2.29924	0.51231	-1.14404
C	-4.65856	-2.40843	-0.49025
C	-4.31012	-3.61105	0.39748
C	-3.11268	-4.34170	-0.22693
C	-1.87271	-3.43710	-0.10510
N	-2.32703	-2.03201	0.18861
C	-2.86845	-1.95413	1.58419
C	-3.89325	-3.08560	1.77928
H	-1.60970	-0.06270	-1.67345
C	-2.04010	1.81098	-0.93924
S	-3.18354	2.88489	-0.23830
N	-0.80285	2.20694	-1.31171
H	-0.17330	1.48219	-1.70622
C	-0.41970	3.59276	-1.47987
C	0.13882	4.26306	-0.18009
N	-0.31791	3.56562	1.01903
C	0.28193	2.57390	1.61927
H	-3.45680	-3.89734	2.37215
H	-3.32368	-4.57612	-1.27655
H	1.23024	4.20705	-0.18553
H	-1.31678	4.15359	-1.76248
H	-3.31224	-0.96172	1.69754
H	-1.99954	-2.03370	2.23977
H	-1.28399	-3.37529	-1.02240
H	-1.21764	-3.71040	0.72396
H	-5.16969	-4.28175	0.48376
H	-5.14201	-2.73153	-1.41747
H	-5.36360	-1.74980	0.03497
H	-2.94838	-1.98082	-1.78372
H	-3.99937	0.25137	0.02304
C	-0.41015	1.88862	2.75305
C	1.55425	2.06813	1.19344
H	-1.23247	2.50095	3.13512
H	-0.82182	0.95683	2.33268
C	2.17865	1.08741	1.89370
C	3.36036	0.36833	1.29501
C	1.70436	0.64746	3.24774
C	4.30078	1.30480	0.52751
H	-2.92680	-5.28853	0.28970

C	0.61358	1.54104	3.83320
H	2.57320	0.60132	3.91668
H	1.05548	2.46364	4.23027
H	1.94432	2.37334	0.22993
H	0.11526	1.03191	4.66266
H	-1.29493	3.74101	1.26780
H	5.23782	0.79211	0.29478
H	4.53586	2.19734	1.11749
H	3.92026	-0.11174	2.10881
H	3.86319	1.62297	-0.42581
H	1.34443	-0.38784	3.15865
C	0.62312	3.68830	-2.58932
H	0.95812	4.72330	-2.71461
H	1.49638	3.06736	-2.35696
H	0.20597	3.34092	-3.53852
C	-0.28676	5.72291	-0.09607
H	0.01110	6.24915	-1.00805
H	-1.37624	5.79822	-0.00373
H	0.17995	6.22279	0.75777
C	-4.56246	0.17078	-2.05617
H	-4.17664	-0.23360	-2.99916
H	-5.54955	-0.26143	-1.86328
H	-4.67971	1.25199	-2.16086
H	-4.76254	-2.70790	2.32724
C	3.95106	-1.40177	-0.42078
C	4.06215	-1.17107	-1.79517
C	4.92942	-2.17603	0.21353
C	5.12626	-1.70639	-2.52168
H	3.30269	-0.56733	-2.29087
C	5.99384	-2.71018	-0.50962
H	4.86448	-2.36171	1.28442
C	6.09555	-2.47676	-1.88173
H	5.19585	-1.52008	-3.59020
H	6.74545	-3.30899	-0.00179
H	6.92475	-2.89465	-2.44619
H	-1.46622	-1.42366	0.16634
O	-0.68102	-1.40549	-2.25709
C	0.51262	-1.00665	-2.24617
O	0.91436	0.17873	-2.33462
H	1.29027	-1.79817	-2.15783

3b-γ′-addition-1

Geometry with 75 atoms:

C	-2.76163	-1.66527	-0.17877
C	-3.34639	-0.28246	0.14269
N	-1.44342	-1.76686	0.40961
C	-4.61939	0.05517	-0.66751
C	-4.32354	1.20553	-1.64114
C	-4.01353	2.47547	-0.83682
C	-2.93375	2.14324	0.21042
N	-2.33438	0.80747	-0.12718
C	-1.85942	0.80907	-1.55219
C	-3.08898	0.83600	-2.47675
H	-1.34086	-1.55721	1.42371
C	-0.36154	-2.35730	-0.15645
S	-0.32356	-2.83223	-1.80156
N	0.66946	-2.49277	0.69108
H	0.52614	-2.07080	1.62392
C	1.99786	-3.00769	0.38997
C	2.98290	-1.84305	0.17630
N	2.50590	-1.03422	-0.92923
C	2.80464	0.28455	-1.09780
H	-2.93095	1.56773	-3.27431
H	-4.91267	2.84301	-0.33387
H	2.96213	-1.21803	1.08479
H	1.92315	-3.57887	-0.54175
H	-1.22856	-0.07231	-1.69753
H	-1.23880	1.70304	-1.65399
H	-3.33383	2.05492	1.22323
H	-2.11141	2.86043	0.23110
H	-5.18586	1.36987	-2.29261
H	-5.44058	0.32652	0.00376
H	-4.93641	-0.82735	-1.23188
H	-3.52771	-0.22047	1.22316
H	-2.65181	-1.77817	-1.26180
C	2.01847	0.99093	-2.17770
C	3.64145	1.01659	-0.31111
H	1.72304	0.28317	-2.96136
H	1.09210	1.35960	-1.70642
C	3.77476	2.46114	-0.51698
C	3.35296	3.03410	-1.66166
H	-3.66473	3.26748	-1.50779
C	2.79663	2.16765	-2.76340
H	3.46791	4.10381	-1.82406
H	3.62257	1.77547	-3.37980
H	4.15758	0.56760	0.53362
H	2.15020	2.74432	-3.43354
H	1.82162	-1.45245	-1.55352
C	-3.68098	-2.76580	0.35419
H	-3.75146	-2.70637	1.44629
H	-4.69002	-2.70135	-0.06517
H	-3.26353	-3.74126	0.08928

H	-3.23042	-0.14158	-2.95068
C	2.43048	-3.93066	1.52561
H	3.37331	-4.43169	1.29163
H	2.55926	-3.36850	2.45886
H	1.66746	-4.69682	1.68938
C	4.41352	-2.33053	-0.06615
H	4.86191	-2.73563	0.84625
H	4.42500	-3.10747	-0.84041
H	5.03765	-1.50098	-0.41154
H	-1.50761	0.66021	0.48121
C	4.38930	3.24962	0.60753
H	5.39938	2.88374	0.83153
H	4.45677	4.31418	0.36312
H	3.79877	3.13990	1.52630
O	-0.46259	-0.97192	2.82155
C	-0.34535	0.30248	2.60559
C	-1.02706	1.26982	3.40443
C	0.44233	0.82916	1.53425
C	-0.88389	2.63460	3.18290
H	-1.63756	0.90258	4.22677
C	0.57841	2.20386	1.32727
H	0.99147	0.13423	0.89934
C	-0.07871	3.12425	2.14633
H	-1.40317	3.33393	3.83633
H	1.22578	2.55193	0.52185
H	0.04212	4.19254	1.99091

3b-γ′-addition-2a

Geometry with 93 atoms:

C	-2.49453	-1.70480	-0.52219
C	-1.49084	-0.88073	-0.19662
N	-0.20270	-1.05019	-0.78848
O	0.61213	-0.14840	-0.57876
O	0.06108	-2.03468	-1.46981
H	-2.29779	-2.49902	-1.23948
H	-1.52228	-0.01436	0.44726
C	4.16017	0.54381	0.84123
C	4.29040	-0.89576	0.32763
N	2.77274	0.81619	1.15952
C	5.66187	-1.21725	-0.30944
C	5.47312	-1.57546	-1.78998
C	4.60901	-2.83938	-1.90293
C	3.30259	-2.62794	-1.11000
N	3.22454	-1.18848	-0.69869
C	3.32508	-0.30424	-1.91014
C	4.74898	-0.41159	-2.48143
H	2.31149	0.22499	1.88769
C	2.11959	1.97278	0.88221
S	2.71416	3.13140	-0.23220
N	0.94971	2.10181	1.52572
H	0.70228	1.31737	2.15238
C	0.09879	3.28253	1.55946
C	-1.17495	3.07921	0.72072
N	-0.79554	2.78678	-0.64919
C	-1.60910	2.12094	-1.51879
H	4.70210	-0.57614	-3.56202
H	5.14559	-3.70645	-1.50641
H	-1.71359	2.20478	1.13135
H	0.66786	4.10594	1.11545
H	3.05285	0.70825	-1.60112
H	2.55847	-0.66661	-2.59970
H	3.27001	-3.21869	-0.19110
H	2.40250	-2.83822	-1.68979
H	6.44795	-1.74337	-2.25560
H	6.14718	-2.03966	0.22583
H	6.31758	-0.34336	-0.22960
H	4.06680	-1.58112	1.15450
H	4.46819	1.24079	0.05530
C	-0.99654	1.81300	-2.86849
C	-2.91653	1.80580	-1.29668
H	-1.19573	2.67427	-3.52346
H	0.09299	1.72806	-2.77305
C	-3.69193	1.07933	-2.30332
C	-3.08172	0.48796	-3.34955
H	4.38576	-3.04530	-2.95469
C	-1.58177	0.54482	-3.49390
H	-3.66087	-0.07226	-4.08122
H	-1.29111	0.49634	-4.54918
H	-3.42020	2.09221	-0.37652
H	-1.13550	-0.34261	-3.01893
H	0.20181	2.76284	-0.84682
C	-3.85588	-1.57840	-0.01109
C	-4.87930	-2.30344	-0.63863
C	-4.17709	-0.74243	1.07108
C	-6.19721	-2.18731	-0.20771
H	-4.63230	-2.94781	-1.47920
C	-5.49347	-0.63348	1.50547
H	-3.39140	-0.19956	1.58950
C	-6.50638	-1.35215	0.86584
H	-6.98242	-2.74647	-0.70805
H	-5.73162	0.00912	2.34820
H	-7.53370	-1.26300	1.20765

C	5.04506	0.74048	2.07325
H	4.69557	0.10728	2.89684
H	6.09376	0.50062	1.86888
H	4.98977	1.78394	2.39603
H	5.29534	0.52356	-2.31547
C	-0.22045	3.60343	3.01838
H	-0.75187	4.55405	3.11081
H	-0.83822	2.81462	3.46646
H	0.70789	3.67382	3.59241
C	-2.08700	4.30818	0.78269
H	-2.60106	4.38300	1.74606
H	-1.49924	5.22051	0.62500
H	-2.84460	4.25907	-0.00414
H	2.29997	-0.98353	-0.28355
O	1.03465	-0.30994	2.93403
C	-5.18161	1.01212	-2.09875
H	-5.62596	2.01486	-2.14236
H	-5.66433	0.38807	-2.85753
H	-5.42106	0.59818	-1.11082
C	0.31655	-1.34840	2.63632
C	0.81639	-2.41007	1.82859
C	-1.02221	-1.50495	3.10265
C	0.04074	-3.51657	1.49809
H	1.85149	-2.34275	1.49140
C	-1.78192	-2.62262	2.78036
H	-1.42850	-0.72192	3.74097
C	-1.27038	-3.63922	1.96554
H	0.46497	-4.29699	0.86781
H	-2.79840	-2.70240	3.16237
H	-1.87421	-4.50500	1.70983

3b-γ′-addition-TS2a-3a

Geometry with 93 atoms:

C	-2.74993	-1.29815	-0.85809
C	-1.68897	-0.69278	-0.20142
N	-0.39766	-0.87462	-0.63217
O	0.50153	-0.17053	-0.11537
O	-0.10859	-1.71280	-1.51631
H	-2.49392	-2.02881	-1.62154
H	-1.75085	-0.05458	0.66870
C	4.30168	0.16343	0.52402
C	4.06205	-1.34665	0.39976
N	3.05481	0.79878	0.89255
C	5.25892	-2.14050	-0.17426
C	4.86703	-2.76743	-1.51936
C	3.73230	-3.77872	-1.30003
C	2.60262	-3.09773	-0.50168
N	2.86347	-1.62259	-0.47168
C	3.03855	-1.10763	-1.87246
C	4.36148	-1.64730	-2.43994
H	2.58006	0.47535	1.76971
C	2.54021	1.92588	0.35985
S	3.14111	2.64745	-1.07970
N	1.48888	2.41079	1.03940
H	1.20265	1.85221	1.86240
C	0.80781	3.66745	0.79719
C	-0.56453	3.45625	0.12995
N	-0.39156	2.64106	-1.06774
C	-1.36790	1.94504	-1.65648
H	4.20040	-2.02557	-3.45405
H	4.09628	-4.65315	-0.75227
H	-1.20151	2.88402	0.82316
H	1.43258	4.24841	0.11096
H	2.99592	-0.01632	-1.82595
H	2.16090	-1.45919	-2.41807
H	2.56854	-3.43114	0.53854
H	1.61452	-3.23208	-0.94399
H	5.73478	-3.26228	-1.96408
H	5.57733	-2.91389	0.53266
H	6.10942	-1.46705	-0.32378
H	3.77525	-1.72563	1.38830
H	4.62391	0.57174	-0.43929
C	-0.92946	1.09763	-2.82842
C	-2.70906	2.03636	-1.29158
H	-0.63542	1.79491	-3.62211
H	-0.00945	0.56947	-2.54570
C	-3.67770	1.15057	-1.81457
C	-3.28860	0.07032	-2.58785
H	3.35647	-4.13075	-2.26643
C	-1.99096	0.10837	-3.36287
H	-4.06383	-0.58050	-2.99087
H	-2.25046	0.39757	-4.38955
H	-3.02082	2.75268	-0.53803
H	-1.55917	-0.89394	-3.43162
H	0.56743	2.47818	-1.37833
C	-4.06033	-1.47312	-0.21020
C	-4.98175	-2.37555	-0.76221
C	-4.42508	-0.76455	0.94386
C	-6.23228	-2.56512	-0.18157
H	-4.70775	-2.93339	-1.65550
C	-5.67577	-0.95444	1.52524
H	-3.73154	-0.05982	1.39360

C	-6.58480	-1.85227	0.96559
H	-6.93105	-3.27185	-0.62044
H	-5.94056	-0.39772	2.42016
H	-7.55926	-1.99939	1.42254
C	5.36925	0.44560	1.58360
H	5.02945	0.09732	2.56577
H	6.32283	-0.03911	1.35157
H	5.53961	1.52419	1.64392
H	5.10778	-0.84719	-2.50246
C	0.67153	4.41235	2.12378
H	0.25391	5.41251	1.98155
H	0.02386	3.85907	2.81526
H	1.65559	4.51538	2.58922
C	-1.21696	4.80180	-0.20560
H	-1.61351	5.28435	0.69253
H	-0.48151	5.47204	-0.66605
H	-2.04010	4.67628	-0.91358
H	2.02815	-1.12103	-0.09564
O	1.41504	0.43211	3.01015
C	-5.11593	1.33250	-1.41415
H	-5.58010	2.09373	-2.05497
H	-5.68802	0.40663	-1.52680
H	-5.20866	1.67482	-0.37806
C	0.43083	-0.41592	2.99285
C	0.58145	-1.74657	2.50848
C	-0.86772	-0.07133	3.46224
C	-0.48096	-2.64167	2.46829
H	1.57087	-2.04923	2.16498
C	-1.91882	-0.98401	3.43933
H	-1.01123	0.93080	3.86275
C	-1.74861	-2.27581	2.93438
H	-0.32123	-3.64347	2.07115
H	-2.89345	-0.68128	3.82047
H	-2.57970	-2.97440	2.90017

3b-γ′-addition-3a

Geometry with 93 atoms:

C	-2.69278	-1.23467	-1.13670
C	-1.54819	-0.65975	-0.37303
N	-0.30946	-0.88856	-0.74018
O	0.64814	-0.23643	-0.15313
O	0.00598	-1.67230	-1.70424
H	-2.33399	-2.14142	-1.63626
H	-1.64150	-0.03498	0.50609
C	4.21758	0.30470	0.45373
C	4.00920	-1.20853	0.33379
N	2.99506	0.95140	0.87731
C	5.26101	-1.95020	-0.18085
C	4.82412	-3.08679	-1.11501
C	3.70614	-3.88061	-0.42387
C	2.46079	-2.97906	-0.33578
N	2.86596	-1.55632	-0.57506
C	3.22780	-1.38563	-2.01500
C	4.26136	-2.46363	-2.40200
H	2.57211	0.67635	1.79217
C	2.39484	1.98862	0.27234
S	2.87284	2.59895	-1.26716
N	1.35786	2.49784	0.96232
H	1.15976	2.01948	1.86471
C	0.66434	3.73236	0.66699
C	-0.67555	3.50293	-0.06942
N	-0.46911	2.53340	-1.15641
C	-1.39130	1.83428	-1.75270
H	3.79600	-3.23955	-3.02038
H	4.03271	-4.19471	0.57403
H	-1.39331	3.05246	0.62900
H	1.30886	4.32400	0.00858
H	3.60783	-0.36867	-2.13573
H	2.28884	-1.46499	-2.56678
H	1.97312	-3.01383	0.64187
H	1.70859	-3.20572	-1.09290
H	5.67317	-3.73665	-1.34489
H	5.83638	-2.33593	0.66672
H	5.91052	-1.25356	-0.72793
H	3.70981	-1.58983	1.31915
H	4.48907	0.71670	-0.52233
C	-0.96622	0.95525	-2.89635
C	-2.80126	1.98165	-1.44622
H	-0.70511	1.63366	-3.71883
H	-0.04123	0.43385	-2.62390
C	-3.68154	1.01208	-1.79165
C	-3.16344	-0.29062	-2.32363
H	3.46587	-4.78604	-0.98969
C	-2.05457	-0.03073	-3.35800
H	-3.98302	-0.82360	-2.82130
H	-2.54013	0.36962	-4.25473
H	-3.14646	2.87632	-0.93748
H	-1.58185	-0.97794	-3.62963
H	0.51063	2.38750	-1.44685
C	-3.87374	-1.60356	-0.25800
C	-4.64667	-2.72186	-0.58734
C	-4.25948	-0.83007	0.84226

C	-5.77568	-3.06180	0.15703
H	-4.35523	-3.33698	-1.43683
C	-5.38705	-1.16533	1.59019
H	-3.67943	0.04463	1.12525
C	-6.15022	-2.28207	1.25054
H	-6.35720	-3.93897	-0.11327
H	-5.66600	-0.55484	2.44514
H	-7.02541	-2.54614	1.83743
C	5.33504	0.60064	1.45701
H	5.06841	0.22065	2.45051
H	6.28571	0.15110	1.15343
H	5.47522	1.68256	1.53290
H	5.06534	-2.01203	-2.99183
C	0.43696	4.48510	1.97666
H	-0.02398	5.46204	1.80956
H	-0.20716	3.90594	2.64875
H	1.39582	4.64081	2.47844
C	-1.20461	4.82151	-0.64044
H	-1.50026	5.50061	0.16328
H	-0.42400	5.30713	-1.23677
H	-2.07332	4.67119	-1.28635
H	1.98563	-0.94527	-0.37584
O	1.43269	0.79663	3.11218
C	-5.15808	1.19021	-1.62594
H	-5.60819	1.31968	-2.61997
H	-5.62106	0.30363	-1.18200
H	-5.40332	2.06761	-1.02084
C	0.40829	-0.00629	3.13707
C	0.52469	-1.39153	2.83672
C	-0.89854	0.45048	3.46399
C	-0.57622	-2.23833	2.83179
H	1.51753	-1.76985	2.59589
C	-1.99308	-0.41160	3.47340
H	-1.01833	1.49898	3.73250
C	-1.85357	-1.76252	3.14956
H	-0.44195	-3.28845	2.57580
H	-2.97491	-0.02061	3.73909
H	-2.71476	-2.42448	3.13643

3b-γ′-addition-2b

Geometry with 93 atoms:

C	2.24447	-1.13529	0.05212
C	1.50765	-1.79532	0.95505
N	0.10391	-1.52698	1.06014
O	-0.52781	-2.18965	1.88386
O	-0.41500	-0.66777	0.35544
H	1.74446	-0.38040	-0.55314
H	1.81760	-2.59221	1.61547
C	3.64704	-1.42239	-0.24466
C	4.23109	-0.80116	-1.35779
C	4.41484	-2.32009	0.51367
C	5.54962	-1.07149	-1.71199
H	3.63895	-0.10396	-1.94689
C	5.73211	-2.58790	0.16114
H	3.99014	-2.79824	1.39151
C	6.30248	-1.96656	-0.95216
H	5.98916	-0.58468	-2.57755
H	6.32033	-3.27751	0.75951
H	7.33319	-2.17783	-1.22251
C	-4.03359	0.98752	-0.71385
C	-4.40813	-0.37598	-0.12165
N	-2.66789	0.95302	-1.19902
C	-5.69866	-0.34975	0.73048
C	-5.35518	-0.64480	2.19743
C	-4.80695	-2.07502	2.30886
C	-3.68753	-2.26067	1.26648
N	-3.29428	-0.90986	0.74455
C	-2.96664	0.01343	1.88571
C	-4.26330	0.33668	2.64642
H	-2.43905	0.29864	-1.98607
C	-1.77612	1.96070	-1.03864
S	-2.05584	3.28706	0.01228
N	-0.64341	1.81109	-1.74865
H	-0.63233	0.99101	-2.37611
C	0.35629	2.84824	-1.97500
C	1.61270	2.68242	-1.09449
N	1.21331	2.47891	0.28203
C	2.02073	1.97720	1.25355
H	-4.08755	0.25085	3.72288
H	-5.59903	-2.80857	2.13183
H	2.15430	1.77799	-1.42475
H	-0.10874	3.80286	-1.70607
H	-2.48121	0.89677	1.46377
H	-2.23683	-0.52396	2.49486
H	-4.01371	-2.84238	0.40072
H	-2.78511	-2.71559	1.67536
H	-6.24807	-0.53080	2.81801
H	-6.42149	-1.08010	0.35225
H	-6.16423	0.63862	0.65500
H	-4.49231	-1.10133	-0.93813
H	-4.08781	1.74941	0.06943
C	1.31342	1.58734	2.53195

C	3.35258	1.70811	1.12257
H	0.43505	2.22579	2.68594
H	0.93826	0.56150	2.38891
C	4.10739	1.09992	2.21856
C	3.57382	0.99954	3.45300
H	-4.41894	-2.24762	3.31828
C	2.23623	1.62912	3.74828
H	4.15428	0.58009	4.27258
H	2.39486	2.68125	4.03860
H	3.87688	1.90007	0.18993
H	1.74443	1.14319	4.59770
H	0.24048	2.65967	0.51461
C	-4.99955	1.34826	-1.84294
H	-4.89220	0.64176	-2.67417
H	-6.04247	1.33739	-1.50924
H	-4.76896	2.35131	-2.21273
H	-4.57538	1.36775	2.44531
C	0.71118	2.85222	-3.46009
H	1.37502	3.68448	-3.70729
H	1.20797	1.91632	-3.74605
H	-0.19730	2.95009	-4.06158
C	2.52927	3.90344	-1.24887
H	3.06647	3.88839	-2.20241
H	1.93767	4.82526	-1.19466
H	3.26838	3.93592	-0.44464
H	-2.43396	-0.99796	0.17440
C	5.52696	0.69443	1.91964
H	6.14904	1.59034	1.78861
H	5.95697	0.10056	2.73254
H	5.59926	0.11883	0.99062
O	-1.48256	-0.50404	-3.14124
C	-1.03382	-1.59326	-2.59913
C	-1.88218	-2.48838	-1.88185
C	0.34052	-1.96523	-2.67484
C	-1.38197	-3.62055	-1.24477
H	-2.95189	-2.28125	-1.88377
C	0.82002	-3.10990	-2.05404
H	1.00623	-1.32300	-3.24987
C	-0.02421	-3.94251	-1.31051
H	-2.06239	-4.27517	-0.70089
H	1.87900	-3.35290	-2.13346
H	0.36225	-4.82930	-0.81668

3b-γ′-addition-TS2b-3b

Geometry with 93 atoms:

C	-2.81210	-1.16840	-0.41924
C	-2.12672	-2.28569	-0.87911
N	-0.74964	-2.31865	-0.90117
O	-0.18390	-3.32912	-1.37974
O	-0.07929	-1.37268	-0.42931
H	-2.20043	-0.40070	0.05298
H	-2.58081	-3.19595	-1.24341
C	-4.19259	-1.29844	0.09544
C	-4.59325	-0.48456	1.16244
C	-5.11445	-2.20887	-0.44018
C	-5.87789	-0.58441	1.69221
H	-3.88738	0.23409	1.57494
C	-6.40129	-2.30125	0.08131
H	-4.83083	-2.83909	-1.27981
C	-6.78737	-1.49185	1.15182
H	-6.16757	0.04848	2.52641
H	-7.10600	-3.00862	-0.34691
H	-7.79026	-1.57122	1.56139
C	4.14954	0.39268	0.26075
C	4.05882	-1.13233	0.36258
N	2.89797	0.98262	0.70015
C	5.22573	-1.86970	-0.33872
C	4.69658	-2.64273	-1.55559
C	3.74839	-3.75133	-1.07725
C	2.74013	-3.14381	-0.08711
N	2.77307	-1.64843	-0.23181
C	2.62135	-1.26730	-1.68001
C	3.90115	-1.66707	-2.43291
H	2.57544	0.77744	1.67616
C	2.39884	2.13936	0.19945
S	2.92458	2.79912	-1.29533
N	1.43429	2.69420	0.95336
H	1.20942	2.18097	1.82730
C	0.82510	3.99995	0.74073
C	-0.55088	3.88952	0.04573
N	-0.41663	2.98879	-1.09273
C	-1.35753	2.14085	-1.51788
H	3.62953	-2.13671	-3.38315
H	4.30493	-4.55503	-0.58591
H	-1.25304	3.41693	0.74818
H	1.49284	4.56557	0.08207
H	2.41497	-0.19423	-1.71667
H	1.73915	-1.80715	-2.02751
H	2.99753	-3.35379	0.95381
H	1.71077	-3.45287	-0.27480
H	5.53279	-3.06771	-2.11748
H	5.72194	-2.55009	0.36140

H	5.97203	-1.14018	-0.66918
H	4.00229	-1.40692	1.42068
H	4.30619	0.68176	-0.78286
C	-0.84024	0.96685	-2.30490
C	-2.70093	2.24733	-1.18335
H	-0.11197	1.31610	-3.04674
H	-0.27882	0.36127	-1.57717
C	-3.63061	1.24950	-1.56598
C	-3.21939	0.08537	-2.20616
H	3.22291	-4.18971	-1.93265
C	-1.91844	0.10155	-2.96280
H	-3.99403	-0.57579	-2.59164
H	-2.12843	0.48023	-3.97405
H	-3.05624	3.10433	-0.61850
H	-1.53755	-0.92029	-3.09194
H	0.53530	2.83922	-1.43307
C	5.31080	0.90853	1.11337
H	5.12714	0.69117	2.17203
H	6.26679	0.45950	0.82574
H	5.39462	1.99263	0.99431
H	4.50672	-0.78326	-2.66343
C	0.71343	4.70384	2.09020
H	0.32339	5.71875	1.97847
H	0.05020	4.14853	2.76454
H	1.69923	4.76732	2.55946
C	-1.08252	5.25770	-0.38205
H	-1.34689	5.87307	0.48281
H	-0.32813	5.78849	-0.97439
H	-1.97689	5.14325	-1.00172
H	1.95877	-1.26608	0.27912
C	-5.08160	1.48217	-1.25164
H	-5.48420	2.20694	-1.97209
H	-5.67237	0.56573	-1.33070
H	-5.21990	1.90681	-0.25175
O	1.49102	0.81691	2.99846
C	0.78845	-0.27293	2.87089
C	1.40118	-1.55725	2.81616
C	-0.63182	-0.25828	2.77511
C	0.65536	-2.72322	2.64760
H	2.47895	-1.60885	2.96839
C	-1.36185	-1.42915	2.61984
H	-1.13377	0.70655	2.84109
C	-0.73337	-2.67613	2.53685
H	1.16461	-3.68583	2.62065
H	-2.44733	-1.38079	2.56240
H	-1.31501	-3.58371	2.40306

3b-γ′-addition-3b

Geometry with 93 atoms:

C	-2.73691	-0.95584	-0.94884
C	-2.00138	-1.99736	-1.72716
N	-0.69120	-1.95995	-1.85196
O	-0.05332	-2.86598	-2.49658
O	-0.00317	-1.00136	-1.30866
H	-1.98533	-0.41200	-0.36609
H	-2.48653	-2.83947	-2.20288
C	-3.72011	-1.58123	0.02453
C	-3.62861	-1.30903	1.39212
C	-4.74984	-2.41550	-0.42644
C	-4.54814	-1.85197	2.29079
H	-2.82476	-0.67331	1.75796
C	-5.67039	-2.95877	0.46708
H	-4.83592	-2.64363	-1.48764
C	-5.57391	-2.67507	1.83059
H	-4.45437	-1.63460	3.35131
H	-6.46193	-3.60671	0.10008
H	-6.28962	-3.09958	2.52904
C	3.89357	0.54449	0.14292
C	3.74690	-0.98001	0.23350
N	2.65111	1.13677	0.60975
C	5.00676	-1.78205	-0.17678
C	4.70303	-2.64462	-1.40880
C	3.61930	-3.67443	-1.05946
C	2.42666	-2.94567	-0.41171
N	2.60442	-1.46758	-0.61580
C	2.79357	-1.19191	-2.08348
C	4.17388	-1.71589	-2.50980
H	2.39127	0.92395	1.59713
C	2.07876	2.26638	0.15048
S	2.44904	2.96044	-1.37292
N	1.14975	2.77056	0.99176
H	1.03381	2.23534	1.87683
C	0.52412	4.07747	0.88674
C	-0.91336	3.96292	0.34043
N	-0.85502	3.14037	-0.87612
C	-1.77385	2.32791	-1.31609
H	4.08009	-2.25227	-3.45911
H	4.01311	-4.42586	-0.36826
H	-1.51669	3.41253	1.07206
H	1.11211	4.67004	0.17694
H	2.66180	-0.11856	-2.23847
H	1.96451	-1.70869	-2.57044

H	2.36413	-3.10383	0.66802
H	1.47025	-3.19919	-0.87531
H	5.61591	-3.14821	-1.73971
H	5.34190	-2.40486	0.65917
H	5.82464	-1.09743	-0.41913
H	3.44964	-1.22358	1.26165
H	4.05899	0.85509	-0.89325
C	-1.40508	1.42938	-2.45603
C	-3.08904	2.27068	-0.72704
H	-0.92026	2.02501	-3.23808
H	-0.64720	0.72846	-2.06579
C	-3.94007	1.25242	-1.01923
C	-3.47468	0.10049	-1.86991
H	3.29483	-4.19727	-1.96577
C	-2.59214	0.63984	-2.99989
H	-4.35008	-0.39660	-2.30615
H	-3.20839	1.27806	-3.64519
H	-3.40269	3.06162	-0.05252
H	-2.22253	-0.18963	-3.60961
H	0.05850	3.12875	-1.35721
C	5.04515	1.04323	1.02108
H	4.89097	0.73603	2.06234
H	6.01829	0.67369	0.68736
H	5.07114	2.13632	0.98755
H	4.87695	-0.88941	-2.66672
C	0.54260	4.74899	2.25689
H	0.15737	5.77068	2.20470
H	-0.05921	4.18301	2.97785
H	1.56930	4.78985	2.63044
C	-1.53686	5.32203	0.03362
H	-1.71531	5.88169	0.95529
H	-0.87442	5.90991	-0.61159
H	-2.49610	5.20564	-0.47988
H	1.70798	-1.02498	-0.34615
C	-5.33628	1.24059	-0.48662
H	-6.03906	1.26330	-1.33011
H	-5.53848	0.31471	0.06317
H	-5.53725	2.09574	0.16376
O	1.44158	0.93232	3.05685
C	0.97581	-0.28372	2.96140
C	1.19291	-1.25567	3.97743
C	0.25806	-0.72615	1.81332
C	0.71991	-2.55749	3.85077
H	1.74062	-0.94650	4.86507
C	-0.20250	-2.03608	1.69484
H	0.06460	-0.01206	1.01217
C	0.01652	-2.96790	2.71177
H	0.90137	-3.26856	4.65510
H	-0.74015	-2.32804	0.79306
H	-0.35263	-3.98527	2.61958