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<Supporting Information>

A potent small-molecule inducer of chondrogenic differentiation of human bone-marrow-derived mesenchymal stem cells

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I. Synthetic procedure and characterization of Δ^5-2-oxopiperazine library

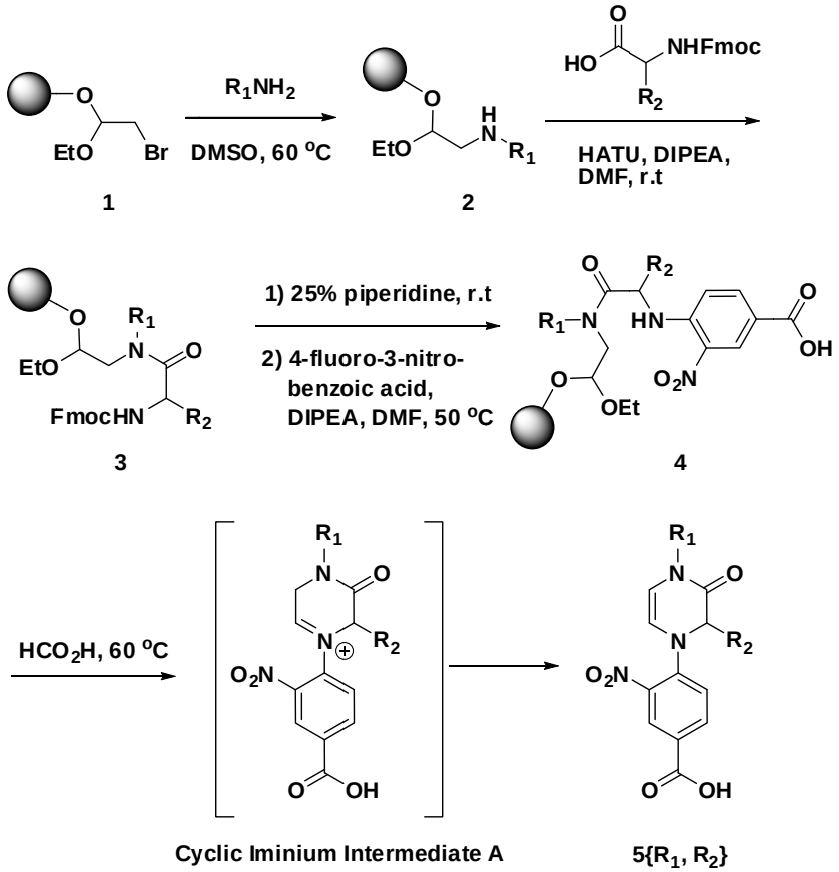
1. General information

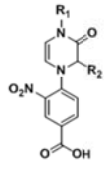
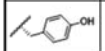
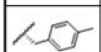
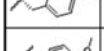
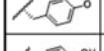
All commercially available reagents and solvents were used without further purification unless noted otherwise. All the solvents were purchased from commercial venders. Bromoacetal resins were obtained from either Advanced ChemTech or Aldrich, but the high loading resins for actual library construction were synthesized in our laboratory.[1] The reaction steps for library construction were performed in parallel using the FlexChem Synthesis System from SciGene [Sunnyvale, CA] in a 96-deep-well filtration block. ^{1}H and ^{13}C NMR spectra were obtained on a Varian Inova-500 (Varian Assoc., Palo Alto, USA) and Bruker DRX-300, AVANCE 600 (Bruker Biospin, Germany). Chemical shifts were reported in ppm from tetramethylsilane (TMS) as internal standard or the residual solvent peak ($CDCl_3$, ^{1}H: 7.26, ^{13}C: 77.23; CD_3OD, ^{1}H: 3.31, ^{13}C: 49.00; DMSO-d_6, ^{1}H: 2.50, ^{13}C: 39.52). Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); dd (doublet of doublet); ddd (doublet of doublet of doublet); dt (triplet of doublet); td (doublet of triplet); br s (broad singlet), etc. Coupling constants were reported in Hz. The purity of all the library members was observed by a LC/MS system equipped with a reverse phase column (C-18, 50 × 2.1 mm, 5 μm) and photodiode array (PDA) detector using electron spray ionization (ESI). Purities were obtained by PDA based LC/MS analysis of final crude products without further purification. The high resolution mass spectrometric analyses were conducted at the Mass Spectrometry Laboratory of Seoul National University using mass spectrometer by direct injection for fast atomic bombardment (FAB).

[1] S.-C. Lee, S. B. Park, *J. Comb. Chem.*, 2006, **5**, 50–57.

2. General solid-phase reaction procedures for the construction of Δ^5-2-oxopiperazine-based small molecule library

Supporting Table 1. Set of buildings blocks and purities [%] of Δ^5-2-oxopiperazines **5**.[a]



			R1												
	R2			a	b	c	d	e	f	g	h	i	j	k	l
			1	77%	76%	82%	88%	81%	84%	84%	79%	82%	84%	86%	80%
			2	67%	70%	93%	92%	81%	72%	80%	83%	85%	81%	84%	79%
			3	88%	82%	88%	89%	92%	93%	86%	84%	84%	87%	90%	86%
			4	80%	85%	83%	83%	90%	81%	80%	88%	87%	82%	82%	80%
			5	82%	74%	86%	82%	88%	90%	84%	88%	77%	79%	85%	88%
			6	85%	86%	74%	90%	81%	67%	72%	95%	81%	83%	67%	87%
			7	66%	71%	73%	69%	79%	73%	70%	82%	86%	79%	73%	75%

[a] Purities were obtained by PDA-based LC/MS analysis of final products without further purification.

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Step 1: Amine Substitution

Bromoacetal resins **1** (40 mg, 1.6 mmol/g, 0.064 mmol) were loaded into each well of a Robbins 96-deep-well filtration block, and solutions of 12 different R_1-amines (20 equiv. in 1.2 mL of DMSO) were dispensed into the designated wells of the reaction block. The reaction mixture was shaken at 60 °C in a rotating oven [Robbins Scientific] for 12 h. The resulting resins **2** thus obtained were washed extensively with DMF, MeOH, and CH_2Cl_2 sequentially (three times each) and dried in vacuo.

Step 2: Amino Acid Coupling

A reaction cocktail of *N*-Fmoc amino acid (3 equiv.), HATU (3 equiv.), and DIPEA (6 equiv.) in DMF (1.2 mL per well) was dispensed into each well of the reaction block charged with resins **2**. The reaction mixture was shaken at room temperature in a rotating oven for 12 h. The resins were then washed extensively with DMF, MeOH and CH_2Cl_2 (three times each) and dried in vacuo. The reaction completion was confirmed by negative chloranil test.

Step 3: Nucleophilic Aromatic Substitution

To the resins **3** in the reaction block was added 25% piperidine in DMF, and the reaction mixture was shaken at room temperature for 1 h to unmask the Fmoc-protected primary amine. The resins were then washed extensively with DMF, MeOH and CH_2Cl_2 (three times each). A reaction cocktail of 4-fluoro-3-nitrobenzoic acid (5 equiv.) and DIPEA (10 equiv.) in DMF (1.2 mL per well) was then dispensed into each well of the reaction block charged with resins. The reaction mixture was shaken at 50 °C in a rotating oven for 12 h. The resins were washed extensively with DMF, MeOH and CH_2Cl_2 (three times each) and dried in vacuo. The reaction completion was confirmed by negative Kaiser test.

Step 4: Cleavage and Cyclization

After the resulting resins **4** in the 96-deep-well reaction blocks were dried under high vacuum, resins were treated with 100% formic acid (1.4 mL per well) for 3 h at 60 °C. Then, the resins were removed by filtration and washed several time with DCM. The filtrate was condensed under reduced pressure using GeneVac [Thermo Savant] and the resulting residues were diluted with 50% H_2O/ACN and freeze-dried, which yielded final products as a pale red powder. The purity of final products was confirmed by LC/MS without further purification.

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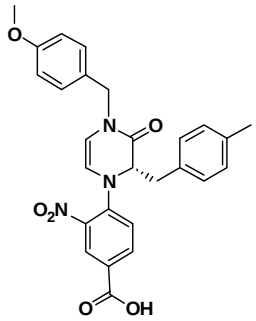
Supporting Table 2. Purity and mass confirmation of representative compounds in Δ^5-2 oxopiperazines library.

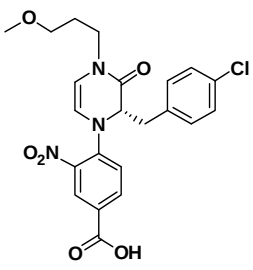
compd	R_1	R_2	Purity[a]	MS[M+H]$^+$ calcd	MS[M+H]$^+$ obs
5{i,2}	4-Methoxybenzyl	4-Methylbenzyl	85%	488.17	488.22
5{h,5}	3-Methoxypropyl	4-Chlorobenzyl	88%	460.12	460.19

[a] Purities were obtained by PDA-based LC/MS analysis of final products without further purification.



5{i,2}

Characterization of Compound 5{i,5}[b]: ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.94 (br s, 1H), 8.34 (d, *J* = 2.1 Hz, 1H), 7.71 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.23 (d, *J* = 8.7 Hz, 2H), 7.07 (s, 4H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.12 (d, *J* = 9.0 Hz, 1H), 5.89 (d, *J* = 5.4 Hz, 1H), 5.39 (dd, *J* = 5.4, *J* = 1.8 Hz, 1H), 4.89 (d, ^2J = 14.7 Hz, 1H), 4.76–4.71 (m, 1H), 4.59 (d, ^2J = 14.7 Hz, 1H), 3.81 (s, 3H), 3.09–3.03 (m, 2H), 2.32 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.4, 163.9, 159.5, 141.8, 140.8, 137.4, 133.7, 133.1, 129.9, 129.6, 129.5, 128.7, 128.1, 122.0, 120.3, 116.0, 114.4, 111.2, 64.9, 55.5, 48.6, 34.4, 21.3; HRMS (FAB+) *m/z* calcd for $C_{27}H_{25}N_3O_6$ $[M+H]^+$: 488.1822; Found: 488.1824.



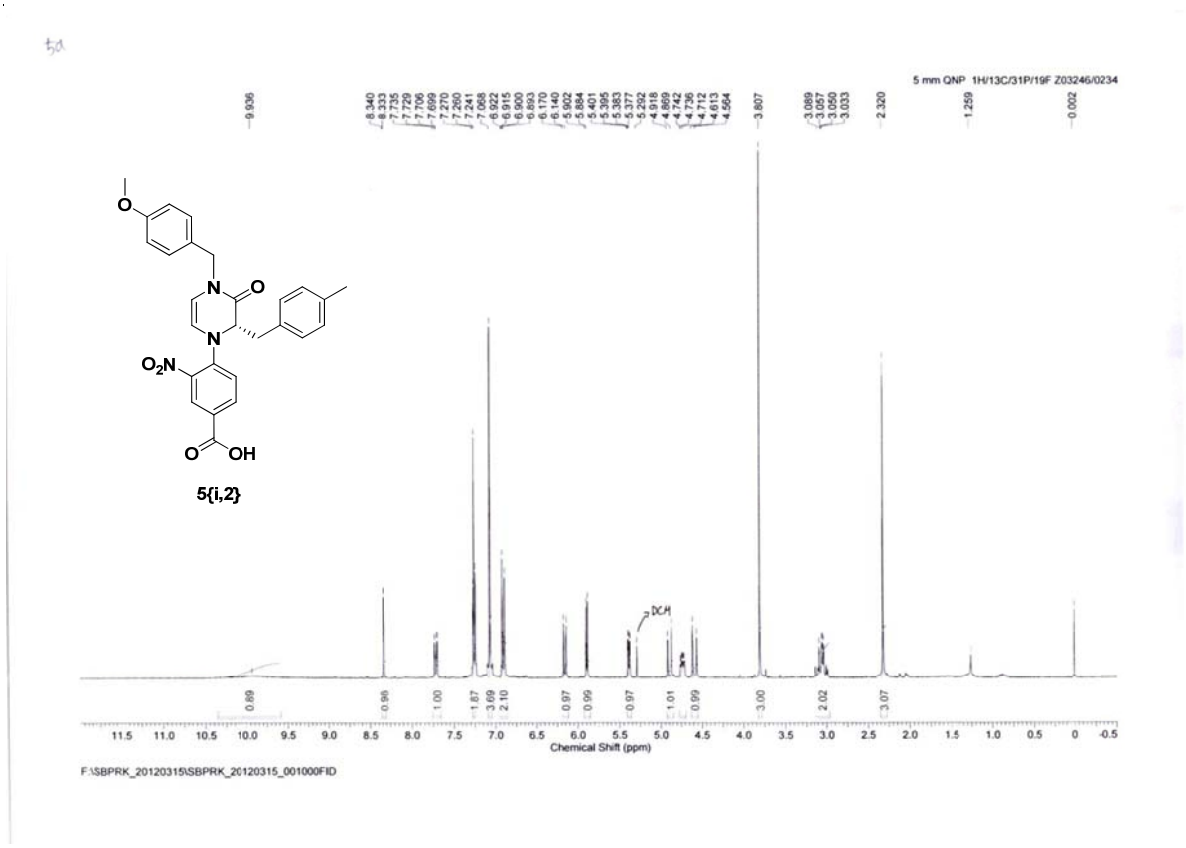
5{h,5}

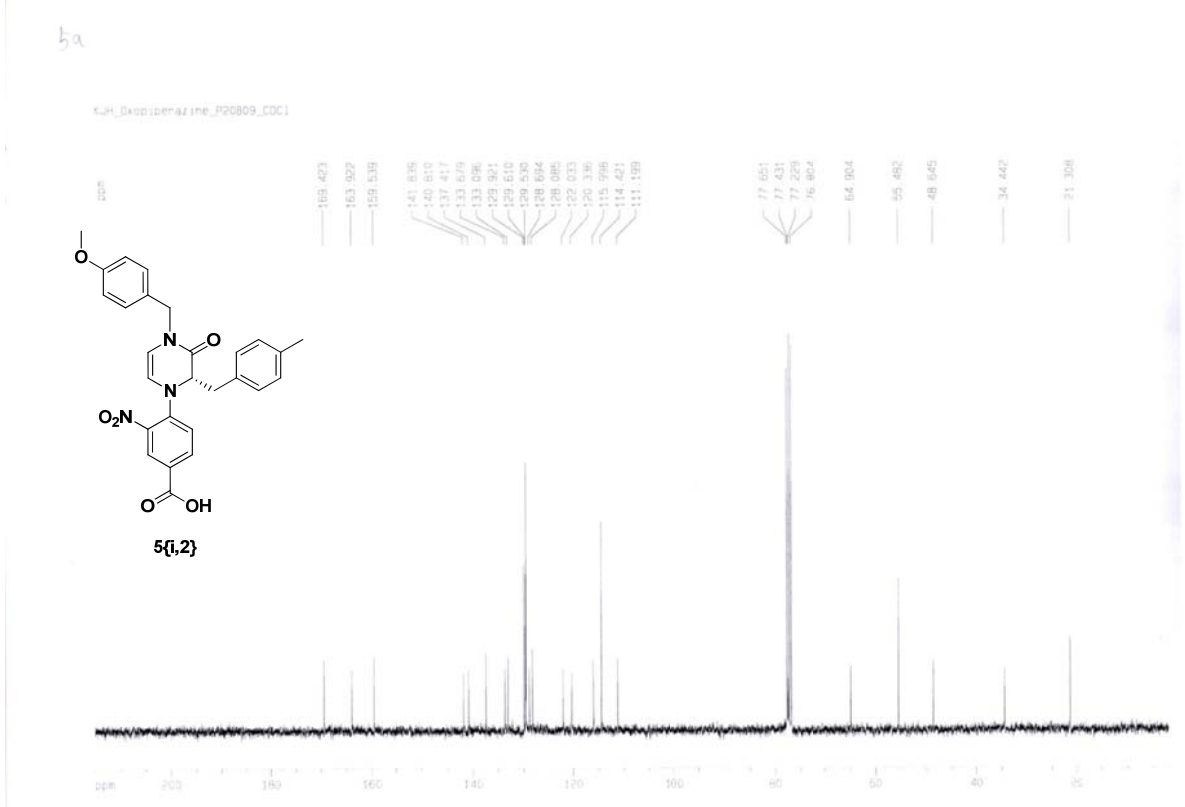
Characterization of Compound 5{h,5}[b]: ^{1}H NMR (500 MHz, CD_3OD) δ 8.27 (d, *J* = 1.5 Hz, 1H), 7.84 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.61 (d, *J* = 9.0 Hz, 1H), 6.03 (d, *J* = 5.0 Hz, 1H), 5.66 (dd, *J* = 5.5, 1.5 Hz, 1H), 4.63–4.61 (m, 1H), 3.85–3.82 (m, 1H), 3.50–3.44 (m, 3H), 3.35 (s, 3H), 3.15 (dd, ^2J = 13.5 Hz, *J* = 9.0 Hz, 1H), 3.00 (dd, ^2J = 13.8 Hz, *J* = 5.8 Hz, 1H), 1.89 (pentet, *J* = 6.5 Hz, 2H); ^{13}C NMR (150 MHz, CD_3OD) δ 164.4, 142.8, 141.5, 136.5, 134.6, 134.1, 132.5, 129.8, 128.4, 122.2, 116.5, 113.4, 70.5, 65.7, 58.8, 44.8, 34.9, 29.5; HRMS (FAB+) *m/z* calcd for $C_{22}H_{23}ClN_3O_6$ $[M+H]^+$: 460.1275; Found: 460.1276.

[b] The ^{1}H and ^{13}C NMR spectroscopy were obtained after purification of samples by silica-gel flash column chromatography .

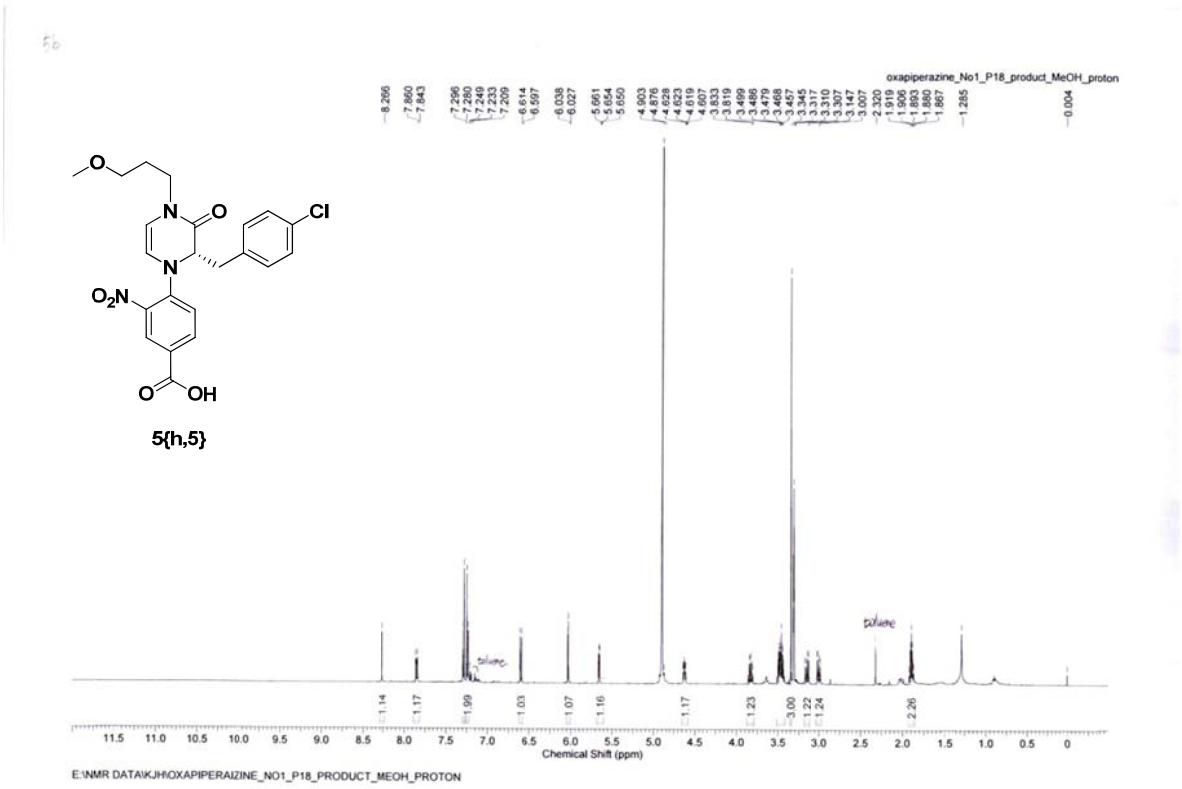
II. NMR spectroscopy

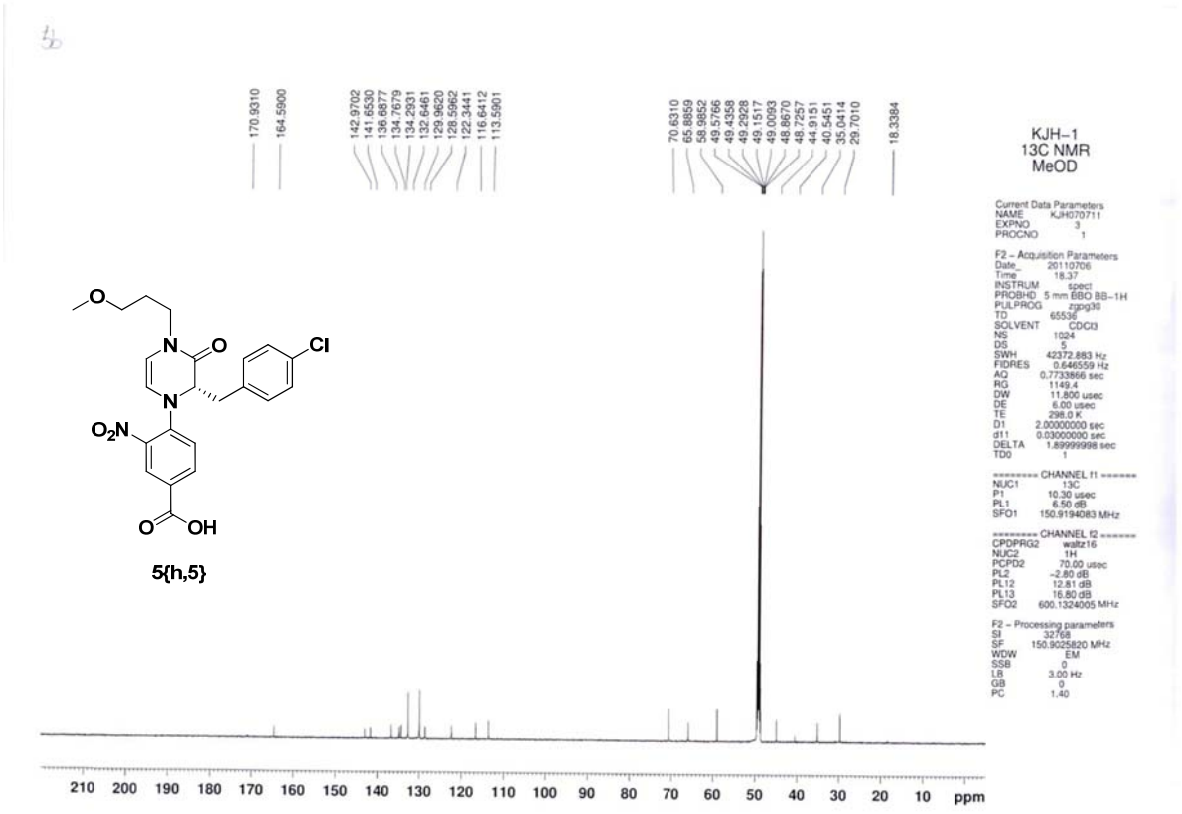
^{1}H and ^{13}C NMR spectra data of 5{i,2}





^{1}H and ^{13}C NMR spectra data of 5{h,5}





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III. Cultivation of human bone-marrow-derived mesenchymal stem cells (hBM-MSCs)

Human bone-marrow-derived MSCs (hBM-MSCs) were obtained from children cardiac surgeries of Seoul National University Hospital, which was approved by the IBR (No.:S-D0090001). hBM-MSCs were maintained and expanded in the medium composed of a high-glucose Dulbecco's modified Eagles medium (DMEM: Welgene, Korea) including 20% Fetal bovine serum (FBS: Hyclon, USA), and 1% Antibiotics-Antimycotics (Gibco, Grand Island, NY) at 37 ^{o}C under 5% CO2. The cells were passaged up to 70% confluency. The cells at passage 7 (P7) were subjected to the chondrogenic differentiation assay.

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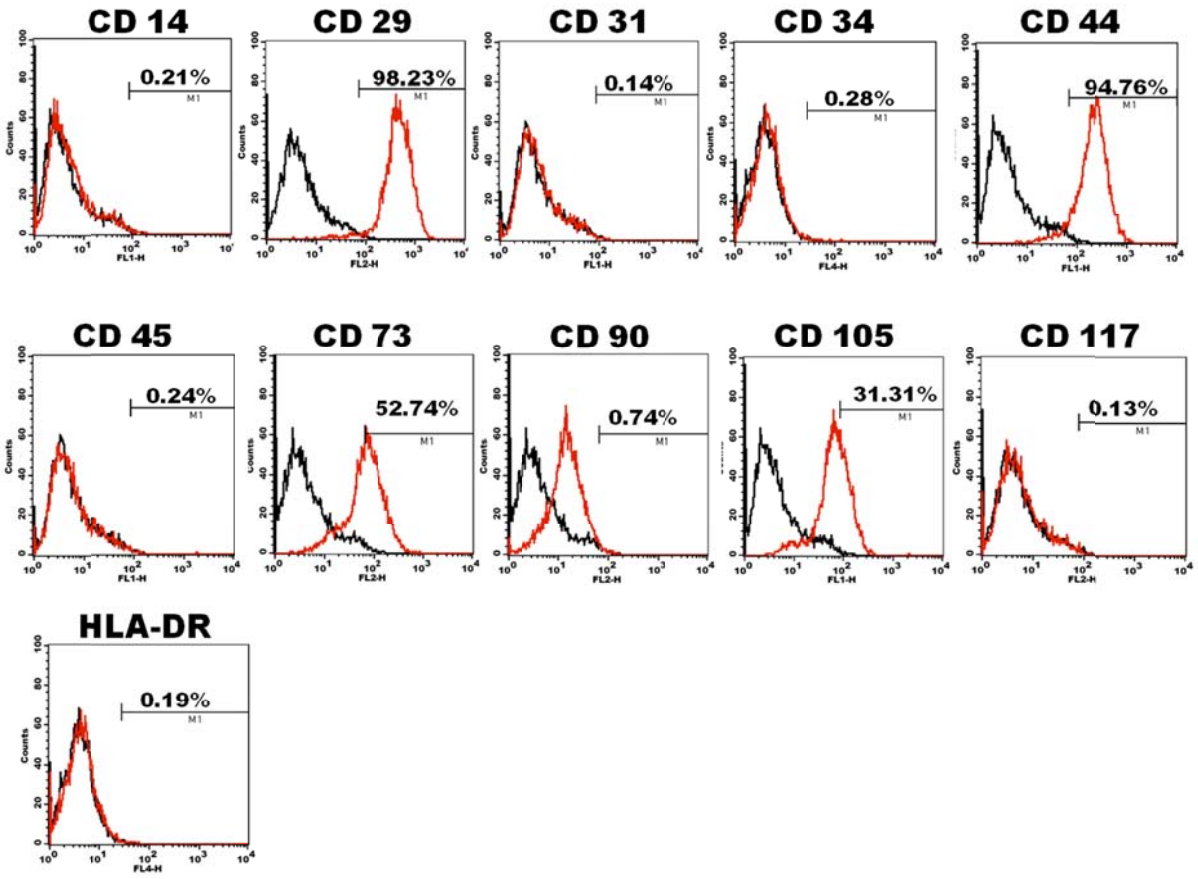
IV. Fluorescence-activated cell sorting (FACS) analysis

For the characterization of the hBM-MSCs, fluorescence-activated cell sorting (FACS) was performed to examine expression status of several stem cell surface markers.

The cells were detached and washed with PBS supplemented with 2% FBS to carry out the FACS analysis. The following antibodies were used; fluorescein isothiocyanate (FITC)-conjugated mouse anti-human CD14, CD31, CD44 and CD45; phycoerythrin (PE)-conjugated mouse anti-human CD29, CD73, and CD117; PE/Cy5-conjugated mouse anti-human CD90; allophycocyanin (APC)-conjugated mouse anti-human CD34; HLA-DR; PE-conjugated streptavidin; biotin-conjugated HLA class II (all from BD PharMingen, San Diego, CA, USA); APC-conjugated mouse anti-human CD105 (eBioscience, USA). Each primary antibody was incubated with 100,000 cells for 30 min on ice. After washing, the secondary antibody was applied for 30 min on ice. Then, cells were fixed with 4% paraformaldehyde at 4 ^{o}C until they were analyzed. The fluorescence intensity was measured by a FACS Calibur^{TM} and data were analyzed with BD CellQuest Pro software (all from Becton Dickinson, San Jose, CA, USA).

As shown in Supporting Figure 1, hBM-MSCs expressed the mesenchymal stem cell markers such as CD29 (98.23%), CD44 (94.76%), CD73 (52.74%), CD90 (0.74%), and CD105 (31.31%), whereas few cells expressed hematopoietic marker such as CD14 (0.21%), , CD34 (0.28%), CD45 (0.24%), CD117 (0.13%), and HLA-DR (0.19%), or the endothelial marker CD31 (0.14%). The homogeneously high expression of CD29 (β1-integrin) and CD44 (hyaluronan receptor) indicates that the used hBM-MSCs are mainly mesenchymal stem cells.[2] However, the lack of hematopoietic cell marker and endothelial cell marker reveals that hBM-MSCs were not contaminated by hematopoietic stem cells or endothelial cells. The relative low level of CD105 (endoglin), which is a specific marker for mesenchymal stem cell, implies that there exists osteogenic differentiation process.[2]

[2] S. P. Burder, M. C. Horowitz, J. D. Mosca, S. E. Haynesworth, *Bone.* 1997, **21**, 225–235.



Supporting Figure 1. Immunophenotypic characterization of hBM-MSC at passage 6 (P6). Data are shown as an overlay plot with immunoglobulin isotype control (in black) and different specific cell-surface markers (in red).

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V. Chondrogenic differentiation of hBM-MSCs

For initiation of chondrogenesis of hBM-MSCs, the cells were enzymatically detached by treating 0.25% trypsin and counted by hemocytometer. Chondrocyte balls were formed in a 15 mL conical polypropylene tube with 250,000 cells. The tubes with cells were centrifuged in 500 g for 5 min. Then, the FBS containing medium was replaced with chemically defined medium which contained a high-glucose DMEM (Welgene, Korea), supplemented with 50 μg/mL ascorbate-2-phosphate, 100 μg/mL sodium pyruvate, 40 μg/mL L-proline, and 1% ITS+Premix (all Sigma-Aldrich, St. Louis, MO, USA). To investigate the effect of TGF-β3 or individual compounds on chondrogenic differenciation of hBM-MSCs, the chondrocyte balls were cultured in three different conditions: chemically defined medium only or defined medium that was supplemented with TGF-β3 (10 ng/mL), or individual compounds **(**10 μM). The chondrocyte balls with each medium were cultured in a 37 ^{o}C, 5% CO_2 incubator and medium change was carried out every 2~3 days.

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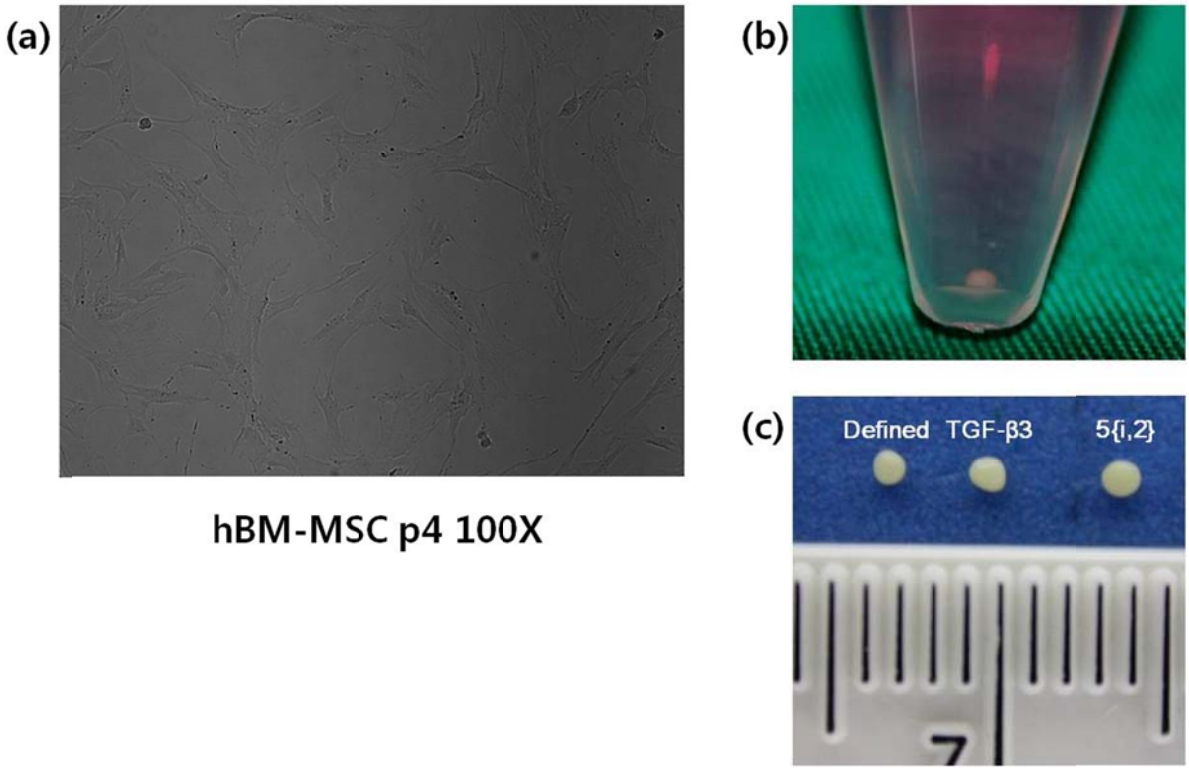
VI. Morphology and chondrocyte ball formation

The hBM-MSCs at passage 4 (P4) exhibited the typical fibroblast-like phenotype and were homogeneous (Supporting Fig. 2a). For inducing chondrogenic differentiation, the cells were aggregated by mechanical force. As shown in Supporting Fig. 2b, the hBM-MSC-derived chondrocyte balls were formed in a tube.



Supporting Figure 2. (a) Morphology of hBM-MSCs at passage 4 (P4) (b,c) Formation of chondrocyte ball upon treatment of TGF-β3(10 ng/mL), **5{i,2}** (10 μM) at Day 14. (a): Original magnitude X100.

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VII. Glycosaminoglycan and DNA measurement

For glycosaminoglycan (GAG) contents assay, we used 3 chondrocyte balls in each group and were measured with Blyscan Sulfate Glycosaminoglycan Assay kit (biocolor, Belfast, Ireland). This experiment was performed according to manufacturer's instructions. Briefly, after putting 3 chondrocyte balls into a new eppendorf tube, papain buffer solution [0.2 M sodium phosphate buffer, 0.1 M sodium acetate, 10 mM EDTA, 5 mM L-cysteine HCl, 7.6 μL/mL papain (Sigma-Aldrich, St. Louis, MO, USA), pH 6.4] was added 500 μL in that tube. This tube was incubated at 65 ^{o}C water bath for 18 h. After that time, the tube was centrifuged for 10 min at 10000 g and 100 μL of supernatant was transferred to a new tube. Then, 1 mL of the Blyscan dye reagent solution was added in the tube. The resulting eppendorf tube was incubated at the room temperature in a gentle mechanical shaker for 30 min. During this time period, a sulphated glycosaminoglycan-dye complex is formed and precipitated out from the soluble unbound dye. The resulting tube was centrifuged for 10 min at 12000 rpm. After the careful removal of all supernatant, a pellet of insoluble sGAG-dye complex at the bottom of the tubes was dried on a paper tissue at the room temperature. After addition of 1 mL of the dissociation reagent, each tube was recapped and vortexed to release the bound dye into the solution. After 10-min mixing, we measured the absorbance of this dissociated solution at 656 nm. For the measurement of total DNA contents, we used Pico-green dsDNA assay kit (Invitrogen, USA) and this experiment was performed according to manufacturer's instructions. The GAG contents were normalized versus the total content of cellular DNA. This experiment was carried out in triplicate.

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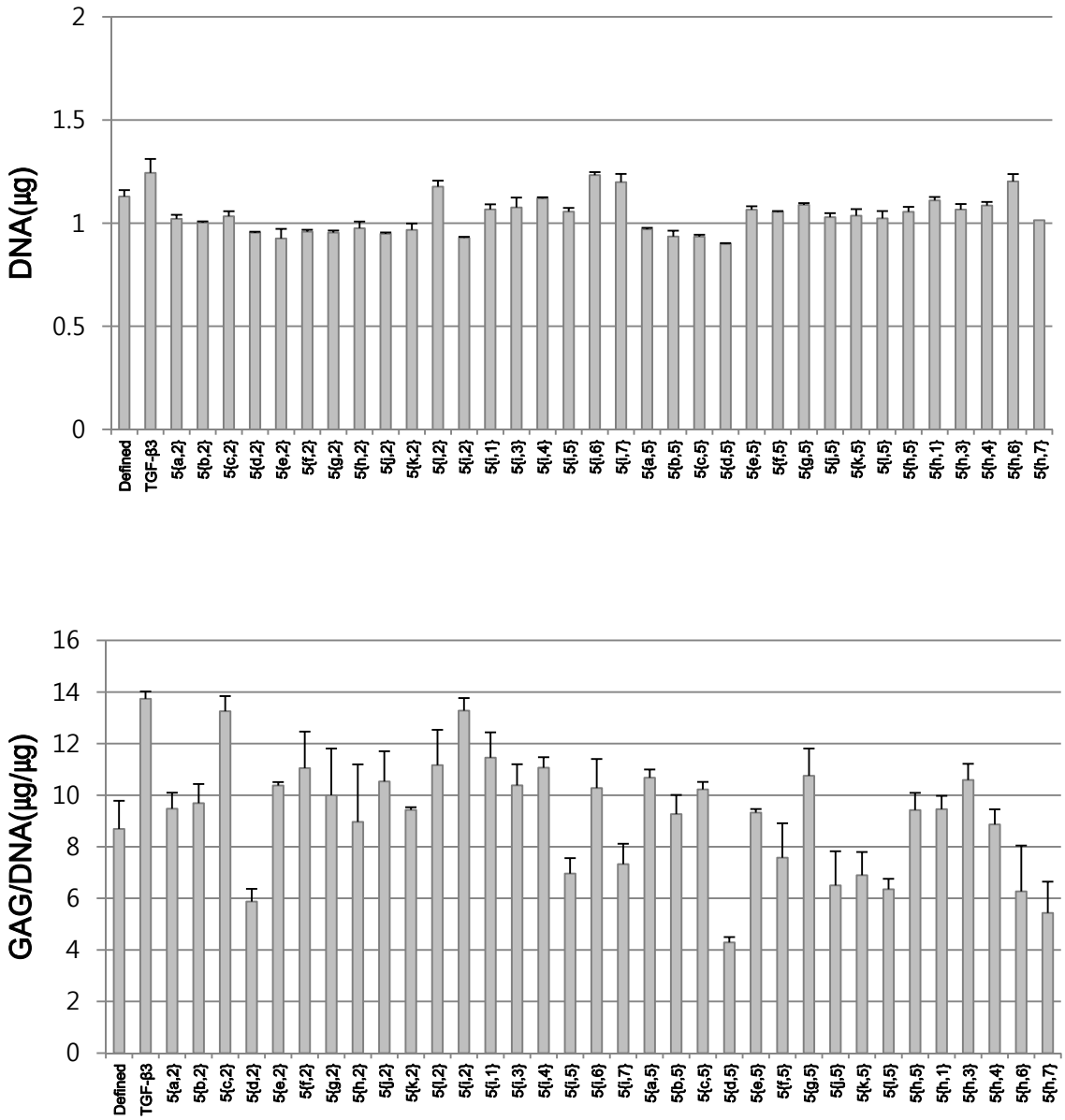

Supporting Figure 3. The measurement of cellular glycosaminoglycan (GAG) contents as a marker that is associated with the chondrogenic capacity at Day 7. Human bone marrow-derived mesenchymal stem cells (hBM-MSCs) were treated with defined medium only or defined medium that was supplemented with TGF-β3 (10 ng/mL), or 34 individual compounds **(**10 μM). Total GAG contents were normalized by dividing with the total DNA contents (n=3).

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VIII. Histological staining and immunohistochemistry

For paraffin section, chondrocyte balls in each different group were fixed in 4% phosphate buffered formalin and embedded in paraffin. Paraffin embedded samples were sectioned by thickness of 4 μm and deparaffinized. Deparaffinized slides were stained by hematoxylin and eosin (H&E) and Safranin O staining to visualize the cellular proteoglycan was carried out. We also performed Von Kossa staining to show the calcium deposition levels in the samples. For the detection of collagen type I and collagen type II, ABC detection kit (Cap-plus detection Kit, Invitrogen) was used and performed according to manufacturer's instructions. Briefly, 3% peroxidase was treated in the samples for 10 min and washed 3 times by PBS. Pepsin solution also was treated for retrieval. Nonspecific binding event was minimized by the treatment of blocking solution of the detection kit. The sample was subjected to the sequential treatment of primary antibody [Rabbit polyclonal antibody for collagen type I (Abcam, UK) and mouse monoclonal antibody for collagen type II (Calbiochem, Germany), diluted by 1:100 and 1:10, respectively], biotinylated secondary antibody (either anti-rabbit IgG or anti-mouse IgG), and streptavidin-HRP (horse-radish peroxidase). The immunohistochemical staining was visualized by the color development of DAB (3,3'-diaminobenzidine) upon peroxidase activity.

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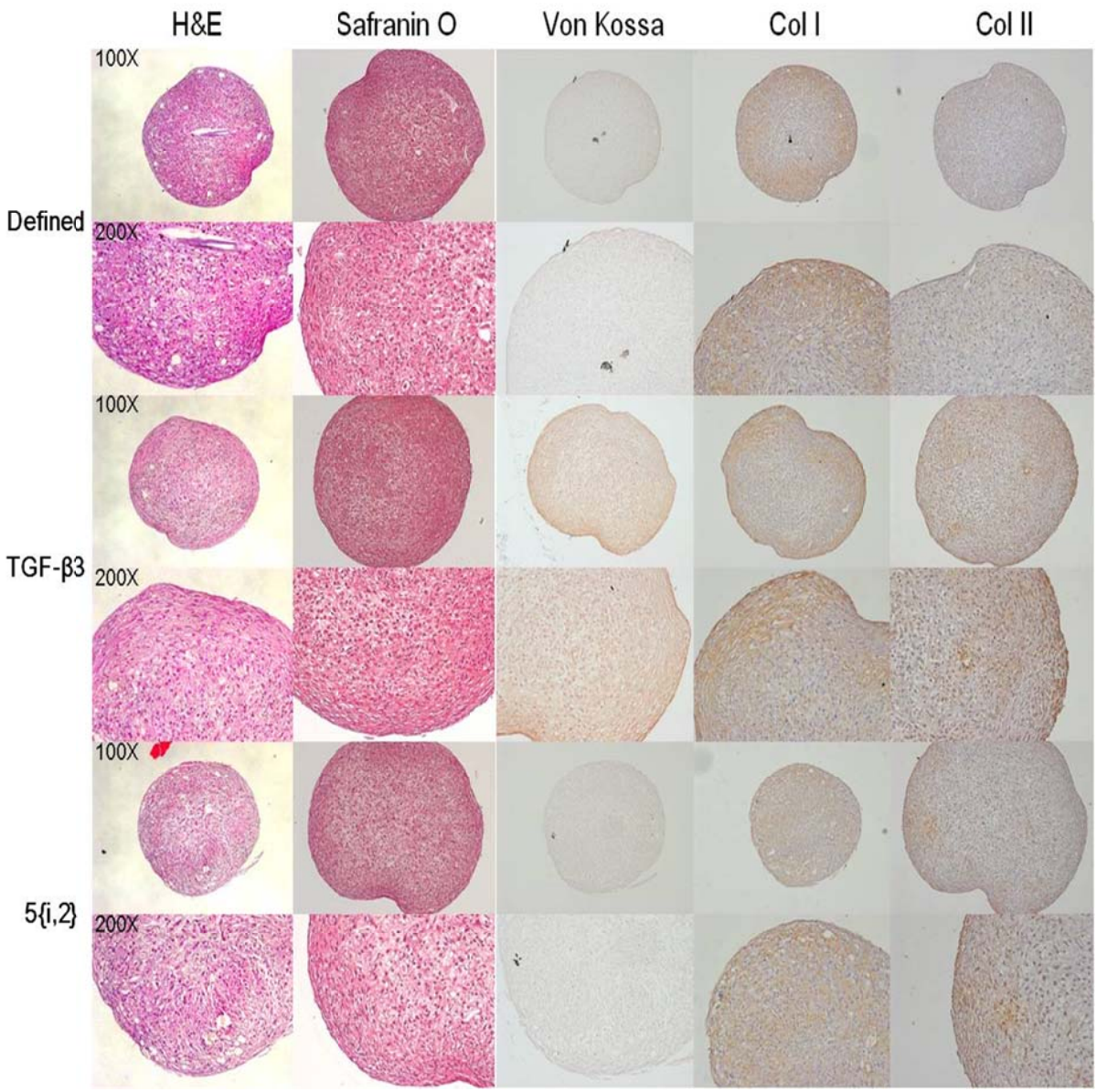

Supporting Figure 4. Histological staining and immunohistochemistry of hBM-MSC-derived chondrocyte balls treated with defined medium only or defined medium that was supplemented either with TGF-β3 (10 ng/mL) or **5{i,2}** (10 μM) for 14 days. H&E staining indicates the morphology changes of chondrocyte balls, Safranin-O staining indicates the level of proteoglycan, and Von Kossa staining indicates the level of deposited calcium. Immunohistochemical staining was performed with collagen type I- and II-specific antibodies.

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IX. Total RNA preparation and RT-PCR

For reverse transcriptase polymerase chain reaction (RT-PCR), chondrocyte balls in 3 different media were gathered at 7, and 14 days. Chondrocyte balls were digested in liquid nitrogen. Then, total RNA was extracted from chondrocyte balls using Trizol Reagent (Invitrogen Life Technologies, USA). To synthesize a complementary DNA (cDNA) used as a template in subsequent PCR reaction, 2 μg of total RNA was reverse-transcribed with cDNA Synthesis Kit (M-MLV RT, Invitrogen, USA) according to manufacturer's instructions. In PCR reactions, the total reaction volume was 20 μl which include 1 μl of 10-fold dilution cDNA, 1 μl of each of primers (5 pmole), PCR premix (Accupower PCR premix, Bioneer, Korea) and sterilized 17 μl of water. PCR amplification was conducted with Mastercycler gradient (Eppendorf, Germany) under followed conditions: denaturation at 94 ^{o}C for 5 min, amplification at 94 ^{o}C for 30 sec, annealing at specific temperature for each primer pair (as shown in supporting table 1) for 30 sec, extension at 72 ^{o}C for 20 sec, and total 28~37 cycles. A final extension step was performed at 72 ^{o}C for 5 min. RT-PCR primer sequences and each annealing temperature are shown in supporting table 1. For analysis of PCR products, DNA gel electrophoresis was carried out in 1.2% agarose gel with 0.01 mg/mL ethidium bromide and quantified by Bio-profil X press zoom 2000 (Vilber Lourmat, Marne-la-Vallee, France).

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Target gene	Primer sequences	Annealing temperature	product size(bp)
SOX9	F: 5`-ATC TGA AGA AGG AGA GCG AG-3`	60 °C	264 bp
	R: 5`-TCA GAA GTC TCC AGA GCT TG-3`		
Aggrecan	F: 5` TCC TCT CCG GTG GCA AAG AAG TTG 3`	60 °C	271 bp
	R: 5` CCA AGT TCC AGG GTC ACT GTT ACC G 3`		
Collagen II	F: 5`-TGGCCTGAGACAGCATGAC-3`	64 °C	373bp
	R: 5`-AGTGTTGGGAGCCAGATTGT-3`		
Collagen X	F: 5`-CCC TTT TTG CTG CTA GTA TCC-3`	58 °C	468 bp
	R: 5`-CTG TTG TCC AGG TTT TCC TGG CAC-3`		
Collagen I	F: 5`-GGACACAATGGATTGCAAGG-3`	54 °C	461bp
	R: 5`-TAACCACTGCTCCACTCTGG-3`		
RUNX2	F: 5`-CAG AAC CCA CGG CCC TCC CT-3`	64 °C	242bp
	R: 5`-TCT GAA GCA CCT GAA ATG CGC CT-3`		
MMP13	F: 5`-TGC GCA TGA GTT CGG CCA CT-3`	60 °C	277bp
	R: 5`-ATG CAG GCG CCA GAA GAA TCT GT-3`		
GPADH	F: 5`-TGT TGC CAT CAA TGA CCC CTT-3`	55 °C	202 bp
	R: 5’-CTC CAC GAC GTA CTC AGC G-3’		

Supporting Table 3. Primer sequence and specific annealing temperature for each primer pair for RT-PCR.

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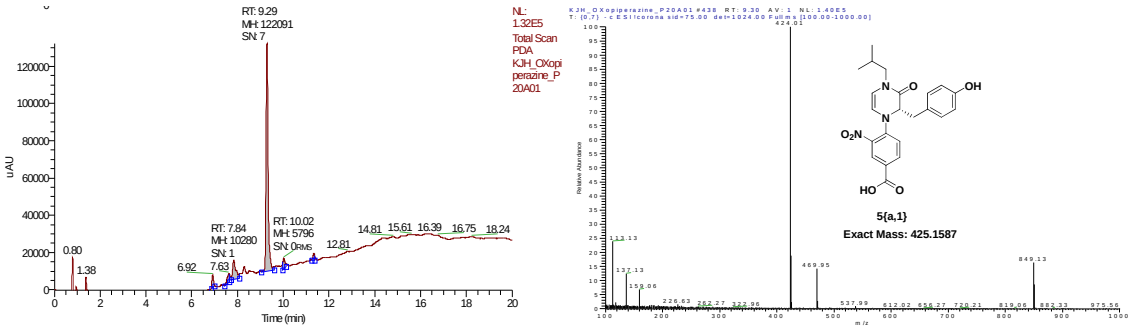
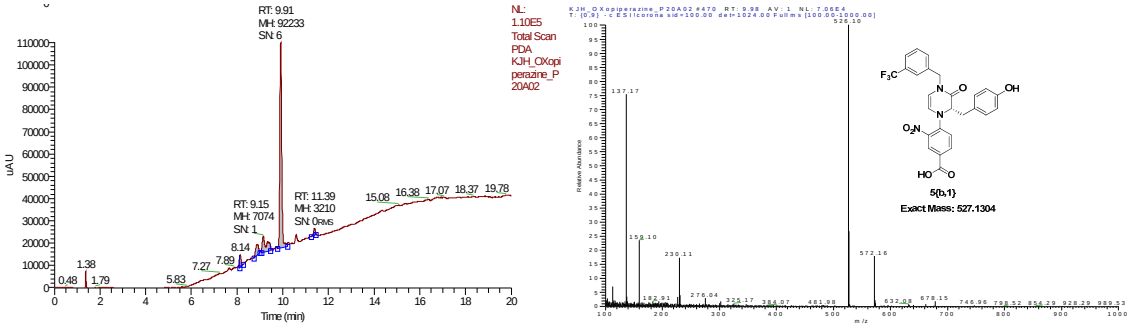
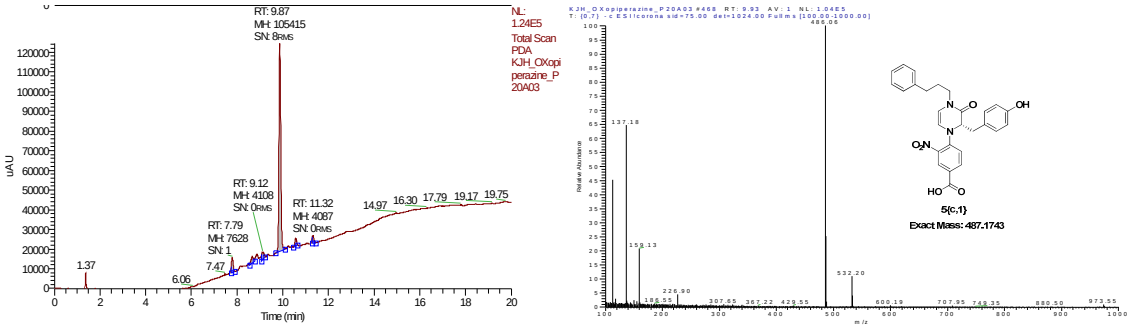
X. Cartilage ball implantation

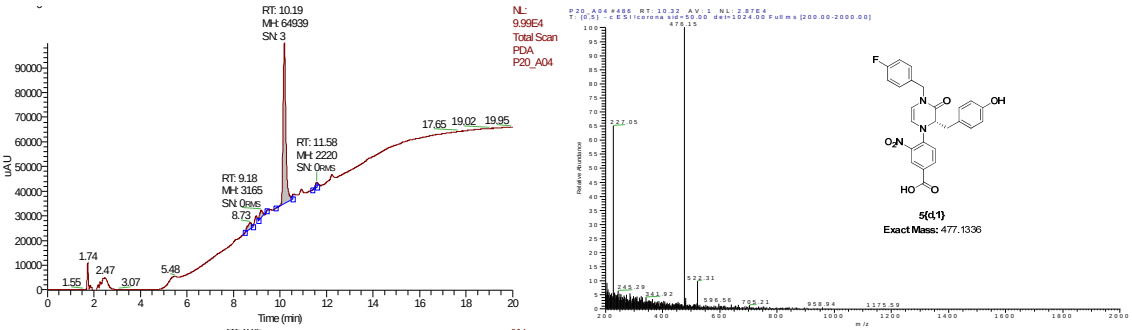
To evaluate the *in vivo* fate of the cartilage balls differentiated with small molecules, complex immunocomprimised NOD/scid/IL-2Rγ$^{-/-}$ (NOG) mice, which lack T, B, and NK cell activities, were anesthesized with intraperitoneal injection of 2.5% Avertin and inhalation of metofane. The parietal peritoneum was exposed in the right lower quadrant of the abdomen and fine incisions along the peritoneum were made using iridectomy scissors. Differentiated cartilage balls with 1~1.5 mm in diameter were inserted into the extraperitoneal fat tissue and the cut peritoneum was sutured using 7-0 nylon. On 14 days following transplantation, mice were sacrificed and the engrafted cartilage balls were exposed. For microscopic analysis, cartilage balls with surrounding tissues were fixed in 4% paraformaldehyde, tissue-processed, and embedded in paraffin. Sections were stained with hematoxylin and eosin (H&E).

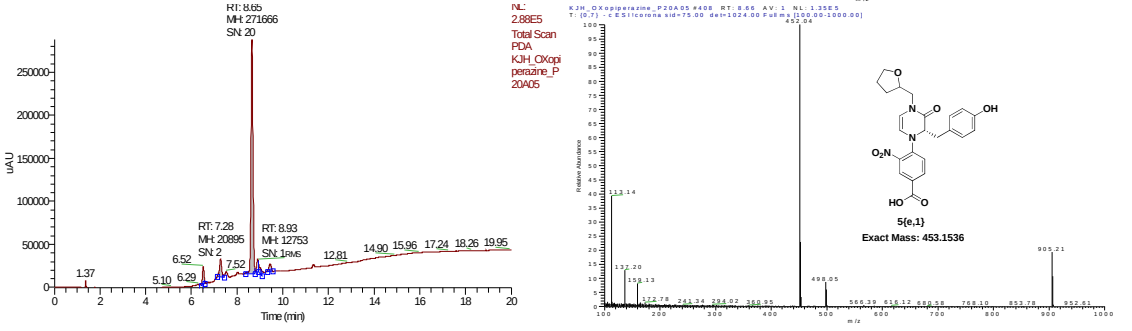
XI. LC/MS analysis data of all library members

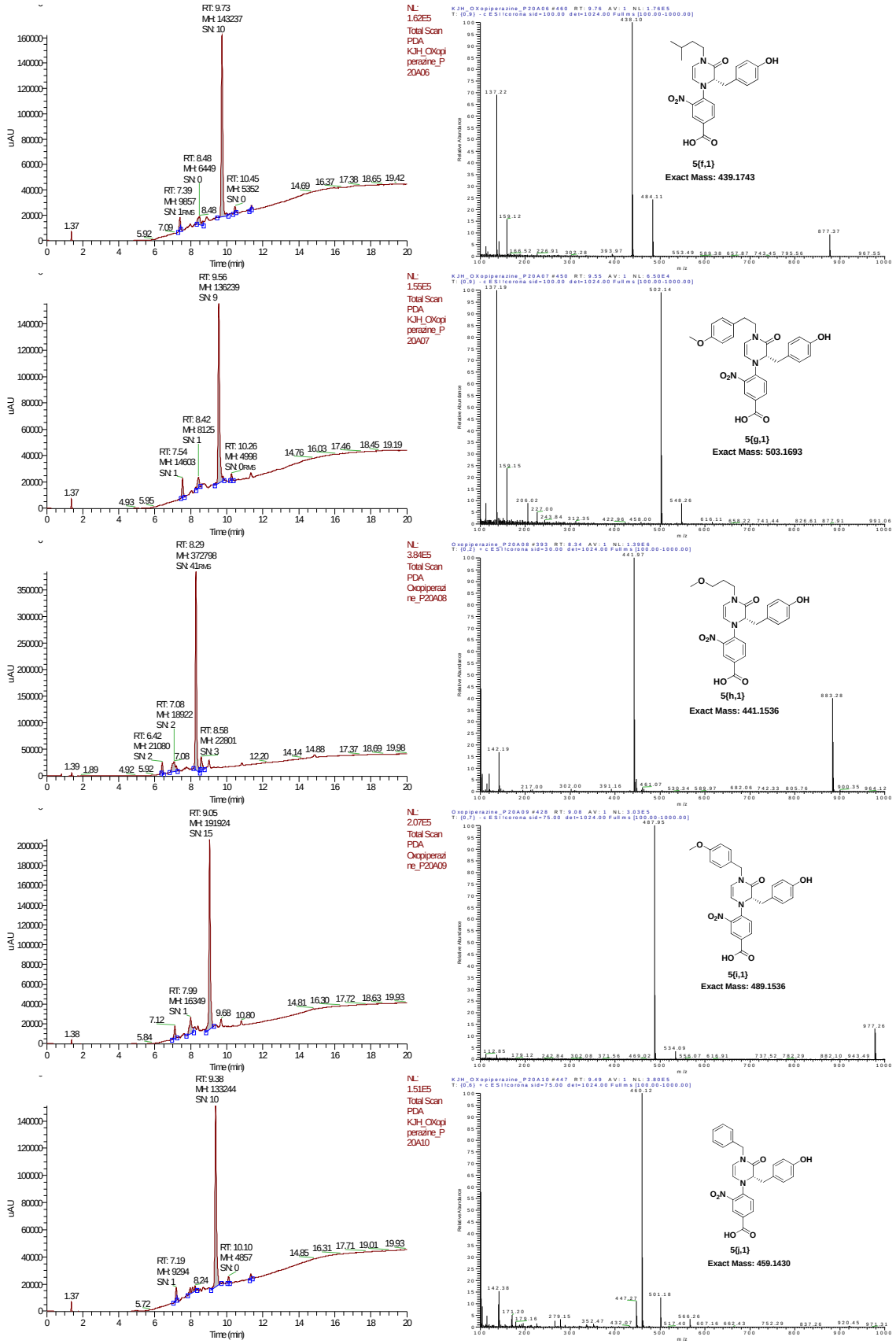








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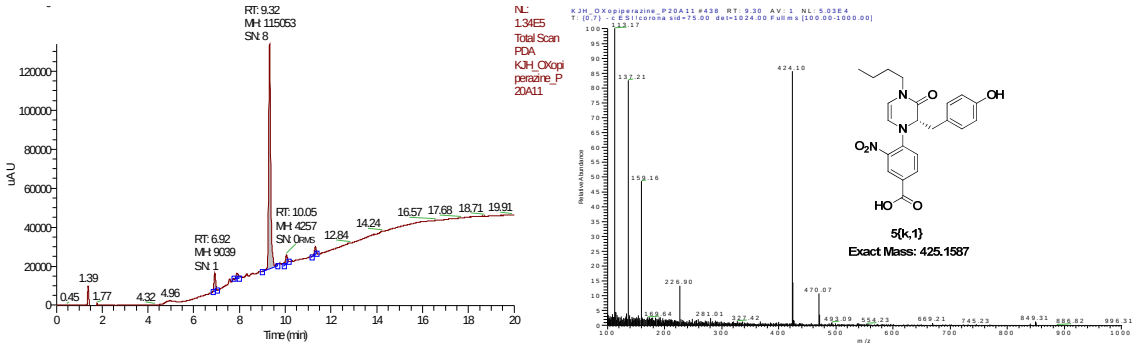
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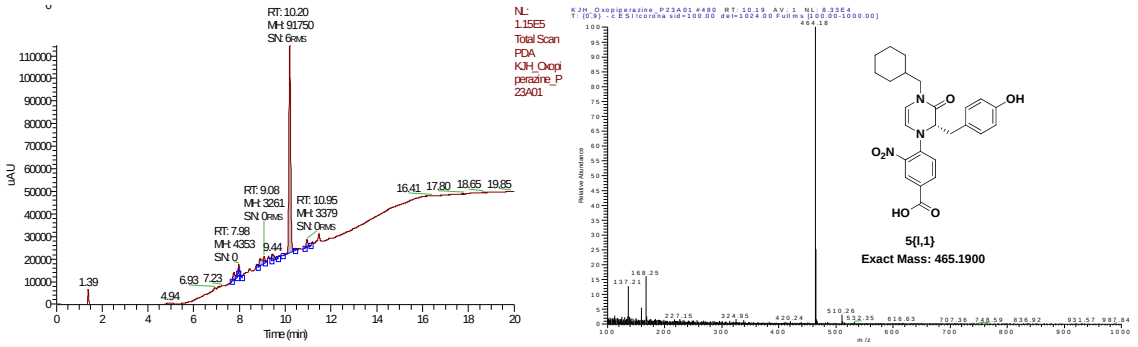
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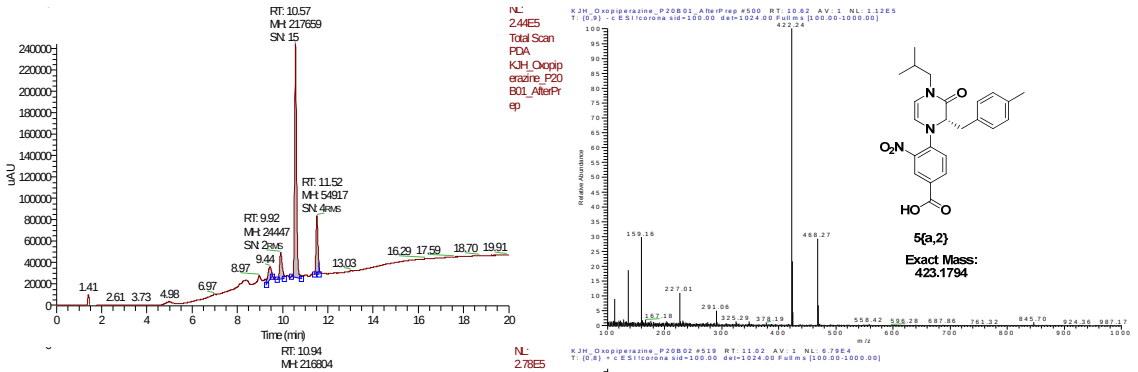
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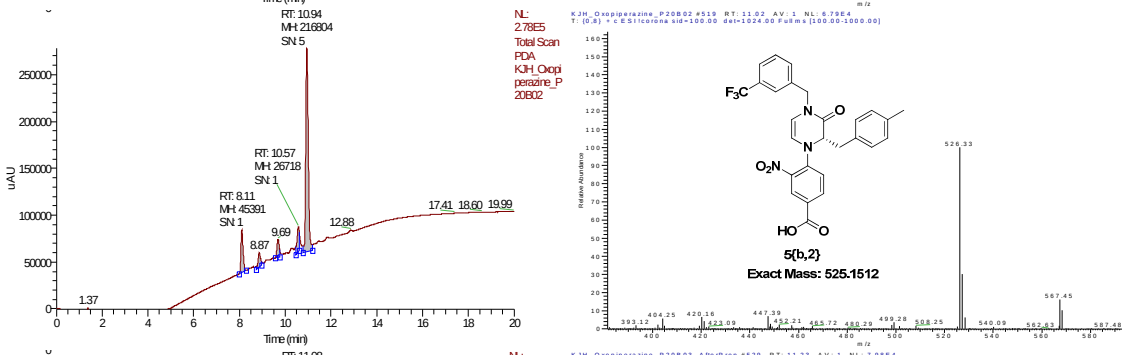
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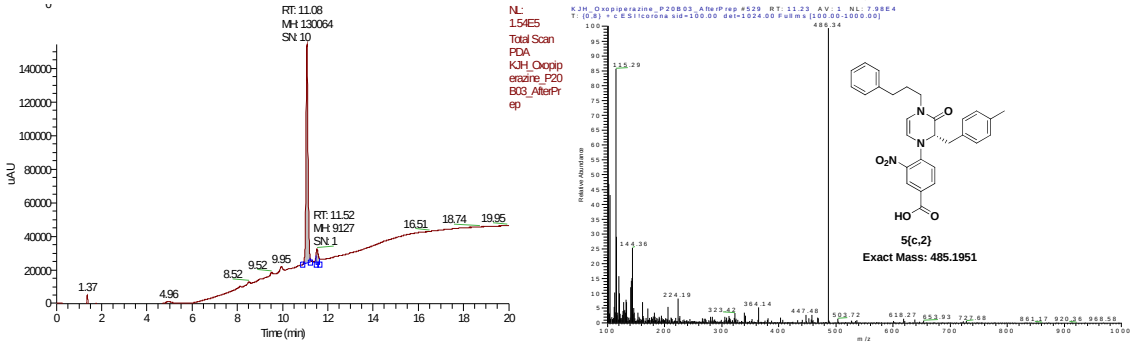
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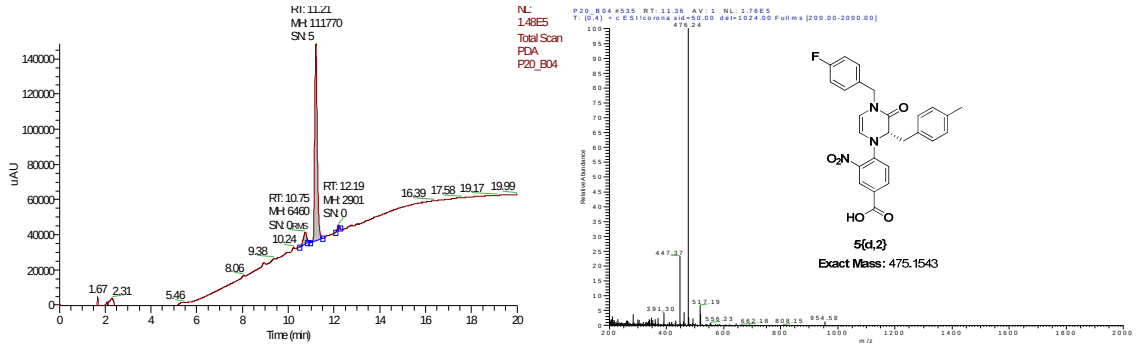
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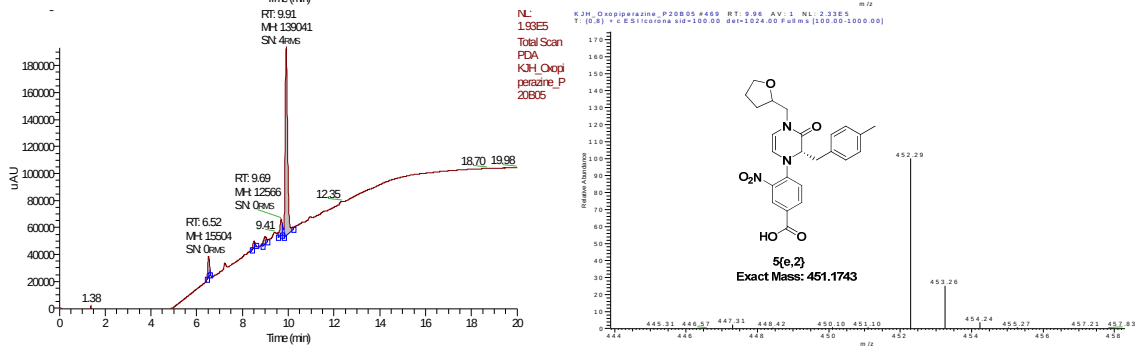
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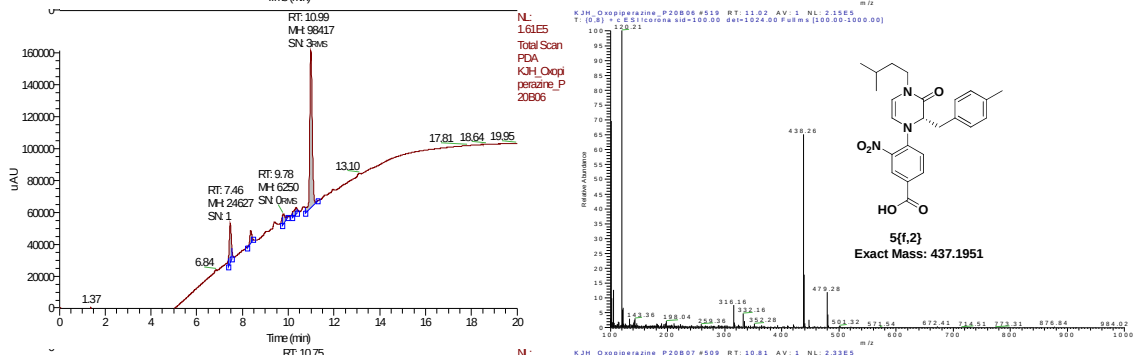
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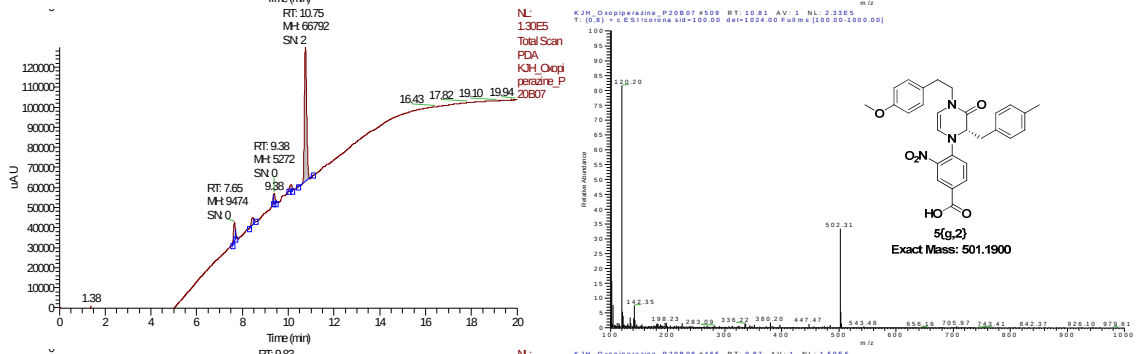
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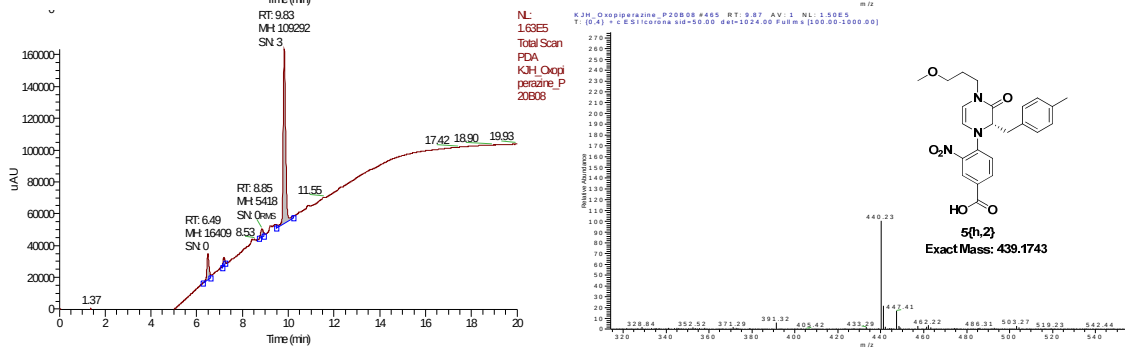
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perazine_P
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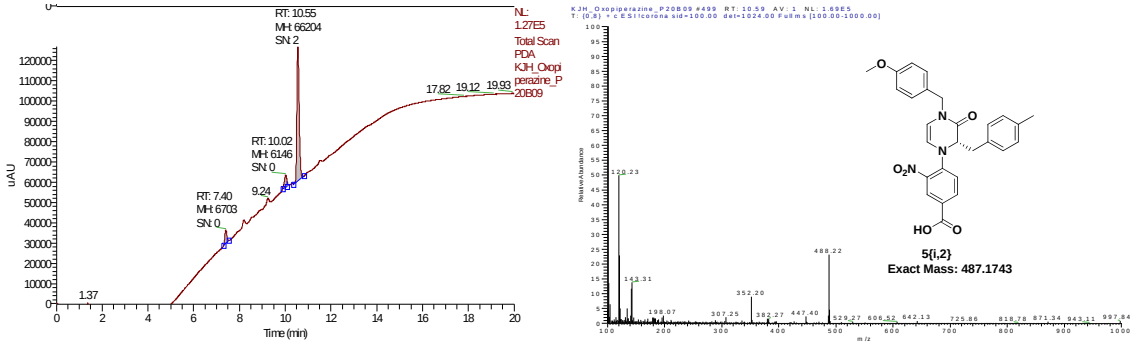
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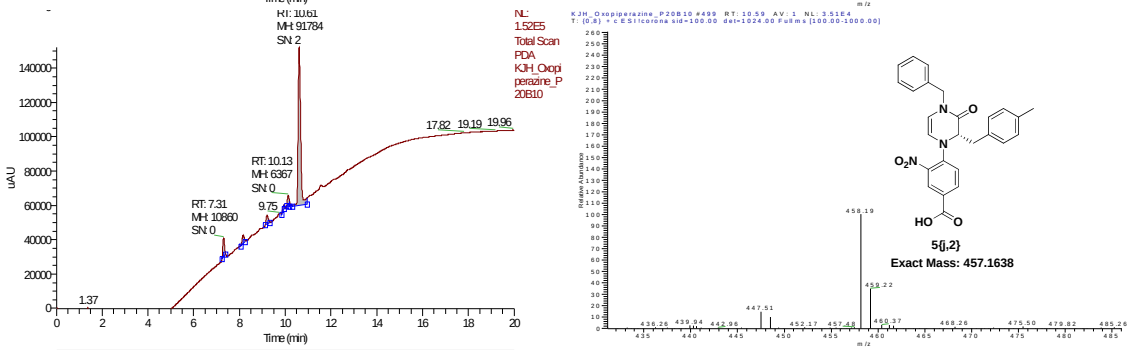
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SN: 0
9.75
17.82 19.19 19.96
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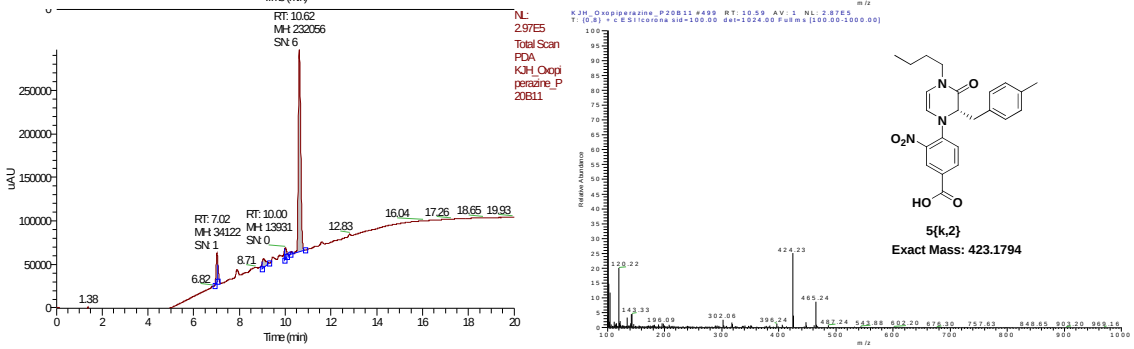
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12.83
16.04 17.26 18.65 19.93
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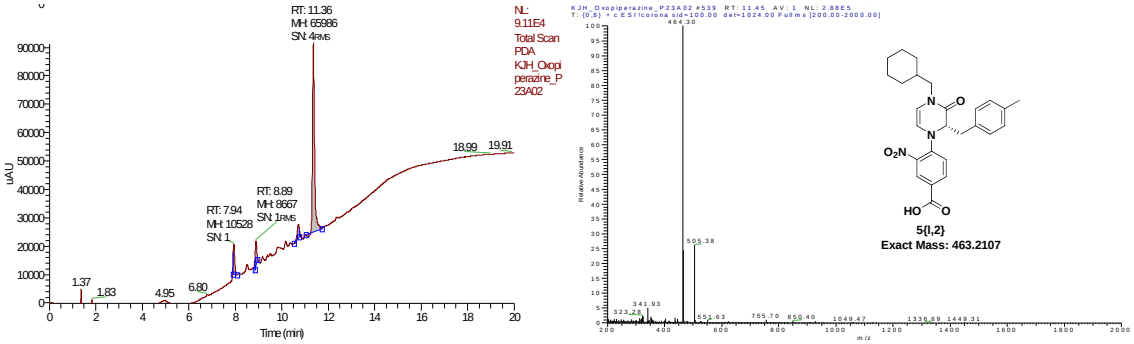
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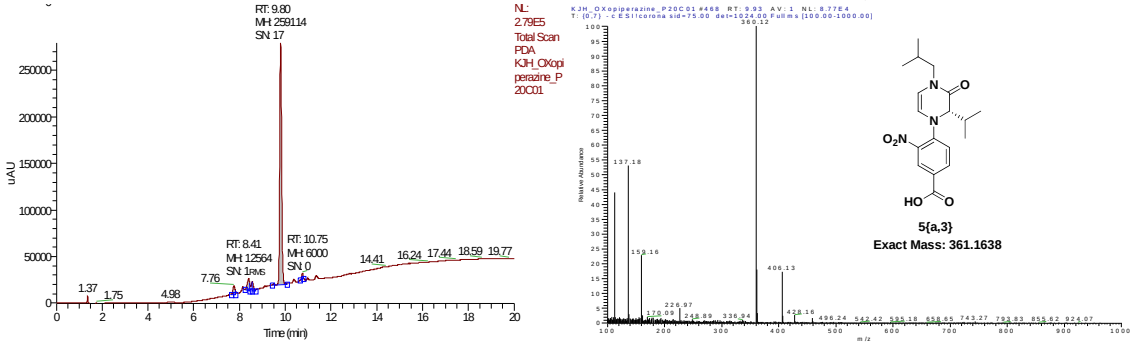
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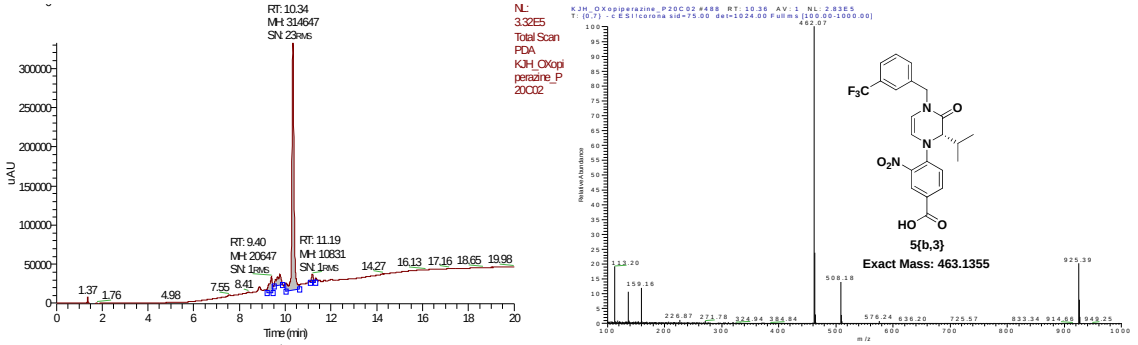
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uAU
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7.55
8.41
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O
N
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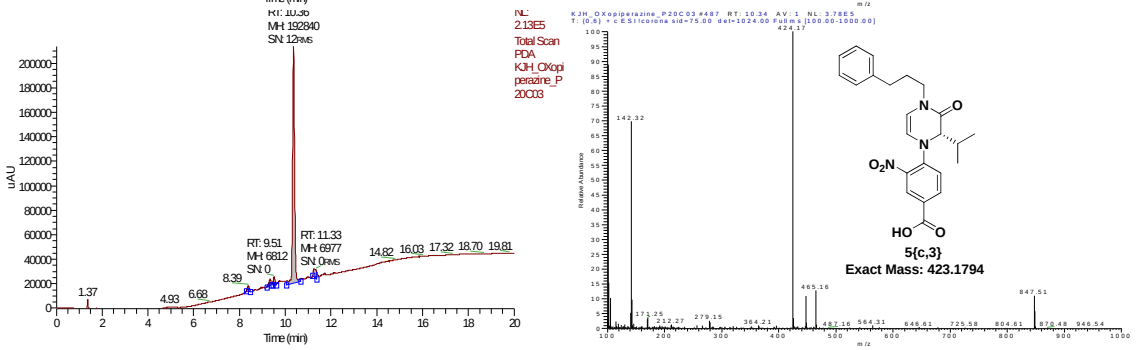
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perazine_P
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uAU
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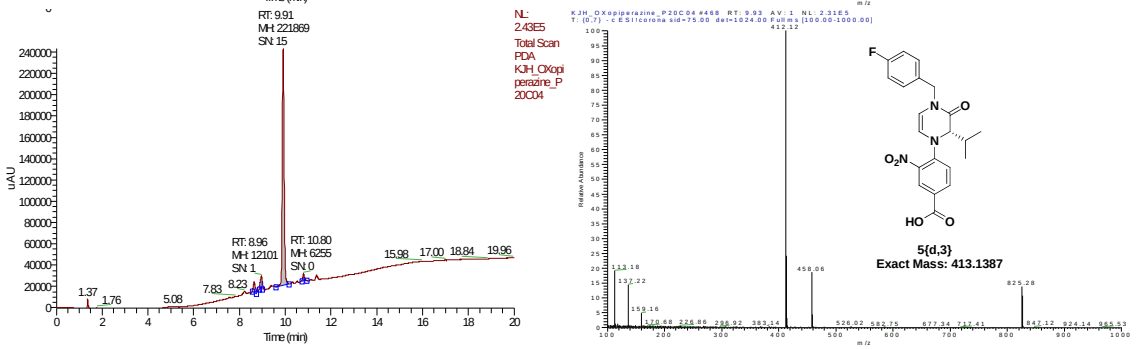
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perazine_P
20C04
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Time (min)
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MH: 12101
SN: 1
RT: 10.80
MH: 6255
SN: 0
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1.76
5.08
7.83
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F
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O
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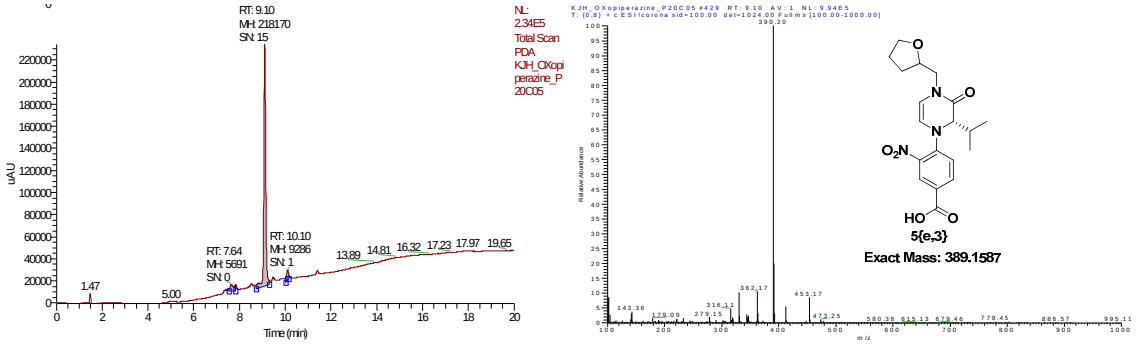
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RT: 10.10
MH: 9286
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HO
O
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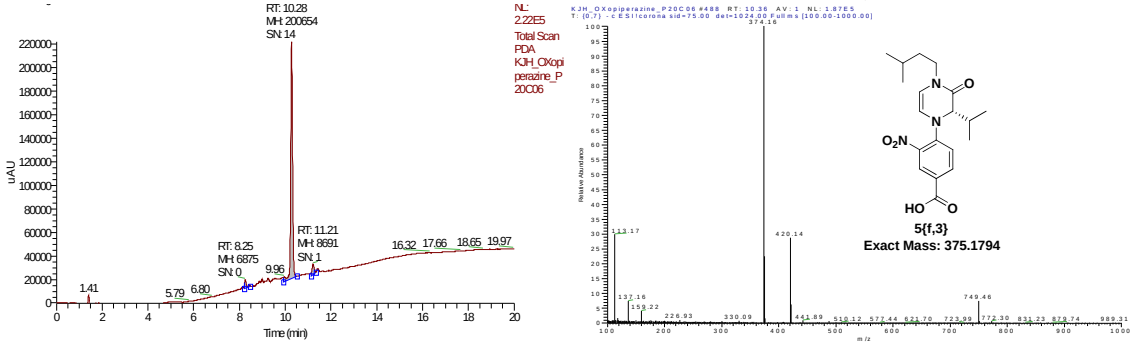
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20C06
uAU
Time (min)
RT: 8.25
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MH: 8691
SN: 1
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5.79
6.80
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HO
O
N
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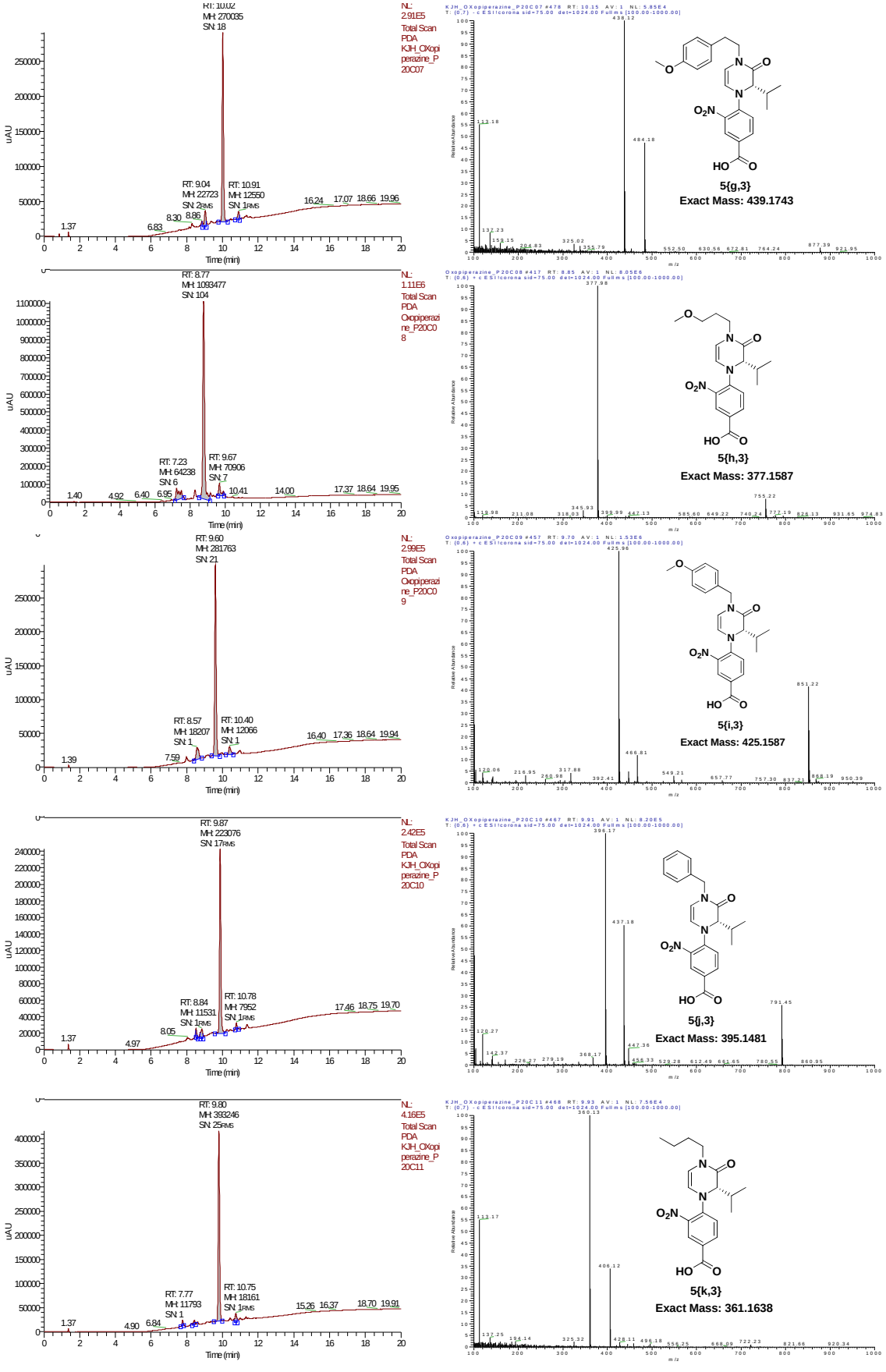
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MH: 22723
SN: 2RMS
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MH: 12550
SN: 1RMS
1.37
6.83
8.30
8.86
16.24
17.07
18.66
19.96
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439.12
484.18
113.18
137.23
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325.02
355.79
552.50
630.56
672.81
764.24
877.39
921.95
Relative Abundance
m/z
5{g,3}
Exact Mass: 439.1743
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NL: 1.11E6
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MH: 64238
SN: 6
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MH: 70906
SN: 7
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4.92
6.40
6.95
10.41
14.00
17.37
18.64
19.95
Oxopiperazine_P20C08 #417 RT: 8.85 AV: 1 NL: 8.05E6
T: {0,0} + c ESI Icorona sid=75.00 det=1024.00 Fullms [100.00-1000.00]
377.98
345.93
755.22
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Exact Mass: 377.1587
RT: 9.60
MH: 281763
SN: 21
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SN: 1
RT: 10.40
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18.64
19.94
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466.81
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Exact Mass: 425.1587
RT: 9.87
MH: 223076
SN: 17RMS
NL: 2.42E5
Total Scan PDA KJH_OXopiperazine_P20C10
RT: 8.84
MH: 11531
SN: 1RMS
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SN: 1RMS
1.37
4.97
8.05
17.46
18.75
19.70
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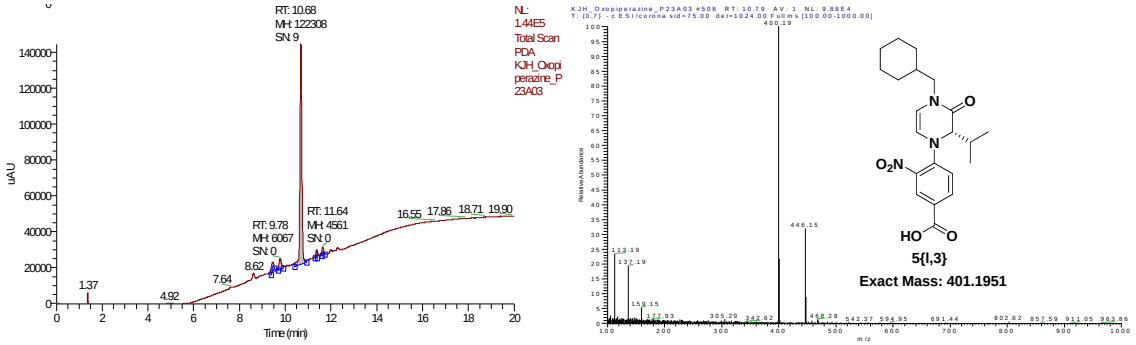
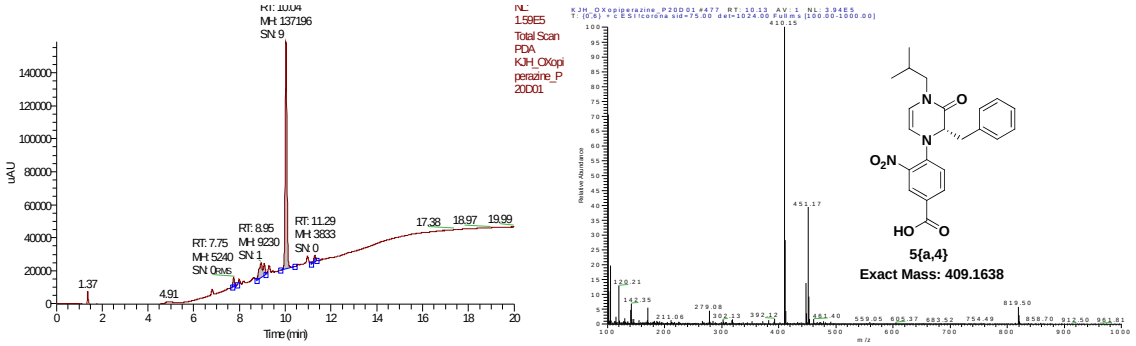
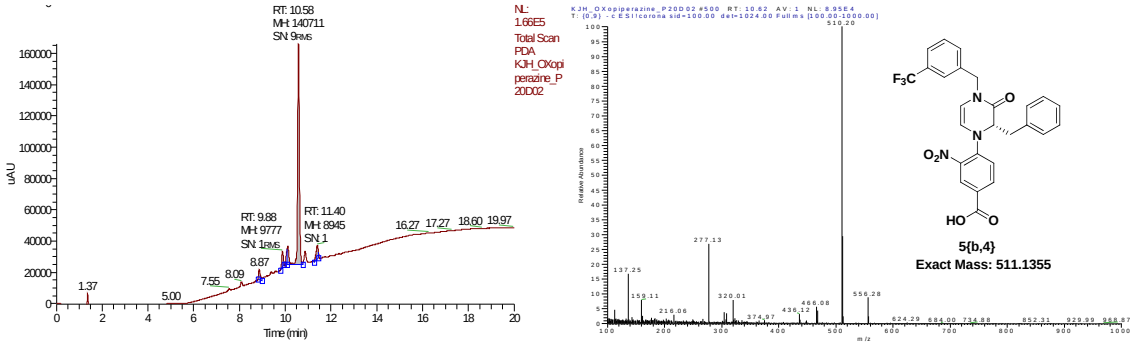
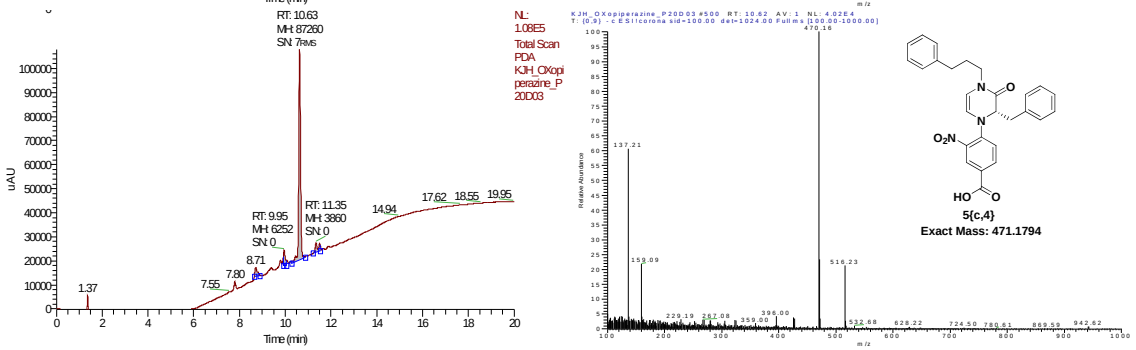
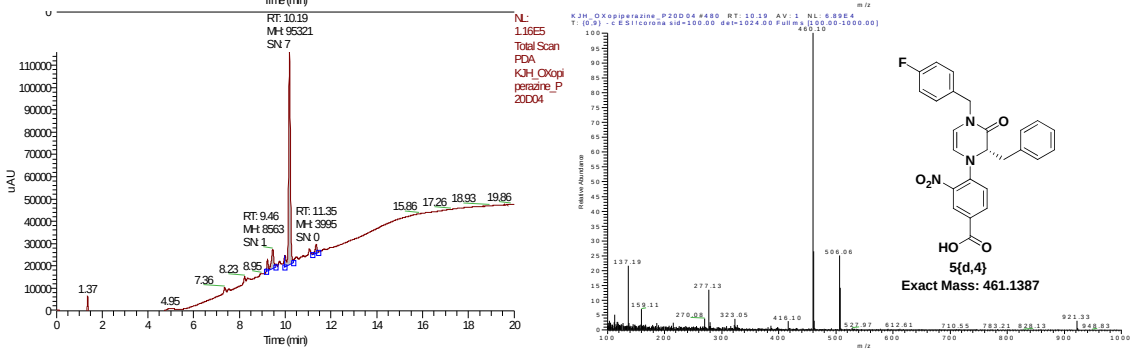
SN: 25RMS
NL: 4.16E5
Total Scan PDA KJH_OXopiperazine_P20C11
RT: 7.77
MH: 11793
SN: 1
RT: 10.75
MH: 18161
SN: 1RMS
1.37
4.90
6.84
15.26
16.37
18.70
19.91
KJH_OXopiperazine_P20C11 #468 RT: 9.93 AV: 1 NL: 7.56E4
T: {0,0} - c ESI Icorona sid=75.00 det=1024.00 Fullms [100.00-1000.00]
360.13
406.12
5{k,3}
Exact Mass: 361.1638

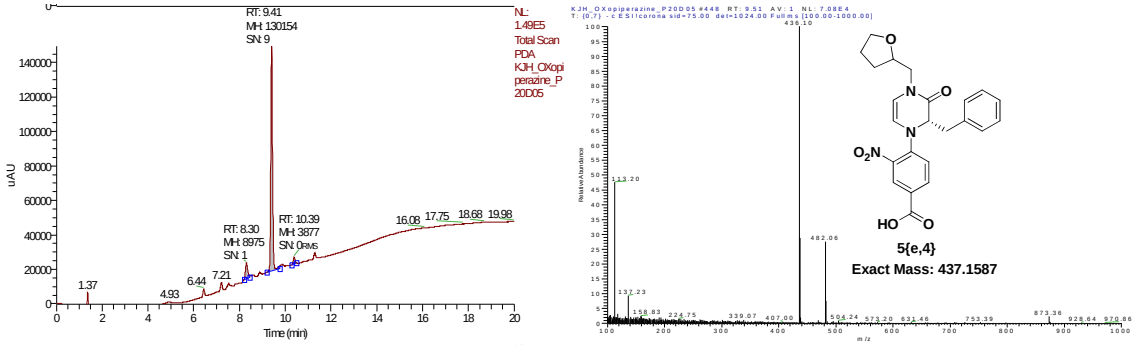

RT: 10.68
MH: 122308
SN: 9
RT: 11.64
MH: 4561
SN: 0
RT: 9.78
MH: 6067
SN: 0
NL:
1.44E5
Total Scan
PDA
KJH_Oxopi
perazine_P
23A03
uAU
Time (min)
5{l,3}
Exact Mass: 401.1951

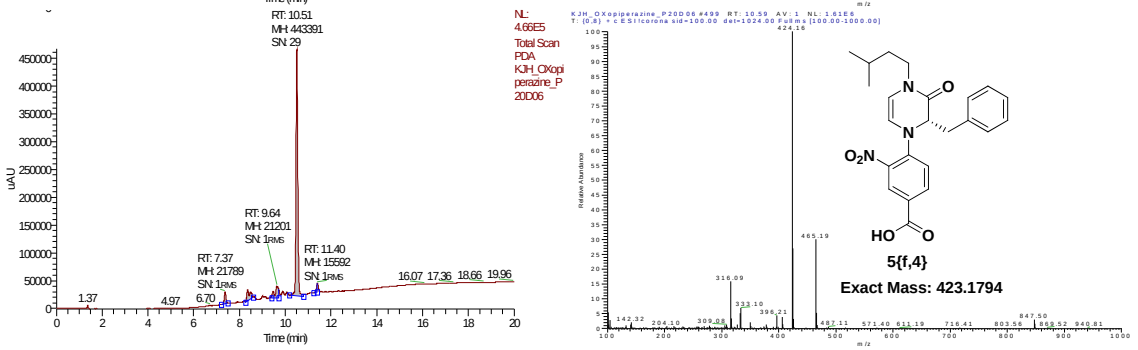

RT: 10.04
MH: 137196
SN: 9
RT: 11.29
MH: 3833
SN: 0
RT: 8.95
MH: 9230
SN: 1
RT: 7.75
MH: 5240
SN: 0
NL:
1.59E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D01
uAU
Time (min)
5{a,4}
Exact Mass: 409.1638

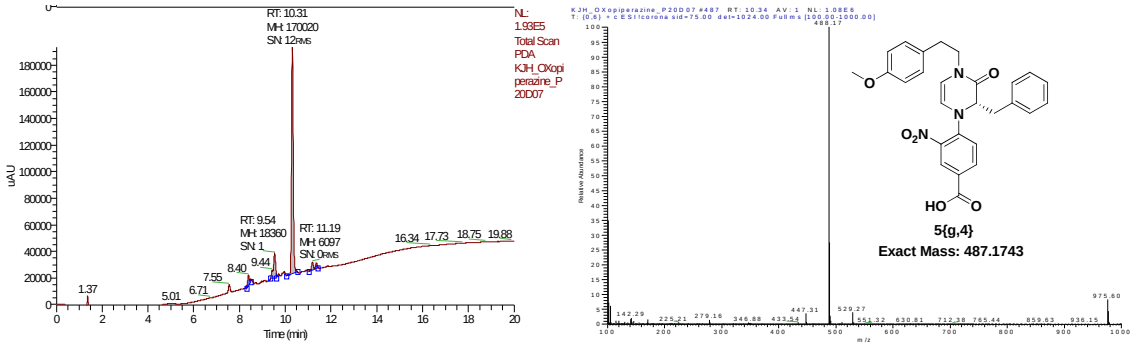

RT: 10.58
MH: 140711
SN: 9
RT: 11.40
MH: 8945
SN: 1
RT: 9.88
MH: 9777
SN: 1
NL:
1.66E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D02
uAU
Time (min)
5{b,4}
Exact Mass: 511.1355

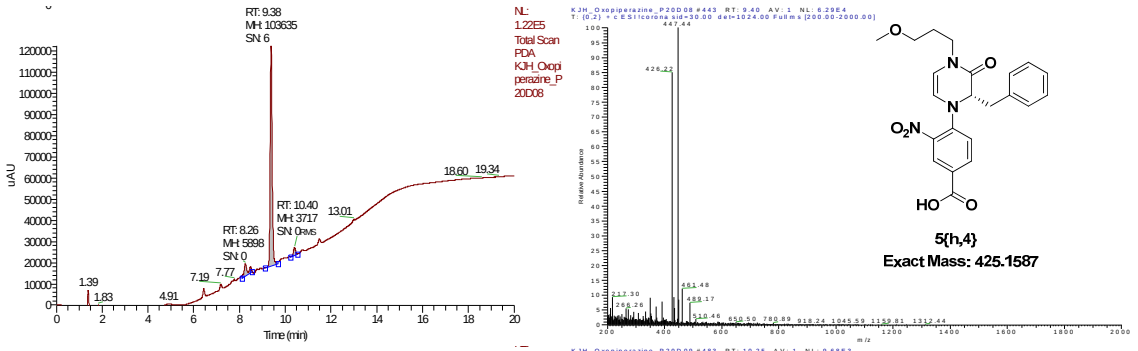

RT: 10.63
MH: 87260
SN: 7
RT: 11.35
MH: 3860
SN: 0
RT: 9.95
MH: 6252
SN: 0
NL:
1.08E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D03
uAU
Time (min)
5{c,4}
Exact Mass: 471.1794

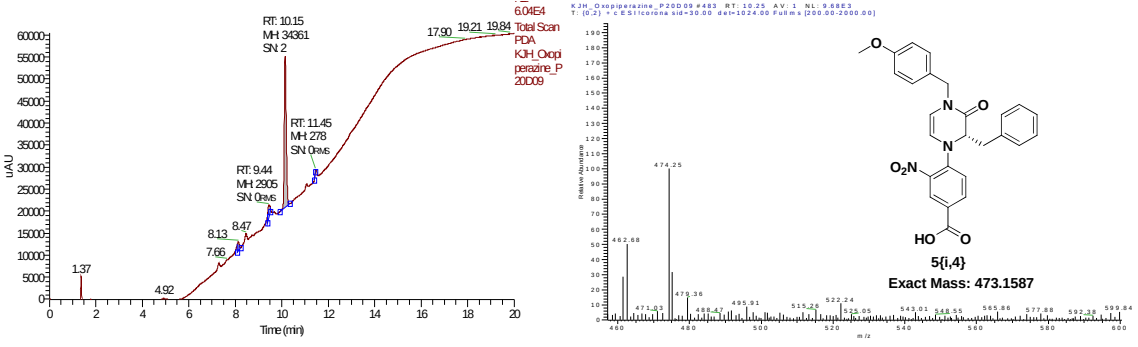

RT: 10.19
MH: 95321
SN: 7
RT: 11.35
MH: 3995
SN: 0
RT: 9.46
MH: 8563
SN: 1
NL:
1.16E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D04
uAU
Time (min)
5{d,4}
Exact Mass: 461.1387

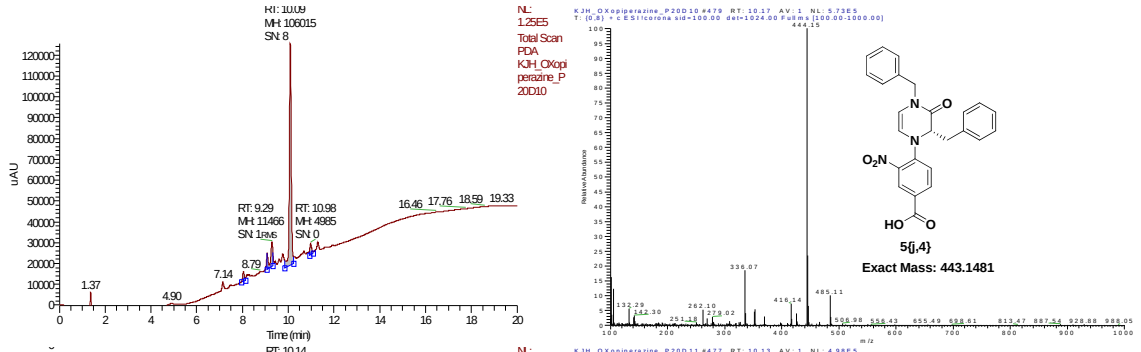

RT: 9.41
MH: 130154
SN: 9
RT: 8.30
MH: 8975
SN: 1
RT: 10.39
MH: 3877
SN: 0RMS
NL:
1.49E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D05
uAU
Time (min)
5{e,4}
Exact Mass: 437.1587


RT: 10.51
MH: 443391
SN: 29
RT: 9.64
MH: 21201
SN: 1RMS
RT: 7.37
MH: 21789
SN: 1RMS
RT: 11.40
MH: 15592
SN: 1RMS
NL:
4.66E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D06
uAU
Time (min)
5{f,4}
Exact Mass: 423.1794

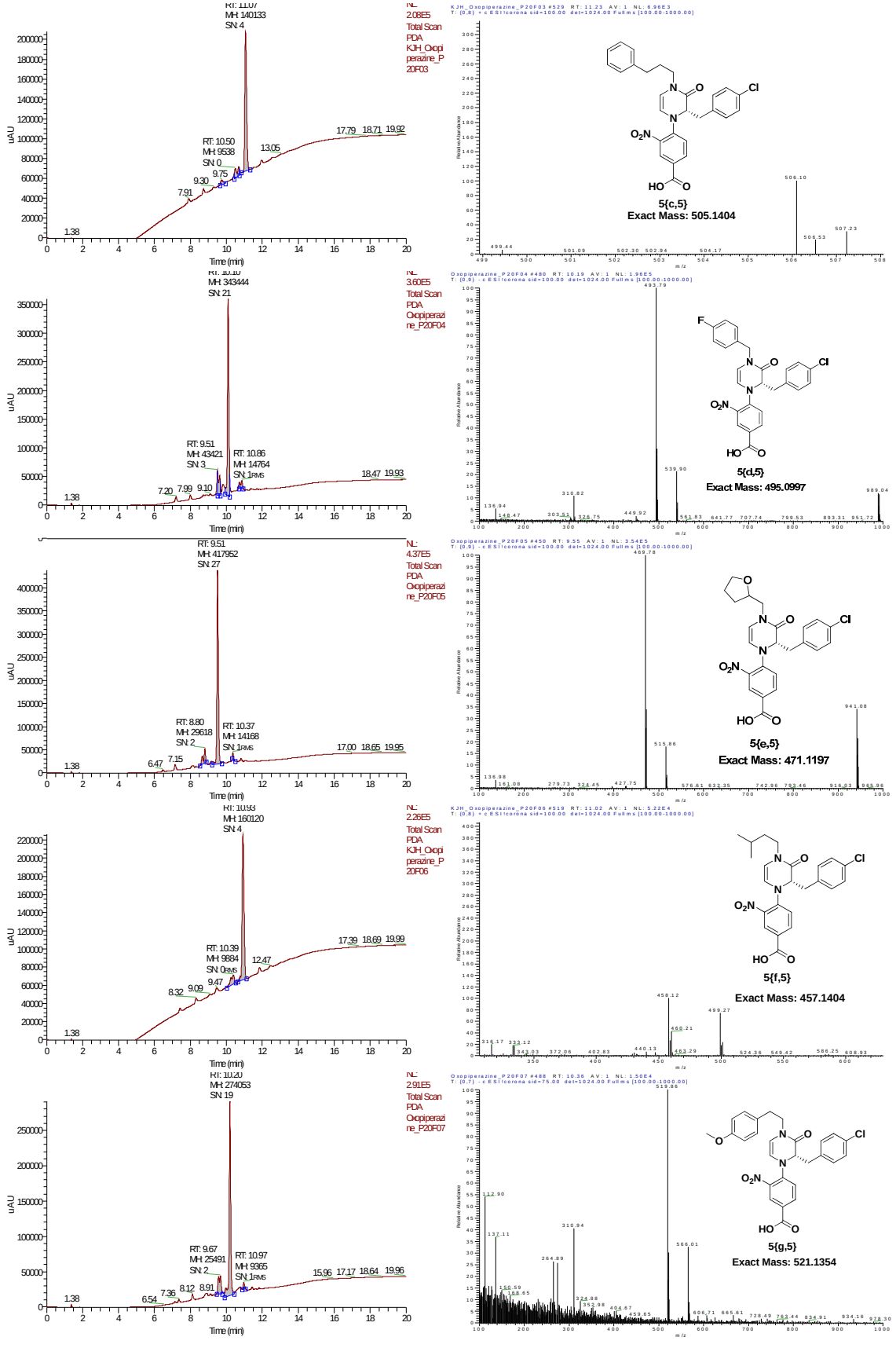

RT: 10.31
MH: 170020
SN: 12RMS
RT: 9.54
MH: 18360
SN: 1
RT: 11.19
MH: 6097
SN: 0RMS
NL:
1.93E5
Total Scan
PDA
KJH_OXopi
perazine_P
20D07
uAU
Time (min)
5{g,4}
Exact Mass: 487.1743

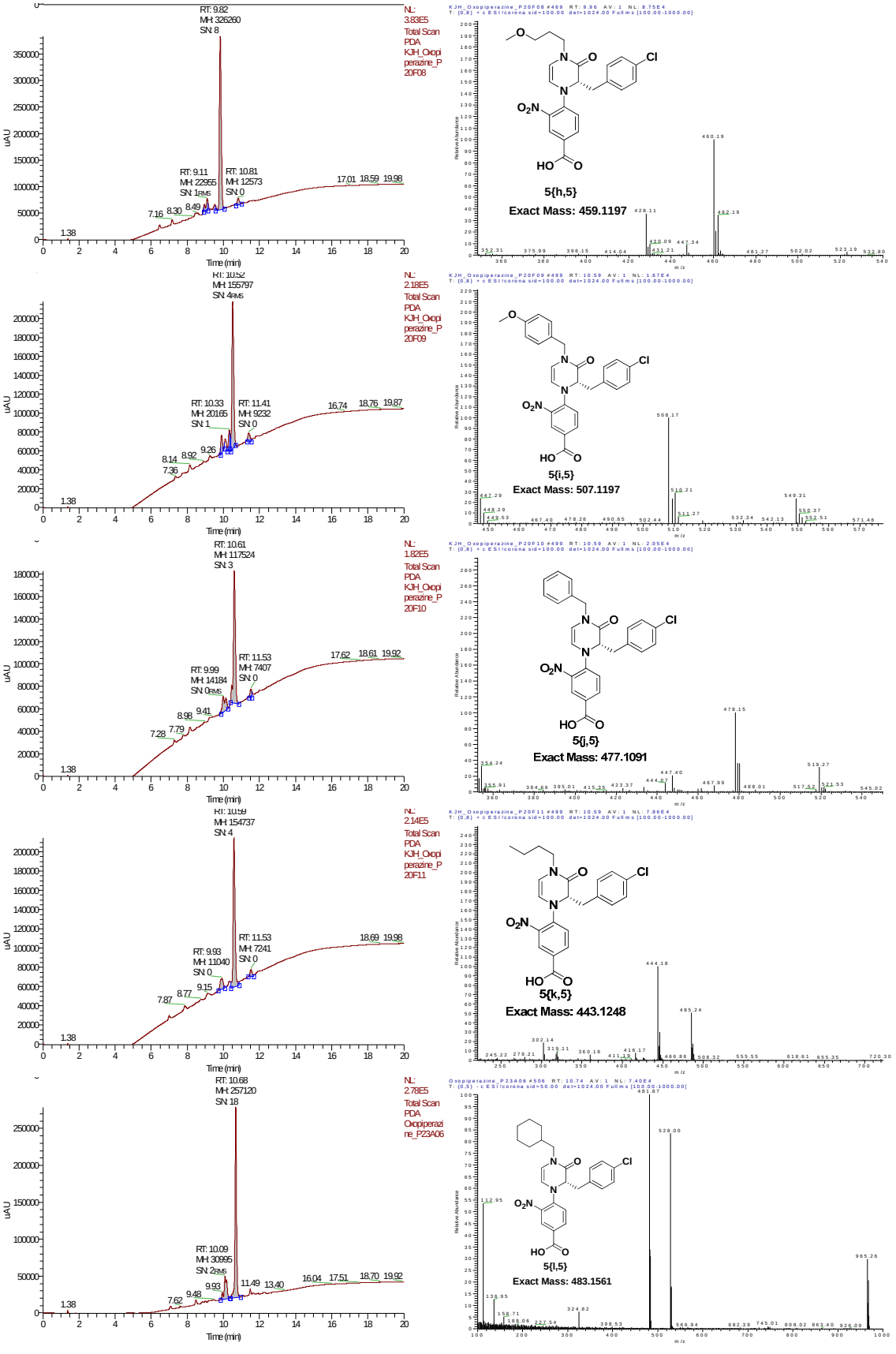

RT: 9.38
MH: 103635
SN: 6
RT: 8.26
MH: 5898
SN: 0
RT: 10.40
MH: 3717
SN: 0RMS
NL:
1.22E5
Total Scan
PDA
KJH_Oxopi
perazine_P
20D08
uAU
Time (min)
5{h,4}
Exact Mass: 425.1587

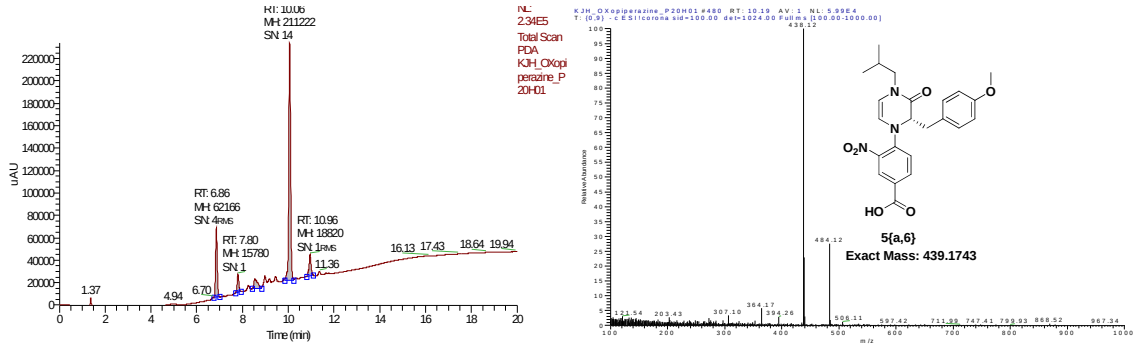

RT: 10.15
MH: 34361
SN: 2
RT: 9.44
MH: 2905
SN: 0RMS
RT: 11.45
MH: 278
SN: 0RMS
6.04E4
Total Scan
PDA
KJH_Oxopi
perazine_P
20D09
uAU
Time (min)
5{i,4}
Exact Mass: 473.1587

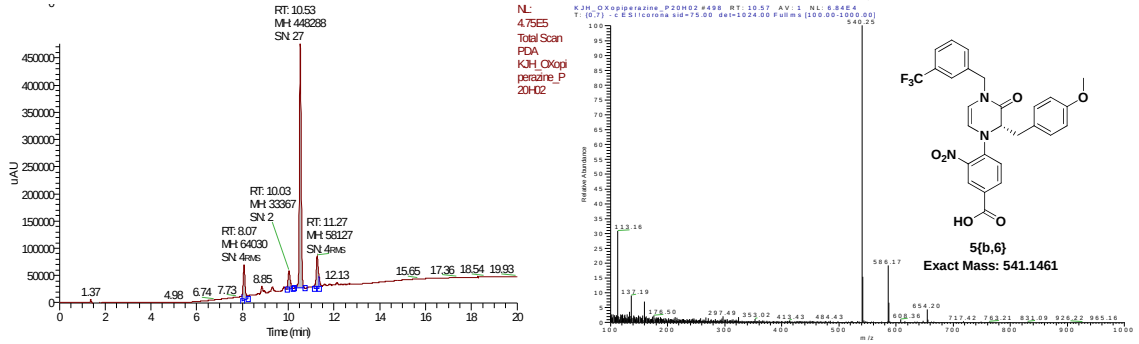

RT: 10.09
MH: 106015
SN: 8
RT: 9.29
MH: 11466
SN: 1RMS
RT: 10.98
MH: 4985
SN: 0
RT: 6.94
MH: 11119
SN: 1
RT: 7.89
MH: 10828
SN: 1
RT: 11.07
MH: 10059
SN: 1RMS
RT: 10.14
MH: 258236
SN: 17RMS
RT: 10.17
MH: 10611
SN: 1RMS
RT: 11.84
MH: 5000
SN: 0RMS
RT: 10.30
MH: 94062
SN: 7
RT: 9.87
MH: 18407
SN: 0
RT: 11.52
MH: 5849
SN: 0RMS
RT: 10.57
MH: 148344
SN: 4
RT: 10.02
MH: 30284
SN: 2RMS
RT: 11.43
MH: 13347
SN: 1RMS
RT: 10.44
MH: 201214
SN: 14
uAU
Time (min)

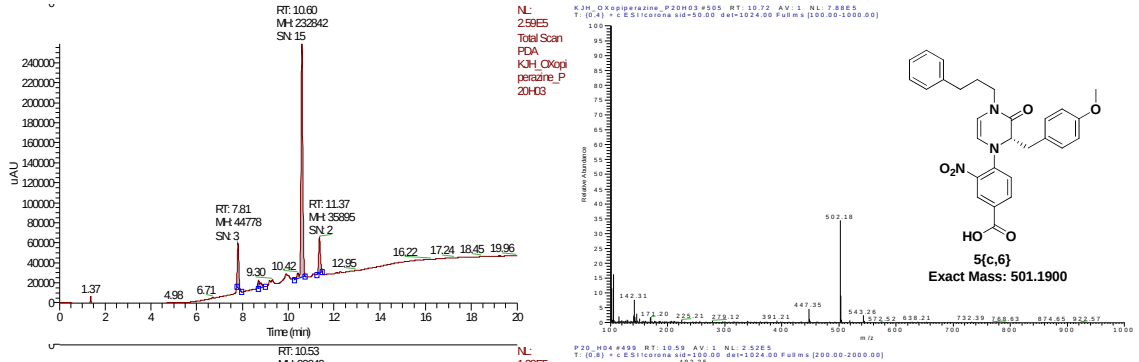
NL: 1.25E5 Total Scan PDA KJH_OXopiperazine_P20D10
NL: 2.80E5 Total Scan PDA KJH_OXopiperazine_P20D11
NL: 1.18E5 Total Scan PDA KJH_Oxopiperazine_P23A04
NL: 2.11E5 Total Scan PDA KJH_Oxopiperazine_P20F01
NL: 2.22E5 Total Scan PDA Oxopiperazine_P20F02
5{j,4}
Exact Mass: 443.1481
5{k,4}
Exact Mass: 409.1638
5{l,4}
Exact Mass: 449.1951
5{a,5}
Exact Mass: 443.1248
5{b,5}
Exact Mass: 545.0965

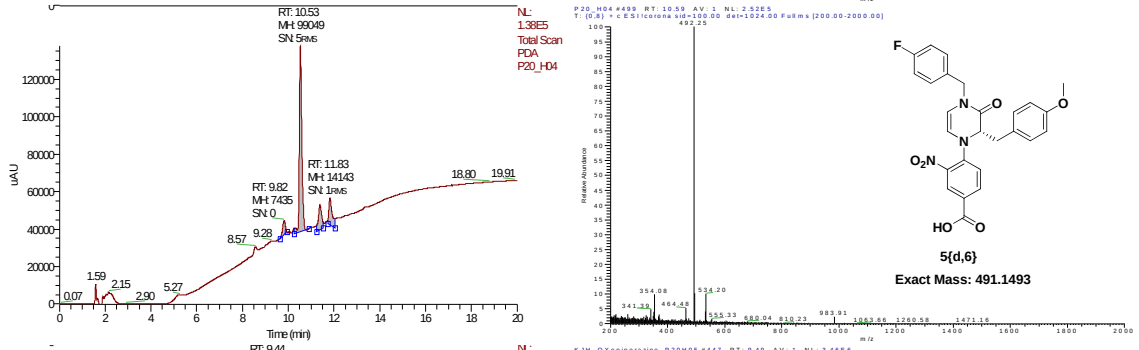

RT: 11.07
MH: 140133
SN: 4
NL: 2.08E5
Total Scan PDA KJH_Oxopiperazine_P20F03
uAU
Time (min)
RT: 10.50
MH: 9538
SN: 0
13.05
17.79
18.71
19.92
9.30
9.75
7.91
1.38
5{c,5}
Exact Mass: 505.1404
RT: 10.10
MH: 343444
SN: 21
NL: 3.60E5
Total Scan PDA Oxopiperazine_P20F04
RT: 9.51
MH: 43421
SN: 3
RT: 10.86
MH: 14764
SN: 1RMS
18.47
19.93
7.20
7.99
9.10
1.38
5{d,5}
Exact Mass: 495.0997
RT: 9.51
MH: 417952
SN: 27
NL: 4.37E5
Total Scan PDA Oxopiperazine_P20F05
RT: 8.80
MH: 29618
SN: 2
RT: 10.37
MH: 14168
SN: 1RMS
17.00
18.65
19.95
6.47
7.15
1.38
5{e,5}
Exact Mass: 471.1197
RT: 10.93
MH: 160120
SN: 4
NL: 2.26E5
Total Scan PDA KJH_Oxopiperazine_P20F06
RT: 10.39
MH: 9884
SN: 0RMS
12.47
17.39
18.69
19.99
8.32
9.09
9.47
1.38
5{f,5}
Exact Mass: 457.1404
RT: 10.20
MH: 274053
SN: 19
NL: 2.91E5
Total Scan PDA Oxopiperazine_P20F07
RT: 9.67
MH: 25491
SN: 2
RT: 10.97
MH: 9365
SN: 1RMS
15.96
17.17
18.64
19.96
6.54
7.36
8.12
8.91
1.38
5{g,5}
Exact Mass: 521.1354

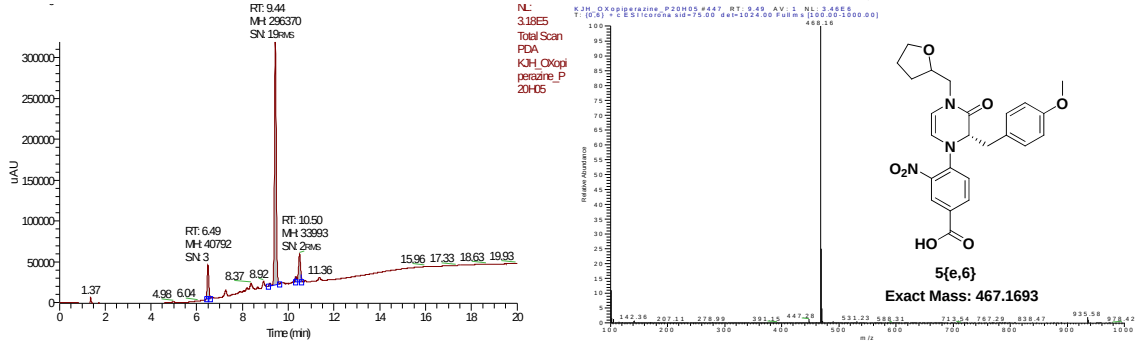

RT: 9.82
MH 326260
SN 8
NL: 3.83E5
Total Scan PDA KJH_Oxopiperazine_P20F08
RT: 9.11
MH 22955
SN 1
RT: 10.81
MH 12573
SN 0
17.01 18.59 19.98
7.16 8.30 8.49
1.38
uAU
Time (min)
5{h,5}
Exact Mass: 459.1197
RT: 10.52
MH 155797
SN 4
NL: 2.18E5
Total Scan PDA KJH_Oxopiperazine_P20F09
RT: 10.33
MH 20165
SN 1
RT: 11.41
MH 9232
SN 0
16.74 18.76 19.87
8.14 8.92 9.26
7.36
1.38
5{i,5}
Exact Mass: 507.1197
RT: 10.61
MH 117524
SN 3
NL: 1.82E5
Total Scan PDA KJH_Oxopiperazine_P20F10
RT: 9.99
MH 14184
SN 0
RT: 11.53
MH 7407
SN 0
17.62 18.61 19.92
8.98 9.41
7.28 7.79
1.38
5{j,5}
Exact Mass: 477.1091
RT: 10.59
MH 154737
SN 4
NL: 2.14E5
Total Scan PDA KJH_Oxopiperazine_P20F11
RT: 9.93
MH 11040
SN 0
RT: 11.53
MH 7241
SN 0
18.69 19.98
7.87 8.77 9.15
1.38
5{k,5}
Exact Mass: 443.1248
RT: 10.68
MH 257120
SN 18
NL: 2.78E5
Total Scan PDA Oxopiperazine_P23A06
RT: 10.09
MH 30995
SN 2
11.49 13.40 16.04 17.51 18.70 19.92
9.93
7.62 9.48
1.38
5{l,5}
Exact Mass: 483.1561

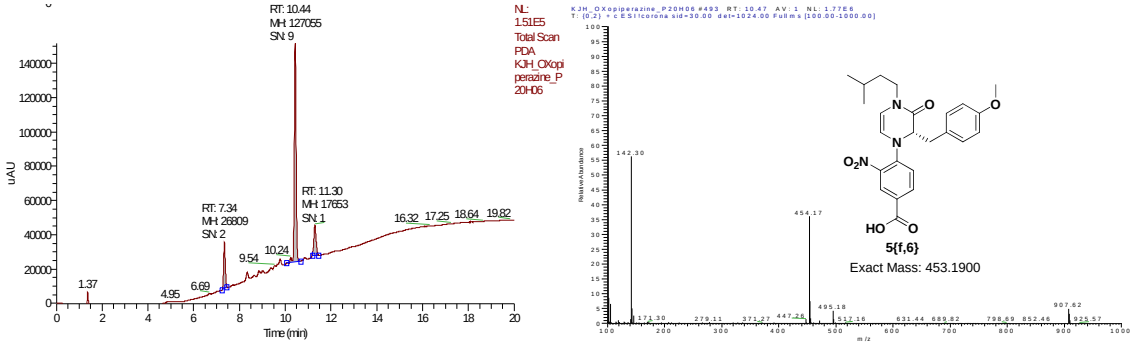

RT: 10.06
MH: 211222
SN: 14
NL:
2.34E5
Total Scan
PDA
KJH_OXopi
perazine_P
20H01
RT: 6.86
MH: 62166
SN: 4RMS
RT: 7.80
MH: 15780
SN: 1
RT: 10.96
MH: 18820
SN: 1RMS
uAU
Time (min)
5{a,6}
Exact Mass: 439.1743

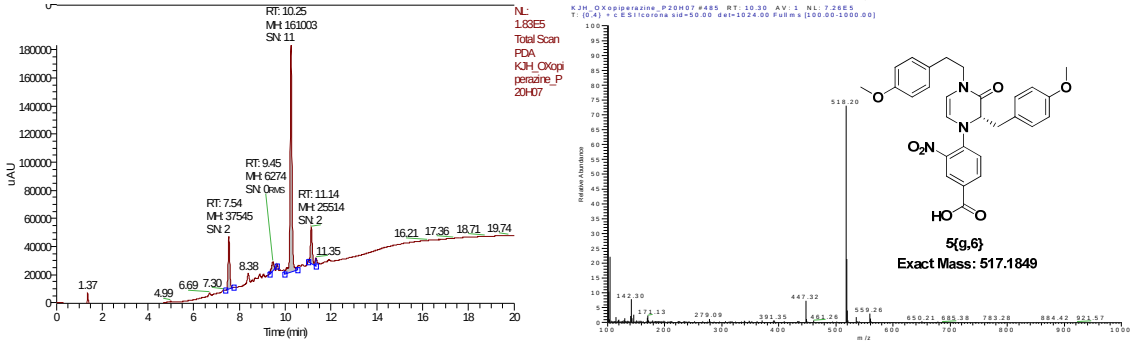

RT: 10.53
MH: 448288
SN: 27
NL:
4.75E5
Total Scan
PDA
KJH_OXopi
perazine_P
20H02
RT: 10.03
MH: 33367
SN: 2
RT: 8.07
MH: 64030
SN: 4RMS
RT: 11.27
MH: 58127
SN: 4RMS
uAU
Time (min)
5{b,6}
Exact Mass: 541.1461

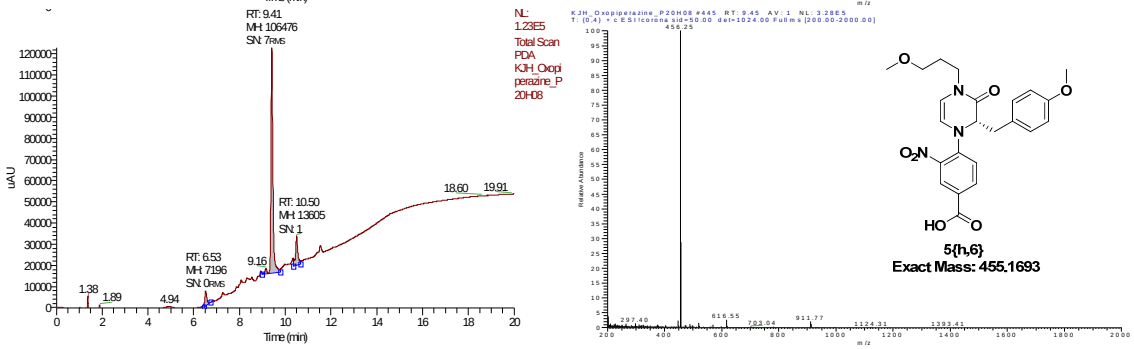

RT: 10.60
MH: 232842
SN: 15
NL:
2.59E5
Total Scan
PDA
KJH_OXopi
perazine_P
20H03
RT: 7.81
MH: 44778
SN: 3
RT: 11.37
MH: 35895
SN: 2
uAU
Time (min)
5{c,6}
Exact Mass: 501.1900

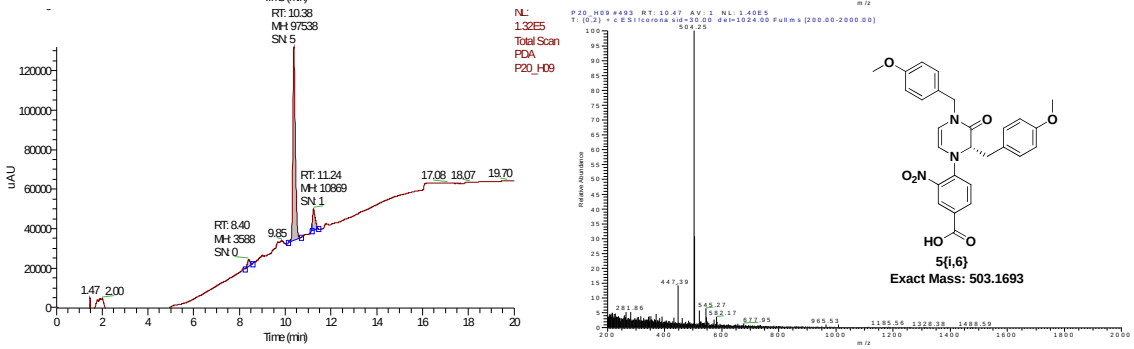

RT: 10.53
MH: 99049
SN: 5RMS
NL:
1.38E5
Total Scan
PDA
P20_H04
RT: 9.82
MH: 7435
SN: 0
RT: 11.83
MH: 14143
SN: 1RMS
uAU
Time (min)
5{d,6}
Exact Mass: 491.1493

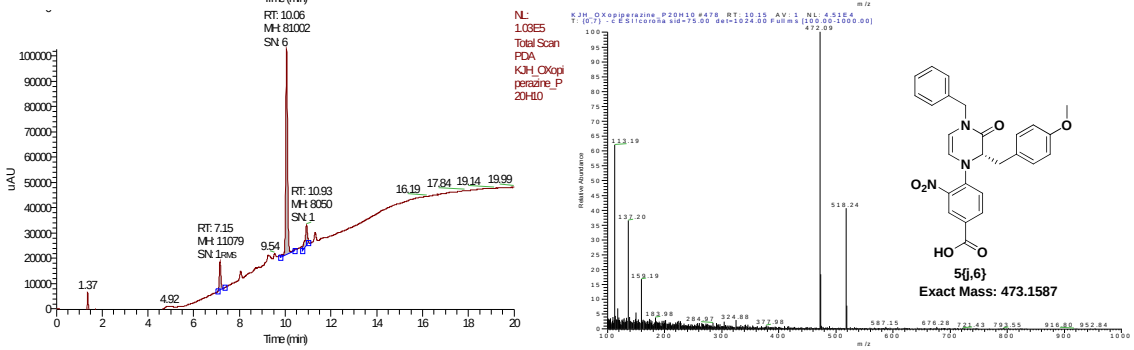

RT: 9.44
MH: 296370
SN: 19RMS
NL:
3.18E5
Total Scan
PDA
KJH_OXopi
perazine_P
20H05
RT: 6.49
MH: 40792
SN: 3
RT: 10.50
MH: 33993
SN: 2RMS
uAU
Time (min)
5{e,6}
Exact Mass: 467.1693

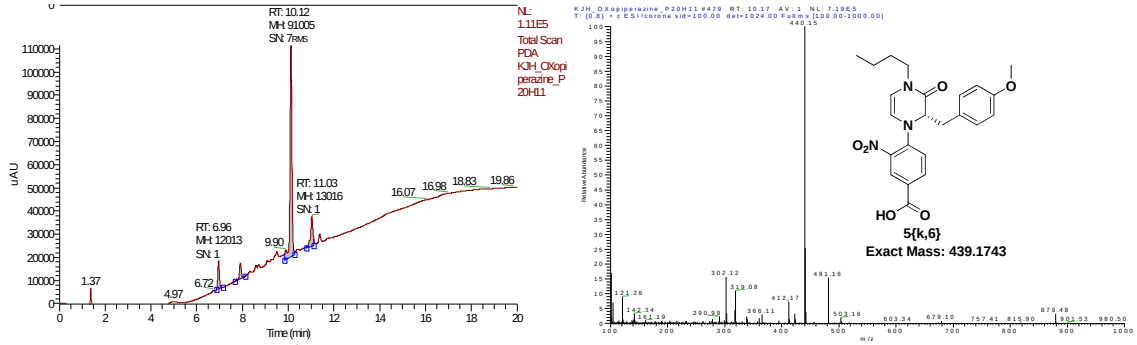

RT: 10.44
MH: 127055
SN: 9
RT: 7.34
MH: 26809
SN: 2
RT: 11.30
MH: 17653
SN: 1
NL: 1.51E5
Total Scan PDA KJH_OXopiperazine_P20H06
uAU
Time (min)
5{f,6}
Exact Mass: 453.1900

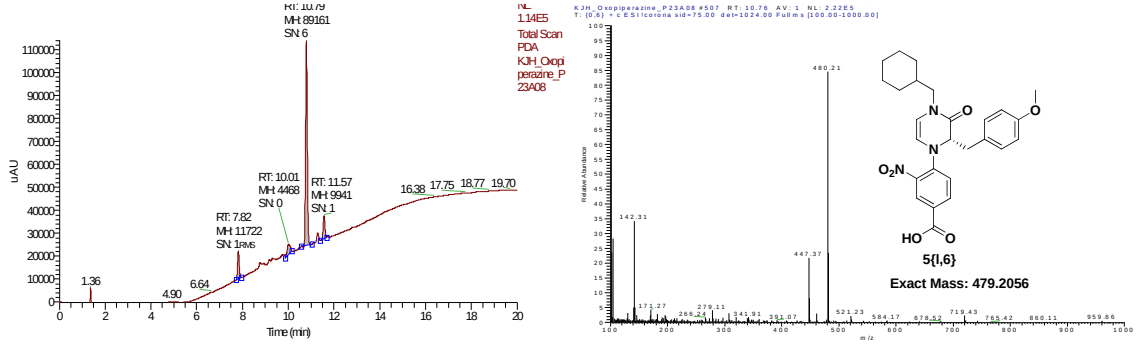

RT: 10.25
MH: 161003
SN: 11
RT: 9.45
MH: 6274
SN: 0rvs
RT: 7.54
MH: 37545
SN: 2
RT: 11.14
MH: 25514
SN: 2
NL: 1.83E5
Total Scan PDA KJH_OXopiperazine_P20H07
uAU
Time (min)
5{g,6}
Exact Mass: 517.1849

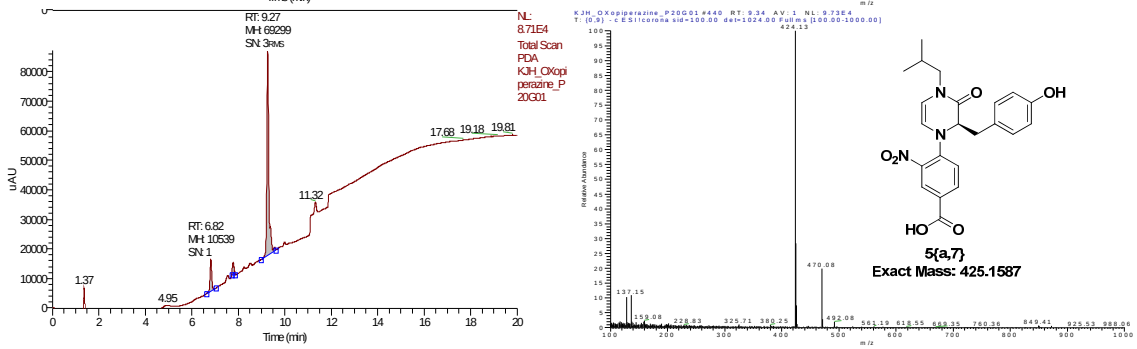

RT: 9.41
MH: 106476
SN: 7rvs
RT: 10.50
MH: 13605
SN: 1
RT: 6.53
MH: 7196
SN: 0rvs
NL: 1.23E5
Total Scan PDA KJH_OXopiperazine_P20H08
uAU
Time (min)
5{h,6}
Exact Mass: 455.1693

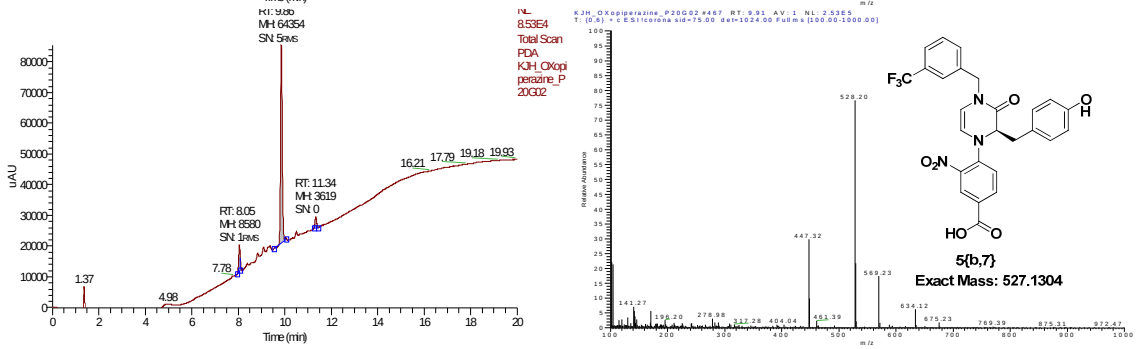

RT: 10.38
MH: 97538
SN: 5
RT: 11.24
MH: 10869
SN: 1
RT: 8.40
MH: 3588
SN: 0
NL: 1.32E5
Total Scan PDA P20_H09
uAU
Time (min)
5{i,6}
Exact Mass: 503.1693

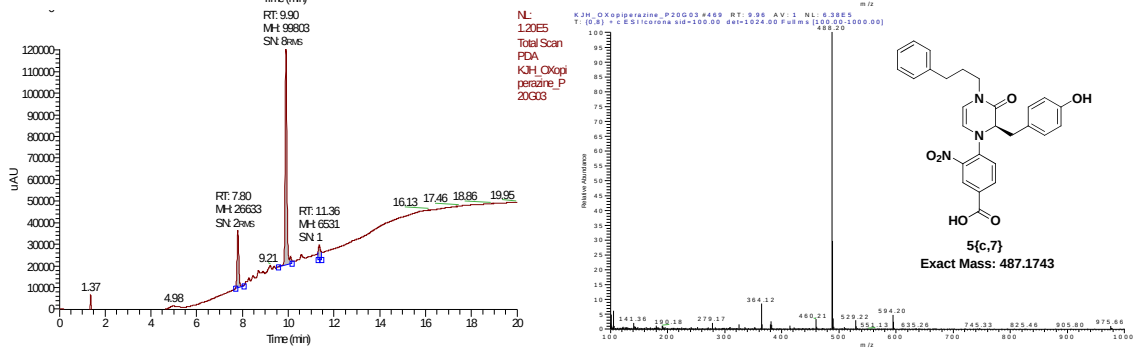

RT: 10.06
MH: 81002
SN: 6
RT: 10.93
MH: 8050
SN: 1
RT: 7.15
MH: 11079
SN: 1rvs
NL: 1.03E5
Total Scan PDA KJH_OXopiperazine_P20H10
uAU
Time (min)
5{j,6}
Exact Mass: 473.1587

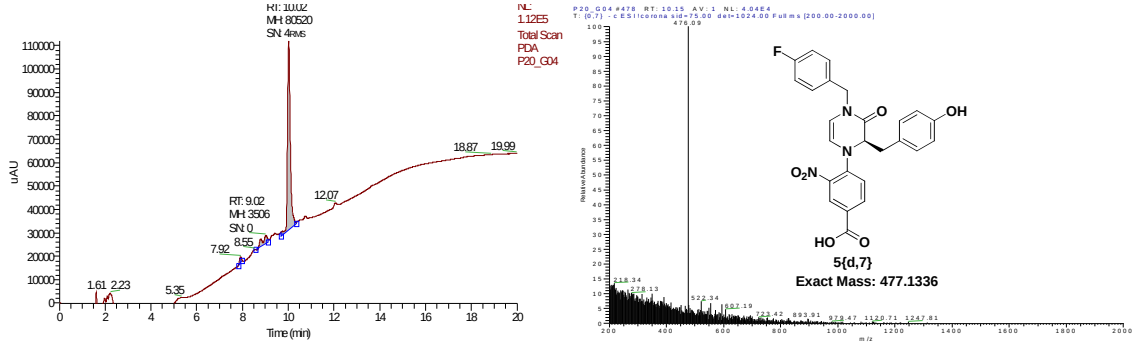

RT: 10.12
MH: 91005
SN: 7RMS
RT: 11.03
MH: 13016
SN: 1
RT: 6.96
MH: 12013
SN: 1
16.07
16.98
18.83
19.86
9.90
1.37
6.72
4.97
uAU
Time (min)
NL:
1.11E5
Total Scan
PDA
KJH_OXopi
perazine_P
20H11
O2N
HO
5{k,6}
Exact Mass: 439.1743

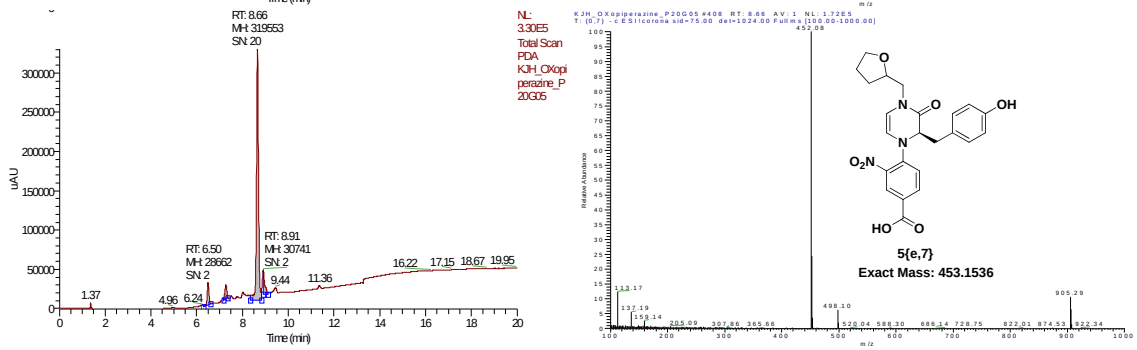

RT: 10.09
MH: 89161
SN: 6
RT: 10.01
MH: 4468
SN: 0
RT: 11.57
MH: 9941
SN: 1
RT: 7.82
MH: 11722
SN: 1RMS
16.38
17.75
18.77
19.70
1.36
6.64
4.90
uAU
Time (min)
NL:
1.14E5
Total Scan
PDA
KJH_Oxopi
perazine_P
23A08
O2N
HO
5{l,6}
Exact Mass: 479.2056

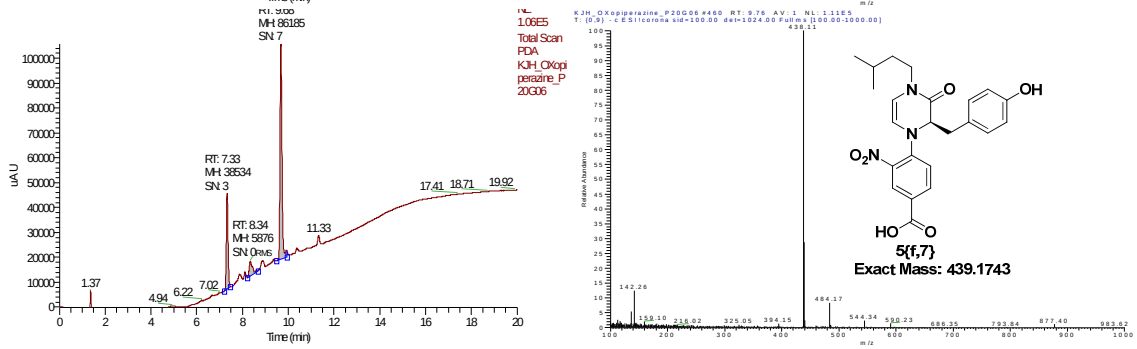

RT: 9.27
MH: 69299
SN: 3RMS
RT: 6.82
MH: 10539
SN: 1
17.68
19.18
19.81
11.32
1.37
4.95
uAU
Time (min)
NL:
8.71E4
Total Scan
PDA
KJH_OXopi
perazine_P
20G01
OH
O2N
HO
5{a,7}
Exact Mass: 425.1587

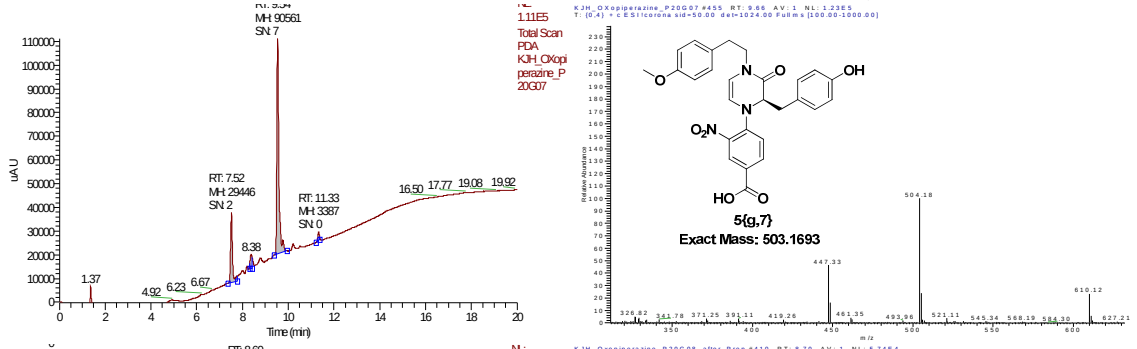

RT: 9.86
MH: 64354
SN: 5RMS
RT: 11.34
MH: 3619
SN: 0
RT: 8.05
MH: 8580
SN: 1RMS
16.21
17.79
19.18
19.93
7.78
1.37
4.98
uAU
Time (min)
NL:
8.53E4
Total Scan
PDA
KJH_OXopi
perazine_P
20G02
F3C
O2N
HO
5{b,7}
Exact Mass: 527.1304

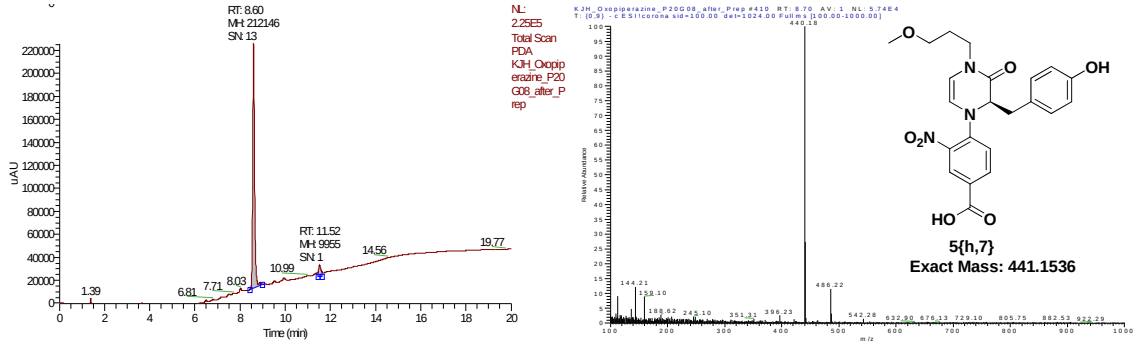

RT: 9.90
MH: 99803
SN: 8RMS
RT: 7.80
MH: 26633
SN: 2RMS
RT: 11.36
MH: 6531
SN: 1
16.13
17.46
18.86
19.95
9.21
1.37
4.98
uAU
Time (min)
NL:
1.20E5
Total Scan
PDA
KJH_OXopi
perazine_P
20G03
OH
O2N
HO
5{c,7}
Exact Mass: 487.1743

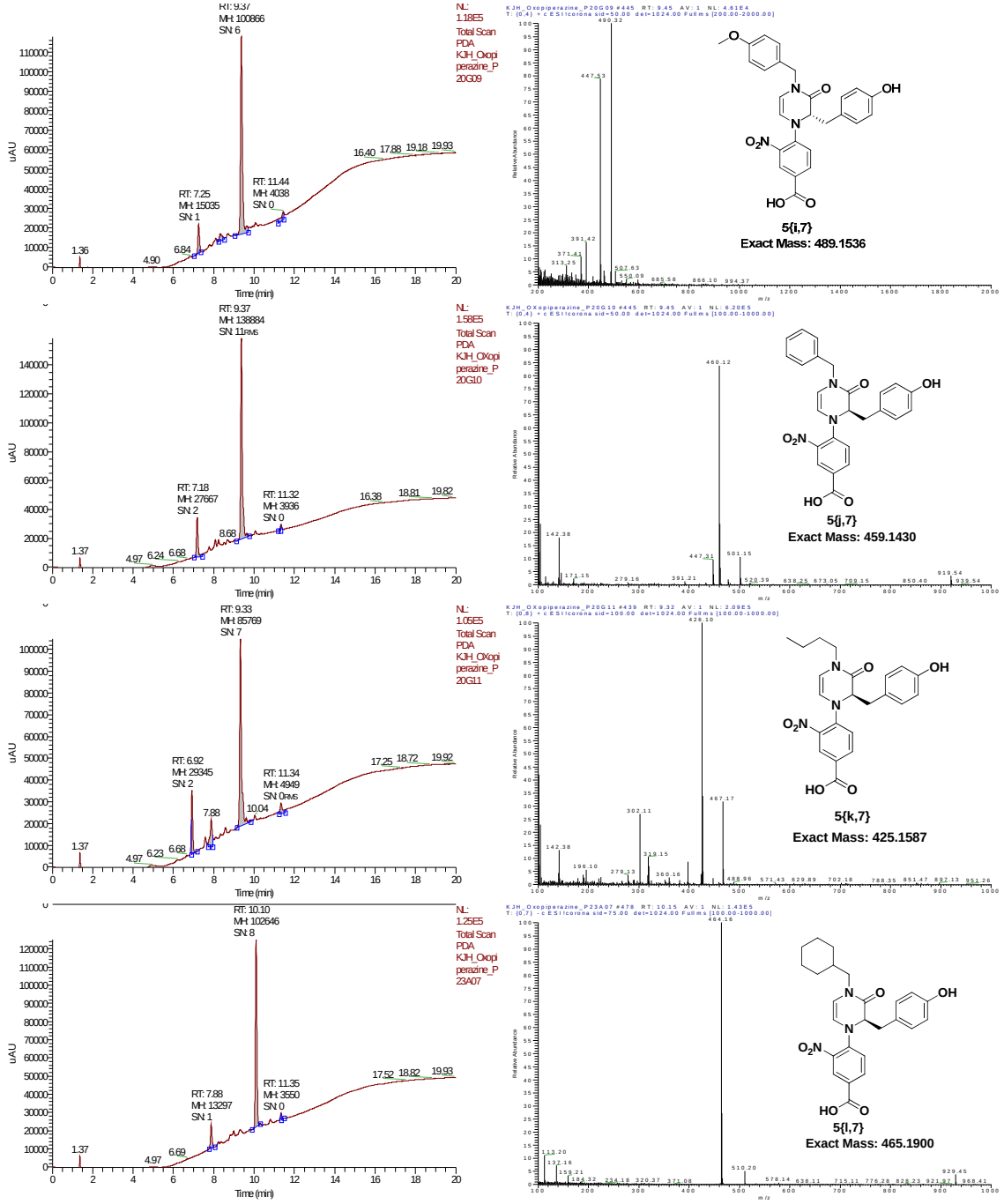

RT: 10.02
MH: 80520
SN: 4rms
RT: 9.02
MH: 3506
SN: 0
RT: 8.55
RT: 7.92
RT: 12.07
RT: 18.87
RT: 19.99
RT: 1.61
RT: 2.23
RT: 5.35
uAU
Time (min)
NL:
1.12E5
Total Scan
PDA
P20_G04
5{d,7}
Exact Mass: 477.1336


RT: 8.66
MH: 319553
SN: 20
RT: 6.50
MH: 28662
SN: 2
RT: 8.91
MH: 30741
SN: 2
RT: 9.44
RT: 11.36
RT: 16.22
RT: 17.15
RT: 18.67
RT: 19.95
RT: 1.37
RT: 4.96
RT: 6.24
uAU
Time (min)
NL:
3.30E5
Total Scan
PDA
KJH_OXopi
perazine_P
20G05
5{e,7}
Exact Mass: 453.1536


RT: 8.66
MH: 86185
SN: 7
RT: 7.33
MH: 38534
SN: 3
RT: 8.34
MH: 5876
SN: 0rms
RT: 11.33
RT: 17.41
RT: 18.71
RT: 19.92
RT: 1.37
RT: 4.94
RT: 6.22
RT: 7.02
uAU
Time (min)
NL:
1.06E5
Total Scan
PDA
KJH_OXopi
perazine_P
20G06
5{f,7}
Exact Mass: 439.1743


MH: 90561
SN: 7
RT: 7.52
MH: 29446
SN: 2
RT: 11.33
MH: 3387
SN: 0
RT: 8.38
RT: 16.50
RT: 17.77
RT: 19.08
RT: 19.92
RT: 1.37
RT: 4.92
RT: 6.23
RT: 6.67
uAU
Time (min)
NL:
1.11E5
Total Scan
PDA
KJH_OXopi
perazine_P
20G07
5{g,7}
Exact Mass: 503.1693


RT: 8.60
MH: 212146
SN: 13
RT: 11.52
MH: 9955
SN: 1
RT: 10.99
RT: 14.56
RT: 19.77
RT: 1.39
RT: 6.81
RT: 7.71
RT: 8.03
uAU
Time (min)
NL:
2.25E5
Total Scan
PDA
KJH_Oxopip
erazine_P20
G08_after_P
rep
5{h,7}
Exact Mass: 441.1536


RT: 9.37
MH: 100866
SN: 6
NL: 1.18E5
Total Scan PDA KJH_Oxopiperazine_P20G09
RT: 7.25
MH: 15035
SN: 1
RT: 11.44
MH: 4038
SN: 0
1.36
4.90
6.84
16.40
17.88
19.18
19.93
uAU
Time (min)
5{i,7}
Exact Mass: 489.1536
RT: 9.37
MH: 138884
SN: 11RMS
NL: 1.58E5
Total Scan PDA KJH_OXopiperazine_P20G10
RT: 7.18
MH: 27667
SN: 2
RT: 11.32
MH: 3936
SN: 0
1.37
4.97
6.24
6.68
8.68
16.38
18.81
19.82
5{j,7}
Exact Mass: 459.1430
RT: 9.33
MH: 85769
SN: 7
NL: 1.05E5
Total Scan PDA KJH_OXopiperazine_P20G11
RT: 6.92
MH: 29345
SN: 2
RT: 11.34
MH: 4949
SN: 0RMS
1.37
4.97
6.23
6.68
7.88
10.04
17.25
18.72
19.92
5{k,7}
Exact Mass: 425.1587
RT: 10.10
MH: 102646
SN: 8
NL: 1.25E5
Total Scan PDA KJH_Oxopiperazine_P23A07
RT: 7.88
MH: 13297
SN: 1
RT: 11.35
MH: 3550
SN: 0
1.37
4.97
6.69
17.52
18.82
19.93
5{l,7}
Exact Mass: 465.1900