Supplementary Material

Appendix A:

Figure 1 depicts an example illustration of 3D BFEN.

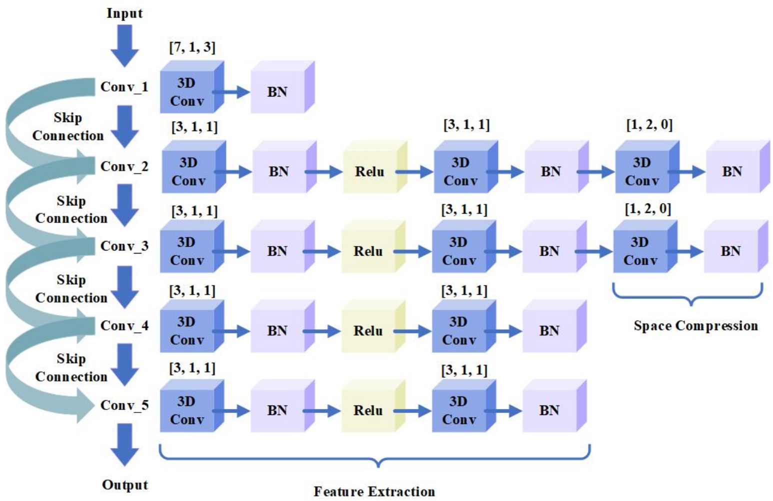

Figure 1: Example illustration of 3D BFEN.

Appendix B:

In this section, we provide the brain tissues contained in the 3D ROI space with a patch size of 8. The specific brain tissues are shown in Table 1. The blue markings indicate the overlap with the main brain regions of a patch size of 4, while the purple markings indicate the overlap with the secondary brain regions of a patch size of 4.

Table 1: Brain tissues included in the interpretable 3D ROI space of MAD-Former with a patch size of 8.

Task	Gyrus(Anatomical and modified Cyto-architectonic descriptions)(left and right brain areas)
AD_NC	FuG, Fusiform Gyrus(A37mv, medioventral area37)(L) MVOcC, MedioVentral Occipital Cortex(rLinG, rostral lingual gyrus)(L) Hipp, Hippocampus(cHipp, caudal hippocampus)(L) FuG, Fusiform Gyrus(A37lv, lateroventral area37)(L) MVOcC, MedioVentral Occipital Cortex(vmPOS,ventromedial parietooccipital sulcus)(L) STG, Superior Temporal Gyrus(A41/42, area 41/42)(L)

	STG, Superior Temporal Gyrus(A22c, caudal area 22)(L) MTG, Middle Temporal Gyrus(A21c, caudal area 21)(L) MTG, Middle Temporal Gyrus(A37dl, dorsolateral area37)(L) ITG, Inferior Temporal Gyrus(A37elv, extreme lateroventral area37)(L) ITG, Inferior Temporal Gyrus(A37vl, ventrolateral area 37)(L) ITG, Inferior Temporal Gyrus(A20cl, caudolateral of area 20)(L) PhG, Parahippocampal Gyrus(TL, area TL (lateral PPHC, posterior parahippocampal gyrus))(L) PhG, Parahippocampal Gyrus(TH, area TH (medial PPHC))(L) pSTS, posterior Superior Temporal Sulcus (rpSTS, rostroposterior superior temporal sulcus)(L) pSTS, posterior Superior Temporal Sulcus (cpSTS, caudoposterior superior temporal sulcus)(L) Tha, Thalamus(Otha, occipital thalamus)(L)
NC_MCIC	FuG, Fusiform Gyrus(A37mv, medioventral area37)(R) MVOcC, MedioVentral Occipital Cortex(rLinG, rostral lingual gyrus)(R) PhG, Parahippocampal Gyrus(TL, area TL (lateral PPHC, posterior parahippocampal gyrus))(R) PhG, Parahippocampal Gyrus(TH, area TH (medial PPHC))(R) CG, Cingulate Gyrus(A23v, ventral area 23)(R) MVOcC, MedioVentral Occipital Cortex(vmPOS,ventromedial parietooccipital sulcus)(R) Hipp, Hippocampus(cHipp, caudal hippocampus)(R) Tha, Thalamus(Otha, occipital thalamus)(R)
NC_MCInc	FuG, Fusiform Gyrus(A37mv, medioventral area37)(R) MVOcC, MedioVentral Occipital Cortex(rLinG, rostral lingual gyrus)(R) PhG, Parahippocampal Gyrus(TL, area TL (lateral PPHC, posterior parahippocampal gyrus))(R) PhG, Parahippocampal Gyrus(TH, area TH (medial PPHC))(R) CG, Cingulate Gyrus(A23v, ventral area 23)(R) MVOcC, MedioVentral Occipital Cortex(vmPOS,ventromedial parietooccipital sulcus)(R) Hipp, Hippocampus(cHipp, caudal hippocampus)(R) Tha, Thalamus(Otha, occipital thalamus)(R)
MCIC_MCInc	IFG, Inferior Frontal Gyrus(A44v, ventral area 44)(L) PrG, Precentral Gyrus(A4tl, area 4(tongue and larynx region))(L) STG, Superior Temporal Gyrus(TE1.0 and TE1.2)(L) STG, Superior Temporal Gyrus(TE1.0 and TE1.2)(L) STG, Superior Temporal Gyrus(A38l, lateral area 38)(L) STG, Superior Temporal Gyrus(A22r, rostral area 22)(L) MTG, Middle Temporal Gyrus(aSTS, anterior superior temporal sulcus)(L) INS, Insular Gyrus(G, hypergranular insula)(L) INS, Insular Gyrus(vIa, ventral agranular insula)(L) INS, Insular Gyrus(dIa, dorsal agranular insula)(L)

	INS, Insular Gyrus(vId/vIg, ventral dysgranular and granular insula)(L) INS, Insular Gyrus(dIg, dorsal granular insula)(L) INS, Insular Gyrus(dId, dorsal dysgranular insula)(L) Amyg, Amygdala(mAmyg, medial amygdala)(L) Amyg, Amygdala(lAmyg, lateral amygdala)(L) Hipp, Hippocampus(rHipp, rostral hippocampus)(L) BG, Basal Ganglia(GP, globus pallidus)(L) BG, Basal Ganglia(NAC, nucleus accumbens)(L) BG, Basal Ganglia(vmPu, ventromedial putamen)(L) BG, Basal Ganglia(dCa, dorsal caudate)(L) BG, Basal Ganglia(dlPu, dorsolateral putamen)(L) Tha, Thalamus(Stha, sensory thalamus)(L) Tha, Thalamus(vCa, ventral caudate)(L) Tha, Thalamus(PPtha, posterior parietal thalamus)(L) Tha, Thalamus(cTtha, caudal temporal thalamus)(L) Tha, Thalamus(lPFtha, lateral pre-frontal thalamus)(L)

Appendix C:

Discussion on Model Generalization Ability. In this section, we investigate the generalization ability of MAD-Former on a non-AD dataset. The Autism Brain Imaging Data Exchange I (ABIDE I) (http://fcon_1000.projects.nitrc.org/indi/abide/abide_I.html) is a project aimed at facilitating autism research, which includes sMRI data from multiple research institutions and laboratories. We extract data provided by the California Institute of Technology, Carnegie Mellon University, Kennedy Krieger Institute, and Ludwig Maximilians University Munich, consisting of 154 subjects (including 77 sujects with autism spectrum disorder (ASD) and 77 HC). We apply the preprocessing methods described in sections 4.2.

In terms of model performance, we compare the experimental results of MAD-Former and 3D ResNet on the ASD vs HC task in ABIDE I (ACC: 0.711 vs 0.694, F1: 0.709 vs 0.681). MAD-Former outperformed 3D ResNet comprehensively. In terms of interpretability, when the patch size is 4, the spatial range of MAD-Former is Coronal () (64-80 (-10.5,-34.5)), Sagittal () (48-64 (-49.5,-25.5)), and Axial () (16-32 (-49.5,-22.5)). By comparing with the AAL, the primary brain tissue is the caudal area 35/36 (A35/36c) of the Parahippocampal Gyrus (PhG) (left), and the secondary brain tissues include the lateral PPHC and posterior parahippocampal gyrus (TL, area TL) (left), the entorhinal cortex (EC, area 28/34) (left), and the rostroventral area 20 (A20rv) of the FuG. Clinical studies have demonstrated a significant increase in gray matter volume of the Parahippocampal Gyrus (PhG) in individuals with ASD [1], particularly showing significant alterations in the left PhG [2]. Additionally, the FuG exhibits both fewer and smaller neurons compared to healthy controls [3]. Our experimental results align closely with these clinical findings. Through analyses of model performance and interpretability, we have demonstrated the effectiveness of MAD-Former across different datasets and its strong generalization capabilities.

[1] Yang X, Si T, Gong Q, et al. Brain gray matter alterations and associated demographic profiles in adults with autism spectrum disorder: A meta-analysis of voxel-based morphometry studies[J]. Australian & New Zealand Journal of Psychiatry, 2016, 50(8): 741-753.

[2] Khundrakpam B S, Lewis J D, Kostopoulos P, et al. Cortical thickness abnormalities in autism spectrum disorders through late childhood, adolescence, and adulthood: a large-scale MRI study[J]. Cerebral Cortex, 2017, 27(3): 1721-1731.

[3] van Kooten I A J, Palmen S J M C, von Cappeln P, et al. Neurons in the fusiform gyrus are fewer and smaller in autism[J]. Brain, 2008, 131(4): 987-999.

Appendix D:

In this section, we have provided the subject sample IDs (ADNI, OASIS, ABIDE) for the dataset used in the manuscript experiments. For more detailed information, please refer to:

https://adni.loni.usc.edu/ for more details and data applications

http://www.oasis-brains.org

http://fcon_1000.projects.nitrc.org/indi/abide/abide_I.html

ADNI

AD:

AD_002_S_0816	AD_023_S_4501	AD_067_S_0110	AD_131_S_0457
AD_002_S_0938	AD_023_S_5120	AD_067_S_0812	AD_131_S_0497
AD_002_S_0955	AD_023_S_5241	AD_067_S_0828	AD_131_S_0691
AD_002_S_1018	AD_024_S_1171	AD_067_S_1185	AD_131_S_5138
AD_002_S_5018	AD_024_S_1307	AD_067_S_1253	AD_133_S_1055
AD_003_S_1059	AD_024_S_4905	AD_067_S_4728	AD_133_S_1170
AD_003_S_1257	AD_024_S_5054	AD_073_S_0565	AD_135_S_4657
AD_005_S_0221	AD_027_S_0404	AD_082_S_1079	AD_135_S_4676
AD_005_S_0814	AD_027_S_0850	AD_082_S_1377	AD_135_S_4954
AD_005_S_0929	AD_027_S_1081	AD_082_S_5029	AD_135_S_5015
AD_005_S_1341	AD_027_S_1254	AD_082_S_5184	AD_135_S_5275
AD_006_S_0547	AD_027_S_1385	AD_094_S_1027	AD_136_S_0194
AD_006_S_0653	AD_029_S_0836	AD_094_S_1090	AD_136_S_0299
AD_006_S_4867	AD_029_S_0999	AD_094_S_1102	AD_136_S_0300
AD_007_S_0316	AD_029_S_1056	AD_094_S_1164	AD_136_S_0426
AD_007_S_1248	AD_029_S_1184	AD_094_S_1397	AD_136_S_4993
AD_007_S_1304	AD_032_S_4755	AD_094_S_1402	AD_137_S_4211
AD_007_S_1339	AD_033_S_0724	AD_098_S_0149	AD_137_S_4258
AD_009_S_5027	AD_033_S_0733	AD_098_S_0884	AD_137_S_4756
AD_009_S_5037	AD_033_S_0889	AD_099_S_0372	AD_141_S_0696
AD_010_S_5163	AD_033_S_1281	AD_099_S_0470	AD_141_S_0790
AD_011_S_0003	AD_033_S_1283	AD_099_S_0492	AD_141_S_0852
AD_011_S_0010	AD_033_S_1285	AD_099_S_1144	AD_141_S_0853
AD_011_S_0053	AD_033_S_1308	AD_099_S_4124	AD_141_S_1024
AD_011_S_0183	AD_033_S_5013	AD_099_S_4994	AD_141_S_1137
AD_011_S_4827	AD_033_S_5017	AD_100_S_5106	AD_141_S_1152
AD_011_S_4845	AD_033_S_5087	AD_109_S_0777	AD_153_S_4172

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AD_011_S_4912	AD_035_S_4783	AD_109_S_1192
AD_011_S_4949	AD_036_S_0577	AD_114_S_0228
AD_013_S_0592	AD_036_S_0759	AD_114_S_0374
AD_013_S_0699	AD_036_S_0760	AD_114_S_0979
AD_013_S_0996	AD_036_S_1001	AD_114_S_4379
AD_013_S_1161	AD_036_S_5063	AD_116_S_4195
AD_013_S_1205	AD_036_S_5112	AD_116_S_4209
AD_013_S_5071	AD_036_S_5149	AD_116_S_4625
AD_014_S_0328	AD_036_S_5210	AD_123_S_4526
AD_014_S_0356	AD_037_S_4001	AD_126_S_0606
AD_014_S_1095	AD_037_S_4770	AD_126_S_0784
AD_014_S_4615	AD_037_S_4879	AD_126_S_0891
AD_016_S_0991	AD_041_S_1368	AD_126_S_1221
AD_016_S_1263	AD_041_S_1391	AD_127_S_0431
AD_018_S_4696	AD_041_S_1435	AD_127_S_0754
AD_019_S_4252	AD_051_S_1296	AD_127_S_0844
AD_019_S_4477	AD_051_S_4980	AD_127_S_1382
AD_019_S_4549	AD_051_S_5005	AD_128_S_1409
AD_019_S_5012	AD_053_S_1044	AD_128_S_1430
AD_019_S_5019	AD_053_S_5070	AD_128_S_4772
AD_020_S_0213	AD_053_S_5208	AD_128_S_4774
AD_022_S_0007	AD_057_S_0474	AD_128_S_4792
AD_022_S_0129	AD_057_S_1371	AD_128_S_5123
AD_022_S_0219	AD_057_S_1373	AD_130_S_0956
AD_022_S_0543	AD_057_S_1379	AD_130_S_1201
AD_023_S_0083	AD_057_S_4110	AD_130_S_1290
AD_023_S_0084	AD_062_S_0535	AD_130_S_1337
AD_023_S_0093	AD_062_S_0690	AD_130_S_4730

AD_023_S_0139	AD_062_S_0730	AD_130_S_4997
AD_023_S_0916	AD_062_S_0793	AD_130_S_5006
AD_023_S_1262	AD_067_S_0029	AD_130_S_5059
AD_023_S_1289	AD_067_S_0076	AD_130_S_5231

HC:

NC_002_S_0295	NC_022_S_0130	NC_062_S_0768	NC_126_S_0506
NC_002_S_0413	NC_023_S_0031	NC_062_S_1099	NC_126_S_0605
NC_002_S_0559	NC_023_S_0058	NC_067_S_0019	NC_126_S_0680
NC_002_S_0685	NC_023_S_0061	NC_067_S_0056	NC_127_S_0259
NC_002_S_1261	NC_023_S_0081	NC_067_S_0059	NC_127_S_0260
NC_002_S_1280	NC_023_S_0926	NC_067_S_0177	NC_127_S_0622
NC_003_S_0907	NC_023_S_0963	NC_067_S_0257	NC_127_S_0684
NC_003_S_0981	NC_023_S_1190	NC_068_S_0210	NC_128_S_0863
NC_003_S_1021	NC_023_S_1306	NC_070_S_4856	NC_128_S_4609
NC_005_S_0553	NC_024_S_0985	NC_073_S_0089	NC_129_S_4422
NC_005_S_0602	NC_024_S_1063	NC_073_S_0311	NC_130_S_0232
NC_005_S_0610	NC_024_S_4084	NC_073_S_0312	NC_130_S_0886
NC_006_S_0484	NC_027_S_0074	NC_073_S_0386	NC_130_S_0969
NC_006_S_0498	NC_027_S_0118	NC_073_S_4155	NC_130_S_1200
NC_006_S_0681	NC_027_S_0120	NC_073_S_4382	NC_131_S_0123
NC_006_S_0731	NC_027_S_0403	NC_073_S_4795	NC_131_S_0319
NC_006_S_4357	NC_029_S_0824	NC_082_S_0304	NC_131_S_0436
NC_006_S_4449	NC_029_S_0843	NC_082_S_0363	NC_131_S_0441
NC_007_S_0068	NC_029_S_0845	NC_082_S_0640	NC_131_S_1301
NC_007_S_0070	NC_029_S_0866	NC_082_S_0761	NC_133_S_0433
NC_007_S_1206	NC_032_S_4277	NC_082_S_1256	NC_133_S_0488
NC_007_S_1222	NC_033_S_0516	NC_082_S_4339	NC_133_S_0493
NC_011_S_0002	NC_033_S_0734	NC_082_S_4428	NC_133_S_0525

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NC_011_S_0021
NC_011_S_0022
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NC_011_S_4222
NC_011_S_4278
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NC_013_S_1035
NC_013_S_1276
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NC_014_S_0558
NC_016_S_0359
NC_016_S_0538
NC_018_S_0055
NC_019_S_4367
NC_020_S_0097
NC_020_S_0883
NC_020_S_0899
NC_020_S_1288
NC_022_S_0014
NC_022_S_0066
NC_022_S_0096
NC_033_S_0741
NC_033_S_0920
NC_033_S_0923
NC_033_S_1016
NC_033_S_1086
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NC_035_S_0156
NC_035_S_0555
NC_036_S_0576
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NC_062_S_0578
NC_094_S_0489
NC_094_S_0526
NC_094_S_0692
NC_094_S_0711
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NC_098_S_0896
NC_099_S_0040
NC_099_S_0090
NC_099_S_0352
NC_099_S_0533
NC_099_S_0534
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NC_941_S_1195
NC_941_S_1197
NC_941_S_1202
NC_941_S_1203
NC_941_S_4292

MCIc:

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MCIc_002_S_1070	MCIc_023_S_0388	MCIc_041_S_1423	MCIc_130_S_0423
MCIc_005_S_0222	MCIc_023_S_0604	MCIc_051_S_1331	MCIc_133_S_0638
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MCIc_011_S_0241	MCIc_027_S_0461	MCIc_067_S_0077	MCIc_141_S_1244
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MCIc_011_S_0861	MCIc_027_S_1387	MCIc_094_S_0434	MCIc_941_S_1311
MCIc_011_S_1282	MCIc_033_S_0567	MCIc_094_S_1015	MCIc_941_S_1363
MCIc_013_S_0240	MCIc_033_S_0723	MCIc_094_S_1398	
MCIc_013_S_0325	MCIc_033_S_0725	MCIc_098_S_0269	
MCIc_013_S_0860	MCIc_033_S_0906	MCIc_099_S_0054	
MCIc_014_S_0658	MCIc_033_S_0922	MCIc_099_S_0111	
MCIc_022_S_0750	MCIc_035_S_0204	MCIc_126_S_1077	
MCIc_022_S_1394	MCIc_035_S_0997	MCIc_127_S_0394	

MCInc:

MCInc_002_S_0782	MCInc_027_S_0307	MCInc_052_S_0989	MCInc_127_S_1032
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MCInc_014_S_0557	MCInc_035_S_0292	MCInc_098_S_0667	MCInc_136_S_0874
MCInc_014_S_0563	MCInc_036_S_0656	MCInc_099_S_0051	MCInc_136_S_1227
MCInc_016_S_0702	MCInc_036_S_0748	MCInc_099_S_0060	MCInc_141_S_0697
MCInc_016_S_0769	MCInc_036_S_0869	MCInc_099_S_0291	MCInc_141_S_0851
MCInc_016_S_1028	MCInc_036_S_0945	MCInc_099_S_1034	MCInc_141_S_1052
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MCInc_022_S_0004	MCInc_036_S_1135	MCInc_109_S_1114	
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MCInc_022_S_0961	MCInc_041_S_0282	MCInc_114_S_0378	
MCInc_022_S_1097	MCInc_041_S_0314	MCInc_114_S_0410	
MCInc_022_S_1351	MCInc_041_S_0598	MCInc_114_S_0458	
MCInc_023_S_0126	MCInc_041_S_0679	MCInc_114_S_1103	
MCInc_023_S_0217	MCInc_041_S_1010	MCInc_114_S_1106	
MCInc_023_S_0331	MCInc_041_S_1260	MCInc_114_S_1118	
MCInc_023_S_0376	MCInc_051_S_1072	MCInc_127_S_0112	
MCInc_023_S_1046	MCInc_051_S_1131	MCInc_127_S_0393	
MCInc_027_S_0116	MCInc_052_S_0671	MCInc_127_S_0925	

OASIS

AD:

OAS30022	OAS30136	OAS30281	OAS30399	OAS30539
OAS30024	OAS30144	OAS30286	OAS30403	OAS30541
OAS30027	OAS30150	OAS30287	OAS30404	OAS30544
OAS30031	OAS30151	OAS30298	OAS30410	OAS30548
OAS30035	OAS30156	OAS30315	OAS30415	OAS30549
OAS30040	OAS30158	OAS30316	OAS30433	OAS30553
OAS30043	OAS30165	OAS30322	OAS30440	OAS30554
OAS30051	OAS30170	OAS30325	OAS30453	OAS30563
OAS30061	OAS30198	OAS30329	OAS30457	OAS30576
OAS30063	OAS30199	OAS30330	OAS30460	OAS30577
OAS30076	OAS30202	OAS30331	OAS30467	OAS30578
OAS30078	OAS30205	OAS30334	OAS30472	OAS30582
OAS30091	OAS30212	OAS30342	OAS30474	OAS30591
OAS30094	OAS30217	OAS30344	OAS30498	OAS30610
OAS30095	OAS30224	OAS30347	OAS30504	OAS30613
OAS30098	OAS30226	OAS30358	OAS30518	OAS30617
OAS30100	OAS30239	OAS30370	OAS30519	OAS30619
OAS30111	OAS30240	OAS30373	OAS30521	
OAS30114	OAS30254	OAS30388	OAS30522	
OAS30120	OAS30262	OAS30394	OAS30527	
OAS30124	OAS30267	OAS30396	OAS30530	
OAS30128	OAS30279	OAS30397	OAS30533	

HC:

OAS30002	OAS30035	OAS30075	OAS30112	OAS30142
OAS30003	OAS30036	OAS30079	OAS30113	OAS30143
OAS30004	OAS30038	OAS30080	OAS30115	OAS30146
OAS30005	OAS30042	OAS30082	OAS30117	OAS30149
OAS30006	OAS30046	OAS30083	OAS30118	OAS30152

OAS30007	OAS30048	OAS30084	OAS30121	OAS30153
OAS30008	OAS30049	OAS30086	OAS30122	OAS30157
OAS30009	OAS30050	OAS30088	OAS30123	OAS30159
OAS30011	OAS30052	OAS30090	OAS30125	OAS30160
OAS30013	OAS30053	OAS30092	OAS30126	OAS30161
OAS30014	OAS30057	OAS30093	OAS30127	OAS30163
OAS30015	OAS30060	OAS30096	OAS30129	
OAS30017	OAS30062	OAS30097	OAS30131	
OAS30025	OAS30065	OAS30099	OAS30132	
OAS30026	OAS30066	OAS30101	OAS30133	
OAS30027	OAS30070	OAS30103	OAS30135	
OAS30028	OAS30071	OAS30104	OAS30137	
OAS30030	OAS30072	OAS30107	OAS30139	
OAS30032	OAS30073	OAS30108	OAS30140	
OAS30034	OAS30074	OAS30109	OAS30141	

ABIDE

ASD:

A0050642	A0050797	A0051323	A0051461
A0050643	A0050799	A0051324	A0051462
A0050644	A0050800	A0051325	A0051463
A0050645	A0050801	A0051326	A0051464
A0050646	A0050802	A0051327	A0051465
A0050647	A0050803	A0051328	A0051466
A0050648	A0050804	A0051329	A0051467
A0050649	A0050805	A0051330	A0051468
A0050650	A0050806	A0051331	A0051469
A0050651	A0050807	A0051348	A0051470
A0050652	A0050815	A0051349	A0051471

A0050653	A0050823	A0051350	A0051472
A0050654	A0050824	A0051351	A0051473
A0050655	A0050825	A0051353	A0051474
A0050791	A0050826	A0051354	A0051606
A0050792	A0051318	A0051355	A0051607
A0050793	A0051319	A0051456	
A0050794	A0051320	A0051457	
A0050795	A0051321	A0051459	
A0050796	A0051322	A0051460	

HC:

T0050656	T0050784	T0051335	T0051364
T0050657	T0050785	T0051336	T0051365
T0050658	T0050786	T0051338	T0051366
T0050659	T0050787	T0051339	T0051367
T0050660	T0050788	T0051340	T0051368
T0050661	T0050789	T0051341	T0051475
T0050663	T0050790	T0051342	T0051476
T0050664	T0050798	T0051343	T0051477
T0050772	T0050808	T0051344	T0051478
T0050773	T0050809	T0051345	T0051479
T0050774	T0050810	T0051346	T0051480
T0050775	T0050811	T0051347	T0051481
T0050776	T0050812	T0051356	T0051482
T0050777	T0050813	T0051357	T0051483
T0050778	T0050814	T0051358	T0051484
T0050779	T0050816	T0051359	T0051485
T0050780	T0050817	T0051360	T0051486
T0050781	T0051332	T0051361	T0051487

T0050782	T0051333	T0051362
T0050783	T0051334	T0051363