Use of Biomimetic Diversity-Oriented Synthesis to Discover Galanthamine-Like Molecules with Biological Properties Beyond Those of the Natural Product

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Supporting Information

I. General Methods

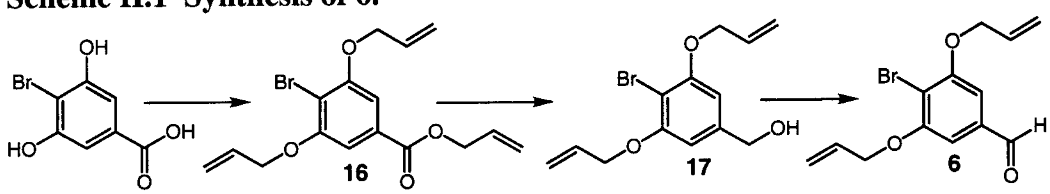
General Procedures. All reactions were performed in oven or flame-dried glassware under a positive pressure of argon unless otherwise noted. Flash chromatography was performed as described by Still et al.[4] employing E. Merck silica gel 60 (230-400 mesh ASTM) unless noted otherwise. All solid phase reactions were performed in either oven-dried glassware under a positive pressure of argon, ChemGlass solid phase reaction vessels (CG-1866) or BioRad Poly-Prep Chromatography Columns. Agitation was provided by a Lab-Line 3-D Rotator. Resin washing was performed with a Promega wash station.

Materials. Starting materials and reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. Tetrahydrofuran and ethyl ether were distilled under nitrogen from sodium-benzophenone ketyl. Toluene was distilled under nitrogen from sodium. Dichloromethane, triethylamine, *N,N*-diisopropylamine, 2,6-lutidine, and diisopropylethylamine were distilled under nitrogen from CaH_2. Alternatively, tetrahydrofuran, ethyl ether, toluene, *N,N*-dimethylformamide, and dichloromethane were purchased as dry solvents from Baker, and filtered through a column charged with activated Al_2O_3.[5] TLC analyses were performed on 250μm Silica Gel $60F_{254}$ plates purchased from EM Science. Wash solvents were used as received. 500-600 μm *p*-bromopolystyrene was obtained from Polymer Laboratories, Inc. and the linker was attached according to the procedure of Tallarico et. al.[6]

Instrumentation. Infrared spectra were recorded using a Nicolet Nexus 400 or a Perkin Elmer Spectrum One FT-IR spectrometer. ^1H and ^{13}C NMR, COSY, NOESY, and GOESY spectra were recorded on a Bruker AM500 or AM400, or a Varian INOVA500 or Mercury400 spectrometer. Chemical shifts for proton and carbon resonances are reported in ppm (δ) relative to chloroform (δ 7.26, 77.1 respectively), acetone (δ 2.05, 29.84 respectively), or DMSO (δ 2.50, 39.52 respectively). Tandem high pressure liquid chromatography/mass spectral (LCMS) analyses were performed on a Micromass Platform II mass spectrometer in atmospheric pressure chemical ionization (APCI) mode or electrospray ionization mode (ES) after separation performed on a Waters Alliance 2690 separations module. A Waters Symmetry® C_{18} column (2.1 mm X 50 mm, 3.5 µm, Protocol A) or a Waters YMC ODS-AQ S3 120A column (2.0 mm x 60mm, Protocol B) were used. In protocol A, samples were eluted using a flow rate of 0.4 mL/min and a 12 minute gradient of 15→100% CH_3CN in H_2O, constant 0.1% formic acid buffer. In protocol B, samples were eluted using a flow rate of 0.4 mL/min and a 12 minute gradient of 0→100% CH_3CN in H_2O, constant 0.1% formic acid buffer. A Waters 996 photodiode array detector was used (scan width 200-450nm, 1 spectra/sec). Automated mass spectral analyses were performed using the above equipment (with column bypassed) at a flow rate of 0.25mL/min of 50% CH_3CN in H_2O, constant 0.1% formic acid buffer for 1.5 minutes per sample. Chiral HPLC data was obtained on a Hewlet Packard Series 1100 HPLC with a Chiracel OD column.

II. Solution Phase Synthesis of Solid-Phase Precursors

Scheme II.1 Synthesis of 6.

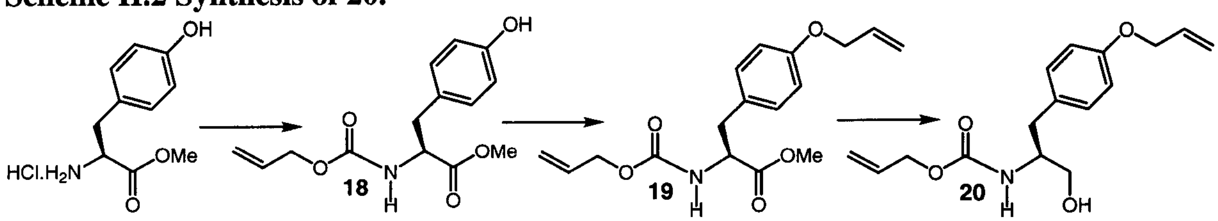


3,5-Bis-allyloxy-4-bromo-benzoic acid allyl ester (16): To a solution of 4-Bromo-3,5-dihydroxybenzoic acid (20.43g, 87.5mmol, 1.0 equiv) in DMF (120mL) at room temperature was added solid K_2CO_3 (60.5g, 438 mmol, 5 equiv). To the suspension was added allylbromide (31ml, 358 mmol, 4.1 equiv) dropwise over 25 minutes. After 15 hours, water (150 mL) was added and the slurry was poured into water (300 mL). The precipitate was separated by filtration, washed with water, and dissolved in ether. The solution was washed with brine, dried over $MgSO_4$, filtered, and concentrated to afford **16** as a white powder (30.1g, 97%). R_f = 0.52 (15% EtOAc/hexane); FTIR (neat, cm^{-1}) 3088, 2900, 1717, 1649, 1582, 1424, 986; ^1H NMR (400 MHz, $CDCl_3$) δ, 7.24 (s, 2H), 6.12-5.98 (m, 3H), 5.51 (dd, J = 17.6, 1.6 Hz, 2H), 5.40 (dd, J = 17.2, 1.2 Hz, 1H), 5.32 (dd, J = 10.2, 1.2 Hz, 2H), 5.30 (dd, J = 8.4, 1.6 Hz, 1H), 4.81 (d, J = 6.0 Hz, 2H), 4.66 (d, J = 3.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.2, 132.0, 129.9, 118.4, 117.9, 107.9, 106.9, 69.9, 65.7; MS EI+ calculated for $C_{16}H_{17}BrO_4$ (M-H^+): 351, found: 351.

(3,5-Bis-allyloxy-4-bromo-phenyl)-methanol (17): To a solution of **16** (30g, 85 mmol) in THF (600 ml) at 0°C was added lithium aluminum hydride (1.0M in THF, 175 mL, 2 equiv) dropwise over 45 minutes. The reaction was stirred at 0°C for 2 hours, after which time saturated aqueous potassium sodium tartrate was added dropwise until bubbling ceased (25 mL, over 45 minutes). To the suspension was added ether (100mL) and additional saturated aqueous potassium sodium tartrate (30 mL). The suspension was filtered through celite, the THF and ether were removed under reduced pressure, and water (250 mL) was added. The aqueous suspension was extracted into EtOAc (4x250mL). The organic layer was washed with brine, dried over $MgSO_4$, filtered, and concentrated. Purification by flash chromatography (20→75% EtOAc/hexane) afforded **17** (11.93g, 47%) as a white oil. R_f = 0.39 (50% EtOAc/hexane); FTIR (neat, cm^{-1}) 3363, 2924, 2869, 1587, 1435, 817; ^1H NMR (400 MHz, $CDCl_3$) δ, 6.56 (s, 2H), 6.10-6.00 (m, 2H), 5.48 (dd, J = 17.4, 1.6 Hz, 2H), 5.29 (dd, J = 10.6, 1.6 Hz, 2H), 4.62 (s, 2H), 4.60 (d, J = 5.2 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2, 141.4, 132.6, 117.6, 104.5, 100.9, 69.8, 65.0; MS EI+ calculated for $C_{13}H_{15}BrO_3$ $(M-H)^+$: 298, found: 298.

3,5-Bis-allyloxy-4-bromo-benzaldehyde (6):[7] To a suspension of pyridinium chlorochromate (17.02g, 79.0 mmol, 2 equiv), celite (17g, 1:1 PCC:Celite), and sodium acetate (1.62g, 19.7 mmol, 0.5 equiv) in CH_2Cl_2 (230 mL) at 0°C was added **17** (11.82g, 39.5 mmol, 1 equiv) in CH_2Cl_2 (115 mL). The reaction was stirred for 4.5 hours at 0°C, after which time the suspension was decanted into ether (600 mL) at room temperature. The suspension was stirred for 2.5 hours at room temperature, after which time it was filtered through celite and concentrated to afford a brown solid. The solid was dissolved in ether with sonocation and filtered through a short column of Florisil which afforded **6** (11.05g, 94%) as a white solid upon concentration. Crystallization from hot hexanes (~60ml/g) prior to solid-phase reductive amination (Section III) afforded **6** as white needles. R_f = 0.38 (20% EtOAc/hexane); FTIR (neat, cm^{-1}) 3079, 2927, 2359, 1699, 1649, 1578, 1436, 1423; ^1H NMR (400 MHz, $CDCl_3$) δ, 9.88 (s, 1H), 7.02 (s, 2H), 6.18-6.00 (m, 2H), 5.50 (dd, J = 17.4, 2.0 Hz, 2H), 5.33 (dd, J = 10.6, 1.2 Hz, 2H), 4.70 (ddd, J = 5.2, 1.6, 1.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 156.7, 136.0, 132.0, 118.1, 109.7, 106.4, 69.9; HRMS (EI^+) calculated for $C_{13}H_{13}BrO_3$: 296.0048, found: 296.0055.

Scheme II.2 Synthesis of 20.



(S)-2-Allyloxycarbonylamino-3-(4-hydroxy-phenyl)-propionic acid methyl ester (18): To a solution of L-Tyrosine methyl ester hydrochloride (25 g, 107.9 mmol, 1.0 equiv) in THF (500 mL) and CH_2Cl_2 (250 mL) at room temperature was added diisopropyl ethylamine (56.5 ml, 322.5 mmol, 3.0 equiv). The solution was cooled to 0°C and allylchoroformate (11.5 ml, 107.9 mmol, 1.0 equiv) was added dropwise. The reaction was stirred at 0°C for 1.5 hours, after which time saturated ammonium chloride (100 mL) was added and the THF and CH_2Cl_2 were removed under reduced pressure. The aqueous suspension was extracted with ether (4 x 300 mL). The organics were combined, washed with brine, dried over $MgSO_4$, and concentrated. Purification by flash chromatography (15→60% EtOAc/hexane) afforded **18** (30g, 96%) as a white solid. R_f = 0.43 (50% EtOAc/hexane); FTIR (neat, cm^{-1}) 3297, 2959, 1734, 1688, 1566, 1518, 1441, 1229; ^1H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, J = 7.9 Hz, 2H), 6.71 (d, J = 8.0 Hz, 2H), 5.85 (m, 1H), 5.24 (m, 3H), 4.6 (m, 1H), 4.53 (d, $J = 5.2$, 2H), 3.71 (s, 3H), 3.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 155.8, 155.2, 132.3, 130.3, 127.0, 118.0, 115.5, 66.0, 54.9, 52.9, 52.4, 37.4; HRMS (ES$^+$) calculated for $C_{14}H_{17}NO_5$ $(M+H)^+$: 280.1107, found: 280.1195.

(S)-2-Allyloxycarbonylamino-3-(4-allyloxy-phenyl)-propionic acid methyl ester (19): To a solution of **18** (30g, 107.4 mmol, 1.0 equiv) in DMF (170 mL) at room temperature was added solid K_2CO_3 (29.6g, 214.2 mmol, 2.0 equiv) then allylbromide (10.2 mL, 116.3 mmol, 1.1 equiv) dropwise. The suspension was stirred at room temperature for 9 hours, after which time water (500 mL) was added and extracted with ether (4 x 250 mL). The organics were combined, washed with brine, dried over $MgSO_4$, and concentrated. Purification by flash chromatography (20→60% EtOAc/hexane) afforded **19** (31.6 g, 92%) as a clear oil. R_f = 0,27 (25% EtOAc/hexane); FTIR (neat, cm^{-1}) 3343, 2919, 1721, 1510, 1239, 1215, 1176, 1052, 1017; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, $J = 8.4$ Hz, 2H), 6.79 (d, $J = 8.8$ Hz, 2H), 5.99 (m, 1H), 5.85 (m, 1H), 5.44 (d, $J = 8.0$ Hz, 1H), 5.36 (dd, $J = 17.4$, 1.2 Hz, 1H), 5.25 (s, 1H), 5.22 (dd, $J =$ 10.2, 1.6 Hz, 1H), 5.15 (dd, $J = 10.4$, 1.2 Hz, 1H), 4.56 (dd, $J = 14.2$, 6.0 Hz, 1H), 4.51 (d, $J =$ 5.6 Hz, 2H), 4.45 (d, $J = 5.2$ Hz, 2H), 3.66 (s, 3H), 3.03 (dd, $J = 14.4$, 5.2 Hz, 1H), 2.96 (dd, $J =$ 14.0, 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 157.5, 155.4, 133.1, 132.5, 130.0, 127.8, 117.4, 117.3, 114.5, 68.4, 65.5, 54.7, 52.0, 37.0; MS (ES$^+$) calculated for $C_{17}H_{21}NO_5$ $(M+H)^+$: 320.1420, found: 320.2.

[(S)-2-(4-Allyloxy-phenyl)-1-hydroxymethyl-ethyl]-carbamic acid allyl ester (20):[8] To a solution of **19** (1.17 g, 3.66 mmol, 1.0 equiv) in THF (10 mL) at room temperature was added ground anhydrous lithium chloride (0.31g, 7.3 mmol, 2.0 equiv), sodium borohydride (0.28 g, 7.3 mmol, 2.0 equiv), and then ethanol (10.2 ml, 176 mmol, 48.0 equiv). The reaction was stirred at room temperature for 19 hours, after which time the mixture was cooled to 0°C and a 10% aqueous citric acid solution (5 mL) was added to achieve pH 3-4. After concentration under reduced pressure, water (20ml) was added and the solution was extracted into ethylacetate (3 x 75 ml). The organics were combined, dried over anhydrous $MgSO_4$, and concentrated. Purification by flash chromatography (30→50% EtOAc/hexane) afforded **20** (0.85 g, 80%) as a white solid. R_f = 0.24 (50% EtOAc/hexane); $[\alpha]^{25}_D$ = -22.3° (c = 0.9, CH_2Cl_2); FTIR (KBr pellet, cm^{-1}) 3324, 2953, 1696, 1613, 1543, 1512, 1240; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, J = 8.8 Hz, 2H), 6.85 (d, $J = 8.4$ Hz, 2H), 6.09-6.00 (m, 1H), 5.92-5.84 (m, 1H), 5.40 (dd, $J = 15.6$, 2.0 Hz, 1 H), 5.28 (dd, $J = 10.4$, 1.2 Hz, 1H), 5.27 (dd, $J = 17.2$, 1.6 Hz, 1H), 5.20 (dd, $J = 10.0$, 1.6 Hz, 1H), 4.97 (d, $J = 7.2$ Hz, 1H), 4.54-4.50 (m, 4H), 3.89-3.86 (m, 1H), 3.68-3.65 (b, 1H), 3.57 (b, 1H), 2.80 (d, $J = 7.2$Hz, 2H) 2.29 (br-s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 156.4, 133.4, 132.8, 130.3, 129.7, 117.8, 117.7, 114.9, 68.9, 65.7, 64.1, 54.2, 36.5; HRMS (ES$^+$) calculated for $C_{16}H_{21}NO_4$ $(M+H)^+$: 292.1471, found: 292.1551.

Enantiomeric Purity of 20 by Chiral HPLC: **rac-20** was synthesized as described above starting from DL-tyrosine methyl ester and compared to **20** by chiral HPLC on Chiracel OD column, 8% isopropanol/hexane at 1 min/mL. Only one enantiomer was observed by Chiral HPLC:

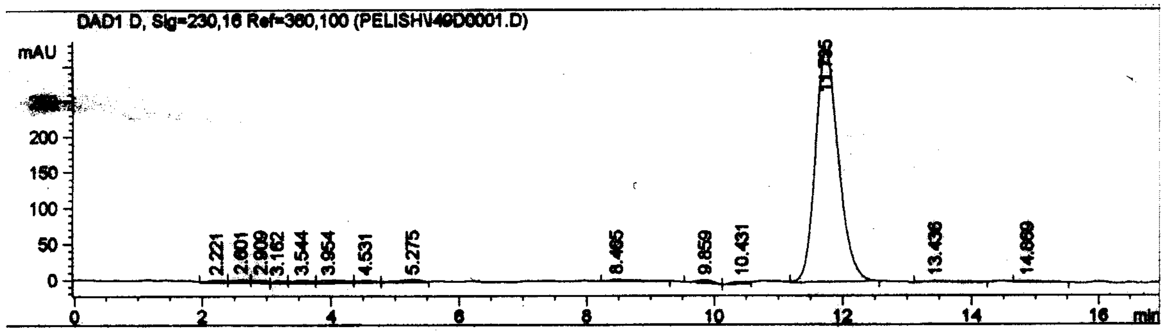


Figure II.1 HPLC of 20 @ 230 nm, major peak retention time = 11.7 minutes.

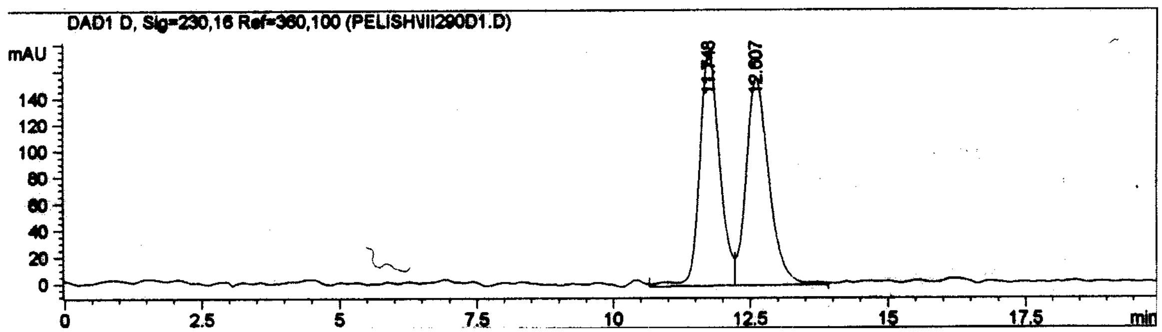
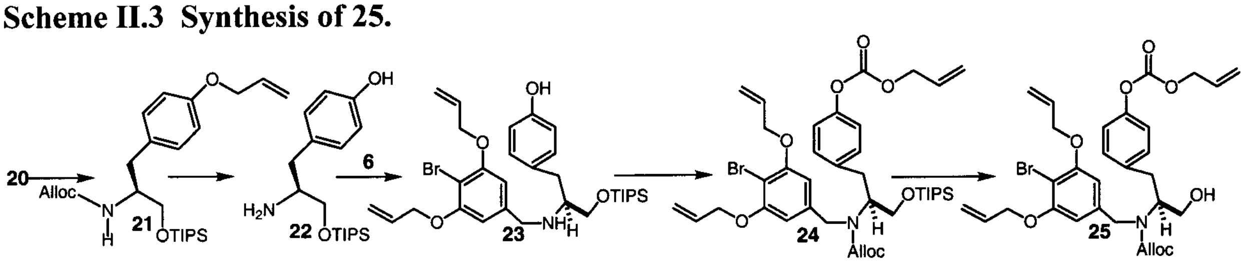


Figure II.2 HPLC of rac-20 @ 230 nm, major peaks retention time = 11.7 minutes and 12.6 minutes.

Scheme II.3 Synthesis of 25.



[(S)-1-(4-Allyloxy-benzyl)-2-(triisopropyl-silanyloxy)-ethyl]-carbamic acid allyl ester (21): To a solution of **20** (4.54 g, 15.6 mmol, 1.0 equiv) in CH_2Cl_2 (150 ml) at 0°C was added diisopropylethylamine (8.1ml, 46.7 mmol, 3.0 equiv) and triisopropylsilyltriflate (5.2 ml, 19.3 mmol, 1.2 equiv) dropwise with stirring. The reaction was stirred at 0°C for 1.5 hours, after which time the reaction was warmed to room temperature. The reaction was stirred at room temperature for 30 minutes, after which time saturated aqueous ammonium chloride (50 mL) was added. The mixture was extracted with CH_2Cl_2 (3 x 100 mL). The organics were combined, washed with brine, dried over $MgSO_4$, filtered, and concentrated. Purification by flash chromatography (5→50% EtOAc/hexane) afforded **21** (6.1 g, 88%) as a yellow oil. R_f = 0.41 (10% EtOAc/hexane); FTIR (neat, cm^{-1}) 3446, 3340, 2943, 2866, 1725, 1612, 1511, 1243; ^1H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, J = 8 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H), 6.08-5.99 (m, 1H), 5.92-5.82 (m, 1H), 5.39 (dd, J = 17.2, 1.6 Hz, 1H), 5.27-5.22 (m, 2H), 5.17 (dd, J = 10.0, 0.8 Hz, 1H), 4.95 (d, J = 8.4 Hz, 1H), 4.52-4.48 (m, 4H), 3.8 (br s, 1H), 3.60 (d, J = 3.6 Hz, 2H), 2.81 (d, J = 7.2 Hz, 2H), 1.1-1.0 (m, 21H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 155.7, 133.3, 133.0, 130.3, 130.2, 117.6, 117.4, 114.6, 68.8, 65.3, 63.1, 53.7, 36.3, 18.0, 11.7; HRMS (ES^+) calculated for $C_{25}H_{41}NO_4Si$ $(M+H)^+$: 448.2805, found: 448.2902.

4-[(S)-2-Amino-3-(triisopropyl-silanoxy)-propyl]-phenol (22): To a solution of **21** (6.05 g, 13.5 mmol, 1.0 equiv) in THF (135 mL) at room temperature, was added morpholine (11.8 mL, 135.6 mmol, 10 equiv), then tetrakis(triphenylphosphine)palladium(0) (1.56 g, 1.35 mmol, 0.1 equiv) in the dark. The solution was warmed to 47°C. The reaction was stirred at 47°C for 10 hours, after which time the solution was cooled to room temperature and the THF was removed under reduced pressure. Purification by flash chromatography (30% EtOAc/hexane→100% EtOAc) afforded **22** (3.9g, 90%) as a brown solid with a minor amount of Ph_3PO. R_f = 0.2 (EtOAc); FTIR (film, cm^{-1}) 2938, 2866, 1515, 1462, 1251, 1105; ^1H NMR (500 MHz, $CDCl_3$) δ 7.01 (d, *J* = 8.5 Hz, 2H), 6.71 (d, *J* = 8.5 Hz, 2H), 4.5 (br s, 2H), 3.75 (dd, *J* = 10.0, 3.5 Hz, 1H), 3.61, (dd, *J* = 9.5, 6.5 Hz, 1H), 3.19 (br s, 1H), 2.79 (dd, *J* = 13.3, 6.0 Hz, 1H), 2.64 (dd, *J* = 13.8, 7.5 Hz, 1H), 1.05 (m, 21H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 130.3, 129.1, 115.8, 115.6, 66.2, 54.9, 37.9, 18.1, 11.9; HRMS (ES^+) calculated for $C_{18}H_{33}NO_2Si$ $(M+H)^+$: 324.2281, found: 324.2374.

4-[(S)-2-(3,5-Bis-allyloxy-4-bromo-benzylamino)-3-(triisopropyl-silanyloxy)-propyl]-phenol (23): A solution of **6** (2.2g, 7.4 mmol, 0.9 equiv) in MeOH (100 mL) was transferred via canula to **22** (2.6g, 8.2 mmol, 1.0 equiv). To the mixture at 0°C was added acetic acid (4.8 mL) followed by sodium cyanoborohydride (250 mg, 4 mmol, 0.5 equiv). The reaction was stirred at 0°C for 30 minutes, after which time additional sodium cyanoborohydride (250 mg, 4 mmol, 0.5 equiv) was added. The reaction was then stirred at room temperature for 15 hours, after which time saturated aqueous sodium chloride (100 mL) and 10% sodium hydroxide in saturated aqueous sodium chloride (150 mL) were added. The mixture was extracted with 5% hexane in EtOAc (4 x 200 mL). The organics were combined, washed with brine, dried over $MgSO_4$, and concentrated. Purification by flash chromatography (20→25% EtOAc/hexane) afforded **23** (2.95 g, 66% from **6**) as a white solid. R_f = 0.2 (30% EtOAc/hexane); FTIR (film, cm^{-1}) 2937, 2865, 1586, 1515, 1456, 1433, 1360, 1246, 1105; ^1H NMR (500 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.0 Hz, 2H), 6.69 (d, *J* = 8.0 Hz, 2H), 6.45 (s, 2H), 6.06-5.99 (m, 2H), 5.46 (dd, *J* = 17.3, 1.5 Hz, 2H), 5.27 (dd, *J* = 11.0, 1.5 Hz, 2H), 4.49, (d, *J* = 5.0 Hz, 4H), 3.8 (d, *J* = 13.0 Hz, 1H), 3.75 (d, *J* = 13.5 Hz, 1H) 3.68-3.61 (m, 2H), 2.93-2.88 (m, 1H), 2.76-2.67 (m, 2H), 1.05 (m, 21H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 154,8, 140.3, 132.7, 130.3, 130.2, 117.6, 115.6, 106.2, 100.6, 69.7, 64.6, 60.5, 51.7, 36.6, 18.1, 11.9; MS (AP^+) calculated for $C_{31}H_{46}BrNO_4Si$ $(M+H)^+$: 604.2380, found: 604.4.

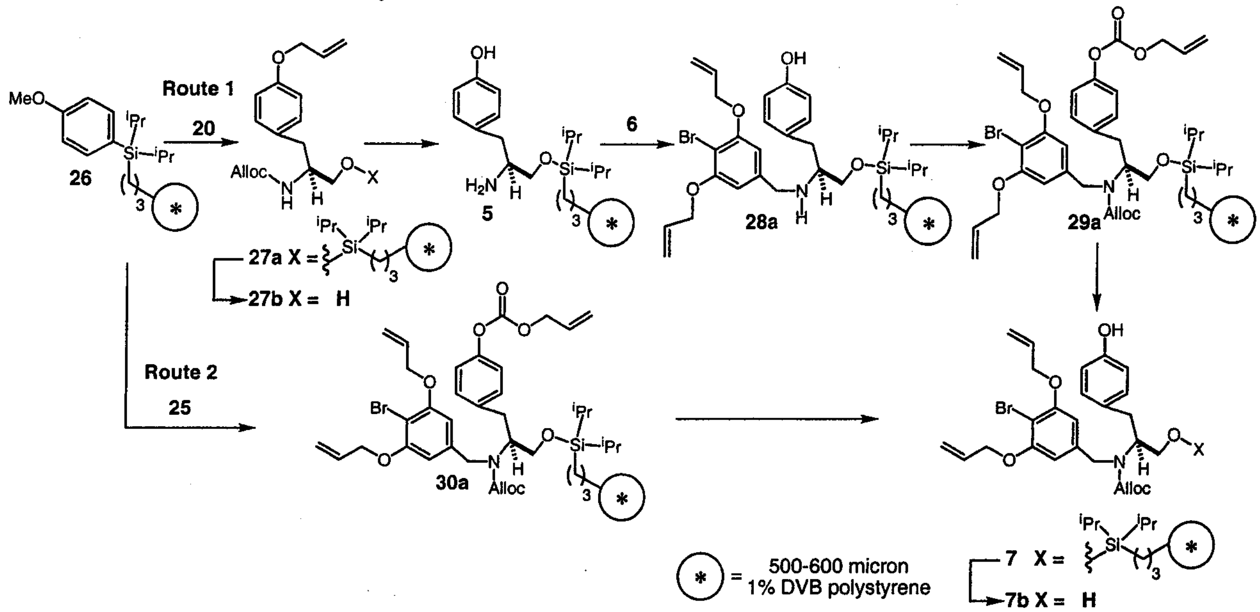
Carbonic acid allyl ester 4-[(S)-2-[allyloxycarbonyl-(3,5-bis-allyloxy-4-bromo-benzyl)-amino]-3-(triisopropyl-silanyloxy)-propyl]-phenyl ester (24): To a solution of **23** (2.74g, 4.53 mmol, 1.0 equiv, azeotropically dried from toluene) in CH_2Cl_2 (80 mL) at room temperature was added 2,6-lutidine (1.85 mL, 15.9 mmol, 3.5 equiv) followed by allylchloroformate (1.44 mL, 13.6 mmol, 3.0 equiv). The reaction was stirred at room temperature for 1.5 hours during which time the solution became pink, and after which time saturated aqueous ammonium chloride was added. The mixture was extracted with CH_2Cl_2 (3 x 100 mL). The organics were combined, washed with brine, dried over Na_2SO_4, and concentrated. Purification by flash chromatography (25% EtOAc/hexane) afforded **24** (3.4 g, 97%) as a yellow oil. R_f = 0.86 (50% EtOAc/hexane); FTIR (film, cm^{-1}) 2938, 2860, 1760, 1701, 1588, 1455, 1419, 1241, 1218, 1104; ^1H NMR (500

MHz, DMSO, 80°C) δ 7.13 (d, *J* = 8.5 Hz, 2H), 7.1 (d, *J* = 9.0 Hz, 2H), 6.56 (s, 2H), 6.05-5.95 (m, 3H), 5.91-5.83 (m, 1H), 5.41 (dd, *J* = 17.3, 1.8 Hz, 2H), 5.39 (dd, *J* = 17.0, 1.5 Hz, 1H), 5.29 (dd, *J* = 10.3, 1.3 Hz, 1H), 5.25 (dd, *J* = 11.0, 1.5 Hz, 2H), 5.20 (d, *J* = 17.0 Hz, 1H), 5.15 (d, *J* = 10.5 Hz, 1H), 4.71 (d, *J* = 5.5 Hz, 2H), 4.52 (d, *J* = 4.5 Hz, 4H), 4.50 (d, *J* = 5.5 Hz, 2H), 4.37 (d, *J* = 16.0 Hz, 1H), 4.28, (d, *J* = 16.0 Hz, 1H), 4.19 (m, 1H), 3.77-3.68 (m, 2H), 2.94-2.86 (m, 2H), 1.0 (m, 21H); ^{13}C NMR (100 MHz, DMSO, 80°C) δ 155.2, 152.2, 148.9, 139.7, 136.0, 132.9, 132.7, 131.5, 129.2, 120.2, 118.1, 116.9, 116.6, 106.0, 105.8, 99.6, 69.3, 69.1, 68.1, 64.9, 63.3, 60.3, 34.0, 17.2, 11.0; HRMS (ES$^+$) calculated for $C_{39}H_{54}BrNO_8Si$ $(M+H)^+$: 772.2802, found: 772.2911.

Carbonic acid allyl ester 4-{(S)-2-[allyloxycarbonyl-(3,5-bis-allyloxy-4-bromo-benzyl)-amino]-3-hydroxy-propyl}-phenyl ester (25): To **24** (1.15g, 1.49 mmol, 1.0 equiv) in THF (20 mL) in a high density polyethylene vial was added hydrogen fluoride-pyridine (1 mL) once an hour for 4 hours (4 mL total), after which time saturated aqueous ammonium chloride was added and the THF was removed under reduced pressure. The remaining solution was extracted with CH_2Cl_2. The organics were combined, washed with brine, dried over Na_2SO_4, and concentrated. Purification by flash chromatography (20→60% EtOAc/hexane) afforded **25** (0.86 g, 94%) as a colorless oil. R_f = 0.23 (50% EtOAc/hexane); $[\alpha]^{28}_D$ = -29.24° (c = 1, CH_2Cl_2); FTIR (neat, cm^{-1}) 3447, 2932, 1761, 1695, 1588, 1435, 1421, 1242; ^{1}H NMR (400 MHz, DMSO, 80°C) δ 7.18-7.12 (m, 2H), 7.10-7.04 (m, 2H), 6.63 (s, 2H), 6.07-5.94 (m, 3H), 5.90-5.78 (m, 1H), 5.42 (dd, *J* = 15.2, 2.0 Hz, 2H), 5.39 (dd, *J* = 14.0, 1.6 Hz, 1H), 5.30 (dd, *J* = 10.4, 1.6 Hz, 1H), 5.25 (dd, *J* = 10.6, 1.8Hz, 2H) 5.18 (d, *J* = 16.8 Hz, 1H), 5.13 (d, *J* = 10.4 Hz), 4.73-4.71 (m, 2H), 4.55-4.54 (m, 4H), 4.72 (d, *J* = 4.0 Hz, 2H), 4.36 (d, *J* = 16.0 Hz, 1H), 4.24 (d, *J* = 16.4 Hz, 1H), 4.21-4.12 (m, 1H), 3.62-3.57 (m, 1H), 3.53-3.49 (m, 1H), 2.90-2.77 (m, 2H); ^{13}C NMR (100 MHz, DMSO, 80°C) δ 155.3, 155.1, 152.2, 148.8, 140.1, 136.3, 132.9, 132.8, 131.5, 129.3, 120.1, 116.8, 116.6, 116.3, 105.8, 105.6, 99.1, 69.2, 69.0, 68.1, 64.7, 61.3, 60.5, 48.1, 34.3; HRMS (ES$^+$) calculated for $C_{30}H_{34}BrNO_8$ $(M+H)^+$: 616.1468, found: 616.1570.

III. Solid-Phase Synthesis of Core Enone (9)

Scheme III.1 Solid-Phase Synthesis of Resin 7.



Resin (27a): To silicon-functionalized resin **26** (3.65g, 1.43 mequiv Si/g, 5.22 mmol Si, 1.0 equiv Si) in a pear-shaped flask (100 mL) was added CH_2Cl_2 (35 mL) at room temperature. After 10 minutes, the solvent was removed via canula and the resin was washed with CH_2Cl_2 (15 mL, 2 x 10 minutes, via canula). CH_2Cl_2 (15 mL) and 2,6-lutidine (1.1 mL, 9.44 mmol, 1.8 equiv) were then added. After 5 minutes with gentle swirling by hand, trimethylsilylchloride (1.1 mL, 8.67 mmol, 1.7 equiv) was added dropwise over 5 minutes. The mixture was swirled gently by hand over 15 minutes, after which time the solvent was removed via canula and the resin was washed with CH_2Cl_2 (15 mL, 3 x 5 minutes, via canula). A 5% trifluoromethanesulfonic acid/ CH_2Cl_2 solution (48 mL, 27.1 mmol, 5.2 equiv) was then added over 10 minutes. The resin turned bright red/orange upon acid treatment. The mixture was swirled gently by hand over 15 minutes, after which time the solvent was removed via canula and the resin was washed with CH_2Cl_2 (15 mL, 3 x 5 minutes, via canula). CH_2Cl_2 (15 mL) and 2,6-lutidene (4.9 mL, 42.1 mmol, 8.1 equiv) were then added. The resin decolorized upon base addition. The mixture was swirled gently by hand over 5 minutes, after which time **6** (2.3 g, 7.9 mmol, 1.5 equiv), azeotroped from toluene and dissolved in CH_2Cl_2 (5 mL) was added. The reaction was swirled gently by hand over 10 minutes and then sealed under argon. The solution was left standing for 20 hours, after which time the heterogeneous mixture was poured into a 100 mL peptide reaction vessel and the solution was drained. The resin was washed with CH_2Cl_2 (3 x 10 minutes), THF (2 x 10 minutes), CH_2Cl_2 (1 x 10 minutes) and hexanes (2 x 5 minutes). Excess **20** was recovered upon concentration of the washings. Air drying afforded **27a** as a colorless resin.

[(S)-2-(4-Allyloxy-phenyl)-1-hydroxymethyl-ethyl]-carbamic acid allyl ester (27b): To vacuum-dried resin **27a** (51.3 mg) in a high density polyethylene vial was added 10% HF-pyridine in THF (1 mL). After 1.5 hours, methoxytrimethylsilane (2 mL) was added to quench unreacted HF. After 30 minutes, the solution was removed and the beads were washed with THF

(2 x 3 mL). The washings and reaction solution were combined and concentrated. Purification by flash chromatography (50% EtOAc/hexane) afforded a white solid (9.2 mg, 0.62 mmol/g) with spectroscopic characteristics identical to **20**. Theoretical Loading Level = 1.13 mmol/g; Loading efficiency = 55%.

Resin (5): To resin **27a** (150 mg, 0.62 mmol/g, 0.093 mmol, 1.0 equiv) in a 2 mL BioRad tube was added 25% morpholine/THF (1.7 mL). After 10 minutes, $Pd(PPh_3)_4$ (87 mg, 0.075 mmol, 0.8 equiv) was added in the dark. The tube was sealed under argon and tumbled for 20 hours, after which time the tube was attached to a Promega wash station. The solvent was drained and the resin was washed with CH_2Cl_2 (2 x 1 minute, 1 x 5 minutes), THF (3 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 0.1 M dimethyldithiocarbamic acid sodium hydrate in 25% H_2O/THF (2 x 15 min with tumbling), 25% CH_3CN/THF (1 x 10 minutes), 50% CH_3CN/THF (1 x 10 minutes), 75% CH_3CN/THF (1 x 10 minutes), 90% CH_3CN/THF (1 x 10 minutes), and CH_3CN (1 x 10 minutes). Air drying afforded **5** white beads.

Resin (28a):[9] To resin **5** (138.5 mg, 0.67 mmol/g, 0.093 mmol, 1.0 equiv) and **6** (411 mg, 1.38 mmol, 14.8 equiv, recrystallized from hexanes) in a 10 mL pear-shaped flask was added CH_2Cl_2 (1.5 mL). After complete dissolution of **6**, $CH(OCH_3)_3$ (1.5 mL) was added. The reaction was sealed under argon at room temperature. After 20 hours, the solvent was drained via canula and the resin was washed (under argon) with 25% $CH(OCH_3)_3$ in CH_2Cl_2 (1 x 10 min), CH_2Cl_2 (4 x 10 min), and 25% $CH(OCH_3)_3$ in CH_2Cl_2 (1 x 10 min). $NaBH_3CN$ (87 mg, 1.38 mmol, 14.8 equiv) dissolved in 10% acetic acid in $CH(OCH_3)_3$ (20 μl in 2 mL) was then added with gentle swirling at room temperature. After 20 hours, the solvent was removed and excess **6** was recovered. The resin was washed with CH_2Cl_2 (2 x 1 minute, 1 x 5 minutes), THF (3 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 25% CH_3CN/THF (1 x 10 minutes), 50% CH_3CN/THF (1 x 10 minutes), 75% CH_3CN/THF (1 x 10 minutes), 90% CH_3CN/THF (1 x 10 minutes), and CH_3CN (1 x 10 minutes). Air drying afforded **28a** as white beads.

Resin (29a): To resin **28a** (89.4 mg, 0.56 mmol/g, 0.05 mmol, 1.0 equiv) in a 10 mL pear-shaped flask was added CH_2Cl_2 (1 mL), *i*Pr_2NEt (467 μL, 2.68 mmol, 53.6 equiv), benzoyl chloride (190 μL, 1.79 mmol, 35.8 equiv) at room temperature. After 20 hours, the solvent was drained and the resin was washed with CH_2Cl_2 (2 x 1 minute, 1 x 5 minutes), THF (3 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 25% CH_3CN/THF (1 x 10 minutes), 50% CH_3CN/THF (1 x 10 minutes), 75% CH_3CN/THF (1 x 10 minutes), 90% CH_3CN/THF (1 x 10 minutes), and CH_3CN (1 x 10 minutes). Air drying afforded **29a** as white beads.

Resin (7, route 1): To **29a** in a 10 mL BioRad tube under argon was added 10% piperidine in THF (10 mL) via at room temperature. The reaction vessel was sealed and tumbled on an orbital stirrer. After 20 hours, the solvent was drained by gravity and washed with THF (3 x 15 minutes), CH_2Cl_2 (1 x 15 minutes), 75% CH_2Cl_2/hexane (1 x 15 minutes), 50% CH_2Cl_2/hexane (1 x 15 minutes), and 25% CH_2Cl_2/hexane (1 x 15 minutes). Air drying afforded **17a** as a white beads.

(3,5-Bis-allyloxy-4-bromo-benzyl)-[(S)-1-hydroxymethyl-2-(4-hydroxy-phenyl)-ethyl]-carbamic acid allyl ester (7b, route 1): To vacuum-dried resin **7** (65.5 mg) in a high density polyethylene vial was added 10% HF-pyridine in THF (1 mL). After 1.5 hours, methoxytrimethylsilane (2 mL) was added to quench unreacted HF. After 30 minutes, the solution was removed and the beads were washed with THF (2 x 3 mL). The washings and reaction solution were combined and concentrated. Purification by flash chromatography (50 % EtOAc/hexane) afforded a clear oil (14.6 mg, 0.42 mmol/g). Theoretical Loading Level[10] (from **27b**) = 0.54 mmol/g; Yield from **27b** = 78% (5 steps). R_f = 0.28 (50% EtOAc/hexane); FTIR (film, cm^{-1}) 3342, 2925, 1670, 1588, 1515, 1432, 1419, 1225; ^1H NMR (400 MHz, DMSO, 80°C) δ 8.88 (s, 1H), 6.90-6.89 (m, 2H), 6.66-6.62 (m, 4H), 6.07-5.96 (m, 2H), 5.83 (br s, 1H), 5.45-5.40 (m, 2H), 5.26-5.23 (m, 2H), 5.20-5.11 (m, 2H), 4.54 (br s, 4H), 4.47 (br s, 2H), 4.34 (dd, J = 16.0, 3.6 Hz, 1H), 4.20 (dd, J = 16.2, 3.2 Hz, 1H), 4.11 (m, 1H), 3.55 (br s, 1H), 3.49-3.45 (m, 1H), 2.74-2.63 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 155.1, 140.3, 133.1, 132.9, 129.2, 128.5, 116.8, 116.3, 114.7, 105.6, 99.0, 69.0, 64.7, 61.3, 60.8, 48.1, 34.2; MS (ES^+) calculated for $C_{26}H_{30}BrNO_6$: 531.1257, found: 531.7.

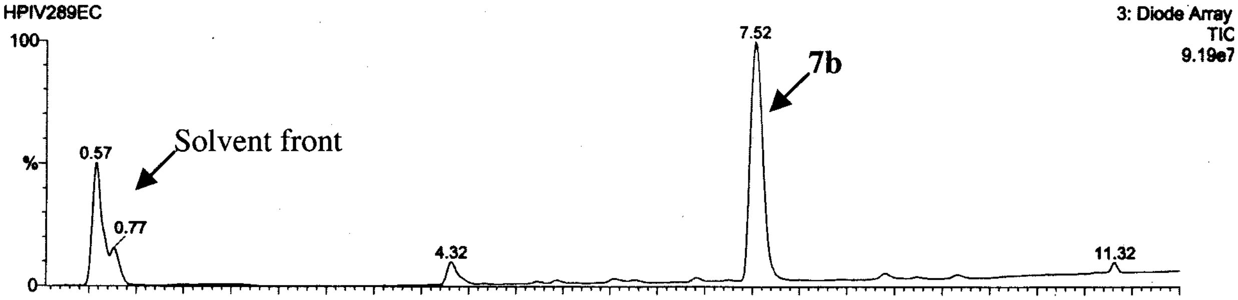


Figure III.1 HPLC of Unpurified 7b, route 1.

Resin (30a): To silicon-functionalized resin **26** (5.87 g, 1.45 mequiv Si/g, 8.51 mmol Si, 1.0 equiv Si) in a pear-shaped flask (200 mL) under positive argon pressure was added CH_2Cl_2 (70 mL) at room temperature. After 10 minutes, the solvent was removed via canula and the resin was washed with CH_2Cl_2 (30 mL, 2 x 10 minutes, via canula). CH_2Cl_2 (30 mL) and 2,6-lutidine (1.8 mL, 15.45 mmol, 1.8 equiv) were then added. After 5 minutes with gentle swirling by hand, trimethylsilylchloride (1.75 mL, 13.79 mmol, 1.6 equiv) was added dropwise over 5 minutes. The mixture was swirled gently by hand over 15 minutes, after which time the solvent was removed via canula and the resin was washed with CH_2Cl_2 (30 mL, 3 x 5 minutes, via canula). A 5% trifluoromethanesulfonic acid/ CH_2Cl_2 solution (90 mL, 50.86 mmol, 6.0 equiv) was then added over 10 minutes. The resin turned bright red/orange upon acid treatment. The mixture was swirled gently by hand over 15 minutes, after which time the solvent was removed via canula and the resin was washed with CH_2Cl_2 (30 mL, 3 x 5 minutes, via canula). CH_2Cl_2 (30 mL) and 2,6-lutidene (7.9 mL, 67.82 mmol, 8.0 equiv) were then added. The resin decolorized upon base addition. The mixture was swirled gently by hand over 5 minutes, after which time **25** (6.3 g, 10.22 mmol, 1.2 equiv), azeotroped from toluene and dissolved in CH_2Cl_2 (30 mL) was added. The reaction was swirled gently by hand over 10 minutes and then sealed under argon. The solution was left standing for 20 hours, after which time the heterogeneous mixture was poured into a 100 mL peptide reaction vessel and the solution was drained. The resin was washed with CH_2Cl_2 (3 x 10 minutes), THF (2 x 10 minutes), CH_2Cl_2 (1 x 10 minutes) and hexanes (2 x 5 minutes). Excess **25** was recovered upon concentration of the reaction solvent and washings. Air drying afforded **30a** as a colorless resin.

Resin (7, route 2): To **30a** in a 100 mL peptide reaction vessel under positive argon pressure was added 10% piperidine in THF (100 mL) via canula at room temperature. The reaction vessel was sealed and tumbled on an orbital stirrer. After 20 hours, the solvent was drained by gravity and washed with THF (3 x 15 minutes), CH_2Cl_2 (1 x 15 minutes), 75% CH_2Cl_2/hexane (1 x 15 minutes), 50% CH_2Cl_2/hexane (1 x 15 minutes), and 25% CH_2Cl_2/hexane (1 x 15 minutes). Air drying afforded **7** as a colorless resin.

(3,5-Bis-allyloxy-4-bromo-benzyl)-[(S)-1-hydroxymethyl-2-(4-hydroxy-phenyl)-ethyl]-carbamic acid allyl ester (7b, route 2): To vacuum-dried resin **7** (46.92 mg, 205 beads, 4369 beads/g and 47.02 mg, 211 beads, 4487 beads/g) in two separate high density polyethylene vials was added 10% HF-pyridine in THF (1 mL). The vials were sealed and gently agitated for 1.5 hours after which time the methoxytrimethylsilane (2 mL) was added to quench unreacted HF. After 30 minutes, the solution was removed and the beads were washed with THF (2 x 3 mL). The washings and reaction solution were combined and concentrated. Purification by flash chromatography (50% EtOAc/hexane) of each afforded a white solid (15.1 mg, 138 nmol/bead and 17.2 mg, 153 nmol/bead, respectively, average loading level = 146 nmol/bead, 0.65 mmol/g) with spectroscopic characteristics identical to **7b, route 1**. Theoretical Loading Level = 0.90 mmol/g; Loading efficiency = 72%.

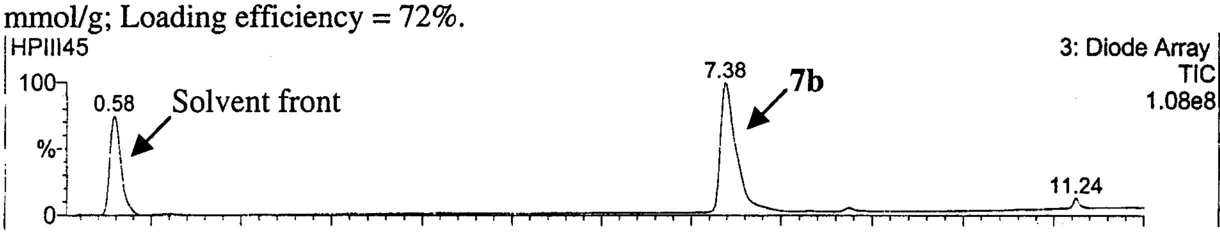
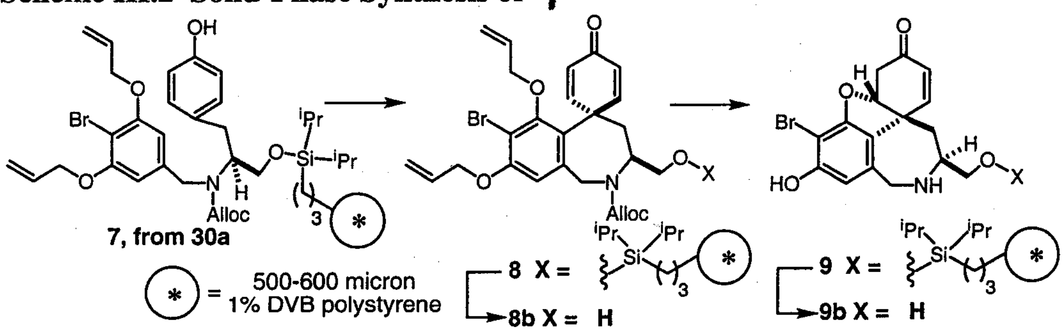


Figure III.2 HPLC of Unpurified 7b, route 2.

Scheme III.2 Solid-Phase Synthesis of 9



Resin (8, from route 2): To resin 7 (from route 2, 6 g, 0.65 mmol/g, 3.88 mmol, 1.0 equiv) in a 100 mL peptide reaction vessel under argon was added 33% CH_2Cl_2/hexafluoroisopropanol (93 mL). After gentle swirling by hand over 15 minutes, $PhI(OAc)_2$ (19g, 59.0 mmol, 15.2 equiv) was added and the mixture was immediately agitated by hand followed by gently tumbling. The resin color changed from clear to green to brown. The resin was tumbled for 4 hours at room temperature, after which time the solution was drained and the resin was washed with THF (2 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 25% CH_3CN/THF (1 x 10 minutes), 50% CH_3CN/THF (1 x 10 minutes), 75% CH_3CN/THF (1 x 10 minutes), 90% CH_3CN/THF (1 x 10 minutes), and CH_3CN (1 x 10 minutes). Air drying afforded **8** as a brown resin.

6,8-Diallyloxy-7-bromo-(S)-3-hydroxymethyl-4'-oxo-5'-spiro-1'cyclohexa-2'5'-diene-1,3,4,5-tetrahydro-benzo[c]azepine-2-carboxylic acid allyl ester (8b): To vacuum-dried resin **8** (41.53 mg, 183 beads, 4406 beads/g and 42.78 mg, 188 beads, 4395 beads/g) in two separate high density polyethylene vials was added 10% HF-pyridine in THF (1 mL). The vials were sealed and gently agitated for 1.5 hours after which time the methoxytrimethylsilane (2 mL) was added to quench unreacted HF. After 30 minutes, the solution was removed and the beads were washed with THF (2 x 3 mL). The washings and reaction were combined and concentrated. Purification by flash chromatography with Florisil (67% EtOAc/hexane) afforded a yellow solid (8.5 mg, 88 nmol/bead and 9.6 mg, 96 nmol/bead, respectively, average loading level = 92 nmol/bead, 0.40 mmol/g). Theoretical Loading Level (from **7**, route 2) = 0.65 mmol/g, Yield = 62%. Some cleavage of product was observed under the acidic conditions of the reaction (refer to Figure III.3 for purity). In a smaller scale reaction (183.4 mg **7**), a yield of 84% was obtained upon cleavage from the resin. R_f = 0.38 (100% EtOAc/hexane); FTIR (film, cm^{-1}) 3411, 2926, 1686, 1657, 1583, 1450, 1412, 1340, 1236; ^1H NMR (400 MHz, $CDCl_3$) At room temperature, 2 rotamers are present in a ratio of 1:1.25 (see Figure III.3 and Section V.1.2) δ 7.06-6.99 (m), 6.93-6.91 (m), 6.59 (s), 6.51 (s), 6.34-6.30 (m), 6.26 (d, J = 10.0 Hz), 6.08-5.78 (m), 5.48 (d, J = 17.2 Hz), 5.33-5.06 (m), 4.79-4.57 (m), 4.49-4.45 (m), 4.39-4.35 (m), 4.27-4.23 (m), 4.12-4.03 (m), 3.73-3.60 (m), 2.76-2.62 (m), 2.4 (br s), 1.75-1.71 (m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.6, 158.0, 157.5, 157.1, 156.9, 156.0, 155.3, 155.2, 152.1, 151.9, 139.4, 139.3, 132.5, 132.4, 132.2, 132.1, 132.0, 131.9, 129.0, 125.2, 125.0, 124.5, 124.2, 118.7, 118.6, 118.4, 118.1, 117.0, 110.2, 110.1, 107.8, 107.7, 74.5, 69.8, 69.7, 66.5, 66.2, 64.6, 64.5, 55.4, 55.3, 47.3, 47.1, 47.0, 41.8, 41.3, 29.7; MS (ES^+) calculated for $C_{26}H_{28}BrNO_6$ ($M+H^+$): 530.1100, found: 530.

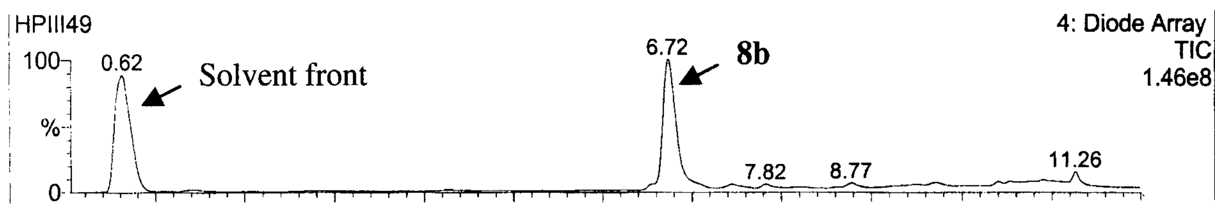


Figure III.3 HPLC of Unpurified 8b

Resin (9): To resin **8** (687 mg, 0.40 mmol/g, 0.28 mmol, 1.0 equiv) in a 10 mL BioRad tube was added 25% morpholine/THF (10 mL). The resin changed color from brown to orange/yellow. After 15 minutes at room temperature, $Pd(PPh_3)_4$ (333 mg, 0.29 mmol, 1.0 equiv) was added in the dark. The tube was sealed under argon and tumbled for 1.5 hours, after which time the tube was attached to a Promega wash station. The solvent was drained and the resin was washed with CH_2Cl_2 (2 x 1 minute, 1 x 5 minutes), THF (3 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 25% CH_3CN/THF (1 x 10 minutes), 50% CH_3CN/THF (1 x 10 minutes), 75% CH_3CN/THF (1 x 10 minutes), 90% CH_3CN/THF (1 x 10 minutes), and CH_3CN (1 x 10 minutes). Air drying afforded **9**.

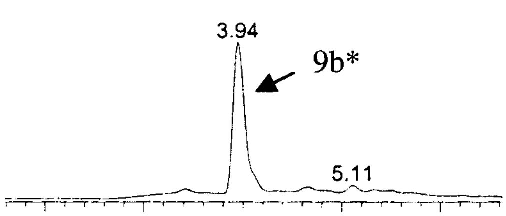
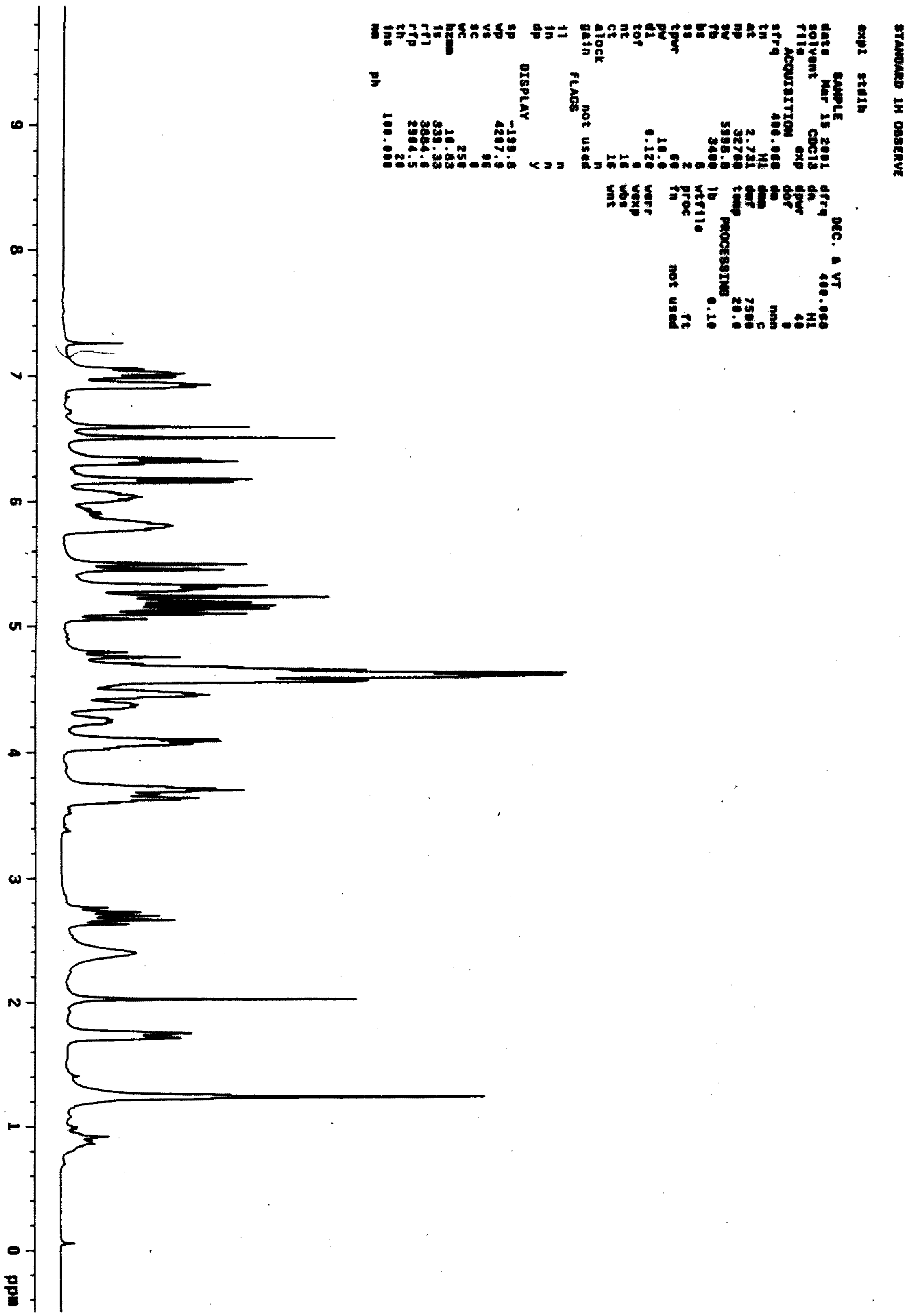


Figure III.4 HPLC of Unpurified 9b. Solvent front omitted for clarity.

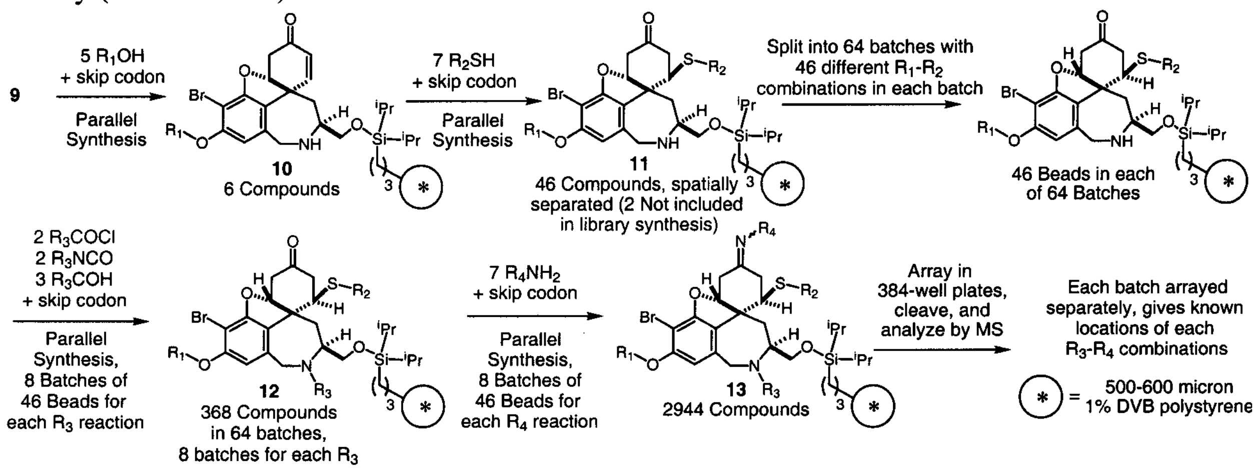
Figure III.5 ^{1}H NMR Spectrum of Spirodienone (8b)



IV. Library Synthesis

IV.1 Introduction

A stepwise approach was taken to the synthesis of a one-bead-one compound galanthamine-like library (Scheme IV.1).



Scheme IV.1 Library Synthetic Sequence

Building blocks were tested for their ability to couple in high yield and purity with a single common substrate. The building blocks are listed in Table IV.1 and their structures are given in Figure IV.1.

Table IV.1 Building Blocks & Identification

R1-	PHENOL FUNCTIONALIZATION	R3-	NITROGEN-FUNCTIONALIZATION
1	3-Nitrobenzyl alcohol	1	Benzoyl chloride
2	Cyclopropylmethanol	2	Benzyl isocyanate
3	3-Phenoxy-1-propanol	3	Ethyl isocyanate
4	3-Cyclopentyl-1-propanol	4	Thiophene-2-carbonyl chloride
5	5-Hexen-1-ol	5	3-(Methylthio)propionaldehyde
6	Skip Codon	6	Undecanal
		7	Cyclopropanecarboxaldehyde
		8	Skip Codon
R2-	**ENONE FUNCTIONALIZATION**	**R4-**	**KETONE FUNCTIONALIZATION**
1	Furfuryl mercaptan	1	*p*-Toluenesulfonhydrazide
2	3-(Trifluoromethyl)benzyl mercaptan	2	Dansyl hydrazine
3	3-Methyl-1-butanethiol	3	Methoxyamine hydrochloride
4	4-Methoxy-alpha-toluenethiol	4	*o*-Benzylhydroxylamine hydrochloride
5	Benzyl mercaptan	5	Carboxymethoxylamine hemihydrochloride
6	2-(*tert* Butyldimethylsilyloxy)ethylmercaptan[11]	6	*p*-Methoxybenzenesulfonylhydrazide
7	Cyclopentanethiol	7	4-Nitrophenylhydrazine
8	Skip Codon	8	Skip Codon

Table IV.1 Building Blocks

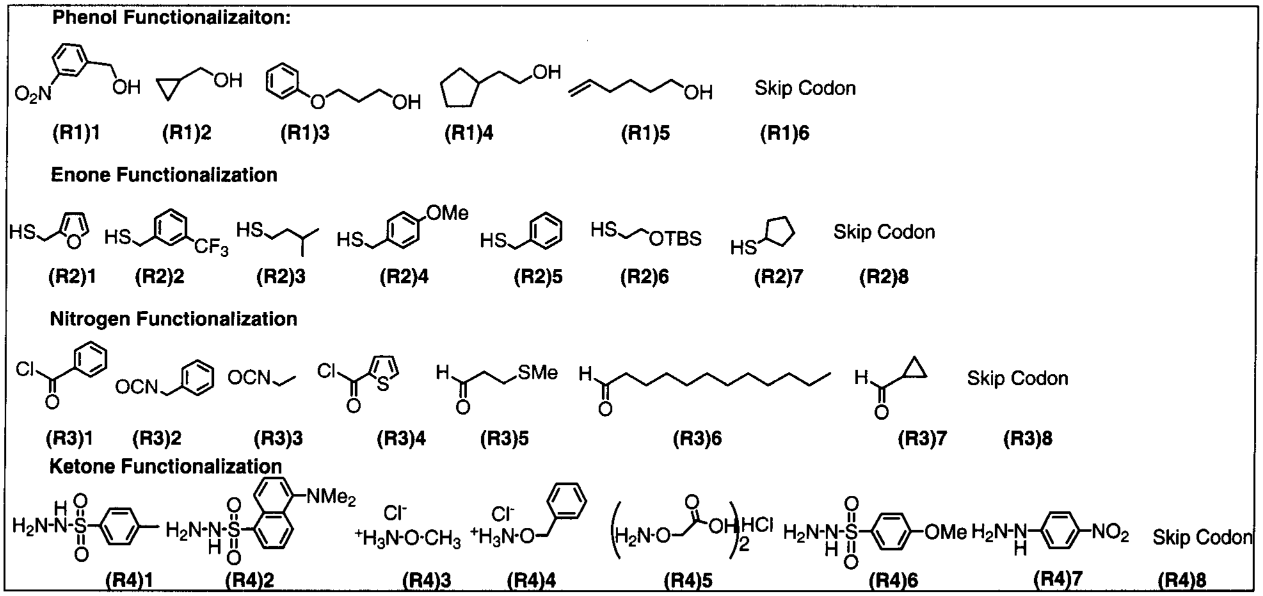


Figure IV.1 Chemical Structure of Building Blocks

In order to identify any undesirable building block interactions during library synthesis, all (R1)(R2) combinations were synthesized in parallel (Scheme IV.1). The purity of all (R1)(R2) combinations was assessed by LCMS analysis (see Section V.3.1, Figures V.3.1.1-V.3.1.6, Table V.3.1.1). LCMS analysis indicated that two combinations of (R1)(R2) ((R1)1(R2)1 and (R1)1(R2)2) resulted in unsuccessful couplings (data not provided) and were therefore not included in the library synthesis. Three compounds from this stage of the library synthesis were characterized by NMR (**(34b)**, **(37b)**, **(38b)**, Section V.4). A single bead from each of the remaining 46 spatially separated R1-R2 combinations was pooled together to form a new batch. This was repeated to generate 64 new batches that each contained all 46 (R1)(R2) combinations. All (R3)(R4) combinations were synthesized in parallel. Each of those batches was sequentially exposed to a different (R3)(R4) combination.

IV.2 Synthetic Procedures

Resin (10) (R1)2: To **9** (687 mg, 0.428 mmol/g, 0.29 mmol, 1.0 equiv) and PPh_3 (946 mg, 3.6 mmol, 12.2 equiv) dissolved THF (8 mL) in a round-bottom flask (25 mL) at room temperature was added cyclopropylmethanol (292 μL, 3.6 mmol, 12.2 equiv). The mixture was gently swirled by hand and cooled to 0°C at which time diisopropylazodicarboxylate (568 μL, 2.9 mmol, 10 equiv) was added in the dark dropwise over 5 minutes with gentle swirling by hand. The reaction was allowed to stand at 0°C for 1 hour in the dark, at which time the mixture was poured into a BioRad tube (20 mL). The tube was attached to a Promega wash station, the solvent was drained, and the resin was washed with CH_2Cl_2 (2 x 1 minute, 1 x 5 minutes), THF (2 x 5 minutes), 10% CH_3CN/THF (1 x 5 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF (1 x 5 minutes), 90% CH_3CN/THF (1 x 5 minutes), and CH_3CN (1 x 5 minutes). Air drying afforded **Resin (10) (R1)2**.

This procedure was repeated twice for full conversion. Conversion was determined by reacting two beads with benzoyl chloride (10 eq.), 2,6-lutidine (10eq.) in DCM overnight at room temperature, detachment of the compound from the solid-support, and analysis by LCMS.

Resin (11) (R1)2(R2)5: To **Resin (10) (R1)2** (80.9mg, 0.418 mmol/g, 0.034 mmol, 1.0 equiv) in a round-bottom flask (25 mL) swollen in THF (1.2 mL) at room temperature was added benzylmercaptan (398 μL, 3.4 mmol, 100 equiv) and 2,6-lutidine (396 μL, 3.4 mmol, 100 equiv). Following gentle swirling by hand over 1 minute, the mixture was cooled to 0°C. The reaction was left at 0°C for 1 hour, after which time nBuLi (40 μL, 2.5 M in hexane, 0.1 mmol, 2.9 equiv) was added dropwise with gentle swirling by hand. The reaction was left at 0°C for 2 hours, after which time it was fitted with a condenser and warmed to 40°C. After 18 hours at 40°C, the reaction was cooled to room temperature and 5% dry acetic acid in THF (500 μL) was added. The mixture was immediately poured into a BioRad tube (20 mL), fitted to a Promega wash station, and drained. The resin was washed with THF (1 x 30 seconds), 10% H_20/THF (2 x 30 seconds), THF (2 x 10 minutes), 10% CH_3CN/THF (1 x 10 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF (1 x 5 minutes), 90% CH_3CN/THF (1 x 5 minutes), and CH_3CN (1 x 5 minutes). Air drying afforded **Resin (11) (R1)2(R2)5**.

Resin (12) (R1)1-6(R2)1-8(R3)1: A single bead from each of the 46 R1-R2 combinations (see above) was placed in a pear-shaped flask (10 mL). To the 46 beads (~92nmol/bead, 0.0042 mmol, 1.0 equiv) was added CH_3CN (2 mL). After 15 minutes, the CH_3CN was removed via canula and replaced with 50% CH_3CN/CH_2Cl_2 (2 mL). After 15 minutes, the solvent was removed via canula and replaced with a stock solution (350 μL) of benzoyl chloride (16.8 μL, 0.051 mmol, 12 equiv) and 2,6-lutidine (16.9 μL, 0.051 mmol, 12 equiv) in CH_2Cl_2 (1 mL). The reaction was allowed to stand at room temperature for 18 hours. For those batches subsequently undergoing imine formation with one of the R4 building blocks, the solvent was removed via canula and the resin was washed under positive argon pressure with a dry solution of 25% $MeOH/CH_2Cl_2$ (3 x 10 minutes) and reacted immediately (before drying) with the appropriate R4 building block. For those batches designated for R4-8 (skip codon), the resin was subsequently washed via canula with THF (1 x 5 minutes), 10% H_20/THF (1 x 5 minutes), 10% CH_3CN/THF (1 x 5 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF (1 x 5 minutes), 90% CH_3CN/THF (1 x 5 minutes), and CH_3CN. The resin was arrayed directly into 384-well plates from the final wash solvent (see Section IV.3).

Resin (12) (R1)1-6(R2)1-8(R3)2: A single bead from each of the 46 R1-R2 combinations (see above) was placed in a pear-shaped flask (10 mL). To the 46 beads (~92nmol/bead, 0.0042 mmol, 1.0 equiv) was added CH_3CN (2 mL). After 15 minutes, the CH_3CN was removed via canula and replaced with 50% CH_3CN/CH_2Cl_2 (2 mL). After 15 minutes, the solvent was removed via canula and replaced with of a stock solution (400 μL) of benzyl isocyanate (54.9 μL, 0.051 mmol, 12 equiv) in CH_2Cl_2 (3.5 mL). The reaction was allowed to stand at room temperature for 18 hours. For those batches subsequently undergoing imine formation with one of the R4 building blocks, the solvent was removed via canula and the resin was washed under positive argon pressure with a dry solution of 25% $MeOH/CH_2Cl_2$ (3 x 10 minutes) and reacted immediately (before drying) with the appropriate R4 building block. For those batches designated for R4-8 (skip codon), the resin was subsequently washed via canula with THF (1 x 5 minutes), 10% H_2O/THF (1 x 5 minutes), 10% CH_3CN/THF (1 x 5 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF (1 x 5 minutes), 90% CH_3CN/THF (1 x 5 minutes), and CH_3CN. The resin was arrayed directly into 384-well plates from the final wash solvent (see Section IV.3).

Resin (12) (R1)1-6(R2)1-8(R3)7: A single bead from each of the 46 R1-R2 combinations (see above) was placed in a pear-shaped flask (10 mL). To the 46 beads (~92nmol/bead, 0.0042 mmol, 1.0 equiv) was added a stock solution (200 μL) of cyclopropanecarboxaldehyde (59.4 μL, 0.064 mmol, 15.1 equiv) and acetic acid (15.1 μL, 0.021 mmol, 5.0 equiv) in 25% MeOH/THF (2.5 mL). The mixture was left standing at room temperature for 2 hours, after which time a stock solution (50 μL) of sodium cyanoborohydride (200 mg, 0.064 mmol, 15.1 equiv) in MeOH (2.5 mL) was added slowly. The reaction was allowed to stand at room temperature for 18 hours. For those batches subsequently undergoing imine formation with one of the R4 building blocks, the solvent was removed via canula and the resin was washed under positive argon pressure with a dry solution of 10% MeOH/THF (2 x 15 minutes) and reacted immediately (before drying) with the appropriate R4 building block. For those batches designated for R4-8 (skip codon), the resin was subsequently washed via canula with THF (1 x 5 minutes), 10% CH_3CN/THF (1 x 5 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF (1 x 5 minutes), 90% CH_3CN/THF (1 x 5 minutes), and CH_3CN. The resin was arrayed directly into 384-well plates from the final wash solvent (see Section IV.3).

Resin (13) (R1)1-6(R2)1-8(R3)1-8(R4)1: To the resin (46 beads, ~92nmol/bead, 0.0042 mmol, 1.0 equiv) and *p*-toluensulfonylhydrazide (59 mg, 0.32 mmol, 75 equiv) in a pear-shaped flask (10 mL) was added AcOH:MeOH:CH_2Cl_2 (1:3.8:10.4, 300 μL) in the dark. The mixture was kept at room temperature in the dark for 20 hours, after which time the solvent was removed via canula and the resin was washed with MeOH:DMSO:THF (1:1:2, 3 x 5 minutes) [Note: additional DMSO was added to dissolve any undissolved reagent], 2.5% 2,6-lutidine in 25% CH_3CN/THF (1 x 5 minutes), MeOH:DMSO:THF (1:1:2, 2 x 10 minutes), 25% CH_3CN/THF (1 x 5 minutes), 10% CH_3CN/THF (1 x 5 minutes), THF (1 x 5 minutes), 10% CH_3CN (1 x 5 minutes), 25% CH_3CN/THF (1 x 5 minutes), 50% CH_3CN/THF (1 x 5 minutes), 75% CH_3CN/THF, 90% CH_3CN/THF (1 x 5 minutes), and left in CH_3CNThe resin was arrayed directly into 384-well plates from the final wash solvent (see Section IV.3).

IV.3 Arraying and Cleavage From Resin

The resin, in CH_3CN, was arrayed into 384-well plates (Genetix, X5005). The bottom 0.5 inches of a 1-200 μL plastic pipette tip was removed and the remaining tip was affixed to a p100 Gilson pipetteman. Each bead was taken up into the tip in a minimal amount of CH_3CN (~40 μL) and dispensed into a well. This was repeated for all the beads in each batch. Bead fragments were also dispensed in a separate well. The resin was dispensed into 17 384-well plates, labelled Plate 1 and Plate 3 through Plate 18. The CH_3CN was allowed to evaporate over 3 hours at atmospheric pressure and room temperature. To each well was then dispensed 10% HF-pyridine in THF (30 μL). The plates were allowed to stand at room temperature, covered with another empty 384-well plate. After 1.5 hours at room temperature, methoxytrimethylsilane (20 μL) was dispensed into each well. After 30 minutes at room temperature, the solution was allowed to evaporate for 2 hours at room temperature and atmospheric pressure. Any remaining solvent was removed from the residue+bead in each well by placing the plate in a vacuum oven at room temperature for 12 hours.

IV.4 Stock Solutions Preparation and Screening

After concentrating *in vacuo* over 12 hours, the residue was dissolved in 6.7 µl of DMSO. The plates were then used directly for biological screening.[12] The plates were stored between screens with an aluminum foil top at –40°C.

IV.5 LC and MS Sample Preparation

Unless otherwise stated LC and MS samples were prepared by removing an aliquot (0.5µl) of DMSO stock from the relevant well of the completed library and diluting this material into analytical grade acetonitrile (16µl).

V. Library Analysis

V.1 Introduction

V.1.1 Use of MS and LC analysis for Library Characterization:

A portion (5μl) of the analytical sample for each well (Section V.5) was introduced into the MS by automated direct infusion (Section I). Using this method it was possible to analyze 24 samples per hour, with a total analysis time of 125 hours for the library. As an example, Figure V.1.1 shows the negative and positive ion mass spectra obtained from the material present in plate 5 well N22. Structural assignments were carried out by manual inspection of the MS data for each well and comparison with tables of theoretical molecular weights for all (R1)1-6(R2)1-8(R3)1-8(R4)1-8 combinations. The chemical structure assigned to each compound is presented in the format (R1)1-6(R2)1-8(R3)1-8(R4)1-8 unless otherwise stated (see Figure V.1.1 for an example of its use). The building block numerical assignments are listed in Table IV.1.

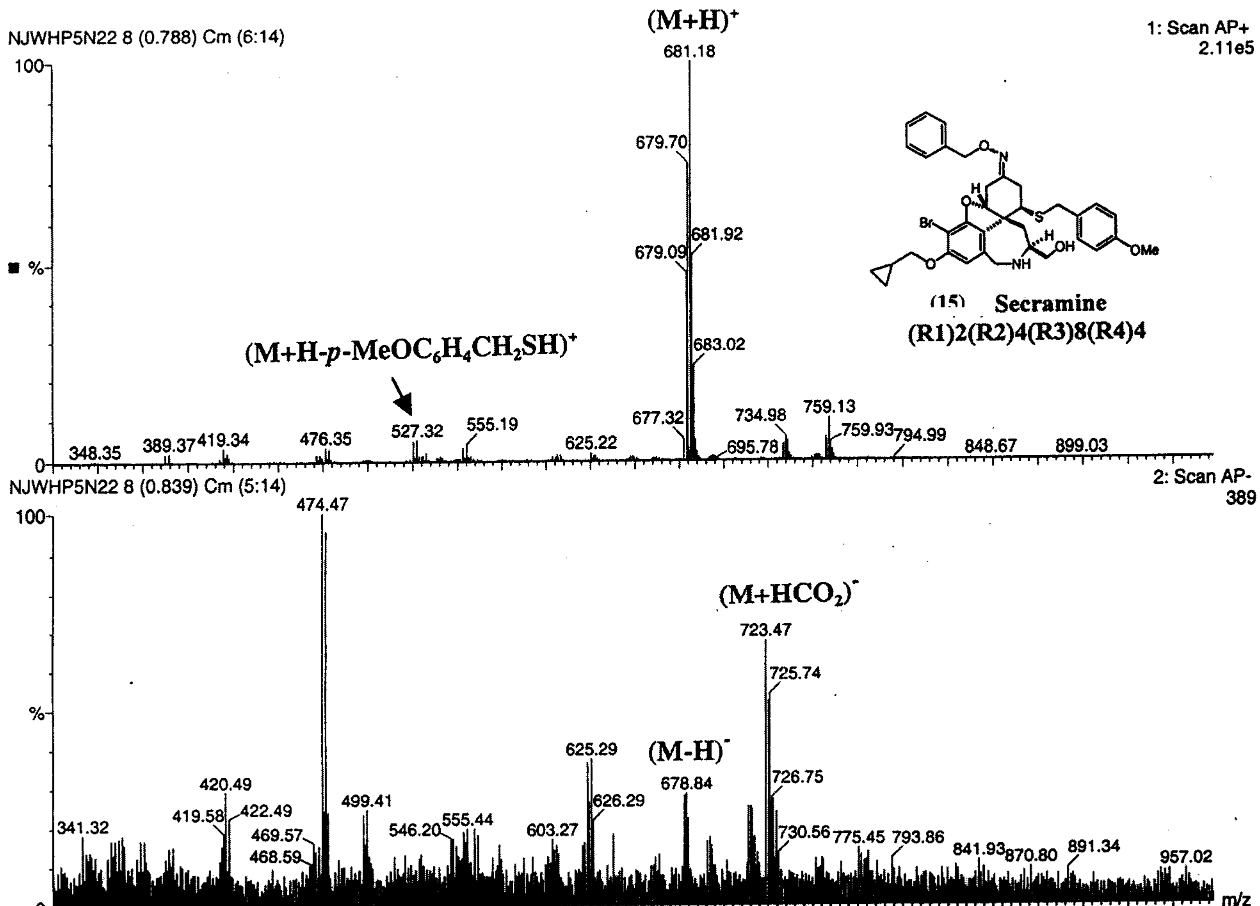
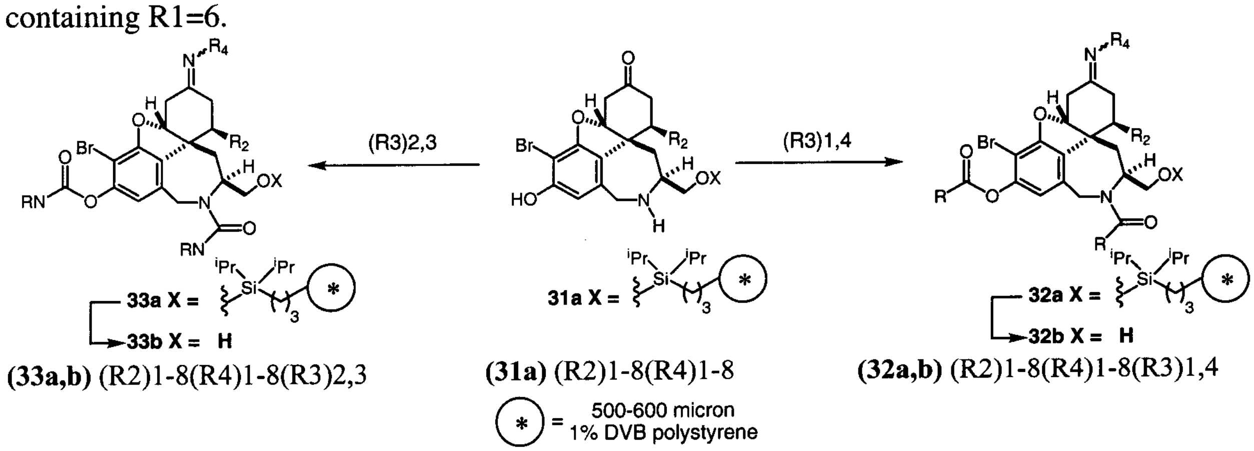


Figure V.1.1 Positive and Negative Ion Mass Spectra Observed for Plate 5 Well N22

The compound in plate 5 well N22 is assigned structure **(15)** and is referred to as secramine (see text of paper). The LCMS data for the compound present in plate 5 well N22 confirms the assignment and purity level of **(15)** (Figure V.1.3). Fragmentations such as the observed 679/681 to 525/527 (positive ion TIC, Figure V.1.3) also aided structure assignment. This particular fragmentation corresponds to loss of 4-methoxy-alpha-toluenethiol from the parent molecular ion, confirming the R2 building block assignment.

Difficulties in structural assignment arising from overlapping theoretical molecular weights were minimized by:
1) keeping final batches of resin spatially separated (in any well of the library both R3 and R4 are already known)
2) imposing an additional constraint on R1 and R2 building blocks. They were selected such that a minimal molecular weight overlap existed for each of the 46 (out of 48) (R1)(R2) combinations.

For (R1)(R3) combinations in which (R1)=6 and (R3)=1,2,3 or 4, the phenol functionality in structure **(31a)** is converted during R3 incorporation in the solid phase to the phenolic ester **(32a)** ((R3)2,3) or phenolic carbamate **(33a)** ((R3)1,4) (Scheme V.1.1). These functional groups typically survived incorporation of the R4 building block and HF.pyridine cleavage conditions to give **(32b)** and **(33b)** respectively. On MS analysis of these compounds, the $(M+H)^+$ ion was observed as the major ion in the positive TIC with a major fragmentation corresponding to loss of one R3 group. On LCMS analysis of these compounds a minor component assigned as the free phenol-containing derivative was occasionally observed (Figures V.3.2.12 and V.3.2.18). The possibility that the phenolic ester or carbamate groups are hydrolyzed under the biological assay conditions is an issue that is being addressed during the resynthesis of preliminary hits containing R1=6.



Scheme V.1.1 R3 Incorporation Leads to Phenolic Ester or Carbamate Formation for (R1)6 examples

A complete structural assignment of the library, broken down by plate, quadrant and (R1)(R2)(R3)(R4) combination is given in Tables V.2.1-V.2.15 (Section V.2). Of the expected 2944 compounds, 2527 have been identified (86%). This information will be incorporated into a structure searchable database designed to link chemical structure with biological screening data.[13] Bead fragmentation during the synthesis may account for the absence of 14% of the expected compounds.

Three stages of LCMS analysis were carried out in order to determine the purity level of the library at key stages (for analytical protocols see Section I). This analysis demonstrated that typically the expected products were obtained at a high level of purity, as judged by this analytical technique. As an example, the diode array trace corresponding to the compound assigned as secramine **(15)** is shown in Figure V.1.2.

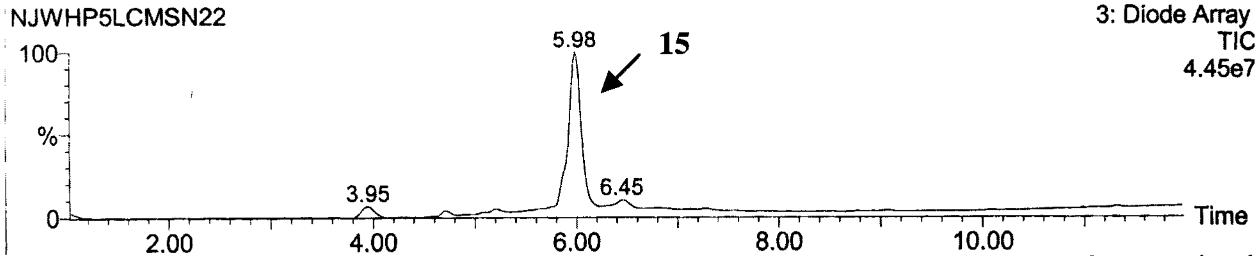


Figure V.1.2 LC (Diode Array) Portion of LCMS of secramine (15). Solvent front omitted for clarity.

For LC data (diode array trace) in support of the successful synthesis of:
1) all (R1)(R2) combinations ((R3)8(R4)8) see Section V.3.1
2) 287 of the possible 322 (R1)(R2)(R3) combinations see Section V.3.2 (excluding (R3)8(R4)8) combinations)
3) Randomly selected (R1)(R2)(R3)(R4) combinations from each library plate (see Section V.3.3; LC traces for Plate 1 are shown in Figures V.3.2.1-6, V.3.2.19-24, V.3.2.37-42). LCMS analysis of the majority of these samples indicates the presence of two major compounds as judged by this analytical technique. Inspection of the mass spectrum of examples in which the two compounds are well resolved indicated that they have identical molecular weights (see Figure V.3.3.6). These structures are currently assigned as the *E*- and *Z*- isomers about the C=N bond (hydrazone, oxime) that may be formed during R4 incorporation. In cases where a peak corresponding to one major compound is observed, it was not determined whether predominantly one isomer was formed or whether the two isomers were not separated under the LC conditions.

Due to the presence of DMSO in the samples a strong signal in the diode array spectrum with a retention time of 0.5-1.0 minutes was typically observed. For clarity of presentation the diode array traces have been cropped to remove this peak. The presence of a UV active impurity that does not ionize in either the positive or negative APCI mode was observed in several wells (retention time 3.5-4.0 minutes, Figures V.3.2.31-36 as an example). The source of this impurity is currently unknown.

V.1.2 NMR Characterization of Representative Compounds

In addition to the use of MS and LC analysis, the synthesis of 6 final compounds has been carried out on the solid phase on an increased scale (Section VI.4.1 for experimental details and full characterization; Section VI.4.2 for accompanying ^{1}H NMR spectra). Interpretation of ^{1}H NMR spectra has been complicated in cases where R4=1-7 by the presence of two compounds which are currently being assigned as *E*- and *Z*- isomers about the C=N bond (hydrazone, oxime). In addition, the presence of rotameric forms that are slow to interconvert on the NMR timescale frequently resulted in broad, unassignable spectra at room temperature ($CDCl_3$ or d_6-DMSO), particularly in cases where R3=1,2,3 or 4. In several cases, recording ^{1}H NMR spectra for these compounds at elevated temperatures in d_6-DMSO, resulted in much sharper signals.

The ^{1}H NMR spectra of spirodienone **(8b)** (Figure III.5) did not simplify in this manner when recorded at temperatures up to 80°C in d_6-DMSO.

V.1.3 Stereochemical Assignments

Only one diastereomer is observed for the formation of Resin **20a**. The stereochemistry at C1 was established by GOESY and NOESY experiments with **29b** (Figure V.1.4, Section V.4.2).

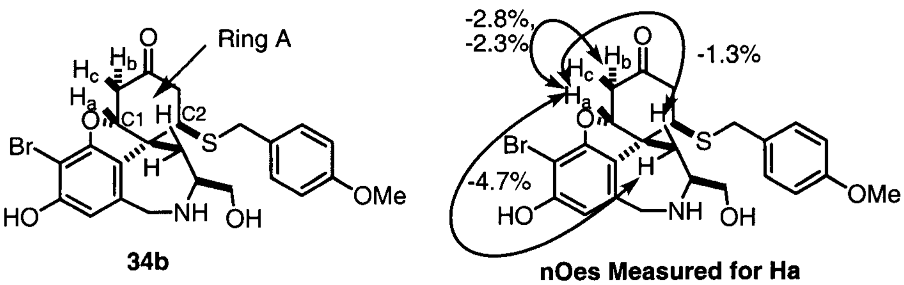
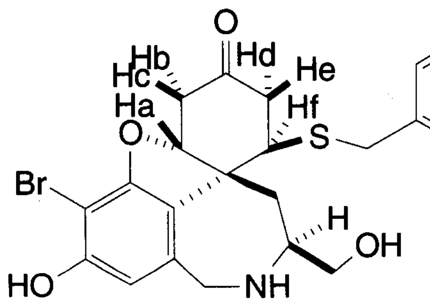
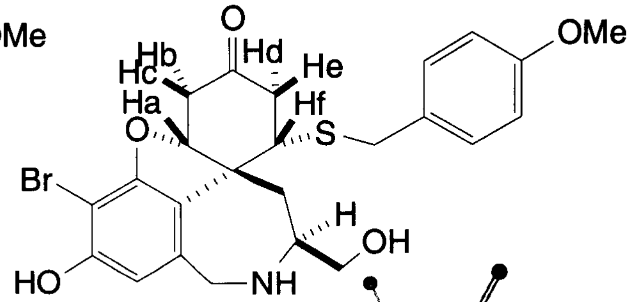


Figure V.1.3 nOe measurements and observations for 34b, H_a

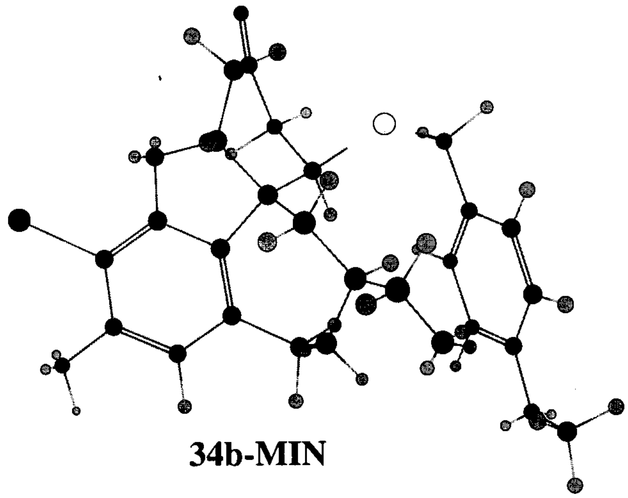
Only one diastereomer was observed for conversion of **10** to **11**. Figure V.4.2.9 and Figure V.4.2.11 present examples of the comparison of ^{1}H NMR spectra obtained with unpurified material cleaved from the resin and the material obtained by flash column chromatography. The presence of a single H_a proton provides evidence of the diastereoselectivity. Molecular modeling was correlated to NMR data to assign the stereochemistry at C2 based on representative structure **34b** (Figure V.1.3). Energy-minimized conformations of **34b** and **34c**, **34b-MIN** and **34c-MIN**, respectively, were calculated using the AMBER force field on 1000 structures generated by a Monte Carlo multiconformer search in chloroform using MacroModel (Version 6.0) (Figure V.1.4). The dihedral angles for H_a-H_b and H_a-H_c differ significantly between **34b-MIN** and **34c-MIN**. The NMR-obtained coupling constant (Figure V.1.5) for the key Ha proton in $CDCl_3$ (dd, J = 2.5, 2.5 Hz) agrees with the theoretical coupling constant based on the Karplus correlation[14] for **34b-MIN** (dd, $J \approx 2$, 2Hz), and not **34c-MIN** (dd, $J \approx 6$, 8-9 Hz).



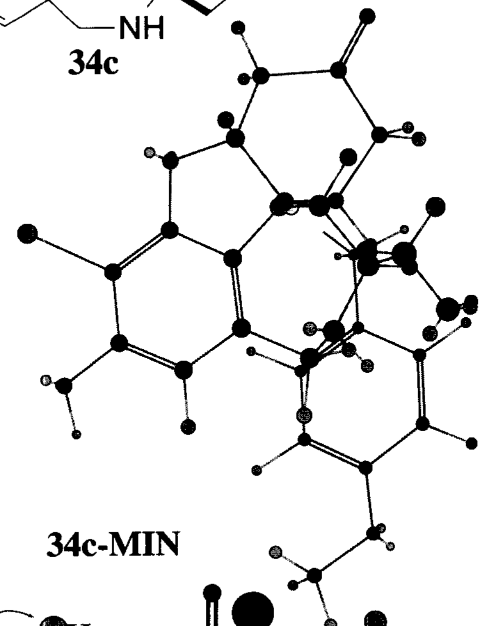
34b



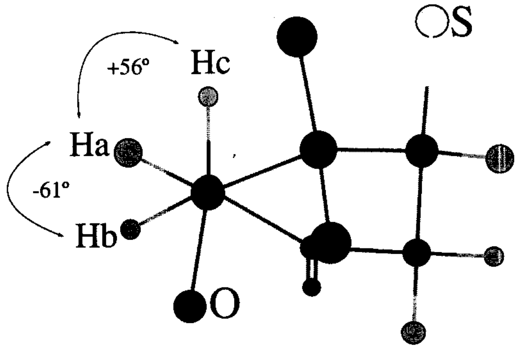
34c

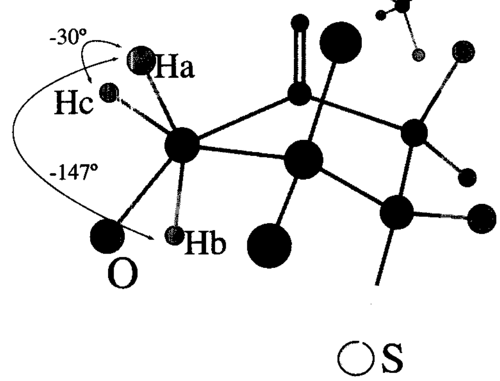


34b-MIN



34c-MIN





34b-MIN, Ring A Higlighted
Expect J_{HaHb} = 2 Hz, J_{HaHc} = 2 Hz

34c-MIN, Ring A Highlighted
Expect J_{HaHc} = 6 Hz, J_{HaHb} = 8-9 Hz

Figure V.1.4 MacroModel Energy Minimization of 34b and 34c in Chloroform

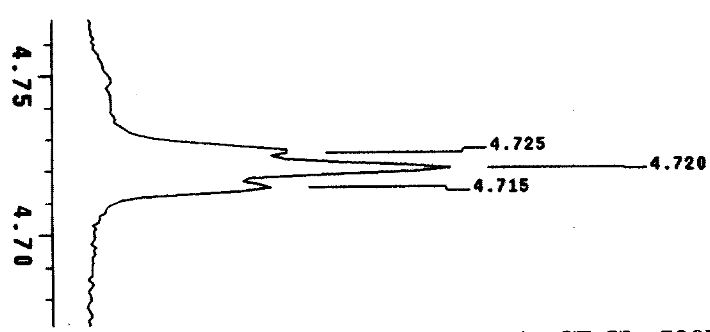


Figure V.1.5 NMR Spectra of Ha, 29b in $CDCl_3$, 500MHz.

V.2 MS analysis for Library Structure Assignment

For structural assignments of compounds in Plate 1 see Tables V.3.2.1, V.3.2.2, V.3.2.4

Table V.2.1	Structural Assignment of Compounds in Plate 3
Table V.2.2	Structural Assignment of Compounds in Plate 4
Table V.2.3	Structural Assignment of Compounds in Plate 5
Table V.2.4	Structural Assignment of Compounds in Plate 6
Table V.2.5	Structural Assignment of Compounds in Plate 7
Table V.2.6	Structural Assignment of Compounds in Plate 8
Table V.2.7	Structural Assignment of Compounds in Plates 9 and 10
Table V.2.8	Structural Assignment of Compounds in Plate 11
See also Tables V.3.2.1 and V.3.2.2 for Structural Assignment of Compounds in Plate 11	
Table V.2.9	Structural Assignment of Compounds in Plate 12
Table V.2.10	Structural Assignment of Compounds in Plate 13
Table V.2.11	Structural Assignment of Compounds in Plate 14
Table V.2.12	Structural Assignment of Compounds in Plate 15
See also Tables V.3.2.3 for Structural Assignment of Compounds in Plate 15	
Table V.2.13	Structural Assignment of Compounds in Plate 16
Table V.2.14	Structural Assignment of Compounds in Plate 17
Table V.2.15	Structural Assignment of Compounds in Plate 18

Z = a compound corresponding to this (R1)(R2)(R3)(R4) combination was not be identified.
* Diode array trace obtained on analysis of the material present in this well is shown in the corresponding Figure V.3.3.X (where X=1-15)

R1	R2	R3	R4	Plate	Loc.
1	3	7	1	3	Z
1	4	7	1	3	C08
1	5	7	1	3	B06
1	6	7	1	3	E09
1	7	7	1	3	B03
1	8	7	1	3	B08
2	1	7	1	3	E05
2	2	7	1	3	E11
2	3	7	1	3	C10
2	4	7	1	3	B05
2	5	7	1	3	Z
2	6	7	1	3	D06
2	7	7	1	3	B09
2	8	7	1	3	C04
3	1	7	1	3	D02
3	2	7	1	3	E06
3	3	7	1	3	B10
3	4	7	1	3	E03
3	5	7	1	3	C07
3	6	7	1	3	D03
3	7	7	1	3	Z
3	8	7	1	3	F02*
4	1	7	1	3	E08
4	2	7	1	3	Z
4	3	7	1	3	D09
4	4	7	1	3	Z
4	5	7	1	3	F05
4	6	7	1	3	D10
4	7	7	1	3	D07*
4	8	7	1	3	D08
5	1	7	1	3	F07
5	2	7	1	3	Z
5	3	7	1	3	B07
5	4	7	1	3	Z
5	5	7	1	3	Z
5	6	7	1	3	Z
5	7	7	1	3	D04
5	8	7	1	3	C02
6	1	7	1	3	E04
6	2	7	1	3	C03
6	3	7	1	3	B04
6	4	7	1	3	C06
6	5	7	1	3	B02
6	6	7	1	3	C09
6	7	7	1	3	E02
6	8	7	1	3	E07

R1	R2	R3	R4	Plate	Loc.
1	3	7	3	3	N11
1	4	7	3	3	K10
1	5	7	3	3	L09
1	6	7	3	3	L02
1	7	7	3	3	N06
1	8	7	3	3	M03
2	1	7	3	3	K08
2	2	7	3	3	N09
2	3	7	3	3	L11
2	4	7	3	3	O07
2	5	7	3	3	K02
2	6	7	3	3	N05*
2	7	7	3	3	K03
2	8	7	3	3	L04
3	1	7	3	3	K06
3	2	7	3	3	O03
3	3	7	3	3	L06
3	4	7	3	3	K05
3	5	7	3	3	O09
3	6	7	3	3	N07
3	7	7	3	3	M08
3	8	7	3	3	K09
4	1	7	3	3	K04
4	2	7	3	3	Z
4	3	7	3	3	M11
4	4	7	3	3	M06
4	5	7	3	3	L08
4	6	7	3	3	N04
4	7	7	3	3	M07
4	8	7	3	3	M09
5	1	7	3	3	N10
5	2	7	3	3	N03
5	3	7	3	3	L07*
5	4	7	3	3	O05
5	5	7	3	3	L03
5	6	7	3	3	O04
5	7	7	3	3	O08
5	8	7	3	3	O06
6	1	7	3	3	O02
6	2	7	3	3	L05
6	3	7	3	3	M04
6	4	7	3	3	M02
6	5	7	3	3	N08
6	6	7	3	3	L10
6	7	7	3	3	N02
6	8	7	3	3	M10

R1	R2	R3	R4	Plate	Loc.
1	3	7	2	3	C18
1	4	7	2	3	F14
1	5	7	2	3	B16
1	6	7	2	3	D19
1	7	7	2	3	Z
1	8	7	2	3	F17
2	1	7	2	3	E18
2	2	7	2	3	D17
2	3	7	2	3	D15
2	4	7	2	3	E23
2	5	7	2	3	E17
2	6	7	2	3	E22
2	7	7	2	3	E21*
2	8	7	2	3	D22
3	1	7	2	3	B18
3	2	7	2	3	D23
3	3	7	2	3	D16
3	4	7	2	3	G14
3	5	7	2	3	C20
3	6	7	2	3	E16
3	7	7	2	3	E14
3	8	7	2	3	C14
4	1	7	2	3	B20
4	2	7	2	3	Z
4	3	7	2	3	B21
4	4	7	2	3	B23
4	5	7	2	3	F19
4	6	7	2	3	B17
4	7	7	2	3	Z
4	8	7	2	3	B22
5	1	7	2	3	D21
5	2	7	2	3	B19
5	3	7	2	3	C17
5	4	7	2	3	D18
5	5	7	2	3	E19
5	6	7	2	3	B14
5	7	7	2	3	E15
5	8	7	2	3	D14*
6	1	7	2	3	B15
6	2	7	2	3	F21
6	3	7	2	3	C16
6	4	7	2	3	F15
6	5	7	2	3	C22
6	6	7	2	3	E20
6	7	7	2	3	F16
6	8	7	2	3	F22

R1	R2	R3	R4	Plate	Loc.
1	3	7	4	3	Z
1	4	7	4	3	L16
1	5	7	4	3	K17
1	6	7	4	3	Z
1	7	7	4	3	K20
1	8	7	4	3	M18
2	1	7	4	3	K18
2	2	7	4	3	N17
2	3	7	4	3	O17
2	4	7	4	3	K23
2	5	7	4	3	M23
2	6	7	4	3	O15
2	7	7	4	3	M15
2	8	7	4	3	L14
3	1	7	4	3	N15
3	2	7	4	3	M20
3	3	7	4	3	K14
3	4	7	4	3	K22
3	5	7	4	3	N23
3	6	7	4	3	N18*
3	7	7	4	3	L18
3	8	7	4	3	L17
4	1	7	4	3	O18
4	2	7	4	3	Z
4	3	7	4	3	K19
4	4	7	4	3	N16
4	5	7	4	3	K16
4	6	7	4	3	L15
4	7	7	4	3	N14
4	8	7	4	3	N19
5	1	7	4	3	L19
5	2	7	4	3	M22
5	3	7	4	3	M16
5	4	7	4	3	O16
5	5	7	4	3	L21
5	6	7	4	3	K15
5	7	7	4	3	M19
5	8	7	4	3	M17*
6	1	7	4	3	M14
6	2	7	4	3	M21
6	3	7	4	3	N22
6	4	7	4	3	L23
6	5	7	4	3	K21
6	6	7	4	3	L20
6	7	7	4	3	N20
6	8	7	4	3	Z

Table V .2.1

R1	R2	R3	R4	Plate	Loc.
1	3	7	5	4	E06
1	4	7	5	4	E02*
1	5	7	5	4	D03
1	6	7	5	4	E10
1	7	7	5	4	B07
1	8	7	5	4	Z
2	1	7	5	4	E05
2	2	7	5	4	D11
2	3	7	5	4	B04
2	4	7	5	4	C10
2	5	7	5	4	E07
2	6	7	5	4	B02
2	7	7	5	4	Z
2	8	7	5	4	B09
3	1	7	5	4	E11
3	2	7	5	4	Z
3	3	7	5	4	E04
3	4	7	5	4	D05
3	5	7	5	4	D08
3	6	7	5	4	Z
3	7	7	5	4	C03
3	8	7	5	4	Z
4	1	7	5	4	B10
4	2	7	5	4	Z
4	3	7	5	4	D02
4	4	7	5	4	F02
4	5	7	5	4	C07
4	6	7	5	4	C08
4	7	7	5	4	B06*
4	8	7	5	4	C02
5	1	7	5	4	Z
5	2	7	5	4	C06
5	3	7	5	4	B03
5	4	7	5	4	D04
5	5	7	5	4	B08
5	6	7	5	4	D10
5	7	7	5	4	C05
5	8	7	5	4	C11
6	1	7	5	4	Z
6	2	7	5	4	E03
6	3	7	5	4	D09
6	4	7	5	4	C04
6	5	7	5	4	B05
6	6	7	5	4	D06
6	7	7	5	4	C09
6	8	7	5	4	D07

R1	R2	R3	R4	Plate	Loc.
1	3	7	7	4	M09
1	4	7	7	4	N02
1	5	7	7	4	L02
1	6	7	7	4	N06
1	7	7	7	4	L09
1	8	7	7	4	M02
2	1	7	7	4	M11
2	2	7	7	4	K06
2	3	7	7	4	K04
2	4	7	7	4	L08
2	5	7	7	4	L03
2	6	7	7	4	O06
2	7	7	7	4	K02*
2	8	7	7	4	O09
3	1	7	7	4	N04
3	2	7	7	4	N11
3	3	7	7	4	L06
3	4	7	7	4	M07
3	5	7	7	4	M04
3	6	7	7	4	Z
3	7	7	7	4	K10
3	8	7	7	4	O08
4	1	7	7	4	M05
4	2	7	7	4	Z
4	3	7	7	4	L05
4	4	7	7	4	N05
4	5	7	7	4	J03
4	6	7	7	4	N03
4	7	7	7	4	L04
4	8	7	7	4	N08
5	1	7	7	4	K09
5	2	7	7	4	L07
5	3	7	7	4	M10*
5	4	7	7	4	L10
5	5	7	7	4	K05
5	6	7	7	4	O07
5	7	7	7	4	K03
5	8	7	7	4	O02
6	1	7	7	4	K11
6	2	7	7	4	L11
6	3	7	7	4	M06
6	4	7	7	4	K07
6	5	7	7	4	M08
6	6	7	7	4	K08
6	7	7	7	4	O03
6	8	7	7	4	Z

R1	R2	R3	R4	Plate	Loc.
1	3	7	6	4	D17
1	4	7	6	4	B15
1	5	7	6	4	E23
1	6	7	6	4	F22
1	7	7	6	4	B14
1	8	7	6	4	E18
2	1	7	6	4	Z
2	2	7	6	4	B22
2	3	7	6	4	G14
2	4	7	6	4	C22
2	5	7	6	4	F21
2	6	7	6	4	Z
2	7	7	6	4	E20
2	8	7	6	4	F18
3	1	7	6	4	E19
3	2	7	6	4	C17
3	3	7	6	4	D20
3	4	7	6	4	F17
3	5	7	6	4	B17*
3	6	7	6	4	C20
3	7	7	6	4	D18
3	8	7	6	4	G15
4	1	7	6	4	C14
4	2	7	6	4	Z
4	3	7	6	4	C21
4	4	7	6	4	D16
4	5	7	6	4	D19
4	6	7	6	4	C16
4	7	7	6	4	B18
4	8	7	6	4	D15
5	1	7	6	4	C18
5	2	7	6	4	E14
5	3	7	6	4	B21
5	4	7	6	4	E21
5	5	7	6	4	E22
5	6	7	6	4	C15
5	7	7	6	4	D22
5	8	7	6	4	E15
6	1	7	6	4	B20
6	2	7	6	4	D14*
6	3	7	6	4	Z
6	4	7	6	4	B16
6	5	7	6	4	B23
6	6	7	6	4	D21
6	7	7	6	4	C19
6	8	7	6	4	E17

Table V .2.2 526

R1	R2	R3	R4	Plate	Loc.
1	3	8	1	5	E10
1	4	8	1	5	B7
1	5	8	1	5	B8
1	6	8	1	5	C8
1	7	8	1	5	E7
1	8	8	1	5	C8
2	1	8	1	5	B3
2	2	8	1	5	E11
2	3	8	1	5	D6
2	4	8	1	5	D5*
2	5	8	1	5	C2
2	6	8	1	5	C6
2	7	8	1	5	C4
2	8	8	1	5	C7
3	1	8	1	5	Z
3	2	8	1	5	C11
3	3	8	1	5	E4
3	4	8	1	5	B10
3	5	8	1	5	F4
3	6	8	1	5	F9
3	7	8	1	5	E8
3	8	8	1	5	E5
4	1	8	1	5	C3
4	2	8	1	5	C10
4	3	8	1	5	D3
4	4	8	1	5	B11
4	5	8	1	5	B9
4	6	8	1	5	D11
4	7	8	1	5	C9
4	8	8	1	5	D7
5	1	8	1	5	F11
5	2	8	1	5	F3*
5	3	8	1	5	G2
5	4	8	1	5	C5
5	5	8	1	5	E3
5	6	8	1	5	F10
5	7	8	1	5	E6
5	8	8	1	5	F8
6	1	8	1	5	D2
6	2	8	1	5	F5
6	3	8	1	5	B2
6	4	8	1	5	E2
6	5	8	1	5	D9
6	6	8	1	5	B4
6	7	8	1	5	D10
6	8	8	1	5	D4

R1	R2	R3	R4	Plate	Loc.
1	3	8	3	5	L9
1	4	8	3	5	N3
1	5	8	3	5	K7
1	6	8	3	5	Z
1	7	8	3	5	M11
1	8	8	3	5	M7
2	1	8	3	5	L7*
2	2	8	3	5	K8
2	3	8	3	5	M5
2	4	8	3	5	K2
2	5	8	3	5	M2
2	6	8	3	5	L6
2	7	8	3	5	K5
2	8	8	3	5	L10
3	1	8	3	5	Z
3	2	8	3	5	K10
3	3	8	3	5	N4
3	4	8	3	5	N6
3	5	8	3	5	K3
3	6	8	3	5	K4
3	7	8	3	5	Z
3	8	8	3	5	N22
4	1	8	3	5	K6
4	2	8	3	5	M9
4	3	8	3	5	L5
4	4	8	3	5	M8
4	5	8	3	5	L3
4	6	8	3	5	Z
4	7	8	3	5	O5
4	8	8	3	5	Z
5	1	8	3	5	Z
5	2	8	3	5	N5
5	3	8	3	5	M6
5	4	8	3	5	O2
5	5	8	3	5	K9
5	6	8	3	5	N8
5	7	8	3	5	M10*
5	8	8	3	5	N9
6	1	8	3	5	K11
6	2	8	3	5	N11
6	3	8	3	5	L2
6	4	8	3	5	N7
6	5	8	3	5	L8
6	6	8	3	5	L11
6	7	8	3	5	L4
6	8	8	3	5	M3

R1	R2	R3	R4	Plate	Loc.
1	3	8	2	5	B18
1	4	8	2	5	B21
1	5	8	2	5	E21
1	6	8	2	5	E14
1	7	8	2	5	E22
1	8	8	2	5	D22
2	1	8	2	5	E19
2	2	8	2	5	Z
2	3	8	2	5	C19
2	4	8	2	5	C23
2	5	8	2	5	E16
2	6	8	2	5	C14
2	7	8	2	5	E20*
2	8	8	2	5	C15
3	1	8	2	5	F15
3	2	8	2	5	D19
3	3	8	2	5	E17
3	4	8	2	5	F17
3	5	8	2	5	D17
3	6	8	2	5	Z
3	7	8	2	5	Z
3	8	8	2	5	E23
4	1	8	2	5	D23
4	2	8	2	5	C22
4	3	8	2	5	D15
4	4	8	2	5	F19
4	5	8	2	5	E15
4	6	8	2	5	D21
4	7	8	2	5	E18
4	8	8	2	5	D16
5	1	8	2	5	F23
5	2	8	2	5	B14
5	3	8	2	5	B15
5	4	8	2	5	Z
5	5	8	2	5	F18
5	6	8	2	5	B22
5	7	8	2	5	D14
5	8	8	2	5	B23*
6	1	8	2	5	C16
6	2	8	2	5	F20
6	3	8	2	5	C20
6	4	8	2	5	F22
6	5	8	2	5	C17
6	6	8	2	5	B20
6	7	8	2	5	Z
6	8	8	2	5	F21

R1	R2	R3	R4	Plate	Loc.
1	3	8	4	5	O20
1	4	8	4	5	M20
1	5	8	4	5	M22
1	6	8	4	5	N21
1	7	8	4	5	Z
1	8	8	4	5	O21
2	1	8	4	5	M19
2	2	8	4	5	O17
2	3	8	4	5	L15
2	4	8	4	5	N22
2	5	8	4	5	N19
2	6	8	4	5	L17*
2	7	8	4	5	O15
2	8	8	4	5	K17
3	1	8	4	5	M21
3	2	8	4	5	O23
3	3	8	4	5	K16
3	4	8	4	5	M15
3	5	8	4	5	K20
3	6	8	4	5	Z
3	7	8	4	5	N23
3	8	8	4	5	K22
4	1	8	4	5	K19
4	2	8	4	5	O18
4	3	8	4	5	K21*
4	4	8	4	5	N14
4	5	8	4	5	L14
4	6	8	4	5	M18
4	7	8	4	5	M23
4	8	8	4	5	K15
5	1	8	4	5	Z
5	2	8	4	5	K14
5	3	8	4	5	L22
5	4	8	4	5	K18
5	5	8	4	5	L20
5	6	8	4	5	L19
5	7	8	4	5	O16
5	8	8	4	5	L16
6	1	8	4	5	L23
6	2	8	4	5	N18
6	3	8	4	5	N17
6	4	8	4	5	M16
6	5	8	4	5	K23
6	6	8	4	5	M17
6	7	8	4	5	L18
6	8	8	4	5	N20

Table V .2.3

R1	R2	R3	R4	Plate	Loc.
1	3	8	5	6	Z
1	4	8	5	6	Z
1	5	8	5	6	Z
1	6	8	5	6	E6
1	7	8	5	6	F6
1	8	8	5	6	C11
2	1	8	5	6	E11
2	2	8	5	6	C6*
2	3	8	5	6	D7
2	4	8	5	6	B8
2	5	8	5	6	E9
2	6	8	5	6	D4
2	7	8	5	6	C5
2	8	8	5	6	C8
3	1	8	5	6	C9
3	2	8	5	6	E7
3	3	8	5	6	F2
3	4	8	5	6	D3
3	5	8	5	6	Z
3	6	8	5	6	B5
3	7	8	5	6	E8
3	8	8	5	6	B2
4	1	8	5	6	Z
4	2	8	5	6	B3
4	3	8	5	6	B6
4	4	8	5	6	C2
4	5	8	5	6	F7
4	6	8	5	6	B9
4	7	8	5	6	B10
4	8	8	5	6	D9
5	1	8	5	6	D6
5	2	8	5	6	F4
5	3	8	5	6	C3
5	4	8	5	6	D10
5	5	8	5	6	D5
5	6	8	5	6	B4*
5	7	8	5	6	D2
5	8	8	5	6	Z
6	1	8	5	6	E10
6	2	8	5	6	E4
6	3	8	5	6	B11
6	4	8	5	6	C10
6	5	8	5	6	D8
6	6	8	5	6	C4
6	7	8	5	6	F5
6	8	8	5	6	F3

R1	R2	R3	R4	Plate	Loc.
1	3	8	7	6	J11
1	4	8	7	6	L8
1	5	8	7	6	M10
1	6	8	7	6	Z
1	7	8	7	6	O10*
1	8	8	7	6	O8
2	1	8	7	6	N3
2	2	8	7	6	M5
2	3	8	7	6	K10
2	4	8	7	6	L7
2	5	8	7	6	K11
2	6	8	7	6	J3
2	7	8	7	6	L5
2	8	8	7	6	J2
3	1	8	7	6	L2
3	2	8	7	6	N6
3	3	8	7	6	N5
3	4	8	7	6	K6
3	5	8	7	6	M4*
3	6	8	7	6	K4
3	7	8	7	6	L3
3	8	8	7	6	L11
4	1	8	7	6	K2
4	2	8	7	6	J9
4	3	8	7	6	K3
4	4	8	7	6	M3
4	5	8	7	6	M6
4	6	8	7	6	M11
4	7	8	7	6	Z
4	8	8	7	6	M9
5	1	8	7	6	Z
5	2	8	7	6	J10
5	3	8	7	6	O11
5	4	8	7	6	J4
5	5	8	7	6	N4
5	6	8	7	6	J7
5	7	8	7	6	M8
5	8	8	7	6	L9
6	1	8	7	6	N7
6	2	8	7	6	K9
6	3	8	7	6	K8
6	4	8	7	6	L6
6	5	8	7	6	O6
6	6	8	7	6	N8
6	7	8	7	6	K5
6	8	8	7	6	Z

R1	R2	R3	R4	Plate	Loc.
1	3	8	6	6	E22*
1	4	8	6	6	B18
1	5	8	6	6	E16
1	6	8	6	6	Z
1	7	8	6	6	D17
1	8	8	6	6	F21
2	1	8	6	6	C23
2	2	8	6	6	B22
2	3	8	6	6	E15
2	4	8	6	6	G15
2	5	8	6	6	B15
2	6	8	6	6	E18
2	7	8	6	6	E23
2	8	8	6	6	E19
3	1	8	6	6	G17
3	2	8	6	6	B16
3	3	8	6	6	B23
3	4	8	6	6	F18
3	5	8	6	6	D21
3	6	8	6	6	C17
3	7	8	6	6	C16
3	8	8	6	6	G22
4	1	8	6	6	E17
4	2	8	6	6	C20
4	3	8	6	6	B19
4	4	8	6	6	C15
4	5	8	6	6	D18
4	6	8	6	6	C19
4	7	8	6	6	F20
4	8	8	6	6	B21
5	1	8	6	6	D19*
5	2	8	6	6	C21
5	3	8	6	6	D20
5	4	8	6	6	Z
5	5	8	6	6	B17
5	6	8	6	6	F23
5	7	8	6	6	D16
5	8	8	6	6	Z
6	1	8	6	6	B20
6	2	8	6	6	F22
6	3	8	6	6	F19
6	4	8	6	6	D15
6	5	8	6	6	F15
6	6	8	6	6	C18
6	7	8	6	6	F17
6	8	8	6	6	E21

R1	R2	R3	R4	Plate	Loc.
1	3	1	1	6	L17
1	4	1	1	6	Z
1	5	1	1	6	M20
1	6	1	1	6	Z
1	7	1	1	6	M22
1	8	1	1	6	L15
2	1	1	1	6	O17
2	2	1	1	6	L23
2	3	1	1	6	N17
2	4	1	1	6	Z
2	5	1	1	6	N18
2	6	1	1	6	N20
2	7	1	1	6	K23
2	8	1	1	6	L21
3	1	1	1	6	Z
3	2	1	1	6	O14
3	3	1	1	6	M17
3	4	1	1	6	M18*
3	5	1	1	6	K21
3	6	1	1	6	K16
3	7	1	1	6	Z
3	8	1	1	6	O21
4	1	1	1	6	M19
4	2	1	1	6	M15
4	3	1	1	6	N16
4	4	1	1	6	K20
4	5	1	1	6	N15
4	6	1	1	6	K19
4	7	1	1	6	L18
4	8	1	1	6	M21
5	1	1	1	6	L22
5	2	1	1	6	L14
5	3	1	1	6	M16
5	4	1	1	6	O18
5	5	1	1	6	K18
5	6	1	1	6	O19
5	7	1	1	6	K17
5	8	1	1	6	L19
6	1	1	1	6	N14*
6	2	1	1	6	K15
6	3	1	1	6	O16
6	4	1	1	6	Z
6	5	1	1	6	M14
6	6	1	1	6	M21
6	7	1	1	6	N19
6	8	1	1	6	K22

Table V .2.4

R1	R2	R3	R4	Plate	Loc.
1	3	1	2	7	C3
1	4	1	2	7	C6
1	5	1	2	7	C5
1	6	1	2	7	C4
1	7	1	2	7	D8*
1	8	1	2	7	C7
2	1	1	2	7	B10
2	2	1	2	7	E3
2	3	1	2	7	C11
2	4	1	2	7	D9
2	5	1	2	7	F4
2	6	1	2	7	G6
2	7	1	2	7	E6
2	8	1	2	7	F8
3	1	1	2	7	D11
3	2	1	2	7	B2
3	3	1	2	7	C8
3	4	1	2	7	B5
3	5	1	2	7	B8
3	6	1	2	7	D5
3	7	1	2	7	E2
3	8	1	2	7	D3
4	1	1	2	7	E5
4	2	1	2	7	D7
4	3	1	2	7	E7
4	4	1	2	7	E9
4	5	1	2	7	F3
4	6	1	2	7	E4
4	7	1	2	7	D6
4	8	1	2	7	E11
5	1	1	2	7	B4*
5	2	1	2	7	D4
5	3	1	2	7	C10
5	4	1	2	7	F2
5	5	1	2	7	F11
5	6	1	2	7	E10
5	7	1	2	7	F10
5	8	1	2	7	B7
6	1	1	2	7	B9
6	2	1	2	7	C2
6	3	1	2	7	E8
6	4	1	2	7	B6
6	5	1	2	7	B3
6	6	1	2	7	F7
6	7	1	2	7	C9
6	8	1	2	7	B11

R1	R2	R3	R4	Plate	Loc.
1	3	1	4	7	K9
1	4	1	4	7	N5
1	5	1	4	7	K4
1	6	1	4	7	M4
1	7	1	4	7	L6
1	8	1	4	7	K6
2	1	1	4	7	K3
2	2	1	4	7	O4
2	3	1	4	7	M10
2	4	1	4	7	M8
2	5	1	4	7	O9*
2	6	1	4	7	M3
2	7	1	4	7	O3
2	8	1	4	7	O10
3	1	1	4	7	K11
3	2	1	4	7	M6
3	3	1	4	7	Z
3	4	1	4	7	K7
3	5	1	4	7	L2
3	6	1	4	7	L3
3	7	1	4	7	L7*
3	8	1	4	7	L9
4	1	1	4	7	N7
4	2	1	4	7	N4
4	3	1	4	7	K8
4	4	1	4	7	M9
4	5	1	4	7	O5
4	6	1	4	7	L10
4	7	1	4	7	K10
4	8	1	4	7	K5
5	1	1	4	7	N8
5	2	1	4	7	M2
5	3	1	4	7	K2...
5	4	1	4	7	Z
5	5	1	4	7	N11
5	6	1	4	7	M7
5	7	1	4	7	L11
5	8	1	4	7	N2
6	1	1	4	7	N9
6	2	1	4	7	L4
6	3	1	4	7	N3
6	4	1	4	7	L8
6	5	1	4	7	J2
6	6	1	4	7	O11
6	7	1	4	7	M5
6	8	1	4	7	Z

R1	R2	R3	R4	Plate	Loc.
1	3	1	3	7	E16
1	4	1	3	7	D22
1	5	1	3	7	B21
1	6	1	3	7	Z
1	7	1	3	7	C16
1	8	1	3	7	D21
2	1	1	3	7	F22
2	2	1	3	7	F16
2	3	1	3	7	B18
2	4	1	3	7	D23
2	5	1	3	7	F21
2	6	1	3	7	E17
2	7	1	3	7	D15
2	8	1	3	7	Z
3	1	1	3	7	D16
3	2	1	3	7	F14
3	3	1	3	7	C19
3	4	1	3	7	C14*
3	5	1	3	7	C22
3	6	1	3	7	B15
3	7	1	3	7	E19
3	8	1	3	7	B19
4	1	1	3	7	D20
4	2	1	3	7	F19
4	3	1	3	7	E20
4	4	1	3	7	E22
4	5	1	3	7	C17
4	6	1	3	7	D17
4	7	1	3	7	B17
4	8	1	3	7	C18
5	1	1	3	7	Z
5	2	1	3	7	C15
5	3	1	3	7	D19
5	4	1	3	7	F15
5	5	1	3	7	B20
5	6	1	3	7	F23
5	7	1	3	7	E21
5	8	1	3	7	C23
6	1	1	3	7	F17
6	2	1	3	7	C21
6	3	1	3	7	F18
6	4	1	3	7	F20
6	5	1	3	7	B16*
6	6	1	3	7	E23
6	7	1	3	7	E18
6	8	1	3	7	E15

R1	R2	R3	R4	Plate	Loc.
2	8	1	5	7	N23
5	8	1	5	7	K15
6	8	1	5	7	M16
4	8	1	5	7	O16
2	6	1	5	7	O18
3	8	1	5	7	L19*
1	8	1	5	7	M20
2	7	1	5	7	O17
2	3	1	5	7	M23
5	6	1	5	7	N22
2	1	1	5	7	K14..
2	5	1	5	7	K21
6	6	1	5	7	M21
5	7	1	5	7	L16
5	3	1	5	7	L21
4	6	1	5	7	N15
5	1	1	5	7	Z
6	7	1	5	7	Z
5	5	1	5	7	L17
6	3	1	5	7	L18
2	4	1	5	7	O21
3	6	1	5	7	K16
4	7	1	5	7	M17
1	6	1	5	7	L20
4	3	1	5	7	N18
6	1	1	5	7	K22*
4	1	1	5	7	K20
6	5	1	5	7	M18
4	5	1	5	7	N17
5	4	1	5	7	L15
3	7	1	5	7	O19
1	7	1	5	7	Z
3	3	1	5	7	L23
1	3	1	5	7	M15
2	2	1	5	7	K18
3	1	1	5	7	M22
6	4	1	5	7	N21
3	5	1	5	7	M19
1	5	1	5	7	O22
4	4	1	5	7	K19
5	2	1	5	7	K23
3	4	1	5	7	N19
1	4	1	5	7	Z
6	2	1	5	7	N20
4	2	1	5	7	L22
3	2	1	5	7	O23

Table V .2.5 529

R1	R2	R3	R4	Plate	Loc.
1	3	1	6	8	C10
1	4	1	6	8	C4
1	5	1	6	8	C3
1	6	1	6	8	Z
1	7	1	6	8	E4
1	8	1	6	8	Z
2	1	1	6	8	E8
2	2	1	6	8	B4
2	3	1	6	8	Z
2	4	1	6	8	C11
2	5	1	6	8	Z
2	6	1	6	8	D8
2	7	1	6	8	B6
2	8	1	6	8	B7
3	1	1	6	8	C9*
3	2	1	6	8	E7
3	3	1	6	8	B5
3	4	1	6	8	B11
3	5	1	6	8	D6
3	6	1	6	8	D7
3	7	1	6	8	D5
3	8	1	6	8	Z
4	1	1	6	8	Z
4	2	1	6	8	D3
4	3	1	6	8	D11
4	4	1	6	8	E2
4	5	1	6	8	E9
4	6	1	6	8	D4
4	7	1	6	8	C6
4	8	1	6	8	E5*
5	1	1	6	8	Z
5	2	1	6	8	Z
5	3	1	6	8	Z
5	4	1	6	8	D9
5	5	1	6	8	B10
5	6	1	6	8	C2
5	7	1	6	8	E3
5	8	1	6	8	E10
6	1	1	6	8	B9
6	2	1	6	8	Z
6	3	1	6	8	E6
6	4	1	6	8	B8
6	5	1	6	8	C5
6	6	1	6	8	C7
6	7	1	6	8	C8
6	8	1	6	8	E11

R1	R2	R3	R4	Plate	Loc.
1	3	4	1	8	N9
1	4	4	1	8	L11
1	5	4	1	8	K3
1	6	4	1	8	Z
1	7	4	1	8	N3
1	8	4	1	8	M11
2	1	4	1	8	O2
2	2	4	1	8	L2
2	3	4	1	8	L10
2	4	4	1	8	L6
2	5	4	1	8	M7
2	6	4	1	8	M9*
2	7	4	1	8	Z
2	8	4	1	8	M5
3	1	4	1	8	N10
3	2	4	1	8	Z
3	3	4	1	8	Z
3	4	4	1	8	N7
3	5	4	1	8	L9
3	6	4	1	8	Z
3	7	4	1	8	M2
3	8	4	1	8	K11*
4	1	4	1	8	M4
4	2	4	1	8	M3
4	3	4	1	8	K2
4	4	4	1	8	N5
4	5	4	1	8	Z
4	6	4	1	8	Z
4	7	4	1	8	O3
4	8	4	1	8	K8
5	1	4	1	8	Z
5	2	4	1	8	M8
5	3	4	1	8	L4
5	4	4	1	8	Z
5	5	4	1	8	N6
5	6	4	1	8	L7
5	7	4	1	8	M6
5	8	4	1	8	K9
6	1	4	1	8	K10
6	2	4	1	8	K6
6	3	4	1	8	L5
6	4	4	1	8	K7
6	5	4	1	8	Z
6	6	4	1	8	M10
6	7	4	1	8	N11
6	8	4	1	8	N4

R1	R2	R3	R4	Plate	Loc.
1	3	1	7	8	B22
1	4	1	7	8	D15*
1	5	1	7	8	G14
1	6	1	7	8	Z
1	7	1	7	8	E14
1	8	1	7	8	Z
2	1	1	7	8	F22
2	2	1	7	8	Z
2	3	1	7	8	C16
2	4	1	7	8	E16
2	5	1	7	8	D14
2	6	1	7	8	D21
2	7	1	7	8	B16
2	8	1	7	8	D16
3	1	1	7	8	C18
3	2	1	7	8	E23
3	3	1	7	8	B14
3	4	1	7	8	B15
3	5	1	7	8	F17
3	6	1	7	8	D18
3	7	1	7	8	C17
3	8	1	7	8	E21
4	1	1	7	8	C19
4	2	1	7	8	B21
4	3	1	7	8	E15
4	4	1	7	8	B17
4	5	1	7	8	E18
4	6	1	7	8	B18
4	7	1	7	8	D23
4	8	1	7	8	B19
5	1	1	7	8	F21
5	2	1	7	8	B20
5	3	1	7	8	E20
5	4	1	7	8	E17
5	5	1	7	8	C22
5	6	1	7	8	F20
5	7	1	7	8	D22
5	8	1	7	8	F14
6	1	1	7	8	B23*
6	2	1	7	8	F16
6	3	1	7	8	E19
6	4	1	7	8	F23
6	5	1	7	8	F19
6	6	1	7	8	D19
6	7	1	7	8	D20
6	8	1	7	8	Z

R1	R2	R3	R4	Plate	Loc.
1	3	4	2	8	M16
1	4	4	2	8	Z
1	5	4	2	8	K16
1	6	4	2	8	O18
1	7	4	2	8	M21
1	8	4	2	8	L18
2	1	4	2	8	K15
2	2	4	2	8	Z
2	3	4	2	8	N19
2	4	4	2	8	M14
2	5	4	2	8	Z
2	6	4	2	8	L19
2	7	4	2	8	M22*
2	8	4	2	8	O15
3	1	4	2	8	O21
3	2	4	2	8	L16
3	3	4	2	8	L20
3	4	4	2	8	K18
3	5	4	2	8	M18
3	6	4	2	8	L15
3	7	4	2	8	O17
3	8	4	2	8	N17
4	1	4	2	8	N18
4	2	4	2	8	N16
4	3	4	2	8	M20
4	4	4	2	8	K22
4	5	4	2	8	N21
4	6	4	2	8	N23
4	7	4	2	8	N22
4	8	4	2	8	K19
5	1	4	2	8	K14
5	2	4	2	8	L23
5	3	4	2	8	O20
5	4	4	2	8	Z
5	5	4	2	8	M15*
5	6	4	2	8	K21
5	7	4	2	8	L21
5	8	4	2	8	L17
6	1	4	2	8	K23
6	2	4	2	8	L14
6	3	4	2	8	M17
6	4	4	2	8	Z
6	5	4	2	8	N20
6	6	4	2	8	L22
6	7	4	2	8	Z
6	8	4	2	8	K17

Table VI.2.6

R1	R2	R3	R4	Plate	Loc.
1	3	4	3	9	D05
1	4	4	3	9	B08
1	5	4	3	9	D02
1	6	4	3	9	F07
1	7	4	3	9	D10
1	8	4	3	9	B06
2	1	4	3	9	F04
2	2	4	3	9	F06
2	3	4	3	9	B11
2	4	4	3	9	E07
2	5	4	3	9	C02
2	6	4	3	9	F03
2	7	4	3	9	D03
2	8	4	3	9	C07
3	1	4	3	9	D08
3	2	4	3	9	D06
3	3	4	3	9	F09
3	4	4	3	9	F08
3	5	4	3	9	E10
3	6	4	3	9	E06
3	7	4	3	9	D07
3	8	4	3	9	D11
4	1	4	3	9	B02
4	2	4	3	9	B07
4	3	4	3	9	D04
4	4	4	3	9	E08
4	5	4	3	9	C10
4	6	4	3	9	B10
4	7	4	3	9	C05
4	8	4	3	9	B03
5	1	4	3	9	B05
5	2	4	3	9	C03
5	3	4	3	9	E05*
5	4	4	3	9	E04
5	5	4	3	9	C04
5	6	4	3	9	B04
5	7	4	3	9	C06
5	8	4	3	9	F05
6	1	4	3	9	F02
6	2	4	3	9	C11
6	3	4	3	9	B09*
6	4	4	3	9	G02
6	5	4	3	9	G03
6	6	4	3	9	C08
6	7	4	3	9	CO9
6	8	4	3	9	C08

R1	R2	R3	R4	Plate	Loc.
1	3	4	5	9	O07
1	4	4	5	9	O03
1	5	4	5	9	M06*
1	6	4	5	9	N11
1	7	4	5	9	N03
1	8	4	5	9	Z
2	1	4	5	9	K11
2	2	4	5	9	L06
2	3	4	5	9	L11
2	4	4	5	9	N09
2	5	4	5	9	O02
2	6	4	5	9	M09
2	7	4	5	9	O10
2	8	4	5	9	K08
3	1	4	5	9	N04
3	2	4	5	9	K10
3	3	4	5	9	O06
3	4	4	5	9	K06
3	5	4	5	9	L10
3	6	4	5	9	L09
3	7	4	5	9	N02
3	8	4	5	9	J02
4	1	4	5	9	K03
4	2	4	5	9	M05
4	3	4	5	9	O09
4	4	4	5	9	M02
4	5	4	5	9	M04
4	6	4	5	9	K04
4	7	4	5	9	L05
4	8	4	5	9	N08
5	1	4	5	9	K09
5	2	4	5	9	L03
5	3	4	5	9	N07
5	4	4	5	9	K05
5	5	4	5	9	M03
5	6	4	5	9	L08
5	7	4	5	9	L02
5	8	4	5	9	K02*
6	1	4	5	9	M07
6	2	4	5	9	M08
6	3	4	5	9	M11
6	4	4	5	9	Z
6	5	4	5	9	Z
6	6	4	5	9	L04
6	7	4	5	9	L05
6	8	4	5	9	O05

R1	R2	R3	R4	Plate	Loc.
1	3	4	4	9	E15
1	4	4	4	9	B17
1	5	4	4	9	B21
1	6	4	4	9	Z
1	7	4	4	9	C14
1	8	4	4	9	F17
2	1	4	4	9	F21
2	2	4	4	9	D19
2	3	4	4	9	F19
2	4	4	4	9	D15
2	5	4	4	9	C16
2	6	4	4	9	F18*
2	7	4	4	9	B15
2	8	4	4	9	C21
3	1	4	4	9	C20
3	2	4	4	9	D21
3	3	4	4	9	E19
3	4	4	4	9	B14
3	5	4	4	9	F23
3	6	4	4	9	B19
3	7	4	4	9	E18
3	8	4	4	9	E21
4	1	4	4	9	B23
4	2	4	4	9	B18
4	3	4	4	9	E14
4	4	4	4	9	C18
4	5	4	4	9	C23
4	6	4	4	9	B22
4	7	4	4	9	B19
4	8	4	4	9	F20
5	1	4	4	9	D22
5	2	4	4	9	Z
5	3	4	4	9	F15
5	4	4	4	9	B20*
5	5	4	4	9	F14
5	6	4	4	9	D17
5	7	4	4	9	F16
5	8	4	4	9	E22
6	1	4	4	9	D18
6	2	4	4	9	C17
6	3	4	4	9	C22
6	4	4	4	9	C19
6	5	4	4	9	C15
6	6	4	4	9	E16
6	7	4	4	9	B16
6	8	4	4	9	E17

R1	R2	R3	R4	Plate	Loc.
1	3	4	6	9	Z
1	4	4	6	9	M16
1	5	4	6	9	Z
1	6	4	6	9	Z
1	7	4	6	9	N17
1	8	4	6	9	N18
2	1	4	6	9	N14*
2	2	4	6	9	O15
2	3	4	6	9	K14
2	4	4	6	9	L22
2	5	4	6	9	N22
2	6	4	6	9	N23
2	7	4	6	9	J20
2	8	4	6	9	M23
3	1	4	6	9	O17
3	2	4	6	9	L18
3	3	4	6	9	K18
3	4	4	6	9	L21*
3	5	4	6	9	L19
3	6	4	6	9	O21
3	7	4	6	9	M21
3	8	4	6	9	O18
4	1	4	6	9	M17
4	2	4	6	9	K16
4	3	4	6	9	M18
4	4	4	6	9	M22
4	5	4	6	9	K15
4	6	4	6	9	M14
4	7	4	6	9	L20
4	8	4	6	9	O16
5	1	4	6	9	L16
5	2	4	6	9	N20
5	3	4	6	9	L23
5	4	4	6	9	L14
5	5	4	6	9	K22
5	6	4	6	9	K17
5	7	4	6	9	O14
5	8	4	6	9	K17
6	1	4	6	9	M19
6	2	4	6	9	N19
6	3	4	6	9	M20
6	4	4	6	9	K21
6	5	4	6	9	Z
6	6	4	6	9	M15
6	7	4	6	9	K19
6	8	4	6	9	Z

R1	R2	R3	R4	Plate	Loc.
1	3	4	7	10	Z
1	4	4	7	10	B02
1	5	4	7	10	D09*
1	6	4	7	10	D07
1	7	4	7	10	Z
1	8	4	7	10	D10
2	1	4	7	10	B07
2	2	4	7	10	Z
2	3	4	7	10	B08
2	4	4	7	10	E07
2	5	4	7	10	B03
2	6	4	7	10	F05
2	7	4	7	10	C05
2	8	4	7	10	E06
3	1	4	7	10	E05
3	2	4	7	10	F10
3	3	4	7	10	Z
3	4	4	7	10	D02
3	5	4	7	10	F07
3	6	4	7	10	C02
3	7	4	7	10	C04*
3	8	4	7	10	E04
4	1	4	7	10	C03
4	2	4	7	10	D03
4	3	4	7	10	B09
4	4	4	7	10	B06
4	5	4	7	10	D06
4	6	4	7	10	B05
4	7	4	7	10	E03
4	8	4	7	10	C11
5	1	4	7	10	F02
5	2	4	7	10	D11
5	3	4	7	10	F04
5	4	4	7	10	B04
5	5	4	7	10	E09
5	6	4	7	10	C10
5	7	4	7	10	C08
5	8	4	7	10	C09
6	1	4	7	10	D08
6	2	4	7	10	F03
6	3	4	7	10	Z
6	4	4	7	10	D05
6	5	4	7	10	Z
6	6	4	7	10	F06
6	7	4	7	10	Z
6	8	4	7	10	E08

Table V .2.7 S31

R1	R2	R3	R4	Plate	Loc.
1	3	2	1	11	L6
1	4	2	1	11	L10
1	5	2	1	11	L3*
1	6	2	1	11	N4
1	7	2	1	11	O8
1	8	2	1	11	L4
2	1	2	1	11	M3
2	2	2	1	11	K7
2	3	2	1	11	M2
2	4	2	1	11	Z
2	5	2	1	11	K9
2	6	2	1	11	L7
2	7	2	1	11	N11
2	8	2	1	11	O3
3	1	2	1	11	O7
3	2	2	1	11	O6
3	3	2	1	11	M4
3	4	2	1	11	N6
3	5	2	1	11	Z
3	6	2	1	11	K4*
3	7	2	1	11	N9
3	8	2	1	11	K10
4	1	2	1	11	M5
4	2	2	1	11	M9
4	3	2	1	11	L2
4	4	2	1	11	Z
4	5	2	1	11	O9
4	6	2	1	11	L5
4	7	2	1	11	K6
4	8	2	1	11	M8
5	1	2	1	11	K5
5	2	2	1	11	M11
5	3	2	1	11	K8
5	4	2	1	11	M6
5	5	2	1	11	Z
5	6	2	1	11	L11
5	7	2	1	11	N7
5	8	2	1	11	L8
6	1	2	1	11	O5
6	2	2	1	11	M7
6	3	2	1	11	N3
6	4	2	1	11	K2
6	5	2	1	11	K11
6	6	2	1	11	N5
6	7	2	1	11	N8
6	8	2	1	11	L9

R1	R2	R3	R4	Plate	Loc.
1	3	2	2	11	O18
1	4	2	2	11	K22
1	5	2	2	11	N16
1	6	2	2	11	N20
1	7	2	2	11	L23
1	8	2	2	11	K17
2	1	2	2	11	N14
2	2	2	2	11	K18
2	3	2	2	11	L21
2	4	2	2	11	O15
2	5	2	2	11	M15
2	6	2	2	11	M21
2	7	2	2	11	M19
2	8	2	2	11	Z
3	1	2	2	11	L22
3	2	2	2	11	N21
3	3	2	2	11	N22
3	4	2	2	11	L15*
3	5	2	2	11	O14
3	6	2	2	11	N15
3	7	2	2	11	N19
3	8	2	2	11	L16*
4	1	2	2	11	N23
4	2	2	2	11	M22
4	3	2	2	11	L18
4	4	2	2	11	L14
4	5	2	2	11	O16
4	6	2	2	11	Z
4	7	2	2	11	K15
4	8	2	2	11	K16
5	1	2	2	11	K23
5	2	2	2	11	L20
5	3	2	2	11	L17
5	4	2	2	11	M18
5	5	2	2	11	K20
5	6	2	2	11	N18
5	7	2	2	11	K14
5	8	2	2	11	M16
6	1	2	2	11	Z
6	2	2	2	11	M14
6	3	2	2	11	M17
6	4	2	2	11	M20
6	5	2	2	11	K21
6	6	2	2	11	K19
6	7	2	2	11	L19
6	8	2	2	11	M23

Table V .2.8

R1	R2	R3	R4	Plate	Loc.
1	3	2	3	12	B9
1	4	2	3	12	D2
1	5	2	3	12	F3
1	6	2	3	12	D10
1	7	2	3	12	Z
1	8	2	3	12	B5
2	1	2	3	12	Z
2	2	2	3	12	B8
2	3	2	3	12	Z
2	4	2	3	12	Z
2	5	2	3	12	Z
2	6	2	3	12	F7
2	7	2	3	12	Z
2	8	2	3	12	Z
3	1	2	3	12	C10
3	2	2	3	12	Z
3	3	2	3	12	Z
3	4	2	3	12	Z
3	5	2	3	12	Z
3	6	2	3	12	Z
3	7	2	3	12	Z
3	8	2	3	12	C2
4	1	2	3	12	Z
4	2	2	3	12	Z
4	3	2	3	12	Z
4	4	2	3	12	Z
4	5	2	3	12	Z
4	6	2	3	12	Z
4	7	2	3	12	Z
4	8	2	3	12	B2
5	1	2	3	12	Z
5	2	2	3	12	Z
5	3	2	3	12	B3
5	4	2	3	12	C6
5	5	2	3	12	Z
5	6	2	3	12	Z
5	7	2	3	12	C7
5	8	2	3	12	Z
6	1	2	3	12	Z
6	2	2	3	12	Z
6	3	2	3	12	Z
6	4	2	3	12	C11
6	5	2	3	12	Z
6	6	2	3	12	Z
6	7	2	3	12	B11
6	8	2	3	12	D4

R1	R2	R3	R4	Plate	Loc.
1	3	2	5	12	K6
1	4	2	5	12	L11
1	5	2	5	12	Z
1	6	2	5	12	K11
1	7	2	5	12	M5
1	8	2	5	12	K10
2	1	2	5	12	L5
2	2	2	5	12	L2
2	3	2	5	12	Z
2	4	2	5	12	N6
2	5	2	5	12	M6
2	6	2	5	12	Z
2	7	2	5	12	N2
2	8	2	5	12	K9
3	1	2	5	12	M4
3	2	2	5	12	L9
3	3	2	5	12	K2
3	4	2	5	12	Z
3	5	2	5	12	O7
3	6	2	5	12	N10
3	7	2	5	12	M3*
3	8	2	5	12	M11
4	1	2	5	12	L3
4	2	2	5	12	L7
4	3	2	5	12	M8
4	4	2	5	12	Z
4	5	2	5	12	Z
4	6	2	5	12	Z
4	7	2	5	12	L10
4	8	2	5	12	M7
5	1	2	5	12	O4
5	2	2	5	12	M2
5	3	2	5	12	N11*
5	4	2	5	12	Z
5	5	2	5	12	N3
5	6	2	5	12	Z
5	7	2	5	12	O9
5	8	2	5	12	L4
6	1	2	5	12	Z
6	2	2	5	12	O3
6	3	2	5	12	K8
6	4	2	5	12	K5
6	5	2	5	12	K4
6	6	2	5	12	Z
6	7	2	5	12	L6
6	8	2	5	12	N8

R1	R2	R3	R4	Plate	Loc.
1	3	2	4	12	D18
1	4	2	4	12	Z
1	5	2	4	12	E23
1	6	2	4	12	D22
1	7	2	4	12	Z
1	8	2	4	12	E20
2	1	2	4	12	E21
2	2	2	4	12	Z
2	3	2	4	12	Z
2	4	2	4	12	B20
2	5	2	4	12	Z
2	6	2	4	12	E19
2	7	2	4	12	Z
2	8	2	4	12	B23
3	1	2	4	12	Z
3	2	2	4	12	C22
3	3	2	4	12	Z
3	4	2	4	12	Z
3	5	2	4	12	C16
3	6	2	4	12	Z
3	7	2	4	12	Z
3	8	2	4	12	Z
4	1	2	4	12	Z
4	2	2	4	12	C21
4	3	2	4	12	Z
4	4	2	4	12	Z
4	5	2	4	12	Z
4	6	2	4	12	Z
4	7	2	4	12	Z
4	8	2	4	12	Z
5	1	2	4	12	Z
5	2	2	4	12	B18
5	3	2	4	12	F17
5	4	2	4	12	Z
5	5	2	4	12	Z
5	6	2	4	12	D16
5	7	2	4	12	C20
5	8	2	4	12	C19
6	1	2	4	12	Z
6	2	2	4	12	E22
6	3	2	4	12	Z
6	4	2	4	12	Z
6	5	2	4	12	C20
6	6	2	4	12	Z
6	7	2	4	12	Z
6	8	2	4	12	Z

R1	R2	R3	R4	Plate	Loc.
1	3	2	6	12	N16
1	4	2	6	12	Z
1	5	2	6	12	N14
1	6	2	6	12	L14
1	7	2	6	12	M22
1	8	2	6	12	N21
2	1	2	6	12	L16
2	2	2	6	12	L15
2	3	2	6	12	M15*
2	4	2	6	12	O17
2	5	2	6	12	K18
2	6	2	6	12	N19
2	7	2	6	12	K17
2	8	2	6	12	L18
3	1	2	6	12	M21
3	2	2	6	12	Z
3	3	2	6	12	N20
3	4	2	6	12	Z
3	5	2	6	12	O21
3	6	2	6	12	Z
3	7	2	6	12	K16
3	8	2	6	12	M20
4	1	2	6	12	M23
4	2	2	6	12	K20
4	3	2	6	12	L17
4	4	2	6	12	O15
4	5	2	6	12	O14
4	6	2	6	12	L21
4	7	2	6	12	Z
4	8	2	6	12	L19
5	1	2	6	12	Z
5	2	2	6	12	M18
5	3	2	6	12	L22
5	4	2	6	12	Z
5	5	2	6	12	Z
5	6	2	6	12	L23
5	7	2	6	12	M14*
5	8	2	6	12	O16
6	1	2	6	12	M17
6	2	2	6	12	N15
6	3	2	6	12	K15
6	4	2	6	12	M19
6	5	2	6	12	K21
6	6	2	6	12	Z
6	7	2	6	12	Z
6	8	2	6	12	N17

Table V.2.9

R1	R2	R3	R4	Plate	Loc.
1	3	2	7	13	C11
1	4	2	7	13	B05
1	5	2	7	13	B06
1	6	2	7	13	B09*
1	7	2	7	13	Z
1	8	2	7	13	F04
2	1	2	7	13	E07
2	2	2	7	13	C07
2	3	2	7	13	C04
2	4	2	7	13	F05
2	5	2	7	13	E05
2	6	2	7	13	B10
2	7	2	7	13	D02*
2	8	2	7	13	E02
3	1	2	7	13	D08
3	2	2	7	13	C03
3	3	2	7	13	E08
3	4	2	7	13	B03
3	5	2	7	13	D06
3	6	2	7	13	C02
3	7	2	7	13	C09
3	8	2	7	13	B02
4	1	2	7	13	B04
4	2	2	7	13	D05
4	3	2	7	13	D04
4	4	2	7	13	C10
4	5	2	7	13	D11
4	6	2	7	13	C05
4	7	2	7	13	E03
4	8	2	7	13	Z
5	1	2	7	13	Z
5	2	2	7	13	F02
5	3	2	7	13	F06
5	4	2	7	13	B08
5	5	2	7	13	F08
5	6	2	7	13	B07
5	7	2	7	13	F03
5	8	2	7	13	Z
6	1	2	7	13	C08
6	2	2	7	13	E09
6	3	2	7	13	E10
6	4	2	7	13	Z
6	5	2	7	13	Z
6	6	2	7	13	Z
6	7	2	7	13	Z
6	8	2	7	13	E11

R1	R2	R3	R4	Plate	Loc.
1	3	3	2	13	M06
1	4	3	2	13	N03
1	5	3	2	13	Z
1	6	3	2	13	Z
1	7	3	2	13	L03
1	8	3	2	13	L11
2	1	3	2	13	K02
2	2	3	2	13	O03
2	3	3	2	13	N02*
2	4	3	2	13	O05
2	5	3	2	13	N05
2	6	3	2	13	L02
2	7	3	2	13	K06
2	8	3	2	13	N04
3	1	3	2	13	L08
3	2	3	2	13	K10
3	3	3	2	13	O02
3	4	3	2	13	N09
3	5	3	2	13	K05
3	6	3	2	13	Z
3	7	3	2	13	N08
3	8	3	2	13	No7*
4	1	3	2	13	M08
4	2	3	2	13	P04
4	3	3	2	13	M04
4	4	3	2	13	N10
4	5	3	2	13	K11
4	6	3	2	13	O04
4	7	3	2	13	K04
4	8	3	2	13	K03
5	1	3	2	13	L06
5	2	3	2	13	M11
5	3	3	2	13	K08
5	4	3	2	13	L07
5	5	3	2	13	L09
5	6	3	2	13	N06
5	7	3	2	13	M07
5	8	3	2	13	L05
6	1	3	2	13	K09
6	2	3	2	13	M05
6	3	3	2	13	M09
6	4	3	2	13	M02
6	5	3	2	13	K07
6	6	3	2	13	N11
6	7	3	2	13	M10
6	8	3	2	13	Z

R1	R2	R3	R4	Plate	Loc.
1	3	3	1	13	E14
1	4	3	1	13	D23
1	5	3	1	13	B21
1	6	3	1	13	F18
1	7	3	1	13	E15
1	8	3	1	13	D19
2	1	3	1	13	B18*
2	2	3	1	13	F14
2	3	3	1	13	D21
2	4	3	1	13	B17
2	5	3	1	13	D15
2	6	3	1	13	B16
2	7	3	1	13	E19
2	8	3	1	13	D20
3	1	3	1	13	F19
3	2	3	1	13	C21
3	3	3	1	13	E18
3	4	3	1	13	B15
3	5	3	1	13	C14*
3	6	3	1	13	B23
3	7	3	1	13	B19
3	8	3	1	13	F21
4	1	3	1	13	D16
4	2	3	1	13	C16
4	3	3	1	13	D14
4	4	3	1	13	F16
4	5	3	1	13	Z
4	6	3	1	13	C23
4	7	3	1	13	E16
4	8	3	1	13	E17
5	1	3	1	13	C20
5	2	3	1	13	B20
5	3	3	1	13	E22
5	4	3	1	13	B22
5	5	3	1	13	D17
5	6	3	1	13	E21
5	7	3	1	13	C17
5	8	3	1	13	E20
6	1	3	1	13	B14
6	2	3	1	13	D18
6	3	3	1	13	F17
6	4	3	1	13	D22
6	5	3	1	13	C19
6	6	3	1	13	C15
6	7	3	1	13	C18
6	8	3	1	13	E23

R1	R2	R3	R4	Plate	Loc.
1	3	3	3	13	Z
1	4	3	3	13	Z
1	5	3	3	13	Z
1	6	3	3	13	Z
1	7	3	3	13	Z
1	8	3	3	13	Z
2	1	3	3	13	Z
2	2	3	3	13	Z
2	3	3	3	13	Z
2	4	3	3	13	K21
2	5	3	3	13	Z
2	6	3	3	13	Z
2	7	3	3	13	Z
2	8	3	3	13	Z
3	1	3	3	13	Z
3	2	3	3	13	Z
3	3	3	3	13	Z
3	4	3	3	13	Z
3	5	3	3	13	N21
3	6	3	3	13	Z
3	7	3	3	13	Z
3	8	3	3	13	Z
4	1	3	3	13	Z
4	2	3	3	13	K23
4	3	3	3	13	Z
4	4	3	3	13	Z
4	5	3	3	13	M18
4	6	3	3	13	Z
4	7	3	3	13	Z
4	8	3	3	13	Z
5	1	3	3	13	Z
5	2	3	3	13	Z
5	3	3	3	13	Z
5	4	3	3	13	Z
5	5	3	3	13	Z
5	6	3	3	13	Z
5	7	3	3	13	Z
5	8	3	3	13	Z
6	1	3	3	13	Z
6	2	3	3	13	Z
6	3	3	3	13	Z
6	4	3	3	13	Z
6	5	3	3	13	Z
6	6	3	3	13	Z
6	7	3	3	13	Z
6	8	3	3	13	Z

Table V.2.10

R1	R2	R3	R4	Plate	Loc.
1	3	3	4	14	Z
1	4	3	4	14	Z
1	5	3	4	14	B11
1	6	3	4	14	Z
1	7	3	4	14	Z
1	8	3	4	14	Z
2	1	3	4	14	Z
2	2	3	4	14	B7
2	3	3	4	14	Z
2	4	3	4	14	Z
2	5	3	4	14	Z
2	6	3	4	14	Z
2	7	3	4	14	Z
2	8	3	4	14	Z
3	1	3	4	14	B10
3	2	3	4	14	Z
3	3	3	4	14	Z
3	4	3	4	14	B9
3	5	3	4	14	B8
3	6	3	4	14	Z
3	7	3	4	14	Z
3	8	3	4	14	Z
4	1	3	4	14	Z
4	2	3	4	14	Z
4	3	3	4	14	Z
4	4	3	4	14	Z
4	5	3	4	14	Z
4	6	3	4	14	Z
4	7	3	4	14	Z
4	8	3	4	14	Z
5	1	3	4	14	Z
5	2	3	4	14	Z
5	3	3	4	14	E3
5	4	3	4	14	Z
5	5	3	4	14	Z
5	6	3	4	14	C10
5	7	3	4	14	Z
5	8	3	4	14	Z
6	1	3	4	14	Z
6	2	3	4	14	Z
6	3	3	4	14	Z
6	4	3	4	14	C3
6	5	3	4	14	Z
6	6	3	4	14	Z
6	7	3	4	14	Z
6	8	3	4	14	Z

R1	R2	R3	R4	Plate	Loc.
1	3	3	6	14	L11
1	4	3	6	14	K02
1	5	3	6	14	L02
1	6	3	6	14	L09
1	7	3	6	14	N10
1	8	3	6	14	N08
2	1	3	6	14	M07
2	2	3	6	14	L08
2	3	3	6	14	M04
2	4	3	6	14	L10
2	5	3	6	14	L05*
2	6	3	6	14	K03
2	7	3	6	14	M09
2	8	3	6	14	Z
3	1	3	6	14	M10
3	2	3	6	14	L06
3	3	3	6	14	M11
3	4	3	6	14	N09
3	5	3	6	14	M02
3	6	3	6	14	N03
3	7	3	6	14	Z
3	8	3	6	14	O03
4	1	3	6	14	N07
4	2	3	6	14	Z
4	3	3	6	14	K08
4	4	3	6	14	N05*
4	5	3	6	14	N02
4	6	3	6	14	O02
4	7	3	6	14	K06
4	8	3	6	14	O06
5	1	3	6	14	M05
5	2	3	6	14	N11
5	3	3	6	14	L07
5	4	3	6	14	K05
5	5	3	6	14	N06
5	6	3	6	14	M03
5	7	3	6	14	L03
5	8	3	6	14	M03
6	1	3	6	14	M06
6	2	3	6	14	K07
6	3	3	6	14	K10
6	4	3	6	14	K04
6	5	3	6	14	M08
6	6	3	6	14	K11
6	7	3	6	14	L04
6	8	3	6	14	K09

R1	R2	R3	R4	Plate	Loc.
1	3	3	5	14	F17
1	4	3	5	14	Z
1	5	3	5	14	C18
1	6	3	5	14	Z
1	7	3	5	14	E20
1	8	3	5	14	D19
2	1	3	5	14	D15
2	2	3	5	14	G14
2	3	3	5	14	Z
2	4	3	5	14	B23
2	5	3	5	14	D17
2	6	3	5	14	F22
2	7	3	5	14	B22
2	8	3	5	14	E15
3	1	3	5	14	F15
3	2	3	5	14	D23*
3	3	3	5	14	E20
3	4	3	5	14	B19
3	5	3	5	14	E21
3	6	3	5	14	B16
3	7	3	5	14	F14
3	8	3	5	14	D22
4	1	3	5	14	B20
4	2	3	5	14	E14
4	3	3	5	14	Z
4	4	3	5	14	D20
4	5	3	5	14	C22
4	6	3	5	14	B15
4	7	3	5	14	E19
4	8	3	5	14	C20
5	1	3	5	14	E18
5	2	3	5	14	C21
5	3	3	5	14	B14*
5	4	3	5	14	C15
5	5	3	5	14	C21
5	6	3	5	14	F20
5	7	3	5	14	Z
5	8	3	5	14	E22
6	1	3	5	14	E16
6	2	3	5	14	B21
6	3	3	5	14	C19
6	4	3	5	14	C23
6	5	3	5	14	D16
6	6	3	5	14	Z
6	7	3	5	14	D14
6	8	3	5	14	F16

R1	R2	R3	R4	Plate	Loc.
1	3	3	7	14	M19
1	4	3	7	14	K15
1	5	3	7	14	K16
1	6	3	7	14	Z
1	7	3	7	14	M20
1	8	3	7	14	M14
2	1	3	7	14	L15
2	2	3	7	14	M22
2	3	3	7	14	M23
2	4	3	7	14	J14
2	5	3	7	14	O17
2	6	3	7	14	L22
2	7	3	7	14	J16
2	8	3	7	14	L21
3	1	3	7	14	O18
3	2	3	7	14	M15
3	3	3	7	14	M18
3	4	3	7	14	N14
3	5	3	7	14	O22
3	6	3	7	14	L18
3	7	3	7	14	L19
3	8	3	7	14	L17*
4	1	3	7	14	Z
4	2	3	7	14	N22
4	3	3	7	14	N15
4	4	3	7	14	M21
4	5	3	7	14	O21
4	6	3	7	14	N23
4	7	3	7	14	M17
4	8	3	7	14	L16
5	1	3	7	14	M16
5	2	3	7	14	O19
5	3	3	7	14	K20
5	4	3	7	14	L14
5	5	3	7	14	K14
5	6	3	7	14	N17
5	7	3	7	14	K22
5	8	3	7	14	O15
6	1	3	7	14	L20
6	2	3	7	14	K21
6	3	3	7	14	N16
6	4	3	7	14	K23
6	5	3	7	14	K17
6	6	3	7	14	K18
6	7	3	7	14	K19*
6	8	3	7	14	L23

Table V.2.11

R1	R2	R3	R4	Plate	Loc.
1	3	5	1	15	N3
1	4	5	1	15	K2*
1	5	5	1	15	L4
1	6	5	1	15	M6
1	7	5	1	15	Z
1	8	5	1	15	O4
2	1	5	1	15	O6
2	2	5	1	15	K9
2	3	5	1	15	M5
2	4	5	1	15	N5
2	5	5	1	15	Z
2	6	5	1	15	L10
2	7	5	1	15	O7
2	8	5	1	15	M4
3	1	5	1	15	N10
3	2	5	1	15	K4
3	3	5	1	15	O2
3	4	5	1	15	K5
3	5	5	1	15	K8
3	6	5	1	15	N9*
3	7	5	1	15	M10
3	8	5	1	15	Z
4	1	5	1	15	M3
4	2	5	1	15	Z
4	3	5	1	15	N2
4	4	5	1	15	N4
4	5	5	1	15	O9
4	6	5	1	15	L5
4	7	5	1	15	N8
4	8	5	1	15	L6
5	1	5	1	15	L3
5	2	5	1	15	M7
5	3	5	1	15	N11
5	4	5	1	15	L9
5	5	5	1	15	L7
5	6	5	1	15	M11
5	7	5	1	15	M2
5	8	5	1	15	K6
6	1	5	1	15	M9
6	2	5	1	15	O3
6	3	5	1	15	K11
6	4	5	1	15	N7
6	5	5	1	15	O5
6	6	5	1	15	K10
6	7	5	1	15	K3
6	8	5	1	15	K7

R1	R2	R3	R4	Plate	Loc.
1	3	5	2	15	L16*
1	4	5	2	15	K14
1	5	5	2	15	N17
1	6	5	2	15	L15
1	7	5	2	15	O16
1	8	5	2	15	N18
2	1	5	2	15	K15
2	2	5	2	15	L14
2	3	5	2	15	N22
2	4	5	2	15	L19
2	5	5	2	15	K21
2	6	5	2	15	M20
2	7	5	2	15	N16
2	8	5	2	15	M21
3	1	5	2	15	K15
3	2	5	2	15	Z
3	3	5	2	15	K18
3	4	5	2	15	M14
3	5	5	2	15	M19
3	6	5	2	15	Z
3	7	5	2	15	K23
3	8	5	2	15	M16
4	1	5	2	15	N19
4	2	5	2	15	Z
4	3	5	2	15	K16
4	4	5	2	15	L18*
4	5	5	2	15	Z
4	6	5	2	15	M15
4	7	5	2	15	M17
4	8	5	2	15	M22
5	1	5	2	15	K20
5	2	5	2	15	L22
5	3	5	2	15	L17
5	4	5	2	15	Z
5	5	5	2	15	O15
5	6	5	2	15	Z
5	7	5	2	15	N14
5	8	5	2	15	N23
6	1	5	2	15	L21
6	2	5	2	15	N15
6	3	5	2	15	K19
6	4	5	2	15	K22
6	5	5	2	15	L20
6	6	5	2	15	O14
6	7	5	2	15	M23
6	8	5	2	15	N20

Table V.2.12

R1	R2	R3	R4	Plate	Loc.
1	3	5	3	16	F06
1	4	5	3	16	D03
1	5	5	3	16	D02
1	6	5	3	16	F03
1	7	5	3	16	B08
1	8	5	3	16	E02*
2	1	5	3	16	B02
2	2	5	3	16	E09
2	3	5	3	16	E05
2	4	5	3	16	D07
2	5	5	3	16	D04
2	6	5	3	16	C10
2	7	5	3	16	F08
2	8	5	3	16	B09
3	1	5	3	16	D05
3	2	5	3	16	E11
3	3	5	3	16	C08
3	4	5	3	16	D11
3	5	5	3	16	B04
3	6	5	3	16	B10
3	7	5	3	16	F04
3	8	5	3	16	B11
4	1	5	3	16	F05
4	2	5	3	16	Z
4	3	5	3	16	E08
4	4	5	3	16	E03
4	5	5	3	16	Z
4	6	5	3	16	B07
4	7	5	3	16	Z
4	8	5	3	16	C06
5	1	5	3	16	B03
5	2	5	3	16	D08*
5	3	5	3	16	F02
5	4	5	3	16	Z
5	5	5	3	16	B06
5	6	5	3	16	DO6
5	7	5	3	16	E10
5	8	5	3	16	F07
6	1	5	3	16	C05
6	2	5	3	16	E04
6	3	5	3	16	C04
6	4	5	3	16	D10
6	5	5	3	16	D09
6	6	5	3	16	B05
6	7	5	3	16	C11
6	8	5	3	16	C07

R1	R2	R3	R4	Plate	Loc.
1	3	5	5	16	O08
1	4	5	5	16	Z
1	5	5	5	16	N07*
1	6	5	5	16	J03
1	7	5	5	16	M11
1	8	5	5	16	Z
2	1	5	5	16	N03
2	2	5	5	16	K10
2	3	5	5	16	L08
2	4	5	5	16	L03
2	5	5	5	16	O07
2	6	5	5	16	O02
2	7	5	5	16	M3
2	8	5	5	16	N05
3	1	5	5	16	MO6*
3	2	5	5	16	K04
3	3	5	5	16	M09
3	4	5	5	16	L05
3	5	5	5	16	N08
3	6	5	5	16	J02
3	7	5	5	16	M02
3	8	5	5	16	J08
4	1	5	5	16	K11
4	2	5	5	16	Z
4	3	5	5	16	L02
4	4	5	5	16	M10
4	5	5	5	16	J07
4	6	5	5	16	O05
4	7	5	5	16	M07
4	8	5	5	16	N02
5	1	5	5	16	K03
5	2	5	5	16	K05
5	3	5	5	16	N04
5	4	5	5	16	K02
5	5	5	5	16	LO9
5	6	5	5	16	N11
5	7	5	5	16	N04
5	8	5	5	16	Z
6	1	5	5	16	N10
6	2	5	5	16	Z
6	3	5	5	16	K06
6	4	5	5	16	N09
6	5	5	5	16	M08
6	6	5	5	16	M05
6	7	5	5	16	L06
6	8	5	5	16	L04

R1	R2	R3	R4	Plate	Loc.
1	3	5	4	16	Z
1	4	5	4	16	C23
1	5	5	4	16	C22
1	6	5	4	16	C20
1	7	5	4	16	C15
1	8	5	4	16	D15
2	1	5	4	16	Z
2	2	5	4	16	D18
2	3	5	4	16	B17
2	4	5	4	16	Z
2	5	5	4	16	D19
2	6	5	4	16	C17
2	7	5	4	16	Z
2	8	5	4	16	E19
3	1	5	4	16	Z
3	2	5	4	16	Z
3	3	5	4	16	Z
3	4	5	4	16	D16
3	5	5	4	16	E14
3	6	5	4	16	D17
3	7	5	4	16	D14*
3	8	5	4	16	E16
4	1	5	4	16	C19
4	2	5	4	16	Z
4	3	5	4	16	C21
4	4	5	4	16	D21
4	5	5	4	16	Z
4	6	5	4	16	C16
4	7	5	4	16	E18*
4	8	5	4	16	B18
5	1	5	4	16	B14
5	2	5	4	16	C18
5	3	5	4	16	D23
5	4	5	4	16	E21
5	5	5	4	16	B16
5	6	5	4	16	B15
5	7	5	4	16	E20
5	8	5	4	16	E23
6	1	5	4	16	D22
6	2	5	4	16	B20
6	3	5	4	16	E17
6	4	5	4	16	B21
6	5	5	4	16	B22
6	6	5	4	16	D20
6	7	5	4	16	C14
6	8	5	4	16	E15

R1	R2	R3	R4	Plate	Loc.
1	3	5	6	16	M18
1	4	5	6	16	L20
1	5	5	6	16	N18*
1	6	5	6	16	M23
1	7	5	6	16	K14
1	8	5	6	16	N23
2	1	5	6	16	Z
2	2	5	6	16	Z
2	3	5	6	16	M19
2	4	5	6	16	K20
2	5	5	6	16	N16
2	6	5	6	16	O20
2	7	5	6	16	M14
2	8	5	6	16	O17
3	1	5	6	16	K16
3	2	5	6	16	O22
3	3	5	6	16	J18
3	4	5	6	16	L22
3	5	5	6	16	M20
3	6	5	6	16	N21
3	7	5	6	16	K22
3	8	5	6	16	L19
4	1	5	6	16	O14
4	2	5	6	16	Z
4	3	5	6	16	N14
4	4	5	6	16	K15
4	5	5	6	16	K17
4	6	5	6	16	O18
4	7	5	6	16	Z
4	8	5	6	16	L17
5	1	5	6	16	L14
5	2	5	6	16	N20*
5	3	5	6	16	K21
5	4	5	6	16	J19
5	5	5	6	16	L23
5	6	5	6	16	Z
5	7	5	6	16	K19
5	8	5	6	16	M17
6	1	5	6	16	M15
6	2	5	6	16	O15
6	3	5	6	16	L21
6	4	5	6	16	N19
6	5	5	6	16	N15
6	6	5	6	16	K18
6	7	5	6	16	Z
6	8	5	6	16	M21

Table V.2.13

R1	R2	R3	R4	Plate	Loc.
1	3	5	7	17	F5
1	4	5	7	17	Z
1	5	5	7	17	F8
1	6	5	7	17	B5*
1	7	5	7	17	B6
1	8	5	7	17	C9
2	1	5	7	17	E9
2	2	5	7	17	E2
2	3	5	7	17	E3
2	4	5	7	17	B9
2	5	5	7	17	C6
2	6	5	7	17	E8
2	7	5	7	17	Z
2	8	5	7	17	F2*
3	1	5	7	17	D3
3	2	5	7	17	D2
3	3	5	7	17	F7
3	4	5	7	17	C8
3	5	5	7	17	C10
3	6	5	7	17	E11
3	7	5	7	17	F3
3	8	5	7	17	E7
4	1	5	7	17	C2
4	2	5	7	17	Z
4	3	5	7	17	C4
4	4	5	7	17	D7
4	5	5	7	17	C5
4	6	5	7	17	B8
4	7	5	7	17	B3
4	8	5	7	17	B4
5	1	5	7	17	D8
5	2	5	7	17	E5
5	3	5	7	17	B2
5	4	5	7	17	E6
5	5	5	7	17	F9
5	6	5	7	17	D6
5	7	5	7	17	E10
5	8	5	7	17	F6
6	1	5	7	17	B7
6	2	5	7	17	B10
6	3	5	7	17	E4
6	4	5	7	17	D9
6	5	5	7	17	D5
6	6	5	7	17	D11
6	7	5	7	17	C3
6	8	5	7	17	D10

R1	R2	R3	R4	Plate	Loc.
1	3	6	2	17	K2
1	4	6	2	17	L3
1	5	6	2	17	M7
1	6	6	2	17	M8
1	7	6	2	17	O6
1	8	6	2	17	M3
2	1	6	2	17	M9
2	2	6	2	17	L6
2	3	6	2	17	M11
2	4	6	2	17	L8
2	5	6	2	17	N10
2	6	6	2	17	O4
2	7	6	2	17	O8
2	8	6	2	17	N8
3	1	6	2	17	O5
3	2	6	2	17	K5
3	3	6	2	17	N6
3	4	6	2	17	K4
3	5	6	2	17	L2*
3	6	6	2	17	K7
3	7	6	2	17	J3
3	8	6	2	17	K10
4	1	6	2	17	L11
4	2	6	2	17	Z
4	3	6	2	17	M2
4	4	6	2	17	L5
4	5	6	2	17	Z
4	6	6	2	17	M6
4	7	6	2	17	N4
4	8	6	2	17	Z
5	1	6	2	17	L9
5	2	6	2	17	N7
5	3	6	2	17	O7
5	4	6	2	17	K6
5	5	6	2	17	L4
5	6	6	2	17	K3
5	7	6	2	17	L7
5	8	6	2	17	K11
6	1	6	2	17	N5*
6	2	6	2	17	N9
6	3	6	2	17	N11
6	4	6	2	17	M4
6	5	6	2	17	K9
6	6	6	2	17	O2
6	7	6	2	17	K8
6	8	6	2	17	L10

R1	R2	R3	R4	Plate	B14
1	3	6	1	17	C22
1	4	6	1	17	Z
1	5	6	1	17	D19
1	6	6	1	17	Z
1	7	6	1	17	E23
1	8	6	1	17	E18
2	1	6	1	17	B14
2	2	6	1	17	E20
2	3	6	1	17	B18
2	4	6	1	17	C19
2	5	6	1	17	F16
2	6	6	1	17	D17
2	7	6	1	17	E19
2	8	6	1	17	B21
3	1	6	1	17	D16
3	2	6	1	17	F15
3	3	6	1	17	Z
3	4	6	1	17	D22
3	5	6	1	17	C17
3	6	6	1	17	B16*
3	7	6	1	17	F21
3	8	6	1	17	D15
4	1	6	1	17	F20
4	2	6	1	17	Z
4	3	6	1	17	F18
4	4	6	1	17	B15
4	5	6	1	17	B23
4	6	6	1	17	D18
4	7	6	1	17	C21
4	8	6	1	17	E22*
5	1	6	1	17	E15
5	2	6	1	17	D21
5	3	6	1	17	C16
5	4	6	1	17	B19
5	5	6	1	17	E14
5	6	6	1	17	D20
5	7	6	1	17	C18
5	8	6	1	17	Z
6	1	6	1	17	C20
6	2	6	1	17	B22
6	3	6	1	17	D23
6	4	6	1	17	C23
6	5	6	1	17	E17
6	6	6	1	17	B20
6	7	6	1	17	C14
6	8	6	1	17	D14

R1	R2	R3	R4	Plate	Loc.
1	3	6	3	17	K19
1	4	6	3	17	N14
1	5	6	3	17	M21
1	6	6	3	17	K16
1	7	6	3	17	L16
1	8	6	3	17	N17
2	1	6	3	17	K18
2	2	6	3	17	K17
2	3	6	3	17	M17
2	4	6	3	17	N18
2	5	6	3	17	N23
2	6	6	3	17	K15
2	7	6	3	17	O23
2	8	6	3	17	N15
3	1	6	3	17	O21
3	2	6	3	17	J15
3	3	6	3	17	J16
3	4	6	3	17	O16
3	5	6	3	17	K21
3	6	6	3	17	M22
3	7	6	3	17	M20*
3	8	6	3	17	M14
4	1	6	3	17	M19
4	2	6	3	17	Z
4	3	6	3	17	L14
4	4	6	3	17	J17
4	5	6	3	17	N16
4	6	6	3	17	L20
4	7	6	3	17	L18
4	8	6	3	17	O22
5	1	6	3	17	J19
5	2	6	3	17	O19
5	3	6	3	17	L21*
5	4	6	3	17	K14
5	5	6	3	17	K20
5	6	6	3	17	O20
5	7	6	3	17	O14
5	8	6	3	17	M16
6	1	6	3	17	M23
6	2	6	3	17	L15
6	3	6	3	17	M18
6	4	6	3	17	J14
6	5	6	3	17	K23
6	6	6	3	17	N22
6	7	6	3	17	K22
6	8	6	3	17	N19

Table V.2.14

R1	R2	R3	R4	Plate	Loc.
1	3	6	4	18	E7
1	4	6	4	18	C10*
1	5	6	4	18	Z
1	6	6	4	18	D11
1	7	6	4	18	D3
1	8	6	4	18	C5
2	1	6	4	18	F4
2	2	6	4	18	E8
2	3	6	4	18	B7
2	4	6	4	18	Z
2	5	6	4	18	C2
2	6	6	4	18	B10
2	7	6	4	18	E2
2	8	6	4	18	C6
3	1	6	4	18	F3
3	2	6	4	18	F5
3	3	6	4	18	Z
3	4	6	4	18	D4*
3	5	6	4	18	D8
3	6	6	4	18	Z
3	7	6	4	18	D9
3	8	6	4	18	D2
4	1	6	4	18	B2
4	2	6	4	18	Z
4	3	6	4	18	B8
4	4	6	4	18	E9
4	5	6	4	18	E3
4	6	6	4	18	E4
4	7	6	4	18	B11
4	8	6	4	18	B6
5	1	6	4	18	C7
5	2	6	4	18	B4
5	3	6	4	18	E5
5	4	6	4	18	C3
5	5	6	4	18	F2
5	6	6	4	18	Z
5	7	6	4	18	Z
5	8	6	4	18	D7
6	1	6	4	18	D6
6	2	6	4	18	C8
6	3	6	4	18	C4
6	4	6	4	18	D10
6	5	6	4	18	C11
6	6	6	4	18	B3
6	7	6	4	18	D5
6	8	6	4	18	B5

R1	R2	R3	R4	Plate	Loc.
1	3	6	6	18	K7
1	4	6	6	18	K8*
1	5	6	6	18	K2
1	6	6	6	18	M7
1	7	6	6	18	L2
1	8	6	6	18	K6
2	1	6	6	18	M4
2	2	6	6	18	N5
2	3	6	6	18	M3
2	4	6	6	18	M11
2	5	6	6	18	L6
2	6	6	6	18	L10
2	7	6	6	18	N6
2	8	6	6	18	M2
3	1	6	6	18	Z
3	2	6	6	18	O4
3	3	6	6	18	K11
3	4	6	6	18	N2*
3	5	6	6	18	N8
3	6	6	6	18	M5
3	7	6	6	18	Z
3	8	6	6	18	N4
4	1	6	6	18	K3
4	2	6	6	18	Z
4	3	6	6	18	N10
4	4	6	6	18	L4
4	5	6	6	18	O8
4	6	6	6	18	O3
4	7	6	6	18	L3
4	8	6	6	18	N7
5	1	6	6	18	O2
5	2	6	6	18	L11
5	3	6	6	18	K5
5	4	6	6	18	N3
5	5	6	6	18	L8
5	6	6	6	18	Z
5	7	6	6	18	O5
5	8	6	6	18	M10
6	1	6	6	18	K10
6	2	6	6	18	K9
6	3	6	6	18	K4
6	4	6	6	18	M6
6	5	6	6	18	M9
6	6	6	6	18	L5
6	7	6	6	18	L7
6	8	6	6	18	L9

R1	R2	R3	R4	Plate	Loc.
1	3	6	5	18	D15
1	4	6	5	18	B23
1	5	6	5	18	C17
1	6	6	5	18	B22
1	7	6	5	18	B19
1	8	6	5	18	B18
2	1	6	5	18	C23
2	2	6	5	18	D23
2	3	6	5	18	B16
2	4	6	5	18	D17
2	5	6	5	18	E15
2	6	6	5	18	E14
2	7	6	5	18	C20
2	8	6	5	18	B15*
3	1	6	5	18	E18
3	2	6	5	18	E16
3	3	6	5	18	D16*
3	4	6	5	18	Z
3	5	6	5	18	F14
3	6	6	5	18	Z
3	7	6	5	18	F15
3	8	6	5	18	F16
4	1	6	5	18	D20
4	2	6	5	18	F23
4	3	6	5	18	D22
4	4	6	5	18	F19
4	5	6	5	18	Z
4	6	6	5	18	F21
4	7	6	5	18	F18
4	8	6	5	18	E21
5	1	6	5	18	C19
5	2	6	5	18	D18
5	3	6	5	18	C15
5	4	6	5	18	B14
5	5	6	5	18	C22
5	6	6	5	18	E17
5	7	6	5	18	D21
5	8	6	5	18	D19
6	1	6	5	18	C18
6	2	6	5	18	B21
6	3	6	5	18	E23
6	4	6	5	18	B20
6	5	6	5	18	B17
6	6	6	5	18	C16
6	7	6	5	18	C21
6	8	6	5	18	C14

R1	R2	R3	R4	Plate	Loc.
1	3	6	7	18	K14
1	4	6	7	18	Z
1	5	6	7	18	L15
1	6	6	7	18	Z
1	7	6	7	18	M21
1	8	6	7	18	M22
2	1	6	7	18	O15
2	2	6	7	18	M23
2	3	6	7	18	M18
2	4	6	7	18	M16
2	5	6	7	18	N18
2	6	6	7	18	Z
2	7	6	7	18	K22
2	8	6	7	18	K19
3	1	6	7	18	N15
3	2	6	7	18	N16
3	3	6	7	18	O20*
3	4	6	7	18	K23
3	5	6	7	18	L23
3	6	6	7	18	K18
3	7	6	7	18	K20
3	8	6	7	18	N17
4	1	6	7	18	L17
4	2	6	7	18	Z
4	3	6	7	18	O16
4	4	6	7	18	M20
4	5	6	7	18	K15
4	6	6	7	18	L20
4	7	6	7	18	L20
4	8	6	7	18	N21
5	1	6	7	18	N14
5	2	6	7	18	Z
5	3	6	7	18	N23
5	4	6	7	18	O18*
5	5	6	7	18	N22
5	6	6	7	18	K17
5	7	6	7	18	N20
5	8	6	7	18	M17
6	1	6	7	18	K21
6	2	6	7	18	N19
6	3	6	7	18	L22
6	4	6	7	18	L16
6	5	6	7	18	M14
6	6	6	7	18	L19
6	7	6	7	18	K16
6	8	6	7	18	M15

Table V.2.15

V.3 LC analysis for Purity Assessment

V.3.1 All (R1)(R2) combinations (46)

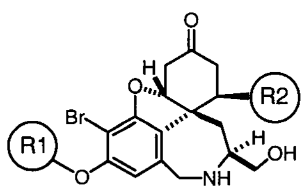


Table V.3.1.1 Structural Assignment of all 46 R1-R2 combinations for (R3)8(R4)8

Figure V.3.1.1	Diode Array Traces for R2 combinations with (R1)1(R3)8(R4)8
Figure V.3.1.2	Diode Array Traces for R2 combinations with (R1)2(R3)8(R4)8
Figure V.3.1.3	Diode Array Traces for R2 combinations with (R1)3(R3)8(R4)8
Figure V.3.1.4	Diode Array Traces for R2 combinations with (R1)4(R3)8(R4)8
Figure V.3.1.5	Diode Array Traces for R2 combinations with (R1)5(R3)8(R4)8
Figure V.3.1.6	Diode Array Traces for R2 combinations with (R1)6(R3)8(R4)8

* these spectra were obtained using LC analysis protocol B (Section I). All other spectra were obtained using LC analysis protocol A (Section I).

R1	R2	R3	R4	MW	Plate	Loc.
1	3	8	8	604.2	4	L20
1	4	8	8	654.2	4	O15
1	5	8	8	624.2	4	L19
1	6	8	8	578.2	4	N18
1	7	8	8	602.2	4	N22
1	8	8	8	500.2	4	N16
2	1	8	8	533.2	4	N21
2	2	8	8	611.2	4	M23
2	3	8	8	523.2	4	K22
2	4	8	8	573.2	4	N15
2	5	8	8	543.2	4	L17
2	6	8	8	497.2	4	K21
2	7	8	8	521.2	19	D8
2	8	8	8	419.1	4	M21
3	1	8	8	613.2	4	L14
3	2	8	8	691.2	4	N14
3	3	8	8	603.3	4	L21
3	4	8	8	653.3	4	M17
3	5	8	8	623.3	4	N20
3	6	8	8	577.2	4	N17
3	7	8	8	601.3	4	K16
3	8	8	8	499.2	4	K20

R1	R2	R3	R4	MW	Plate	Loc.
4	1	8	8	589.3	4	K23
4	2	8	8	667.3	19	B10
4	3	8	8	579.3	4	K19
4	4	8	8	629.3	4	N19
4	5	8	8	599.3	4	O16
4	6	8	8	553.3	4	M18
4	7	8	8	577.3	4	L16
4	8	8	8	475.2	4	L15
5	1	8	8	561.2	4	L23
5	2	8	8	639.2	4	M22
5	3	8	8	551.3	4	M14
5	4	8	8	601.2	4	N23
5	5	8	8	571.2	4	M16
5	6	8	8	525.2	4	O14
5	7	8	8	549.2	4	L18
5	8	8	8	447.2	4	K14
6	1	8	8	479	4	M20
6	2	8	8	557.1	4	M19
6	3	8	8	469.1	4	K15
6	4	8	8	519.1	4	L22
6	5	8	8	489.1	4	M15
6	6	8	8	443	4	K18
6	7	8	8	467.1	4	O17
6	8	8	8	365	19	E5

Table V .3.1.1

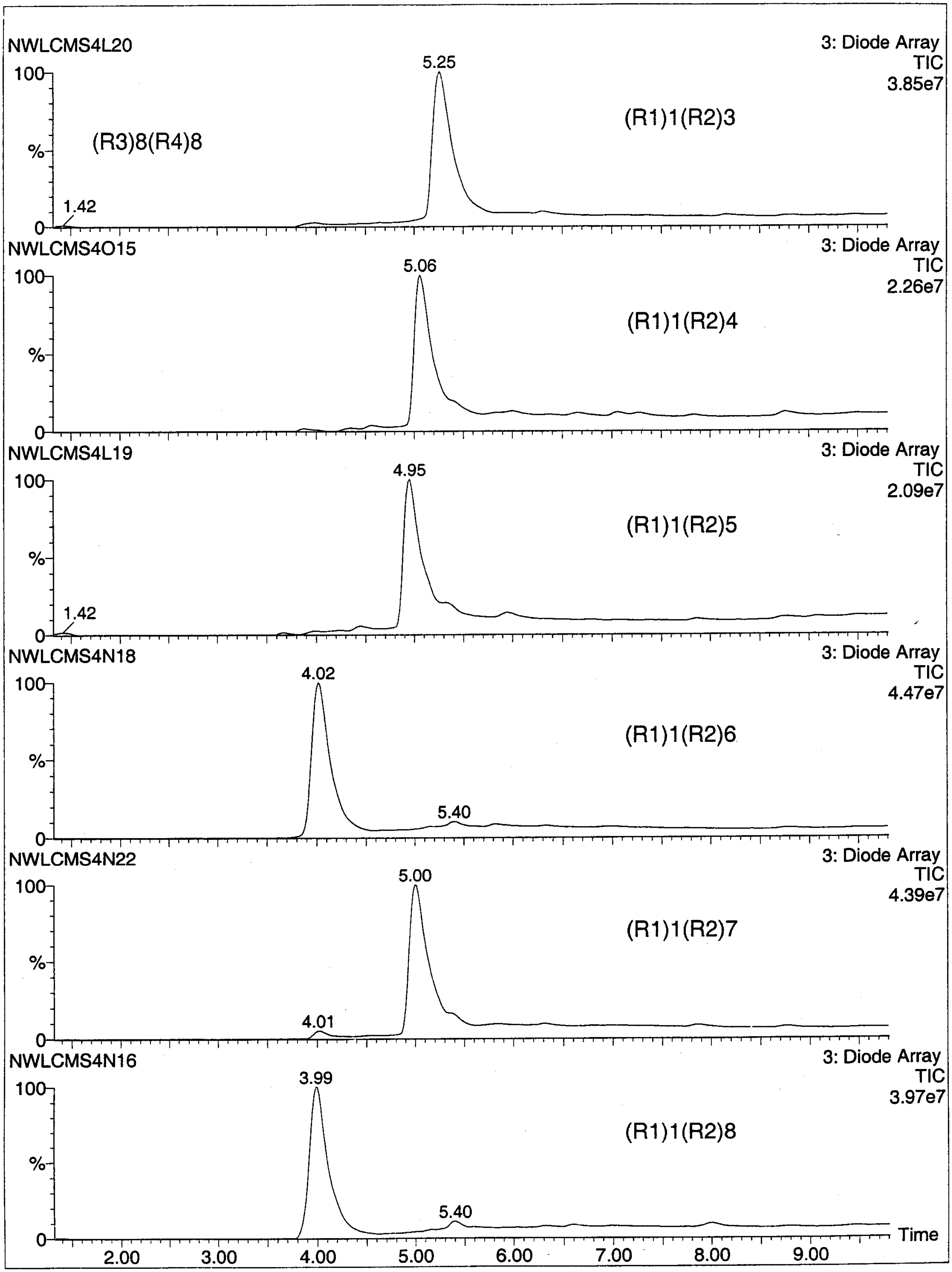


Figure V .3.1.1 S42

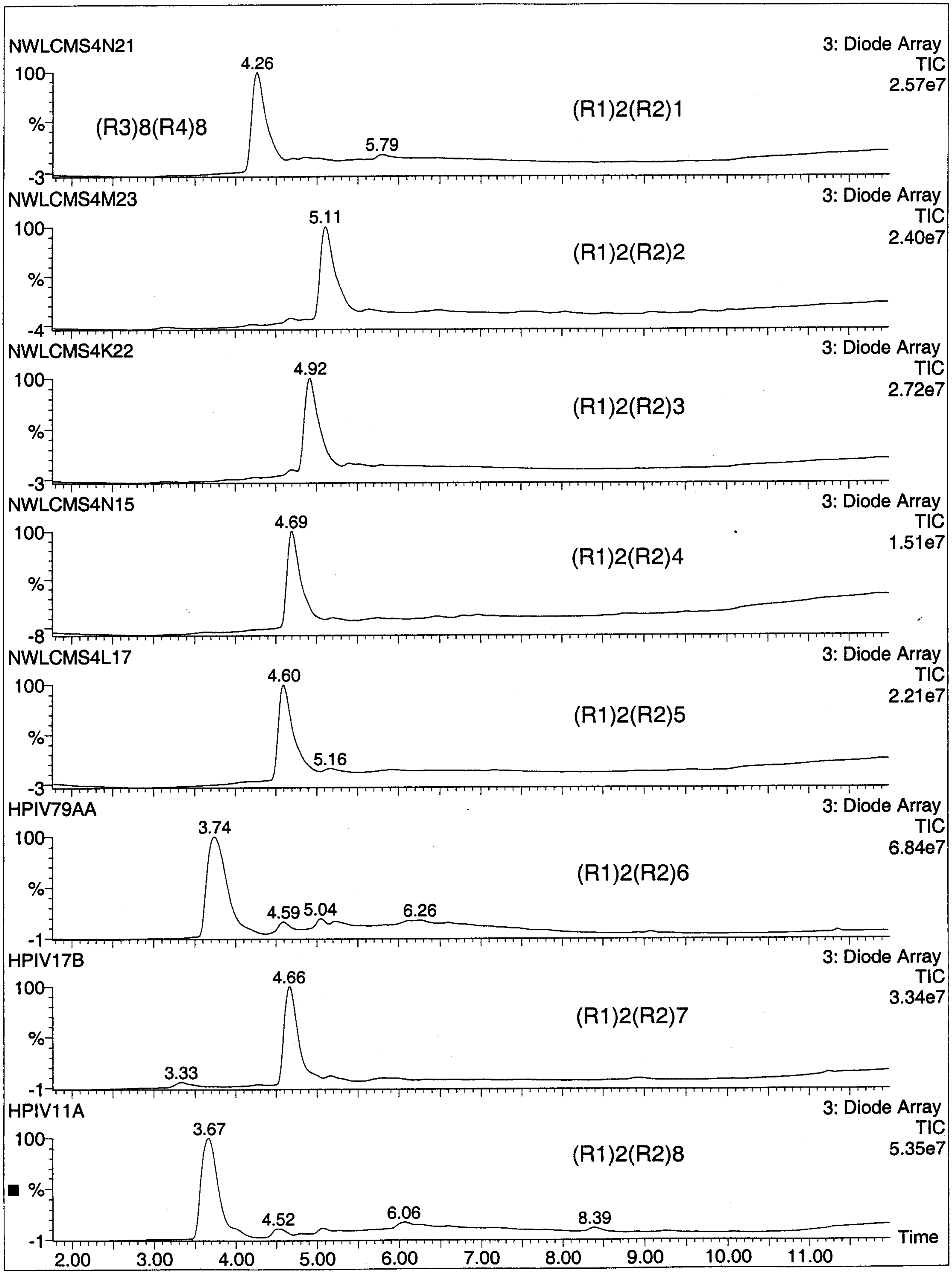
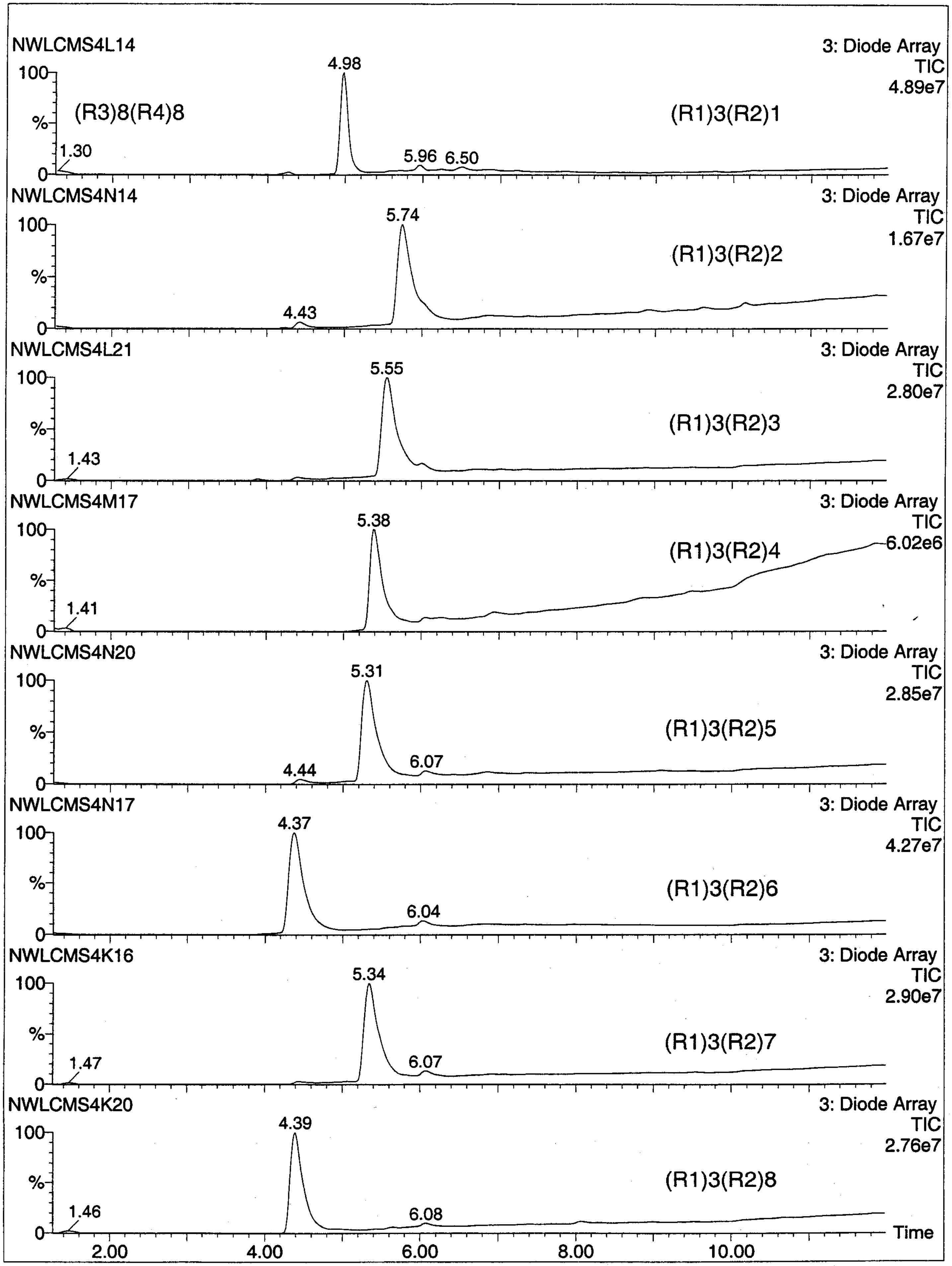


Figure V .3.1.2 543



NWLCMS4L14
3: Diode Array
TIC
4.89e7
(R3)8(R4)8
(R1)3(R2)1
4.98
1.30
5.96
6.50
NWLCMS4N14
3: Diode Array
TIC
1.67e7
(R1)3(R2)2
5.74
4.43
NWLCMS4L21
3: Diode Array
TIC
2.80e7
(R1)3(R2)3
5.55
1.43
NWLCMS4M17
3: Diode Array
TIC
6.02e6
(R1)3(R2)4
5.38
1.41
NWLCMS4N20
3: Diode Array
TIC
2.85e7
(R1)3(R2)5
5.31
4.44
6.07
NWLCMS4N17
3: Diode Array
TIC
4.27e7
(R1)3(R2)6
4.37
6.04
NWLCMS4K16
3: Diode Array
TIC
2.90e7
(R1)3(R2)7
5.34
1.47
6.07
NWLCMS4K20
3: Diode Array
TIC
2.76e7
(R1)3(R2)8
4.39
1.46
6.08
100
%
0
Time
2.00
4.00
6.00
8.00
10.00

Figure V .3.1.3

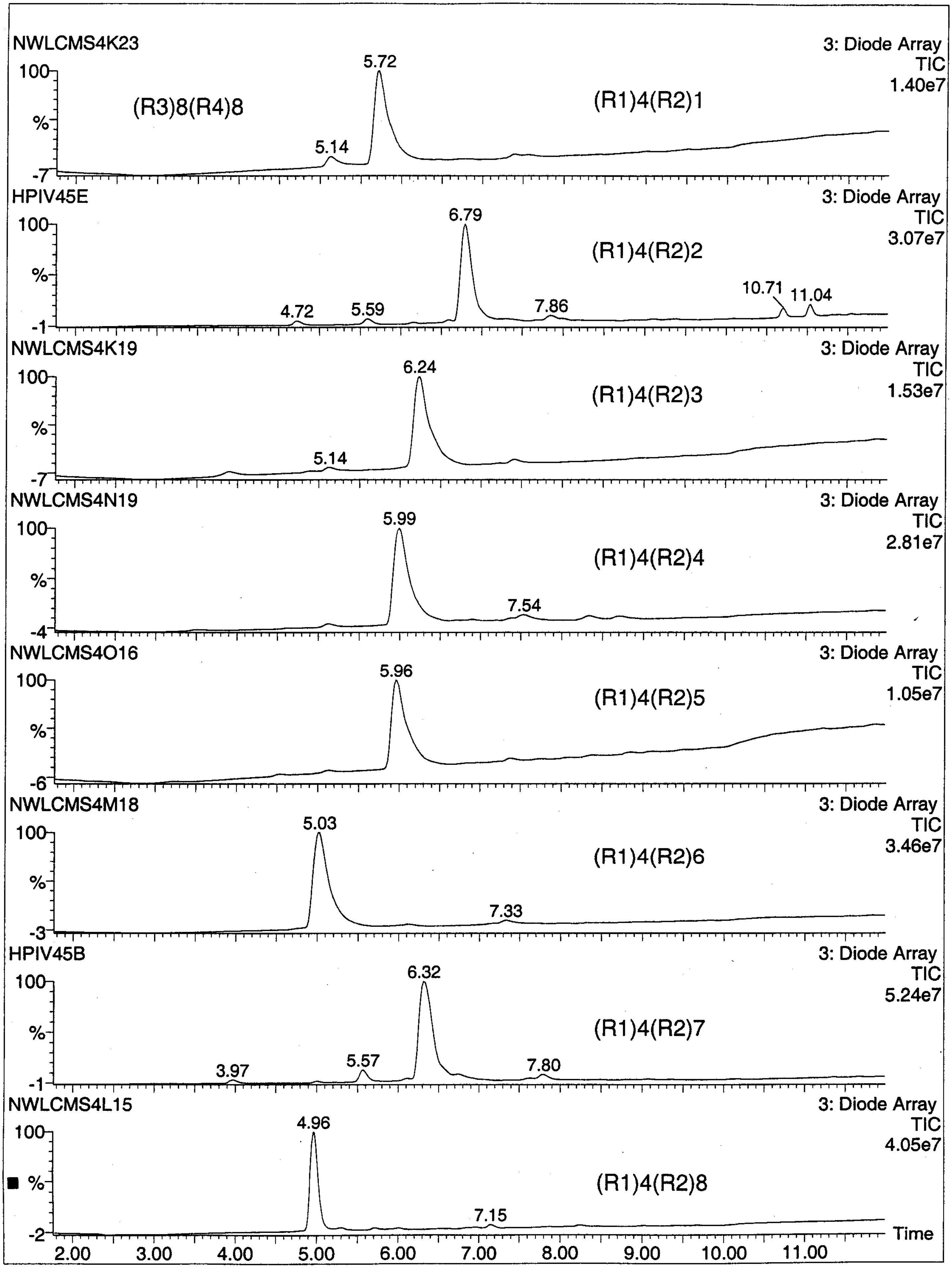


Figure V..3.1.4 545

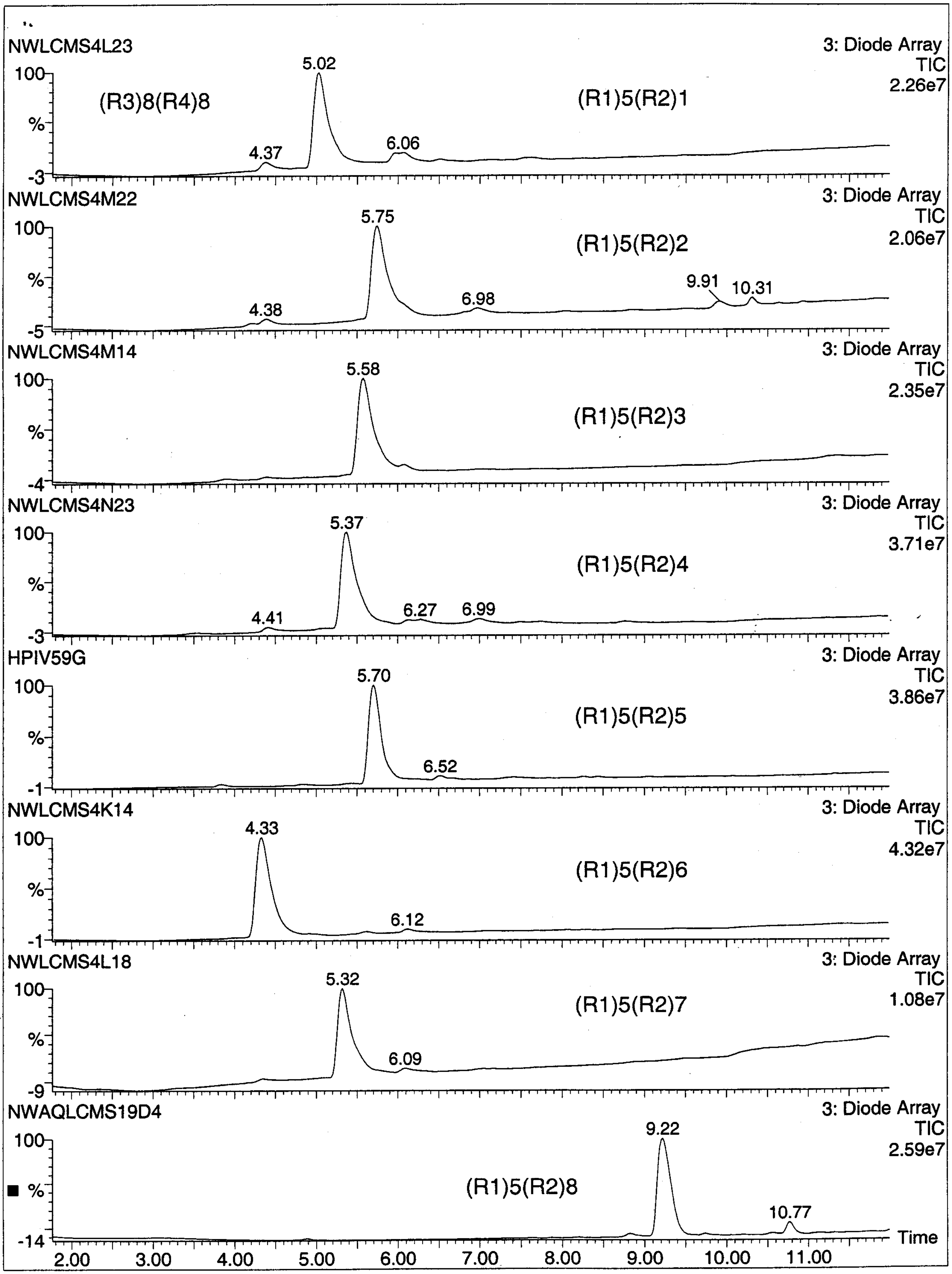


Figure V .3.1.5 546

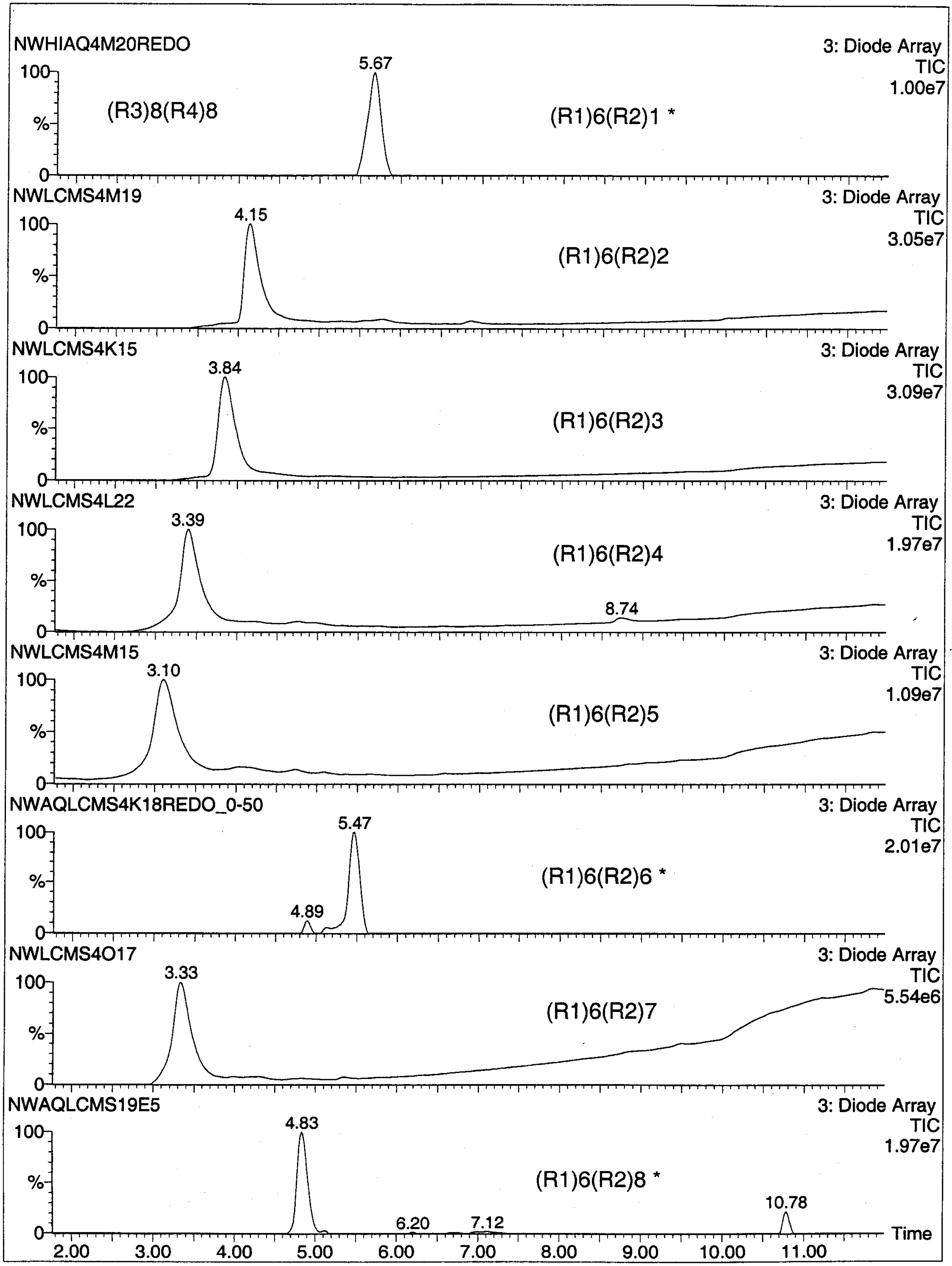
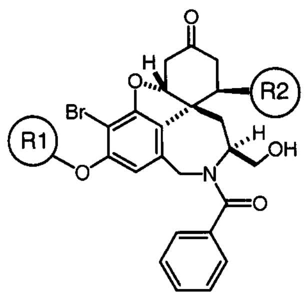
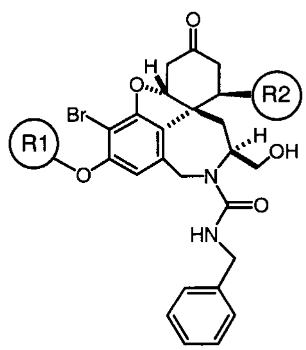


Figure V .3.1.6 S47

V.3.2 (R1)(R2)(R3) Combinations

287 compounds of the theoretical maximum of 322 compounds were identified.





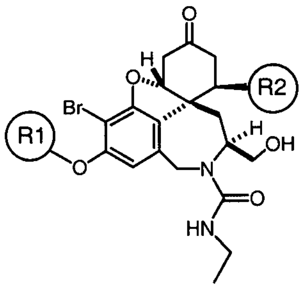


Figure V.3.2.13 Diode Array Traces for R2 combinations with (R1)1(R3)3(R4)8
Figure V.3.2.14 Diode Array Traces for R2 combinations with (R1)2(R3)3(R4)8
Figure V.3.2.15 Diode Array Traces for R2 combinations with (R1)3(R3)3(R4)8
Figure V.3.2.16 Diode Array Traces for R2 combinations with (R1)4(R3)3(R4)8
Figure V.3.2.17 Diode Array Traces for R2 combinations with (R1)5(R3)3(R4)8
Figure V.3.2.18 Diode Array Traces for R2 combinations with (R1)6(R3)3(R4)8

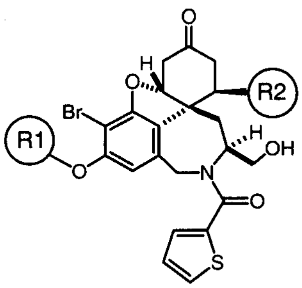


Figure V.3.2.19 Diode Array Traces for R2 combinations with (R1)1(R3)4(R4)8
Figure V.3.2.20 Diode Array Traces for R2 combinations with (R1)2(R3)4(R4)8
Figure V.3.2.21 Diode Array Traces for R2 combinations with (R1)3(R3)4(R4)8
Figure V.3.2.22 Diode Array Traces for R2 combinations with (R1)4(R3)4(R4)8
Figure V.3.2.23 Diode Array Traces for R2 combinations with (R1)5(R3)4(R4)8
Figure V.3.2.24 Diode Array Traces for R2 combinations with (R1)6(R3)4(R4)8

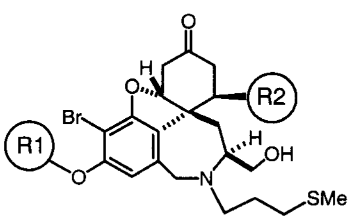
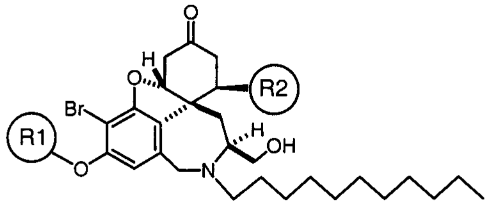
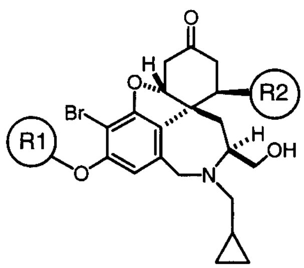


Figure V.3.2.25 Diode Array Traces for R2 combinations with (R1)1(R3)5(R4)8
Figure V.3.2.26 Diode Array Traces for R2 combinations with (R1)2(R3)5(R4)8
Figure V.3.2.27 Diode Array Traces for R2 combinations with (R1)3(R3)5(R4)8
Figure V.3.2.28 Diode Array Traces for R2 combinations with (R1)4(R3)5(R4)8
Figure V.3.2.29 Diode Array Traces for R2 combinations with (R1)5(R3)5(R4)8
Figure V.3.2.30 Diode Array Traces for R2 combinations with (R1)6(R3)5(R4)8





* these spectra were obtained using LC analysis protocol B (Section I). All other spectra were obtained using LC analysis protocol A (Section I).

					Figs VI.3.2.1-6
R1	R2	R3	R4	Plate	Loc
1	3	1	8	1	K02
1	4	1	8	1	K03
1	5	1	8	1	K07
1	6	1	8	1	O05
1	7	1	8	1	L05
1	8	1	8	1	N04
2	1	1	8	1	K04
2	2	1	8	1	K09
2	3	1	8	1	L06
2	4	1	8	1	L08
2	5	1	8	1	M08
2	6	1	8	1	N02
2	7	1	8	1	L09
2	8	1	8	1	M11
3	1	1	8	1	N09
3	2	1	8	1	Z
3	3	1	8	1	Z
3	4	1	8	1	O09
3	5	1	8	1	Z
3	6	1	8	1	M02
3	7	1	8	1	M07
3	8	1	8	1	Z
4	1	1	8	1	L07
4	2	1	8	1	K11
4	3	1	8	1	O02
4	4	1	8	1	M03
4	5	1	8	1	Z
4	6	1	8	1	Z
4	7	1	8	1	N11
4	8	1	8	1	K06
5	1	1	8	1	K05
5	2	1	8	1	L03
5	3	1	8	1	Z
5	4	1	8	1	L10
5	5	1	8	1	Z
5	6	1	8	1	Z
5	7	1	8	1	N06
5	8	1	8	1	K10
6	1	1	8	1	N07
6	2	1	8	1	L02
6	3	1	8	1	M10
6	4	1	8	1	O03
6	5	1	8	1	N10
6	6	1	8	1	M04
6	7	1	8	1	M06
6	8	1	8	1	N05

					Figs VI.3.2.7-12
R1	R2	R3	R4	Plate	Loc
1	3	2	8	11	C11
1	4	2	8	11	F11
1	5	2	8	11	E11
1	6	2	8	11	D6
1	7	2	8	11	C5
1	8	2	8	11	E9
2	1	2	8	11	D11
2	2	2	8	11	C2
2	3	2	8	11	Z
2	4	2	8	11	F4
2	5	2	8	11	B3
2	6	2	8	11	B11
2	7	2	8	11	F9
2	8	2	8	11	B9
3	1	2	8	11	D8
3	2	2	8	11	F7
3	3	2	8	11	B7
3	4	2	8	11	B8
3	5	2	8	11	D10
3	6	2	8	11	E4
3	7	2	8	11	E7
3	8	2	8	11	Z
4	1	2	8	11	D9
4	2	2	8	11	C10
4	3	2	8	11	F3
4	4	2	8	11	E3
4	5	2	8	11	Z
4	6	2	8	11	Z
4	7	2	8	11	C9
4	8	2	8	11	Z
5	1	2	8	11	B2
5	2	2	8	11	B4
5	3	2	8	11	F10
5	4	2	8	11	E2
5	5	2	8	11	C4
5	6	2	8	11	D7
5	7	2	8	11	F2
5	8	2	8	11	E5
6	1	2	8	11	F6
6	2	2	8	11	C6
6	3	2	8	11	F8
6	4	2	8	11	D5
6	5	2	8	11	E10
6	6	2	8	11	E6
6	7	2	8	11	D3
6	8	2	8	11	B5

Table V .3.2.1

					Figs VI.3.2.13-18
R1	R2	R3	R4	Plate	Loc
1	3	3	8	11	D23
1	4	3	8	11	D21
1	5	3	8	11	E23
1	6	3	8	11	Z
1	7	3	8	11	F17
1	8	3	8	11	D18
2	1	3	8	11	E16
2	2	3	8	11	F15
2	3	3	8	11	Z
2	4	3	8	11	C21
2	5	3	8	11	C15
2	6	3	8	11	E20
2	7	3	8	11	G22
2	8	3	8	11	B14
3	1	3	8	11	C14
3	2	3	8	11	B18
3	3	3	8	11	F23
3	4	3	8	11	C19
3	5	3	8	11	D20
3	6	3	8	11	C23
3	7	3	8	11	C16
3	8	3	8	11	F19
4	1	3	8	11	B17
4	2	3	8	11	G17
4	3	3	8	11	Z
4	4	3	8	11	F18
4	5	3	8	11	G18
4	6	3	8	11	E22
4	7	3	8	11	H16
4	8	3	8	11	G15
5	1	3	8	11	G21
5	2	3	8	11	F20
5	3	3	8	11	G20
5	4	3	8	11	G19
5	5	3	8	11	G23
5	6	3	8	11	D15
5	7	3	8	11	B20
5	8	3	8	11	B23
6	1	3	8	11	D19
6	2	3	8	11	C22
6	3	3	8	11	H14
6	4	3	8	11	B22
6	5	3	8	11	D16
6	6	3	8	11	B16
6	7	3	8	11	E15
6	8	3	8	11	H15

					Figs VI.3.2.19-24
R1	R2	R3	R4	Plate	Loc
1	3	4	8	1	L17
1	4	4	8	1	M23
1	5	4	8	1	L22
1	6	4	8	1	L16
1	7	4	8	1	N17
1	8	4	8	1	O15
2	1	4	8	1	K16
2	2	4	8	1	K18
2	3	4	8	1	L15
2	4	4	8	1	N15
2	5	4	8	1	O16
2	6	4	8	1	K17
2	7	4	8	1	L21
2	8	4	8	1	K20
3	1	4	8	1	Z
3	2	4	8	1	Z
3	3	4	8	1	N16
3	4	4	8	1	M16
3	5	4	8	1	Z
3	6	4	8	1	M14
3	7	4	8	1	N14
3	8	4	8	1	Z
4	1	4	8	1	N21
4	2	4	8	1	L14
4	3	4	8	1	L23
4	4	4	8	1	O17
4	5	4	8	1	O18
4	6	4	8	1	K14
4	7	4	8	1	N23
4	8	4	8	1	M20
5	1	4	8	1	M18
5	2	4	8	1	K15
5	3	4	8	1	K19
5	4	4	8	1	L18
5	5	4	8	1	M17
5	6	4	8	1	L19
5	7	4	8	1	M19
5	8	4	8	1	K22
6	1	4	8	1	M21
6	2	4	8	1	K21
6	3	4	8	1	M15
6	4	4	8	1	M22
6	5	4	8	1	Z
6	6	4	8	1	K23
6	7	4	8	1	L20
6	8	4	8	1	Z

Table V .3.2.2 552

					Figs VI.3.2.25-30
R1	R2	R3	R4	Plate	Loc
1	3	5	8	15	Z
1	4	5	8	15	B2
1	5	5	8	15	B7
1	6	5	8	15	Z
1	7	5	8	15	B5
1	8	5	8	15	F9
2	1	5	8	15	B3
2	2	5	8	15	D9
2	3	5	8	15	E6
2	4	5	8	15	B6
2	5	5	8	15	F5
2	6	5	8	15	C6
2	7	5	8	15	F7
2	8	5	8	15	F6
3	1	5	8	15	Z
3	2	5	8	15	C10
3	3	5	8	15	E8
3	4	5	8	15	D3
3	5	5	8	15	D4
3	6	5	8	15	F4
3	7	5	8	15	Z
3	8	5	8	15	E9
4	1	5	8	15	D6
4	2	5	8	15	Z
4	3	5	8	15	B9
4	4	5	8	15	D11
4	5	5	8	15	D7
4	6	5	8	15	E2
4	7	5	8	15	C3
4	8	5	8	15	C8
5	1	5	8	15	B10
5	2	5	8	15	B11
5	3	5	8	15	C5
5	4	5	8	15	Z
5	5	5	8	15	C4
5	6	5	8	15	D5
5	7	5	8	15	B8
5	8	5	8	15	F3
6	1	5	8	15	Z
6	2	5	8	15	C11
6	3	5	8	15	E3
6	4	5	8	15	C9
6	5	5	8	15	E4
6	6	5	8	15	Z
6	7	5	8	15	B4
6	8	5	8	15	D2

					Figs VI.3.2.31-36
R1	R2	R3	R4	Plate	Loc
1	3	6	8	15	C20
1	4	6	8	15	D18
1	5	6	8	15	B19
1	6	6	8	15	F20
1	7	6	8	15	E19
1	8	6	8	15	E17
2	1	6	8	15	B16
2	2	6	8	15	F15
2	3	6	8	15	E14
2	4	6	8	15	E16
2	5	6	8	15	E22
2	6	6	8	15	C22
2	7	6	8	15	E23
2	8	6	8	15	B15
3	1	6	8	15	B22
3	2	6	8	15	D23
3	3	6	8	15	F14
3	4	6	8	15	B18
3	5	6	8	15	E18
3	6	6	8	15	B17
3	7	6	8	15	B21
3	8	6	8	15	D20
4	1	6	8	15	B20
4	2	6	8	15	Z
4	3	6	8	15	C17
4	4	6	8	15	F19
4	5	6	8	15	F16
4	6	6	8	15	D19
4	7	6	8	15	C23
4	8	6	8	15	D15
5	1	6	8	15	C19
5	2	6	8	15	B14
5	3	6	8	15	C14
5	4	6	8	15	E21
5	5	6	8	15	E15
5	6	6	8	15	F18
5	7	6	8	15	F17
5	8	6	8	15	D17
6	1	6	8	15	C15
6	2	6	8	15	C16
6	3	6	8	15	E20
6	4	6	8	15	D14
6	5	6	8	15	B23
6	6	6	8	15	C18
6	7	6	8	15	D16
6	8	6	8	15	C21

Table V .3.2.3

					Figs VI.3.2.37-42
R1	R2	R3	R4	Plate	Loc
1	3	7	8	1	D07
1	4	7	8	1	C06
1	5	7	8	1	F03
1	6	7	8	1	E07
1	7	7	8	1	E10
1	8	7	8	1	C03
2	1	7	8	1	D11
2	2	7	8	1	Z
2	3	7	8	1	Z
2	4	7	8	1	E09
2	5	7	8	1	Z
2	6	7	8	1	E05
2	7	7	8	1	D05
2	8	7	8	1	D06
3	1	7	8	1	E11
3	2	7	8	1	Z
3	3	7	8	1	B06
3	4	7	8	1	C02
3	5	7	8	1	Z
3	6	7	8	1	E04
3	7	7	8	1	D04
3	8	7	8	1	B08
4	1	7	8	1	B07
4	2	7	8	1	E08
4	3	7	8	1	D08
4	4	7	8	1	D09
4	5	7	8	1	F04
4	6	7	8	1	C07
4	7	7	8	1	D10
4	8	7	8	1	F02
5	1	7	8	1	B04
5	2	7	8	1	F06
5	3	7	8	1	C04
5	4	7	8	1	C05
5	5	7	8	1	C08
5	6	7	8	1	E03
5	7	7	8	1	D02
5	8	7	8	1	C11
6	1	7	8	1	B09
6	2	7	8	1	B02
6	3	7	8	1	B03
6	4	7	8	1	E02
6	5	7	8	1	C10
6	6	7	8	1	B10
6	7	7	8	1	B11

Table V .3.2.4

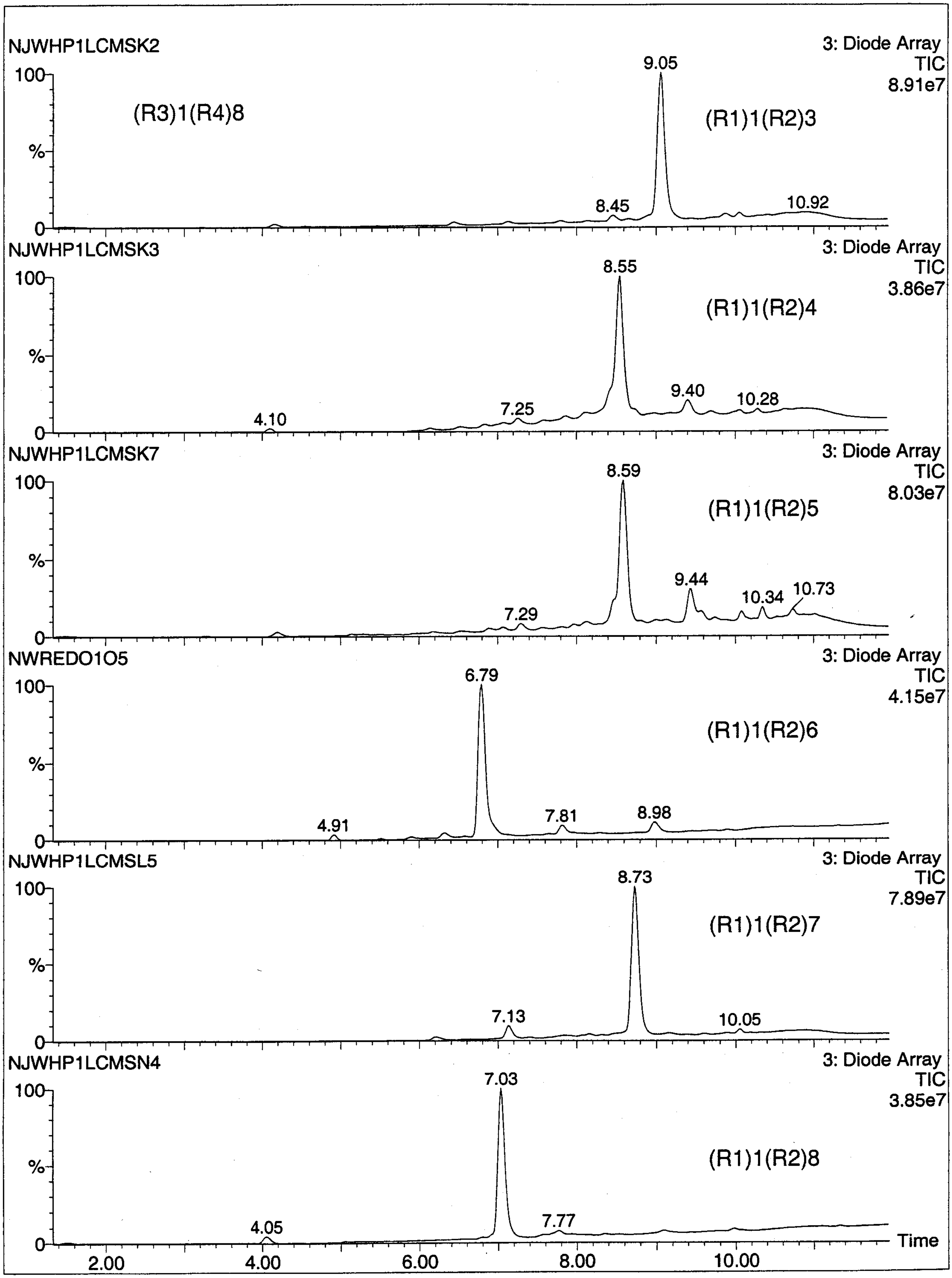


Figure V .3.2.1 555

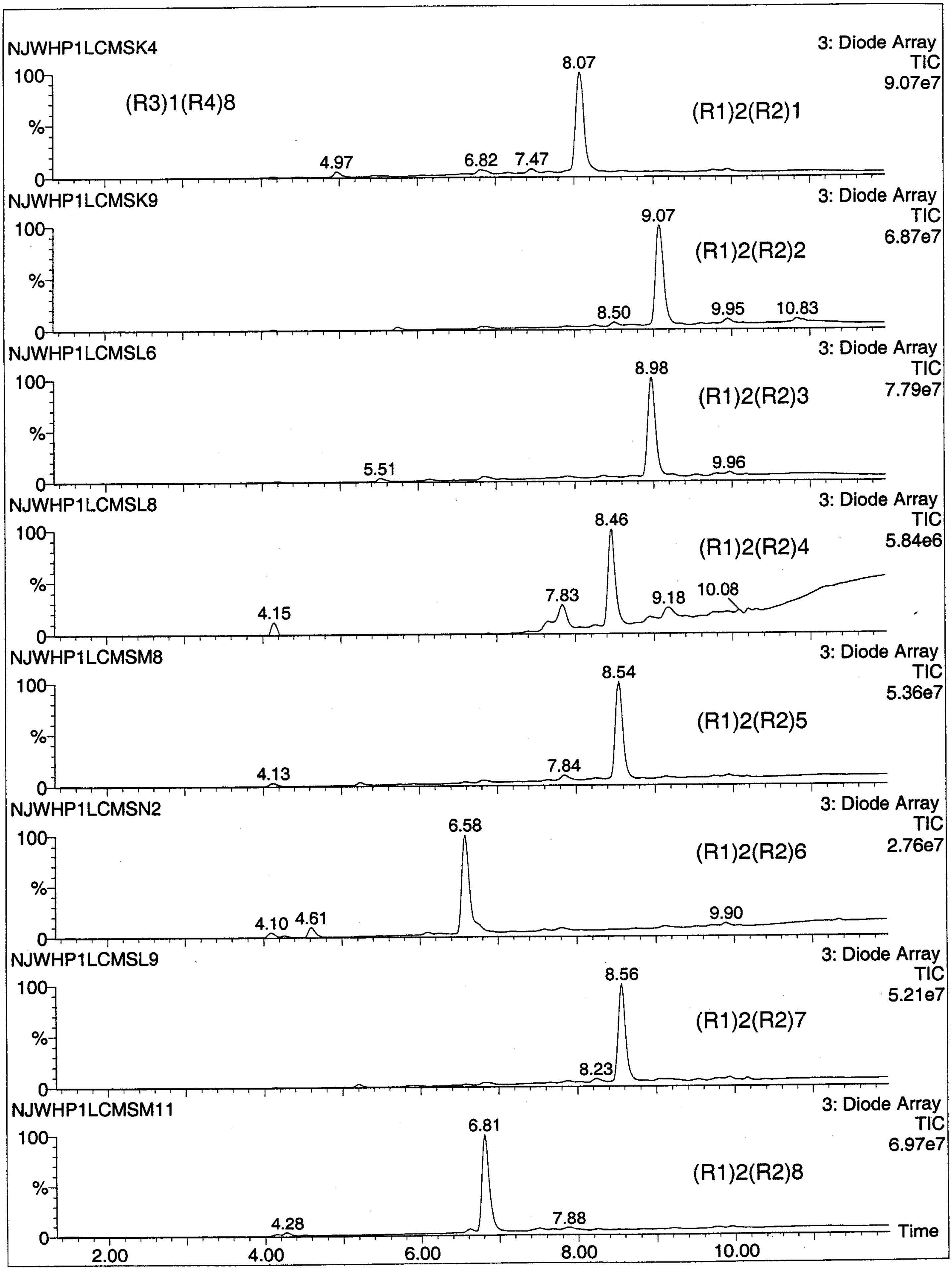


Figure V .3.2.2 556

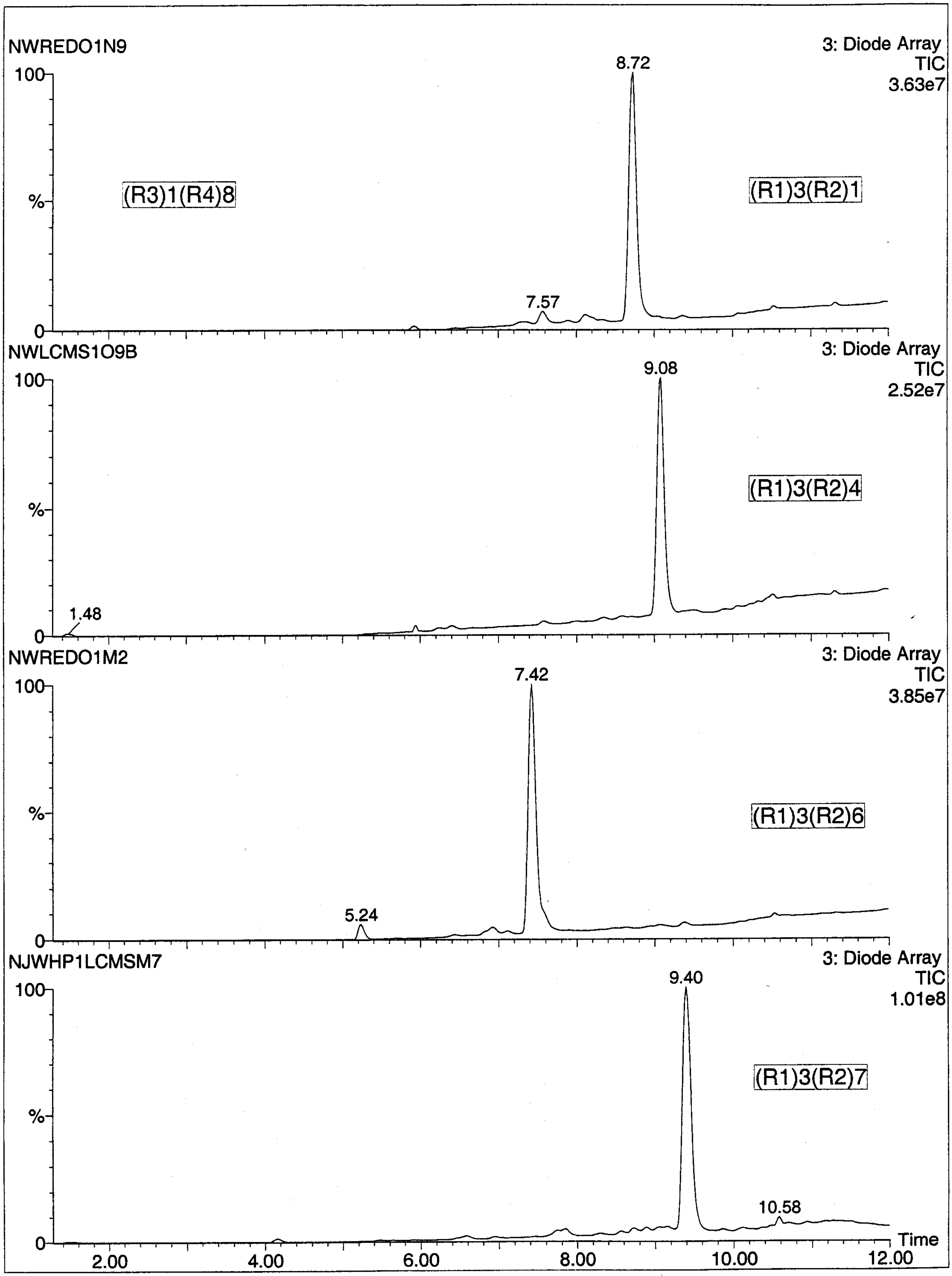


Figure V .3.2.3 557

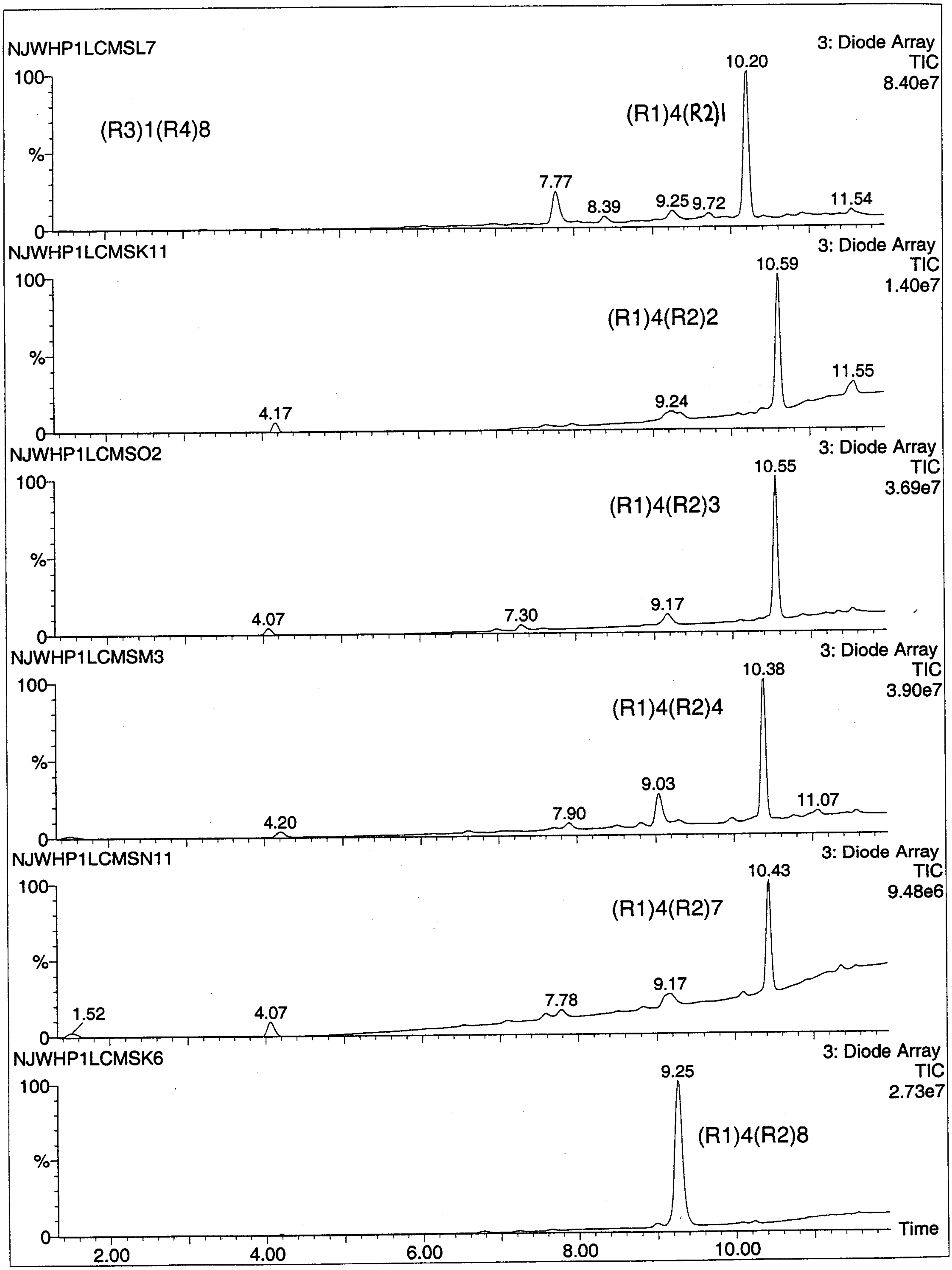


Figure V .3.2.4 S58

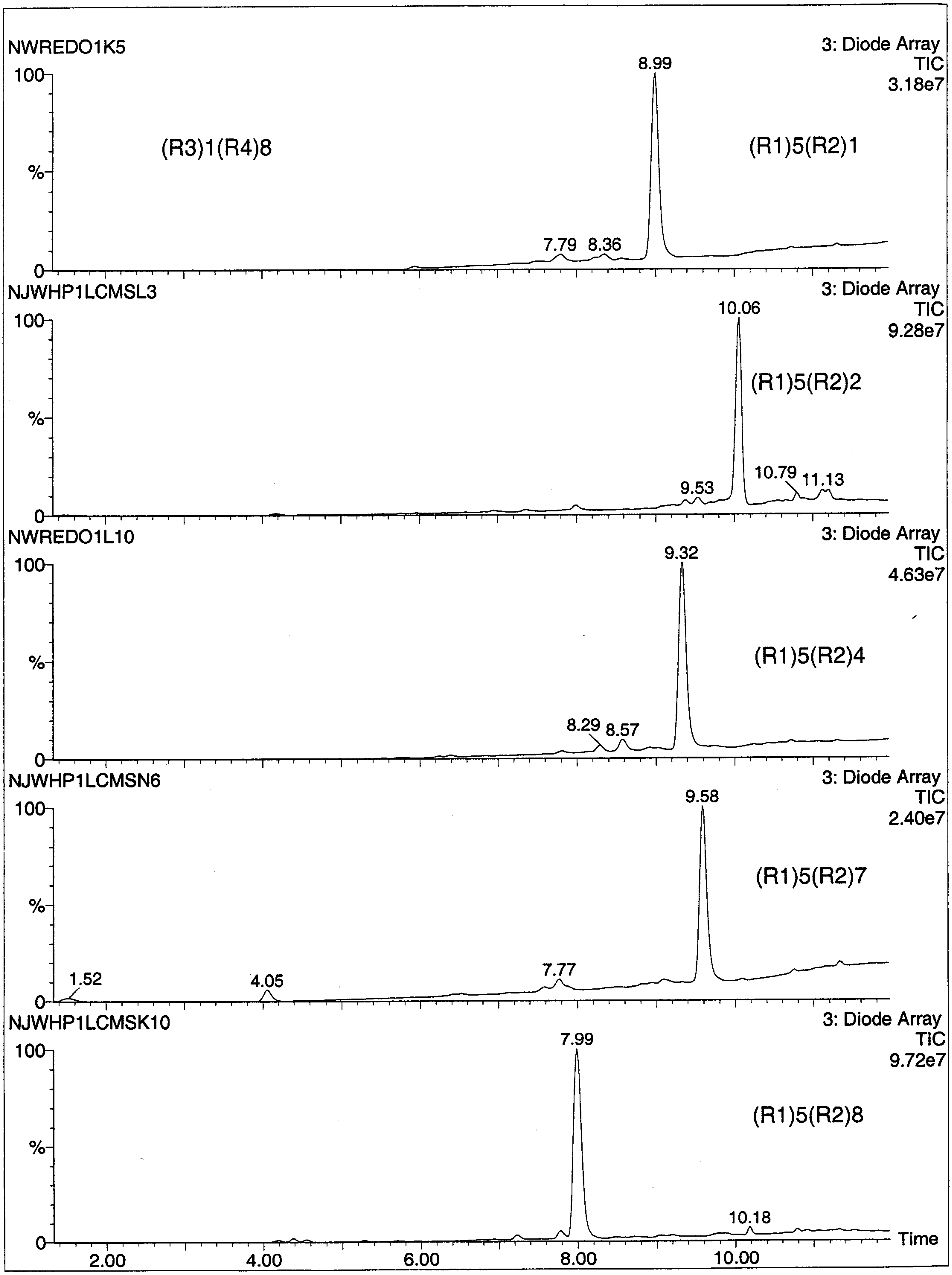


Figure V .3.2.5 559

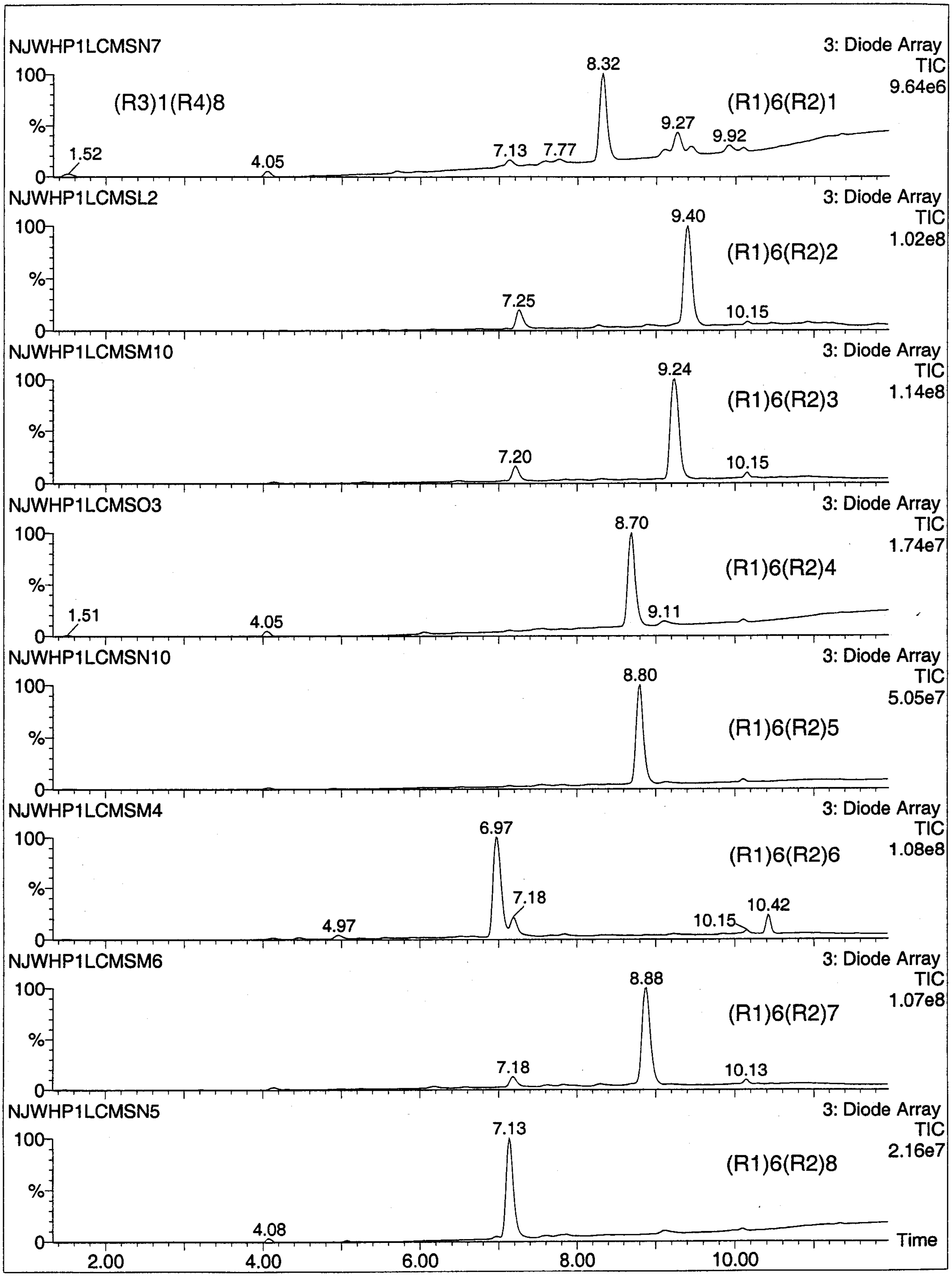


Figure V .3.2.6 560

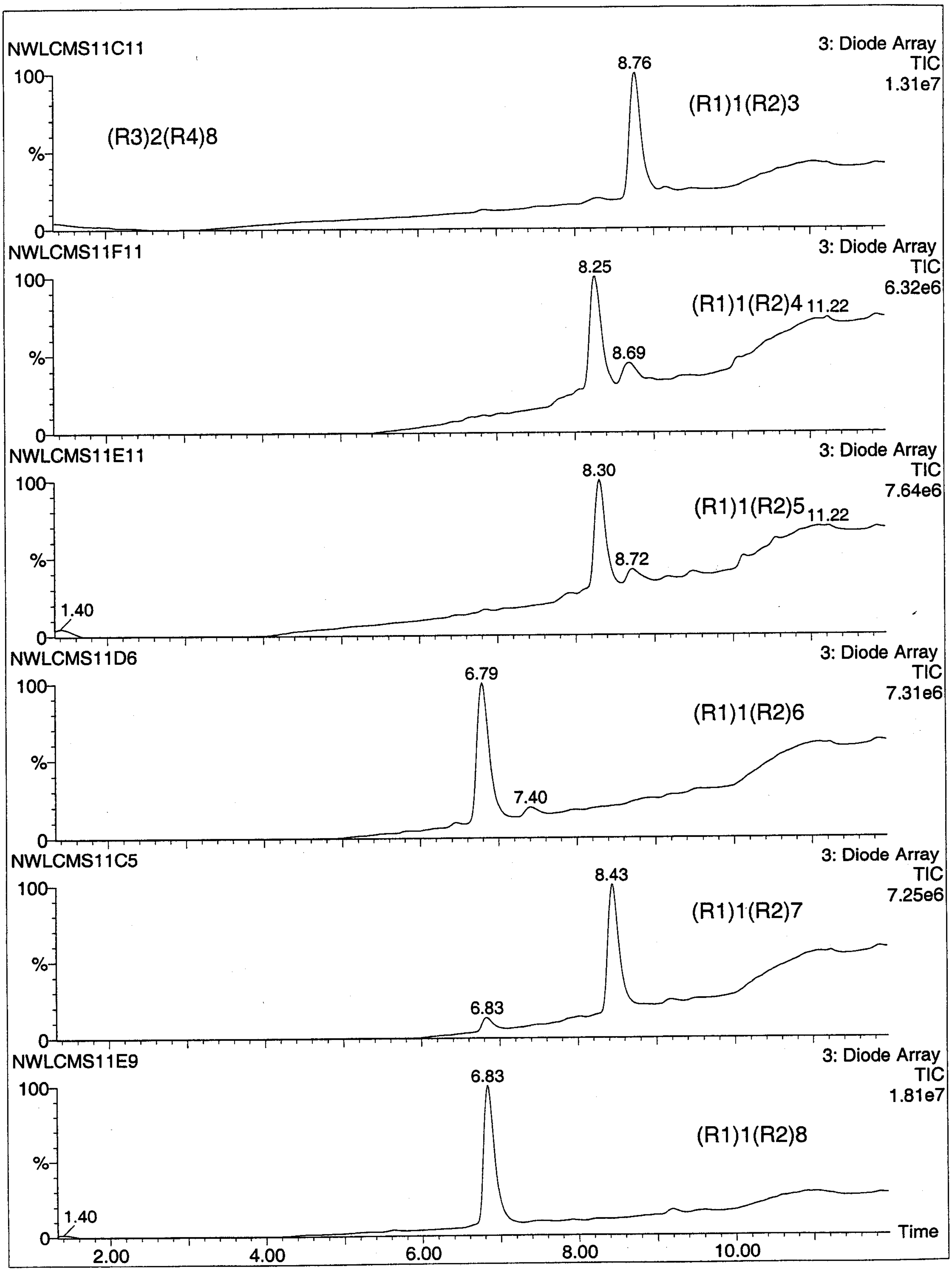


Figure V .3.2.7 S61

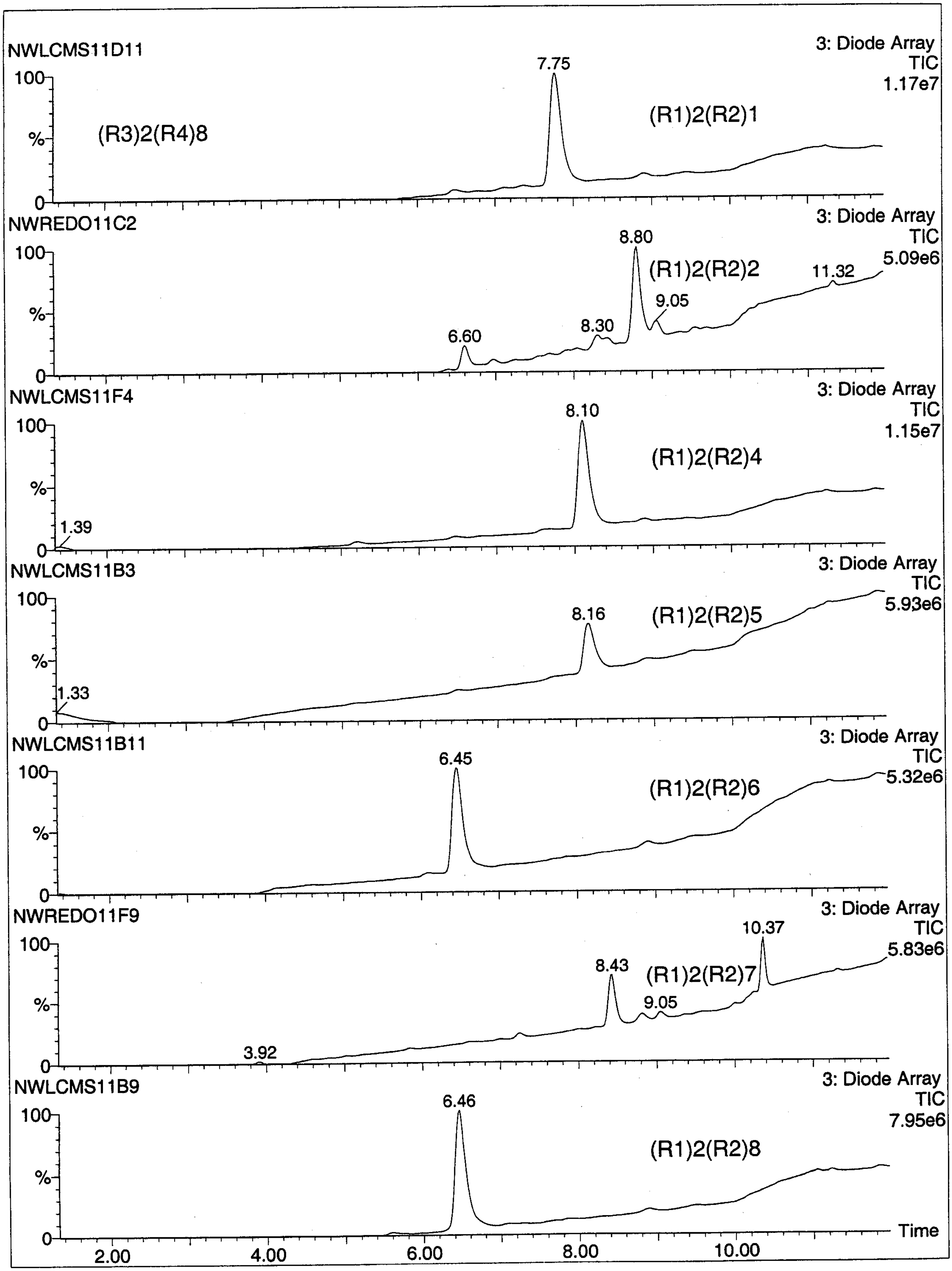


Figure V .3.2.8 S62

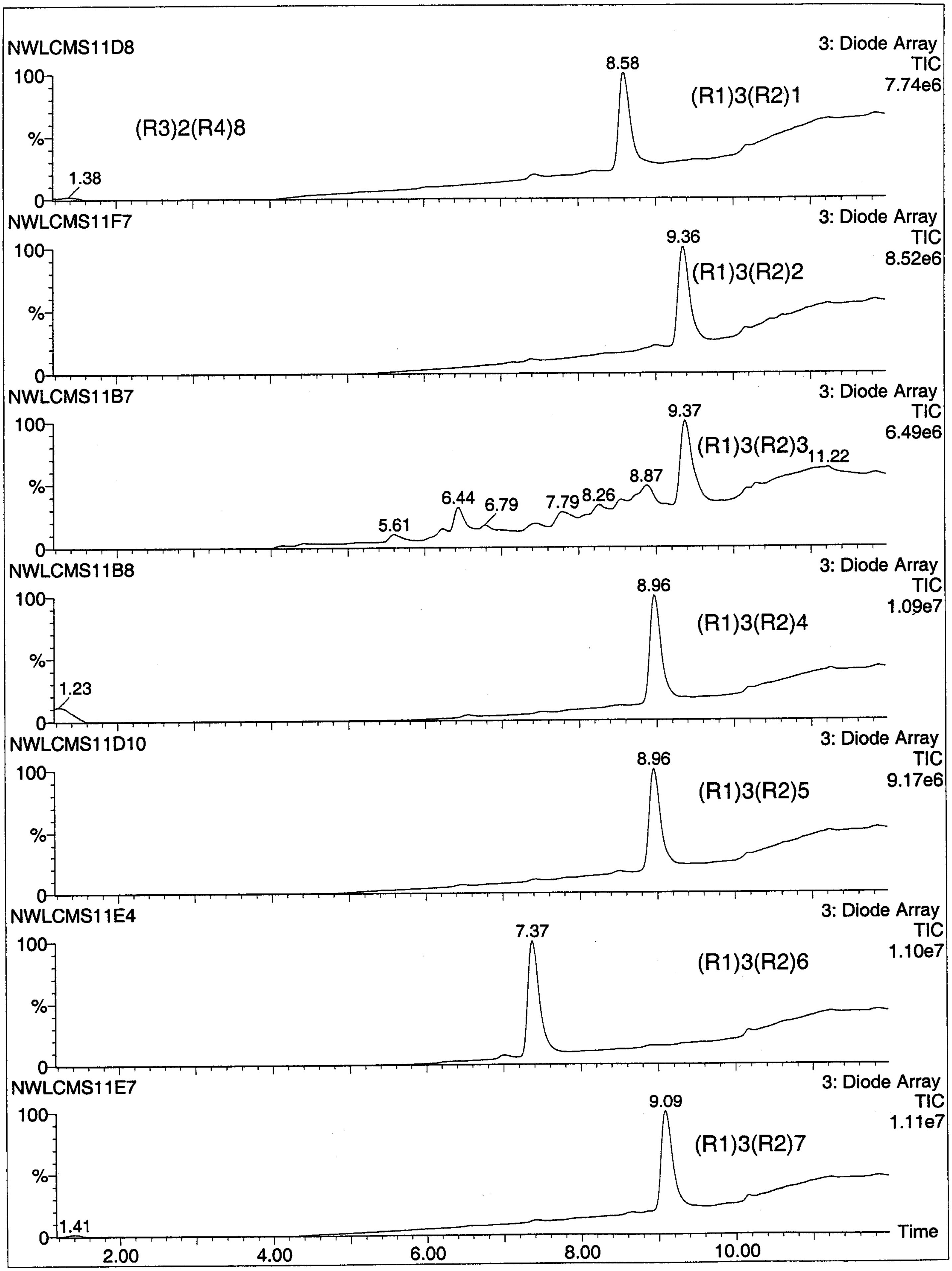


Figure V .3.2.9 S63

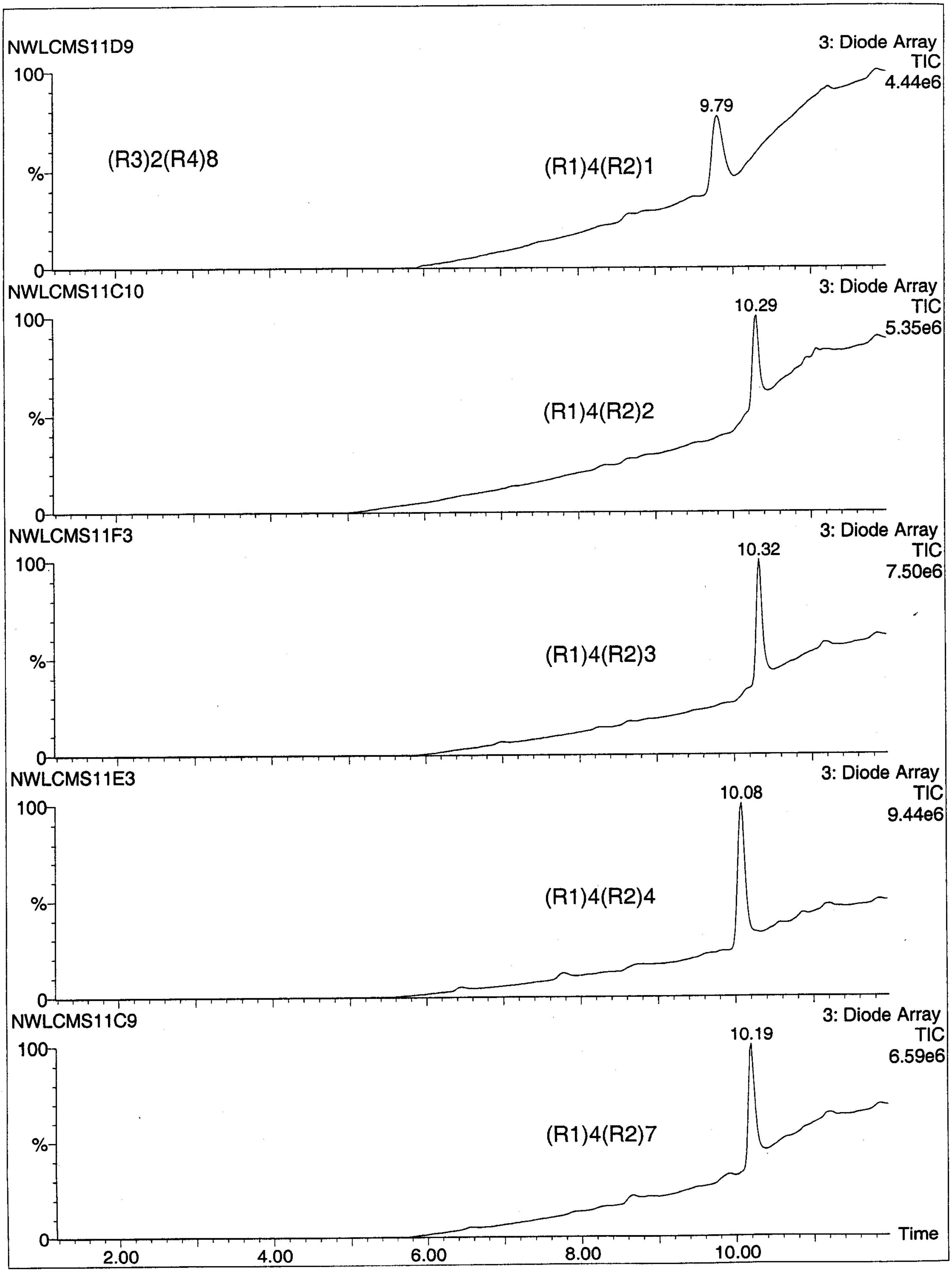


Figure V .3.2.10

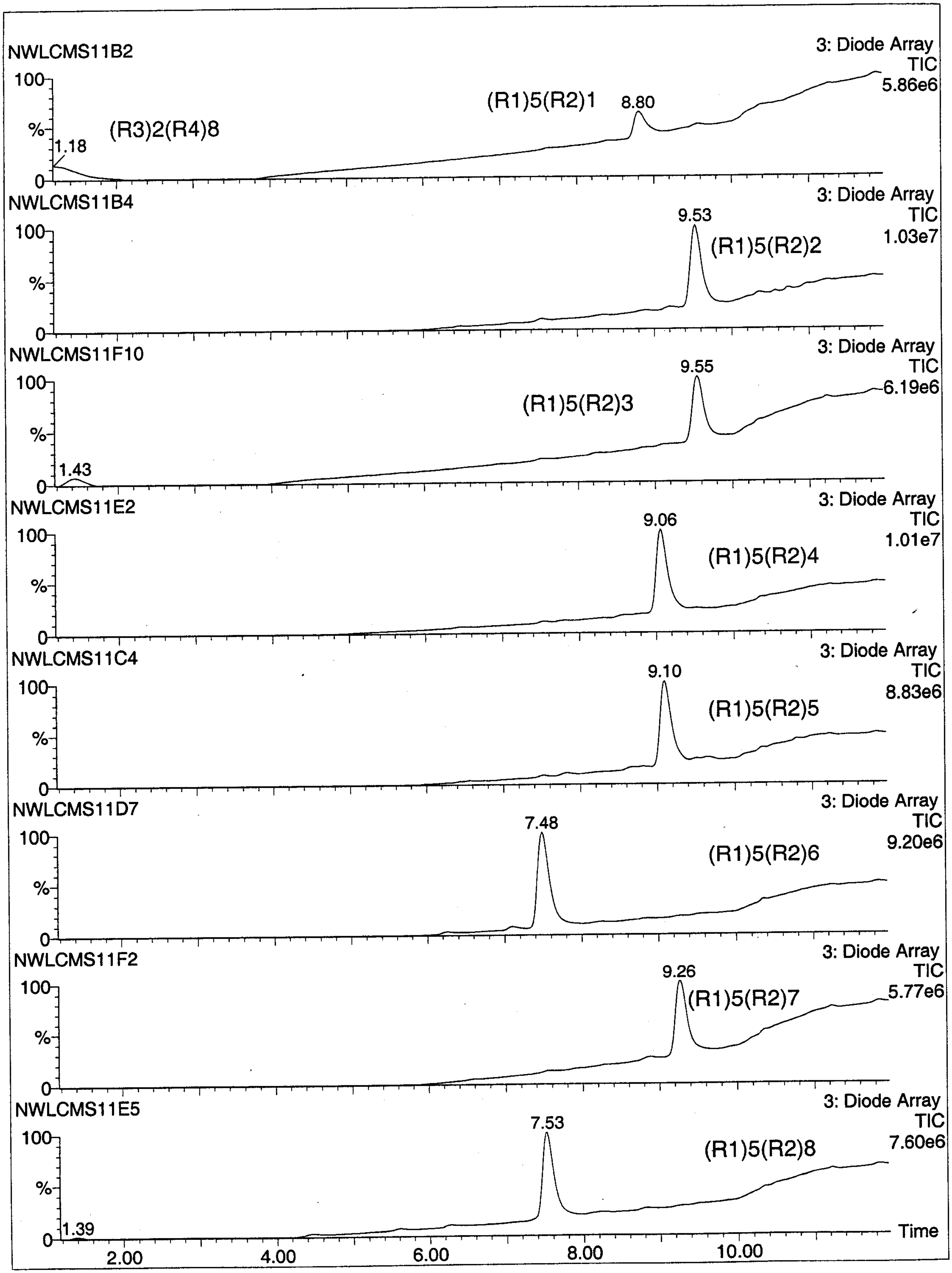


Figure V .3.2.11

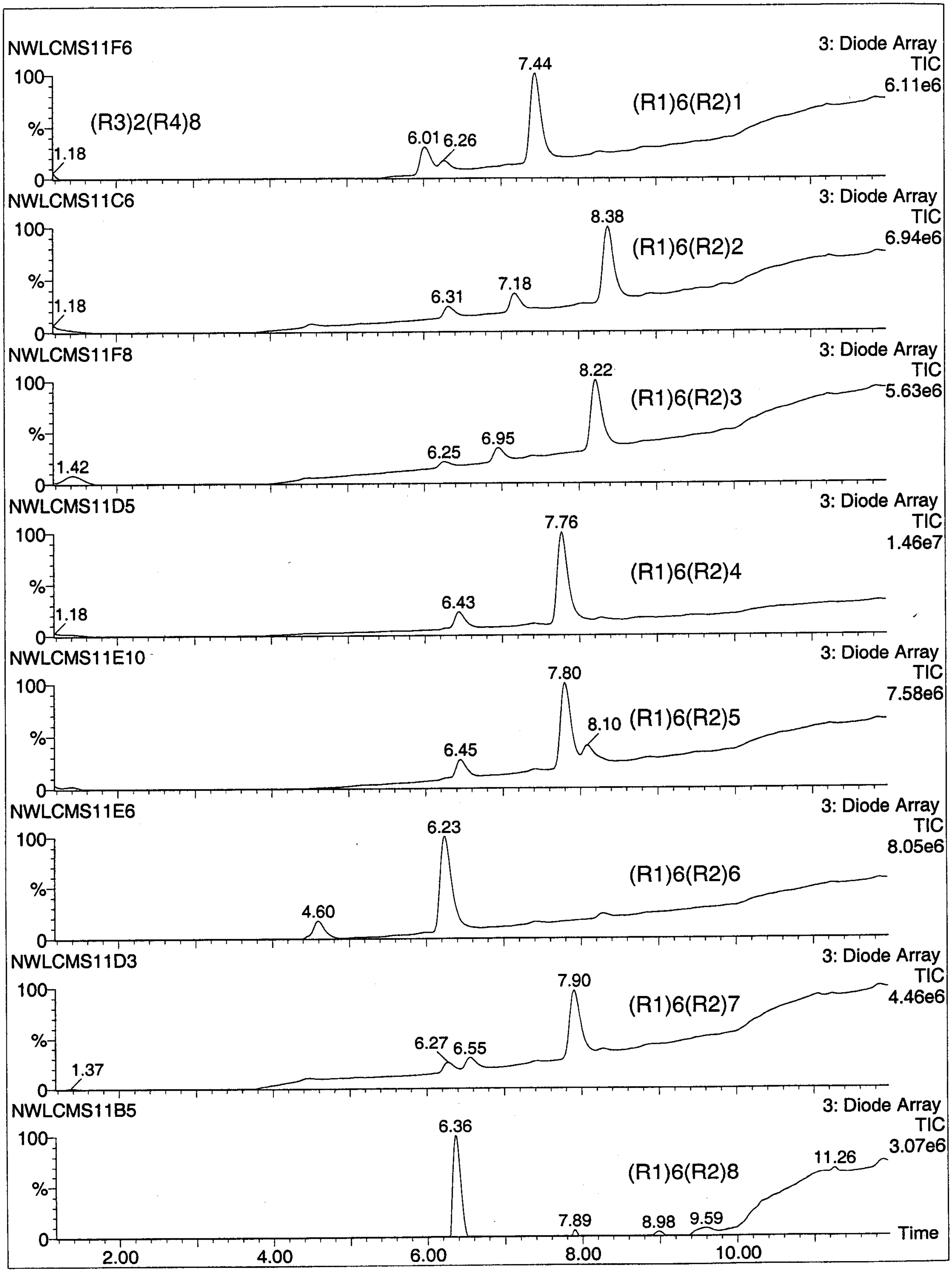


Figure V .3.2.12

S66

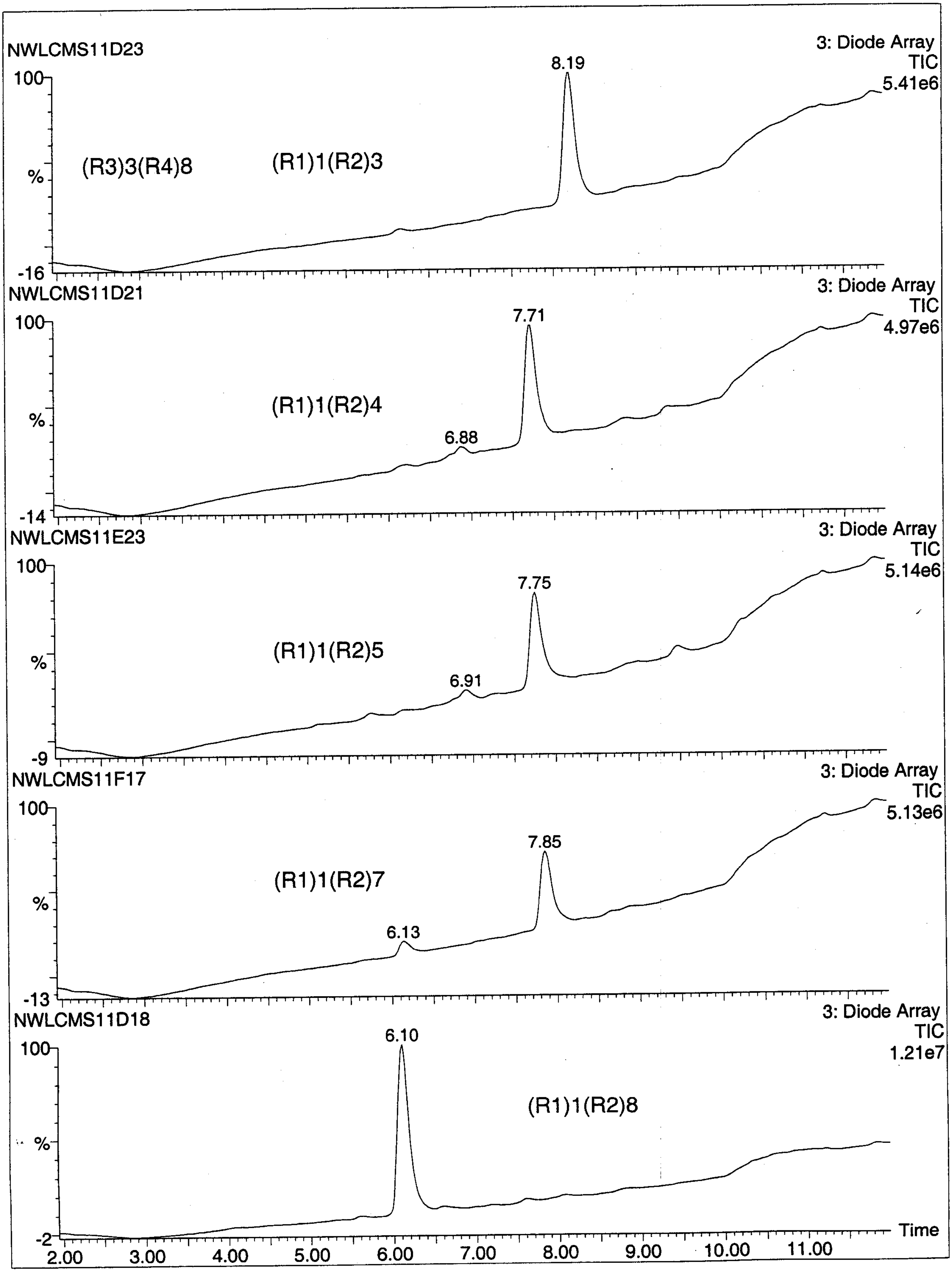


Figure V .3.2.13 567

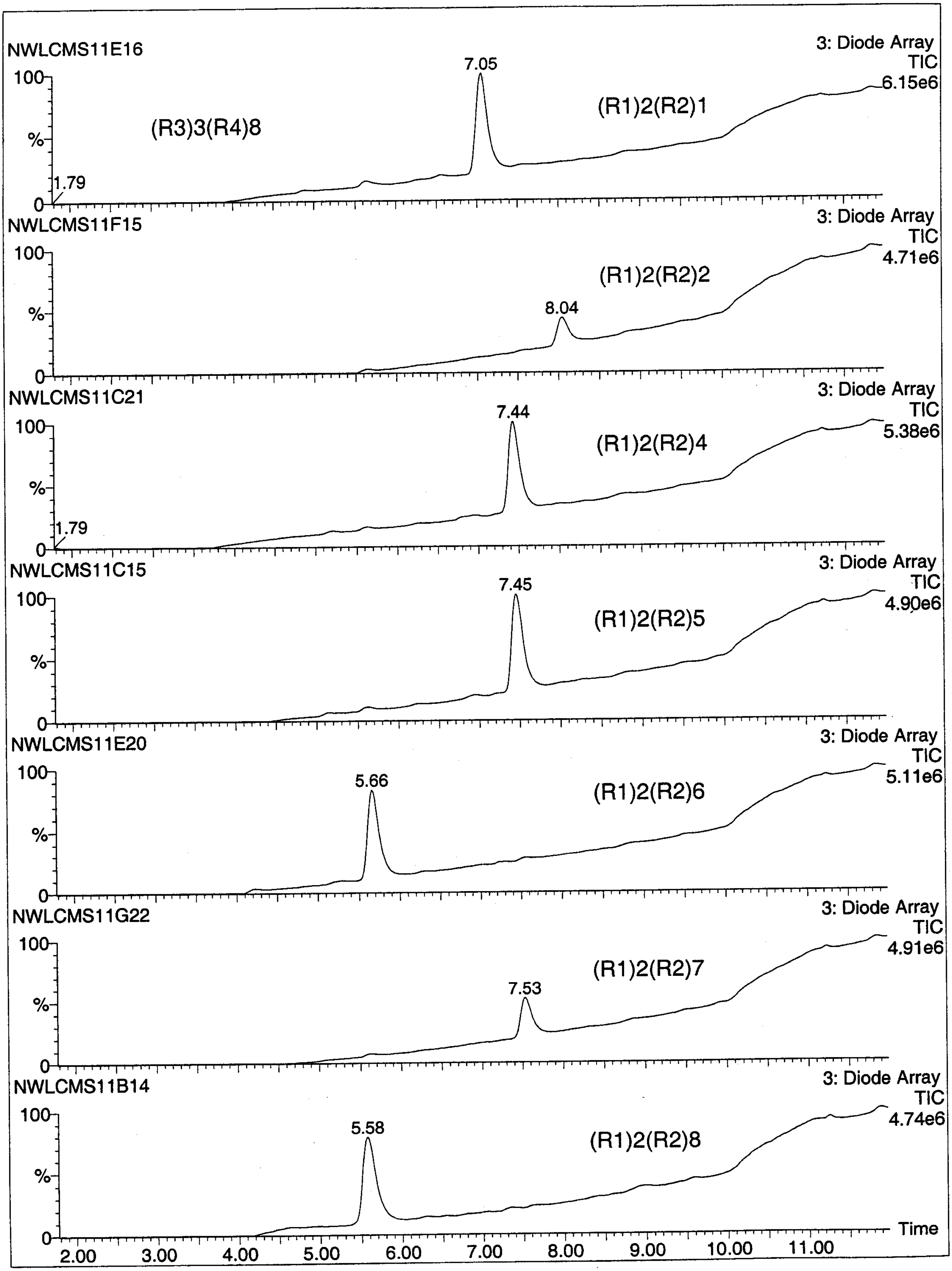


Figure V .3.2.14

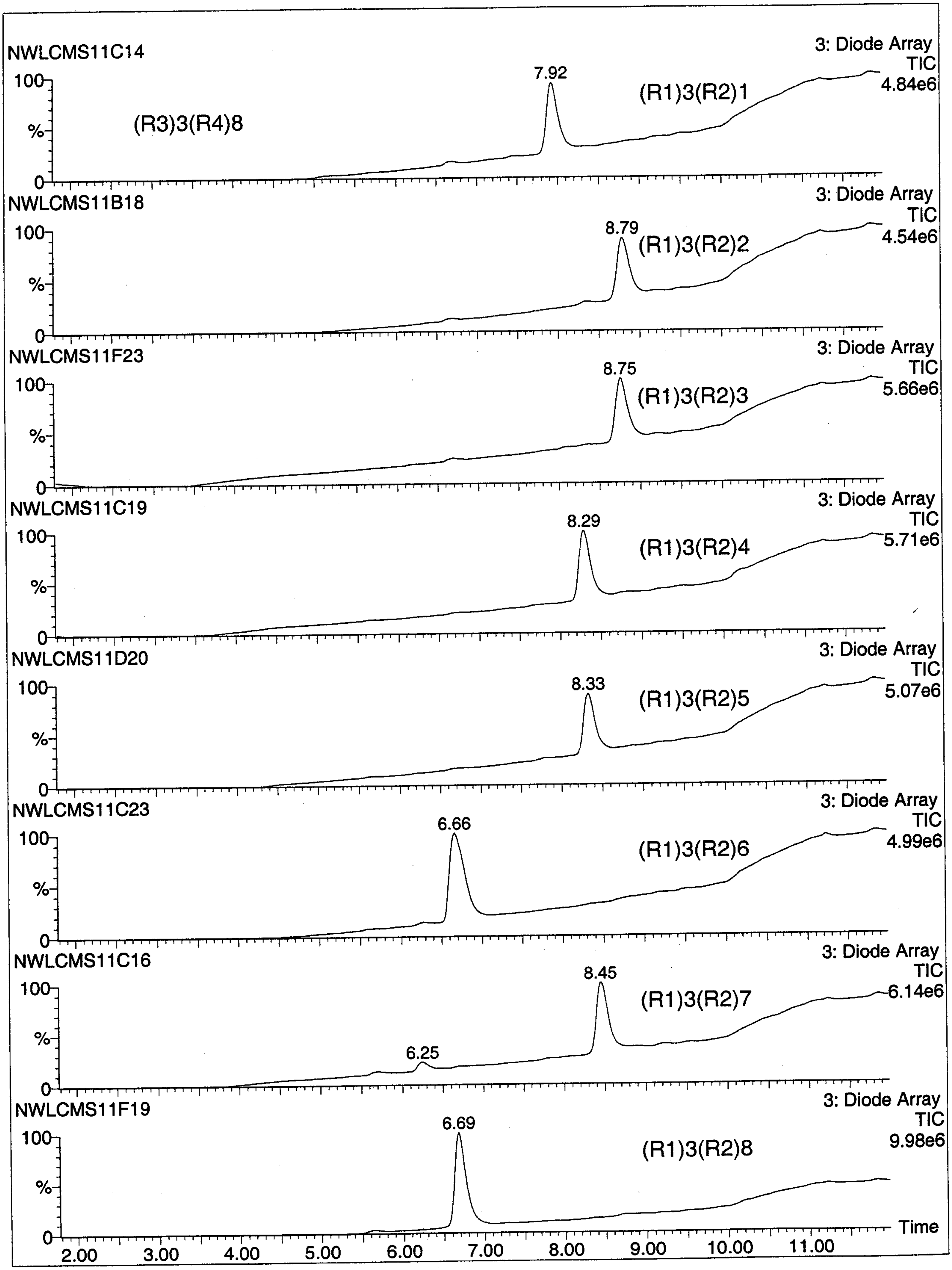


Figure V .3.2.15 S69

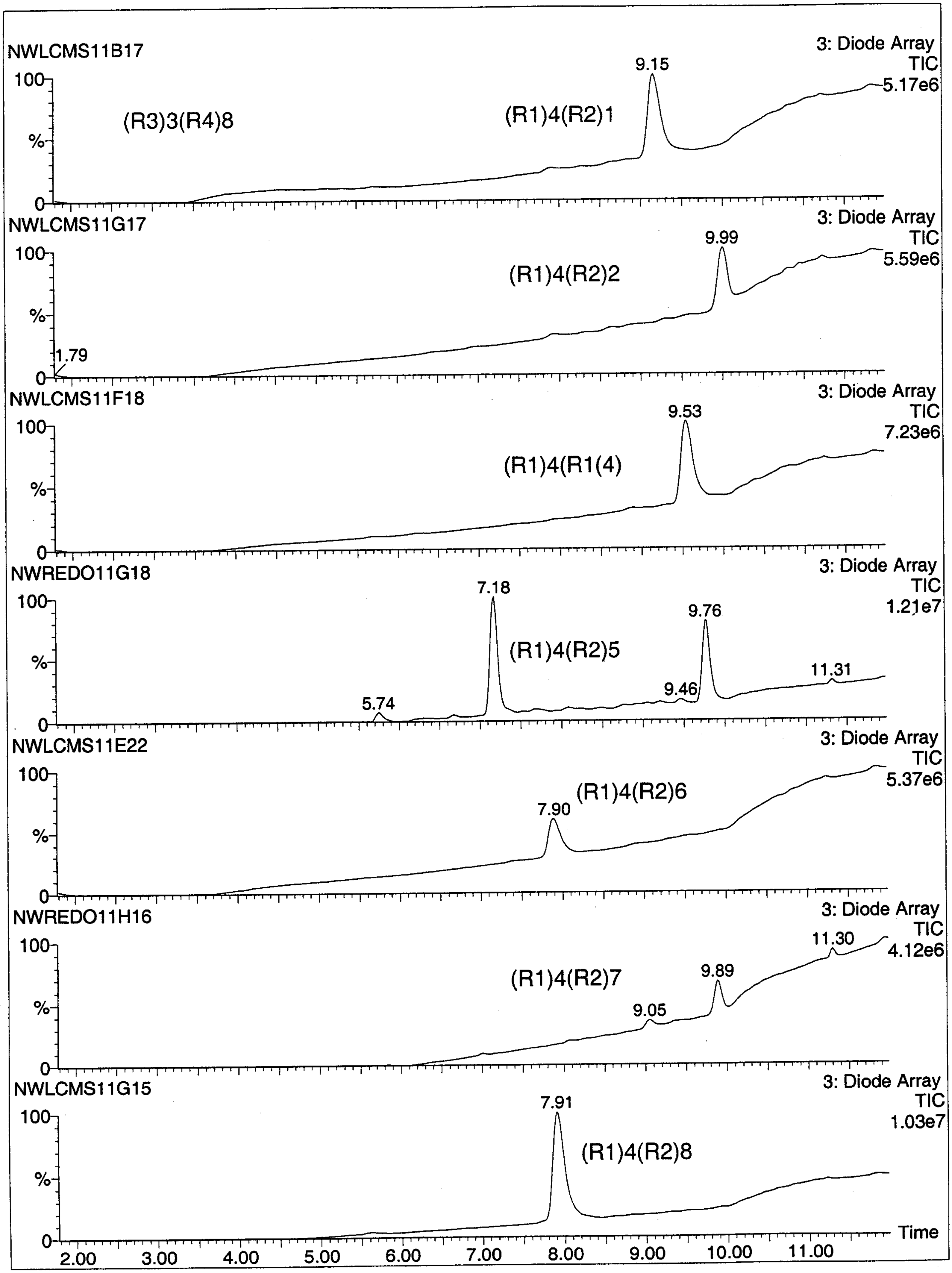


Figure V .3.2.16 570

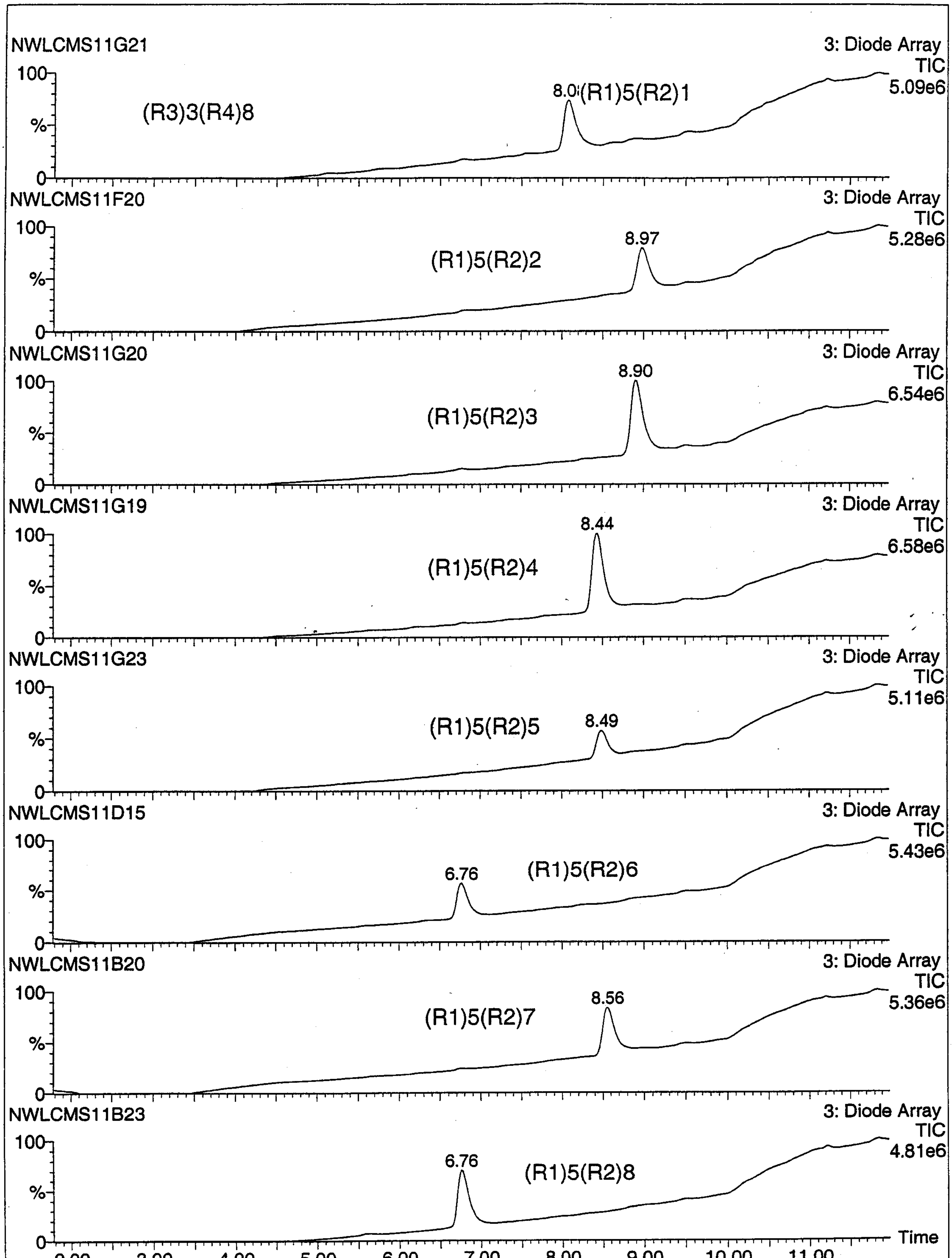


Figure V .3.2.17 S71

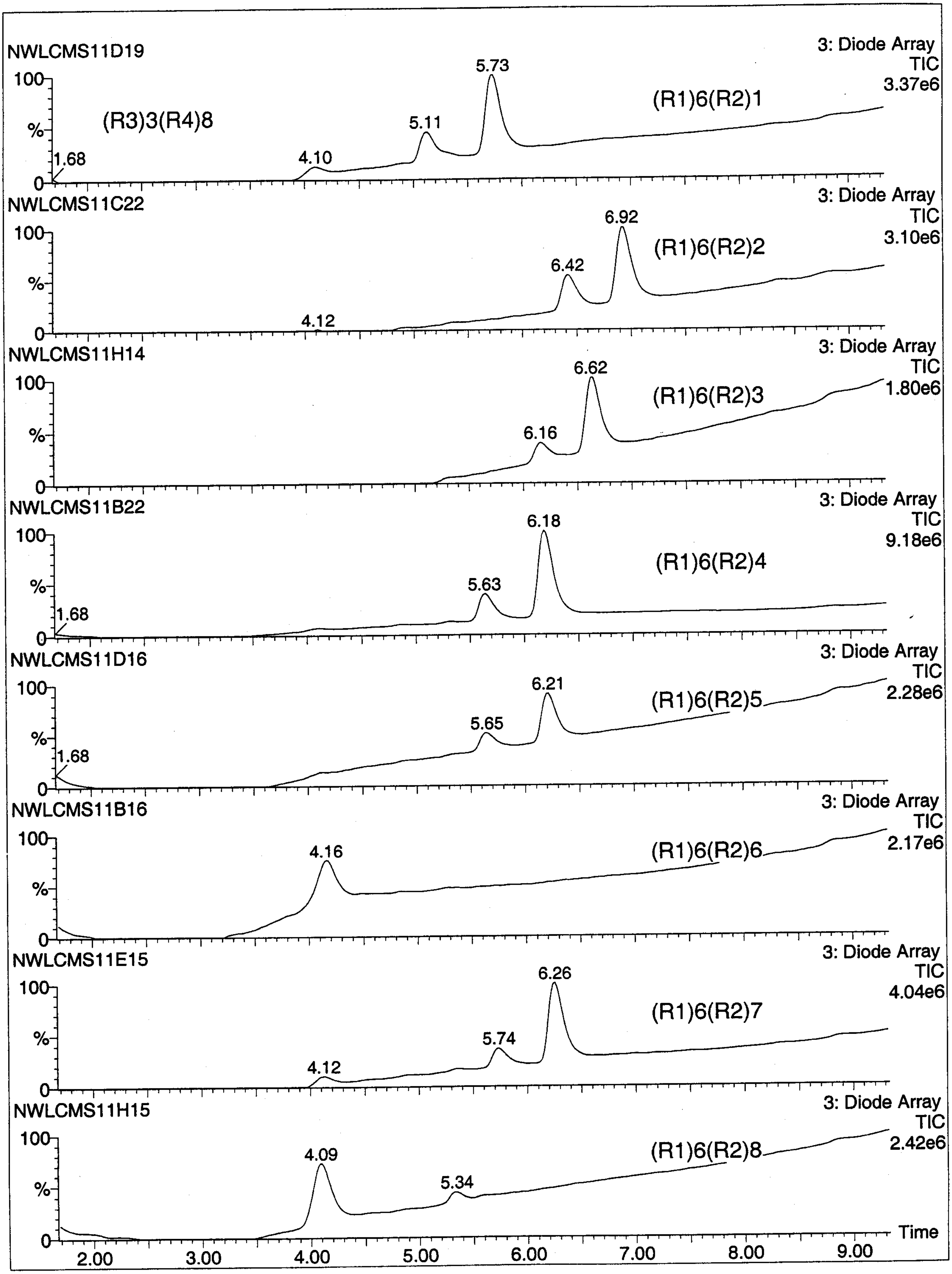


Figure V .3.2.18 S72

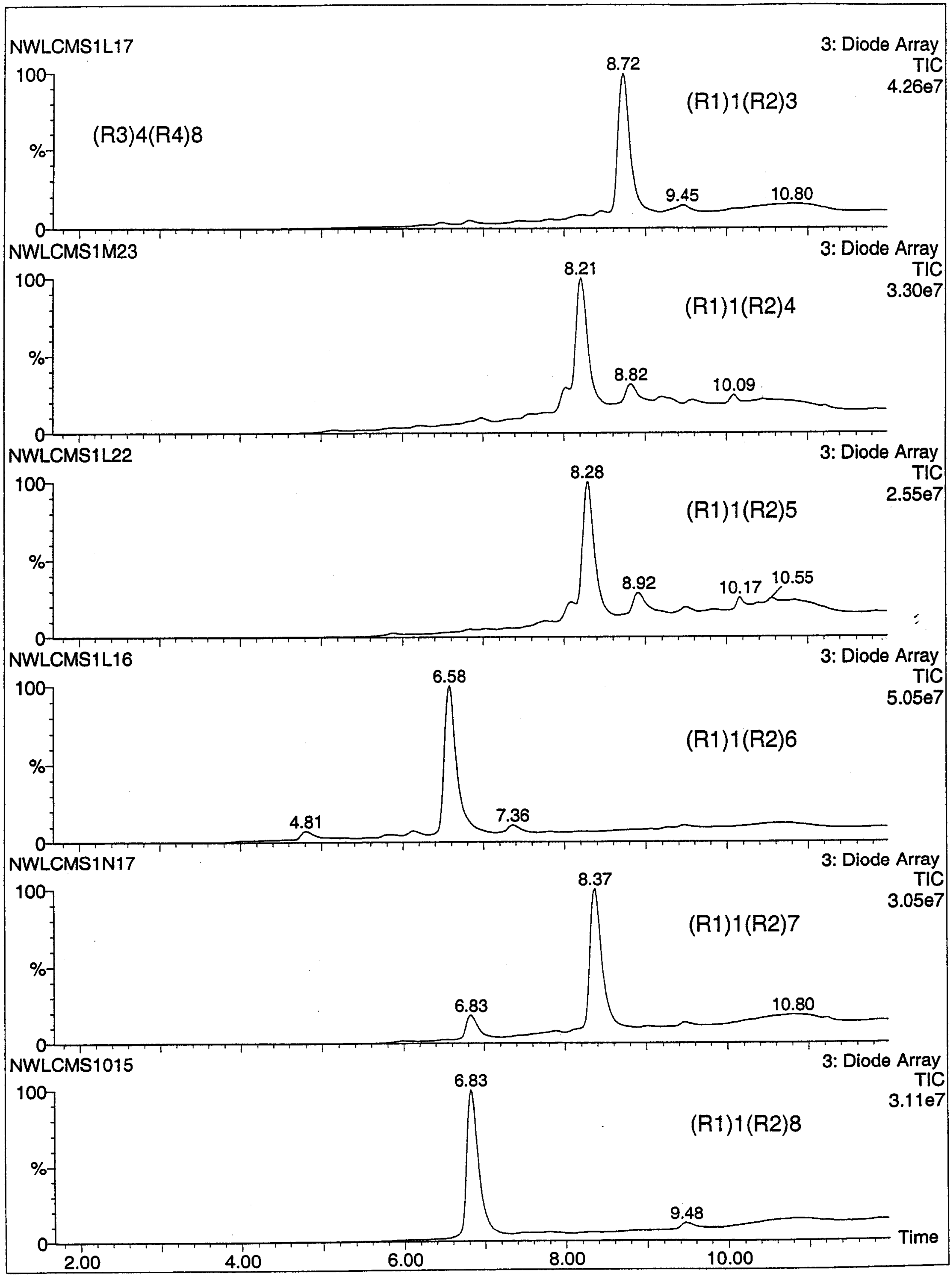


Figure V .3.2.19 S73

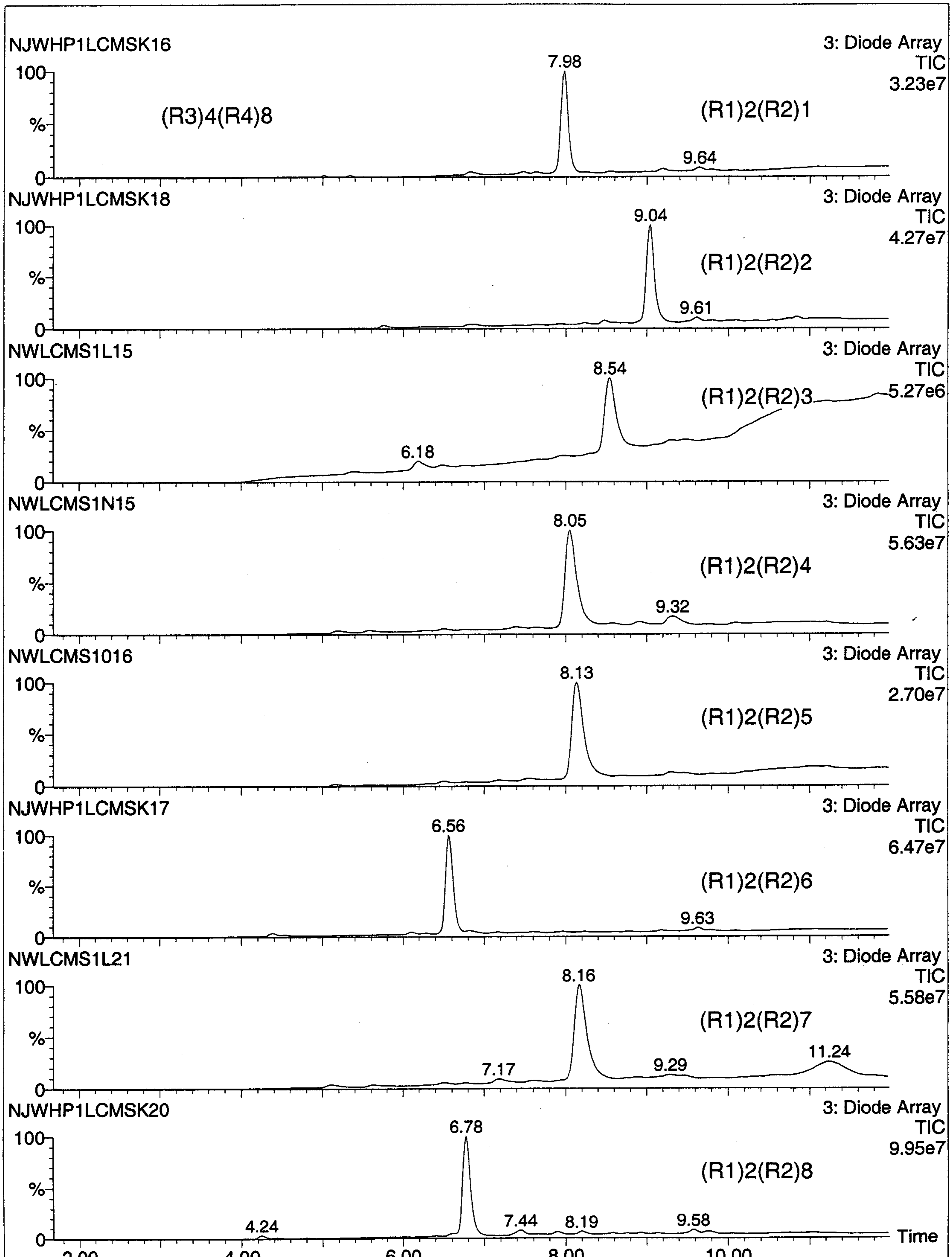


Figure V .3.2.20 S74

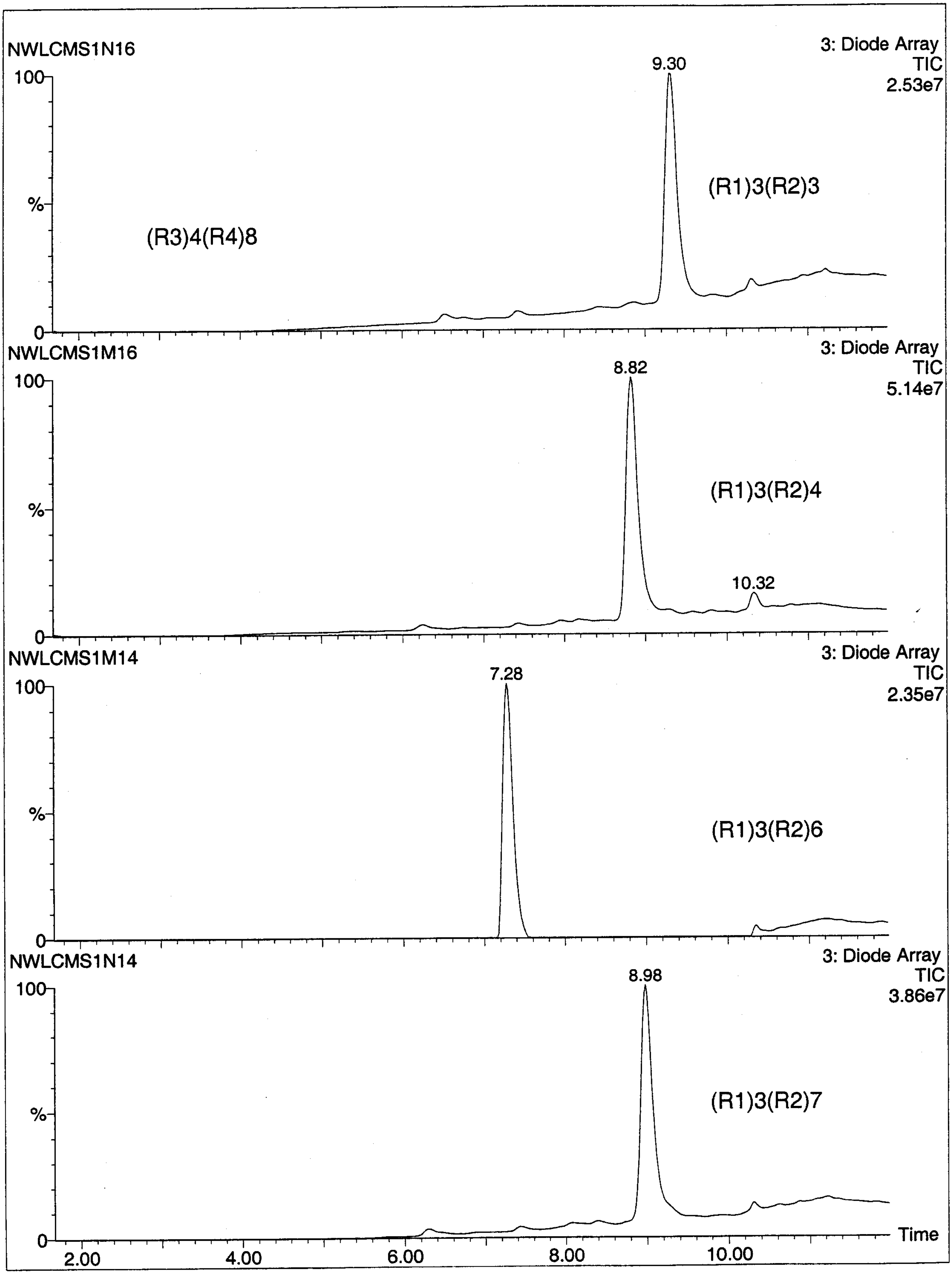


Figure V .3.2.21 S75

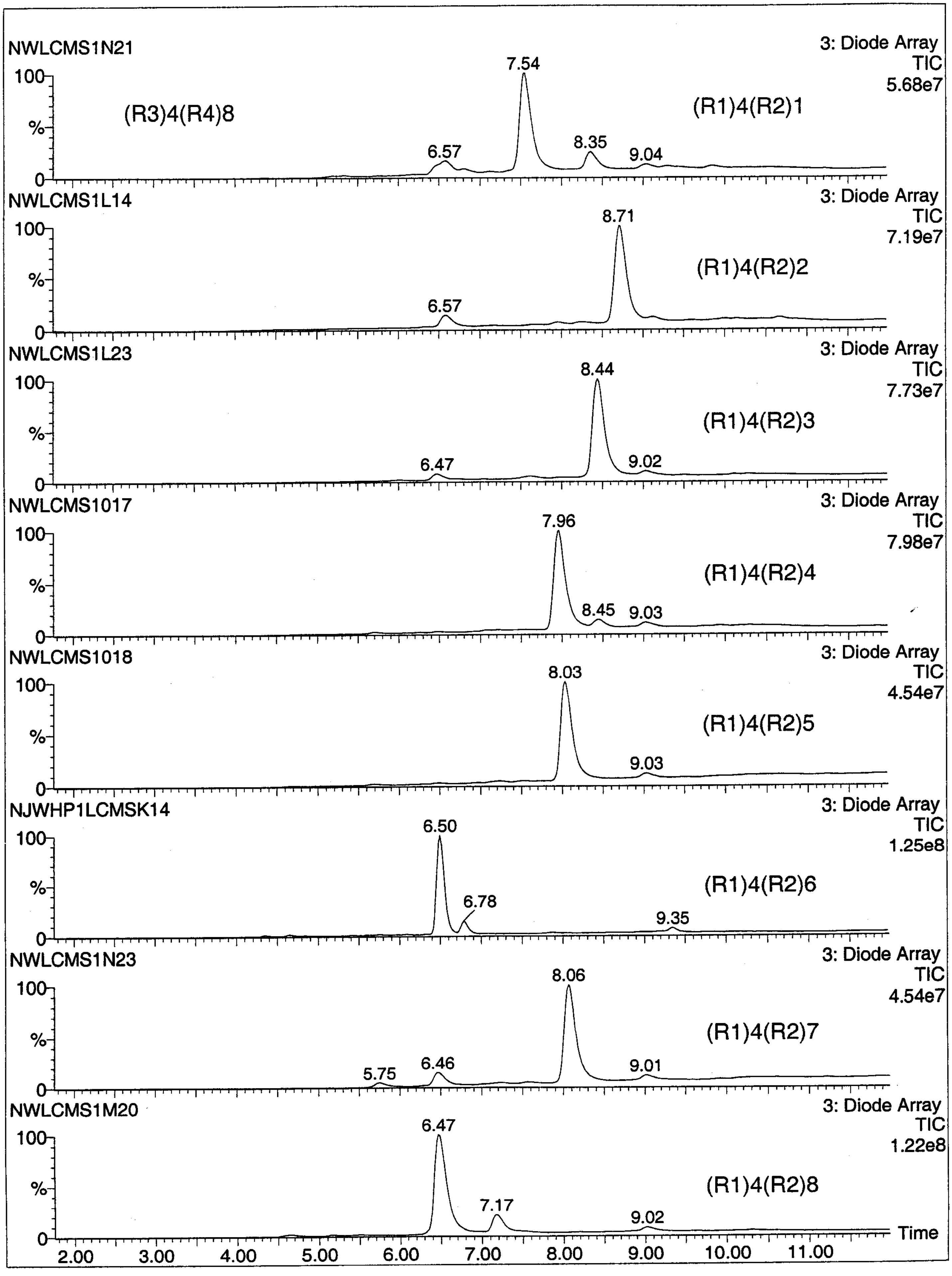


Figure VI.3.2.22

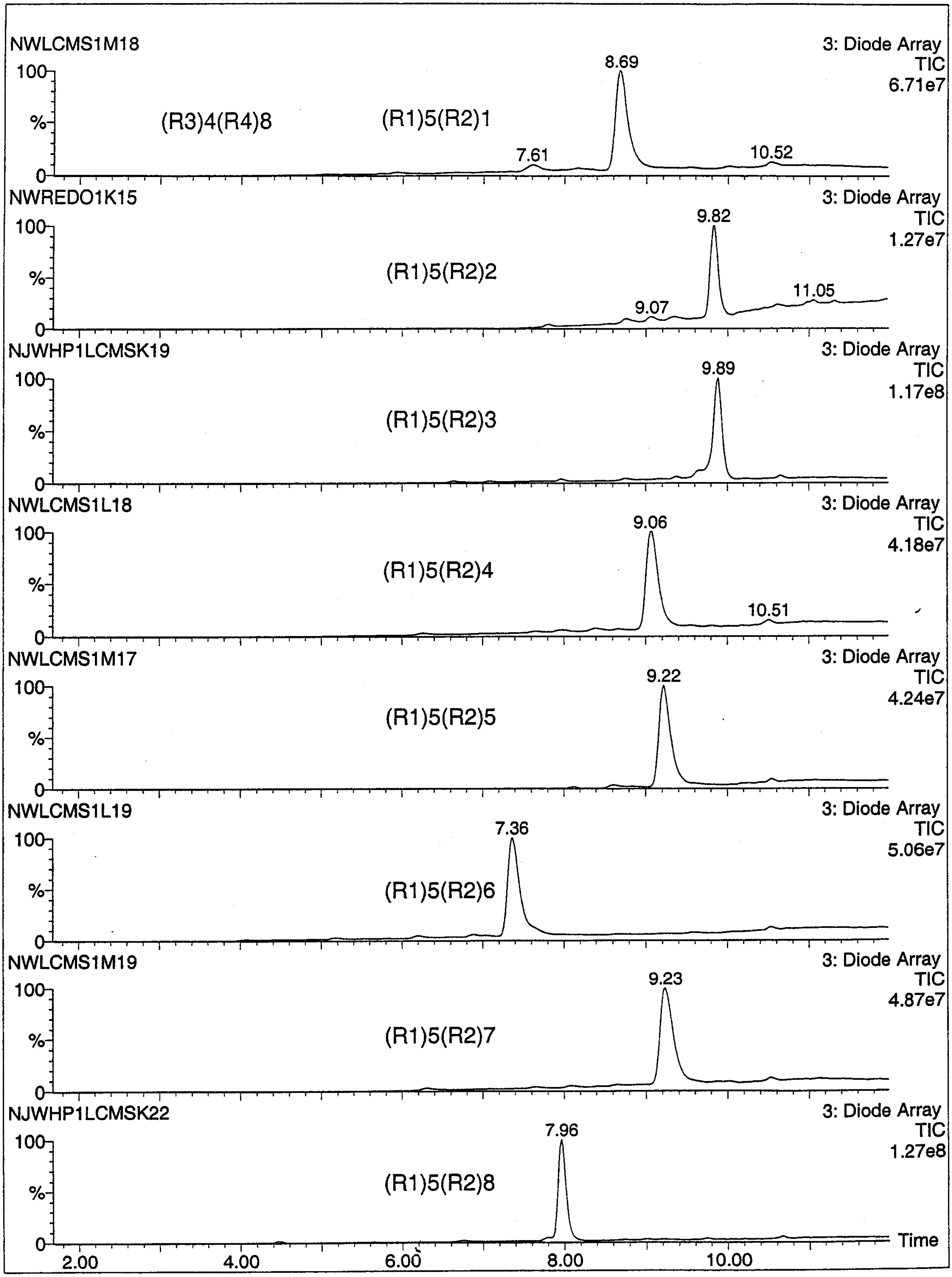


Figure V .3.2.23 577

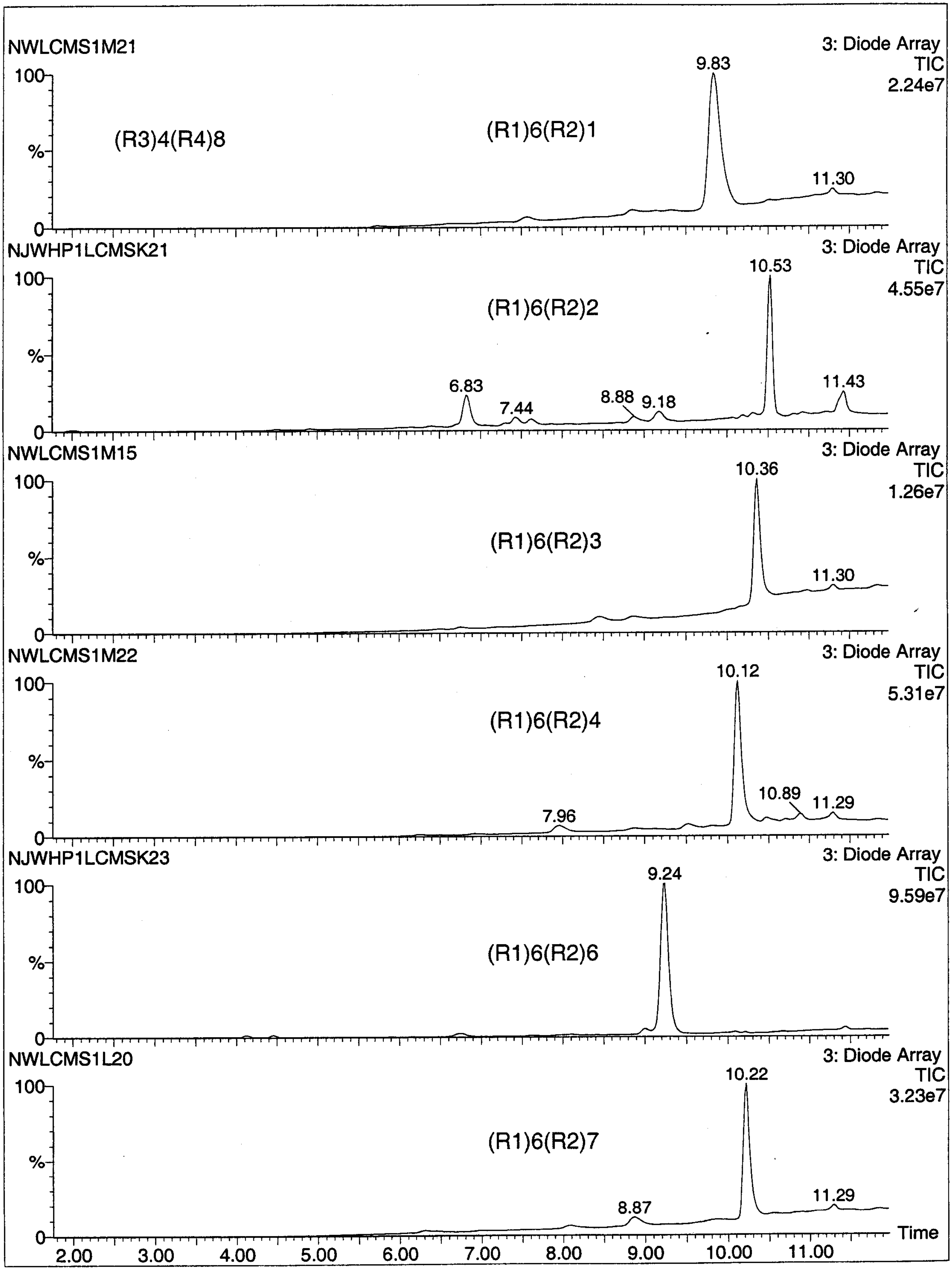


Figure V .3.2.24 S78

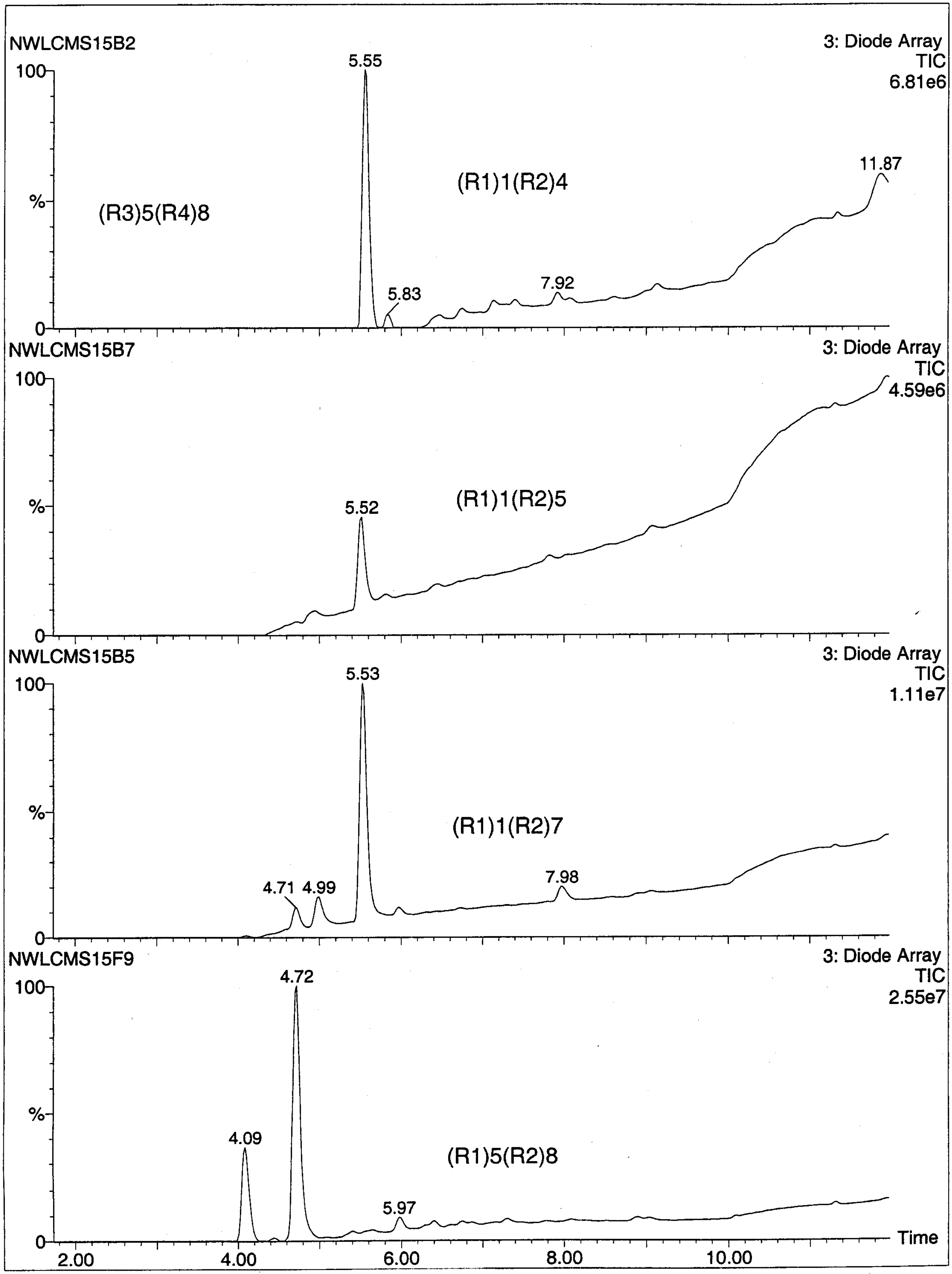


Figure V.3.2.25 S79

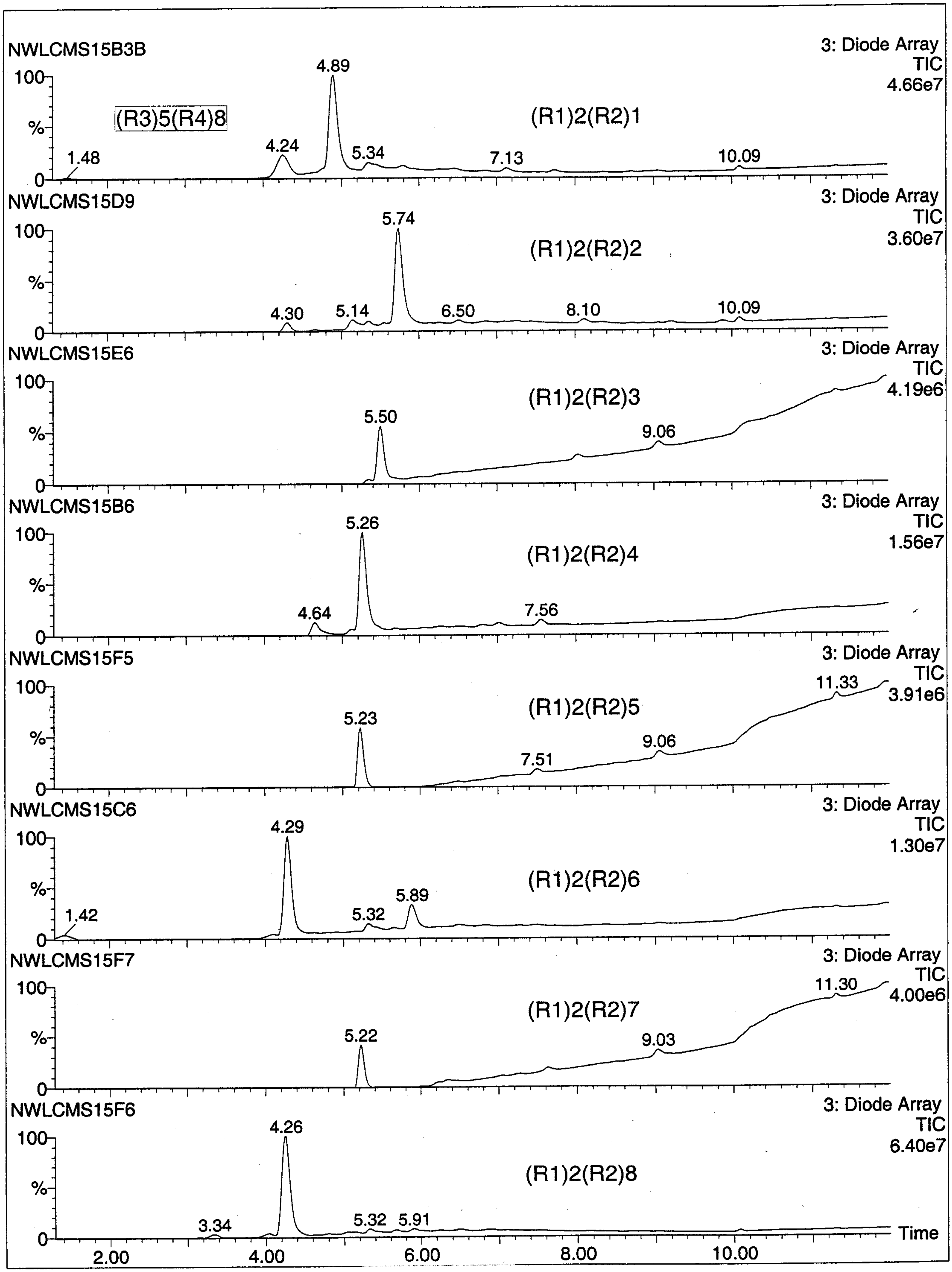


Figure V.3.2.26

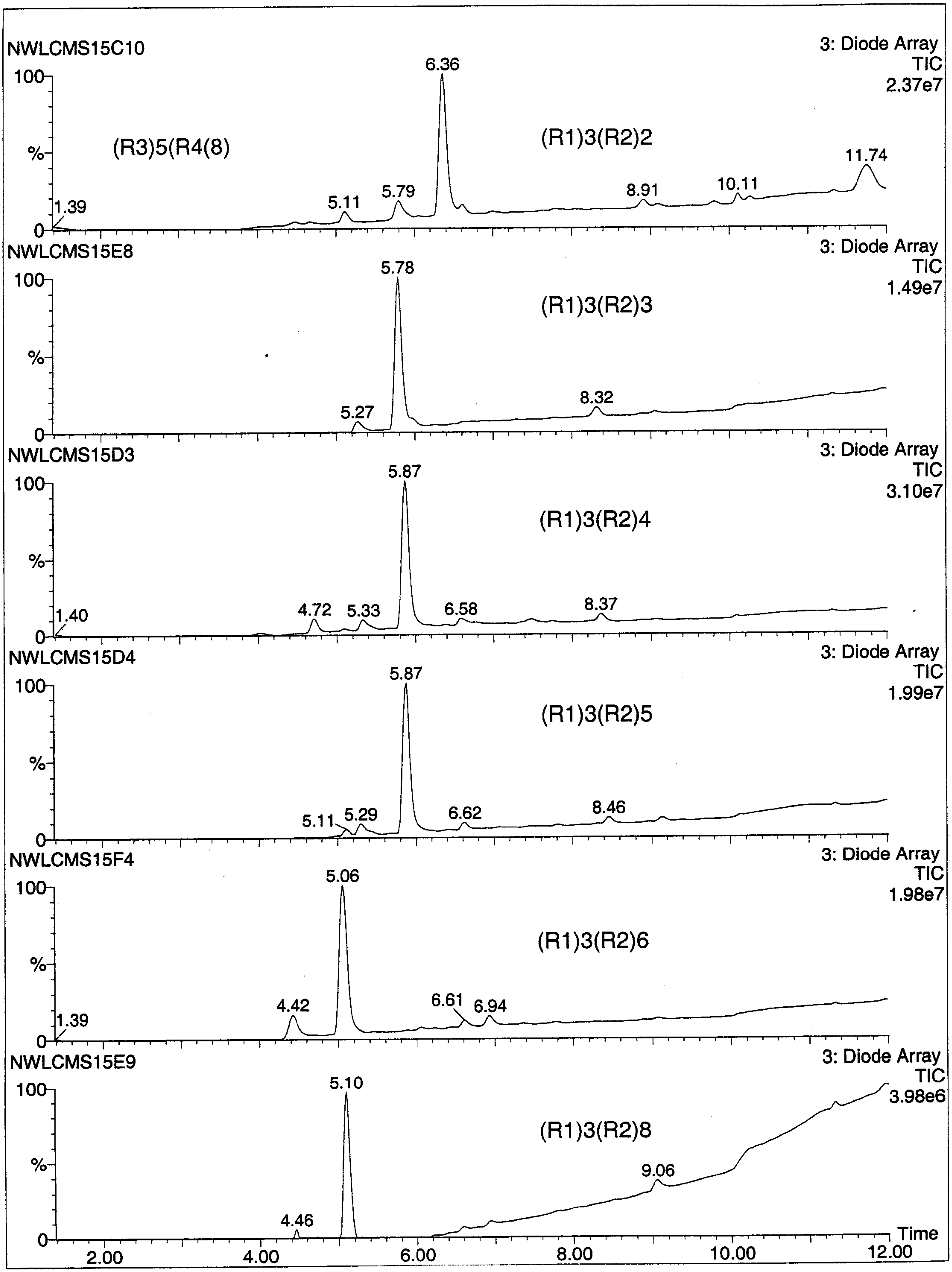


Figure V.3.2.27 581

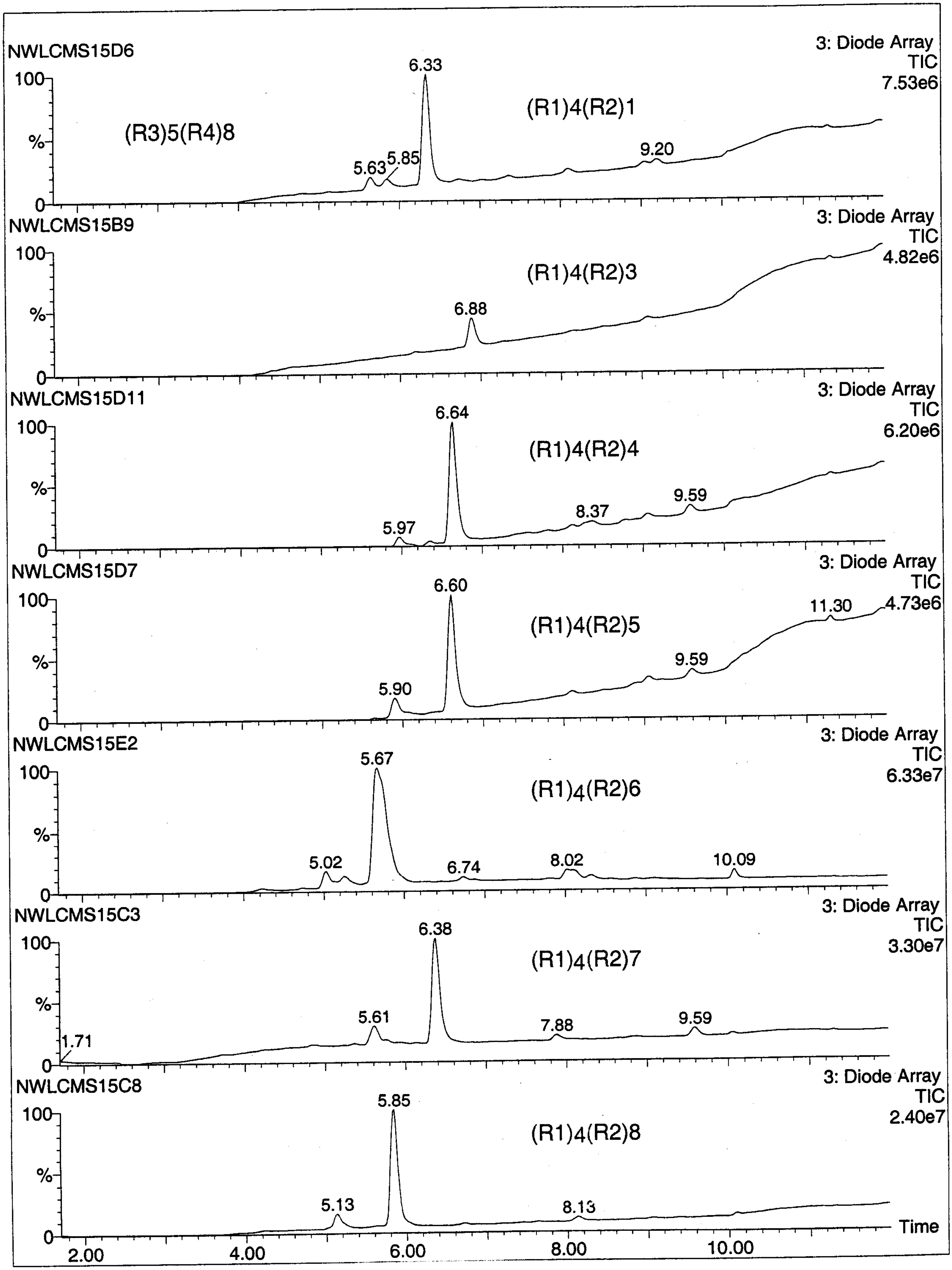


Figure V.3.2.28 S82

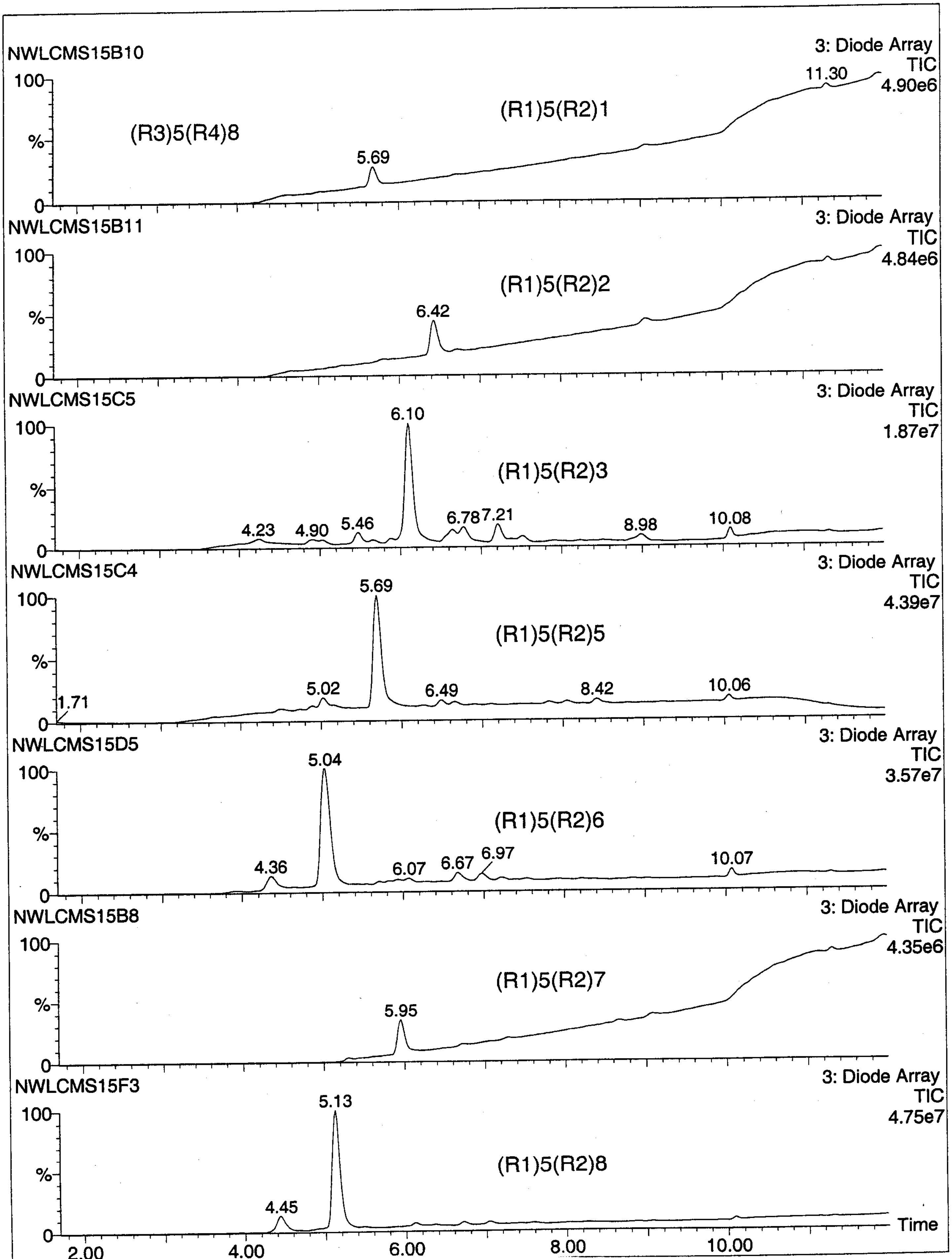


Figure V.3.2.29, 583

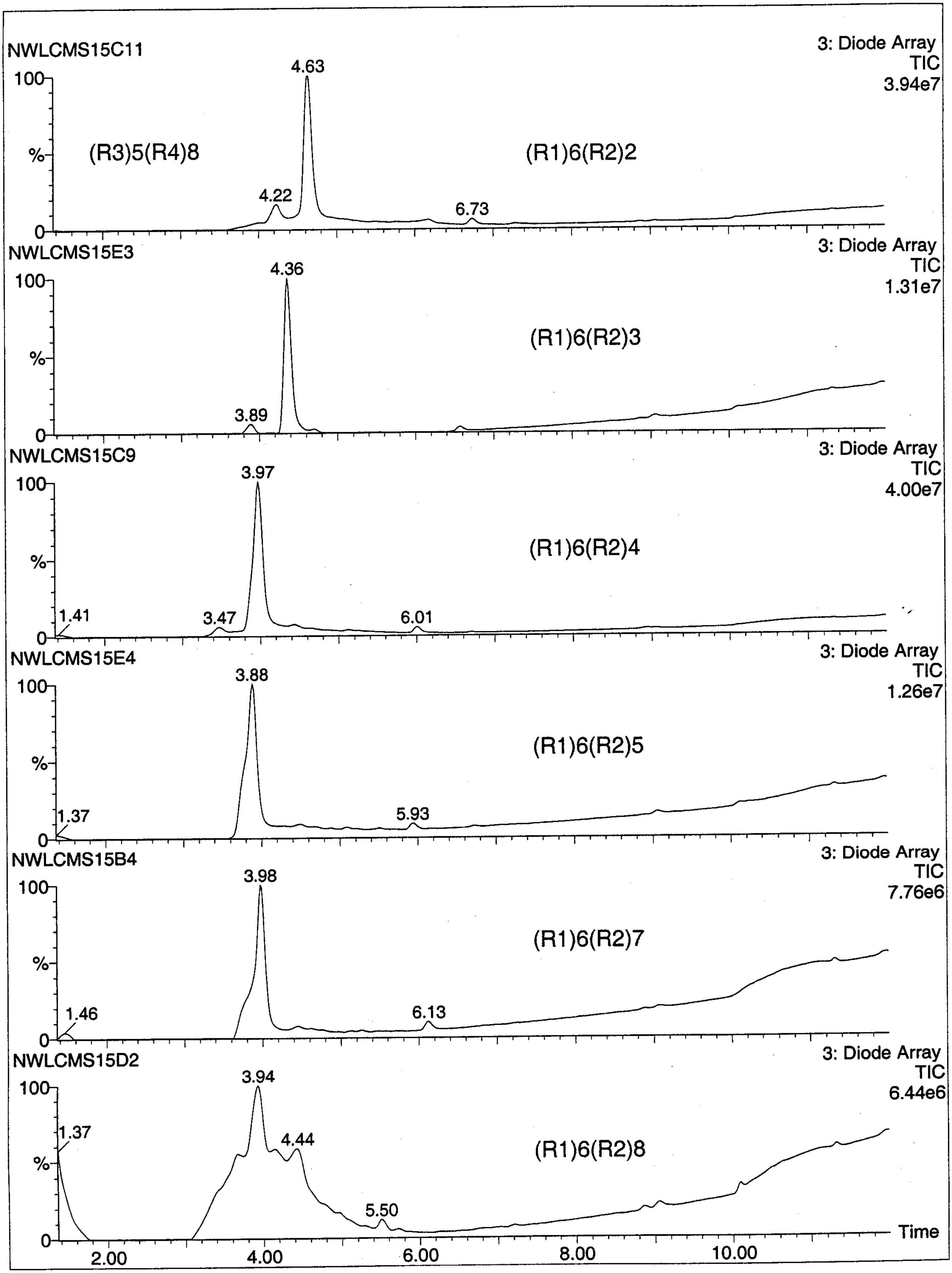


Figure V.3.2.30 S84

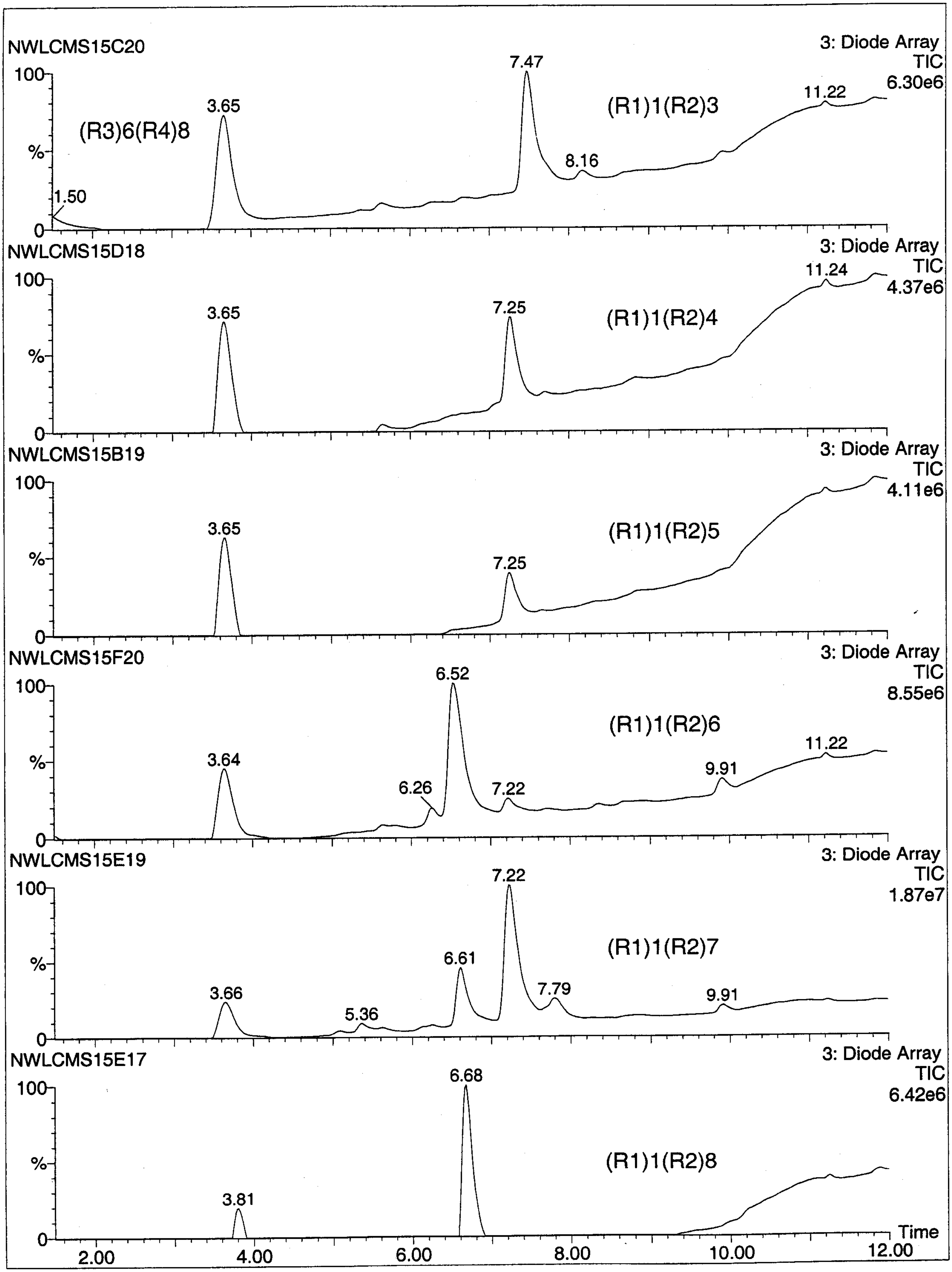


Figure V.3.2.31

S85

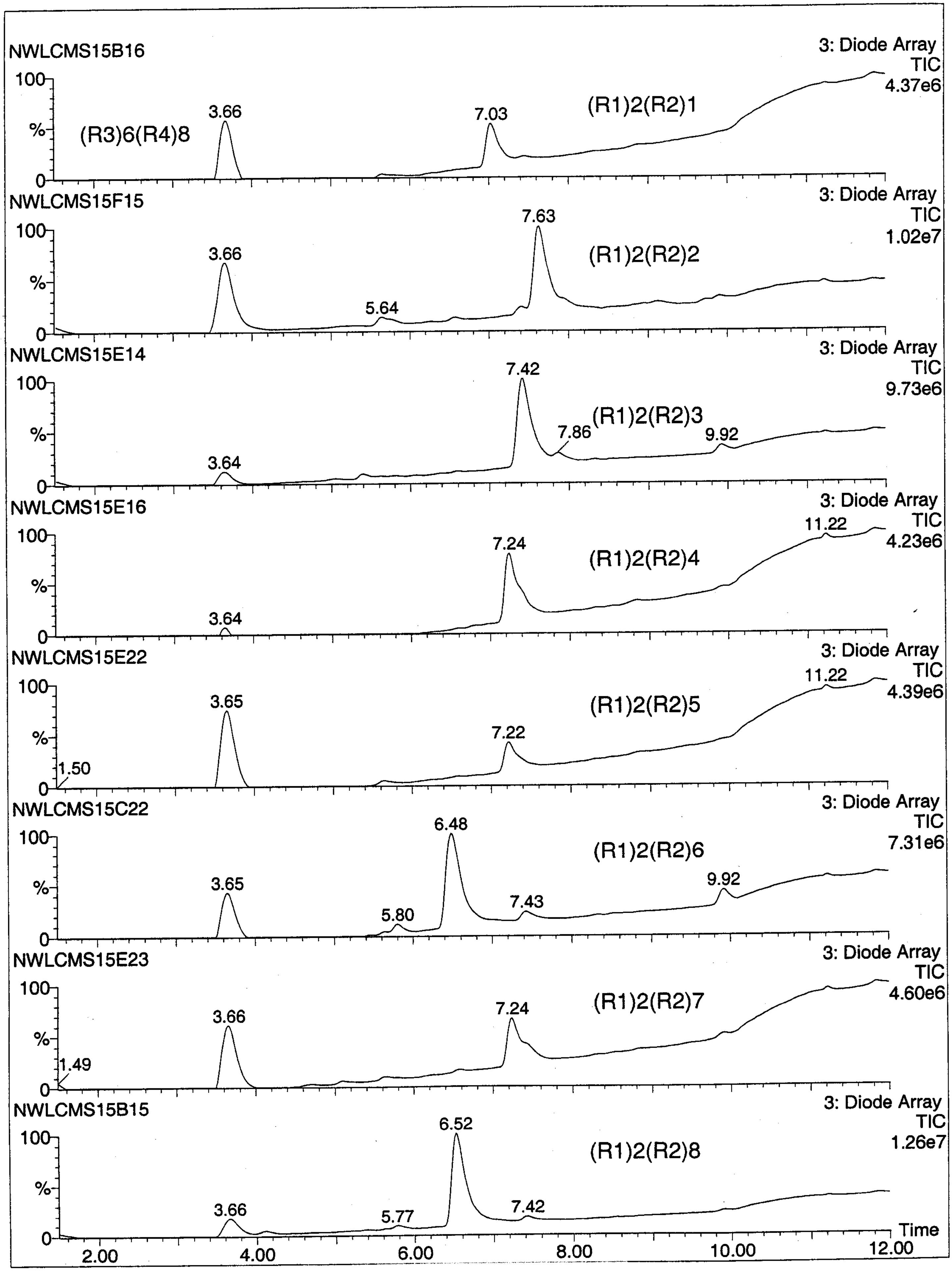


Figure V.3.2.32

S86

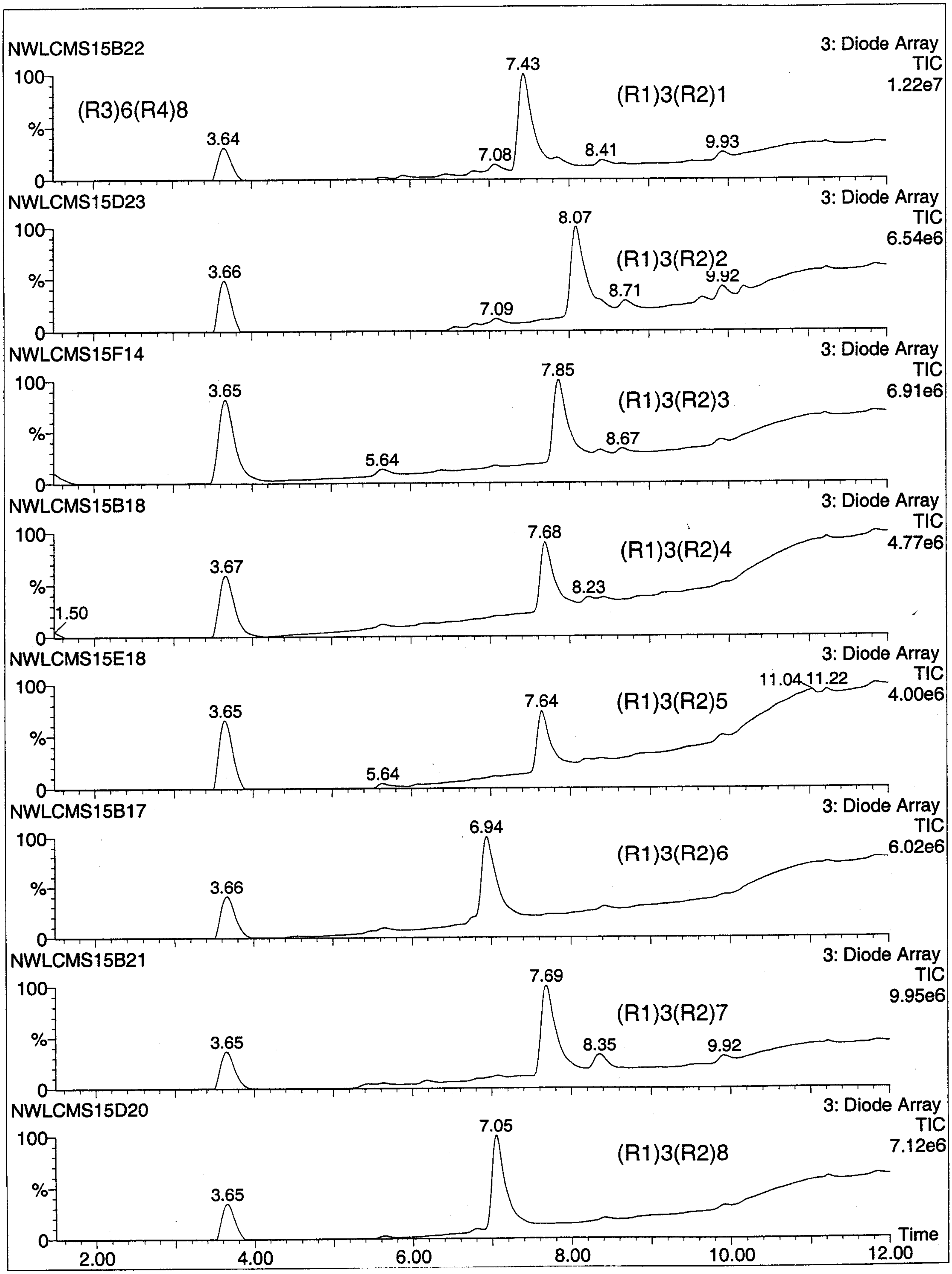
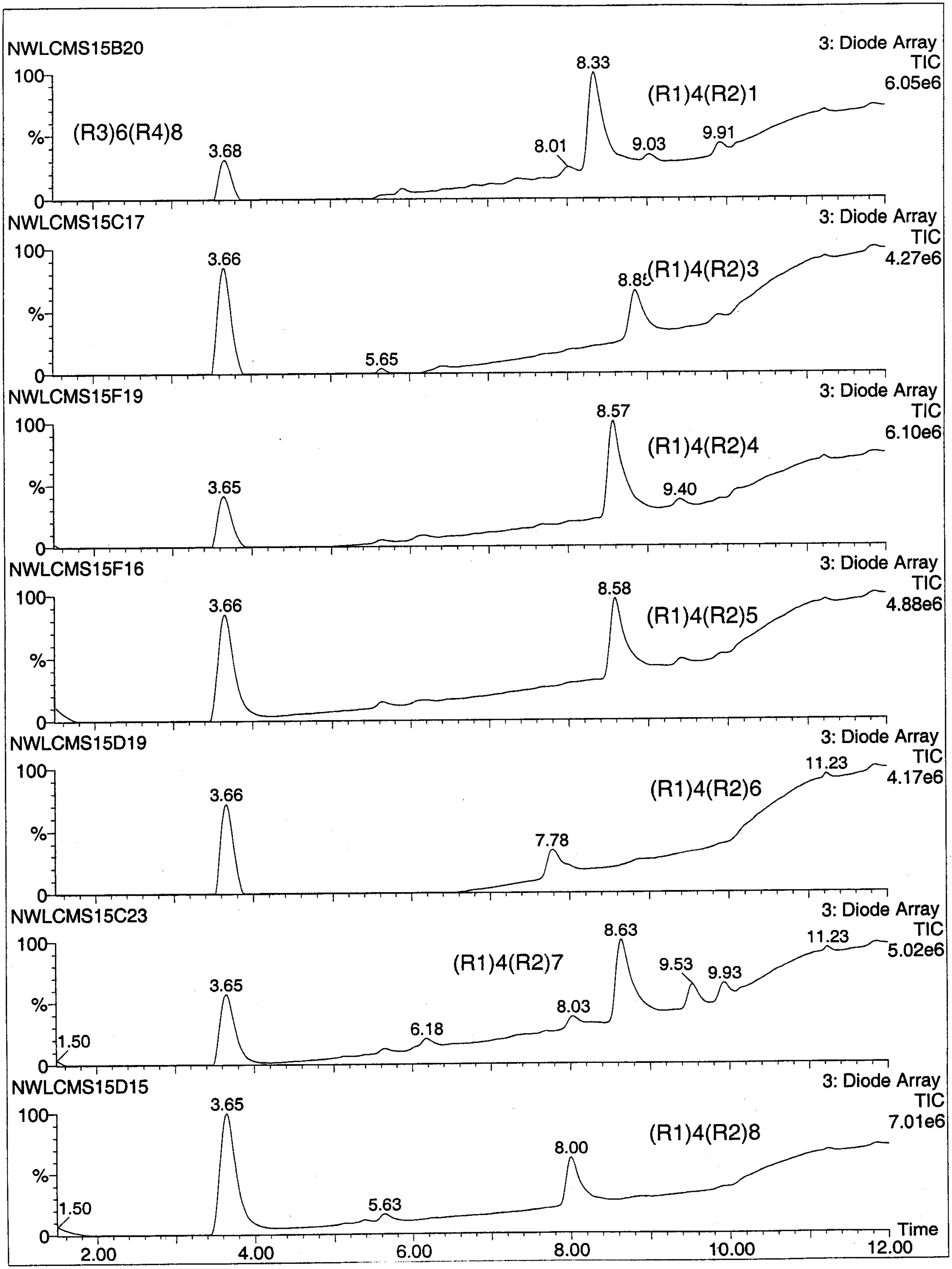


Figure V.3.2.33



]Figure V.3.2.34

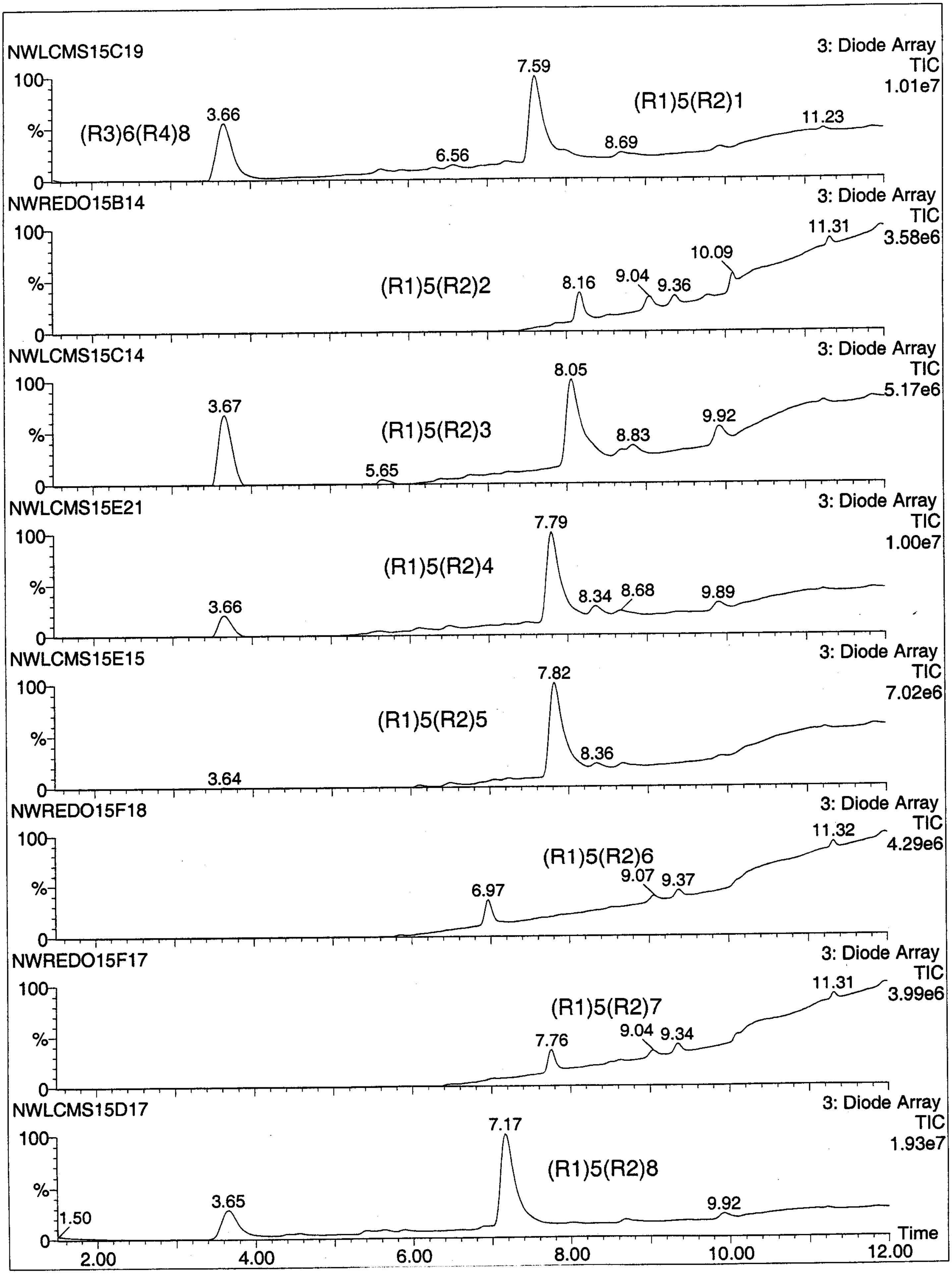


Figure V.3.2.35 589

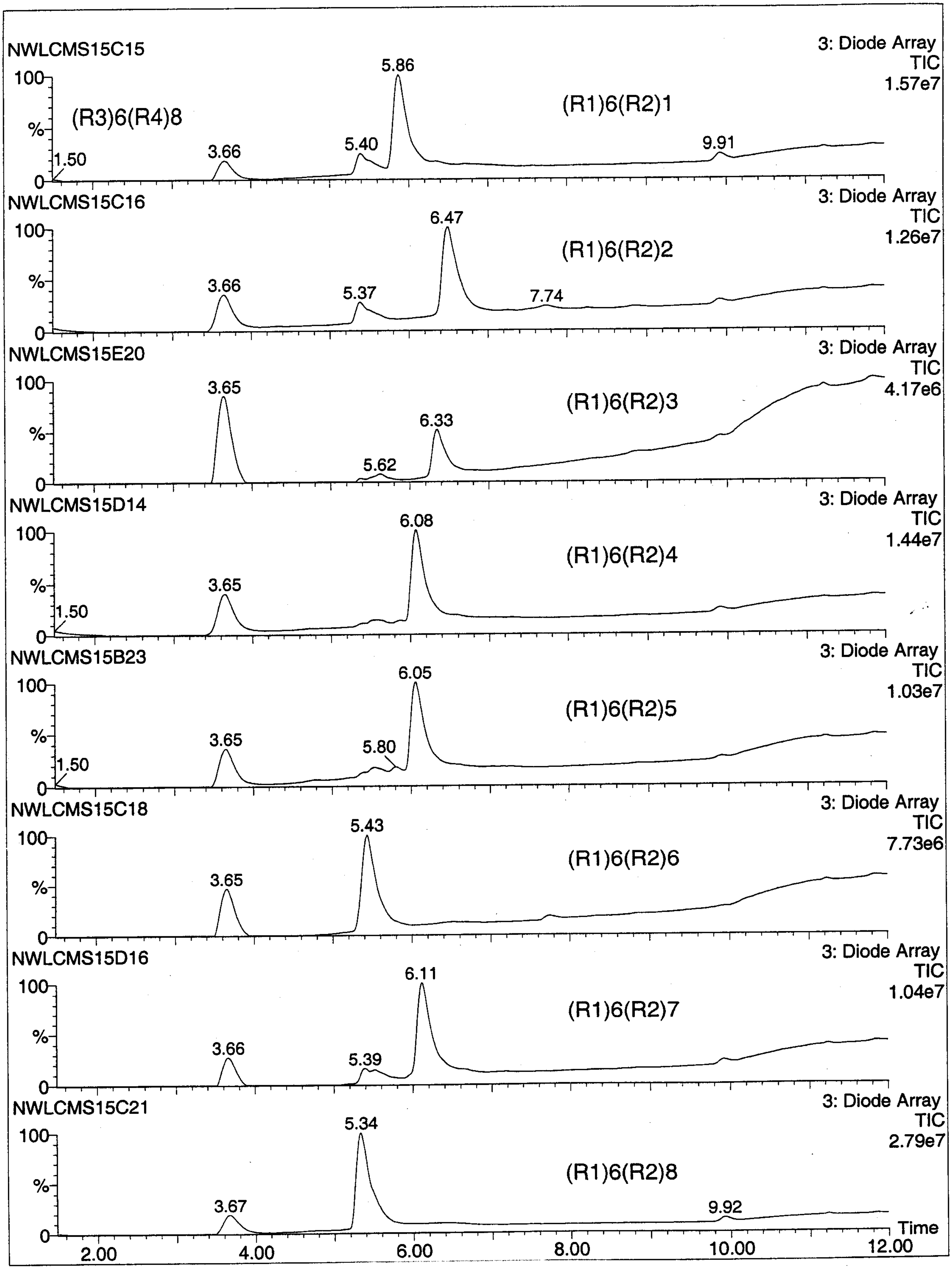


Figure V.3.2.36 S90

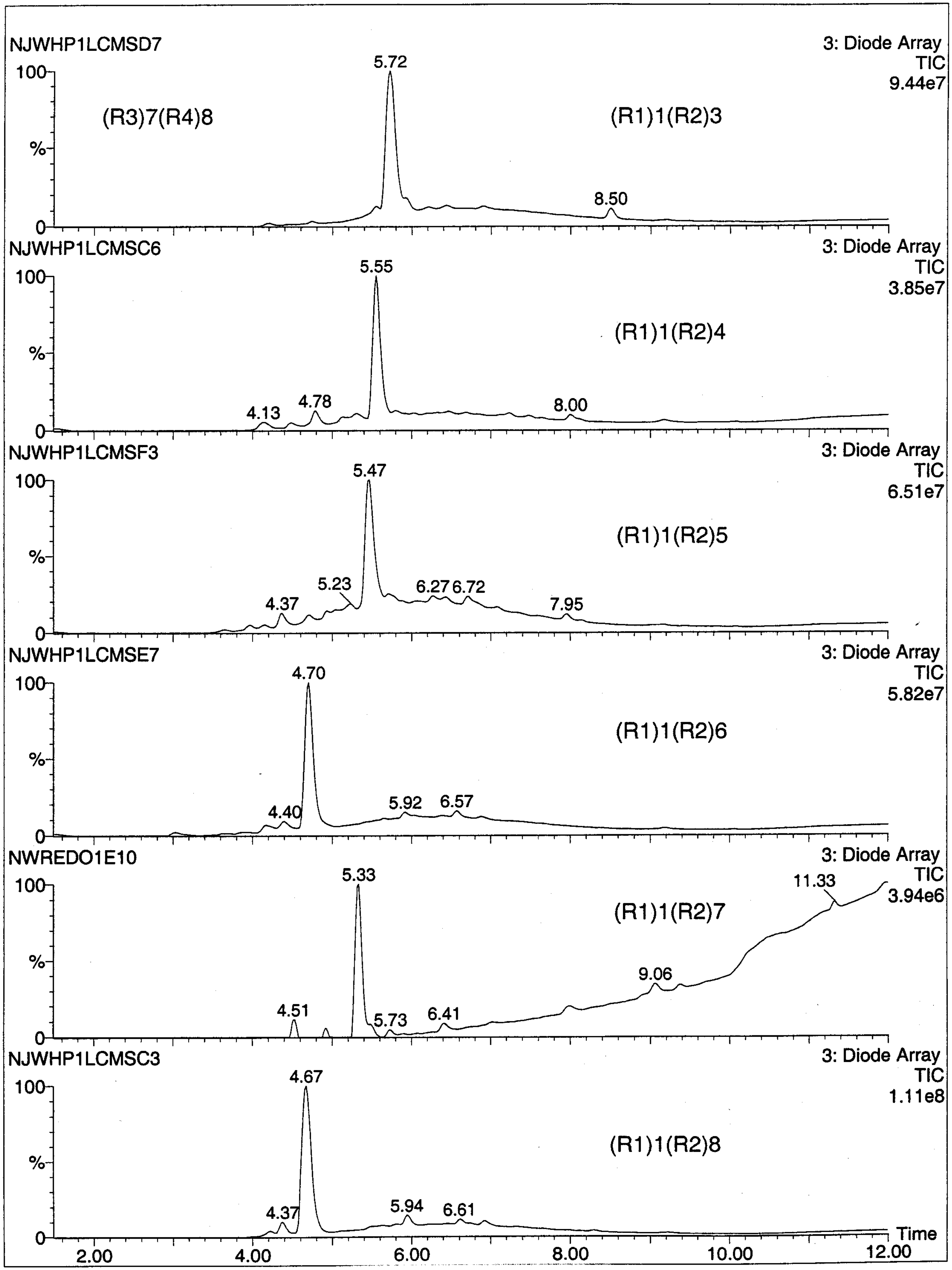


Figure V.3.2.37 591

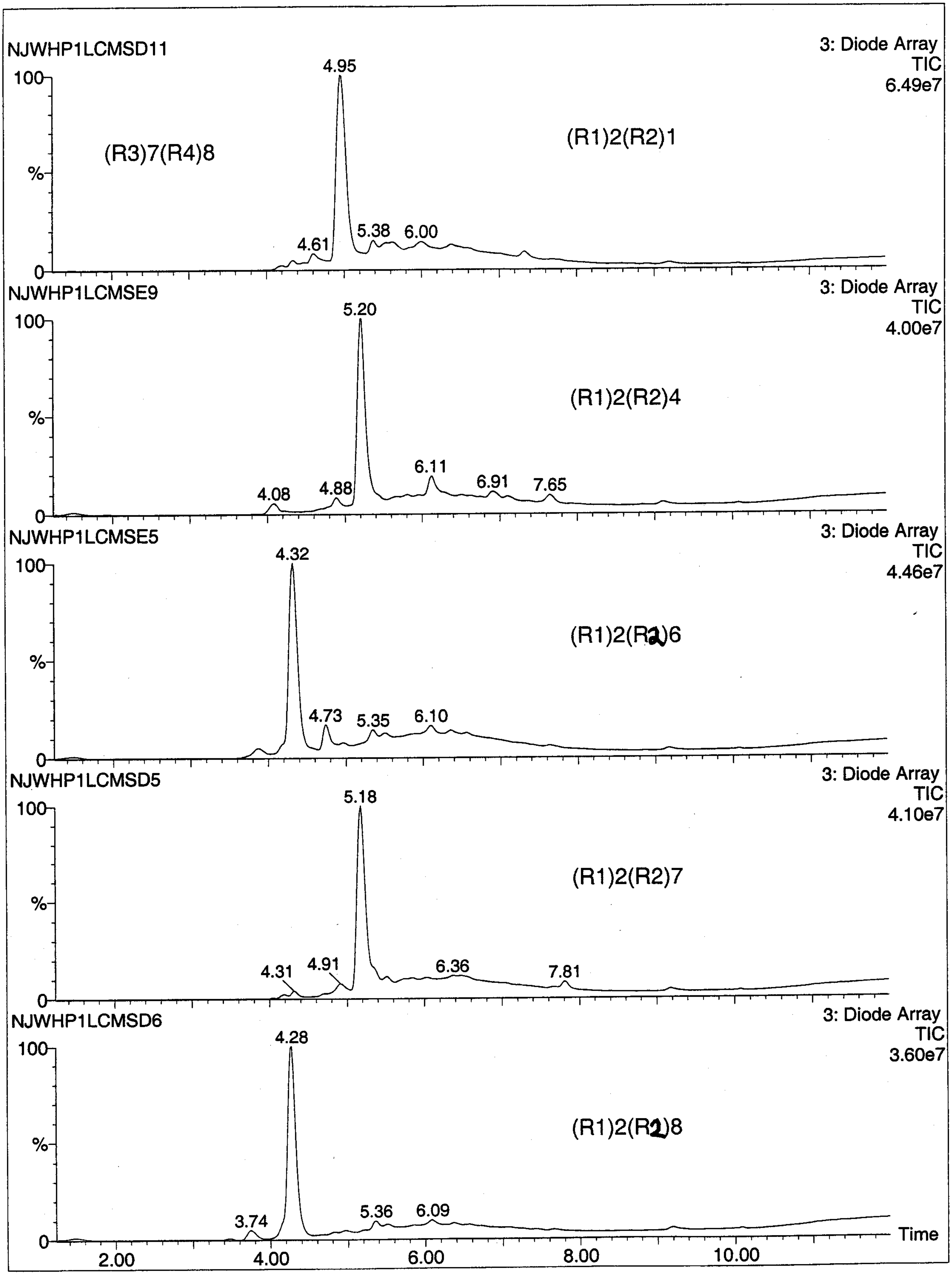


Figure V.3.2.38 592

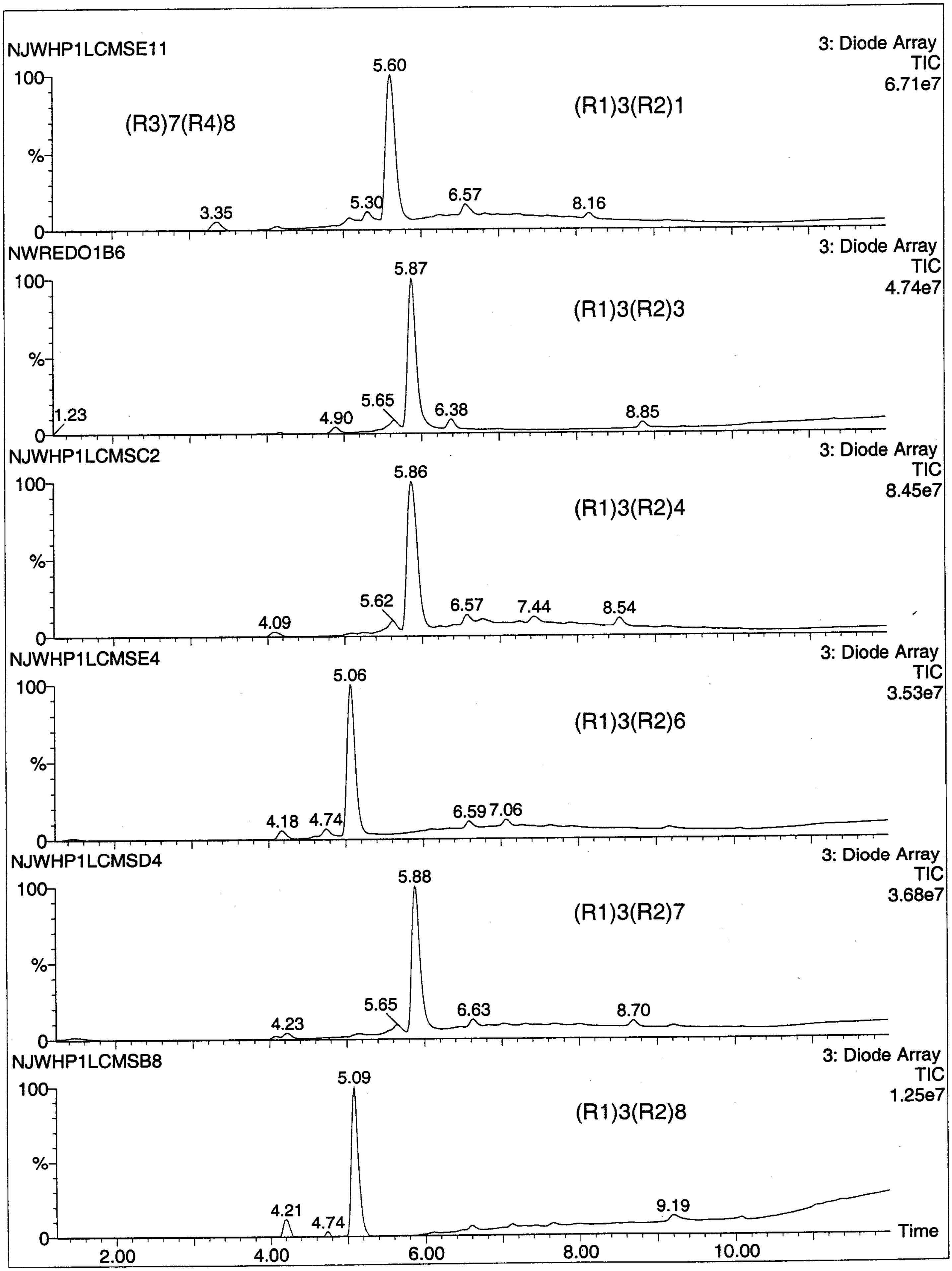


Figure V.3.2.39 593

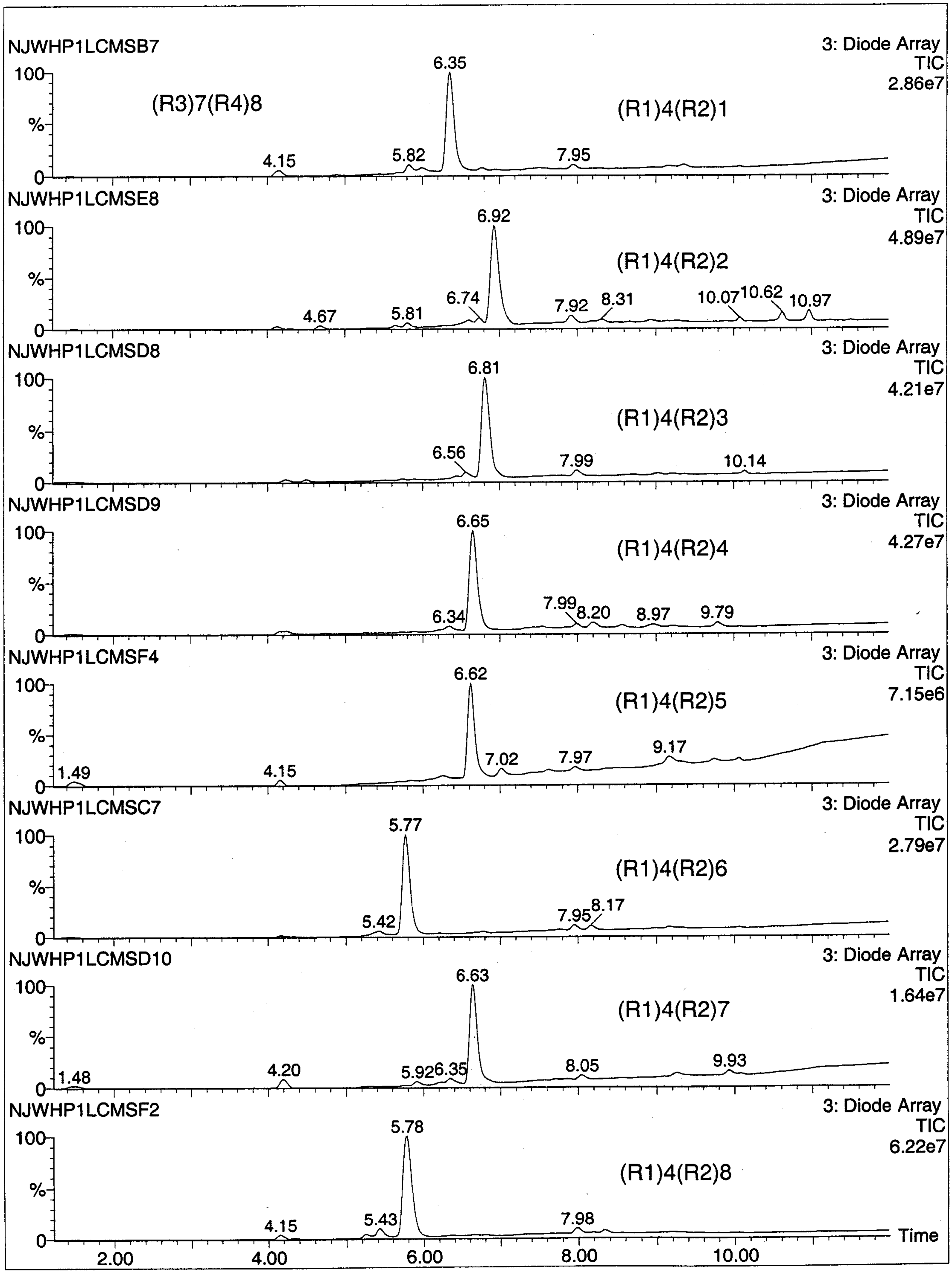


Figure V.3.2.40 S94

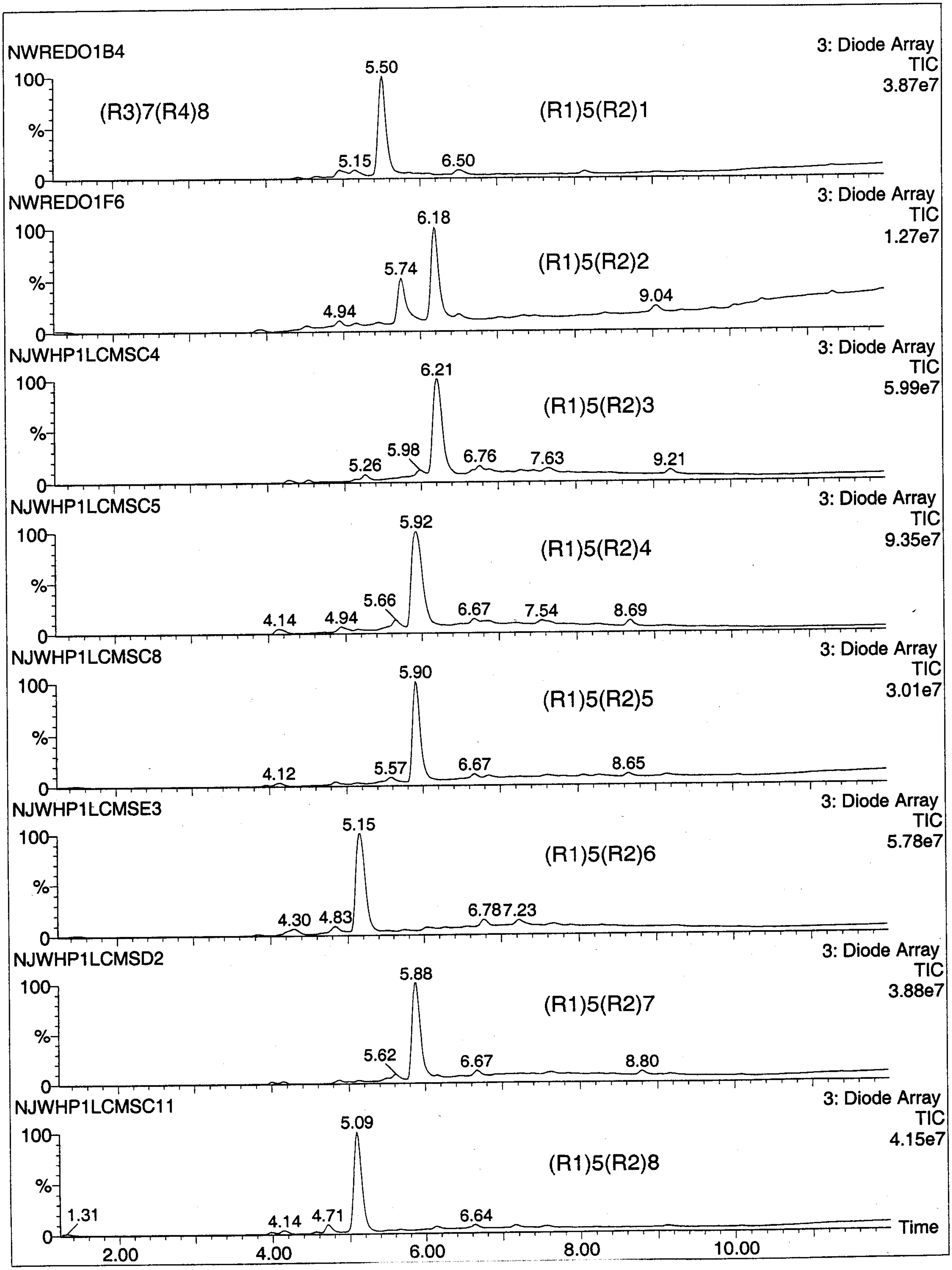


Figure V.3.2.41 S95

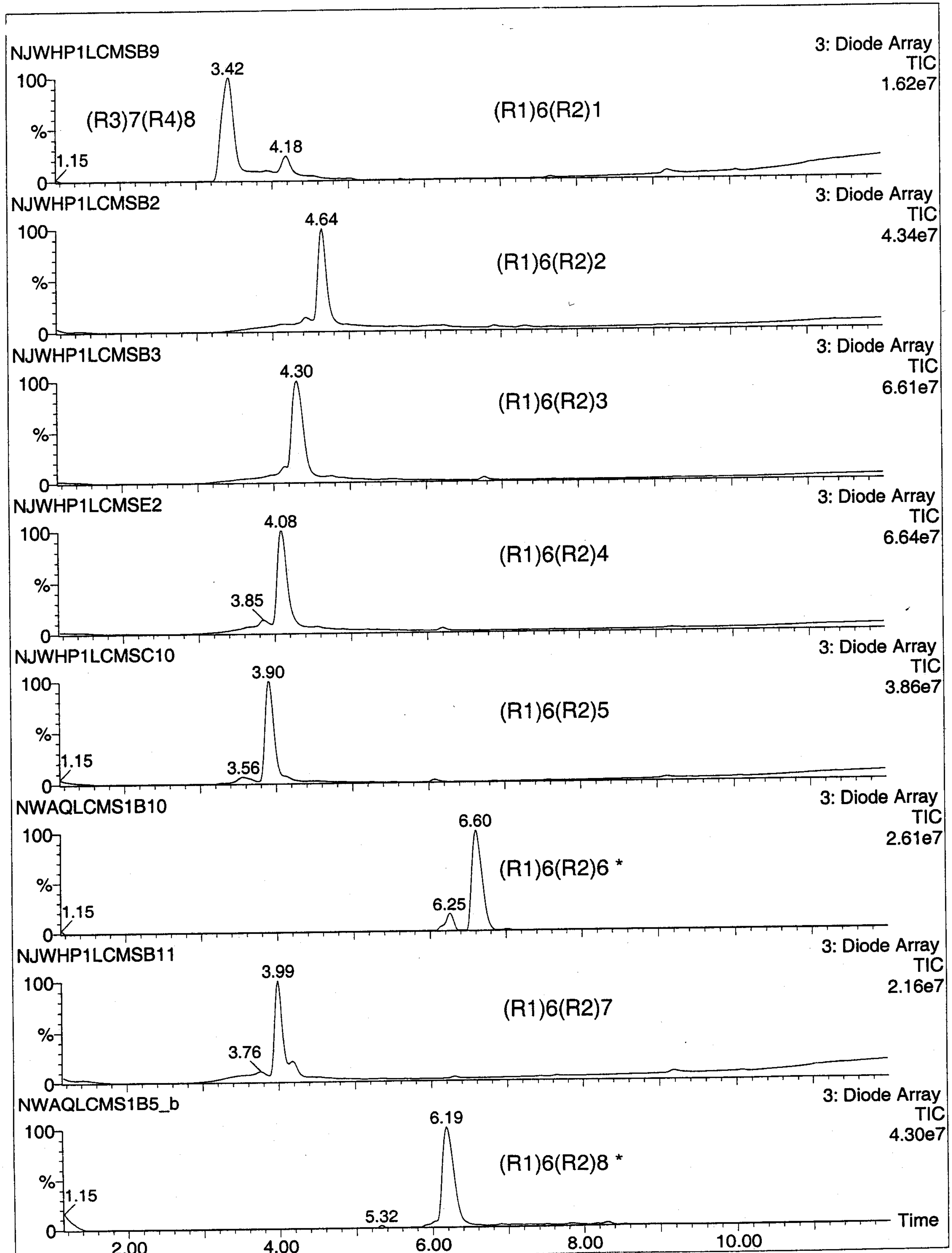
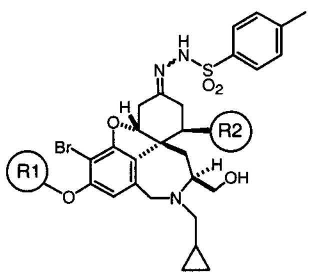


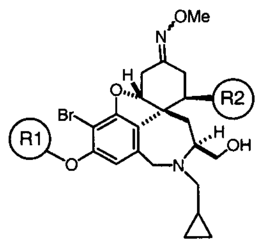
Figure V.3.2.42 S96

V.3.3 Representative Final Compounds From Library Plates 3-18

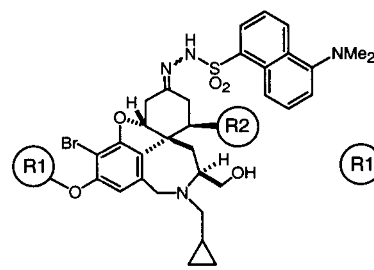
Figure V.3.3.1 - Plate 3



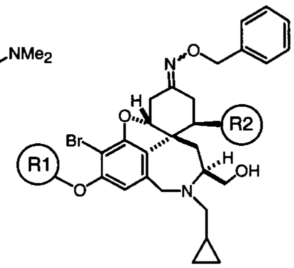
(R3)7(R4)1



(R3)7(R4)3

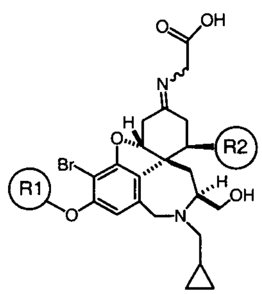


(R3)7(R4)2

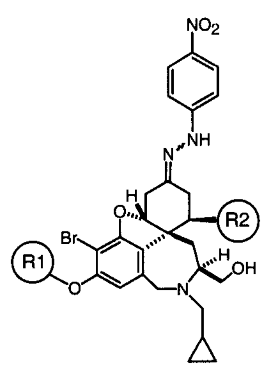


(R3)7(R4)4

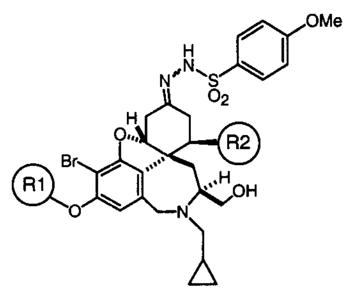
Figure V.3.3.2 - Plate 4



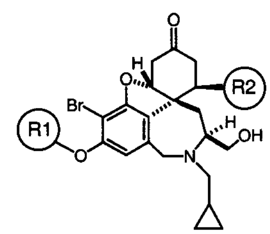
(R3)7(R4)5



(R3)7(R4)7

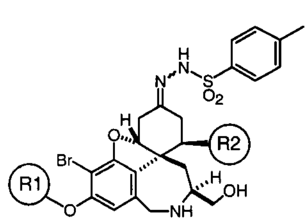


(R3)7(R4)6

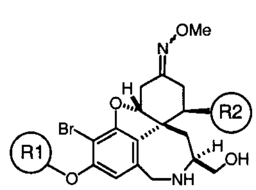


(R3)7(R4)8
(see Figure VI.3.2.37-42)

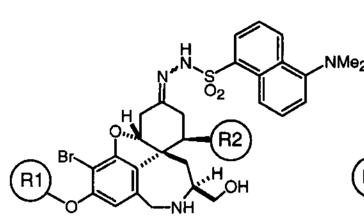
Figure V.3.3.3 - Plate 5



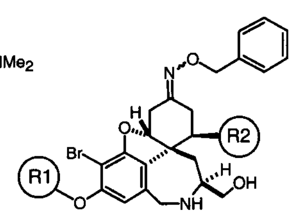
(R3)8(R4)1



(R3)8(R4)3

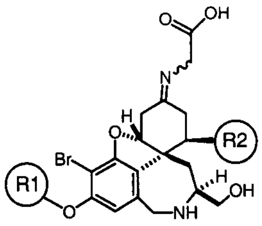


(R3)8(R4)2

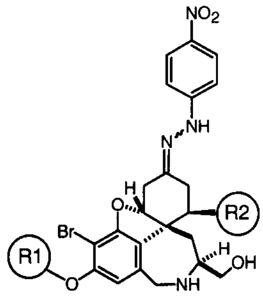


(R3)8(R4)4

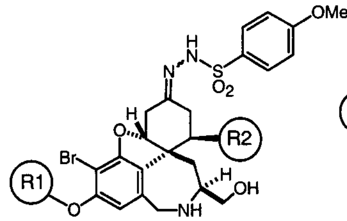
Figure V.3.3.4 - Plate 6



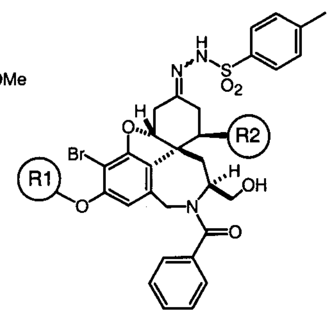
(R3)8(R4)5



(R3)8(R4)7

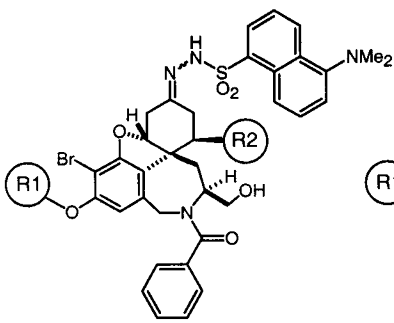


(R3)8(R4)6

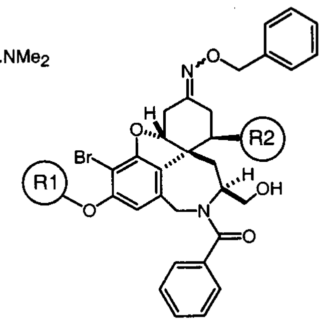


(R3)1(R4)1

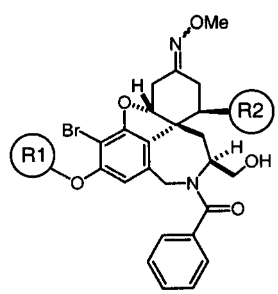
Figure V.3.3.5 - Plate 7



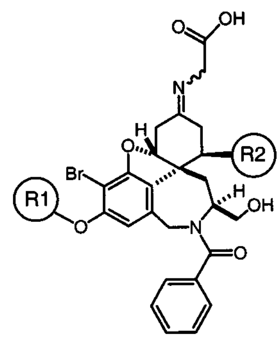
(R3)1(R4)2



(R3)1(R4)4

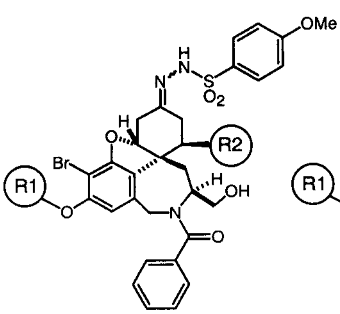


(R3)1(R4)3

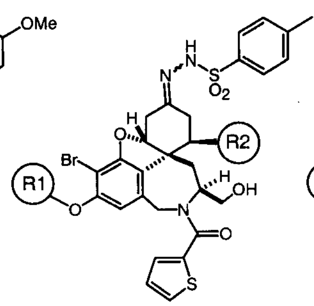


(R3)1(R4)5

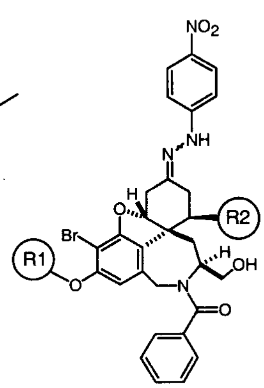
Figure V.3.3.6 - Plate 8



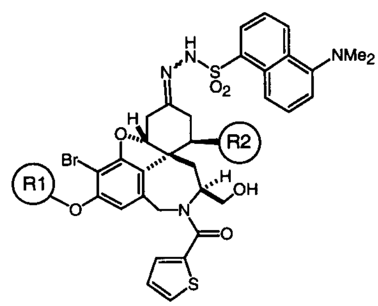
(R3)1(R4)6



(R3)4(R4)1

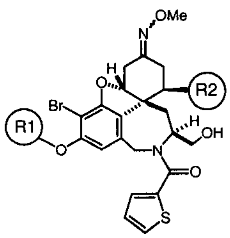


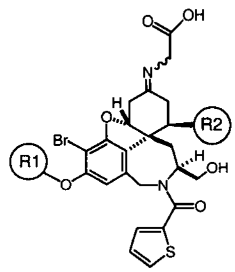
(R3)1(R4)7

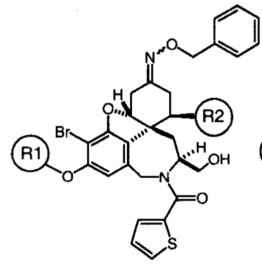


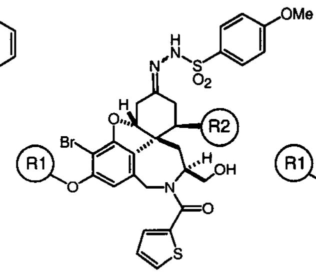
(R3)4(R4)2

Figure V.3.3.7 – Plates 9 and 10


(R3)4(R4)3


(R3)4(R4)5


(R3)4(R4)4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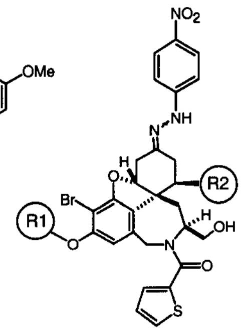
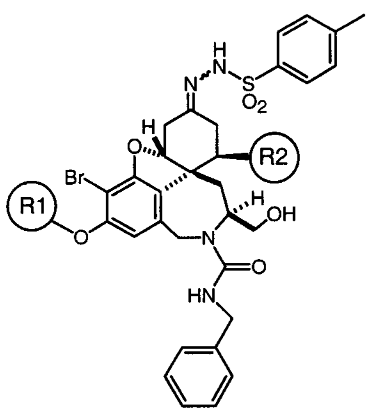

(R3)4(R4)7

Figure V.3.3.8 – Plate 11


(R3)2(R4)1

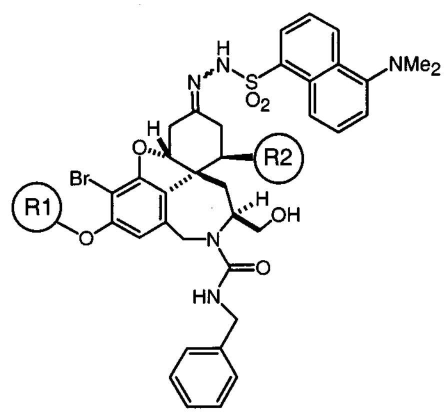
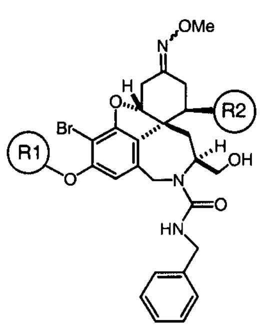

(R3)2(R4)2

Figure V.3.3.9 – Plate 12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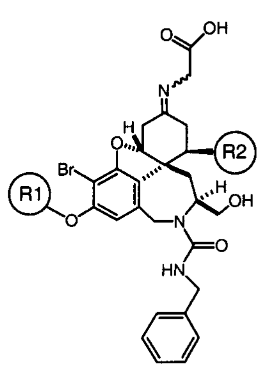
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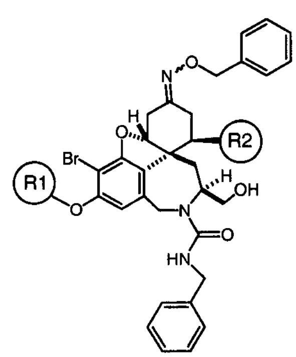

(R3)2(R4)4

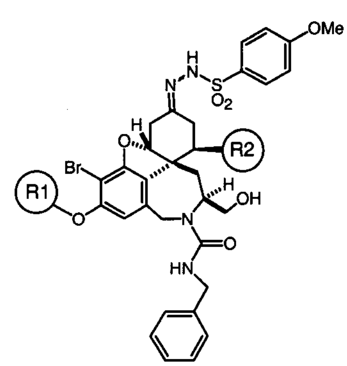
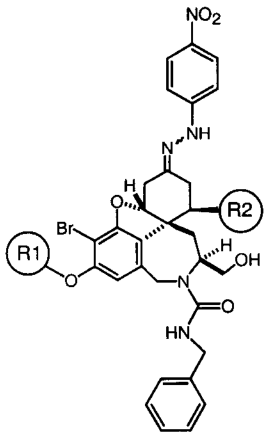
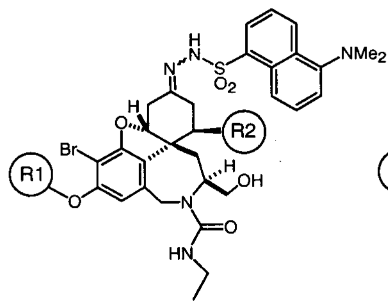

(R3)2(R4)6

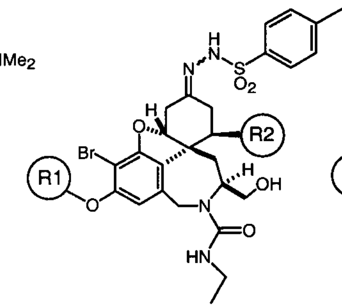
Figure V.3.3.10 – Plate 13



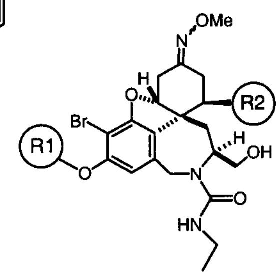
(R3)2(R4)7



(R3)3(R4)2

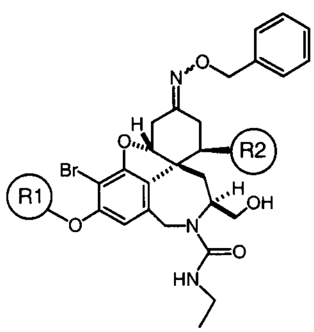


(R3)3(R4)1

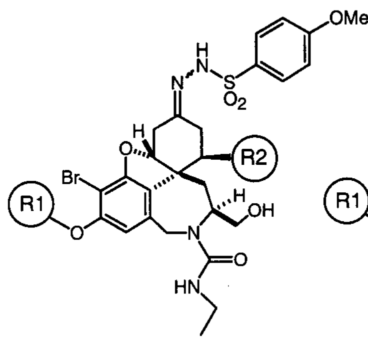


(R3)3(R4)3

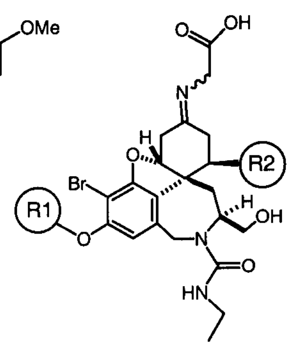
Figure V.3.3.11 – Plate 14



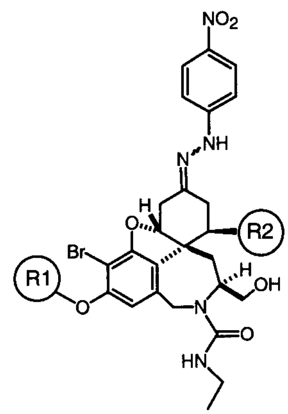
(R3)3(R4)4



(R3)3(R4)6

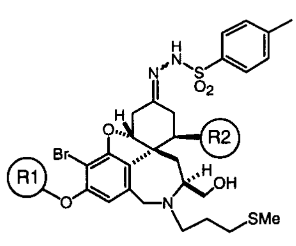


(R3)3(R4)5

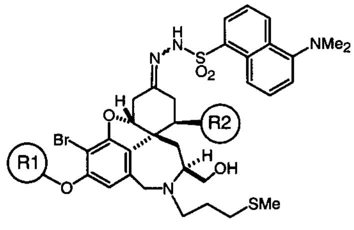


(R3)3(R4)7

Figure V.3.3.12 – Plate 15

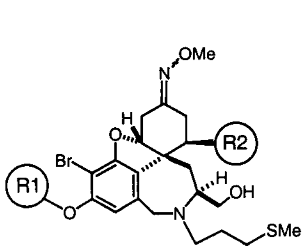


(R3)5(R4)1

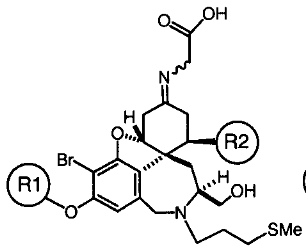


(R3)5(R4)2

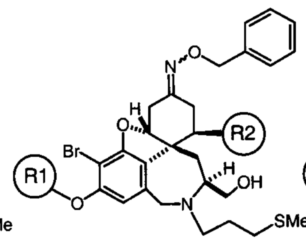
Figure V.3.3.13 – Plate 16



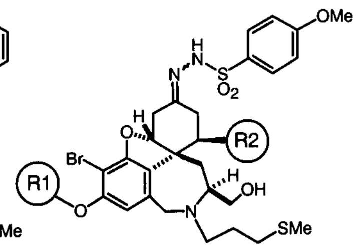
(R3)5(R4)3



(R3)5(R4)5

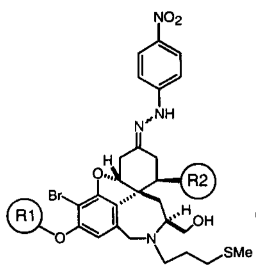


(R3)5(R4)4

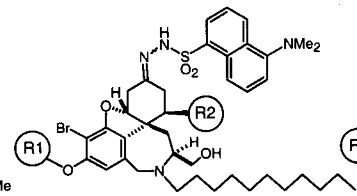


(R3)5(R4)6

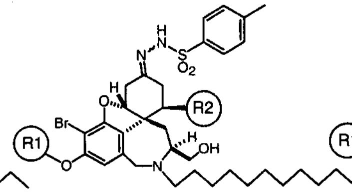
Figure V.3.3.14 – Plate 17



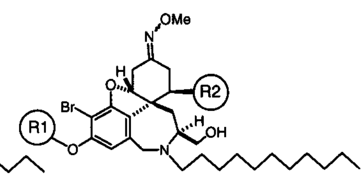
(R3)5(R4)7



(R3)6(R4)2

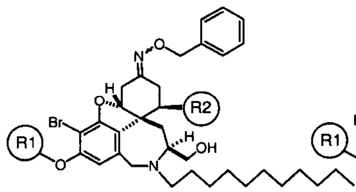


(R3)6(R4)1

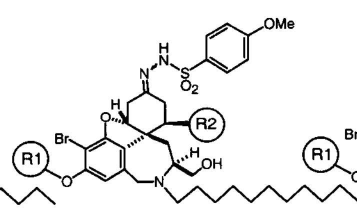


(R3)6(R4)3

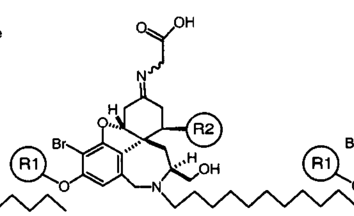
Figure V.3.3.15 – Plate 18



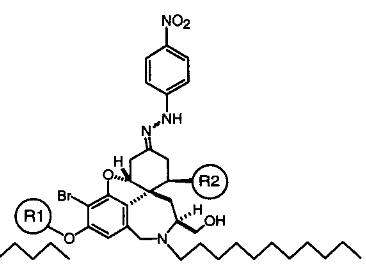
(R3)6(R4)4



(R3)6(R4)6



(R3)6(R4)5



(R3)6(R4)7

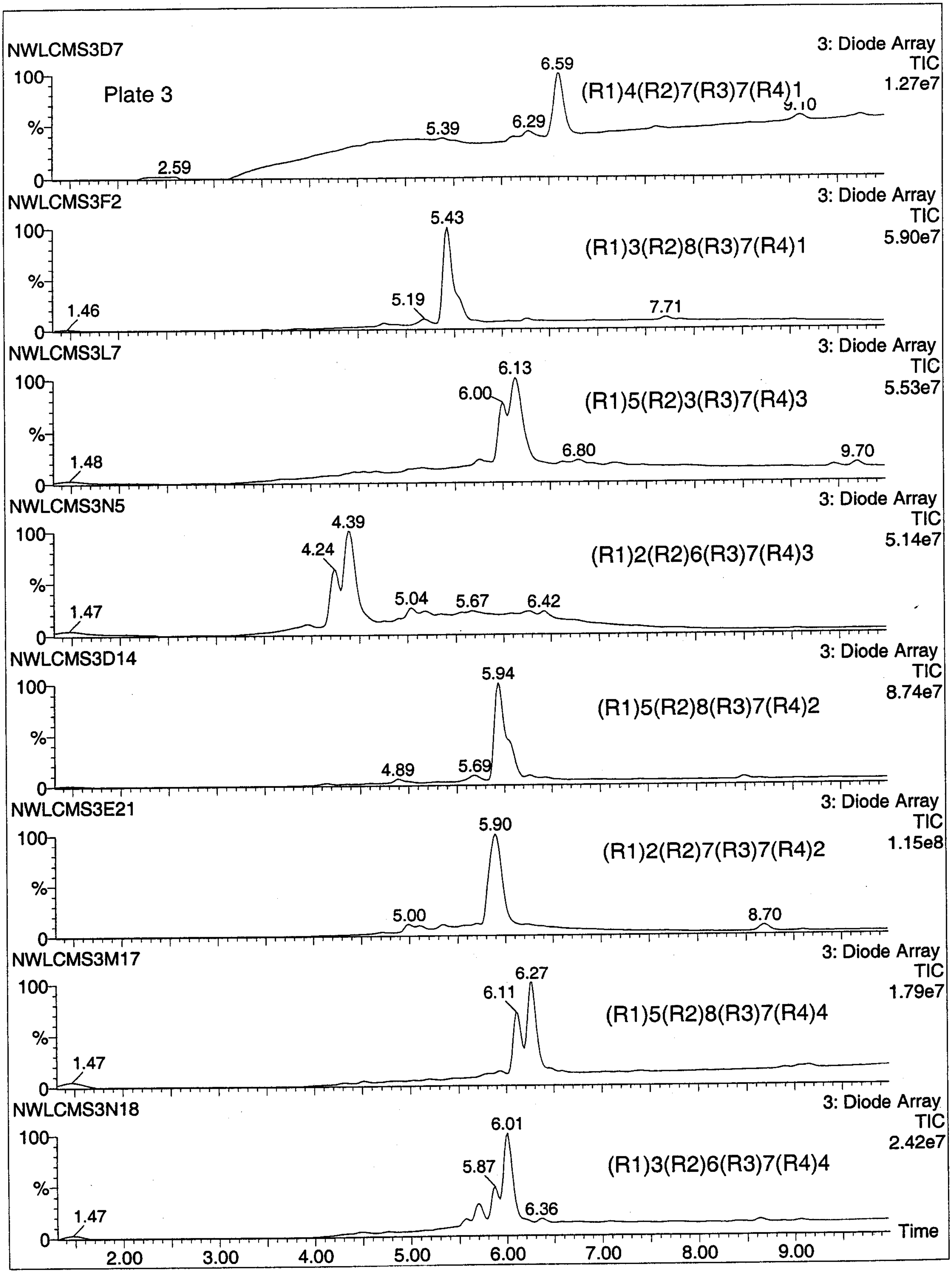


Figure V.3.3.1 S102

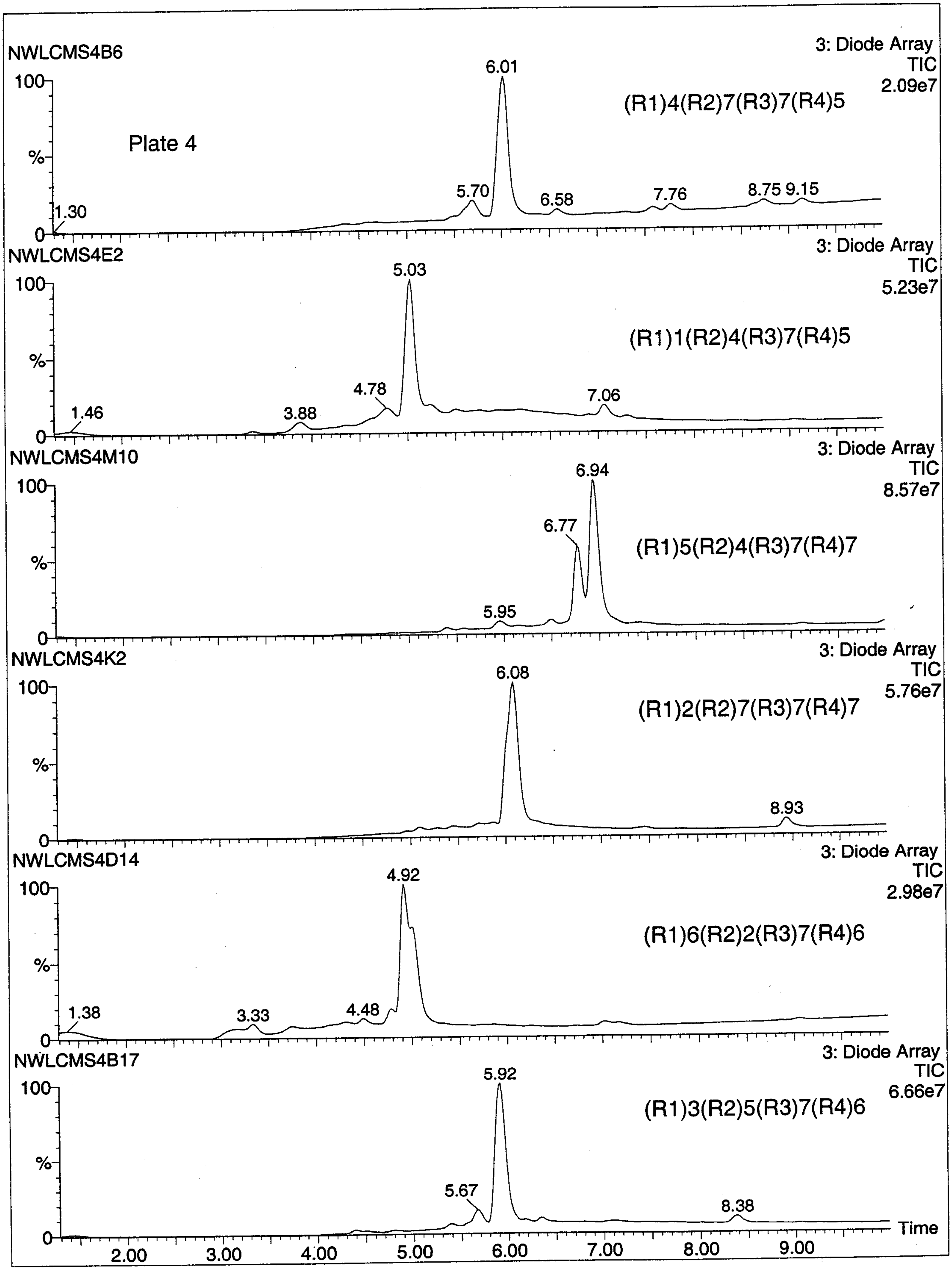
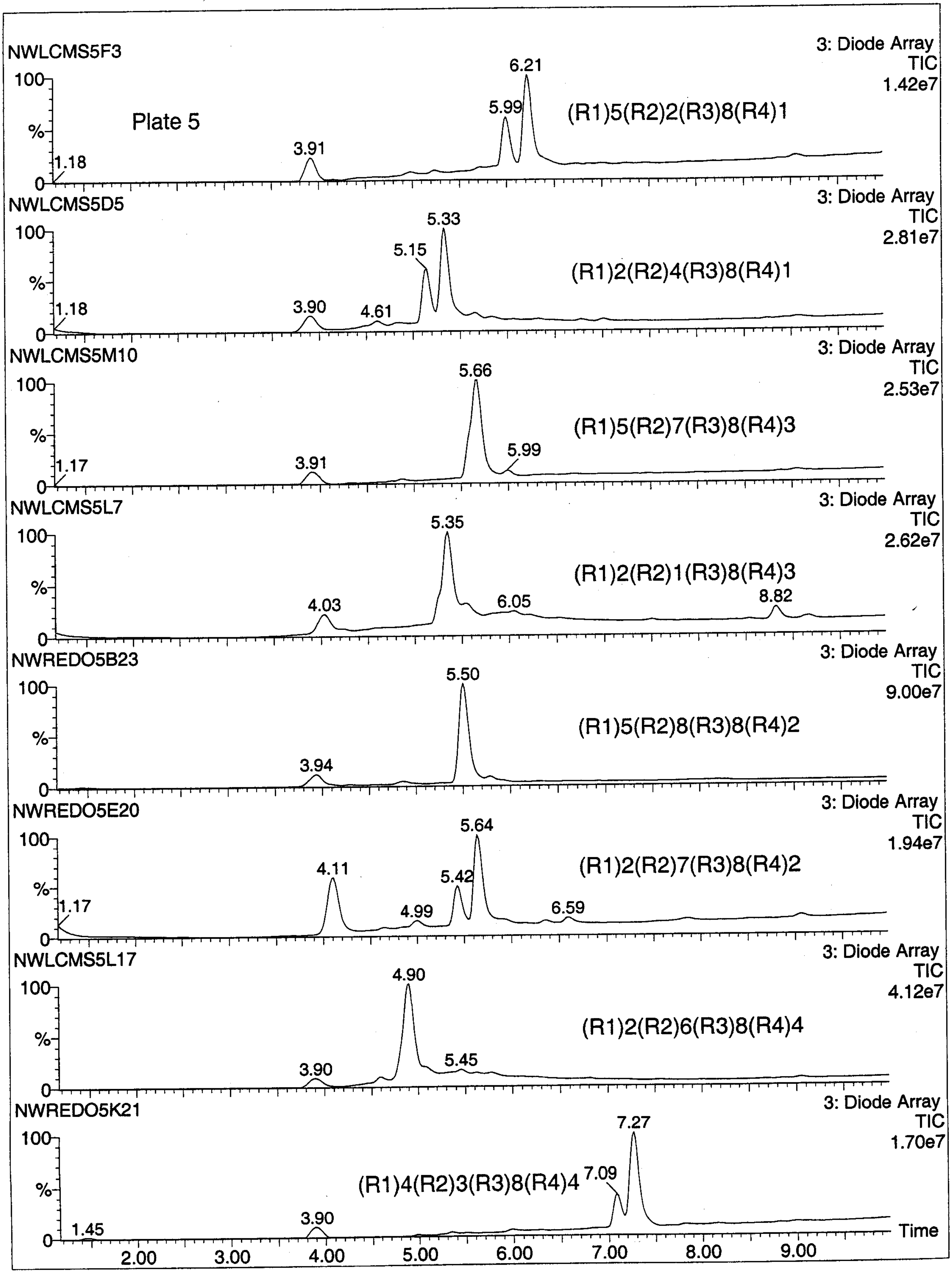


Figure V.3.3.2 S103



NWLCMS5F3
3: Diode Array
TIC
1.42e7
Plate 5
(R1)5(R2)2(R3)8(R4)1
6.21
5.99
3.91
1.18
NWLCMS5D5
3: Diode Array
TIC
2.81e7
(R1)2(R2)4(R3)8(R4)1
5.33
5.15
3.90
4.61
1.18
NWLCMS5M10
3: Diode Array
TIC
2.53e7
(R1)5(R2)7(R3)8(R4)3
5.66
5.99
3.91
1.17
NWLCMS5L7
3: Diode Array
TIC
2.62e7
(R1)2(R2)1(R3)8(R4)3
5.35
4.03
6.05
8.82
NWREDO5B23
3: Diode Array
TIC
9.00e7
(R1)5(R2)8(R3)8(R4)2
5.50
3.94
NWREDO5E20
3: Diode Array
TIC
1.94e7
(R1)2(R2)7(R3)8(R4)2
5.64
4.11
5.42
4.99
6.59
1.17
NWLCMS5L17
3: Diode Array
TIC
4.12e7
(R1)2(R2)6(R3)8(R4)4
4.90
3.90
5.45
NWREDO5K21
3: Diode Array
TIC
1.70e7
(R1)4(R2)3(R3)8(R4)4
7.27
7.09
3.90
1.45
Time
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00

Figure V.3.3.3

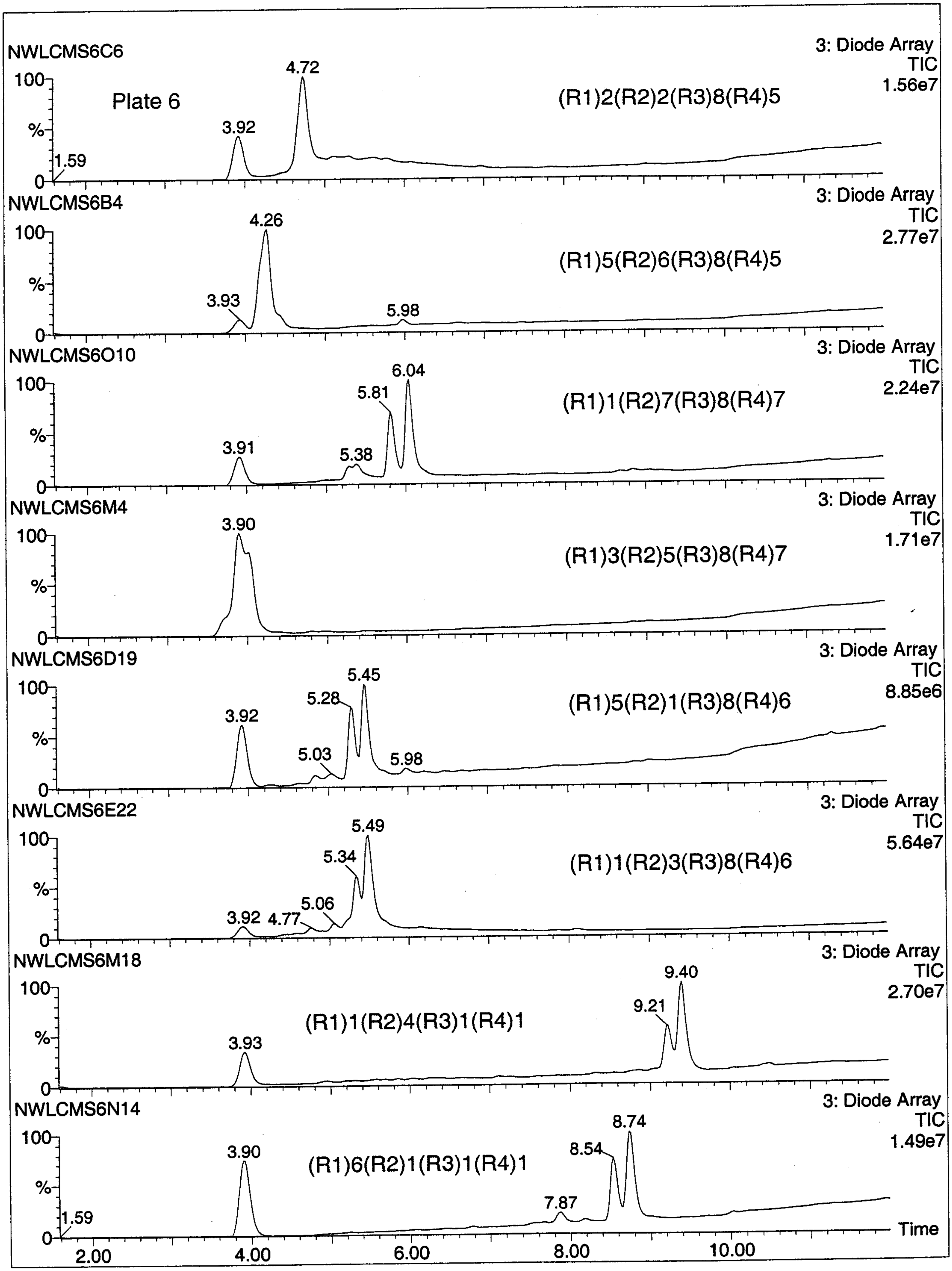


Figure V.3.3.4 S105

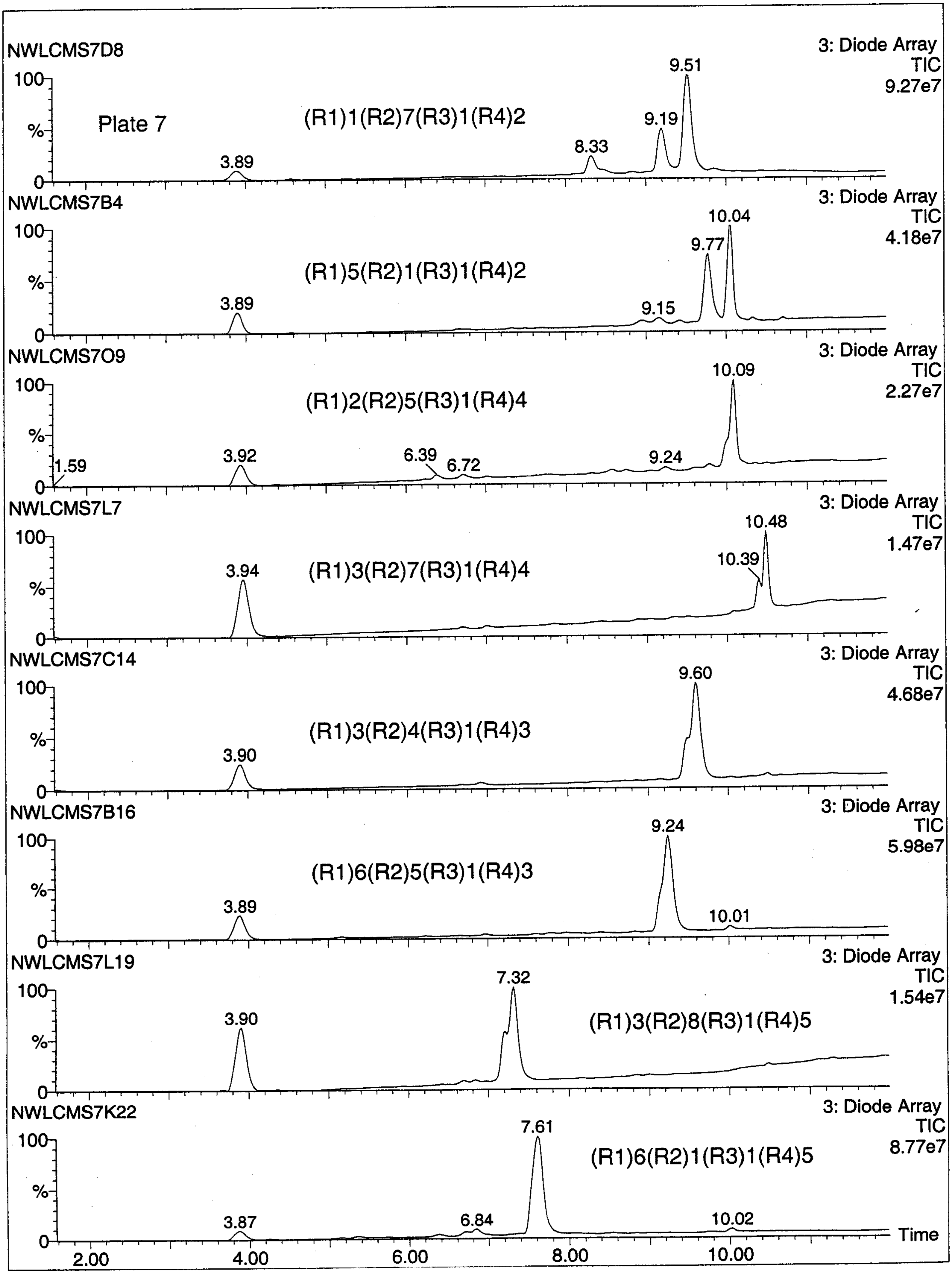


Figure V.3.3.5 S106

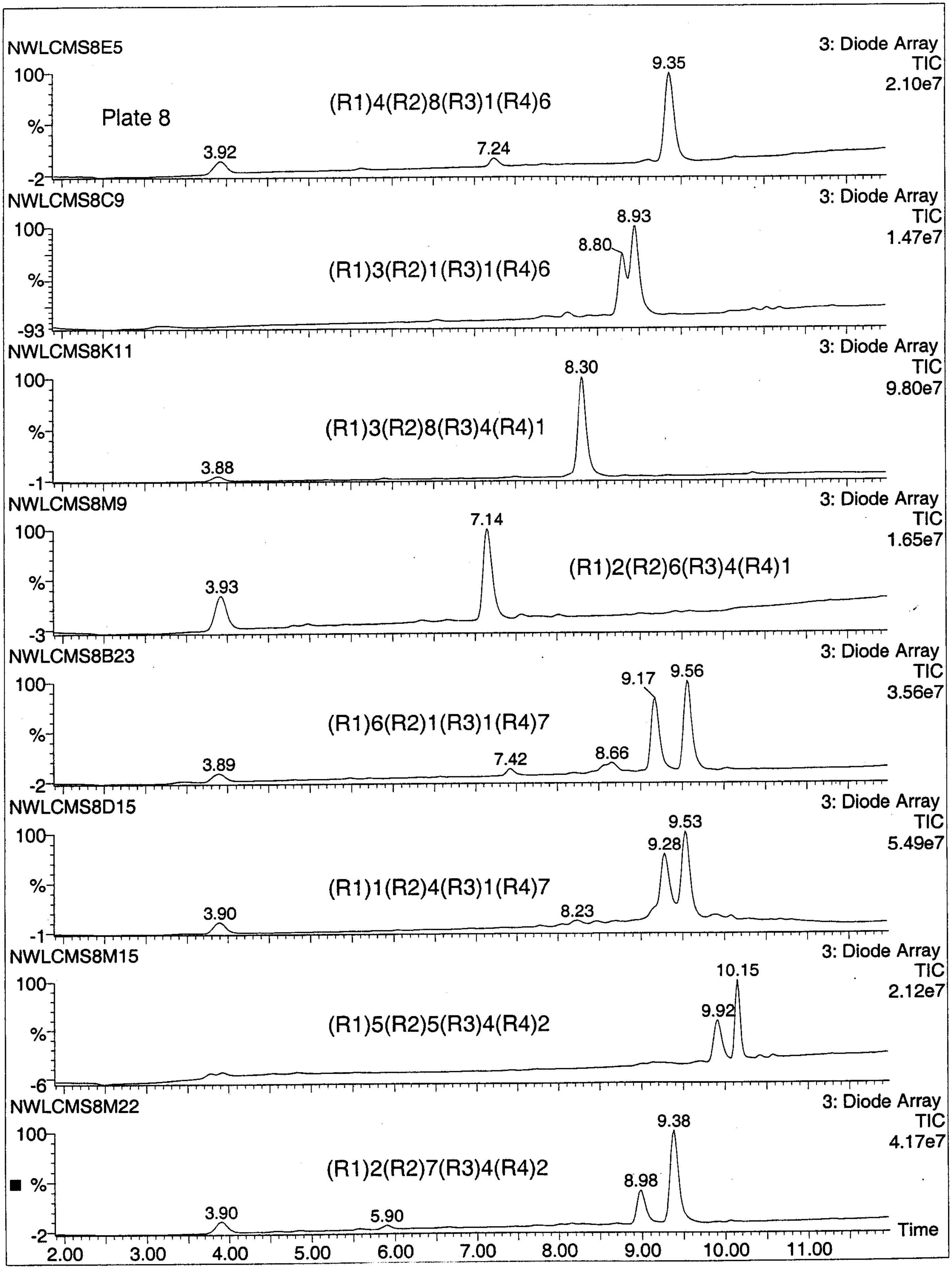


Figure V.3.3.6 S107

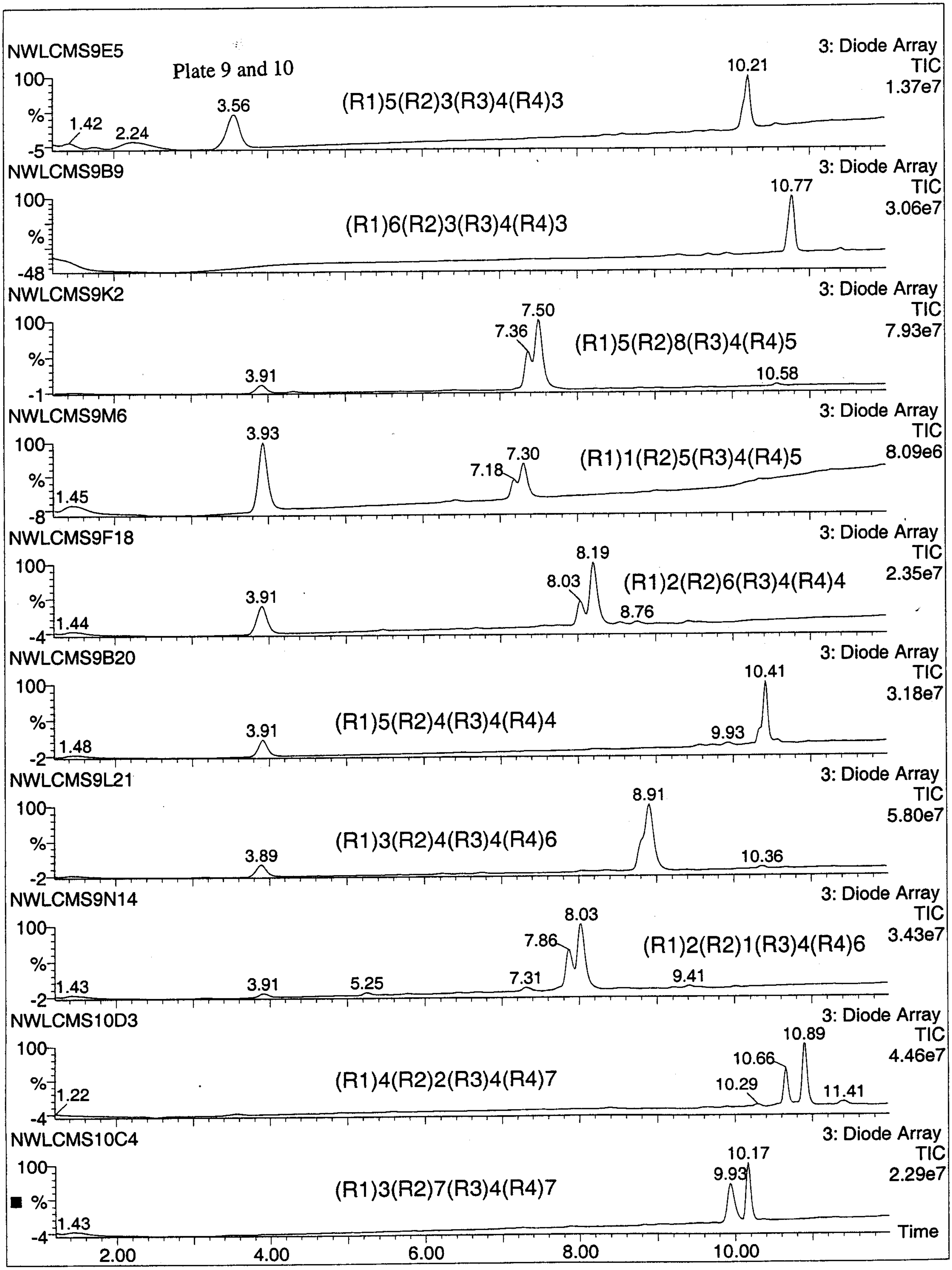


Figure V.3.3.7 S108

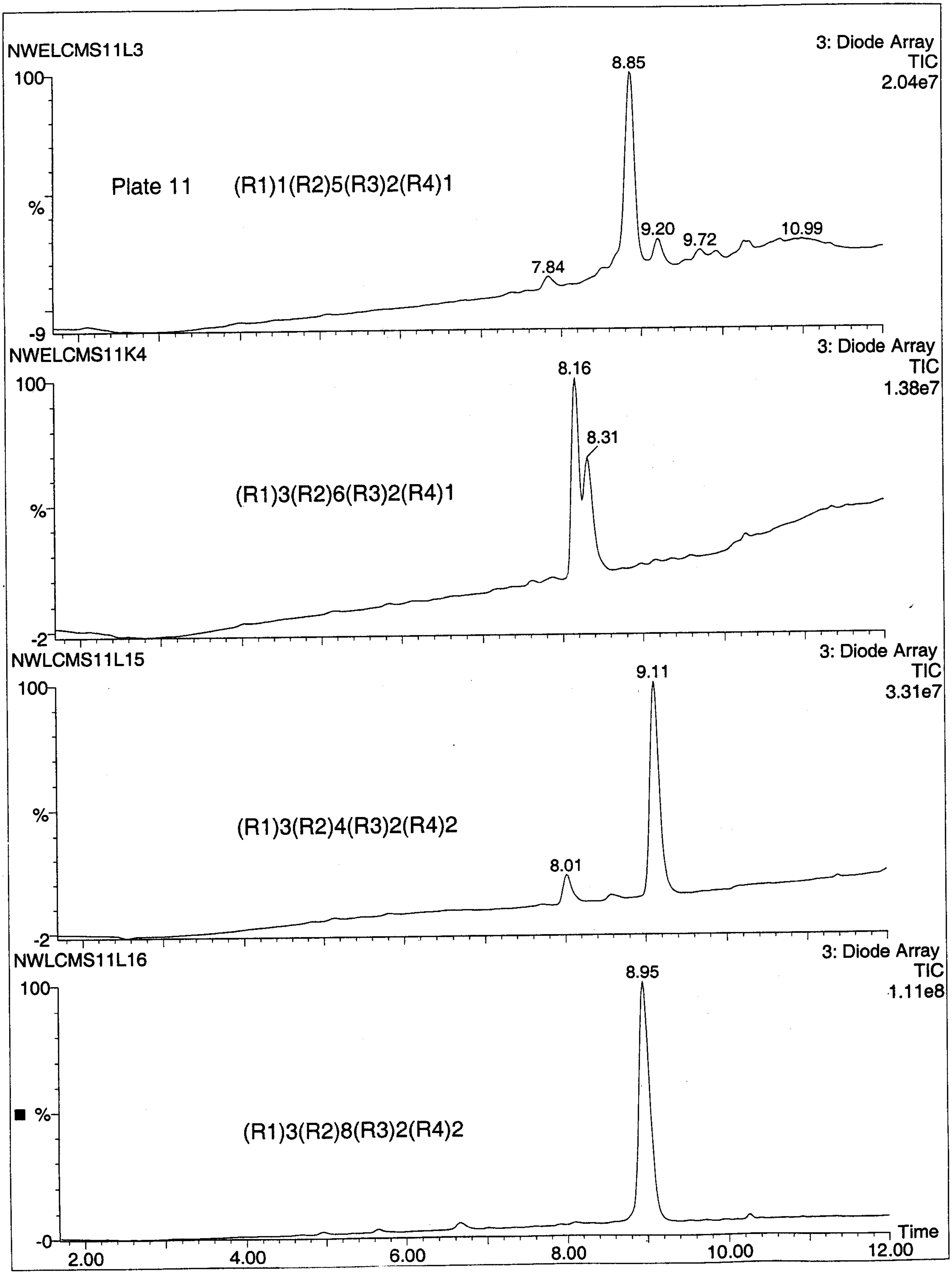


Figure V.3.3.8 S109

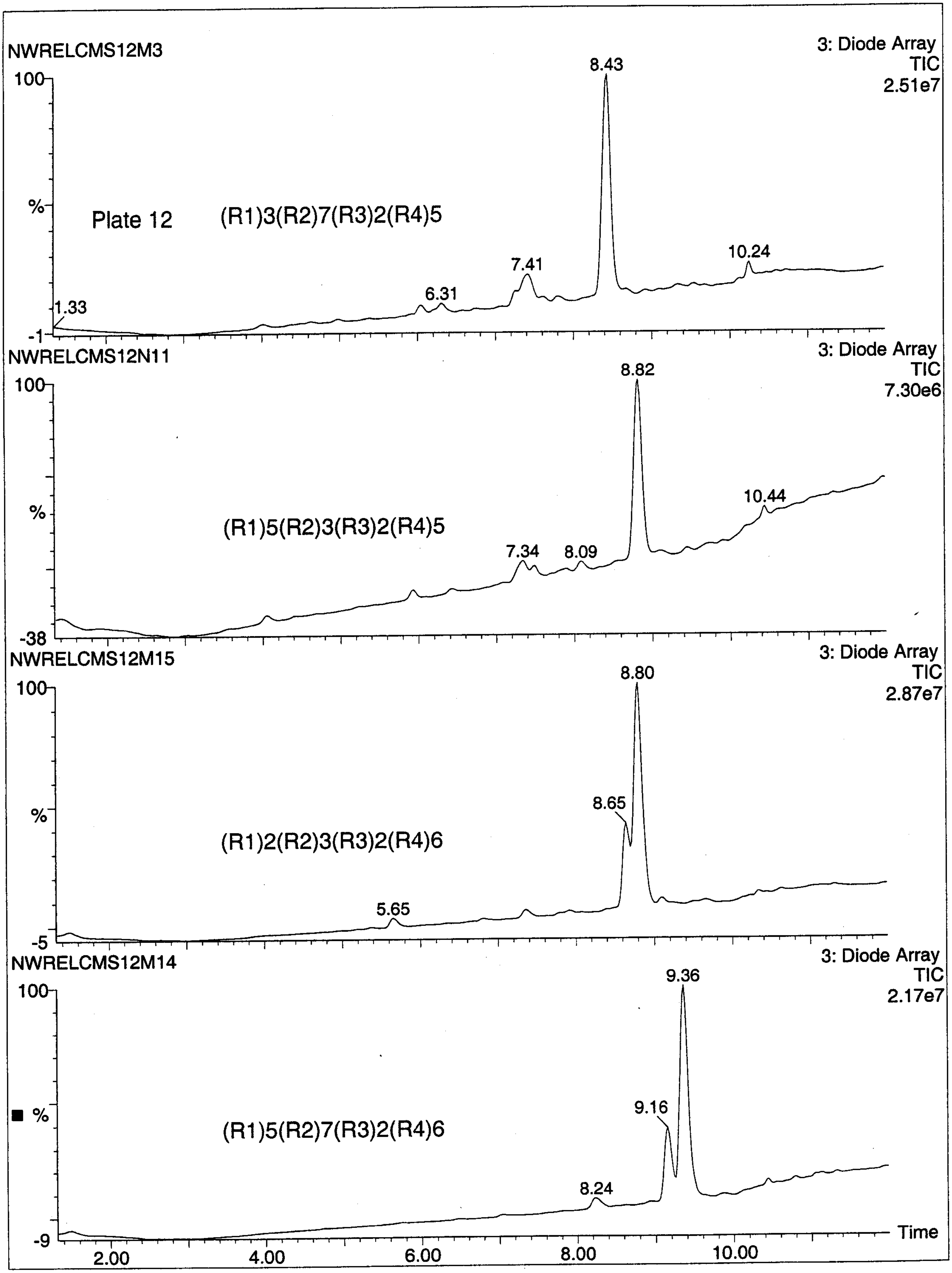


Figure V .3.3.9 S110

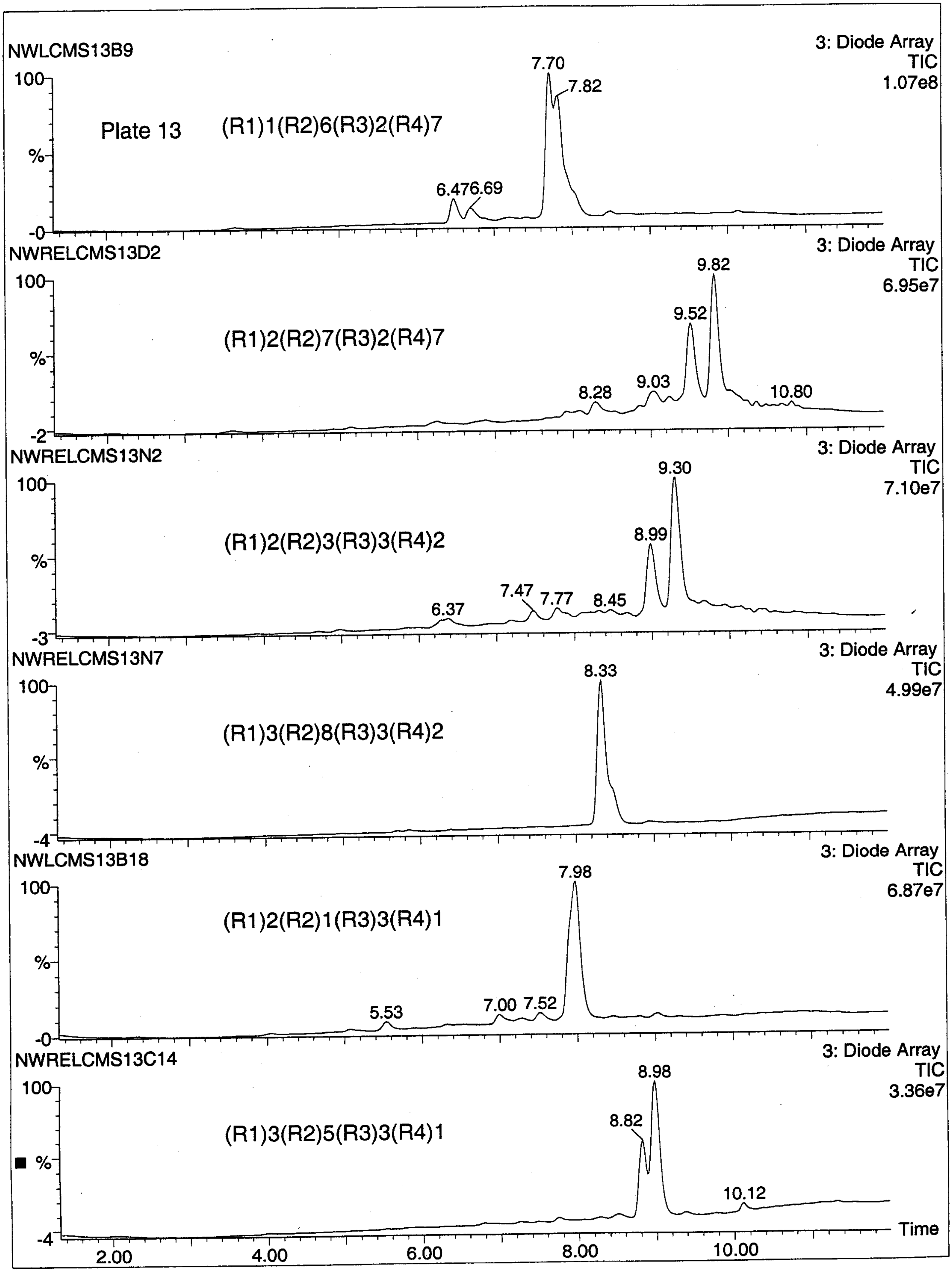


Figure V .3.3.10 S111

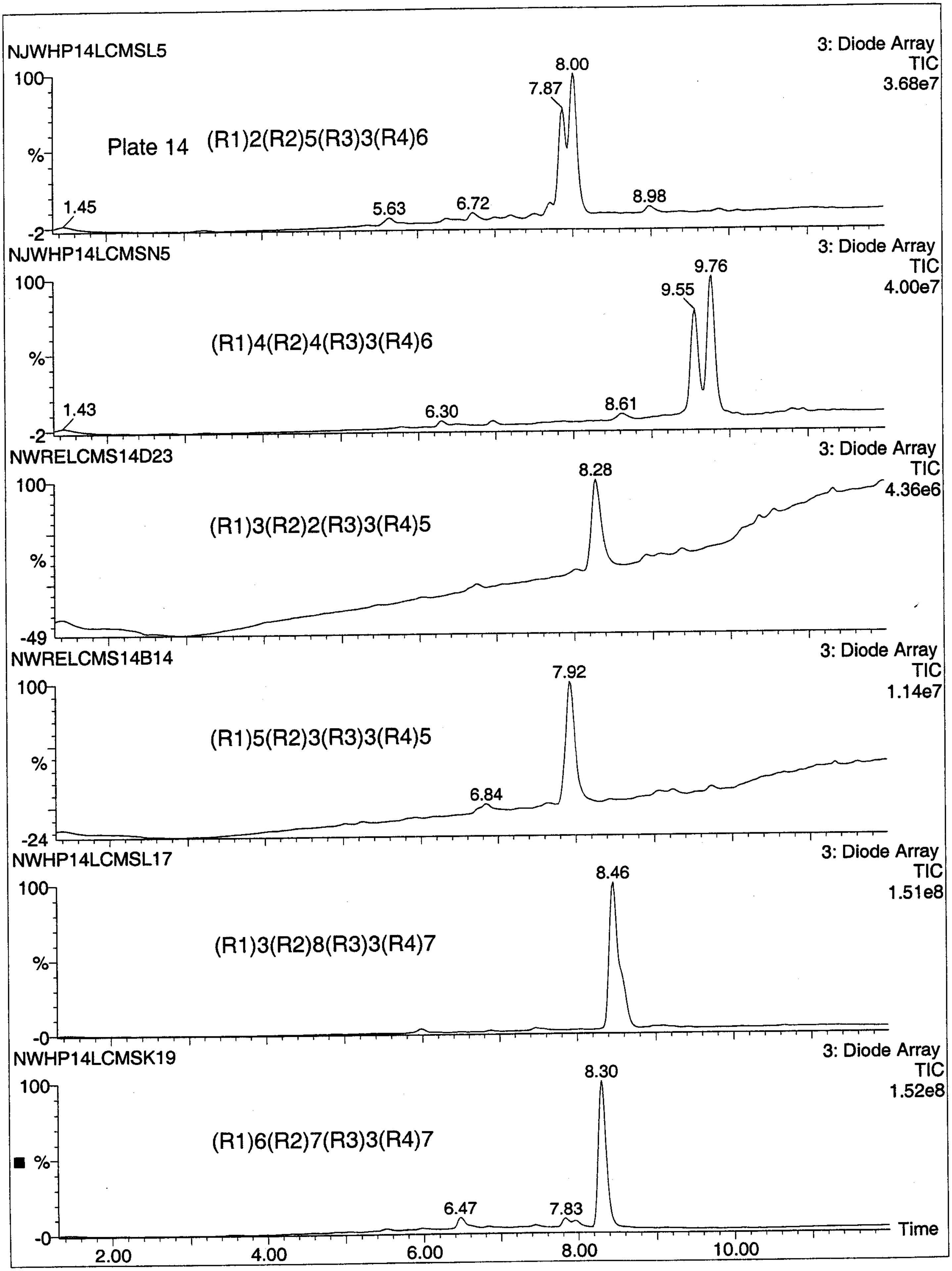


Figure V.3.3.11 S112

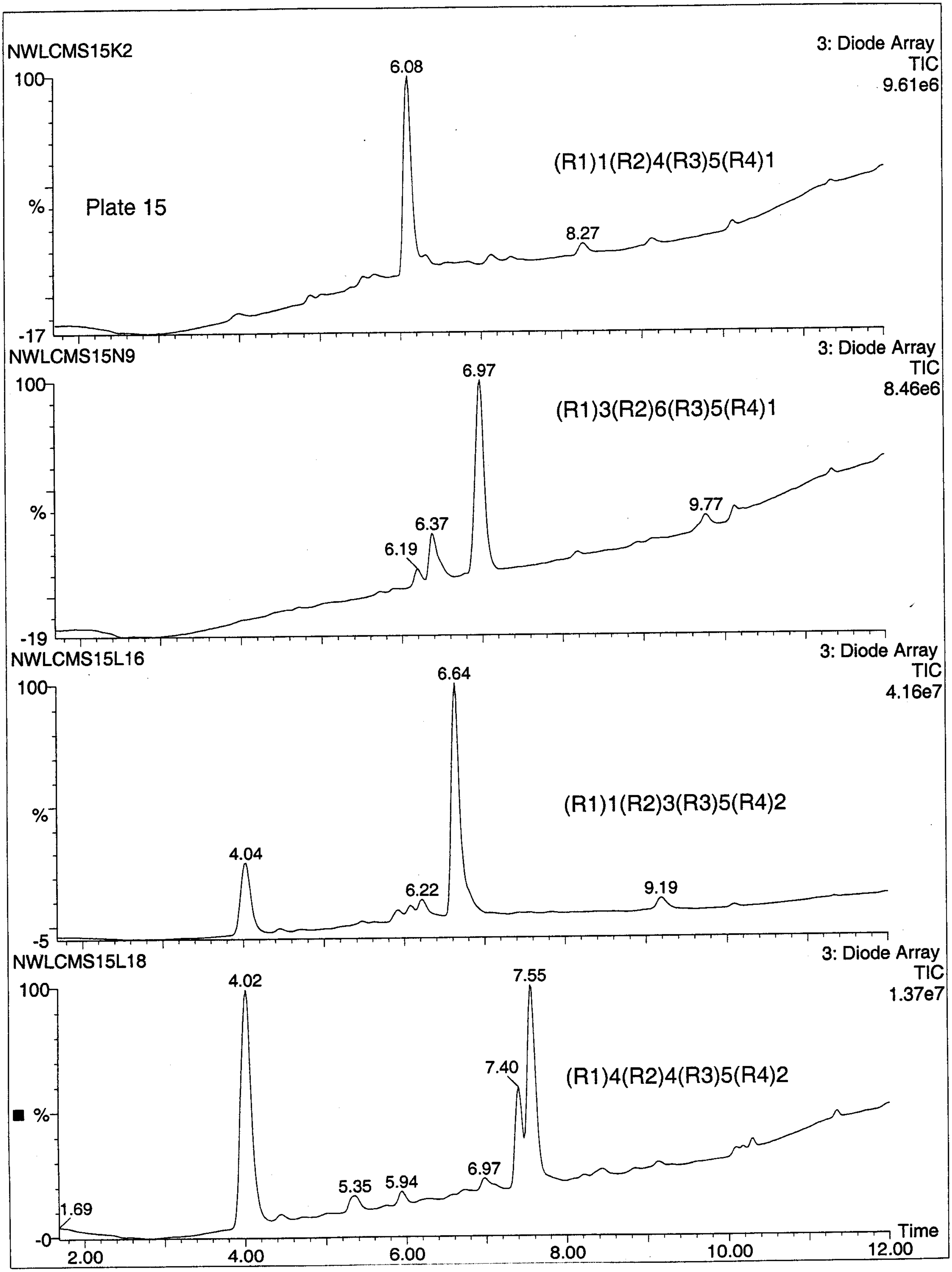


Figure V.3.3.12 S113

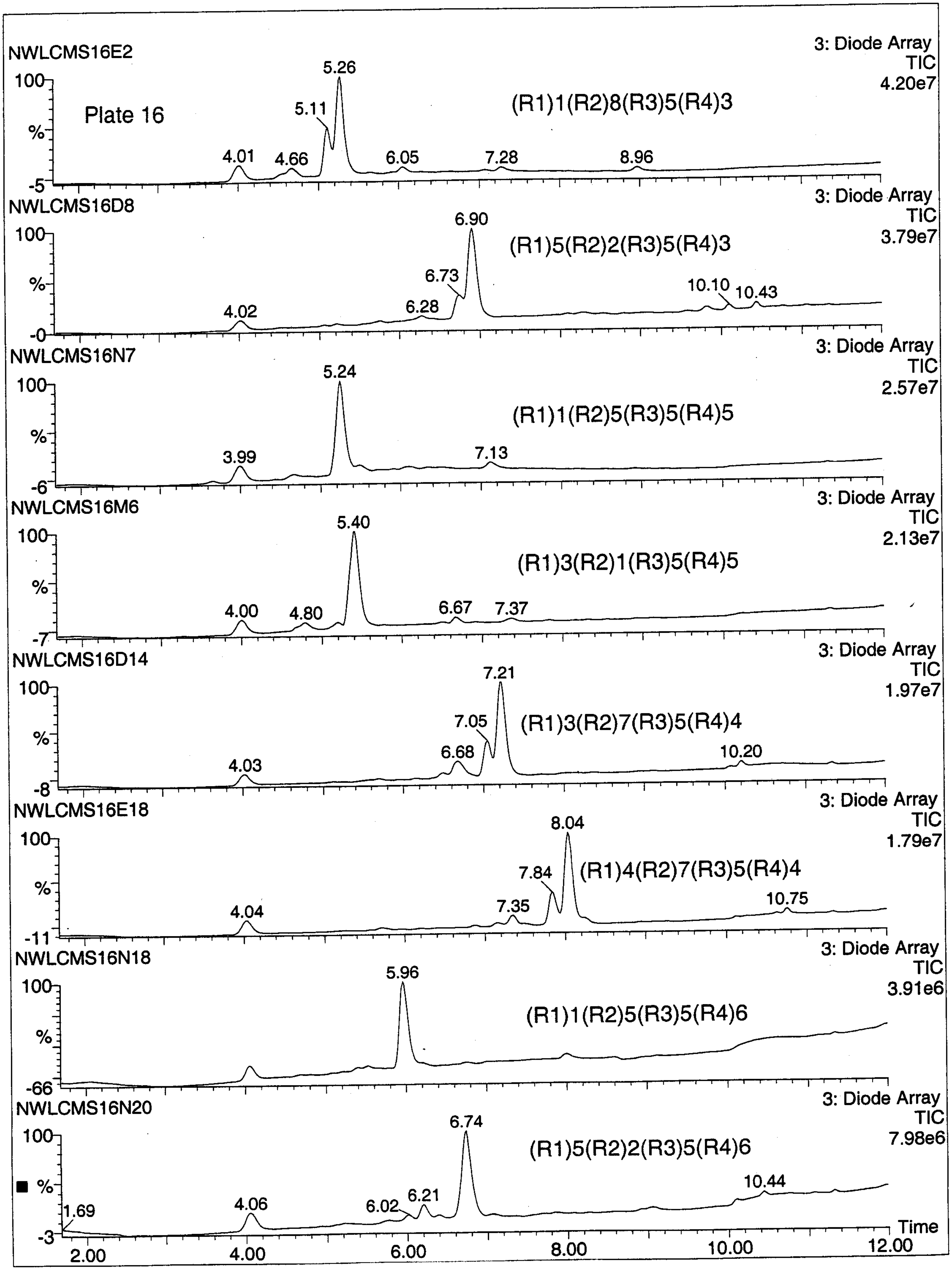


Figure V.3.3.13

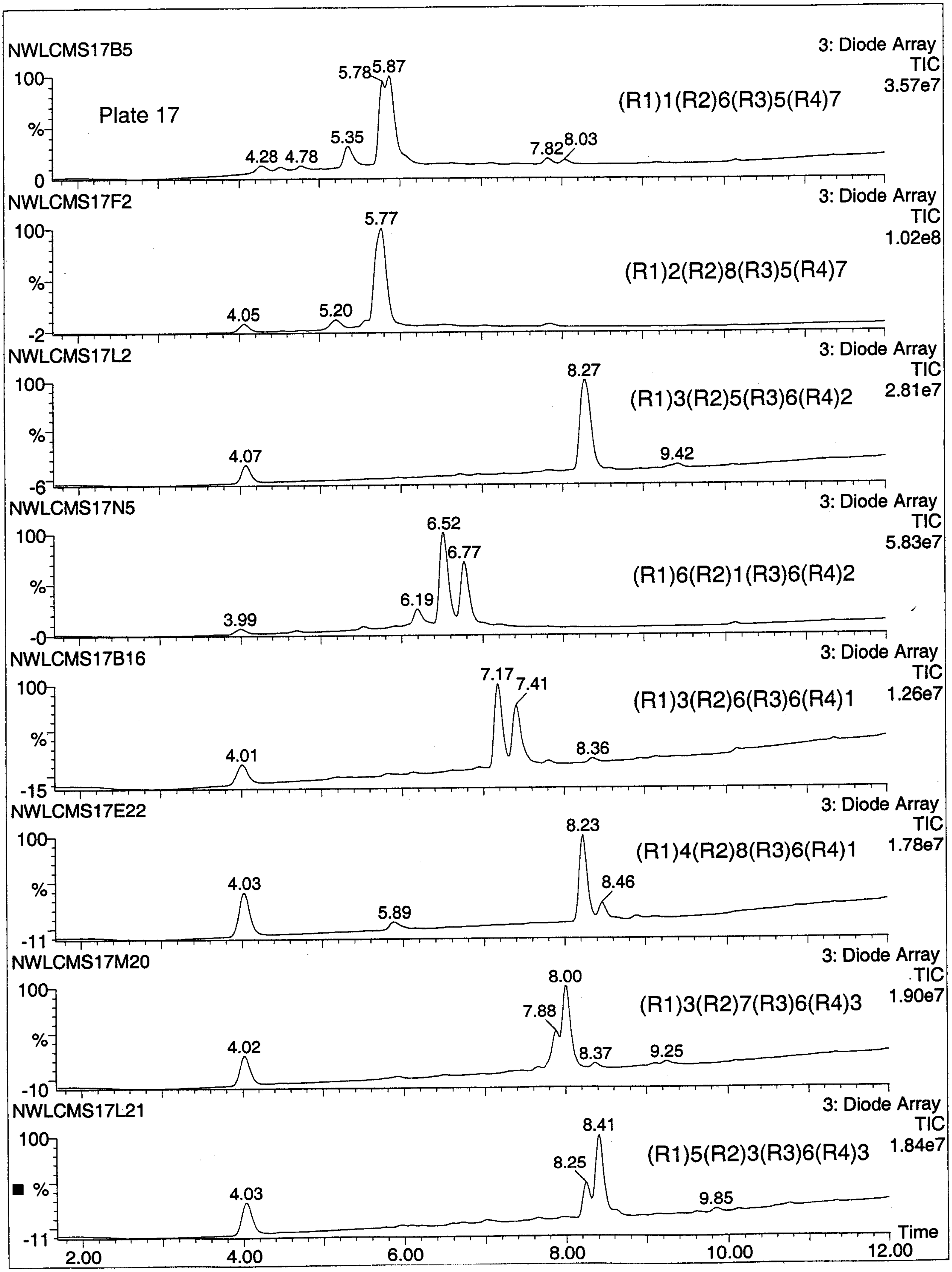


Figure V.3.3.14

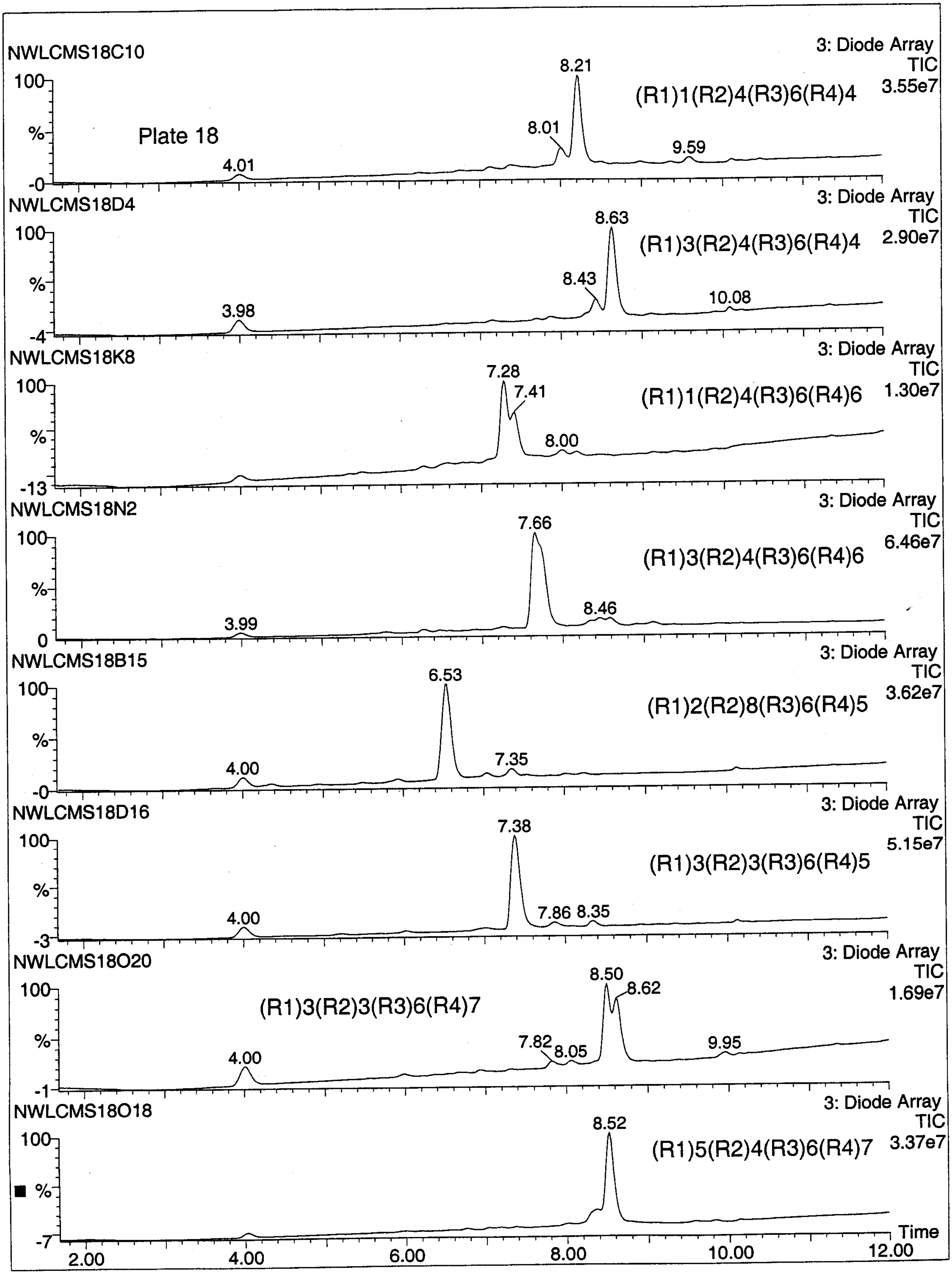
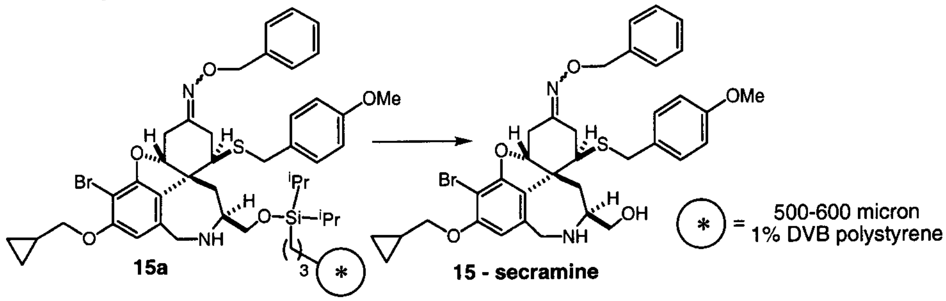


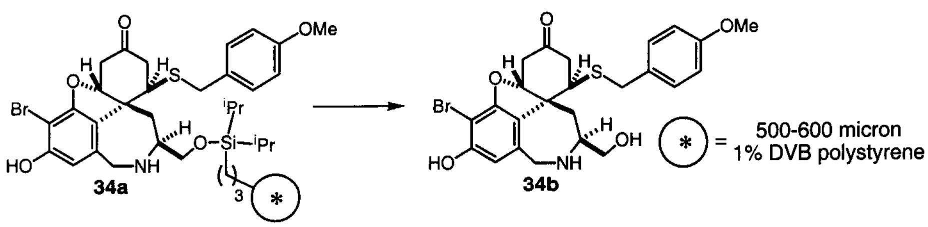
Figure V.3.3.15 5116

V.4 Representative Compound Synthesis and Analytical Data



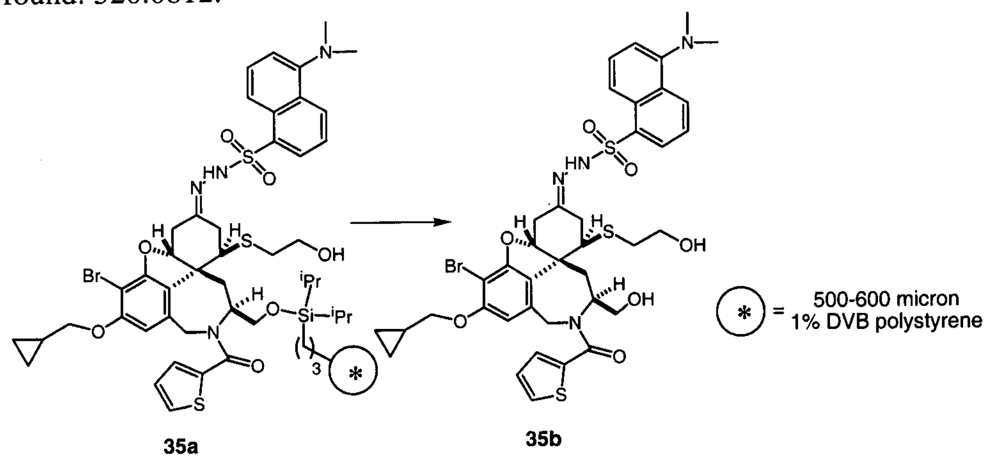
Scheme V.4.1

15: Resin **15a** (40 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (100% EtOAc → 5% MeOH/EtOAc) afforded a yellow film (7.4 mg, loading level = 0.27 mmol/g, theoretical loading level = 0.38 mmol/g, Yield (from **8b**) = 71%. R_f = 0.18 (5% MeOH/CH_2Cl_2); FTIR (film, cm^{-1}) 3368, 2938, 2873, 2306, 1607, 1510, 1429, 1364, 1250, 1176; ^1H NMR (500 MHz, $CDCl_3$) Two isomers are present in a ratio of 1:5. δ 7.42-7.34 (m), 7.31-7.28 (m), 7.19 (d, J = 8.5 Hz), 6.87-6.84 (m), 6.13 (s), 6.10 (s), 5.20 (d, J = 12.5 Hz), 5.16 (d, J = 5 Hz), 5.15 (d, J = 12.5 Hz), 5.13 (d, J = 5 Hz), 4.61 (dd, J = 3.0, 3.0 Hz), 4.56 (dd, J = 3.0, 3.0 Hz), 3.85-3.76 (m), 3.73-3.55 (m), 3.52 (d, J = 13.5 Hz), 3.30 (d, J = 15.5 Hz), 3.13-3.05 (m), 3.00-2.99 (m), 2.96 (dd, J = 3.7, 2.0 Hz), 2.93 (m), 2.74 (m), 2.56 (dd, J = 15.7, 4.0 Hz), 2.34 (d, J = 15.5 Hz), 2.08-2.05 (m), 2.01 (d, J = 14.0 Hz), 1.32-1.18 (m), 1.01 (d, J = 6.5 Hz), 0.96 (d, J = 6.5 Hz), 0.94 (d, J = 3.0 Hz), 0.65-0.61 (m), 0.40-0.35 (m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 157.5, 156.3, 154.6, 140.3, 138.3, 130.5, 130.3, 128.5, 128.4, 127.8, 127.7, 127.6, 124.3, 114.2, 114.1, 106.0, 92.3, 87.6, 75.7, 75.6, 74.2, 65.6, 59.3, 55.5, 52.6, 51.5, 43.3, 41.2, 33.9, 29.4, 27.1, 10.3, 3.3; HRMS (ES^+) calculated for $C_{35}H_{39}BrN_2O_5S$ $(M+H)^+$: 679.1763, found: 679.1816.



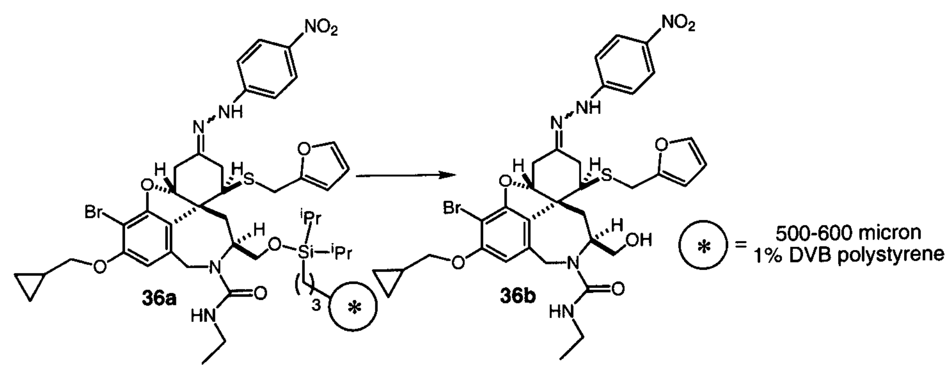
Scheme V.4.2

34b: Resin **34a** (20 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (100% EtOAc; 100% CH_2Cl_2; 10% MeOH/CH_2Cl_2) afforded a yellow film (2.3 mg, loading level = 0.22 mmol/g, theoretical loading level = 0.40 mmol/g, Yield (from **8b**) = 55%. R_f = 0.14 (10% MeOH/CH_2Cl_2); FTIR (film, cm^{-1}) 3407, 2931, 1724, 1701, 1607, 1513, 1426, 1247; ^1H NMR (500 MHz, $(CD_3)_2C(O)$) δ 7.34 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.5 Hz, 2H), 6.34 (s, 1H), 4.80-4.79 (dd, J = 3.0, 3.0 Hz, 1H), 3.87 (d, J = 13.7 Hz, 1H), 3.82 (s, 3H), 3.76 (d, J = 13.5 Hz, 1H), 3.67 (d, J = 15.0 Hz, 1H), 3.52, (dd, J = 10.2, 4.5 Hz, 1H), 3.38, (d, J = 15.0 Hz, 1H), 3.27-3.252 (m, 1H), 3.22 (dd, J = 10.5, 9.0 Hz, 1H), 3.05 (dd, J = 18.5, 3.0 Hz, 1H), 2.97 (m, 1H), 2.82 (dd, J = 18.0, 3.0 Hz, 1H), 2.70 (dd, J = 17.0, 3.50 Hz, 1H), 2.28 (dd, J = 17.5, 3.0 Hz, 1H), 2.16 (d, J = 14.0 Hz, 1H), 1.50-1.40 (m, 1H); ^{13}C NMR (100 MHz, $(CD_3)_2C(O)$) δ 160.0, 158.1, 155.5, 142.2, 131.3, 129.6, 123.6, 114.8, 109.3, 90.1, 89.4, 66.4, 59.6, 55.6, 52.6, 51.9, 44.2, 41.6, 41.2, 41.1, 35.1; HRMS (ES$^+$) calculated for $C_{24}H_{26}NO_5S$ (M+H)$^+$: 520.0715, found: 520.0812.



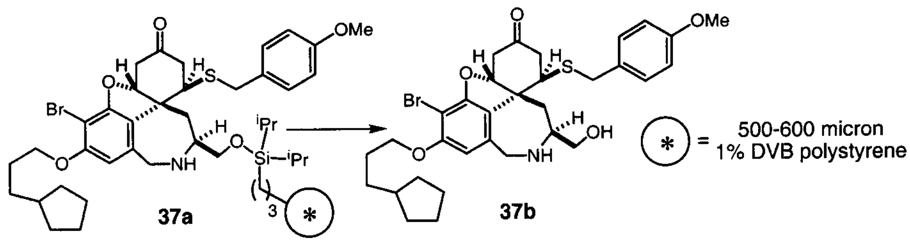
Scheme V.4.3

35b: Resin **35a** (47.5 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (50% EtOAc/hexanes → 100% EtOAc) afforded a yellow solid (12 mg, loading level = 0.30 mmol/g, theoretical loading level = 0.35 mmol/g, Yield (from **8b**) = 86%. R_f = 0.16 (100% EtOAc); FTIR (film, cm^{-1}) 3433, 2925, 2866, 2230, 1604, 1455, 1422, 1331, 1250; ^{1}H NMR (400 MHz, 75°C DMSO) Rotamers and isomers (ratio of 1:1.8) are present. δ 8.51-8.45 (m), 8.41 (d, J = 8.4 Hz), 8.10 (d, J = 7.2 Hz), 7.70 (d, J = 5.2 Hz), 7.67 (d, J = 5.2 Hz), 7.64-7.53 (m), 7.24 (d, J = 7.6 Hz), 7.11-7.06 (m), 4.74 (br s), 4.70 (br s), 3.81 (br s), 3.69-3.65 (m), 3.17 (dd, J = 19.0, 3.2 Hz), 3.04 (s), 2.85-2.74 (m), 2.29 (br s), 2.26-2.14 (m), 2.08 (s), 1.26-1.17 (m), 0.86-0.82 (m), 0.56-0.54 (m), 0.32 (br s); HRMS (ES$^+$) calculated for $C_{39}H_{43}BrN_4O_7S_3$ (M+H)$^+$: 855.1477, found: 855.1515.



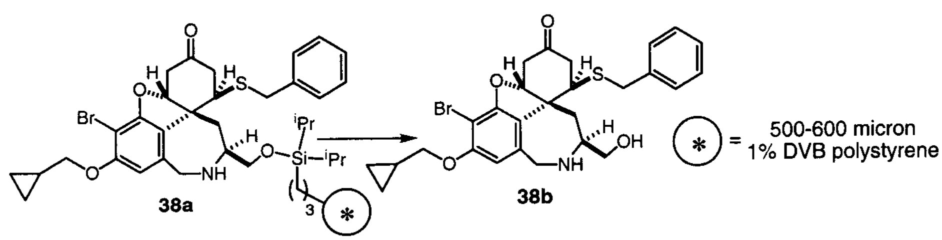
Scheme V.4.4

36b: Resin **36a** (44.1 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (25% EtOAc/hexanes → 100% EtOAc) afforded a yellow solid (8.6 mg, loading level = 0.26 mmol/g, theoretical loading level = 0.37 mmol/g, Yield (from **8b**) = 70%. Two isomers about the C=N are present. R_f = 0.22 (100% EtOAc); FTIR (film, cm^{-1}) 3296, 2932, 2866, 1594, 1494, 1322, 1261; ^{1}H NMR (400 MHz, 65°C DMSO) Two isomers are present in a ratio of 1:2.2 δ 9.93 (s), 9.67 (s), 8.10-8.06 (m), 7.55 (s), 7.52 (s), 7.18 (d, J = 8.8 Hz), 7.12 (d, J = 8.8 Hz), 6.66 (s), 6.65 (s), 6.39-6.36 (m), 6.31, (d, J = 2.8 Hz), 4.82 (s), 4.78 (s), 4.56-4.50 (m), 3.95-3.84 (m), 3.8 (s), 3.78-3.70 (m), 3.62-3.59 (m), 3.37 (dd, J = 18.8, 2.4 Hz), 3.23 (m), 3.04-2.90 (m), 2.65 (d, J = 20.0 Hz), 2.36 (d, J = 16.0 Hz), 2.20 (d, J = 14.0 Hz), 2.14-2.09 (m), 1.98-1.92 (m), 1.25-1.16 (m), 0.93-0.90 (m), 0.86-0.81 (m), 0.60-0.55 (m), 0.37-0.33 (m); ^{13}C NMR (100 MHz, 70°C DMSO) δ 155.1, 150.4, 142.2, 138.1, 125.3, 111.2, 110.2, 73.2, 63.8, 50.7, 34.4, 27.6, 14.7, 9.6, 2.5; HRMS (ES$^+$) calculated for $C_{34}H_{38}BrN_5O_7S$ $(M+H)^+$: 740.1675, found: 740.1726.



Scheme V.4.5

37b: Resin **37a** (19.8 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (100% EtOAc) afforded a yellow foam (3.2 mg, loading level = 0.26 mmol/g, theoretical loading level = 0.38 mmol/g, Yield (from **8b**) = 68%. R_f = 0.29 (100% EtOAc); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, J = 8.5 Hz, 2H), 6.89 (d, J = 8.5 Hz, 2H), 6.2 (s, 1 H), 4.70 (br s, 1H), 3.98-3.90 (m, 2H), 3.82 (s, 3H), 3.81-3.75 (m, 3H), 3.63 (dd, J = 10.3 Hz, 4.5 Hz, 1H), 3.57 (d, J = 13.5 Hz, 1H), 3.22 (d, J = 16.0 Hz, 1H), 3.17 (d, J = 10.0 Hz, 1H), 3.01 (m, 1H), 3.00 (m, 2H), 2.96-2.92 (m, 1H), 2.12 (d, J = 2.12 Hz, 1H), 1.85-1.45 (m, 20H), 1.39-1.24 (m, 3H), 1.11 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.6, 159.1, 156.5, 130.3, 127.9, 114.2, 105.7, 94.3, 88.2, 83.7, 79.2, 69.9, 58.9, 58.9, 55.5, 50.8, 42.5, 40.5, 40.2, 39.8, 34.5, 32.7, 32.4, 28.3, 25.2; MS (APCI$^+$) calculated for $C_{32}H_{40}BrNO_5S$ $(M+H)^+$: 630.1811, found: 630.



Scheme V.4.6

38b: Resin **38a** (19.1 mg) was cleaved as described for **7b**. Purification by flash chromatography with Florisil (100% EtOAc) afforded a yellow oil (3.2 mg, loading level = 0.31 mmol/g, theoretical loading level = 0.39 mmol/g, Yield (from **8b**) = 79%. R_f = 0.23 (100% EtOAc); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.27 (m, 5H), 6.14 (s, 1H), 4.70 (dd, J = 3.2, 3.2 Hz, 1H), 3.86-3.77 (m, 4H), 3.66 (d, J = 15.6 Hz, 1H), 3.61 (d, J = 14.0 Hz, 1H), 3.60 (d, J = 4.4 Hz), 3.58 (d, J = 4.4 Hz, 1H), 2.64 (dd, J = 16.0, 3.6 Hz, 1H), 2.38 (dd, J = 16.0, 2.8 Hz, 1H), 2.11 (d, J = 14.0 Hz, 1H), 1.32-1.24 (m, 3H), 0.66-0.61 (m, 2H), 0.38-0.34 (m, 2H); MS (APCI$^+$) calculated for $C_{27}H_{30}BrNO_4S$ $(M+H)^+$: 544.1079, found: 544.

V.4.3 NMR Spectra for Structure, Purity Assessment, and Diastereoselectivity

Crude and Purified Compound NMR Spectra are provided for 3 representative compounds – **15** (secramine), **37b**, and **38b** to establish purity of crude material. Comparison of the crude NMR to the purified compound NMR for **37b**, and **38b** (see proton H_a) demonstrates that only one diastereomer is present.

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[3] Department of Cell Biology, Harvard Medical School

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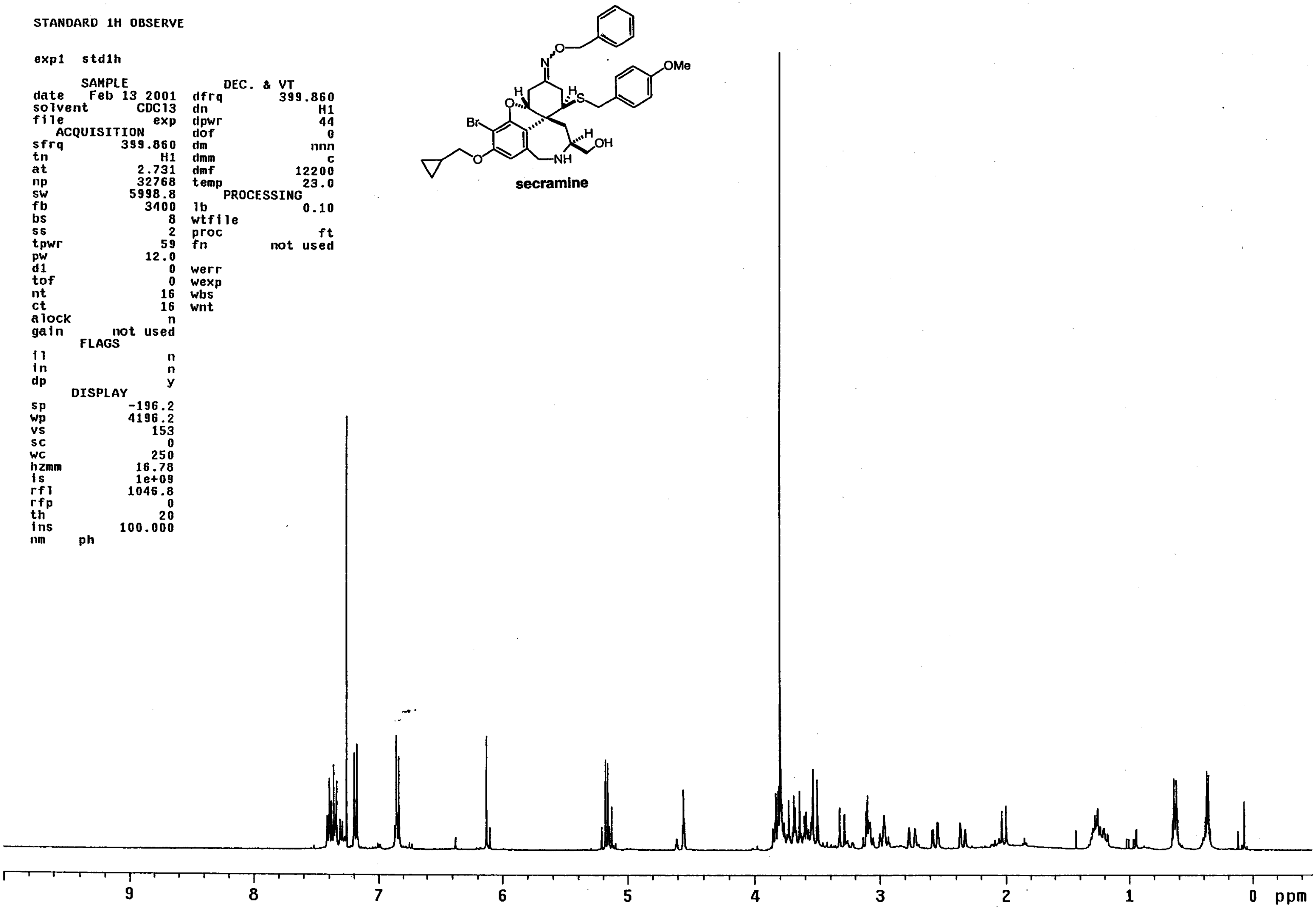
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sw 5998.8
fb 3400
bs 8
ss 2
tpwr 59
pw 12.0
d1 0
tof 0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
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sc 0
wc 250
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is 1e+09
rfl 1046.8
rfp 0
th 20
ins 100.000
nm ph
DEC. & VT
dfrq 399.860
dn H1
dpwr 44
dof 0
dm nnn
dmm c
dmf 12200
temp 23.0
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
OMe
N
O
H
S
Br
OH
NH
secramine
9
8
7
6
5
4
3
2
1
0 ppm

Figure V.4.2.1

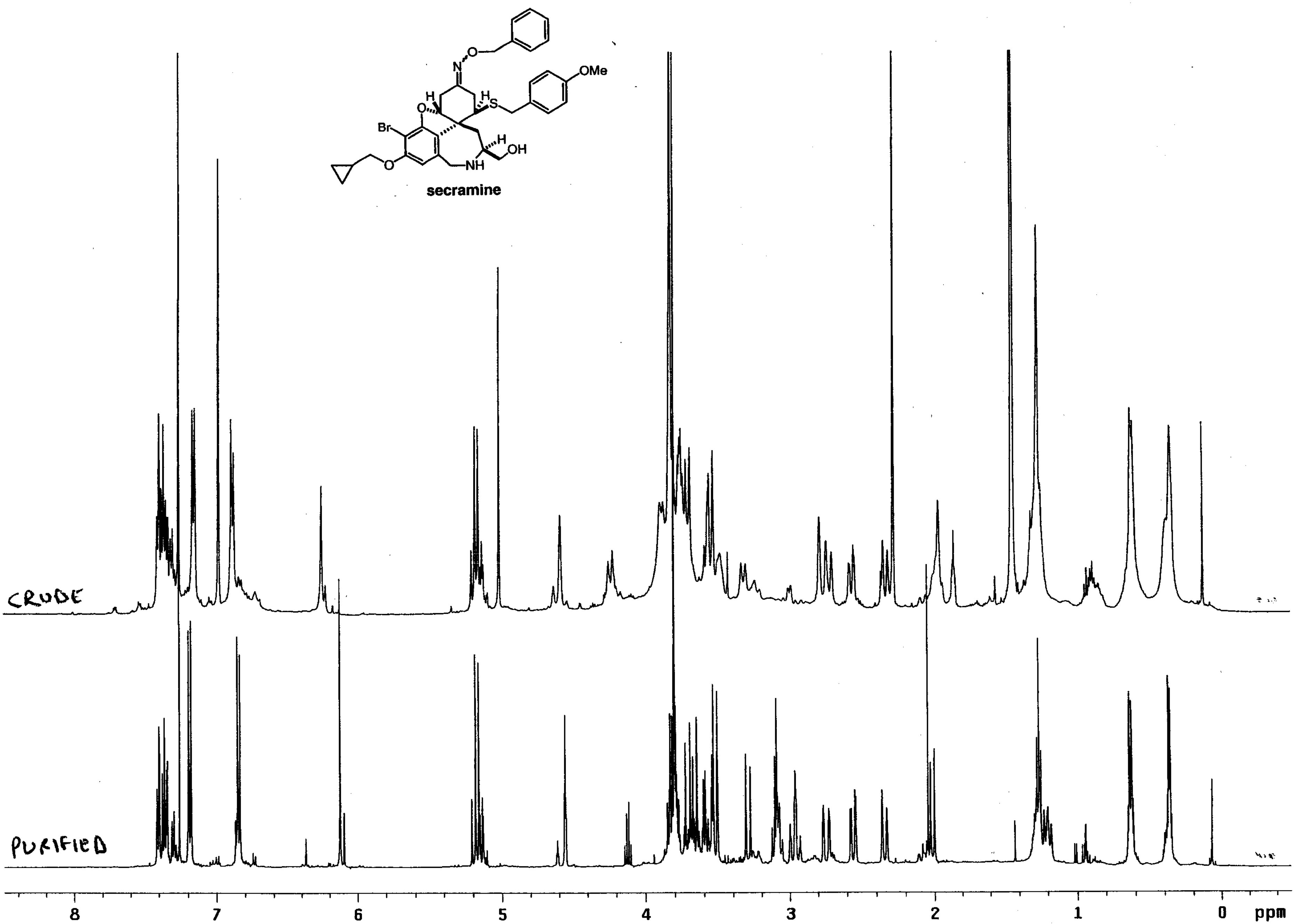
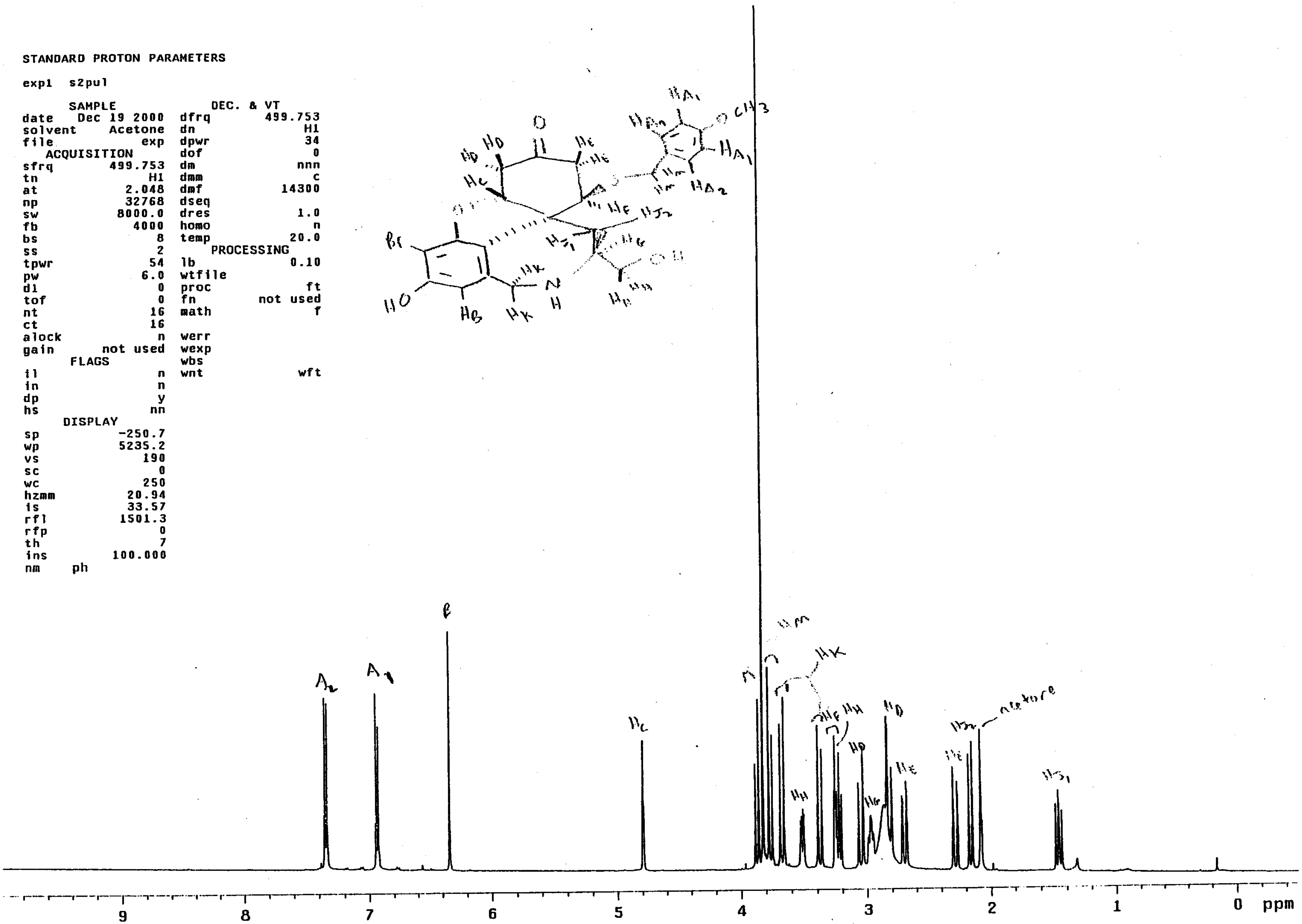


Figure V.4.2.2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SAMPLE
date Dec 19 2000
solvent Acetone
file exp
ACQUISITION
sfrq 499.753
tn H1
at 2.048
np 32768
sw 8000.0
fb 4000
bs 8
ss 2
tpwr 54
pw 6.0
d1 0
tof 0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.7
wp 5235.2
vs 190
sc 0
wc 250
hzmm 20.94
is 33.57
rfl 1501.3
rfp 0
th 7
ins 100.000
nm ph
DEC. & VT
dfrq 499.753
dn H1
dpwr 34
dof 0
dm nnn
dmm c
dmf 14300
dseq
dres 1.0
homo n
temp 20.0
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
math f
werr
wexp
wbs
wnt wft
9
8
7
6
5
4
3
2
1
0 ppm

Figure V.4.2.3

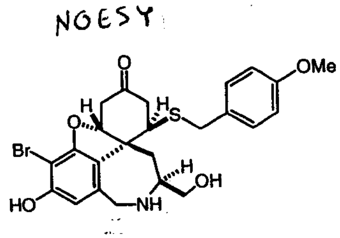
STANDARD PROTON PARAMETERS

Pulse Sequence: NOESY

Solvent: Acetone
Temp. 22.0 C / 295.1 K
INOVA-500 "inova500b"

PULSE SEQUENCE: NOESY
Relax. delay 1.000 sec
Mixing 0.400 sec
Acq. time 0.155 sec
Width 3304.4 Hz
2D Width 3304.4 Hz
48 repetitions
2 x 200 increments
OBSERVE H1, 500.2111386 MHz
DATA PROCESSING
Gauss apodization 0.072 sec
F1 DATA PROCESSING
Gauss apodization 0.056 sec
FT size 2048 x 2048
Total time 8 hr, 32 min, 26 sec

NOESY



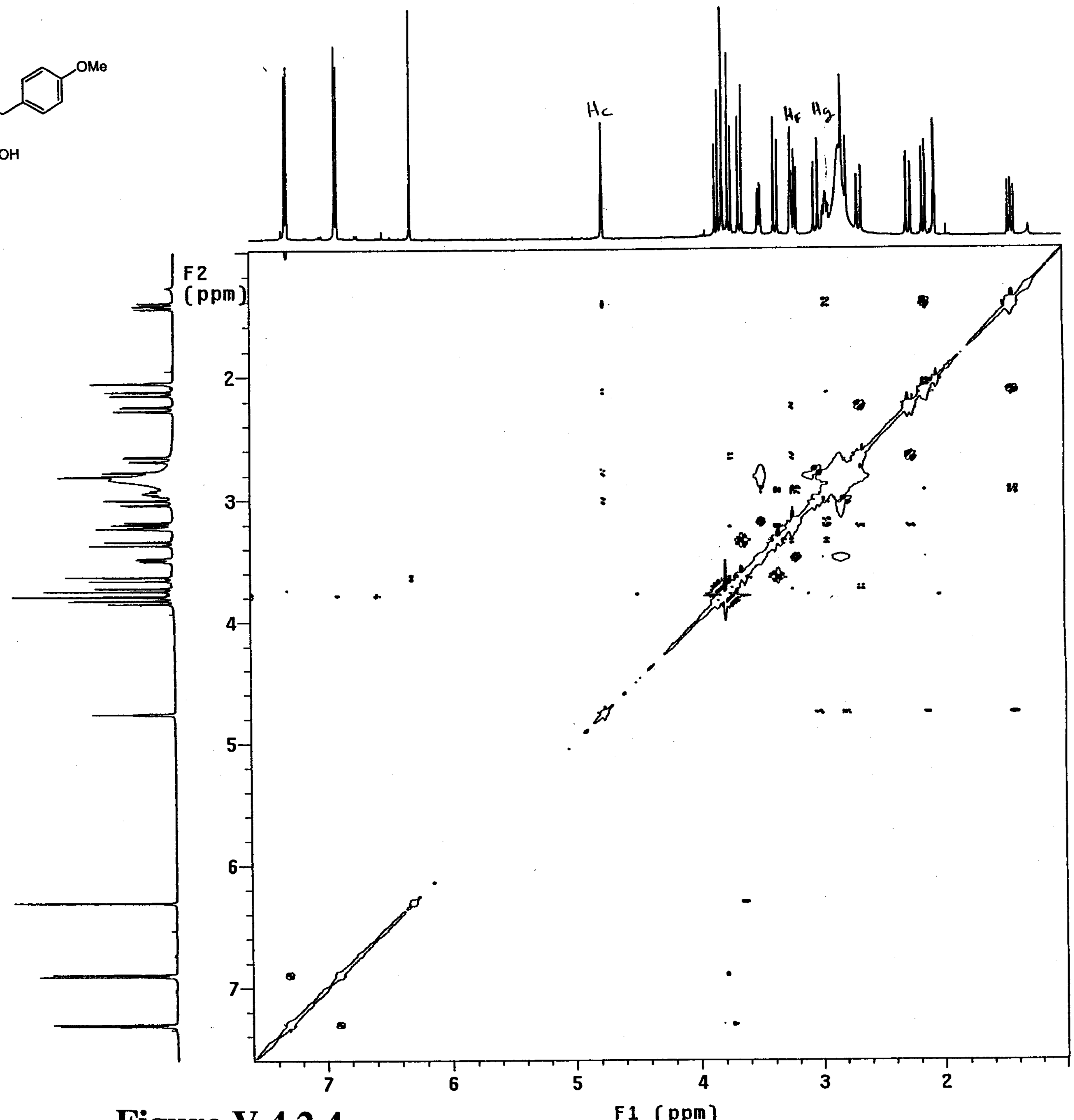


Figure V.4.2.4

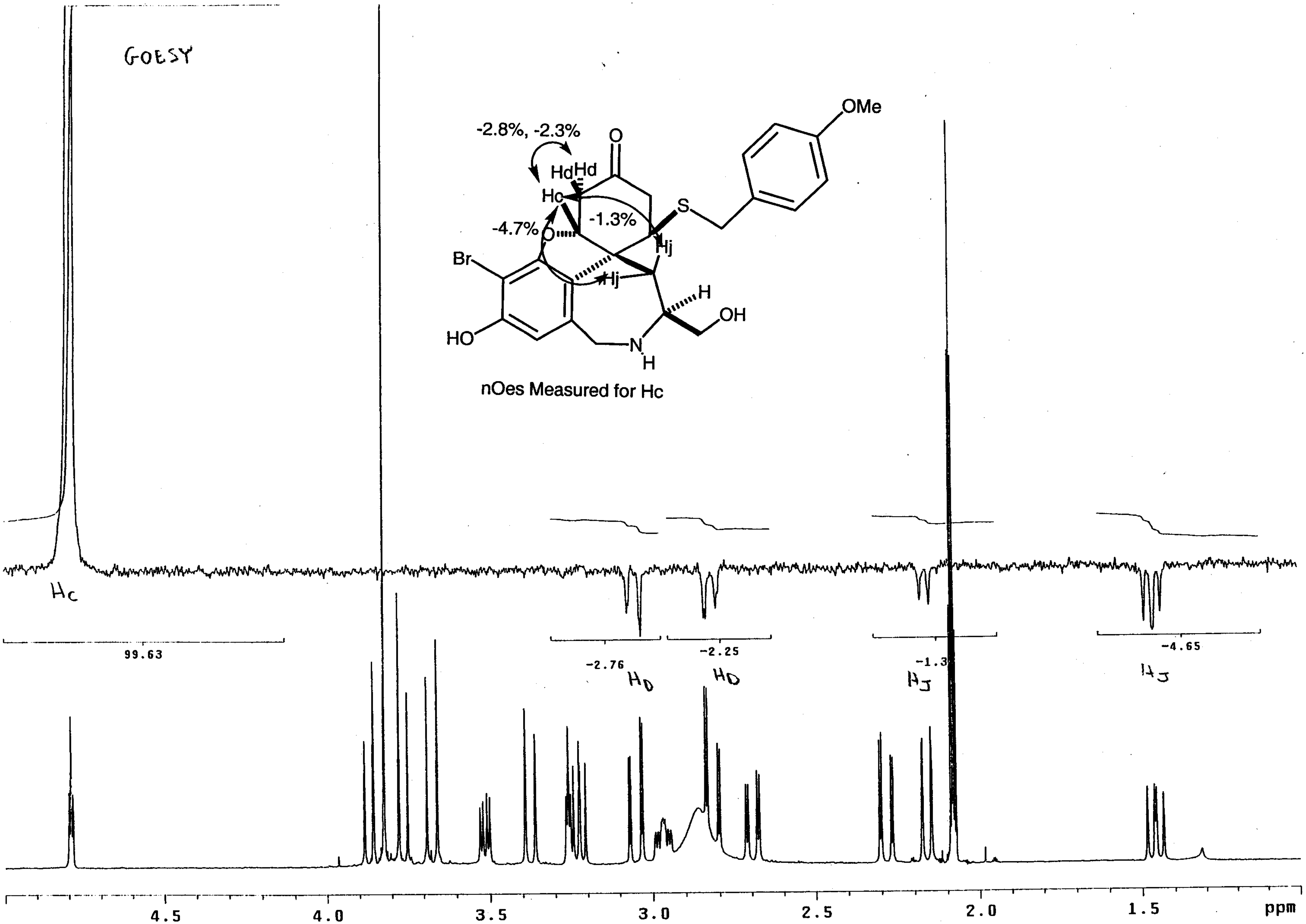
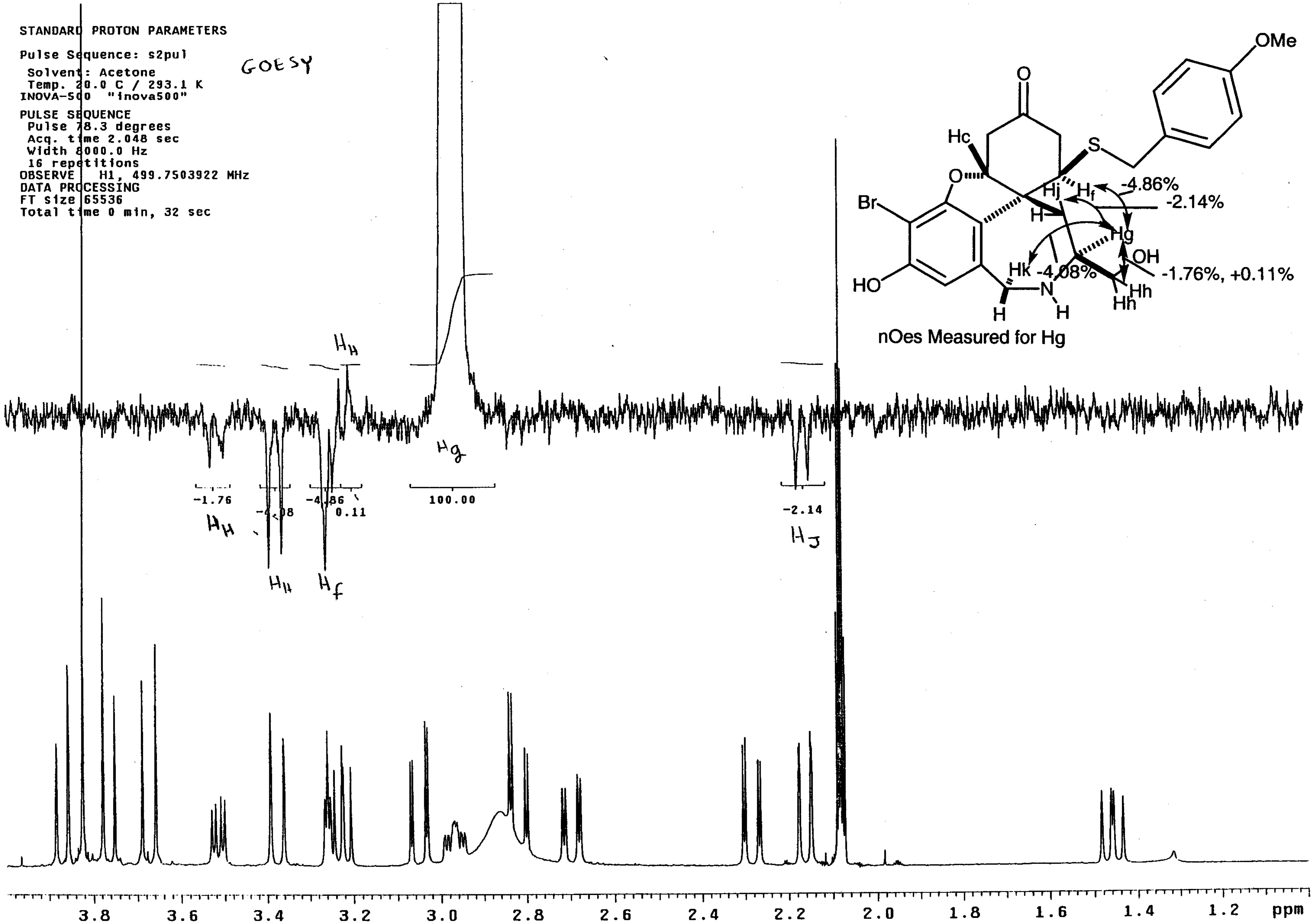

GOESY
-2.8%, -2.3%
Hd
Hd
Hc
-4.7%
-1.3%
Hj
Hj
O
S
OMe
Br
HO
H
OH
N
H
nOes Measured for Hc
Hc
99.63
-2.76
HD
-2.25
HD
-1.3
HJ
-4.65
HJ
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

Figure V.4.2.5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Pulse Sequence: s2pul
Solvent: Acetone
Temp. 20.0 C / 293.1 K
INOVA-500 "inova500"
PULSE SEQUENCE
Pulse 78.3 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7503922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 32 sec
GOESY
OMe
O
Hc
S
Br
HO
Hj
Hf
-4.86%
-2.14%
H
Hg
OH
Hk
-4.08%
-1.76%, +0.11%
N
H
Hh
nOes Measured for Hg
-1.76
-4.08
-4.86
0.11
100.00
-2.14
Hg
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
ppm

Figure V.4.2.6

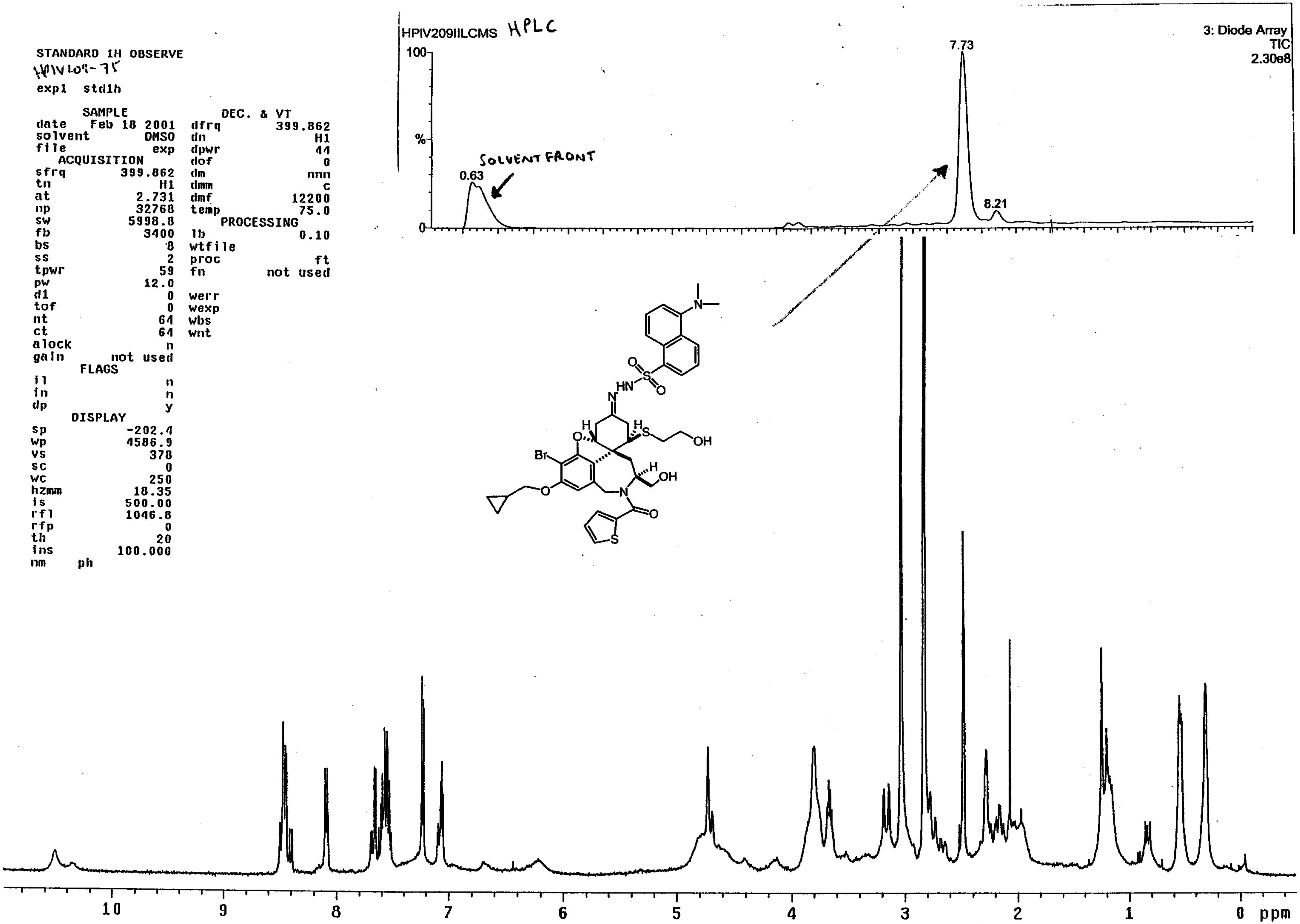

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Feb 18 2001
solvent DMSO
file exp
ACQUISITION
sfrq 399.862
tn H1
at 2.731
np 32768
sw 5998.8
fb 3400
bs 8
ss 2
tpwr 59
pw 12.0
d1 0
tof 0
nt 64
ct 64
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -202.4
wp 4586.9
vs 378
sc 0
wc 250
hzmm 18.35
is 500.00
rfl 1046.8
rfp 0
th 20
ins 100.000
nm ph
DEC. & VT
dfrq 399.862
dn H1
dpwr 44
dof 0
dm nnn
dmm c
dmf 12200
temp 75.0
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
HPIV209IILCMS HPLC
3: Diode Array
TIC
2.30e8
100
%
0
0.63
SOLVENT FRONT
7.73
8.21
10
9
8
7
6
5
4
3
2
1
0 ppm

Figure V.4.2.7

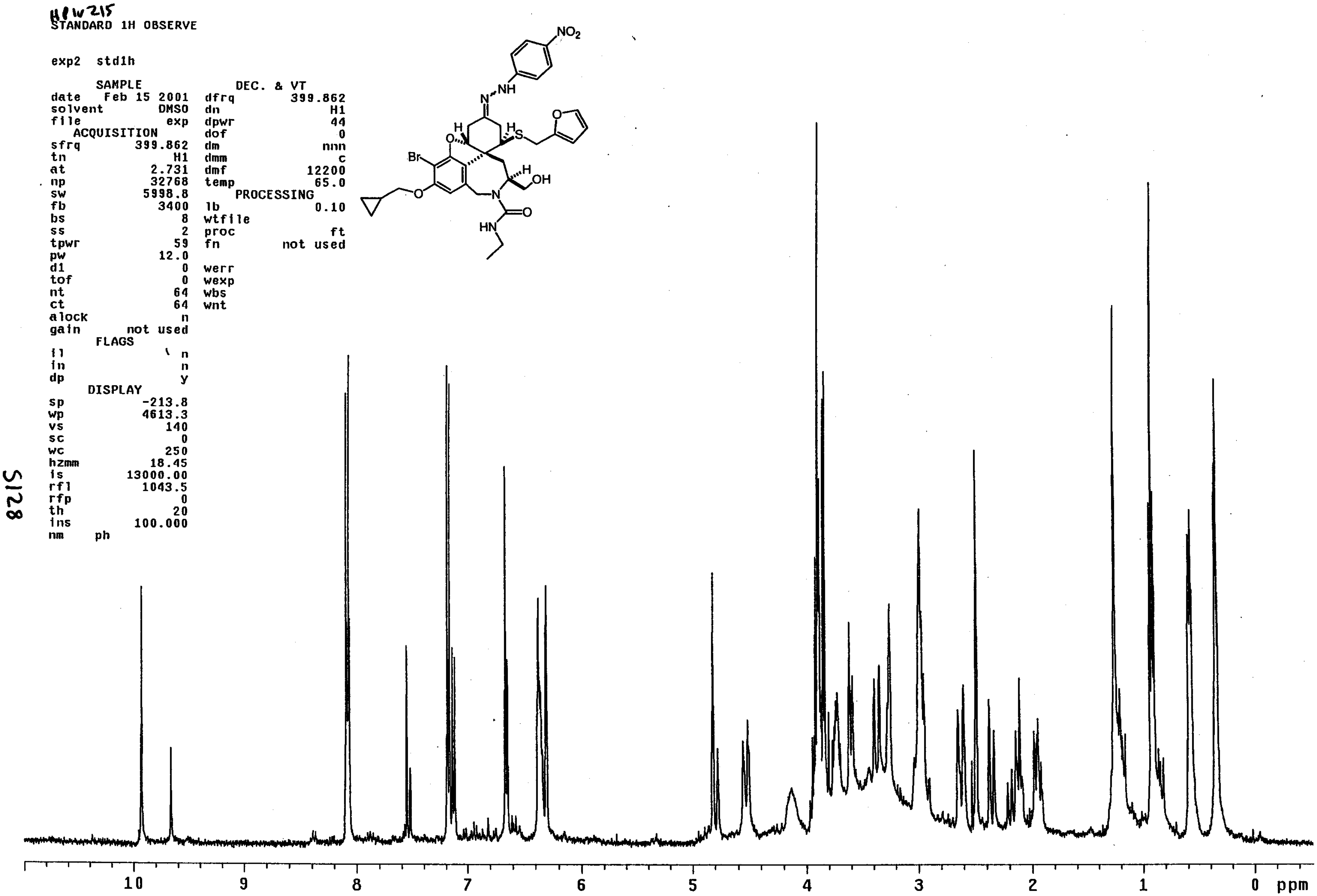

HPW215
STANDARD 1H OBSERVE
exp2 std1h
SAMPLE
date Feb 15 2001
solvent DMSO
file exp
ACQUISITION
sfrq 399.862
tn H1
at 2.731
np 32768
sw 5998.8
fb 3400
bs 8
ss 2
tpwr 59
pw 12.0
d1 0
tof 0
nt 64
ct 64
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -213.8
wp 4613.3
vs 140
sc 0
wc 250
hzmm 18.45
is 13000.00
rfl 1043.5
rfp 0
th 20
ins 100.000
nm ph
DEC. & VT
dfrq 399.862
dn H1
dpwr 44
dof 0
dm nnn
dmm c
dmf 12200
temp 65.0
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
NO2
NH
N
O
H
S
Br
OH
N
O
HN
10
9
8
7
6
5
4
3
2
1
0 ppm

Figure V.4.2.8

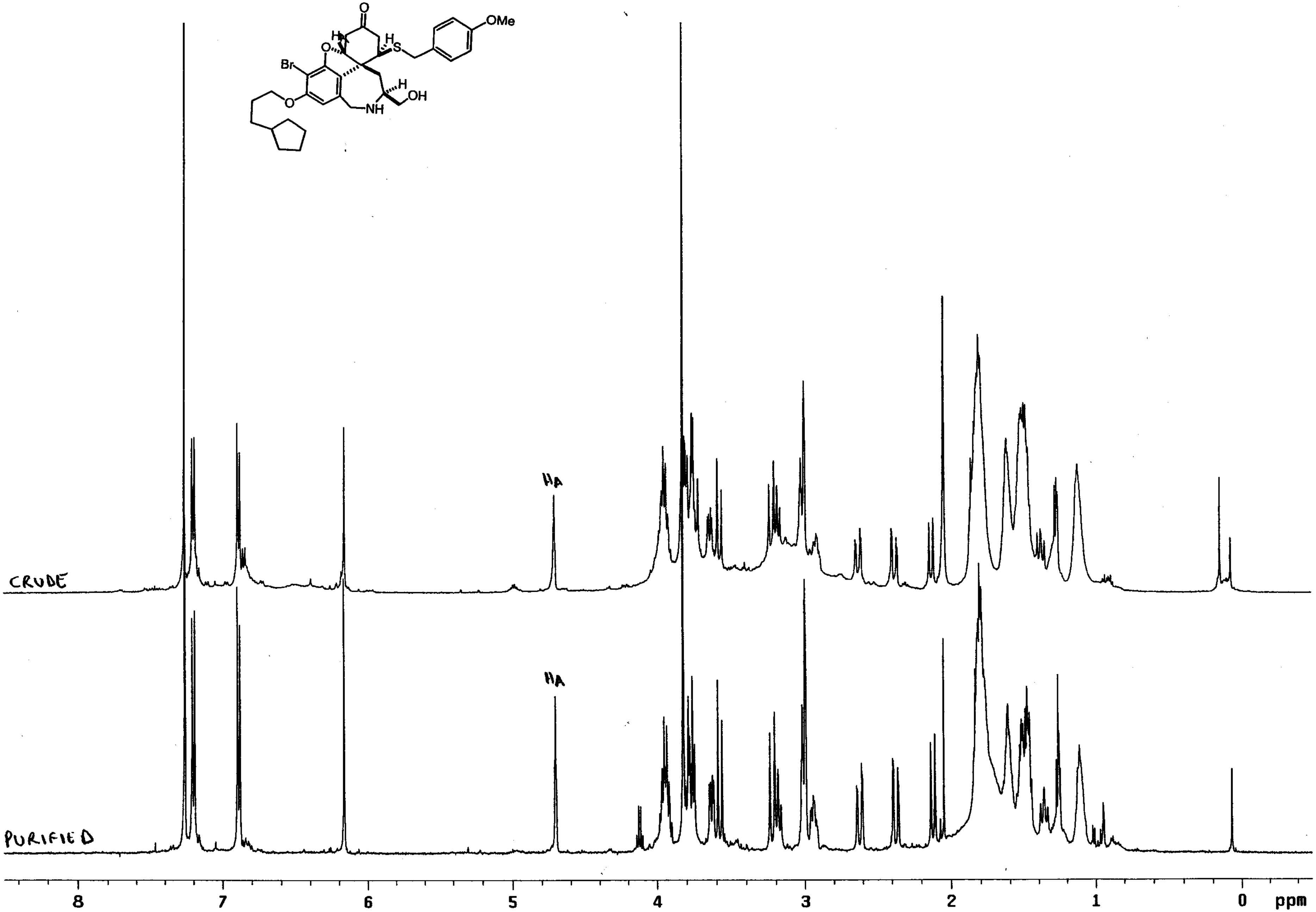
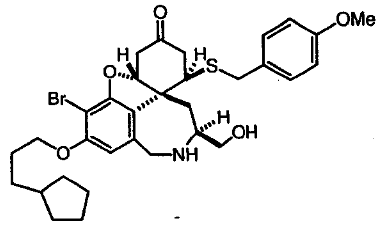


Figure V.4.2.9

STANDARD 1H OBSERVE

Pulse Sequence: gCOSY
 Solvent: CDCl3
 Temp. 23.0 C / 296.1 K
Mercury-400BB "mercury400b"
PULSE SEQUENCE: gCOSY
 Relax. delay 1.000 sec
 Acq. time 0.171 sec
 Width 5998.8 Hz
 2D Width 5998.8 Hz
 Single scan
 128 increments
OBSERVE H1, 399.8581284 MHz
DATA PROCESSING
 Sq. sine bell 0.085 sec
F1 DATA PROCESSING
 Sq. sine bell 0.021 sec
FT size 2048 x 2048
Total time 3 min, 46 sec



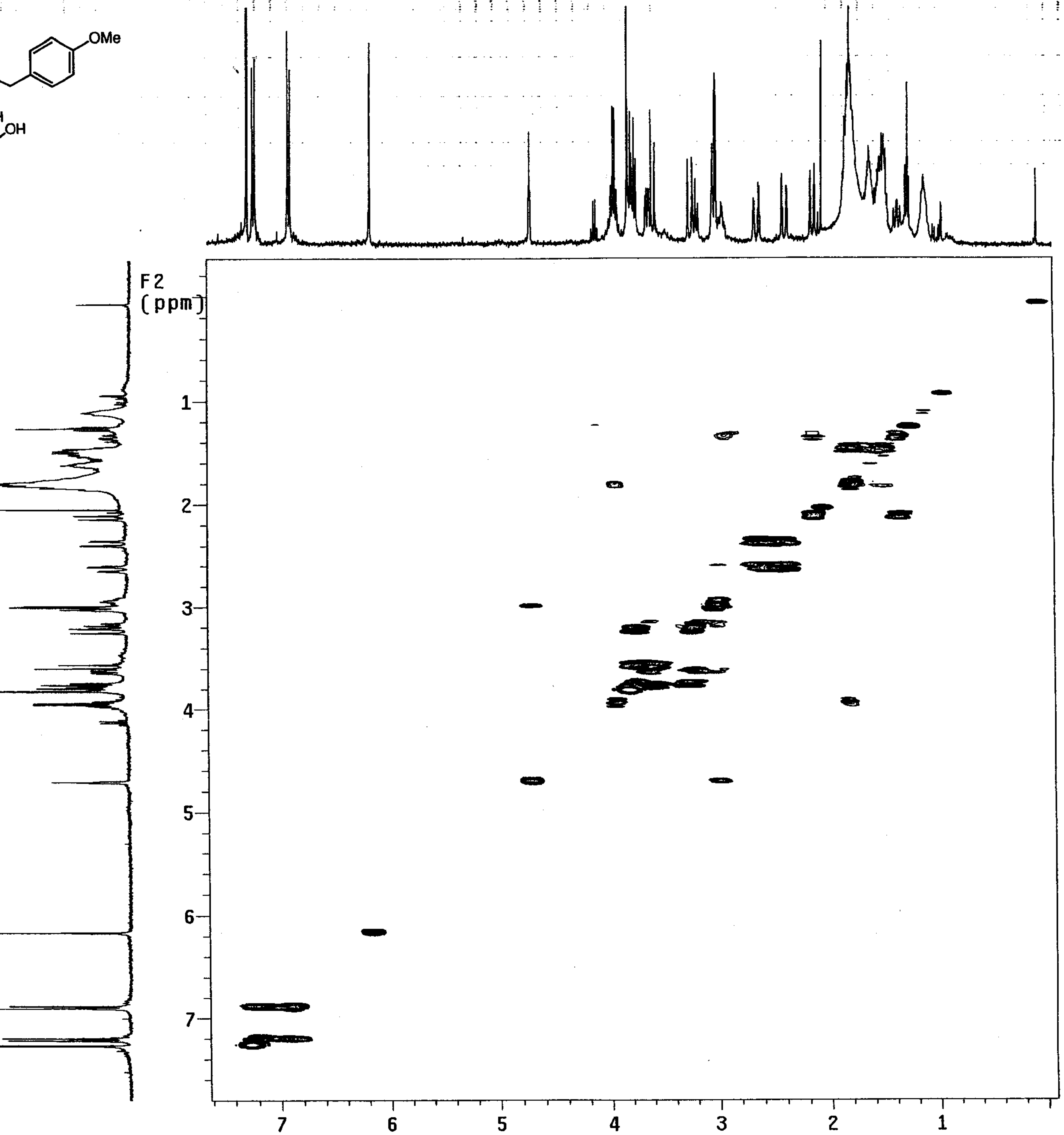


Figure V.4.2.10

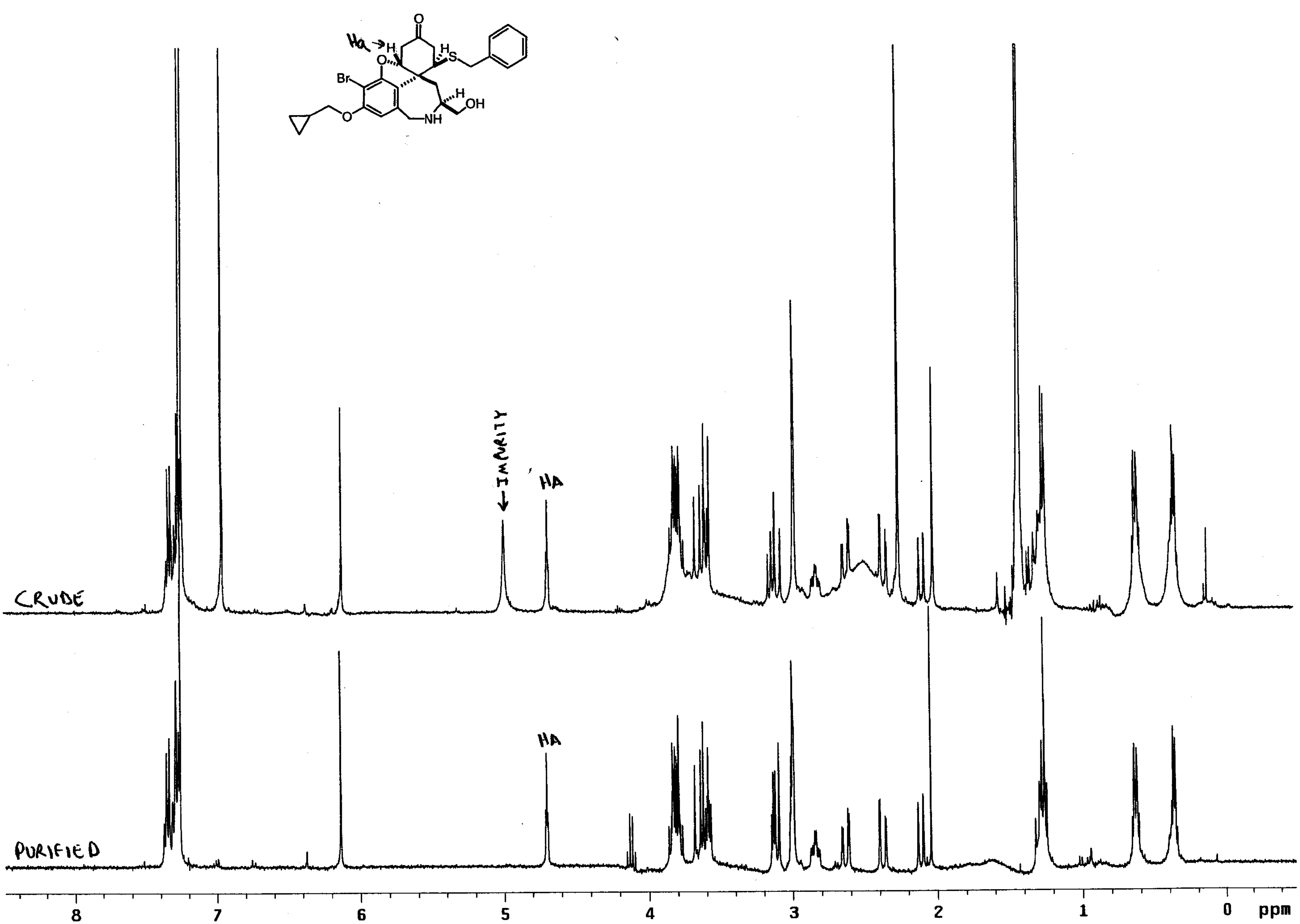


Figure V.4.2.11