RosettaCon
Workshop
2008

"Bridging Industry and Academia"

David Baker at the white board.

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ROSETTA's Origins

In 1999, a collection of scripts and programs used to predict the tertiary structures of proteins from their amino acid sequences was christened **ROSETTA** by David Baker and colleagues at the University of Washington in their paper entitled, '*Ab Initio Protein Structure Prediction of CASP III Targets Using ROSETTA*'. The Critical Assessment of Techniques for Protein Structure Prediction (CASP) is a biennial competition of computational protein structure prediction technologies that was established in 1994. In the competition, protein sequences are provided for which crystal structures have been solved but not yet released to the public, eliminating the potential bias that arises from algorithms trained or developed to produce specific structures. The CASP competitions have always played a central role accelerating the development of Rosetta. The innovative drive will be particularly evident this year, as Rosetta developers will be submitting predictions for CASP8 during the month of July.

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Rosetta Design Group

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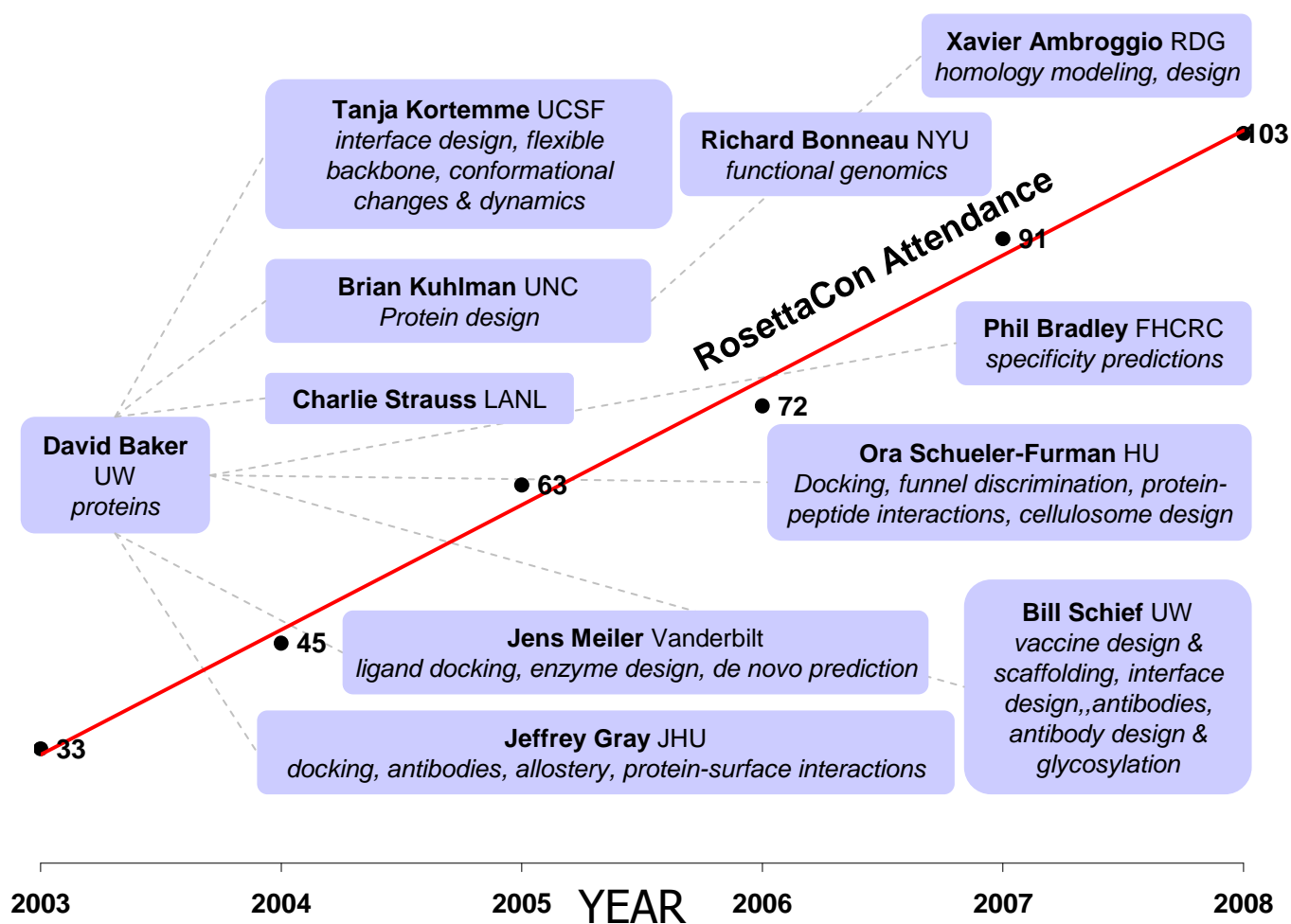
Development of ROSETTA

The Rosetta algorithms and community grew in subsequent years as post-doctoral scholars from the Baker laboratory began their own laboratories (see below) and interests in macromolecular modeling developed beyond structure prediction.

Xavier Ambroggio RDG
homology modeling, design

Tanja Kortemme UCSF
interface design, flexible backbone, conformational changes & dynamics

Richard Bonneau NYU
functional genomics

Brian Kuhlman UNC
Protein design

Phil Bradley FHCRC
specificity predictions

Charlie Strauss LANL

David Baker
UW
proteins

Ora Schueler-Furman HU
Docking, funnel discrimination, protein-peptide interactions, cellulosome design

Bill Schief UW
vaccine design & scaffolding, interface design,,antibodies, antibody design & glycosylation

Jens Meiler Vanderbilt
ligand docking, enzyme design, de novo prediction

Jeffrey Gray JHU
docking, antibodies, allostery, protein-surface interactions

RosettaCon Attendance

103
91
72
63
45
33

| 2003 | 2004 | 2005 | YEAR | 2006 | 2007 | 2008 |

Gabrielle Campbell and colleagues at the University of Washington's Tech Transfer Office worked with the Rosetta developers to establish the Rosetta Commons consortium to allow for continued collaboration. The consortium is governed by an executive committee composed of the principle investigators of each laboratory. Revenues from licensing Rosetta go directly towards supporting code development by funding RosettaCon and allowing for dedicated support staff. This unique arrangement allows for cutting-edge innovation through combining the strengths of the open source model of development with a coherent organizational structure. Since inception of the Rosetta Commons, the Rosetta Algorithms have been widely adopted by hundreds of academic labs in more than 35 countries. Many of the top pharmaceutical companies are also licensing the Rosetta suite.

Agenda RC2008

TUE, July 22nd

11:00AM	Check in
12:00PM	Buffet Lunch
01:00PM	Introductions
03:30PM	**Session 1: Rosetta Science I** Moderated by Jeff Gray
	High resolution protein refinement and the crystallographic phase problem Srivatsan Rama (Baker lab)
	Design and Characterization of 2-Fold Symmetric TIM Barrels Carie Fortenberry (Meiler lab)
	Computational enzymology: Hypotheses about success and failures in enzyme design Alex Zanghellini (Baker lab)
06:00PM	Buffet Dinner
07:20PM	**After Dinner Keynote Lecture** David Baker

07:50PM		
	Rosetta Tutorials I Moderated by Xavier Ambroggio	
	Tutorial 1: A framework for understanding Rosetta Xavier Ambroggio (RDG)	**Poster Session I**
	Tutorial 2: High-resolution design of a protein loop. A Case Study by Jenny Hu (Kuhlman Lab)	
	Tutorial 3: Command lines and Options Session Chu Wang (Baker lab) and Glenn Butterfoss (Bonneau lab, RDG)	

09:00PM	Drinks

★ Beverage & Snack Breaks

Breaks will be interspersed with the talks.
The following complimentary beverages and snacks will be available during breaks:

BEVERAGES
Regular and Decaffeinated Coffees
Hot Water for Teas, Cider and Hot Chocolate
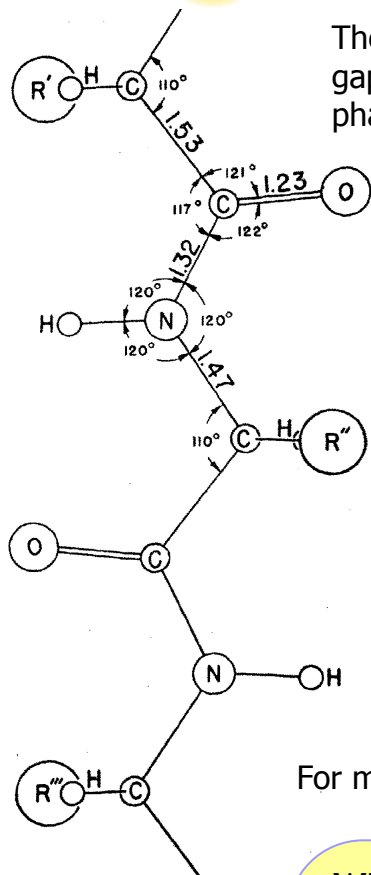Assorted Fruit Juices, Soft Drinks and Water

SNACKS
Sliced Seasonal Fresh Fruit Tray
Freshly Baked Cookies and Brownies
Assorted Domestic and Imported Cheeses Displayed with Fresh Fruits and Vegetables
Cracker Basket

Rosetta Design Group

The Rosetta Design Group LLC was established in 2007 to bridge the gap between the Rosetta Commons academic community and the pharmaceutical industry. A sampling of RDG activities are listed below:

★**On-site Training Seminars**
Two days of Instruction and Hands-on Tutorials

★**Contract Modeling Services**

Antibody Modeling	Loop Modeling
Epitope Mapping	Protein Design and Stabilization
Homology Modeling	Protein-protein Docking
Ligand Docking	Protein-protein Interface Design

★**RosettaCon Workshops**
Networking and the Cutting Edge of Rosetta Development

★**Rosetta Design Group Website**
http://www.rosettadesigngroup.com
Rosetta Support Resources

For more information, please contact: **info@rosettadesigngroup.com**

WED A.M., July 23nd

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07:30AM	Buffet Breakfast
9:00AM	**Session 2: "Rosetta Science: Structure prediction"** Moderated by Brian Kuhlman
	Solution and Adsorbed-State Ensembles of Biomineralization Proteins with RosettaSurface David Masica (Gray lab)
	(Re)discovering missing physics in Rosetta, through RNA Rhiju Das (Baker lab)
	Protein Function Prediction Using Structural Homology Kevin Drew (Bonneau lab)
	Understanding amphetamines by modeling the interaction of MDMA with the serotonin transporter from C. elegans Keith Henry (Meiler lab)
10:30AM	**Session 3:"Moving to Mini: Structure prediction"** Moderated by Charlie Strauss
	Comparative Modeling of Protein Structures James Thompson (Baker lab)
	Predicting Protein-DNA Interaction Specificity Phil Bradley (Bradley lab)
	Ligand Docking with MiniRosetta Ian Davis (Baker lab)
12:00PM	Buffet Lunch

RC2008

01:15PM	**Session 4: "Sampling techniques"** Moderated by Bill Schief
	PathRover: sampling dynamic molecular motion with Rosetta Barak Raveh (Furman lab)
	Backrub News Colin Smith (Kortemme lab)
	Analytical Loop Closure & Flexible BB Interface Design Dan Mandell (Kortemme lab)
02:50PM	**Session 5: "Rosetta Science: Protein Design"** Moderated by Phil Bradley
	Design of Beta Sheet Proteins Jenny Hu (Kuhlman lab)
	HIV Immunogens Design - Targeting (Dis)continuous Motifs Bruno Correia (Schief lab)
	OF rescuing MICE AND MEN: Structure-based computational design of superantigen inhibitors Nir London (Furman lab)
	De Novo Design of Protein-Protein Interfaces John Karanicolas (Baker lab)
04:30PM	**Session 6: "Moving to Mini: Protein Design"** Moderated by Rich Bonneau
	Protein Design with Non-Canonical Amino Acids in MiniRosetta Doug Renfrew (Kuhlman lab)
	Alteration of Enzyme Specificity by Computational Loop Remodeling and Design Paul Murphy (Baker lab)
	Small Molecules as Rotamers: Generation and Docking in ROSETTALIGAND Kristian Kaufmann (Meiler lab)
06:00PM	Buffet Dinner
07:20PM	**After Dinner Keynote Lecture** Andrew Leaver-Fay (Baker Lab)

07:50PM	**Rosetta Tutorials II** Moderated by Xavier Ambroggio	
	Tutorial 4: So you've done docking. What now? Nir London (Furman lab)	**Poster Session II**
	Tutorial 5: Simulating localized backbone flexibility with backrub moves Colin Smith (Kortemme lab)	
	Tutorial 6: Kinematic loop closure and flexible backbone interface modeling Dan Mandell (Kortemme lab)	
09:00PM	Drinks	

NOTES

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07:30AM	Buffet Breakfast
9:00AM	**Session 7: "Mini: Technical Details and Discussion"** Moderated by Tanja Kortemme
	Computational Experiments with a Lone-Pair Based Hydrogen-Bonding Potential in Mini Chris Sheldahl (Snoeyink lab)
	Smoothed high-resolution backbone-dependent rotamer libraries for protein structure prediction Roland Dunbrack
	Loop Modeling: Trimming the Fat Steven Lewis (Kuhlman lab)
	Testing infrastructure and procedures in Mini Sergey Lyskov (Gray lab)
	Discussion of Mini project release Yi Liu (Kuhlman lab)
12:00PM	Buffet Lunch

Rosetta Design Group

Scientific Advisory Board

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Jeffrey J. Gray
Assistant Professor of Chemical Engineering
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Management

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Gabrielle Campbell
Rosetta Design Group Executive Adviser

VP of Business Development
American Association of Medical Colleges

Glenn Butterfoss
Associate Member
Rosetta Design Group LLC

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01:15PM	**Session 8: "Interfaces to Rosetta"** Moderated by Jens Meiler
	Rosetta Design Wizard: Protein Design Through PyMol Matt O'Meara (Kuhlman lab)
	FoldIt Seth Cooper (Baker-affiliated)
	Pysetta? PyRosetta? Will Sheffler (Baker lab)
03:30PM	**Session 9: Macromolecular Modeling Outside of the Commons** Moderated by Jens Meiler
	Redesign of galactose oxidase substrate specificity Shaun Lippow (Codon Devices)
	Strand-Exchange Engineered Dimers: A platform for multifunctional biotherapeutics and bispecific antibodies Jeff Way (EMD Serono)
	Trying to Make Better Drugs with Molecular Modeling: Structure-Guided Design of Therapeutic Antibodies Deping Wang (Biogen Idec)
	NanoEngineer-1: An extensible, open-source, multi-scale modeling and simulation program for DNA and protein structures Mark Sims (Nanorex)
06:00PM	Buffet Dinner
07:30PM	Discussions, Conclusions, Outlook and Hike Organization
09:00PM	Drinks

FRI, July 25th

07:30AM	Buffet Breakfast
	Cascades Hike Departures!
	Check out
08:00AM	Box Lunch
01:00PM	Non-Hikers Departure

Rosetta Design Group

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The Rosetta Design Group would like to extend a special thanks to RosettaCon2008 Participants, the Rosetta Commons Community, the University of Washington, Merck Research Laboratories, and Nanorex for making this event possible.

Rosetta Commons Participants

Rosetta Design Group

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Eva-Maria Strauch

Paul Murphy

David Kim

Will Sheffler

Justin Siegel

Sarel Fleishman

James Thompson

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Ling Wang

Ingemar Andre

Nobuyasu Koga

Seth Cooper

TJ Brunette

Oliver Brock

Frank DiMaio

Chris King

Chu Wang

Sagar Khare

Justin Ashworth

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Kevin Drew

Glenn Butterfoss

FHCRC, Seattle

Phil Bradley

Chen Yanover

Fox Chase Cancer Center

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Guoli Wang

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Furman Lab

Nir London

Barak Raveh

University of Washington

Goodlett Lab

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Johns Hopkins University

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Karplus Lab

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University of California
San Francisco

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Sen Liu

Dan Mandell

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Florian Lauck

Greg Friedland

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Steven Lewis

Grant Murphy

Matthew O'Meara

Doug Renfrew

Jenny Hu

Ron Jacak

Ramesh Jha

Ben Stranges

Yi Liu

Oana Lungu

Eun Jung Choi

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Chapel Hill

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Vanderbilt University

Jens Meiler

Steven Combs

Kristian Kaufmann

Andrew Morin

Gordon Lemmon

Jens Krause

Will Proffitt

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Chemical Research and Development
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Your Stay at Sleeping Lady

We look forward to welcoming you as our guest. To ensure you feel at home during your stay with us, we've provided the following information about our site. Please do not hesitate to contact us at 800-574-2123 if you have any questions.

- **Check-in** time is 3:00 p.m.; **Checkout** is 11:00 a.m.

- Our **Registration Desk** and **Gift Shop** are staffed 24 hours a day and look forward to serving you.

- We have a **non-smoking policy** indoors and out. Guests not adhering to the policy will be charged a minimum of $150. Please help us keep Sleeping Lady smoke-free.

- Due to the four seasons we experience and our natural environment we recommend **business casual attire** and **non-slip footwear**. High heels are strongly discouraged.

- Sleeping Lady is a walking site. Please park your **vehicles** in the guest parking lot. No motor vehicles may be driven on site. A wheelchair is available upon request.

- **Luggage carts** are available directly outside the main office for the convenience of our guests.

- The **Woodland Rock Pool** is open 24 hours a day seasonally (mid April-September) and the adjoining **hot pool** is open year round. Both are accessible via your room key. Swimsuits are required.

- The **Sauna** and cold plunge is open 24 hours a day.

- If you would like to schedule a **massage,** please call us at the number above. 24-hour advance reservation is recommended.

- **Grasshopper Fitness Center** adjacent to the Sauna building is open 24 hours a day and is accessible via your room key.

- Roki, our resident Icelandic Sheep Dog will likely welcome you upon your arrival or make your acquaintance some time during your stay. Those with pet allergies should note that Sleeping Lady also hosts a resident cat, Kiska. Dog lovers – Ask about our Canine Companion Program.

- There are **no televisions** in our guest rooms. We invite you to take our self guided art walk, a leisurely stroll down by the river or through our organic garden.   We offer **seasonal equipment rental** including snowshoes, cross-country skis, bicycles and trail passes and information on the seemingly endless recreational opportunities surrounding our site.

- There are **telephones, wireless and dial up Internet access** in all the guest rooms and meeting spaces.

- Our friendly barkeep at **The Grotto Bar** keeps the music and beverages flowing, with wine, beer, spirits and soft drinks to choose from. Open daily at 4:30 – 10:00 p.m., or later at the barkeep's discretion.

- **Dining Hours**: Dinner is served from 6-7 p.m. Breakfast, 7:30-8:30 a.m. weekdays, 8-9 a.m. weekends. Lunch is served from noon-1 p.m. All meals are served in the Kingfisher Dining Lodge.

- **O'Grady's Pantry,** offers in between meal snacks, espresso, a wide selection of teas and juices, as well as a fine collection of Northwest wines, beers and spirits.
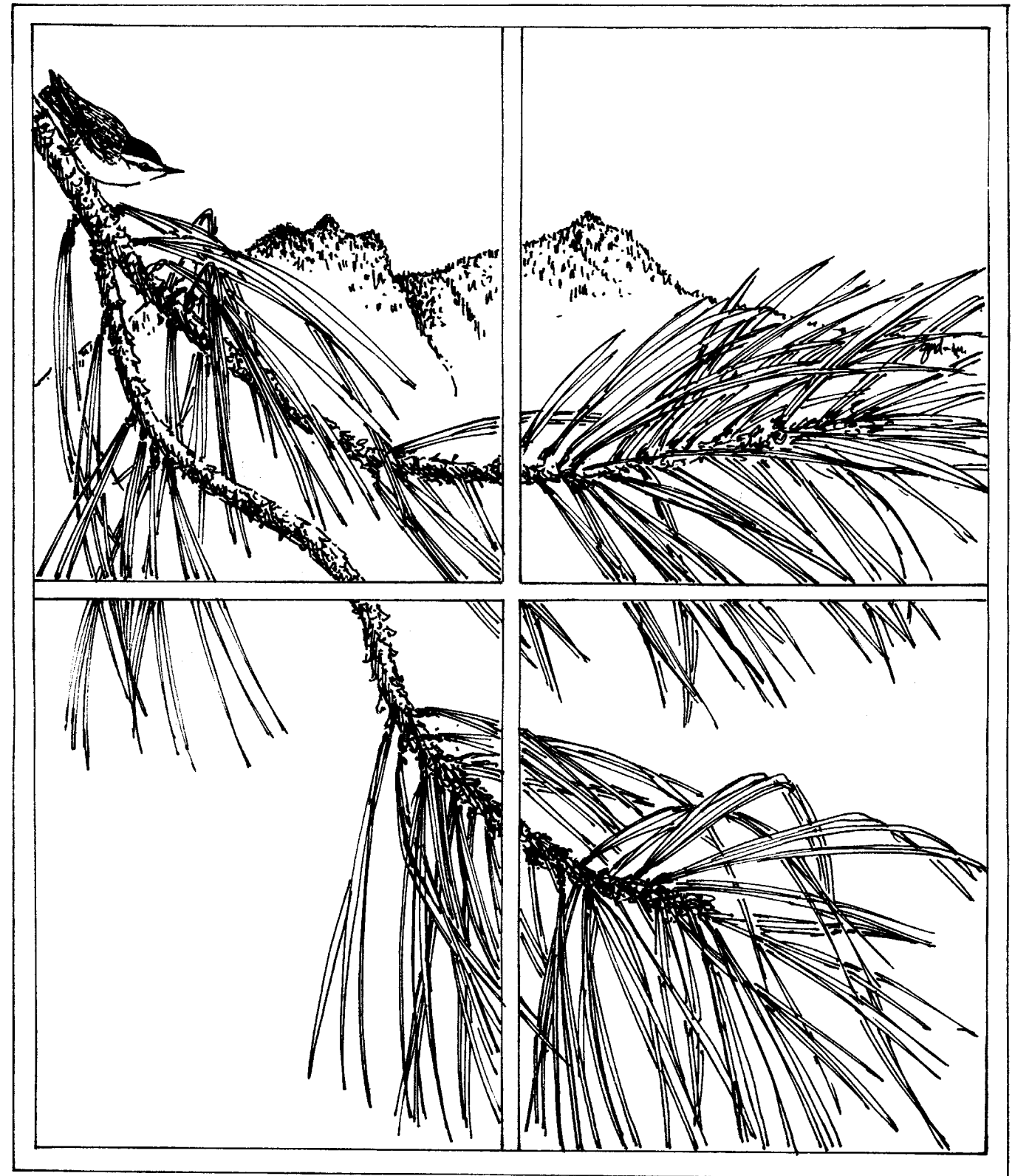
SLEEPING LADY
MOUNTAIN RETREAT

1. **OFFICE & GIFT SHOP**
   Registration and guest services include check-in desk, gift shop, management office, and faxing and copying. Adjacent luggage depot offers carts for guests to transport luggage to rooms and bicycles for guest's rental.

2. **MERGANSER**
   Administrative offices.

3. **FLICKER**
   Comfortable meeting cabin with space for up to 40.

4. **WOODPECKER**
   Seats up to 150. Built in audio-visual system.

5. **CHIHULY'S "ICICLES"**
   Dale Chihuly's blown glass sculpture, dedicated in December 1996, is his only permanent outdoor installation.

6. **KINGFISHER DINING LODGE & TERRACE**
   Menus feature Northwest cuisine with an international flair and offer fresh seasonal herbs, complimented by vegetables and fruits grown in the organic garden. Meals served buffet style. Breakfast starting at 7:30, lunch at 12, dinner at 6:00. Saturday & Sunday breakfast at 8:00.

7. **RIVER MEADOW**
   Barbecue and picnic area. Outdoor stage for seasonal performances.

8. **FIRE CIRCLES**
   One circle is located behind Kingfisher Dining Lodge overlooking the Icicle River, another is adjacent to the office and the third is outside of the Grotto Bar.

9. **CHAPEL THEATER & SALMON GALLERY**
   A 185-seat performing arts theater. A grand piano, audio-visual conference equipment, a 12-foot projection screen and meeting/dressing rooms. The Salmon Gallery has a fireplace and piano, and accommodates receptions for up to 180.

10. **NUTHATCH**
    Cozy meeting cabin with wood stove and space for up to 30.

11. **ROCK CLUSTER #100-109**
    Ten units with private baths in a setting of granite boulders. Each unit sleeps 2-4

12. **GROTTO BAR**
    An evening gathering place around a rocky fireplace for guests to relax over wine, beer and spirits. Seats 35.
    Seasonal outdoor beer garden and fire circle.

13. **SOFT DRINK & ICE MACHINE**

14. **ROOKERY #157**
    On Woodpecker Hill, this cabin accommodates up to eight in a large room with double-decker beds. Two showers.

15. **EYRIE #158**
    On Woodpecker Hill, this secluded lookout cabin features a king-size bed, one queen Murphy bed, wood stove, whirlpool bath and refrigerator.

16. **WOODLAND ROCK POOLS**
    Up the hill in a clearing is the boulder-lined swimming pool and year-round hot pool. Extra towels in Sauna House.

17. **DANCE**
    A meeting space accommodating up to 60.

18. **SAUNA & MASSAGE ROOM**
    Relax in the sauna or schedule a massage. This cabin has a sitting room and an outdoor, screened terrace with a cold plunge pool. Open 24 hours. Towels provided.

19. **QUAIL**
    Quail features state-of-the-art AV equipment, a wood stove, and seats up to 125. Large windows frame the mountains.

20. **TADPOLE**
    Tadpole features state-of-the-art AV equipment, a wood stove, and seats up to 80. Large windows look out on pond, meadow and mountains.

21. **FOREST CLUSTER #151-156**
    These three cabins have two units each, all with private baths. Each unit sleeps 2-4. One wheelchair accessible unit.

22. **LIBRARY & GUEST COMPUTER WORKSTATION**
    Lined with hand-crafted bookshelves, this cozy cabin has a wood stove and comfortable seating. Curl up with a book.

23. **POND CLUSTER #140-149**
    Ten units with private baths. Each unit sleeps 2-5. A pond extends into the courtyard.

24. **FOUNTAIN CLUSTER #130-139**
    Ten units with private baths. Each unit sleeps 2-5. Includes two connecting units and a wheelchair accessible unit. Built around a Tsutakawa fountain.

25. **TSUTAKAWA FOUNTAIN**
    Gerard Tsutakawa's water sculpture is a cast bronze column within the courtyard pool of Fountain Cluster. Forms and symmetry in nature provide the inspiration for this artwork.

26. **MEADOW CLUSTER #120-129**
    Ten units with private baths. Each unit sleeps 2-5. Includes two connecting units and a wheelchair accessible unit.

27. **DIPPER**
    Cozy meeting cabin with wood stove and space for up to 30.

28. **COTTONWOOD CLUSTER #110-119**
    Ten units with private baths. Each unit sleeps 2-5.

29. **ORGANIC GARDEN**
    Seasonal produce for Kingfisher Dining Lodge. Guests are welcome to visit the garden.

30. **O'GRADY'S PANTRY**
    The Pantry, at the entrance to Sleeping Lady, sells espresso, soups, salads, sandwiches, ice cream and other desserts from Kingfisher Dining Lodge, seasonal produce and flowers from our organic garden, beer, wine, and spirits.

31. **FITNESS ROOM & COIN LAUNDRY**
    Features cardiovascular, weight and stretching equipment, coin operated washer and dryer, changing rooms and shower. Open 24 hours, use room key for access.

32. **ICICLE BROADCASTING CO.**
    Home of KOHO radio, 101.1 FM, local music and news station for Leavenworth and Central Washington.

PUBLIC TELEPHONES are located at the entrances to Kingfisher Dining Lodge, the main office, and the rear entrance to the Salmon Gallery.
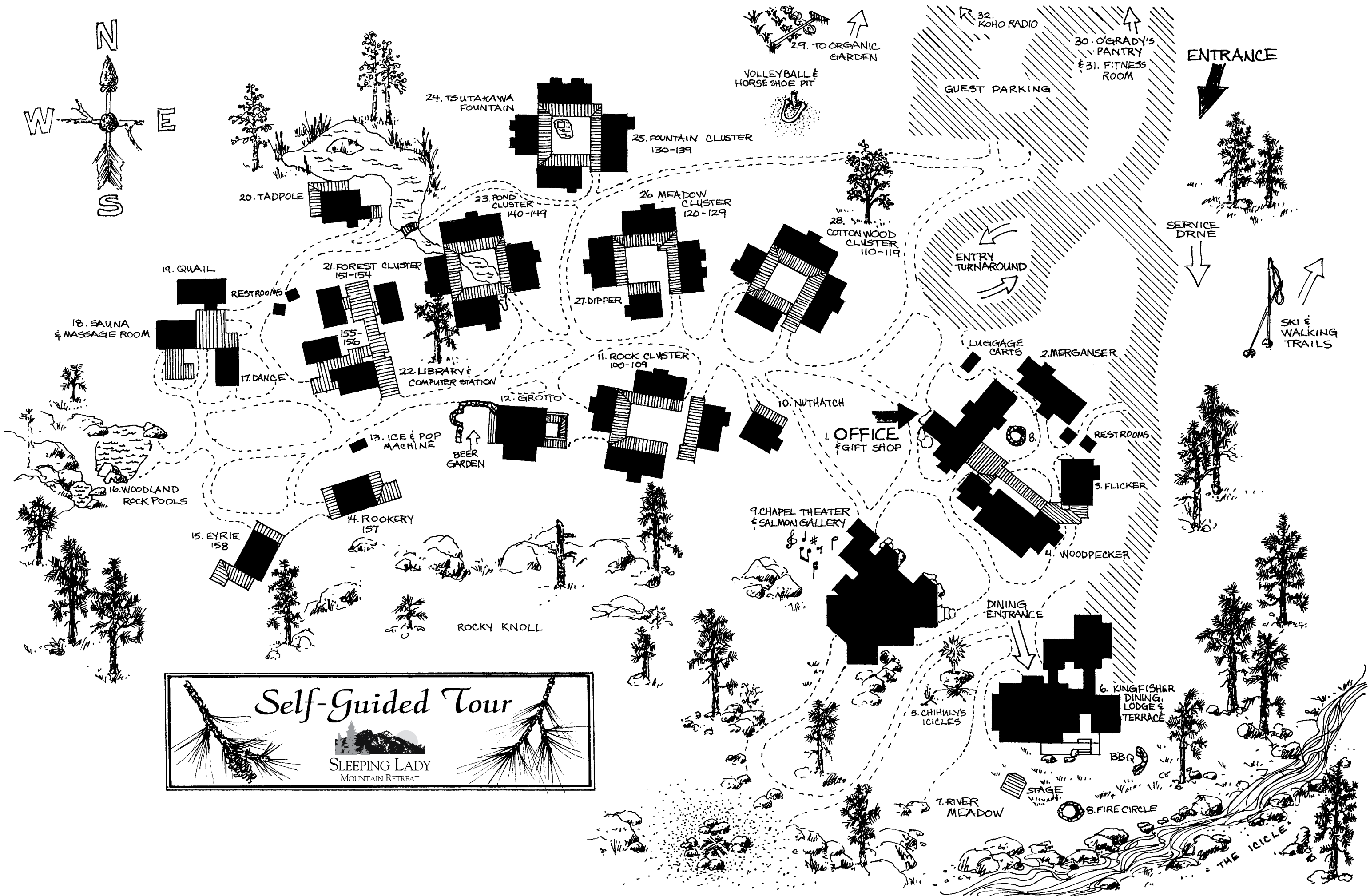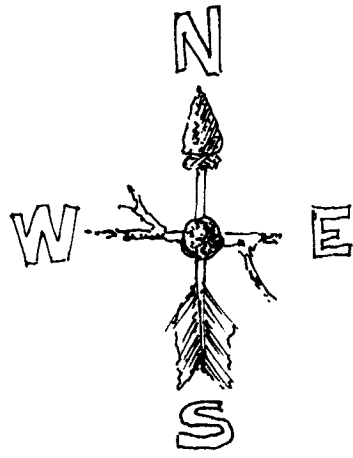

VOLLEYBALL AND HORSESHOES
Located near the organic garden entrance. Equipment is available at the front desk.

7375 Icicle Road, Leavenworth, WA 98826
(509) 548-6344 • (800) 574-2123 • Fax (509) 548-6312
e-mail: info@sleepinglady.com • www.sleepinglady.com

SLEEPING LADY
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The music of her rivers, the fragrance of her trees and the mystery of her rocks, combine to welcome visitors and restore the human spirit.

Self-Guided Tour
SLEEPING LADY
MOUNTAIN RETREAT

N W E S

ENTRANCE

32. KOHO RADIO

30. O'GRADY'S PANTRY & 31. FITNESS ROOM

GUEST PARKING

29. TO ORGANIC GARDEN

VOLLEYBALL & HORSE SHOE PIT

24. TSUTAKAWA FOUNTAIN

25. FOUNTAIN CLUSTER 130-139

SERVICE DRIVE

20. TADPOLE

23. POND CLUSTER 140-149

26. MEADOW CLUSTER 120-129

28. COTTONWOOD CLUSTER 110-119

ENTRY TURNAROUND

21. FOREST CLUSTER 151-154

19. QUAIL

RESTROOMS

27. DIPPER

SKI & WALKING TRAILS

18. SAUNA & MASSAGE ROOM

155-156

17. DANCE

22. LIBRARY & COMPUTER STATION

11. ROCK CLUSTER 100-109

10. NUTHATCH

LUGGAGE CARTS

2. MERGANSER

1. OFFICE & GIFT SHOP

8.

RESTROOMS

3. FLICKER

12. GROTTO

13. ICE & POP MACHINE

BEER GARDEN

16. WOODLAND ROCK POOLS

14. ROOKERY 157

4. WOODPECKER

9. CHAPEL THEATER & SALMON GALLERY

15. EYRIE 158

DINING ENTRANCE

ROCKY KNOLL

5. CHIHULY'S ICICLES

6. KINGFISHER DINING, LODGE & TERRACE

BBQ

STAGE

7. RIVER MEADOW

8. FIRE CIRCLE

THE ICICLE

Directions

From Seattle via Interstate 90

Travel east on Interstate 90 past Cle Elum. Take the Wenatchee Exit 85 Go east on State Rt. 970 for 11.9 miles to US 97. Follow Highway 97 north over Blewett Pass for 35 miles to the junction of Highway 2. Turn left and travel west on Highway 2 for 5.6 miles through downtown Leavenworth to the west edge of town. Turn left on Icicle Road (just before milepost 99) and travel approximately 2.5 miles and past the Leavenworth National Fish Hatchery. Turn left into Sleeping Lady. Do not follow the major curve to the right which leads into Icicle Canyon.

From Seattle via Highway 2

Travel north on Interstate 405 from Seattle/Bellevue to Bothell where it meets Highway 522 east to Monroe. Head east on Highway 2 for 85 miles over Stevens Pass to the west boundary of Leavenworth. Turn right on Icicle Road. Follow directions above.

From Spokane via Interstate 90

Travel west on Interstate 90 to the junction of Highway 281 near George. Travel north on Highway 281 to Quincy. Turn left on Highway 28 and travel west to Wenatchee to Highway 2. Travel on Highway 2 to the west boundary of Leavenworth. Turn left on Icicle Road. Follow directions above.

From Portland, Oregon

Take I-5 north to Seattle. Go east on I-90 over Snoqualmie Pass. Past Cle-Elum follow signs to US-97 and Wenatchee over Blewett Pass. Turn left on Hwy 2 and travel 5 miles to Leavenworth. At the west end of town turn left on Icicle Road. Follow directions above. An alternative is Hwy 2 over Stevens Pass.

Want to know the road conditions before you go?

Find pass conditions, construction reports, and other transportation information on the traffic by clicking on HTTP://traffic.WSDOT.WA.Gov/Sno-info/

Airports

Sea-Tac International Airport is located south of Seattle and is 131 miles from Sleeping Lady. A wide range of airline carriers provides service to this international hub.   Pangborn Memorial Airport in East Wenatchee is located 34 miles from Sleeping Lady. Horizon Airlines provides five direct flights per day between Seattle and East Wenatchee.