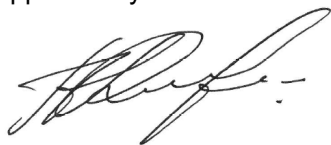


Name:	(S)-Ibuprofen Acyl-β-D-Glucuronide
Lot#:	GR-15-185
Test Date:	02/02/2024 (re-test date: 02/02/2027)
CAS No.:	98649-76-4
MF:	C ₁₉ H ₂₆ O ₈
MW:	382.41
Appearance:	Pink solid
Purity:	98.4% by HPLC (average of two sample preparations, sum of alpha- and beta-epimers)
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 381.16 [M-H] ⁻)
Storage	Long term store at -20° C in a dry place away from direct sunlight

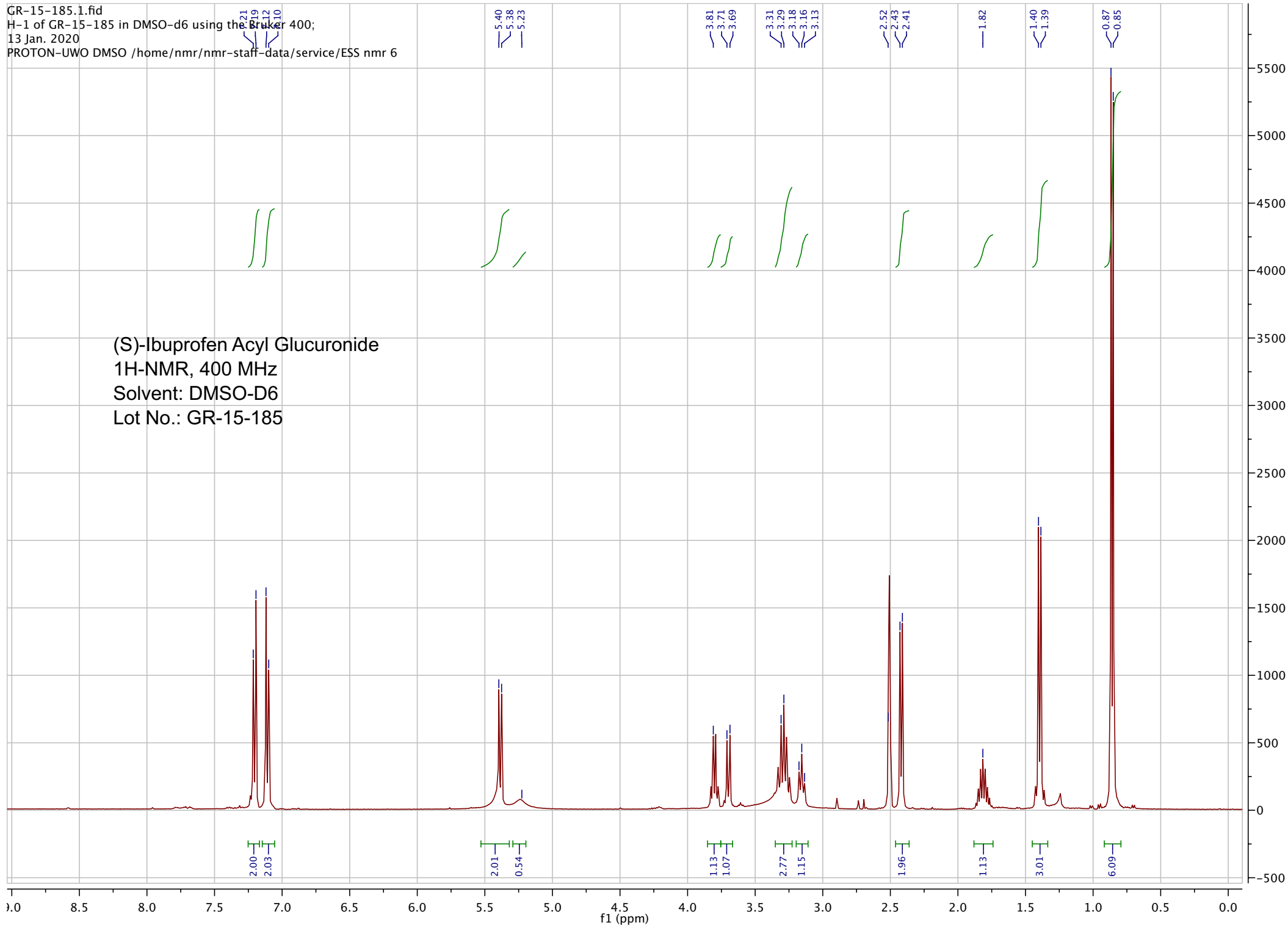
Approved by:

Date: 02/02/2024

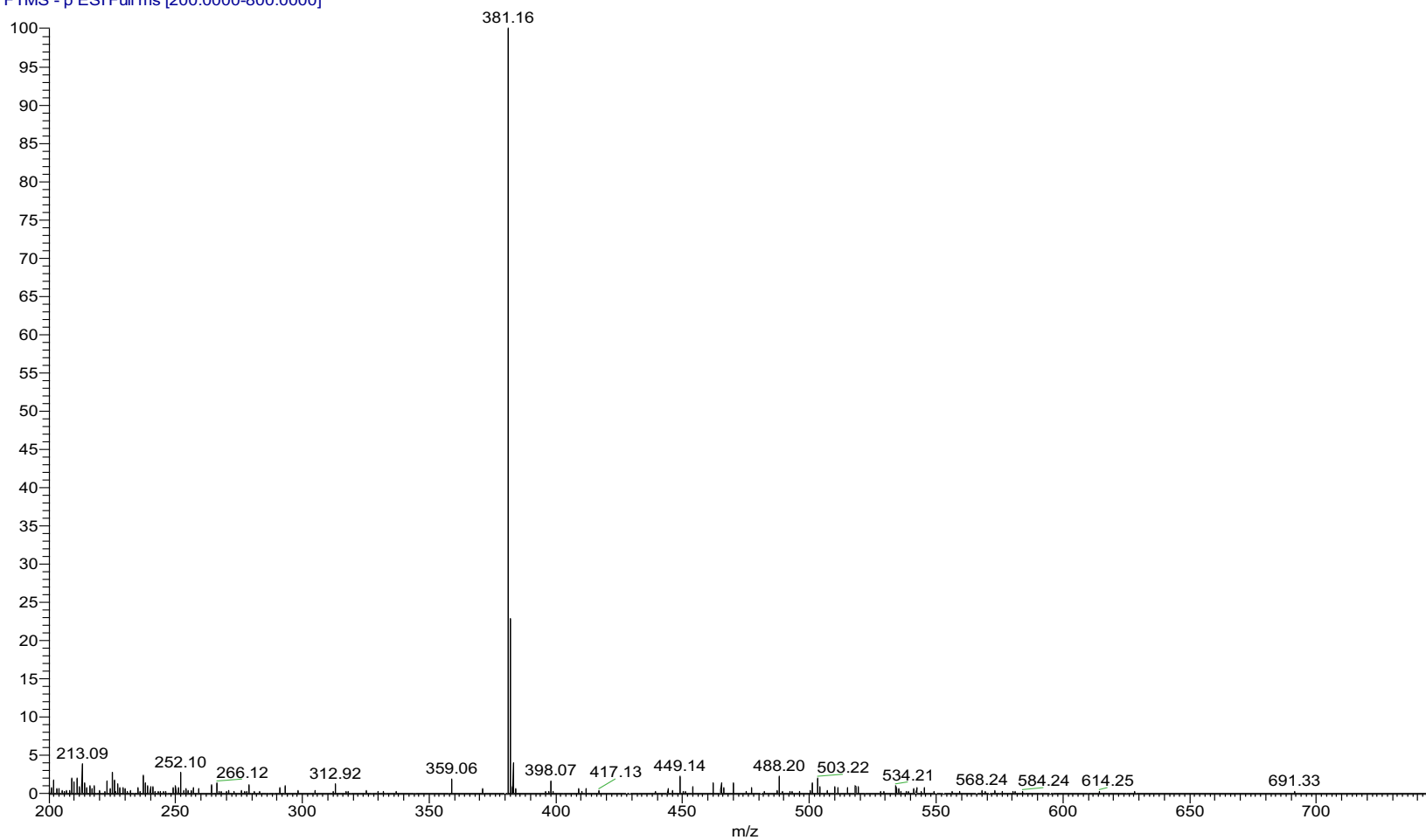


Viorica Rusu, QC/QA Manager

GR-15-185.1.fid
H-1 of GR-15-185 in DMSO-d6 using the Bruker 400;
13 Jan. 2020
PROTON-UWO DMSO /home/nmr/nmr-staff-data/service/ESS nmr 6



pp_2021_001_GR_15_185_1 #925 RT: 2.08 AV: 1 NL: 1.05E8
T: FTMS - p ESI Full ms [200.0000-800.0000]



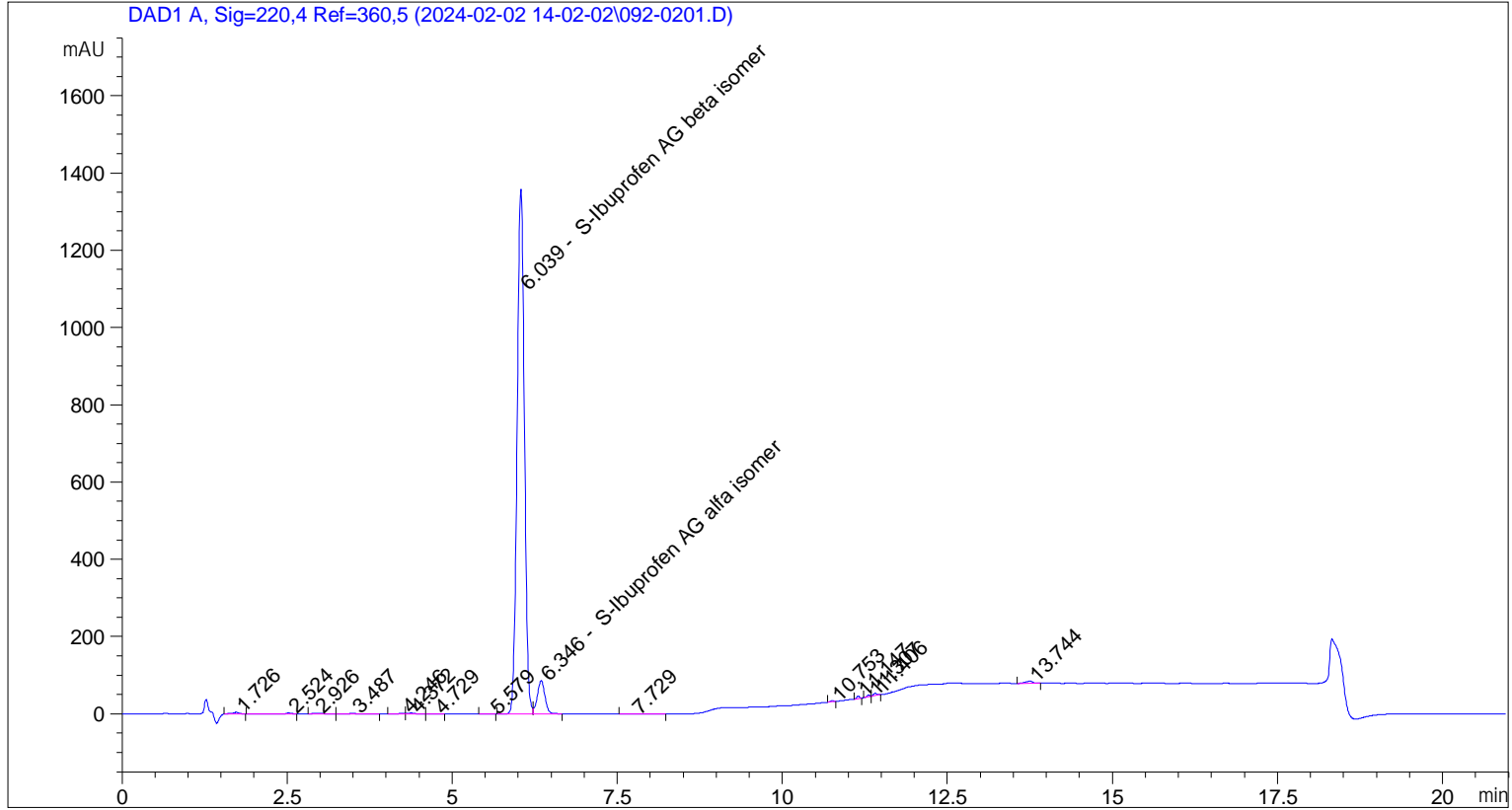
ESI-MS spectrum for sample 2021-001, GR-15-185. Shows monoisotopic [M-H]⁻ mass.

Sample Name: GR-15-185

```

=====
Acq. Operator   : vrusu                               Seq. Line :    2
Acq. Instrument : Instrument 1                         Location  : Vial 92
Injection Date  : 2/2/2024 2:25:34 PM                 Inj       :    1
                                                    Inj Volume: 5.0 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\DATA\2024-02-02 14-02-02\VR020224_185.M
Last changed    : 2/2/2024 2:01:34 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR020224_185_PM.M
Last changed    : 2/2/2024 3:44:45 PM by vrusu
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By           :      Signal
Calib. Data Modified :      Friday, February 02, 2024 3:42:17 PM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	6.039	BV	0.1215	1.04074e4	92.1936	S-Ibuprofen AG beta isomer
2	6.346	VB	0.1203	681.03241	6.0329	S-Ibuprofen AG alfa isomer

```
Totals :                               1.10884e4   98.2265
```

Uncalibrated Peaks:

Sample Name: GR-15-185

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.726	BB	0.0919	27.88124	0.2470	?
2	2.524	BB	0.0916	13.83162	0.1225	?
3	2.926	BB	0.1157	12.69649	0.1125	?
4	3.487	BB	0.1734	7.57256	0.0671	?
5	4.246	BV	0.1006	7.81044	0.0692	?
6	4.372	VB	0.0927	13.66774	0.1211	?
7	4.729	BB	0.1408	2.93523	0.0260	?
8	5.579	BB	0.1263	1.36395	0.0121	?
9	7.729	BB	0.3163	6.46038	0.0572	?
10	10.753	BB	0.0491	10.01347	0.0887	?
11	11.147	BB	0.0524	17.80913	0.1578	?
12	11.307	BV	0.0537	13.21035	0.1170	?
13	11.406	VB	0.0565	23.66593	0.2096	?
14	13.744	BB	0.1070	41.28446	0.3657	?

Uncalib. totals : 200.20298 1.7735

1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

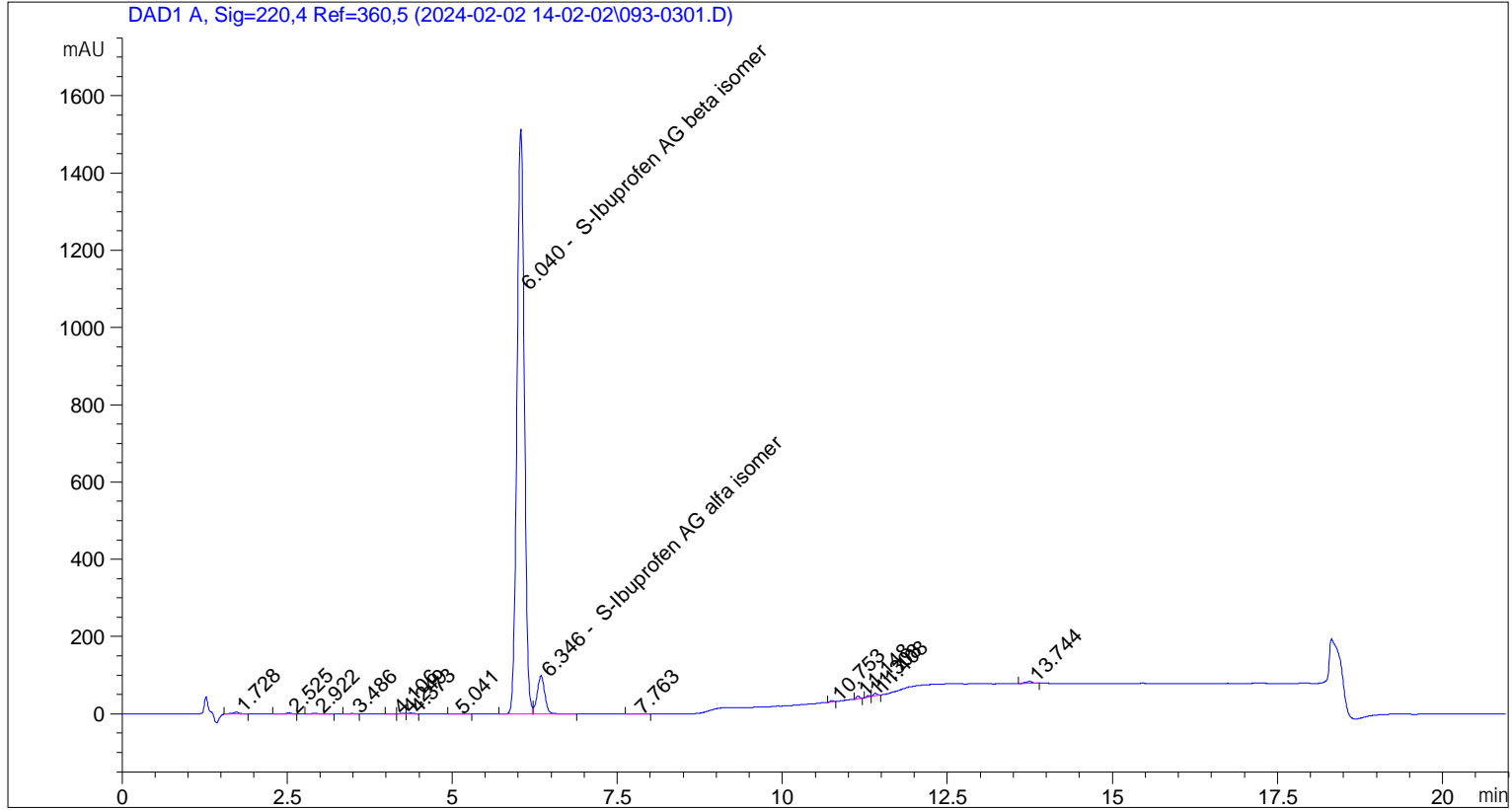
=====
*** End of Report ***

Sample Name: GR-15-185

```

=====
Acq. Operator   : vrusu                               Seq. Line :    3
Acq. Instrument : Instrument 1                         Location  : Vial 93
Injection Date  : 2/2/2024 2:47:56 PM                 Inj       :    1
                                                    Inj Volume: 5.0 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 10.0 µl
Acq. Method    : C:\CHEM32\1\DATA\2024-02-02 14-02-02\VR020224_185.M
Last changed   : 2/2/2024 2:01:34 PM by vrusu
Analysis Method: C:\CHEM32\1\METHODS\VR020224_185_PM.M
Last changed   : 2/2/2024 3:44:45 PM by vrusu
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By           :      Signal
Calib. Data Modified :      Friday, February 02, 2024 3:42:17 PM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	6.040	BV	0.1226	1.17470e4	92.2915	S-Ibuprofen AG beta isomer
2	6.346	VB	0.1251	787.07898	6.1838	S-Ibuprofen AG alfa isomer

```
Totals :                               1.25341e4   98.4753
```

Uncalibrated Peaks:

Sample Name: GR-15-185

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.728	BB	0.0916	32.93357	0.2587	?
2	2.525	BB	0.0783	12.92515	0.1015	?
3	2.922	BB	0.0944	9.38752	0.0738	?
4	3.486	BB	0.0883	3.37184	0.0265	?
5	4.106	BV	0.0757	1.60943	0.0126	?
6	4.249	VV	0.0821	6.04730	0.0475	?
7	4.373	VB	0.0859	13.06031	0.1026	?
8	5.041	BB	0.1591	3.62949	0.0285	?
9	7.763	BB	0.1824	3.69207	0.0290	?
10	10.753	BB	0.0492	11.58766	0.0910	?
11	11.148	BB	0.0528	20.92033	0.1644	?
12	11.308	BV	0.0524	13.60703	0.1069	?
13	11.408	VB	0.0553	25.31574	0.1989	?
14	13.744	BB	0.0995	35.97825	0.2827	?

Uncalib. totals : 194.06571 1.5247

1 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)

=====
*** End of Report ***